

## Publications year 2022-2023 acknowledging the Italian centre of Instruct ERIC

### 2023

1. Shukla R, Peoples AJ, Ludwig KC, Maity S, Derk MGN, De Benedetti S, Krueger AM, Vermeulen BJA, Harbig T, Lavoie F, Kumar R, Honorato RV, Grein F, Nieselt K, Liu Y, Bonvin AMJJ, Baldus M, Kubitscheck U, Breukink E, Achorn C, Nitti A, Schwalen CJ, Spoering AL, Ling LL, Hughes D, Lelli M, Roos WH, Lewis K, Schneider T, Weingarth M. An antibiotic from an uncultured bacterium binds to an immutable target. *Cell* 2023 Aug 16:S0092-8674(23)00853-X. doi: 10.1016/j.cell.2023.07.038 (IF 66.85)
2. Bellomo G, Paciotti S, Concha-Marambio L, Rizzo D, Wojdała A.L, Chiasserini D, Gatticchi L, Cerfolini L, Giuntini S, De Luca C.M.G, Ma Y, Farris C.M, Pieraccini G, Bologna S, Filidei M, Ravera E, Lelli M, Moda F, Fragai M, Parnetti L, Luchinat C, Cerebrospinal fluid lipoproteins inhibit  $\alpha$ -synuclein aggregation by interacting with oligomeric species in seed amplification assays. *Mol Neurodegeneration* 2023, 18, 20, <https://doi.org/10.1186/s13024-023-00613-8> (IF 18.879)
3. Schiavina M, Bracaglia L, Rodella MA, Kümmerle R, Konrat R, Felli IC, Pierattelli R. Optimal  $^{13}\text{C}$  NMR investigation of intrinsically disordered proteins at 1.2 GHz. *Nat Protoc.* 2023, doi: 10.1038/s41596-023-00921-9. Epub ahead of print. (IF 17.021)
4. Cerfolini L, Vasa K, Bianconi E, Salobehaj M, Cappelli G, Bonciani A, Licciardi G, Pérez-Ràfols A, Padilla-Cortés L, Antonacci S, Rizzo D, Ravera E, Viglianis, C, Calderone V, Parigi G, Luchinat C, Macchiarulo A, Menichetti S, Fragai M. Combining Solid-State NMR with Structural and Biophysical Techniques to Design Challenging Protein-Drug Conjugates. *Angew. Chem. Int. Ed.* 2023, 62, e202303202, doi.org/10.1002/anie.202303202 (IF 16.6)
5. Lan B. T. Pham, A Costantino, L Barbieri, V Calderone, E Luchinat, L, Banci. Direct expression of fluorinated proteins in human cells for 19F in-cell NMR spectroscopy. *J. Am. Chem. Soc.* 2023, 145, 2, 1389–1399, doi.org/10.1021/jacs.2c12086 (IF 16.383)
6. Tang H, Li H, Yuan C, Parigi G, Luchinat C, Meade T.J. Molecular Engineering of Self-Immulative Bioresponsive MR Imaging Probes, *J. Am. Chem. Soc.* 2023 145, 10045–10050 (IF 16.383)
7. Carniato F, Ricci M, Tei L, Garello F, Furlan C, Terreno E, Ravera E, Parigi G, Luchinat C, Botta M. (2023), Novel Nanogels Loaded with Mn(II) Chelates as Effective and

Biologically Stable MRI Probes. *Small* 2023, 2302868.  
doi.org/10.1002/smll.202302868 (IF 15.153)

8. David R, Rybina A, Burel JM, Heriche JK, Audergon P, Boiten JW, Coppens F, Crockett S, Exter K, Fahrner S, Fratelli M, Goble C, Gormanns P, Grantner T, Grüning B, Gurwitz KT, Hancock JM, Harmse H, Holub P, Juty N, Karnbach G, Karoune E, Keppler A, Klemeier J, Lancelotti C, Legras JL, Lister AL, Longo DL, Ludwig R, Madon B, Massimi M, Matser V, Matteoni R, Mayrhofer MT, Ohmann C, Panagiotopoulou M, Parkinson H, Perseil I, Pfander C, Pieruschka R, Raess M, Rauber A, Richard AS, Romano P, Rosato A, Sánchez-Pla A, Sansone SA, Sarkans U, Serrano-Solano B, Tang J, Tanoli Z, Tedds J, Wagener H, Weise M, Westerhoff HV, Wittner R, Ewbank J, Blomberg N, Gribbon P. "Be sustainable": EOSC-Life recommendations for implementation of FAIR principles in life science data handling. *EMBO J.* 2023 Dec 1;42(23):e115008. doi: 10.15252/embj.2023115008. (IF 11.4)
9. Parigi G, Ravera E, Piccioli M, Luchinat C. Paramagnetic NMR restraints for the characterization of protein structural rearrangements, *Curr. Opin. Struct. Biol.* (2023) 80, 102595. (IF 7.786)
10. Cerfolini L, Ravera E, Fischer C, Trovato A, Sacco F, Palinsky W, Angiuoni G, Fragai M, Baroni F. Integration of NMR Spectroscopy in an Analytical Workflow to Evaluate the Effects of Oxidative Stress on Abituzumab: Beyond the Fingerprint of mAbs *Anal. Chem.* 2023, 95, 24, 9199–9206, doi.org/10.1021/acs.analchem.3c00317 (IF 7.4)
11. Riccardi C, Calvanese M, Ghini V, Alonso-Vásquez T, Perrin E, Turano P, Giurato G, Weisz A, Parrilli E, Tutino M L, Fondi M. Metabolic robustness to growth temperature of a cold adapted marine bacterium. *mSystems*, 2023; e0112422. doi: 10.1128/msystems.01124-22. (IF 7.328).
12. Bargagna B, Matteucci S, Ciofi Baffoni S, Camponeschi F, Banci L. Unraveling the mechanism of [ 4Fe-4S ] cluster assembly on the N-terminal cluster binding site of NUBP1 DOI: 10.1002/pro.4625. *Protein Science*. 2023 (IF 6.725)
13. Ghini V, Vieri W, Celli T, Pecchioli V, Boccia N, Alonso-Vásquez T, Pelagatti L, Fondi M, Luchinat C, Bertini L, Vannucchi V, Landini G, Turano P. COVID-19: A complex disease with a unique metabolic signature. *PLoS Pathog.* 2023 Nov 9;19(11):e1011787. doi: 10.1371/journal.ppat.1011787 (IF 6.7)
14. Fallarini S, Cerfolini L, Salobehaj M, Rizzo D, Gheorghita GR, Licciardi G, Capialbi DE, Zullo V, Sodini A, Nativi C, Fragai M. Site-Selective Functionalized PD-1 Mutant

for a Modular Immunological Activity against Cancer Cells. *Biomacromolecules*. 2023 Nov 13;24(11):5428-5437. doi: 10.1021/acs.biomac.3c00893 (IF 6.2)

15. Da Vela S., Saudino G., Lucarelli F., Banci L., Svergun D.I., Ciofi-Baffoni S. Structural plasticity of NFU1 upon interaction with binding partners: insights into the mitochondrial [4Fe-4S] cluster pathway. DOI: 10.1016/j.jmb.2023.168154 *J Mol Biol.* 2023 (IF 6.151)
16. Ghini V, Meoni G, Vignoli A, Di Cesare F, Tenori L, Turano P, Luchinat C. Fingerprinting and profiling in metabolomics of biosamples. *Prog Nucl Magn Reson Spectrosc.* 2023 Nov-Dec;138-139:105-135. doi: 10.1016/j.pnmrs.2023.10.002. Epub 2023 Oct 18. (IF 6.1)
17. Cerofolini L, Ramberg KO, Padilla LC, Antonik P, Ravera E, Luchinat C, Fragai M, Crowley PB, Solid-state NMR - a complementary technique for protein framework characterization, *Chem.Commun.*, 2023, 56, 6, 776-779 10.1039/d2cc05725e (IF 6.065)
18. Donati G, D'Amore VM, Russomanno P, Cerofolini L, Amato J, Marzano S, Salobehaj M, Rizzo D, Assoni G, Carotenuto A, La Pietra V, Arosio D, Seneci P, Fragai M, Brancaccio D, Di Leva FS, Marinelli L. Theoretical and experimental studies on the interaction of biphenyl ligands with human and murine PD-L1: Up-to-date clues for drug design, *Comput. Struct. Biotechnol. J.*, 2023, 21, 3355-3368, doi.org/10.1016/j.csbj.2023.06.006 (IF 6)
19. Laveglia V, Bazayeva M, Andreini C, Rosato A. Hunting down zinc(II)-binding sites in proteins with distance matrices. *Bioinformatics*. 2023 Nov 1;39(11):btad653. doi: 10.1093/bioinformatics/btad653. (IF 5.8)
20. Vignoli A, Miolo G, Tenori L, Buonadonna A, Lombardi D, Steffan A, Scalzone S, Luchinat C, Corona G. Novel metabolomics-biohumoral biomarkers model for predicting survival of metastatic soft-tissue sarcomas. *iScience*. 2023 Aug 19;26(10):107678. doi: 10.1016/j.isci.2023.107678. (IF 5.8)
21. Bargagna B, Banci L, Camponeschi F. Understanding the Molecular Basis of the Multiple Mitochondrial Dysfunctions Syndrome 2: The Disease-Causing His96Arg Mutation of BOLA3. *Int. J. Mol. Sci.* 2023, 24(14), 11734, doi.org/10.3390/ijms241411734 (IF 5.6)
22. Brunetti A, Pintus A, Lombardi L, Kovtun A, Mascietti F, Bruno F, Ravera E, Melucc Mi, Bertuzzi G, Bandini M. Graphene-Oxide Mediated Chemodivergent Ring-Opening

of Cyclobutanols, *Chinese Journal of Chemistry*, 2023, 41(11), 1333-1340, doi.org/10.1002/cjoc.202200757 (IF 5.56)

23. Licari C, Tenori L, Di Cesare F, Luchinat C, Giusti B, Kura A, De Cario R, Inzitari D, Piccardi B, Nesi M, Sarti C, Arba F, Palumbo V, Nencini P, Marcucci R, Gori AM, Sticchi E, Nuclear Magnetic Resonance-Based Metabolomics to Predict Early and Late Adverse Outcomes in Ischemic Stroke Treated with Intravenous Thrombolysis, *J Proteome Res.*, 2023, vol. 22, no. 1, pp. 16-25, <https://doi.org/10.1021/acs.jproteome.2c00333> (IF 5.370)
24. Di Cesare F, Calgaro M, Ghini V, Squarzanti DF, De Prisco A, Visciglia A, Zanetta P, Rolla R, Savoia P, Amoruso A, Azzimonti B, Vitulo N, Tenori L, Luchinat C, Pane M. Exploring the Effects of Probiotic Treatment on Urinary and Serum Metabolic Profiles in Healthy Individuals. *J Proteome Res.* 2023 Dec 1;22(12):3866-3878. doi: 10.1021/acs.jproteome.3c00548. Epub 2023 Nov 16 (IF 5.370)
25. Cosottini L, Massai L, Ghini V, Zineddu S, Geri A, Mannelli M, Ciambellotti S, Severi M, Gamberi T, Messori L, Turano P. Bioconjugation of the gold drug auranofin to human ferritin yields a potent cytotoxin, *J. Drug Deliv. Sci. Technol.*, 2023, doi.org/10.1016/j.jddst.2023.104822 (IF 5)
26. Vitali V, Torricella F, Massai L, Messori L, Banci L. Enlarging the scenario of site directed <sup>19</sup>F labeling for NMR spectroscopy of biomolecules. *Sci Rep.* 2023 Dec 12;13(1):22017. doi: 10.1038/s41598-023-49247-2. (IF 4.997)
27. Cerfolini L, Ramberg KO, Padilla L C, Antonik P, Ravera E, Luchinat C, Fragai M, Crowley PB. Solid-state NMR – a complementary technique for protein framework characterization, *Chem. Commun.*, 2023, 59, 776-779 doi.org/10.1039/D2CC05725E (IF 4.9)
28. M.A. Kaster, M.D. Levasseur, T.G.W. Edwardson, M.A. Caldwell, D. Hofmann, G. Licciardi, G. Parigi, C. Luchinat, D. Hilvert, T.J. Meade, Engineered NonViral Protein Cages Modified for MR Imaging, *ACS Appl. Bio Mater.* 2023, 6, 2, 591–602, doi.org/10.1021/acsabm.2c00892 (IF 4.7)
29. Malanho Silva J, Cerfolini L, Carvalho A.L., Ravera E, Fragai M, Parigi G, Macedo A.L., Geraldes C.F.G.C., Luchinat C. Elucidating the concentration-dependent effects of thiocyanate binding to carbonic anhydrase, *J. Inorg. Biochem.* (2023) 244, 112222. (IF 4.336) <https://doi.org/10.1016/j.jinorgbio.2023.112222>

30. Cosottini, L.; Zineddu, S.; Massai, L.; Ghini, V.; Turano, P. 19F: A Small Probe for a Giant Protein. *Journal of Inorganic Biochemistry* 2023, 112236. <https://doi.org/10.1016/j.jinorgbio.2023.112236>. (IF: 4.336)
31. Ghini V., Mannelli M., Massai L., Geri A., Zineddu S., Gamberi T., Messori L., Turano P. The effects of two cytotoxic gold(i) carbene compounds on the metabolism of A2780 ovarian cancer cells: mechanistic inferences through NMR analysis, *RSC Adv.*, 2023, **13**, 21629-21632, doi.org/10.1039/D3RA04032A (IF 3.9)
32. Ribolla LM, Sala K, Tonoli D, Ramella M, Bracaglia L, Bonomo I, Gonnelli L, Lamarca A, Brindisi M, Pierattelli R, Provenzani A, de Curtis I. (2023) Interfering with the ERC1–LL5β interaction disrupts plasma membrane–Associated platforms and affects tumor cell motility. *PLoS ONE*, 2023, 18(7): e0287670. doi.org/10.1371/journal.pone.0287670 (IF 3.752)
33. Bruno F, Gigli L, Ravera E. Spin Label Study of the Orientational Preferences of Lysozyme in a Bioinspired Silica Composite. *Journal of Composites Science*. 2023; 7(5):188. doi.org/10.3390/jcs7050188 (IF 3.3)
34. Mulder, F.A.A., Tenori, L., Licari, C. & Luchinat, C. 2023, Practical considerations for rapid and quantitative NMR-based metabolomics, *Journal of Magnetic Resonance*, 2023 vol. 352, <https://doi.org/10.1016/j.jmr.2023.107462> (IF 2.734)
35. Schiavina M, Konrat R, Ceccolini I, Mateos B, Konrat R, Felli IC, Pierattelli R. Studies of proline conformational dynamics in IDPs by <sup>13</sup>C-detected cross-correlated NMR relaxation, *J Magn Reson.* 2023, 11;354:107539. doi: 10.1016/j.jmr.2023.107539 (IF 2.734)
36. Villarruel Dujovne M, Bringas M, Felli I C, Ravera E, Di Lella S, Capdevila D A, Introducing NMR strategies to define water molecules that drive metal binding in a transcriptional regulator, *Journal of Magnetic Resonance Open*, 2023, doi.org/10.1016/j.jmro.2023.100114. (IF 2.734)
37. Schiavina M, Bracaglia L, Bolognesi T, Rodella MA, Tagliaferro G, Tino AS, Pierattelli R, Felli IC. Intrinsically disordered proteins studied by NMR spectroscopy., doi.org/10.1016/j.jmro.2023.100143, *Journal of Magnetic Resonance Open* (IF 2.734)
38. Querci L, Trindade IB, Invernici M, Silva JM, Cantini F, Louro RO, Piccioli M. NMR of Paramagnetic Proteins: <sup>13</sup>C Derived Paramagnetic Relaxation Enhancements Are an Additional Source of Structural Information in Solution. *Magnetochemistry*. 2023; 9(3):66, doi.org/10.3390/magnetochemistry9030066 (IF 2.7)

39. Querci L, Grifagni D, Trindade IB, Silva JM, Louro RO, Cantini F, Piccioli M. Paramagnetic NMR to study iron sulfur proteins:  $^{13}\text{C}$  detected experiments illuminate the vicinity of the metal center. *J Biomol NMR*. 2023 Dec;77(5-6):247-259. doi: 10.1007/s10858-023-00425-4. (IF 2.58)
40. Bruno F, Fiorucci L, Ravera E, Sensitivity considerations on denoising series of spectra by singular value decomposition, *Magn Reson Chem*, 2023, doi: 10.1002/mrc.5338 (IF 2.392)
41. Luchinat E, Banci L. In-cell NMR: recent progresses and future challenges, *Rend. Fis. Acc. Lincei*, 2023, doi: 10.1007/s12210-023-01168-y (IF 1.810)
42. Villarruel Dujovne M, Bringas M, Felli I C, Ravera E, Di Lella S, Capdevila D A, Introducing NMR strategies to define water molecules that drive metal binding in a transcriptional regulator, *Journal of Magnetic Resonance Open*, 2023, doi.org/10.1016/j.jmro.2023.100114. (IF 2.734)
43. Schiavina M, Bracaglia L, Bolognesi T, Rodella MA, Tagliaferro G, Tino AS, Pierattelli R, Felli IC. Intrinsically disordered proteins studied by NMR spectroscopy., doi.org/10.1016/j.jmro.2023.100143, *Journal of Magnetic Resonance Open* (IF 2.734)

## 2022

1. Luchinat E, Cremonini M, Banci L. Radio Signals from Live Cells: The Coming of Age of In-Cell Solution NMR, *Chem. Rev.* DOI: 10.1021/acs.chemrev.1c00790. (IF 60.622).
2. Felli IC, Pierattelli R.  $^{13}\text{C}$  Direct Detected NMR for Challenging Systems. *Chem. Rev.* DOI: 10.1021/acs.chemrev.1c00871. (IF 60.622)
3. Rhythm Shukla, Lavore F, Maity S, Lelli M, Weingarth M, et al. Teixobactin kills bacteria by a two-pronged attack on the cell envelope. doi.org/10.1038/s41586-022-05019-y. *Nature* 608, 390–396 (2022) (IF 49.962)
4. Berg H. et al. Comprehensive Fragment Screening of the SARS-CoV-2 Proteome Explores Novel Chemical Space for Drug Development. *Angew Chem Int Ed Engl.* 2022 Nov 14;61(46):e202205858. doi: 10.1002/anie.202205858. (IF 16.823)

5. Saudino G, Ciofi-Baffoni S, Banci L. Protein-Interaction Affinity Gradient Drives [4Fe-4S] Cluster Insertion in Human Lipoyl Synthase. *J Am Chem Soc.* 2022, 144, 5713-5717. doi: 10.1021/jacs.1c13626. (IF 14.419)
6. Rizzo D, Cerfolini L, Giuntini S, Iozzino L, Pergola C, Sacco F, Palmese A, Ravera E, Luchinat C, Baroni F, Fragai M. Epitope Mapping and Binding Assessment by Solid-State NMR Provide a Way for the Development of Biologics under the Quality by Design Paradigm. *J Am Chem Soc.* 2022, 144, 10006-10016. doi: 10.1021/jacs.2c03232. (IF 14.419)
7. Santana FS, Perfetti M, Briganti M, Sacco F, Poneti G, Ravera E, Soares JF, Sessoli R. A dysprosium single molecule magnet outperforming current pseudocontact shift agents. *Chem Sci.* 2022 Apr 26;13(20):5860-5871. doi: 10.1039/d2sc01619b. (IF 9.825).
8. Meoni G, Tenori L, Schade S, Licari C, Pirazzini C, Bacalini MG, Garagnani P, Turano P; PROPAG-AGEING Consortium, Trenkwalder C, Franceschi C, Mollenhauer B, Luchinat C. Metabolite and lipoprotein profiles reveal sex-related oxidative stress imbalance in de novo drug-naive Parkinson's disease patients. *NPJ Parkinsons Dis.* 2022; 8, 14. doi: 10.1038/s41531-021-00274-8. (IF. 8.651)
9. Tricomi J, Cacaci M, Biagiotti G, Caselli L, Niccoli L, Torelli R, Gabbani A, Di Vito M, Pineider F, Severi M, Sanguinetti M, Menna E, Lelli M, Berti D, Cicchi S, Bugli F, Richichi B. Ball milled glyco-graphene oxide conjugates markedly disrupted *Pseudomonas aeruginosa* biofilms. *Nanoscale.* 2022 Jul 21;14(28):10190-10199. doi: 10.1039/d2nr02027k. (IF. 8.307)
10. Luchinat E, Banci L. In-cell NMR: From target structure and dynamics to drug screening. *Curr Opin Struct Biol.* 2022 doi:10.1093/gerona/glab335 (IF 7.25)
11. Parigi G, Ravera E, Luchinat C. Paramagnetic effects in NMR for protein structures and ensembles: Studies of metalloproteins. *Curr Opin Struct Biol.* 2022, 102386. doi: 10.1016/j.sbi.2022.102386. (IF 7.25)
12. Di Cesare F, Luchinat C, Tenori L, Saccenti E. Age- and Sex-Dependent Changes of Free Circulating Blood Metabolite and Lipid Abundances, Correlations, and Ratios. *J Gerontol A Biol Sci Med Sci.* 2022 5;77(5):918-926. doi: 10.1093/gerona/glab335. (IF 6.591)
13. Conti L, S. Ciambellotti, G. E. Giacomazzo, V. Ghini, L. Cosottini, E. Puliti, M. Severi, E. Fratini, F. Cencetti, P. Bruni, B. Valtancoli, C. Giorgi and P. Turano, Ferritin nanocomposites for the selective delivery of photosensitizing ruthenium-polypyridyl

compounds to cancer cells, *Inorg. Chem. Front.*, 2022, DOI:10.1039/D1QI01268A (IF 6.569)

14. Cantini F, Andreano E, Paciello I, Ghini V, Berti F, Rappuoli R Banci L. 2D NMR Analysis as a Sensitive Tool for Evaluating the Higher-Order Structural Integrity of Monoclonal Antibody against COVID-19. *Pharmaceutics* 2022, 14, 1981 doi.org/10.3390/pharmaceutics14101981. (IF 6.525)
15. Ghini V, Meoni G, Pelagatti L, Celli T, Veneziani F, Petrucci F, Vannucchi V, Bertini L, Luchinat C, Landini G, Turano P. Profiling metabolites and lipoproteins in COMETA, an Italian cohort of COVID-19 patients. *PLoS Pathog*, 2022, 18: e1010443. (IF 6.51)
16. Beniamino Y, Cenni V, Piccioli M, Ciurli S, Zambelli B. The Ni(II)-Binding Activity of the Intrinsically Disordered Region of Human NDRG1, a Protein Involved in Cancer Development. *Biomolecules* 2022. doi:10.3390/biom12091272. (IF 6.064)
17. Massai L, Grifagni D, De Santis A, Geri A, Cantini F, Calderone V, Banci L, Messori L. Gold-Based Metal Drugs as Inhibitors of Coronavirus Proteins: The Inhibition of SARS-CoV-2 Main Protease by Auranofin and Its Analogs. *Biomolecules*. 2022 Nov 11;12(11):1675. doi: 10.3390/biom12111675. (IF 6.064)
18. Vignoli, A. et al. Metabolomics Fingerprint Predicts Risk of Death in Dilated Cardiomyopathy and Heart Failure. *Front. Cardiovasc. Med.* 9, 2022. (IF 6.050)
19. Hricovíni M, Owens RJ, Bak A, Kozik V, Musiał W, Pierattelli R, Májeková M, Rodríguez Y, Musioł R, Slodek A, Štarha P, Piętak K, Słota D, Florkiewicz W, Sobczak-Kupiec A, Jampílek J. Chemistry towards Biology-Instruct: Snapshot. *Int J Mol Sci.* 2022 Nov 26;23(23):14815. doi: 10.3390/ijms232314815. (IF 6.009)
20. Di Cesare F , Tenori L, Luchinat C , Saccenti E. Association of Plasma Metabolites and Lipoproteins with Rh and ABO Blood Systems in Healthy Subjects. *J. Proteome Res.* 2022, 21, 11, 2655–2663. doi: 10.1021/acs.jproteome.2c00375. (IF 5.370)
21. Ghini V, Maggi L, Mazzoni A, Spinicci M, Zammarchi L, Bartoloni A, Annunziato F, Turano P. Serum NMR Profiling Reveals Differential Alterations in the Lipoproteome Induced by Pfizer-BioNTech Vaccine in COVID-19 Recovered Subjects and Naïve Subjects. *Front. Mol. Biosci.*, 2022, 9:839809. (IF 5.246)
22. Ghini V, Abuja PM, Polasek O, Kozera L, Laiho P, Anton G, Zins M, Klovins J, Metspalu A, Wichmann HE, Gieger C, Luchinat C, Zatloukal K, Turano P. Impact of the pre-examination phase on multicenter metabolomic studies. *New Biotech.* 2022, doi: 10.1016/j.nbt.2022.01.006. (IF 5.079)

23. Torricella F, Barbieri L, Bazzurro V, Diaspro A, Banci L. Protein delivery to living cells by thermal stimulation for biophysical investigation. *Sci Rep.* 2022 Oct 13;12(1):17190. doi: 10.1038/s41598-022-21103-9. (IF 4.996)
24. Camponeschi F, Piccioli M, Banci L. The Intriguing mitoNEET: Functional and Spectroscopic Properties of a Unique [2Fe-2S] Cluster Coordination Geometry. *Molecules.* 2022 Nov 25;27(23):8218. doi: 10.3390/molecules27238218. (IF 4.927)
25. Licciardi G, Rizzo D, Salobehaj M, Massai L, Geri A, Messori L, Ravera E, Fragai M, Parigi G. Large Protein Assemblies for High-Relaxivity Contrast Agents: The Case of Gadolinium-Labeled Asparaginase. *Bioconjug Chem.* 2022 Dec 21;33(12):2411-2419. doi: 10.1021/acs.bioconjchem.2c00506. (IF 4.774)
26. Schiavina M, Pontoriero L, Tagliaferro G, Pierattelli R, Felli IC. The Role of Disordered Regions in Orchestrating the Properties of Multidomain Proteins: The SARS-CoV-2 Nucleocapsid Protein and Its Interaction with Enoxaparin. *Biomolecules.* 2022 12, 1302. doi: 10.3390/biom12091302. (IF 4.569)
27. Pontoriero L, Schiavina M, Korn SM, Schlundt A, Pierattelli R, Felli IC. MR Reveals Specific Tracts within the Intrinsically Disordered Regions of the SARS-CoV-2 Nucleocapsid Protein Involved in RNA Encountering. *Biomolecules.* 2022 12, 929. doi: 10.3390/biom12070929 (IF 4.569)
28. Camponeschi F, Ciofi-Baffoni S, Calderone V, Banci L. Molecular Basis of Rare Diseases Associated to the Maturation of Mitochondrial [4Fe-4S]-Containing Proteins, *Biomolecules*, 12(7), 1009-1037, doi.org/10.3390/biom12071009, 2022. (IF 4.569)
29. Ghini V, Magherini F, Massai L, Messori L, Turano P. Comparative NMR metabolomics of the responses of A2780 human ovarian cancer cells to clinically established Pt-based drugs. *Dalton Trans.* 2022 Aug 23;51(33):12512-12523. doi: 10.1039/d2dt02068h. (IF 4.569)
30. Vignoli A, Tenori L, Morsiani C, Turano P, Capri M, Luchinat C. Serum or Plasma (and Which Plasma), That Is the Question. *J. Proteome Res.* 21, 1061–1072 (2022). (IF 4.466)
31. Bruno F, Gigli L, Ferraro G, Cavallo A, Michaelis VK, Goobes G, Fratini E, Ravera E. Lysozyme is Sterically Trapped Within the Silica Cage in Bioinspired Silica-Lysozyme Composites: A Multi-Technique Understanding of Elusive Protein-Material Interactions. *Langmuir.* 2022 Jul 5;38(26):8030-8037. doi: 10.1021/acs.langmuir.2c00836. (IF 4.331)

32. Trindade IB, Coelho A, Cantini F, Piccioli M, Louro RO. NMR of paramagnetic metalloproteins in solution: Ubi venire, quo vadis? *J Inorg Biochem.* 2022, 234:111871. doi: 10.1016/j.jinorgbio.2022.111871. (IF 4.155)
33. Camponeschi F, Banci L. Metal trafficking in the cell: Combining atomic resolution with cellular dimension. *FEBS Letters* 2022, doi.org/10.1002/1873-3468.14524 (IF 4.124)
34. Licciardi G, Rizzo D, Ravera E, Fragai M, Parigi G, Luchinat C. Not only manganese, but fruit component effects dictate the efficiency of fruit juice as an oral magnetic resonance imaging contrast agent. *NMR Biomed.* 2022, 35, e4623. doi: 10.1002/nbm.4623. (IF 4.044)
35. Caputo S, Kovtun A, Bruno F, Ravera E, Lambruschini C, Melucci M, Moni L. Study and application of graphene oxide in the synthesis of 2,3-disubstituted quinolines via a Povarov multicomponent reaction and subsequent oxidation. *RSC Adv.* 2022 May 26;12(25):15834-15847. doi: 10.1039/d2ra01752k. (IF 4.036)
36. Ravera E, Gigli L, Fiorucci L, Luchinat C, Parigi G. The evolution of paramagnetic NMR as a tool in structural biology. *Phys Chem Chem Phys.* 2022 Jul 27;24(29):17397-17416. doi: 10.1039/d2cp01838a. (IF 3.676)
37. Gallorini R, Ciuffi B, Real Fernández F, Carozzini C, Ravera E, Papini AM, Rosi L. Subcritical Hydrothermal Liquefaction as a Pretreatment for Enzymatic Degradation of Polyurethane, doi.org/10.1021/acsomega.2c04734. *ACS Omega* 2022. (IF 3.512)
38. Cerofolini L, Parigi G, Ravera E, Fragai M, Luchinat C. Solid-state NMR methods for the characterization of bioconjugations and protein-material interactions. *Solid State Nucl Magn Reson.* 2022 Dec; 122:101828. doi: 10.1016/j.ssnmr.2022.101828. (IF 2.97)
39. Silva JM, Grifagni D, Cantini F, Piccioli M. 1H, 13C and 15N assignment of the human mitochondrial paramagnetic iron-sulfur protein CISD3. *Biomol NMR Assign.* 2022 Dec 15. doi: 10.1007/s12104-022-10113-3. (IF 0.746)