CERM Publications

(December 2022)

1. Luchinat E, Cremonini M, Banci L. Radio Signals from Live Cells: The Coming of Age of In-Cell Solution NMR, *Chem. Rev.* 2022 DOI: 10.1021/acs.chemrev.1c00790. (IF 72.087).

2. Felli IC, Pierattelli R. 13C Direct Detected NMR for Challenging Systems. DOI: 10.1021/acs.chemrev.1c00871. *Chem. Rev*. 2022. (IF 72.087)

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* 2022, 608, 390–396,. (IF 69.504)

4. Honarmand Ebrahimi K, Ciofi-Baffoni S, Hagedoorn PL, Nicolet Y, Le Brun NE, Hagen WR, Armstrong FA. Iron-sulfur clusters as inhibitors and catalysts of viral replication. doi: 10.1038/s41557-021-00882-0. *Nat Chem.* 2022, 14.. (IF 24.274)

5. Varadi M, Armastrong D, Carazo JM, Andreini C, Rosato A, et al. (PDBe-KB Consortium). PDBe-KB: collaboratively defining the biological context of structural data. DOI 10.1093/nar/gkab988. *Nucleic Acids Research*, 50, D534-D542, , 2022, (IF 19.160)

6. Saudino G, Ciofi-Baffoni S, Banci L. Protein-Interaction Affinity Gradient Drives [4Fe-4S] Cluster Insertion in Human Lipoyl Synthase*.* doi: 10.1021/jacs.1c13626. *J Am Chem Soc*. 2022, 144, 5713-5717. (IF 16.383).

7. Abelein A, Ciofi-Baffoni S, Mörman C, Kumar R, Giachetti A, Piccioli M, Biverstål H. Molecular Structure of Cu(II)-Bound Amyloid-β Monomer Implicated in Inhibition of Peptide Self-Assembly in Alzheimer's Disease. doi: 10.1021/jacsau.2c00438 *J Am Chem Soc.* 2022, 11, 2571-2584, (IF 16.383).

8. Rizzo D, Cerofolini 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. doi: 10.1021/jacs.2c03232. *J Am Chem Soc*. 2022,144, 10006-10016. (IF 16.383)

9. Jabbour R, Renom-Carrasco M, Chan KW, Völker L, Berruyer P, Wang Z, Widdifield CM, Lelli M, Gajan D, Copéret C, Thieuleux C, Lesage A. Multiple Surface Site Three-Dimensional Structure Determination of a Supported Molecular Catalyst. doi: 10.1021/jacs.2c01013. *J Am Chem Soc*. 2022, 144, 10270-10281. (IF 16.383)

10. Assoni G, La Pietra V., Digilio R, Ciani C, Nausicaa Valentina Licata, Mariachiara Micaelli, Elisa Facen, Weronika Tomaszewska, Linda Cerofolini, Anna Pérez-Ràfols, Marta Varela Rey, Marco

Fragai, Ashwin Woodhoo, Luciana Marinelli, Daniela Arosio, Isabelle Bonomo, Alessandro Provenzani, Pierfausto Seneci. HuR-targeted agents: An insight into medicinal chemistry, biophysical, computational studies and pharmacological effects on cancer models. ***Adv Drug Deliv Rev***. 2022, 181, 114088. (IF 15.47)

11. Castagneto-Gissey L, Angelini G, Mingrone G, Cavaretta E, Tenori L, Licari C. The early reduction of left ventricular mass after sleeve gastrectomy depends on the fall of branched-chain amino acid circulating levels, Doi:10.1016/j.ebiom.2022.103864. ***eBioMedicine (Open Access)*** 2022, 76, 103864 (IF 11.205)

12. De Sousa Santana F, Perfetti M, Briganti M, Sacco F, Poneti G, Ravera E, Soares J, Sessoli R. A textbook Single Molecule Magnet outperforming current pseudocontact shift agents. Doi:10.1039/d2sc01619b ***Chem Sci***, 2022 13, 5860, (IF 9.969)

13. Theillet, FX, Luchinat E. In-cell NMR: Why and how? ***Prog. Nucl. Magn. Reson. Spectrosc.*** (2022) DOI: 10.1016/j.pnmrs.2022.04.002. (IF 9.447).

14. 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 doi: 10.1038/s41531-021-00274-8. ***NPJ Parkinsons Dis***. 2022; 8, 14. (IF. 9.304).

15. Tricomi J, Cacaci M, Biagiotti G, Caselli L, Niccoli L, Torelli R, Gabbani A, Di Vito M, Pineider F, Severi Mi, 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 Doi: 10.1039/D2NR02027K ***Nanoscale,*** 2022, 14, 10190-10199 (IF 8.307)

16. 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 7.786)

17. Luchinat, E., Banci L. In-cell NMR: From target structure and dynamics to drug screening. DOI: 10.1016/j.sbi.2022.102374. ***Curr. Op. Struct. Biol***. 74 (2022), 102374.. (IF 7.786)

18. 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 DOI:10.1039/D1QI01268A, ***Inorg. Chem. Front***., 2022, 9, 1070 (IF 7.779)

19. Bernacchioni C, Squecco R, Gamberi T, Ghini V, Schumacher F, Mannelli M, Garella R, Idrizaj E, Cencetti F, Puliti E, Bruni P, Turano P, Fiaschi T, Donati C. S1P Signalling Axis Is Necessary for Adiponectin-Directed Regulation of Electrophysiological Properties and Oxidative Metabolism in C2C12 Myotubes. ***Cells***. 2022, 11, 713. doi: 10.3390/cells11040713. (IF 7.666)

20. Di Cesare F., Tenori L., Meoni G., et al. Lipid and metabolite correlation networks specific to clinical and biochemical covariate show differences associated with sexual dimorphism in a cohort of nonagenarians***. GeroScience*** (2022). doi.org/10.1007/s11357-021-00404-3 (IF 7.581)

21. 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 7.464)

22. 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, *The Journals of Gerontology*: Series A, Volume 77, 5, 2022, 918–926, doi.org/10.1093/gerona/glab335 (IF 6.591)

23. 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)

24. Burgalassi S, Fragai M, Francesconi O, Cerofolini L, Monti D, Leone G, Lamponi S, Greco G, Magnani A, Nativi C. Functionalized Hyaluronic Acid for " In Situ" Matrix Metalloproteinase Inhibition: A Bioactive Material to Treat the Dry Eye Sydrome. *ACS Macro Lett.* (2022), 11, 1190-1194. ISSN : 2161-1653 (IF : 6.434).

25. 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 6.409)

26. Andreini C, A Rosato Structural bioinformatics and deep learning of metalloproteins: recent advances and applications. *Int.J Mol Sci* 23 (14), 7684, (IF 6.208)

27. Hricovíni, M.; Owens, R.J.; 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, 23, 14815. (IF 6.208)

28. Laveglia V, Giachetti A, Sala D, Andreini C, Rosato A Learning to Identify Physiological and Adventitious Metal-Binding Sites in the Three-Dimensional Structures of Proteins by Following the Hints of a Deep Neural Network doi.org/10.1021/acs.jcim.2c00522 *J. Chem. Inf. Model*. 2022, 62, 12, 2951–2960 (IF 6.162)

29. 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 6.113)

30. Zinga, M.M., Abdel-Shafy, E., Melak, T., Vignoli, A., Piazza, S., Zerbini, L.F., Tenori, L. & Cacciatore, S., "KODAMA exploratory analysis in metabolic phenotyping", *Frontiers in Molecular Biosciences*, 2022, vol. 9. https://doi.org/10.3389/fmolb.2022.1070394 (IF 6.113)

31. Invernici, M; Selvolini, G; Silva, J M; Marrazza, G; Ciofi-Baffoni, S; Piccioli, M; Interconversion between [2Fe-2S] and [4Fe-4S] cluster glutathione complexes *Chem. Commun*., 2022, 58, 3533-3536 (IF 6.065)

32. 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 6.064)

33. 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 6.064)

34. 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 6.064)

35. Ciani C, Pérez-Ràfols A, Bonomo I, Micaelli M, Esposito A, Zucal C, Belli R, D'Agostino V G, Bianconi I, Calderone V, Cerofolini L, Massidda O, Whalen M B, Fragai M, Provenzani A. Identification and Characterization of an RRM-Containing, RNA Binding Protein in *Acinetobacter baumannii*. *Biomolecules* (2022), 12, 922. ISSN : 2218273X (IF 5.88)

36. Vignoli, A. et al. Metabolomics Fingerprint Predicts Risk of Death in Dilated Cardiomyopathy and Heart Failure. *Front. Cardiovasc. Med*. 9, 2022. (IF 5.848)

37. Carniato F, Ricci M Tei L, Garello F, Terreno E, Ravera E, Parigi G, Luchinat C, Botta M. High Relaxivity with No Coordinated Waters: A Seemingly Paradoxical Behavior of [Gd(DOTP)]$^{5-}$ Embedded in Nanogels. doi.org/10.1021/acs.inorgchem.2c00225 *Inorg Chem*, 2022, 61, 13, 5380-5387 (IF 5.436)

38. Vignoli A, Tenori L, Morsiani C, Turano P, Capri M, Luchinat C. Serum or Plasma (and Which Plasma), That Is the Question. doi.org/10.1021/acs.jproteome.1c00935 *J. Proteome Res.* 21, 1061–1072 (2022). (IF 5.370)

39. 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.org/10.1021/acs.jproteome.2c00375 (IF 5.370)

40. 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 A.M., Sticchi E., NMR-based metabolomics to predict early and late adverse outcomes in ischemic stroke treated with intravenous thrombolysis, doi.org/10.1021/acs.jproteome.2c00333 *J. Proteome Res.* 2022 (IF 5.370)

41. Torricella F, L Barbieri, V Bazzurro, A Diaspro, L Banci; Protein delivery to living cells by thermal stimulation for biophysical investigation. *Scientific Reports* 12, 1-10 DOI 10.1038/s41598-022-21103-9 (IF. 4.996)

42. Niero G.; Meoni G.; Tenori L.; Luchinat C.; Visentin G.; Callegaro S.; Visentin E; Cassandro M.; De Marchi M.; Penasa M. Grazing affects metabolic pattern of individual cow milk. *Journal of Dairy Science*, 2022, 105(12), pp. 9702-9712. 10.3168/jds.2022-22072. (IF 4.987)

43. Camponeschi F., Piccioli M., Banci L. The Intriguing mitoNEET: Functional and Spectroscopic Properties of a Unique [2Fe-2S] Cluster Coordination Geometry, doi.org/10.3390/molecules27238218 *Molecules*, 2022, *27*, 8218 (IF 4.927)

44. Micaelli M, Dalle Vedove A, Cerofolini L, Vigna J, Sighel D, Zaccara S, Bonomo I, Poulentzas G, Rosatti EF, Cazzanelli G, Alunno L, Belli R, Peroni D, Dassi E, Murakami S, Jaffrey SJ, Fragai M, Mancini I, Lolli G, Quattrone A, Provenzani A. Small-Molecule Ebselen Binds to YTHDF Proteins Interfering with the Recognition of N6-Methyladenosine-Modified RNAs. *ACS Pharmacol Transl Sci.* (2022), 5, 872-891. (IF 4.88)

45. Vignoli, A., Tenori, L. & Luchinat, C. An omics approach to study trace metals in sera of hemodialysis patients treated with erythropoiesis stimulating agents. *Metallomics* (2022). doi.org/10.1093/mtomcs/mfac028 (IF 4.636)

46. Andreini C, Arnesano F, Rosato R.The zinc proteome of SARS-CoV-2. doi.org/10.1093/mtomcs/mfac047 *Metallomics*, 14, 2022, mfac047, (IF 4.636)

47. Ji Y, Wei L, Da A, Stark H, Hagedoorn PL, Ciofi-Baffoni S, Cowley SA, Louro RO, Todorovic S, Mroginski MA, Nicolet Y, Roessler MM, Le Brun NE, Piccioli M, James WS, Hagen WR, Ebrahimi KH Radical-SAM dependent nucleotide dehydratase (SAND), rectification of the names of an ancient iron-sulfur enzyme using NC-IUBMB recommendations. doi: 10.3389/fmolb.2022.1032220 *Front Mol Biosci*. 9:1032220 (IF 4.615)

48. 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 4.478)

49. 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 4.336)

50. Bazayeva, M, V Laveglia, C Andreini, A Rosato Metal-induced structural variability of mononuclear metal-binding sites from a database perspective. *J Inorg Biochem*, 2022, 238, 112025, https://doi.org/10.1016/j.jinorgbio.2022.112025 (IF 4.336)

51. Lang L., Ravera E., Parigi G., Luchinat C., Neese F.; Theoretical analysis of the long-distance limit of NMR chemical shieldings. *J. Chem. Phys*., 2022, 156, 15, 154115 (IF 4.304)

52. Bobbo T, Meoni G, Niero G, Tenori L, Luchinat C, Cassandro M, Penasa M. Nuclear magnetic resonance spectroscopy to investigate the association between milk metabolites and udder quarter health status in dairy cows. *J Dairy Sci*. 2022; 105:535-548. doi: 10.3168/jds.2021-20906. (IF 4.225)

53. Lang SH, Camponeschi F, Joya E, Borjas-Mendoza P, Tekin M, Thorson W. Multiple Mitochondrial Dysfunction Syndrome Type 3: A Likely Pathogenic Homozygous Variant Affecting a Patient of Cuban Descent and Literature Review. 10.3390/genes13112044. *Genes (Basel)*;13, 2044.(IF 4.141).

54. 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 4.132)

55. Camponeschi, F. and Banci, L, Metal trafficking in the cell: Combining atomic resolution with cellular dimension. **FEBS Lett.** doi.org/10.1002/ 2022, 1873-3468.14524. (IF 4.124)

56. Del Duca S, Puglia AM, Calderone V, Bazzicalupo M, Fani R. Effect of Non-Lethal Selection on Spontaneous Revertants of Frameshift Mutations: The *Escherichia coli* hisF Case. Doi: 10.3390/microorganisms10040692. **Microorganisms**. 2022,10, 692. (IF 3.864)

57. Ravera E, L. Gigli, L. Fiorucci, C. Luchinat, G. Parigi, The evolution of paramagnetic NMR as a tool in structural biology**, Phys. Chem. Chem. Phys.** 2022, 24, 17397-17416. (IF 3.676)

58. Dimitri G.M.; Meoni G.; Tenori L.; Luchinat C.; Pietro L.; PROPAG-AGEING Consortium. NMR Spectroscopy Combined with Machine Learning Approaches for Age Prediction in Healthy and Parkinson's Disease Cohorts through Metabolomic Fingerprints. **Applied Sciences**, 2022, 2(18), 8954; https://doi.org/10.3390/app12188954. (IF 2.838)

59. Vignoli A.; Meoni G.; Tenori L. Applications and Challenges for Metabolomics via Nuclear Magnetic Resonance Spectroscopy. **Applied Sciences**, 2022, 12 (9), 4655. https://doi.org/10.3390/app12094655. (IF 2.838)

60. 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, 122, 101828. doi: 10.1016/j.ssnmr.2022.101828. (IF : 2.812)

61. Martellini, T ; Sposato, L; Pucci, S; Meoni, G; Marinelli, C; Tenori, L; Luchinat, C; Giorgi, R; Sarti, C; Cincinelli, A. Influence of in-amphorae vinification on the molecular profile of Sangiovese and Cabernet Franc. **Flavour and Fragrances Journal**, 2022 Volume37, 219-233; https://doi.org/10.1002/ffj.3697. (IF 2.5)

BOOK chapters

Titolo: Fast 2D NMR to investigate dynamic events in biomolecules.
Autori: Francesco Bruno, Enrico Luchinat, Krzysztof Kazimierczuk and Enrico Ravera.
Libro: Fast 2D solution-state NMR: concepts and applications.
Editors: Jean-Nicolas Dumez and Patrick Giraudeau

Titolo: NMR-Based Metabolomics to Evaluate Individual Response to Treatments.
Autori: Vignoli A.; Meoni G.; Ghini V.; Di Cesare F.; Tenori L.; Luchinat C.; Turano P.
Libro: Handbook of Experimental Pharmacology
Editors: Claudio Luchinat, Veronica Ghini, Kathleen Stringer