

CERM Publications
(December 2017)

1. Liu, G., Levien, M., Karschin, N., Parigi, G., Luchinat, C., and Bennati, M., One-thousand fold enhancement of high field liquid nuclear-magnetic resonance signals at room temperature, **Nat.Chem.**, 9, 676-680, 2017 (IF 27.893).
2. Brancaccio, D., Gallo, A., Piccioli, M., Novellino, E., Ciofi-Baffoni, S., and Banci, L., [4Fe-4S] Cluster Assembly in Mitochondria and Its Impairment by Copper, **J.Am.Chem.Soc.**, 139, 719-730, 2017 (IF 13.858).
3. Camponeschi, F., Ciofi-Baffoni, S., and Banci, L., Anamorsin/Ndor1 Complex Reduces [2Fe-2S]-MitoNEET via a Transient Protein-Protein Interaction, **J.Am.Chem Soc.**, 139, 9479-9482, 2017 (IF 13.858).
4. Berruyer, P; Lelli, M.; Conley, MP; Silverio, DL; Widdifield, CM; Siddiqi, G; Gajan, D; Lesage, A; Coperet, C; Emsley, L. Three-Dimensional Structure Determination of Surface Sites **J.Am.Chem.Soc.** 139, 849-855, 2017 (IF 13.858)
5. Chaudhari, SR, Wisser, D, Pinon, AC; Berruyer, P, Gajan, D; Tordo, P ; Ouari, O, Reiter, C; Engelke, F; Coperet, Lelli, M.; C Dynamic Nuclear Polarization Efficiency Increased by Very Fast Magic Angle Spinning, **J.Am.Chem.Soc.** 139, 10609-10612, 2017 (IF 13.858)
6. Dubiela P, Aina R, Polak D, Geiselhart S, Humeniuk P, Bohle B, Alessandri S, Del Conte R, Cantini F, Borowski T, Bublin M, Hoffmann-Sommergruber K., Enhanced Pru p 3 IgE-binding activity by selective free fatty acid-interaction. **J Allergy Clin Immunol.** 2017 , S0091-6749(17)31094-1 (IF 13.081)
7. Takis, PG; Schaefer,H.; Spraul, M.; Luchinat,C.; Deconvoluting interrelationships between concentrations and chemical shifts in urine provides a powerful analysis tool **Nat.Comm.**, doi:10.1038/ s41467 -017-01587-0, 1662, 2017, (IF 12.124)
8. Giuntini, S., Balducci, E., Cerofolini, L., Ravera, E., Fragai, M., and Berti, F., Luchinat,C., Characterization of conjugation pattern in large polysaccharide-protein conjugates by NMR, **Angewandte Chemie**, 56, 14997-15001, 2017 (IF 11.994)
9. Lal, P., Cerofolini, L., D'Agostino, VG, Zucal, C., Fuccio, C., Bonomo, I, Dassi, E., Giuntini, S., Di Maio, D., Vishwakarma, V., Preet, R., Williams, SN, Fairlamb, MS, Munk, R, Lehrmann, E, Abdelmohsen, K, Elezgarai, SR, Luchinat, C., Novellino, E., Quattrone, A., Biasini, E, Manzoni, L, Gorospe,

- M, Dixon, DA, Seneci, P, Marinelli, L., Fragai, M., and Provenzani, A., Regulation of HuR structure and function by dihydrotanshione-I, **Nucleic Acids Res**, Doi: 10.1093/nar/gkx623, 2017 (IF 10.162).
10. Putignano V, Rosato A, Banci L, Andreini C., MetalPDB in 2018: a database of metal sites in biological macromolecular structures., **Nucleic Acids Res**. 2017, doi: 10.1093/nar/gkx989 (IF 10.162).
 11. Andralojc, W., Hiruma, Y., Liu, W.-M., Ravera, E., Nojiri, M., Parigi, G., Luchinat, C., and Ubbink, M., Identification of productive and futile encounters in an electron transfer protein complex, **Proc.Natl.Acad.Sci.USA**, 114, E1840-E1847, 2017 (IF 9.423).
 12. Moreno-Beltran, B., Guerra-Castellano, A., Diaz-Quintana, A., Del Conte, R., Garcia-Maurino, SM, Diaz-Moreno, S., Gonzalez-Arzola, K., Santos-Ocana, C., Velazquez-Campoy, A., De la Rosa, M. A., Turano, P., and Diaz-Moreno, I, Structural basis of mitochondrial dysfunction in response to cytochrome c phosphorylation at tyrosine 48, **Proc.Natl.Acad.Sci.USA**, 114, E3041-E3050, 2017 (IF 9.423).
 13. Pozzi, C., Ciambellotti, S., Bernacchioni, C., Di Pisa, F., Mangani, S., and Turano, P., Chemistry at the protein-mineral interface in L-ferritin assists the assembly of a functional (μ^3 -oxo)tris [(μ^2 -peroxo)] triiron(III) cluster, **Proc.Natl.Acad.Sci.USA**, 114, 2580-2585, 2017 (IF 9.423).
 14. Hart, CD, Vignoli, A., Tenori, L., Uy, G, Ta Van, T, Adebamowo, C., Hossain, SM, Biganzoli, L., Risi, E., Love, R, Luchinat, C., and Di Leo, A., Serum metabolomic profiles identify ER-positive early breast cancer patients at increased risk of disease recurrence in a multicentre population, **Clin Cancer Res**, doi 10.1158/1078-0432.CCR-16-1153, 2017 (IF 8.738).
 15. Cacciatore, S., Tenori, L., Tyekucheva, S., Luchinat, C., Bennett, RP, and MacIntyre, DA, KODAMA: an R package for knowledge discovery and data mining, **Bioinformatics**, 33, 621-623, Doi: 10.1093/bioinformatics/btw705, 2017 (IF 7.307).
 16. Kay, KL., Zhou, L., Tenori, L., Bradley, J., Singleton, C., Kihlken, M. A., Ciofi-Baffoni, S., and Le Brun, N. E., Kinetic analysis of copper transfer from a chaperone to its target protein mediated by complex formation, **Chem Commun.(Camb.)**, 53, 1397-1400, 2017 (IF 6.567).
 17. Jarvis, JA; Haies, I; Lelli, M; Rossini, AJ; Kuprov, I; Carravetta, M; Williamson, PTF Measurement of N-14 quadrupole couplings in biomolecular solids using indirect-detection ^{14}N solid-state NMR with DNP, **CHEMICAL COMMUNICATIONS**, 53, 12116-12119, 2017 (IF 6.319)
 18. Giustiniano, M., Daniele, S, Pelliccia, S., La Pietra, V, Pietrobono, D, Brancaccio, D, Cosconati, S., Messere, A, Giuntini, S., Cerofolini, L., Fragai,

- M., Luchinat, C., Taliani, S., La Regina, G, Da Settimo, F, Silvestri, R, Martini, C, Novellino, E., and Marinelli, L., Computer-aided identification and lead optimization of dual murine double minute 2 and 4 binders: structure-activity relationship studies and pharmacological activity, **J Med Chem**, doi: 10.1021/acs.jmedchem.7b00912, 2017 (IF 6.259).
19. Takis, PG, Tenori, L., Ravera, E., and Luchinat, C., Gelified biofluids for HRMAS 1H NMR analysis: the case of urine, **Anal.Chem.**, doi: 10.102/acs.analchem.6b04318, 2017 (IF 5.886).
20. Nasta, V., Giachetti, A., Ciofi-Baffoni, S., and Banci, L., Structural insights into the molecular function of human (2Fe-2S) BOLA1-GRX5 and (2Fe-2S) BOLA3-GRX5 complexes, **Biochim Biophys Acta** , 1861, 2119-2131, 2017 (IF 5.34).
21. Zanzoni, S., Pagano, K, D'Onofrio, M., Assfalg, M., Ciambellotti, S., Bernacchioni, C., Turano, P., Aime, S., Ragona, L., and Molinari, H., Unsaturated long chain fatty acids are preferred ferritin ligands enhancing iron biomineralization, **Chemistry**, 23, 9879-9887, 2017 (IF 5.317).
22. Vilona, D; Lachkar, D; Dumont, E; Lelli, M; Lacote, E. Elucidation of the Conformation of Polyglycine Organo-Polyoxotungstates: Evidence for Zipper Folding, **CHEMISTRY**, 23, 13323-13327, 2017 (IF 5.317)
23. Banci, L. and Luchinat, E., In cell NMR - a topical review, **IUCrJ**, 4, 108-118, 2017 (IF 5.316).
24. Bernacchioni, C., Ghini, V., Cencetti, F., Japtok, L., Donati, C., Bruni, P., and Turano, P., NMR metabolomics highlights sphingosine kinase-1 as a new molecular switch in the orchestration of aberrant metabolic phenotype in cancer cells, **Mol.Oncol.**, 11, 517-533, 2017 (IF 5.314).
25. Bertarello, A., Schubeis, T., Fuccio, C., Ravera, E., Fragai, M., Parigi, G., Emsley, L., Pintacuda, G., and Luchinat, C., Paramagnetic properties of a crystalline iron-sulfur protein by magic-angle spinning NMR spectroscopy, **Inorg Chem**, 56, 6624-6629, 2017 (IF 4.857).
26. Chatzikonstantinou, AV, Chatziathanasiadou, MV, Ravera, E., Fragai, M., Parigi, G., Gerothanassis, I. P., Luchinat, C., Stamatidis, HL, and Tzakos, AG, Enriching the biological space of natural products, through real time biotransformation monitoring: the NMR tube bioreactor, **Biochim Biophys Acta**, 17, 30321-30325, 2017 (IF 4.702).
27. Coletti A, Camponeschi F, Albini E, Greco FA, Maione V, Custodi C, Ianni F, Grohmann U, Orabona C, Cantini F, Macchiarulo A., Fragment-based approach to identify IDO1 inhibitor building blocks, **Eur J Med Chem**. 2017, 141:169-177 (IF 4.519)

28. van Zundert, GCP, Trellet, M., Schaarschmidt, J, Kurkcuoglu, Z, David, M, Verlato, M., Rosato, A., and Bonvin, A. M. J. J., The DisVis and powerFit web servers: explorative and integrative modeling of biomolecular complexes, **J Mol Biol**, 429, 399-407, 2017 (IF 4.517).
29. Suarez-Diez, M., Adam, J., Adamski, J, Chasapi, SA, Luchinat, C., Peters, A, Prehn, C, Santucci, C., Spyridonidis, A., Spyroulias, G. A., Tenori, L., Wang-Sattler, R, and Saccenti, E., Plasma and Serum Metabolite Association Networks: Comparability within and between Studies Using NMR and MS Profiling., **J. Proteome Res.**, 16, 2547-2559, 2017 (IF 4.268).
30. Hou, MM., Polykretis, P., Luchinat, E., Wang, X., Chen, SN, Zuo, HH, Yang, Y., Chen, JL, Ye, Y, Li, C., Banci, L., and Su, X. C., Structural insights into the first BIR domain of XIAP in solution and interaction with copper in vitro and in living cells, **Scientific Reports** 7, 16630, 2017, doi:10.1038/s41598-017-16723-5, (IF 4.259)
31. Luchinat, E., Barbieri, L., and Banci, L., A molecular chaperone activity of CCS restores the maturation of SOD1 fALS mutants, **Scientific Reports** 2017 7(1):17433. doi: 10.1038/s41598-017-17815-y (IF 4.259)
32. Sala, D., Ciambellotti, S., Giachetti, A., Turano, P., and Rosato, A., Investigation of the Iron(II) Release Mechanism of Human H-Ferritin as a Function of pH, **J.Chem Inf.Model.**, 57, 2112-2118, 2017 (IF 3.760).
33. Baronti, L., Hosek, T., Gil-Caballero, S., Raveh-Amit, H, Calçada, E. O., Ayala, I., Dinnyes, A., Felli, I. C., Pierattelli, R., and Brutscher, B., Fragment-based NMR study of the conformational dynamics in the bHLH transcription factor ASC11, **Biophys J.**, 112, 1366-1373, 2017 (IF 3.632).
34. Bemporad, F., Elia, F., Cantini, F., Chiti, F., and Dobson, C. M., Direct conversion of a globular protein from native-like to amyloid-like aggregates within bacterial inclusion bodies, **Biophys J.**, 112, 2540-2551, 2017 (IF 3.632).
35. Andreini, C., Rosato, A., and Banci, L., The relationship between environmental dioxygen and iron-sulfur proteins explored at the genome level, **PLoS ONE**, 12, e0171279-, 2017 (IF 3.54).
36. Canales Á, Rösinger M, Sastre J, Felli IC, Jiménez-Barbero J, Giménez-Gallego G, Fernández-Tornero C., Hidden α -helical propensity segments within disordered regions of the transcriptional activator CHOP. **PLoS One**, 12, e0189171. 2017 (IF 3.54).
37. Vignoli, A., Rodio, D. M., Bellizzi, A., Sobolev, A., Anzivino, E., Mischitelli, M., Tenori, L., Marini, F., Scrivo, R., Valensini, G., Francia, A., Morreale, M., Ciardi, MR, Iannetta, M., Capanella, C., Capitani, D., Mannina, L., Luchinat,

- C., and Pietropaolo, V., Nuclear magnetic resonance based metabolomic approach to study urines of chronic inflammatory rheumatic diseases, **Analytical and Bioanalytical Chemistry**, 409, 1405-1413, 2017 (IF 3.431)
38. Valasatava Y, Rosato A, Furnham N, Thornton JM, Andreini C., To what extent do structural changes in catalytic metal sites affect enzyme function? **J Inorg Biochem.** 79, 40-53, (IF 3.348)
39. Ghini, V., Di Nunzio, M., Tenori, L., Valli, V., Danesi, F., Capozzi, F., Luchinat, C., and Bordoni, A., Evidence of a DHA signature in the lipidome and metabolome of human hepatocytes, **Int.J.Mol.Sci.**, 18, E359-, 2017 (IF 3.257).
40. Belli, G., Busoni, S., Ciccarone, A., Coniglio, A., Esposito, M., Giannelli, M., Mazzoni, LN, Nocetti, L., Sghedoni, R., Tarducci, R., Zatelli, G., Anoja, RA, Belmonte, G., Bertolino, N., Betti, M., Biagini, C., Ciarmatori, A., Cretti, F., Fabbri, E., Fedeli, L., Filice, S., Fulcheri, CPL, Gasperi, C., Mangili, P., Mazzocchi, S., Meliado', G., Morzenti, S., Noferini, L., Oberhofer, N., Orsingher, L., Paruccini, N., Princigalli, G., Quattrocchi, M., Rinaldi, A, Scelfo, D., Freixas, GV, Tenori, L., Zucca, I., Luchinat, C., Gori, C., and Gobbi, G., Quality assurance multicenter comparison of different MR scanners for quantitative diffusion-weighted imaging, **J.Magn.Reson.Imaging**, 43, 213-219, 2017 (IF 3.25).
41. Brizzolara, S., Santucci, S., Tenori, L., Hertog, M., Nicolai, B., Stuerz, S., Zanella, A., and Tonutti, P., A metabolomics approach to elucidate apple fruit responses to static and dynamic controlled atmosphere storage, **Postharvest Biol.Tech.**, 127, 76-87, 2017 (IF3.248).
42. Cerofolini, L., Giuntini, S., Louka, A., Ravera, E., Fragai, M., and Luchinat, C., High-resolution solid state NMR characterization of ligand binding to a protein immobilized in a silica matrix, **J.Phys.Chem B**, 121, 8094-8101, 2017 (IF 3.302).
43. Pinon, AC; Schlagnitweit, J; Berruyer, P ; Rossini, AJ; Lelli, M ; Socie, E ; Tang, MX ; Pham, T ; Lesage, A; Schantz, S.; Measuring Nano- to Microstructures from Relayed Dynamic Nuclear Polarization NMR **J.Phys.Chem. B**, 121, 15993-16005, 2017 (IF 3.302).
44. Nogueira, O. M., Hosek, T., Calçada, E. O., Castiglia, F., Massimi, P., Banks, L., Felli, I. C., and Pierattelli, R., Monitoring HPV-16 E7phosphorylation events, **Virology**, 503, 70-75, 2017 (IF 3.200).
45. Barbieri, L., Luchinat, E., and Banci, L., Intracellular metal binding and redox behavior of human DJ-1, **J Biol Inorg Chem** doi: 10.1007/ s00775-017, 1509-5, 2017, (IF 2.894)

46. Calderone, V., Fragai, M., Gallo, G., and Luchinat, C., Solving the crystal structure of human calcium-free S100Z: the siege and conquer of one of the last S100 family strongholds, **J Biol Inorg Chem**, 22, 519-526, 2017 (IF 2.894)
47. McCartney, A., Vignoli, A., Hart, C., Tenori, L., Luchinat, C., Biganzoli, L., and Di Leo, A., De-escalating and escalating treatment beyond endocrine therapy in patients with luminal breast cancer, **Breast**, epub ahead of print, 2017 (IF 2.801).
48. Ravera, E., Parigi, G., and Luchinat, C., Perspectives on paramagnetic NMR from a life sciences infrastructure, **J. Magn Reson.**, 282, 154-169, 2017 (IF 2.432).
49. Lescanne, M, Skinner, S. P., Blok, A, Timmer, M., Cerofolini, L., Fragai, M., Luchinat, C., and Ubbink, M., Methyl group assignment using pseudocontact shifts with PARAssign, **J Biomol NMR**, doi: 10.1007/s10858-017-0136-3, 2017 (IF 2.410)
50. Basoglu, A., Baspinar, N., Tenori, L., Vignoli, A., and Gulersoy, E., Effects of boron supplementation on peripartum dairy cow's health, **Biol.Trace Elem.Res.**, Doi:10.1007/s12011-017-0971-9, 1-8, 2017 (IF 2.399).
51. Emsley J. W., M. Lelli, G. R. Luckhurst, and H. Zimmermann, ¹³C NMR study of the director distribution adopted by the modulated nematic phases formed by liquid-crystal dimers with odd numbers of atoms in their spacers **PHYSICAL REVIEW E** 96, 062702 (2017) (IF 2.366)
52. Doucet M, Becker KF, Björkman J, Bonnet J, Clément B, Daidone MG, Duyckaerts C, Erb G, Haslacher H, Hofman P, Huppertz B, Junot C, Lundeberg J, Metspalu A, Lavitrano M, Litton JE, Moore HM, Morente M, Naimi BY, Oelmueller U, Ollier B, Parodi B, Ruan L, Stanta G, Turano P, Vaught J, Watson P, Wichmann HE, Yuille M, Zaomi M, Zatloukal K, Dagher G. Quality Matters: 2016 Annual Conference of the National Infrastructures for **Biobanking, Biopreserv Biobank**. 2017, 3, :270-276 (IF 1.698)

BOOKS

1. P. Turano, NMR of Paramagnetic Species in Encyclopedia of Spectroscopy and Spectrometry (3rd Edition), vol 3, pp. 164-169, Editors JC Lindon, GE Tranter, DW Koppenaal, AP

2. Bertini, C. Luchinat, G. Parigi, E. Ravera, NMR of Paramagnetic Molecules, Elsevier, 2017.
3. Analytical Chemistry: Developments, Applications and Challenges in Food Analysis. Editors: Marcello Locatelli and Christian Celia, Chapter 5. NMR Methodologies in Food Analysis, Chapter 6. NMR Applications in Food Analysis: Part A; Chapter 7. NMR Applications in Food Analysis: Part B; Nova Science Publishers, 2017: