Справка за забелязаните цитирания (без автоцитати) върху

трудовете на проф. Тодор Дудев

(общ брой: 4236)

IF = 30

Монография: B.S. Galabov and **T. Dudev**, “Vibrational Intensities”, Elsevier, 1996

1. W.E. Richter, L.J. Duarte, R.E. Bruns, J. Chem. Inf. Model. 2021, 61, 3881–3890.
2. Yan-Li Chen et al., Journal of Electroanalytical Chemistry 914, 2022, 116267.
3. H.Y. Seuret-Hernández et al., J. Mol. Graphics and Modelling 115, 2022, 108234.
4. Wagner E. Richter et al., J. Phys. Chem. A 2021, 125, 15, 3219–3229.
5. Prasanta Das, Infrared Spectroscopy, Edited by Marwa El-Azazy, Khalid Al-Saad and Ahmed S. El-Shafie, IntechOpen, 2023.
6. J.E. Bertie, S.L.L. Zhang, J. Mol. Struct. 413 (1997) 33.
7. S. Tai, K.H. Illinger, S. Papasavva, J. Phys. Chem. A 101 (1997) 9749.
8. R. Garrett, Anal. Chem. (1997) 618.
9. D. C. McKean, Spectrochim. Acta A 53 (1997) 2189.
10. W.J. Orville-Thomas, J. Mol. Struct. 443 (1998) 273.
11. M. Bakiler, I.M. Maslov, S. Akyuz, J. Mol. Struct. 475 (1999) 83.
12. L. A. Gribov, D. I. Sidelov and I. V. Maslov, J. Appl. Spectrosc. (Russ.) 66 (1999) 15.
13. J. Wang, C.Y. Chen, S.M. Buck, J. Phys. Chem. B 105 (2001) 12118.
14. G. Maroulis, P. Karamanis, Chem. Phys. 269 (2001) 137.
15. Y. I. Binev, J. Mol. Struct. (Theochem) 535 (2001) 93.
16. I. G. Binev, D. Sc. Thesis, Institute of Organic Chemistry, Bulgarian Academy of Sciences, Sofia, 2001.
17. L. Khriantchev, H. Tanskanen, M. Pettersson, J. Chem. Phys. 116 (2002) 5649.
18. J. Neugebauer, M. Reiher, C. Kind, J. Comput. Chem. 23 (2002) 895.
19. M. Gussoni, C. Castiglioni, G. Zerbi, in “Handbook of Vibrational Spectroscopy”, P. Griffiths, J. M. Chalmers (Eds.) Wiley, New York, 2002.
20. G. Maroulis, J. Chem. Phys. 118 (2003) 2673.
21. M. Moran, J. Dreyer, S. Mukamel, J. Chem. Phys. 118 (2003) 1347.
22. J. Fernandez, S. Montero, J. Chem. Phys. 118 (2003) 2657.
23. C. Sammon, C. S. Deng, J. Yarwood, Polymer 44 (2003) 2669.
24. J. Dreyer, A. M. Moran, S. Mukamel, J. Phys. Chem. B 107 (2003) 5967
25. Y. Xie, D. Y. Wu, G. K. Liu, J. Electroanal. Chem. 554 (2003) 417.
26. P. Karamanis, G. Maroulis, Chem. Phys. Lett. 376 (2003) 417.
27. J. Neugebauer, Ph.D. Thesis, Universitat Erlangen, 2003.
28. G. Maroulis, J. Mol. Struct. (Theochem) 633 (2003) 177.
29. D. T. Durig, Z. H. Yu, C. H. Pan, Spectrochim. Acta A 59 (2003) 1579.
30. L.A. Gribov, E.V. Alekseev, J. Appl. Spectrosc. 70 (2003) 327.
31. A. Haskopoulis, G. Maroulis, Chem. Phys. Lett. 397 (2004) 253.
32. S. R. Banks, C. Sammon, C. D. Melia, P. Timmins, Appl. Spectrosc. 59 (2005) 452.
33. D. Xenides, J. Mol. Struct. (Theochem) 764 (2006) 41.
34. C. Carteret, Spectrochim. Acta A 64 (2006) 670.
35. C. Sammon, C. Li, S. P. Armes, A. L. Lewis, Polymer 47 (2006) 6123.

36. Z. Mielke, L. Sobczyk, in “Isotope Effects in Chemistry and Biology”, A. Kohen, H. H. Limbach, Eds., Taylor & Francis, 2006, p. 281.
37. L. Daskalova, Ph.D. Thesis, Institute of Organic Chemistry, Bulgarian Academy of Sciences, 2007.
38. A. G. Markelz, J. R. Knab, J. Y. Chen, Y. He, Chem. Phys. Lett. 442 (2007) 413.
39. G. Maroulis, Chem. Phys. Lett. 442 (2007) 265.
40. D. Rappoport, Dissertation, Universität Karlsruhe (TH), Fakultät für Chemie und Biowissenschaften, 2007.
41. S. Pehkonen, K. Marushkevich, L. Khriachtchev, M. Räsänen, B.L. Grigorenko, A.V. Nemukhin, J. Phys. Chem. A 111 (2007) 11444.
42. Z.-Q. Tian, B. Ren, J.-F. Li and Z.-L. Yang, Chem.Commun. (2007) 3514.
43. C.A. Jimenez-Hoyos, B.G. Janesko and G.E. Scuseria, Phys. Chem. Chem. Phys. 10 (2008) 6621.
44. P. Das, E. Arunan, P. K. Das. Vibr. Spectrosc. 47 (2008) 1.
45. S. Pehkonen, Academic Dissertation, Department of Chemistry, University of Helsinki, 2008.
46. Y. He, J.-Y. Chen, J. R. Knab, W. Zheng, A. G. Markelz, Terahertz Sci. Tech. 3 (2010) 149.
47. E.E. Zvereva, A.R. Shagidullin, S.A. Katsyuba, J. Phys. Chem. A 115 (2011) 63.
48. F.S. Karoui, A. Karoui, J. Appl. Phys. 108 (2010) 033513.
49. L.B. Zhao, R. Huang, Y.-F. Huang, D.-Y. Wu, B. Ren, Z.-Q. Tian, J. Chem. Phys. 135 (2011) 134707.
50. P. Das, E. Arunan, P. K. Das, J. Phys. Chem. A (2011) DOI: 10.1021/jp2045542.
51. M. Alipour, A. Mohajeri, Chem. Phys. 387 (2011) 5.
52. G. Maroulis, Int. J. Quant. Chem. 111 (2011) 807.
53. E.G. Lewars, “Computational Chemistry”, Springer Netherlands, 2011, pp. 175-390.
54. Y.F. He, J.Y. Chen, J.R. Knab, W.J. Zheng, A.G. Markelz, Biophys. J. 100 (2011) 1058.
55. H. F. Schaefer III, J. Mol. Struct. 1009 (2012) 1.
56. S.S. Stoyanov, J.A. Tsenov, D.Y. Yancheva, J. Mol. Struct. 1009 (2012) 42.
57. D. Cheshmedzhieva, et al., J. Mol. Struct. 1009 (2012) 69.
58. C. D. Keefe, T. Wilcox, E. Campbel, J. Mol. Struct. 1009 (2012) 111.
59. A. Milani, C. Castiglioni, L. Brambilla, G. Zerbi, J. Mol. Struct. 1009 (2012) 130.
60. N.-T. Van-Oanh, C. Falvo, F. Calvo, D. Lauvergnat, M. Basire, M.-P. Gaigeot, P. Parneix, Phys. Chem. Chem. Phys. 14 (2012) 2381.
61. F.S. Karoui, A. Karoui, in “Some Applications of Quantum Mechanics”, M.R. Pahlavani (Ed.), InTech, Rijeka, 2012, pp. 131-166.
62. S. Chakraborty, P. Das and P.K. Das, Ind. J. Phys. 86 (2012) 209.
63. T. Furtenbacher, A.G. Császár, J. Mol. Struct. 1009 (2012) 123.
64. S. Ilieva, Bulg. J. Chem. 1 (2012) 9.
65. A. Γ. Kalampoynia, Ph.D. thesis, University of Patra, Greece, 2003.
66. G. Maroulis, T. Simos, Eds., Trends and Perspectives in Modern Computational Science, Brill Academic Publ., Leiden, The Netherlands, 2006, p. 403.
67. L. A. Gribov, in Computer Appluications in Scientific Researches, IVTN Session – 2008, Proceedings, P. Gabusu, N. Voronina, Eds., Moscow, 2008, p. 5 .
68. G. Maroulis, J. Comp. Theor. Nanosci. 6 (2009) 886.
69. С. С. Стоянов, Дисертация, Институт по органична химия с център по фитохимия, БАН, 2009.
70. S. S. Stoyanov, J. Phys. Chem. A 114 (2010) 5149.
71. Y. Yamaguchi, H. F. Schaefer, in Handbook of High-Resolution Spectroscopy, M. Quack, F. Merkt, Eds., Wiley, 2011.

72. M. Yildiz, M. Karabacak, M. Kurt, J. Mol. Struct. 1006 (2011) 642.
73. M. Yildiz, M. Karabacak, M. Kurt, S. Akkoyuna, Sp. Acta A 90 (2012) 55.
74. P. Das, E. Arunan, P. K. Das, J. Phys. Chem. A 115 (2012) DOI: 10.1021/jp2045542.
75. Шагидуллин, Артур Рифгатович, Диссертация, Ученая степень: кандидат физико-математических наук, Казань, 2011.
76. V. Barone, M. Biczysko, J. Bloino, Phys. Chem. Chem. Phys., 2014, 16, 1759-1787.
77. Wenli Zou and Dieter Cremer, Theoretical Chemistry Accounts 2014, 133:1451.
78. J. Sjöqvist et al. Phys. Chem. Chem. Phys., 2014, 16, 24841-24852.
79. Li-Kun Yang et al. J. Phys. Chem. C, 2014, 118, 25987–25993.
80. F. N. N. Pansini et al. J. Phys. Chem. A, 2015, 119, 1208–1217.
81. Seo Young Kim et al. ECS Trans. 2015, 69, 101-110.
82. Derek Pletcher, Zhong-Qun Tian and David E. Williams, in Developments in Electrochemistry: Science Inspired by Martin Fleischmann (Zhong-Qun Tian andXue-Min Zhang, Eds.), Wiley, 2014, DOI: 10.1002/9781118694404.ch7.
83. SU Ya-Qiong, WU De-Yin, TIAN Zhong-Qun, Acta Phys.-Chim. Sin., 2014, 30, 1993.
84. Бурганов Тимур Ильдарович, Диссертация на соискание ученой степени кандидата химических наук, Федеральное государственное бюджетное учреждение науки, Институт органической и физической химии им. А. Е. Арбузова Казанского научного центра Российской академии, Казань –2015.
85. A. Bende, C. M. Muntean, J. Mol. Mod. 20 (2014) 2113.
86. T. Jin, F. M. Kong, R. Q. Bai, Chem. Lett. 44 (2015) 943.
87. Errol G. Lewars, Chapter, Computational Chemistry, Springer, 2016, pp 193-419.
88. Jian-Feng Li et al., *Chem. Rev.* 2017, 117, 5002–5069.
89. Zou W., Cremer D. (2015) Properties of local vibrational modes: the infrared intensity. In: Wilson A., Peterson K., Woon D. (eds) Thom H. Dunning, Jr. Highlights in Theoretical Chemistry, vol 10. Springer, Berlin, Heidelberg.
90. Yunwen Tao, Wenli Zou, Dieter Cremer, J. Comp. Chem. 39, Issue6, 2018, 293-306.
91. Goutam Brahmachari, Avijit Mondal, Nayana Nayek, Abhishek Kumar, Ambrish Kumar Srivastava, Neeraj Misra, J. Mol. Struct. 1143 (2017) 184-191.
92. D.Yancheva, et al. Vib. Spectrosc. 92, 2017, 200-214.
93. K. Kondo et al. Processing Materials of 3D Interconnects, Damascene, and Electronics Packaging 6, The Electrochemical Society, Pennington, New Jersey, U.S.A., 2015.
94. F. Zapata et al. (2020) Appl. Spectrosc. Rev. DOI: 10.1080/05704928.2020.1797761,
95. P. Pracht, D.F. Grant and S. Grimme**,** J. Chem. Theory Comput. 2020, 16, 7044–7060.
96. A. Kalampoynia, Ph. D. Thesis, University of Patra, Greece,2003.
97. W.E. Richter, J. Phys. Chem. A 2024, 128, https://doi.org/10.1021/acs.jpca.4c02167.
98. L.J. Duarte, Ph.D. Thesis, University of Campinas, Campinas, Brazil, 2023.

Глава от книга: C. Lim and **T. Dudev**, "Potassium Versus Sodium Selectivity in Monovalent Ion Channel Selectivity Filters" in The Alkali Metal Ions: Their Role for Life, Vol. 16 of Metal Ions in Life Sciences (Eds. A. Sigel, H. Sigel, R.K.O. Sigel), Springer International, Cham, Switzerland, 2016, pp. 325-347.

99. Xiaolin Zhang, Chen Huang, Xiangyu Jin, J. Appl. Polym. Sci., 2017, 134, 44396.
100. B. Alshukri et al. Pest Manag. Sci., 75 (2019) 2505-2516.
101. Y. A. Perez Sirkin, I. Szleifer**,** M. Tagliazucchi**,** Macromolecules, 2020, 53, 7, 2616.
102. Y.A.Perez Sirkin, M.Tagliazucchi, I.Szleifer, Materialstoday Advances, 5, 2020, 100047.
103. Alshukri, Baida Mohsen Hemed, Ph. D. Thesis, Newcastle University, UK, 2018.

104. Robert Eisenberg, Luigi Catacuzzeno , Fabio Franciolini, : Science Open Preprints, 2022, DOI: 10.14293/S2199-1006.1.SOR-.PPD7MCA.v1.
105. S. Zaheri, F. Hassanipour, Int. J. Heat and Mass Transfer, 177, 2021, 121423.
106. Mandresy Ivan Ny Hanitra, Ph.D. Thesis, EPFL, Lausanne, 2022.
107. Oleg V. Gradov, Margaret A. Gradova, Radioelectronics. Nanosystems. Information Technologies, 8:154-170, 2016.
108. Blockley, Alix Dawn (2017) Doctoral thesis, Birkbeck, University of London.
109. L. Samineni et al. Cell Systems, 14 (2023) 676.

N. Kircheva, S. Dobrev, V. Petkova, V. Nikolova, S. Angelova and T. Dudev, “Complexation of metal cations (mono-, di- and trivalent) to cucurbiturils: Insights from a DFT/SMD study”, Int. Sci. J. Science. Business. Society 8 (2023) 3-6.

110. S. He at al., Angew. Chemie 62, 2023, e202313864.

V. Petkova, V. Nikolova, N. Kircheva, S. Dobrev, S. Angelova and T. Dudev, “Theoretical study of β-cyclodextrin inclusion complexes with vitamin K”, Innovations 11 (2023) 37-40

111. S.Saffarionpour, et al. Drug Deliv. and Transl. Res. (2024) https://doi.org/10.1007/s13346-024-01586-x

N. Kircheva, S. Dobrev, L. Dasheva, V. Nikolova, S. Angelova and T. Dudev, “Metal-assisted complexation of fluorogenic dyes by cucurbit[7]uril and cucurbit[8]uril: a DFT/SMD evaluation of the key factors governing the host–guest recognition”, Molecules 28 (2023) 1540

112. S. He at al., Angew. Chemie 62, 2023, e202313864.
113. X. Zhang et al., J. Mol. Liquids, 384, 2023, 122266.

V. Nikolova, N. Kircheva, S. Dobrev, S. Angelova and T. Dudev, “Lanthanides as Calcium Mimetic Species in Calcium-Signaling/Buffering Proteins: The Effect of Lanthanide Type on the Ca2+/Ln3+ Competition”, Int. J. Mol. Sci. 24 (2023) 6297

114. I.F. Costa et al. Coord. Chem. Rev. 502, 2024, 215590.
115. Z. Chen et al. J Nanobiotechnol 22, 185 (2024). https://doi.org/10.1186/s12951-024-02442-3
116. C. Shuai, et al. Bio-des. Manuf. 7, 105 (2024) https://doi.org/10.1007/s42242-023-00264-0
117. T. Malcomson et al. RSC Adv., 2023, 13, 28426-28433.
118. N. Grosjean, et al. pp.19-61, 2024, Advances in Botanical Research, 978-0-443-15825-4.
119. S.N. Voicu et al., Polymers 2024, 16(8), 1064.

V. Nikolova, S. Dobrev, N. Kircheva, V. Yordanova, T. Dudev and S. Angelova, "Host-guest complexation of cucurbit[7]uril and cucurbit[8]uril with the antimuscarinic drugs tropicamide and atropine", J. Mol. Graph. Modell., 119 (2023) 108380

120. F. Meng at al. Chem. Eng. J. 474, 2023, 145805.
121. Y. Hamidian, et al. Food Measure 17, 4870–4880 (2023)
122. H. Wang et al. Energy 288, 2024, 129779.

N. Kircheva, S. Dobrev, L. Dasheva, V. Nikolova, S. Angelova and T. Dudev, "Metal-assisted complexation of fluorogenic dyes by cucurbit[7]uril and cucurbit[8]uril: a DFT/SMD evaluation of the key factors governing the host–guest recognition", Molecules 28 (2023) 1540

123. S. He at al., Angew. Chemie 62, 2023, e202313864.
124. X. Zhang et al., J. Mol. Liquids, 384, 2023, 122266.

N. Kircheva, S. Dobrev, V. Nikolova, S. Angelova and T. Dudev, "Theoretical Insight into the Phosphate-Targeted Silver's Antibacterial Action: Differentiation between Gram (+) and Gram (-) Bacteria", Inorg. Chem. 61 (2022) 10089-10100

125. Z. Shen, Polymers 2023, 15, 2000.
126. S. Jieying, et al. Comprehensive Rev. Food Sci. Food Safety, 2024 https://doi.org/10.1111/1541-4337.13373.
127. S. Jafarnia, et al. J. Mol. Struct. 1289, 2023, 135870.
128. T.A. Fernandes et al., RSC Appl. Interfaces, 2024, 1, 98.
129. T. Suzuki et al., Cardiovasc Intervent Radiol 46, 1696–1702 (2023).

N. Kircheva, N. Toshev and T. Dudev, "Holo-chromodulin: Competition between the native Cr^{3+} and other biogenic cations (Fe^{3+}, Fe^{2+}, Mg^{2+} and Zn^{2+}) for the binding sites", Metallomics 14 (2022) mfac082

130. Vincent, J.B. Chromium: Sources, Speciation, Toxicity, and Chemistry. In: Kumar, N.,
131. Walther, C., Gupta, D.K. (eds) Chromium in Plants and Environment. Environmental Science and Engineering. Springer, Cham, 2023.

S. Dobrev, N. Kircheva, V. Nikolova, S. Angelova and T. Dudev, "Competition between Ag^{+} and Ni^{2+} in nickel enzymes: Implications for the Ag^{+} antibacterial activity", *Comp. Biol. Chem*. **101** (2022) 107785

132. A.Matic et al., Int. J. Mol. Sci. 2023, 24(16), 12747.
133. A. Matic, Ph.D. Thesis, University of Zagreb, Croatia, 2024.

I.Z. Koleva, S. Dobrev, N. Kircheva, L. Dasheva, V. Nikolova, S. Angelova and T. Dudev, „Complexation of trivalent metal cations (Al^{3+}, Ga^{3+}, In^{3+}, La^{3+}, Lu^{3+}) to cucurbiturils: a DFT/SMD evaluation of the key factors governing the host–guest recognition“, Phys. Chem. Chem. Phys., 24 (2022) 6274

134.I-Y. Izato, et al. Phys. Chem. Chem. Phys., 2023,25, 8082-8089.

T. Dudev, “How theoretical evaluations can generate guidelines for designing/engineering metalloproteins with desired metal affinity and selectivity”, Molecules 28 (2023) 249

135.Kimia Noroozi, Laura R Jarboe, J. Ind. Microbiol. Biotechnol. 50, 2023, kuad011

T. Dudev, D. Cheshmedzhieva, P. Dorkov and I. Pantcheva, “A DFT/PCM Study on the Affinity of Salinomycin to Bind Monovalent Metal Cations”, Molecules 27 (2022) 532.

136. Zarzeczańska Dorota et al., Wiadomosci Chemiczne, 76, 2022, 7-8.
137. L. Qin et al. Analytica Chimica Acta, 1287, 2024, 342086.
138. T.I. Rokitskaya et al., Biochim. Biophys. Acta (BBA) – Biomembranes1865, 2023, 184182
139. K. Hirata et al., J. Phys. Chem. Lett. 2023, 14, 24, 5567–5572.

D. Cheshmedzhieva, S. Ilieva, E.A. Permyakov, S.E. Permyakov and **T. Dudev**, „Ca^{2+}/Sr^{2+} Selectivity in Calcium-Sensing Receptor (CaSR): Implications for Strontium’s Anti-Osteoporosis Effect“, Biomolecules 11 (2021) 1576.

140. Ayla Hassani et al., J Nanobiotechnol **20**, 310 (2022).
141. Abu Shufian Ishtiaq Ahmed et al., Am J Physiol Cell Physiol 322: C977–C990, 2022
142. Niko Putra et al., *Int. J. Mol. Sci.* 2022, *23*(21), 13239.
143. Gen Li et al., J. Mater. Chem. B, 2023,11, 1115-1130.
144. Wen-Hao Ren et al., Adv. NanoBiomed Res.2022,2, 22000182200018.
145. Jiaqian You et al. Front Bioeng Biotechnol. 2022; 10: 928799.
146. Домнина А. П. и др. Трансляционная Медицина, 9, 2022, 41-61.
147. X. Sheng et al., Materials Today Bio 20, 2023, 100636.
148. X. Liu et al. Bioengineering 2023, 10, 414.
149. P. Tan et al., Int. J. Mol. Sci. 2023, 24(11), 9383.
150. Y. Zhao et al. ACS Nano 2024, 18, 7204–7222.
151. Y. Weng at al., J. Biomed. Materials Res. 111, 2023, 1447.
152. H. Wang, et al. Biol Trace Elem Res 202, 900–912 (2024).
153. H. Qiu et a., ACS Biomater. Sci. Eng. 2024, https://doi.org/10.1021/acsbiomaterials.4c00228.
154. S. Qin et al., Biomacromolecules 2024, https://doi.org/10.1021/acs.biomac.3c01072.
155. W. Liu et al., J. Biomed. Materials Res, 112, 2024, 1083-1092.
156. W. Xie et al., Technology in Cancer Research & Treatment. 2024,

https://doi.org/10.1177/15330338241254

157. S. Sathyanarayanan and S. Kannan, Int. J. Materials Res. 115 (2024) https://doi.org/10.1515/ijmr-2023-0089.

T. Dudev, C. Grauffel and C. Lim, "Calcium in Signaling: Its Specificity and Vulnerabilities toward Biogenic and Abiogenic Metal Ions", J. Phys. Chem. B 125 (2021) 10419-10431.

158. Md Shofiul Alam et al., Metallomics, 14, 2022, mfac039.
159. Robert Eisenberg, Journal of Molecular Liquids, 361, 2022, 119574.
160. Joanna Masternak et al., Eur. J. Inorg. Chem. 2022, 29, e202200353.
161. X. Hu et al., Chemical Engineering Journal, 2024, 152317; https://doi.org/10.1016/j.cej.2024.152317
162. R. Lai et al., J. Am. Chem. Soc. 2024, 146, 7628–7639.
163. M.S. Alam et al., Phys. Chem. Chem. Phys., 2023,25, 9500-9512.

C. Grauffel, **T. Dudev** and C. Lim, "Metal Affinity/Selectivity of Monophosphate-Containing Signaling/Lipid Molecules", J. Chem. Theor. Comput. 17 (2021) 2444-2456.

164. Kateryna Kostenkova et al., Current Opinion Chem. Biol. 69, 2022, 102155.
165. W. Maret, Appl. Sci. 2021, 11, 10846.
166. L.W. Njenga et al., Dalton Trans., 2023,52, 5823-5847.
167. M. Fortino et al., J. Phys. Chem. B 2024, https://doi.org/10.1021/acs.jpcb.4c01026.
168. B.T.A. Boychuk et al., Front. Chem., 2023, 11 https://doi.org/10.3389/fchem.2023.1296787
169. M. Fortino et al., Inorganica Chimica Acta 550, 2023, 121452.

N. Kircheva and **T. Dudev**, „Competition between abiogenic and biogenic metal cations in biological systems: Mechanisms of gallium's anticancer and antibacterial effect", *J. Inorg. Biochem.* **214** (2021) 111309.

170. Fupeng Li et al., Front. Bioeng. Biotechnol. 2022, 10:827960.
171. Marika Mosina et al., Acta Biomaterialia 150, 2022, Pages 48-57.
172. Yangyang Li et al., ACS Nano 2022, 16, 12786–12800.
173. Jie Zhaoet al., Food Chemistry 385, 2022, 132656.
174. Youjun Zhang, Molecules 2022, 27(11), 3443.
175. Marika Mosina et al., J. Funct. Biomater. 2023, 14(2), 51.
176. Chun-Chun Qu et al., Bioengineering 2022, 9(9), 416.
177. Xiaotong Yang et al. Ceramics International 48, Part A, 2022, 34148-34168.
178. Irena Kostova, Inorganics 2023, 11(2), 56.
179. Yangyang Li et al., Research 2023, article ID: 0070; DOI: 10.34133/research.0070.
180. D. Romani et al. J. Med. Chem. 2023, 66, 5, 3212–3225

181.Y. Liu et al., Matarialstoday 67, 2023, 548-565
182.S. Liu et al., J. Mater. Chem. B, 2023, 11, 10446-10454.
183.A.P. Sharif, et al., J Clust Sci 34, 1065–1075 (2023).
184.L.M. O'Ferrall et al. Dalton Trans., 2023, 52, 11958-11964.
185.Y. Han et al., Materialstoday Chemistry 36, 2024, 101984.
186.H. Kitagawa, et al., (2023). Biomaterial Investigations in Dentistry, 10(1). https://doi.org/10.1080/26415275.2023.2284372.
187.G. Song et al., Heliyon 10, E31788, 2024
188.F. Mehraban et al., Inorg. Chem. Commun. 157, 2023, 111307.
189.I. Kostova, JAFSB, 1(1), 23-34, 2023.

V. Nikolova, A. Velinova, S. Dobrev, N. Kircheva, S. Angelova and **T. Dudev**, "Host−GuestComplexation of Cucurbit[7]Uril and Cucurbit[8]Uril with the Antineoplastic and Multiple Sclerosis Agent Mitoxantrone (Novantrone)", *J. Phys. Chem. A* **125** (2021) 536-542.

190. Gao, J. et al. Chem. Res. Chin. Univ. (2021) doi.org/10.1007/s40242-021-1045-2.
191. Fatine Ali Messiad et al., Nanomaterials 2022, 12, 2517.
192. H. Roithmeyer, H., et al. (2023). Supramolecular Chemistry, 34, 77–86

A.A. Vologzhannikova, M.P. Shevelyova, A.S. Kazakov, A.S. Sokolov, N.I. Borisova, E. A. Permyakov, N. Kircheva, V. Nikolova, T. Dudev and S.E. Permyakov, "Strontium Binding to α-Parvalbumin, a Canonical Calcium-Binding Protein of the "EF-Hand" family", Biomolecules 11 (2021) 1158

193. P. Tan et al., Int. J. Mol. Sci. 2023, 24(11), 9383.
194. O.P. Gerzen et al., Int. J. Mol. Sci. 2023, 24(13), 10579.

D. Damyanov, V. Nikolova, S. Angelova and T. Dudev, "Halide anion solvation and recognition by bambusurils: a DFT study", J. Mol. Liq. 335 (2021) 116160.

195. M. Purgel, J. Mol. Liquids 403, 2024, 124863

N. Kircheva, S. Dobrev, L. Dasheva, I. Koleva, V. Nikolova, S. Angelova and **T. Dudev**, "Complexation of biologically essential (mono- and divalent) metal cations to cucurbiturils: DFT/SMD evaluation of the key factors governing the host-guest recognition", *RSC Advances* **10** (2020) 28139-28147

196.Yurii A.Borisov, Sergey S.Kiselev, Comp. Theor. Chemistry 1197, 2021, 113141.
197.Abdelkarim Litim et al. Molecules 2021, 26, 7479.
198. BORISOV YU. A., KISELEV S.S., INEOS OPEN, 4, 2021, 70-77.
199. Rafaela da Silva Bechara Soares, M.Sc. Thesis, Univesidade de Sao Paulo, 2021.
200. Alenzo Murray et al. ChemistrySelect 9, 2024, e202304161.

N. Kircheva and **T. Dudev**, "Gallium as an Antibacterial Agent: A DFT/SMD Study of The Ga^{3+}/Fe^{3+} Competition for Binding Bacterial Siderophores", *Inorg. Chem*. **59** (2020) 6242-6254.

201. A. Donnadio, et al. ACS Biomater. Sci. Eng. 2021, 7, 1361–1373.
202. Alvin L. Crumbliss, Sambuddha Banerjee, J. Inorg. Biochem. 219, 2021, 111411.
203. Marika Mosina et al., Acta Biomaterialia 150, 2022, 48-57.
204. Nailin Yang et al., Coordination Chemistry Reviews, 471, 2022, 214731.
205. Fan Wang et al., Biomaterials Advances 135, 2022, 212736.
206. Chunyi Hu et al., ACS Appl. Nano Mater. 2022, 5, 12.
207. Marika Mosina et al., J. Funct. Biomater. 2023, 14, 51.
208. Jingze Li et al., 2022 Nanotechnology 33 075706.
209. Agnese D'Agostino et al., Applied Surface Science 609, 2023, 155300.
210. Mingyi Kang et al., J. Photochem. Photobiol. A: Chemistry 438, 2023, 114510.
211. Patrick R. W. J. Davey and Brett M. Paterson, Molecules 2023, 28, 203.
212. Salazar-Alemán, D.A., Turner, R.J. (2022). Challenges. In: Hurst, C.J. (eds) Microbial Metabolism of Metals and Metalloids. Advances in Environmental Microbiology, vol 10. Springer, Cham.
213. Cojocari, Ș. et al. (2022). Zinc Oxide and Gallium Nitride Nanoparticles Application in Biomedicine: A Review. In: Tiginyanu, I., Sontea, V., Railean, S. (eds) 5th International Conference on Nanotechnologies and Biomedical Engineering. ICNBME 2021. IFMBE Proceedings, vol 87. Springer, Cham.
214. George Northover, Ph.D. thesis, Imperial College London, UK, 2022.
215. Kang, Mingyi et al., J. Photochem. Photobiol. A: Chemistry 438, 2023, 114510
216. Jan Diettrich, Ph.D. thesis, Technischen Universität Dortmund, Germany, 2022
217. S. Fahde et al., Agriculture 2023, 13(7), 1279.
218. Y. Liu et al., Materialstoday 67, 2023, 548-565.
219. S. Liu et al., J. Mater. Chem. B, 2023, 11, 10446-10454
220. A. Rodríguez-Contreras et al., Int. J. Mol. Sci. 2023, 24, 8762.
221. Y.C. Xu, et al., Environ Sci Pollut Res 30, 91780–91793 (2023).
222. T. Xu et al., ACS Nano 2024, 18, 9, 7123–7135.
223. M. Guo et al. Microbiol Spectr 2023, 11:e00334-23.
224. M. Hajfathalian et al., WIREs 16, 2024, e1959.
225. A. Mular et al., Coordination Chemistry Reviews 501, 2024, 215551.
226. W. Guan et al., Science of The Total Environment 900, 2023, 165850.
227. K. Kharga, (2024) Critical Reviews in Microbiology, 1–40.
228. C. Chantarangkul, Arab J Sci Eng (2024) https://doi.org/10.1007/s13369-023-08650-7
229. S. Lavian et al., Current Medicinal Chemistry, 2024; DOI: https://doi.org/10.2174/0109298673264118231228042816
230. P. Jewula et al. EurJIC 26, 2023, e202300038

S. Pereva, V. Nikolova, T. Sarafska, S. Angelova, T. Spassov, **T. Dudev**, “Inclusion complexes of ibuprofen and β-cyclodextrin: Supramolecular structure and stability”, *J. Mol. Struct*. **1205** (2020) 127575.

231. L. Taouzinet, et al. Cryoletters, 42, 2021, 1-12.
232. A. Puentes Parra, et al., J. Drug Delivery Sci. Technol., 63, 2021, 102509.
233. A. Buczek, et al. Int. J. Quantum Chem. 121 (2021) e26487.
234. Y. Zeng, et al. Spectrochim. Acta A, 246, 2021, 119002.
235. G.S. Hameed et al., Int. J. Pharm. Res. 2020, 12, 3038-3044.
236. M.A.Chouker, et al., J.Mol. Struct. 1235, 5 2021, 130273.
237. S. Nazerdeylami, et al. Diamond and Related Materials, 109, 2020, 108032.
238. Linfan Shi et al. Carbohydrate Polymers 274, 2021, 118596.
239. Anna Helena Mazurek and Łukasz Szeleszczuk, Molecules 2022, 27, 3874.
240. Yan Feng et al. 2021, Critical Reviews in Food Science and Nutrition DOI: 10.1080/10408398.2021.2007352.
241. Katarzyna Betlejewska-Kielak et al., Molecules 2021, 26(13), 4089.
242. Fahad Abdulaziz1, Dina Salah, J. Biomaterials & Nanobiotechnology, 2021, 12, 79.
243. Ke Chen et al., Computational and Theoretical Chemistr, 1206, 2021, 113496.
244. Paulo Gabriel de Lima et al., Comp. Theoretical Chemistry, 1206, 2021, 113465
245. Mejías C and Ginés-Dorado JM, Rev Esp Cien Farm. 2022;3(1):72-81.
246. M. Liu et al. Int. J. Pharmaceutics 637, 2023, 122876.
247. X. Bao et al. Phys. Chem. Chem. Phys., 2023,25, 13923.
248. M. Orsagh et al., ACS Appl. Nano Mater. 2023, 6, 17, 16055.
249. F. Pinelli et al., Int. J. Biological Macromolecules, 252, 2023, 126284.
250. M. Amirinejad et al., ChemistrySelect 8, 2023, e202204396.
251. I.M. Vasincu et al., Pharmaceutics 2023, 15(10), 2492.

T. Dudev, L.M. Frutos and O. Castano, “How mechanical forces can modulate the metal affinity and selectivity of metal binding sites in proteins”, Metallomics 12 (2020) 363-370.

252. Jingyuan Nie et al., Chem.Lett. 2021, 50, 1667–1675.
253. Shengchao Shi, Tao Wu and Peng Zheng, ChemBioChem, 23, 2022, e202200165

T. Dudev, D. Cheshmedzhieva, R. Dimitrova, P. Dorkov and I. Pantcheva, “Factors governing the competition between group IA and IB cations for monensin A: a DFT/PCM study”, RSC Advances 10 (2020) 5734-5741.

254. K. Hirata et al., J. Phys. Chem. Lett. 2023, 14, 5567–5572.
255. L. Bai et al., Materials Today Bio 26, 2024, 101056.

N. Kircheva, S. Dobrev, V. Nikolova, S. Angelova, and **T. Dudev**, “Zinc and Its Critical Role in Retinitis pigmentosa: Insights from DFT/SMD Calculations”, Inorg. Chem. 59 (2020) 17347-17355.

256. Ye Z, et al. Front Med (Lausanne). 2022, 28;9:877752.

257. J. Gujar, et al. Current Nanoscience, 20, 2024, 314-327.
258. A. Matic et al., Int. J. Mol. Sci. 2023, 24(16), 12747.
259. F. Wang et al., Int. J. Mol. Sci. 2023, 24(13), 11231;
260. J.D. Lemme et al. Front. Med., 2022, 9, https://doi.org/10.3389/fmed.2022.857079.
261. Antonia Matic, Ph.D. Thesis, University of Zagreb, Croatia, 2024.

S. Yordanova-Tomova, D. Cheshmedzhieva, S. Stoyanov, T. Dudev and I. Grabchev, „Synthesis, Photophysical Characterization, and Sensor Activity of new 1,8-Naphtalimide Derivatives", Sensors 20 (2020) 3892.

262. P. Murugaperumal et al., J. Mol. Liquids 398, 2024, 124335.
263. N. Bagherzadeh and A.R. Sardarian, J. Photochem. Photobiol. A: Chemistry 449, 2024, 115345
264. Y. Zagranyarski et al., Sensors 2023, 23(6), 2902.
265. K. Prsir et al., Molecules 2023, 28(3), 1275.
266. C.H. Jeong, et al., J Fluoresc 32, 427–433 (2022)
267. A. Mendoza, M.Sc. Thesis, Ohio State University, U.S.A., 2022.

V.K. Nikolova, C.V. Kirkova, S.E. Angelova and **T.M. Dudev**, "Host-guest interactions between p-sulfonatocalix[4]arene and p-sulfonatothiacalix[4]arene and group IA, IIA and f-block metal cations: a DFT/SMD study", *Beilstein J. Org. Chem.* **15** (2019) 1321-1330

268. L.V. Shmygleva, et al. Nanotechnol Russia 15, 301–307 (2020).
269. Shanthini Priscilla A et al., Phys. Chem. Chem. Phys., 2022,24, 21812-21821.
270. Hamid Hadi & Reza Safari (2022), Molecular Physics, 120:17.
271. W. Lan et al., Appl. Organometallic Chem. 37, 2023, e7168.
272. S. Chaurasiya et al., Medicine in Drug Discovery 22, 2024, 100180.

S. Ilieva, D. Cheshmedzhieva and **T. Dudev**, "Electric field influence on the helical structure of peptides: insights from DFT/PCM computations", *Phys. Chem. Chem. Phys*. **21** (2019) 16198-16206.

273. Riancho, J., et al. Int J Biometeorol 65, 107–117 (2021).
274. Yao Sun, et al., Journal of Applied Physics 128, 235111 (2020).
275. Y. Lee, K. Won Kim, , et al., Small, **16,** 2020, 2003986.
276. M. Wang, et al. Soft Matter, 2020, 16, 8547-8553.
277. Benjamin B. Noble et al., Phys. Chem. Chem. Phys., 2022, 24, 6327-6348.
278. Anastasia Kraskov et al., Biochemistry 2021, 60, 2967–2977.
279. Venelin Enchev, Nadezhda Markova, Int. J. Quantum Chem. 121, 2021, e26760.
280. B. Li et al., J. Agric. Food Chem. 2023, 71, 5614–5629.

T. Dudev, K. Mazmanian, W.-H. Weng, C. Grauffel and C. Lim, "Free and bound lithium in brain signaling", *Acc. Chem. Res*. **52** (2019) 2960-2970.

281. M.S. Shashidhar, N.T.Patil, Carbohydrates Drug Discov Devel. 2020, 283-329.
282. И.С. Лосенков, Е.В. Плотников, Е.В. Епимахова, Н.А. Бохан, Журнал неврологии и психиатрии им С.С. Корсакова, 120 (2020) 108-115.
283. F.X. Theillet, E. Luchinat, Progress in NMR Spectroscopy, 132–133, 2022, 1-112.
284. Bidisha Rajkhowa et al., Pharmaceuticals 2022, 15, 959.
285. Patrick Reith et al., Microorganisms 2022, 10, 590.
286. Lv Wangqiang et al., ALTERNATIVE THERAPIES, 2022, VOL. 28, 58.
287. Stephan Betz, The World in 1 D: The Music of Physics and the Physics of Music, Walnut Creek Consulting, 2021.
288. S.I. Hamstra et al., Curr Neuropharmacol. 2023;21(4):891-910.
289. E. Plotnikov et al., Current Pharm. Biotechnol. 24, 2023, 1623-1629.
290. A.M. Iordache et al., Foods 2024, 13(4), 592.

N. Kircheva and **T. Dudev**, "Novel insights into gallium's mechanism of therapeutic action: a DFT/PCM study of the interaction between Ga^{3+} and ribonucleotide reductase substrates*", J. Phys. Chem. B* **123** (2019) 5444-5451.

291. J. Medina-Franco, et al. (2020) Computational Molecular Bioscience, 10, 1-11.
292. Y. Ding et al. J. Hazard. Mater. 415, 2021, 125719.
293. Alvin L. Crumbliss, Sambuddha Banerjee, J. Inorganic Biochem. 219, 2021, 111411.
294. Yangyang Li et al., ACS Nano 2022, 16, 12786–12800.
295. Ning Yang et al., Front Bioeng Biotechnol. 2023; 11: 1124944.
296. M. Piatek, Ph.D. Thesis, Maynooth University, Ireland, 2023.

S. Pereva, V. Nikolova, S. Angelova, T. Spassov and **T. Dudev**, "Water inside β Cyclodextrin cavity: amount, stability and mechanism of binding", *Beilstein J. Org. Chem*. **15** (2019) 1592-1600.

297. J. Wankar, et al., Adv. Funct. Mater. 30, 2020, 1909049.
298. A. Matencio, et al., Trends in Food Science & Technology, 104, 2020, 132-143.
299. I. Munar, et al. J. Phys. Chem. A 2020, 124, 13, 2580–259.
300. A. Buczek, et al., Int. J. Quantum Chem. 121 (2021) e26487.
301. A.Ignaczak, et al. J. Mol. Liquids, 315, 2020, 113767.
302. D.L. Melnikova et al. Molecules 2020, *25*, 5706.
303. M. Durante et al., Foods 2020, *9*(11), 1553.

304.J. Avvadukkam, et al., J. Heterocyclic Chem. 58, 2021, Pages 724-736.

305.Benkovics, G., Malanga, M., Cutrone, G. et al. Nat Protoc 16, 965–987 (2021)

306.Brian D. Wagner, Host–Guest Chemistry, Supramolecular Inclusion in Solution, In: De Gruyter Textbook, De Gruyter, 2020.

307.O.V. de Oliveira, R.G. Viegas, J. Incl. Phenom. Macrocycl. Chem. 98, 93 (2020).S

308.A.A. Sandilya, et al. ACS Omega, 2020, 5, 25655–25667.

309.L. dos Santos Silva Araújo, et al. Adv. Coll. Interface Science, 289,2021, 102375.

310.Benjamin Gabriel Poulson et al., Polysaccharides 2022, 3(1), 1-31.

311.Meng Yang et al., J. Agric. Food Chem. 2022, 70, 16, 5126–5136.

312.Pooyan Makvandi et al., ACS Omega 2022, 7, 12, 10039–10048.

313.Qonita Kurnia Anjani et al., Pharmaceuticals 2022, 15, 20.

314.T. Sugiyama, S-F. Wang, J. Photochem. Photobiol. C: Photochem. Rev., 52, 2022, 100530.

315.Tsung-Wei Shih et al., Cryst. Growth Des. 2021, 21, 12, 6913–6923.

316.Sakhiran Sakulwech et al., Colloids and Surfaces B: Biointerfaces 220, 2022, 112920.

317.Xingran Kou et al., LWT, 178, 2023, 114589.

318.C.Muñoz-Shugulí et al., Front. Nutr. 2022, 8, doi.org/10.3389/fnut.2021.799779.

319.Chotima Seripracharat et al., J. Drug Delivery Sci. Technol. 68, 2022, 103052.

320.C.P.A. Ancon, L.C.A.Souza, Computat. Theor. Chem. 1217, 2022, 113916.

321.Mary K. Chaves et al. (2022) Pharm. Development Technol., 27:5, 511-524.

322.GholamReza Jafari et al. (2022) Molecular Simulation, 48:2, 168-175.

323.Wanrong Song et al., Molecules 2022, 27(9), 2998.

324.Tânia F. Cova et al., Book “Applications of Biodegradable and Bio-Based Polymers for Human Health and a Cleaner Environment”, Apple Academic Press, 2021.

325.Nuh Yaman, M.Sc. thesis, Trakya Universitesi, Turkey, 2022.

326.Ipek Munar, M.Sc. thesis, Boˇgazi¸ci University, Turkey, 2020.

327.N. Goyal et al., ACS Appl. Nano Mater. 2023, 6, 13766–13791.

328.C. Zagni et al., Mater. Chem. Front., 2023, 7, 2693-2705.

329.Y. Park et al., nd. Eng. Chem. Res. 2023, 62, 11595–11605.

330.C.T.H Tran et al., J Food Sci Technol 60, 1521–1529 (2023).

331.Na Li et al., J. Mol. Structure 1295, 2024, 136686.

332.A.H. Mazurek et al., Molecules 2023, 28(9), 3747.

333.G.S. Varalakshmi et al., Inorg. Chem. Commun. 156, 2023, 111159.

334.B. Chen et al., J.Mol. Liquids 391, 2023, 123362.

335.H. Poudel et al., Bioengineering 2023, 10(9), 1088.

336.Y.-D. Yin et al., Anal. Chem. 2024, 96, 8325–8331.

337.L. Lan et al., Int. J. Biological Macromolecules 262, 2024, 130108.

338.J. Huang et al., Carbohydrate Polymers 333, 2024, 121985.

339.C.T.H. Tran et al., Food Chemistry 433, 2024, 137394.
340.N.S. Alsadun et al., Molecules 2024, 29(11), 2535.
341.L. Alonso et al., Molecules 2023, 28(12), 4709.
342.Y.-X. Ge et al., Int. J. Mol. Sci. 2024, 25(5), 3047.
343. J. Muñoz-Espinoza, G. Barriga-González, J. Chil. Chem. Soc. 68, 2023; http://dx.doi.org/10.4067/s0717-97072023000205857.
344.I.N.I. Ibrahim, S. Asman, Enhanced Knowledge in Sciences and Technology 3 (2023)432-441.

C. Grauffel, **T. Dudev** and C. Lim, „Why Cellular Di/Triphosphates Preferably Bind Mg^{2+} and Not Ca^{2+}", J. Chem. Theor. Comput. 15 (2019) 6992-7003.

345.K.K. Grotz and N. Schweirz, J. Chem. Theory Comput. 2022, 18, 1, 526–537.
346.Hu, X., Lenz-Himmer, MO. & Baldauf, C. Better force fields start with better data: A data set of cation dipeptide interactions. Sci Data 9, 327 (2022).
347.Emma Rossi et al., Phys. Chem. Chem. Phys., 2023, 25, 6102-6111.
348. Rajwinder Kaur et al., Phys. Chem. Chem. Phys., 2022, 29130-29140.
349. R. Lai et al., J. Am. Chem. Soc. 2024, 146, 7628–7639.
350. F. Paoletti et al., Protein Science 32, 2023, e4563

D. Cheshmedzhieva, N. Toshev, M. Gerova, O. Petrov and **T. Dudev**, "Sulfur and Selenium derivatives of suberoyl anilide hydroxamic acid (SAHA) as a plausible HDAC inhibitors: a DFT study of their tautomerism and metal affinity/selectivity", *Bulg. Chem. Commun*. **50** (2018) 228-236.

351. J.S. Alotaibi et al. Pharmaceuticals 2023, 16(3), 367

T. Dudev, S. Ilieva and L. Doudeva, "How an electric field can modulate the metal ion Selectivity of protein binding sites: insights from DFT/PCM calculations", *Phys. Chem. Chem. Phys*. **20** (2018) 24633-24640.

352.Croix J. Laconsay, Ka Yi Tsui and Dean J. Tantillo, Chem. Sci., 2020, 11, 2231-2242.
353.J. Haiech, et al., Biochim. Biophys. Acta (BBA) - Molecular Cell Research, 1866, 2019, 1046-1053.
354.Cheng, Youji, M. Sc. Thesis, Saint Marry's University, Canada, 2019.
355.X.-L.Zhan, et al. ACS Omega 2020, 5, 15325–15334.
356.Catharine Shipps et al., PNAS, 2021 118, e2014139118.
357.Croix J. Laconsay et al. J. Org. Chem. 2021, 86, 1, 731–738.
358.Amina Abula et al., J. Chem. Inf. Model. 2020, 60, 12, 6242–6250.
359.Benjamin B. Noble et al., Phys. Chem. Chem. Phys., 2022, 24, 6327-6348.
360.Caio B. Castro et al. Current Research in Chemical Biology 1, 2021, 100004.

361.Sunayana Mitra et al., J. Phys. Chem. A 2021, 125, 22, 4867–4881.
362.Yubo Liu et al., Progress in Organic Coatings 174, 2023, 107311.
363.Garima Chanana, Kriti Batra; Comput. Theor. Chemistry 1222, 2023, 114051.
364.C. D. Radka and S. G. Aller, Acta Cryst. (2021). F77, 286-293.
365.Sampaio, I.C.F., et al. (2022). Pulsed Electric Field and Ultrasound Applied to Proteins, Enzymes and Peptides. In: Taft, C.A., de Lazaro, S.R. (eds) Research Topics in Bioactivity, Environment and Energy. Engineering Materials. Springer, Cham.
366.Sunayana Mitra, Ph.D. thesis, University of Pittsburgh, 2021
367.F. Gao et al., Small Methods 8, 2024, 2300753.
368. R. Lai et al., J. Am. Chem. Soc. 2024, 146, 7628–7639.
369.G. Chanana, K. Batra, Comput. Theor. Chem. 1222, 2023, 114051.
370.P. Yadav, et al., J Chem Sci 135, 43 (2023).

D. Cheshmedzhieva, N. Toshev, M. Gerova, O. Petrov and T. Dudev, "Hydroxamic acid derivatives as histone deacetylase inhibitors: a DFT study of their tautomerism and metal affinities/selectivities", J. Mol. Modeling 24 (2018) 114

371. S. Geurs et al., J. Med. Chem. 2023, 66, 12, 7698–7729.
372.S. Khatun et al., Computers in Biology and Medicine 175, 2024, 108468.
373. A.I. Uba, K. Yelekçi, Comp. Biol. Chem. 77, 2018, 318.
374. T. Adimulam et al., Int. J. Mol. Sci. 2021, 22, 12952.
375. H. Song et al., Int. J. Mol. Sci. 2020, 21, 4589
376. M. Woźniczka, M. Świątek, Synthesis and Applications in Chemistry and Materials, 107-141 (2024); https://doi.org/10.1142/9789811283208_0004
377. M. Woźniczka, et al. Acta Chimica Slovenica, 66 (2019) 5194.
378. V. Jakubkiene et al., Beilstein J. Org. Chem. 2022, 18, 837–844.
379. P. Kobauri, Ph.D. Thesis, University of Groningen, 2022.
380. J.H. Ma, Ph.D. Thesis, University of California, Berkeley, 2021.

T. Dudev, D. Cheshmedzhieva and L. Doudeva, "Competition between abiogenic Al^{3+} and native Mg^{2+}, Fe^{2+} and Zn^{2+} ions in protein binding sites: Implications for aluminium toxicity", *J. Mol. Modeling* **24** (2018) 55

381.Xiaojun He et al., Dyes and Pigments 174, 2020, 108059.
382.Sandy Sgorlon et al., Italian Journal of Animal Science, 18, 2019 , 1126-1134.
383.Zhigen Li, Ph.D. thesis, The University of Queensland, Australia, 2019.
384.Hina Goyal et al., Sensors 2023, 23(4), 1798.
385.Feng, R., Chen, L. & Chen, K. Ecotoxicology 30, 2056–2070 (2021).
386.M.N. Karpenko et al., Antioxidants 2023, 12(9), 1654.

T. Dudev, C. Grauffel and C. Lim, "How Pb^{2+} Binds and Modulates Properties of Ca^{2+}

Signaling Proteins", *Inorg. Chem.* **57** (2018) 14798-14809.

387. Sachin Katti, Tatyana I Igumenova, Metallomics 12, 2020, 164–172.
388. Cristiano Farace et al., NeuroToxicology, 81, 2020, 80-88.
389. Luca Sauser, Michal S. Shoshan, J. Inorg. Biochem. 212, 2020, 111251.
390. Yuanyuan Fang et al., Food and Chemical Toxicology, 150, 2021, 112063.
391. Dutta, S. et al. Environ Sci Pollut Res 29, 62067 (2022).
392. Gonzalo Ferreira et al. Molecular Aspects of Medicine 87, 2022, 101048.
393. Li, S., Yang, C., Yi, X. et al. Biol Trace Elem Res 201, 282–293 (2023).
394. Qing Han et al., The Journal of Toxicological Sci. 46 (2021) 8.
395. Tagwa A. Mohammed et al. Angew. Chemie Int. Ed. 133, 25, 2021, 12489.
396. Sunayana Mitra et al. J. Phys. Chem. A 2021, 125, 22, 4867–4881.
397. Sohom Kundu et al. Inorg. Chem. 2022, 61, 43, 17007–17011.
398. Azadeh Hekmat et al. Pharmaceutics 2022, 14(12), 2640.
399. Luca Sauser et al. ChemMedChem 17, 2022, e202200152.
400. M. Wyparło-Wszelaki et al., J. Biochem. Mol. Toxicol. 36, 2022, e22964.
401. Farace, C., Fiorito, G., Pisano, A. et al. Neurol Sci 43, 5851–5859 (2022).
402. Claudia S. Cox et al. Australian Journal of Chemistry 75(2) 142-154.
403. Zakharova, M.N et al. Neurochem. J. 15, 410 (2021).
404. Sunayana Mitra, Ph.D. thesis, University of Pittsburgh, 2021.
405. Y.-Y. Zhang et al., Ageing Research Reviews 87, 2023, 101931.
406. L. Ranno, et al., Nat Commun 15, 3820 (2024).
407. F.Takele Geldasa et al., 2023 Phys. Scr. 98 065701.
408. R. Lai et al., J. Am. Chem. Soc. 2024, 146, 7628–7639.
409. T. Kalvoda et al., J. Chem. Phys. 160, 084308 (2024).
410. A. Hekmat, et al., BioNanoSci. (2024); https://doi.org/10.1007/s12668-024-01423-y.
411. M.A. Gallegos-reyes et al., J. Toxicol. Sci., 48 (2023) 481.
412. J.X.B. Sia et al., Nature Commun., 2024; https://doi.org/10.21203/rs.3.rs-3486416/v1

T. Dudev, K. Mazmanian and C. Lim, "Competition between Li^+ and Na^+ in sodium transporters and receptors: Which Na^+-binding sites are "therapeutic" Li^+ targets?", *Chem. Sci.* **9** (2018) 4093-4103.

413. Barbara Zarzycka et al. Pharmacol. Rev. 2019, 71, 571-595.
414. M. Giladi et al., Biochim. Biophys. Acta (BBA) - Bioenergetics, 1860, 2019, 189.
415. Jean Jules Fifen, Noam Agmon, J. Chem. Phys. 150, 034304 (2019).
416. Esteban Suárez-Picado et al., Angew. Chem. Intl. Ed. 59, 2020, 4537-4543.
417. Alexey A. Dyshin**,** Michael G. Kiselev, J. Chem. Eng. Data 2019, 64, 2536–2541.
418. Benjamin C.McIlwain et al., J. Mol. Biol. 432, 2020,1098-1108.
419. Jayasree, E.G., Sukumar, C., Struct Chem (2021). https://doi.org/10.1007/s11224-021-01761-7.
420. Jiali Wang et al., J. Gen. Physiol. (2020) 152: e202012577.
421. Rongfeng Zou et al. WIREs Comp. Mol. Sci. 12, 2022, e1565.
422. Kamil Wojtkowiak et al. Symmetry 2022, 14(4), 691.
423. Patrick Reith et al., Microorganisms 2022, 10(3), 590.
424. K.E. Brock et al., NeuroSci 2023, 4(4), 280-295.

425.M. Bazayeva, et al., Structural Biology 80 (2024) 362.

K. Mazmanian, **T. Dudev** and C. Lim, "How first shell – second shell interactions and metal substitution modulate protein function", Inorg. Chem. 57 (2018) 14052-14061.

426. Yongtong Lao et al., ACS Chem. Biol. 2022, 17, 8, 2088–2098.
427. Vamsi Nallapareddy et al. Proteins 89, 2021, 745-761.
428. R. Malamaci et al., Foods 2024, 13(3), 419.
429. J.E.P. Brandis, Ph.D. Thesis, University of Maryland, Baltimore, 2020

S. Angelova, V. Nikolova and **T. Dudev**, "Divalent metal ions binding to lactose: a DFT computational study", Bulg. Chem. Commun. 50 (2018) 130-134.

430. Jelić, D., et al. J Therm Anal Calorim 148, 4281–4305 (2023)

T. Dudev, C. Grauffel, S.-T. D. Hsu and C. Lim, "How native and non-native cations bind and modulate the properties of GTP/ATP", J. Chem. Theor. Comput. 14 (2018) 3311-3320.

431.E. Rossi et al., Phys. Chem. Chem. Phys., 2023, 25, 6102-6111.

T. Dudev and L. Doudeva, "How the extra methylene group affects the ligation properties of Glu vs. Asp and Gln vs. Asn amino acids: a DFT/PCM study", *J. Mol. Modeling* **23** (2017) 45.

432.Chan Zhong et al., Food Funct., 2018, 9, 594-603.
433.Huimin Guo et al., J. Sci. Food Agricult. 100, 2020, 5569-5576.
434.Xian Chen et al., J. Comp. Chem. 39, 2018, 2307-2315.
435.Ryota Yamagami et al. Biochemistry 2021, 60, 31, 2374–2386.
436.Y. Dong et al. Food Chemistry 430, 2024, 137074.

S.E. Angelova, V.K. Nikolova and **T.M. Dudev**, "Determinants of the host-guest interactions between α-, β- and γ-cyclodextrins and group IA, IIA and IIIA metal cations: a DFT/PCM study", *Phys. Chem. Chem. Phys.* **19** (2017) 15129-15136.

437.Xin Chen et al., Carbohydrate Research, 492, 2020, 107987.
438.Nan Li et al., Environ. Sci.: Nano, 2020,7, 3124-3135.
439.Héloïse Dossmann et al., Inorg. Chem. 2021, 60, 2, 930–943.
440.Liancheng Gu et al., Rapid Commun. Mass Spectr. 35, 2021, e9052.
441.Jordan M. Rabus et al., Phys. Chem. Chem. Phys., 2021, 23, 13714-13723.
442.Shutong Yang et al., Analytica Chimica Acta 1184, 2021, 339017.
443.Cédric Przybylski and Véronique Bonnet, Carbohydrate Polymers 297, 2022, 120019.

444.Robert Paul PELLEGRINELLI, Ph.D. thesis, EPFL, Lausanne, 2021.
445.E. Zlibut et al., Anal. Chem. 2023, 95, 21, 8180–8188.
446.N. Li et al., Separation and Purification Technology 330, Part A, 2024, 125206.

S. Angelova, V. Nikolova, S. Pereva, T. Spassov and **T. Dudev**, "α-Cyclodextrin: How Effectively Can Its Hydrophobic Cavity Be Hydrated?", *J. Phys. Chem. B* **121** (2017) 9260-9267

447.Julia Gebhardt et al., J. Phys. Chem. B 2018, 122, 5, 1608–1626.
448.Shiwei Wang et al., J. Mater. Chem. B, 2018, 6, 4972-4984.
449.Tânia F.Cova et al., Carbohydrate Polymers, 205, 2019, 42-54.
450.Manoj Kumar Banjare et al., J.Mol. Liquids, 299, 2020, 112204.
451.Askar K. Gatiatulin et al., RSC Adv., 2019, 9, 37778-37787.
452.A. Buczek, et al. , Int. J. Quantum Chem. 121 (2021) e26487.
453.A. Ignaczak, et al. J. Mol. Liquids, 315, 2020, 113767.
454.D.L. Melnikova et al. Molecules 2020, 25, 5706.
455.Tanmoy Ghosh *et al*. 2021 Nanotechnology 32 025208.
456.Zhang Zhuge, M. Sc. thesis, Univ. Calgary, Canada, 2019.
457.A.A. Sandilya, et al. ACS Omega, 2020, 5, 25655–25667.
458.Benjamin Gabriel Poulson et al. Polysaccharides 2022, 3(1), 1-31.
459.S. Paolacci et al. Eur. Review Medical Pharmacol. Sci. 2021; 25 (1 Suppl): 90-100.
460.Aditi Roy et al. Journal of Molecular Structure 1247, 2022, 131371.
461.Zhang, S., Li, W., Luan, J. et al. Nat. Chem. 15, 240–247 (2023).
462.M.M.H. Desoky et al., Materials 2023, 16(16), 5540.
463.K. Adachi et al., ACS Omega 2024, 9, 17, 18957–18972.
464.M.F. Mojdehi et al., Results in Engineering 21, 2024, 102020.
465.B. Saha et al., ChemistrySelect 2024, 9, e202302895.
466.A. Sharma et al., ChemistrySelect 2023, 8, e202300417.

S. Angelova, V. Nikolova, N. Molla and **T. Dudev**, "Factors Governing the Host−Guest Interactions between IIA/IIB Group Metal Cations and α-Cyclodextrin: A DFT/CDM Study", *Inorg. Chem*. **56** (2017) 1981-1987.

467.Quevedo, M.A., Zoppi, A., J Incl Phenom Macrocycl Chem 90, 1–14 (2018).
468.Anna Haynes et al. ACS Omega 2019, 4, 18361–18369.
469.Shiwei Yang et al., Anal. Methods**,** 2019, 11, 3829-3836.
470.Xin Chen et al., Carbohydrate Research, 492, 2020, 107987.
471.Siyun Zhang et al., Chinese Chemical Letters, 32, 2021, 642-648.
472.S. Thijs, et al. Phytomanagement of Pollutants in Soil and Groundwater, in Soil and Groundwater Remediation Technologies, CRC Press, 2020.
473.Héloïse Dossmann et al., Inorg. Chem. 2021, 60, 2, 930–943.
474.Liancheng Gu et al., Rapid Commun. Mass Spectr. 35, 2021, e9052.
475.Anna Helena Mazurek and Łukasz Szeleszczuk, Molecules 2022, 27(12), 3874.
476.Cédric Przybylski and Véronique Bonnet, Carbohydrate Polymers 297, 2022, 120019.
477.N. Li et al., Separation and Purification Technology 330, 2024, 125206.

T. Dudev, C. Grauffel and C. Lim, "How Native and Alien Metal Cations Bind ATP: Implications for Lithium as a Therapeutic Agent", *Sci. Rep.* **7** (2017) 42377.

478. Nicholas A. Meanwell, Bioorg. Medicinal Chem. Lett., 27, (2017) 5355-5372.
479. Motahare Sadeghi Googheri et al., J. Mol. Liquids 263 (2018) 158-173.
480. M. Vosahlikova, et al. Biochem. Pharmacol., 156, 2018, 396-397.
481. R. Yamagami et al., Biochemistry 2019, 58, 3971–3979.
482. Amin Hosseinian et al., J. Mol. Liquids 277 (2019) 631-640.
483. Jinrok Oh and Jong-In Hong, Bull. Korean Chem. Soc. 2018, 39, 899–901.
484. Vered Wineman-Fisher et al., J. Chem. Phys. 153, 104113 (2020).
485. Haimovich, A; Goldbourt, A.; Biochimica et Biophysica Acta (BBA) - General Subjects,1864, 2020, 129456.
486. Sean A.Sullivan et al., Arch. Biochem. Biochem. 683 (2020) 108276.
487. Zhou Tian ann Feng Qian, Mol. Pharmaceutics 2021, 18, 1, 267–274.
488. Ewa D. Raczyńska et al., J. Mol. Model. 26 (2020) 93.
489. Anagh Mukherjee et al., J. Phys. Chem. A 2020, 124, 8040–8049.
490. Zuzana Tatarkova et al., Int. J. Mol. Sci. 2020, 21, 8221.
491. Michal Cibulka et al. Int. J. Mol. Sci. 2022, 23(3), 1604.
492. Foroutannejad, S., Good, L.L., Lin, C. et al. Nat Commun 14, 1057 (2023).
493. Anne Labarre et al. J. Chem. Inf. Model. 2022, 62, 4, 1061–1077.
494. Xuanye Leng et al. CHEMNANOMAT 8, 2022, e202200041.
495. Camila Gherardelli et al. Int. J. Mol. Sci. 2022, 23(15), 8733.
496. Emma Rossi et al., Phys. Chem. Chem. Phys., 2023, 25, 6102-6111.
497. Ryan M. L. McFadden et al. Angew. Chemie Intl. Ed. 134, 2022, e202207137.
498. Biao Li et al. Biology of Reproduction, 107, 2022, 1059–1071.
499. Kalyan Immadisetty et al. Biophys. J. 121, 2022, 1134-1142.
500. Patrick Reith et al., Microorganisms 2022, 10(3), 590.
501. David J. Reilley et al. J. Phys. Chem. B 2021, 125, 33, 9480–9489.
502. Torsten Schmenger, Ph.D. thesis, Ruprecht - Karls – University, Heidelberg, 2022.
503. J.M. Delgado et al., J. Chem. Inf. Model. 2024, 64, 2, 378–392.
504. R. Lai et al., J. Am. Chem. Soc. 2024, 146, 11, 7628–7639.
505. J.D. Livingstone et al. Biochemistry and Biophysics Reports 34, 2023, 101461.
506. F. Gao et al., Small, 2024; https://doi.org/10.1002/smll.202310248.
507. F. Paoletti, Biochem Soc Trans (2024) BST20231089; https://doi.org/10.1042/BST20231089
508. S.D. Hiremath et al., Chemistry – An Asian Journal, 2024, e202400291; https://doi.org/10.1002/asia.202400291
509. N. Bgatova et al., Behavioural Brain Research 456, 2024, 114679.
510. T. Schmenger, Ph.D. Thesis, Ruprecht - Karls – University Heidelberg, 2022.

V. Nikolova, S. Angelova and **T. Dudev**, "IIA/IIB group metal cations hosted by β-cyclodextrin: a DFT study", Bulg. Chem. Commun. 49 (2017) 189-194.

511.Shutong Yang et al. Talanta 243, 2022, 123363.

T. Dudev, C. Grauffel and C. Lim, "Influence of the Selectivity Filter Properties on Proton Selectivity in the Influenza A M2 Channel", *J. Am. Chem. Soc*. **138** (2016) 13038-13047.

512.Paul Santner et al., Biochemistry 2018, 57, 5957–596.
513.A.M. Kariev and M.E. Green, Sensors 2018, 18(9), 3143.
514.Juan J. Nogueira and Ben Corry, The Oxford Handbook of Neuronal Ion Channels Edited by Arin Bhattacharjee, Oxford University Press, 2021.
515.Alisher M. Kariev and Michael E. Green, Membranes 2022, 12(7), 718.

T. Dudev and V. Nikolova, "Determinants of Fe^{2+} over M^{2+} (M = Mg, Mn, Zn) Selectivity in Non-Heme Iron Proteins", *Inorg. Chem.* **55** (2016) 12644–12650.

516.Laura Dalle Carbonare et al., Plant Physiol. 2019. DOI: https://doi.org/10.1104/pp.18.01458.
517.Luca Belmonte and Sheref S. Mansy, J. Chem. Inf. Model. 2017, 57, 3162–3171.
518.Xian Chen et al., J. Comp. Chem. 39 (2018) 2307-2315.
519.J.H. Frisk et al. Nucleosides, Nucleotides & Nucleic Acids, 41:12, 1305-1317 (2022).
520.X. Cao et al., Environ Sci Pollut Res 30, 65392–65400 (2023).

T. Dudev, K. Mazmanian, and C. Lim, "Factors controlling the selectivity for Na^{+} over Mg^{2+} in sodium transporters and enzymes", *Phys. Chem. Chem. Phys.* **18** (2016) 16986-16997.

521.Jing-Han Hu et al., RSC Adv., 2017, 7, 29697-29701.
522.A.M. Kariev and M.E. Green, Sensors 2018, 18(9), 3143.
523.Benjamin C. McIlwain et al., J. Mol. Biol. 432 (2020) 1098-1108.
524.Qi Li et al., J. Am. Chem. Soc. 2023, 145, 28038–28048.

V. Nikolova, S. Angelova, N. Markova, and **T. Dudev**, "Gallium as a Therapeutic Agent: A Thermodynamic Evaluation of the Competition between Ga^{3+} and Fe^{3+} Ions in Metalloproteins", *J. Phys. Chem. B* **120** (2016) 2241-2248.

525.Jacek L. Kolanowski et al., Chem. Soc. Rev., 2018, 47, 195-208.
526.Irina Velikyan, Contrast Media & Molecular Imaging, vol. 2018, Article ID 9713691, 24 pages, 2018.
527.Jinxu Qi et al., New J. Chem., 2018,42, 10226-10233.
528.Zhichao Zeng et al., Sensors and Actuators B: Chemical, 250 (2017) 267-273.
529.Natalie Gugala et al., Genes 2019, 10, 34.
530.Jinxu Qi et al., J. Inorg. Biochem. 186 (2018) 42-50.
531.Gugala, Natalie; Ph.D. thesis, University of Calgary, Calgary, Canada, 2019.
532.Jinxu Qi et al., RSC Adv., 2020, 10, 18553-18559.
533.A. Rodríguez-Contreras et al., Surface and Coatings Technology, 403 (2020) 126381.

534.Hao-Yan Yin et al., Angew. Chem. Intl. Ed. 59 (2020) 20147-20153.
535.Alvin L. Crumbliss, Sambuddha Banerjee; J. Inorg. Biochem. 219 (2021) 111411.
536.Mark G. Best, ACS Appl. Bio Mater. 2020, 3, 7589–7597.
537.Christina Eleftheria Tzeliou et al. Molecules 2022, 27(9), 2660.
538.Marika Mosina et al., Acta Biomaterialia 150, 2022, 48-57.
539.Chun-Chun Qu et al., Bioengineering 2022, 9(9), 416.
540.Diego S. Vazquez et al., Dalton Trans., 2022, 51, 17587-17601.
541.Zheng H. et al., (2022), Front. Chem. 10:1017548.
542.F.-Y. Ye et al., Coordination Chemistry Reviews 493, 2023, 215328.
543.A. Rodríguez-Contreras et al., Int. J. Mol. Sci. 2023, 24(10), 8762.
544.B. Murphy et al., Colloids and Surfaces B: Biointerfaces 227, 2023, 113378.
545.M.N. Zavalishin et al., Dyes and Pigments 219, 2023, 111621.
546.O.J. Hills et al., PLoS ONE 2023, 18: e0287191.
547.H. Xu et al. National Science Review, 11, 2024, nwad302.
548.F. Zhao et al., Chemical Physics Letters 839, 2024, 141123.
549.Qi Zhao et al., Biochem. Biophys. Research Commun. 679, 2023, Pages 52-57.

K. Mazmanian, K. Sargsyan, C. Grauffel, **T. Dudev**, and C. Lim, "Preferred Hydrogen-Bonding Partners of Cysteine: Implications for Regulating Cys Functions", *J. Phys. Chem. B* **120** (2016) 10288–10296.

550.Vangelis Agouridas et al., Chem. Rev. 2019, 119, 7328–7443.
551.Saba Parvez et al., Chem. Rev. 2018, 118, 8798–8888.
552.Joana Reis et al., J. Med. Chem. 2018, 61, 4203–4212.
553.Jagpreet Singh Sidhu et al., Sensors and Actuators B: Chemical, 282 (2019) 515-522.
554.Helena W. Qi et al., J. Chem. Inf. Model. 2019, 59, 2199–2211.
555.Emmanuelle Bignon et al., Front. Oncol., 2018, https://doi.org/10.3389/fonc.2018.00272.
556.Esam A. Orabi and Ann M. English, J. Phys. Chem. B 2018, 122, 3760–3770.
557.Katelyn M. Dreux Gregory S. Tschumper, J. Comp. Chem. 40 (2019) 229-236.
558.Bo Yuan et al., Analyst, 2020,145, 1179-1183.
559.Eric S. Wiedner, J. Am. Chem. Soc. 2019, 141, 7212–7222.
560.Segawa, K., et al. Eur Biophys J 48, 361–369 (2019).
561.Teruyuki Miyake et al., Bioconjugate Chem. 2020, 31, 794–802.
562.Victor Yim, Ph.D. thesis, University of Auckland, New Zealand, 2019.
563.Vyshnavi Vennelakanti et al., Chem. Sci., 2021, 12, 1147-1162.
564.Marcello Pignataro et al., Redox Biology, Volume 37, October 2020, 101691.
565.H. van den Bedem and M. A. Wilson, J. Synchrotron Rad. (2019). 26, 958-966.
566.Paul Brünker et al., J. Chem. Phys. 154, 134305 (2021).
567.Batoul Hosseinzadeh at al., Colloids and Surfaces A: Physicochemical and Engineering Aspects, 612 (2021) 125978.
568.Nicholas McGregor, Ph.D. thesis, University of British Columbia, Vancouver, Canada, 2019.
569.Joseph Senan O'Brien, M.Sc. thesis, Georgia Institute of Technology, U.S.A. 2020.
570.Teresa Duda et al., Front. Mol. Neurosci., 2018 https://doi.org/10.3389/fnmol.2018.00430.
571.Debbie S. Retnoningrum et al., J. Struct. Biol. 213 (2021) 107731.

572. Amrita Singh et al., IUBMB Life, 2021, https://doi.org/10.1002/iub.2466.
573. Katelyn Mae Dreux, Ph.D. thesis, University of Mississippi, U.S.A. 2019.
574. Eduard Mas Claret, Ph.D. thesis, University of Surrey, UK, 2020.
575. Helena Qi, Ph.D. thesis, Massachusetts Institute of Technology, U.S.A., 2019.
576. Brunker, P. et al.; J. Chem. Phys. 154 (2021) 134305.
577. Peter A. Ajibade and Solomon O. Oloyede, Int. J. Mol. Sci. 2022, 23(14), 7980.
578. Zamir G. Khan, Pravin O. Patil; Materials Chemistry and Physics 276, 2022, 125383.
579. Diego Garrido Ruiz et al. Biochemistry 2022, 61, 20, 2165–2176.
580. Anukool A. Bhopatkar et al. Biophys. J. 121, 2022, 2107-2126.
581. Jelena M. Živković et al. Cryst. Growth Des. 2022, 22, 1, 148–158.
582. Santiago Movilla et al., J. Chem. Inf. Model. 2021, 61, 9, 4582–4593.
583. Brunella Grassiri et al. Polymers 2022, 14(15), 3170.
584. Mariafrancesca Scalise et al. Int. J. Mol. Sci. 2022, 23(3), 1127.
585. Debashis Ghosh, J. Steroid Biochemistry and Molecular Biology 227, 2023, 106228.
586. Elfriede Dall et al. ACS Catal. 2021, 11, 19, 11885–11896.
587. D.T. S. Ranathunga, H. Torabifard, Phys. Chem. Chem. Phys., 2023,25, 3361-3374.
588. Ishwar Patidar et al. (2023) Journal of Biomolecular Structure and Dynamics, DOI: 10.1080/07391102.2023.2167112.
589. Shamasoddin Shekh et al. Journal of Sulfur Chemistry, 44:1, 74-89 (2023).
590. Oliviero Carugo, Proteins 91, 2023, 395-399.
591. Wai-Po Kong et al. Journal of Structural Biology 214, 2022, 107922.
592. Cecilia Chávez-García et al., J. Chem. Inf. Model. 2022, 62, 3, 668–677.
593. Jelena M. Živković et al., Cryst. Growth Des. 2022, 22, 9, 5198–5205.
594. Marlène Le Tertre et al., Int. J. Mol. Sci. 2021, 22(12), 6412.
595. Gerardo Ferrer-Sueta, Redox Chemistry and Biology of Thiols, 2022, 19-58.
596. Y. Bodnar, C.H. Lillig, Redox Biology 65, 2023, 102832.
597. J.-K. Wang et al., J. Am. Chem. Soc. 2024, 146, 5, 3125–3135.
598. Vidhya Rajalakshmi V. et al., PLoS ONE 18(3): e0282263.
599. L. Huang et al., Biomacromolecules 2024, 25, 5, 2953–2964.
600. L. Héja, et al., Cell Commun Signal 22, 185 (2024).
601. A. Bertrand, et al., Human Molecular Genetics, 33, 2024, Pages 612–623.
602. A.E. Cannon, P.J. Horn, Plant and Cell Physiology, 2023;, pcad163, https://doi.org/10.1093/pcp/pcad163.
603. T. Abaffy et al., Molecular Pharmacology 2024, MOLPHARM-AR-2023-000843; https://doi.org/10.1124/molpharm.123.000843.
604. S. Xu et al. Chem. Commun., 2024, 60, 5606-5609.
605. G.H. Ta et al., Toxicology 503, 2024, 153739.
606. Y. Guo et al., Appl Microbiol Biotechnol 107, 4533–4542 (2023).
607. A.F.T. Waffo et al. J. Am. Chem. Soc. 2023, 145, 25, 13674.
608. M. Takayama, Molecules 2023, 28(23), 7700.
609. S. Shekh, (2022) Journal of Sulfur Chemistry, 44(1), 74–89.
610. N.P.F. Mueller et al. Front. Pharmacol., 2023, Sec. Predictive Toxicology 14. | https://doi.org/10.3389/fphar.2023.1125871
611. P. Ponraj et al. BioRxivm 2024, https://doi.org/10.1101/2024.04.26.591287.
612. L. Heja et al., BioRxivm 2023, https://doi.org/10.1101/2023.07.19.549697

Todor Dudev and Carmay Lim, “Ion selectivity in the selectivity filters of acid-sensing ion channels”, *Sci Rep*. **5** (2015) 7864.

613.Brioche, Julien, et al., J. Am. Chem. Soc. 137 (2015): 6680-6691.
614.Rossana Morabito et al., Sci. Rep. 7, Article number: 41065 (2017).
615.Kai Wang et al., Biophys. J. 119 (2020) 2335-2348.
616.Anping Ji and Yunfei Chen, RSC Adv., 2021, 11, 13806-13813**.**
617.Cédric Vallée et al. Int. J. Mol. Sci. 2021, 22(20), 10998.
618.Fatima R. Ulhuq, Giuseppina Mariano; Microbiology 2022;168:001154.
619.Cédric Vallée et al., Phys. Chem. Chem. Phys., 2022, 24, 13824-13830.
620.Chen, X. et al. Biomedical Materials & Devices (2022).
621.X. Chen et al. Biomedical Materials & Devices 1, 269–285 (2023).

Todor Dudev, Mike Devereux, Markus Meuwly, Carmay Lim, Jean-Philip Piquemal and Nohad Gresh, Todor Dudev, “Quantum-chemistry based calibration of the alkali metal cation series (Li^+ - Cs^+) for large-scale polarizable molecular mechanics/dynamics simulations”, *J. Comp. Chem*. **36** (2015) 285-302.

622.Liu, Jinfeng, et al., J. Chem. Theory Comp. 11 (2015): 5897-5905.
623.Lukas Vlcek and Ariel A. Chialvo, Fluid Phase Equilibria 407 (2016) 58–75.
624.Q. Cui, Journal of Chemical Physics 145, 140901 (2016).
625.Nikolai Manin et al., Phys. Chem. Chem. Phys. 18 (2016) 4191-4200.
626.Zhifeng Jing et al., J. Chem. Phys. **147**, 161733 (2017).
627.Léa El Khoury et al., J. Comp. Chem. 38 (2017) 1897-1920.
628.Emma Ahlstrand et al., J. Chem. Phys. 147, 194102 (2017).

Todor Dudev, Boris Musset, Deri Morgan, Vladimir V Cherny, Susan ME Smith, Karine Mazmanian, Thomas E DeCoursey, Carmay Lim, “Selectivity mechanism of the voltage-gated proton channel, HV1”, *Sci. Rep*. **5** (2015) 10320.

629.Gustavo Chaves et al., The FEBS Journal 283 (2016) 1453–146.
630.Luisa Ribeiro-Silva et al., ACS Chem. Neurosci. 2016, 7 864–869.
631.Okamura Kazuo, Biophysics (Japan) 56 (2016) 154.
632.Siri C. van Keulen et al., J. Phys. Chem. B 2016, DOI: 10.1021/acs.jpcb.6b08339.
633.Aaron L. Randolph et al., eLife 2016;5:e18017.
634.Siri C. van Keulen et al., J. Phys. Chem. B 2017, 121, 15, 3340–3351.
635.Johannes Vierock et al., Sci. Rep. 7, Article number: 9928 (2017).
636.Jens Kuhne et al., PNAS 2019, 116, 9380-9389.
637.Gustavo Chaves et al., FEBS J. 283 (2016) 1453-1464.
638.Ashley L. Bennett and Ian Scott Ramsey, J Physiol. 2017; 595: 6797–6799.
639.Saotome, K., Teng, B., Tsui, C.C. et al. Nat Struct Mol Biol **26,** 518–525 (2019).
640.Myungjin Lee et al., PNAS 2018 115 10321-10326.

641. Roman Fudim et al., Science Signaling 2019: 12, eaav4203.
642. Xingya Li et al., Adv. Mater. 32 (2020) 2001777.
643. Gabriel Kigundu et al., J. Eukar. Microbiol. 65 (2018) 928-933.
644. Alisher M. Kariev and Michael E. Green, J. Phys. Chem. B 2019, 123, 7984–7998.
645. Ashley L. Bennett and Ian Scott Ramsey, J Physiol. 2017; 595: 6803.
646. Zhao, C., Tombola, F., Commun Biol **4,** 261 (2021).
647. J.R. Groome, L. Bayless-Edwards, Front. Pharmacol., 2020 | https://doi.org/10.3389/fphar.2020.00160.
648. Azat Gabdulkhakov et al., J. Biomol. Struct. Dyn.; https://doi.org/10.1080/07391102.2021.1911852.
649. Gustavo Chaves Barboza, Ph.D. thesis, Heinrich Heine University Düsseldorf, 2017.
650. Lea Wobig, Ph.D. thesis, Rheinischen Friedrich-Wilhelms-Universität Bonn, 2020.
651. Erika Artukka, Ph.D. thesis, University of Turku, Finland, 2018.
652. Saleh Riahi Samani, Ph.D. thesis, University of California, Irvine, U.S.A., 2019.
653. Lee, Myungjin; Ph.D. thesis, University of Southern California, U.S.A., 2019.
654. Haq, Saddef, Ph.D. thesis, University of Maryland, Baltimore, U.S.A., 2018.
655. J.T.T. Vierock, Ph.D. thesis, Humboldt-Universität, Berlin, Germany, 2020.
656. V.S. Sokolov et al. Biochim. Biophys Acta (BBA) – Bioenergetics 1862, 2021, 148480.
657. Haonan Qu et al. ACS Appl. Nano Mater. 2022, 5, 10, 14970–14977.
658. Thi Tuong Vy Phan and Myunggi Yi, Molecules 2022, 27(7), 2277.
659. Alisher M. Kariev and Michael E. Green, Membranes 2022, 12(7), 718.
660. Azat Gabdulkhakov et al. J. Biomolecular Structure and Dynamics, 40:18, 8324-8331.
661. Danila Boytsov et al., (2023) Smal l19, 2205968.
662. J.J. Alvear-Arias et al., Front. Pharmacol., 2023, 14 | https://doi.org/10.3389/fphar.2023.11757.
663. Themis Lazaridis, J. Phys. Chem. B 2023, 127, 37, 7937–7945.
664. Gustavo Chaves et al., FEBS Journal 2023, 290, 3436-3447.
665. J.J.A. Arias, Ph.D. Thesis, UNIVERSIDAD DE VALPARAÍSO, Chile, 2023.

S. Pereva, T. Himitliiska, T. Spassov, S.D. Stoyanov, L.N. Arnaudov and **T. Dudev,** “Cyclodextrin-Based Solid-Gas Clathrates”, *J. Agric. Food Chem.* **63** (2015) 6603-6613.

666. Linfan Shi et al., J. Agric. Food Chem. 2017, 65, 2189–2197.
667. Haoqing Ji et al., J. Phys. Chem. C 2017, 121, 20967–20975.
668. Tianxiang Guo et al., Energy Fuels 2017, 31, 4186–4192.
669. Thao M. Ho et al., Food Chemistry 206 (2016) 92-101.
670. Linfan Shi et al., International J. Biol. Macromol. 141 (2019) 947-954.
671. Thao M. Ho et al., International J. Food Properties, 19, 2016, 1696-1707.
672. Thao M. Ho et al., J. Microencapsulation, 33 (2016) 763-772.
673. Linfan Shi et al., International J. Biol. Macromol. 156 (2020) 10-17.
674. Minh Thao Ho, Ph.D. thesis, University of Queensland, Australia, 2017.
675. Thao M. Ho, et al., J. Food Proc. Preserv. 42 (2018) e13514.

676.Xiaolu Cai et al. Gels 2023, 9(2), 83.
677.Ho, T.M., Bhandari, B.R. (2021). Encapsulation of Gases. In: Ho, T.M., Yoshii, H., Terao, K., Bhandari, B.R. (eds) Functionality of Cyclodextrins in Encapsulation for Food Applications. Springer, Cham.
678.T.M. Ho et al., Drying Technology, 2022, 41, 843–858.
679.X. Guo et al., Journal of Renewable Materials . 2023, 11, 777-789.

T. Dudev and C. Lim, "Competition among metal ions for protein binding sites: determinants of metal ion selectivity in proteins", *Chem. Rev.* 114 (2014) 538-556.

680.A.K. Yetisen, et al. Anal. Chem., 2015, 87, 5101–5108.
681.M.J. van Oosten, A. Maggio, Environ. Exp. Botany 111 (2015) 135–146.
682.P. Sun, et al. Scientific Reports 2014, 4, Article number: 5528.
683.P. Li et al. J. Chem. Theory Comput., 2015, 11, 1645–1657.
684.Giulia Palermo et al., Acc. Chem. Res., 2015, 48, 220–228.
685.A.K. Yetisen, Chapter Holographic Sensors, Part of the series Springer Theses pp 85-99, 2014.
686.H.A. Alhazmi et al., J. Pharmaceutical and Biomedical Analysis 107 (2015) 311.
687.Ganga Ram Chaudhary et al., Inorg. Chem., 2015, 54, 9002–9012.
688.M. Salamone, et al. J. Org. Chem., 2015, 80, 9214–9223.
689.Teng-Yao Shih and Shen-Long Tsai, RSC Adv., 2014, 4, 40994-40998.
690.A.W. Foster, et al. J. Biol. Chem. 289 (2014) 28095-28103.
691.P. Li, et al. J. Phys. Chem. B, 2015, 119, 883–895.
692.Chih-Chiang Chang et al., Nucl. Acids Res. 2015, 43: 7612-7623.
693.Robert W. Wheatley et al., Phys. Chem. Chem. Phys., 2015, 17, 10899-10909.
694.Zahra Jafari Chermahini et al., Structural Chemistry 2015, 26, 675-684.
695.Dimitrios Nianios et al., BMC Biochemistry 2015, 16:10.
696.A. Hagège, et al. TrAC Trends in Analytical Chemistry 64 (2015) 64–74.
697.Shinya Tashiro et al., Biochemistry, 2014, 53, 2218–2220.
698.Ondrej Gutten, Lubomír Rulíšek, Phys. Chem. Chem. Phys., 2015, 17, 14393-14404.
699.Y. Valasatava,et al. Scientific Reports 2015, 5, Article number: 9486.
700.Paul Linsdell, Biomolecular Concepts 6 (2015) 191–203.
701.Taka-aki Okamura, et al. J. Am. Chem. Soc., 2014, 136, 14639–14641.
702.Neeru, Dolly Yadav et al., Inorg. Chem., 2014, 53, 5887–5889.
703.H. Choi, et al. Acta Cryst. 2015, D71, 2054-2065.
704.Amr Atef El-Sayed, et al. Desalination and Water Treatment, 2015, 56, 1010-1019.
705.Taka-aki Okamura, et al. Dalton Trans., 2015, 44, 7512-7523.
706.E.T. Mendenhall, M.Sc. Thesis, Paper 927, Marshall University, U.S.A., 2015.
707.Chanel R. Easley et al., Eur. J. Inor. Chem. 2015 (2015) 2092–2100.
708.Matthias J. Knape et al., ACS Chem. Biol., 2015, 10, 2303–2315.
709.M. Cianci, et al. RSC Adv., 2014, 4, 36771-36776.
710.Caidan Zhang et al., Dyes and Pigments 123 (2015) 380–385.
711.Maguerroski, Kamila dos Santos, MS thesis, University of Sao Paolo, Brazil, 2014.

712.Hendrik Küpper and Elisa Andresen, Metallomics 8 (2016) 269-285.
713.F. Leonarskia, et al. Inorganica Chimica Acta 452 (2016) 82–89.
714.P. Koley, et al. ACS Appl. Mater. Interfaces, 2016, 8, 2380–2392.
715.Elisa Andresen et al., New Phytologist 210 (2016) 1244.
716.R.D. Parra, Mol. Phys. 114 (2016) 1485.
717.Bosmat Refaeli et al., Biochemistry 2016, 55, 1673–1676.
718.M. Ropo, V. Blum and C. Baldauf, Sci. Rep. 2016; 6: 35772.
719.Remi Poirot et al. ChemPhysChem 17 (2016) 2112.
720.Yuri Kutin et al., Journal of Inorganic Biochemistry 162 (2016) 164–177.
721.Kim, Woo-Sik et al., J. Nanoscience and Nanotechnology 16 (2016) 6930-6935.
722.Gurpreet Kaur et al., RSC Advances 62 (2016) 57084-57097.
723.C. Ing and R. Pomès, Current Topics in Membranes 78 (2016) 215–260.
724.C. E. Bartman, H. Metwally, L. Konermann, Anal. Chem. 2016, 88, 6905–6913.
725.W. Maret, Metallomics: A Primer of Integrated Biometal Sciences, Imperial; College Press, London, UK, 2016.
726.Matthew L. Harty, M.Sc. Thesis, Dalhousie University, Halifax, Nova Scotia, 2015.
727.Saba Pirnia, Ph.D. Thesis, Brock University, St. Catharines, ON, U.S.A. 2016.
728.Michael J. Mashock, Ph.D. Thesis, Milwaukee, Wisconsin, U.S.A., 2016.
729.Jiong Wang et al., Chem. Commun. 2016, 52, 13409-13412.
730.R.W. Wheatley, et al. Archives of Biochemistry and Biophysics 590 (2016) 125–137.
731.Nikolai Manin et al., Phys. Chem. Chem. Phys. 18 (2016) 4191-4200.
732.A. Rosato, Y. Valasatava, C. Andreini, Int. J. Mol. Sci. 2016, 17, 671.
733.Pradyot Koley et al., RSC Adv. 89 (2016) 86607-86616.
734.S.L. Gupta et al., Rapid Comm. Mass Spectrometry 30 (2016) 1313.
735.S.M. Wagoner et al., J. Mass Spectr. 51 (2016) 1120.
736.Marco de Vivo, Workshop Modeling activity vs. selectivity in metalloproteins, CECAM-FR-IDF, 2015.
737.Daniel Bim et al., Chem. Listy 110 (2016) 354-364.
738.Zao Wang et al., Adv. Sci. 6 (2019) 1801182.
739.Baile Wu et al., Environ. Sci. Technol. 2020, 54, 50–66.
740.J. Zhang, et al. Briefings in Bioinformatics, Volume 20, 2019, 1250–1268.
741.Mario Prejanò et al., Chem. Eur. J. 23 (2017) 8652-8657.
742.Bloom, A.J., Lancaster, K.M. Nature Plants **4,** 414–422 (2018).
743.Zhifeng Jing et al., PNAS 2018, 115, E7495-E7501.
744.Wei Yang and Luhua Lai, Curr. Opin. Struct. Biol. 45 (2017) 67-73.
745.R.M.Freire et al., Sensors and Actuators B: Chemical, 255 (2018) 2725-2732.
746.Zhifeng Jing et al., J. Chem. Phys. **147**, 161733 (2017).
747.Agnès Hagège et al., TrAC Trends in Analytical Chemistry, 64 (2015) 64-74.
748.Matthias J Knape et al., Metallomics, 9, 2017, 1576–1584.
749.Nicholas J. Schnicker et al., Biochemistry 2017, 56, 2873–2885.
750.Jiazhi He et al., Chem. Eur. J. 24 (2018) 3052-3057.
751.Chunlei Su et al., Environmental and Experimental Botany 142 (2017) 24-33.
752.P. Zhang,et al. Briefings in Bioinformatics, 19, 2018, 524–536.
753.Xiaoran Roger Liu et al., Chem. Rev. 2020, 120, 4355–4454.

754. M. Jeżowska-Bojczuk, K. Stokowa-Sołtys, Eur. J. Med. Chem. 143 (2018) 997-1009.
755. Lukas Gritsch et al., J. Mater. Chem. B, 2019, 7, 6109-6124.
756. Jingjing Guo et al., Anal. Chem. 2018, 90, 12292–12298.
757. Yetisen A.K. (2015) Holographic Metal Ion Sensors. In: Holographic Sensors. Springer Theses (Recognizing Outstanding Ph.D. Research). Springer, Cham.
758. Romana Schober et al., Science Signaling, 2019: 12, eaax3194.
759. Zhifeng Jing et al., J. Chem. Phys. **147**, 161733 (2017).
760. Agnès Hagège et al., TrAC Trends in Analytical Chemistry, 64 (2015) 64-74.
761. Matthias J Knape et al., Metallomics, 9, 2017, 1576–1584.
762. Nicholas J. Schnicker et al., Biochemistry 2017, 56, 2873–2885.
763. Jiazhi He et al., Chem. Eur. J. 24 (2018) 3052-3057.
764. Chunlei Su et al., Environmental and Experimental Botany 142 (2017) 24-33.
765. Akshaya K. Das et al., J. Chem. Theory Comput. 2018, 14, 6722–6733.
766. Zeling Xu et al., J. Biol. Chem. 294 (2019) 16978-16991.
767. Xiankun Cheng, et al., Nucleic Acids Research, 47, 2019, 4308–4318.
768. Vladimir Sladek and Igor Tvaroška, J. Phys. Chem. B 2017, 121, 6148–6162.
769. Sidsel Birkelund Schmidt et. al., Plants 2019, 8, 381.
770. Caidan Zhang et al., ACS Omega 2019, 4, 14633–14639.
771. Elisa Bellomo et al., J. Am. Chem. Soc. 2018, 140, 4446–4454.
772. Wenli Huang et al., Ecotoxicology and Environmental Safety, 171 (2019) 894-903.
773. Suma K. Pawar and Seetharamappa Jaldappagari, J. Pharm. Anal. 9 (2019) 274-283.
774. Rui Qi et al., J. Phys. Chem. B 2018, 122, 6371–6376.
775. Damaris Lorenzo-Gutiérrez et al., Metallomics 11, 2019, 1230–1240.
776. Jiong Wang et al., Chem. Commun., 2016, 52, 13409-13412.
777. Ganasen, M., Togashi, H., Takeda, H. et al. Commun Biol 1, 120 (2018).
778. Eom, H., Song, W.J., J Biol Inorg Chem 24, 517–531 (2019).
779. Suman Kalyan et al., ACS Sustainable Chem. Eng. 2019, 7, 12304–12314.
780. Yu Qiao et al., Chem. Phys. Lett. 709 (2018) 116-124.
781. Fuchs, A.C.D., Maldoner, L., Wojtynek, M. et al. Nat Commun 9, 2696 (2018).
782. Nogueira LS et al., 2017. *PeerJ* 5:e3141.
783. Jun Ohta and Masako Ohmura, Legal Medicine 28 (2017) 54-58.
784. Itziar Guerrero and Prof. Arkaitz Correa, Asian J. Org. Chem. 9 (2020) 898-909.
785. H. Li, D. Pi, Y. Wu and C. Chen, IEEE Access, 5, 14647-14656, 2017.
786. Arnold J. Bloom, Current Opin. Struct. Biol. 49 (2019) 33-38.
787. Shailender Kumar Verma et al., J. Inorg. Biochem. 170 (2017) 63-74.
788. M.J. Knape, F.W. Herberg; Biochem Soc Trans 15 June 2017; 45: 653–663.
789. Agnieszka Rodzik et al., Int. J. Mol. Sci. 2020, 21, 2156.
790. E. Duboué-Dijon et al., J. Chem. Phys. 153, 050901 (2020).
791. Ramesh Singh et al., Chem. Select 4 (2019) 5810-5816.
792. Shanti Swaroop Srivastava et al., Biochemistry 2017, 56, 1299–1310.
793. R.S. Eisenberg, 2019 Classical Physics arXiv:1904.09695; DOI: 10.31224/osf.io/urxgs.
794. De Lillo, A., Cardi, M., Landi, S. et al. Sci Rep 8, 13481 (2018).
795. Griese, J.J., Kositzki, R., Haumann, M. et al. J Biol Inorg Chem 24, 211–221 (2019).

796. Król E, et al. (2017) PLoS ONE 12(3): e0174713.
797. Eva-Maria Schneeberger and Kathrin Breuker, Chem. Sci., 2018, 9, 7338-7353.
798. Bin Sun et al., J. Chem. Theory Comput. 2019, 15, 2692–2705.
799. Alhazmi, H. A. et al. Die Pharmazie - An International Journal of Pharmaceutical Sciences, 72, 2017, 243-248.
800. Jung, Jaejoon; Lee, Sang Jun, J. Microbiol. Biotechnol. (2019) 29,1522 - 1542.
801. Urbina, J., Patil, A., Fujishima, K. et al. Sci Rep **9,** 16422 (2019).
802. Amolegbe, S.A., et al. J Biol Inorg Chem 22, 1–18 (2017).
803. Rui Qi et al., J. Phys. Chem. B 2019, 123, 6034–6041**.**
804. Laurel Hoffman et al., Biochemistry 2017, 56, 2149–2160.
805. Lee, M., Rozeboom, H.J., Keuning, E. et al. Biotechnol Biofuels 13, 5 (2020).
806. Oksana Danylyuk, CrystEngComm, 2017, 19, 3892-3897.
807. Christina Marie Burden, Ph.D. thesis, Arizona State University, U.S.A., 2016.
808. Shuangli Du et al., J. Chem. Theory Comput. 2019, 15, 1841–1847.
809. Xin Xu et al., Langmuir 2019, 35, 15564–15572.
810. Maria de Andrade Gomes et al., J. Nanomaterials, 2018, Article ID 5167182.
811. Kazutaka Kusunoki et al., Soil Sci. Plant Nutrition 64 (2018) 469-481.
812. Irene O'Callaghan et al., Chemisphere 235 (2019) 498-509.
813. William Foster et al., Nanoscale, 2020, 12, 5452-5463.
814. Elisa Andresen et al., J. Exp. Botany, 71, 2020, 1628–1644.
815. Harald Zänker et al., Inorg. Chem. 2019, 58, 4173–4189.
816. Geoffrey W. Grime et al., J. Am. Chem. Soc. 2020, 142, 185–197.
817. Rima Roy et al., Metallomics, 2018,10, 1476-1500.
818. Lygia Sega Nogueira et al., Marine Environ. Res. 135 (2018) 136-144.
819. Soha Ahmadi et al., J. Inorg. Biochem. 205 (2020) 110987.
820. Shiran Barber-Zucker et al., FEBS J. 286 (2019) 2193-2215.
821. Susmita De et al., Phys. Chem. Chem. Phys**.**, 2018, 20, 17517-17529.
822. CJ. J. Griese and M. Högbom, Acta Cryst. (2019). D75, 764-771.
823. Lili Zhang et al., New J. Chem**.**, 2019, 43, 3071-3077.
824. Deliang Chen et al., Phys. Chem. Chem. Phys., 2019, 21, 205-216.
825. G. Berggren, et al., in Encyclopedia of Inorganic and Bioinorganic Chemistry, Wiley, 2017,doi.org/10.1002/9781119951438.eibc2480.
826. Effie C. Kisgeropoulos et al., J. Am. Chem. Soc. 2020, 142, 5338–5354.
827. Yaqin Zhao Xiaojuan Guo and Binsheng Yang, RSC Adv., 2017, 7, 10206-10214.
828. Pejaver, V., Urresti, J., Lugo-Martinez, J. et al. Nat Commun 11**,** 5918 (2020).
829. Nor Ain Fathihah Abdullah, Lee Sin Ang, Acta Chim. Slovenica, 65 (2018) 231-238.
830. Leanne M. Martin; Lars Konermann, J. Am. Soc. Mass Spectrom. 2020, 31, 25–33.
831. Lin Frank Song et al., J. Am. Chem. Soc. 2020, 142, 6365–6374.
832. Karl J. Koebke et al., J. Inorg. Biochem. 203 (2020) 110882.
833. Sharma A, Sharma D, Verma SK. 2019, R. Soc. open sci. 6: 19036.
834. Shelley D Copley 2020 Phys. Biol. 17, 051001.
835. Jiří Janda and Jitka Tichá, J. Environ. Radioact. 192 (2018) 181-186.
836. Barber-Zucker, S., Shahar, A., Kolusheva, S. et al., Sci Rep 10, 14022 (2020).

837.Yousef, E.N. et al., J. Vis. Exp. (151), e60102.
838.Sarah Höhn et al., Adv. Mater. Interfaces 7 (2020) 2000420.
839.Yuki Amano et al., Polymer 137 (2018) 169-172.
840.Jure Borišek and Alessandra Magistrato, ACS Catal. 2021, 11, 4319–4326.
841.A.T Yuan, et al. Metallomics, 12, 2020, 767–783.
842.Toshiyuki Kowada et al., Cell Chem. Biol. 27 (2020) 1521-1531.
843.Li, M., Henderson, K.L., Martinez, S. *et al.* J Biol Inorg Chem 23, 785–793 (2018).
844.Sirikan Maneesuwannarat et al., Minerals Engin. 137 (2019) 207-216.
845.Mahsa Abareghi and Ezat Keshavarzi, J. Mol. Liquids 302 (2020) 112283.
846.Xin Lin et al., Microorganisms 2019, 7, 232.
847.Al Mokhtar Lamsabhi et al., J. Phys. Chem. A 2019, 123, 6241–6250.
848.Lalita Uribe et al., Chem. Eur. J. 24 (2018) 5074-5077.
849.Daniel G.J. Smethurst et al., J. Biol. Chem. 295 (2020) 17200-17214.
850.J.S. BALDUINO, Ph.D. thesis, Universidade Federal de Alfenas, Brasil, 2018.
851.John P. Lisher, Ph.D. thesis, Indiana University, U.S.A. 2016.
852.Enxian Shi et al., J. Rare Earths 36 (2018) 203-208.
853.X. Yu et al., Xenobiotica 2021, https://doi.org/10.1080/00498254.2021.1922781.
854.Zhihao Li et al., ACS Nano 2020, 14, 16085–16095.
855.Nadine Freifrau Von Maltzahn et al., Eur Endod J. 2020; 5: 40–45.
856.Shiran Barber-Zucker et al., RSC Chem. Biol., 2021, 2, 486-498.
857.Knop, Matthias, Doctoral Thesis, University of Basel, Switzerland, 2017.
858.M.O. Fashola, Ph.D. thesis, North-West University, South Africa, 2017.
859.Hong Zhang et al., J. Phys. Chem. Lett. 2021, 12, 3281–3287.
860.Mörman, Cecilia, Ph.D. thesis, Stockholm University, Sweden, 2020.
861.M.D. Ritz, Undergraduate Honors Thesis, College of William and Mary, U.S.A., 2017.
862. Gugala, Natalie; Ph.D. thesis, University of Calgary, Calgary, Canada, 2019.
863.Hui Li, Ph.D. thesis, University of Akron, U.S.A., 2019.
864.Sushanta Debnath, Abhijit Chakrabarti, Biophys. Chem. 269 (2021) 106527.
865.Noah Belkhayat, M.Sc. thesis, Virginia Commonwealth University, U.S.A. 2016.
866.Zhen Li et al., J. Chem. Theory Comput. 2021, 17, 2342–2354.
867.Rui Qi, Ph.D. thesis, University of Texas at Austin, U.S.A. 2018.
868.R. Balhara, R. Chatterjee, G. Jindal, Phys. Chem. Chem. Phys., 2021,23, 9500-9511.
869.Alexander E. Yarawsky, Andrew B. Herr, J. Biol. Chem. 295 (2020) 12840-12850.
870.Markus SCHNEIDER, Ph.D. thesis, ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE, Switzerland, 2018.
871.Alessia De Lillo, Ph.D. thesis, Università Degli studi di NAPOLI “FEDERICO II”, Italy.
872.R.S. Eisenberg, arXiv, https://arxiv.org/abs/1904.09695, DOI: 10.13140/RG.2.2.30402.02249, 2019.
873.E.D. Spoerke, Programmable Nanocomposite Membranes for Ion-Based Electrical Energy Storage. United States: N. p., 2016. Web. doi:10.2172/1599531.
874.G. Wróblewski, et al J Mater Sci: Mater Electron 30, 12465–12474 (2019).
875.Jana Královičová, et al., Nucleic Acids Research, 49, 2021, 2460–2487.

876.Patrick Diep et al., Anal. Biochem. 609 (2020) 113836.
877.Elison Kalman, Grim; M.SC. thesis, Uppsala University, Sweden, 2019.
878.Zhen Li et al., J. Chem. Theory Comput. 2020, 16, 4429–4442.
879.Barwinska-Sendra, Anna Maria, Ph.D. thesis, Newcastle University, UK, 2018.
880.SCOTT, ANDREW, JAMES, PETER, Ph.D. thesis, Durham University, UK, 2018.
881.Vieira, J.C.S., et al. Biol Trace Elem Res 197, 667–675 (2020).
882.Zhenyang Zhang et al. (2021) Biofouling, 37:2, 222-234.
883.S.Houwaart, Ph.D. thesis, Albert-Ludwigs-Universität Freiburg, Germany, 2016.
884.Yusong Tu et al., Phys. Rev. E 101, 022410 (2020).
885.Abdul Malik et al., Phys. Chem. Chem. Phys.**,** 2020, 22, 14551-14559.
886.Pabbathi, N.P.P., Velidandi, A., Tavarna, T. et al. Biomass Conv. Bioref. (2021).
887.Hassan A. Alhazmi et al., Acta Biochim. Polonica, Vol. 68 No. 1 (2021).
888.Sérgio F. Sousa et al., ACS Catal. 2020, 10, 8444–8453.
889.Erika Bellini et al., Plants 2021, *10*, 770.
890.Bower, Edward Kenneth Merrick, Ph.D. thesis, University of Edinburgh, UK, 2017.
891.Ashfaq Ur Rehman et al., Phys. Chem. Chem. Phys.**,** 2021, https://doi.org/10.1039/D0CP06360F.
892.Nicholas Jay Schnicker, Ph.D. thesis, University of Iowa, U.S.A., 2017.
893.Stefan Schmollinger et al., PNAS 2021, 118, e2026811118.
894.Ziyu Deng et al., J. Agric. Food Chem. 2020, 68, 13990–14000.
895.L. Gritsch, Ph.D. thesis, Friedrich-Alexander-Universität Erlangen-Nürnberg, 2019.
896.L. Bütof, Lucy, Ph.D. thesis, Martin-Luther-Universität Halle-Wittenberg, 2018.
897.Denise Pinkert, Ph.D. thesis, Humboldt-Universität zu Berlin, Germany, 2018.
898.Francois-Xavier Theillet, Chem. Rev. 2022, 122, 10, 9497–9570.
899.Meng Du et al., Chemical Engineering Journal 442, 2022, 136147.
900.Choi, T.S., Tezcan, F.A. Nature 603, 522–527 (2022).
901.Emily R. Featherston et al. J. Am. Chem. Soc. 2021, 143, 35, 14287–14299.
902.Lin Wei et al. J. Med. Chem. 2022, 65, 7, 5528–5538.
903.Mitchell R. Slobodian et al. Toxics 2021, 9(10), 269.
904.Feehan, R., Franklin, M.W. & Slusky, J.S.G. Nat Commun 12, 3712 (2021).
905.Stephan Clemens, Journal of Experimental Botany, 73, 2022, 1688–1698.
906.Chenghao Ge et al. Science of The Total Environment 838, Part 3, 2022, 156401.
907.Tae Su Choi, and F. Akif Tezcan, J. Am. Chem. Soc. 2022, 144, 39, 18090–18100.
908.Sina Hassanjani Saravi et al. J. Phys. Chem. B 2022, 126, 15, 2891–2898.
909.Andrew W Foster et al. Metallomics, 14, 2022, mfac058.
910.Jackson Geary at al. J. Am. Chem. Soc. 2021, 143, 27, 10317–10323.
911.Yue Yu et al. Molecules 2022, 27(4), 1277.
912.Elisa Andresen et al. Journal of Hazardous Materials 442, 2023, 130062.
913.Shaopei Jia et al. International Journal of Hydrogen Energy 47, 2022, 24796-24806.
914.Md Shofiul Alam et al. Metallomics, 14, 2022, mfac039.
915.Liang Yao et al. Nanoscale, 2022,14, 17277-17289.
916.Diessl, J., Berndtsson, J., Broeskamp, F. et al. Nat Commun 13, 6061 (2022).
917.Jana Královičová et al. Nucleic Acids Research, 49, 2021, 2460–2487.
918.Johan Pääkkönen et al. Biochemistry 2021, 60, 41, 3046–3049.

919.Abdul Basit et al. J. Chem. Inf. Model. 2022, 62, 11, 2821–2834.
920.Abhishek Kumar and Priyadarshi Satpati, J. Phys. Chem. B 2021, 125, 11943–11954.
921.Jure Borišek and Alessandra Magistrato, ACS Catal. 2021, 11, 7, 4319–4326.
922.Ali Mawof et al. Sustainability 2022, 14(9), 5665.
923.Zhen Li et al. J. Chem. Theory Comput. 2023, 19, 2, 619–625.
924.Briana T. A. Boychuk et al. J. Chem. Theory Comput. 2021, 17, 8, 5392–5408.
925.Sunayana Mitra et al. J. Phys. Chem. A 2021, 125, 22, 4867–4881.
926.Xiao-Lan Huang, New J. Chem., 2022,46, 15273-15291.
927.Mezbah Uddin et al. Coatings 2022, 12(5), 673.
928.Rosario Valenti et al. Protein Science 31, 2022, e4423.
929.Xiuxiu Jia et al. Separation and Purification Technology 306, 2023, 122713.
930.Theodore Gerard et al. ACS Omega 2023, 8, 4, 3835–3841.
931.Rajwinder Kaur et al. Phys. Chem. Chem. Phys., 2022,24, 29130-29140.
932.A. Kumar, P. Satpati, Phys. Chem. Chem. Phys., 2022,24, 24192-24202.
933.J. Čapek, B. Večerek, Front. Cell. Infect. Microbiol., 2023, 13, https://doi.org/10.3389/fcimb.2023.943390.
934.Carvalho, L. (2022). Copper-Organic Complexes Synthetized Electrochemically. In: Beyond Copper Soaps. SpringerBriefs in Applied Sciences and Technology. Springer, Cham.
935.Xinyu Teng et al. iScience 25, 2022, 105565.
936.Irena Kostova, Inorganics 2023, 11(2), 56.
937. M. Lella, R. Mahalakshmi, Protein Science 113 , 2021, e24240.
938.Saini, R., et al. Bioenerg. Res. (2022), https://doi.org/10.1007/s12155-022-10521-2
939.Victoria N. Syryamina et al. Chemosensors 2022, 10(2), 71.
940.A. Gołębiowski et al. Journal of Molecular Structure 1270, 2022, 133940.
941.J. Zhang, F. Zhou, X. Liang and G. Yang, "SCAMPER: accurate type-specific prediction of calcium-binding residues using sequence-derived features," in IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2022, doi: 10.1109/TCBB.2022.3173437.
942.Moosavi-Movahedi et al. *J IRAN CHEM SOC* **19**, 475–487 (2022).
943.M. Li, et al., Machine Learning in Bioinformatics of Protein Sequences, pp. 265-287 (2023), World Scientific
944.Manran Wu et al., Chinese Chemical Letters 33, 2022, 3492-3496
945.K. Balamurugan and M.T. Pisabarro, ACS Omega 2021, 6, 39, 25350–25360.
946.Junmei Hu Frisk, et al. (2022) Nucleosides, Nucleotides & Nucleic Acids, 41:12, 1305.
947.Shuwei Jin at al. Chinese Journal of Chemical Physics **34**, 741 (2021)
948.M. S. Shoshan, Chimia 2022, 76, 744, DOI: 10.2533/chimia.2022.744.
949.Norhafiza Ilyana Yatim et al., Malaysian J. Analytical Sciences, 26 (2022): 16 - 28
950.Paul W. Johns et al. International Dairy Journal Volume 114, March 2021, 104912
951.O'Callaghan, I. 2022. PhD Thesis, University College Cork.
952.РОЖКОВ С.П, АКТУАЛЬНЫЕ ВОПРОСЫ БИОЛОГИЧЕСКОЙ ФИЗИКИ И ХИМИИ Том: 6, 2021 Страницы: 330-339.
953.Jutta Diessl, Ph.D. thesis, Stokholm University, 2021.
954.Sunayana Mitra, Ph.D. thesis, University of Pittsburgh, 2021.

955.Stephanie Michelle Thibert, Ph.D. thesis, Arizona State University, 2021.
956.Ali Mawof, Ph.D. thesis, McGill University, 2021.
957.Jurković, J., et al. (2022). Trichloroacetic and Nitric Acid Extraction of Ca, Mg, Fe, Zn, Na and K from Whey Samples. In: , *et al.* 10th Central European Congress on Food. CE-Food 2020. Springer, Cham.
958.Johan Pääkkönen, Ph.D. thesis, University of Eastern Finland, 2021.
959.MENILLA MARIA ALVES DE MELO, Ph.D. thesis, Universidade Federal do Rio Grande do Norte, Brazil, 2021.
960.Feng H et al. Front Microbiol. 2022 Nov 29;13:1084530.
961.S. Ray et al., (2023) eLife 12:e84006.
962.Hyunuk Eom et al., J. Am. Chem. Soc. 2023, 145, 10, 5880–5887.
963.J. Wang et al., Advances in Colloid and Interface Science 318, 2023, 102964.
964.Elisa Andresen et al., Journal of Hazardous Materials 442, 2023, 130062.
965.Omar Naneh et al., Front. Immunol., 2023, 14| https://doi.org/10.3389/fimmu.2023.1181020.
966. Dara Bakhtiar et al., Nucleic Acids Research, 52, 2024, 1090–1106.
967.X. Fang et al., Environmental Research 243, 2024, 117816.
968.X. Jia et al., Separation and Purification Technology 306, 2023, 122713.
969.X. Xu et al., Advanced Functional Materials 2023, 33, 2306215.
970.J. Ma et al., Environmental Research 236, 2023, 116798.
971.P. Zhang et al., Nat Commun 14, 5592 (2023).
972.M. Pan et al., J. dental Res., 2023, 102, https://doi.org/10.1177/0022034523116.
973.A.M. Hoffnagle, F.A. Tezcan, J. Am. Chem. Soc. 2023, 145, 26, 14208–14214.
974.W.J. Jeong et al., Acc. Chem. Res. 2023, 56, 18, 2416–2425.
975.H. Fu et al., J. Am. Chem. Soc. 2023, 145, 36, 19554–19560.
976.Y. Ding, J. Huang, J. Phys. Chem. Lett. 2024, 15, 2, 616–627.
977.R. Lai et al., J. Am. Chem. Soc. 2024, 146, 11, 7628–7639.
978.Y. Tian et al., Appl Microbiol Biotechnol 107, 5269–5279 (2023).
979.S. Zhao et al., ACS Materials Lett. 2024, 6, 3, 738–747.
980.Rashmi R. Samal, Umakanta Subudhi, Chemosphere 357, 2024, 142090.
981.X. Ma et al., International Journal of Hydrogen Energy 60, 2024, 845-866.
982.X. Hu et al., Chemical Engineering Journal, Available online 24 May 2024, 152317.
983.Versha Pandey et al., Journal of Hazardous Materials Advances 10, 2023, 100274.
984.P. Kumar, S. Das, ACS Appl. Eng. Mater. 2023, 1, 5, 1343–1355.
985.J. Gao et al., Inorg. Chem. 2023, 62, 34, 13812–13823.
986.Hieu D. Nguyen et al., Chem. Sci., 2023, 14, 10264-10272.
987.X. Liu et al., Journal of Hazardous Materials 473, 2024, 134662.
988.M.N. Afridi et al., J. Water Process Engineering 63, 2024, 105530.
989.M. Hou et al., Front. Bioeng. Biotechnol. 2023, 11, | https://doi.org/10.3389/fbioe.2023.1142873.
990.Y. Yang et al., J. Environmental Chemical Engineering 12, 2024, 112571.
991.K.A. Shisler et al. (2024) mBio 15:e02987-23.
992.X. Hu et al., J. Chem. Theory Comput. 2024, 20, 3, 1448–1464.
993.Y. Matsui et al., Chem. Commun., 2023, 59, 7048-7051.

994.R. Saini et al., Bioenerg. Res. 16, 1769–1776 (2023).
995.T. Zhang et al., Ecotoxicology and Environmental Safety 264, 2023, 115394.
996.Max Klotzsche et al., Analyst, 2023,148, 4668-4676.
997.Mantas Liutkus et al., Protein Science 2024, 33, e4971.
998.P. Diep et al., The FEBS Journal 2024, https://doi.org/10.1111/febs.17125.
999.M.J. Stevens, S.L.B. Rempe, Phys. Chem. Chem. Phys., 2023,25, 29881-29893.
1000. Kiomars Zargoosh et al., Reactive and Functional Polymers 193, 2023, 105757.
1001. Y. Liu et al., Food Chemistry: X 18, 2023, 100692.
1002. Siti Fatimah Nur Abdul Aziz et al., Enzyme Microbial Technol. 178, 2024, 110439.
1003. Sai S. Patkar et al., Chemistry – A European Journal 2024, 30, e202400582.
1004. Upendra Nayek et al., RSC Adv., 2023, 13, 36261-36279.
1005. P. Diep et al., Analytical Biochemistry 676, 2023, 115182.
1006. José P. Leite et al., Journal of Structural Biology 215, 2023, 108038.
1007. Q. Wen et al., Sustainability 2023, 15(22), 16053.
1008. X.-L. Huang, iScience 27, 2024, https://doi.org/10.1016/j.isci.2024.109555.
1009. L. Leone et al., Journal of Peptide Science, 2024, e3606; https://doi.org/10.1002/psc.3606.
1010. S. Schmollinger et al., Metallomics, 15, 2023, mfad025.
1011. T. Gerard et al., ACS Omega 2023, 8, 4, 3835–3841.
1012. Li, Zhen, Ph.D. Thesis, Michigan State University, 2023.
1013. Diep, Patrick, Ph.D. Thesis, University of Toronto, 2023.
1014. Anna Kravchenko, Ph.D. Thesis, l'Universit´e de Lorraine, 2023.
1015. Francisco Javier Marcos-Torres et al., Biochem Soc Trans 2023; 51 (3): 1319–1329.

Delphine Meffre, Julien Grenier, Sophie Bernard, Françoise Courtin, **Todor Dudev,** Mehrnaz Jafarian-Tehrani, Charbel Massaad, "Wnt and lithium: a common destiny in the therapy of nervous system pathologies?", *Cellular and Molecular Life Sciences* **71** (2014) 1123-1148.

1016. Sergi Bayod et al., Neurobiology of Aging 36 (2015) 720-729.
1017. M. Alda, Molecular Psychiatry (2015) 20, 661–671.
1018. Ashley M. Fortress et al., Hippocampus 25 (2015) 616–629.
1019. Anna M. Siebel et al., ACS Chem. Neurosci., 2014, 5, 468–476.
1020. Li-Jin Chew and Cynthia A. DeBoy, Neuropharmacology, 110 (2016) 605-625.
1021. Yang Gao, Ph.D. Thesis, University of Arizona, U.S.A., 2014.
1022. Xiaoheng Li et al., PNAS 113 (2016) 2666.
1023. Li-Jin Chewa and Cynthia A. DeBoy, Neuropharmacology 110 (2016) 605–625.
1024. Shim Seong S. and Stutzmann Grace E., Journal of Neurotrauma 2016, 33: 2065-2076.
1025. Murat İlhan Atagün, Neuropsychiatr Dis Treat. 2016; 12: 589–601.

1026. Xin-Yu Fang et al., Neuroscience 329 (2016) 213–225.
1027. Gonzalo Piñero et al., Mol Neurobiol 2016, DOI 10.1007/s12035-016-0262-z.
1028. Yuzhen Xu et al., Neuroscience 330 (2016) 100–108.
1029. Hoseth, E.Z., Krull, F., Dieset, I. et al. Transl Psychiatry 8, 55 (2018).
1030. Ather Muneer, Clin Psychopharmacol Neurosci. 2017, 15: 100–114.
1031. Flory, J., Donohue, D., Muhie, S. et al. Transl Psychiatry **7,** e1226 (2017).
1032. Papadima, E.M., Niola, P., Melis, C. et al., J Mol Neurosci 62, 304–308 (2017).
1033. Sarah Kittel-Schneider et al., (2019) The World J. Biol. Psychiatry, 20:6, 462-475.
1034. Piñero, G., Berg, R., Andersen, N. et al., Mol Neurobiol 54, 8287–8307 (2017).
1035. Yuzhen Xu et al., Brain Res. Bull. 149 (2019) 168-174.
1036. Helen C. Causton, Eur. J. Neurosci. 51 (2020) 1-12.
1037. Qian Wang et al., Cancer Medicine 8 (2019) 2360-2371.
1038. Carlos González-Fernández et al., Neural Regen Res. 2020; 15: 1580–1589.
1039. Sandra K. Bopp et al., European Neuropsychopharmacology 29 (2019) 211-221.
1040. Emanuela Stampone et al., Int. J. Mol. Sci. 2020, 21, 1169.
1041. Mengke Ge et al., Connective Tissue Research, 2019, 60, 444-451.
1042. Dena A.-E. Mohammed, et al., Int. J. Developmental Neurosci. 80 (2020) 123-138.
1043. Zheng Hongyun et al., Stroke and Neurological Diseases; 2015, 03, 3-5.
1044. Mengmeng Wang et al., Front. Cell. Neurosci. 13 (2019) Article 447.
1045. Liu, Zj., Liu, Yh., Huang, Sy. et al., Stem Cell Rev and Rep (2021). https://doi.org/10.1007/s12015-021-10133-x.
1046. Alparslan Cansız and Bahri İnce, Early Human Develop. 143 (2020) 104971.
1047. Li, M., et al. Mol Psychiatry (2020). https://doi.org/10.1038/s41380-020-00968-0.
1048. Xin Jiang et al., Cells 2021, 10, 839.
1049. Sinha, Priyanka; Ph.D. thesis, University of Otago, New Zealand, 2019.
1050. Filippa V.P., Mohamed F.H. (2019) Lithium Therapy Effects on the Reproductive System. In: Gargiulo P., Mesones Arroyo H. (eds) Psychiatry and Neuroscience Update. Springer, Cham. https://doi.org/10.1007/978-3-319-95360-1_16.
1051. F.B. Basmanav, Ph.D. thesis, Rheinische Friedrich-Wilhelms-Universität, Bonn, 2015.
1052. Ya-Bin Ji et al., Neuropharmacology 186 (2021) 108474.
1053. Seh Hyun Kim et al., Seizure 81 (2020) 47-52.
1054. И.С. Лосенков, Е.В. Плотников, Е.В. Епимахова, Н.А. Бохан, Журнал неврологии и психиатрии им С.С. Корсакова, 120 (2020) 108-115.
1055. Shuai Shi et al., Volume 2022, Article ID 1649605.
1056. Xinyu Shi et al., Folia Neuropathologica 60, 2022, 92-104.
1057. Du H, et al. Front Pharmacol. 2022 Dec 22;13:1078464.
1058. Han M, et al. Front Psychiatry. 2022 Aug 23;13:980315
1059. Wang B, Liu W, Sun F., Front Mol Neurosci. 2022 Dec 8;15:1034766.
1060. R. Kumar et al., Cellular Signalling 112, 2023, 110915.
1061. E. Delangre et al., Biomedicine & Pharmacotherapy 164, 2023, 114895.

1062. Marina Zafrilla-López et al., European Neuropsychopharmacology 85, 2024, 23-31.

Todor Dudev, "Modeling metal binding sites in proteins by quantum chemical calculations", Comp. Chem. 2 (2014) 19-21.

1063. M. Pivato, et al. Archives of biochemistry and biophysics 560 (2014): 83-99.
1064. B. Sadhu, et al. Journal of Physical Chemistry B 119 (2015): 12783-12797.
1065. B. Sadhu, et al.Phys. Chem. Chem. Phys.**,** 2017,19**,** 27611-27622.
1066. Jing Qu et al. Comput. Math. Methods Medicine Volume 2021, Article ID 2327832.
1067. B. Buszewski and I. Baranowska (Eds), Handbook of Bioanalytics, Springer, 2022.

Todor Dudev and Carmay Lim, "Ion selectivity strategies of sodium channel selectivity filters", Acc. Chem. Res. 47 (2014) 3580-3587.

1068. Salamone, Michela, et al., Journal of organic chemistry 80 (2015): 9214-9223.
1069. R.W. Wheatley, et al. Phys. Chem. Chem. Phys., 2015, 17, 10899-10909.
1070. Ngo, Van, et al., Journal of chemical theory and computation 11 (2015): 4992-5001.
1071. Noh, Sujin, et al., Integrative Medicine Research 4 (2015): 142-146.
1072. M. Giladi, et al. Int. J. Mol. Sci. 2016, 17, 1949.
1073. In-Joon Byun et al., Polymer Chemistry 54 (2016) 1713.
1074. James C. Gumbart and Sergei Noskov, BBA – Biomembranes 1858 (2016) 1553.
1075. Xuan Zhang et al., Advanced Materials 31 (2019) 1804540.
1076. Fabio Fusi et al., Eur. J. Pharmacol. 796 (2017) 158-174.
1077. Hristina R. Zhekova et al., Coord. Chem. Rev. 345 (2017) 108-136.
1078. Emelie Flood et al., Chem. Rev. 2019, 119, 7737–7832.
1079. Magali Roux, Anthony Dosseto, Metallomics, 9 (2017) 1326–1351.
1080. Marawan Ahmed et al., Drug Des Devel Ther. 2017; 11: 2301–2324.
1081. Flood E, Boiteux C, Allen TW (2018) PLoS Comput Biol 14: e1006398.
1082. Debajyoti Basak et al., Bioorg. Medicinal Chem. Lett. 27 (2017) 2886-2889.
1083. ШПАКОВ А.О., ДЕРКАЧ К.В., БАСОВА Н.Е. "С-ПЕПТИД ПРОИНСУЛИНА", Тип: монография Язык: русский ISBN: 978-5-7422-6720-1; Год издания: 2019 Место издания: Санкт-Петербург, Число страниц: 210; Издательство: ПОЛИТЕХ-ПРЕСС.
229.Encinas AC, et al. (2020) PLoS ONE 15: e0238121.
1084. Kim, S., Choi, S., Lee, H.G. et al. Nat Commun 12**,** 47 (2021).
1085. Xianfeng Zhou et al., Life 2020, 10, 39.
1086. Juan J. Nogueira and Ben Corry, The Oxford Handbook of Neuronal Ion Channels
Edited by Arin Bhattacharjee, Oxford University Press, 2021.

1087. Fanning, J. K., M.Sc. thesis, University of Calgary, Calgary, AB, Canada, 2018.
1088. Bahiru P. Benke et al., Eur. J. Org. Chem. 2020 (2020) 6898-6902.
1089. Sohail, MI et al.; in CADMIUM TOLERANCE IN PLANTS: AGRONOMIC, MOLECULAR, SIGNALING, AND OMIC APPROACHES (Edited by: Hasanuzzaman, M; Prasad, MNV; Nahar, K); 2019; pp 19-67.
1090. JUN LU**,** SCIENCE ADVANCES 2022, Vol 8, Issue 14, DOI: 10.1126/sciadv.abl5070
1091. K-D Kreuer and A. Münchinger, Ann. Rev. Mater. Res. 51, 2021 , 21-46.
1092. Miles Sasha Dickinson et al. PNAS February 24, 2022, 119 (9) e2110936119.
1093. Jun Lu and Huanting Wang, Matter 4, 2810–2830, September 1, 2021.
1094. Stevie N. Bush et al., *ACS Nano* 2022, 16, 5, 8338–8346.
1095. Qing Zhu et al.Journal of Membrane Science Volume 659, 5 October 2022, 120805.
1096. Xuechen Zhou et al. ACS Nano 2021, 15, 10, 16828–16838.
1097. Jun Lu et al., Sci. Adv.2023, 9, Issue 4 DOI: 10.1126/sciadv.abq1369
1098. D.M Echevarria-Cooper et al. Human Molecular Genetics, 31, 2022, 2964–2988
1099. Cédric Vallée et al. Int. J. Mol. Sci. **2021**, 22(20), 10998.
1100. Jun Lu et al. Acc. Mater. Res. 2022, 3, 7, 735–747.
1101. Zhang, XG., Wang, JH., Yang, WH. *et* al. BMC Neurol **22**, 111 (2022).
1102. Kamil Wojtkowiak et al. Symmetry **2022**, *14*(4), 691.
1103. Cédric Vallée et al. Phys. Chem. Chem. Phys., 2022, **24**, 13824-13830.
1104. N. Bielopolski et al. Epilepsy ResearchVolume 186, October 2022, 107002.
1105. Andrew Bogard et al. Membranes **2021**, 11(11), 897.
1106. Patrick Menzel, Ph.D. thesis, Georg-August University Göttingen, 2020.
1107. Yajia Li et al., Front. Nutr., 2021, 8, https://doi.org/10.3389/fnut.2021.754663.
1108. M. Xu et al., J. Mater. Chem. B, 2023,11, 3295-3306.
1109. G. Xing et al., Chem. Soc. Rev., 2024,53, 1495-1513.
1110. T. Ye et al., Angew. Chemie 136, 2024, e202316161.
1111. C.M. Ives et al., J Gen Physiol (2023) 155 (5): e202213226.
1112. Q. Li et al., J. Am. Chem. Soc. 2023, 145, 28038–28048.
1113. J.R. Groome, Mar. Drugs 2023, 21(4), 209.
1114. X. Qiu et al., 29, 2023, e202300976.
1115. A. Bertaud et al., J Gen Physiol (2024) 156 (5): e202313509.
1116. Z. Song et al., IMA J. Applied Mathematics, 88, 2023, Pages 805–836.
1117. D.M. Echevarria-Cooper, Ph.D. Thesis, Northwestern University, Evanston, Illinois, 2023.
1118. J. Dian et al., Neural Regeneration Research 10.4103/NRR.NRR-D-23-01444, 2024.
1119. Ives, Callum Matthew, Ph.D. Thesis, University of Dundee, UK, 2023.

Todor Dudev and Carmay Lim, "Evolution of eukaryotic ion channels: Principles underlying the conversion of Ca2+-selective to Na+-selective channels", J. Am. Chem. Soc. 136 (2014) 3553-3559.

1120. Kaufman, I. Kh, et al. New Journal of Physics 17 (2015): 083021.
1121. Li, Yang, and Haipeng Gong, Protein & cell 6 (2015): 413-422.
1122. Amey, Joanna S., et al., FEBS letters 589 (2015): 598-607.
1123. Yang Li, et al. PLoS ONE 11 (2016) e0162413.
1124. Hristina R. Zhekova et al., Coord. Chem. Rev. 345 (2017) 108-136.
1125. Han, M., Kopec, W., Solov'yov, I. et al. Sci Rep **7,** 39829 (2017).
1126. O.A. Fedorenko et al., Biochim. Biophys. Acta (BBA) – Biomembranes 1862 (2020) 183301.
1127. Carlos A. Cañas et al. Journal of Translational Autoimmunity 5, 2022, 100146.
1128. Miles Sasha Dickinson et al. PNAS February 24, 2022 119 (9) e2110936119.
1129. A. Bertaud et al., J Gen Physiol (2024) 156 (5): e202313509.

C. Satheesan Babu, Y.-M. Lee, **Todor Dudev** and Carmay Lim, "Modeling Zn2+ Release from Metallothionein", *J. Phys. Chem. A* **118** (2014) 9244-9252.

1130. Xiaomeng Liang et al., Current Opin. Chem. Biol. 31 (2016) 120-125.
1131. Agnieszka Drozd et al., Metallomics 10 (2018) 595–613.
1132. Miguel Angel Merlos Rodrigo et al., Int. J. Mol. Sci. 2017, 18, 610.
1133. Savasci, G., Borges-Martínez, M., Berger, R.J.F. et al. J Mol Model 25, 258 (2019).
1134. J. M.G. Evers, et al. Proteins, Wiley Periodicals, 2015.
1135. Manuel David Peris-Díaz et al. J. Am. Chem. Soc. 2021, 143, 40, 16486–16501.
1136. A.G. Hall et al., Int. J. Mol. Sci. 2023, 24(7), 6561.
1137. X. Hu et al., J. Chem. Theory Comput. 2024, 20, 3, 1448–1464.
1138. S. Ma et al., Science of The Total Environment 901, 2023, 166187.

C. Satheesan Babu, **Todor Dudev** and Carmay Lim, "Differential Role of the Protein Matrix on the Binding of a Catalytic Aspartate to Mg^{2+} vs Ca^{2+}: Application to Ribonuclease H", *J. Am. Chem. Soc*. **135** (2013) 6541-6548.

1139. Kevin M. N. Burgess et al., Inorg. Chem., 2014, 53, 552–561.
1140. Jin-Hua Wang et al., Journal of Solid State Chemistry 219 (2014) 55–66
1141. Giulia Palermo et al., Acc. Chem. Res., 2015, 48, 220–228.
1142. A. Krah, S. Takada, Biochim. Biophys. Acta (BBA) – Bioenergetics 1847 (2015) 1101.
1143. Michela Salamone and al., J. Org. Chem., 2015, 80, 9214–9223.
1144. Taka-aki Okamura, et al. Dalton Trans., 2015, 44, 7512-7523.
1145. G. SURESH, U DEVA PRIYAKUMAR, J. Chem. Sci. 2015, 127, 1701-1713.
1146. Marjorie Fournier et al., Nat Commun. 2016; 7: 13227.

1147. H. Thie, K. Reck and V. Nolle, Generating metal ion binding proteins, US Patent US 9518131 B2, 2016.
1148. Zhifeng Jing et al., PNAS 2018, 115, E7495-E7501.
1149. Kevin M. N. Burgess et al., J. Phys. Chem. A 2013, 117, 6561–6570.
1150. Taka-aki Okamura and Junko Nakagawa, Inorg. Chem. 2013, 52, 10812–10824.
1151. Hwang, W., Yoo, J., Lee, Y. et al. Nat Commun 9, 4404 (2018).
1152. Tong, C., Zhou, T., Zhao, C. et al., Microchim Acta 186, 335 (2019).
1153. Jiarong Peng et al. J. Chem. Inf. Model. 2021, 61, 6, 2981–2997.
1154. Rajwinder Kaur et al. Phys. Chem. Chem. Phys., 2022,24, 29130-29140.
1155. Zhifeng Jing, Ph.D. thesis, University of Texas at Austin, 2021.
1156. Pang J, Guo Q, Lu Z. Front Microbiol. 2022 Nov 21;13:1034811.
1157. R. Lai, et al., J. Am. Chem. Soc. 2024, 146, 7628–7639.
1158. K. Noroozi, L.R. Jarboe, J. Ind. Microbiol. Biotechnol. 50, 2023, kuad011.

Todor Dudev and Carmay Lim, “Importance of metal hydration on the selectivity of Mg2+ versus Ca2+ in magnesium ion channels”, *J. Am. Chem. Soc*. **135** (2013) 17200-17208.

1159. Olivier Dalmas et al., PNAS 111 (2014) 3002-3007.
1160. A. Crémazy, et al. Environ. Sci. Technol., 2014, 48, 9754–9761.
1161. S. Chandra Shekar and R. S. Swathi, J. Phys. Chem. C, 2015, 119, 8912–8923.
1162. M. Moirangthem et al., Advanced Functional Materials 26 (2016) 1154.
1163. Sidsel-Marie Glasdam et al., Advances in Clinical Chemistry 73 (2016) 169–193.
1164. J.M. Andric et al., ChemPhysChem 17 (2016) 2035.
1165. D.H. Dagade et al., ChemPhysChem 17 (2016) 902.
1166. Toshio Yamaguchi et al., BUNSEKI KAGAKU 64 (2015) 295.
1167. Thirupathi Ravula et al., Langmuir 2017, 33, 10655–10662.
1168. Eric V. Bukovsky et al., Inorg. Chem. 2017, 56, 4369–4379.
1169. Nicolas Schaeffer et al., Phys. Chem. Chem. Phys., 2018, 20, 9838-9846.
1170. Gati, C., Stetsenko, A., Slotboom, D.J. et al., Nat Commun 8, 1313 (2017).
1171. Nawavi Naleem et al., J. Chem. Phys. 148, 222828 (2018).
1172. Bernette M. Oosterlaken et al., Adv. Funct. Mater. 30 (2020) 1907456.
1173. M. Mahmoudvand et al., Coll. Surf. A, 579 (2019) 123665.
1174. M.I. Chaudhari et al., Annual Review of Physical Chemistry 2020, 71, 461-484.
1175. Vipin Nautiyal and R.C .Dubey, Saudi J. Biol. Sci. 28 (2021) 2432-2437.
1176. E.D. Spoerke, Programmable Nanocomposite Membranes for Ion-Based Electrical Energy Storage. United States: N. p., 2016. Web. doi:10.2172/1599531.
1177. Xiao-Feng Xu et al., Front. Plant Sci., 2021; https://doi.org/10.3389/fpls.2020.621338.
1178. Mostafavi, N., Ebrahimi, A.; Theor Chem Acc 137, 117 (2018).
1179. K. Kosev et al., J. Mol. Struct. 1224 (2021) 129009.

1180. Yoonsun Jang et al., Particle 35 (2018) 1800132.
1181. Huacheng Zhang et al. Chem. Soc. Rev., 2022,51, 2224-2254.
1182. Diego T. Gomez et al. Acc. Chem. Res. 2022, 55, 16, 2201–2212.
1183. Mohsen Mahmoudvand et al. J. Petroleum Sci. Eng. 206, 2021, 108970.
1184. Rukuan Chai et al. Energy Fuels 2021, 35, 12, 9860–9872
1185. Sedigheh Mahdavi et al.Energy Fuels 2021, 35, 23, 19211–19247.
1186. Caio B. Castro et al. Current Research in Chemical Biology 1, 2021, 100004.
1187. Akhilesh Jaiswar et al. J. Phys. Chem. B 2021, 125, 24, 6479–6490.
1188. Mohsen Ramezani et al. J. Petroleum Sci. Eng. 219, 2022, 111117.
1189. Jelena Gitarić et al. (2022) Journal of Coordination Chemistry, 75:11-14, 1899-1914.
1190. Nishith Ghosh et al. Liquids 2023, *3*(1), 19-39.
1191. Milica G. Nikolić, Ph.D. thesis, University of Nish, 2022.
1192. Jan-Niklas Boyn, Emily A. Carter, J. Am. Chem. Soc. 2023, 145, 37, 20462–20472.
1193. J. Hou et al., Small 8, 2024, 2300278.
1194. Lai, L.T.F., et al., Nat Commun 14, 7207 (2023).
1195. A. Vlieghe et al., Biomolecules 2023, 13(9), 1341.
1196. Rani S, et al., Pharmacognosy Research. 2023;15(4):705-715.
1197. M.N. Moia, M.Sc. Thesis, Univ. Federal do Rio Grande do Norte, Brazil, 2023.
1198. Sara Filipa Matos dos Santos, M.Sc. Thesis, Univ. de São João, Brazil, 2023.

Todor Dudev and Carmay Lim, "Competition among Ca^{2+}, Mg^{2+} and Na^{+} for model ion channel selectivity filters: determinants of ion selectivity", *J. Phys. Chem. B* **116** (2012) 10703-10714.

1199. Yibo Wang et al., J. Phys. Chem. B 2014, 118, 2041–2049.
1200. Alisher M. Kariev, Philipa Njau, Michael E. Green, Biophys. J.106 (2014) 548–555.
1201. David Feakins et al., Journal of Solution Chemistry 2014, 43, 40-58.
1202. Yang Li et al. PLoS ONE 11 (2016) e0162413.
1203. Song Ke et al., Biochem. Biophys. Res. Commun. 430 (2013) 1272-1276.
1204. M.R. Gunner et al., Biochim. Biphys. Acta (BBA) – Bioenergetics 1827 (2013) 892.
1205. Mengdie Xia et al. Biophys. J. 104 (2013) 2401-2409.
1206. Jiali Wang et al., Biomaterials 157 (2018) 86-97.
1207. Zuozhen Han et al., Minerals 2018, 8, 585.
1208. Sakipov, S., Sobolevsky, A.I. & Kurnikova, M.G. Sci Rep 8, 5715 (2018).
1209. R.S. Eisenberg, 2019 Classical Physics arXiv:1904.09695; DOI: 10.31224/osf.io/urxgs.
1210. Chakraborty, Manjusha et al., Adv. Sci., Engin. Medicine, 8, 2016, 450-459.
1211. Yang Li et al., Biochim. Biphys. Acta (BBA) – Biomembranes 1859 (2017) 879-887.
1212. Mohammad Ashrafuzzaman, Nanoscale Biophysics of the Cell, Springer, 2018.
1213. Yurie Chatzikyriakidou, Ph.D. thesis, Stockholm University, 2021.

1214. M.J. Stevens, S.L.B. Rempe, Phys. Chem. Chem. Phys., 2023,25, 29881-29893.
1215. X. Zhao et al., in IEEE Transactions on Plasma Science, 2024, doi: 10.1109/TPS.2024.3384434.

Todor Dudev and Carmay Lim, "The effect of metal binding on the characteristic infrared band intensities of ligands of biological interest", *J. Mol. Struct*. **1009** (2012) 83-88.

1216. Kim, Inhye, et al., Journal of Materials Chemistry B 2 (2014): 6478-6486.
1217. M. Moirangthem et al., Advanced Functional Materials 26 (2016) 1154.
1218. M. Nara et al., Biochim. Biophys. Acta – Biomembranes 1828 (2013) 2319.
1219. Rakesh K. Pathak et al., Anal. Chem. 2012, 84, 8294–8300.
1220. M. Moirangthem A.P.H.J. Schenning, ACS Appl. Mater. Interfaces 2018, 10, 4, 4168.
1221. Joseph W. DePalma et al., J. Phys. Chem. Lett. 2017, 8, 484–488.
1222. Joanna K. Denton et al., PNAS 2019, 116, 14874-14880.
1223. Kelleher, Patrick Joseph; Ph.D. thesis, Yale University, U.S.A., 2018.
1224. Ye-Ji Kim, Soo-Young Park, ACS Appl. Mater. Interfaces 2020, 12, 47342.
1225. Belen Reig-Vano et al., Int. J. Biological Macromolecules 246, 2023, 125659.

Todor Dudev and Carmay Lim, "Why voltage-gated Ca^{2+} and bacterial Na^{+} channels with the same EEEE motif in their selectivity filters confer opposite metal selectivity", *Physical Chemistry Chemical Physics* **14** (2012) 12451-12456.

1226. Todd Scheuer, Voltage Gated Sodium Channels, Volume 221 of the series Handbook of Experimental Pharmacology, Springer, pp 269-291, 2014.
1227. O. Gutten and L. Rulíšek, Phys. Chem. Chem. Phys., 2015, 17, 14393-14404.
1228. Yang Li, Haipeng Gong, Protein & Cell 2015, 6, 413-422.
1229. A. M. Kariev, et al. Biophysical Journal 106 (2014) 548–555.
1230. Valentina Taiakina, Ph.D. Thesis, University of Waterloo, Canada, 2014.
1231. C. Ing and R. Pomès, Current Topics in Membranes 78 (2016) 215–260.
1232. Mark J. Stevens, Susan L. B. Rempe, J. Phys. Chem. B 2016, 120, 12519–12530.
1233. Y. Li, et al. PLoS ONE 11 (2016) e0162413.
1234. Daniel Bim et al., Chem. Listy 110 (2016) 354-364.
1235. Zhang, X., Xia, M., Li, Y. et al. Cell Res 23, 409–422 (2013).
1236. Simone Furini and Carmen Domene, Biphys. J. 105 (2013) 1737-1745.
1237. Song Ke et al., Biochem. Biophys. Res. Commun. 430 (2013) 1272-1276.
1238. Mengdie Xia et al. Biophys. J. 104 (2013) 2401-2409.
1239. Hristina R. Zhekova et al., Coord. Chem. Rev. 345 (2017) 108-136.
1240. Thévenod, F., Fels, J., Lee, WK. et al., Biometals 32, 469–489 (2019).

1241. M. Ashrafuzzaman, Nanoscale Biophysics of the Cell, Springer, 2018.
1242. Olena A. Fedorenko et al., Entropy 2020, 22(12), 1390.
1243. Bernadett Bacsa et al., Curr. Opin. Physiol. 17 (2020) 25-33.
1244. Junliang Zhu et al. Biophys J. 122, 2023, Pages 496-505.
1245. M. Liutkus et al., Protein Science 33, 2024, e4971.

Todor Dudev and Carmay Lim, "Competition between Li^{+} and Mg^{2+} in metalloproteins. Implications for lithium therapy", *J. Am. Chem. Soc.* **133** (2011) 9506-9515.

1246. Eleonore Beurel et al., Pharmacology & Therapeutics 148 (2015) 114–131.
1247. Vincent Balter and Nathalie Vigier, Metallomics 2014, 6, 582-586.
1248. Michela Salamone et al., J. Org. Chem., 2015, 80, 9214–9223.
1249. A. Dutta et al., FEBS Journal 281 (2014) 5309-5324.
1250. G. Zanni, Ph.D. Thesis, University of Gothenburg, Goteborg, Sweden, 2015.
1251. M.C. Duff et al. Plant Science 229 (2014) 262–279.
1252. Anna I. Erickson et al., 2015, 54, 6830–6841.
1253. Philip G. Janicak and Bradley R. Cutler, Encyclopedia of Inorganic and Bioinorganic Chemistry, DOI: 10.1002/9781119951438.eibc2346, 2015.
1254. D. Mota de Freitas, et al. The Alkali Metal Ions: Their Role for Life, Volume 16 of the series Metal Ions in Life Sciences, Springer, 2016, pp 55 e
1255. Jiyeon Park et al., Ind. Eng. Chem. Res. 2016, 55, 4278–4284.
1256. Kim, Woo-Sik et al., J. Nanosci.Nanotechnol. 16 (2016) 6930-6935.
1257. Piñero, G., et al. Mol. Neurobiol. (2016) doi:10.1007/s12035-016-0262-z.
1258. Kiełczykowska, M., et al. Biol. Trace Elem. Res. (2016) doi:10.1007/s12011-016-0906-x.
1259. Kiełczykowska, M., Musik, I., Żelazowska, R. et al., Biometals (2016) 29: 873.
1260. Richard S. Jope and Charles B. Nemeroff, Cerebrum. 2016, cer-02-16.
1261. Vladan Sekulić, Ph.D. Thesis, Nis, Serbia, 2016.
1262. K.M. Brown, D.K. Tracy, Therapeutic Adv. Psychopharmacology 3 (2013) 163.
1263. Anat Haimovich et al., J. Am. Chem. Soc. 2012, 134, 5647–5651.
1264. Hasmukh A. Patel et al., J. Am. Chem. Soc. 2017, 139, 11020–11023.
1265. Shao-Yong Lu et al., Proteins 81 (2013) 740-753.
1266. Shaoyong Lu et al., J. Chem. Inf. Model. 2012, 52, 2398–2409.
1267. Xiaoqing Wang and Hajime Hirao, J. Phys. Chem. B 2013, 117, 833–842.
1268. Piñero, G., Berg, R., Andersen, N. et al., Mol Neurobiol 54, 8287–8307 (2017).
1269. Ozerdem, A. et al. Current Drug Metabolism, 19 (2018) 653-662.
1270. Kiełczykowska, M. et al., Biol Trace Elem Res 178, 79–85 (2017).
1271. Nicholas A. Meanwell, Bioorg. Med. Chem. Lett. 27 (2017) 5355-5372.
1272. I.Yu. Torshin et al., Neurology, neuropsychiatry and psychosomatics 9, 2017,78.
1273. A.V. Pronin et al., Neurology, neuropsychiatry and psychosomatics 9,2017, 111.

1274. БОРОДИН Ю.И., РОБИНСОН М.В., ДАРНЕВА И.С., РАЧКОВСКАЯ Л.Н., КОРОЛЕВ М.А., ЛЕТЯГИН А.Ю., “СОЕДИНЕНИЯ ЛИТИЯ В БИОЛОГИИ И МЕДИЦИНЕ” (монография), Новосибирск; ООО Азарт, 2016.
1275. A. K. Singha Deb et al., Mol. Syst. Des. Eng., 2019,4, 616-625.
1276. A. Khayachi et al., Neuroscience & Biobehavioral Reviews, 127, (2021) 424.
1277. Arthur Ernst van Woerkom, Neuropsychiatr Dis Treat. 2017; 13: 275–302.
1278. J.F. Stoddart et al., US patent, Publication of US20200164342A1, 2020.
1279. Carugo, Oliviero, Protein and Peptide Letters, 27, 2020, 763-769.
1280. M. V. Robinson et al., Siberian Scientific Med. J. Vol 39, No 5 (2019).
1281. Arthur Ernst van Woerkom, Neuropsychiatr Dis Treat. 2017; 13: 275–302.
1282. Samuel Tetteh, J. Chem. Volume 2019, Article ID 5675870.
1283. Samiol Azam et al., ACS Chem. Neurosci. 2020, 11, 2543–2548.
1284. Ana Bravo et al., Chem. Biol. Drug Design 93 (2019) 965-969.
1285. Jesse Lee Goossens, Ph.D. thesis, Loyola University Chicago, U.S.A. 2018.
1286. Anagh Mukherjee et al., J. Phys. Chem. A 2020, 124, 8040–8049.
1287. K. M. Brown, D.K. Tracy; Ther Adv Psychopharmacol (2013), 3, 163–176.
1288. R.M.M. Oliveira, Ph.D. thesis, Universidade federal de Sao Carlos, Brazil, 2012.
1289. Heng Zhang et al. Angew. Chemie Intl. Ed. 61, 2022, e202214054.
1290. Sun Hae Ra Shin et al. *ACS Materials Lett.* 2023, 5, 2, 330–335.
1291. David J. Reilley et al. *J. Phys. Chem. B* 2021, 125, 33, 9480–9489.
1292. Torshin I.Yu., et al., *Neurology, Neuropsychiatry, Psychosomatics*. 2022;14(5):60-68. (In Russ.)
1293. David John Reilley, Ph.D. thesis, University of California, Los Angeles, 2021.
1294. H.M. Díaz-Alejo Guerrero, Ph.D. thesis, Univ. Complutense de Madrid, 2022.
1295. James Fraser, Stoddar Hasmukh, A. Patel Zhichang Liu Siva Krishna Mohan NALLURI, Patent application, Publication of US11298677B2, 2022.
1296. J.D. Livingstone et al., Biochem. Biophys. Reports 34, 2023, 101461.
1297. Mekkawy MH, et al., Dose-Response 2023;21(4); https://doi.org/10.1177/1559325823121.
1298. T.R. Memhave, Ph.D. Thesis, Georg-August-Universität Göttingen, 2023.
1299. J.F. Stoddart et al., US patent US11890591B2, 2024.

Todor Dudev and Carmay Lim, “Factors governing the Na^+ vs K^+ selectivity in sodium ion channels” *J. Am. Chem. Soc.* **132** (2010) 2321-2332.

1300. Jin-Hua Wang et al., Journal of Solid-State Chemistry 219 (2014) 55–66.
1301. Jukic, Mark et al., Current Medicinal Chemistry, 21 (2014) 164-186.
1302. Todd Scheuer, Voltage Gated Sodium Channels, Volume 221 of the series Handbook of Experimental Pharmacology, pp 269-291, 2014.
1303. O. Gutten, L. Rulíšek, Phys. Chem. Chem. Phys., 2015, 17, 14393-14404.
1304. Yang Li, Haipeng Gong, Protein & Cell 2015, 6, 413-422.
1305. A.M. Kariev, Philipa Njau, Michael E. Green, Biophys. J. 106 (2014) 548–555.
1306. Biswajit Sadhu et al., J. Phys. Chem. B, 2015, 119, 12783–12797.
1307. Yasser A. Mahmmoud et al., J. Biol. Chem. 290 (2015) 3720-3731.

1308. Ruhong Zhou, Molecular Modeling at Atomic Scale: Methods and Applications in Quantitative Biology, CRC Press, Boca Raton, 2015.
1309. Jeng-Yang Lin et al., Anal.Chem. 2016, 88, 1176.
1310. Jean Jules Fifen,Noam Agmon, J. Chem. Theory Comput. 2016, 12, 1656–1673.
1311. Yang Li et al., PLoS ONE 11 (2016) e0162413.
1312. Zhongjin He et al., ACS Nano 2013, 7, 10148–10157.
1313. Ben Corry and Michael Thomas, J. Am. Chem. Soc. 2012, 134, 1840–1846.
1314. Y. Marcus, Ions in Water and Biophysical Implications: From Chaos to Cosmos, Springer, 2012.
1315. Zhang, X., Xia, M., Li, Y. et al. Cell Res 23, 409–422 (2013).
1316. Li Rao et al., J. Am. Chem. Soc. 2010, 132, 18092–18102.
1317. Mengdie Xia et al. Biophys. J. 104 (2013) 2401-2409.
1318. Aurore Lenglet et al., New Phytologist 216 (2017) 1161-1169.
1319. Xue-Bin Wang, J. Phys. Chem. A 2017, 121, 1389–1401.
1320. Garold Murdachaew et al., J. Phys. Chem. A 2012, 116, 2055–2061.
1321. Hristina R. Zhekova et al., Coord. Chem. Rev. 345 (2017) 108-136.
1322. Benoît Roux, J. Phys. Chem. B 2012, 116, 6966–6979.
1323. Dieterich, J.M., et al., J Mol Model 17, 3195–3207 (2011).
1324. Bogdan Lev, Sergei Yu. Noskov, Phys. Chem. Chem. Phys., 2013, 15, 2397.
1325. Flood E, Boiteux C, Allen TW (2018) PLoS Comput Biol 14: e1006398.
1326. B. Sadhu, et al. Phys. Chem. Chem. Phys., 2017,19, 27611-27622.
1327. Ren-Zhong L. et al., Phys. Chem. Chem. Phys., 2018, 20, 29051-29060.
1328. Bo Xu et al., Plant Direct 4 (2020) e00275.
1329. H. Farrokhpour, S. Khoshkhou, Int. J. Quantum Chem. 120 (2020) e26104.
1330. Pengju Wang et al., Front. Chem., 2019, https://doi.org/10.3389/fchem.2019.00624.
1331. Mahdi Khatibi et al., Anal. Chimica Acta 1122 (2020) 48-60.
1332. M. Ashrafuzzaman, Nanoscale Biophysics of the Cell, Springer, 2018.
1333. Boris S. Zhorov, J. Phys. Chem. B 2021, 125, 2074–2088.
1334. Xianfeng Zhou et al., Life 2020, 10, 39.
1335. S. Lifa et al., Acta Cryst. (2021). C77, 90-99.
1336. Charlotte Hölscher, Ph.D. thesis, University of Lubeck, Germany, 2017.
1337. A.A. Linhares, M.Sc. thesis, Univ. Federal de Santa Catarina, Brazil, 2020.
1338. Huacheng Zhang et al. Chem. Soc. Rev., 2022,51, 2224-2254.
1339. Ilan, Y. Mol Cell Biochem 478, 375–392 (2023).
1340. M. Karimzadeh et al. Electrochimica Acta Volume 399, 2021, 139376.
1341. Rafael Furlan de Oliveira et al. Small Volume18, Issue27 July 7, 2022, 2201861
1342. Cédric Vallée et al. Int. J. Mol. Sci. 2021, 22(20), 10998.
1343. Cao, L., Chen, IC., Li, Z. et al. Nat Commun 13, 7894 (2022).
1344. Mohammad Karimzadeh et al., Physics of Fluids 34, 122008 (2022).
1345. Linsen Yang and Liping Wen, Cell Report Physical Science, 3, 2022, 101167.
1346. J. Hou, H. Zhang, Advanced Materials Technologies, 2023, https://doi.org/10.1002/admt.202201433.
1347. M. Khosravikia, Electrophoresis 2023, https://doi.org/10.1002/elps.202300006.

1348. Sunayana Mitra, Ph.D. thesis, University of Pittsburgh, 2021.
1349. J. Lu et al., SCIENCE ADVANCES 2023, 9, DOI: 10.1126/sciadv.abq136.
1350. Goutham, S. et al., Nat. Nanotechnol. 18, 596–601 (2023).
1351. J. Hou et al., Small 8, 2024, 2300278.
1352. Amirhossein Heydari et al., Phys. Chem. Chem. Phys., 2023,25, 26716-26736.
1353. G. Alberini et al., J. Chem. Theory Comput. 2023, 19, 2953–2972.
1354. L. Zhang et al., J. Am. Chem. Soc. 2024, 146, 8500–8507.
1355. T.-X. Cao et al., Ind. Eng. Chem. Res. 2023, 62, 37, 14772–14790.
1356. Y. Feng et al., ACS Appl. Mater. Interfaces 2024, 16, 20, 26817–26823.
1357. Gopika Sabu, Susmita De, J. Phys. Chem. B 2023, 127, 48, 10326–10337.
1358. A. Mohammadi, M. Roostaei, Int. Commun. Heat Mass Transfer 150, 2024, 107176.
1359. A.D. Veloso et al., Nano Materials Science 2023, https://doi.org/10.1016/j.nanoms.2023.12.002.
1360. Z. Song et al., IMA J. Applied Mathematics, 88, 2023, 805–836.
1361. Thijs Rudolf ter Rele, M.Sc. Thesis, Utrecht University, 2022.
1362. Mirna Damergi, M.Sc. Thesis, University of Calgary, Canada, 2022.
1363. O. ARUN, Ph.D. Thesis, SELÇUK ÜNİVERSİTESİ, Konya, Turkey, 2023.

Todor Dudev and Carmay Lim, “Factors controlling the mechanism of NAD+ non-redox reactions”, *J. Am. Chem. Soc.* **132** (2010) 16533-16543.

1364. Kuhn, Isabelle, et al., Biochimica et Biophysica Acta (BBA)-Proteins and Proteomics 1844 (2014): 1317-1331.
1365. Hou, Shuhua et al., Chin. J. Org. Chem. 2016, 36, 297.
1366. Roy, Swarup; Das, Tapan Kumar; Adv. Sci., Engin. Medicine 7 (2015) 729.
1367. Guangquan Li et al., Int. J. Mol. Sci. 2012, 13, 466-476.
1368. Bernhard Lüscher et al., Chem. Rev. 2018, 118, 1092–1136.
1369. Dwivedi S, et al. (2013) PLoS ONE 8: e57404.
1370. Gaikwad Sagar and Bhosale Ashok, Eur. J.Exp. Biol. 2012, 2:1654-1658.
1371. Carlo Nervi and Alceo Macchioni, ACS Catal. 2017, 7, 7788–7796.
1372. Egea PF et al., PLoS ONE (2012) 7: e34918.
1373. Ruibo Wu et al., J. Phys. Chem. B 2012, 116, 1984–1991.
1374. Zarrin Haris, Iqbal Ahmad, Int. J. Life Sci. Scienti. Res., 2017, 3: 1020-1030.
1375. Bruce G. Szczepankiewicz et al., J. Org. Chem. 2011, 76, 6465–6474.
1376. Q. Husain, Biointerface Research in Applied Chemistry, 9, (2019) 4255 – 4271.
1377. S. Chandrasekaran, S.P. Sivasamy, Int. J. Sci. Devel. Res. 5 (2020) issue 9.
1378. Simeon Dimitrov Draganov. Ph.D. thesis, Imperial College London, 2022.
1379. RYAN THOMAS HOWARD, Ph.D. thesis, Imperial College London, 2021.
1380. Q. Song et al., Advances in Nutrition 14, 2023, 1416-1435.
1381. Y. Zhang et al., BIOCELL 2023 47(4): 859-868.

Commented [1]:

Todor Dudev and Carmay Lim, “Metal-binding affinity and selectivity of nonstandard natural amino acid residues from DFT/CDM calculations”, *J. Phys. Chem. B* **113** (2009) 11754-11764.

1382. Shilpi Mandal, Gunajyoti Das and Hassan Askari, Struct. Chem. 2014, 25, 43.
1383. Shilpi Mandal et al., J. Chem. Inf. Model., 2014, 54, 2524–2535.
1384. Ondrej Gutten, Lubomír Rulíšek, Phys. Chem. Chem. Phys., 2015, 17, 14393.
1385. Tanya Singh et al., Mol. BioSyst., 2015, 11, 1041-1051.
1386. Milan Remko et al., Chem. Phys. Lett. 614 (2014) 214–219.
1387. Gunajyoti Das and Shilpi Mandal, Chemical Papers 69 (2015) 616–626.
1388. Marcela Hurtado et al., ARKIVOC 2014 (ii) 207-223.
1389. Ondrej Gutten et al., J. Phys. Chem. A 2011, 115, 11394–11402.
1390. Demian Riccardi et al., J. Chem. Theory Comput. 2013, 9, 555–569.
1391. M.R. Gunner et al., Biochimica et Biophysica Acta (BBA) – Bioenergetics, 1827, 2013, 892-913.
1392. Federico Mazur et al., Sensors and Actuators B: Chemical 268, 2018, 182-187.
1393. Yan Ling et al., J. Phys. Chem. B 2011, 115, 2663–2670.
1394. Mandal, S., Das, G.; J Mol Model 19, 2613–2623 (2013).
1395. Das, G.; J Mol Model 19, 1901–1911 (2013).
1396. Matthias J. Knape; Friedrich W. Herberg; Biochem Soc Trans (2017) 45: 653.
1397. Das, G., Mandal, S.; J Mol Model 19, 1695–1704 (2013.
1398. Das, G.; J Mol Model 19, 2981–2991 (2013).
1399. Markus SCHNEIDER, Ph.D. thesis, ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE, Switzerland, 2018.
1400. Zhuang Huiying, M.Sc. thesis, Kaohsiung Medical University, Taiwan, 2012.
1401. Wenbin Yao et al. Appl. Sci. 2022, 12(3), 1114.
1402. U. Yoon et al. RSC Adv., 2024, 14, 1051-1055.
1403. N.N. Golosova et al., Viruses 2024, 16(1), 93.

Todor Dudev and Carmay Lim, “Determinants of K^+ vs Na^+ selectivity in potassium channels”, *J. Am. Chem. Soc*. **131** (2009) 8092-8101.

1404. Benoît Roux et al., J Gen Physiol (2011) 137: 415–426.
1405. Zhongjin He et al., ACS Nano 2013, 7, 11, 10148–10157.
1406. Hao Lin and Hui Ding, J. Theor. Biol. 269 (2011) 64-69.
1407. Bob Eisenberg, in Stuart A. Rice, Aaron R. Dinner (Eds) Advances in Chemical Physics, vol. 148, John Wiley &Sons, 2012.
1408. Mehabaw G. Derebeet al., PNAS 2011, 108, 598-602.
1409. Sameer Varma et al., J Gen Physiol (2011) 137: 479–488.
1410. Tomoyuki Matsuda et al., J. Am. Chem. Soc. 2010, 132, 12206–12207.

1411. Y. Marcus, Ions in Water and Biophysical Implications: From Chaos to Cosmos, Springer, 2012.
1412. Vicente M. Aguilella et al., Integrative Biology, 3 (2011) 159–172.
1413. Sameer Varma and Susan B. Rempe, Biophys. J. 99 (2010) 3394-3401.
1414. Michael Zwolak et al., 2010 J. Phys.: Condens. Matter 22 454126.
1415. David B. Sauer et al., PNAS 2011 108 16634-16639.
1416. Richard D. Carpenter and A. S. Verkman, Org. Lett. 2010, 12, 1160–1163.
1417. Zhu, Y., Zhou, J., Lu, X. et al., Microfluid Nanofluid 15, 191–205 (2013).
1418. Li Rao et al., J. Am. Chem. Soc. 2010, 132, 51, 18092–18102.
1419. Amer Alam; Youxing Jiang, J Gen Physiol (2011) 137: 397–403.
1420. Jelena M. Andrić et al., Phys. Chem. Chem. Phys., 2012,14, 10896-10898.
1421. Yudan Zhu et al., Fluid Phase Equilibria, 297 (2010) 215-220.
1422. D.L. Bostick; C.L. Brooks, III, J. Am. Chem. Soc. 2010, 132, 13185–13187.
1423. Xue-Bin Wang, J. Phys. Chem. A 2017, 121, 7, 1389–1401.
1424. Garold Murdachaew et al., J. Phys. Chem. A 2012, 116, 2055–2061.
1425. Christopher J. R. Illingworth et al., J. Chem. Theory Comput. 2010, 6, 3780.
1426. Benoît Roux, J. Phys. Chem. B 2012, 116, 6966–6979.
1427. Michael Thomas et al., Biophys. J. 100 (2011) 60-69.
1428. Gang Yang et al., J. Mass Spectrometry 47 (2012) 1372-1383.
1429. Thomas M, Jayatilaka D, Corry B (2013) PLoS Comput Biol 9: e1002914.
1430. Justin J. Finnerty et al., J. Chem. Theory Comput. 2013, 9, 766–773.
1431. Biswas, S., Avan, I., Basak, A.K. et al. Amino Acids 45, 159–170 (2013).
1432. Li-Long Dang et al., Chem. Sci., 2020, 11, 1226-1232.
1433. Michael Thomas et al., Biophys. Chem. 172 (2013) 37-42.
1434. Joanne Carney et al., Current Topics in Membranes 66, 2010, 49-67.
1435. Han, M., Kopec, W., Solov'yov, I. et al. Sci Rep 7, 39829 (2017).
1436. Chun-Hung Wang et al., Front. Chem., 2018, https://doi.org/10.3389/fchem.2018.00062
1437. Xiaomin Wu et al., Comp. Biol.Chem. 38 (2012) 1-9.
1438. Biswajit Sadhu et al., Phys. Chem. Chem. Phys., 2017,19, 27611-27622.
1439. Miedema H. (2011) Ion-Selective Biomimetic Membranes. In: Hélix-Nielsen C. (eds) Biomimetic Membranes for Sensor and Separation Applications. Biological and Medical Physics, Biomedical Engineering. Springer, Dordrecht.
1440. Ren-Zhong Li et al., Phys. Chem. Chem. Phys., 2018, 20, 29051-29060.
1441. Susmita De et al., Phys. Chem. Chem. Phys., 2018,20, 17517-17529.
1442. Brewster, Daniel L; M.Sc. thesis, University of Alberta, Canada, 2012.
1443. Kenichiro Mita et al., PNAS 2021, 118, e2017168118.
1444. M. Ashrafuzzaman, Nanoscale Biophysics of the Cell, Springer, 2018.
1445. Y. Marcus, Ions in Water and Biophysical Implications: From Chaos to Cosmos, Springer, 2012.
1446. Wilson, James Michael; Ph.D. thesis, University of California, San Diego, 2013.
1447. Julia Braunagel, Ph.D. thesis, Johannes Gutenberg-Universität Mainz, 2009.
1448. M. Soniat,et al. J. Chem. Theory Comput., 2015, 11, 2958–2967.
1449. Caterina Fraschetti et al., J. Am. Soc. Mass Spectrom. 2015, 26, 1186-1190.

1450. Alisher M. Kariev et al. Biophys. J. 106 (2014) 548–555.
1451. Biswajit Sadhu et al., J. Phys. Chem. B, 2015, 119, 12783–12797.
1452. H. Lin, W. Chen, The Scientific World Journal, 2015 (2015) Article ID 945927.
1453. Yasser A. Mahmmoud et al., J. Biol. Chem. 290 (2015) 3720-3731.
1454. Ruhong Zhou, Molecular Modeling at Atomic Scale: Methods and Applications in Quantitative Biology, CRC Press, Boca Raton, 2015.
1455. J.M. Andric et al., ChemPhysChem 17 (2016) 2035.
1456. Fabien Archambault, Ph.D. thesis, Université Henri Poincaré, France, 2011.
1457. Li-Long Dang et al., Chem. Sci., 2020, 11, 1226-1232.
1458. Chun-Hung Wang et al., Front. Chem., 2018, https://doi.org/10.3389/fchem.2018.00062
1459. Ren-Zhong Li et al., Phys. Chem. Chem. Phys., 2018, 20, 29051-29060.
1460. Susmita De et al., Phys. Chem. Chem. Phys., 2018,20, 17517-17529.
1461. Kenichiro Mita et al., PNAS 2021, 118, e2017168118.
1462. M. Ashrafuzzaman, Nanoscale Biophysics of the Cell, Springer, 2018.
1463. A.A. Linhares, M.Sc. thesis, Univ. Federal de Santa Catarina, Brazil, 2020.
1464. Seifi, M., Soltanmanesh, A. & Shafiee, A. *Sci Rep* **12**, 9237 (2022).
1465. Matthew Colledge, Ph.D. thesis, Birkbeck, University of London, 2021.
1466. Y. Hou et al., J. Phys. Chem. Lett. 2023, 14, 2660–2664.
1467. J. Xu et al., Int. J. Mol. Sci. 2023, 24(19), 14414.
1468. L. Zhang et al., J. Am. Chem. Soc. 2024, 146, 8500–8507.
1469. Y. Feng et al., ACS Appl. Mater. Interfaces 2024, 16, 26817–26823.
1470. Y.-N. Chen et al., Molecules 2024, 29(4), 853.
1471. M.J. Stevens, S. L.B. Rempe, Faraday Discuss., 2024, 249, 195-209.
1472. Chen YN et al. Molecules (Basel, Switzerland). 2024 Feb;29(4):853.

Todor Dudev and Carmay Lim, "Metal binding affinity and selectivity in metalloproteins: insights from computational studies", *Annu. Rev. Biophys*. **37** (2008) 97-116.

1473. Anne Hong-Hermesdorf et al., Nature Chem. Biol. 10, 2014, 1034–1042.
1474. E. Degtyar et al. Angewandte Chemie International Edition, 53, 2014, 12026.
1475. Stephan Schmidt et al., Biomacromolecules, 2014, 15, 1644–1652.
1476. Shilpi Mandal et al., Struct Chem (2014) 25:43–51.
1477. Edina Rosta et al., J. Am. Chem. Soc., 2014, 136, 3137–3144.
1478. Haining Liu et al., J. Phys. Chem. A, 2014, 118, 3944–3951.
1479. Shilpi Mandal et al., J. Chem. Inf. Model., 2014, 54, 2524–2535.
1480. Michael D. L. Johnson et al., Infect. Immun. 2015, 83, 1684-1694.
1481. Adriana Ilie andManfred T. Reetz, Israel J. Chem. 55 (2015) 51–60.
1482. H.A. Alhazmi et al., J. Pharmaceutical Biomedical Analysis 107 (2015) 311.
1483. Ming Guo et al., Chemosphere 112 (2014) 472–480.
1484. Irina Galkina et al., Cryst. Eng. Comm, 2014,16, 9010-9024.

1485. Irfan Manzoor et al., Front Microbiol. 2015; 6: 748.
1486. Shilpi Mandal et al., RSC Adv., 2014, 4, 24796-24809.
1487. Haochen Ke et al., J. Phys. Chem. A, 2015, 119, 2037–2051.
1488. Ran Friedman, Dalton Trans., 2014, 43, 2878-2887.
1489. Samuel O. Odoh et al., J. Am. Chem. Soc., 2014, 136, 17484–17494.
1490. Noelia B. Luque et al., Phys. Chem. Chem. Phys., 2014, 16, 20107-2011.
1491. Zexian Liu et al., Biochimica et Biophysica Acta (BBA) - Proteins and Proteomics 1844 (2014) 171–180.
1492. Balasubramanian Sangeetha et al., Eur. Biophys. J. 2014, 43, 485-498.
1493. Elena Degtyar et al., Angewandte Chemie 126 (2014) 12220–12240.
1494. Shilpi Mandal et al., Journal of Molecular Structure 1100 (2015) 162–173.
1495. Paul Linsdell, Biomolecular Concepts 6 (2015) 191–203.
1496. Benjamin D. Greenbaum et al., PLoS ONE 2014, 9: e113943.
1497. Ran Friedman, Proteins 85, 2017, 2143-2152.
1498. Sikdar et al., Chemical Physics Letters 605–606 (2014) 103–107.
1499. Marco Flores et al., J. Phys. Chem. B, 2015, 119, 13825–13833.
1500. A. Kreider-Mueller et al., Journal of Organometallic Chemistry 792 (2015) 177.
1501. Bogdan F. Ion, Erum Kazim and James W. Gauld, Molecules 2014, 19, 15735.
1502. Hardeep Singh Tuli et al., Life Sciences 143 (2015) 71–79.
1503. Andrew G. P. Maloney et al., Cryst. Eng. Comm, 2015, 17, 9300-9310.
1504. Biswajit Sadhu et al., J. Phys. Chem. B, 2015, 119, 12783–12797.
1505. Caidan Zhang et al., Dyes and Pigments 123, 2015, 380–385.
1506. Samapan Sikda et al., J. Phys. Chem. B, 2015, 119, 14652–146d
1507. M. Ropo, V. Blum and C. Baldauf, Sci. Rep. 2016; 6: 35772.
1508. Ruhong Zhou, Molecular Modeling at Atomic Scale: Methods and Applications in Quantitative Biology, CRC Press, Boca Raton, 2015.
1509. Tomáš Rajský and Miroslav Urban, J. Phys. Chem. A, 2016, 120, 3938–3949.
1510. B. Sharma et al., J. Comp. Chem. 37 (2016) 992.
1511. Sharon L. Guffy et al., Protein Eng. Des. Sel. (2016) 29, 327-338.
1512. Rafael Grande-Aztatzi et al., Phys. Chem. Chem. Phys. 2016, 18, 7197-7207.
1513. Васина Дарья Владимировна, Ph.D. Thesis, Москва, 2015.
1514. A.Rosato, Y. Valasatava, C. Andreini, Int. J. Mol. Sci. 2016, 17, 671.
1515. Ichhuk Karki et al., J. Phys. Chem. B, 2016, 120, 12420.
1516. S.R. Garapati, Ph.D. Thesis, East Carolina University, U.S.A. 2014.
1517. J. Nyland, Honor Thesis, University of Tennessee, Knoxville, U.S.A., 2014.
1518. Gemma Aragay, et al., Chem. Rev. 2011, 111, 3433–3458.
1519. Waldron, K., Rutherford, J., Ford, D. et al. Nature 460, 823–830 (2009).
1520. Ya-Nan Chang et al., Materials 2012, 5(12), 2850-2871.
1521. N.J. Robinson, D.R. Winge, Annu. Rev. Biochem. 79:537-562 (2010).
1522. Marjorie M. Harding et al., (2010) Crystallography Reviews, 16:4, 247-302
1523. Zhou, Ting et al.; Current Topics in Medicinal Chemistry, 10, 2010, 33-45.
1524. Shavkat Mamatkulov et al, J. Chem. Phys. 138, 024505 (2013).
1525. F. Ruipérez et al., J. Inorg. Biochem. 117, 2012, 118-123.
1526. Claudia Andreini et al., Nucleic Acids Research, 41, 2013, D312–D319.

1527. Deborah G. Conrady et al., PNAS 2013 110 (3) E202-E211.
1528. Jing Hou et al., Environmental Pollution 221, 2017, 209-217.
1529. Steven M Yannone et al., Curr. Op. Biotechnology 23, 2012, 89-95.
1530. Andreini C. et al., (2011) PLoS ONE 6(10): e26325.
1531. J. I. Mujika et al., J. Phys. Chem. A 2011, 115, 6717–6723.
1532. Erin S. Honsa et al., Front. Cell. Infect. Microbiol., 2013; https://doi.org/10.3389/fcimb.2013.00092.
1533. Chen K, Kurgan L (2009) PLoS ONE 4(2): e4473.
1534. Claudia Andreini et al., J. Nol. Biol. 388, 2009, 356-380.
1535. Petr Sklenovský et al., J. Chem. Theory Comput. 2011, 7, 2963–2980.
1536. Sérgio F. Sousa et al., J. Comp. Chem. 30, 2009, 2752-2763.
1537. Ondrej Gutten and Lubomír Rulíšek, Inorg. Chem. 2013, 52, 10347–10355.
1538. Baile Wu et al., Environ. Sci. Technol. 2020, 54, 50–66.
1539. Ondrej Gutten et al., J. Phys. Chem. A 2011, 115, 11394–11402.
1540. Jiří Šponer et al., Methods 64, 2013, 3-11.
1541. Tong Zhu et al., J. Chem. Theory Comput. 2013, 9, 1788–1798.
1542. Milan Vašák and Gabriele Meloni, Int. J. Mol. Sci. 2017, 18(6), 1117.
1543. Dhruva K. Chakravorty et al., J. Am. Chem. Soc. 2012, 134, 3367–3376.
1544. Demian Riccardi et al., J. Chem. Theory Comput. 2013, 9, 555–569.
1545. Foster, A.W., Robinson, N.J. BMC Biol 9, 25 (2011).
1546. Orazio Amata et al., Phys. Chem. Chem. Phys., 2011,13, 3468-3477.
1547. Li Rao et al., J. Am. Chem. Soc. 2010, 132, 18092–18102.
1548. Melinda Wales and C. Steven McDaniel, US patent US20110070376A1, 2011.
1549. Peng Wang et al., Mol. Microbiol. 86, 2012, 1441-1451.
1550. M.R. Gunner et al., Biochim. Biophys. Acta – Bioenergetics 1827, 2013, 892.
1551. Bhaskar Sharma et al., J. Phys. Chem. A 2011, 115, 1971–1984.
1552. Shao-Yong Lu et al., Proteins 81, 2013, 740-753.
1553. Amit Das et al., Biophys. J. 104, 2013, 1274-1284.
1554. Zhifeng Jing et al., PNAS 2018 115 (32) E7495-E7501.
1555. George N. Khairallah et al., Organometallics 2013, 32, 2319–2328.
1556. Hai Lei et al., J. Am. Chem. Soc. 2017, 139, 1538–1544.
1557. Gaetano Invernizzi et al., J. Struct. Biol. 168, 2009, 562-570.
1558. Stefan Zechel et al., Biomimetics 2019, 4(1), 20.
1559. Peng Zheng et al., J. Am. Chem. Soc. 2013, 135, 7992–8000.
1560. S. Sruthi et al., Materials Today Chemistry 10, 2018, 175-186.
1561. Lawrence C. Thompson et al., Protein Sci. 20, 2011, 366-378.
1562. Adebayo A. Adeniyi et al., Drug Discovery Today 22, 2017, 1216-1223.
1563. Bingpeng Guo et al., Sensors and Actuators B: Chemical 256, 2018, 632-638.
1564. Yuanqiang Hao et al., Nanomaterials 2019, 9(7), 974.
1565. Antoine Ziller et al., J. Inorg. Biochemistry 167, 2017, 1-11.
1566. Lancaster, W.A., et al., BMC Bioinformatics 12, 64 (2011).
1567. Kenichi Shimada et al., Cell Chemical Biology 25, 2018, 585-594.e7.
1568. Neela, Y.I., Mahadevi, A.S. & Sastry, G.N. Struct Chem 24, 67–79 (2013).
1569. Ivano Bertini, Gabriele Cavallaro; Metallomics 2, 2010, 39–51.

1570. Richard P. Matthews and Kevin J. Naidoo, J. Phys. Chem. B 2010, 114, 7286.
1571. Yi Cao et al., ChemPhysChem 10, 2009, 1450-1454.
1572. Amit Das et al., Chem. Phys. Lett. 581, 2013, 91-95.
1573. Georgia C. Boles et al., Phys. Chem. Chem. Phys., 2017,19, 12394-12406.
1574. Tiwari, M.K., et al. Appl Microbiol Biotechnol 87, 571–581 (2010).
1575. Sergei Y. Ponomarev et al., J. Phys. Chem. B 2011, 115, 10079–10085.
1576. Yang, X., Li, Q., Cheng, J. et al. J Mol Model 19, 247–253 (2013).
1577. Grasso, G., Spoto, G. Anal Bioanal Chem 405, 1833–1843 (2013).
1578. Suseung Lee et al., Chem. Commun., 2009, 6171-6173.
1579. Pena L.B., Azpilicueta C.E., Benavides M.P., Gallego S.M. (2012) Protein Oxidative Modifications. In: Gupta D., Sandalio L. (eds) Metal Toxicity in Plants: Perception, Signaling and Remediation. Springer, Berlin, Heidelberg.
1580. Edwards, B.F., Fernando, R., Martin, P.D. et al. Biochem 14, 36 (2013).
1581. Gaoxiang Liu et al., J. Phys. Chem. A 2017, 121, 5817–5822.
1582. Oliver Schalk et al., Z. Phys. Chem.227(2013) 35–47.
1583. Koohi-Moghadam, M., et al. Nat Mach Intell 1, 561–567 (2019).
1584. Claudia Andreini et al., J. Chem. Inf. Model. 2013, 53, 3064–3075.
1585. Besnik Krasniqi, Jeremy S Lee; Metallomics 4, 2012, 539–544.
1586. Annaleizle Ferranco et al., Dalton Trans., 2017,46, 4844-4859.
1587. Taka-aki Okamura and Junko Nakagawa, Inorg. Chem. 2013, 52, 10812–10824.
1588. Joseph, D., Chakraborty, K. Appl Biochem Biotechnol 185, 55–71 (2018).
1589. Kenneth D. Karlin (Ed.) Progress in Inorganic Chemistry, Volume 57, ISBN 9781118010631, John Wiley & Sons, Inc. 2012.
1590. Maojie Xu et al., Chemical Physics Letters 537, 2012, 101-106.
1591. Shanti Swaroop Srivastava, et al., Biochemistry 2017, 56, 1299–1310.
1592. Alberto Ciferri and Angelo Perico (Eds.) Ionic Interactions in Natural and Synthetic Macromolecules, ISBN:9780470529270, 2012 John Wiley & Sons, Inc.
1593. Miroslav A. Rangelov et al., J. Mol. Graphics Model. 29, 2010, 246-255.
1594. Sha Wang et al., Chem. Sci., 2020, 11, 879-887.
1595. Yi Wang et al., J. Am. Chem. Soc. 2013, 135, 6084–6091.
1596. Phillip C. Wright et al., IUBMB Life 65, 2013, 17-27.
1597. Saumen Chakraborty et al., Acc. Chem. Res. 2017, 50, 92225–2232.
1598. Teng Wang et al., Phys. Chem. Chem. Phys., 2011,13, 1140-1151.
1599. Elena Papaleo, Gaetano Invernizzi; Biopolymers 95, 2011, 117-126.
1600. Amolegbe, S.A. et al. J Biol Inorg Chem 22, 1–18 (2017).
1601. Maryam Akbari et al., Ceramics International 46, Part A, 2020, 9979-9989.
1602. Ahmad Motaharia and Alireza Fattahi; New J. Chem., 2017,41, 15110-15119.
1603. Mahmoud Khadem-Maaref et al., J. Mol. Graphics Model. 73, 2017, 24-29.
1604. Moulahoum, H.,et al. Probiotics & Antimicro. Prot. 12, 48–63 (2020).
1605. Cecilia Wallin et al., J. Biol. Chem. 295, 2020, 7224-7234.
1606. Q.D. Le et al., Coastal Mirine Sci. 35 (2012) 136-141.
1607. Liliana Pacureanu et al., Rev. Roum. Chim. 2011, 56(4), 289-298.
1608. Mahadevi A.S., Sastry G.N. (2011) In: Leszczynski J., Shukla M. (Eds) Practical Aspects of Computational Chemistry I. Springer, Dordrecht.

1609. Nezar H. Khdary et al., New J. Chem., 2017,41, 11556-11567.
1610. K. Eskandari & F. Ebadinejad (2018) Molecular Physics, 116:10, 1369-1376.
1611. Colleen M. Doyle et al., Analytical Biochemistry 579, 2019, 44-56.
1612. Zia, M., et al. Plant Cell Tiss Organ Cult 145, 261–274 (2021).
1613. Tavallali, H., et al. Appl Biochem Biotechnol 187, 913–937 (2019).
1614. Xiaohua Ma et al., J. Anal. Met. Chem., vol. 2018, Article ID 1986468, 2018.
1615. Christina Wegeberg et al., Inorg. Chem. 2019, 58, 8983–8994.
1616. Zhenyao Luo et al., J. Bacteriol. 2019, DOI: 10.1128/JB.00580-19.
1617. Ang, TF., Salleh, A.B., Normi, Y.M. et al. Biotech 8, 314 (2018).
1618. Šponer J., Šponer J.E., Leontis N.B. (2012) In: Leontis N., Westhof E. (eds) RNA 3D Structure Analysis and Prediction. Nucleic Acids and Molecular Biology, vol 27. Springer, Berlin, Heidelberg.
1619. Ilic, S., Akabayov, S.R., Froimovici, R. et al. Sci Rep 7, 5797 (2017).
1620. Gui-Feng Li et al., Chemical Engineering Journal 393, 2020, 124800.
1621. Liliana Beatriz Pena et al. In book: Metal Toxicity in Plants: Perception, Signaling and Remediation (pp.207-225) Chapter: 10, Publisher: Springer-Verlag, 2012.
1622. Chyuan-Chuan Wu et al., Trends Biochem. Sci. 45, 2020, 935-946.
1623. Claude Steven McDaniel, US patent US20200354588A1, 2020.
1624. KIRAN KUMAR NALLA, M.Sc. thesis, Texas A&M University, U.S.A. 2012.
1625. Thach, Chia Tha, Ph.D. thesis, University of Rochester, New York, 2012.
1626. Rafael Grande-Aztatzi et al., J. Inorg. Biochem. 210, 2020, 111169.
1627. Tyler B. J. Pinter et al., Angew. Chem. Intl. Ed. 59, 2020, 20445-20449.
1628. Dixit, Purushottam D.; Ph.D. thesis, Johns Hopkins University, U.S.A. 2011.
1629. Mohammed Ismael et al., New J. Chem. 2019, 43(19) DOI:10.1039/C9NJ00859D.
1630. Gugala, Natalie; Ph.D. thesis, University of Calgary, Canada, 2019.
1631. A. Mudhoo and R. Mohee, Dynamic Soil, Dinamyc Plant 5 (2011) 25-35.
1632. Lohse, Jonas; Ph.D. thesis, University of Groningen, Germany, 2018.
1633. Jerzy Leszczynski and Manoj K. Shukla (Eds.) Practical Aspects of Computational Chemistry I, ISBN: 978-94-007-0919-5, Springer, 2012.
1634. Azam Javadi et al. J Fasa Univ Med Sci 2020, 10(1): 1998-2011.
1635. Lee Soo-seung, Ph.D. thesis, Seoul National University, Korea, 2013.
1636. Zhang, Yaofang; Ph.D. thesis, University of Cincinnati, U.S.A. 2012.
1637. Armelle Vigouroux et al., FEBS J., 287, 2020, 295-309.
1638. A.M. Haase, M.Sc. thesis, Western Michigan University, U.S.A., 2012.
1639. Sérgio F. Sousa et al., ACS Catal. 2020, 10, 8444–8453.
1640. Samapan Sikdar, Ph.D. thesis, University of Calcutta, India, 2016.
1641. A.M. Oertel, Ph.D. thesis, Univesrsite de Strasbourg, France, 2010.
1642. C.E. BLABY-HAAS, Ph.D. thesis, University of Florida, 2011.
1643. Dong Wang, Ph.D. thesis, Arizona State University, U.S.A. 2014.
1644. Zheng, Peng; Ph.D. thesis, THE UNIVERSITY OF BRITISH COLUMBIA (Vancouver), Canada, 2013.
1645. Ran Friedman, J. Phys. Chem. B 2021, 125, 2251–2257.

1646. A. Mangavelu, M.Sc. thesis, University Putra Malaysia, 2018.
1647. Guenther, Joel Michael; Ph.D. thesis, University of California, Berkeley, 2010.
1648. Claude Steven McDaniel, Melinda Wales; US patent US20210017402A1, 2021.
1649. Javadi, Azam Farzaneh et al.; J. Fasa University of Medical Sciences / Majallah-i Danishgah-i Ulum-i Pizishki-i Fasa, 2020, 10, 1998-2011.
1650. Isabell Tunn, Ph.D. thesis, Potsdam University, Germany, 2020.
1651. Zhuang Huiying, M.Sc. thesis, Kaohsiung Medical University, Taiwan, 2012.
1652. Yi Wang, Ph.D. thesis, Duke University, U.S.A. 2012.
1653. S. Jachimoviciute, M. Sc. Thesis, Vilniaus Gedimino Technikos Universitetas, Vilnius, Lithuania, 2008.
1654. Lin Liyang, Ph. D. Thesis, National Chung Hsing University, Taiwan, 2010.
1655. Y. el Khoury, Ph. D. Thesis, University of Strasbourg, France, 2010.
1656. T. Shen, M.Sc. Thesis, University of British Columbia, Canada, 2012.
1657. Guillermo Bahr et al. *Chem. Rev.* 2021, 121, 13, 7957–8094.
1658. Majed Nejati et al. Inorg. Chem. Communications 136, 2022, 109107.
1659. Abrar Muhammad et al. Science of The Total Environment, 813, 2022, 152608.
1660. Lu Zhang et al. European J. Medicinal Chemistry Volume 230, 2022, 114101.
1661. Jackson Gearyet al. J. Am. Chem. Soc. 2021, 143, 27, 10317–10323.
1662. Jinho Yoon et al.Biosensors and Bioelectronics 212, 2022, 114427.
1663. Joanna I. Lachowicz et al. Int. J. Mol. Sci. 2022, 23(1), 551.
1664. Sunayana Mitra et al. J. Phys. Chem. *A* 2021, 125, 22, 4867–4881.
1665. Isah, T., Qurratul & Umar, S. Plant Cell Tiss Organ Cult 149, 563–587 (2022).
1666. Kai Wang, Briefings in Bioinformatics, 24, 2023, bbac620, https://doi.org/10.1093/bib/bbac620.
1667. Salvatore La Gatta et al., Molecules 2021, 26(17), 5221.
1668. Maureen Bilinga Tendwa et al. Molecules 2021, 26(10), 2929.
1669. Zhifeng Jing, Ph.D. thesis, University of Texas at Austin, 2021.
1670. Sunayana Mitra, Ph.D. thesis, University of Pittsburgh, 2021.
1671. Alina Beșliu and Nadejda Efremova, Scientific Study & Researc 2021, 22, 383.
230. Claude Steven McDaniel and Melinda Wales, US patent, Publication of US20210017402A1, 2021.
231. OLADAPO S FALOKUN, M.Sc. Thesis, Texas A&M University, 2021.
232. Wenjia Wang, Ph.D. thesis, University of Groningen, 2021.
1672. OUARI Malika, M.Sc. Thesis,Université de Tissemsilt, Algerie, 2022.
1673. Abedini A, et al. Front Chem. 2022;10:893793.
1674. Y. Wu et al., Water Research 239, 2023, 120031.
1675. H. Sajjad et al., Comparative Biochem. Physiol. Part C 271, 2023, 109682.
1676. Shirin Malehmir et al., Inorg. Chem. Commun. 156, 2023, 111306.
1677. A.M. Hoffnagle and F.A. Tezcan, J. Am. Chem. Soc. 2023, 145, 14208–14214.
1678. Julen Aduriz-Arrizabalaga et al., Phys. Chem. Chem. Phys., 2023, 25, 27618.
1679. R. Lai et al., J. Am. Chem. Soc. 2024, 146, 11, 7628–7639.
1680. P. Potok et al., Inorg. Chem. 2023, 62, 45, 18425–18439.
1681. Mantas Liutkus et al., Protein Science 33, 2024, e4971.
1682. David Silva-Brea et al., Phys. Chem. Chem. Phys., 2023,25, 26429-26442.

1683. Tadeáš Kalvoda et al., J. Chem. Phys. 160, 084308 (2024).
1684. I.-A. Vagena et al., Nanomaterials 2024, 14(5), 397.
1685. L. Zhang et al., Molecules 2024, 29(5), 1096.
1686. Alabbası A, et al. JOTCSA. 2023;10(2):325-38.
1687. Bruno Hay Mele, et al., Essays Biochem 11, 2023; 67 (4): 653–670.
1688. M.-A. Gatou et al., Crystals 2024, 14(3), 215.
1689. J.P. Leite et al., Journal of Structural Biology 215, 2023, 108038.
1690. A. Motahari, A. Fattahi, JPOC 37, 2024, e4571.
1691. S. Wang et al., Water 2023, 15(23), 4080.

Tsung-Ying Yang, **Todor Dudev** and Carmay Lim, "Mononuclear versus binuclear metal-binding sites: metal-binding affinity and selectivity from PDB survey and DFT/CDM calculations", *J. Am. Chem. Soc.* **130** (2008) 3844-3852.

1692. A.W. Foster, et al. J. Biol. Chem. 289 (2014) 28095-28103.
1693. Shiyan Xiao at al., J. Phys. Chem. B 2014, 118, 873–889.
1694. C. Pozzi et al., Acta Cryst. (2015). D71, 941-953.
1695. A. Krah, S. Takada, Biochim. Biophys. Acta – Bioenergetics 1847 (2015) 1101.
1696. Ran Friedman, Dalton Trans., 2014, 43, 2878-2887.
1697. Claudia Sissi, Manlio Palumbo; Nucleic Acids Research, 37, 2009, 702–711.
1698. Joseph, A.P., Agarwal, G., Mahajan, S. et al. Biophys Rev 2, 137–145 (2010).
1699. Tuo Zhang et al., Science Advances 2017: 3, e1700344.
1700. Dominga Rogolino et al., Coord. Chem. Rev. 256, 2012, 3063-3086.
1701. Tong Zhu et al., J. Chem. Theory Comput. 2013, 9, 1788–1798.
1702. Bojana Savić et al., Plant and Cell Physiology, 50, 2009, 1587–1599.
1703. Johannes Gregor Matthias Rack et al., Cell Chem. Biol. 25, 2018, 1533-1546.
1704. Ran Friedman, Proteins 85, 2017, 2143-2152.
1705. Marcos Mandado et al., J. Comput. Chem. 31, 2010, 2735-2745.
1706. Tuo Zhang et al., FASEB J. 34, 2020, 237-247.
1707. Alberto Ciferri and Angelo Perico (Eds.) Ionic Interactions in Natural and Synthetic Macromolecules, ISBN:9780470529270, 2012 John Wiley & Sons, Inc.
1708. Saliu A. Amolegbe et al., J Biol Inorg Chem (2017) 22:1–18.
1709. J.F. Scortecci et al., Biochim. Biophys. Acta - Proteins and Proteomics 1865, 2017, 1326-1335.
1710. Taiho Kambe et al., J Biol Chem. 2021; 296: 100320.
1711. David J. Eide (2020) Critical Rev. Biochem. Mol. Biol., 55:1, 88-110.
1712. Li, M., Henderson et al. J Biol Inorg Chem 23, 785–793 (2018).
1713. Ilic, S., Akabayov, S.R., Froimovici, R. et al. Sci Rep 7, 5797 (2017).
1714. Chen, Shilu; Ph.D. thesis, Royal Institute of Technology, Stockholm, 2008.

1715. O. Maglio, F. Nastri, A. Lombardi, in IONIC INTERACTIONS IN NATURAL AND SYNTHETIC MACROMOLECULES (A. Ciferri, A. Perico, Eds.), John Wiley & Sons, 2012, Ch. 11, pp. 361-449.
1716. A.W. Foster et al. Current Opinion Chem. Biology, Volume 66, 2022, 102095.
1717. G. Sharma et al., Biochemistry 2021, 60, 36, 2727–2738.
1718. Gaurav Sharma et al., Methods in Enzymology 687, 2023, 263-278.

Todor Dudev and Carmay Lim, “Effect of carboxylate-binding mode on metal binding/selectivity and function in proteins”, *Acc. Chem. Res*. **40** (2007) 85-93.

1719. Matthew R. Berwick et al., J. Am. Chem. Soc., 2014, 136, 1166–1169.
1720. K.E. Dalle and Franc Meyer, Eur. J. Inorg. Chem. 2015 (2015) 3391–3405.
1721. Edward Greinera et al. Geochimica et Cosmochimica Acta 133 (2014) 142–155.
1722. Jia-Jia Xu et al., Phys. 112 (2014) 1710-1723.
1723. Nam-Ho Kim et al. J. Korean Soc. Appl. Biol. Chem. 2014, 57, 91-95.
1724. Ying-Hua Zhou et al., Inorganica Chimica Acta 426 (2015) 211–220.
1725. S.F. Sousa et al. Int. J. Quantum Chem. 114 (2014) 1253-1256.
1726. O. Gutten and L. Rulíšek, Phys. Chem. Chem. Phys., 2015, 17, 14393-14404.
1727. Xue Cheng et al., RSC Adv., 2015, 5, 4511-4523.
1728. Taka-aki Okamura et al., J. Am. Chem. Soc., 2014, 136, 14639–14641.
1729. Lingling Liu et al., Scientific Reports 5, Article number: 11121 (2015).
1730. Samapan Sikdar et al., Chemical Physics Letters 605–606 (2014) 103–107.
1731. L. I. N. Tomé et al., RSC Adv., 2015, 5, 15024-15034.
1732. Adam E. Brummett et al., PLoS ONE 10 (2015): e012728.
1733. Taka-aki Okamura et al., Dalton Trans., 2015, 44, 7512-7523.
1734. T. A. Babushkina et al., Russian J. Coord. Chem. 2015, 41, 43-46.
1735. Sneha R. Wankar et al., Journal of Luminescence 177 (2016) 416–424.
1736. B.I. Okeleye et al., Iranian J. Pharm. Res. (2016) Available Online from 06 March 2016.
1737. Adewale Adewuyia; Fabiano Vargas Pereira, J. Adv. Res. 7 (2016) 947–959.
1738. A.F.A. Peacock, Methods in Enzymology 580 (2016) 557–580.
1739. Hassan A. Azab et al., Journal of Luminescence 176 (2016) 181–192.
1740. Virender K. Sharma (2009) J. Environ. Sci. Health, Part A, 44:14, 1485-1495.
1741. Sergei Y. Noskov and Benoît Roux, J. Mol. Biol. 377, 2008, 804-818.
1742. Yu-Hao Lin et al., Science of The Total Environment 408, 2010, 2260-2267.
1743. Jaibir Kherb et al., J. Phys. Chem. B 2012, 116, 7389–7397.
1744. John Podtetenieff et al., Angew. Chem. 122, 2010, 5277-5281.
1745. Sung Hee Joo et al., Environ. Sci. Technol. 2009, 43, 4954–4959.
1746. Lung Wa Chung et al., J. Am. Chem. Soc. 2008, 130, 12299–12309.
1747. Clark Zhang et al., J. Controlled Release 263, 2017, 112-119.

1748. M. Tyagi et al., Proteins 71, 2008, 920-937.
1749. Yukihiro Kimura et al., J. Biol. Chem. 283, 2008, 13867-13873.
1750. YukihiroKimura et al., J. Biol. Chem. 284, 2009, 93-99.
1751. Jessica N. Malin et al., J. Phys. Chem. C 2009, 113, 2041–2052.
1752. Changlin Liu and Li Wang, Dalton Trans., 2009, 227-239.
1753. Kirberger, M. et al.; J Biol Inorg Chem 13, 1169–1181 (2008).
1754. Ondrej Gutten and Lubomír Rulíšek, Inorg. Chem. 2013, 52, 10347–10355.
1755. Ondrej Gutten et al., J. Phys. Chem. A 2011, 115, 11394–11402.
1756. Tong Zhu et al., J. Chem. Theory Comput. 2013, 9, 1788–1798.
1757. Ezzat M. Soliman et al., Desalination 278, 2011, 18-25.
1758. Bhuvaneshwari Mahalingam et al., J Immunol 2011, 187, 6393-6401.
1759. Zhifeng Jing et al., PNAS August 7, 2018 115 (32) E7495-E7501.
1760. George N. Khairallah et al., Organometallics 2013, 32, 2319–2328.
1761. Sergio Navalon et al., J. Hazardous Materials 169, 2009, 901-906.
1762. Lucie Ducháčková et al., Inorg. Chem. 2011, 50, 3153–3158.
1763. Congmeng Wu et al., Cryst. Growth Des. 2011, 11, 3153–3162.
1764. Rutkowska-Zbik et al., J Mol Model 19, 4661–4667 (2013).
1765. Tanskanen, A. et al.; Sci Rep 8, 8976 (2018).
1766. Milan Kožíšek et al., Chem. Eur. J. 14, 2008, 7836-7846.
1767. Adam R. Offenbacher et al., J. Am. Chem. Soc. 2013, 135, 6380–6383.
1768. Kaur, G., Guruprasad, K., Temple, B.R.S. et al. Amino Acids 50, 79–94 (2018).
1769. Joseph W. DePalma et al., J. Phys. Chem. Lett. 2017, 8, 484–488.
1770. D. Rutkowska-Zbik; T. Korona, J. Chem. Theory Comput. 2012, 8, 2972–2982.
1771. Xueqin Pang et al., J. Comp. Chem. 34, 2013, 1620-1635.
1772. Gilles Frison; Gilles Ohanessian; Phys. Chem. Chem. Phys., 2009,11, 374-383.
1773. Dohyun Moon et al., Polyhedron 27, 2008, 447-452.
1774. Sebastian T. Le Quement et al., J. Comb. Chem. 2008, 10, 546–556.
1775. Umesh Kumar et al., Polyhedron 55, 2013, 233-240.
1776. KaushikGhosh et al., Inorganica Chimica Acta 405, 2013, 24-30.
1777. Richard Tjörnhammar and Olle Edholm, J. Chem. Phys. 132, 205101 (2010).
1778. Kirberger, Michael et al., Current Bioinformatics, 5, 2010, 68-80.
1779. Lung Wa Chung et al., in Quantum Biochemistry, Chérif F. Matta (Ed.) 2010 Wiley-VCH Verlag GmbH & Co. KGaA.
1780. Feng-Mei Nie et al., Inorganica Chimica Acta 362, 2009, 763-770.
1781. C.D. Quarles Jr.; R.K. Marcus; Spectrochim. Acta B, 64, 2009, 1185.
1782. Marc Donald Parrent, M.Sc. thesis, University of Alberta, Canada, 2012.
1783. Taka-aki Okamura and Junko Nakagawa, Inorg. Chem. 2013, 52, 10812–10824.
1784. Willis Kwun Hei Ho et al., J. Phys. Chem. Lett. 2019, 10, 4692–4698.
1785. Ezzatollah Najafi et al., Inorg. Chim. Acta 463, 2017, 61-69.
1786. Alberto Ciferri and Angelo Perico (Eds.) Ionic Interactions in Natural and Synthetic Macromolecules, ISBN:9780470529270, 2012 John Wiley & Sons, Inc.
1787. Bikash K. Dey et al., J. Mol. Catal. A: Chemical 303, 2009, 137-140.
1788. Teng Wang et al., Phys. Chem. Chem. Phys., 2011,13, 1140-1151.
1789. Yang, L., Liao, RZ., Ding, WJ. et al. Theor Chem Acc 131, 1275 (2012).

1790. Elena Papaleo, Gaetano Invernizzi; Biopolymers 95, 2011, 117-126.
1791. Subramaniam Kavitha et al., J. Mol. Graphics Model. 85, 2018, 13-24.
1792. Feng Xiang et al., J. Phys. Chem. B 2007, 111, 12282–12293.
1793. Daniel E. Bacelo; R. C. Binning, Jr.; J. Phys. Chem. A 2009, 113, 1189–1198.
1794. Ahmad Motaharia; Alireza Fattahi; New J. Chem., 2017,41, 15110-15119.
1795. Susmita De et al., Phys. Chem. Chem. Phys., 2020,22, 799-810.
1796. Chunchun Zhang et al., Biochemistry 2018, 57, 4504-4517.
1797. Goswami, Shyamaprosad; Jana, Subrata, Lett. Org. Chem. 7, 2010, 399-405.
1798. Patricija Hriberšek and Ksenija Kogej, Polymers 2019, 11(4), 605.
1799. Tufan Singha Mahapatra et al., Eur. J. Inorg. Chem. 2017, 2017, 769-779.
1800. Rachel E. Bongini et al., J. Inorg. Biochem. 101, 2007, 1251-1264.
1801. Patricija Hriberšek, Macromolecules 2019, 52, 7028–7041.
1802. Benjamin Ifeoluwa Okeleye et al., Iran J Pharm Res. 2017, 16(2): 714–724.
1803. Kai Wang et al., Bioinformatics, 36, 2020, 4004–4011.
1804. Dipjyoti Kalita et al., Polyhedron 44, 2012, 52-58.
1805. D.M. de Oliveira et al., Phys. Chem. Chem. Phys., 2020,22, 24014-24027.
1806. JAIBIR KHERB, Ph.D. thesis, Texas A&M University, U.S.A. 2011.
1807. Tanskanen, Anne’ Ph.D. thesis, Aalto University, Finlnd, 2018.
1808. Michelle Marian Turco, Ph.D. thesis, University of Colorado, U.S.A. 2013.
1809. Patricija Hriberšek, Ksenija Kogej; Acta Chimica Slovenica 66, 4 (2019).
1810. Michael Kirberger, Ph.D. thesis, Georgia State University, U.S.A. 2011.
1811. Hai Deng, Ph.D. thesis, Georgia State University, U.S.A. 2007.
1812. Samapan Sikdar, Ph.D. thesis, University of Calcutta, India, 2016.
1813. Gutten, Ondrej; Diploma thesis, Charles University, Prague, 2010.
1814. Фомина, Е.К.; Бутовская, Г.В.; Круль, Л.П.; Гринюк, Е.В.; Якименко, О.В.; "Журнал Белорусского государственного университета" Химия 2017, 2, 94-109.
1815. Stefan Kluge, Ph.D. thesis, Friedrich-Schiller-Universität Jena, Germany, 2007.
1816. Yu-Hao Lin, Ph.D. Thesis, National Chung Hsing University, Taiwan, 2010.
1817. S.N. Oltra, Ph.D. Thesis, Universidad Politécnica de Valencia, Spain, 2010.
1818. C.D. Quarles, Jr., Ph.D. Thesis, Clemson University, USA, 2011.
1819. E. Duboué-Dijon *and* J. Hénin, J. Chem. Phys. 154, 204101 (2021).
1820. Kunlin Chu et al. J. Phys. Chem. Lett. 2021, 12, 33, 8003–8008.
1821. A.F. Ferreira et al. Solid State Sciences Volume 128, June 2022, 106870.
1822. Hui Zhou et al. Chemosphere Volume 308, Part 2, December 2022, 136324.
1823. Ahmed Mohamed et al. J. Phys. Chem. A 2023, 127, 6, 1413–1421.
1824. Mehriban Aliyeva et al. J. Chem. Eng. Data 2022, 67, 6, 1565–1572.
1825. Kai Wang, Briefings in Bioinformatics, 24, 2023, bbac620, https://doi.org/10.1093/bib/bbac620.
1826. Alyssa A. DeLucia et al. Inorg. Chem. 2021, 60, 20, 15599–15609.
1827. Denilson Mendes de Oliveira, Ph.D. thesis, Purdue University, 2021.
1828. Vishal Kumar Porwal et al., J. Compt. Chem. 44, 2023, 1898-1911.
1829. S. Shanjitha et al., Appl. Organometallic Chem. 38, 2024, e7465.
1830. S. Shanjitha et al., Inorganica Chimica Acta 553, 2023, 121541.
1831. do Nascimento, R.F.F., et al., J Nanopart Res 26, 59 (2024).

1832. Ahmad Motahari, Alireza Fattahi, JPOC 37, 2024, e4571.
1833. Milana Bazayeva et al., Acta Cryst. (2024). D80, 362–376.
1834. X.-M. Du et al., Appl. Organometallic Chem., 2024, https://doi.org/10.1002/aoc.7522.
1835. S.J. Firth, Ph.D. Thesis, Durham University, UK, 2023.

Todor Dudev and Carmay Lim, "All-electron calculations of the nucleation structures in metal-induced zinc-finger folding: Role of the peptide backbone", *J. Am. Chem. Soc.* **129** (2007) 12497-12504.

1836. Wenfei Li et al., Current Opinion in Structural Biology 30 (2015) 25–31.
1837. A. Gerard Daniela and Nicholas P. Farrell, Metallomics, 2014, 6, 2230-2241.
1838. Borko M. Matijević et al., Spectrochim. Acta Part A 117 (2014) 568–575.
1839. Wenfei Li et al., J. Am. Chem. Soc. 2008, 130, 892–900.
1840. Shan Chang et al., Int. J. Mol. Sci. 2010, 11(10), 4014-4034.
1841. Gábor Nagy et al., J. Mol. Graphics Model. 29, 2011, 928-934.
1842. Madhumita Mukherjee et al., Inorg. Chem. 2008, 47, 4430–4432.
1843. Mori, S. et al., Theor Chem Acc 130, 279–297 (2011).
1844. DriciNedjoua et al., Comput. Biol. Chem. 74, 2018, 86-93.
1845. Mori, Seiji et al., Theoretical Chemistry Accounts: Theory, Computation, & Modeling, 2011, 130, 279-297.
1846. N. Drici, Ph.D. thesis, University of Oran, Algeria, 2017.

M. Dudev, J. Wang, T. Dudev and C. Lim, "Factors governing the metal coordination number in metal complexes from Cambridge Structural Database analyses", *J. Phys. Chem. B* **110** (2006) 1889-1895.

1847. Jason Tien et al., eLife 2014:e02772.
1848. Md. Elius Hossain et al., Spectrochimica Acta Part A 138 (2015) 499–508.
1849. Emanueli do Nascimento da Silva et al., Microchemical J. 119 (2015) 152–158.
1850. Ran Friedman, Dalton Trans., 2014, 43, 2878-2887.
1851. Ryota Mizushima et al., PLOS ONE 2014, 9, e98554.
1852. R. Jesu Jaya Sudan & C. Sudandiradoss, J. Coord. Chem. 67 (2014) 1888-1904.
1853. Alexandre C. Bertoli et al., J. Inorganic Biochemistry 144 (2015) 31–37.
1854. Anirudha Dutta et al., FEBS Journal 281 (2014) 5309–5324.
1855. María del Carmen Ramírez Avi et al. Theor. Chem. Acc. 2015, 134:52.
1856. Joshua H. Palmer et al., J. Mol. Struct. 1091 (2015) 177–182.
1857. Alain Manceau et al., Inorg. Chem., 2015, 54, 11776–11791.

1858. Monika Fuxreiter, Computational Approaches to Protein Dynamics, CRC Press, Boka Raton, 2015.
1859. Elisa Bellomo et al., Coordination Chemistry Reviews 327–328 (2016) 70–83.
1860. Faulkner, Robert A.; Ph.D. thesis, University of Huddersfield, UK, 2016.
1861. Keyan Li and Dongfeng Xue, J. Phys. Chem. A 2006, 110, 11332–11337.
1862. Christopher M. Micklitsch et al., Angew. Chem. Intl. Ed. 50, 2011, 1577-1579.
1863. Félix Freire et al., J. Am. Chem. Soc. 2012, 134, 19374–19383.
1864. Darren M. Griffith et al., Journal of Inorganic Biochemistry 105, 2011, 763-769.
1865. Sonja M. Schwarzl et al., Biochemistry 2006, 45, 5830–5847.
1866. Gilles Frison, Gilles Ohanessian; J. Comp. Chem. 29, 2008, 416-433.
1867. Robin Taylor and Peter A. Wood, Chem. Rev. 2019, 119, 9427–9477.
1868. Asnake Lealem Berhanu et al., TrAC Trends Anal. Chem. 116, 2019, 74-91.
1869. Alba Guarné, Progress Mol. Biol. Trans. Sci. 110, 2012, 41-70.
1870. Christophe Gourlaouen Ing et al., Chem. Eur. J. 12, 2006, 5024-5032.
1871. Demian Riccardi et al., J. Chem. Theory Comput. 2013, 9, 555–569.
1872. Keyan Li, Dongfeng Xue; Physica Status Solidi 44, 2007, 1982-1987.
1873. M.R. Gunner et al., Biochim. Biophys. Acta – Bioenergetics 1827, 2013, 892.
1874. Niloufar J. Ataie et al., Biochemistry 2008, 47, 7673–7683.
1875. Patrick Frank et al., Inorg. Chem. 2012, 51, 2086–2096.
1876. Anna Adach et al., Polyhedron 47, 2012, 104-111.
1877. Barak Akabayov et al., Biochemistry 2009, 48, 1763–1773.
1878. Md. R. Shakil et al., Inorg. Chem. 2018, 57, 9977–9987.
1879. Alain Manceau et al., Environ. Sci. Technol. 2018, 52, 10286–10296.
1880. da Costa, L.M. et al; J Mol Model 17, 2061–2067 (2011).
1881. Leonardo Moreirada Costa et al., THEOCHEM 911, 2009, 46-51.
1882. Matthew J. Eibling et al., J. Am. Chem. Soc. 2017, 139, 17811–17823.
1883. Delphine Picot et al., Chem. Asian J. 5, 2010, 1445-1454.
1884. George Pontikis et al., J. Phys. Chem. A 2009, 113, 3588–3593.
1885. C. Gourlaouen, O. Parisel; Int. J. Quantum Chem. 108, 2008, 1888-1897.
1886. Albano N. Carneiro Neto et al., J. Luminescence 201, 2018, 451-459.
1887. da Costa, L.M. et al.; J Mol Model 19, 2669–2677 (2013).
1888. Moreira da Costa et al., J Mol Model 18, 4389–4396 (2012).
1889. Jiří Rais and Tatsuhiro Okada, J. Phys. Chem. B 2008, 112, 5393–5402.
1890. Aurora Jiménez et al., Chem. Eur. J. 15, 2009, 1422-1428.
1891. Kyle W. Roskamp et al., Biochemistry 2019, 58, 4505–4518.
1892. L. Rigamontiac & A. Fornibc, Inorg. Chim. Acta 473, 2018, 216-222.
1893. Alhazmi, H. A. et al.; Die Pharmazie – Intl. J. Pharm. Sci. 72, 2017, 243-248.
1894. Quattrociocchi, D.G.S. et al. J Mol Model 23, 60 (2017).
1895. Feng Xiang et al., J. Phys. Chem. B 2007, 111, 12282–12293.
1896. V.P. Cuenca-Gotor et al., Phys. Chem. Chem. Phys. 2020,22, 3352-3369.
1897. Hassan A. Alhazmi et al., Microchemical J. 145, 2019, 259-265.
1898. da Silva, V.H.M. et al.; J Mol Model 24, 39 (2018).
1899. Jonathan M Dilger et al., J Am Soc Mass Spectrom . 2017, 28:1293-1303.
1900. Gantt, Stephanie L., Ph.D. thesis, University of Michigan, U.S.A. 2006.

1901. Nihar Ranjan Jena, ChemistrySelect, 4, 2019, 6945-6953.
1902. Karl J. Koebke et al., J. Inorg. Biochem. 203, 2020, 110882.
1903. Glauber S. Melengate et al., J. Braz. Chem. Soc. 30, 2019; https://doi.org/10.21577/0103-5053.20190011.
1904. Rachel E. Bongini et al., J. Inorg. Biochem. 101, 2007, 1251-1264.
1905. Sonja M. Schwarzl, Ph.D. thesis, Ruprecht-Karls-Universitat, Heidelberg, 2006
1906. Niloufar J. Ataie, Ph.D. thesis, Brandeis University, U.S.A. 2008.
1907. Fellner, M., Huizenga, K.G., Hausinger, R.P. et al. Sci Rep 10, 5830 (2020).
1908. Samuel Tetteh, J. Chem., Volume 2019, Article ID 5675870.
1909. Mykyta Tretiakov et al., Catalysts 2019, 9(3), 238.
1910. Li Chen, Ph.D. thesis, Rice University, U.S.A. 2017.
1911. da Silva, V.H.M. et al., J Mol Model 26, 146 (2020).
1912. Marina Justi et al., J. Mol. Struct. 1237, 2021, 130405.
1913. Sopbué Fondjo Emmanuel et al., IOSR Journal of Applied Chemistry (IOSR-JAC) e-ISSN: 2278-5736.Volume 13, Issue 3 Ser. I (March. 2020), PP 08-15.
1914. Marina Justi et al., (2021) Archives of Agronomy and Soil Science, DOI: 10.1080/03650340.2020.1870678.
1915. Christopher M. Micklitsch, Ph.D. thesis, University of Delaware, U.S.A. 2007.
1916. Crysten Elizabeth Blaby-Haas, Ph.D. thesis, University of Florida, 2011.
1917. Shu-Wei Xia et al., Chinese J. Inorg. Chem. 24, (2008), 1748-1752.
1918. S.C.A.D.L. Solano, Ph.D. Thesis, Univ. Nova de Lisboa, Portugal, 2008.
1919. K. Dvorakova, B.Sc. Thesis, Jihoceska Univerzita v Ceskyh Budejovicich, Czech Republic, 2007.
1920. L. Guimaraes, Ph. D. Thesis, Universidade Federal de Minas Gerais, Belo Horizonte, Brazil, 2009.
1921. A. Guarne, in “MECHANISMS OF DNA REPAIR”, Vol. 1 (P. Doetsch, Ed.), Academic Press, Oxford, 2012, pp. 41-70.
1922. Aditya Nandy et al. Chem. Rev. 2021, 121, 16, 9927–10000.
1923. C. Immanuel David et al. Microchemical Journal Volume 169, 2021, 106590.
1924. Franziska Riedel et al. Int. J. Environ. Res. Public Health **2021**, 18(20), 10867.
1925. Cheng Hao Lin et al. Materials Today Nano 20, 2022, 100246.
1926. B. Hosseinzadeh, M. Ahmadi,Coord. Chem. Reviews, 471, 2022, 214733.
1927. Marine Boudias et al. Chem. Engineering J.2022, 138395.
1928. C. Immanuel David et al. J. Photochem. Photobiol. A: 422, 2022, 113558.
1929. Nicholas Andrikopoulos et al. ACS Appl. Mater. Interfaces 2023, 15, 6, 7777.
1930. Penche, G.et al. Top Catal 65, 1541–1555 (2022).
1931. M. Boudias et al. Advances in Sample Preparation Volume 5, 2023, 100049.
1932. Austin D. Ready et al. Dalton Trans., 2022,51, 11547-11557.
1933. Okke Melse et al. J. Comp. Chem. Volume44, Issue8, 2023, Pages 912-926.
1934. Nqayi, S., Gulumian, M., Cronjé, S. et al. J Mol Model 28, 376 (2022).
1935. Mona Jalali et al. (2022) Molecular Physics, 121(9–10).
1936. G. Suneetha et al. Results in Chemistry Volume 5, January 2023, 100688.
1937. Thongsri, O. et al. J Mater Sci **57**, 633–650 (2022).
1938. J. Rine et al.,Acta Cryst. (2022). B**78**, 589-592.

1939. M. Vakarelska-Popovska et al. J. Chem. Technol. Metallurgy, 57, 2022, 419.
1940. Steven Kiyabu, Ph.D. thesis, University of Michigan, 2022.
1941. Marina Justi et al. (2022) Archives of Agronomy and Soil Science, 68:8, 1131.
1942. Ethan P. Stevenson, M.Sc. thesis, University of Otago, New Zealand, 2021.
1943. MARINA JUSTI, Ph.D. thesis, Universidade Federal de Lavras, Brazil, 2021.
1944. Alexander Carvalho Vendite, M.Sc. thesis, University of Sao Paulo, 2021.
1945. Amalia Garcia Garcia, Ph.D. thesis, University of Granada, Spain, 2021.
1946. Marine Boudias, Ph.D. thesis, University of Paris, 2022.
1947. J.J. Alcázar Jiménez; Ph.D. thesis, Pontificia Univ. Católica de Chile, 2021.
1948. S. Ray et al., (2023) eLife 12:e84006.
1949. J. Yoo et al., RSC Chem. Biol., 2023, 4, 548-563.
1950. J. Gao et al., Inorg. Chem. 2023, 62, 13812–13823.
1951. A. Taha et al., Journal of Molecular Liquids 401, 2024, 124678.
1952. M. Iqbal et al., Polyhedron 246, 2023, 116698.
1953. Munro, T.A., BMC Biol 21, 213 (2023).
1954. Martin Lutz, Journal of Molecular Structure 1284, 2023, 135362.
1955. Amy Alexandra Bowyer, Ph.D. Thesis, University of Sydney, 2023.
1956. B. Messaoudı et al., Turkish Comp. Theor. Chem. 2024, 8, 65 – 79.

Todor Dudev and Carmay Lim, "A DFT/CDM study of metal-carboxylate interactions in metalloproteins: Factors governing the maximum number of metal-bound carboxylates", *J. Am. Chem. Soc.* **128** (2006) 1553-1561.

1957. Ran Friedman, Dalton Trans., 2014, 43, 2878-2887.
1958. O. Gutten & L. Rulíšek, Phys. Chem. Chem. Phys., 2015, 17, 14393-14404.
1959. Mayhan, Collin M., Ph.D. Thesis, University of Missouri, U.S.A., 2014.
1960. Matthew L. Harty, M.Sc. Thesis, Dalhousie University, Halifax, Canada, 2015.
1961. M.J. Stevens & S.L.B. Rempe, J. Phys. Chem. B 2016, 120, 12519–12530.
1962. Sergei Y. Noskov and Benoît Roux, J. Mol. Biol. 377, 2008, 804-818.
1963. Ondrej Gutten et al., J. Phys. Chem. A 2011, 115, 11394–11402.
1964. Li Rao et al., J. Am. Chem. Soc. 2010, 132, 18092–18102.
1965. M.-M. Blum, J.C.-H. Chen; Chemico-Biological Inter., 187, 2010, 373-379.
1966. M.R. Gunner et al., Biochim. Biphys. Acta – Bioenergetics 1827 (2013) 892.
1967. Elixabete Rezabal et al., J. Inorg. Biochem. 101, 2007, 1192-1200.
1968. Xiaohua Chen and Yuxiang Bu, J. Am. Chem. Soc. 2007, 129, 9713–9720.
1969. Zhifeng Jing et al., PNAS 2018 115 (32) E7495-E7501.
1970. Elixabete Rezabal et al., ChemPhysChem 2007, 8, 2119 – 2124.
1971. Xiaohua Chen et al., J. Comp. Chem. 30, 2009, 2694-2705.
1972. Vladimir Sladek and Igor Tvaroška, J. Phys. Chem. B 2017, 121, 6148–6162.
1973. Collin M. Mayhan et al., Comp. Theor. Chem. 984, 15 2012, 19-35.
1974. Marcin Hoffmann et al., New J. Chem., 2010,34, 2020-2026.
1975. Taka-aki Okamura and Junko Nakagawa, Inorg. Chem. 2013, 52, 10812–10824.

1976. James Weston, in The Chemistry of Organomagnesium Compounds, Zvi Rappoport and Ilan Marek (Eds.), 2008 John Wiley & Sons, Ltd.
1977. Subramaniam Kavitha et al., J. Mol. Graphics Model. 85, 2018, 13-24.
1978. Liliana Pacureanu et al., Rev. Roum. Chim. 2011, 56(4), 289-298.
1979. Xiaohua Chen et al., ChemPhysChem 13, 2012, 183-192.
1980. Usenobong Friday Ufot, Ph.D. thesis, University of Sussex, UK, 2010.
1981. Y. Z. X. Guo and B. Yang, RSC Adv., 2017, 7, 10206-10214.
1982. Feng Xiang et al., New J. Chem., 2006, 30, 890-900.
1983. J. McMaster, Annu. Rep. Prog. Chem., Sect. A; 2007,103, 492-517.
1984. Elixabete Rezabal, Ph.D. thesis, University of the Basque Country, Spain, 2007.
1985. Ran Friedman, J. Phys. Chem. B 2021, 125, 2251–2257.
1986. Stefan Kluge, Ph.D. thesis, Friedrich-Schiller-Universität Jena, 2007.
1987. K. Dvorakova, B.Sc. Thesis, Jihoceska Univerzita v Ceskyh Budejovicich, Czech Republic, 2007.
1988. M. Jafari et al., J. Phys. Chem. B 2024, 128, 684–697.

Todor Dudev and Carmay Lim, "Competition between protein ligands and cytoplasmic inorganic anions for the metal cation: a DFT/CDM study", *J. Am. Chem. Soc***. 128** (2006) 10541-10548.

1989. A. Krah, S. Takada, Biochim. Biophys. Acta – Bioenergetics 1847 (2015) 1101.
1990. M.R. Gunner et al., Biochim. Biphys. Acta – Bioenergetics 1827 (2013) 892.
1991. Elixabete Rezabal et al., J. Inorg. Chem. 101, 2007, 1192-1200.
1992. Michael Appell et al., J. Mol. Struct. THEOCHEM 894, 2009, 23-31.
1993. Feng Xiang et al., J. Phys. Chem. B 2007, 111,12282–12293.
1994.
1995. Derek R. Case et al., Molecules 2021, 26(9), 2419.
1996. Gugala, Natalie; Ph.D. thesis, University of Calgary, Calgary, Canada, 2019.
1997. David Eisner et al., Physiol. Rev. 103, 2023, 2767-2845.

Todor Dudev, Li-Ying Chang, Carmay Lim, "Factors governing the substitution of La^{3+} for Ca^{2+} and Mg^{2+} in metalloproteins: a DFT/CDM study", *J. Am. Chem. Soc.* **127** (2005) 4091-4103.

1998. Rebecca O. Fuller et al., Dalton Trans., 2015, 44, 2132-2137.
1999. Ruhong Zhou, Molecular Modeling at Atomic Scale: Methods and Applications in Quantitative Biology, CRC Press, Boca Raton, 2015.
2000. E.A. Amin and D.G. Truhlar, J. Chem. Theory Comput. 2008, 4, 75–85.
2001. Yun Huang et al., J. Biol. Chem. 282, 2007, 19000-19010.

2002. Claude Vidaud et al., Chem. Res. Toxicol. 2012, 25, 1161–1175.
2003. Anastassia Sorkin et al., J. Chem. Theory Comput. 2009, 5, 1254–1265.
2004. Sandra B. Gabelli et al., Structure 15, 2007, 1014-1022.
2005. Cristina Trujillo et al., Org. Biomol. Chem., 2008,6, 3695-3702.
2006. Martin Lepšík and Martin J. Field, J. Phys. Chem. B 2007, 111, 10012–10022.
2007. Simon A.J. Messing et al., Structure 17, 2009, 472-481.
2008. Li Rao et al., J. Am. Chem. Soc. 2010, 132, 18092–18102.
2009. M.R. Gunner et al., Biochim. Biphys. Acta (BBA) – Bioenergetics 1827 (2013) 892.
2010. Anna Wilkins Maniccia et al., Biochemistry 2006, 45, 5848–5856.
2011. Eichmüller, C., Skrynnikov, N.R.; J Biomol NMR 37, 79–95 (2007).
2012. Elixabete Rezabal et al., J. Inorg. Biochem. 101, 2007, 1192-1200.
2013. J.P. Yuan et al., Materials Science and Engineering: C 33, 2013, 446-452.
2014. Christopher W. am Ende et al., ChemBioChem 11, 2010, 1738-1747.
2015. Tujin Shi et al., J. Phys. Chem. A 2007, 111, 11562–11571.
2016. Chunyang Guo et al., Anal. Chem. 2019, 91, 1416–1423.
2017. Maniccia, A.W., Yang, W., Johnson, J.A. et al. PMC Biophys 2, 11 (2009).
2018. Zichun J. Lu and George D. Markham, Biochemistry 2007, 46, 27, 8172–8180.
2019. S.-Y. Ku et al., Acta Cryst. (2007). D63, 493-499.
2020. Stavros K. Dimitriou et al., Polyhedron 29, 2010, 2213-2219.
2021. Buz’ko, V.Y., Sukhno, I.V. et al. Russ. J. Inorg. Chem. 53, 1249–1255 (2008).
2022. Sara Espinosa et al., Methods 125, 2017, 55-62.
2023. Zdzislaw Paryzek et al., J. Rare Earths 28, 2010, 56-60.
2024. Kotrba P., Rulíšek L., Ruml T. (2011) Bacterial Surface Display of Metal-Binding Sites. In: Kotrba P., Mackova M., Macek T. (eds) Microbial Biosorption of Metals. Springer, Dordrecht.
2025. Ana-Mădălina Măciucă et al., Molecules 2020, 25(6), 1347.
2026. Rachel E. Bongini et al., J. Inorg. Biochem. 101, 2007, 1251-1264.
2027. T.A. da Silva Brandão, Ph.D. thesis, Univ. Federal de Santa Catarina, Brazil, 2007.
2028. Wojciech Jurkowski et al., ACS Omega 2020, 5, 42, 27050–27056.
2029. Samapan Sikdar, Ph.D. thesis, University of Calcutta, India, 2016.
2030. Simon A. Messing, Ph.D. thesis, Johns Hopkins University, Baltimore, 2008.
2031. C. Immanuel David et al. Microchemical Journal,169, October 2021, 106590.
2032. C. Immanuel David et al. Journal of Photochemistry and Photobiology A: Chemistry 422, 2022, 113558.
2033. Sokhuoy Sam et al. J. Phys. Chem. B 2022, 126, 3, 643–649.
2034. R. Liu et al., Front. Microbiol., 2024, 15 - 2024; https://doi.org/10.3389/fmicb.2024.1298154.

Todor Dudev and Carmay Lim, “Monodentate versus bidentate carboxylate binding in magnesium and calcium proteins: what are the basic principles?”, *J. Phys. Chem. B* **108** (2004) 4546-4557.

2035. Jens Kahlen et al., J. Phys. Chem. B, 2014, 118, 3960–3972.
2036. Matthew B. Stewart et al., Carbohydrate Polymers 102 (2014) 246–253.
2037. Edward Greinera et al., Geochimica et Cosmochimica Acta 133 (2014) 142–155.
2038. Matthew B. Stewart et al., Carbohydrate Polymers 112 (2014) 486–493.
2039. Francesco Zonta et al., Biochem. Biophys. Res. Commun. 445 (2014) 10–15.
2040. Alexander Krah and Shoji Takada, Biochim. Biophys. Acta (BBA) – Bioenergetics 1847 (2015) 1101–1112.
2041. Marek J. Kobylarz et al. J. Biol. Chem. 289 (2014) 33797-33807.
2042. Andrew T. Church et al., RSC Adv., 2015, 5, 67820-67828.
2043. М.О. Анікєєва и др., БІОФІЗИЧНИЙ ВІСНИК Вип. 31, 2014, 29-39.
2044. Ruhong Zhou, Molecular Modeling at Atomic Scale: Methods and Applications in Quantitative Biology, CRC Press, Boca Raton, 2015.
2045. M. Moirangthem et al., Advanced Functional Materials 26 (2016) 1154.
2046. Amir N. Kucharski et al., J. Phys. Chem. B 2016, 120, 8617–8630.
2047. Michael D. Dail et al. J. Phys. Chem. B 2016, 120, 2198–2208.
2048. Giulia Mancardi et al., Cryst. Growth Des. 2016, 16, 3353–3358.
2049. J.P. McEvoya and G.W. Brudvig, Phys. Chem. Chem. Phys., 2004,6, 4754-4763.
2050. Koji Nakano et al., Macromolecules 2009, 42, 18, 6972–6980.
2051. Eugenia Iskrenova-Tchoukova et al., Langmuir 2010, 26, 20, 15909–15919.
2052. Dezső Boda et al., J. Gen Physiol (2009) 133 (5): 497–509.
2053. Zhao Qin Bao et al., Structure 19, 2011, 675-690.
2054. Dezső Boda et al., Biophys. J. 94, 2008, 3486-3496.
2055. Kunhi Mouvenchery et al., Rev Environ Sci Biotechnol 11, 41–54 (2012).
2056. Jessica N. Malin et al., J. Phys. Chem. C 2009, 113, 6, 2041–2052.
2057. Joseph K. Gallaher et al., Chem. Commun., 2012,48, 7961-7963.
2058. M. Lepšík and M.J. Field, J. Phys. Chem. B 2007, 111, 33, 10012–10022.
2059. Filip Leonarski et al., Nucleic Acids Research, 45, 2017, 987–1004.
2060. Elixabete Rezabal et al., J. Inorg. Biochem. 100, 2006, 374-384.
2061. Laura A. Clapp et al., Inorg. Chem. 2005, 44, 23, 8495–8502.
2062. JuniasAdusei-Gyamfi et al., Water Research 160, 2019, 130-147.
2063. Li Rao et al., J. Am. Chem. Soc. 2010, 132, 51, 18092–18102.
2064. Bhuvaneshwari Mahalingam et al., J Immunol 15, 2011, 187 (12) 6393-6401.
2065. Shao-Yong Lu et al., Proteins 81, 2013, 740-753.
2066. Elixabete Rezabal et al., J. Inorg. Chem. 101, 2007, 1192-1200.
2067. Francis E. Appoh et al., J. Organometallic Chem. 690, 2005, 1209-1217.
2068. Christopher M. Micklitsch et al., Tetrahedron Letters 47, 2006, 6277-6280.
2069. Congmeng Wu et al., Cryst. Growth Des. 2011, 11, 7, 3153–3162.
2070. Elixabete Rezabal et al., ChemPhysChem 2007, 8, 2119 – 2124.
2071. Franco King-Chi Leung et al., J. Am. Chem. Soc. 2018, 140, 50, 17724–17733.
2072. E. Fernández-de Gortari, L. M. Espinoza-Fonseca, J. Biol. Chem. 293, 2018, 12405.
2073. Francesco Cilurzo et al., Mol. Pharmaceutics 2010, 7, 2, 421–430.
2074. Umesh Kumar et al., Polyhedron 55, 2013, 233-240.
2075. Feng Xiang et al., J. Phys. Chem. B 2004, 108, 45, 17628–17638.

2076. M.M. Aboelnga, S.D. Wetmore, J. Am. Chem. Soc. 2019, 141, 21, 8646–8656.
2077. Spencer E. Taylor et al., Colloids Interfaces 2018, 2(3), 40.
2078. Shixun Bai et al., J. Colloid Interface Sci. 569, 2020, 128-139.
2079. K. Subramanian et al., Biomolecules 2019, 9(6), 212.
2080. Willis Kwun Hei Ho et al., J. Phys. Chem. Lett. 2019, 10, 16, 4692–4698.
2081. James Weston, in The Chemistry of Organomagnesium Compounds, Zvi Rappoport and Ilan Marek (Eds.), 2008 John Wiley & Sons, Ltd.
2082. Alberto Ciferri and Angelo Perico (Eds.) Ionic Interactions in Natural and Synthetic Macromolecules, ISBN:9780470529270, 2012 John Wiley & Sons, Inc.
2083. Bernette M. Oosterlaken et al., Adv. Funct. Mater. 30, 2020, 1907456.
2084. Yang, L., et al.; Theor Chem Acc 131, 1275 (2012).
2085. M. Mahmoudvand et al., Coll. Surf. A 579, 20, 2019, 123665.
2086. V. Rimsa et al., Acta Cryst. (2011). F67, 442-445.
2087. T. Balakrishnan et al., CrystEngComm, 2019,21, 4063-4071.
2088. André C. Dumetz, Ph.D. thesis, University of Delaware, 2007.
2089. F. M. de Wit et al. J. Adhesion Science and Technology, 22:10-11, 1089-1104.
2090. Zhicheng Zuo and Jin Liu, J. Chem. Inf. Model. 2019, 59, 1, 399–408.
2091. Brax, M. et al.; Biogeochemistry 147, 35–52 (2020).
2092. Janusz Lewiński et al., Eur. J. Inorg. Chem. 2005, 2005, 4490-4492.
2093. Ahmad Fuad, Fazia Adyani; Ph.D. thesis, University of Edinburgh, UK, 2012.
2094. Patricija Hriberšek et al., Polymers 2019, 11(4), 605.
2095. Tufan Singha Mahapatra et al., Eur. J. Inorg. Chem. 2017, 2017, 769-779.
2096. Chi Ming Yang et al., Chem. Eur. J. 13, 2007, 3120-3130.
2097. William A. McHale and Dale G. Brown, US patent US9585818B2, 2017.
2098. Feng Xiang et al., New J. Chem., 2006,30, 890-900.
2099. Patricija Hriberšek and Ksenija Kogej, Macromolecules 2019, 52, 7028–7041.
2100. Kang, Sun-Kil et al.; Bull. Korean Chem. Soc. 32, 793-799, 2011.
2101. Y.K. Mouvenchery et al., J. Plant Nutr. Soil Sci. 181, 2018, 453-461.
2102. D. Mendes de Oliveira et al., Phys. Chem. Chem. Phys., 2020,22, 24014-24027.
2103. Patricija Hriberšek, Ksenija Kogej; Acta Chimica Slovenica 66, 4 (2019).
2104. Appoh F.E., Kraatz HB. (2008) Metal Binding Studies of Ferrocene Peptides in Solution. In: Abd-El-Aziz A.S., Carraher C.E., Pittman C.U., Zeldin M. (eds) Inorganic and Organometallic Macromolecules. Springer, New York, NY.
2105. Fellner, M., Huizenga, K.G., Hausinger, R.P. et al. Sci Rep 10, 5830 (2020).
2106. Giulia MANCARDI, Ph.D. thesis, University College London, UK, 2018.
2107. Elixabete Rezabal, Ph.D. thesis, University of the Basque Country, Spain, 2007.
2108. Itab Youssef et al., Am. J. Anal. Chem. 10 (2019), Article ID:92338.
2109. Valentin Nelea et al., Cryst. Growth Des. 2021, 21, 5, 2898–2910.
2110. Rafael C. Marchi et al., ACS Omega 2020, 5, 7, 3504–3512.
2111. Isabelle K.V. Gonçalves et al., Polyhedron 198, 2021, 115068.
2112. Mauro Torsello, Ph.D. thesis, Università degli Studi di Padova, Italy, 2016.
2113. M. J. Kobylarz, Ph.D. thesis, University of British Columbia, Canada, 2016.
2114. Yuexian Hong et al., CrystEngComm, 2020,22, 2585-2592.
2115. C.M. Micklitsch, Ph.D. thesis, University of Delaware, U.S.A. 2007.

2116. Remya Korah, Ph.D. thesis, Indian Institute of Technology-Bombay, 2008.
2117. Tromans, Robert; Ph.D. thesis, University of Bristol, UK, 2018.
2118. K. Subramanian et al., Biomolecules 2019, 9, 212.
2119. C.I. David et al. Microchemical Journal Volume 169, October 2021, 106590.
2120. Ruochen Lan et al. Advanced Funct. Materials, 31, 2021, 2106419.
2121. Gefei Ma et al. Journal of Hazardous Materials, 424, Part B, 2022, 127408.
2122. A.P. Isfahani et al. J. Hazardous Materials 434, 2022, 128780.
2123. Hanifrahmawan Sudibyo et al. Ind. Eng. Chem. Res. 2022, 61, 20, 6894–6908.
2124. Moses Egor et al. ACS Sustainable Chem. Eng. 2021, 9, 38, 12788–12799.
2125. C. Immanuel David et al. Journal of Photochemistry and Photobiology A: Chemistry,Volume 422, 1 January 2022, 113558.
2126. Sainan Peng et al. Water Research Volume 232, 1 April 2023, 119675.
2127. Naoya Ohara et al. J. Am. Chem. Soc. 2023, 145, 1, 216–223.
2128. Ahmed Mohamed et al. J. Phys. Chem. A 2023, 127, 6, 1413–1421.
2129. Judith Rose et al. Protein Science Volume31, Issue3 March 2022 Pages 602.
2130. Bishoy Khairalla and Izabella Brand, Langmuir 2022, 38, 1, 446–457.
2131. Jihyun Choi, Sungho Yoon; Bull. Kor. Chem. Soc.Volume43, 2022 Pages 299.
2132. Natália Cristina Zanotelli et al. J. Chem. Educ. 2023, 100, 2, 844–851.
2133. Quentin Chevalier et al. Metabolites 2021, 11(9), 571.
2134. Xingyue Guan et al. PLOS Comp. Biol. 2022 doi.org/10.1371/journal.pcbi.1010195.
2135. Alisa A. Vologzhannikova et al. Biomolecules 2021, 11(12), 1823.
2136. Tyson Alexander Rietz, Ph.D. thesis,Vanderbilt University, 2022.
2137. Denilson Mendes de Oliveira, Ph.D. thesis, Purdue University, 2021.
2138. Z. Zhou et al., Water Research 238, 2023, 120007.
2139. S. Peng et al., Science of The Total Environment 906, 2024, 167719.
2140. M. Jafari et al., J. Phys. Chem. B 2024, 128, 3, 684–697.
2141. J. Becker et al., Adv. Funct. Materials 34, 2024, 2312159.
2142. Vishal Kumar Porwal et al., J. Comput. Chem. 44, 2023, 1898-1911.
2143. Elisa González-Fernández et al., Chemistry - A European Journal, 2024, https://doi.org/10.1002/chem.202401215.
2144. V.K. Porwal et al., Molecules 2024, 29(8), 1853.
2145. M. Herzberg et al., Acta Cryst. B 79, 2023, 330-335.
2146. Milana Bazayeva et al., Acta Cryst. (2024). D80, 362–376.

Todor Dudev and Carmay Lim, "Oxyanion selectivity in sulfate and molybdate transport proteins: an ab initio/CDM study", *J. Am. Chem. Soc.* **126** (2004) 10296-10305.

2147. M. Jake Pushie et al., Metallomics, 2014, 6, 15-24.
2148. Sami Virolainen et al., Hydrometallurgy 158 (2015) 74–82.
2149. Anne Maillard et al., PLoS ONE 11(11): e0166910.
2150. Anne Maillard et al., J. Exp. Bot. (2016) 67: 5631-5641.

2151. I. Dokmanic et al., Acta Cryst. (2008). D64, 257-263.
2152. Kate L. Fitzpatrick et al., FEBS Lett. 582, 2008, 1508-1513.
2153. M. Schiavon et al., Environ. Exp. Botany 75, 2012, 41-51.
2154. Andrea Balan et al., Biochimica et Biophysica Acta - Proteins and Proteomics 1784, 2008, 393-399.
2155. Hristina R. Zhekova et al., Coord. Chem. Rev. 345 (2017) 108-136.
2156. Graham N. George et al., Adv. Mol. Toxicology 2, 2008, 123-152.
2157. Schmitt, AD. Et al.; Biogeochemistry 137, 197–217 (2018).
2158. Loes E. Bevers et al., J. Bacteriol. 2011, 193, 4999–5001.
2159. C.T. Pereira et al., Mol. Plant-Microbe Interact. 30 (2017) 578-588.
2160. Matilde Fernández et al., Int. J. Mol. Sci. 2019, 20(20), 5156.
2161. Geoffrey C. Anderson et al., Agronomy 2020, 10(8), 1213.
2162. Souad Moumène, Ph.D. thesis, University of Manchester, UK, 2012.
2163. Yadav P.K., Singh A., Agrawal S.B. (2020) An Overview on Management of Micronutrients Deficiency in Plants Through Biofortification: A Solution of Hidden Hunger. In: Mishra K., Tandon P.K., Srivastava S. (eds) Sustainable Solutions for Elemental Deficiency and Excess in Crop Plants. Springer, Singapore.
2164. Alexandre Moutran, Ph.D. thesis, University of São Paulo, Brazil, 2009.
2165. C.T. Pereira, Ph.D. thesis, Univ. Estadual de Campinas, Brazil, 2017.
2166. K.L. Fitzpatrick, Ph.D. Thesis, University of Adelaide, Australia, 2008.
2167. A. Gasber, Ph.D. Thesis, Technischen Universität Kaiserslautern, 2010.
2168. A. Kabata-Pendias, TRACE ELEMENTS IN SOILS AND PLANTS (4th Edition), CRC Press, 2011.
2169. Cécile Jacques et al. Front. Plant Sci., 23 December 2021 Volume 12 - 2021 | https://doi.org/10.3389/fpls.2021.785221.
2170. Li, Y. Et al., J Soil Sci Plant Nutr 23, 5438–5453 (2023).
2171. J. Jang et al., Journal of Chromatography A 1705, 2023, 464192.
2172. G.C. Anderson, N.Bolan, J. Easton, D.J.M. Hall, R. Sharma, S. Pathan, R.W. Bell , Acidity and Aluminum Toxicity Measurement, Formation, and Management Strategies in Conservation Farming Systems, in Soil Constraints and Productivity, CRC press, 2023.
2173. Shun Liu, Ph.D. Thesis, Université Paris-Saclay, 2023.

T. Dudev and C. Lim, "Principles governing Mg, Ca, and Zn binding and selectivity in proteins", *Chem. Rev.* **103** (2003) 773-788.

2174. Xin Su and Ivan Aprahamian, Chem. Soc. Rev., 2014, 43, 1963-1981.
2175. Luke A. Tatum et al., Acc. Chem. Res., 2014, 47 (7), 2141–2149.
2176. Jason Tien et al., eLife 2014:e02772.
2177. Crystal E. Valdez et al., Acc. Chem. Res., 2014, 47 (10), 3110–3117.
2178. Gyeong Jin Park et al., Sensors and Actuators B 215 (2015) 568–576.
2179. Miriam Kohagen et al., J. Phys. Chem. B, 2014, 118 (28), 7902–7909.
2180. Shilpi Mandal, Gunajyoti Das, Hassan Askari, Struct Chem (2014) 25:43–51.

2181. Pengfei Li et al., J. Chem. Theory Comput., 2015, 11, 1645–1657.
2182. Marion J. Limo et al., Chem. Mater., 2015, 27, 1950–1960.
2183. Dingguo Xua et al., Intl. Reviews in Physical Chemistry 33, 2014, 1-41.
2184. Miriam Kohagen et al., J. Phys. Chem. Lett., 2014, 5, 3964–3969.
2185. P. Umadevia and L. Senthilkumar, RSC Adv., 2014, 4, 49040-49052.
2186. Miriam Kohagen et al., J. Phys. Chem. Lett., 2015, 6, 1563–1567.
2187. Sung Ryul Lee et al., Korean J Physiol Pharmacol. 2015, 19:389-399.
2188. Irina Galkina et al. Cryst. Eng. Comm, 2014,16, 9010-9024.
2189. Catherine M. Guzzo et al., PLOS ONE 2014, 9, e105271.
2190. Isti Yunita, Ekasith Somsook; Indonesian J. Chem. Sci. 9(2) (2020) 71-84.
2191. Shilpi Mandal et al., RSC Adv., 2014, 4, 24796-24809.
2192. Pengfei Li et al., J. Phys. Chem. B, 2015, 119, 883–895.
2193. Dwight D. Lane et al., Soft Matter, 2015, 11, 6981-6990.
2194. Ryota Mizushima et al., PLOS ONE 2014, 9, e98554.
2195. Robert W. Wheatley et al., Phys. Chem. Chem. Phys., 2015, 17, 10899-10909.
2196. Ranjitha Singh et al., Enzyme and Microbial Technology, 72 (2015) 56–64.
2197. Agnieszka Kania et al., Inorg. Chem., 2014, 53, 8473–8484.
2198. Ana Paula S. F. Farias et al., Intl. J. Astrobiology 13 (2014) 259-270.
2199. A. Subhasri and C. Anbuselvan, RSC Adv., 2015, 5, 2576-2585.
2200. Li, Fang-zhen et al., Progr. React. Kinetics Mechanism, 39 (2014) 209-232.
2201. O. Gutten and L. Rulíšek, Phys. Chem. Chem. Phys., 2015, 17, 14393-14404.
2202. Deepika Saini et al., Inorganica Chimica Acta 419 (2014) 13–18.
2203. L. I. N. Tomé et al., RSC Adv., 2015, 5, 15024-15034.
2204. P. Sappidia & U. Natarajan, Mol. Simulations 41 (2015) 1476-1487.
2205. Ava Kreider-Mueller et al., J. Organometallic Chem. 792 (2015) 177–183.
2206. Andrew S. Thomsoa et al., PNAS 111 (2014) E1713–E1722.
2207. Kristen Grinstead et al., Chapter Bioluminescence: Fundamentals and Applications in Biotechnology, Volume 154 of the series Advances in Biochemical Engineering/Biotechnology, pp 149-179, 2015.
2208. Bogdan F. Ion et al., Molecules 2014, 19, 15735-15753.
2209. B. Herguedas et al., Acta Cryst. (2015). D71, 2526-2542.
2210. Shilpi Mandal et al., Journal of Molecular Structure 1081 (2015) 281–292.
2211. Claudia Vicari, Ph.D. Thesis, Università degli Studi di Napoli Federico II, Naple, Italy, 2014.
2212. Ruhong Zhou, Molecular Modeling at Atomic Scale: Methods and Applications in Quantitative Biology, CRC Press, Boca Raton, 2015.
2213. Monika Fuxreiter, Computational Approaches to Protein Dynamics, CRC Press, Boka Raton, 2015.
2214. Andrey N. Istrate et al., Scientific Reports 6, Article number: 21734 (2016).
2215. M. Moiranghtem et al., Advanced Functional Materials 26 (2016) 1154.
2216. Toshiki G. Nakashige et al., J. Am. Chem. Soc. 2016, 138, 12243–12251
2217. Dominic J. Hare et al., Systems Biology of Alzheimer's Disease, Volume 1303 of the series Methods in Molecular Biology, New Yotk, 2016, pp 379-389.
2218. Khalili, B.; J. Mol. Model. (2016) 22: 11.

2219. M. Ropo, V. Blum and C. Baldauf, Sci. Rep. 2016; 6: 35772.
2220. Joann M. Butkus et al., Intl. J. Spectrosc., 2016 (2016), Article ID 1378680.
2221. Feng Qiu et al., PNAS 113 (2016) E5962–E5971.
2222. V. Kljucaric et al., J. Mass Spectrometry 51 (2016) 998.
2223. Patra N, Ioannidis EI, Kulik HJ; PLoS ONE 11 (2016) e0161868.
2224. A. Pantazis and R. Olcese, International Review of Neurobiology 128 (2016) 1.
2225. Tamalika Ash et al., J. Phys. Chem. B, 2016, 120, 3467–3478.
2226. P. Sappidi, U. Natarajan; J. Mol. Graphics and Model. 64 (2016) 60–74.
2227. Sivaiah Areti et al., ACS Omega, 2016, 1, 626–635.
2228. P. Umadevi and L. Senthilkumar, RCS Advances 45 (2016) 38919.
2229. W. G. Touw et al., Acta Cryst. (2016). D72, 1110-1118.
2230. Behzad Khalili and Mehdi Rimaz, Canadian J. Chem. 2016, 94(5): 501-508.
2231. Gerard Parkin, Chem. Rev. 2004, 104, 2, 699–768.
2232. Changlin Liu et al., Coord. Chem. Rev. 248, 2004, 147-168.
2233. Won Jun Lee et al., Molecular Pharmacology October 2005, 68 (4) 1018-1030.
2234. Haibo Yu et al., J. Chem. Theory Comput. 2010, 6, 3, 774–786.
2235. Kenneth D. Westover et al., Cell 119, 2004, 481-489.
2236. Sergei Yu. Noskov et al., J. Phys. Chem. B 2005, 109, 14, 6705–6713.
2237. Cui, J., Yang, H. & Lee, U.S. Cell. Mol. Life Sci. 66, 852–875 (2009).
2238. I. Dokmanic et al., Acta Cryst. (2008). D64, 257-263.
2239. Decroly E et al., PLoS Pathog 7(5): e1002059.
2240. E.A. Amin and D.G. Truhlar, J. Chem. Theory Comput. 2008, 4, 75–85.
2241. HermesReyes-Caballero et al., Biophysical Chemistry 156, 2011, 103-114.
2242. Helga C. Lichtenegger et al., PNAS 2003 100 (16) 9144-9149.
2243. Julie Torruellas et al., Mol. Microbiol. 57, 2005, 1719-1733.
2244. Halil I. Okur et al., J. Am. Chem. Soc. 2013, 135, 13, 5062–5067.
2245. Wolfgang Maret, Metallomics, 2, Issue 2, 2010, 117–125.
2246. Eugenia Iskrenova-Tchoukova et al., Langmuir 2010, 26, 20, 15909–15919.
2247. Zhou, Ting; Huang, Danzhi; Caflisch, Amedeo; Current Topics in Medicinal Chemistry, Volume 10, Number 1, 2010, pp. 33-45; Bentham Science Publishers.
2248. A. McSkimming & S.B. Colbran; Chem. Soc. Rev., 2013,42, 5439-5488.
2249. Jiaobing Wang et al., J. Mater. Chem., 2005,15, 2836-2839.
2250. Yatsunyk, L.A. et al., J Biol Inorg Chem 13, 271–288 (2008).
2251. Hendrik Küpper and Peter M. H. Kroneck, in Metal Ions in Biological Systems (Astrid Sigel, Helmut Sigel, Roland K. O. Sigel, Eds.), CRC Press, 2005.
2252. E.M.W.M. van Dongen et al., J. Am. Chem. Soc. 2006, 128, 33, 10754–10762.
2253. Yang, H. et al.; Nat Struct Mol Biol 15, 1152–1159 (2008).
2254. Shavkat Mamatkulov et al., J. Chem. Phys. 138, 024505 (2013).
2255. Andreas A. Zavitsas, J. Phys. Chem. B 2005, 109, 43, 20636–20640.
2256. Xin Su et al., Angew. Chem. Intl. Ed. 50, 2011, 1841-1844.
2257. Deborah G. Conrady et al., PNAS January 15, 2013 110 (3) E202-E211.
2258. Tarun Jain, B. Jayaram; Proteins 67, 2007, 1167-1178.
2259. Roeland Boer et al., J. Mol. Biol. 358, 2006, 857-869.
2260. Penmatsa Aravind et al., J. Mol. Biol. 376, 2008, 1100-1115.

2261. Rakesh Kumar Pathak et al., Inorg. Chem. 2012, 51, 9, 4994–5005.
2262. Gabor Bunkoczi et al., Chemistry & Biology 14, 2007, 1243-1253.
2263. Dirk Rothenstein et al., J. Am. Chem. Soc. 2012, 134, 30, 12547–12556.
2264. Toon H. Evers et al., J. Nol. Biol. 374, 2007, 411-425.
2265. M.M. Rohani & A.L. Zydney, Adv. Coll. Interface Sci. 160, 2010, 40-48.
2266. Barbara Barszcz, Coord. Chem. Rev. 249, 2005, 2144-2155.
2267. Joseph I. Kliegman et al., Biochemistry 2006, 45, 11, 3493–3505.
2268. Ivan Aprahamian, Chem. Commun., 2017,53, 6674-6684.
2269. Michael Kirberger, Jenny J. Yang; J. Inorg. Biochem. 102, 2008, 1901-1909.
2270. Holger Fleischer; Coord. Chem. Rev. 249, 2005, 799-827.
2271. Anastassia Sorkin et al., J. Chem. Theory Comput. 2009, 5, 5, 1254–1265.
2272. G.J. Fleming et al., Surface Sci. 602, 2008, 2029-2038.
2273. Xue Wang et al., Proteins 75, 2009, 787-798.
2274. Gilles Frison, Gilles Ohanessian; J. Comp. Chem. 29, 2008, 416-433.
2275. Guohui Zhang et al., PNAS 2010 107 (43) 18700-18705.
2276. Luciana I. N. Tomé et al., J. Phys. Chem. B 2013, 117, 20, 6116–6128.
2277. Fabiana Fantinel et al., Langmuir 2004, 20, 7, 2539–2542.
2278. Amy K. Petros et al., Inorg. Chem. 2006, 45, 25, 9941–9958.
2279. Remko, M. et al.; J Mol Model 17, 3117–3128 (2011).
2280. Stefan Kluge and Jennie Weston, Biochemistry 2005, 44, 12, 4877–4885.
2281. Chen K, Kurgan L (2009) PLoS ONE 4(2): e4473.
2282. Sérgio Filipe Sousa et al., Dalton Trans., 2009, 7946-7956.
2283. O. Pible et al., Biochimie 88, 2006, 1631-1638.
2284. Changlin Liu and Li Wang, Dalton Trans., 2009, 227-239.
2285. Kirberger, M. et al.; J Biol Inorg Chem 13, 1169–1181 (2008).
2286. E. Constantino et al., J. Phys. Chem. A 2005, 109, 1, 224–230.
2287. Marion J. Limo et al., Chem. Rev. 2018, 118, 22, 11118–11193.
2288. Valeria A. Campos-Bermudez et al., Biochemistry 2007, 46, 39, 11069–11079.
2289. Petr Sklenovský et al., J. Chem. Theory Comput. 2011, 7, 9, 2963–2980.
2290. R.I. Cukier, Biochim. Biophys. Acta (BBA) – Bioenergetics 1656, 2004, 189.
2291. E.A. Permyakov; R.H. Kretsinger; J. Inorg. Biochem. 103, 2009, 77-86.
2292. Sérgio F. Sousa et al., J. Comp. Chem. 30, 2009, 2752-2763.
2293. Sungwon Lee; C. Dale Poulter; J. Am. Chem. Soc. 2006, 128, 11545–11550.
2294. Andrew J. Bordner; Bioinformatics, 24, 2008, 2865–2871.
2295. Alba Guarné, Progr. Mol. Biol. Translational Sci. 110, 2012, 41-70.
2296. Lauren R. Sheckler et al., J. Mol. Biol. 281, 2006, 22896-22905.
2297. Ondrej Gutten and Lubomír Rulíšek, Inorg. Chem. 2013, 52, 18, 10347–10355.
2298. R. Shankar et al., J. Phys. Org. Chem. 24, 2011, 553-567.
2299. Martin Lepšík and Martin J. Field; J. Phys. Chem. B 2007, 111, 10012–10022.
2300. Lyudmila G. Doudeva et al., Protein Science 15, 2006, 269-280.
2301. Wen-Lin Lai et al., J. Biol. Chem. 279, 2004, 13962-13967.
2302. Amit R. Reddi and Brian R. Gibney, Biochemistry 2007, 46, 12, 3745–3758.
2303. Elixabete Rezabal et al., J. Inorg. Biochem. 100, 2006, 374-384.
2304. Ondrej Gutten et al., J. Phys. Chem. A 2011, 115, 41, 11394–11402.

2305. Jiří Šponer et al., Methods 64, 2013, 3-11.
2306. Koiri, R.K., Trigun, S.K., Dubey, S.K. et al. Biometals 21, 117–126 (2008).
2307. B. T. Zhu et al., (2008) Xenobiotica, 38:2, 130-146.
2308. Yun Xiang and Arieh Warshel, J. Phys. Chem. B 2008, 112, 3, 1007–1015.
2309. Victor P. T. Pau et al., PNAS 2011 108 (43) 17684-17689.
2310. Laura A. Clapp et al., Inorg. Chem. 2005, 44, 23, 8495–8502.
2311. James W. Torrance et al., Proteins 71, 2008, 813-830.
2312. Olivier Pible et al., Protein Sci. 19, 2010, 2219-2230.
2313. ThomasVorup-Jensen, Adv. Drug Delivery Rev. 64, 2012, 1759-1781.
2314. Eider San Sebastian et al., J. Am. Chem. Soc. 2006, 128, 11, 3554–3563.
2315. Hu Hou et al., Food Chemistry 243, 2018, 389-395.
2316. ThomasVorup-Jensen et al., Biochimica et Biophysica Acta (BBA) - Proteins and Proteomics 1774, 2007, 1148-1155.
2317. Lizbeth Edmonds et al., J. Mol. Biol. 365, 2007, 175-186.
2318. Judit E. Šponer et al., Phys. Chem. Chem. Phys., 2004,6, 2772-2780.
2319. Li Rao et al., J. Am. Chem. Soc. 2010, 132, 51, 18092–18102.
2320. Emilia L. Wu et al., J. Phys. Chem. B 2009, 113, 8, 2477–2485.
2321. M.-M. Blum; J.C.-H. Chen; Chemico-Biological Interactions 187, 2010, 373-379.
2322. Catherine H. Schein et al., Proteins 58, 2005, 200-210.
2323. Sun Hee Kim et al., J. Am. Chem. Soc. 2004, 126, 23, 7228–7237.
2324. Kathryn A. McMenimen et al., ACS Chem. Biol. 2006, 1, 4, 227–234.
2325. Michelle W.Y. Szeto et al., J. Mol. Struct.: THEOCHEM 898, 2009, 106-114.
2326. M.R. Gunner et al., Biochim. Biophys. Acta– Bioenergetics 1827, 2013, 892-913.
2327. Malene Ringkjøbing Jensen et al., Biochemistry 2005, 44, 33, 11014–11023.
2328. Srigokul Upadhyayula et al., J. Phys. Chem. B 2011, 115, 30, 9473–9490.
2329. A.B. Hickman et al., EMBO J. (2010)29:3840-3852.
2330. Jan L. Vinkenborg et al., Chem. Commun., 2011,47, 11879-11881.
2331. Shao-Yong Lu et al., Proteins 81, 2013, 740-753.
2332. Manish Kumar Tiwari et al., J. Biol. Chem. 287, 2012, 19429-19439.
2333. Christopher Larkin et al., J. Biol. Chem. 282, 2007, 33707-33713.
2334. HuangheYang et al., Biophys. J. 91, 8, 2006, 2892-2900.
2335. Zhifeng Jing et al., PNAS 2018 115 (32) E7495-E7501.
2336. Mey Khalili et al., Protein Science 13, 2004, 2725-2735.
2337. Ewa Matczak-Jon et al., J. Inorg. Biochem. 100, 2006, 1155-1166.
2338. Rebecca K. Donegan et al., J. Mol. Biol. 287, 2012, 43370-43377.
2339. Torres Martin de Rosales et al., J Biol Inorg Chem 15, 717–728 (2010).
2340. Yong L. Li et al., J. Phys. Chem. B 2011, 115, 33, 10154–10162.
2341. L.A. Levine, M.E. Williams, Curr. Opin. Chem. Biology 13, 2009, 669-677.
2342. Zhifeng Jing et al., J. Chem. Phys. 147, 161733 (2017).
2343. D. Mukhopadhyay et al., Acta Cryst. (2004). D60, 638-645.
2344. Hristina R. Zhekova et al., Coord. Chem. Rev. 345 (2017) 108-136.
2345. Barbara Barszcz et al., Polyhedron 24, 2005, 627-637.

2346. Jose M. Mercero et al., Intl. J. Quantum Chem. 98, 2004, 409-424.
2347. Supriya Saha et al., J. Comp. Chem. 33, 2012, 1165-1178.
2348. G. J. Fleming et al., J. Phys. Org. Chem. 20, 2007, 1032-1042.
2349. Xiaoyang Wang et al., J. Org. Chem. 2010, 75, 10, 3358–3370.
2350. Rutkowska-Zbik, D. et al., J Mol Model 19, 4661–4667 (2013).
2351. L.L. Thio and H.X. Zhang, Neuroscience 139, 2006, 1315-1327.
2352. Barak Akabayov et al., Biochemistry 2009, 48, 8, 1763–1773.
2353. Julia T. Warren et al., J. Mol. Biol. 374, 2007, 517-527.
2354. Karen E. Christensen et al., J. Biol. Chem. 280, 2005, 34316-34323.
2355. Anita Lagutschenkov et al., Intl. J. Mass Spectrom. 308, 2011, 316-329.
2356. De Courcy, B. et al., Interdiscip Sci Comput Life Sci 1, 55–60 (2009).
2357. Matthew S. Glover et al., Intl. J. Mass Spectrom. 354–355, 2013, 318-325.
2358. R. Shankar et al., Inorganica Chimica Acta 387, 2012, 125-136.
2359. Sulagna De et al., Phys. Chem. Chem. Phys., 2009,11, 8285-8294.
2360. William R. Silverman et al., Biophys. J. 87, 2004, 3110-3121.
2361. Vincent Breukels et al., Biochemistry 2011, 50, 41, 8804–8812.
2362. Remko, M., Šoralová, S. J Biol Inorg Chem 17, 621–630 (2012).
2363. Yu Liu et al., Chem. Commun., 2004, 2266-2267.
2364. Solov'ev, V. et al., J Incl Phenom Macrocycl Chem 72, 309–321 (2012).
2365. D.P. Linder and K.R. Rodgers, J. Phys. Chem. B 2004, 108, 36, 13839–13849.
2366. Georgia C. Boles et al., Phys. Chem. Chem. Phys., 2017,19, 12394-12406.
2367. D. Rutkowska-Zbik; T. Korona; J. Chem. Theory Comput. 2012, 8, 2972–2982
2368. Roy R. Hantgan et al., Biochemistry 2008, 47, 9, 2884–2892.
2369. Hongshan He et al., J. Inorg. Biochem. 98, 2004, 667-676.
2370. John Burgess; Emma Raven; Adv. Inorg. Chem. 61, 2009, 251-366.
2371. Thereza A. Soares et al., J. Chem. Theory Comput. 2007, 3, 4, 1569–1579.
2372. Mats Eriksson et al., J. Chem. Phys. 128, 105105 (2008).
2373. Nadav Elad et al., PNAS 2017 114 (42) 11139-11144.
2374. Lyubov V. Parfenova et al., J. Biol. Chem. 282, 2007, 24302-24309.
2375. Albert Guskov; Said Eshaghi; Current Topics in Membranes 69, 2012, 393-414
2376. Basam M. Alzoubi et al., Austral. J. Chem. 63(2) 236-244; 2010.
2377. Junqiu Yang et al., J Gen Physiol (2013) 141 (2): 217–228.
2378. F. Wiesbrock; H. Schmidbaur; CrystEngComm, 2003,5, 503-505.
2379. F. Wiesbrock; H. Schmidbaur; J. Inorg. Biochem. 98, 2004, 473-484.
2380. Zdeněk Chval et al., J. Phys. Chem. B 2011, 115, 37, 10943–10956.
2381. Sergei E. Permyakov et al., Proteins 78, 2010, 2609-2624.
2382. Pena L.B., Azpilicueta C.E., Benavides M.P., Gallego S.M. (2012) Protein Oxidative Modifications. In: Gupta D., Sandalio L. (eds) Metal Toxicity in Plants: Perception, Signaling and Remediation. Springer, Berlin, Heidelberg.
2383. Zhongyue Yang et al., React. Chem. Eng., 2019, 4, 298-315.
2384. M. Hassan Khodabandeh et al., ChemPhysChem 14, 2013, 1733-1745.
2385. Vladimir Sladek and Igor Tvaroška, J. Phys. Chem. B 2017, 121, 6148–6162.
2386. Hai-Chuan Liu et al., J. Am. Chem. Soc. 2003, 125, 40, 12351–12357.
2387. K. Krambrock et al. Phys. Rev. B 75, 104205, 2007.

2388. Elisa Bellomo et al., J. Am. Chem. Soc. 2018, 140, 12, 4446–4454.
2389. Otero, L.H., Beassoni, P.R., Lisa, A.T. et al. Biometals 23, 307–314 (2010).
2390. George Pontikis et al., J. Phys. Chem. A 2009, 113, 15, 3588–3593.
2391. Dimas Suárez et al., J. Phys. Chem. A 2011, 115, 41, 11331–11343.
2392. Rovira C. (2005) Study of Ligand-Protein Interactions by Means of Density Functional Theory and First-Principles Molecular Dynamics. In: Ulrich Nienhaus G. (eds) Protein-Ligand Interactions. Methods in Molecular Biology™, vol 305. Humana Press.
2393. Yawei Shi et al., J. Neurochemistry 106, 2008, 1027-1034.
2394. Kirberger, Michael et al., Current Bioinformatics, 5, 2010, 68-80.
2395. Maniccia, A.W. et al., PMC Biophys 2, 11 (2009).
2396. Anil Boda; Sk. Musharaf Ali; J. Mol. Liquids 179, 2013, 34-45.
2397. Parthasarathi Karmakar et al., New J. Chem., 2018, 42, 76-84.
2398. Rebecca A. Bozym et al., Proc. SPIE 5318, Advanced Biomedical and Clinical Diagnostic Systems II, (2004).
2399. Heather A. Behanna, Samuel I. Stupp; Chem. Commun., 2005, 4845-4847.
2400. S. Xia, J.D. Robertus; Arch. Biochem. Biophys. 488, 2009, 42-47.
2401. Jared J. Paul et al., Inorg. Chem. 2006, 45, 13, 5126–5135.
2402. E. Constantino et al., J. Phys. Chem. A 2008, 112, 48, 12385–12392.
2403. Ya-Wei Shi et al., Arch. Biochem. Biophys. 494, 2010, 1-6.
2404. Milin, Č. et al.; Biol Trace Elem Res 108, 225–243 (2005).
2405. Philipp O. Tsvetkov et al., Front. Mol. Neurosci., 2018, 11, 459.
2406. Arulandu Arockiasamy et al., Protein Science 20, 2011, 827-833.
2407. Tiziana Marino et al., Intl. J. Quantum Chem. 111, 2011, 1152-1162.
2408. Sonya J. Franklin & Joel T. Welch, Comm. Inorg. Chem. 26:3-4, 127-164.
2409. Zichun J. Lu and George D. Markham, Biochemistry 2007, 46, 27, 8172–8180.
2410. M. Hassan Khodabandeh et al., Intl. J. Mass Spectrom. 313, 2012, 47-57.
2411. Temitope Aiyejorun et al., J. Chem. Educ. 2006, 83, 8, 1208.
2412. Aurora Jiménez et al., Chem. Eur. J. 15, 2009, 1422-1428.
2413. C.E. Domenech et al., Enzyme Res. Volume 2011, Article ID 561841.
2414. G. Prehna and C. E. Stebbins, Acta Cryst. (2007). D63, 628-635.
2415. Pengzhi Zhang et al., 112, 2017, 1105-1119.
2416. M.M. RIPPEL, Ph.D. thesis, Univ. Estadual de Campinas, Brazil, 2005.
2417. Xiaohua Zhu et al., ACS Nano 2020, 14, 2, 2172–2182.
2418. Atsushi Miyazaki et al., Bioorg. Med. Chem. 17, 2009, 7978-7986.
2419. Kui Cheng et al., Thin Solid Films 519, 2011, 4647-4651.
2420. Alberto Ciferri and Angelo Perico (Eds.) Ionic Interactions in Natural and Synthetic Macromolecules, ISBN:9780470529270, 2012 John Wiley & Sons, Inc.
2421. C.J. Siddonsa and R.D. Hancock, Chem. Commun., 2004, 1632-1633.
2422. Sha Wang et al., Chem. Sci., 2020, 11, 879-887.
2423. Basam M. Alzoubi et al., J. Inorg. Gen. Chem. 635, 2009, 1536-1540.
2424. Lukas Nejdl et al., Analytica Chimica Acta 1017, 2018, 41-47.
2425. Teng Wang et al., Phys. Chem. Chem. Phys., 2011,13, 1140-1151.
2426. Pochodylo, A.L. et al.; Environ Chem Lett 15, 695–701 (2017).

2427. Subramaniam Kavitha et al., J. Mol. Graphics Model. 85, 2018, 13-24.
2428. Das, G. J Mol Model 19, 2981–2991 (2013).
2429. S. M. Bakalova et al., Bulg. Chem. Commun. 35, 245–251, 2003.
2430. Ignatyev, I.S. et al.; J Mol Model 19, 1819–1834 (2013).
2431. Dénes Berta et al., Current Opinion in Structural Biology 61, 2020, 198-206.
2432. Xin Xu et al., Langmuir 2019, 35, 48, 15564–15572.
2433. Ahmad Motaharia; Alireza Fattahi; New J. Chem., 2017,41, 15110-15119.
2434. Christopher E. R. Richardson et al., Biochemistry 2018, 57, 50, 6807–6815.
2435. Gabriele Macari et al., Int. J. Mol. Sci. 2019, 20(10), 2499.
2436. Joan Bertran et al., in Encyclopedia of Computational Chemistry, Wiley, 2005.
2437. Meera Kumari et al., Biochem J (2018) 475 (21): 3393–3416.
2438. Amanda Andersen et al., J. Phys. Chem. B 2018, 122, 43, 10062–10067.
2439. Lokpati Mishra et al., J. Phys. Chem. B 2019, 123, 13, 2729–2744.
2440. Onur Gokce, M.Sc. thesis, Sabanci University, Turkey, 2006.
2441. Hercend C et al., PLoS ONE 6(10): e26245.
2442. Liliana Pacureanu et al., Rev. Roum. Chim. 2011, 56(4), 289-298.
2443. Šramko, M., Šille, J., Ježko, P. et al. Chem. Pap. 64, 395–404 (2010).
2444. James Weston, in PATAI's Chemistry of Functional Groups, 2009, John Wiley & Sons, Ltd.
2445. Nicholas A. Meanwell, Bioorg. Med. Chem. Lett. 27, 2017, 5355-5372.
2446. Slavoljub C. Živanović et al., New J. Chem., 2018,42, 6256-6263.
2447. Bhargab Borah; Th Gomti Devi; J. Mol. Struct. 1210, 2020, 128022.
2448. Kotrba P., Rulíšek L., Ruml T. (2011) In: Kotrba P., Mackova M., Macek T. (eds) Microbial Biosorption of Metals. Springer, Dordrecht.
2449. Zhang, H., Wang, J., Lu, X. et al. Biol Trace Elem Res 107, 101–111 (2005).
2450. Usenobong Friday Ufot, Ph.D. thesis, University of Sussex, UK, 2010.
2451. Xuanting Liu et al., Food Hydrocolloids 101, 2020, 105450.
2452. Pengbo Cui et al., J. Agric. Food Chem. 2019, 67, 44, 12283–12292.
2453. B. Dhakshnamoorthy et al., J. Struct. Biol. 183, Issue 3, 2013, 512-518.
2454. Jinping Tian, Yingwu Yin; MRC 42, 2004, 641-647.
2455. James William Torrance, Ph.D. thesis, Robinson College, Cambridge, 2008.
2456. Dominic Hare et al., Biochem (Lond) (2009) 31 (1): 46–49.
2457. Patricija Hriberšek; Ksenija Kogej; Polymers 2019, 11(4), 605.
2458. Kenton Meronard et al., Electroanalysis 31, 2019, 1934-1942.
2459. Chi Ming Yang et al., Chem. Eur. J. 13, 2007, 3120-3130.
2460. Jon I. Mujika, Adrian J. Mulholland, Jeremy N. Harvey, in Encyclopedia of Inorganic and Bioinorganic Chemistry, Wiley, 2011.
2461. Feng Xiang et al., New J. Chem., 2006,30, 890-900.
2462. L.L. Boone, M.Sc. thesis, University of North Carolina Wilmington, 2006.
2463. Lokpati Mishra et al., JBIC J. Biol. Inorg. Chem. 25, 213–231 (2020).
2464. Roberto López et al., ChemPhysChem 21, 2020, 99-112.
2465. İbrahim ŞEN, Ph.D. thesis, BALIKESİR ÜNİVERSİTESİ, Turkey, 2011.
2466. Patricija Hriberšek, Macromolecules 2019, 52, 7028–7041.
2467. A.I. Denesyuk et al., Biochem. Biophys. Res. Commun. 494, 2017, 311-317.

2468. L. Li, S.O. Meroueh, in Wiley Encyclopedia of Chemical Biology, 2008.
2469. Šponer J., Šponer J.E., Leontis N.B. (2012) In: Leontis N., Westhof E. (eds) RNA 3D Structure Analysis and Prediction. Nucleic Acids and Molecular Biology, vol 27. Springer, Berlin, Heidelberg.
2470. Florence Reddish, Ph.D. thesis, Georgia State University, U.S.A. 2017.
2471. Anahita Daneshyar et al., Electrochimica Acta 324, 2019, 134893.
2472. Merkx M. In: Geddes C.D. (eds) Reviews in Fluorescence 2008. Reviews in Fluorescence 2008, vol 2008. Springer, New York, NY.
2473. Georgia C. Boles et al., J. Mass Spectrom. 56, 2021, e4580.
2474. Arndt, Joseph W., Ph.D. thesis, Ohio State University, U.S.A. 2003.
2475. Xin Lin et al., Microorganisms 2019, 7(8), 232.
2476. Lee, Jong-min, Ph.D. thesis, University of Auckland, NZ, 2006.
2477. Reeves, Tony Elvern, Ph.D. thesis, Texas A&M University, 2007.
2478. Michael Patrick Kirberger, M.Sc. thesis, Georgia State University, 2008.
2479. Petersson, Ernest James; Ph.D. thesis, California Institute of Technology, 2005.
2480. D.M. de Oliveira et al., Phys. Chem. Chem. Phys., 2020,22, 24014-24027.
2481. Monika Michaelis et al., Langmuir 2019, 35, 44, 14230–14237.
2482. Hatun Barut et al., Çukurova J.l Agricult. Food Sci. 2017, 32, 1 – 14.
2483. JAIBIR KHERB, Ph.D. thesis, Texas A&M University, U.S.A. 2011.
2484. Sara Omar, M.Sc. thesis, University of Manitoba, Canada, 2013.
2485. Thach Ngoc Vo, M.Sc. thesis, University of Manitoba, Canada, 2008.
2486. Patricija Hriberšek, Ksenija Kogej; Acta Chimica Slovenica 66, 4 (2019).
2487. Michael Kirberger, Ph.D. thesis, Georgia State University, U.S.A. 2011.
2488. Simon R. Collinson, Martin Schröder, in Encyclopedia of Inorganic and Bioinorganic Chemistry, John Wiley & Sons, 2011.
2489. Pengbo Cui et al., Food Funct., 2019,10, 8240-8249.
2490. Heung-Chin Cheng, Robert Z. Qi, Hemant Paudel, and Hong-Jian Zhu (Eds.), Regulation and Function of Protein Kinases and Phosphatases, 2011 SAGE-Hindawi Access to Research.
2491. Chronopoulou E.G., Ioannou E., Perperopoulou F., Labrou N.E. (2020) Protein Nanostructures with Purpose-Designed Properties in Biotechnology and Medicine. In: Shukla P. (eds) Microbial Enzymes and Biotechniques. Springer, Singapore.
2492. Yang, Huanghe, Ph.D. thesis, Washington University, Missouri, 2008.
2493. Kim, J.K., Lee, C., Lim, S.W. et al. Nat Commun 11, 4557 (2020).
2494. Heather Alisa Behanna, Ph.D. thesis, Northwestern University, Illinois, 2005.
2495. P. Lasitha et al., ChemPhysChem 2020, 21, 1564– 1570.
2496. Alexander I. Denesyuk et al., Biomolecules 2020, 10(4), 588.
2497. Kay, Laura; Ph.D. thesis, Northumbria University, UK, 2016.
2498. Pengzhi Zhang et al., J. Chem. Phys. 154, 124104 (2021).
2499. Zhen Li et al., J. Chem. Theory Comput. 2021, 17, 4, 2342–2354.
2500. Vincent Breukels, Ph.D. thesis, Universiteit Nijmegen, The Netherlands, 2012.
2501. Xue Wang, Ph.D. thesis, Georgia State University, U.S.A. 2009.
2502. Evlampia-Kyriaki Dimitriadou, Ph.D. thesis, University College London, 2014.
2503. Jessica Lear, Ph.D. thesis, University of Technology, Sydney, 2012.

2504. Gerd Prehna, Student thesis, The Rockefeller University, U.S.A. 2007.
2505. Areti Sivaiah et al., ChemistrySelect 6, 2021, 2051-2079.
2506. Juan Zou, Ph.D. thesis, Georgia State University, 2016.
2507. Lokpati Mishra et al., Proteins 89, 2021, 193-206.
2508. GermánPérez-Sánchez et al., J. Mol. Liquids 310, 2020, 113044.
2509. Jacob Litman et al., J. Chem. Theory Comput. 2019, 15, 8, 4602–4614.M
2510. Čedomila Milin et al., Croatica Chemica Acta, Vol. 78 No. 3, 2005.
2511. Nuvjeevan Singh Dosanjh, Ph.D. thesis, University of Leicester, UK, 2005.
2512. Maria Magdalena Kamm, M.Sc. thesis, Loyola University Chicago, 2012.
2513. Ezhumalai Dhineshkumar et al., Intl. J. Adv. Chem. 6 (1) (2018) 37-45.
2514. Chen, Ke; Ph.D. thesis, University of Alberta, Canada, 2011.
2515. Donegan, Rebecca Kristen; Ph.D. thesis, Georgia Institute of Technology, 2015.
2516. Niaz Shahed Ahmed et al., (2020) Platelets, DOI: 10.1080/09537104.2020.1840540.
2517. Zhang, Xin-Hao; Ph.D. thesis, Hong Kong University of Science and Technology, 2007.
2518. HERMES REYES CABALLERO, Ph.D. thesis, Texas A&M University, 2011.
2519. Baha’a H. Jabali, M.Sc. thesis, Birzeit University, Palestine, 2014.
2520. Ayobami B. Ilesanmi et al., Intl. J. Mass Spectrom. 455, 2020, 116369.
2521. Neena Chakrabarti et al., J. Mex. Chem. Soc. 61 no.2 México abr./jun. 2017.
2522. Xian Chen et al., J. Comp. Chem. 39, 2018, 2307-2315.
2523. Christopher James Larkin, Ph.D. thesis, Johns Hopkins University, U.S.A. 2007.
2524. Roberto E. Bruna et al., PNAS 2021 118 (11) e2021370118.
2525. Won Jun Lee, Ph.D. thesis, University of South Carolina, U.S.A. 2005.
2526. Helga C. Lichtenegger et al., PNAS 2003, 100, 9144–9149.
2527. Sérgio F. Sousa et al., ACS Catal. 2020, 10, 15, 8444–8453.
2528. Samapan Sikdar, Ph.D. thesis, University of Calcutta, India, 2016.
2529. Jia Tang, Ph.D. thesis, University of Pennsylvania, U.S.A. 2008.
2530. Eugene A. Permyakov, Encyclopedia 2021, 1(1), 261-292.
2531. Harvey, Christine Marie; Ph.D. thesis, Boston University, U.S.A. 2012.
2532. Jason Roland Whitehead, M.Sc. thesis, University of North Carolina, 2007.
2533. Micklitsch, Christopher M.; Ph.D. thesis, University of Delaware, 2007.
2534. Remko, Milan et al.; J. Mol. Model. 2011, 17, 3117-3128.
2535. Keegan, Brenna C., Ph.D. thesis, University of Nevada, Reno, 2019.
2536. S.R. Garapati, Ph.D. thesis, East Carolina University, U.S.A. 2014.
2537. Michelle Daniela Gardner, Ph.D. thesis, University of London, 2009.
2538. J.M. Guenther, Ph.D. thesis, University of California, Berkeley, 2010.
2539. Malin J. Allert & Homme W. Hellinga, Biochemistry 2020, 59, 39, 3725–3740
2540. Heer, Florian; Ph.D. thesis, University of Basel, Switzerland, 2016.
2541. Gutten, Ondrej; Diploma thesis, Charles University, Prague, 2010.
2542. Miroslav A. Rangelov et al., J. Mol. Graphics Model. 30, 2011, 10-14.
2543. Malek Bou Kallaba, Ph.D. thesis, Universite de Montpellier, France, 2017.
2544. Jacques, Benoit; M.Sc. thesis, Universite de Montreal, Canada, 2016.
2545. Russi, Silvia; Ph.D. thesis, Universitat Autònoma de Barcelona, 2009.

2546. M. Reinisalo, Ph. D. thesis, Univ. Eastern Finland, Kuopio, Finland, 2012.
2547. M. Faiella, Ph.D. Thesis, University of Naples, Italy, 2010.
2548. K. Dvorakova, B.Sc. Thesis, Jihoceska Univerzita v Ceskyh Budejovicich, Czech Republic, 2007.
2549. F. Wiesbrock, Ph.D. Thesis, Technischen Universitat Munchen, Germany, 2003.
2550. S. Schiller, Ph.D. Thesis, Johannes Gutenberg Universitat Mainz, 2008.
2551. Chalkley, M.J., Mann, S.I. & DeGrado, W.F. *Nat Rev Chem* **6**, 31–50 (2022).
2552. Ragotte, R.J., Pulido, D., Lias, A.M. *et al.* Heterotypic interactions drive antibody synergy against a malaria vaccine candidate. *Nat Commun* **13**, 933 (2022).
2553. Emily R. Featherston et al. J. Am. Chem. Soc. 2021, 143, 35, 14287–14299.
2554. Giovanni Barone et al. COMPREHENSIVE REVIEWS IN FOOD SCIENCE AND FOOD SAFETY Volume20, Issue6 November 2021Pages 5616-5640.
2555. Michael E. O'Brien et al. Int. J. Mol. Sci. 2022, 23(5), 2441.
2556. Himansu S. Biswal et al. J. Chem. Inf. Model. 2021, 61, 8, 3945–3954.
2557. Maria G. Vazquez de Vasquez et al. J. Phys. Chem. B 2021, 125, 40, 11308.
2558. Alexandra Lešková et al. Journal of Experimental Botany, Volume 73, Issue 6, 15 March 2022, Pages 1751–1765.
2559. T. Zhang et al. Food Hydrocolloids 124, Part A, March 2022, 107221.
2560. B. Mohan et al. Tetrahedron Letters 109, 26 October 2022, 154155.
2561. Neelam Chetry et al. Journal of Molecular Structure 1250, 2022, 131670.
2562. Zongfan Yang et al. J. Chem. Inf. Model. 2021, 61, 11, 5658–5672.
2563. Maria G. Khrenova et al. ACS Catal. 2021, 11, 15, 8985–8998.
2564. YONIKA A. LARASATI et al. SCIENCE ADVANCES 7 Oct 2022 Vol 8, Issue 40 DOI: 10.1126/sciadv.abn9350.
2565. C.K. Zagal-Padilla at al. Journal of Alloys and Compounds Volume 891, 25 January 2022, 162087.
2566. Sainan Peng et al. Water Research Volume 232, 1 April 2023, 119675.
2567. Ammar, A., Cavill, R., Evelo, C. et al. J Cheminform 14, 8 (2022).
2568. Niaz Shahed Ahmed et al. (2021) Platelets, 32:7, 880-887.
2569. Maxim B. Gindele et al. Langmuir 2022, 38, 47, 14409–14421.
2570. Sharon L. Guffy et al. Biochemistry 2023, 62, 3, 770–781.
2571. Yu-Ying Chen et al. J. Biol. Chem. 299 (2023) 102731.
2572. Vilde Leipart et al. Insect Molecular Biology 31, 2022, 810-820.
2573. Rajwinder Kaur et al. Phys. Chem. Chem. Phys., 2022, 24, 29130-29140.
2574. Davletshina, N.V., Dolgova, D.R., Ermakova, E.A. et al. Structure and Complexing Properties of Butyl [(N-Benzyl-N,N-dibutylammonio)methyl] Phosphonate. Russ J Gen Chem 92, 1221–1227 (2022).
2575. Mehriban Aliyeva et al. J. Chem. Eng. Data 2022, 67, 6, 1565–1572.
2576. Kenzo Aki et al.J. Molecular Liquids Volume 364, 15 October 2022, 120050
2577. Magdalena Wyparło-Wszelaki et al. Biochem. Mol. Toxicol. 36, 2022 e22964.
2578. Lokpati Mishra et al. ProteinsVolume89, Issue2 February 2021 Pages 193-206
2579. Aboumanei, M.H.et al. BioNanoSci. 13, 13–25 (2023)
2580. Gurleen Singh et al. J. Molecular Structure Volume 1277, 2023, 134823.
2581. Shuwei Jin et al. Chinese Journal of Chemical Physics 34, 741 (2021).

2582. Lipska, A.G., Antoniak, A.M., Wesołowski, P. et al. J Mol Model 28, 201 (2022).
2583. Jin Kyun Kim, Ph.D. thesis, Ulsan National Institute of Science and Technology, Korea, 2022.
2584. Shuwei Jin et al. Chinese Journal of Chemical Physics , 2021, 34(6): 741-750.
2585. M.G.V. de Vasquez, Ph.D. thesis, Ohio State University, 2022
2586. Denilson Mendes de Oliveira, Ph.D. thesis, Purdue University, 2021.
2587. Хорн Полина Александровна, Диссертация на соискание ученой степени кандидата биологических наук, Пущинский научный центр биологических исследований Российской академии наук, Москва, 2021.
2588. D. Eisner et al., Physiol. Rev. 10, 2023, 2767-2845.
2589. Q. Han et al., J. Colloid and Interface Science 650, 2023, 1393-1405.
2590. J. Zhou et al., Phys. Rev. Lett. 2023, 130, 233001.
2591. Dara Bakhtiar et al., Nucleic Acids Research, 52, Issue 3, 2024, 1090–1106.
2592. Katarzyna Sołtys et al., Biochimica et Biophysica Acta - Molecular Cell Research 1870, 2023, 119567.
2593. R. Lai et al., J. Am. Chem. Soc. 2024, 146, 7628–7639.
2594. Edoardo Jun Mattioli et al., J. Mater. Chem. B, 2024, 12, 5162-5170.
2595. Skorupska-Stasiak, A. et al., Cell Commun Signal 21, 165 (2023).
2596. Vishnu Verman Rajasekaran et al., ChemSystemsChem 5, 2023, e202300009.
2597. Ahmad Motahari, Alireza Fattahi; JPOC 37, 2024, e4571.
2598. Elvina Clarie Dullah et al., 3 (2023): Borneo International Journal of Biotechnology https://doi.org/10.51200/bijb.v3i.4719.
2599. Z. Li, Ph.D. Thesis, Michigan State University, 2023.
2600. P.I.K. Peiris, Ph.D. Thesis, La Trobe University, Australia, 2023 .

Todor Dudev, Yen-lin Lin, Minko Dudev, Carmay Lim, "First-second shell interactions in metal binding sites in proteins: a PDB survey and DFT/CDM calculations", *J. Am. Chem. Soc*. **125** (2003) 13168–3180.

2601. Elena Degtyar et al., Angew. Chem. Intl. Ed., 53, 2014, 12026–12044.
2602. Hindurao Barage et al. Protein and Peptide Letters, 21, 2014, 140-152.
2603. Marcel Enke et al., Polymer 69 (2015) 274–282.
2604. Shiyan Xiao et al., J. Phys. Chem. B, 2014, 118, 873–889.
2605. Birgit Eisenhabera et al., Cell Cycle 13 (2014) 1912-1917.
2606. A. Krah & S. Takada, Biochim. Biophys. Acta (BBA) – Bioenergetics 1847 (2015) 1101–1112.
2607. Manish Kumar Tiwari et al., Mol. BioSyst. 2014, 10, 3255-3263.
2608. Ryota Mizushima et al., PLOS ONE 2014, 9, e98554.
2609. Elena Degtyar et al., Angewandte Chemie 126 (2014) 12220–12240.
2610. María-Rocío Meinia et al., FEBS Lett. 589 (2015) 3419–3432.
2611. Mathias Gruber et al., J. Phys. Chem. B, 2014, 118, 1207–1215.

2612. O. Gutten and L. Rulíšek, Phys. Chem. Chem. Phys., 2015, 17, 14393-14404.
2613. Van Ngo et al., J. Chem. Theory Comput., 2015, 11, 4992–5001.
2614. Marharyta Petukh and Emil Alexov, Asian J. Phys. 2014, 23, 735–744.
2615. William B. O'Dell et al., Arch. Biochem. Biophys. (2015) 1-13.
2616. Peng Wang et al., Dalton Trans., 2015, 44, 18057-18064.
2617. Kaustuv Mittra et al., J. Inorg. Biochem. 155 (2016) 82–91.
2618. Filip Leonarski et al., Inorganica Chimica Acta 452 (2016) 82–89.
2619. Peng Wang et al., J. Mater. Chem. B 2016,4, 4526-4533.
2620. Sunan Kitjaruwankul et al., J. Phys. Chem. B 2016, 120, 406–417.
2621. Dhruva K. Chakravorty et al., Biochemistry, 2016, 55, 501–509.
2622. Feng Qiu et al., PNAS 113 (2016) E5962–E5971.
2623. Sharon L. Guffy et al., Protein Eng. Des. Sel. (2016) 29: 327-338.
2624. Morán-Barrio J. et al.; Antimicrob Agents Chemother. 2016, 60:6013–6022.
2625. William B. O'Dell, et al., Arch. Biochem. Biophys. 602 (2016) 48–60.
2626. Kaustuv Mittra et al., Dalton Transactions 47 (2016) 18796.
2627. Antonio Rosato et al., Int. J. Mol. Sci. 2016, 17, 671.
2628. M.M. González & A.J. Vila, Zinc Enzyme Inhibitors 22 (2016) 1-34.
2629. Gerard Parkin, Chem. Rev. 2004, 104, 2, 699–768.
2630. Wolfgang Maret and Yuan Li, Chem. Rev. 2009, 109, 10, 4682–4707.
2631. Argüello, J.; J. Membrane Biol. 195, 93–108 (2003).
2632. I. Dokmanic et al., Acta Cryst. (2008). D64, 257-263.
2633. Kasper P. Kepp, Coord. Chem. Rev. 257, Issue 1, 2013, 196-209.
2634. Marjorie M. Harding et al., (2010) Crystallography Reviews, 16:4, 247-302.
2635. C.M. Micklitsch et al., Angew. Chem. Intl. Ed. 50, 2011, 1577-1579.
2636. Andreini C. et al., (2011) PLoS ONE 6(10): e26325.
2637. Mariana Babor et al., Proteins 70, 2008, 208-217.
2638. Fu Lin and Renxiao Wang, J. Chem. Theory Comput. 2010, 6, 6, 1852–1870.
2639. Offmann, Bernard et al.; Current Bioinformatics, 2, 2007, 165-202.
2640. Catherine L. Tooke et al., J. Mol. Biol. 431, 2019, 3472-3500.
2641. Tanya A. Murphy et al., J. Mol. Biol. 357, 2006, 890-903.
2642. Yang, H., Shi, J., Zhang, G. et al. Nat Struct Mol Biol 15, 1152–1159 (2008).
2643. Satya P. Gupta, Chem. Rev. 2007, 107, 7, 3042–3087.
2644. Toon H. Evers et al., J. Mol. Biol. 374, 2007, 411-425.
2645. Michael Kirberger & Jenny J. Yang, J. Inorg. Biochem. 102, 2008, 1901-1909.
2646. Anastassia Sorkin et al., J. Chem. Theory Comput. 2009, 5, 5, 1254–1265.
2647. Mariana Babor et al., Proteins 59, 2005, 221-230.
2648. Xue Wang et al., Proteins 75, 2009, 787-798.
2649. Gilles Frison, Gilles Ohanessian; J. Comp. Chem. 29, 2008, 416-433.
2650. Stefan Kluge and Jennie Weston, Biochemistry 2005, 44, 12, 4877–4885.
2651. Sérgio Filipe Sousa et al., Dalton Trans., 2009, 7946-7956.
2652. Kirberger, M. et al.; J Biol Inorg Chem 13, 1169–1181 (2008).
2653. Claudia Andreini et al., J. Mol. Biol. 388, 2009, 356-380.
2654. E. Constantino et al., J. Phys. Chem. A 2005, 109, 1, 224–230.
2655. Abdelhamid, R.F. et al.; J Biol Inorg Chem 12, 165–173 (2007).

2656. Davide Marini et al., US patent US20060148104A1, 2006.
2657. Alba Guarné, Progress Mol. Biol. Translational Sci. 110, 2012, 41-70.
2658. Zoran D. Tomić et al., Eur. J. Inorg. Chem. 2004, 2004, 2215-2218.
2659. Martin Lepšík and Martin J. Field, J. Phys. Chem. B 2007, 111, 10012–10022.
2660. Ronen Levy et al., Proteins 76, 2009, 365-374.
2661. Elixabete Rezabal et al., J. Inorg. Biochem. 100, 2006, 374-384.
2662. Koiri, R.K. et al.; Biometals 21, 117–126 (2008).
2663. Grit D. Straganz et al., Biochemistry 2010, 49, 5, 996–1004.
2664. Barber-Zucker, S., Shaanan, B. & Zarivach, R. Sci Rep 7, 16381 (2017).
2665. N. Peica et al., Spectrochim. Acta A 66, 2007, 604-615.
2666. Emilia L. Wu et al., J. Phys. Chem. B 2009, 113, 8, 2477–2485.
2667. Okada, Chiaki et al.; Proteins 63 (2006) 1119-1122.
2668. Matthew L. Reback et al., Chem. Eur. J. 19, 2013, 1928-1941.
2669. Antonio De Riso et al., Biophys J. 91 2006, 1999-2008.
2670. Marharyta Petukh et al., Biophys. J. 102, 2012, 2885-2893.
2671. Manish KumarTiwari et al., J. Biol. Chem. 287, 2012, 19429-19439.
2672. Niloufar J. Ataie et al., Biochemistry 2008, 47, 29, 7673–7683.
2673. Lok Nath Neupane et al., Biosensors and Bioelectronics, 92, 2017, 179-185.
2674. Zhifeng Jing et al., PNAS 2018 115 (32) E7495-E7501.
2675. Mey Khalili et al., Protein Science 13, 2004, 2725-2735.
2676. Sriharsha Vemana et al., Cell Physiol. 295, 2008, C557-C565.
2677. Christopher M. Micklitsch et al., Tetrahedron Letters 47, 2006, 6277-6280.
2678. Bridgette A. Barry et al., Biophys. J. 89, 2005, 393-401.
2679. Peng Wang; JiangWu; Spectrochim. Acta A 208, 2019, 140-149.
2680. Jones PM et al., PLoS ONE 6(12): e28589.
2681. Jose M. Mercero et al., Int. J. Quantum Chem. 98, 2004, 409-424.
2682. Lisa M. Miller Jenkins et al., J. Am. Chem. Soc. 2006, 128, 36, 11964–11976.
2683. Riccardo Chelli et al., Proteins 55, 2004, 139-151.
2684. Ioannis N. Kasampalidis et al., Proteins 68, 2007, 123-130.
2685. Rutkowska-Zbik, D. et al., J Mol Model 19, 4661–4667 (2013).
2686. Małgorzata Sikorska et al., J. Inorg. Biochem. 115, 2012, 28-35.
2687. Mautin A. Kappo et al., J. Biol. Chem. 287, 2012, 7146-7158.
2688. Marharyta Petukh et al., Bioinformatics, 29, 2013, 805–806.
2689. Elixabete Rezabal et al., ChemPhysChem 2007, 8, 2119 – 2124.
2690. Ivano Bertini, Gabriele Cavallaro, Metallomics, 2, 2010, 39–51.
2691. Ronen Levy et al., Human Mutation 32, 2011, 1309-1318.
2692. D.P. Linder and K.R. Rodgers, J. Phys. Chem. B 2004, 108, 36, 13839–13849.
2693. Ann Schmiedekampa, Vikas Nanda; J. Inorg. Biohem. 103, 2009, 1054-1060.
2694. Kun Zhao et al., Proteins 80, 2012, 2666-2679.
2695. Jee-Loon Foo et al., Biochem J (2010) 429 (2): 313–321.
2696. J.J. Yang, W. Yang; in Encyclopedia of Inorganic Chemistry, Wiley, 2006.
2697. Zhiqiang Jiang et al., Carbohydrate Research 461, 2018, 11-18.
2698. Jun Takahashi et al., Gene 499, 2012, 130-134.
2699. M. S. Santosh et al., J. Phys. Chem. B 2010, 114, 49, 16632–16640.

2700. Gilles Frison; Gilles Ohanessian; Phys. Chem. Chem. Phys., 2009,11, 374-383.
2701. Manjula Pandey et al., J. Biol. Chem. 279, 2004, 47840-47848.
2702. Eli Fernández-de Gortari et al., J. Biol. Chem. 293, 2018, 12405-12414.
2703. Victor De La Rosa et al., J Gen Physiol (2018) 150 (6): 863–881.
2704. Matthieu Rouffet et al., Org. Biomol. Chem., 2009,7, 3817-3825.
2705. Marijana Đaković et al., Journal of Coordination Chemistry, 65:6, 1017-1032.
2706. Aleksandar Višnjevac et al., Org. Lett. 2010, 12, 9, 2044–2047.
2707. Piero Procacci, Annu. Rep. Prog. Chem., Sect. C, 2011,107, 242-262.
2708. George Pontikis et al., J. Phys. Chem. A 2009, 113, 15, 3588–3593.
2709. Rodrigo Diaz-Espinoza et al., Arch. Biochem. Biophys. 621, 2017, 46-53.
2710. Kirberger, Michael et al., Current Bioinformatics, 5, 2010, 68-80.
2711. Vladimir Sobolev, Marvin Edelman; Israel J. Chem. 53, 2013, 166-172.
2712. Claudia Andreini et al., J. Chem. Inf. Model. 2013, 53, 11, 3064–3075.
2713. P.J. Almhjell, J.H. Mills; Curr. Op. Struct. Biol. 51, 2018, 170-176.
2714. Bruno Therrien, Front. Chem., 2018, 6, Art. 602.
2715. Francesco Musiani et al., J. Phys. Chem. B 2004, 108, 22, 7495–7499.
2716. Marc A. Walters et al., Inorg. Chem. 2005, 44, 5, 1172–1174.
2717. Peng-Hua Qin et al., Comput. Theor. Chem. 1021, 2013, 164-170.
2718. Liang Qiao; Dongqing Xie; Anal. Biochem. 566, 2019, 75-88.
2719. James Weston, in The Chemistry of Organomagnesium Compounds, Zvi Rappoport and Ilan Marek (Eds.), 2008 John Wiley & Sons, Ltd.
2720. Tee Bordelon et al., Proteins 74, 2009, 808-819.
2721. Ekaterina D. Kots et al 2019 Russ. Chem. Rev. 88 1.
2722. Marvin Edelman et al., Structural Proteomics and Its Impact on the Life Sciences, pp. 181-205 (2008).
2723. Liao, Si-Ming et al., Medicinal Chemistry 15, 2019, 510-520.
2724. Elena Sugrue et al., Australian J. Chem. 69(12) 1383-1395, 2016.
2725. Niculina Peica, Ph.D. thesis, Universität Würzburg, Germany, 2006.
2726. Yong An et al., J. Advanced Research 24, 2020, 363-370.
2727. Shenghui Xue, Ph.D. thesis, Georgia State Unuversity, U.S.A. 2013.
2728. Benoit Jacques et al., J. Biol. Chem. 293, 2018, 7737-7753.
2729. Gantt, Stephanie L., Ph.D. thesis, University of Michigan, U.S.A. 2006.
2730. Ben Hamida-Rebaï M, Robert CH (2010) PLoS ONE 5(2): e9142.
2731. Chi Ming Yang et al., Chem. Eur. J. 13, 2007, 3120-3130.
2732. Louise N. Slope et al., Chem. Commun., 2020, 56, 3729-3732.
2733. M. Ajitha et al., Proteins 86, 2018, 322-331.
2734. Christina Wegeberg et al., Inorg. Chem. 2019, 58, 14, 8983–8994.
2735. Feng Xiang et al., New J. Chem., 2006,30, 890-900.
2736. Vladimir Sobolev et al., http://www.beilstein-institut.de/escec2011/Proceedings/Sobolev/Sobolev.pdf.
2737. A.I. Denesyuk et al., Biochem. Biophys. Res. Commun. 494, 2017, 311-317.
2738. Acharya, Shveta et al.; Current Physical Chemistry, 9, 2019, 151-162.
2739. Reeves, Tony Elvern, Ph.D. thesis, Texas A&M University, 2007.
2740. Acharya, Shveta et al.; Current Physical Chemistry, 10, 2020, 47-64.

2741. Michael Patrick Kirberger, M.Sc. thesis, Georgia State University, 2008.
2742. Clemens Nikolaus Zeno Schmitt, Ph.D. thesis, University of Potsdam, 2015.
2743. Bryan Shroyer Der, Ph.D. thesis, Univ. of North Carolina, Chapel Hill, 2013.
2744. Mariana Babor, Ph.D. thesis, Weizmann Institute of Science (Israel), 2006.
2745. Mani Salarian, Ph.D. thesis, Georgia State University, U.S.A. 2018.
2746. Michael Kirberger, Ph.D. thesis, Georgia State University, U.S.A. 2011.
2747. Mario Prejanò et al., Catalysts 2020, 10(9), 1038.
2748. Hsin, Kun-Yi; Ph.D. thesis, University of Edinburgh, UK, 2010.
2749. Niloufar J. Ataie, Ph.D. thesis, Brandeis University, U.S.A. 2008.
2750. Su, C.TT. et al., Biol Direct 15, 14 (2020).
2751. S. Acharya & A.K. Sharma, Nat. Environ. Pol. Technol. 19 (2020) 577-586.
2752. Dixit, Purushottam D.; Ph.D. thesis, Johns Hopkins University, U.S.A. 2011.
2753. Yang, Huanghe; Ph.D. thesis, Washington University in St. Louis, 2008.
2754. Mathieu Coinçon, Ph.D. thesis, Université de Montréal, Canada, 2010.
2755. Wang, Xue; Ph.D. thesis, Georgia State University, U.S.A. 2009.
2756. Petukh, Marharyta; Ph.D. thesis, Clemson University, U.S.A. 2015.
2757. Barwinska-Sendra, Anna Maria; Ph.D. thesis, Newcastle University, UK, 2018.
2758. Hai Deng, Ph.D. thesis, Georgia State University, U.S.A. 2007.
2759. Samapan Sikdar, Ph.D. thesis, University of Calcutta, India, 2016.
2760. Micklitsch, Christopher M; Ph.D. thesis, University of Delaware, U.S.A. 2007.
2761. Ioannis N. Kasampalidis et al., in Proceedings of the 4th TICSP Workshop on Computational Systems Biology, WCSB 2006, Tampere University of Technology, Tampere, Finland (Edited by Pekka Ruusuvuori, Tiina Manninen, Heikki Huttunen, Marja-Leena Linne, Olli Yli-Harja), pp. 41-44.
2762. Korah, Remya; Ph.D. thesis, Indian Institute of Technology, Bombay, 2008.
2763. María-Belen Reyes et al., Int. J. Mol. Sci. 2020, 21(11), 4132.
2764. Olasunkanmi O. Olaoye et al., J. Med. Chem. 2021, 64, 5, 2691–2704.
2765. Stefan Kluge, Ph.D. thesis, Friedrich-Schiller-Universität Jena, 2007.
2766. Jason Cooper, Ph.D. thesis, Weizmann Institute of Science (Israel), 2016.
2767. Regina M.M. Oliveira et al., Braz. J. Develop. 6, 87828-87842, 2020.
2768. Evdokia Katsemi, Ph.D. thesis, Johann Wolfgang Goethe-Universität, 2003.
2769. Raleb Taher, Ph.D. thesis, Université Grenoble Alpes, France, 2018.
2770. M.R. Meini, Ph.D. thesis, Universidad Nacional de Rosario, Argentina, 2014.
2771. A. Guarne, in “MECHANISMS OF DNA REPAIR”, Vol. 1 (P. Doetsch, Ed.), Academic Press, Oxford, 2012, pp. 41-70.
2772. Yue Yu et al. Molecules 2022, 27(4), 1277.
2773. Feehan, R. Et al., Nat Commun 12, 3712 (2021).
2774. Huayong Xie et al. J. Am. Chem. Soc. 2022, 144, 48, 22229–22241.
2775. Zongfan Yang et al. J. Chem. Inf. Model. 2021, 61, 11, 5658–5672.
2776. Yongtong Lao et al. ACS Chem. Biol. 2022, 17, 8, 2088–2098.
2777. John K. Barrows et al. J. Bacteriology 204 (2022) https://doi.org/10.1128/jb.00303-22.
2778. Seulgi Kim et al. Inorg. Chem. 2021, 60, 17, 13637–13645.
2779. Rikuri Morita et al. J. Phys. Chem. B 2021, 125, 46, 12712–12717.

2780. Zhifeng Jing, Ph.D. thesis, University of Texas at Austin, 2021.
2781. Alexander Boldt, Ph.D. thesis, Technische Universität Dresden, 2021.
2782. B. Roy, T. Govindaraju, Bull. Chem. Society Japan, 97, 2024, bcsj.20230224.
2783. J.M. Delgadoet al., J. Chem. Inf. Model. 2024, 64, 378–392.
2784. Li, Dongjun et al. Investigative Radiology 59(2):p 170-186, 2024.
2785. X. Hu et al., J. Chem. Theory Comput. 2024, 20, 3, 1448–1464.
2786. M.C. Simpson et al., Biochemistry 2023, 62, 22, 3188–3205.
2787. Ryan Feehan et al. Protein Science 32, 2023, e4626.
2788. J.P. Leite et al., Journal of Structural Biology 215, 2023, 108038.
2789. Ryan Feehan, Ph.D. Thesis, University of Kansas, 2023.
2790. S.J. Firth, Ph.D. Thesis, Durham University, UK, 2023.
2791. Ives, Callum Matthew, Ph.D. Thesis, University foo Dundee, UK, 2023.
2792. : María Belén Reyes Cuevas, M.Sc. Thesis, Univ. de Concepción, Chile, 2023.

C.S. Babu, **T. Dudev**, R. Casareno, J.A. Cowan and C. Lim, "A combined experimental and theoretical study of divalent metal ion selectivity and function in proteins: application to E. coli ribonuclease H1" *J. Am. Chem. Soc.* **125** (2003) 9318-9328.

2793. Edina Rosta et al., J. Am. Chem. Soc., 2014, 136, 3137–3144.
2794. Jens Kahlen et al. J. Phys. Chem. B, 2014, 118, 3960–3972.
2795. Alexander Krah and Shoji Takada, Biochimica et Biophysica Acta (BBA) – Bioenergetics 1847 (2015) 1101–1112.
2796. Natércia F. Brás et al., Journal of Molecular Modeling 2014, 20:2271.
2797. Makoto Kita et al., Molecular Physics 112 (2014) 355-364.
2798. Jens Kahlen, Ph.D. thesis, Johannes Gutenberg-University at Mainz, 2014.
2799. Andrew T. Church et al., RSC Adv., 2015, 5, 67820-67828.
2800. Tamalika Ash et al., J. Phys. Chem. B 2016, 120, 3467–3478.
2801. Xu, C., Yang, L., Yu, JG. et al. Theor. Chem. Acc. (2016) 135: 138.
2802. Hui Li et al., Proteins 61, 2005, 704-721.
2803. I. Dokmanic et al., Acta Cryst. (2008). D64, 257-263.
2804. Jiří Šponer et al., Chem. Rev. 2018, 118, 8, 4177–4338.
2805. Edina Rosta et al., J. Am. Chem. Soc. 2011, 133, 23, 8934–8941.
2806. Jaibir Kherb et al., J. Phys. Chem. B 2012, 116, 25, 7389–7397.
2807. Fabien Cailliez, Richard Lavery; Biophys. J. 89, 2005, 3895-3903.
2808. Anastassia Sorkin et al., J. Chem. Theory Comput. 2009, 5, 5, 1254–1265.
2809. Xue Wang et al., Proteins 75, 2009, 787-798.
2810. Eric C. Dykeman and Otto F. Sankey, Phys. Rev. Lett. 100, 028101, 2008.
2811. Kirberger, M. et al.; J Biol Inorg Chem 13, 1169–1181 (2008).
2812. Alba Guarné, Progr.Mol. Biol. Translational Sci. 110, 2012, 41-70.
2813. Ming-Hsun Ho et al., J. Am. Chem. Soc. 2010, 132, 39, 13702–13712.
2814. Kevin J. Travers et al., RNA 2007. 13: 1205-1213.

2815. Christopher Etzkorn; Nancy C. Horton; Biochemistry 2004, 43, 13256–13270.
2816. M.R. Gunner et al., Biochimica et Biophysica Acta (BBA) – Bioenergetics 1827, 2013, 892-913.
2817. Yasuo Tsunaka et al., J. Mol. Biol. 345, 2005, 1171-1183.
2818. Shao-Yong Lu et al., Proteins 81, 2013, 740-753.
2819. Huanghe Yang et al., Biophys. J. 91, 2006, 2892-2900.
2820. Zhifeng Jing et al., PNAS 2018 115 (32) E7495-E7501.
2821. Christopher Etzkorn, Nancy C. Horton; J. Mol. Biol. 343, 2004, 833-849.
2822. Elixabete Rezabal et al., ChemPhysChem 2007, 8, 2119 – 2124.
2823. Kommireddy Vasu et al., Nucleic Acids Res. 41, 2013, 9812–9824.
2824. Kirberger, Michael; Current Bioinformatics, 5, 2010, 68-80.
2825. Corral I. et al., (2010) Challenges and Advances in Computational Chemistry and Physics, vol 12. Springer, Dordrecht.
2826. M.M. RIPPEL, Ph.D. thesis, Universidade Estadual de Campinas, Brazil, 2005.
2827. James Weston, in The Chemistry of Organomagnesium Compounds, Zvi Rappoport and Ilan Marek (Eds.), 2008 John Wiley & Sons, Ltd.
2828. Teng Wang et al., Phys. Chem. Chem. Phys., 2011, 13, 1140-1151.
2829. Yang, L. et al.; Theor Chem Acc 131, 1275 (2012).
2830. Easa Nagamalleswari et al., Biochemistry 2012, 51, 44, 8939–8949.
2831. Yao Wang, Ph.D. thesis, University of Wollongong, Australia, 2015.
2832. Xin Xu et al., Langmuir 2019, 35, 48, 15564–15572.
2833. Willemsen T. et al. (2008) Protein Engineering. In: Walker J.M., Rapley R. (eds) Molecular Biomethods Handbook. Springer Protocols Handbooks.
2834. Lui, Lauren Michelle; Ph.D. thesis, Univ. California, Santa Cruz, 2015.
2835. Kotrba P., Rulíšek L., Ruml T. (2011) Bacterial Surface Display of Metal-Binding Sites. In: Kotrba P., Mackova M., Macek T. (eds) Microbial Biosorption of Metals. Springer, Dordrecht.
2836. Feng Xiang et al., New J. Chem., 2006,30, 890-900.
2837. Eric Charles Dykeman, Ph.D. thesis, Arizona State University, 2008.
2838. T. Rios-Carvajal et al., Langmuir 2019, 35, 49, 16153–16163.
2839. JAIBIR KHERB, Ph.D. thesis, Texas A&M University, U.S.A. 2011.
2840. Michael Kirberger, Ph.D. thesis, Georgia State University, 2011.
2841. Thomas Willemsen et al., in Molecular Biomethods Handbook, 2nd Edition (J. M. Walker and R. Rapley, Eds.) Humana Press, Totowa, NJ, 2008, p. 587-629.
2842. Wang, Xue, Ph.D. thesis, Georgia State University, 2009.
2843. Hai Deng, Ph.D. thesis, Georgia State University, 2007.
2844. Fabien Cailliez, Ph.D. thesis, Univeristé Paris Diderot Paris 7, 2006.
2845. Pen-Yuan Chen, M.Sc. Thesis, National Cheng Kung University, Taiwan 2004
2846. Jachimoviciute, M. Sc. Thesis, Vilniaus Gedimino Technikos Universitetas, Vilnius, Lithuania, 2008.
2847. Zhifeng Jing, Ph.D. thesis, University of Texas at Austin, 2021.
2848. Mantas Liutkus et al., Protei Science 33, 2024, e4971.

Todor Dudev and Carmay Lim, “Metal binding and selectivity in zinc proteins”, *J. Chin. Chem. Soc.* **50** (2003) 1093-1102.

2849. Nirupama Singh et al., J. Solid State Electrochemistry 2014, 18, 523-533.
2850. P. Pomastowski et al., Colloids and Surfaces B 120 (2014) 21–27.
2851. K. Mahnam et al., Research in Pharmaceutical Sciences 2014; 9: 69-82.
2852. A. Gerard Daniel and Nicholas P. Farrell, Metallomics 2014, 6, 2230-2241.
2853. Pik Mun Foong et al., Metallomics 2015, 7, 156-164.
2854. T. Sreevaram et al., Intl. J. Pharm. Drug Analys. 4 (2016) 35 – 43.
2855. N.J. Ataie et al., Biochemistry 2008, 47, 29, 7673–7683.
2856. Renjie Chen et al., Sustainable Energy Fuels, 2018, 2, 1093-1100.
2857. Samia Richards et al., J. Environ. Manag. 231, 2019, 275-281.
2858. Orlova, M.A. et al.; J Radioanal Nucl Chem 311, 1177–1183 (2017).
2859. S.R. Pedada et al., Bull. Chem. Soc. Ethiopia 23 (2009) 3.
2860. Srikanth Bathula et al., J. Serbian Chem. Soc. 2009, 74, 745-754.
2861. Vaddadi Usha Rani et al., Acta Chim. Slov. 2010, 57, 916–921.
2862. Ivan G. Pallares et al., Biochemistry 2017, 56, 2, 364–375.
2863. B. Veeraswami et al., (2013) Chem. Speciation & Bioavailability, 25:2, 147-151
2864. Yan-Dong Huang, Jian-Wei Shuai; J. Phys. Chem. B 2013, 117, 20, 6138–6148.
2865. M. Ajitha et al., Proteins 86, 2018, 322-331.
2866. N. Vijaya Kumar et al. (2013) Chem. Speciation & Bioavailability, 25:1, 43-51.
2867. B.Y. Hirpaye et al., J. Chem. Pharmaceut. Res. 2012, 4, 1725-1733.
2868. B. Veeraswami; G. Nageswara Rao; Der Pharma Chemica, 2018, 10(5): 1-5.
2869. Der, Bryan S.; Ph.D. thesis, Univ. North Carolina at Chapel Hill, 2013.
2870. Niloufar J. Ataie, Ph.D. thesis, Brandeis University, U.S.A. 2008.
2871. Dixit Sharma et al., Front. Genet., 2019, https://doi.org/10.3389/fgene.2019.00797.
2872. Renjie Chen et al., Journal of Alloys and Compounds 866, 2021, 158969.
2873. Omar, Suhad Nizar; M.Sc. thesis, Birzeit University, Palestine, 2013.
233. C.S. Weyessa, Ph.D. thesis, Adama Science and Technology Univ., Ethiopia, 2020.
2874. R. Srinivasu et al., J. Engin. Sci. 11 (2020) 1018-1028.
2875. Hulugalle, Dhakshinari, Ph.D. thesis, UNSW Australia, 2013.
2876. S.R. Garapati, Ph.D. Thesis, East Carolina University, U.S.A. 2014.
2877. Hussien, H. Et al., J Mater Sci: Mater Electron 34, 1596 (2023).

Todor Dudev and Carmay Lim, “Factors governing the protonation state of cysteines in proteins: an Ab initio/CDM study”, *J. Am. Chem. Soc*. **124** (2002) 6759-6766.

2878. Jana Mládková et al., Proteins 82 (2014) 2552–2564.
2879. A. Gerard Daniel and Nicholas P. Farrell, Metallomics, 2014, 6, 2230-2241.
2880. Mathias Gruber et al., J. Phys. Chem. B, 2014, 118, 1207–1215.
2881. Justin A. Lemku et al., PLoS ONE 10 (2015) e0123984.
2882. Victoria E. J. Berryman et al., J. Phys. Chem. A, 2014, 118, 4565–4574.
2883. Sunan Kitjaruwankul et al., J. Phys. Chem. B 2016, 1 20, 406–417.

2884. Raffaella Breglia et al., Protein Eng. Des. Sel. 2016 1-6.
2885. Tomasz Kochańczyk et al., Sci. Rep. 2016; 6: 36346.
2886. T. Sreevaram et al., International Journal of Science and Research 5 (2016) 361.
2887. Mathias F. Gruber, Ph.D. Thesis, Technical University of Denmark, 2016.
2888. M.A. Castiglione Morelli et al., Inorg. Chim. Acta 453 (2016) 330–338.
2889. W. G. Touw et al., Acta Cryst. (2016) D72, 1110-1118.
2890. Francisco Hidalgo and Cecilia Noguez, Nanoscale 2016, 8, 14457-14466.
2891. Hess, D. et al.; Nat Rev Mol Cell Biol 6, 150–166 (2005).
2892. Gerard Parkin, Chem. Rev. 2004, 104, 2, 699–768.
2893. Wolfgang Maret, Biochemistry 2004, 43, 12, 3301–3309.
2894. I. Dokmanic et al., Acta Cryst. (2008). D64, 257-263.
2895. Bradford G. Hill, Aruni Bhatnagar; J. Mol. Cell. Cardiol. 52, 2012, 559-567.
2896. Susana M Quintal et al., Metallomics, 3, 2011, 121–139.
2897. John S. Magyar, Hilary Arnold Godwin; Anal. Biochem. 320, 2003, 39-54.
2898. Tomáš Zimmermann et al., J. Inorg. Biochem. 99, 2005, 2184-2196.
2899. Lubomír Rulíšek et al., Inorg. Chem. 2005, 44, 16, 5612–5628.
2900. Douglas A. Mitchell et al., Biochemistry 2005, 44, 12, 4636–4647.
2901. Erik G. Brandt et al., Phys. Chem. Chem. Phys., 2009,11, 975-983.
2902. Melissa M. Morlok et al., J. Am. Chem. Soc. 2005, 127, 40, 14039–14050.
2903. Anne M. Rich et al., J. Am. Chem. Soc. 2012, 134, 25, 10405–10418.
2904. Thomas Simonson, Nicolas Calimet; Proteins, 49, 2002, 37-48.
2905. Michelle M. Dicus et al., J. Am. Chem. Soc. 2010, 132, 6, 2037–2049.
2906. Gilles Frison, Gilles Ohanessian; J. Comp. Chem. 9, 2008, 416-433.
2907. Amy K. Petros et al., Inorg. Chem. 2006, 45, 25, 9941–9958.
2908. Michael L. Hayes et al., J. Biol. Chem. 288, 2013, 36519-36529.
2909. Jason L. Larabee et al., Chem. Res. Toxicol. 2005, 18, 12, 1943–1954.
2910. Jaroslav V. Burda et al., J. Phys. Chem. B 2003, 107, 22, 5349–5356.
2911. Riccardo Spezia etal., J. Phys. Chem. A 2006, 110, 31, 9727–9735.
2912. Koiri, R.K. et al.; Biometals 21, 117–126 (2008).
2913. Cecilio Giménez et al., J. Biol. Chem. 287, 2012, 28986-29002.
2914. Olivier Sénèque et al., Chem. Eur. J. 15, 2009, 4798-4810.
2915. Delphine Picot et al., Inorg. Chem. 2008, 47, 18, 8167–8178.
2916. Stepan Sklenak et al., J. Am. Chem. Soc. 2004, 126, 45, 14879–14889.
2917. Lishan Yao et al., J. Phys. Chem. B 2005, 109, 15, 7500–7510.
2918. Manish K. Tiwari et al., J. Biol. Chem. 287, 2012, 19429-19439.
2919. Lishan Yao et al., J. Phys. Chem. B 2007, 111, 16, 4200–4210.
2920. Mironel Enescu et al., Phys. Chem. Chem. Phys., 2003,5, 3762-3767.
2921. Sandip Panicker et al., J. Biol. Chem. 279, 2004, 28149-28158.
2922. Nohad Gresh, P. Derreumaux; J. Phys. Chem. B 2003, 107, 20, 4862–4870.
2923. Dirk V. Deubel, J. Am. Chem. Soc. 2002, 124, 41, 12312–12318.
2924. Barak Akabayov et al., Biochemistry 2009, 48, 8, 1763–1773.
2925. Ahmad G. Nozad et al., Biophys. Chem. 141, 2009, 49-58.
2926. Milan Kožíšek et al., Chem. Eur. J. 14, 2008, 7836-7846.
2927. Mautin A. Kappo et al., J. Biol. Chem. 287, 2012, 7146-7158.

2928. D.P. Linder and K.R. Rodgers, J. Phys. Chem. B 2004, 108, 36, 13839–13849.
2929. Hanas J.S. et al.; (2005) Zinc Finger Interactions with Metals and Other Small Molecules. In: Iuchi S., Kuldell N. (eds) Zinc Finger Proteins. Molecular Biology Intelligence Unit. Springer, Boston, MA; pp 39-46.
2930. M.D. Stewart, T.I. Igumenova; Biochemistry 2012, 51, 37, 7263–7277.
2931. Patrick J. Desrochers et al., Inorg. Chem. 2007, 46, 22, 9221–9233.
2932. Safwat Abdel-Azeim et al., J. Comp. Chem. 32, 2011, 3154-3167.
2933. Emma Ahlstrand et al., J. Phys. Chem. A 2017, 121, 13, 2643–2654.
2934. Aurélie Jacques et al., Chem. Eur. J. 19, 2013, 3921-3931.
2935. Ryan Hufschmid et al., Nanoscale, 2019,11, 13098-13107.
2936. M.C. Hernández-Galindo et al., J. Organometallic Chem. 692, 2007, 5295-5302.
2937. Haobo Wang et al., Biochemistry 2018, 57, 4, 451–460.
2938. Debasmita Biswal, Peter G. Kusalika; J. Chem. Phys. 147, 044702 (2017).
2939. Bo-Xue Tian et al., J. Phys. Chem. B 2012, 116, 40, 12105–12112.
2940. Sha Wang et al., Chem. Sci., 2020, 11, 879-887.
2941. Ava Kreider-Mueller et al., Inorg. Chem. 2017, 56, 8, 4643–4653.
2942. Teng Wang et al., Phys. Chem. Chem. Phys., 2011,13, 1140-1151.
2943. D. Dutta, S. Mishra; J. Mol. Graphics Model. 84, 2018, 82-89.
2944. Douglas A. Mitchell et al., Adv. Exp. Biol. 2007, 151-179, 456.
2945. Dandamudi Usharani et al., J. Chem. Theory Comput. 2008, 4, 6, 974–984.
2946. R. Breglia et al., Protein Engineering, Design and Selection, 30, 2017, 169–174.
2947. Ly H. Nguyen et al., Biochemistry 2020, 59, 13, 1378–1390.
2948. Lindsay Zumwalt et al., ChemPhysChem 21, 2020, 2384-2387.
2949. Hitoshi Goto et al., Modern Methods for Theoretical Physical Chemistry of Biopolymers, 2006, Pages 227-248.
2950. J. McMaster, Annu. Rep. Prog. Chem., Sect. A: Inorg. Chem., 2003,99, 565-588
2951. Lang, Eric Jean Maurice; Ph.D. thesis, University of Canterbury, UK, 2016.
2952. Jie Cai et al., NanoImpact 22, 2021, 100305.
2953. Sharma, Bharat Kumar; Ph.D. thesis, Concordia University, Canada, 2016.
2954. Biswal, Debasmita; Ph.D. thesis, University of Calgary, Canada, 2017.
2955. R. Elijah; Ph.D. thesis, University of Illinois at Urbana-Champaign, 2010.
2956. Y. Bu, R. I. Cukier; in Encyclopedia of Inorganic and Bioinorganic Chemistry, Wiley, 2011; https://doi.org/10.1002/9781119951438.eibc0378.
2957. Victoria E. J. Berryman, Ph.D. thesis, Dalhousie University, Canada, 2015.
2958. Ryan Dean Hufschmid, Ph.D. thesis, University of Washington, U.S.A. 2019.
2959. Panicker, Sandip; Ph.D. thesis, University of California, San Diego, 2004.
2960. Yumi Azumako, Ph.D. thesis, University of Tsukuba, Japan, 2013.
2961. Toledo Porteros, Héctor; Ph.D. thesis, Universidad de Salamanca, 2017.
2962. Matthijs L. A. Hakkennes et al., . Chem. Inf. Model. 2023, 63, 7816–7825.
2963. L.-A. Chen et al., J. Med. Chem. 2023, 66, 10604–10616.
2964. Nuno M. S. Almeida et al., J. Chem. Inf. Model. 2023, 63, 7423.
2965. Y.-H. Yu et al., Advanced Science 11, 2024, 2307852.
2966. Cueny RR, et al., (2023) PLoS ONE 18(6): e0281524.

R. Escribano, J.J. Sloan, N. Siddique, N. Sze and **T. Dudev**, "Raman spectroscopy of carbon-containing particles", *Vibrational Spectroscopy* **26** (2001) 179–186.

2967. B. Sahoo and B. Kandasubramanian, RSC Adv., 2014, 4, 11331-1134.
2968. Matthew Genovese et al., J. Mater. Chem. A, 2015, 3, 2903-2913.
2969. S. Sobanska et al., Microchemical Journal 114 (2014) 89–98.
2970. Yui Kouketsu et al., Island Arc 23 (2014) 33–50.
2971. Dairene Uy et al., Tribology International 80 (2014) 198–209.
2972. Betina M. Faroldi et al., Applied Catalysis B 150–151 (2014) 126–137.
2973. V. Švorčíka et al., Carbon 69 (2014) 361–371.
2974. Qin Yu et al., J. Molecular Catalysis A: Chemical 392 (2014) 89–96.
2975. Jacco Hoekstra et al., J. Phys. Chem. C, 2015, 119, 10653–10661.
2976. B.N. Sahoo; B. Kandasubramanian, Mater. Chem. Phys. 148 (2014) 134–142.
2977. Kazuhiro Hayashida et al., Fuel 128 (2014) 148–154.
2978. Ismail Karacan et al., Journal of Materials Science 2014, 49, 7462-7475.
2979. Qingfeng Wang et al., Materials Letters 128 (2014) 279–283.
2980. Cheng Huang and Yi Ming Gong, Science China Earth Sci. 2014, 57, 943-956.
2981. Jacco Hoekstra et al., New J. Chem., 2015, 39, 6593-6601.
2982. Fang Wang et al., Journal of Fluorine Chemistry 166 (2014) 78–83.
2983. PING HE et al., Surf. Rev. Lett. 22 (2015) 1550018.
2984. Raina Chao et al., Studies in Conservation 59 (2014) 102-112.
2985. M. Patel, P.B. Aswath; Tribology – Mater. Surf. Interfac. 9 (2015) 1-18.
2986. Maghsoumi, L. Brambilla et al.; J. Raman Spectroscopy 46 (2015) 757–764.
2987. Wang, Fang et al.; Indian Journal of Chemistry 54A (2015) 1192-1197.
2988. Anna Ferrugiari et al., J. Raman Spectroscopy 46 (2015) 1215–1224.
2989. Pallavi Arod and S. A. Shivashankar, RSC Adv., 2015, 5, 59463-59471.
2990. T.C. Santos Evangelista et al., J. Spectroscopy 2015 (2015), Article ID 329730.
2991. Jessirie Dilag et al., Polymer International 64 (2015) 884–891.
2992. Markus Grafena et al., Aerosol Science and Technology 49 (2015) 997-1008.
2993. Reznickova, A. et al.; J. Nanosci. Nanotechnol. 15 (2015) 10053-10073.
2994. I. Karacan and L. Erzurumluoğlu, Fibers and Polymers 2015, 16, 961-974.
2995. Fang Wang et al., Chem. Res. Chinese Universities 2015, 31, 1003-1006.
2996. Eugenia P. Tomasini et al., Herit. Sci. (2015) 3:19.
2997. Vibhu Sharma et al., Carbon 103 (2016) 327–338.
2998. Julius Rischard et al., Applied Catalysis A: General 511 (2016) 23–30.
2999. Vibhu Sharma et al., Energy Fuels, 2016, 30, 2276–2284.
3000. Enzhu Hu et al., Applied Surface Science 366 (2016) 372–382.
3001. K.S. Rao et al., Sensors and Actuators B: Chemical 231 (2016) 830–836.
3002. Huayan Sun et al., Materials Research Bulletin 80 (2016) 316–320.
3003. Mattias Kruskopf et al., 2D Mater. 3 (2016) 041002.
3004. Jacco Hoekstra et al., Carbon 107 (2016) 248–260.

3005. Zhi-Hao Ma et al., Energy and Mechanical Engineering (S.Y. Liang, Ed.), World Scientific, Danvers, U.S.A., 2016.
3006. Guofu Ma et al., RSC Adv. 2016, 6, 103508-103516.
3007. Huayan Sun et al., Electrochimica Acta 213 (2016) 752–760.
3008. Federico Consonni, Ph.D. Thesis, Politecnico di Milano, Milano, Italy, 2016.
3009. M. Matti Maricq, J. Aerosol Sci. 38, 2007, 1079-111.
3010. Chiara Castiglioni et al., Phylosoph. Trans. Royal Soc. A 2004, 362, 1824.
3011. K. Al-Qurashi, A.L. Boehman; Combustion and Flame 155, 2008, 675-695.
3012. Yongzhi Wang et al., Materials Letters 59, 2005, 3046-3049.
3013. Jill Dill Pasteris and Brigitte Wopenka, .Astrobiology.Dec 2003.727-738.
3014. T.V. Reshetenko et al., Carbon 41, 2003, 1605-1615.
3015. Yo-Rhin Rhim et al., Carbon 48, 2010, 1012-1024.
3016. Natalia P. Ivleva et al., Environ. Sci. Technol. 2007, 41, 10, 3702–3707.
3017. Yongzhi Wang et al 2006 Nanotechnology 17 3304.
3018. Craig P. Marshall et al., Precambrian Research 138, 2005, 208-224.
3019. N.P. Ivleva et al., Aerosol Science and Technology, 41:7, 655-671.
3020. Mihir Patel et al., Tribology International 52, 2012, 29-39.
3021. S.J. Tinnemans et al., Phys. Chem. Chem. Phys., 2005, 7, 211-216.
3022. Jennifer D. Herdman et al., Carbon 49, 2011, 5298-5311.
3023. Hee Je Seong and André L. Boehman, Energy Fuels 2013, 27, 3, 1613–1624.
3024. Eugenia P. Tomasini et al., J. Raman Spectroscopy 43, 2012, 1671-1675.
3025. L.M. Cornaglia et al., Applied Catalysis A: General 263, 2004, 91-101.
3026. Yijin Cai et al., J. Power Sources 353, 2017, 260-269.
3027. Albert Dato and Michael Frenklach, New J. Phys. 12, 2010, 125013.
3028. Stephan Mertes et al., J. Aerosol Science 35, 2004, 347-361.
3029. M.P. Ruiz et al., Chemical Engineering Journal 127, 2007, 1-9.
3030. Christine Esangbedo et al., Tribology International 47, 2012, 194-203.
3031. Roh, Jae-Seung et al.; Carbon letters 9, 127-130, 2008.
3032. A. Guedes et al., Intl. J. Coal Geology 73, 2008, 359-370.
3033. Chong Han et al., J. Phys. Chem. A 2012, 116, 16, 4129–4136.
3034. M. Pilar Ruiz et al., Ind. Eng. Chem. Res. 2007, 46, 23, 7550–7560.
3035. Dong, G. et al., J Nanopart Res 12, 1319–1329 (2010).
3036. Wilm Schumacher et al., J. Raman Spectroscopy, 42, 2011, 383-392.
3037. Upare, D.P. et al.; Korean J. Chem. Eng. 28, 731–743 (2011).
3038. Ruth Signorell, Jonathan P. Reid (Eds.), Fundamentals and Applications in Aerosol Spectroscopy, CRC Press, 2011.
3039. E.A. Stefaniak et al., Spectrochimica Acta Part B 61, 2006, 824-830.
3040. Pablo Beato et al., Catalysis Today 205, 2013, 128-133.
3041. Marcelo Zuleta et al 2005 J. Electrochem. Soc. 152 A270.
3042. Chuanyong Zhang et al., Chem. Asian J. 8, 2013, 2714-2720.
3043. Brett G. Diehl et al., Carbon 60, 2013, 531-537.
3044. G.D.J. Guerrero Peña et al., Fuel 222, 2018, 42-55.
3045. Hiranuma, N. et al.; Atmos. Chem. Phys., 11, 8809–8823.
3046. Dang Sheng Su et al., Adv. Mater. 20, 2008, 3597-3600.

3047. Zaoxue Yan et al., J. Mater. Chem., 2012,22, 5072-5079.
3048. A. Guedes et al., Journal of Aerosol Science 40, 2009, 81-86.
3049. S. S. Potgieter-Vermaak, R. Van Grieken; Appl. Spectrosc. 60, 39-47, 2006.
3050. Xie, GQ., Luo, MF., He, M. et al. J Nanopart Res 9, 471–478 (2007).
3051. Nasir K. Memon et al., Combustion and Flame 160, 2013, 1848-1856.
3052. O.F.-K. Schlüter et al., Applied Catalysis A: General 274, 2004, 71-77.
3053. J.A. Gómez-Cuaspud, M. Schmal; Intl. J. Hyd. Energy 38, 2013, 7458-7468.
3054. George Ting-Kuo Fey et al., Pure Appl. Chem., 82, 2157–2165, 2010.
3055. Bohumil Barda et al., Applied Surface Science 257, 2010, 414-422.
3056. Y. Cao et al., (2006) Mater. Sci. Technol., 22:10, 1227-1234.
3057. B. Wopenka et al., Geochimica et Cosmochimica Acta 106, 2013, 463-489.
3058. Swanson, M., Pushkarev, V.V., et al. Catal Lett 116, 41–45 (2007).
3059. I. Martínez-Arkarazo et al., Spectrochimica Acta Part A 68, 2007, 1058-1064.
3060. Z.F. Zhang et al., Intl. J. Refract. Metals Hard Mater. 38, 2013, 111-117.
3061. Saheed A. Ganiyu et al., Chemical Engineering Journal 321, 2017, 651-661.
3062. Jun He et al., Journal of Catalysis 253, 2008, 1-10.
3063. Wen-Zhi Jia et al., J. Mater. Chem., 2011,21, 8987-8990.
3064. Nord, K. et al., SAE Technical Paper 2004-01-1987, 2004.
3065. Chen Jin-Yang et al 2008 Chinese Phys. Lett. 25 780.
3066. Ho Ting Luk et al., ACS Catal. 2018, 8, 10, 9604–9618.
3067. Bo Li et al., J. Industr. Engin. Chem. 19, 2013, 250-255.
3068. Taek-Seung Kim et al., Small 14, 2018, 1801284.
3069. Qiang Huang et al., Atmospheric Environment 66, 2013, 17-24.
3070. Deepa Kathiravan et al., J. Mater. Chem. C, 2017,5, 5239-5247.
3071. Ki Chul Park et al., J. Phys. Chem. Solids 69, 2008, 2481-2486.
3072. James A. Sullivan et al., Appl. Catal. B 108–109, 2011, 134-139.
3073. Bo Li et al., Applied Surface Science 280, 2013, 179-185.
3074. Md Zakir Hossain et al., Energy Fuels 2017, 31, 4, 4013–4023.
3075. Marwa Mahmoudi et al., Intl. J. Hyd. Energy 42, 2017, 8712-8720.
3076. Y.H. Lee et al., Mater. Chem. Phys. 82, 2003, 750-757.
3077. Dairene Uy, Ann E. O'Neill; J. Raman Spectroscopy 36, 2005, 988-995.
3078. Vladimir A. Bershtein et al., RSC Adv., 2012, 2, 1424-1431.
3079. Tomita, T., Okada, T., Kawahara, H. et al. Appl. Phys. A 100, 113–117 (2010).
3080. Ali, Ashraf Abd El-Fattah; Ph.D. thesis, Drexel University, U.S.A. 2002.
3081. G.T.K. Fey et al., Intl. J. Chem. Engin. Appl. 2, 2011, 20-25.
3082. Dairene Uy et al., Lubrication Sci. 22, 2010, 19-36.
3083. Sultan Ahmed et al 2018 Mater. Res. Express 5 045601.
3084. Li-bo Zhang et al., Materials & Design 29, 2008, 2066-2071.
3085. Yuanfu Deng et al., Small 2, 2018, 1700332.
3086. Ahmad Mukhtar et al., Microporous Mesoporous Mater. 294, 2020, 109883.
3087. Bijoy Tudu et al., ACS Appl. Mater. Interfaces 2019, 11, 36, 32869–32878.
3088. Ayumi Iwata, Atsushi Matsuki; Atmos. Chem. Phys., 18, 1785–1804, 2018.
3089. Shazam Williams, Ph.D. thesis, University of Toronto, Canada, 2008.
3090. Jianbing Gao et al., Fuel 219, 2018, 62-68.

3091. Seung-Hyun Kim et al., Anal. Chem. 2010, 82, 6, 2243–2252.
3092. Jinyang Chen et al., Geochem J. 2007, 41, 283-290.
3093. S. Nordmann et al., Gefahrstoffe - Reinhaltung der Luft 69 (2009) 469-474.
3094. Seung-Hyun Kim et al., Anal. Chem. 2008, 80, 20, 7661–7669.
3095. Da-Sol Kim et al., J. Alloys Compounds 769, 15 2018, 1113-1120.
3096. Srikanth Dama et al., Journal of Catalysis 360, 2018, 27-39.
3097. Yafan Wan et al., J. Anal. Appl. Pyrolysis 127, 2017, 223-228.
3098. Pranay P. Morajkar et al., Energy Fuels 2019, 33, 12, 12852–12864.
3099. Nikhil Sharma et al., J. Energy Resour. Technol. 2019, 141(2): 022201.
3100. Yinhui Li et al., ACS Appl. Mater. Interfaces 2017, 9, 6, 5653–5659.
3101. Seong, Hee Je; Ph.D. thesis, Pennsylvania State University, U.S.A. 2010.
3102. Sujay Bagi et al., Carbon 136, 2018, 395-408.
3103. Roh, Jae-Seung et al.; Carbon letters 10, 38-42, 2009.
3104. A.M. Katzenmeyer et al., J. Nanomaterials, 2009, Article ID 832327, 2009.
3105. Al-Qurashi, Khalid; Ph.D. thesis, Pennsylvania State University, U.S.A. 2007.
3106. Tomasz Powolny et al., Ore Geology Reviews 114, 2019, 103130.
3107. U. Böttger et al., Planetary and Space Science 144, 2017, 106-111.
3108. Jörg Fischer et al., (2010) Journal of Sports Sciences, 28:5, 555-562.
3109. Md. ZakirHossain et al., Fuel 231, 2018, 253-263.
3110. Haoran Wu et al 2019 J. Electrochem. Soc. 166 A821.
3111. Willemien Anaf et al., Talanta 101, 2012, 420-427.
3112. K.S. Rao, A.K. Chaudhary; Optics & Laser Technol. 109, 2019, 149-156.
3113. XING, Li-Qiong et al., Acta Physico-Chimica Sinica, 25, 2009, 1928-1932.
3114. Yang Wang et al 2017 Mater. Res. Express 4 095601.
3115. Keisuke Nagai et al., J. Tribol. Feb 2019, 141(2): 022201.
3116. Piergrossi, V. et al.; Int. J. Environ. Sci. Technol. 16, 1227–1238 (2019).
3117. Patel, Mihir; Ph.D. thesis, University of Texas at Arlington, 2011.
3118. Deise M Santos et al., Orbital - Vol. 9 No. 3 (2017).
3119. Rair Driss et al., Mediterranean Journal of Chemistry 2018, 7(5), 337-345.
3120. Chenxi Sun, Ph.D. thesis, University of Michigan, U.S.A. 2017.
3121. Markus Knauer, Ph.D. thesis, Technischen Universität München 2010.
3122. Pranay P. Morajkar et al., Fuel 280, 2020, 118631.
3123. Meghan Elizabeth Swanson, Ph.D. thesis, University of Pittsburgh, 2008.
3124. Rabia Amen et al., Cleaner Engineering and Technology 1, 2020, 100006.
3125. Damir Starešinić et al., Carbon 124, 2017, 708-721.
3126. Woojin Kim et al., Fuel 89, 2010, 2047-2053.
3127. Adhimoorthy Saravanan et al., Chem. Eur. J. 24, 2018, 12574-12583.
3128. Moataz K. Abdrabou et al., Fuel 275, 2020, 117918.
3129. Rajkumar Sadasivam et al., ChemistrySelect 4, 2019, 5044-5054.
3130. Harpale, V.M. et al.; Aerosol Air Qual. Res. 6: 295-304, 2006.
3131. Kouki Oka et al., Cell Reports Physical Science 2, 2021, 100306.
3132. K. Hayashida et al., Japan Soc. Mechan. Engin. Proc. B, 2013, 806, 2228-2238.
3133. Решетенко, Т.В., диссертация кандидат химических наук, Институт катализа им. Г.К. Борескова СО РАН, Новосибирск, 2003.

3134. V.M. Harpale et al., Global NEST Journal, Vol 8, No 3, pp 260-264, 2006.
3135. Fusheng Li et al., Dalton Trans., 2020,49, 588-592.
3136. Sadaf Tahmasebi et al., ACS Appl. Energy Mater. 2020, 3, 8, 7294–7305.
3137. M. Udayakumar et al., Arabian J. Chem.; Available online 20 May 2021, 103214
3138. Wei Ma et al., Colloids and Surfaces A 610, 5 February 2021, 125724.
3139. Pacley, Shanee Danyale; Ph.D. thesis, University of Dayton, U.S.A. 2012.
3140. Magdalena Dumańska-Słowik et al., Lithos 334–335, 2019, 231-244.
3141. Sujay Bagi et al., Fuel 282, 2020, 118878.
3142. Tinnemans, Stanislaus Josephus; Ph.D. thesis, Utrecht University, 2006.
3143. A.M. Dato, Ph.D. thesis, University of California, Berkeley, 2009.
3144. A. M. Katzenmeyer et al., 2008 8th IEEE Conf. Nanotechnol., 2008, 297-299.
3145. Zhang, D. et al.; J. Wuhan Univ. Technol.-Mat. Sci. Edit. 28, 358–361 (2013).
3146. Grasso, G. et al.; Anal Bioanal Chem 409, 3943–3950 (2017).
3147. Pasi P. Paalanen et al., ACS Catal. 2020, 10, 17, 9837–9855.
3148. Xing Li-Qiong et al., Acta Phys -Chim. Sin., 2009, 25, 1928-1932.
3149. Sourov K. Sajib, Sushil Adhikari; Trans. ASABE. 63, 485-493, 2020.
3150. V.S. Sedov et al., Diamond and Related Materials 74, 2017, 65-69.
3151. Choi, S.C.; Park, S.H.; J. Nanosci. Nanotechnol. 18, 2018, pp. 2148-2151.
3152. Nasir K. Memon et al., "One-Step Combustion Synthesis of Carbon-Coated Nanoparticles using Multiple-Diffusion Flames" (5 pages); Proceedings of the 8th U. S. National Combustion Meeting Organized by the Western States Section of the Combustion Institute and hosted by the University of Utah, May 19-22, 2013.
3153. Amritpal Singh Chaddha et al., J. Archaeol. Sci. 36, 2021, 102799.
3154. Jiangjun Wei, Yuncheng Wang; Scie.Total Environ. 788, 2021, 147753.
3155. Zhi-Hao Ma et al., in Energy and Mechanical Engineering, pp. 37-46 (2016).
3156. Matthew Genovese, Ph.D. thesis, University of Toronto, Canada, 2017.
3157. Xueai Li et al., Composites Part A: 140, 2021, 106202.
3158. Yanan Zhang et al., ACS Nano 2021, 15, 4, 7021–7031.
3159. Kim, Seung-Hyun; Ph.D. thesis, University of California, Davis. 2009..
3160. Ayumi Iwata, Atsushi Matsuki; Atmos. Chem. Phys. Discuss., https://doi.org/10.5194/acp-2017-301.
3161. Mera, K. et al.; J. Immumol. Methods 334(1-2):82-90 (2008).
3162. M.A. Paviotti et al., J. Environ. Chem. Engin. 9, 2021, 105173.
3163. Chiara Castiglioni y Matteo Tommasini, Opt. Pura Apl. 40 (2) 169-174 (2007).
3164. Kazemimanesh, Mohsen; Ph.D. thesis, University of Alberta, Canada, 2020.
3165. Zhao He et al., Anal. Chem. 2020, 92, 14, 9583–9590.
3166. Hongbo Yu et al., Indian J. Chem. 51A (2012) 927-939.
3167. S. Zhao et al., Optoelectronics and Advanced Materials - Rapid Communications, 6, 1-2, January-February 2012, pp.249-252 (2012).
3168. Yavuz Bayam et al., J. Nanomaterials 2009, Article ID 832327, 4 pages.
3169. Sharad Pachpute, B. Premachandran; J. Heat Transfer. Feb 2019, 141: 022201.
3170. Harahap, Mahyuni; M.Sc. thesis, Unoversity of Birmingham, 2018.
3171. Zhang, Wen Biao, et al., Applied Mechanics and Materials, 189, 2012, 80–86.
3172. Ling-Yun Jin et al., Indian J. Chem. 41A (2010) 49-53.

3173. N.P. Levitt, M.Sc. thesis, Texas A&M University, 2007.
3174. Cosey, Whitney K.; Ph.D. thesis, University of Texas at Dallas, 2020.
3175. Hammonds, Mark David; Ph.D. thesis, University of Edinburgh, 2012.
3176. Qiang Huang, M.Sc. thesis, University of Maryland, 2011.
3177. Harpale V.M. et al., in Proceeding of NONEQUILIBRIUM PROCESSES, COMBUSTION, AND ATMOSPHERIC PHENOMENA, Sochi, 03–07 October 2005; pp.337-342.
3178. Pranay P. Morajkar et al., Energy Fuels 2020, 34, 10, 12960–12971.
3179. A Nagyné Szép, Ph.D. thesis, Budapest University, 2006.
3180. Zeynep Ferial ÇAVDAR, M.Sc. thesis, İSTANBUL TEKNİK ÜNİV. 2008.
3181. Pereira García, Fernando Jose; Ph.D. thesis, Universidad de Leon, Spain, 2014.
3182. Ohlig, Dominik; Ph.D. thesis, Technische Universität Darmstadt 2020.
3183. Alexander Rinkenburger, Ph.D. thesis, Technische Universität München, 2018.
3184. K. Nord, Ph.D. Thesis, Lulea University of Technology, Sweden, 2005.
3185. S.H. Park, Ph.D. Thesis, Drexel University, USA, 2007.
3186. S.J. Tinnemans, Ph.D. Thesis, University of Utrecht, The Netherlands, 2006.
3187. W. Xia, Ph.D. Thesis, Ruhr Universitat Bochum, Germany, 2006.
3188. S.-G. Moon, Ph.D. Thesis, Texas A&M University, USA, 2010.
3189. J.-O. Muller, Ph.D. Thesis, Technischen Universitat Berlin, Germany, 2005.
3190. Luo Kong et al., Carbon Volume 193, 30 June 2022, Pages 216-229.
3191. Kajal Sharma et al., J. Environ. Chem. Eng.10, 2022, 107674.
3192. Cedeño Estefany et al. Ecotoxicol. Environ. Safety 249, 2023, 114405.
3193. Runjing Mao et al. Dalton Trans., 2022, 51, 8705-8713.
3194. Marrot, L., et al. Waste Biomass Valor 13, 2267–2285 (2022).
3195. Pengfei Cheng et al. ACS Appl. Mater. Interfaces 2023, 15, 6, 8761–8769.
3196. Chenbo Yuan et al. ACS Appl. Energy Mater. 2023, 6, 3, 1897–1905.
3197. Samantha Da Costa et al. Fuel Volume 309, 1 February 2022, 122141.
3198. Jiachun Chai et al. Journal of CatalysisVolume 416, 2022, Pages 289-300.
3199. Manuel J. Pinzón C. et al.J. Energy Storage Volume 62, June 2023, 106858
3200. Kaiyue Hu et al. Molecules 2023, 28(2), 565.
3201. A. Bumajdad, P. Hasila; Arabian J. Chemistry 16, 2023, 104403.
3202. Jeffrey T. Osterhout et al. Astrobiology 22 (2022) 1239-1254.
3203. Franca Caucia et al. Minerals 2022, 12(11), 1449.
3204. Natalia Zioła et al. Atmosphere 2021, 12(6), 768.
3205. Rawat, S., Kottaichamy, A.R., Bhat, Z.M. et al. Biomass Conv. Bioref. (2022).
3206. Kim, J., Kwon, W., Bai, B.C. et al. Carbon Lett. 32, 1315–1327 (2022).
3207. Melo, H.P., Valadas, S., Cruz, A.J. et al. Herit Sci 10, 23 (2022).
3208. Woranan Netkueakul et al. NanoImpact Volume 27, July 2022, 100414.
3209. Li-lai Liu et al. Int. J. Electrochem. Sci., 17 (2022) Article Number: 221058.
3210. Hyeon Ji Kim et al. J. Indust.Eng. Chem. 119, 2023, Pages 428-438.
3211. Khushboo Kumari et al., J. Analyt. Applied Pyrolysis 171, 2023, 105961
3212. K. Prabhu et al., Sensors and Actuators A: Physical 357, 2023, 114419
3213. C. Russo et al., Energy Fuels 2023, 37, 12525–12540.
3214. L. Sun et al., SusMat 3, 2023, 207-221.

3215. Chen, C. et al., Biochar 5, 51 (2023).
3216. J.S. Rodrigues et al., Internat. J. Biological Macromolecules 240, 2023, 124460.
3217. M. Zlatar et al., ACS Catal. 2023, 13, 15375–15392.
3218. G. Chen et al., Reactive and Functional Polymers 193, 2023, 105744.
3219. Recep Yuksel, Naile Karakehya, Carbon 221, 2024, 118934.
3220. Manuel J. Pinzón C. et al., Journal of Energy Storage 62, 2023, 106858
3221. A.S. May et al., Green Chem., 2023, 25, 8687-8697.
3222. H. Xiong et al., Chemical Engineering Research and Design 194, 2023, 756-767.
3223. F. Ren et al., ACS Appl. Energy Mater. 2023, 6, 6773.
3224. J.S. Rodrigues et al. Internat. J. Biological Macromolecules 268, 2024, 131883.
3225. Alireza Heidarian et al., Journal of Power Sources 569, 2023, 233026.
3226. N. Yadav et al., Langmuir 2024, 40, 8474–8482.
3227. Sun, Z. et al., Int J Coal Sci Technol 11, 5 (2024).
3228. K. Chen et al., Journal of the Geological Society 2024, 181, https://doi.org/10.1144/jgs2024-005.
3229. Y. Kim et al., Journal of Industrial and Engineering Chemistry 119, 2023, 376-385.
3230. Charles D. Brewster et al., Energy Adv., 2023, 2, 398-409.
3231. Chongrui Zhuang et al 2023 J. Electrochem. Soc. 170 102503.
3232. David M. Freire-Lista et al., Heritage 2023, 6(12), 7277-7292.
3233. S. Chae et al., ACS Appl. Mater. Interfaces 2023, 15, 11652–11661.
3234. S. K. Murtaza et al., IEEE 11th International Conference on Smart Energy Grid Engineering (SEGE), Oshawa, ON, Canada, 2023, pp. 48-52.
3235. Partha Protim Bakal, et al., J. Water Chem. Technol. 45, 200–210 (2023).
3236. S. Da Costa et al., Advances in Nano and Biochemistry 2023, Pages 199-231.
3237. Alireza Heidarian, Ph.D. Thesis, RMIT University, Australia, 2023.
3238. K. Inaba et al., Transactions of the Society of Automotive Engineers of Japan 54 (2023) 970.

Todor Dudev and Carmay Lim, "Metal selectivity in metalloproteins: Zn^{2+} vs Mg^{2+}", *J. Phys. Chem. B* **105** (2001) 4446-4452.

3239. Yanyan Du et al., Catalysis Communications 57 (2014) 73–77.
3240. Marharyta Petukh and Emil Alexov, Asian J. Phys. 2014, 23: 735–744.
3241. Paola R. Beassoni et al., Enzyme Research 2015 (2015), Article ID 404607.
3242. Marharyta Petukh et al., J. Comput. Chem. 36 (2015) 2381–2393.
3243. I. Dokmanic et al., Acta Cryst. (2008). D64, 257-263.
3244. Chia-Lung Li et al., EMBO J (2003)22:4014-4025.
3245. Tarun Jain, B. Jayaram; Proteins 67, 2007, 1167-1178.
3246. Lubomír Rulíšek and Jiří Šponer, J. Phys. Chem. B 2003, 107, 8, 1913–1923.
3247. María J. Maté, Colin Kleanthous; J. Biol. Chem. 279, 2004, 34763-34769.
3248. Wen-Yen Ku et al., Nucleic Acids Research, 30, 2002, 1670–1678.
3249. Meng-Jiun Sui et al., Protein Sci. 11, 2002, 2947-2957.

3250. Mariana Babor et al., Proteins 59, 2005, 221-230.
3251. Stefan Kluge and Jennie Weston, Biochemistry 2005, 44, 12, 4877–4885.
3252. U.C. Chaturvedi et al., FEMS Immunol. Medical Microbiol. 43, 2005, 105–114.
3253. Lubomír Rulíšek, Zdeněk Havlas; J. Phys. Chem. B 2003, 107, 10, 2376–2385.
3254. Alessandra Magistrato et al., J. Phys. Chem. B 2003, 107, 17, 4182–4188.
3255. Emilia L. Wu et al., J. Phys. Chem. B 2009, 113, 8, 2477–2485.
3256. Jason R. Wickham et al., J. Phys. Chem. B 2009, 113, 7, 2177–2183.
3257. Catherine H. Schein et al., Proteins 58, 2005, 200-210.
3258. Marharyta Petukh et al., Biophys. J. 102, 2012, 2885-2893.
3259. Shao-Yong Lu et al., Proteins 81, 2013, 740-753.
3260. Piovesan, D. et al.;
3261. BMC Bioinformatics 13, S10 (2012).
3262. D. Mukhopadhyay et al., Acta Cryst. (2004). D60, 638-645.
3263. Yu Zhang, Kaixun Huang; J. Mol. Struct. THEOCHEM 812, 2007, 51-62.
3264. Hongshan He et al., J. Inorg. Biochem. 98, 2004, 667-676.
3265. M. Smiesko, M. Remko; Chem. Pap. 59 (5) 310—315 (2005).
3266. Gilles Frison, Gilles Ohanessian; Phys. Chem. Chem. Phys., 2009,11, 374-383.
3267. M. Kanthimathi et al., Langmuir 2003, 19, 8, 3398–3402.
3268. Otero, L.H., Beassoni, P.R., Lisa, A.T. et al. Biometals 23, 307–314 (2010).
3269. D. Nayak et al., J. Radioanalytical Nuclear Chemistry 271 (2007) 387–390.
3270. Cheryl L. Wojciechowski, Evan R. Kantrowitz; Biochimica et Biophysica Acta (BBA) - Proteins and Proteomics 1649, 2003, 68-73.
3271. M. Cepeda-Plaza, A. Peracchi; Org. Biomol. Chem., 2020,18, 1697-1709.
3272. Carlos Eduardo Domenech et al., Enzyme Research 2011, Article ID 561841.
3273. G. Prehna, C. E. Stebbins; Acta Cryst. (2007). D63, 628-635.
3274. Nilson Nunes-Tavares et al., Med Sci Monit 2005; 11(4): BR100-105.
3275. Teng Wang et al., Phys. Chem. Chem. Phys., 2011,13, 1140-1151.
3276. Amolegbe, S.A. et al.; J Biol Inorg Chem 22, 1–18 (2017).
3277. Kotrba P., Rulíšek L., Ruml T. (2011), In: Kotrba P., Mackova M., Macek T. (eds) Microbial Biosorption of Metals. Springer, Dordrecht.
3278. Usenobong Friday Ufot, Ph.D. thesis, University of Sussex, UK, 2010.
3279. Daniela Cajado-Carvalho et al., Toxins 2019, 11(4), 194.
3280. Aborode Abdullahi Tunde; Intl. J. Current Res. Appl. Chem. & Chem. Engin. Vol. 4, Issue 2 – 2020, 1-13.
3281. Silvia Morante et al., Front Mol Biosci. 2020; 7: 222.
3282. Heung-Chin Cheng, Robert Z. Qi, Hemant Paudel, and Hong-Jian Zhu (Eds.), Regulation and Function of Protein Kinases and Phosphatases, 2011 SAGE-Hindawi Access to Research.
3283. De Santiago, Luis M.; M.Sc. thesis, The University of Texas, U.S.A. 2015.
3284. Gerd Prehna, Ph.D. thesis, Rockefeller University, U.S.A., 2007.
3285. Petukh, Marharyta; Ph.D. thesis, Clemson University, U.S.A. 2015.
3286. Yang, Bowei and Yao, Hebang and Li, Dianfan and Liu, Zhenfeng, Phosphatidylglycerol Phosphate Biosynthesis at the Membrane-Cytosol Interface. Available at SSRN: http://dx.doi.org/10.2139/ssrn.3802022.

3287. Y. Tian et al., Materials Today Energy 20, 2021, 100649.
3288. Stefan Kluge, Ph.D. thesis, Friedrich-Schiller-Universität Jena, Germany 2007.
3289. C. Chaingam, M. Sc. Thesis, Kasetsart University, Thailand, 2005.
3290. D. Poger, Ph. D. Thesis, Universite Joseph Fourier, Grenoble, France, 2005.
3291. A.W. Foster et al. Curr. Opin. Chem. Biol. 66, 2022, 102095.
3292. Theodore Gerard et al. ACS Omega 2023, 8, 4, 3835–3841.
3293. Bowei Yang et al. Curr. Res. Struct. Biol. 3, 2021, 312-323.
3294. Deborah E. Shalev, Int. J. Mol. Sci. 2022, 23(24), 15957.
3295. Groves, Nicole, Ph.D. thesis, University of Sydney, 2021.
3296. Daniella dos Santos Courrol et al. Front. Cell. Infect. Microbiol., 2022, 12, https://doi.org/10.3389/fcimb.2022.966370.
3297. S. Utrera-Barrios et al., Mater. Horiz., 2024, 11, 708-725.

Todor Dudev and Carmay Lim, “Modeling Zn2+-cysteinate complexes in proteins”, *J. Phys. Chem. B* **105** (2001) 10709-10714.

3298. Ramadan M. Ramadan et al., Spectrochim. Acta Part A 132 (2014) 417–422.
3299. O. Gutten, L. Rulíšek; Phys. Chem. Chem. Phys., 2015, 17, 14393-14404.
3300. Tamalika Ash et al., J. Phys. Chem. B 2016, 120, 3467–3478.
3301. Marcus Elstner et al., J. Comp. Chem. 24, 2003, 565-581.
3302. Dirk V. Deubel, J. Am. Chem. Soc. 2002, 124, 20, 5834–5842.
3303. Joseph, A.P., Agarwal, G., Mahajan, S. et al. Biophys Rev 2, 137–145 (2010).
3304. Thomas Simonson, Nicolas Calimet; Proteins 49, 2002, 37-48.
3305. Gilles Frison, Gilles Ohanessian; J. Comp. Chem. 29, 2008, 416-433.
3306. Markos Koutmos et al., PNAS 2008 105 (9) 3286-3291.
3307. Demian Riccardi et al., Biochimica et Biophysica Acta (BBA) - Proteins and Proteomics 1804, 2010, 342-351.
3308. Ondrej Gutten and Lubomír Rulíšek, Inorg. Chem. 2013, 52, 18, 10347–10355.
3309. Lubomír Rulíšek, Zdeněk Havlas; J. Phys. Chem. B 2003, 107, 10, 2376–2385.
3310. Amit R. Reddi and Brian R. Gibney, Biochemistry 2007, 46, 12, 3745–3758.
3311. Ondrej Gutten et al., J. Phys. Chem. A 2011, 115, 41, 11394–11402.
3312. Delphine Picot et al., Inorg. Chem. 2008, 47, 18, 8167–8178.
3313. Stepan Sklenak et al., J. Am. Chem. Soc. 2004, 126, 45, 14879–14889.
3314. B.H. Shankar, D. Ramaiah; J. Phys. Chem. B 2011, 115, 45, 13292–13299.
3315. Lishan Yao et al., J. Phys. Chem. B 2005, 109, 15, 7500–7510.
3316. Cory C. Pye et al., Phys. Chem. Chem. Phys., 2006,8, 5428-5436.
3317. Andrew S. Lipton et al., J. Am. Chem. Soc. 2008, 130, 19, 6224–6230.
3318. Mironel Enescu et al., Phys. Chem. Chem. Phys., 2003,5, 3762-3767.
3319. Dirk V. Deubel, J. Am. Chem. Soc. 2002, 124, 41, 12312–12318.
3320. Nicolas Calimet, Thomas Simonson; J. Mol. Graphics Model. 24, 2006, 404-411
3321. A.K. Abu Al-Nasr, R.M. Ramadan; Spectrochim. Acta Part A 105, 2013, 14-19.

3322. Milan Kožíšek et al., Chem. Eur. J. 14, 2008, 7836-7846.
3323. Ahmed M. Abu-Dief et al., Appl. Organometallic Chem. 34, 2020, e5373.
3324. Parveez Gull et al., J. Mol. Struct. 1134, 2017, 734-741.
3325. Parveez Gull et al., Microbial Pathogenesis 104, 2017, 212-216.
3326. Lishan Yao et al., J. Phys. Chem. B 2006, 110, 51, 26320–26326.
3327. Nicholas Dimakis et al., J. Chem. Phys. 128, 115104 (2008).
3328. Emma Ahlstrand et al., Intl. J. Quantum Chem. 113, 2013, 2554-2562.
3329. Delphine Picot et al., Chem. Asian J. 5, 2010, 1445-1454.
3330. A. Mohajeri and M. Abasi, J. Theor. Comput. Chem. 5, 87-98 (2006).
3331. N. Drici; M.A. Krallafa; J Biol Inorg Chem (2017) 22:109–119.
3332. Anil K. Jamithireddy et al., J. Phys. Chem. B 2017, 121, 29, 7005–7015.
3333. R.M. Ramadan, A. Al-Nasr; Intl. J. Org. Chem. 2 (2012) Article ID: 17862.
3334. Markus SCHNEIDER, Ph.D. thesis, ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE, Switzerland, 2018.
3335. A. Gerard Daniel, Ph.D. thesis, Virginia Commonwealth University, 2013.
3336. Gutten, Ondrej; Diploma thesis, Charles University, Prague, 2010.
3337. Doha S. Ali et al., Journal of Molecular Structure 1292, 2023, 136113.

S. Ilieva, B. Galabov, **T. Dudev**, T.K. Gounev and J.R. Durig, “Effective bond charges from infrared intensities in CH_4, SiH_4, GeH_4 and SnH_4”, *J. Mol. Struct*. **565** (2001) 395-398.

3338. Arguilla, Maxx Q., et al, Chemistry of Materials 26 (2014): 6941-6946.
3339. Пономарева Алина Александровна, Диссертация на соискание ученой степени кандидата технических наук; Работа выполнена на кафедре микро и наноэлектроники СанктПетербургского государственного электротехнического университета «ЛЭТИ» им. В. И. Ульянова (Ленина), 2013.
3340. Batsanov S., Batsanov A. (2012) Chemical Bond. In: Introduction to Structural Chemistry. Springer, Dordrecht; https://doi.org/10.1007/978-94-007-4771-5_2.
3341. Spectroscopic Properties of Inorganic and Organometallic Compounds: Volume 35 (G. Davidson, Ed.) Royal Society pf Chemistry, 2002.
3342. Michalčíková, Regina; Diploma thesis, Charles University, Prague, 2012.
3343. O.N. Ulenikov et al. Spectrochim. Acta A: 284, 5 2023, 121796.

Gholam H Hakimelahi, Ali A Moosavi-Movahedi, Shwu-Chen Tsay, Fu-Yuan Tsai, Jon D Wright, **Todor Dudev**, Shahram Hakimelahi, Carmay Lim, “Design, Synthesis, and SAR of Novel Carbapenem Antibiotics with High Stability to Xanthomonas m altophilia Oxyiminocephalosporinase Type II”, *J. Med. Chem*. **43** (2000) 3632-3640.

3344. Jin Liu et al., RSC Adv., 2014, 4, 27582-27590.
3345. Fu Xinbo et al., J. Chem. Res. 27 (2016) 587.
3346. Francisco Palacios et al., Chem. Rev. 2005, 105, 3, 899–932.
3347. Franck Meyer et al., Tetrahedron 60, 2004, 3593-3597.
3348. Qiang Yao, Tetrahedron Letters 48, 2007, 2749-2753.
3349. Nader Zabarjad-Shiraz et al., (2009) Phosphorus, Sulfur, and Silicon and the Related Elements, 184:11, 3023-3037.
3350. Michael J. Gallagher, Matthew L. Crawley, in Encyclopedia of Reagents for Organic Synthesis, 2007.
3351. T. Salih, et al. J. Pharmaceut. Scie. 2020, Vol. 20, No.3, 35-50.
3352. Es Sbai, Zouhair; Ph.D. thesis, Universidad del Pais Vasco, Spain, 2017.
3353. Arif Mermer, M.Sc. thesis, Karadeniz Technical University, Turkey, 2014.
3354. Dmitriy Yu. Vandyshev et al. Molecules 2022**,** 27(16), 5268.
3355. ASHJAEE YASAMAN et al. ADV. J. SCI. ENG. 2 (2021) 99-102

Todor Dudev and Carmay Lim, "Tetrahedral vs octahedral zinc complexes with ligands of biological interest: A DFT/CDM study", *J. Am. Chem. Soc. 122* (2000) 11146-11153.

3356. Hindurao Barage, et al., Protein and Peptide Letters, 21 (2014) 140-152.
3357. L.P. Nitha et al., Spectrochimica Acta Part A 118 (2014) 154–161.
3358. Mohammed Enamullah et al., Inorganica Chimica Acta 427 (2015) 103–111.
3359. David P. Martin et al., J. Am. Chem. Soc., 2014, 136, 5400–5406.
3360. David P. Martin et al., J. Med. Chem., 2014, 57, 7126–7135.
3361. A. Gerard Daniel and Nicholas P. Farrell, Metallomics 2014, 6, 2230-2241.
3362. M.A. Gabal et al., J. Mol. Struct. 1097 (2015) 45–51.
3363. D. Wyrzykowski et al., Journal of Molecular Recognition 27 (2014) 722–726.
3364. K. Aruna et al., WORLD J. PHARM. PHARMACEUT. SCI. 2014, 3, 784-793.
3365. Alexandr V. Vinogradov et al., Chem. Commun., 2015, 51, 17764-17767.
3366. Werner Kaminsky et al., Peptide Science 104 (2015) 84–90.
3367. Muhammad Shabbir et al., J. Chem. Soc. Pak., 36 (2014) 56-62.
3368. Swathy, S S; Biju, R; Mohanan, K., Asian J. Chemistry 27 (2015): 4679-4685.
3369. R. Tokarz-Sobieraj et al., Catalysis Today 257 (2015) 72–79.
3370. Kazuhiro Akutsu et al., Talanta 146 (2016) 575–584.
3371. Nidhi Sharma et al., Biochimica et Biophysica Acta - Proteins and Proteomics 1864 (2016) 1649–1657.
3372. E. Ortega Carrasco, Ph.D. Thesis, Universitat Autonoma de Barcelona, 2015.
3373. G Gutiérrez, MA Gordillo, MN Chaur; Revista Colombiana de Química, 2016.
3374. Varughese P. Daniel et al., Spectrochimica Acta Part A 70, 2008, 403-410.
3375. Dirk V. Deubel, J. Am. Chem. Soc. 2002, 124, 20, 5834–5842.
3376. Safaa Eldin H. Etaiw et al., Spectrochimica Acta Part A 79, 2011, 1331-1337.
3377. Lubomír Rulíšek and Jiří Šponer, J. Phys. Chem. B 2003, 107, 8, 1913–1923.
3378. Anne-Christine Chamayou et al., Inorg. Chem. 2011, 50, 22, 11363–11374.

3379. A. J. Stace, Phys. Chem. Chem. Phys., 2001,3, 1935-1941.
3380. Murukan, B. et al., Transition Met Chem 31, 441–446 (2006).
3381. Thomas Simonson, Nicolas Calimet; Proteins 49, 2002, 37-48.
3382. Gilles Frison, Gilles Ohanessian; J. Comp. Chem. 29, 2008, 416-433.
3383. Zhan Zhang et al., Geochim. Cosmochim. Acta 70, 2006, 4039-4056.
3384. Erendra Manandhar et al., Chem. Commun., 2011,47, 8796-8798.
3385. Anne-Christine Chamayou et al., Inorganica Chimica Acta 365, 2011, 447-450.
3386. Kideok D. Kwon et al., Geochimica et Cosmochimica Acta 73, 2009, 1273-1284
3387. Changlin Liu; Huibi Xu; J. Inorg. Biochem. 88, 2002, 77-86.
3388. M.S. Sujamol et al., Spectrochimica Acta Part A 75, 2010, 106-112.
3389. Lubomír Rulíšek, Zdeněk Havlas; J. Phys. Chem. B 2003, 107, 10, 2376–2385.
3390. Beatriz González et al., J. Mol. Biol. 338, 2004, 771-782.
3391. Emilia L. Wu et al., J. Phys. Chem. B 2009, 113, 8, 2477–2485.
3392. Hazel Cox et al., J. Am. Chem. Soc. 2003, 125, 1, 233–242.
3393. Saeed-ur-Rehman Rehman et al., Bull. Chem. Soc. Ethiop. 2010, 24, 201-207.
3394. Min Liu et al., J. Mater. Chem. C, 2017,5, 2936-2941.
3395. Cory C. Pye et al., Phys. Chem. Chem. Phys., 2006,8, 5428-5436.
3396. Lars Olsen et al., J. Phys. Chem. B 2003, 107, 10, 2366–2375.
3397. Tamer Shoeib, J. Chem. Phys. 117, 2762 (2002).
3398. Sladjana B. Novaković et al., J. Phys. Chem. A 2007, 111, 51, 13492–13505.
3399. Abdul Wahab and Sekh Mahiuddin, J. Chem. Eng. Data 2004, 49, 1, 126–132.
3400. Manish Kumar Tiwari et al., J. Biol. Chem. 287, 2012, 19429-19439.
3401. Niloufar J. Ataie et al., Biochemistry 2008, 47, 29, 7673–7683.
3402. Anup Pandith et al., Sensors and Actuators B: Chemical 247, 2017, 840-849.
3403. M. Qaiser Fatmi et al., Phys. Chem. Chem. Phys., 2010,12, 9713-9718.
3404. Saeed–Ur–Rehman et al., J. Mex. Chem. Soc vol.55 no.3 México 2011.
3405. Michael Thutewohl et al., Bioorg. Med. Chem. 11, 2003, 2617-2626.
3406. Mehdi Tabatabaei majd et al., J. Mol. Liquids 294, 2019, 111550.
3407. Gouvea, L.R. et al. Biometals 26, 813–825 (2013).
3408. Nicolas Calimet; ThomasSimonson; J. Mol. Graphics Model. 24, 2006, 404-411
3409. Ahmad K. Abu Al-Nasr et al., Spectrochim. Acta Part A 105, 2013, 14-19.
3410. Sabrina Conrad et al., Angew. Chem. Intl. Ed. 57, 2018, 13592-13597.
3411. K. Mohanan & B. Murukan (2005) Synthesis and Reactivity in Inorganic, Metal-Organic, and Nano-Metal Chemistry, 35:10, 837-844.
3412. Yu Zhang; Kaixun Huang; J. Mol. Struct. THEOCHEM 812, 2007, 51-62.
3413. B. Lenarcik; A. Kierzkowska (2005) Separ. Sci. Technol. 39:15, 3485-3508.
3414. M. Smiesko & M. Remko (2003) J. Biomolecul. Struct. Dynam. 20:6, 759-770.
3415. Thereza A. Soares et al., J. Chem. Theory Comput. 2007, 3, 4, 1569–1579.
3416. Hanas J.S. et al., (2005) In: Iuchi S., Kuldell N. (eds) Zinc Finger Proteins. Molecular Biology Intelligence Unit. Springer, Boston, MA.
3417. D. Wyrzykowski et al., Inorganica Chimica Acta 405, 2013, 163-168.
3418. Safwat Abdel-Azeim et al., J. Comp. Chem. 32, 2011, 3154-3167.
3419. Martin Šramko et al., J. Mol. Struct. THEOCHEM 869, 2008,19-28.
3420. Emma Ahlstrand et al., J. Phys. Chem. A 2017, 121, 13, 2643–2654.

3421. Zdeněk Chval et al., J. Phys. Chem. B 2011, 115, 37, 10943–10956.
3422. Collin M. Mayhan et al., Comput. Theor. Chem. 984, 2012, 19-35.
3423. Saša Petriček; Alojz Demšar; 18, 2010, 3329-3334.
3424. Han, Min-Su et al., Bull. Korean Chem. Soc. 25, 1151-1155, 2004.
3425. Oliver Schalk ety al., Z. Phys. Chem. 227 (2013) 35–47.
3426. Sakina Bootwala et al., JPBS 3, 2013, 345-354.
3427. Fatemeh Poshtiban et al., Applied Surface Science 495, 2019, 143582.
3428. Kishimoto, S., Hara, K., Hashimoto, H. et al. Nat Commun 9, 2826 (2018).
3429. M. Trachtman; C.W. Bock; J. Mol. Struct. THEOCHEM 672, 2004,75-96.
3430. Najmeh Asadi et al., J. Mol. Liquids 310, 2020, 113220.
3431. Cheryl L. Wojciechowski; Evan R. Kantrowitz; Biochimica et Biophysica Acta (BBA) - Proteins and Proteomics 1649, 2003, 68-73.
3432. Jingqiu Hua; Michael S. Elioff; Talanta 188, 2018, 552-561.
3433. Andrés F. Posada et al, Polymers 2018, 10(11), 1239.
3434. Nina Winkler et al., J. Mater. Chem. C, 2019, 7, 3889-3900.
3435. Tanja V. Soldatović et al., (2019) J. Coordination Chemistry, 72:4, 690-706.
3436. Saša Petriček, Croat. Chem. Acta 84 (4) (2011) 515–520.
3437. Dick, B.L. et al.; J Biol Inorg Chem 22, 605–613 (2017).
3438. Laura Escorihuela et al., Food and Chemical Toxicology 112, 2018, 518-525.
3439. V. J. Klema et al., Acta Cryst. (2012). F68, 501-510.
3440. Bujdošová, Z. et al.; J Chem Crystallogr 41, 443–448 (2011).
3441. J.G. Krabbe et al., Journal of Chromatography A 1093, 2005, 36-46.
3442. Liji John et al., J. Mol. Struct. 1198, 2019, 126934.
3443. Sheeja Mathews et al., (2008) Spectroscopy Letters, 41:4, 154-16.
3444. Hok Hei Tam et al., J. Chem. Phys. 137, 164504 (2012).
3445. Francesco Stellato et al., Phys. Chem. Chem. Phys., 2018,20, 24775-24782.
3446. Jeralyne B. Padilla Mercado et al., Microchem. J. 134, 2017, 119-124.
3447. Šramko, M., Šille, J., Ježko, P. et al. Chem. Pap. 64, 395–404 (2010).
3448. Swayam Prakash et al., Chemosphere 265, 2021, 129189.
3449. Paolo Piazzetta et al., Molecules 2017, 22(6), 1009.
3450. Corey L. Jones et al., Royal Soc. Open Sci. 2017, 4, 12.
3451. Adedibu C. Tella et al., Comptes Rendus Chimie 22, 2019, 3-12.
3452. Sujamol, M.S., et al. Russ. J. Inorg. Chem. 56, 1276 (2011).
3453. T. Soldatović; E. Selimović; Progr. Reaction Kinetics Mech. 2018, 43(1), 53–61
3454. Mohammad Azama et al., Inorganica Chimica Acta 487, 2019, 97-106.
3455. Aswathy, R., Mohanan, K.; J Fluoresc 27, 1171–1181 (2017).
3456. Michał Abendrot et al., Molecules 2020, 25(4), 951.
3457. Md Ikbal Ahmed Talukdar et al., Food Chemistry 284, 2019, 213-218.
3458. Sandipan Chakraborty, Biman Jana, Metallomics 11, 2019, 1387–1400.
3459. Liji John et al., Journal of Coordination Chemistry, 72:16, 2669-2687.
3460. Saeed-Ur-Rehman et al., J. Mex. Chem. Soc. 2011, 55(3), 164-16.
3461. Shadia A. Elsayed et al., Appl. Organometallic Chem. 34, 2020, e5643.
3462. Pujari Chandrasekhar et al., Eur. J. Inorg. Chem. 2017, 2017, 1163-1170.
3463. Md Ikbal Ahmed Talukdar et al., J. Mol. Struct. 1225, 2021, 129091.

3464. Ramadan M. Ramadan, Intl. J. Org. Chem. 2 (2012) 17862.
3465. Ang, TF. et al. Biotech 8, 314 (2018).
3466. E.T. Yukl, in Encyclopedia of Inorganic and Bioinorganic Chemistry, Wiley, 2011.
3467. Vedran Milosavljevic et al., Bioconjugate Chem. 2018, 29, 9, 2954–2969.
3468. R. Reshma et al., (2019) J. Coordination Chemistry, 72:19-21, 3326-3337.
3469. Benjamin A. Link et al., Phys. Chem. Chem. Phys., 2020,22, 9290-9300.
3470. L.R. Gouvea, Ph.D. thesis, Universidade Federal de Minas Gerais, Brazil, 2013.
3471. Lars Kissau, Ph.D. thesis, University of Dortmund, 2002.
3472. Shing Bo Peh et al., Inorg. Chem. 2020, 59, 13, 9350–9355.
3473. Collin M. Mayhan, Ph.D. thesis, University of Missouri, 2014.
3474. A. Temidayo Odularu, Ph.D. thesis, University of Fort Hare, South Africa 2016.
3475. Pan, Lurong, Ph.D. thesis, University of Alabama at Birmingham, 2013.
3476. Shin Aoki et al., Eur. J. Inorg. Chem. 2019, 2019, 4740-4751.
3477. Niloufar J. Ataie, Ph.D. thesis, Brandeis University, U.S.A. 2008.
3478. Mattia Battistin et al., Molecules 2019, 24(24), 4546.
3479. Ulf Molich, Ph.D. thesis, Technical University of Denmark, 2020.
3480. Rasouli, Z. et al., Sci Rep 11, 6465 (2021).
3481. Erendra Manandhar, Ph.D. thesis, University of Southern Mississippi, 2014
3482. Ilesanmi, Ayobami Babajide, M.Sc. thesis, Texas A&M University, 2020.
3483. Arvind Kumar et al., J. Mol. Structure 1235, 2021, 130233.
3484. Bin Nazri, Ahmad, Ph.D. thesis, University of Southampton, UK, 2016.
3485. Navarro, Maribel et al., Current Pharmaceutical Design, 2021, DOI: https://doi.org/10.2174/1381612826666201113104633.
3486. Sridarala Ramu; Int. J. Adv. Res. 5(5), 1444-1457, 2017.
3487. Liji John et al., (2020) J. Biomol. Struct. Dynamics, DOI: 10.1080/07391102.2020.1794964.
3488. Abdulaziz Ali Alomari, Asian J. Adv. Basic Sci.: 2015, 3(2), 74-78.
3489. Anna Szemik-Hojniak et al., Spectrochimica Acta Part A 239, 2020, 118464
3490. Eveline J. Krab et al., Soil Biology and Biochemistry 59 (2013) 16-24.
3491. Julieta Reyna-Luna et al., J. Phys. Chem. B 2020, 124, 16, 3355–3370.
3492. Xiaodan Huang et al., Nanoscale, 2021,13, 8514-8523.
3493. Thomas W. Lyons et al., Org. Process Res. Dev. 2020, 24, 8, 1457–1466.
3494. Patrick Diep et al., Analytical Biochemistry 609, 2020, 113836.
3495. Preethy, Soosan Thomas et al., Oriental J. Chem. 33 (2017): 2787-2795.
3496. Stephanie Anne Avola, M.Sc. thesis, York University, Toronto, 2008.
3497. Valerie Jane Klema, Ph.D. thesis, University of Minnesta, U.S.A. 2012.
3498. Esra Bozkurt et al., J. Chem. Theory Comput. 2017, 13, 12, 6382–6390.
3499. Ashley L Hollings et al., Metallomics, 12, 2020, 2134–2144.
3500. Sridarala Ramu et al., Intl. J. Engin. Res. Devel. 13, (July 2017), 13-24.
3501. S.Z. Bootwala, J. Interdisciplinary Cycle Research Volume XII, 2020, 6-15.
3502. S.S. Swathy et al., Arabian Journal of Chemistry 9, 2016, S1847-S1857.
3503. Trilochan Sahoo et al 2020 Mater. Res. Express 7 035701.
3504. Cristina I. Fernandes et al., Applied Clay Science 190, 2020, 105562.

3505. Buff, Carolyn Elizabeth; Ph.D. thesis, University of Missouri-Columbia, 2004
3506. John, L. et al., SN Appl. Sci. 2, 500 (2020).
3507. Johannes Gerardus Krabbe, Ph.D. thesis, Vrije Universiteit Amsterdam, 2007.
3508. M.S. Sujamol et al., Chemical Data Collections 31, 2021, 100634.
3509. Li Zhiqua et al., J. Huazhong Normal University, 2013, 52, 646-645.
3510. Ibrahim, Mohamed M.M., Ph.D. thesis, University of Malaya, 2010.
3511. Malek Bou Kallaba, Ph.D. thesis, Université Montpellier, France, 2017.
3512. A.-C. Chamayou, Ph.D. thesis, Albert-Ludwigs-Universität zu Freiburg, 2010.
3513. Jana Anhäuser, Ph.D. thesis, Friedrich-Wilhelms-Universität Bonn, 2019.
3514. К.О. Степанюк, Хімія, фізика та технологія поверхні. 2020. Т. 11. No 3. С. 304-318.
3515. Barbara Czaplińska, Ph.D. thesis, Uniwersytet Śląski, Poland, 2019.
3516. K. Dvorakova, B.Sc. Thesis, Jihoceska Univerzita v Ceskyh Budejovicich, Czech Republic, 2007.
3517. Ariana C. F. Santos et al. Int. J. Mol. Sci. **2022**, 23(5), 2855.
3518. Shing Bo Peh et al. Chem. Eng. Sci. Volume 250, 15 March 2022, 117399.
3519. Marcin H. Kudzin et al. Antibiotics 2021, 10(11), 1327.
3520. M. Nematzadeh et al. Science of The Total Environment 820, 2022, 153376.
3521. Zongfan Yang et al. J. Chem. Inf. Model. 2021, 61, 11, 5658–5672.
3522. Amstrup, S.K., Ong, S.C., Sofos, N. et al. Nat Commun 14, 1001 (2023).
3523. Abhishek Kumar et al. J. Phys. Chem. B 2021, 125, 43, 11943–11954.
3524. Tanzimjahan A. Saiyed et al. Open Chemistry 19 (2021) 974.
3525. Somaye Nilouyal et al. Chem. Mater. 2023, 35, 4, 1610–1623.
3526. N. Andrikopoulos et al. ACS Appl. Mater. Interfaces 2023, 15, 6, 7777–7792.
3527. Salvador R. G. Balestra et al. Nanoscale, 2023,15, 3504-3519.
3528. Juan Ramón Avilés-Moreno et al. Phys. Chem. Chem. Phys., 2022,24, 27136.
3529. Angelo Pio Sebaaly et al. Int. J. Mol. Sci. 2023, 24(3), 2123.
3530. Franz A. Mautner et al. Inorganics 2021, 9(7), 53.
3531. Ye-hui-zi WU et al. Trans. Nonferrous Metals Soc. China 32, 2022, 1336.
3532. Alla V. Marukhlenko et al. Pharmaceutics 2023, 15(2), 590.
3533. M. Graves et al. Spectrochim. Acta A: 282, 2022, 121702.
3534. M. Sumi et al. Inorganica Chimica Acta Volume 549, 1 May 2023, 121397.
3535. Abeer A Sharfalddin et al. (2021) Front. Chem. 9:644691. doi: 10.3389/fchem.2021.644691.
3536. Bandar A. Babgi et al. Chemistry 2021, 3(4), 1178-1188.
3537. Jan Mohammad Mir et al. J. Indian Chem. Soc.99, 2022, 100743.
3538. Ipsita Mondal et al. J. Mol. Struct. Volume 1249, 5 February 2022, 131598.
3539. A. Khadivi Asenjan et al. J. Mol. Struct. 1244, 15 November 2021, 130882.
3540. Youzhi Li et al. J. Mol. Struct.1251, 5 March 2022, 132078.
3541. Ashley Louise Hollings, Ph.D. thesis, Curtin University, 2022.
3542. OLADAPO S FALOKUN, M.Sc. thesis, Texas A&M University, 2021.
3543. Dewi Mariyam et al. Jurnal Riset Kimia, 13(1), 100–110 (2022).
3544. ELSA MATHEWS, N., & K, M. (2021). Scholar: National School of Leadership, 10(1.0).

3545. Puspendu Middya et al., New J. Chem., 2023,47, 9346-9363.
3546. Jorge L. Martinez et al., ACS Catal. 2023, 13, 12673–12680.
3547. Jake Seymour et al., Faraday Discuss. 2024 DOI: 10.1039/D4FD00029C.
3548. K. Garstka et al., Molecules 2023, 28(10), 3985.
3549. Julen Aduriz-Arrizabalaga et al., Phys. Chem. Chem. Phys., 2023, 25, 27618.
3550. Corrêa, R.L.G.Q. et al. J Mol Model 29, 166 (2023).
3551. Z. Guan et al., J. Environmental Chemical Engineering 12, 2024, 112488.
3552. N. Ansari et al., Materials Sci. Semiconductor Processing 173, 2024, 108087.
3553. Panyakorn Taweechat et al., J. Phys. Chem. B 2024, 128, 19, 4670–4684.
3554. Binitha Sreedharan Daisylet et al., J. Inorganic Biochem. 257, 2024, 112603.
3555. Bruno Martínez-Haya et al., Phys. Chem. Chem. Phys., 2024, 26, 198-208.
3556. Khalfan Almarzooqi et al., 2024 Nanotechnology 35 305606.
3557. Reyna-Luna, J. et al., J Comput Aided Mol Des 37, 279–299 (2023).
3558. D.S. Ali et al., Journal of Molecular Structure 1292, 2023, 136113.
3559. H. Deng et al., Metals 2023, 13(6), 1021.
3560. Mezna Saleh Altowyan et al., Crystals 2023, 13(9), 1375.
3561. de Miranda, D.B. et al., J Mol Model 29, 203 (2023).
3562. Zerrouk, A. et al., J Chem Sci 135, 91 (2023).
3563. J. Song et al., Macromolecular Rapid Commun. 44, 2023, 2300077.
3564. E. Muller et al., Acta Cryst. F 79, 2023, 240-246.
3565. Eesha Khare, Ph.D. Thesis, MIT, U.S.A., 2023.
3566. Diep, Patrick, Ph.D. Thesis, University of Toronto, 2023.
3567. Itxaso Anso, Ph.D. Thesis, University of Basque Country, Spain, 2023.
3568. Марухленко Алла, Ph.D. Thesis, РОССИЙСКИЙ УНИВЕРСИТЕТ ДРУЖБЫ НАРОДОВ ИМЕНИ ПАТРИСА ЛУМУМБЫ, 2023.

Todor Dudev and Carmay Lim, "Metal binding in proteins: the effect of the dielectric medium", *J. Phys. Chem. B* **104** (2000) 3692-3694.

3569. M.A. Gabal et al., Journal of Molecular Structure 1097 (2015) 45–51.
3570. Ping Yin et al., Food Chemistry 148 (2014) 307–313.
3571. Metalloproteins: Theory, Calculations, and Experiments, edited by Art E. Cho, William A. Goddard III, CRC Press, London, 2015.
3572. Nicholas E. Jackson et al., Ratner, Israel J. Chem. 54 (2014) 454–466.
3573. Mahdieh Jalalian et al., Journal of Cluster Science 2015, 26, 703-711.
3574. Elisabeth O. Carrasco, Ph.D. thesis, Universitat Autonoma de Barcelona, 2015.
3575. Monika Fuxreiter, Computational Approaches to Protein Dynamics, CRC Press, Boka Raton, 2015.
3576. Roland K.O. Sigel; Anna M. Pyle; Chem. Rev. 2007, 107, 1, 97–113.
3577. Vinod K. Misra and David E. Draper, PNAS 2001 98 (22) 12456-12461.
3578. Akash Khandelwal et al., J. Med. Chem. 2005, 48, 17, 5437–5447.
3579. B.R. Schone et al., Geochem. J. 44 (2010) 23-37.

3580. Art E. Cho, David Rinaldo; J. Comp. Chem. 30, 2009, 2609-2616.
3581. Stefan Kluge and Jennie Weston, Biochemistry 2005, 44, 12, 4877–4885.
3582. Mayaan, E., Range, K. & York, D.M. J Biol Inorg Chem 9, 807–817 (2004).
3583. M. Kanthimathi et al., Materials Letters 58, 2004, 2914-2917.
3584. Monica Farcas et al., J. Electroanal. Chem. 649, 2010, 206-21.
3585. Henry M. Heitzer et al., J. Am. Chem. Soc. 2013, 135, 26, 9753–9759.
3586. Laurens Vandebroek et al., Chem. Eur. J. 2018, 24, 1 – 11.
3587. Subha Kalyaanamoorthy, J. Mol. Graphics Model. 44, 2013, 44-53.
3588. Jose M. Mercero et al., Intl. J. Quantum Chem. 98 (2004) 409-424.
3589. Rutkowska-Zbik, D. et al. J Mol Model 19, 4661–4667 (2013).
3590. Emanuela M. Bianchi et al., Helv. Chim. Acta 88, 2005, 406-425.
3591. Elixabete Rezabal et al., ChemPhysChem 2007, 8, 2119 – 2124.
3592. Alessandra Ricca; J. Phys. Chem. A 2002, 106, 13, 3219–3223.
3593. Barroso daSilva, F., Dias, L. Biophys Rev 9, 699–728 (2017).
3594. Sidney Jurado de Carvalho et al., J. Phys. Chem. B 2008, 112, 51, 16766–16776.
3595. Mesbahi-Vasey S, (2017) PLoS ONE 12(6): e0177686.
3596. Jiménez, A. et al., J Mol Model 14, 735–746 (2008).
3597. Otero, L.H., Beassoni, P.R., Lisa, A.T. et al. Biometals 23, 307–314 (2010).
3598. Zengjie Zhang, Ph.D. thesis, Goethe-Universität in Frankfurt am Main, 2009.
3599. T. Marino et al., J. Chem. Theory Comput. 2007, 3, 5, 1830–1836.
3600. Akash Khandelwal et al., Mol. Inform. 23, 2004, 754-766.
3601. Aurora Jiménez et al., Chem. Eur. J. 15, 2009, 1422-1428.
3602. Cheryl L. Wojciechowski et al., Biochimica et Biophysica Acta - Proteins and Proteomics 1649, Issue 1, 2003, 68-73.
3603. Carlos Eduardo Domenech et al., Enzyme Res., Vol. 2011, Article ID 561841.
3604. Elisabeth Ortega-Carrasco, J. Inorg. Biochem. 117, 2012, 230-236.
3605. A. Mohajeri; J. Theor. Comput. Chem. 5, 87-98 (2006).
3606. Liliana M. Pacureanu et al., Rev. Roum. Chim., 2011, 56, 289-298.
3607. Šramko, M., Šille, J., Ježko, P. et al. Chem. Pap. 64, 395–404 (2010).
3608. James A. Snyder, J. Phys. Chem. B 2005, 109, 37, 17757–17761.
3609. Kevin M. Peese et al., Bioorg. Med. Chem. Lett. 30, 2020, 126784.
3610. Ping Yang et al., J. Phys. Chem. A 2007, 111, 18, 3602–3612.
3611. Heung-Chin Cheng, Robert Z. Qi, Hemant Paudel, and Hong-Jian Zhu (Eds.), Regulation and Function of Protein Kinases and Phosphatases, 2011 SAGE-Hindawi Access to Research.
3612. Xun Liu et al., Ceramics International 45, 2019, 23869-23889.
3613. E D Barbosa et al., Metallomics, 13, 2021, mfab017.
3614. Kay, Laura; Ph.D. thesis, Northumbria University, UK, 2016.
3615. Delboni, Lariani Aparecida, M.Sc. thesis, Univ. de Sao Paolo, Brazil, 2016.
3616. Laurens Vandebroek, Ph.D. thesis, KU Leuven, Belgium, 2020.
3617. Stefan Kluge, Ph.D. thesis, Friedrich-Schiller-Universität Jena, Germany, 2007.
3618. Yue Yu et al. Molecules 2022, 27(4), 1277.
3619. Zhifeng Jing et al. Chem. Sci., 2021, 12, 8920-8930.
3620. Feehan, R., Franklin, M.W. & Slusky, J.S.G. Nat Commun 12, 3712 (2021).

Todor Dudev, JA Cowan, Carmay Lim, "Competitive binding in magnesium coordination chemistry: water versus ligands of biological interest", *J. Am. Chem. Soc.* **121** (1999) 7665-7673.

3621. Mauro Carcelli et al., Mol. Pharmaceutics, 2014, 11, 304–316.
3622. Ian M. Power et al., Minerals 2014, 4, 399-436.
3623.
3624. Xiya Lu et al., J. Phys. Chem. B, 2015, 119, 1062–1082.
3625. Alexander Krah and Shoji Takada, Biochimica et Biophysica Acta (BBA) – Bioenergetics 1847 (2015) 1101–1112.
3626. Gaurao V. Dhoke et al., ACS Catal., 2015, 5, 3207–3215.
3627. Ondrej Gutten; Phys. Chem. Chem. Phys., 2015, 17, 14393-14404.
3628. Taka-aki Okamura et al., J. Am. Chem. Soc. 2014, 136, 14639–14641.
3629. Quin R. S. Miller et al., Environ. Sci. Technol., 2015, 4, 4724–4734.
3630. Taka-aki Okamura et al., Dalton Trans., 2015, 44, 7512-7523.
3631. Duarte Mota de Freitas et al., Chapter, The Alkali Metal Ions: Their Role for Life, Volume 16 of the series Metal Ions in Life Sciences, 2016, pp 557-584.
3632. Matthew Lloyd Harty, M.Sc. Thesis, Dalhousie University, Canada, 2015.
3633. D.G. Jones et al., Intl. J. Greenhouse Gas Control 40 (2015) 350–377.
3634. Uluğ M. Ünligil; James M. Rini; Curr. Opin. Struct. Biol. 10, 2000, 510-517.
3635. Wei Li et al., Molecular Physics 119:8, 2016.
3636. Michael A. Duncan (2003) Intl. Reviews in Physical Chemistry, 22:2, 407-435.
3637. C. Desfrançois et al., Chem. Rev. 2000, 100, 11, 3943–3962.
3638. Hao Zhou, David E. Clapham; PNAS 2009 106 (37) 15750-15755.
3639. U. Wehrmeister et al., J. Raman Spectroscopy 41, 2010, 193-201.
3640. Snežana D. Zarić et al., Chem. Eur. J. 6, 2000, 3935-3942.
3641. Ian M. Power et al., Rev. Mineralogy and Geochemistry (2013) 77 (1): 305–360.
3642. Power, I.M. et al., Geochem Trans 8, 13 (2007).
3643. Hoober, J.K. et al., Photosynth Res 94, 387–400 (2007).
3644. B.R. Schone et al., Geochem. J. 44 (2010) 23-37.
3645. N. Walker et al., J. Am. Chem. Soc. 2000, 122, 45, 11138–11145.
3646. James K. Bashkin, Curr. Op. Chem. Biol. 3, 1999, 752-758.
3647. Lubomír Rulíšek and Jiří Šponer; J. Phys. Chem. B 2003, 107, 8, 1913–1923.
3648. Wen-Yen Ku et al., Nucleic Acids Research, 30, 2002, 1670–1678.
3649. Sladjana Prisic and Reuben J. Peters, Plant Physiol. 2007, 144, 445–454.
3650. Dongfeng Xue et al., Powder Technology 191, Issues 1–2, 2009, 98-106.
3651. Ian M. Power et al., Intl. J. Greenhouse Gas Control 16, 2013, 145-155.
3652. Lindsay S. Cahill et al., Chem. Eur. J. 15, 2009, 9785-9798.
3653. Stefan Kluge and Jennie Weston; Biochemistry 2005, 44, 12, 4877–4885.
3654. Yuri G. Abashkin et al., J. Phys. Chem. B 2001, 105, 1, 287–292.
3655. A. Erxleben, D. Schumacher; Eur. J. Inorg. Chem. 2001, 2001, 3039-3046.
3656. Pradeep R. Varadwaj et al., J. Phys. Chem. A 2008, 112, 42, 10657–10666.

3657. Lubomír Rulíšek, Zdeněk Havlas; J. Phys. Chem. B 2003, 107, 10, 2376–2385.
3658. Elixabete Rezabal et al., J. Inorg. Biochem. 100, 2006, 374-384.
3659. Robert C. Rittenhouse et al., Proteins 53, 2003, 667-682.
3660. Rajput N.N. et al., (2018) Elucidating Solvation Structures for Rational Design of Multivalent Electrolytes—A Review. In: Korth M. (ed) Modeling Electrochemical Energy Storage at the Atomic Scale. Topics in Current Chemistry Collections. Springer, Cham.
3661. Yang, P., Ren, R., Guo, M. et al. J Biol Inorg Chem 9, 495–506 (2004).
3662. Wei Zheng et al., J. Mol. Biol. 366, 2007, 1447-1458.
3663. Agnieszka Kania and Leszek Fiedor, J. Am. Chem. Soc. 2006, 128, 2, 454–458.
3664. Lizbeth Edmonds et al., J. Mol. Biol. 365, 2007, 175-186.
3665. Mauro Carcelli et al., Mol. Pharmaceutics 2014, 11, 1, 304–316.
3666. Judit E. Šponer et al., Phys. Chem. Chem. Phys., 2004,6, 2772-2780.
3667. Ian M. Power et al., Cryst. Growth Des. 2017, 17, 11, 5652–5659.
3668. Jason R. Wickham et al., J. Phys. Chem. B 2009, 113, 7, 2177–2183.
3669. Glen Akibo-Betts et al., J. Am. Chem. Soc. 2002, 124, 31, 9257–9264.
3670. Thomas S. Peat et al., Mol. Mocrobiol. 88, 2013, 1149-1163.
3671. Brian L. Scott et al., J. Inorg. Biochem. 94, 2003, 5-13.
3672. C.M. Dupureur; L.H. Conlan, Biochemistry 2000, 39, 35, 10921–10927.
3673. Simon Petrie, J. Phys. Chem. A 2002, 106, 30, 7034–7041.
3674. Elixabete Rezabal et al., J. Inorg. Biochem. 101, 2007, 1192-1200.
3675. Manish Kumar Tiwari et al., J. Biol. Chem. 287, 2012, 19429-19439.
3676. Piovesan, D. et al. BMC Bioinformatics 13, S10 (2012).
3677. Xingchen Zhang et al., J. Mol. Struct.: THEOCHEM 594, 2002, 19-30.
3678. M.R. Ganjalikhany et al., J. Mol. Catal. B: Enzymatic 62, 2010, 127-132.
3679. Petra Imhof et al., J. Chem. Theory Comput. 2006, 2, 4, 1050–1056.
3680. Bart M. J. M. Suijkerbuijk et al., Dalton Trans., 2010,39, 6198-6216.
3681. Iván Solt et al., J. Phys. Chem. B 2007, 111, 22, 6272–6279.
3682. D. Mukhopadhyay et al., Acta Cryst. (2004). D60, 638-645.
3683. Jose M. Mercero et al., Intl. J. Quantum Chem. 98, 2004, 409-424.
3684. Keiji Takamoto et al., Structure 15, 2007, 39-51.
3685. Xiaoyang Wang et al., J. Org. Chem. 2010, 75, 10, 3358–3370.
3686. Nicolas Calimet; Thomas Simonson; J. Mol. Graphics Model. 24, 2006, 404-411
3687. Rutkowska-Zbik et al., J Mol Model 19, 4661–4667 (2013).
3688. Vadapalli Chandrasekhar et al., Chem. Commun., 2005, 459-461.
3689. Elixabete Rezabal et al., ChemPhysChem 2007, 8, 2119 – 2124.
3690. Judit E. Šponer et al., J. Phys. Chem. B 2001, 105, 48, 12171–12179.
3691. Quin R. S. Miller et al., Environ. Sci. Technol. 2018, 52, 12, 7138–7148.
3692. V. Sladek and I. Tvaroška, J. Phys. Chem. B 2017, 121, 25, 6148–6162.
3693. Hoober J.K. (2007) Chloroplast Development: Whence and Whither. In: Wise R.R., Hoober J.K. (eds) The Structure and Function of Plastids. Advances in Photosynthesis and Respiration, vol 23. Springer, Dordrecht.
3694. George Pontikis et al., J. Phys. Chem. A 2009, 113, 15, 3588–3593.
3695. Zengjie Zhang, Ph.D. thesis, Goethe-Universität in Frankfurt am Main, 2009.

3696. Neela, Y.I., Mahadevi, A.S. & Sastry, G.N.; Struct Chem 24, 637–650 (2013).
3697. Spencer E. Taylor et al., Colloids Interfaces 2018, 2(3), 40.
3698. M.A. Peterson et al., Nucleosides, Nucleotides & Nucleic Acids, 2007,26:5, 499.
3699. L.M. da Costa et al., J Mol Model 19, 2669–2677 (2013).
3700. Christopher A. Dunlap et al., Carbohydrate Research 338, 2003, 2367-2373.
3701. Cheryl L. Wojciechowski; Biochimica et Biophysica Acta (BBA) - Proteins and Proteomics 1649, 2003, 68-73.
3702. Teng Wang et al., Phys. Chem. Chem. Phys., 2011,13, 1140-1151.
3703. Subramaniam Kavitha et al., J. Mol. Graphics Model. 85, 2018, 13-24.
3704. In Taek Songa and Russell J. Stewart, Soft Matter, 2018,14, 379-386.
3705. Sanchez, E.R., Caudle, M.T. J Biol Inorg Chem 9, 724–732 (2004).
3706. Hoober J.K., Eggink L.L., Chen M., Larkum A.W.D. (2010) Chapter 15 The Chemistry and Biology of Light-Harvesting Complex II and Thylakoid Biogenesis: raison d'etre of Chlorophylls b and c. In: Rebeiz C.A. et al. (eds) The Chloroplast. Advances in Photosynthesis and Respiration, vol 31. Springer, Dordrecht.
3707. R.L. Mancera; B.J. Carrington; J. Mol. Struct: THEOCHEM 755,2005, 151-159
3708. Mangesh I. Chaudhari et al., Annu. Rev. Phys. Chem. 71, 2020, 461-484.
3709. Ali Riahi-Madvar et al., Intl. J. Biol. Macromolecules 52, 2013, 157-163.
3710. James Weston, in PATAI's Chemistry of Functional Groups, 2009, John Wiley.
3711. Jose M. Mercero et al., Chemical Physics 295, 2003, 175-184.
3712. Sławomir J. Grabowski; ChemistrySelect 3, 2018, 3147-3154.
3713. Stern, N. et al.; J Biol Inorg Chem 17, 861–879 (2012).
3714. Xuanting Liu et al., Food Hydrocolloids 101, 2020, 105450.
3715. Matteo Mori et al., J. Med. Chem. 2020, 63, 13, 7066–7080.
3716. Patricija Hriberšek; Ksenija Kogej; Polymers 2019, 11(4), 605.
3717. Tejral G et al., 2017, PeerJ 5:e3087.
3718. Hyeong-Hwan Lee et al., Chem. Sci., 2017, 8, 2592-2596.
3719. Hughes, Sean; Ph.D. thesis, Concordia University, Canada, 2006.
3720. Ping Yang et al., J. Phys. Chem. A 2007, 111, 18, 3602–3612.
3721. B.M.J.M.Suijkerbuijk, Ph.D. thesis, Universiteit Utrecht, The Netherlands, 2007
3722. Florence Reddish, Ph.D. thesis, Georgia State University, U.S.A. 2017.
3723. Dr. Robert W. Molt, Jr. et al., Chemistry. 2019 Jun 26; 25(36): 8484–8488.
3724. Hattab, A. et al. Theor Chem Acc 138, 71 (2019).
3725. Lee, Jong-min; PhD Thesis - University of Auckland, New Zealand, 2010.
3726. Christopher A. Dunlap, Ph.D. thesis, The Ohio State University, 2002.
3727. I. B. Gorrella, Annu. Rep. Prog. Chem., Sect. A: Inorg. Chem., 2000,96, 5-22.
3728. Shehla Yousuf et al., Metallomics, 12, 2020, 1791–1801.
3729. Juliana Morais Missina et al., Inorganica Chimica Acta 523, 2021, 120319.
3730. Zixuan Huang et al., AIP Advances 11, 025308 (2021).
3731. Dimitrios Toroz et al., CrystEngComm, 2021, Advance Article; DOI: 10.1039/D1CE00052G.
3732. Rafael C. Marchi et al., ACS Omega 2020, 5, 7, 3504–3512.
3733. Kurz, Jeffrey Crossen; Ph.D. thesis, Duke University, 2001.
3734. Frank C. Sciavolino, US patent US10130719B2, 2018.

3735. Mehdi D. Esrafili and Sirous Yourdkhani, Can. J. Chem. 90, 10, 2012.
3736. Heidrich, Jennifer; Ph.D. thesis, Johannes Gutenberg-Universität, Mainz, 2018.
3737. Lea Veras, Ph.D. thesis, Carnegie Mellon University, 2014.
3738. Remya Korah, Ph.D. thesis, Indian Institute of Technology-Bombay, 2008.
3739. Heinonen, Reija; M.Sc. thesis, University of Helsinki, 2020.
3740. Isti Yunita, Ekasith Somsook; Indonesian J. Chem. Sci. 9(2) (2020) 71-84.
3741. Stefan Kluge, Ph.D. thesis, Friedrich-Schiller-Universität Jena, Germany, 2007
3742. C. Chaingam, M. Sc. Thesis, Kasetsart University, Thailand, 2005.
3743. J.L. Vinkenborg, Ph.D. Thesis, Technical University of Eindhoven, 2010.
3744. T.D. Jaeger, Ph.D. Thesis, University of Georgia, USA, 2004.
3745. Arpita Varadwaj et al. Int. J. Mol. Sci. 2022, 23(15), 8816.
3746. Wouter Lindeboom et al. Chem. Eur. J. 27 (2021) 12224.
3747. Yuto Yoshida et al. J. Phys. Chem. C 2021, 125, 38, 21124–21130.
3748. Yunyan Han et al. Tribology International Volume 179, January 2023, 108197.
3749. M. Wyparło-Wszelaki et al. J. Biochem. Mol. Toxicol. 36 (2022) e22964.
3750. Tomasz Sierański et al. Crystals 2022, 12(10), 1434.
3751. Deborah E. Shalev, Int. J. Mol. Sci. 2022, 23(24), 15957.
3752. Kurz, Julia Leanne, Ph.D. thesis, University of Queensland, 2022.
3753. Z. Zhao et al., Advanced Materials 36, 2024, 2313211.
3754. Durnian C. Parulski-Seager et al., ACS Appl. Polym. Mater. 2023, 5, 6143.
3755. D. Singh et al., Cement and Concrete Research 175, 2024, 107367.
3756. P. Zhang et al., Construction and Building Materials 433, 2024, 136611.
3757. Gopika Sabu, Susmita De, J. Phys. Chem. B 2023, 127, 10326–10337.
3758. Géssica Domingos da Silveira et al., Int. J. Pharmaceutics 648, 2023, 123559.
3759. Gaurab Chowdhury et al., Biochimica et Biophysica Acta (BBA) - Proteins and Proteomics 1872, 2024, 140964.
3760. Kouhei Aoki et al., Dalton Trans., 2023, 52, 15313-15316.
3761. Mikkel Herzberg et al., Acta Cryst. B 79, 2023, 330-335.
3762. Durnian Chen Chang Li Parulski-Seager, M.Sc. Thesis, Rice University, 2023.
3763. P.I.K. Peiris, Ph.D. Thesis, La Trobe University, Australia, 2023.

Todor Dudev and Carmay Lim, "Incremental binding free energies in Mg2+ complexes: a DFT study", *J. Phys. Chem. A* **103** (1999) 8093-8100.

3764. Evangelos Miliordos et al., Theoretical Chemistry Accounts 2014, 133:1450.
3765. Sukhjinder Singh et al., Inorganica Chimica Acta 419 (2014) 13–18.
3766. E. Bruzzi and A. J. Stace, J. Phys. Chem. A 2014, 118, 9357–9363.
3767. Quin R. S. Miller et al., Environ. Sci. Technol., 2015, 49, 4724–4734.
3768. Felice C. Lightstone et al., Chemical Physics Letters 343, 2001, 549-555.
3769. George D. Markham et al., J. Phys. Chem. B 2002, 106, 19, 5118–5134.
3770. N. Walker et al., J. Am. Chem. Soc. 2000, 122, 45, 11138–11145.
3771. Stefan Kluge and Jennie Weston et al., Biochemistry 2005, 44, 12, 4877–4885.
3772. Christian Krekeler; Luigi Delle Site; 2007 J. Phys.: Condens. Matter 19 192101.

3773. M. Lepšík and M.J. Field, J. Phys. Chem. B 2007, 111, 33, 10012–10022.
3774. L. Rulíšek and Z. Havlas, J. Phys. Chem. B 2003, 107, 10, 2376–2385.
3775. Elixabete Rezabal et al., J. Inorg. Biochem. 100, 2006, 374-384.
3776. Mayaan, E., Range, K. & York, D.M. J Biol Inorg Chem 9, 807–817 (2004).
3777. Sebastien Kerisit et al., Chemical Geology 359, 2013, 81-89.
3778. Michel Masella and Philippe Cuniasse, J. Chem. Phys. 119, 1866 (2003).
3779. Simon Petrie, J. Phys. Chem. A 2002, 106, 30, 7034–7041.
3780. Damon R. Carl, Peter B. Armentrou; ChemPhysChem 14, 2013, 681-697.
3781. Cristian Faralli et al., J. Chem. Theory Comput. 2008, 4, 1, 156–163.
3782. Jose M. Mercero et al., Intl. J. Quantum. Chem. 98, 2004, 409-424.
3783. Rutkowska-Zbik, D., Witko, M. & Fiedor, J Mol Model 19, 4661–4667 (2013).
3784. da Costa, L.M., J Mol Model 17, 2061–2067 (2011).
3785. Eli Fernández-de Gortari; J. Biol. Chem. 293, 2018, 12405-12414.
3786. Quin R. S. Miller et al., Environ. Sci. Technol. 2018, 52, 12, 7138–7148.
3787. Christin P. Morrow et al., J. Phys. Chem. C 2010, 114, 12, 5417–5428.
3788. George Pontikis et al., J. Phys. Chem. A 2009, 113, 15, 3588–3593.
3789. Miliordos E., Xantheas S.S. (2015) In: Wilson A., Peterson K., Woon D. (eds) Thom H. Dunning, Jr., Highlights in Theoretical Chemistry, vol 10. Springer, Berlin, Heidelberg.
3790. M. Trachtman; C.W. Bock; J. Mol. Struct.: THEOCHEM 672, 2004, 75-96.
3791. Christopher A. Dunlap et al., Carbohydrate Research 338, 2003, 2367-2373.
3792. A. Mohajero; M. Abasi; J. Theor. Comput. Chem. 5, 87-98 (2006).
3793. Charles W. Bock and Mendel Trachtman, Inorg. Chem. 2002, 41, 18, 4680–4688
3794. Jose M. Mercero et al., Chemical Physics 295, 2003, 175-184.
3795. Hattab, A., Dhaouadi, Z., Malloum, A. et al. Theor Chem Acc 138, 71 (2019).
3796. Christopher A. Dunlap, Ph.D. thesis, The Ohio State University, 2002.
3797. Christian Krekeler, Ph.D. thesis, Johannes Gutenberg-Universität, Mainz, 2008.
3798. Stefan Kluge, Ph.D. thesis, Friedrich-Schiller-Universität Jena, Germany, 2007
3799. F. Tavani et al. ACS Appl. Mater. Interfaces 2022, 14, 33, 38370–38378.

Todor Dudev and Carmay Lim, “Ring Strain Energies from Ab Initio Calculations”, *J. Am. Chem. Soc.* **120** (1998) 4450-4458.

3800. Ujjal Das et al., J. Phys. Chem. Lett., 2014, 5, 813–819.
3801. Zhaobin Wang et al., Org. Biomol. Chem., 2014, 12, 6028-6032.
3802. Zhaobin Wang et al., J. Am. Chem. Soc., 2015, 137, 5895–5898.
3803. Sasidhar Kantheti et al., Ind. Eng. Chem. Res., 2014, 53, 8357–8365.
3804. Murray G. Rosenberg et al., J. Org. Chem., 2014, 79, 8786–8799.
3805. N. Kasyapi; A.K. Bhowmick, J. Phys. Chem. C, 2014, 118, 22325–22338.
3806. Akihiro Kimura et al., Org. Biomol. Chem., 2014, 12, 6717-6724.
3807. Swapnil Shukla et al., RSC Adv., 2015, 5, 78071-78080.
3808. Jian-ying Zhang and Xue-dong Gong, J. Phys. Org. Chem. 28, (2015) 577–585.

3809. Dorian Didier et al., Chemistry - A European Journal 20 (2014) 1038–1048.
3810. Ujjal Das et al., ACS Catal., 2015, 5, 7177–7185.
3811. Hannelore Goossens et al., Bonding and Reactivity of Heterocyclic Compounds, Volume 38 of the series Topics in Heterocyclic Chemistry, pp 1-34, 2014.
3812. Huiting Bian et al., Intl. J. Chemical Kinetics 47, (2015) 685–694.
3813. Jana Herzberger et al., Chem. Rev. 2016, 116, 2170–2243.
3814. Michele Aresta et al., Chapter, Reaction Mechanisms in Carbon Dioxide Conversion, Springer-Verlag, Berlin, 2016, pp 183-235.
3815. Alejandro Vásquez-Espinal et al., New J. Chem., 2016,40, 2007-2013.
3816. M.J. Houghton, D.B. Collum; J. Org. Chem. 2016; 81: 11057–11064.
3817. Yirong Mo et al., Chem. Sci., 2016, 7, 5872-5878.
3818. Qunfei Zhou et al., J. Phys. Chem. A, 2016, 120, 7101–7111.
3819. Murray G. Rosenberg et al., J. Org. Chem. 2016, 8, 12388–12400.
3820. Michael R. Douglass et al., J. Am. Chem. Soc. 2001, 123, 42, 10221–10238.
3821. Peter R. Khoury et al., Tetrahedron 60, Issue 37, 2004, 8103-8112.
3822. Robert D. Bach; Olga Dmitrenko, J. Am. Chem. Soc. 2004, 126, 13, 4444–4452
3823. Rebecca N. Loy; Eric N. Jacobsen, J. Am. Chem. Soc. 2009, 131, 8, 2786–2787
3824. Kristin N. Bauer et al., Progress in Polymer Science 73, 2017, 61-122.
3825. Kevin Range et al., J. Am. Chem. Soc. 2004, 126, 6, 1654–1665.
3826. B. Sirjean et al., J. Phys. Chem. A 2006, 110, 46, 12693–12704.
3827. Robert D. Bach, J. Am. Chem. Soc. 2009, 131, 14, 5233–5243.
3828. Robert D. Bach; Olga Dmitrenko, J. Am. Chem. Soc. 2006, 128, 14, 4598–4611
3829. Zhaobin Wang et al., Angew. Chem. 125, 2013, 6817-6820.
3830. Thach-Mien Nguyen et al., Ind. Eng. Chem. Res. 2013, 52, 13, 4715–4724.
3831. Robert D. Bach et al., J. Am. Chem. Soc. 2003, 125, 4, 924–934.
3832. Robert D. Bach and Olga Dmitrenko, J. Org. Chem. 2002, 67, 8, 2588–2599.
3833. Stefan A. Ruider et al., Angew. Chem. Intl. Ed. 52, 2013, 11908-11911.
3834. Zhen-Hua Li et al., J. Phys. Chem. A 2005, 109, 16, 3711–3716.
3835. Robert D. Bach and Olga Dmitrenko, J. Org. Chem. 2002, 67, 11, 3884–3896.
3836. Oliveira, B.G. et al. J Mol Model 15, 123–131 (2009).
3837. Xabier Lopez et al., J. Am. Chem. Soc. 2001, 123, 47, 11755–11763.
3838. Stephane Quideau et al., J. Org. Chem. 1998, 63, 9597-9600.
3839. Kelvin Y. T. Ho, Christophe Aïssa; Chem. Eur. J. 18, 2012, 3486-3489.
3840. Martina Schömer et al., J. Polym. Sci. 51, 2013, 995-1019.
3841. Xin Cheng, Shengming Ma; Angew. Chem. 120, 2008, 4657-4659.
3842. Sara Kenis et al., J. Org. Chem. 2012, 77, 14, 5982–5992.
3843. Sze Ming Ng et al., Organometallics 2003, 22, 19, 3898–3904.
3844. Scott E. Denmark et al., J. Am. Chem. Soc. 2006, 128, 35, 11620–11630.
3845. Harold D. Banks, J. Org. Chem. 2006, 71, 21, 8089–8097.
3846. Harold D. Banks, J. Org. Chem. 2003, 68, 7, 2639–2644.
3847. Jennifer Howell et al., Tetrahedron 65, 2009, 4562-4568.
3848. Metin Zora; J. Org. Chem. 2005, 70, 15, 6018–6026.
3849. Y.-Y.T. Tsao; K.L. Wooley; J. Am. Chem. Soc. 2017, 139, 15, 5467–5473.
3850. Pablo Wessig and Annika Matthe, J. Am. Chem. Soc. 2011, 133, 8, 2642–2650.

3851. Antonio Vila; Ricardo A. Mosquera; Tetrahedron 57, 2001, 9415-9422.
3852. Yanwei Li et al., ChemPhysChem 7, 2006, 2593-2600.
3853. A.S. Burns; S.D. Rychnovsky; J. Am. Chem. Soc. 2019, 141, 34, 13295–13300.
3854. Enrique Marcos et al., J. Chem. Theory Comput. 2008, 4, 1, 49–63.
3855. Mark L. G. Borst et al., J. Org. Chem. 2005, 70, 20, 8110–8116.
3856. Christopher J. Hagedorn et al., J. Am. Chem. Soc. 2001, 123, 5, 929–940.
3857. Peter Hanson et al., New J. Chem., 2010, 34, 65-84.
3858. Antonio Vila, Ricardo A. Mosquera; J. Phys. Chem. A 2006, 110, 11752–11759
3859. Truong N. Nguyen and Jeremy A. May, Org. Lett. 2018, 20, 12, 3618–3621.
3860. Harold D. Banks, J. Org. Chem. 2008, 73, 7, 2510–2517.
3861. Ye Sha et al., Macromolecules 2018, 51, 22, 9131–9139.
3862. Giuseppe Cassone et al., Phys. Chem. Chem. Phys., 2017,19, 1817-1825.
3863. Leah S. Alconcel; Robert E. Continetti; Chem. Phys. Lett. 366, 2002, 642-649
3864. Zrinka Rajic et al., J. Inorg. Biochem. 169, 2017, 50-60.
3865. Malgorzata Chwatko; Nathaniel A. Lynd; Macromolecules 2017, 50, 2714–2723
3866. Jeong-il Park; Dong H. Kim; Bioorg. Med. Chem. Lett. 11, 2001, 2967-2970.
3867. Dong Pan et al., Org. Lett. 2017, 19, 13, 3584–3587.
3868. M.A. Ali and M.S. Krishnan, J. Org. Chem. 2010, 75, 17, 5797–5809.
3869. Mohamad A. Ali & Mangala S. Krishnan (2009) Mol. Phys. 107:20, 2149-2158
3870. Diego Núñez-Villanueva et al., Chem. Sci., 2019, 10, 5258-5266.
3871. Tan, B., Long, X., Li, J. et al. J Mol Model 18, 5127–5132 (2012).
3872. Ching-Yeh Lin and Jia-Jen Ho; J. Phys. Chem. A 2002, 106, 16, 4137–4144.
3873. Silvia Rinaldi et al., ACS Catal. 2018, 8, 7, 5698–5707.
3874. José E. Gómez, Arjan W. Kleij; Adv. Organometallic Chem. 71, 2019, 175-226.
3875. Masha Elkin, Timothy R. Newhouse; Chem. Soc. Rev., 2018,47, 7830-7844.
3876. Illan Kim et al., Org. Lett. 2017, 19, 20, 5509–5512.
3877. Carsten Dingels et al., Chemie in unserer Zeit, 45, 2011, 338-349.
3878. Li Yang et al 2011 ECS Trans. 33 57.
3879. Wangshui Cai et al., Org. Lett. 2018, 20, 13, 3833–3837.
3880. Michele Aresta et al., Advances in Catalysis 62, 2018, 49-111.
3881. Akihiro Kimura et al., J. Org. Chem. 2013, 78, 7, 3086–3094.
3882. Tibor Höltzl et al., J. Mol. Struct.: THEOCHEM 811, 2007, 27-35.
3883. Steven M. Cope et al., J. Org. Chem. 2011, 76, 2, 380–390.
3884. Collins U. Ibeji et al., ChemPhysChem 20, 2019, 1126-1134.
3885. Antonio J. Mota et al., Eur. J. Org. Chem. 2005, 2005, 4346-4358.
3886. Angela Marinetti et al., Eur. J. Org. Chem. 2000, 2000, 1815-1820.
3887. Joaquim J. Queralt et al., Chemical Physics 280, 2002, 1-14.
3888. Jennifer Imbrogno et al., ACS Catal. 2018, 8, 9, 8796–8803.
3889. Sudipta Raha Roy et al., Chem. Sci., 2017, 8, 334-339.
3890. Konstantin L. Kaygorodov et al., (2018) Cogent Chemistry, 4:1.
3891. James P. Lajiness; Dale L. Boger; J. Am. Chem. Soc. 2010, 132, 13936–13940
3892. Xingpeng Chen, Jiaxi Xu; Progress in Chemistry 2017, 29, 181-197.
3893. Wujie Wang et al., Chem. Commun., 2020, 56, 8920-8923.
3894. Harold D. Banks, Org. Biomol. Chem., 2009,7, 4496-4501.

3895. Peter Finkbeiner et al., J. Med. Chem. 2020, 63, 13, 7081–7107.
3896. Conner M. Farley et al., J. Am. Chem. Soc. 2020, 142, 10, 4598–4603.
3897. Younes Valadbeigi, Robert Vianello; ChemistrySelect 5, 2020, 5794-5798.
3898. Matthias R. Bauer et al., RSC Med. Chem., 2021,12, 448-471.
3899. Lara Martínez-Fernández; Photochem. Photobiol. Sci., 2018,17, 586-591.
3900. Dhivya Manogaran, J. Comp. Chem. 40, 2019, 1556-1569.
3901. Chitranjan Sah et al., J. Phys. Chem. A 2018, 122, 24, 5464–5476.
3902. Stefan A. Ruider, Angew. Chem. 125, 2013, 12125-12128.
3903. Jian-Miao Fan et al., J. Mol. Struct.: THEOCHEM 617, 2002, 209-217.
3904. Harold D. Banks, Org. Biomol. Chem., 2011,9, 6335-6342.
3905. Michael M. Bobek et al., J. Org. Chem. 2003, 68, 6, 2129–2134.
3906. C.C. De Silva, T.A. Holme; Comp. Theor. Chem. 1019, 2013, 78-84.
3907. Wanno, B., Ruangpornvisuti, V. Struct Chem 21, 715–725 (2010).
3908. Mohamad A. Ali and Mohammad A. Alam; RSC Adv., 2017, 7, 40189-40199.
3909. M.T. Rayez et al., J. Mol. Struct. THEOCHEM 487, 1999, 241-250.
3910. Kaki Raveendra Babu et al., Synlett 2020, 31, 117–124.
3911. Erkki Kolehmainen et al., in PATAI'S Chemistry of Functional Groups, 2009.
3912. Sonhwan Kim et al., Synthesis 2019; 51(04): 885-888.
3913. Romero, A.H., Struct Chem 29, 1623–1636 (2018).
3914. Jesús Jara-Cortés et al., Phys. Chem. Chem. Phys., 2018,20, 27558-27570.
3915. P.B. Sherly mole et al., Tetrahedron 75, Issue 46, 15 November 2019, 130676.
3916. Niklas Volk et al., Coord. Chem. Rev. 437, 2021, 213818.
3917. Janis Jermaks et al., Chem. Sci., 2020, 11, 7884-7895.
3918. Roger Machín Rivera et al., Org. Lett. 2020, 22, 16, 6510–6515.
3919. Nicola Helen Powell, Ph.D. thesis, University of Warwick, UK, 2014.
3920. Michael A. E. Townsend, Ph.D. thesis, University of Canterbury, NZ, 2006.
3921. Ching-Yeh Lin, Jia-Jen Ho; Intl. J. Quantum Chem. 91, 2003, 461-466.
3922. Hai Huang et al., Angew. 133, 2021, 2700-2705.
3923. Kazuya Maruyama et al., Polym. Chem., 2019,10, 5304-5314.
3924. Kristin N. et al. Polyphosphoesters: An Old Biopolymer in a New Light (Pages: 191-241) in: Polymers for Biomedicine: Synthesis, Characterization, and Applications (Carmen Scholz, Ed.), 2017 John Wiley & Sons, Inc.
3925. Virginia R. Ward, Ph.D. thesis, University of Adelaide, Australia, 2012.
3926. Christopher M. Poteat et al., Angew. Chem. 132, 2020, 18814-18820.
3927. Xin Wang et al., Chem. Sci., 2020, 11, 11307-11314.
3928. Pierre-Antoine Nocquet, Ph.D. thesis, Université de Strasbourg, France, 2013.
3929. Xingpeng Chen, Jiaxi Xu; Progress in Chemistry 2017, 29, 181-197.
3930. Waqar Rizvi, Ph.D. thesis, City University of New York, 2018.
3931. Bohdan Biletskyi et al., Chem. Soc. Rev., 2021, Advance article, https://doi.org/10.1039/D0CS01396J.
3932. H. Merouani et al., Canadian J. Chem. 2013, https://doi.org/10.1139/cjc-2012-0521.
3933. Nils L. Ahlburg et al., Org. Lett. 2020, 22, 11, 4255–4260.
3934. Kenson Ambrose et al., Inorg. Chem. 2020, 59, 20, 15375–15383.

3935. J. Nicolas Rödel, Ph.D. thesis, Ludwig-Maximilians-Universität München 2008
3936. Steven Stanton, Ph.D. thesis, University of Bristol, UK, 2019.
3937. Alexander Sandvoß and Johannes M. Wiest, Chemistry 2021 27: 5871–5879.
3938. E. Quintanilla et al., in PATAI'S Chemistry of Functional Groups, Wiley, 2009.
3939. Paul R. Rablen, Chemistry 2020, 2(2), 347-360.
3940. Jeroen Dolfen, Ph.D. thesis, Ghent University, Belgium, 2017.
3941. Madison Taylor Timmons, M.Sc. thesis, University of Calgary, Canada, 2020.
3942. Jieun Choi et al., Molecules 2021, 26(6), 1703.
3943. Prof. Qinqin Shi et al., Angew. Chem. Intl. Ed. 60, 2021, 2924-2928.
3944. Anja Röder et al., Phys. Chem. Chem. Phys., 2020,22, 26241-26254.
3945. H. Babiz, M.Sc. thesis, Middle East Technical University, Turkey, 2010.
3946. Mingyang Ma, Younghwan Kwon; Eur. Polymer J. 123, 2020, 109414.
3947. Kondapi, Venkata Pavan Kumar; Ph.D. thesis, University of Alberta, 2016.
3948. Wendell Steven Grainger, Ph.D. thesis, Auburn University, U.S.A. 2015.
3949. Auvil, Tyler Jay; Ph.D. thesis, Ohio State University, 2014.
3950. Waqar Rizvi et al., Chemistry. 2019 Nov 18; 25(64): 14517–14521.
3951. M. Bierenstiel, Ph.D. thesis, Ludwig-Maximilians-Universität München, 2005
3952. Adriana Luque et al., Chemistry. 2021 Mar 8; 27(14): 4500–4516.
3953. Thomas James Carey, Ph.D. thesis, University of Colorado, 2018.
3954. Xinghan Li, M. Sc. thesis, University of Toronto, 2008.
3955. Jan Paternoga et al., J. Org. Chem. 2021, 86, 4, 3232–3248.
3956. Haseeb Mughal and Michal Szostak, Org. Biomol. Chem., 2021,19, 3274-3286.
3957. Jala Ranjith et al., Molecules 2021, 26(6), 1774.
3958. Yi-Yun Tsao, Ph.D. thesis, Texas A&M University, U.S.A. 2018.
3959. HaixinWang et al., Eur. Polymer J. 140, 2020, 109999.
3960. Hyun-Joon Ha, Molecules 2021, 26(6), 1525.
3961. Yang, Zheren Jim, Ph.D. thesis, Columbia University, U.S.A. 2017.
3962. Yujin Jang; Ph.D. thesis, North Carolina State University, U.S.A., 2021.
3963. Manoj K. Kesharwani et al., Organometallics 2020, 39, 17, 3146–3159.
3964. Yuko Otani et al., Chirality 32, 2020, 790-807.
3965. Yujin Jang and Vincent N. G. Lindsay, Org. Lett. 2020, 22, 22, 8872–8876.
3966. Licheng Wu et al., ACS Catal. 2021, 11, 3, 1774–1779.
3967. Lawal, N.S. et al.; Monatsh Chem 152, 275–285 (2021).
3968. Arturo Espinosa Ferao et al., Eur. J. Inorg. Chem. 2021, 2021, 348-353.
3969. Zongying Wang et al., Comput. Theor. Chem. 1150, 2019, 49-56.
3970. Christopher Michael Poteat, Ph.D. thesis, North Carolina State University, 2021
3971. Wilkinson, Christopher T., M.Sc. thesis, University of Huddersfield, UK, 2014
3972. Patrick Walther, Ph.D. thesis, Universität Stuttgart, Germany, 2020.
3973. Paternoga, Jan N., Ph.D. thesis, Johannes Gutenberg-Universität Mainz, 2021.
3974. Annika Matthes, Ph.D. thesis, Universität Potsdam, Germany, 2013.
3975. Kazuhiro Okamoto et al., J. Synthetic Org. Chem. 78 (2020) 1126-1137.
3976. Ching-Yeh Lin, M.Sc. Thesis, National Taiwan Normal University, Taipei, Taiwan, 2000.
3977. W. Disadee, Ph.D. Thesis, Chiba University, Japan, 2006.

3978. J.A. Burkhard, Ph.D. Thesis, ETH Zurich, Switzerland, 2011.
3979. H. Babiz, M.Sc. Thesis, Middle East Technical University, Turkey, 2010.
3980. B. Sirjean, Ph.D. Thesis, Institut National Polytechnique de Lorraine E.N.S.I.C., France, 2007.
3981. Nelson Y. S. Lam et al. *J. Am. Chem. Soc.* 2022, 144, 6, 2793–2803.
3982. M. Jung, V.N. G. Lindsay; *J. Am. Chem. Soc.* 2022, 144, 11, 4764–4769.
3983. Huan Tran et al. J. Phys. Chem. Lett. 2022, 13, 21, 4778–4785.
3984. S.S. Dindorkar, A. Yadav; Comput. Theor. Chemistry, May 2022, 113676.
3985. Jeonguk Kweon et al. J. Am. Chem. Soc. 2022, 144, 4, 1872–1880.
3986. Wen Zhang et al. Chem. Soc. Rev., 2021,50, 9430-9442.
3987. Tomsmith O. Unimuke et al. ACS Omega 2022, 7, 16, 13704–13720.
3988. Luc-Sy Tran et al. Progress Ener. Combust. Sci. 92, 2022, 101019.
3989. Anshul Yadav et al.Chemical Physics Volume 562, 1 October 2022, 111629.
3990. Baljit Kaur, Palwinder Singh; Bioorganic Chemistry 125, 2022, 105862.
3991. Xiaoyang Lei et al. Combustion and Flame Volume 237, March 2022, 111881.
3992. Kien P. Malarney et al. Org. Biomol. Chem., 2021,19, 8425-8441.
3993. Khursan, S.L., Ismagilova, A.S., Ziganshina, F.T. et al. Constructing a Complete Set of Homodesmic Reactions Using the Depth-First Search Procedure. Russ. J. Phys. Chem. **95**, 1386–1393 (2021).
3994. M.P. Confer et al. ChemPhysChem 23, ,2022, e202200133.
3995. C.M. Poteat,V.N.G. Lindsay; Org. Lett. 2021, 23, 16, 6482–6487.
3996. Luning Tang et al. Org. Lett. 2022, 24, 17, 3259–3264.
3997. Joseph M. Parr et al. *Chem. Sci.*, 2023, 14, 1590-1597.
3998. S. Sinhababu, N.P. Mankad; Organometallics 2022, 41, 15, 1917–1921.
3999. Yan Jiang et al. Nanoscale Adv., 2021**,** 3, 4079-4088.
4000. Craig Hardy et al. Polym. Chem., 2023, 14, 623-632.
4001. D. Núñez-Villanueva and C.A. Hunter; Org. Biomol. Chem., 2022**,** 20, 8285.
4002. B.M. Coia et al. J. Polymer Sci. 60, 2022, 3391-3403.
4003. Y.Valadbeigi, R. Taheri, Comp. Theor. Chem. 1222, 2023, 114076.
4004. Jala Ranjith and Hyun-Joon Ha, in More Synthetic Approaches to Nonaromatic Nitrogen Heterocycles, Volume I, Ana Maria M.M. Faisca Phillips (Eds), Ch. 15, John Wiley & Sons, 2022.
4005. Fareed Bhasha Sayyed et al. Org. Process Res. Dev. 2022, 26, 1, 183–194.
4006. N. Srivastava, H.-J.Ha; Asian J. Org. Chem. 11, 2022 e202100567.
4007. A. Akhmetyanova and A. Ismagilova, "Development and Automation of an Algorithm for Determining the Basis of Homodesmic Reactions," 2021 3rd International Conference on Control Systems, Mathematical Modeling, Automation and Energy Efficiency (SUMMA), Lipetsk, Russian Federation, 2021, pp. 27-31.
4008. Srivastava, N., Ha, H. J., J. Vis. Exp. (184), e63705, doi:10.3791/63705 (2022).
4009. Akhmetyanova, A., Ismagilova, A., Ziganshina, F. (2022). Mathematical Modeling of Cyclic Chemical Compounds. In: Smirnov, N., Golovkina, A. (eds) Stability and Control Processes. SCP 2020. Lecture Notes in Control and Information Sciences - Proceedings. Springer, Cham.
4010. Jasper Tyler, Ph.D. thesis, University of Bristol, 2022.

4011. Roger Machín Rivera, Ph.D. thesis, North Carolina State University, 2022.
4012. Wujie Wang, Ph.D. thesis, Massachusetts Institute of Technology, 2022.
4013. Nuwan Asanka Pannilawithana, Ph.D. thesis, Marquette University, 2021.
4014. Yujin Jang, Ph.D. thesis, North Carolina State University, 2021.
4015. Christopher Michael Poteat, Ph.D. thesis, North Carolina State University, 2021.
4016. Nils Frank, M.Sc. thesis, University of Oxford, 2022.
4017. J.N. Paternoga, Ph.D. thesis, Johannes Gutenberg-Universität Mainz, 2021.
4018. Matthew Charles O'Reilly, US patent, application US17/574,998; 2022.
4019. S. Sun et al., Chem 9, P2128-2143, 2023.
4020. Y. Deng et al., Macromolecular Rapid Commun. 44, 2023, 2200941.
4021. Q.-B. Zhang et al., Adv. Synth. Catalys. 365, 2023, 3556-3571.
4022. W. Ma et al., J. Am. Chem. Soc. 2023, 145, 26611–26622.
4023. E. Matador et al., J. Am. Chem. Soc. 2023, 145, 27810–27820.
4024. K. Wang et al., Angew. Chemie 135, 2023, e202307249.
4025. Q. Li et al., J. Am. Chem. Soc. 2023, 145, 7580–7591.
4026. B.M. Coia et al., J. Phys. Chem. A 2023, 127, 5005–5017.
4027. Yadav, A., Silicon 15, 1847–1857 (2023).
4028. U. Yolsal et al., ACS Catal. 2024, 14, 1050–1074.
4029. Daniel Del Angel Cruz et al., Phys. Chem. Chem. Phys. 2023, 25, 27276-27292.
4030. T. Hansen et al., Chemistry – A European Journal 29, 2023, e202301308.
4031. Wijitra Meelua et al., Phys. Chem. Chem. Phys., 2023,25, 8767-8778.
4032. D. Lebedeva et al., Green Chem., 2024, DOI: 10.1039/D4GC01257G.
4033. A. Toland et al., J. Phys. Chem. A 2023, 127, 10709–10716.
4034. Joseph M. Parr, Mark R. Crimmin, Chem. Sci., 2023, 14, 11012-11021.
4035. G. Jhaa et al., J. Chem. Inf. Model. 2024, 64, 178–188.
4036. X. Liu et al., Cell Rep. Phys. Sci. 5, 101910, 2024.
4037. L.-C. Cheng et al., Org. Biomol. Chem., 2024,22, 2554-2557.
4038. Mingtao Zhou, Nikos Hadjichristidis, Angew. Chemie 2024, https://doi.org/10.1002/ange.202403527
4039. P. Kumar et al., Angew. Chemie 135, 2023, e202305005.
4040. Z. Ding et al., Macromolecules 2024, 57, 98–109.
4041. Rosario C. Sausa, Iskander G. Batyrev, J. Phys. Chem. C 2024, 128, 927–940.
4042. J. Mi et al., Sustainable Energy Fuels, 2023,7, 5374-5384.
4043. Loc T. Nguyen et al., Phys. Chem. Chem. Phys., 2023,25, 19126-19138.
4044. Ya-Chu Chan, David J. Nesbitt, Phys. Chem. Chem. Phys., 2024,26, 3081-3091.
4045. O. Stephen Ojo et al., Org. Biomol. Chem., 2023, 21, 6738-6742.
4046. W. Cai et al., Advanced Synthesis and Catalysis., 2024 https://doi.org/10.1002/adsc.202400263.
4047. J. Choi et al., Materials 2023, 16(21), 6995.
4048. E. Kersten et al., Macromolecular Chemistry and Physics 224, 2023, 2300097.
4049. Chen, LY., Li, YP. (2023). Machine Learning Applications in Chemical Kinetics and Thermochemistry. In: Qu, C., Liu, H. (eds) Machine Learning in Molecular Sciences. Challenges and Advances in Computational Chemistry and Physics, vol 36. Springer.

4050. Lebedeva, Daria, Ph.D. Thesis, Stockholm University, 2024.
4051. Simon Kolb, Ph.D. Thesis, Albert-Ludwigs University of Freiburg, 2023.
4052. Qing-Bao Zhang et al., Chemistry – A European Journal 2024, https://doi.org/10.1002/chem.202401501.
4053. Hatice Seher Korkmaz, M.Sc. Thesis, BILKENT UNIVERSITY, Turkey, 2023.
4054. Alena Häfner, Ph.D. Thesis, JULIUS-MAXIMILIANS-UNIVERSITÄT, WÜRZBURG, 2023.

B Galabov, **T Dudev**, S Ilieva, JR Durig, "Creation of intensity theory in vibrational spectroscopy: Key role of ab initio quantum mechanical calculations" *International Journal of Quantum Chemistry* **70** (1998) 331-339.

4055. B. Sivaraman et al., Phys. Chem. Chem. Phys., 2011,13, 421-427.
4056. W.O. George et al., J. Mol. Struct. 550–551, 2000, 281-296.
4057. Beata W. Domagalska et al., Computers & Chemistry 24, 2000, 359-367.
4058. Х. Ш. Абдулов, Расчет ИК-спектров ориентированных и неориентированных полимеров, Дис. Канд. физ.-мат. наук, Душанбе, 2009.

V. Koleva, **T. Dudev**, I. Wawer, "1 H and 13 C NMR study and AM1 calculations of some azobenzenes and N-benzylideneanilines: effect of substituents on the molecular planarity", *Journal of Molecular Structure* **412** (1997) 153-159.

4059. Mehmet Cinara et al., Spectrochimica Acta Part A 122 (2014) 682–689.
4060. Linyan Wang et al., Magnetic Resonance in Chemistry 53 (2015) 520–525.
4061. Asit K. Chakraborti et al., Tetrahedron Letters 45, October 2004, 7641-7644.
4062. Helmi Neuvonen et al., J. Org. Chem. 2006, 71, 8, 3141–3148.
4063. I. Kraicheva et al., Eur. J. Medicinal Chem. 44, 2009, 3363-3367.
4064. Shaw-Tao Lin et al., Tetrahedron 56, December 2000, 9619-9623.
4065. Wei-Dong Wang and James H. Espenson, Organometallics 1999, 18, 5170–5175
4066. Y.M. Issa et al., Spectrochimica Acta Part A 74, 2009, 902-910.
4067. Antonín Lyčka, Annu. Rep. NMR Spectroscopy 42, 2000, 1-57.
4068. Helmi Neuvonen et al., J. Mol. Struct. THEOCHEM 815, 2007, 95-104.
4069. Sun-Young Han et al., (2003) J. Enzyme Inhibition Med. Chem. 18:3, 279-283.
4070. Vildan Güner & Sevgi Bayari (2002) Spectroscopy Letters, 35:1, 83-98.
4071. Mehmet Cinar et al., Spectrochimica Acta Part A 105, 2013, 80-87.
4072. Chao-tun Cao et al., Chinese Journal of Chemical Physics 31, 45 (2018).
4073. Hynek Balcar et al., Collect. Czech. Chem. Commun. 2000, 65, 203-215.
4074. V. Proks and M. Holík, Collect. Czech. Chem. Commun. 2004, 69, 1566-1576.
4075. Bamidele Joseph Okoli, et al., Antioxidants 2018, 7(9), 113.
4076. Vladimír Proks, J. Mol. Struct. THEOCHEM 725, 2005, 69-73.

4077. V. Güner et al., J. Mol. Struct., 526, 2000, 151-157.
4078. Manuel A. Leiva et al., Spectroscopy Letters, 35:4, 611-624.
4079. H.-L. Peng, Ph.D. thesis, Case Western Reserve University, U.S.A. 2007.
4080. Guo Yanshen et al., Acta Chimica 2002, 02, 228 – 233.
4081. Chuan-Chen Lee et al., J. Chin. Chem. Soc. 53, 2006, 915-921.
4082. Gamal A. Gohar, J. Chem. Res. 2003 (2003) 188-190.
4083. Khor Ke Xin, B.Sc. thesis, Universiti Tunku Abdul Rahman, Malaysia, 2011.
4084. Bamidele J. Okoli et al., (2019) In: Ramasami P., Gupta Bhowon M., Jhaumeer Laulloo S., Li Kam Wah H. (eds) Chemistry for a Clean and Healthy Planet. ICPAC 2018. Springer, Cham.
4085. Okoli Bamidele Joseph et al., Asian J. Pharmaceutics 2018, 12, S1-S10.
4086. M. Yamaguchi, in Nuclear Magnetic Resonance: Volume 25 (G.A. Webb, Ed.) Royal Society of Chemistry, 2007.
4087. Melle Elhassasna Kawther, M.Sc. thesis, Université du Guelma, Algeria, 2010.
4088. M.A.L. Guzman, Ph. D. Thesis, Universidad de Chile, Santiago, Chile, 2002.
4089. Zhong-Heng Yu, QUESTIONING THE FUNDAMENTAL PRINCIPLES OF ORGANIC CHEMISTRY, Chapter 2, http://blog.sciencenet.cn/home.php?mod=space&uid=94786&view=yuzh, Beijing, 2012.
4090. Z.-H. Yu, Z.-Q. Xuan, Y.-S. Guo, T.-X., X.-Q. Peng, T.-X. Wang, X.N. Xiang-Lin, CHEM. J. CHIN. UNIV. 22, 122, 2001.

Boris Galabov, Petia Bobadova-Parvanova, **Todor Dudev**, "Interpretation of carbonyl stretching band intensities in the infrared spectra: an ab initio MO study", *J. Mol. Struct*. **406** (1997) 119-125.

4091. I.M.M. Oliveira et al., Journal of Molecular Structure 1099 (2015) 226–231.
4092. Wagner E. Richter et al., Phys. Chem. Chem. Phys. 2016,18, 17575-17585.
4093. W.E. Richter, Ph.D. Thesis, Universidade Estudial de Campinas, Brazil, 2016.
4094. Jens Dreyer and Andreas Kummrow, J. Am. Chem. Soc. 2000, 122, 2577–2585
4095. E. Meaurio et al., Macromolecules 2009, 42, 15, 5717–5727.
4096. Andrew M. Moran et al., J. Chem. Phys. 118, 1347 (2003).
4097. Sergey Vasenkov and Heinz Frei, J. Phys. Chem. A 2000, 104, 18, 4327–4332.
4098. Jens Dreyer et al., J. Phys. Chem. B 2003, 107, 24, 5967–5985.
4099. D. Aureau et al., J. Phys. Chem. C 2009, 113, 32, 14418–14428.
4100. R.N.S. Santiago et al., J. Mol. Struct., 1171, 2018, 815-826.
4101. V.H. Rusu et al., J. Mol. Struct. 993, 2011, 86-90.
4102. N.B. de Lima, M.N. Ramos; J. Mol. Struct. 1008, 2012, 29-34.
4103. Renata X. D. Nascimento et al., Int. J. Quantum Chem. 112, 2012, 3147-3151.
4104. R.N.S. Santiago, Ph.D. thesis, Universidade Federal do Ceara, Brazil, 2018.

B. Galabov, S. Ilieva, B. Hadjieva and **T. Dudev**, "N–H stretching frequencies and the conformation of substituted ureas: an ab initio MO study", *J. Mol. Struct*. **407** (1997) 47-51.

4105. Wang, Jianping, et al. Journal of Chemical Physics 143 (2015): 185102.
4106. Wang, Jianping et al. Journal of Physical Chemistry B 119 (2015): 15451-15459.
4107. Loeffler, J.R. et al., J. Comput. Aided Mol. Des. (2016) 30: 391.
4108. Ewa Daniela Raczyńska et al., Chem. Rev. 2005, 105, 10, 3561–3612.
4109. Frédéric Lortie et al., Chem. Eur. J. 9, 2003, 3008-3014.
4110. Christopher Baddeley et al., J. Org. Chem. 2007, 72, 19, 7270–7278.
4111. Frédéric Lecomte et al., Phys. Chem. Chem. Phys., 2003,5, 3120-3125.
4112. R. Keuleers et al., J. Phys. Chem. A 2000, 104, 25, 5946–5954.
4113. János Mink et al., Applied Spectroscopy Reviews, 45:4, 274-326.
4114. Shijing Xia, Ph.D. thesis, Ohio State University, U.S.A. 2008.
4115. P. Baddeley, M. Sc. Thesis, Ohio State University, 2009.
4116. S. Xia, Ph.D. Thesis, Ohio State University, USA, 2008.

T. Dudev, P. Bobadova-Parvanova, D. Pencheva and B. Galabov, "Molecular geometry, vibrational frequencies, infrared intensities and C≡N effective bond charges in a series of simple nitrile compounds: HF/6–31+ G (d, p) molecular orbital study", *Journal of Molecular Structure* **436** (1997) 427-433.

4117. D. Begue et al., J. Phys. Chem. A 2005, 109, 20, 4611–4616.
4118. Justin M. Rhinehart et al., J. Phys. Chem. B 2012, 116, 35, 10522–10534.
4119. M.K. Georgieva, E.A. Velcheva; Intl. J. Quantum. Chem. 106, 2006, 1316-1322
4120. Bogusław Buszewski et al., J. Separation Sci., 33, 2010, 2060-2068.
4121. Wei Lin and Stewart E. Novick, J. Mol. Struct. 243, 2007, 32-36.
4122. V.H. Rusu et al., J. Mol. Struct., 993, 2011, 86-90.
4123. R. Bharathi and N. Santhi, J. Theor. Comp. Chem. 16, 1750057 (2017).
4124. Malose J. Mphahlele et al., J. Mol. Struct. 1238, 2021, 130447.
4125. С. С. Стоянов, Дисертация, ИОХЦФ, БАН, 2009.

T Dudev, B Galabov, "Ab initio calculations of Raman intensity parameters and geometry of polyynes and polyynenitriles" *Spectrochimica Acta Part A* **53** (1997) 2053-2059

4126. Roman Dembinski et al., J. Am. Chem. Soc. 2000, 122, 5, 810–822.
4127. Thomas Gibtner et al., Chem. Eur. J. 8, 2002, 408-432.
4128. Vladimir A. Basiuk, Spectrochimica Acta Part A 55, 1999, 2771-2782.
4129. Pual J. Low and Michael I. Bruce, in Advances in Organometallic Chemistry, Vol. 48 (Robert C. West, Anthony F. Hill, Eds.), Academic Press, 2001.
4130. C. Agisilaos, Ph.D. Thesis, University of Patras, Greece, 2011.
4131. H. Tabata, Ph. D. Thesis, Kobe University, 2007.

S Ilieva, M Krusteva, **T Dudev**, B Galabov, T Gounev, JR Durig, "Effective bond charges from infrared intensities: ab initio calculations" *Journal of Molecular Structure* **377** (1996) 75-79.

4132. M Penza et al 2009 J. Phys. D: Appl. Phys. 42 072002.
4133. V.H. Rusu et al., J. Mol. Struct. 993, 2011, 86-90.

B Galabov, **T Dudev**, S Ilieva, "Effective bond charges from experimental IR intensities" *Spectrochimica Acta Part A* **51** (1995) 739-754.

4134. V. B. Kazansky et al., J. Phys. Chem. B 2006, 110, 15, 7975–7978.
4135. Martin Jetzki et al., J. Chem. Phys. 120, 11775 (2004).
4136. H. Winterling et al., Phys. Chem. Chem. Phys., 2001,3, 4592-4599.
4137. V.H. Rusu et al., J. Mol. Struct. 993, 2011, 86-90.
4138. Alberto Milani et al., J. Mol. Struct. 1009, 2012, 130-140.
4139. A.M. Coatsa, D.C. McKean; Spectrochimica Acta Part A 61, 2005, 455-469.
4140. Batsanov S., Batsanov A. (2012) Chemical Bond. In: Introduction to Structural Chemistry. Springer, Dordrecht.
4141. M. Jetzki, Ph. D. Thesis, Universitat Göttimgen, Cuvillier Verlag Göttimgen, 2005.
4142. Субботина ИР, "Новые подходы к использованию ИК-спектроскопии для изучения механизма превращений углеводородов на кислотных гетерогенных катализаторах", Диссертация (доктор химических наук), Москва, 2010.

S Metsov, **T Dudev**, V Koleva, "Infrared and NMR study of some 2-styrylindolium dyes", *Journal of Molecular Structure* **350** (1995) 241-246.

4143. Zhiyong Li et al., Biomaterials 34, 2013, 6473-6481.
4144. Na Li et al., Bioorganic & Medicinal Chemistry 27, 2019, 2845-2856.
4145. Alexis Perry, Org. Biomol. Chem., 2019,17, 4825-4834.
4146. Lowe, Jonathan; Ph.D. thesis, Northumbria University, UK, 2016.

B Galabov, **T Dudev**, S Ilieva, "Interpretation of vibrational absorption intensities: effective bond charges from rotation free atomic polar tensors" *Spectrochimica Acta Part A* **49** (1993) 373-385.

4147. W. F. Murphy et al., J. Raman Spectroscopy 26, 1995, 763-770.
4148. V.H. Rusu et al., J. Mol. Struct. 993, 2011, 86-90.

B Galabov, S Ilieva, **T Dudev**, HV Phan, JR Durig, "Interpretation and prediction of vibrational absorption intensities: methylethyl ether and diethyl ether" *Spectrochimica Acta Part A* **49** (1993) 2093-2103.

4149. Keijiro Taga et al., J. Mol. Struct. 788, 2006, 159-175.

4150. Shubhra Sarkar et al., Spectrochimica Acta Part A 213, 2019, 361-369.

R. Ionov, **T. Dudev**, "Raman and infrared study of amorphous SeTe/CdSe superlattices" *Applied Physics A* **55** (1992) 203-206.

4151. Svoboda, Roman et al., Journal of Alloys and Compounds 644 (2015): 40-46.
4152. Gurevits, Jelena, et al., MRS Proceedings. Vol. 1707. Cambridge University Press, 2014.
4153. Yuval Golan et al., J. Phys. Chem. 1996, 100, 6, 2220–2228.
4154. Roman Svoboda et al., J. Non-Crystalline Solids 357, 2011, 2163-2169.
4155. Roman Svoboda, Acta Materialia 61, 2013, 4534-4541.
4156. Wu, Yi-Chyi, Ph.D. thesis, University of California, Berkeley, 1996.
4157. Keiji Tanaka, Encyclopedia of Nanoscience and Nanotechnology (H.S. Nalwa, Ed.) Vol. 7, American Scientific Publishers, 2004; pp. 629-640.
4158. R. Svoboda and J. Malek, Sci. Pepers Univ. Pardubice Ser. A 18 (2012) 47-65.
4159. Roman Svoboda et al., Sci. Pepers Univ. Pardubice Ser. A 17 (2011) 97-128.
4160. Gurevits, J. et al.; MRS Online Proceedings Library 1707, 13–18 (2014).

G Georgieva, **T Dudev**, B Galabov, JR Durig, "Vibrational intensity analysis of 1, 2-dichloroethane and 1-chloropropane" *Vibrational Spectroscopy* **3** (1992) 9-21.

4161. A. Martucci et al., Microporous Mesoporous Materials 151, 2012, 358-367.
4162. Robert J. Sabharwal et al., J. Phys. Chem. B 2007, 111, 25, 7267–7273.
4163. Y.O. Aochi, W.J. Farmer, Environ. Sci. Technol. 1995, 29, 7, 1760–1765.
4164. Xiaoyan Xiang et al. Journal of Analytical Methods in Chemistry; Volume 2023 | Article ID 1894505 | https://doi.org/10.1155/2023/1894505

Angelina Angelova, Jordan G Petrov, **Todor Dudev**, Boris Galabov, "Infrared spectra of Langmuir—Blodgett multilayers of docosylammonium phosphate", *Colloids and surfaces* **60** (1991) 351-368.

4165. Joe Forth et al., Langmuir, 2015, 31, 9312–9324.
4166. Victor M. Starov (Ed.) Nanoscience: Colloidal and Interfacial Aspects, CRC Press, 2017.
4167. M. Bardosova et al., Langmuir 1995, 11, 4, 1273–1276.
4168. P. Ganguly et al., Langmuir 1997, 13, 20, 5433–5439.
4169. Robin H. A. Ras et al., Chem. Commun., 2005, 4095-4097.
4170. V.I. Kovalchuk, D. Vollhardt; Adv. Coll. Interface Sci. 114–115, 2005, 267.
4171. Serge Bourbigot et al., 31 (2012) 112-130.
4172. V.I. Kovalchuk et al., Adv. Coll. Interface Sci. 168, 2011, 114-123.
4173. Annette Murphy et al., Colloids and Surfaces A 102, 1995, 1-19.

4174. V. I. Kovalchuk, E. K. Zholkovskiy, M. P. Bondarenko, D. Vollhardt; in Nanoscience: Colloidal and Interfacial Aspects (Victor M. Starov, Ed.) CRC Press, 2010.

T Dudev, T Kamisuki, N Akamatsu, C Hirose, "Transient resonance coherent anti-Stokes Raman scattering spectra of ion radicals of all-trans-1, 4-diphenyl-1, 3-butadiene" *Journal of Physical Chemistry* **95** (1991), 4999-5002.

4175. Maurer, J. et al.; J Solid State Electrochem 9, 738–749 (2005).
4176. J. Oberlé et al., J. Phys. Chem. 1996, 100, 24, 10179–10186.
4177. Takakazu Nakabayashi et al., J. Phys. Chem. A 2001, 105, 38, 8605–8614.
4178. María S. Galletero et al., J. Phys. Chem. B 2003, 107, 5, 1135–1141.
4179. Jin-Yeol Kim et al., Chemical Physics Letters, 276, 1997, 418-422.
4180. Yutaka Sasaki, J. Chem. Phys. 110, 9179 (1999).
4181. Rullière C., Amand T., Marie X. (1998) Spectroscopic Methods for Analysis of Sample Dynamics. In: Rullière C. (eds) Femtosecond Laser Pulses. Springer, Berlin, Heidelberg.
4182. J. Oberlé et al., J. Photochem. Photobiol. A: 105, 1997, 217-223.
4183. Jin-Yeol Kim et al., Synthetic Metals 129, Issue 3, 2002, 235-238.
4184. J. Oberle, E. Abraham, A. Ivanov and G. Jonusauskas, "Picosecond Cars and Transient Absorption Studies of Monophotonic Ionization of Diphenylbutadiene and Trans-stilbene in Solution," EQEC'96. 1996 European Quantum Electronic Conference, 1996, pp. 194-194.
4185. Masao Takayanagi; Hiromi Okamoto; Spectrosc. Res. 1997, 46, 131-145.
4186. Mizuho Kajita et al. Phys. Chem. Chem. Phys., 2022,24, 5411-5418

T Kamisuki, **T Dudev**, C Hirose, "Photoionization of diphenylhexatriene and diphenylbutadiene ion radicals in various polar solvents by using time-resolved resonance CARS" *Journal of Physical Chemistry* **95** (1991), 5845-5849.

4187. J. Oberlé et al., J. Phys. Chem. 1996, 100, 24, 10179–10186.
4188. Takakazu Nakabayashi et al., J. Phys. Chem. A 2001, 105, 38, 8605–8614.
4189. F. Schael, H.-G. Löhmannsröben; Chem. Phys. 206, 1996, 193-210.
4190. J.-M. Funk et al., Applied Spectroscopy 52, 1541-1553 (1998).
4191. Yutaka Sasaki, J. Chem. Phys. 110, 9179 (1999).
4192. J.-M. Funk et al., J. Raman Spectroscopy 31, 2000, 743-753.
4193. Juan Carlos del Valle et al., J. Phys. Chem. B 1999, 103, 43, 9350–9355.
4194. J.-M. Funk, A. Materny; J. Raman Spectroscopy 29, 1998, 1071-1078.
4195. J.-M. Funk et al., (2003) Spectroscopy Letters, 36:1-2, 1-23.
4196. J. Oberlé et al., J. Photochem. Photobiol. A 105, 1997, 217-223.
4197. Masao Takayanagi; Hiromi Okamoto; Spectrosc. Res. 1997, 46, 131-145.
4198. R.B. Cundall, in PHOTOCHEMISTRY (D. Bryce-Smith, A. Gilbert, Eds.), Atheneaum Press, 1993, Ch. 1, pp. 3-49.

B Galabov, **T Dudev**, JR Durig, WJ Orville-Thomas, "Computations in vibrational intensity spectroscopy" *Journal of Molecular Structure* **173** (1988) 111-128.

4199. R. Superfine et al., Chem. Phys. Lett. 172, 1990, 303-306.
4200. D. L. Gerrard and J. Birnie, Anal. Chem. 1990, 62, 12, 140–150.
4201. U. Hohm et al., J. Mol. Struct. 1054–1055, 2013, 282-292.
4202. J.D. Miller et al., Colloids and Surfaces A 154, 1999, 137-147.
4203. A. Kindness et al., J. Mol. Struct. 224, 1990, 363-384.
4204. Xiao-Hua Hu et al., J. Phys. Chem. C 2019, 123, 24, 15071–15086.
4205. Mason Gardner, Honors thesis, University of Mississippi, 2021.
4206. R. Superfine, Ph.D. Thesis, University of California, USA, 1991.
4207. J. V. Jouanne, D. Koschel, Gmelin Handbook of Inorganic and Organometallic Chemistry, 8th Ed., Bromine, Suppl. Vol. Springer, Berlin, 1990.

B Galabov, **T Dudev**, JR Durig, "Bond properties and molecular conformation from vibrational intensity analysis" *Croatica Chemica Acta* **61** (1988), 569-587.

4208. S.D. Williams et al., J. Quant. Spectrosc. Rad. Transfer 129, 2013, 298-307.
4209. S. Lopez-Zamora et al., Chem. Engin. Sci. 192, 2018, 788-802.
4210. Sandra Milena López Zamora, Ph.D. thesis, Universidad Nacional de Colombia, Medellín, Colombia 2018.
4211. Asim Kumar Das et al. J. Mol. Struct.1245, 2021, 131126.

T. Dudev, B. Galabov and W.J. Orville-Thomas, "Interpretation of infrared intensities of some simple hydrides", *Journal of Molecular Structure* **157** (1987) 289-294.

4212. Czarnecki, Mirosław Antoni, et al., Chemical Reviews 115 (2015): 9707-9744.
4213. Yoshisuke Futami et al., J. Mol. Struct. 1018, 2012, 102-106.
4214. Willis B. Person; Kuhalim Kubulat; J. Mol. Struct. 224, 1990, 225-244.
4215. J. V. Jouanne, D. Koschel, Gmelin Handbook of Inorganic and Organometallic Chemistry, 8th Ed., Bromine, Suppl. Vol. Springer, Berlin, 1990.

B. Galabov, **T. Dudev** and W.J. Orville-Thomas, "Interpretation and prediction of vibrational intensities in infrared spectra: fluorinated methanes", *Journal of Molecular Structure* **145** (1986) 1-13.

4216. Mirosław Antoni Czarnecki et al., Chem. Rev., 2015, 115, 9707–9744.
4217. Khlifi, M. et al., J. Mol. Struct. 174, 1995, 116-122.
4218. M.M.C. Ferreira and Elisabete Suto, J. Phys. Chem. 1992, 96, 22, 8844–8849.
4219. Dusan Papousek et al., J. Phys. Chem. 1995, 99, 42, 15387–15395.
4220. Yoshisuke Futami et al., J. Mol. Struct. 1018, 2012, 102-106.
4221. Li Zhou et al., Planetary and Space Science, 57, 2009, 830-835.
4222. A. Tabyaoui et al., J. Raman Spectroscopy 25, 1994, 255-260.

4223. Kwan Kim, Cheol Woo Park; J. Mol. Struct. 161, 1987, 297-309.
4224. Kim, Kwan et al.; Bull. Korean Chem. Society 10, 161-167, 1989.
4225. Yongxuan Zhu, M.Sc. thesis, Lamar University, U.S.A. 2005.
4226. Thomas J. Cronin, Ph.D. thesis, University of Akron, U.S.A., 1999.
4227. Bolotova, Irina; Ph.D. thesis, ETH Zurich, 2017.
4228. Christophorou L.G., Olthoff J.K. (2004) Physics of Atoms and Molecules. Springer, Boston, MA.
4229. Cheol Ho Choi; Kwan Kim; J. Mol. Struct. 269, 1992, 309-327.

B. Galabov, **T. Dudev**, B. Nikolova and W.J. Orville-Thomas, "Predicted infrared intensities of diacetylene and 1,3-pentadiyne" *Journal of Molecular* Spectroscopy **120** (1986) 276-283.

4230. CRAW JS; et al. J. MOL. STRUCT.-THEOCHEM 60, 69, 1989.
4231. SUZUKI I; ATAKA S; TASUMI M, J. MOL. STRUCT. 171, 1, 1987.
4232. M. Khlifi, P. Paillous, C. Delpesh, J. Mol. Spetrosc. 174 (1995) 116.
4233. P. J. Low, M. I. Bruce, in Advances in Organometallic Chemistry, v. 48, Academic Press, Ed. R. West, A. F. Hill., San Diego, 2001, p.71.

B Galabov, **T Dudev**, C Lozanova, WJ Orville-Thomas, "Infrared intensities. an MO study of the transferability of bond polar parameters" *Journal of Molecular Structure* **129** (1985), 27-33.

4234. Stefanova, V. et al.; Veget Hist Archaeobot 15, 333–343 (2006).
4235. Shinoda Hiroyuki, Bull. Chem. Soc. Jpn. 60 (1987) 2355-2360.
4236. L.J. Duarte; Roy E. Bruns; J. Phys. Chem. A 2020, 124, 17, 3407–3416.