

1. Ghafouri, H.; Lazar, T.; Del Conte, A.; Ku, L.G.T.; Aspromonte, M.C.; Bernadó, P.; Chaves-Arquero, B.; Chemes, L.B.; Clementel, D.; Cordeiro, T.N.; Elena-Real, C.A.; Feig, M.; Felli, I.C.; Ferrari, C.; Forman-Kay, J.D.; Gomes, T.; Gondelaud, F.; Gradinaru, C.C.; Ha-Duong, T.; Head-Gordon, T.; Heidarsson, P.O.; Janson, G.; Jeschke, G.; Leonardi, E.; Liu, Z.H.; Longhi, S.; Lund, X.L.; Macias, M.J.; Martin-Malpartida, P.; Mercadante, D.; Mouhand, A.; Nagy, G.; Nugnes, M.V.; Pérez-Cañadillas, J.M.; Pesce, G.; Pierattelli, R.; Piovesan, D.; Quaglia, F.; Ricard-Blum, S.; Robustelli, P.; Sagar, A.; Salladini, E.; Séricourt, L.; Sibille, N.; Teixeira, J.M.C.; Tsangaris, T.E.; Varadi, M.; Tompa, P.; Tosatto, S.C.E.; Monzon, A.M., PED in 2024: improving the community deposition of structural ensembles for intrinsically disordered proteins, *Nucleic Acids Res.*, 2024, 52, D536–D544. DOI: 10.1093/nar/gkad947 (IF 19.16)
2. Di Carluccio C., Cerofolini L., Moreira M., Rosu F., Padilla-Cortés L., Gheorghita G.R., Xu Z., Santra A., Yu H., Yokoyama S., Gray T.E., St. Laurent C.D., Manabe Y., Chen X., Molecular Insights into O-Linked Sialoglycans Recognition by the Siglec-Like SLBR-N (SLBRUB10712) of *Streptococcus gordonii*, *ACS Central Sci.*, 2024, 10 (2), pp. 447 – 459, DOI: 10.1021/acscentsci.3c01598 (IF 18.2)
3. Cosottini L., Geri A., Ghini V., Mannelli M., Zineddu S., Di Paco G., Giachetti A., Massai L., Severi M., Gamberi T., Rosato A., Turano P., Messori L., Unlocking the Power of Human Ferritin: Enhanced Drug Delivery of Aurothiomalate in A2780 Ovarian Cancer Cells, *Angewandte Chemie - International Edition*, 2024, 63 (40), art. no. e202410791, DOI: 10.1002/anie.202410791 (IF 16.1)
4. Schiavina M., Bracaglia L., Rodella M.A., Kümmerle R., Konrat R., Felli I.C., Pierattelli R., Optimal <sup>13</sup>C NMR investigation of intrinsically disordered proteins at 1.2 GHz, *Nat. Protoc.*, 2024, 19 (2), pp. 406 - 440, DOI: 10.1038/s41596-023-00921-9 (IF 14.8)
5. Garcia-Vello P., Tytgat H.L.P., Elzinga J., Van Hul M., Plovier H., Tiemblo-Martin M., Cani P.D., Nicolardi S., Fragai M., De Castro C., Di Lorenzo F., Silipo A., Molinaro A., de Vos W.M., The lipooligosaccharide of the gut symbiont *Akkermansia muciniphila* exhibits a remarkable structure and TLR signaling capacity, *Nature Communications*, 2024, 15 (1), art. no. 8411, DOI: 10.1038/s41467-024-52683-x (IF 14.7)
6. Mao J., Jin X., Shi M., Heidenreich D., Brown L.J., Brown R.C.D., Lelli M., He X., Glaubitz C., Molecular mechanisms and evolutionary robustness of a color switch in proteorhodopsins, *Sci. Adv.*, 2024, 10 (4), DOI: 10.1126/sciadv.adj0384 (IF 13.6)
7. Staderini T., Bigi A., Lagrève C., Marzi I., Bemporad F., Chiti F. Biophysical characterization of the phase separation of TDP-43 devoid of the C-terminal domain. DOI: 10.1186/s11658-024-00615-4. *Cellular and Molecular Biology Letters*, 29, 104, (IF 8.1).

8. Niccoli L, Casano G, Menzildjian G, Yulikov M, Robinson T, Akrial SE, Wang Z, Reiter C, Porea A, Siri D, Venkatesh A, Emsley L, Gajan D, Lelli M, Ouari O, Lesage A. Efficient DNP at high fields and fast MAS with antenna-sensitized dinitroxides. *Chem Sci*. 2024 Sep 12;15(40):16582–93. doi: 10.1039/d4sc04473h. Epub ahead of print. PMID: 39309076; PMCID: PMC11411413 (IF 7.6)
9. Luchinat E., Barbieri L., Davis B., Brough P.A., Pennestri M., Banci L., Ligand-Based Competition Binding by Real-Time <sup>19</sup>F NMR in Human Cells, *J. Med. Chem.*, 2024, 67 (2), pp. 1115 – 1126, DOI: 10.1021/acs.jmedchem.3c01600 (IF 7.3)
10. Pelliccia S., Russomanno P., Barone S., Mateu B., Alfano A.I., Miranda M., Coretti L., Lembo F., Piccolo M., Irace C., Friggeri L., Hargrove T.Y., Curtis A., Lepesheva G.I., Kavanagh K., Buommino E., Brindisi M. A First-in-Class Pyrazole-isoxazole Enhanced Antifungal Activity of Voriconazole: Synergy Studies in an Azole-Resistant *Candida albicans* Strain, Computational Investigation and in Vivo Validation in a *Galleria mellonella* Fungal Infection Model. DOI: 10.1021/acs.jmedchem.4c01109. *J of Med Chem*, 2024, 67, 14256 – 14276 (IF 7.3).
11. Alburquerque-González B., Montoro-García S., Bernabé-García A., Bernabé-García M., Campioni-Rodrigues P., Rodríguez-Martínez A., Luque I., Salo T., Pérez-Garrido A., Pérez-Sánchez H., Cayuela M.L., Luengo-Gil G., Luchinat E., Postigo-Corrales F., Staderini T., Nicolás F.J., Conesa-Zamora P., Monastrol suppresses invasion and metastasis in human colorectal cancer cells by targeting fascin independent of kinesin-Eg5 pathway, *Biomedicine and Pharmacotherapy*, 2024, 175, art. no. 116785, DOI: 10.1016/j.biopha.2024.116785 (IF 6.9)
12. Costantino A, Pham LBT, Barbieri L, Calderone V, Ben-Nissan G, Sharon M, Banci L, Luchinat E. Controlling the incorporation of fluorinated amino acids in human cells and its structural impact. *Protein Sci*. 2024, 33(3):e4910, Doi: 10.1002/pro.4910. (IF 6.725)
13. Dolcemascolo R., Heras-Hernández M., Goiriz L., Montagud-Martínez R., Requena-Menéndez A., Ruiz R., Pérez-Ràfols A., Higuera-Rodríguez R.A., Pérez-Ropero G., Vranken W.F., Martelli T., Kaiser W., Buijs J., Rodrigo G. Repurposing the mammalian RNA-binding protein Musashi-1 as an allosteric translation repressor in bacteria. DOI: 10.7554/eLife.91777. *eLife*, 13, art. no. RP91777 (IF 6.4)
14. Flood R.J., Cerofolini L., Fragai M., Crowley P.B., Multivalent Calixarene Complexation of a Designed Pentameric Lectin, *Biomacromolecules*, 2024, 25 (2), pp. 1303 – 1309, DOI: 10.1021/acs.biomac.3c01280 (IF 6.2)
15. Ghini V, Sorbi F, Fambrini M, Magherini F. NMR Metabolomics of Primary Ovarian Cancer Cells in Comparison to Established Cisplatin-Resistant and -Sensitive Cell Lines. *Cells*. 2024 Apr 9;13(8):661. doi: 10.3390/cells13080661. (IF 6.0)
16. Muzzioli R., Gallo A., The Interaction and Effect of a Small MitoBlock Library as Inhibitor of ALR Protein–Protein Interaction Pathway, *Int. J. Mol. Sci.*, 2024, 25 (2), art. no. 1174, DOI: 10.3390/ijms25021174 (IF 5.6)

17. La Guidara C., Adamo R., Sala C., Micoli F., Vaccines and Monoclonal Antibodies as Alternative Strategies to Antibiotics to Fight Antimicrobial Resistance, *Int. J. Mol. Sci.*, 2024, 25 (10), art. no. 5487, DOI: 10.3390/ijms25105487 (IF 5.6)
18. Fiorucci L., Schiavina M., Felli I.C., Pierattelli R., Ravera E. Are Protein Conformational Ensembles in Agreement with Experimental Data? A Geometrical Interpretation of the Problem. DOI: 10.1021/acs.jcim.4c00582. *J of Chem Information and Modeling*, 64, 5392 – 5401 (IF 5.6).
19. Fiorucci L., Schiavina M., Felli I.C., Pierattelli R., Ravera E. Are Protein Conformational Ensembles in Agreement with Experimental Data? A Geometrical Interpretation of the Problem. DOI: 10.1021/acs.jcim.4c00582 *J of Chem Information and Modeling*, 64, 5392 – 5401 (IF 5.6).
20. Gigli, L; Silva, J; Cerofolini, L; Macedo, A; Geraldes, C; Suturina, E; Calderone, V; Fragai, M; Parigi, G; Ravera, E; Luchinat, C. Machine Learning-Enhanced Quantum Chemistry-assisted Refinement of the Active Site Structure of Metalloproteins, *Inorganic Chemistry*, In Press (IF 5.436)
21. Vignoli A., Gori A.M., Berteotti M., Cesari F., Giusti B., Bertelli A., Kura A., Sticchi E., Salvadori E., Barbato C., Formelli B., Pescini F., Marcucci R., Tenori L., Poggesi A. The serum metabolomic profiles of atrial fibrillation patients treated with direct oral anticoagulants or vitamin K antagonists. DOI: 10.1016/j.lfs.2024.122796. *Life Sciences*, 351, art. no. 122796. (IF 5.2)
22. Di Nisio A., De Toni L., Sabovic I., Vignoli A., Tenori L., Dall'Acqua S., Sut S., La Vignera S., Condorelli R.A., Giacone F., Ferlin A., Foresta C., Garolla A. Lipidomic Profile of Human Sperm Membrane Identifies a Clustering of Lipids Associated with Semen Quality and Function DOI: 10.3390/ijms25010297, *Int. Journal of Molecular Sciences*, 25 art. no. 297, (IF 4.9)
23. Di Pietro B., Villata S., Dal Monego S., Degasperi M., Ghini V., Guarnieri T., Plaksienko A., Liu Y., Pecchioli V., Manni L., Tenori L., Licastro D., Angelini C., Napione L., Frascella F., Nardini C., Differential Anti-Inflammatory Effects of Electrostimulation in a Standardized Setting, *Int. Journal of Molecular Sciences*, 2024, 25 (18), art. no. 9808, DOI: 10.3390/ijms25189808 (IF 4.9)
24. Bargagna B., Staderini T., Lang S.H., Banci L., Camponeschi F., Defects in the Maturation of Mitochondrial Iron–Sulfur Proteins: Biophysical Investigation of the MMDS3 Causing Gly104Cys Variant of IBA57, *In. Journal of Molecular Sciences*, 2024, 25 (19), art. no. 10466, DOI: 10.3390/ijms251910466 (IF 4.9)
25. Grifagni D, Silva JM, Querci L, Lepoivre M, Vallières C, Louro RO, Banci L, Piccioli M, Golinelli-Cohen MP, Cantini F. Biochemical and cellular characterization of the CISD3 protein: Molecular bases of cluster release and destabilizing effects of nitric oxide. *J Biol Chem*. 2024, 300(3):105745, doi: 10.1016/j.jbc.2024.105745 (IF 4.8)

26. De Santis A., Grifagni D., Orsetti A., Lenci E., Rosato A., D'Onofrio M., Trabocchi A., Ciofi-Baffoni S., Cantini F., Calderone V., A Structural Investigation of the Interaction between a GC-376-Based Peptidomimetic PROTAC and Its Precursor with the Viral Main Protease of Coxsackievirus B3, *Biomolecules*, 2024, 14 (10), art. no. 1260, DOI: 10.3390/biom14101260 (IF 4.8)
27. Querci L., Piccioli M., Ciofi-Baffoni S., Banci L Structural aspects of iron-sulfur protein biogenesis: An NMR view. DOI: 10.1016/j.bbamcr.2024.119786. *Biochimica et Biophysica Acta - Molecular Cell Research*, 187, no. 119786 (IF 4.6)
28. Di Maro M., Giraldi D., Menichetti S., Losio S., Stagnaro P., Utzeri R., Cerofolini L., Fragai M., Viglianisi C., Mechanochemical synthesis of polypropylene-based macromolecular stabilizers, *Reactive and Functional Polymers*, 2024, 197, art. no. 105858, DOI: 10.1016/j.reactfunctpolym.2024.105858 (IF 4.5)
29. Grifagni D., Doni D., Susini B., Fonseca B.M., Louro R.O., Costantini P., Ciofi-Baffoni S., Unraveling the molecular determinants of a rare human mitochondrial disorder caused by the P144L mutation of FDX2, *Protein Science*, 2024, 33 (11), art. no. e5197, DOI: 10.1002/pro.5197 (IF 4.5)
30. Shimshoni E, Solomonov I, Sagi I, Ghini V. Integrated Metabolomics and Proteomics of Symptomatic and Early Presymptomatic States of Colitis. *J Proteome Res.* 2024 Apr 5;23(4):1420-1432. doi: 10.1021/acs.jproteome.3c00860. Epub 2024 Mar 18. (IF 4.4)
31. Macchiagodena M, Fragai M, Gallo A, Pagliai M, Ravera E. The Role of Lysozyme in the Formation of Bioinspired Silicon Dioxide" *Chemistry: a European journal.* 2024, e202401249, doi: 10.1002/chem.202401249, (IF 4.3)
32. Toscano G., Rosati M., Barbieri L., Maier K., Banci L., Luchinat E., Konrat R., Lichtenecker R.J., The synthesis of specifically isotope labelled fluorotryptophan and its use in mammalian cell-based protein expression for 19F-NMR applications, *Chemical Communications*, 2024, DOI: 10.1039/d4cc04789c (IF 4.3)
33. Grifagni D., Lenci E., De Santis A., Orsetti A., Barracchia C.G., Tedesco F., Bellini Puglielli R., Lucarelli F., Lauriola A., Assfalg M., Cantini F., Calderone V., Guardavaccaro D., Trabocchi A., D'Onofrio M., Ciofi-Baffoni S., Development of a GC-376 Based Peptidomimetic PROTAC as a Degradator of 3-Chymotrypsin-like Protease of SARS-CoV-2, *ACS Med. Chem. Lett.*, 2024, 15 (2), pp. 250 - 257, DOI: 10.1021/acsmchemlett.3c00498. (IF 4.2)
34. Altincekic N, Jores N, Löhr F, Richter C, Ehrhardt C, Blommers MJJ, Berg H, Öztürk S, Gande SL, Linhard V, Orts J, Abi Saad MJ, Bütikofer M, Kaderli J, Karlsson BG, Brath U, Hedenström M, Gröbner G, Sauer UH, Perrakis A, Langer J, Banci L, Cantini F, Fragai M, Grifagni D, Barthel T, Wollenhaupt J, Weiss MS, Robertson A, Bax A, Sreeramulu S, Schwalbe H. Targeting the Main Protease (Mpro, nsp5) by Growth of Fragment Scaffolds Exploiting Structure-Based Methodologies. doi: 10.1021/acschembio.3c00720, *ACS Chem Biol.* 2024, 19(2):563-574 (IF 4.2)

35. Wan Z., Shi M., Gong Y., Lucci M., Li J., Zhou J., Yang X.-L., Lelli M., He X., Mao J. Multitasking Pharmacophores Support Cabotegravir-Based Long-Acting HIV Pre-Exposure Prophylaxis (PrEP). *Molecules*, 29, 376,(IF 4.2)
36. Pérez-Ropero G., Pérez-Ràfols A., Martelli T., Danielson U.H., Buijs J., Unraveling the Bivalent and Rapid Interactions Between a Multivalent RNA Recognition Motif and RNA: A Kinetic Approach, *Biochemistry*, 2024, 63 (21), pp. 2816 – 2829, DOI: 10.1021/acs.biochem.4c00301 (IF 2.9)
37. Badoni S., Berruyer P., Niccoli L., Lesage A., Emsley L. Maximizing Relayed 1H Hyperpolarization Transfer by Slow-Fast MAS NMR Spectroscopy DOI: 10.1021/acs.jpca.4c02452. *J of Physical Chem A*, 128, 7005 - 7012, (IF 2.8)
38. Rosati M., Barbieri L., Hlavac M., Kratzwald S., Lichtenecker R.J., Konrat R., Luchinat E., Banci L., Towards cost-effective side-chain isotope labelling of proteins expressed in human cells, *Journal of Biomolecular NMR*, 2024, DOI: 10.1007/s10858-024-00447-6 (IF 2.4)
39. Bazayeva M, Andreini C, Rosato A. A database overview of metal-coordination distances in metalloproteins. doi: 10.1107/S2059798324003152, *Acta Crystallogr D Struct Biol.*, 2024; 80, 362-376, (IF 2.2)
40. Schiavina M., Bracaglia L., Bolognesi T., Rodella M.A., Tagliaferro G., Tino A.S., Pierattelli R., Felli I.C. Intrinsically disordered proteins studied by NMR spectroscopy, *J. Magn. Reson. Open*, 2024, 18, 100143, doi: 10.1016/j.jmro.2023.100143 (IF 2.2)
41. Casoria M., Macchiagodena M., Rovero P., Andreini C., Papini A.M., Cardini G., Pagliai M., Upgrading of the general AMBER force field 2 for fluorinated alcohol biosolvents: A validation for water solutions and melittin solvation, *Journal of Peptide Science*, 2024, 30 (2), art. no. e3543, DOI: 10.1002/psc.3543 (IF 1.8)
42. Vitali V., Ackermann K., Hagelueken G., Bode B.E. Spectroscopically Orthogonal Labelling to Disentangle Site-Specific Nitroxide Label Distributions DOI: 10.1007/s00723-023-01611-1. *Applied Magnetic Resonance*, 2024, 55, 187 – 205 (IF 1.1).
43. Monaci V., Gasperini G., Banci L., Micoli F., Cantini F. 1H, 13C and 15N assignment of self-complemented MrkA protein antigen from Klebsiella pneumonia DOI: 10.1007/s12104-024-10185-3 . *Biomolecular NMR Assignments* 2024. (IF 0.8)
44. Coelho A., Silva J.M., Cantini F., Piccioli M., Louro R.O., Paquete C.M. Resonance assignments of cytochrome MtoD from the extracellular electron uptake pathway of sideroxydans lithotrophicus ES-1. DOI: 10.1007/s12104-024-10180-8. *Biomolecular NMR Assignments* 2024, (IF 0.8)
45. Adam A.A.-A., Baspinar N., Vignoli A., Meoni G., Tenori L., Basoglu A., Gulersoy E., Bicipi R.O., Effects of Boron Supplementation on Dairy Calves' Health: a Metabolomic Study,

*Assiut Veterinary Medical Journal (Egypt)*, 2024, 70 (180), pp. 10 - 25, DOI: 10.21608/AVMJ.2023.218730.1157.

46. Jekhmane S., Derks M.G.N., Maity S., Slingerland C.J., Tehrani K.H.M.E., Medeiros-Silva J., Charitou V., Ammerlaan D., Fetz C., Consoli N.A., Cochrane R.V.K., Matheson E.J., van der Weijde M., Elenbaas B.O.W., Lavore F., Cox R., Lorent J.H., Baldus M., Künzler M., Lelli M., Cochrane S.A., Martin N.I., Roos W.H., Breukink E., Weingarh M. Host defence peptide plectasin targets bacterial cell wall precursor lipid II by a calcium-sensitive supramolecular mechanism. DOI: 10.1038/s41564-024-01696-9. **Nature Microbiology**, 9 1778 - 1791, 2024