

Publications

153. 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) doi.org/10.1021/acsabm.2c00892
152. G. Licciardi, D. Rizzo, M. Salobehaj, L. Massai, A. Geri, L. Messori, E. Ravera, M. Fragai, G. Parigi, “Large protein assemblies for high relaxivity contrast agents: the case of gadolinium-labeled asparaginase”, *Bioconj. Chem.* (2022) 33, 2411-2419.
151. L. Cerofolini, G. Parigi, E. Ravera, M. Fragai, C. Luchinat, “Solid-state NMR methods for the characterization of bioconjugations and protein-material interactions”, *Solid State Nucl. Magn. Reson.* (2022) 122, 101828 (14 pages).
150. E. Ravera, 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 (Perspective article).
149. G. Parigi, E. Ravera, C. Luchinat, “Paramagnetic effects in NMR for protein structures and ensembles: studies of metalloproteins”, *Curr. Opin. Struct. Biol.* (2022) 74, 102386 (9 pages).
148. L. Lang, E. Ravera, G. Parigi, C. Luchinat, F. Neese, “Theoretical analysis of the long-distance limit of NMR chemical shieldings”, *J. Chem. Phys.* (2022) 156, 154115 (21 pages).
147. F. Carniato, M. Ricci, L. Tei, F. Garello, E. Terreno, E. Ravera, G. Parigi, C. Luchinat, M. Botta, “High relaxivity with no coordinated waters: a seemingly paradoxical behavior of [Gd(DOTP)]⁵⁻ embedded into nanogels”, *Inorg. Chem.* (2022) 61, 5380-5387.
146. G. Licciardi, D. Rizzo, E. Ravera, M. Fragai, G. Parigi, C. Luchinat, “Not only manganese, but fruit component effects dictate the efficiency of fruit juice as oral magnetic resonance imaging contrast agent”, *NMR in Biomed.* (2021) e4623.
145. L. Gigli, S. Di Grande, E. Ravera, G. Parigi, C. Luchinat, “NMR for Single Ion Magnets”, *Magnetochemistry* (2021) 7, 96.
144. Z. Wang, S. Pisano, V. Ghini, P. Kadeřávek, M. Zachrdla, P. Pelupessy, M. Kazmierczak, T. Marquardsen, J.-M. Tyburn, G. Bouvignies, G. Parigi, C. Luchinat, F. Ferrage, “Detection of metabolite-protein interactions in complex biological samples by high-resolution relaxometry: towards interactomics by NMR”, *J. Am. Chem. Soc.* (2021) 143, 9393–9404.
143. G. Parigi, E. Ravera, M. Fragai, C. Luchinat, “Unveiling protein dynamics in solution with field-cycling NMR relaxometry”, *Prog. NMR Spectrosc.* (2021), 124–125, 85–98.
142. M. Yon, S. Gineste, G. Parigi, Lonetti, B., L. Gibot, D. Talham, J.-D. Marty, C.

Mingotaud, “Hybrid Polymeric Nanostructures Stabilized by Zirconium and Gadolinium ions for Use as Magnetic Resonance Imaging Contrast Agents”, *ACS Applied Nano Materials* (2021), 4, 4974-4982.

141. E. Ravera, L. Cerofolini, M. Fragai, G. Parigi, C. Luchinat, “Characterization of lanthanoid-binding proteins using NMR spectroscopy”, *Methods Enzymol.* (2021) 651, 103-137. In: “Rare-Earth Element Biochemistry: Characterization and Applications of Lanthanide-Binding Biomolecules”, J. A. Cotruvo Jr. (serial volume editor), Elsevier.

140. E. Ravera, L. Gigli, E.A. Sutura, V. Calderone, M. Fragai, G. Parigi, C. Luchinat, “A high-resolution view of the coordination environment in a paramagnetic metalloprotein from its magnetic properties” *Angew. Chem. Int. Ed.* (2021) 60, 14960-14966.

139. E. Ravera, L. Gigli, B. Czarniecki, L. Lang, R. Kümmerle, G. Parigi, M. Piccioli, F. Neese, C. Luchinat, “A Quantum Chemistry View on Two Archetypical Paramagnetic Pentacoordinate Nickel(II) Complexes Offers a Fresh Look on Their NMR Spectra”, *Inorg. Chem.* (2021) 60, 2068–2075.

138. G. Bellomo, E. Ravera, V. Calderone, M. Botta, M. Fragai, G. Parigi, C. Luchinat, “Revisiting paramagnetic relaxation enhancements in slowly rotating systems: how long is the long range?”, *Magn. Reson.* (2021) 2, 25–31.

137. D. Rizzo, E. Ravera, M. Fragai, G. Parigi, C. Luchinat, “Origin of the MRI contrast in natural and hydrogel formulation of pineapple juice”, *Bioinorg. Chem. Appl.* (2021) 6666018 (12 pages)

136. D. M. Selegato, C. Bracco, C. Giannelli, G. Parigi, C. Luchinat, L. Sgheri, E. Ravera, “Comparison of Different Reweighting Approaches for the Calculation of Conformational Variability of Macromolecules from Molecular Simulations”, *ChemPhysChem* (2021) 22, 127–138.

135. F. Carniato, L. Tei, M. Botta, E. Ravera, M. Fragai, G. Parigi, C. Luchinat, “¹H NMR Relaxometric Study of Chitosan-Based Nanogels Containing Mono- and Bis-Hydrated Gd(III) Chelates: Clues for MRI Probes of Improved Sensitivity”, *ACS Appl. Bio Mater.* (2020) 3, 9065–9072.

134. L. Lang, E. Ravera, G. Parigi, C. Luchinat, F. Neese, “Solution of a Puzzle: High-Level Quantum-Chemical Treatment of Pseudocontact Chemical Shifts Confirms Classic Semiempirical Theory”, *J. Phys. Chem. Lett.* (2020) 11, 8735-8744.

133. E. Ravera, M. Fragai, G. Parigi, C. Luchinat, “Different flavors of diffusion in paramagnetic systems: Unexpected NMR signal intensity and relaxation enhancements”, *J. Magn. Reson. Open* (2020) 2-3, 100003 (Concept paper).

132. S.M. McLeod, L. Robison, G. Parigi, A. Olszewski, R.J. Drout, X. Gong, T. Islamoglu, C. Luchinat, O.K. Farha, T.J. Meade, “Maximizing Magnetic Resonance Contrast in Gd(III) Nanoconjugates: Investigation of Proton Relaxation in Zirconium Metal–Organic Frameworks”, *ACS Appl. Mater. Interfaces* (2020), 12, 41157-41166.

131. E.I. Vrettos, I.E. Valverde, A. Mascarini, P.N. Pallier, L. Cerofolini, M. Fragai, G. Parigi, B. Hirmiz, N. Bekas, N.M. Grob, E. Stylos, H. Shaye, M. Del Borgo, M.-I. Aguilar, F. Magnani, N. Syed, T. Crook, E. Waqif, E. Ghazaly, V. Cherezov, R.E. Widdop, C. Luchinat, A.T. Michael-Titus, T.L. Mindt, A.G. Tzakos, "Single Peptide Backbone Surrogate Mutations to Regulate Angiotensin GPCR Subtype Selectivity", *Chem. Eur. J.* (2020) 26, 10690-10694.
130. A.V. Chatzikonstantinou, A. Tsailanis, I.P. Gerothanassis, H. Stamatis, E. Ravera, M. Fragai, C. Luchinat, G. Parigi, A.G. Tzakos, "The NMR tube bioreactor", *Methods Enzymol.* (2020) 633, 71-101. In "Chemical and Synthetic Biology Approaches to Understand Cellular Functions", Part C, A. Shukla (serial volume editor), Elsevier.
129. 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 photocatalysed thiol-ene reaction: a new tag to yield fast, selective and reversible paramagnetic tagging of proteins", *ChemPhysChem* (2020) 21, 863-869.
128. A. Schirò, A. Carlon, G. Parigi, G. Murshudov, V. Calderone, E. Ravera, C. Luchinat, "On the complementarity of X-ray and NMR data", *J. Struct. Biol.: X* (2020) 4, 100019.
127. A. Carlon, L. Gigli, E. Ravera, G. Parigi, A.M. Gronenborn, C. Luchinat, "Assessing structural preferences of unstructured protein regions by NMR", *Biophys. J.* (2019) 117, 1948-1953.
126. 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, 2204-2209.
125. G. Parigi, E. Ravera, C. Luchinat, "Magnetic susceptibility and paramagnetism-based NMR" *Prog. NMR Spectrosc.* (2019) 114-115, 211-236.
124. 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.
123. A. Carlon, E. Ravera, G. Parigi, G.N. Murshudov, C. Luchinat, "Joint X-ray/NMR structure refinement of multidomain/multisubunit systems", *J. Biomol. NMR* (2019) 73, 265-278.
122. L. Cerofolini, J. Malanho Silva, E. Ravera, M. Romanelli, C.F.G.C. Geraldes, 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, 3610-3614.
121. N. Rezaei-Ghaleh, G. Parigi, M. Zweckstetter, "Reorientational Dynamics of Amyloid- β from NMR Spin Relaxation and Molecular Simulation", *J. Phys. Chem. Lett.* (2019) 10, 3369-3375.
120. H. Li, G. Parigi, C. Luchinat, T.J. Meade, "Bimodal Fluorescence-Magnetic Resonance Contrast Agent for Apoptosis Imaging", *J. Am. Chem. Soc.* (2019) 141, 6224-6233.
119. G. Parigi, L. Benda, E. Ravera, M. Romanelli, C. Luchinat, "Pseudocontact shifts and paramagnetic susceptibility in semiempirical and quantum chemistry theories", *J. Chem. Phys.* (2019) 150, 144101 (1-11) [arXiv:1804.09055].

118. J. Malanho Silva, L. Cerofolini, S. Giuntini, V. Calderone, C. Geraldès, A. Macedo, G. Parigi, M. Fragai, E. Ravera, C. Luchinat, “Metal centers in biomolecular solid-state NMR”, *J. Struct. Biol.* (2019) 206, 99-109.
117. G. Parigi, E. Ravera, M. Bennati, C. Luchinat, “Understanding Overhauser Dynamic Nuclear Polarisation through NMR relaxometry”, *Mol. Phys.* (2019) 117, 888-897.
116. 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”, *Chemistry Eur. J.* (2019) 25, 1984-1991.
115. L. Gigli, W. Andrałójć, 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.
114. E. Ravera, P.G. Takis, M. Fragai, G. Parigi, C. Luchinat, “NMR Spectroscopy and Metal Ions in Life Sciences”, *Eur. J. Inorg. Chem.* (2018) 4752-4770.
113. B. Wienen-Schmidt, H.R.A. Jonker, T. Wulsdorf, H.-D. Gerber, K. Saxena, D. Kudlinzki, S. Sreeramulu, G. Parigi, C. Luchinat, A. Heine, H. Schwalbe, G. Klebe, “Paradoxically, Most Flexible Ligand Binds Most Entropy-Favored: Intriguing Impact of Ligand Flexibility and Solvation on Drug-Kinase Binding”, *J. Med. Chem.* (2018) 61, 5922-5933.
112. N. Rezaei-Ghaleh, G. Parigi, A. Soranno, A. Holla, S. Becker, B. Schuler, C. Luchinat, M. Zweckstetter, “Local and Global Dynamics in Intrinsically Disordered Synuclein”, *Angew.Chem.Int.Ed.* (2018) 57, 15262-15266.
111. L.M. Lilley, K. Du, M.D. Krzyaniak, G. Parigi, C. Luchinat, T.D. Harris, T.J. Meade, “Effect of magnetic coupling on water proton relaxivity in a series of transition metal Gd^{3+} complexes”, *Inorg. Chem.* (2018) 57, 5810-5819.
110. 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, 19-28.
109. S. Gineste, E. Di Cola, B. Amouroux, U. Till, J.-D. Marty, A.-F. Mingotaud, C. Mingotaud, F. Violleau, D. Berti, G. Parigi, C. Luchinat, S. Balor, M. Sztucki, B. Lonetti, “Mechanistic insights into polyion complex associations”, *Macromolecules* (2018) 51, 1427-1440.
108. 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.* (2018) 23, 71-80.
107. A. Chatzikonstantinou, M. Chatziathanasiadou, E. Ravera, M. Fragai, G. Parigi, I. Gerothanassis, C. Luchinat, H. Stamatis, A. Tzakos, “Enriching the biological space of natural products, through real time biotransformation monitoring: the NMR tube bioreactor”, *BBA - General Subjects* (2018) 1862, 1-8.
106. E. Ravera, G. Parigi, C. Luchinat, “Perspectives on paramagnetic NMR from a life sciences infrastructure”, *J. Magn. Reson.* (2017) 282, 154-169.
105. A. Bertarello, T. Schubeis, C. Fuccio, E. Ravera, M. Fragai, G. Parigi, L. Emsley, G. Pintacuda, C. Luchinat, “Paramagnetic Properties of a Crystalline Iron-Sulfur Protein by Magic-Angle Spinning NMR Spectroscopy”, *Inorg. Chem.* (2017) 56, 6624-6629.
104. W. Andrałójć, 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. Natl. Acad. Sci. USA* (2017) 114, E1840-E1847.
103. G. Liu, M. Levien, N. Karschin, G. Parigi, C. Luchinat, M. Bennati, “One-thousand fold enhancement of high field liquid nuclear-magnetic resonance signals at room temperature”, *Nat. Chem.* (2017) 9, 676-680.
102. L. Benda, J. Mareš, E. Ravera, G. Parigi, C. Luchinat, M. Kaupp, J. Vaara, “Pseudo-contact NMR shifts over a paramagnetic metalloprotein (CoMMP-12) from first

principles”, *Angew.Chem.Int.Ed.* (2016) 55, 14713-14717.

101. N. Rammohan, K.W. MacRenaris, L.K. Moore, G. Parigi, D.J. Mastarone, L.M. Manus, L.M. Lilley, A.T. Preslar, E.A. Waters, A. Filicko, C. Luchinat, D. Ho, T.J. Meade, “Nanodiamond-Gadolinium(III) Aggregates for Tracking Cancer Growth *In Vivo* at High Field”, *Nano Letters* (2016) 16, 7551–7564.

100. A. Carlon, E. Ravera, J. Hennig, G. Parigi, M. Sattler, C. Luchinat, “Improved accuracy from joint X-ray and NMR refinement of a protein-RNA complex structure”, *J. Am. Chem. Soc.* (2016) 138, 1601-1610.

99. E. Ravera, C. Luchinat, G. Parigi, “Basic facts and perspectives of Overhauser DNP NMR”, *J. Magn. Reson.* (2016) 264, 78-87.

98. 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”, *Prog. NMR Spectrosc.* (2016) 92-93, 54-70.

97. E. Ravera, L. Sgheri, G. Parigi, C. Luchinat, “A critical assessment of methods to recover information from averaged data”, *Phys. Chem. Chem. Phys.* (2016) 18, 5686-5701.

96. W. Andrałojć, E. Ravera, L. Salmon, G. Parigi, H.M. Al-Hashimi, C. Luchinat, “Interhelical conformational preferences of HIV-1 TAR-RNA from Maximum Occurrence analysis of NMR data and Molecular Dynamics simulations”, *Phys. Chem. Chem. Phys.* (2016) 18, 5743-5752.

95. E. Ravera, D. Shimon, A. Feintuch, D. Goldfarb, S. Vega, A. Flori, C. Luchinat, L. Menichetti, G. Parigi, “The Effect of Gd on trityl-based Dynamic Nuclear Polarisation in Solids”, *Phys. Chem. Chem. Phys.* (2015) 17, 26969-26978.

94. E. Ravera, M. Fragai, G. Parigi, C. Luchinat, “Differences in dynamics between cross-linked and non-cross-linked hyaluronates measured by using fast-field-cycling relaxometry”, *ChemPhysChem* (2015) 16, 2803-2809.

93. W. Andrałojć, 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, 353-371.

92. M. Rotz, K. Culver, G. Parigi, K. MacRenaris, C. Luchinat, T. Odom, T.J. Meade, “High Relaxivity Gd(III)-DNA Gold Nanostars: Investigation of Shape Effects on Proton Relaxation”, *ACS Nano* (2015) 9, 3385-3396.

91. J.-H. Ardenkjaer-Larsen, G.S. Boebinger, A. Comment, S. Duckett, A. Edison, F. Engelke, C. Griesinger, R.G. Griffin, C. Hilty, H. Maeda, G. Parigi, T. Prisner, E. Ravera, J. van Bentum, S. Vega, A. Webb, C. Luchinat, H. Schwalbe, L. Frydman, “Facing and overcoming sensitivity challenges in biomolecular NMR spectroscopy”, *Angew.Chem.Int.Ed* (2015) 54, 9162–9185.

90. 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.

89. 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, 21-34.

88. G. Parigi, N. Rezaei-Ghaleh, A. Giachetti, S. Becker, C. Fernandez, M. Blackledge, C. Griesinger, M. Zweckstetter, C. Luchinat, “Long-Range Correlated Dynamics in Intrinsically Disordered Proteins”, *J. Am. Chem. Soc.* (2014) 136, 16201–16209.

87. E. Ravera, L. Salmon, M. Fragai, G. Parigi, H. Al-Hashimi, C. Luchinat, “Insights into Domain-Domain Motions in Proteins and RNA from Solution NMR”, *Acc. Chem. Res.* (2014) 47, 3118–3126.

86. P. Neugebauer, J.G. Krummenacker, V.P. Denysenkov, C. Helmling, C. Luchinat, G. Parigi, T.F. Prisner, "High-field liquid state NMR hyperpolarization: A combined DNP/NMRD approach", *Phys. Chem. Chem. Phys.* (2014) 16, 18781-18787.
85. A.T. Preslar, G. Parigi, M.T. McClendon, S.S. Sefick, T.J. Moyer, C. Haney, E.A. Waters, K.W. MacRenaris, C. Luchinat, S.I. Stupp, T.J. Meade, "Gd(III) Labeled Peptide Nanofibers for Reporting on Biomaterial Localization In Vivo", *ACS Nano* (2014) 8, 7325-7332.
84. E. Ravera, A. Carlon, G. Parigi, "Pairwise binding competition experiments for sorting hub-protein/effector interaction hierarchy and simultaneous equilibria", *J. Biomol. NMR* (2014) 60, 29-36.
83. W. Andralojc, C. Luchinat, G. Parigi, E. Ravera, "Exploring Regions of Conformational Space Occupied by Two-domain Proteins" *J. Phys. Chem. B* (2014) 118, 10576-10587.
82. C. Luchinat, G. Parigi, E. Ravera, "NMR technology: The competitive world of RAS biology", *Nat. Chem. Biol. News & Views* (2014) 10, 173-174.
81. M. Rinaldelli, E. Ravera, V. Calderone, G. Parigi, G. Murshudov, C. Luchinat, "Simultaneous Use of Solution NMR and X-ray Data in REFMAC5 for Joint Refinement/Detection of Structural Differences", *Acta Crystallographica D* (2014) 70, 958-967.
80. C. Luchinat, G. Parigi, E. Ravera, "Can metal ion complexes be used as polarizing agents for solution DNP? A theoretical discussion", *J. Biomol. NMR* (2014) 58, 239-249.
79. A. Bhaumik, C. Luchinat, G. Parigi, E. Ravera, M. Rinaldelli, "NMR crystallography on paramagnetic systems: solved and open issues", *CrystEngComm* (2013) 15, 8639-8656.
78. A.H. Hung, M.C. Duch, G. Parigi, M.W. Rotz, L.M. Manus, D.J. Mastarone, K.T. Dam, C.C. Gits, K.W. MacRenaris, C. Luchinat, M.C. Hersam, T.J. Meade, "Mechanisms of gadographene-mediated proton spin relaxation", *J. Phys. Chem. C* (2013) 117, 16263-16273.
77. M. Fragai, C. Luchinat, G. Parigi, E. Ravera, "Practical considerations over spectral quality in solid state NMR spectroscopy of soluble proteins", *J. Biomol. NMR* (2013) 57, 155-166.
76. C. Luchinat, G. Parigi, E. Ravera, "Water and protein dynamics in sedimented systems: a relaxometric investigation", *ChemPhysChem* (2013) 14, 3156-3161.
75. P. Neugebauer, J.G. Krummenacker, V.P. Denysenkov, G. Parigi, C. Luchinat, T.F. Prisner, "Liquid State DNP of Water at 9.2 T: An Experimental Access to Saturation" *Phys. Chem. Chem. Phys.* (2013) 15, 6049-6056.
74. E. Ravera, G. Parigi, A. Mainz, T.L. Religa, B. Reif, C. Luchinat, "Experimental determination of microsecond reorientation correlation times in protein solutions", *J. Phys. Chem. B* (2013) 117, 3548-3553.
73. I. Bertini, C. Luchinat, G. Parigi, E. Ravera, "SedNMR: on the edge between solution and solid state NMR", *Acc. Chem. Res.* (2013) 46, 2059-2069.
72. M. Fragai, C. Luchinat, G. Parigi, E. Ravera, "Conformational freedom of metalloproteins revealed by paramagnetism-assisted NMR", *Coord. Chem. Rev.* (2013) 257, 2652-2667.
71. L. Cerofolini, G.B. Fields, M. Fragai, C.F.G.C. Geraldès, C. Luchinat, G. Parigi, E. Ravera, D.I. Svergun, J.M.C. Teixeira, "Examination of matrix metalloproteinase-1 (MMP-1) in solution: a preference for the pre-collagenolysis state", *J. Biol. Chem.* (2013) 288, 30659-30671.
70. I. Bertini, L. Ferella, C. Luchinat, G. Parigi, M.V. Petoukhov, E. Ravera, A. Rosato, D.I. Svergun, "MaxOcc: a web portal for Maximum Occurrence Analysis", *J. Biomol.*

NMR (2012) 53, 271-280.

69. I. Bertini, C. Luchinat, M. Nagulapalli, G. Parigi, E. Ravera, "Paramagnetic relaxation enhancement for the characterization of the conformational heterogeneity in two-domain proteins", *Phys. Chem. Chem. Phys.* (2012) 14, 9149-9156.

68. C. Luchinat, M. Nagulapalli, G. Parigi, L. Sgheri, "Maximum occurrence analysis of protein conformations for different distributions of paramagnetic metal ions within flexible two-domain proteins", *J. Magn. Reson.* (2012) 215, 85-93.

67. C. Luchinat, G. Parigi, E. Ravera, M. Rinaldelli, "Solid state NMR crystallography through paramagnetic restraints", *J. Am. Chem. Soc.* (2012) 134, 5006-5009.

66. I. Bertini, F. Engelke, C. Luchinat, G. Parigi, E. Ravera, C. Rosa, P. Turano, "NMR properties of sedimented solutes", *Phys. Chem. Chem. Phys.* (2012) 14, 439-447.

65. M. Nagulapalli, G. Parigi, J. Yuan, J. Gsponer, G. Deraos, V.V. Bamm, G. Harauz, J. Matsoukas, M.R.R. de Planque, I.P. Gerothanassis, M.M. Babu, C. Luchinat, A.G. Tzacos, "Recognition Pliability is Coupled to Structural Heterogeneity: a Calmodulin-Intrinsically Disordered Binding Region Complex", *Structure* (2012) 20, 522-533.

64. M.-T. Türke, G. Parigi, C. Luchinat, M. Bennati, "Overhauser DNP with ¹⁵N labelled Frémy's salt at 0.35 Tesla", *Phys. Chem. Chem. Phys.* (2012) 14, 502-510.

63. C. Griesinger, M. Bennati, H.M. Vieth, C. Luchinat, G. Parigi, P. Höfer, F. Engelke, S.J. Glaser, V. Denysenkov, T.F. Prisner, "Dynamic Nuclear Polarization at High Magnetic Fields in Liquids", *Prog. NMR Spectrosc.* (2012) 64, 4-28.

62. I. Bertini, V. Calderone, L. Cerofolini, M. Fragai, C.F.G.C. Geraldes, P. Hermann, C. Luchinat, G. Parigi, J.M.C. Teixeira, "The catalytic domain of MMP-1 studied through tagged lanthanides", *FEBS Letters* (2012) 586, 557-567.

61. S. Das Gupta, X. Hu, P.H.J. Keizers, W.-M. Liu, C. Luchinat, M. Nagulapalli, M. Overhand, G. Parigi, L. Sgheri, M. Ubbink, "Narrowing the conformational space sampled by two-domain proteins with paramagnetic probes in both domains", *J. Biomol. NMR* (2011) 51, 253-263.

60. I. Bertini, C. Luchinat, G. Parigi, E. Ravera, B. Reif, P. Turano, "Solid State NMR of proteins sedimented by ultracentrifugation", *Proc. Natl. Acad. Sci. USA* (2011) 108, 10396-10399.

59. J.E. Jones, A.J. Amoroso, I.M. Dorin, G. Parigi, B.D. Ward, N.J. Buurma, S.J.A. Pope, "Bimodal, dimetallic lanthanide complexes that bind to DNA: the nature of binding and its influence on water relaxivity", *ChemComm* (2011) 47, 3374-3376.

58. D.J. Mastarone, V.S.R. Harrison, A.L. Eckermann, G. Parigi, C. Luchinat, T.J. Meade, "A Modular System for the Synthesis of Multiplexed Magnetic Resonance Probes", *J. Am. Chem. Soc.* (2011) 133, 5329-5337.

57. E. Babini, X. Hu, G. Parigi, M. Vignali, "Human multiprotein bridging factor 1 and calmodulin do not interact in vitro as confirmed by NMR spectroscopy and CaM-agarose affinity chromatography", *Protein Expression and Purification* (2011) 80, 1-7.

56. I. Bertini, C. Luchinat, G. Parigi, "Moving the frontiers in solution and solid state bioNMR", *Coord. Chem. Rev.* (2011) 255, 649-663.

55. E. Babini, I. Bertini, V. Borsi, V. Calderone, X. Hu, C. Luchinat, G. Parigi, "Structural characterization of human S100A16, a low affinity calcium binder", *J. Biol. Inorg. Chem.* (2011) 16, 243-256.

54. I. Bertini, A. Giachetti, C. Luchinat, G. Parigi, M.V. Petoukhov, R. Pierattelli, E. Ravera, D.I. Svergun, "Conformational space of flexible biological macromolecules from average data", *J. Am. Chem. Soc.* (2010) 132, 13553-13558.

53. M. Bennati, C. Luchinat, G. Parigi, M.-T. Türke, "Water proton relaxation dispersion analysis on a nitroxide radical provides information on the maximal signal enhancement in Overhauser Dynamic Nuclear Polarization experiments", *Phys.Chem.Chem.Phys.*

(2010) 12, 5902-5910.

52. M. Reese, M.-T. Türke, I. Tkach, G. Parigi, C. Luchinat, T. Marquardsen, A. Tavernier, P. Höfer, F. Engelke, C. Griesinger, M. Bennati, “ ^1H and ^{13}C Dynamic Nuclear Polarization in Aqueous Solution with a Two-Field (0.35T/14T) Shuttle DNP Spectrometer”, *J. Am. Chem. Soc.* (2009) 131, 15086-15087.
51. V. Borsi, C. Luchinat, G. Parigi, “Global and local mobility of apocalmodulin monitored through fast field cycling relaxometry”, *Biophys. J.* (2009) 97, 1765-1771.
50. I. Bertini, S. Das Gupta, X. Hu, T. Karavelas, C. Luchinat, G. Parigi, J. Yuan, “Solution structure and dynamics of S100A5 in the apo and Ca^{2+} -bound states”, *J. Biol. Inorg. Chem.* (2009) 14, 1097-1107.
49. I. Bertini, P. Kursula, C. Luchinat, G. Parigi, J. Vahokoski, M. Wilmanns, J. Yuan, “Accurate solution structures of proteins from X-ray data and a minimal set of NMR data: calmodulin-peptide complexes as examples”, *J. Am. Chem. Soc.* (2009) 131, 5134-5144.
48. J. Kowalewski, A. Egorov, D. Kruk, A. Laaksonen, S. Nikkhou Aski, G. Parigi and P.-O. Westlund, “Extensive NMRD studies of Ni(II) salt solutions in water and water-glycerol mixtures”, *J. Magn. Reson.* (2008) 195, 103-111.
47. I. Bertini, C. Luchinat, G. Parigi, R. Pierattelli, “Perspectives in paramagnetic NMR of metalloproteins”, *Dalton Trans.* (2008) 3782-3790.
46. C. Luchinat, G. Parigi, “Nuclear relaxometry helps designing systems for solution DNP on proteins”, *Appl. Magn. Reson.* -Special volume on DNP- (2008) 34, 379-392.
45. P. Höfer, G. Parigi, C. Luchinat, P. Carl, G. Guthausen, M. Reese, T. Carlomagno, C. Griesinger, M. Bennati, “Field Dependent Dynamic Nuclear Polarization with Radicals in Aqueous Solution”, *J. Am. Chem. Soc.* (2008) 130, 3254-3255.
44. L.M. Urbanczyk-Pearson, F.J. Femia, J. Smith, G. Parigi, J.A. Duimstra, A.L. Eckermann, C. Luchinat, T.J. Meade, “Mechanistic Investigation of β -galactosidase-activated MR Contrast Agents”, *Inorg. Chem.* (2008) 47, 56-68.
43. P. Caravan, G. Parigi, J.M. Chasse, N.J. Cloutier, J.J. Ellison, R.B. Lauffer, C. Luchinat, S.A. McDermid, M. Spiller, T.J. McMurry, “Albumin binding, relaxivity, and water exchange kinetics of the diastereoisomers of MS-325, a gadolinium(III) based magnetic resonance angiography contrast agent”, *Inorg. Chem.* (2007) 46, 6632-6639.
42. I. Bertini, Y.K. Gupta, C. Luchinat, G. Parigi, M. Peana, L. Sgheri, J. Yuan, “Paramagnetism-based NMR restraints provide maximum allowed probabilities for the different conformations of partially independent protein domains”, *J. Am. Chem. Soc.* (2007) 129, 12786-12794.
41. J.L. Major, G. Parigi, C. Luchinat, T.J. Meade, “The synthesis and in vitro testing of a zinc-activated MRI contrast agent”, *Proc. Natl. Acad. Sci. USA* (2007) 104, 13881-13886.
40. I. Bertini, I.C. Felli, C. Luchinat, G. Parigi, R. Pierattelli, “Towards a protocol for solution structure determination of copper(II) proteins: the case of Cu(II)Zn(II) superoxide dismutase”, *ChemBioChem* (2007) 8, 1422-1429.
39. C. Luchinat, G. Parigi, “Collective relaxation of protein protons at very low magnetic field: a new window on protein dynamics and aggregation”, *J. Am. Chem. Soc.* (2007) 129, 1055-1064.
38. S. Balayssac, I. Bertini, C. Luchinat, G. Parigi, M. Piccioli, “ ^{13}C direct detected NMR increases the detectability of residual dipolar couplings”, *J. Am. Chem. Soc.* (2006) 128, 15042-15043.
37. M. Longinetti, C. Luchinat, G. Parigi, L. Sgheri, “Efficient determination of the most favored orientations of protein domains from paramagnetic NMR data”, *Inv. Probl.* (2006) 22, 1485-1502.

36. M. Fragai, C. Luchinat, G. Parigi, "Four dimensional protein structures: examples from metalloproteins", *Acc. Chem. Res.* (2006) 39, 909-917.
35. I. Bertini, M. Fragai, A. Giachetti, C. Luchinat, M. Maletta, G. Parigi, K.J. Yeo, "Combining in silico tools and NMR data to validate protein-ligand structural models: application to matrix metalloproteinases", *J. Med. Chem.* (2005) 48, 7544-7559.
34. I. Bertini, C. Luchinat, G. Parigi, R. Pierattelli, "NMR Spectroscopy of Paramagnetic Metalloproteins", *ChemBioChem* (2005) 6, 1536-1549.
33. I. Bertini, Y.K. Gupta, C. Luchinat, G. Parigi, C. Schlörb, H. Schwalbe, "NMR Spectroscopic Detection of Protein Protons and Longitudinal Relaxation Rates between 0.01 and 50 MHz", *Angew. Chem. Int. Ed.* (2005) 44, 2223-2225.
32. E. Libralesso, K. Nerinovski, G. Parigi, P. Turano, "¹H nuclear magnetic relaxation dispersion of Cu,Zn superoxide dismutase in the native and guanidinium-induced unfolded forms", *Biochem. Biophys. Res. Comm.* (2005) 328, 633-639.
31. J. Kowalewski, D. Kruk, G. Parigi, "NMR relaxation in solution of paramagnetic complexes: recent theoretical progress for $S \geq 1$ ", *Adv. Inorg. Chem.* (2005) 57, 41-104. In R. van Eldik and I. Bertini, "Relaxometry of water-metal ion interactions".
30. I. Bertini, C. Luchinat, G. Parigi, "¹H NMRD profiles of paramagnetic aquo-complexes and metalloproteins", *Adv. Inorg. Chem.* (2005) 57, 105-172. In R. van Eldik and I. Bertini, "Relaxometry of water-metal ion interactions".
29. R. Barbieri, C. Luchinat, G. Parigi, "Backbone-only protein solution structures with a combination of classical and paramagnetism-based constraints: a method that can be scaled to large molecules", *Chem. Phys. Chem.* (2004) 5, 797-806.
28. I. Bertini, C. Del Bianco, I. Gelis, N. Katsaros, C. Luchinat, G. Parigi, M. Peana, A. Provenzani, M.A. Zoroddu, "Experimentally exploring the conformational space sampled by domain reorientation in calmodulin", *Proc. Natl. Acad. Sci. USA* (2004) 101, 6841-6846.
27. I. Bertini, J. Faraone-Mennella, H.B. Gray, C. Luchinat, G. Parigi, J.R. Winkler, "NMR-validated structural model for oxidized *Rhodospseudomonas palustris* cytochrome *c556*", *J. Biol. Inorg. Chem.* (2004) 9, 224-230.
26. L. Banci, I. Bertini, G. Cavallaro, A. Giachetti, C. Luchinat, G. Parigi, "Paramagnetism-based restraints for Xplor-NIH", *J. Biomol. NMR* (2004) 28, 249-261.
25. I. Bertini, C. Luchinat, K. Nerinovski, G. Parigi, M. Cross, Z. Xiao, A.G. Wedd, "Application of NMRD to Hydration of Rubredoxin and a Variant Containing a (Cys-S)₃Fe^{III}(OH) Site", *Biophys. J.* (2003) 84, 545-551.
24. M. Longinetti, G. Parigi, L. Sgheri, "Uniqueness and degeneracy in the localization of rigid domains in paramagnetic proteins", *J. Phys. A: Math. Gen.* (2002) 35, 8153-8169.
23. W. Li, G. Parigi, M. Fragai, C. Luchinat, T.J. Meade, "Mechanistic studies of a calcium-dependent MRI contrast agent", *Inorg. Chem.* (2002) 41, 4018-4024.
22. I. Bertini, C. Luchinat, G. Parigi, "Magnetic susceptibility in paramagnetic NMR", *Prog. NMR Spectrosc.* (2002) 40, 249-273.
21. J. Kowalewski, C. Luchinat, T. Nilsson, G. Parigi, "Nuclear spin relaxation in paramagnetic systems: electron spin relaxation effects under near-Redfield limit conditions and beyond", *J. Phys. Chem. A* (2002) 106, 7376-7382.
20. T. Nilsson, G. Parigi, J. Kowalewski, "Experimental NMRD profiles for some low-symmetry Ni(II) complexes (S=1) in solution and their interpretation using slow-motion theory", *J. Phys. Chem. A* (2002) 106, 4476-4488.
19. I. Bertini, M. Longinetti, C. Luchinat, G. Parigi, L. Sgheri, "Efficiency of paramagnetism-based constraints to determine the spatial arrangement of α -helical secondary structure elements", *J. Biomol. NMR* (2002) 22, 123-136.

18. F. Alhaique, I. Bertini, M. Fragai, M. Carafa, C. Luchinat, G. Parigi, "Solvent ^1H NMRD study of biotinylated paramagnetic liposomes containing Gd-bis-SDA-DTPA or Gd-DMPE-DTPA" (Dedicated to G. Sykes), *Inorg. Chim. Acta* (2002) 331, 151-157.
17. I. Bertini, C. Luchinat, G. Parigi, "Paramagnetic constraints: an aid for quick solution structure determination of paramagnetic metalloproteins", *Concepts in Magn. Reson.* (2002) 14, 259-286.
16. I. Bertini, A. Donaire, B. Jimenez, C. Luchinat, G. Parigi, M. Piccioli, L. Poggi, "Paramagnetism-based versus classical constraints: an analysis of the solution structure of Ca Ln calbindin D_{9k} ", *J. Biomol. NMR* (2001) 21, 85-98.
15. I. Bertini, J. Kowalewski, C. Luchinat, G. Parigi, "Cross-correlation between the dipole-dipole interaction and the Curie spin relaxation: the effect of anisotropic magnetic susceptibility", *J. Magn. Reson.* (2001) 152, 103-108.
14. I. Bertini, M. Fragai, C. Luchinat, G. Parigi, "Solvent ^1H NMRD study of hexaaquochromium(III): inferences on hydration and electron relaxation", *Inorg. Chem.* (2001) 40, 4030-4035.
13. I. Bertini, F. Castellani, C. Luchinat, G. Martini, G. Parigi, S. Ristori, "Partial orientation of cytochrome c in a lyotropic liquid crystal: residual H-H dipolar coupling", *J. Phys. Chem. B* (2000) 104, 10653-10658.
12. I. Bertini, M. Fragai, C. Luchinat, G. Parigi, " ^1H NMRD profiles of diamagnetic proteins: a model free analysis" (Dedicated to Harald Günther), *Magn. Reson. Chem.* (2000) 38, 543-550.
11. I. Bertini, C. Luchinat, G. Parigi, "Hyperfine shifts in low spin iron(III) hemes: a ligand field analysis", *Eur. J. Inorg. Chem.* (2000) 2473-2480.
10. P.L. Anelli, I. Bertini, M. Fragai, L. Lattuada, C. Luchinat, G. Parigi, "Sulfonamide-functionalised Gadolinium DTPA complexes as possible contrast agents for MRI: a relaxometric investigation", *Eur. J. Inorg. Chem.* (2000) 625-630.
9. I. Bertini, C. Luchinat, G. Parigi, F.A. Walker, "Heme methyl ^1H chemical shifts as structural parameters in some low spin ferriheme proteins", *J. Biol. Inorg. Chem.* (1999) 4, 515-519.
8. I. Bertini, J. Kowalewski, C. Luchinat, T. Nilsson, G. Parigi, "Nuclear spin relaxation in paramagnetic complexes of $S=1$: electron spin relaxation effects", *J. Chem. Phys.* (1999) 111, 5795-5807.
7. S.W.A. Bligh, A.H.M.S. Chowdhury, D. Kennedy, C. Luchinat, G. Parigi, "Non-ionic bulky Gd(III) DTPA-Bisamide complexes as potential contrast agents for magnetic resonance imaging", *Magn. Reson. Med.* (1999) 41, 767-773.
6. I. Bertini, O. Galas, C. Luchinat, G. Parigi, G. Spina, "Nuclear and electron relaxation in magnetic exchange coupled dimers: implications for NMR spectroscopy", *J. Magn. Reson.* (1998) 130, 33-44.
5. I. Bertini, C. Luchinat, G. Parigi, G. Quacquarelli, P. Marzola, F.M. Cavagna, "Off-resonance experiments and contrast agents to improve magnetic resonance imaging", *Magn. Reson. Med.* (1998) 39, 124-131.
4. S. J. Kroes, J. Salgado, G. Parigi, C. Luchinat, G.W. Canters, "Electron relaxation and solvent accessibility of the metal site in wild-type and mutated azurins as determined from nuclear magnetic relaxation dispersion experiments", *J. Biol. Inorg. Chem.* (1996) 1, 551-559.
3. I. Bertini, C. Luchinat, G. Mincione, G. Parigi, G.T. Gassner, D.P. Ballou, "NMRD studies on phthalate dioxygenase: evidence for displacement of water on binding substrate", *J. Biol. Inorg. Chem.* (1996) 1, 468-475.
2. I. Bertini, O. Galas, C. Luchinat, L. Messori, G. Parigi, "A theoretical analysis of the H Nuclear Magnetic Relaxation Dispersion profiles of diferric transferrin", *J. Phys. Chem.*

(1995) 99, 14217-14222.

1. I. Bertini, O. Galas, C. Luchinat, G. Parigi, "A computer program for the calculation of paramagnetic enhancements of nuclear relaxation rates in slowly rotating systems", *J. Magn. Reson., Series A* (1995) 113, 151-158.

Books:

1. I. Bertini, C. Luchinat, G. Parigi, *Solution NMR of Paramagnetic Molecules*, Elsevier, Amsterdam, 2001.
2. I. Bertini, C. Luchinat, G. Parigi, E. Ravera, *NMR of Paramagnetic Molecules*, Elsevier, 2017.

Book chapters:

1. I. Bertini, K.S. McGreevy, G. Parigi, "NMR and its Place in Mechanistic Systems Biology" in "NMR of Biomolecules: Towards Mechanistic Systems Biology", Bertini I, McGreevy KS, Parigi G (Eds.), Wiley-VCH, Weinheim, Germany, 2012, pag. 3-5.
2. I. Bertini, C. Luchinat, G. Parigi, "Paramagnetic molecules" in "NMR of Biomolecules: Towards Mechanistic Systems Biology", Bertini I, McGreevy KS, Parigi G (Eds.), Wiley-VCH, Weinheim, Germany, 2012, pag. 155-171.
3. 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", Bertini I, McGreevy KS, Parigi G (Eds.), Wiley-VCH, Weinheim, Germany, 2012, pag. 377-392.
4. G. Parigi, C. Luchinat, "NMR Consequences of the Nucleus–Electron Spin Interactions" in "Paramagnetism in Experimental Biomolecular NMR", Luchinat C, Parigi G, Ravera E (Eds.), RSC, 2018, pag. 1-41.

Other publications:

1. C. Luchinat, G. Parigi, "Structural determination of metalloproteins", In G. Bassani, G. Liedl, P. Wyder, "Encyclopedia of Condensed Matter Physics", Elsevier Academic Press, Oxford, 2005, pag. 369-378.
2. I. Bertini, C. Luchinat, G. Parigi, R. Pierattelli, "NMR Spectroscopy of Paramagnetic Metalloproteins", in "Wiley Encyclopedia of Chemical Biology, 4 volume set" (WECB), Wiley-Interscience, 2009, pag. 408-423.
3. C. Luchinat, G. Parigi, "Paramagnetic Systems in Biochemistry: Solution NMR Studies", in "Encyclopedia of Magnetic Resonance" on-line edition, eds-in-chief R. K. Harris and R. E. Wasylshen, John Wiley & Sons Ltd., Chichester. DOI: 10.1002/9780470034590.emrstm1088. Published online 15th December 2010.

4. I. Bertini, G. Parigi, "Paramagnetic metalloproteins" in "Encyclopedia of Biophysics", Gordon C. K. Roberts (Editor), Springer-Verlag Berlin Heidelberg, 2013, pag. 1824.
5. I. Bertini, G. Parigi, "Hyperfine shifts" in "Encyclopedia of Biophysics", Gordon C. K. Roberts (Editor), Springer-Verlag Berlin Heidelberg, 2013, pag. 1030-1031.
6. C. Luchinat, G. Parigi, "Metalloproteins, Structural Determination of". In "Reference Module in Materials Science and Materials Engineering", Saleem Hashmi (editor-in-chief), Elsevier, Oxford; 2016.
7. G. Parigi, "Hyperfine shifts" in "Encyclopedia of Biophysics" (2nd edition), Roberts G., Watts A., European Biophysical Societies (eds), Springer, Berlin, Heidelberg, 2018.
8. L. Banci, L. Barbieri, V. Calderone, F. Cantini, L. Cerofolini, S. Ciofi-Baffoni, I.C. Felli, M. Fragai, M. Lelli, C. Luchinat, E. Luchinat, G. Parigi, M. Piccioli, R. Pierattelli, E. Ravera, A. Rosato, L. Tenori, P. Turano, "Biomolecular NMR at 1.2 GHz", arXiv: 1910.07462, 2019.
9. G. Parigi, I. Bertini, L. Banci, "Paramagnetic Metalloproteins" in "Encyclopedia of Biophysics" (2nd edition), Roberts G., Watts A., European Biophysical Societies (eds), Springer, Berlin, Heidelberg, 2021.