

**PUBLICATIONS** (\* indicates corresponding/co-corresponding authorship)

- 1) F. Bruno, R. Francischello, G. Bellomo, L. Gigli, A. Flori, L. Menichetti, L. Tenori, C. Luchinat, E. Ravera\* "Multivariate Curve Resolution for 2D solid-state NMR spectra", *Analytical Chemistry*, in press
- 2) M. Denis, C. Softley, S. Giuntini, M. Gentili, E. Ravera, G. Parigi, M. Fragai, G. Popowicz, M. Sattler, C. Luchinat, L. Cerofolini, C. Nativi "The photo-catalysed thiol-ene reaction: a new tag to yield fast, selective and irreversible paramagnetic tagging of proteins", *ChemPhysChem*, in press
- 3) A. Schirò, A. Carlon, G. Parigi, G. Murshudov, V. Calderone, E. Ravera\*, C. Luchinat "On the complementarity of X-ray and NMR data", *Journal of Structural Biology* :X 2020, 100019 IF not available
- 4) A. Carlon, L. Gigli, E. Ravera, G. Parigi, A.M. Gronenborn, C. Luchinat "Assessing structural preferences of unstructured protein regions by NMR", *Biophysical Journal*, 2019, 117 (10), 1948-1953, IF2018=3.665
- 5) M. Fragai, E. Ravera, F. Tedoldi, C. Luchinat, G. Parigi "Relaxivity of Gd-Based MRI Contrast Agents in Crosslinked Hyaluronic Acid as a Model for Tissues", *ChemPhysChem*, 2019, 20 (17), 2204-2209, IF2018=3.077
- 6) E. Ravera, G. Parigi, C. Luchinat "What are the methodological and theoretical prospects for paramagnetic NMR in structural biology? A glimpse into the crystal ball", *J. Magn. Reson.*, 2019, 306, 173-179, IF2018=2.689
- 7) L. Cerofolini, M. Fragai, E. Ravera, C.A. Diebolder, L. Renault, V. Calderone "Integrative Approaches in Structural Biology: A More Complete Picture from the Combination of Individual Techniques", *Biomolecules*, 2019, 9 (8), 370
- 8) G. Parigi, E. Ravera, C. Luchinat "Magnetic susceptibility and paramagnetism-based NMR", *Progress in NMR spectroscopy*, 2019, 114-115, 211-236, IF2018=8.848
- 9) L. Cerofolini, J.M. Silva, E. Ravera, M. Romanelli, C.F.G.C. Geraldès, A. Macedo, M. Fragai, G. Parigi, C. Luchinat "How Do Nuclei Couple to the Magnetic Moment of a Paramagnetic Center? A New Theory at the Gauntlet of the Experiments", *J. Phys. Chem. Lett.*, 2019, 10(13),3610-3614, IF2018=7.329
- 10) L. Cerofolini, S. Giuntini, E. Ravera, C. Luchinat, F. Berti, M. Fragai "Structural characterization of a protein adsorbed on aluminum hydroxide adjuvant in vaccine formulation", *npj Vaccines*, 2019, 4, 20, IF2018=5.020.
- 11) G. Bellomo, S. Bologna, L. Cerofolini, S. Paciotti, L. Gattichi, E. Ravera, L. Parnetti, M. Fragai, C. Luchinat, "Dissecting the Interactions between Human Serum Albumin and  $\alpha$ -Synuclein: New Insights on the Factors Influencing  $\alpha$ -Synuclein Aggregation in Biological Fluids", *J. Phys. Chem. B*, 2019, 123(20), 4380-4386, IF2018=2.932
- 12) G. Parigi, L. Benda, E. Ravera, M. Romanelli, C. Luchinat, "Pseudocontact shifts and paramagnetic susceptibility in classical and quantum chemistry theories", *J Chem Phys*, 2019, 150 (14), 144101, IF2017=2.997, preprint arXiv:1804.09055
- 13) J.M. Silva, L. Cerofolini, S. Giuntini, V. Calderone, C.F.G.C. Geraldès, A.L. Macedo, M. Fragai, G. Parigi, E.Ravera, C. Luchinat, "Metal centers in biomolecular solid-state NMR", *J. Struct. Biol.*, 2019, 206(1), 99-109, IF2018=3.02
- 14) L. Cerofolini, S. Giuntini, L. Barbieri, M. Pennestri, A. Codina, M. Fragai, L. Banci, E. Luchinat, E. Ravera\*, "Real-time insights into biological events: in-cell processes and protein-ligand interactions", *Biophys. J.*, 2019, 116 (2), 239-247, IF2018=3.665

- 15) L. Cerofolini, S. Giuntini, A. Carlon, E. Ravera\*, V. Calderone, M. Fragai, G. Parigi, C. Luchinat, "Characterization of PEGylated asparaginase: new opportunities from NMR analysis of large pegylated therapeutics", *Chem. Eur. J.*, 2019, 25(8), 1984-1991, IF2018=5.160
- 16) E. Ravera, P.G. Takis, M. Fragai, G. Parigi, C. Luchinat, "NMR Spectroscopy and Metal Ions in Life Sciences", *European Journal of Inorganic Chemistry* 2018 (44), 4752-4770, IF2017=2.507
- 17) J.M. Silva, S. Giuntini, L. Cerofolini, C.F.G.C. Geraldes, A.L. Macedo, E. Ravera, M. Fragai, C. Luchinat, V. Calderone, "Non-crystallographic symmetry in proteins: Jahn–Teller-like and Butterfly-like effects?", *J. Biol. Inorg. Chem.*, IF2017=2.952
- 18) A. Karmakar, M.S. Dodd, S. Agnihotri, E. Ravera, V.K. Michaelis, "Cu(II)-Doped Cs<sub>2</sub>SbAgCl<sub>6</sub> Double Perovskite: A Lead-Free, Low-Bandgap Material", *Chem. Mater.*, 2018, 30, 8280-8290, IF2017=9.890
- 19) L. Gigli, W. Andralojc, A. Dalaloyan, G. Parigi, E. Ravera, D. Goldfarb, C. Luchinat, "Assessing protein conformational landscapes: integration of DEER data in Maximum Occurrence analysis", *Phys. Chem. Chem. Phys.*, 2018, 20, 27429-27438 IF2017=3.906
- 20) A. Carlon, E. Ravera, G. Parigi, G.N. Murshudov, C. Luchinat, "Joint X-ray/NMR structure refinement of multidomain/multisubunit systems", *J. Biomol. NMR*, 2018, in press, IF2017=2.534
- 21) G. Bellomo, S. Bologna, L. Gonnelli, E. Ravera, M. Fragai, M. Lelli, C. Luchinat, "Aggregation kinetics of the Aβ<sub>1–40</sub> peptide monitored by NMR", *Chem. Commun.*, 2018, 54, 7601-7604, IF2017=6.290
- 22) G. Parigi, E. Ravera, M. Bennati, C. Luchinat, "Understanding Overhauser Dynamic Nuclear Polarisation through NMR relaxometry", *Mol. Phys.*, 2018, in press, IF2017=1.704
- 23) E. Ravera, A. Carlon, M. Fragai, G. Parigi, C. Luchinat, "Paramagnetic NMR as a new tool in structural biology", *Emerging topics in Life Sciences*, 2018, 2(1), 19-28 IF not available
- 24) A. Louka, I Matlahov, S. Giuntini, L. Cerofolini, A. Cavallo, S. Pillozzi, E. Ravera\*, M. Fragai, A. Arcangeli, A. Ramamoorthy, G. Goobes, C. Luchinat, "Engineering L-asparaginase for spontaneous formation of calcium phosphate bioinspired microreactors", *Phys.Chem.Chem.Phys.*, 2018, 20, 12719-12726, IF2017=3.906
- 25) S. Rumpel, E. Ravera, C. Sommer, E. Reijerse, C. Farès, C. Luchinat, W. Lubitz, "1H NMR Spectroscopy of [FeFe] Hydrogenase: Insight into the Electronic Structure of the Active Site, *J. Am. Chem. Soc.*, 2018, 140, 131-134, IF2017=14.357
- 26) A.V.Chatzikonstantinou, M.V.Chatziathanasiadou, E. Ravera, M. Fragai, G. Parigi, I.P. Gerothanassis, C. Luchinat, H.L. Stamatis, A.G. Tzakos, "Enriching the biological space of natural products, through real time biotransformation monitoring: the NMR tube bioreactor", *B.B.A. General Subjects*, 2018, 1862, 1-8, IF2017=3.679
- 27) L. Cerofolini, T. Staderini, S. Giuntini, E. Ravera, M. Fragai, G. Parigi, R. Pierattelli, C. Luchinat, "Long-Range paramagnetic NMR data can provide a closer look on metal coordination in metalloproteins", *J.Biol.Inorg.Chem.*, 23, 71-80, IF2017=2.952
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- 29) S. Giuntini, L. Cerofolini, E. Ravera\*, M. Fragai, C. Luchinat, "Atomic structural details of a protein grafted onto gold nanoparticles", *Sci. Rep.*, 2017, 7, 17934, IF2017=4.122
- 30) E. Ravera, G. Parigi, C. Luchinat, "Perspectives on paramagnetic NMR from a life sciences infrastructure", *J. Magn. Reson.*, 2017, 282, 154-169, IF2017=2.586
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- 32) A. Bertarello, T. Schubeis, C. Fuccio, E. Ravera, M. Fragai, G. Parigi, C. Luchinat, G. Pintacuda, *Inorganic Chemistry*, 2017, 56, 6624-6629, IF2017 = 4.700;
- 33) W. Andrałojć, Y. Hiruma, W.-M. Liu, E. Ravera, M. Nojiri, G. Parigi, C. Luchinat, M. Ubbink, "Identification of productive and futile encounters in an electron transfer protein complex", *Proc. Nat. Acac. Sci. USA*, 2017, 114 (10), E1840-E1847, IF2017=9.504;
- 34) P.G. Takis, L. Tenori, E. Ravera, C. Luchinat, "Gelified biofluids for HRMAS 1H NMR analysis: the case of urine", *Analytical Chemistry*, 2017, 89 (2), 1054-1058, IF2017 = 6.042;
- 35) L. Benda, J. Mares, E. Ravera, G. Parigi, C. Luchinat, M. Kaupp, J. Vaara, "Pseudo-Contact NMR Shifts over the Paramagnetic Metalloprotein CoMMP-12 from First Principles", *Angewandte Chemie*, 2016, 55 (47), 14713-14717, IF2016=11.994;
- 36) E. Ravera, T. Martelli, Y. Geiger, M. Fragai, G. Goobes, C. Luchinat, "Biosilica and bioinspired silica studied by solid-state NMR", *Coord. Chem. Rev.* 2016, in press, IF2015=13.324;
- 37) E. Ravera\*, L. Cerofolini, T. Martelli, A. Louka, M. Fragai, C. Luchinat, "1H-detected solid-state NMR of proteins entrapped in bioinspired silica: a new tool for biomaterials characterization" *Scientific Reports* , 2016, 6, 27851, IF2016=4.259;
- 38) E. Ravera, G. Parigi, C. Luchinat, "Basic facts and perspectives of Overhauser DNP NMR", *J. Magn. Reson.*, 2016, 264,78-87, IF2016=2.432;
- 39) A. Carlon, E. Ravera, W. Andrałojć, G. Parigi, G.N. Murshudov, C. Luchinat, "How to tackle protein structural data from solution and solid state: An integrated approach", *Progress in NMR spectroscopy*, 2016, 92–93, 54–70, IF2016=5.971;
- 40) A. Carlon, E. Ravera, J. Hennig, G. Parigi, M. Sattler and C. Luchinat, "Improved accuracy from joint X-ray and NMR refinement of a protein-RNA complex structure", *J. Am. Chem. Soc.*, 2016, 38,1601–1610, IF2016=13.858;
- 41) E. Ravera, S. Ciambellotti, L. Cerofolini, T. Martelli, T. Kozyreva, C. Bernacchioni, S. Giuntini, M. Fragai, P. Turano, C. Luchinat, "Solid-state NMR of PEGylated Proteins", *Angewandte Chemie*, 2016, 128, 2492–2495, IF2016=11.994;
- 42) E. Ravera, L. Sgheri, G. Parigi, C. Luchinat, "A critical assessment of methods to recover information from averaged data", *PCCP*, 2016, 18, 5686-5701, IF2016=4.123;
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- 44) T. Martelli, E. Ravera, A. Louka, L. Cerofolini, M. Hafner, M. Fragai, C.F.W. Becker, C. Luchinat, "Atomic-Level Quality Assessment of Enzymes Encapsulated in Bioinspired Silica", *Chem. Eur. J.*, 2016, 22 (1), 425-432, IF2015=5.317;

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- 48) W. Andralojc, K. Berlin, D. Fushman, C. Luchinat, G. Parigi, E. Ravera, L. Sgheri, "Information content of long-range NMR data for the characterization of conformational heterogeneity", *J. Biomol. NMR*, 2015, 62 (3), 353-371, IF2015=3.439;
- 49) J.-H. Ardenkjaer-Larsen, G.S. Boebinger, A. Comment, S.B. Duckett, A.S. Edison, F. Engelke, C. Griesinger, R.G. Griffin, C. Hilty, H. Maeda, G. Parigi, T.F. Prisner, E. Ravera, G.J.M. van Bentum, S. Vega, A. Webb, C. Luchinat, H. Schwalbe, and L. Frydman, "Facing and overcoming biomolecular NMR's sensitivity challenges", *Angewandte Chemie*, 2015, 54 (32), 9162-9185, IF2015=11.709;
- 50) E. Ravera, T. Schubeis, T. Martelli, M. Fragai, G. Parigi, C. Luchinat, "NMR of sedimented, fibrillized, silica-entrapped and microcrystalline (metallo)proteins", *J. Magn. Reson* 2015, 253, 60-70, IF2015=2.889;
- 51) M. Rinaldelli, A. Carlon, E. Ravera, G. Parigi, C. Luchinat, "FANTEN: a new web-based interface for the analysis of magnetic anisotropy-induced NMR data", *J. Biomol. NMR* 2015, 61 (1), 21-34, IF2015=3.439;
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- 53) W. Andralojc, C. Luchinat, G. Parigi, E. Ravera, "Exploring Regions of Conformational Space Occupied by Two-Domain Proteins", *J. Phys. Chem. B* 2014, 47 (10), 3118-3126, IF2014=3.302;
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- 62) C.Luchinat, G.Parigi and E.Ravera, "Can metal ion complexes be used as polarizing agents for solution DNP? A theoretical discussion", *J. Biomol. NMR* 2014, 58(4), 239-249, IF2014=3.141;
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- 66) A. Bhaumik, C. Luchinat, G. Parigi, E. Ravera and M. Rinaldelli, "NMR crystallography on paramagnetic systems: solved and open issues", *CrystEngComm* 2013, 15(43), 8639-8656, IF2013=3.858;
- 67) M. Fragai, C.Luchinat, G.Parigi and E.Ravera, "Practical considerations over spectral quality in solid state NMR spectroscopy of soluble proteins", *J. Biomol. NMR* 2013, 57(2), 155-166, IF2013=3.305;
- 68) C.Luchinat, G.Parigi and E.Ravera, "Water and Protein Dynamics in Sedimented Systems: a Relaxometric Investigation", *ChemPhysChem.* 2013, 14(13), 3156-3161, IF2013=3.360;
- 69) E.Ravera, G.Parigi, A.Mainz, T.L.Religa, B.Reif and C.Luchinat, "Experimental Determination of Microsecond Reorientation Correlation Times in Protein Solutions", *J. Phys. Chem. B*, 2013, 117(13), 3548-3553, IF2013=3.377;
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- 76) C.Luchinat, G.Parigi, E.Ravera and M.Rinaldelli, "Solid-State NMR Crystallography through Paramagnetic Restraints", *J.Am.Chem.Soc.* 2012, 134(11), 5006-5009, IF2012=10.677;
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- 79) I.Bertini, A.Giachetti, C.Luchinat, G.Parigi, M.V.Petoukhov, R.Pierattelli, E.Ravera and D.I.Svergun, "Conformational Space of Flexible Biological Macromolecules from Average Data", *J.Am.Chem.Soc.* 2010, 132(38), 13553-8, IF2010=9.023.

### Non-Peer Reviewed Publications

- 1) G. Parigi, L. Benda, E. Ravera, M. Romanelli, C. Luchinat, "Pseudocontact shifts and paramagnetic susceptibility in classical and quantum chemistry theories", *ArXiv*, 2018
- 2) E.Ravera, "Paramagnetic NMR in structural biology: from the specialist's toolbox to everyday research", *Biotechniques*, 2018
- 3) C. Luchinat, G. Parigi, E. Ravera, "The competitive world of RAS biology", *Nature Chemical Biology* 2014, 10 (3), 173-174, IF2014=12.996;

### Authored books

- 1) I. Bertini, C. Luchinat, G. Parigi and E. Ravera, "NMR of Paramagnetic Molecules: Applications to Metallobiomolecules and Models", Elsevier, 2016

### Edited books

- 1) C. Luchinat, G. Parigi and E. Ravera, "Paramagnetism in Experimental Biomolecular NMR", RSC, 2018

### Book chapters

- 1) L. Cerofolini, E. Ravera\*, M. Fragai, C. Luchinat "NMR of Immobilized Enzymes", *Methods in Molecular Biology - "Immobilization of Enzymes and Cells"* – Editors: J.M. Guisan, J.M.Bolivar, F. Lopez-Gallego, J. Rocha-Martin, 2020, 363-383
- 2) A.V. Chatzikonstantinou, A.D. Tsailanis, I.P. Gerothanassis, H. Stamatis, E. Ravera, M. Fragai, C. Luchinat, G. Parigi, A. G. Tzakos "The NMR tube bioreactor", *Methods in Enzymology – "Chemical and Synthetic Biology Approaches To Understand Cellular Functions - Part C"* – Editor: A.K.Shukla, 2019, 633, 71-101
- 3) W. Andralojc, E. Ravera\* "Treating Biomolecular Conformational Variability" in "Paramagnetism in Experimental Biomolecular NMR", see above
- 4) W.T. Franks, B.-J. van Rossum, B. Bardiaux, E. Ravera, G. Parigi, C. Luchinat, H. Oschkinat "Microcrystalline Proteins—An Ideal Benchmark for Methodology Development" in "NMR

of Biomolecules: Towards Mechanistic Systems Biology” – Editors: I. Bertini, K. McGreevy,  
G. Parigi, 2012, 376-392