

## Prof. Claudio Luchinat

### Complete list of publications

#### 2020 (update May)

692. Bruno F, Francischello R, Bellomo G, Gigli L, Flori A, Menichetti L, Tenori L, Luchinat C, Ravera E. Multivariate Curve Resolution for 2D Solid-State NMR spectra **Anal Chem.** 2020 Mar 17;92(6):4451-4458. doi: 10.1021/acs.analchem.9b05420 (IF 6.350)
691. Vignoli, A.; Muraro, E.; Miolo, G.; Tenori, L.; Turano, P.; Di Gregorio, E.; Steffan, A.; Luchinat, C.; Corona, G. Effect of Estrogen Receptor Status on Circulatory Immune and Metabolomics Profiles of Her2-Positive Breast Cancer Patients Enrolled for Neoadjuvant Targeted Chemotherapy. **Cancers** 2020, 12 (2). doi.org/10.3390/cancers12020314. (IF: 6.162)
690. Sala, D, Cerofolini L, Fragai L, Giachetti A, Luchinat C, Rosato A, A protocol to automatically calculate homo-oligomeric protein structures through the integration of evolutionary constraints and NMR ambiguous contacts. **Computational and Structural Biotechnology Journal** 18, 2020, 114-124 (IF 4.720)
689. Ghini, V.; Tenori, L.; Capozzi, F.; Luchinat, C.; Bub, A.; Malpuech-Brugere, C.; Orfila, C.; Ricciardiello, L.; Bordoni, A. DHA-Induced Perturbation of Human Serum Metabolome. Role of the Food Matrix and Co-Administration of Oat  $\beta$ -Glucan and Anthocyanins. **Nutrients** 2020, 12 (1). doi.org/10.3390/nu12010086. (IF: 4.171)
688. Vignoli A, Santini G, Tenori L, Macis G, Mores, Macagno N, Pagano F, Higenbottam T Luchinat C, Montuschi P, NMR-Based Metabolomics for the Assessment of Inhaled Pharmacotherapy in Chronic Obstructive Pulmonary Disease Patients, **J. Proteom Res.** 2020, 19, 64-74. doi: 10.1021/acs.jproteome.9b00345 (IF 3.78)
687. Vignoli, A.; Tenori, L.; Giusti, B.; Valente, S.; Carrabba, N.; Balzi, D.; Barchielli, A.; Marchionni, N.; Gensini, G. F.; Marcucci, R.; Gori, A. M.; Luchinat, C.; Saccenti, E. Differential Network Analysis Reveals Metabolic Determinants Associated with Mortality in Acute Myocardial Infarction Patients and Suggests Potential Mechanisms Underlying Different Clinical Scores Used to Predict Death. **J. Proteom Res.** 2020, 19 (2), 949-961. doi.org/10.1021/acs.jproteome.9b00779. (IF 3.78)
686. Vignoli A, Paciotti S, Tenori L, Eusebi P, Biscetti L, Chiasserini D, Scheltens P, Turano P, Teunissen C, Luchinat C, Parnetti L., Fingerprinting Alzheimer's Disease by <sup>1</sup>H Nuclear Magnetic Resonance Spectroscopy of Cerebrospinal Fluid., **J Proteome Res.** 2020, 19, 1696-1705. doi: 10.1021/acs.jproteome.9b00850. Epub 2020 Mar 12 (IF 3.78)
685. Schirò A, 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 (IF 3.754)
684. Denis M, Softley C, Giuntini S, Gentili M, Ravera E, Parigi G, Fragai M, Popowicz G, Sattler M, Luchinat C, Cerofolini L, Nativi C., The Photocatalyzed Thiol-ene reaction: A New Tag to Yield Fast, Selective and reversible Paramagnetic Tagging of Proteins **ChemPhysChem.** 2020, doi: 10.1002/cphc.202000071. (IF 3.077)
683. Chatzikonstantinou AV, Tsiailanis AD, Gerothanassis IP, Stamatis H, Ravera E, Fragai M, Luchinat C, Parigi G, Tzakos AG. The NMR tube bioreactor **Methods Enzymol.** 2020; 633:71-101. doi: 10.1016/bs.mie.2019.10.032. (IF 2.002)
682. Cerofolini L, Ravera E, Fragai M, Luchinat C. NMR of Immobilized Enzymes. **Methods Mol Biol.** 2020, 2100:363-383. doi: 10.1007/978-1-0716-0215-7\_24 (IF 1.698)

#### 2019

681. Mulder FAA, Tenori L, Luchinat C, Fast and Quantitative NMR Metabolite Analysis Afforded by a Paramagnetic Co-Solute. **Angew Chem Int Ed Engl.** 2019 doi: 10.1002/anie.201908006. (IF 12.257)
680. Amato J, Cerofolini L, Brancaccio D, Giuntini S, Iaccarino N, Zizza P, Iachettini S, Biroccio A, Novellino E, Rosato A, Fragai M, Luchinat C, Randazzo A, Pagano B. Insights into telomeric G-quadruplex DNA recognition by HMGB1 protein. **Nucleic Acids Res.** 2019, 47, 9950-9966 (IF 11.147)
679. Parigi, G., Ravera E., Luchinat C., Magnetic susceptibility and paramagnetism-based NMR **Prog. NMR Spectrosc.** 2019, 114-115, 211-236. (IF 8.848)
678. Cerofolini L, Silva JM, Ravera E, Romanelli M, Geraldès CFGC, Macedo AL, Fragai M, Parigi G, Luchinat C., 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. (IF 7.329)
677. 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. (IF 3.665)
676. Dourou, AM, S. Brizzolara, G. Meoni, L. Tenori, F. Famiani, C. Luchinat, P. Tonutti. The inner temperature of the olives before processing affects the volatile profile and the composition of the oil. doi.org/10.1016/j.foodres.2019.108861 **Food Res Int.** (IF 3.579)
675. Cerofolini L, Fragai M, Luchinat C. Mechanism and Inhibition of Matrix Metalloproteinases. **Curr Med Chem.** 2019; 26, 2609-2633. (IF 3.469).
674. Cerofolini L, Giuntini S, Ravera E, Luchinat C, Berti F, Fragai M., [Structural characterization of a protein adsorbed on aluminum hydroxide adjuvant in vaccine formulation.](#) **NPJ Vaccines.** 2019 May 28;4:20. doi: 10.1038/s41541-019-0115-7. eCollection 2019. (IF 3.143)
673. Carlon A, Ravera E, Parigi G, Murshudov GN, Luchinat C., [Correction to: Joint X-ray/NMR structure refinement of multidomain/multisubunit systems.](#) **J Biomol NMR.** 2019 May 8. doi: 10.1007/s10858-019-00238-4. [Epub ahead of print] (IF 2.534)
672. Bellomo G, Bologna S, Cerofolini L, Paciotti S, Gatticchi L, Ravera E, Parnetti L, Fragai M, Luchinat C., [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 May 23;123(20):4380-4386. doi: 10.1021/acs.jpcc.9b02381. Epub 2019 May 9. (IF 3.146)
671. Ghini V, Quaglio D, Luchinat C, Turano P., [NMR for sample quality assessment in metabolomics.](#) **New Biotechnol.** 2019 Apr 22;52:25-34. doi: 10.1016/j.nbt.2019.04.004. [Epub ahead of print] (IF 3.733)
670. Meoni G, Lorini S, Monti M, Madia F, Corti G, Luchinat C, Zignego AL, Tenori L, Gagnani L., [The metabolic fingerprints of HCV and HBV infections studied by Nuclear Magnetic Resonance Spectroscopy.](#) **Sci Rep.** 2019 Mar 11;9(1):4128. doi: 10.1038/s41598-019-40028-4.

(IF 4.122)

669. Calderone V, Fragai M, Luchinat C., [Reviewing the Crystal Structure of S100Z and Other Members of the S100 Family: Implications in Calcium-Regulated Quaternary Structure](#). *Methods Mol Biol*. 2019;1929:487-499. doi: 10.1007/978-1-4939-9030-6\_30.
668. Parigi G, Ravera E, Ravera M, Bennati, C, Luchinat, Understanding Overhauser Dynamic Nuclear Polarisation through NMR relaxometry, *Mol. Phys.* 2019 117, 888-897.(IF 1.704)
667. McCartney A, Vignoli A, Tenori L, Fornier M, Rossi L, Risi E, Luchinat C, Biganzoli L, Di Leo A. Metabolomic analysis of serum may refine 21-gene expression assay risk recurrence stratification. *NPJ Breast Cancer*. 2019 Aug 29;5:26. doi: 10.1038/s41523-019-0123-9. eCollection 2019.
666. Li H, Parigi G, Luchinat C, Meade TJ. Bimodal Fluorescence-Magnetic Resonance Contrast Agent for Apoptosis Imaging. *J Am Chem Soc*. 2019, 141, 6224-6233. doi: 10.1021/jacs.8b13376. Epub 2019 Apr 4. (IF 14.357)
665. Parigi G, Benda L, Ravera E, Romanelli M, Luchinat C., Pseudocontact shifts and paramagnetic susceptibility in semiempirical and quantum chemistry theories. *J Chem Phys*. 2019 Apr 14;150(14):144101. doi: 10.1063/1.5037428 (IF 2.843)
664. Malanho Silva J, Cerofolini L, Giuntini S, Calderone V, Galdes CFGC, Macedo AL, Parigi G, Fragai M, Ravera E, Luchinat C. Metal centers in biomolecular solid-state NMR. *J Struct Biol*. 2019 Apr 1;206(1):99-109. doi: 10.1016/j.jsb.2018.11.013. Epub 2018 Nov 28 (IF 3.433)
663. Vignoli A, Tenori L, Giusti B, Takis PG, Valente S, Carrabba N, Balzi D, Barchielli A, Marchionni N, Gensini GF, Marcucci R, Luchinat C, Gori AM. NMR-based metabolomics identifies patients at high risk of death within two years after acute myocardial infarction in the AMI-Florence II cohort. *BMC Med*. 2019 Jan 7;17(1):3. doi: 10.1186/s12916-018-1240-2. (IF 9.088)
662. PG Takis, V Ghini, L Tenori, P Turano, C Luchinat Uniqueness of the NMR approach to metabolomics, *TrAC Trends in Analytical Chemistry*, <https://doi.org/10.1016/j.trac.2018.10.036> (IF 7.030)
661. Trimigno A, Khakimov B, Savorani F, Tenori L, Hendrixson V, Čivilis A, Glibetic M, Gurinovic M, Pentikäinen S, Sallinen J, Garduno Diaz S, Pasqui F, Khokhar S, Luchinat C, Bordoni A, Capozzi F, Balling Engelsen S. Investigation of Variations in the Human Urine Metabolome Amongst European Populations. An Exploratory Search for Biomarkers of People at Risk-of-Poverty. *Mol Nutr Food Res*. (2018) e1800216. (IF 4.323)
660. Fragai M, Ravera E, Tedoldi F, Luchinat C, Parigi G., Relaxivity of Gd-based MRI contrast agents in crosslinked hyaluronic acid as a model for tissues. *Chemphyschem*. 2019, 20, 2204-2209 (IF 1.66)
659. Vignoli A, Ghini V, Meoni G, Licari C, Takis PG, Tenori L, Turano P, Luchinat C. High-Throughput Metabolomics by 1D NMR. *Angew Chem Int Ed Engl*. 2019 Jan 21;58(4):968-994. doi: 10.1002/anie.201804736. Epub 2018 Nov 11. Review. (IF 12.102)
658. Cerofolini L, Giuntini S, Carlon A, Ravera E, Calderone V, Fragai M, Parigi G, Luchinat C. Characterization of PEGylated Asparaginase: New Opportunities from NMR Analysis of Large PEGylated Therapeutics. *Chemistry*. 2019 Feb 6;25(8):1984-1991. doi: 10.1002/chem.201804488. Epub 2019 Jan 9. (IF 5.16)
657. Silva JM, Giuntini S, Cerofolini L, Galdes CFGC, Macedo AL, Ravera E, Fragai M, Luchinat C, Calderone V. Non-crystallographic symmetry in proteins: Jahn-Teller-like and Butterfly-like effects? *J Biol Inorg Chem*. 2019 Feb;24(1):91-101. doi: 10.1007/s00775-018-1630-0. Epub 2018 Nov 23. (IF 2.952)
656. Vignoli A, Orlandini B, Tenori L, Biagini MR, Milani S, Renzi D, Luchinat C, Calabrò AS. Metabolic Signature of Primary Biliary Cholangitis and Its Comparison with Celiac Disease. *J Proteome Res*. 2019 Mar 1;18(3):1228-1236. doi: 10.1021/acs.jproteome.8b00849. Epub 2019 Jan 10. (IF 3.950)

## 2018

655. Takis PG, Taddei A, Pini R, Grifoni S, Tarantini F, Bechi P, Luchinat C. Fingerprinting Acute Digestive Diseases by Untargeted NMR Based Metabolomics. *Int J Mol Sci*. 2018 Oct 23;19(11). pii: E3288. doi: 10.3390/ijms19113288. (IF )
654. Rittweger J, Albracht K, Flück M, Ruoss S, Brocca L, Longa E, Moriggi M, Seynnes O, Di Giulio I, Tenori L, Vignoli A, Capri M, Gelfi C, Luchinat C, Franceschi C, Bottinelli R, Cerretelli P, Narici M. Erratum: Author Correction: Sarcolab pilot study into skeletal muscle's adaptation to longterm spaceflight. *NPJ Microgravity*. 2018 Oct 24;4:23. doi: 10.1038/s41526-018-0058-8. eCollection 2018 (IF )
653. Jörn Rittweger, Kirsten Albracht, Martin Flück, Severin Ruoss, Lorenza Brocca, Emanuela Longa, Manuela Moriggi, Olivier Seynnes, Irene Di Giulio, Leonardo Tenori, Alessia Vignoli, Miriam Capri, Cecilia Gelfi, Claudio Luchinat, Claudio Francheschi, Roberto Bottinelli, Paolo Cerretelli, Marco Narici, "Sarcolab pilot study into skeletal muscle's adaptation to long-term spaceflight", *NPJ Microgravity*, (2018) 4:18. doi: 10.1038/s41526-018-0052-1 (IF 2.00)
652. Calderone, V., Fragai, M. Luchinat, C. When molecular replacement has no trivial solution: the importance of model editing in humanS100Z X-ray structure solution. *Inorg Chim Acta* 470, 402-406 (2018) (IF 2.002)
651. Fedeli L, Belli G, Ciccarone A, Coniglio A, Esposito M, Giannelli M, Mazzoni LN, Nocetti L, Sghedoni R, Tarducci R, Altabella L, Belligotti E, Benelli M, Betti M, Caivano R, Carni' M, Chiappiniello A, Cimolai S, Cretti F, Fulcheri C, Gasperi C, Giacometti M, Levrero F, Lizio D, Maieron M, Marzi S, Mascaro L, Mazzocchi S, Meliado' G, Morzenti S, Noferini L, Oberhofer N, Quattrocchi MG, Ricci A, Taddeucci A, Tenori L, Luchinat C, Gobbi G, Gori C, Busoni S. Dependence of apparent diffusion coefficient measurement on diffusion gradient direction and spatial position - A quality assurance intercomparison study of forty-four scanners for quantitative diffusion-weighted imaging.; Italian Association of Physics in Medicine (AIFM) Working Group on MR Intercomparison. *Phys Med*. (2018) Nov;55:135-141. doi: 10.1016/j.ejmp.(2018).09.007 (IF=2.240)
650. Ravera E., P.G. Takis, M. Fragai, G. Parigi, C. Luchinat, "NMR Spectroscopy and Metal Ions in Life Sciences", *Eur. J. Inorg. Chem.* (2018) 4752-4770 DOI 10.1002/ejic.201800875, (IF 2.507)
649. Carlon A, Ravera E, Parigi G, Murshudov GN, Luchinat C. Joint X-ray/NMR structure refinement of multidomain/multisubunit systems. *J Biomol NMR* (2018) doi: 10.1007/s10858-018-0212-3. (IF 2.534)
648. Cerofolini L, Staderini T, Giuntini S, Ravera E, Fragai M, Parigi G, Pierattelli R, Luchinat C Long-range paramagnetic NMR data can provide a closer look on metal coordination in metalloproteins. *J. Biol. Inorg. Chem* 23, 71-80 (2018) (IF 2.894)
647. 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. DOI: 10.1042/ETLS20170084 (IF 2.906)
646. Cerofolini L, Fragai M, Luchinat C. Mechanism and Inhibition of Matrix Metalloproteinases *Current Medicinal Chemistry*, (2018),

DOI: 10.2174/0929867325666180326163523, (IF: 3.469)

645. Tenori, L., Santucci, C., Meoni, G., Morrocchi, V., Matteucci, G., Luchinat, C. NMR metabolomic fingerprinting distinguishes milk from different farms, **Food Research Int.**, 113, (2018), 131-139. (IF 3.520)
644. Baggio, C., Cerofolini, L., Fragai, M., Luchinat, C. & Pellecchia, M. HTS by NMR for the Identification of Potent and Selective Inhibitors of Metalloenzymes. **ACS Med. Chem Lett** 9, 137-142 (2018) (IF 3.746).
643. Louka A, Matlahov I, Giuntini S, Cerofolini L, Cavallo A, Pillozzi S, Ravera E, Fragai M, Arcangeli A, Ramamoorthy A, Goobes G, Luchinat C. Engineering l-asparaginase for spontaneous formation of calcium phosphate bioinspired microreactors.. (2018), 20, 12719-12726. doi: 10.1039/c8cp00419f. **Phys Chem Chem Phys** (IF 3.906)
642. Gigli L, Andrałojć W, Dalaloyan A, Parigi G, Ravera E, Goldfarb D, Luchinat C. Assessing protein conformational landscapes: integration of DEER data in Maximum Occurrence analysis. **Phys Chem Chem Phys.** (2018), 43, 27429-27438. doi: 10.1039/c8cp06195e. (IF 3.906)
641. Vignoli, A., Orlandini, B., Tenori, L., Biagini, M. R., Milani, S., Renzi, D., Luchinat, C., Calabrò, A. "The metabolic signature of Primary Biliary Cholangitis and its comparison with Coeliac Disease", **J. Proteome Res.** doi: 10.1021/acs.jproteome.8b00849 (2018), (IF 3.950)
640. Caracausi M, Ghini V, Locatelli C, Mericio M, Piovesan A, Antonaros F, Pelleri MC, Vitale L, Vacca RA, Bedetti F, Mimmi MC, Luchinat C, Turano P, Strippoli P, Cocchi G., Plasma and urinary metabolomic profiles of Down syndrome correlate with alteration of mitochondrial metabolism, **Sci Rep.** 8(1):2977. doi: 10.1038/s41598-018-20834-y.(2018) (IF 4.122)
639. Vignoli, A., Tenori, L., Luchinat, C., Saccenti, E. Age and sex effects on plasma metabolite association networks in healthy subjects. **J. Proteome Res** (2018)17, 97-107 (IF 4.268)
638. Montuschi P, Santini G, Mores N, Vignoli A, Macagno F, Shoreh R, Tenori L, Zini G, Fuso L, Mondino C, Di Natale C, D'Amico A, Luchinat C, Barnes PJ, Higenbottam T, Breathomics for Assessing the Effects of Treatment and Withdrawal With Inhaled Beclomethasone/Formoterol in Patients With COPD, **Frontiers in pharmacology** (2018); 9: 258 (IF 4.40)
637. Lilley, L.M., 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<sup>3+</sup> complexes", **Inorg. Chem.** (2018) 57, 5810-5819 (IF 4.700)
636. Chatzikonstantinou, A., M. Chatziathanasiadou, E. Ravera, M. Fragai, G. Parigi, I. Gerotheranassis, 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. (IF 4.702)
635. Marra A, Dong J, Ma T, Giuntini S, Crescenzo E, Cerofolini L, Martinucci M, Luchinat C, Fragai M, Nativi C, Dondoni A Protein Glycosylation via Sulfur Fluoride Exchange (SuFEx) Chemistry: The Key Role of a Fluorosulfate Thiolactoside. **Chemistry** (2018) 24, 18981-18987 (IF 5.16)
634. Cutrin JC, Alberti D, Bernacchioni C, Ciambellotti S, Turano P, Luchinat C, Crich SG, Aime S. Cancer cell death induced by ferritins and the peculiar role of their labile iron pool. **Oncotarget.** 46, 27974-27984. (2018) doi: 10.18632/oncotarget.25416. (IF 5.168)
633. Checcucci A, diCenzo GC, Ghini V, Bazzicalupo M, Becker A, Decorosi F, Döhlemann J, Fagorzi C, Finan TM, Fondi M, Luchinat C, Turano P, Vignolini T, Viti C, Mengoni A. Creation and Characterization of a Genomically Hybrid Strain in the Nitrogen-Fixing Symbiotic Bacterium *Sinorhizobium meliloti*. **ACS Synth Biol.** (2018), 7:2365-2378. doi: 10.1021/acssynbio.8b00158. (IF 5.316)
632. Gineste, S., 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. (IF 5.835)
631. Manzoni L, Zucal C, Di Maio D, D'Agostino VG, Thongon N, Bonomo I, Lal P, Miceli M, Baj V, Brambilla M, Cerofolini L, Elezgarai S, Biasini E, Luchinat C, Novellino E, Fragai M, Marinelli L, Provenzani A, Seneci. Interfering with HuR-RNA Interaction: Design, Synthesis and Biological Characterization of Tanshinone Mimics as Novel, Effective HuR Inhibitors, **J. Med. Chem.**, (2018), 61, 1483-1498, (IF: 6.253).
630. B. Wiene-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. (IF 6.253)
629. Merlino F, Daniele S, La Pietra V, Di Maro S, Di Leva FS, Brancaccio D, Tomassi S, Giuntini S, Cerofolini L, Fragai M, Luchinat C, Reichart F, Cavallini C, Costa B, Piccarducci R, Taliani S, Da Settimo F, Martini C, Kessler H, Novellino E, Marinelli L. Simultaneous Targeting of RGD-Integrins and Dual Murine Double Minute Proteins in Glioblastoma Multiforme, **J Med Chem.** (2018) 61, 4791-4809. (IF 6.253)
628. Bellomo G, Bologna S, Gonnelli L, Ravera E, Fragai M, Lelli M, Luchinat C. Aggregation kinetics of the Aβ<sub>1-40</sub> peptide monitored by NMR. **Chem Commun (Camb)**. (2018) 7601-7604. doi: 10.1039/c8cc01710g. (IF 6.290)
627. Schober D, Jacob D, Wilson M, Cruz JA, Marcu A, Grant JR, Moing A, Deborde C, de Figueiredo LF, Haug K, Rocca-Serra P, Easton J, Ebbels TMD, Hao J, Ludwig C, Günther UL, Rosato A, Klein MS, Lewis IA, Luchinat C, Jones AR, Grauslys A, Larralde M, Yokochi M, Kobayashi N, Porzel A, Griffin JL, Viant MR, Wishart DS, Steinbeck C, Salek RM, Neumann S nmrML: a community supported open data standard for the description, storage, and exchange of NMR data. **Anal. Chem** 90, 649-656 (2018). (IF 6.320)
626. McCartney A, Vignoli A, Biganzoli L, Love R, Tenori L, Luchinat C, Di Leo A Metabolomics in breast cancer: A decade in review. **Cancer Treat Rev.** (2018); 67:88-96. doi: 10.1016/j.ctrv.2018.04.012. (IF 8.122)
625. 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. (IF 11.994)
624. Rumpel S, Ravera E, Sommer C, Reijerse E, Farès C, Luchinat C, Lubitz W, 1H NMR Spectroscopy of [FeFe] Hydrogenase: Insight into the Electronic Structure of the Active Site, **J Am Chem Soc.** (2018), 140, 131-134. doi: 10.1021/jacs.7b11196 (IF 14.357)

## 2017

623. Giuntini, S.; Cerofolini, L.; Ravera, E.; Fragai, M.; Luchinat, C.; Atomic structural details of a protein grafted onto gold nanoparticles, **Scientific Reports** 7, 17934, 2017 (IF 4.259)
622. 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, M.R., Iannetta, M., Capanella, C., Capitani, D., Mannina, L., Luchinat, C., and Pietropaolo, V., NMR-based metabolomic approach to study urines of chronic inflammatory rheumatic diseases, **Analytical and Bioanalytical Chemistry**, 409, 1405-1413, 2017 (IF 3.431)
621. 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)
620. 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)
619. 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).
618. 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).
617. 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).
616. 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**, 34 Suppl 1:S13-S18, 2017 (IF 2.801).
615. 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).
614. 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**, 69, 183-195. doi: 10.1007/s10858-017-0136-3. Epub 2017 Nov 27. 2017 (IF 2.410)
613. 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 Provenzano, A., Regulation of HuR structure and function by dihydrotanshione-I, **Nucleic Acids Res**, Doi: 10.1093/nar/gkx623, 2017 (IF 10.162).
612. 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).
611. 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).
610. 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).
609. Chatzikonstantinou, AV, Chatziathanasiadou, MV, Ravera, E., Fragai, M., Parigi, G., Gerotheranassis, I. P., Luchinat, C., Stamatis, 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).
608. 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).
607. 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 2.495).
606. Calderone, V., Fragai, M., and Luchinat, C., When molecular replacement has no trivial solution: the importance of model editing in human S100Z X-ray structure solution, **Inorg Chim Acta**, 2017 (IF 2.002).
605. Cacciatore, S., Tenori, L., Tyekucheva, S., Luchinat, C., Bennett, RP, and MacIntyre, DA, KODAMA: an R package for knowledge discovery and data mining, **Bioinformatics**, 10.1093/bioinformatics/btw705, 2017 (IF 4.981).
604. 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).
603. 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).
602. 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).

## 2016

601. Wallner-Liebmann, S., Tenori, L., Mazzoleni, A., Dieber-Rotheneder, M., Konrad, M., Hofmann, P., Luchinat, C., Turano, P., and Zatloukal, K., The individual metabolomic phenotype analyzed by 1H-NMR of saliva samples, **J.Proteome.Res.**, 15, 1787-1793, 2016 (IF 5.001).
600. Sala, D., Giachetti, A., Luchinat, C., and Rosato, A., A protocol for therefinement of NMR structures using simultaneously pseudocontact shift restraints from multiple lanthanide ions, **J.Biomol.NMR**, 66, 175-185, 2016 (IF 3.439).
599. Saccenti, E., Menichetti, G., Ghini, V., Remondini, D., Tenori, L., and Luchinat, C., Entropy-Based Network Representation of the Individual Metabolic Phenotype, **J.Proteome.Res.**, 15, 3298-3307, 2016 (IF 5.001).
598. Ravera, E., Sgheri, L., Parigi, G., and Luchinat, C., A critical assessment of methods to recover information from averaged data, **Phys.Chem.Chem.Phys.**, 2016, 5686-5701, 2016 (IF 4.493).
597. Ravera, E., Parigi, G., and Luchinat, C., Basic facts and perspectives of Overhauser DNP NMR, **J.Magn Reson.**, 264, 78-87, 2016 (IF 2.510).
596. Ravera, E., Cerofolini, L., Martelli, T., Louka, A., Fragai, M., and Luchinat, C., 1H detected solid state NMR of proteins entrapped in bioinspired silica: a new tool for biomaterials, **Sci.Rep.**, 6, 27851-doi: 10.1038/srep27851, 2016 (IF 5.578).
595. Ravera, E., Martelli, T., Geiger, Y., Fragai, M., Goobes, G., and Luchinat, C., Biosilica and bioinspired silica studied by solid-state nmr,

**Coord.Chem.Rev.**, 327, 110-122, 2016 (IF 12.239).

594. Ravera, E., Ciambellotti, S., Cerofolini, L., Martelli, T., Kozyreva, T., Bernacchioni, C., Giuntini, S., Fragai, M., Turano, P., and Luchinat, C., Solid-state NMR of PEGylated proteins, **Angew.Chem.Int.Ed.**, 55, 1-5, 2016 (IF 11.336).
593. Rammohan, N., MacRenaris, K. W., Moore, LK, Parigi, G., Mastarone, D. J., Manus, L. M., Lilley, LM, Preslar, AT, Waters, E. A., Filicko, A., Luchinat, C., Ho, D, and Meade, T. J., Nanodiamond-gadolinium(III) aggregates for tracking cancer growth in vivo at high field, **Nano Letters**, 16, 7551-7564, 2016 (IF 13.779).
592. Martelli, T., Ravera, E., Louka, A., Cerofolini, L., Hafner, M., Fragai, M., Becker, C. F. W., and Luchinat, C., Atomic level quality assessment of biosilica encapsulated and autoencapsulated enzymes, **Chem.Eur.J.**, 22, 425-432, 2016 (IF 5.771).
591. Luchinat, C., Exploring the conformational heterogeneity of biomolecules: theory and experiments, **Phys.Chem Chem Phys.**, 18, 5684-5685, 2016 (IF 4.493).
590. Hart, CD, Tenori, L., Luchinat, C., and Di Leo, A., Metabolomics in breast cancer: current status and perspectives, **Adv.Exp.Med.Biol.**, 882, 217-234, 2016 (IF 1.953).
589. Emwas, A. H., Roy, R., McKay, R. T., Ryan, D., Brennan, L., Luchinat, C., Tenori, L., Gao, X., Zeri, A. C., Gowda, G. A. N., Raftery, D., and Wishart, D. S., Recommendations and standardization of biomarker quantification using NMR-based metabolomics with particular focus on urinary analysis, **J.Proteome Res.**, 15, 360-373, 2016 (IF 5.001).
588. Cukrov, D., Zemiani, M., Brizzolara, S., Cestaro, A., Licausi, F., Luchinat, C., Santucci, C., Tenori, L., Van Veen, H., Zuccolo, A., Ruperti, B., and Tonutti, P., Extreme hypoxic conditions induce selective molecular responses and metabolic reset in detached apple fruit, **Front Plant Sci**, 7, 146-, 2016 (IF 3.360).
587. Cerofolini, L., Amar, S., Lauer, L., Martelli, T., Fragai, M., Luchinat, C., and Fields, G. B., Bilayer membrane modulation of membrane type 1 matrix metalloproteinase (MT1-MMP) Structure and proteolytic activity, **Sci.Rep.**, 6, 29511-, 2016 (IF 5.228).
586. Carlon, A., Ravera, E., Hennig, J., Parigi, G., Sattler, M., and Luchinat, C., Improved accuracy from joint X-ray and NMR refinement of a protein-RNA complex structure, **J.Am.Chem.Soc.**, 138, 1601-1610, 2016 (IF 13.038).
585. Carlon, A., Ravera, E., Andralojc, W., Parigi, G., Murshudov, G. N., and Luchinat, C., How to tackle protein structural data from solution and solid state: An integrated approach, **Progress in NMR Spectroscopy**, 92-93, 54-70, 2016 (IF 7.237).
584. Bertini, I., Luchinat, C., Parigi, G., and Ravera, E., NMR of Paramagnetic Molecules, 2016
583. Benda, L., Mare, J., Ravera, E., Parigi, G., Luchinat, C., Kaupp, M., and Vaara, J., Pseudo-contact NMR shifts over a paramagnetic metalloprotein (CoMMP-12) from first principles, **Angew.Chem.Int.Ed.**, 5, 14713-14717, 2016 (IF 11.336).
582. Baldoneschi, V., Cerofolini, L., Dragoni, E., Storai, A., Luchinat, C., Fragai, M., Richichi, B., and Nativi, C., Active-site targeting paramagnetic probe for matrix metalloproteinase, **Chempluschem**, 81, 1333-1338, 2016 (IF 2.44).
581. Andralojc, W., Ravera, E., Salmon, L., Parigi, G., Al-Hashimi, H. M., and Luchinat, C., Inter-helical conformational preferences of HIV-1 TAR-RNA from Maximum Occurrence analysis of NMR data and Molecular Dynamics simulations, **Phys.Chem.Chem.Phys.**, 18, 5743-5752, 2016 (IF 4.493).

## 2015

580. Wallner-Liebmann, S., Gralka, E., Tenori, L., Konrad, M., Hofman, P., Dieber-Rotheneder, M., Turano, P., Luchinat, C., and Zatloukal, K., The impact of free or standardized lifestyle and urine sampling protocol on metabolome recognition accuracy, **Genes&Nutrition**, 10, 441-443, 2015 (IF 3.419).
579. van Ommen, G. B., Tomwall, O., Brechot, C., Dagher, G., Galli, J., Hveem, K., Landegren, U., Luchinat, C., Metspalu, A., Nilsson, C., Solesvik, O. V., Perola, M., Litton, J. E., and Zatloukal, K., BBMRI-ERIC as a resource for pharmaceutical and life science industries: the development of biobank-based expert centres, **Eur.J.Hum.Genet.**, doi: 10.1038/ejhg.2014.235, 2015 (IF 4.225).
578. Tenori, L., Oakman, C., Morris, P. G., Gralka, E., Turner, N., Cappadona, S., Fournier, M., Hudis, C., Norton, C., Luchinat, C., and Di Leo, A., Serum metabolomic profiles evaluated after surgery may identify patients with estrogen receptor negative early breast cancer at increased risk of disease recurrence. Results from a retrospective study, **Mol.Oncol.**, 9, 128-139, 2015 (IF 5.331).
577. Santucci, C., Tenori, L., and Luchinat, C., NMR fingerprinting as a tool to evaluate post-harvest time-related changes of three agricultural products, **Food res.Intl.**, 75, 106-114, 2015 (IF 3.050).
576. Salek, R. M., Neumann, S., Schober, D., Hummel, J., Billiau, K., Kopka, J., Correa, E., Reijmers, T., Rosato, A., Tenori, L., Turano, P., Marin, S., Deborde, C., Jacob, D., Rolin, D., Dartigues, B., Conesa, P., Haug, K., Rocca-Serra, P., O'Hagan, S., Hao, J., vanVliet, M., ysi-Aho, M., udwing, C., ouwman, J., ascante, M., bbels, T., riffin, J. L., oing, A., ikolski, M., resc, M, anson, S.-A, iant, M. R., oodacre, R., unther, U. L., ankemeier, T., Luchinat, C., Walther, D., and Steinbeck, C., Coordination of standards in metabolomics (COSMOS): facilitating integrated metabolomics data access, **Metabolomics**, 11, 1587-1597, 2015 (IF 3.965).
575. Saccenti, E., Suarez-Diez, M., Luchinat, C., Santucci, A., and Tenori, L., Probabilistic networks of blood metabolites in healthy subjects as indicators of latent cardiovascular risk, **J.Proteome Res.**, 14, 1011-1111, 2015 (IF 5.001).
574. Rotz, M. W., Culver, K. S. B., Parigi, G., MacRenaris, K. W., Luchinat, C., Odom, T. W., and Meade, T. J., High relaxivity Gd(III)-DNA gold nanostars: investigation of shape effects on proton relaxation, **ACS nano**, 9, 3385-3396, 2015 (IF 12.033).
573. Rinaldelli, M., Carlon, A., Ravera, E., Parigi, G., and Luchinat, C., FANTEN: a new web-based interface for the analysis of magnetic anisotropy-induced NMR data, **J Biomol NMR**, 61, 21-34, 2015 (IF 3.141).
572. Ravera, E., Shimon, D., Feintuch, A., Goldfarb, D., Vega, S., Flori, A., Menichetti, L., Luchinat, C., and Parigi, G., The effect of Gd on trityl-based dynamic nuclear polarisation in solids, **Phys.Chem.Chem.Phys.**, 17, 26969-26978, 2015 (IF4.493).
571. Ravera, E., Michaelis, V. K., Ong, T. C., Keeler, E. G., Martelli, T., Fragai, M., Griffin, R. G., and Luchinat, C., Biosilica-entrapped enzymes can be studied by DNP-enhanced high-field NMR, **ChemPhysChem**, 16, 2751-2754, 2015 (IF 3.419).
570. Ravera, E., Schubeis, T., Martelli, T., Fragai, M., Parigi, G., and Luchinat, C., NMR of sedimented, fibrillized, silica-entrapped and microcrystalline (metallo)proteins, **J.Magn Reson.**, 253, 60-70, 2015 (IF 2.300).
569. Ravera, E., Fragai, M., Parigi, G., and Luchinat, C., Differences in dynamics between cross-linked and non-cross-linked hyaluronates measured by fast-field-cycling relaxometry, **ChemPhysChem**, 16, 2803-2809, 2015 (IF 3.419).
568. Ravanbakhsh, S., Liu, P., Bjorndahl, T. C., Mandal, R., Grant, J. R., Wilson, M., Eisner, R., Sineelnikov, I., Hu, X., Luchinat, C., Greiner, R., and Wishart, D. S., Accurate, fully-automated NMR spectral profiling for metabolomics, **Plos ONE**, 10, e0124219-, 2015 (IF 3.534).

567. Luchinat, C. and Tenori, L., Applications of <sup>1</sup>H-NMR metabolomics: from individual fingerprints to food analysis, in: *Magnetic Resonance in Food Science*, <[05] Date, primary>
566. Gralka, E., Luchinat, C., Tenori, L., Ernst, B., Thumheer, M., and Schultes, B., The metabolomic fingerprint of severe obesity is dynamically affected by bariatric surgery in a procedure-dependent manner, **Am.J.Clin.Nutr.**, 102, 1313-1322, 2015 (IF 6.77).
565. Ghini, V., Saccenti, E., Tenori, L., Assfalg, M., and Luchinat, C., Allostasis and resilience of the human individual metabolic phenotype, **J.Proteome.Res.**, 14, 2951-2962, 2015 (IF 4.245).
564. Fragai, M. and Luchinat, C., Matrix metalloproteinase: from structure to function, in: *Matrix metalloproteinase biology*, <[05] Date, primary>
563. Emwas, A. H., Luchinat, C., Turano, P., Tenori, L., Roy, R., Salek, R., Ryan, D., Merzaban, J. S., Kaddurah-Daouk, R., Zeri, A. C., Gowda, G. A. N., Raftery, D., Wang, Y., Brennan, L., and Wishart, D. S., Standardizing the experimental conditions for using urine in NMR-based metabolomic studies with a particular focus on diagnostic studies: a review, **Metabolomics**, 11, 872-894, 2015 (IF 3.965).
562. Carotenuto, D., Luchinat, C., Marcon, G., Rosato, A., and Turano, P., The Da Vinci European BioBank: a metabolomics driven infrastructure, **J.Pers.Med.**, 5, 107-119, 2015 (IF 1.132).
561. Ardenkjaer-Larsen, J.-H., Boebinger, G. S., Comment, A., Duckett, S. B., Edison, A. S., Engelke, F., Griesinger, C., Griffin, R. G., Hilty, C., Maeda, H., Parigi, G., Prisner, T. F., Ravera, E., van Bentum, G. J. M., Vega, S., Webb, A., Luchinat, C., Schwalbe, H., and Frydman, L., Facing and overcoming biomolecular NMR's sensitivity challenges, **Angew.Chem.Int.Ed.**, 54, 9162-9185, 2015 (IF 11.336).
560. Andralojc, W., Berlin, K., Fushman, D., Luchinat, C., Parigi, G., Ravera, E., and Sgheri, L., Information content of long-range NMR data for the characterization of conformational heterogeneity, **J.Biomol.NMR**, 62, 353-371, 2015 (IF 3.305).

## 2014

559. Tenori, L., Oakman, C., Morris, P. G., Gralka, E., Cappadona, S., Fomier, M., Hudis, C., Norton, L., Luchinat, C., and Di Leo, A., Serum metabolomic profiles evaluated after surgery identify early breast cancer patients with increased risk of disease recurrence, **Mol.Oncol.**, 14, 00167-00174, 2014 (IF 5.935).
558. Tarocchi, M., Polvani, S., Peired, A.J., Marroncini, G., Calamante, M., Ceni, E., Rhodes, D., Mello, G., Pieraccini, G., Quattrone, A., Luchinat, C., and Galli, A., Telomerase activated thymidine analogue pro-drug is a new molecule targeting hepatocellular carcinoma, **J.Hepatol.**, 14, 1064-1072, 2014 (IF 10.401).
557. Saccenti, E., Tenori, L., Verbruggen, P., Timmerman, M.A., Bouwman, J., van der Greef, J., Luchinat, C., and Smilde, A. K., Of monkeys and men: a metabolomic analysis of static and dynamic urinary metabolic phenotypes in two species, **PLoS ONE**, 9, e106077, 2014 (IF 3.534).
556. Rinaldelli, M., Ravera, E., Calderone, V., Parigi, G., Murshudov, G. N., and Luchinat, C., Simultaneous use of solution NMR and X-ray data REFMAC5 for joint refinement/detection of structural differences, **Acta Cryst.D**, D70, 958-967, 2014 (IF 14.103).
555. Ravera, E., Salmon, L., Fragai, M., Parigi, G., Al-Hashimi, H. M., and Luchinat, C., Insights into domain-domain motions in proteins and RNA from solution NMR, **Acc.Chem.Res.**, 47, 3118-3126, 2014 (IF 24.348).
554. Ravera, E., Corzilius, B., Michaelis, V. K., Luchinat, C., Griffin, R. G., and Bertini, I., DNP-enhanced MAS NMR of Bovine Serum Albumin Sediments and Solutions, **J.Phys.Chem.B**, 118, 2957-2965, 2014 (IF 3.607).
553. Ravanbakhsh, S., Liu, P., Bjorn Dahl, T. C., Mandal, R., Grant, J. R., Wilson, M., Eisner, R., Sinelnikov, I., Hu, X., Luchinat, C., Greiner, R., and Wishart, D. S., Accurate, fully-automated NMR spectral profiling for metabolomics, **arXiv**, 1409.1456v3, 2014
552. Preslar, A. t., Parigi, G., McClendon, M. T., Sefick, S. S., Moyer, T. J., Haney, C. R., Waters, E. A., MacRenaris, K. W., Luchinat, C., Stupp, S. I., and Meade, T. J., Gd(III)-labeled peptide nanofibers for reporting on biomaterial localization in vivo, **ACS nano**, 8, 7325-7332, 2014 (IF 12.033).
551. Parigi, G., Rezaei-Ghaleh, N., Giachetti, A., Becker, S., Fernandez, C., Blackledge, M., Griesinger, C., Zweckstetter, M., and Luchinat, C., Long-Range Correlated Dynamics in Intrinsically Disordered Proteins, **J.Am.Chem.Soc.**, 136, 16201-16209, 4-11-2014 (IF 11.444).
550. Padeletti, L., Modesti, P.A., Cartei, S., Checchi, L., Ricciardi, G., Pieragnoli, P., Alterini, B., Padeletti, M., Hu, X., Tenori, L., and Luchinat, C., Metabolomic does not predict response to cardiac resynchronization therapy in patients with heart failure, **J.Cardiov.Med.**, 15, 295-300, 2014 (IF 2.657).
549. Neugebauer, P., Krummenacker, J. G., Denysenkov, V. P., Helmling, C., Luchinat, C., Parigi, G., and Prisner, T. F., High-field liquid state NMR hyperpolarization: a combined DNP/NMRD approach, **Phys.Chem.Chem.Phys.**, 16, 18781-18787, 2014 (IF 4.198).
548. Michaelis, V. K., Ong, T. C., Kiesewetter, M. K., Frantz, D. K., Walsh, J. J., Ravera, E., Luchinat, C., Swager, T. M., and Griffin, R. G., Topical developments in high-field dynamic nuclear polarization, **Israel J.Chem.**, 54, 207-221, 2014 (IF 1.535).
547. Luchinat, C., Parigi, G., and Ravera, E., NMR technology: the competitive world of RAS biology, **Nature Chemical Biology**, 10, 173-174, 2014 (IF 12.948).
546. Luchinat, C., Parigi, G., and Ravera, E., Can metal ion complexes be used as polarizing agents for solution DNP? A theoretical discussion., **J.Biomol.NMR**, 58, 239-249, 2014 (IF 3.305).
545. Fragai, M., Luchinat, C., Martelli, T., Ravera, E., Sagi, I., Solomonov, I., and Udi, Y., SSNMR of biosilica-entrapped enzymes permits an easy assessment of preservation of native conformation in atomic detail, **Chem.Commun.**, 50, 421-423, 2014 (IF 6.2).
544. Dani, C., Bresci, C., Berti, E., Mello, G., Hu, X., Tenori, L., and Luchinat, C., Metabolomic profile of term infants of gestational diabetic mothers, **J.Matern.Fetal.Neonatal.Med.**, 27, 537-542, 2014 (IF 1.518).
543. Corzilius, B., Michaelis, V. K., Penzel, S., Ravera, E., Smith, A., Luchinat, C., and Griffin, R. G., Dynamic nuclear polarization of <sup>1</sup>H, <sup>13</sup>C and <sup>59</sup>Co in a Co(III) tris-ethylenediamine crystalline lattice doped with Cr(III), **J.Am.Chem.Soc.**, 136, 11716-11727, 2014 (IF 11.444).
542. Cerofolini, L., Amato, J., Fragai, M., Giachetti, A., Limongelli, V., Luchinat, C., Novellino, E., Parrinello, M., and Randazzo, A., G-triplex structure and formation propensity, **Nucleic Acids Res.**, 42, 13393-13404, 2014 (IF 8.808).
541. Calabro, A., Gralka, E., Luchinat, C., Saccenti, E., and Tenori, L., A metabolomic perspective on coeliac disease, **Autoimmune diseases**, 2014, 756138, 2014
540. Cacciatore, S., Luchinat, C., and Tenori, L., Knowledge discovery by accuracy maximization, **Proc.Natl.Acad.Sci.USA**, 111, 5117-5122, 2014 (IF 9.771).
539. Bertini, I., Hu, X., and Luchinat, C., Metabolomics characterization of bacteria: pre-analytical treatments and profiling, **Metabolomics**,

10, 241-249, 2014 (IF 4.433).

538. Bertini, I., Luchinat, C., Miniati, M., Monti, S., and Tenori, L., Phenotyping COPD by 1H-NMR metabolomics of exhaled breath condensate, **Metabolomics**, 10, 302-311, 2014 (IF 4.433).

537. Banci, L. and Luchinat, C., Biological inorganic chemists pay tribute to Ivano Bertini, **J.Biol.Inorg.Chem.**, 19, 487-489, 2014 (IF 3.353).

536. Banci, L., Blazevits, O., Cantini, F., Danielsson, J., Lang, L., Luchinat, C., Mao, J., Oliveberg, M., and Ravera, E., Solid-state NMR studies of metal free SOD1 fibrillar structures, **J.Biol.Inorg.Chem.**, 19, 659-666, 2014 (IF 3.353).

535. Andralojc, W., Luchinat, C., Parigi, G., and Ravera, E., Exploring regions of conformational space occupied by two-domain proteins, **J.Phys.Chem.B**, 118, 10576-10587, 2014 (IF 3.607).

## 2013

534. Udi, Y., Fragai, M., Grossman, M., Mitternacht, S., Arad-Yellin, R., Calderone, V., Melikian, M., Toccafondi, M., Berezovsky, I. N., Luchinat, C., and Sagi, I., Unraveling hidden regulatory sites in structurally homologous metalloproteases, **J.Mol.Biol.**, 425, 2330-2346, 10-7-2013 (IF 4.008).

533. Tenori, L., Hu, X., Pantaleo, P., Alterini, B., Castelli, G., Olivetto, I., Bertini, I., Luchinat, C., and Gensini, G., Metabolomic fingerprint of heart failure in humans: a nuclear magnetic resonance spectroscopy analysis, **In.J.Cardiol.**, 164, e113-115, 2013 (IF 5.509).

532. Ravera, E., Parigi, G., Mainz, A., Religa, T. L., Reif, B., and Luchinat, C., Experimental determination of microsecond reorientation correlation times in protein solutions, **J.Phys.Chem.B**, 117, 3548-3553, 2013 (IF 3.696).

531. Ravera, E., Corzilius, B., Michaelis, V. K., Rosa, C., Griffin, R. G., Luchinat, C., and Bertini, I., Dynamic Nuclear Polarization of Sedimented Solutes, **J.Am.Chem.Soc.**, 135, 1641-1644, 2013 (IF 9.907).

530. Neugebauer, P., Krummenacker, J. G., Denysenkov, V. P., Parigi, G., Luchinat, C., and Prisner, T. F., Liquid state DNP of water at 9.2 T: an experimental access to saturation, **Phys.Chem.Chem.Phys.**, 15, 6049-6056, 2013 (IF 3.57).

529. Mori, M., Massaro, A., Calderone, V., Fragai, M., Luchinat, C., and Mordini, A., Discovery of a new class of potent MMP inhibitors by structure-based optimization of the arylsulfonamide scaffold, **ACS Medicinal Chemistry Letters**, 4, 565-569, 2013 (IF 3.073).

528. Mori, M., De Lorenzo, E., Torre, E., Fragai, M., Nativi, C., Luchinat, C., and Arcangeli, A., A highly soluble matrix metalloproteinase-9 inhibitor for potential treatment of dry eye syndrome, **Basic.Clin.Pharmacol.Toxicol.**, 111, 289-295, 2013 (IF 2.124).

527. Luchinat, C., Parigi, G., and Ravera, E., Water and protein dynamics in sedimented systems: a relaxometric investigation, **Chem.Phys.Chem.**, 14, 3156-3161, 2013 (IF 3.412).

526. Limongelli, V., De Tito, S., Cerofolini, L., Fragai, M., Pagano, B., Trotta, R., Cosconati, S., Marinelli, L., Novellino, E., Bertini, I., Randazzo, A., Luchinat, C., and Parrinello, M., The G-triplex DNA, **Angew.Chem.Int.Ed.**, 52, 2269-2273, 18-2-2013 (IF 13.734).

525. Hung, A. H., Duch, M. C., Parigi, G., Rotz, M. W., Manus, L. M., Mastarone, D. J., Dam, K. T., Gits, C. C., MacRenaris, K. W., Luchinat, C., Hersam, M. C., and Meade, T. J., Mechanisms of gadographene-mediated proton spin relaxation, **J.Phys.Chem.C**, 117, 16263-16273, 2013 (IF 4.814).

524. Fragai, M., Luchinat, C., Parigi, G., and Ravera, E., Practical considerations over spectral quality in solid state NMR spectroscopy of soluble proteins, **J.Biomol.NMR**, 57, 155-166, 2013 (IF 3.612).

523. Fragai, M., Luchinat, C., Parigi, G., and Ravera, E., Conformational freedom of metalloproteins revealed by paramagnetism-assisted NMR, **Coord.Chem.Rev.**, 257, 2652-2667, 2013 (IF 12.110).

522. Ferella, L., Luchinat, C., Ravera, E., and Rosato, A., SEDNMR: A web tool for optimizing sedimentation of macromolecular solutes for SSNMR, **J.Biomol.NMR**, 57, 319-326, 2013 (IF 2.845).

521. Czarny, B., Stura, E. A., Devel, L., Vera, L., Cassar-Lajeunesse, E., Beau, F., Calderone, V., Fragai, M., Luchinat, C., and Dive, V., Molecular determinants of a selective matrix metalloprotease-12 inhibitor: insights from crystallography and thermodynamic studies, **J.Med.Chem.**, 56, 1149-1159, 14-2-2013 (IF 5.614).

520. Cerofolini, L., Fields, G. B., Fragai, M., Gheraldes, C. F. G. C., Luchinat, C., Parigi, G., Ravera, E., Svergun, D. I., and Teixeira, J. M. C., Examination of Matrix Metalloproteinase-1 (MMP-1) in solution: a preference for the pre-collagenolysis state, **J.Biol.Chem.**, 288, 30659-30671, 2013 (IF 4.651).

519. Cacciatore, S., Hu, X., Viertler, C., Kap, M., Bernhardt, G. A., Mischinger, H. J., Riegman, P., Zatloukal, K., Luchinat, C., and Turano, P., The effects of intra- and postoperative ischemia on the metabolic profile of clinical tissue specimens monitored by NMR, **J.Proteome Res.**, 12, 5723-5729, 2013 (IF 5.056).

518. Bhaumik, A., Luchinat, C., Parigi, G., Ravera, E., and Rinaldelli, M., NMR crystallography on paramagnetic systems: solved and open issues, **Cryst.Eng.Comm.**, 15, 8639-8656, 2013 (IF 3.879).

517. Bertini, I., Luchinat, C., Parigi, G., and Ravera, E., SedNMR: on the edge between solution and solid state NMR, **Acc.Chem.Res.**, 46, 2059-2069, 2013 (IF 21.640).

516. Bertini, I., Gallo, G., Korsak, M., Luchinat, C., Mao, J., and Ravera, E., Formation Kinetics and Structural Features of Beta-Amyloid Aggregates by Sedimented Solute NMR, **ChemBioChem**, 14, 1891-1897, 2013 (IF 3.944).

515. Bertini, I., Borsi, V., Cerofolini, L., Das Gupta, S., Fragai, M., and Luchinat, C., Solution structure and dynamics of human S100A14, **J.Biol.Inorg.Chem.**, 2, 183-194, 2013 (IF 3.353).

514. Bertini, I., Borsi, V., Cerofolini, L., Das, Gupta S., Fragai, M., and Luchinat, C., Solution structure and dynamics of human S100A14, **J.Biol.Inorg.Chem.**, 18, 2013

513. Bartoloni, M., Dominiquez, B. E., Dragoni, E., Richichi, B., Fragai, M., Andre', S., Gabius, H.-J., Ardà, A., Luchinat, C., Jimenez-Barbero, J., and Nativi, C., Targeting matrix metalloproteinases: design of a bifunctional inhibitor of presentation by tumor-associated galectins, **Chem.Eur.J.**, 19, 1896-1902, 2013 (IF 5.925).

## 2012

512. Turke, MT, Parigi, G., Luchinat, C., and Bennati, M., Overhauser DNP with 15N labelled Fremy's salt as polarizer, **Phys.Chem.Chem.Phys.**, 14, 502-510, 2012 (IF 3.453).

511. Tenori, L., Oakman, C., Claudino, W., Bernini, P., Cappadona, S., Nepi, S., Biganzoli, L., Arbushites, M. C., Luchinat, C., Bertini, I.,

- and Di Leo, A., Exploration of serum metabolomic profiles and outcomes in women with metastatic breast cancer: A pilot study, **Mol.Oncol.**, 6, 437-444, 2012 (IF 4.25).
510. Oakman, C., Tenori, L., Cappadona, S., Luchinat, C., Bertini, I., and Di Leo, A., Targeting metabolomics in breast cancer, **Curr.Breast Cancer Reports**, 4, 249-256, 2012 (IF 3.696).
509. Nagulapalli, M., Parigi, G., Yuan, J., Gsponer, J., Deraos, S., Bamm, V. V., Harauz, G., Matsoukas, J., de Planque, MRR, Gerothanassis, I. P., Babu, M. M., Luchinat, C., and Tzakos, A. G., Recognition pliability is coupled to structural heterogeneity: a calmodulin-intrinsically disordered binding region complex, **Structure**, 20, 522-533, 2012 (IF 6.337).
508. Mori, M., De Lorenzo, E., Torre, E., Fragai, M., Nativi, C., Luchinat, C., and Arcangeli, A., A highly soluble matrix metalloproteinase-9 inhibitor for potential treatment of dry eye syndrome, **Basic.Clin.Pharmacol.Toxicol.**, 111, 289-295, 2012 (IF 2.179).
507. Maccaferri, S., Klinder, A., Cacciato, S., Chitarrari, R., Honda, H., Luchinat, C., Bertini, I., Carnevali, P., Gibson, G. F., Brigidi, P., and Costabile, A., In Vitro fermentation of potential prebiotic flours from natural sources: impact of the human colonic microbiota and metabolome, **Mol Nutr Food Res.**, 56, 1342-1352, 2012 (IF 4.3).
506. Luchinat, C., Parigi, G., Ravera, E., and Rinaldelli, M., Solid state NMR crystallography through paramagnetic restraints, **J.Am.Chem.Soc.**, 134, 5006-5009, 2012 (IF 9.019).
505. Luchinat, C., Nagulapalli, M., Parigi, G., and Sgheri, L., Maximum occurrence analysis of protein conformations for different distributions of paramagnetic metal ions within flexible two-domain proteins, **J.Magn.Reson.**, 215, 85-93, 2012 (IF 2.333).
504. Griesinger, C., Bennati, M., Vieth, H.-M., Luchinat, C., Parigi, G., Hofer, P., Engelke, F., Glaser, S. J., Denysenkov, V., and Prisner, T. F., Dynamic nuclear polarization at high magnetic fields in liquids, **Progr.NMR Spectrosc.**, 64, 4-28, 2012 (IF 4.933).
503. Franks, W. T., van Rossum, B.-J., Bardiaux, B., Ravera, E., Parigi, G., Luchinat, C., and Oschkinat, H., Microcrystalline Proteins—An Ideal Benchmark for Methodology Development, in: *NMR of Biomolecules: Towards Mechanistic Systems Biology*, Bertini, I., McGreevy, K. S., and Parigi, G., 376, <[05] Date, primary>
502. Borsi, V., Cerofolini, L., Fragai, M., and Luchinat, C., NMR characterization of the C-terminal tail of full-length RAGE in a membrane mimicking environment, **J.Biomol.NMR**, 54, 285-290, 2012 (IF 3.612).
501. Bertini, I., Engelke, F., Gonnelli, L., Knott, B., Luchinat, C., Osen, D., and Ravera, E., On the use of ultracentrifugal devices for sedimented solute NMR, **J.Biomol.NMR**, 54, 123-127, 2012 (IF 3.612).
500. Bertini, I., Ferella, L., Luchinat, C., Parigi, G., Petoukhov, M. V., Ravera, E., Rosato, A., and Svergun, D. I., MaxOcc: a web portal for Maximum Occurrence Analysis, **J.Biomol.NMR**, 53, 271-280, 2012 (IF 3.612).
499. Bertini, I., Engelke, F., Luchinat, C., Parigi, G., Ravera, E., Rosa, C., and Turano, P., NMR properties of sedimented solutes, **Phys.Chem.Chem.Phys.**, 14, 439-447, 2012 (IF 3.453).
498. Bertini, I., Luchinat, C., and Tenori, L., Metabolomics for the future of personalized medicine through information and communication technologies, **J.Pers.Med.**, 9, 133-136, 2012 (IF 0.783).
497. Bertini, I., Luchinat, C., Nagulapalli, M., Parigi, G., and Ravera, E., Paramagnetic relaxation enhancements for the characterization of the conformational heterogeneity in two-domain proteins, **Phys.Chem.Chem.Phys.**, 14, 9149-9156, 2012 (IF 3.453).
496. Bertini, I., Fragai, M., Luchinat, C., Melikian, M., Toccafondi, M., Lauer, J. L., and Fields, G. B., Structural Basis for Matrix Metalloproteinase 1-Catalyzed Collagenolysis, **J.Am.Chem.Soc.**, 134, 2100-2110, 2012 (IF 9.019).
495. Bertini, I., Cacciato, S., Jensen, B. V., Schou, J. V., Johansen, J. S., Kruhøffer, M., Luchinat, C., Nielsen, D. L., and Turano, P., Metabolomic NMR fingerprinting to identify and predict survival of patients with metastatic colorectal cancer, **Cancer Res.**, 356-364, 2012 (IF 8.234).
494. Bertini, I., Calderone, V., Cerofolini, L., Fragai, M., Gherdes, C. F. G. C., Hermann, P., Luchinat, C., Parigi, G., and Teixeira, J. M. C., The catalytic domain of MMP-1 studied through tagged lanthanides. Dedicated to Prof. A.V. Xavier, **FEBS Lett.**, 586, 557-567, 2012 (IF 3.264).
493. Banci, L. and Luchinat, C., Ivano Bertini 1940-2012., **Nat.Chem.Biol.**, 8, 807-, 2012 (IF 14.690).

## 2011

492. Polvani, S., Calamante, M., Foresta, V., Ceni, E., Mordini, A., Quattrone, A., D'Amico, M., Luchinat, C., Bertini, I., and Galli, A., Acycloguanosyl 5'-thymidyltriphosphate, a new thymidine analogue prodrug activated by telomerase, reduces pancreatic tumor growth in mice, **Gastroenterology**, 140, 709-720, 2011 (IF 12.403).
491. Oakman, C., Tenori, L., Claudino, W. M., Cappadona, S., Nepi, S., Battaglia, A., Bernini, P., Zafarana, E., Saccenti, E., Fomier, M., Morris, P. G., Biganzoli, L., Luchinat, C., Bertini, I., and Di Leo, A., Identification of a serum-detectable metabolomic fingerprint potentially correlated with the presence of micrometastatic disease in early breast cancer patients at varying risks of disease relapse by traditional prognostic methods, **Ann.Oncol.**, 22, 1295-1301, 2011 (IF 6.452).
490. Mastarone, D. J., Harrison, V. S. R., Eckermann, A. L., Parigi, G., Luchinat, C., and Meade, T. J., A modular system for the synthesis of multiplexed MR probes, **J.Am.Chem.Soc.**, 133, 5329-5337, 2011 (IF 9.019).
489. Das Gupta, S., Hu, X., Keizers, P. H. J., Liu, W.-M., Luchinat, C., Nagulapalli, M., Overhand, M., Parigi, G., Sgheri, L., and Ubbink, M., Narrowing the conformational space sampled by two-domain proteins with paramagnetic probes in both domains, **J.Biomol.NMR**, 51, 253-263, 2011 (IF 3.047).
488. Corzilius, B., Smith, A. A., Barnes, A. B., Luchinat, C., Bertini, I., and Griffin, R. G., High-field dynamic nuclear polarization with high spin transition metal ions, **J.Am.Chem.Soc.**, 133, 5648-5651, 2011 (IF 9.019).
487. Bertini, I., Luchinat, C., Parigi, G., Ravera, E., Reif, B., and Turano, P., Solid-state NMR of proteins sedimented by ultracentrifugation, **Proc.Natl.Acad.Sci.USA**, 108, 10396-10399, 2011 (IF 9.771).
486. Bertini, I., Luchinat, C., and Parigi, G., Moving the frontiers in solution solid state bioNMR. A celebration of Harry Gray's 75th birthday, **Coord.Chem.Rev.**, 255, 649-663, 2011 (IF 10.018).
485. Bertini, I., Gonnelli, L., Luchinat, C., Mao, J., and Nesi, A., A new structural model A $\beta$ 40 fibrils, **J.Am.Chem.Soc.**, 133, 16013-16022, 2011 (IF 9.019).
484. Bernini, P., Bertini, I., Luchinat, C., Tenori, L., and Tognaccini, A., The cardiovascular risk of healthy individuals studied by NMR metabolomics of plasma samples, **J.Proteome Res.**, 10, 4983-4992, 2011 (IF 5.460).
483. Bernini, P., Bertini, I., Calabro, A., La Marca, G., Lami, G., Luchinat, C., Renzi, D., and Tenori, L., Are patients with potential celiac



- disease really potential? The answer of metabonomics, **J.Proteome Res.**, 10, 714-721, 2011 (IF 5.460).
482. Bernini, P., Bertini, I., Luchinat, C., Nincheri, P., Staderini, S., and Turano, P., Standard operating procedures for pre-analytical handling of blood and urine for metabolomic studies and biobanks, **J.Biomol.NMR**, 49, 231-243, 2011 (IF 3.047).
481. Banci, L., Bertini, I., Blazevits, O., Cantini, F., Lelli, M., Luchinat, C., Mao, J., and Vieru, M., NMR characterization of a "fibril-ready" state of demetallated wild-type superoxide dismutase, **J.Am.Chem.Soc.**, 133, 345-349, 2011 (IF 9.019).
480. Babini, E., Bertini, I., Borsi, V., Calderone, V., Hu, X., Luchinat, C., and Parigi, G., Structural characterization of human S100A16, a low-affinity calcium binder, **J.Biol.Inorg.Chem**, 16, 2011
479. Babini, E., Bertini, I., Borsi, V., Calderone, V., Hu, X., Luchinat, C., and Parigi, G., Structural characterization of human S100A16, a low affinity calcium binder, **J.Biol.Inorg.Chem.**, 16, 243-256, 2011 (IF 3.287).

## 2010

478. Oakman, C., Tenori, L., Biganzoli, L., Santaripa, L., Cappadona, S., Luchinat, C., and Di Leo, A., Uncovering the metabolomic fingerprint of breast cancer, **Int.J.Biochem.Cell Biol.**, 10-5-2010 (IF 4.178).
477. Luchinat, C. and Parigi, G., Paramagnetic systems in biochemistry: solution NMR studies Harris, R. K. and Wasylishen, R. E., DOI: 10.1002/9780470034590.emrstm.1088, <[05] Date, primary>
476. Borsi, V., Calderone, V., Fragai, M., Luchinat, C., and Sarti, N., Entropic contribution to the linking coefficient in fragment based drug design: a case study, **J.Med.Chem.**, 53, 4285-4289, 2010 (IF 4.898).
475. Bertini, I., Giachetti, A., Luchinat, C., Parigi, G., Petoukhov, M. V., Pierattelli, R., Ravera, E., and Svergun, D. I., Conformational space of flexible biological macromolecules from average data, **J.Am.Chem.Soc.**, 132, 13553-13558, 2010 (IF 8.580).
474. Bertini, I., Bhaumik, A., De Paepe, G., Griffin, R. G., Lelli, M., Lewandowski, J. R., and Luchinat, C., High-Resolution Solid-State NMR Structure of a 17.6 kDa Protein, **J.Am.Chem.Soc.**, 132, 1032-1040, 27-1-2010
473. Bertini, I., Emsley, L., Lelli, M., Luchinat, C., Mao, J., and Pintacuda, G., Ultra-Fast MAS solid-state NMR permits extensive <sup>13</sup>C and <sup>1</sup>H detection in paramagnetic metalloproteins, **J.Am.Chem.Soc.**, 132, 5558-5559, 2010 (IF 8.580).
472. Bennati, M., Luchinat, C., Parigi, G., and Türke, M.-T., Water proton relaxation dispersion analysis on a nitroxide radical provides information on the maximal signal enhancement in overhauser dynamic nuclear polarization experiments, **PhysChemChemPhys**, 12, 5902-5910, 2010 (IF 4.064).
471. Banci, L., Bertini, I., Luchinat, C., and Mori, M., NMR in structural proteomics and beyond, **Prog.NMR Spectrosc.**, 56, 247-266, 2010 (IF 6.162).
470. Attolino, E., Calderone, V., Dragoni, E., Fragai, M., Richichi, B., Luchinat, C., and Nativi, C., Structure-based approach to nanomolar, water soluble matrix metalloproteinases inhibitors (MMPis), **Eur.J.Med.Chem.**, 45, 5919-5925, 2010 (IF 2.882).

## 2009

469. Reese, M., Türke, M.-T., Tkach, I., Parigi, G., Luchinat, C., Marquardsen, T., Tavernier, A., Höfer, P., Engelke, F., Griesinger, C., and Bennati, M., <sup>1</sup>H and <sup>13</sup>C dynamic nuclear polarization in aqueous solution with a two-field (0.35T/14T) shuttle DNP spectrometer, **J.Am.Chem.Soc.**, 131, 15086-15087, 2009 (IF 8.091).
468. Luchinat, C. and Parigi, G., Paramagnetic systems in biochemistry: solution NMR studies <[05] Date, primary>
467. Isaksson, J., Nystroem, S., Derbishire, W., Wallberg, H., Agback, T., Kovacs, H., Bertini, I., Giachetti, A., and Luchinat, C., Does a fast nuclear magnetic resonance spectroscopy- and X-ray crystallography hybrid approach provide reliable structural information of ligand-protein complexes? A case study of metalloproteinases, **J.Med.Chem.**, 1712-1722, 2009 (IF 4.898).
466. Dragoni, E., Calderone, V., Fragai, M., Jaiswal, R., Luchinat, C., and Nativi, C., Biotin-tagged probes for MMP expression and activation: design, synthesis and binding properties, **Bioconjug.Chem.**, 4, 719-727, 2009 (IF 4.584).
465. Borsi, V., Luchinat, C., and Parigi, G., Global and local mobility of apocalmodulin monitored through fast field cycling relaxometry, **Biophys.J.**, 97, 1765-1771, 2009 (IF 4.683).
464. Bertini, I., Dasgupta, S., Hu, X., Karavelas, T., Luchinat, C., Parigi, G., and Yuan, J., Solution structure and dynamics of S100A5 in the apo and Ca<sup>2+</sup>-bound states, **Ravanbakhsh**, 14, 1097-1107, 2009 (IF 3.6).
463. Bertini, I., Fragai, M., Luchinat, C., Melikian, M., and Venturi, C., Characterization of the MMP-12-elastin adduct, **Chem.Eur.J.**, 15, 7842-7845, 2009 (IF 5.454).
462. Bertini, I., Luchinat, C., Parigi, G., and Pierattelli, R., NMR spectroscopy of paramagnetic metalloproteins, in: Encyclopedia of Chemical Biology, Begley, T. P., 408, <[05] Date, primary>
461. Bertini, I., Calderone, V., Fragai, M., Luchinat, C., and Talluri, E., Structural basis of serine/threonine phosphatase inhibition by the archetypal small molecules cantharidin and norcantharidin, **J.Med.Chem.**, 15, 4838-4843, 2009 (IF 4.898).
460. Bertini, I., Fragai, M., and Luchinat, C., Intra- and Interdomain Flexibility in Matrix Metalloproteinases: Functional Aspects and Drug Design, **Curr.Pharm.Des.**, 15, 3592-3605, 2009 (IF 4.399).
459. Bertini, I., Calabro, A., De carli, V., Luchinat, C., Nepi, S., Porfirio, B., Renzi, D., Saccenti, E., and Tenori, L., The metabonomic signature of celiac disease, **J.Proteome Res.**, 1, 170-177, 2009 (IF 5.684).
458. Bertini, I., Kursula, P., Luchinat, C., Parigi, G., Vahokoski, J., Wilmanns, M., and Yuan, J., Accurate solution structures of proteins from X-ray data and minimal set of NMR data: calmodulin peptide complexes as examples, **J.Am.Chem.Soc.**, 131, 5134-5144, 2009 (IF 8.091).
457. Bertini, I., Das, Gupta S., Hu, X., Karavelas, T., Luchinat, C., Parigi, G., and Yuan, J., Solution structure and dynamics of S100A5 in the apo and Ca<sup>2+</sup>-bound states, **J.Biol.Inorg.Chem**, 14, 2009
456. Bertini, I., Fragai, M., Luchinat, C., Melikian, M., Mylonas, E., Sarti, N., and Svergun, D., Interdomain flexibility in full-length matrix metalloproteinase-1 (MMP-1), **J.Biol.Chem.**, 284, 12821-12828, 2009 (IF 5.520).

## 2008

455. Urbanczyk-Pearson, L. M., Femia, F. J., Smith, J., Parigi, G., Luchinat, C., and Meade, T. J., Mechanistic Investigation of b-galactosidase-activated MR Contrast Agents, **Inorg.Chem.**, 47, 56-68, 2008 (IF 4.123).

454. Pellecchia, M., Bertini, I., Cowburn, D., Dalvit, C., Giralt, E., Jahnke, W., James, T. L., Homans, S. W., Kessler, H., Luchinat, C., Meyer, B., Oschkinat, H., Peng, J., Schwalbe, H., and Siegal, G., Perspectives on NMR in drug discovery: a technique comes of age, **Nat.Rev.Drug Discov.**, 7, 738-745, 2008 (IF 23.308).
453. Luchinat, C. and Parigi, G., Nuclear relaxometry helps designing systems for solution DNP on proteins, *Appl.Magn.Reson.-A special volume on DNP*, 34, 379-392, 2008 (IF 0.706).
452. Höfer, P., Parigi, G., Luchinat, C., Carl, P., Guthausen, G., Reese, M., Carlomagno, T., Griesinger, C., and Bennati, M., Field dependent dynamic nuclear polarization with radicals in aqueous solution, **J.Am.Chem.Soc.**, 130, 3254-3255, 2008 (IF 7.885).
451. Bertini, I., Fragai, M., Luchinat, C., and Talluri, E., Water-based ligand screening for paramagnetic metalloproteins, **Angew.Chem.Int.Ed.**, 47, 4533-4537, 2008 (IF 10.031).
450. Bertini, I., Luchinat, C., and Parigi, G., Solution NMR of paramagnetic molecules, <[05] Date, primary>
449. Bertini, I., Calderone, V., Fragai, M., Jaiswal, R., Luchinat, C., Melikian, M., Mylonas, E., and Svergun, D., Evidence of reciprocal reorientation of the catalytic and hemopexin-like domains of full-length MMP-12, **J.Am.Chem.Soc.**, 130, 7011-7021, 2008 (IF 7.885).
448. Bertini, I., Luchinat, C., Parigi, G., and Pierattelli, R., Perspectives in NMR of paramagnetic proteins, **Dalton Trans.**, 2008, 3782-3790, 2008 (IF 3.212).
447. Balayssac, S., Bertini, I., Bhaumik, A., Lelli, M., and Luchinat, C., Paramagnetic shifts in solid-state NMR of proteins to elicit structural information., **Proc.Natl.Acad.Sci.USA**, 105, 17284-17289, 2008 (IF 9.598).
446. Assfalg, M., Bertini, I., Colangiuli, D., Luchinat, C., Schafer, H., Schutz, B., and Spraul, M., Evidence of different metabolic phenotypes in humans, **Proc.Natl.Acad.Sci.USA**, 105, 1420-1424, 5-2-2008

## 2007

445. Major, J. L., Meade, T. J., Parigi, G., and Luchinat, C., The Synthesis and In-Vitro testing of a Zn(II)-Activated MR contrast agent, **Proc.Natl.Acad.Sci.USA**, 104, 13881-13886, 2007 (IF 9.643).
444. Luchinat, C. and Parigi, G., Collective relaxation of protein protons at very low magnetic field: a new window on protein dynamics and aggregation., **J.Am.Chem.Soc.**, 129, 1055-1064, 2007 (IF 7.696).
443. Dolderer, B., Echner, H., Beck, A., Hartmann, H. J., Weser, U., Luchinat, C., and Del Bianco, C., Coordination of three and four Cu(I) to the alpha- and beta-domain of vertebrate Zn- metallothionein-1, respectively, induces significant structural changes, **FEBS J.**, 274, 2349-2362, 2007 (IF 3.033).
442. Caravan, P., Cloutier, N.J., McDermid, S.A., Ellison, J. J., Chasse, J. M., Lauffer, R. B., Luchinat, C., McMurry, T. J., Parigi, G., and Spiller, M., Albumin binding, relaxivity and water exchange kinetics of the diastereoisomers of MS-325 a gadolinium(III) based magnetic resonance angiography contrast agent, **Inorg.Chem.**, 46, 6632-6639, 2007 (IF 3.81).
441. Capozzi, F., Luchinat, C., Micheletti, C., and Pontiggia, F., Essential dynamics of helices provide a functional classification of EF-hand proteins, **J.Proteome.Res.**, 6, 2007
440. Capozzi, F., Luchinat, C., Micheletti, C., and Pontiggia, F., Essential dynamics of helices provide a functional classification of EF-hand proteins, **J.Proteome Res.**, 6, 4245-4255, 2007 (IF 5.15).
439. Bertini, I., Gupta, Y. K., Luchinat, C., Parigi, G., Peana, M., Sgheri, L., and Yuan, J., Paramagnetism-Based NMR Restraints Provide Maximum Allowed Probabilities for the Different Conformations of Partially Independent Protein Domains, **J.Am.Chem.Soc.**, 129, 12786-12794, 2007 (IF 7.696).
438. Bertini, I., Calderone, V., Fragai, M., Giachetti, A., Loconte, M., Luchinat, C., Maletta, M., Nativi, C., and Yeo, K. J., Exploring the subtleties of drug-receptor interactions: the case of matrix metalloproteinases, **J.Am.Chem.Soc.**, 129, 2466-2475, 2007 (IF 7.696).
437. Bertini, I., Felli, I. C., Luchinat, C., Parigi, G., and Pierattelli, R., Towards a protocol for solution structure determination of copper(II) proteins: the case of Cu(II)Zn(II) superoxide dismutase, **ChemBioChem**, 8, 1422-1429, 2007 (IF 4.100).
436. Balayssac, S., Bertini, I., Falber, K., Fragai, M., Jehle, S., Lelli, M., Luchinat, C., Oschkinat, H., and Yeo, K. J., Solid-state NMR of matrix metalloproteinase 12: an approach complementary to solution NMR, **ChemBioChem**, 8, 486-489, 2007 (IF 4.100).
435. Balayssac, S., Bertini, I., Lelli, M., Luchinat, C., Maletta, M., and Yeo, K. J., Paramagnetic ions provide precious structural restraints in solid-state NMR of proteins, **J.Am.Chem.Soc.**, 129, 2218-2219, 2007 (IF 7.696).
434. Arendt, Y., Bhaumik, A., Del Conte, R., Luchinat, C., Mori, M., and Porcu, M., Fragment docking to S100 proteins reveals a wide diversity of weak interaction sites, **ChemMedChem**, 2, 1648-1654, 2007

## 2006

433. Longinetti, M., Luchinat, C., Parigi, G., and Sgheri, L., Efficient determination of the most favored orientations of protein domains from paramagnetic NMR data, **Inv.Probl.**, 22, 1485-1502, 2006 (IF 1.541).
432. Fragai, M., Luchinat, C., and Parigi, G., "Four-dimensional" protein structures: examples from metalloproteins, **Acc.Chem.Res.**, 39, 909-917, 2006 (IF 13.141).
431. Capozzi, F., Casadei, F., and Luchinat, C., EF-hand protein dynamics and evolution of calcium signal transduction: an NMR view, **J.Biol.Inorg.Chem.**, 11, 949-962, 2006 (IF 3.224).
430. Calderone, V., Fragai, M., Luchinat, C., Nativi, C., Richichi, B., and Roelens, S., A high-affinity carbohydrate-containing inhibitor of matrix metalloproteinases, **ChemMedChem**, 1, 598-601, 2006
429. Bertini, I., Grassi, E., Luchinat, C., Quattrone, A., and Saccenti, E., Monomorphism of human Cytochrome c, **Genomics**, 88, 669-672, 2006 (IF 3.181).
428. Bertini, I., Calderone, V., Fragai, M., Luchinat, C., and Maletta, M., Snapshots of the reaction mechanism of Matrix metalloproteinases, **Angew.Chem.Int.Ed.**, 45, 7952-7955, 2006 (IF 9.596).
427. Bermeil, W., Bertini, I., Felli, I. C., Lee, Y.-M., Luchinat, C., and Pierattelli, R., Protonless NMR experiments for sequence-specific assignment of backbone nuclei in unfolded proteins, **J.Am.Chem.Soc.**, 128, 3918-3919, 2006 (IF 7.419).
426. Banci, L., Bertini, I., Luchinat, C., and Turano, P., Electron transfer proteins, in: *Biological Inorganic Chemistry: Structure & Reactivity*, Bertini, I., Gray, B. H., Valentine, J. S., and Stiefel, E. I., 229, <[05] Date, primary>
425. Banci, L., Bertini, I., Luchinat, C., and Turano, P., Special Cofactors and Metal Clusters, in: *Biological Inorganic Chemistry: Structure*

& Reactivity, Bertini, I., Gray, B. H., Valentine, J. S., and Stiefel, E. I., 43, <[05] Date, primary>

424. Balayssac, S., Bertini, I., Luchinat, C., Parigi, G., and Piccioli, M., <sup>13</sup>C direct detected NMR increases the detectability of residual dipolar couplings, **J.Am.Chem.Soc.**, 128, 15042-15043, 2006 (IF 7.419).
423. Babini, E., Bertini, I., Capozzi, F., Chirivino, E., and Luchinat, C., A structural and dynamic characterization of the EF-hand protein CLSP, **Structure**, 14, 1029-1038, 2006 (IF 5.543).
422. Arnesano, F., Banci, L., Bertini, I., Capozzi, F., Ciurli, S., Luchinat, C., Mangani, S., Ciofi-Baffoni, S., Rosato, A., Turano, P., and Viezzoli, M. S., An Italian contribution to structural genomics: understanding metalloproteins., **Coord.Chem.Rev.**, 250, 1419-1450, 2006 (IF 9.779).
421. Albeck, S., Alzari, P., Andreini, C., Banci, L., Berry, I. M., Bertini, I., Cambillau, C., Canard, B., Carter, L., Cohen, S.X., Diprose, J.M., Dym, O., Esnouf, R.M., Felder, C., Ferron, F., Guillemot, F., Hamer, R., Ben Jelloul, M., Laskowski, R.A., Laurent, T., Longhi, S., Lopez, R., Luchinat, C., Malet, H., Mochel, T., Morris, R. J., Moulinier, L., Oinn, T., Pajon, A., Peleg, Y., Perrakis, A., Poch, O., Prilusky, J., Rachedi, A., Ripp, R., Rosato, A., Silman, I., Stuard, D. I., Sussman, J. L., Thierry, J. C., Thompson, J. D., Thornton, J. M., Unger, T., Vaughan, B., Vranken, W., Watson, J. D., Whamond, G., and Herik, K., SPINE bioinformatics and data-management aspects of high-throughput structural biology, **Acta Crystallogr D Biol Crystallogr**, 62, 1184-1195, 2006 (IF 1.401).
420. Ab, E., Atkinson, A. R., Banci, L., Bertini, I., Ciofi-Baffoni, S., Brunner, K., Diercks, T., Dötsch, V., Engelke, F., Folkers, G., Griesinger, C., Gronwald, W., Gunther, H., Habeck, M., de Jong, R., Kalbitzer, H. R., Kieffer, B., Lee, B. R., Loss, S., Luchinat, C., Marquardsen, T., Moskau, D., Neidig, K. P., Nilges, M., Piccioli, M., Pierattelli, R., Rieping, W., Schippmann, T., Schwalbe, H., Trave, G., Trenner, J. M., Wohnert, J., Zweckstetter, M., and Kaptein, R., NMR in structural proteomics, **Acta Crystallogr D Biol Crystallogr**, 62, 1161-, 2006 (IF 1.401).

## 2005

419. Priem, A. H., Klaassen, A. A. K., Reijerse, E. J., Meyer, T. E., Luchinat, C., Capozzi, F., Dunham, W. R., and Hagen, W. R., EPR analysis of multiple forms of [4Fe-4S]<sup>3+</sup> clusters in HiPIPs, *Ravanbakhsh*, 10, 417-424, 2005 (IF 3.300).
418. Luchinat, C. and Parigi, G., Structural determination of metalloproteins, *Encyclopedia of Condensed Matter Physics*, ACADEMIC PRESS, 2005
417. Calderone, V., Del Bianco, C., Dolderer, B., Echner, H., Hartmann, H. J., Luchinat, C., Mangani, S., and Weser, U., The crystal structure of yeast copper thionein: The solution of a long-lasting enigma, **Proc.Natl.Acad.Sci.USA**, 102, 51-56, 2005 (IF 10.272).
416. Bertini, I., Luchinat, C., Parigi, G., and Pierattelli, R., NMR of paramagnetic metalloproteins, **ChemBioChem**, 6, 1536-1549, 2005 (IF 3.474).
415. Bertini, I., Luchinat, C., and Parigi, G., <sup>1</sup>H NMRD profiles of paramagnetic complexes and metalloproteins, **Adv.Inorg.Chem.**, 57, 105-172, 2005 (IF 3.769).
414. Bertini, I., Calderone, V., Cosenza, M., Fragai, M., Lee, Y.-M., Luchinat, C., Mangani, S., Terni, B., and Turano, P., Conformational variability of MMPs: beyond a single 3D structure, **Proc.Natl.Acad.Sci.USA**, 102, 5334-5339, 2005 (IF 10.272).
413. Bertini, I., Fragai, M., Giachetti, A., Luchinat, C., Maletta, M., Parigi, G., and Yeo, K. J., Combining in silico tools and NMR data to validate protein-ligand structural models: application to matrix metalloproteinases, **J.Med.Chem.**, 48, 7544-7559, 2005 (IF 5.076).
412. Bertini, I., Gupta, Y. K., Luchinat, C., Parigi, G., Schlörb, C., and Schwalbe, H., NMR spectroscopic detection of protein protons and longitudinal relaxation rates between 0.01 and 50 MHz, **Angew.Chem.Int.Ed.**, 44, 2223-2225, 2005 (IF 9.161).
411. Babini, E., Bertini, I., Capozzi, F., Luchinat, C., Quattrone, A., and Turano, M., Principal component analysis of a comprehensive structural database of EF-hand domains to describe the conformational freedom within the EF-hand superfamily, **J.Proteome Res.**, 4, 1961-1971, 2005 (IF 6.917).
410. Babini, E., Bertini, I., Capozzi, F., Luchinat, C., Quattrone, A., and Turano, M., Principal component analysis of the conformational freedom within the EF-hand superfamily, **J.Proteome.Res.**, 4, 2005
409. Babini, E., Felli, I. C., Lelli, M., Luchinat, C., and Pierattelli, R., Backbone and side-chains <sup>1</sup>H, <sup>13</sup>C and <sup>15</sup>N NMR assignment of human  $\alpha$ -parvalbumin, **J.Biomol.NMR**, 33, 137-137, 2005 (IF 2.918).

## 2004

408. Desvaux, H., Kümmerle, R., Kowalewski, J., Luchinat, C., and Bertini, I., Direct measurement of dynamic frequency shift of cross-correlation in <sup>15</sup>N enriched proteins, **Chem.Phys.Chem.**, 5, 959-965, 2004 (IF 2.070).
407. Chary, K. V. R., Del Bianco, C., Luchinat, C., Sulakshana, M., and Mustafi, S. M., Ca<sup>2+</sup> displacement by lanthanides in protozoan calcium binding protein by NMR, thermodynamics and simulations, **Biochemistry**, 43, 9320-9331, 2004 (IF 3.922).
406. Bertini, I., Del Bianco, C., Gelis, I., Katsaros, N., Luchinat, C., Parigi, G., Peana, M., Provenzani, A., and Zoroddu, M. A., Experimentally exploring the conformational space sampled by domain reorientation in calmodulin, **Proc.Natl.Acad.Sci.USA**, 101, 6841-6846, 2004 (IF 10.272).
405. Bertini, I., Luchinat, C., and Mani, F., *Chimica*, 2004
404. Bertini, I., Bianchini, F., Calorini, L., Colagrande, S., Fragai, M., Franchi, A., Gallo, O., Gavazzi, C., and Luchinat, C., Persistent contrast enhancement by paramagnetic PEG-stabilized liposomes in murine melanoma, **Magn Reson Med**, 52, 669-672, 2004 (IF 3.313).
403. Bertini, I., Felli, I. C., Kümmerle, R., Luchinat, C., and Pierattelli, R., <sup>13</sup>C-<sup>13</sup>C NOESY: a constructive use of <sup>13</sup>C-<sup>13</sup>C spin-diffusion, **J.Biomol.NMR**, 30, 245-251, 2004 (IF 2.420).
402. Bertini, I., Fragai, M., Lee, Y.-M., Luchinat, C., and Terni, B., Paramagnetic metal ions in ligand screening: the Coll matrix metalloproteinase 12, **Angew.Chem.Int.Ed.**, 43, 2254-2256, 2004 (IF 8.427).
401. Bertini, I., Calderone, V., Fragai, M., Luchinat, C., Mangani, S., and Terni, B., Crystal structure of the catalytic domain of human matrix metalloproteinase 10, **J.Mol.Biol.**, 336, 707-716, 2004 (IF 5.359).
400. Bertini, I., Duma, L., Felli, I. C., Fey, M., Luchinat, C., Pierattelli, R., and Vasos, P. R., A heteronuclear direct detection NMR experiment for protein backbone assignment, **Angew.Chem.Int.Ed.**, 43, 2257-2259, 2004 (IF 8.427).
399. Bertini, I., Faraone-Mennella, J., Gray, B. H., Luchinat, C., Parigi, G., and Winkler, J. R., NMR-validated structural model for oxidized *Rhodospseudomonas palustris* cytochrome c556, **J.Biol.Inorg.Chem.**, 9, 224-230, 2004 (IF 3.905).
398. Berti, F., Costantino, P., Fragai, M., and Luchinat, C., Water accessibility, aggregation and motional features of polysaccharide-protein

conjugate vaccines., **Biophys.J.**, 86, 3-9, 2004 (IF 4.463).

397. Barbieri, R., Luchinat, C., and Parigi, G., Backbone-only protein solution structures with a combination of classical and paramagnetism-based constraints: a method that can be scaled to large molecules., **ChemPhysChem**, 21, 797-806, 2004 (IF 3.316).

396. Banci, L., Bertini, I., Cavallaro, G., Giachetti, A., Luchinat, C., and Parigi, G., Paramagnetism-based restraints for Xplor-NIH, **J.Biomol.NMR**, 28, 249-261, 2004 (IF 2.420).

395. Baig, I., Bertini, I., Del Bianco, C., Gupta, Y. K., Lee, Y.-M., Luchinat, C., and Quattrone, A., Paramagnetism-based refinement strategy for the solution structure of human alpha-parvalbumin, **Biochemistry**, 43, 5562-5573, 2004 (IF 3.922).

394. Babini, E., Bertini, I., Capozzi, F., Felli, I. C., Lelli, M., and Luchinat, C., Direct carbon detection in paramagnetic metalloproteins to further exploit pseudocontact shift restraints, **J.Am.Chem.Soc.**, 126, 10496-10497, 2004 (IF 6.516).

393. Babini, E., Bertini, I., Capozzi, F., Del Bianco, C., Holleder, D., Kiss, T., Luchinat, C., and Quattrone, A., Solution structure of human  $\alpha$ -parvalbumin and structural comparison with its paralog  $\beta$ -parvalbumin and with their rat orthologs., **Biochemistry**, 43, 16076-16085, 2004 (IF 3.922).

392. Andreini, C., Banci, L., Bertini, I., Luchinat, C., and Rosato, A., A bioinformatic comparison of structures and homology-models of matrix metalloproteinases, **J.Proteome Res.**, 3, 21-31, 2004 (IF 5.611).

## 2003

391. Luchinat, C., Dolderer, B., Del Bianco, C., Echner, H., Hartman, HJ, Voelter, W., and Weser, U., The Cu(1)7-cluster in yeast copper thionein survives major shortening of the polypeptide backbone as deduced from electronic absorption, circular dichroism, luminescence and 1H-NMR., **J.Biol.Inorg.Chem.**, 8, 353-359, 2003 (IF 3.911).

390. Geraldes, C. F. G. C. and Luchinat, C., Lanthanides as shift and relaxation agents in elucidating the structure of proteins and nucleic acids., **Met.Ions Biol.Syst.**, 40, 513-588, 2003 (IF 2.486).

389. Gelis, I., Katsaros, N., Luchinat, C., Piccioli, M., and Poggi, L., A Simple Protocol to Study Blue Copper Proteins by NMR., **Eur.J.Biochem.**, 270, 600-609, 2003 (IF 2.999).

388. Bertini, I., Gelis, I., Katsaros, N., Luchinat, C., and Provenzani, A., Tuning the Affinity for Lanthanides of Calcium Binding Proteins., **Biochemistry**, 42, 8011-8021, 2003 (IF 4.064).

387. Bertini, I., Luchinat, C., Turano, P., Battaini, G., and Casella, L., The magnetic properties of myoglobin as studied by NMR spectroscopy., **Chem.Eur.J.**, 9, 2316-2322, 2003 (IF 4.238).

386. Bertini, I., Calderone, V., Fragai, M., Luchinat, C., Mangani, S., and Terzi, B., X-ray structures of ternary enzyme-product-inhibitor complexes of MMP., **Angew.Chem.Int.Ed.**, 42, 2673-2676, 2003 (IF 7.671).

385. Bertini, I., Luchinat, C., and Sola, M., Zinc enzymes/models, *Encyclopaedia of Chemistry*, DOI: 10.1002/0471227617.EOC205, 2003

384. Bertini, I., Cavallaro, G., Luchinat, C., and Poli, I., A use of ramachandran potentials in protein solution structure determinations, **J.Biomol.NMR**, 4, 355-366, 2003

383. Bertini, I., Capozzi, F., and Luchinat, C., Electronic isomerism in oxidized HiPIPs revisited, *ACS series*, 858, 272-286, 2003

382. Bertini, I., Cowan, J. A., Del Bianco, C., Luchinat, C., and Mansy, S. S., Thermotoga maritima IscU. Structural characterization and dynamics of a new class of metallochaperone., **J.Mol.Biol.**, 331, 907-924, 2003 (IF 5.359).

381. Bertini, I., Luchinat, C., Nerinovski, K., Parigi, G., Cross, M., Xiao, Z., and Wedd, A. G., Application of NMRD to hydration of rubredoxin and a variant containing a (Cys-S)3Fell(OH) site., **Biophys.J.**, 84, 545-551, 2003 (IF 4.643).

380. Banci, L., Bertini, I., Ciulli, A., Fragai, M., Luchinat, C., and Terzi, B., Expression and high yield production of matrix metalloproteinase 12 and of an active mutant with increased solubility., **J.Mol.Catal.A: Chemical**, 204-205, 401-408, 2003 (IF 1.729).

379. Atreya, H. S., Mukherjee, S., Chary, K. V. R., Lee, Y.-M., and Luchinat, C., Structural basis for the sequential displacement of Ca<sup>2+</sup> by Yb<sup>3+</sup> in a protozoan EF-hand calcium binding protein., **Protein Sci.**, 12, 412-425, 2003 (IF 3.546).

378. Amesano, F., Banci, L., Bertini, I., Felli, I. C., Luchinat, C., and Thompsett, A. R., A strategy for the NMR characterization of type II copper(II) proteins: the case of the copper trafficking protein CopC from Pseudomonas syringae. **J.Am.Chem.Soc.**, 125, 7200-7208, 2003 (IF 6.201).

## 2002

358. Aime, S., D'Amelio, N., Fragai, M., Lee, Y.-M., Luchinat, C., Terreno, E., and Valensin, G., A paramagnetic probe to localize residues next to carboxylates on protein surface, **J.Biol.Inorg.Chem.**, 7, 617-622, 2002

359. Alhaique, F., Bertini, I., Fragai, M., Carafa, M., Luchinat, C., and Parigi, G., Solvent 1H NMRD study of biotinylated paramagnetic liposomes containing gd-bis-SDA-DTPA or Gd-DMPE-DTPA. Dedicated to G. Sykes., **Inorg.Chim.Acta**, 331, 151-157, 2002

360. Allegrozzi, M., Bertini, I., Choi, S. N., Lee, Y.-M., and Luchinat, C., Detecting small structural changes in metalloproteins by the use of NMR pseudocontact shifts, **Eur.J.Inorg.Chem.**, 2121-2127, 2002

361. Antonkine, M. L., Liu, G., Bentrup, D., Bryant, D. A., Bertini, I., Luchinat, C., Stehlik, D., and Golbeck, J. H., Solution Structure of the unbound, photosystem I subunit PsaC, containing [4Fe-4S] clusters FA and FB . A conformational change occurs upon binding to photosystem I, **J.Biol.Inorg.Chem.**, 7, 461-472, 2002

362. Banci, L., Bertini, I., Cavallaro, G., and Luchinat, C., Chemical shift-based constraints for solution structure determination of paramagnetic low spin heme proteins with bis-His and His-Cn axial ligands. The cases of oxidized cytochrome b5 and Met80Ala cytochrome c, **J.Biol.Inorg.Chem.**, 7, 416-426, 2002

377. Li, C., Parigi, G., Fragai, M., Luchinat, C., and Meade, T. J., Mechanistic studies of a calcium-dependent MRI contrast agent, **Inorg.Chem.**, 41, 4018-4024, 2002

376. Lehmann, T. E., Luchinat, C., and Piccioli, M., Redox-related chemical shift perturbations on backbone nuclei of high-potential iron sulfur proteins, **Inorg.Chem.**, 41, 1679-1683, 2002

375. Kowalewski, J., Luchinat, C., Nilsson, T., and Parigi, G., Nuclear Spin Relaxation in Paramagnetic Systems: Electron Spin Relaxation Effects under Near-Redfield Limit Conditions and Beyond, **J Phys Chem A**, 106, 7376-7382, 2002

374. Dilg, A. W. E., Grantner, K., Iakovleva, O., Parak, F., Babini, E., Bertini, I., Capozzi, F., Luchinat, C., and Meyer-Klaucke, W., Dynamics

- of wild type HiPIP's a Cys77Ser-mutant and a partially unfolded HiPIP, **J.Biol.Inorg.Chem.**, 7, 691-703, 2002
373. Bertini, I., Luchinat, C., and Parigi, G., Magnetic susceptibility in paramagnetic NMR, **Progr.NMR Spectrosc.**, 40, 249-273, 2002
372. Bertini, I., Luchinat, C., and Parigi, G., Paramagnetic constraints: an aid for quick solution structure determination of paramagnetic metalloproteins, **Concepts Magn.Reson.**, 14, 259-286, 2002
371. Bertini, I., Cavallaro, G., Cosenza, M., Kümmerle, R., Luchinat, C., Piccioli, M., and Poggi, L., Cross Correlation Rates Between Curie Spin and Dipole-Dipole relaxation in Paramagnetic Proteins: the Case of Cerium Substituted Calbindin D9k, **J.Biomol.NMR**, 23, 115-125, 2002
370. Bertini, I., Luchinat, C., Provenzani, A., Rosato, A., and Vasos, P. R., Browsing gene banks for Fe<sub>2</sub>S<sub>2</sub> ferredoxins and structural modeling of 87 plant-type sequences: an analysis of fold and function, **Proteins Struct.Funct.Genet.**, 46, 110-127, 2002
369. Bertini, I., Carrano, C. J., Luchinat, C., Piccioli, M., and Poggi, L., A 15N NMR mobility study on the Di-calcium P43M calbindin D9K and its mono La 3+ substituted form, **Biochemistry**, 41, 5104-5111, 2002
368. Bertini, I., Dilg, A. W. E., Iakovleva, O., Luchinat, C., Mincione, G., and Parak, F., Simultaneous interpretation of Mössbauer, EPR and 57Fe ENDOR spectra of the [Fe<sub>4</sub>S<sub>4</sub>] cluster in the high-potential iron protein I Ectothiorhodospira halophila, **J.Biol.Inorg.Chem.**, 4, 727-741, 2002
367. Bertini, I., Longinetti, M., Luchinat, C., Parigi, G., and Sgheri, L., Efficiency of paramagnetism-based constraints to determine the spatial arrangement of  $\alpha$ -helical secondary structure elements, **J.Biomol.NMR**, 22, 123-136, 2002
366. Bernado, P., Barbieri, R., Padros, E., Luchinat, C., and Pons, M., Lanthanide modulation of the orientation of macromolecules induced by purple membrane., **J.Am.Chem.Soc.**, 124, 374-375, 2002
365. Barbieri, R., Bertini, I., Cavallaro, G., Lee, Y.-M., Luchinat, C., and Rosato, A., Paramagnetically induced residual dipolar couplings for solution structure determination of lanthanide-binding proteins, **J.Am.Chem.Soc.**, 124, 5581-5587, 2002
364. Barbieri, R., Hore, P. J., Luchinat, C., and Pierattelli, R., An NMR tool for studying the kinetics of metal exchange in biomolecular processes, **J.Biomol.NMR**, 23, 303-309, 2002
363. Barbieri, R., Bertini, I., Lee, Y.-M., Luchinat, C., and Velders A.H., Structure-independent cross-validation of residual dipolar couplings originating from internal and external orienting media, **J.Biomol.NMR**, 22, 365-368, 2002

## 2001

357. Luchinat, C., Piccioli, M., Pierattelli, R., Engelke, F., Marquardsen, T., and Ruin, R., Development of NMR instrumentation to achieve excitation of large bandwidths in high resolution spectra at high-fields, **J.Magn.Reson.**, 150, 161-166, 2001
356. Luchinat, C., Capozzi, F., and Bentrop, D., Iron-Sulfur Proteins, in: Handbook on Metalloproteins, Bertini, I., Sigel, A., and Sigel, H., 357, <[05] Date, primary>
355. Hollender, D., Nerinovski, K., Kiss, T., Luchinat, C., and Bertini, I., Interaction of insulin-mimetic VO(IV) complexes with albumin and apotransferrin, **J Inorg Biochem**, 86, 267-, 2001
354. Fragai, M., Luchinat, C., Nerinovski, K., and Parigi, G., 1H NMRD dispersions of porous media: a model-free analysis, **Magn.Res.Imaging**, 19, 580, 2001
353. Dilg, A. W. E., Capozzi, F., Mentler, M., Iakovleva, O., Luchinat, C., Bertini, I., and Parak, F. G., Comparison and characterization of the (Fe<sub>4</sub>S<sub>4</sub>)<sup>2+/3+</sup> centre in the wild-type and C77S mutated HiPIPs from Chromatium vinosum monitored by Mössbauer, 57Fe ENDOR and EPR spectroscopies, **J.Biol.Inorg.Chem.**, 6, 232-246, 2001
352. Bertini, I., Ciurli, S., Dikiy, A., Fernández, C. O., Luchinat, C., Safarov, N., Shumilin, S., and Vila, A. J., The first solution structure of an oxidized paramagnetic copper (II) protein : the case of plastocyanin from the cyanobacterium Synechocystis PCC6803, **J.Am.Chem.Soc.**, 123, 2405-2413, 2001
351. Bertini, I., Luchinat, C., and Parigi, G., Solution NMR of paramagnetic molecules, 2001
350. Bertini, I., Fragai, M., Luchinat, C., and Parigi, G., Solvent 1H NMRD Study of Hexaaquochromium(III): Inferences on Hydration and Electron Relaxation, **Inorg.Chem.**, 40, 4030-4035, 2001
349. Bertini, I., Janik, M. B. L., Lee, Y.-M., Luchinat, C., and Rosato, A., Magnetic Susceptibility Tensor Anisotropies for a Lanthanide Ion Series in a Fixed Protein Matrix, **J.Am.Chem.Soc.**, 123, 4181-4188, 2001
348. Bertini, I., Lee, Y.-M., Luchinat, C., Piccioli, M., and Poggi, L., Locating the metal ion in calcium-binding proteins by using cerium(III) as a probe, **ChemBioChem**, 2, 550-558, 2001
347. Bertini, I., Luchinat, C., and Piccioli, M., Paramagnetic Probes in Metalloproteins. Turning Limitations into Advantages, **Methods Enzymol.**, 339, 314-340, 2001
346. Bertini, I., Janik, M. B. L., Liu, G., Luchinat, C., and Rosato, A., Solution structure calculations through self-orientation in a magnetic field of cerium (III) substituted calcium-binding protein, **J.Magn.Reson.**, 148, 23-30, 2001
345. Bertini, I., Bryant, D. A., Ciurli, S., Dikiy, A., Fernández, C. O., Luchinat, C., Safarov, N., Vila, A. J., and Zhao, J., Backbone dynamics of plastocyanin in both oxidation states. Solution structure of the reduced form and comparison with the oxidized state, **J.Biol.Chem.**, 276, 47217-47226, 2001
344. Bertini, I., Donaire, A., Jiménez, B., Luchinat, C., Parigi, G., Piccioli, M., and Poggi, L., Paramagnetism-based Versus Classical Constraints: An Analysis of the Solution Structure of Ca Ln Calbindin D9k., **J.Biomol.NMR**, 21, 85-98, 2001
343. Bertini, I., Kowalewski, J., Luchinat, C., and Parigi, G., Cross-correlation between the dipole-dipole interaction and the Curie spin relaxation. The effect of anisotropic magnetic susceptibility, **J.Magn.Reson.**, 152, 103-108, 2001
342. Bertini, I., Hajieva, P., Luchinat, C., and Nerinovski, K., Redox/dependent hydration of cytochrome c and cytochrome b5 studied through 17O NMRD, **J.Am.Chem.Soc.**, 123, 12925-12926, 2001
341. Aime, S., Barge, A., Botta, M., Casnati A., Fragai, M., Luchinat, C., and Ungaro R., A new calix(4)arene GdIIIComplex Endowed with High Stability, Relaxivity and Ninding Affinity to Serum Albumin, **Angew.Chem.Int.Ed.**, 40, 4737-4739, 2001

## 2000

340. Mannina, L., Luchinat, C., Patumi, M., Emanuele, M. C., Rossi, E., and Segre, A., Concentration dependence of 13C NMR spectra of triglycerides: implications for the NMR analysis of olive oils, **Magn.Reson.Chem.**, 38, 886-890, 2000

339. Im, S.-C., Worrall, J. A. R., Liu, G., Aliverti, A., Zanetti, G., Luchinat, C., Bertini, I., and Sykes, A. G., Reduction of [2Fe-2S] Ferredoxins and Site of Attachment of Cr(III) using 1H-NMR and Site-Directed Mutagenesis, **Inorg.Chem.**, 39, 1755-1764, 2000
338. Bertini, I., Hartmann, H. J., Klein, T., Liu, G., Luchinat, C., and Weser, U., High resolution solution structure of the protein part of Cu7 metallothionein, **Eur.J.Biochem.**, 267, 1008-1018, 2000
337. Bertini, I., Luchinat, C., and Turano, P., 15N chemical shift changes in cytochrome b5: redox-dependent vs. guanidinium chloride-induced changes, **J.Biol.Inorg.Chem.**, 5, 761-764, 2000
336. Bertini, I., Fernández, C. O., Karlsson, B. G., Leckner, J., Luchinat, C., Malmström, B. G., Nersissian, A. M., Pierattelli, R., Shipp, E., Valentine, J. S., and Vila, A. J., Structural information through NMR hyperfine shifts in blue copper proteins, **J.Am.Chem.Soc.**, 122, 3701-3707, 2000
335. Bertini, I., Felli, I. C., and Luchinat, C., Lanthanide induced residual dipolar couplings for the conformational investigation of peripheral 15NH2 moieties, **J.Biomol.NMR**, 18, 347-355, 2000
334. Bertini, I., Luchinat, C., and Rosato, A., The use of propionate  $\alpha$ -proton contact shifts as structural constraints (Dedicated to Steve Lippard), **Inorg.Chim.Acta**, 297, 199-205, 2000
333. Bertini, I., Huber, J. G., Luchinat, C., and Piccioli, M., Protein hydration and location of water molecules in oxidized horse heart cytochrome c by 1H NMR, **J.Magn.Reson.**, 147, 1-8, 2000
332. Bertini, I., Faraone-Mennella, J., Luchinat, C., and Rosato, A., The use of the electron-nucleus hyperfine interaction for solution structure determination, in: Metal-ligand interactions in chemistry, physics and biology, Russo, N. and Salahub, D. R., 1, <[05] Date, primary>
331. Bertini, I., Fragai, M., Luchinat, C., and Parigi, G., 1H NMRD profiles of diamagnetic proteins: a model-free analysis, **Magn.Reson.Chem.**, 38, 543-550, 2000
330. Bertini, I., Luchinat, C., and Parigi, G., The hyperfine shifts in low spin iron(III) hemes: a ligand field analysis, **Eur.J.Inorg.Chem.**, 2473-2480, 2000
329. Bertini, I., Luchinat, C., Niikura, Y., and Presenti, C., Model-free analysis of a thermophilic Fe7S8 protein as compared to a mesophilic Fe4S4 protein, **Proteins Struct.Funct.Genet.**, 41, 75-85, 2000
328. Bertini, I., Castellani, F., Luchinat, C., Martini, G., Parigi, G., and Ristori, S., Partial Orientation of Cytochrome-c in a Lyotropic Liquid Crystal: Residual H-H Dipolar Coupling, **J.Phys.Chem.**, 104, 10653-10658, 2000
327. Bentrop, D., Bertini, I., Borsari, M., Cosenza, G., Luchinat, C., and Niikura, Y., A refined model for [Fe3S4]0 clusters in proteins, **Angew.Chem.Int.Ed**, 39, 3620-3622, 2000
326. Banci, L., Bertini, I., Luchinat, C., and Turano, P., Solution structures of hemoproteins, in: The Porphyrin Handbook, Kadish, K. M., Smith, K. M., and Guilard, R., 323, <[05] Date, primary>
325. Babini, E., Bertini, I., Borsari, M., Capozzi, F., Luchinat, C., Zhang, X., Moura, G. L. C., Kurnikov, I. V., Beratan, D. N., Ponce, A., Di Bilio, A. J., Winkler, J. R., and Gray, H. B., Bond-Mediated Electron Tunneling in Ruthenium-Modified High-Potential Iron-Sulfur Protein, **J.Am.Chem.Soc.**, 122, 4532-4533, 2000
324. Antonkine, M. L., Bentrop, D., Bertini, I., Luchinat, C., Shen, G., Bryant, D. A., Stehlik, D., and Golbeck, J. H., Paramagnetic 1H NMR spectroscopy of the reduced, unbond photosystem I subunit PsaC: sequence specific assignment of contact-shifted resonances and identification of mixed and equal valence Fe-Fe pairs in (4Fe-4S) centers FA- and FB-, **J.Biol.Inorg.Chem.**, 5, 381-392, 2000
323. Anelli, P. L., Bertini, I., Fragai, M., Lattuada, L., Luchinat, C., and Parigi, G., Sulfonamide-functionalised gadolinium DTPA complexes as possible contrast agents for MRI: a relaxometric investigation, **Eur.J.Inorg.Chem.**, 625-630, 2000
322. Allegrozzi, M., Bertini, I., Janik, M. B. L., Lee, Y.-M., Liu, G., and Luchinat, C., Lanthanide induced pseudocontact shifts for solution structure refinements of macromolecules in shells up to 40 Å from the metal ion, **J.Am.Chem.Soc.**, 122, 4154-4161, 2000

## 1999

321. Tierney, D. L., Gassner, G. T., Luchinat, C., Bertini, I., Ballou, D. P., and Penner-Hahn, J. E., NMR characterization of substrate binding in the Phtalate Dioxygenase system, **Biochemistry**, 38, 11051-11061, 1999
320. Parisini, E., Capozzi, F., Lubini, P., Lamzin, V., Luchinat, C., and Sheldrick, G. M., Ab initio solution and refinement of two high-potential iron protein structures at atomic resolution., **Acta Crystallogr D Biol Crystallogr**, 55, 1773-1784, 1999
319. Mulliez, E., Ollagnier-de Choudens, S., Meier, C., Cremonini, M. A., Luchinat, C., Trautwein, A. X., and Fontecave, M., Iron-sulfur interconversions in the anaerobic ribonucleotide reductase from *Escherichia coli*, **JBIC**, 4, 614-620, 1999
318. Mannina, L., Luchinat, C., Emanuele, M. C., and Segre, A. L., Acyl Positional Distribution of Glycerol Tri-Esters in Vegetable Oils: a 13C NMR Study, **Chem.Phys.Lipids**, 103, 47-55, 1999
317. Kappl, R., Ciurli, S., Luchinat, C., and Huttermann, J., Probing Structural and Electronic Properties of the Oxidized [Fe 4S4]3+ Cluster of *Ectothiorhodospira halophila* iso-II High-Potential Iron-Sulfur Protein by ENDOR Spectroscopy, **J.Am.Chem.Soc.**, 121, 1925-1935, 1999
316. Dilg, A. W. E., Mincione, G., Achterhold, K., Iakovleva, O., Mentler, M., Luchinat, C., Bertini, I., and Parak, F. G., Simultaneous interpretation of Mössbauer, EPR, and 57Fe ENDOR spectra of the [Fe4S4] cluster in the high-potential iron protein I from *Ectothiorhodospira halophila*, **J.Biol.Inorg.Chem.**, 4, 727-741, 1999
315. Capozzi, F., Cremonini, M. A., Luchinat, C., Placucci, G., and Vignali, C., A Low Frequency 1H-NMR External Unit for the Analysis of Large Foodstuff Samples, **J.Magn.Reson.**, 138, 277-280, 1999
314. Bligh, S. W. A., Chowdhury, A. H. M. S., Kennedy, D., Luchinat, C., and Parigi, G., Non-ionic Bulky Gd(III) DTPA-Bisamide Complexes as Potential Contrast Agents for Magnetic Resonance Imaging, **Magn.Res.Med.**, 41, 767-773, 1999
313. Bertini, I., Kowalewski, J., Luchinat, C., Nilsson, T., and Parigi, G., Nuclear spin relaxation in paramagnetic complexes of S=1: Electron spin relaxation effects, **J.Chem.Phys.**, 111, 5795-5807, 1999
312. Bertini, I. and Luchinat, C., New Applications of Paramagnetic NMR in Chemical Biology, **Curr.Opin.Chem.Biol.**, 3, 145-151, 1999
311. Bertini, I., Luchinat, C., and Rosato, A., NMR spectra of iron-sulfur proteins, in: *Adv.Inorg.Chem.*, Sykes, A. G. and Cammack, R., 251, <[05] Date, primary>
310. Bertini, I., Ciurli, S., Dikiy, A., Gasanov, R., Luchinat, C., Martini, G., and Safarov, N., High-field NMR studies of oxidized blue copper proteins: the case of spinach plastocyanin, **J.Am.Chem.Soc.**, 121, 2037-2046, 1999
309. Bertini, I., Luchinat, C., Parigi, G., and Walker, F. A., Heme methyl 1H chemical shifts as structural parameters in some low spin

ferriheme proteins, **J.Biol.Inorg.Chem.**, 4, 515-519, 1999

308. Bentrop, D., Bertini, I., Iacoviello, R., Luchinat, C., Niikura, Y., Piccioli, M., Presenti, C., and Rosato, A., Structural and dynamical properties of a partially unfolded Fe4S4 protein: the role of the cofactor in protein folding, **Biochemistry**, 38, 4669-4680, 1999

307. Babini, E., Borsari, M., Capozzi, F., Eltis, L. D., and Luchinat, C., Experimental evidence for the role of buried polar groups in determining the reduction potential of metalloproteins: the S79P variant of Chromatium vinosum HiPIP, **JBIC**, 4, 692-700, 1999

306. Babini, E., Bertini, I., Borsari, M., Capozzi, F., Luchinat, C., Di Bilio, A. J., Gray, H. B., and Ponce, A., Electron transfer in ruthenium-modified high-potential iron sulfur proteins, **J Inorg Biochem**, 74, 266-, 1999

## 1998

305. Im, S.-C., Liu, G., Luchinat, C., Sykes, A. G., and Bertini, I., The solution structure of parsley [2Fe-2S] ferredoxin, **Eur.J.Biochem.**, 258, 465-477, 1998

304. Cremonini, M. A., Tacconi, D., Clementi, V., and Luchinat, C., Accurate Determination of Deuterium/Hydrogen Ratios in Natural Organic Compounds through a Nuclear Magnetic Resonance Time-Domain Reference Convolution Method: Application to Ethanol from Three Botanical Sources and Critical Analysis of Systematic Inaccur, **J.Agric.Food.Chem.**, 46, 3943-3946, 1998

303. Clementi, V. and Luchinat, C., NMR and spin relaxation in dimers, **Acc.Chem.Res.**, 31, 351-361, 1998

302. Capozzi, F., Ciurli, S., and Luchinat, C., Coordination sphere versus protein environment as determinants of electronic and functional properties of iron-sulfur proteins, **Struct.Bonding**, 90, 127-160, 1998

301. Bertini, I., Kurtz, D. M., Jr., Eidsness, M. K., Liu, G., Luchinat, C., Rosato, A., and Scott, R. A., Solution structure of reduced Clostridium pasteurianum rubredoxin, **J.Biol.Inorg.Chem.**, 3, 401-410, 1998

300. Bertini, I., Luchinat, C., Mincione, G., and Soriano, A., 2H NMR Investigation of [Fe3S4]0 cluster in 7Fe8S ferredoxin from Bacillus schlegelii, **Inorg.Chem.**, 37, 969-972, 1998

299. Bertini, I., Luchinat, C., and Soriano, A., NMR of FeS proteins, in: Spectroscopic methods in bioinorganic chemistry, Solomon, E. I. and Hodgson, K. O., 302, <[05] Date, primary>

298. Bertini, I., Dikiy, A., Luchinat, C., Macinai, R., and Viezzoli, M. S., 1H NMR study of the reduced cytochrome c' from Rhodopseudomonas palustris containing a high spin iron(II) heme moiety, **Inorg.Chem.**, 37, 4814-4821, 1998

297. Bertini, I., Galas, O., Luchinat, C., Parigi, G., and Spina, G., Nuclear and electron relaxation in magnetic exchange coupled dimers, **J.Magn.Reson.**, 130, 33-44, 1998

296. Bertini, I., Felli, I. C., and Luchinat, C., High magnetic field consequences on the NMR hyperfine shifts in solution, **J.Magn.Reson.**, 134, 360-364, 1998

295. Bertini, I., Luchinat, C., Parigi, G., Quacquarelli, G., Marzola, P., and Cavagna, F. M., Off-resonance experiments and contrast agents to improve magnetic resonance imaging, **Magn.Res.Med.**, 39, 124-131, 1998

294. Bertini, I., Luchinat, C., Piccioli, M., and Soriano, A., Folding properties of iron sulfur proteins. (Dedicated to Prof. O. Yamauchi), **Inorg.Chim.Acta**, 283, 12-16, 1998

293. Bertini, I. and Luchinat, C., NMR of paramagnetic proteins. (<http://biosci.umn.edu/biophys/OLTB/NMR.html#10>), in: Nuclear Magnetic Resonance, Gorenstein, D., <[05] Date, primary>

292. Bertini, I., Luchinat, C., Macinai, R., Martinuzzi, S., Pierattelli, R., and Viezzoli, M. S., Isolation and characterization of a cytochrome c2 from Rhodopseudomonas palustris. Dedicated to Prof. W.Beck, **Inorg.Chim.Acta**, 269, 125-134, 1998

291. Banci, L. and Luchinat, C., Selective versus non-selective T1 experiments to determine metal-nucleus distances in paramagnetic proteins, **Inorg.Chim.Acta**, 373-379, 1998

290. Banci, L., Bertini, I., Cremonini, M. A., Gori Savellini, G., Luchinat, C., Wüthrich, K., and Güntert, P., PSEUDODYANA for NMR structure calculation of paramagnetic metalloproteins using torsion angle molecular dynamics, **J.Biomol.NMR**, 12, 553-557, 1998

289. Banci, L., Bertini, I., Luchinat, C., Pierattelli, R., Shokhirev, N. V., and Walker, F. A., Analysis of the temperature dependence of the 1H and 13C isotropic shifts of horse heart ferricytochrome c: explanation of Curie and anti-Curie temperature dependence and nonlinear pseudocontact shifts in a two-level framework, **J.Am.Chem.Soc.**, 120, 8472-8479, 1998

288. Banci, L., Bertini, I., Huber, J. G., Luchinat, C., and Rosato, A., Partial orientation of oxidized and reduced cytochrome b5 at high magnetic fields: Magnetic susceptibility anisotropy contributions and consequences for protein solution structure determination, **J.Am.Chem.Soc.**, 120, 12903-12909, 1998

287. Banci, L., Bertini, I., Turano, P., and Luchinat, C., The solution structure of redox proteins and beyond, in: Biological electron transfer chains: genetics and mode of operation, Canters, G. W. and Vijgenboom, E., 225, <[05] Date, primary>

286. Banci, L., Berners-Price, S., Bertini, I., Clementi, V., Luchinat, C., Spyroulias, G. A., and Turano, P., Water-protein interaction in native and partially unfolded equine cytochrome c. (Dedicated to Prof. R.R. Ernst), **Mol.Phys.**, 95, 797-808, 1998

285. Aono, S., Bentrop, D., Bertini, I., Donaire, A., Luchinat, C., Niikura, Y., and Rosato, A., Solution structure of the oxidized Fe7S8 ferredoxin from the thermophilic bacterium Bacillus schlegelii by 1H NMR spectroscopy, **Biochemistry**, 37, 9812-9826, 1998

284. Aono, S., Bentrop, D., Bertini, I., Cosenza, G., and Luchinat, C., Solution structure of an artificial Fe8S8 ferredoxin: the D13C variant of Bacillus schlegelii Fe7S8 ferredoxin, **Eur.J.Biochem.**, 258, 502-514, 1998

## 1997

283. Murthy, N. N., Karlin, K. D., Bertini, I., and Luchinat, C., NMR and electronic relaxation in paramagnetic Dicopper(II) compounds, **J.Am.Chem.Soc.**, 119, 2156-2162, 1997

282. Luchinat, C., Soriano, A., Djinic-Carugo, K., Saraste, M., Malmström, B. G., and Bertini, I., Electronic and geometric structure of the CuA site studied by 1H NMR in a soluble domain of cytochrome c oxidase from paracoccus denitrificans, **J.Am.Chem.Soc.**, 119, 11023-11027, 1997

281. Bertini, I., Dikiy, A., Luchinat, C., Macinai, R., Viezzoli, M. S., and Vincenzini, M., An NMR study of the 7Fe-8S ferredoxin from Rhodopseudomonas palustris and reinterpretation of data on similar systems, **Biochemistry**, 36, 3570-3579, 1997

280. Bertini, I., Cowan, J. A., Luchinat, C., Natarajan, K., and Piccioli, M., Characterization of a partially unfolded high potential iron protein relevant to the folding pathway and cluster stability, **Biochemistry**, 36, 9332-9339, 1997

279. Bertini, I., Donaire, A., Felli, I. C., Luchinat, C., and Rosato, A., <sup>1</sup>H and <sup>13</sup>C NMR studies on an oxidized HiPIP, **Inorg.Chem.**, 36, 4798-4803, 1997
278. Bertini, I., Donaire, A., Luchinat, C., and Rosato, A., Paramagnetic relaxation as a tool for solution structure determination: Clostridium pasteurianum ferredoxin as an example, **Proteins Struct.Funct.Genet.**, 29, 348-358, 1997
277. Bertini, I., Gori Savellini, G., and Luchinat, C., Are unit charges always negligible?, **J.Biol.Inorg.Chem.**, 2, 114-118, 1997
276. Bertini, I., Dalvit, C., Huber, J. G., Luchinat, C., and Piccioli, M., ePHOGSY experiment on a paramagnetic protein: location of the catalytic water molecule in the heme crevice of the oxidized form of horse heart Cytochrome c., **FEBS Lett.**, 415, 45-48, 1997
275. Bentrop, D., Bertini, I., Cremonini, M. A., Forsén, S., Luchinat, C., and Malmendal, A., The solution structure of the paramagnetic complex of the N-terminal domain of calmodulin with two Ce<sup>3+</sup> ions by <sup>1</sup>H NMR, **Biochemistry**, 36, 11605-11618, 1997
274. Bentrop, D., Bertini, I., Luchinat, C., Nitschke, W., and Mühlhoff, U., Characterization of the unbound 2[Fe<sub>4</sub>S<sub>4</sub>]-ferredoxin-like photosystem I subunit Psac from the cyanobacterium Synechococcus elongatus, **Biochemistry**, 36, 13629-13637, 1997
273. Banci, L., Bertini, I., Gori Savellini, G., Romagnoli, A., Turano, P., Cremonini, M. A., Luchinat, C., and Gray, H. B., Pseudocontact shifts as constraints for energy minimization and molecular dynamic calculations on solution structures of paramagnetic metalloproteins, **Proteins Struct.Funct.Genet.**, 29, 68-76, 1997
272. Banci, L., Bertini, I., Gray, H. B., Luchinat, C., Reddig, T., Rosato, A., and Turano, P., Solution structure of oxidized horse heart cytochrome c, **Biochemistry**, 36, 9867-9877, 1997
271. Aono, S., Bentrop, D., Bertini, I., Luchinat, C., and Macinai, R., The D13C variant of Bacillus schlegelii 7Fe ferredoxin is an 8 Fe ferredoxin as revealed by <sup>1</sup>H-NMR spectroscopy, **FEBS Lett.**, 412, 501-505, 1997

## 1996

270. Luchinat, C. and Sola, M., Transferrins, in: Encyclopedia of Nuclear Magnetic Resonance, Grant, D. M. and Harris, R. K., 4811, <[05] Date, primary>
269. Kroes, S. J., Salgado, J., Parigi, G., Luchinat, C., and Canters, G. W., Electron relaxation and solvent accessibility of the metal site in wild-type and mutated azurins as determined from nuclear magnetic relaxation dispersion experiments, **JBIC**, 1, 551-559, 1996
268. Ciurli, S., Cremonini, M. A., Kofod, P., and Luchinat, C., <sup>1</sup>H NMR of high potential iron-sulfur protein from the purple non-sulfur bacterium Rhodospirillum rubrum, **Eur.J.Biochem.**, 236, 405-411, 1996
267. Bertini, I., Bren, K. L., Clemente, A., Fee, J. A., Gray, H. B., Luchinat, C., Malmström, B. G., Richards, J. H., Sanders, D., and Slutter, C. E., The Cua center of a soluble domain from thermus cytochrome ba<sub>3</sub>: an NMR investigation of the paramagnetic protein, **J.Am.Chem.Soc.**, 46, 11658-11659, 1996
266. Bertini, I., Luchinat, C., Mincione, G., Parigi, G., Gassner, G. T., and Ballou, D. P., NMR studies on Phtalate Dioxygenase: evidence for displacement of water on binding substrate, **J.Biol.Inorg.Chem.**, 1, 468-475, 1996
265. Bertini, I. and Luchinat, C., Iron-sulfur proteins, in: Encyclopedia of Magnetic Resonance, Grant, D. M. and Harris, R. K., 2621, <[05] Date, primary>
264. Bertini, I., Donaire, A., Felli, I. C., Luchinat, C., and Rosato, A., From NOESY Cross-Peaks to Structural Constraints in a Paramagnetic Metalloprotein, **Magn.Reson.Chem.**, 34, 948-950, 1996
263. Bertini, I. and Luchinat, C., NMR of paramagnetic substances, 1, 1, 1996
262. Bertini, I., Cremonini, M. A., Ferretti, S., Lozzi, I., Luchinat, C., and Viezzoli, M. S., Arene hydroxylases: metalloenzymes catalyzing dioxygenation of aromatic compounds, **Coord.Chem.Rev.**, 151, 145-160, 1996
261. Bertini, I., Briganti, F., Luchinat, C., and Scozzafava, A., Dioxygen activation in biodegradation reactions, **New J.Chem.**, 20, 187-193, 1996
260. Bertini, I., Couture, M. M. J., Donaire, A., Eltis, L. D., Felli, I. C., Luchinat, C., Piccioli, M., and Rosato, A., The solution structure refinement of the paramagnetic reduced HiPIP I from Ectothiorhodospira halophila by using stable isotope labeling and nuclear relaxation, **Eur.J.Biochem.**, 241, 440-452, 1996
259. Bertini, I. and Luchinat, C., Electronic isomerism in oxidized Fe<sub>4</sub>S<sub>4</sub> HiPIPs, in: Transition metal sulfur chemistry: biological and industrial significance, Stiefel, E. I. and Matsumoto, K., 57, <[05] Date, primary>
258. Bertini, I. and Luchinat, C., Experimental data and calculated parameters in FeS polymetallic centers in proteins, **J.Biol.Inorg.Chem.**, 1, 183-185, 1996
257. Bertini, I., Coutsolelos, A. G., Dikiy, A., Luchinat, C., Spyroulias, G. A., and Troganis, A., Structural Yb<sup>3+</sup> and Dy<sup>3+</sup> porphyrin double decker complexes. What can be obtained from <sup>1</sup>H NMR spectroscopy in solution through <sup>1</sup>H NMR, **Inorg.Chem.**, 35, 6308-6315, 1996
256. Bertini, I., Felli, I. C., Luchinat, C., and Rosato, A., A Complete Relaxation Matrix Refinement of the Solution Structure of a Paramagnetic Metalloprotein: Reduced HiPIP I from E. halophila, **Proteins Struct.Funct.Genet.**, 24, 158-164, 1996
255. Bertini, I., Luchinat, C., and Rosato, A., Evaluation of paramagnetic relaxation rates in a J-coupled two-spin system, **Chem.Phys.Lett.**, 250, 495-504. Erratum: (1997) 265, 677, 1996
254. Bertini, I., Borsari, M., Bosi, M., Eltis, L. D., Felli, I. C., Luchinat, C., and Piccioli, M., The influence of a surface charge on the electronic and steric structure of a high potential iron sulfur protein, **J.Biol.Inorg.Chem.**, 1, 257-263, 1996
253. Bertini, I., Luchinat, C., and Rosato, A., The solution structure of paramagnetic metalloproteins, **Progr.Biophys.Mol.Biol.**, 66, 43-80, 1996
252. Bentrop, D., Bertini, I., Luchinat, C., Mendes, J., Piccioli, M., and Teixeira, M., Paramagnetic NMR of the 7Fe ferredoxin from the hyperthermoacidophilic archaeon Desulfurolobus ambivalens reveals structural similarity to other dicluster ferredoxins, **Eur.J.Biochem.**, 236, 92-99, 1996
251. Bentrop, D., Bertini, I., Capozzi, F., Dikiy, A., Eltis, L. D., and Luchinat, C., Three dimensional structure of the reduced C77S mutant of the Chromatium vinosum high potential iron-sulfur protein through NMR. Comparison with the solution structure of the wild-type protein., **Biochemistry**, 35, 5928-5936, 1996
250. Belinskii, M. I., Bertini, I., Galas, O., and Luchinat, C., An exchange coupling model for Fe<sub>4</sub>S<sub>4</sub><sup>3+</sup> polymetallic center present in proteins and model compounds. Dedicated to Prof. H.B. Gray, **Inorg.Chim.Acta**, 243, 91-99, 1996
249. Banci, L., Bertini, I., Gori Savellini, G., and Luchinat, C., Individual Reduction Potentials of the Iron-Ions in Fe<sub>2</sub>S<sub>2</sub> and high potential



Fe<sub>4</sub>S<sub>4</sub> ferredoxins, **Inorg.Chem.**, 35, 4248-4253, 1996

248. Banci, L., Bertini, I., Bren, K. L., Cremonini, M. A., Gray, H. B., Luchinat, C., and Turano, P., The use of pseudocontact shifts to refine solution structures of paramagnetic metalloproteins: Met80Ala cyano-cytochrome c as an example, **J.Biol.Inorg.Chem.**, 1, 117-126, 1996
247. Babini, E., Bertini, I., Borsari, M., Capozzi, F., Dikiy, A., Eltis, L. D., and Luchinat, C., A Serine → Cysteine Ligand Mutation in the High Potential Iron-Sulfur Protein from *Chromatium vinosum* Provides Insight into the Electronic Structure of the [4Fe-4S] Cluster, **J.Am.Chem.Soc.**, 118, 75-80, 1996
246. Aono, S., Bertini, I., Cowan, J. A., Luchinat, C., Rosato, A., and Viezzoli, M. S., <sup>1</sup>H NMR studies of the Fe<sub>7</sub>S<sub>8</sub> ferredoxin from *Bacillus schlegelii*: a further attempt to understand Fe<sub>3</sub>S<sub>4</sub> clusters, **J.Biol.Inorg.Chem.**, 1, 523-528, 1996

## 1995

245. Piccioli, M., Luchinat, C., Mizoguchi, T. J., Ramirez, B. E., Gray, H. B., and Richards, J. H., Paramagnetic NMR spectroscopy and coordination structure of cobalt(II) Cys112Asp azurin, **Inorg.Chem.**, 34, 737-742, 1995
244. Luchinat, C. and Piccioli, M., New Approaches to NMR of Paramagnetic Molecules, in: NMR of Paramagnetic Macromolecules. NATO ASI Series, La Mar, G. N., 1, <[05] Date, primary>
243. Ferretti, S., Luchinat, C., Sola, M., and Battistuzzi, G., Polymetallic hydrolytic zinc enzymes. Probing the site of nuclease P1 through cobalt(II) substitution, **Inorg.Chim.Acta**, 234, 9-11, 1995
242. Davy, S. L., Osborne, M. J., Breton, J., Moore, G. R., Thomson, A. J., Bertini, I., and Luchinat, C., Determination of the (Fe<sub>4</sub>S<sub>4</sub>)Cys<sub>4</sub> cluster geometry of *Desulfovibrio africanus* ferredoxin I by <sup>1</sup>H NMR spectroscopy, **FEBS Lett.**, 363, 199-204, 1995
241. Bertini, I., Luchinat, C., and Rosato, A., Principi di chimica al calcolatore, 1995
240. Bertini, I., Capozzi, F., Dikiy, A., Happe, B., Luchinat, C., and Timmis, K. N., Evidence of histidine coordination to the catalytic ferrous ion in the ring-cleaving 2,2'-trihydroxybiphenyl dioxygenase from the dibenzofuran-degrading bacterium *Sphingomonas* sp strain RW1, **Biochem.Biophys.Res.Comm.**, 215, 855-860, 1995
239. Bertini, I., Capozzi, F., Eltis, L. D., Felli, I. C., Luchinat, C., and Piccioli, M., Sequence specific assignment of ligand cysteine protons of oxidized, recombinant HiPIP I from *Ectothiorhodospira halophila*, **Inorg.Chem.**, 34, 2516-2523, 1995
238. Bertini, I., Ciurli, S., and Luchinat, C., The electronic structure of FeS centers in proteins and models. A contribution to the understanding of their electron transfer properties., **Struct.Bonding**, 83, 1-54, 1995
237. Bertini, I., Luchinat, C., Mangani, S., and Pierattelli, R., Carbonic anhydrase: an example of how the cavity governs the reactivity at the zinc ion, **Comments Inorg.Chem.**, 17, 1-15, 1995
236. Bertini, I., Galas, O., Luchinat, C., and Parigi, G., A computer program for the calculation of paramagnetic enhancements of nuclear relaxation rates in slowly rotating systems, **J.Magn.Reson.Ser.A**, 113, 151-158, 1995
235. Bertini, I., Dikiy, A., Kastrau, D. H. W., Luchinat, C., and Sompompisut, P., The three dimensional solution structure of the oxidized HiPIP from *Chromatium vinosum* through NMR. Comparative analysis with the solution structure of the reduced species., **Biochemistry**, 34, 9851-9858, 1995
234. Bertini, I., Eltis, L. D., Felli, I. C., Kastrau, D. H. W., Luchinat, C., and Piccioli, M., The solution structure of oxidized HiPIP I from *Ectothiorhodospira halophila*, can NMR probe rearrangements associated to electron transfer processes?, **Chem.Eur.J.**, 1, 598-607, 1995
233. Bertini, I., Galas, O., Luchinat, C., Messori, L., and Parigi, G., A theoretical analysis of the <sup>1</sup>H nuclear magnetic relaxation dispersion profiles of diferric transferrin, **J.Phys.Chem.**, 99, 14217-14222, 1995
232. Bertini, I., Donaire, A., Feinberg, B. A., Luchinat, C., Piccioli, M., and Yuan, H., Solution structure of the oxidized 2[Fe<sub>4</sub>S<sub>4</sub>] ferredoxin from *Clostridium pasteurianum*, **Eur.J.Biochem.**, 232, 192-205, 1995
231. Benini, S., Ciurli, S., and Luchinat, C., NMR and the electronic structure of selenium-substituted Fe<sub>2</sub>S<sub>2</sub> proteins, **Inorg.Chem.**, 34, 417-420, 1995
230. Belinskii, M. I., Bertini, I., Galas, O., and Luchinat, C., The electronic structure of the Fe<sub>4</sub>S<sub>4</sub><sup>3+</sup> cluster in proteins: the importance of double exchange parameter. Dedicated to Prof. Hitoshi Ohtaki, **Z.Naturforsch.**, 50a, 75-80, 1995
229. Battistuzzi, G., Borsari, M., Ferretti, S., Luchinat, C., and Sola, M., Magnetic resonance of Fe-S clusters: isolation and characterization of a 7Fe ferredoxin from *Rhodospseudomonas palustris*, **Arch.Biochem.Biophys.**, 320, 149-154, 1995
228. Banci, L., Bertini, I., Ciurli, S., Luchinat, C., and Pierattelli, R., Rationalization of the reduction potentials within the series of the high potential iron-sulfur proteins. Dedicated to Prof. F.Basolo, **Inorg.Chim.Acta**, 240, 251-256, 1995
227. Banci, L., Bertini, I., Dikiy, A., Kastrau, D. H. W., Luchinat, C., and Sompompisut, P., The three-dimensional solution structure of the reduced high potential iron sulfur protein *Chromatium vinosum* through NMR, **Biochemistry**, 34, 206-219, 1995

## 1994

226. Luchinat, C. and Sola, M., Zinc enzymes, in: Encyclopedia of Inorganic Chemistry, <[05] Date, primary>
225. Luchinat, C., Capozzi, F., Borsari, M., Battistuzzi, G., and Sola, M., Influence of surface charges on redox properties in high potential iron-sulfur proteins, **Biochem.Biophys.Res.Comm.**, 203, 436-442, 1994
224. Ciurli, S., Luchinat, C., and Scozzafava, A., Iron-sulfur Proteins: Part II. Valence-specific Assignment in Oxidized HiPIP through <sup>1</sup>H NMR Spectroscopy, in: Properties and Chemistry of Biomolecular Systems, Russo, N., Anastassopoulou, J., and Barone, G., 143, <[05] Date, primary>
223. Cavagna, F. M., Luchinat, C., Scozzafava, A., and Xia, Z., Polymetallic macromolecules are potential contrast agents of improved efficiency, **Magn.Res.Med.**, 31, 58-60, 1994
222. Cavagna, F. M., Marzola, P., Daprà, M., Maggioni, F., Vicinanza, E., Castelli, P. M., De Haen, C., Luchinat, C., Wendland, M. F., Saeed, M., and Higgins, C. B., Binding of gadobenate dimeglumine to proteins extravasated into interstitial space enhances conspicuity of reperused infarcts, **Invest.Radiol.(Suppl.2)**, 29, S50-S53, 1994
221. Bertini, I., Luchinat, C., Piccioli, M., and Tarchi, D., COSY spectra of paramagnetic macromolecules, observability, scalar effects, cross correlation effects, relaxation allowed coherence transfer, **Concepts Magn.Reson.**, 6, 307-335, 1994
220. Bertini, I. and Luchinat, C., The reaction pathway of zinc enzymes and related biological catalysts, in: Bioinorganic chemistry, Bertini, I., Gray, H. B., Lippard, S. J., and Valentine, J. S., 37, <[05] Date, primary>

219. Bertini, I., Dikiy, A., Luchinat, C., Piccioli, M., and Tarchi, D., NOE-NOESY, a further tool in NMR of paramagnetic metalloproteins, **J.Magn.Reson.Ser.B**, 103, 278-283, 1994
218. Bertini, I., Luchinat, C., Macinai, R., Piccioli, M., Scozzafava, A., and Viezzoli, M. S., Paramagnetic metal centers in proteins can be investigated through heterocorrelated NMR spectroscopy, **J.Magn.Reson.Ser.B**, B104, 95-98, 1994
217. Bertini, I., Felli, I. C., Kastrau, D. H. W., Luchinat, C., Piccioli, M., and Viezzoli, M. S., Sequence-specific assignment of the <sup>1</sup>H and <sup>15</sup>N Nuclear Magnetic Resonance spectra of the reduced recombinant high potential iron sulfur protein (HiPIP) I from *Ectothiorhodospira halophila*, **Eur.J.Biochem.**, 225, 703-714, 1994
216. Bertini, I., Luchinat, C., and Piccioli, M., Copper zinc superoxide dismutase a paramagnetic protein that provides a unique frame for the NMR investigations, **Progr.NMR Spectrosc.**, 26, 91-141, 1994
215. Bertini, I., Luchinat, C., and Martini, G., Electron relaxation (data tabulation), in: Handbook of electron spin resonance, Poole, C. P., 79, <[05] Date, primary>
214. Bertini, I., Jonsson, B.-H., Luchinat, C., and Martini, G., Electron relaxation (background and theory), in: Handbook of electron spin resonance, Poole, C. P., 51, <[05] Date, primary>
213. Bertini, I., Capozzi, F., Luchinat, C., Piccioli, M., and Vila, A. J., The Fe<sub>4</sub>S<sub>4</sub> centers in ferredoxins studied through proton and carbon hyperfine coupling. Sequence specific assignments of cysteines in ferredoxins from *Clostridium aciduroides* and *Clostridium pasteurianum*, **J.Am.Chem.Soc.**, 116, 651-660, 1994
212. Bertini, I., Luchinat, C., and Pierattelli, R., NMR and unpaired electrons in biomolecules, in: NMR of biological macromolecules. NATO ASI Series., Stassinopoulou, C. I., 199, <[05] Date, primary>
211. Bertini, I., Jonsson, B.-H., Luchinat, C., Pierattelli, R., and Vila, A. J., Strategies of signal assignments in paramagnetic metalloproteins. An NMR investigation of the thiocyanate adduct of the cobalt(II)-substituted human carbonic anhydrase II, **J.Magn.Reson.Ser.B**, 104, 230-239, 1994
210. Benelli, B., Bertini, I., Capozzi, F., and Luchinat, C., <sup>1</sup>H NMR studies of the CoFe<sub>3</sub>S<sub>4</sub> derivative of ferredoxin from *Clostridium aciduroides*. Dedicated to Prof. Luigi Sacconi, **Gazz.Chim.Ital.**, 124, 469-474, 1994
209. Banci, L., Bertini, I., and Luchinat, C., 2D NMR spectra of paramagnetic systems, in: Methods in enzymology, James, T. L. and Oppenheimer, N. J., 485, <[05] Date, primary>
208. Banci, L., Bertini, I., Eltis, L. D., Felli, I. C., Kastrau, D. H. W., Luchinat, C., Piccioli, M., Pierattelli, R., and Smith, M., The three dimensional structure in solution of the paramagnetic protein high-potential iron-sulfur protein I from *Ectothiorhodospira halophila* through nuclear magnetic resonance, **Eur.J.Biochem.**, 225, 715-725, 1994
207. Banci, L., Bertini, I., Bruni, B., Carloni, P., Luchinat, C., Mangani, S., Orioli, P. L., Piccioli, M., Rypniewski, W., and Wilson, K., X-ray structure, NMR and molecular dynamics of the reduced form of copper-zinc superoxide dismutase, **Biochem.Biophys.Res.Comm.**, 202, 1088-1095, 1994

### 1993

206. Luchinat, C. and Ciurli, S., NMR of polymetallic systems in proteins, **Biological Magnetic Resonance**, 12, 357-420, 1993
205. Luchinat, C., Relaxometry and paramagnetic metal ions in biological systems, **Magn.Reson.Chem.**, 31, S145-S153, 1993
204. Capozzi, F., Cremonini, M. A., Luchinat, C., and Sola, M., Assignment of pseudo-contact-shifted <sup>1</sup>H NMR resonances in the EF-site of Yb<sup>3+</sup>-substituted rabbit parvalbumin through a combination of 2D techniques and magnetic susceptibility tensor determination, **Magn.Reson.Chem.**, 31, S118-S127, 1993
203. Capozzi, F., Ciurli, S., and Luchinat, C., Applicazioni della spettroscopia NMR in agricoltura, **Agric.Ricerca**, 149, 3-22, 1993
202. Bertini, I., Campos, A. P., Luchinat, C., and Teixeira, M., A Mössbauer investigation of oxidized Fe<sub>4</sub>S<sub>4</sub> HiPIP II from *Ectothiorhodospira halophila*, **J.Inorg.Biochem.**, 52, 227-234, 1993
201. Bertini, I., Luchinat, C., and Tarchi, D., Are true scalar proton-proton connectivities ever measured in COSY spectra of paramagnetic macromolecules?, **Chem.Phys.Lett.**, 203, 445-449, 1993
200. Bertini, I., Ciurli, S., Dikiy, A., and Luchinat, C., The electronic structure of the [Fe<sub>4</sub>Se<sub>4</sub>]<sup>3+</sup> clusters in *Chromatium vinosum* HiPIP and *Ectothiorhodospira halophila* HiPIP II through NMR and EPR studies, **J.Am.Chem.Soc.**, 115, 12020-12028, 1993
199. Bertini, I., Capozzi, F., Luchinat, C., and Xia, Z., Nuclear and electron relaxation of Fe(OH<sub>2</sub>)<sup>63+</sup>, **J.Phys.Chem.**, 97, 1134-1137, 1993
198. Bertini, I., Gaudemer, A., Luchinat, C., and Piccioli, M., Electron self-exchange in HiPIPs. A characterization of HiPIP I from *Ectothiorhodospira vacuolata*, **Biochemistry**, 32, 12887-12893, 1993
197. Bertini, I., Gori, G., Luchinat, C., and Vila, A. J., 1D and 2D NMR characterization of oxidized and reduced cytochrome c' from *Rhodocyclus gelatinosus*, **Biochemistry**, 32, 776-783, 1993
196. Bertini, I., Capozzi, F., Luchinat, C., Nicastro, G., and Xia, Z., Water proton relaxation for some lanthanide aqua ions in solution, **J.Phys.Chem.**, 101, 198-201, 1993
195. Bertini, I., Briganti, F., Luchinat, C., and Xia, Z., Nuclear magnetic relaxation dispersion studies of hexaquo Mn(II) ions in water-glycerol mixtures, **J.Magn.Reson.**, 101, 198-201, 1993
194. Bertini, I., Capozzi, F., Luchinat, C., and Piccioli, M., <sup>1</sup>H NMR investigation of oxidized and reduced HiPIP from *R. globiformis*, **Eur.J.Biochem.**, 212, 69-78, 1993
193. Bertini, I., Luchinat, C., Messori, L., and Vasak, M., A two-dimensional NMR study of cobalt(II)<sub>7</sub> rabbit liver metallothionein, **Eur.J.Biochem.**, 211, 235-240, 1993
192. Banci, L., Bertini, I., Capozzi, F., Carloni, P., Ciurli, S., Luchinat, C., and Piccioli, M., The iron-sulfur cluster in the oxidized high potential iron sulfur protein from *Ectothiorhodospira halophila*, **J.Am.Chem.Soc.**, 115, 3431-3440, 1993
191. Banci, L., Bertini, I., Ciurli, S., Ferretti, S., Luchinat, C., and Piccioli, M., The electronic structure of (Fe<sub>4</sub>S<sub>4</sub>)<sup>3+</sup> clusters in proteins. An investigation of the oxidized high-potential iron-sulfur protein II from *Ectothiorhodospira vacuolata*, **Biochemistry**, 32, 9387-9397, 1993
190. Banci, L., Bertini, I., Luchinat, C., Messori, L., and Turano, P., Frontiers in 2D NMR of paramagnetic metalloproteins, **Appl.Magn.Reson.**, 4, 461-476, 1993
189. Banci, L., Bermel, W., Luchinat, C., Pierattelli, R., and Tarchi, D., <sup>1</sup>H 3D NOE-NOE spectrum of met-myoglobin-CN: the first 3D NMR

- spectrum of a paramagnetic protein. Special issue devoted to Bioinorganic Chemistry, **Magn.Reson.Chem.**, 31, S3-S7, 1993
188. Banci, L., Bertini, I., Capozzi, F., Ciurli, S., Gori Savellini, G., and Luchinat, C., NMR and MD Investigation on the Structure-Function Relationship in HiPIP, in: The development of science for the improvement of human life. Proceedings of the II Kyoto-Siena Symposium., <[05] Date, primary>
187. Banci, L., Bertini, I., Luchinat, C., and Viezzoli, M. S., pH dependent properties of SOD studied through mutants on Lys 136, **Inorg.Chem.**, 32, 1403-1406, 1993
186. Banci, L., Bertini, I., Ferretti, S., Luchinat, C., and Piccioli, M., The structure of iron-sulfur clusters in proteins as monitored by NMR, Mössbauer, EPR and molecular dynamics, **J.Mol.Struct.**, 292, 207-220, 1993
185. Banci, L., Bertini, I., Luchinat, C., Piccioli, M., and Scozzafava, A., 1D versus 2D 1H NMR experiments in dicopper, dicobalt superoxide dismutase: a further mapping of the active site. Dedicated to Prof. Lamberto Malatesta, **Gazz.Chim.Ital.**, 123, 95-100, 1993
- 1992**
184. Luchinat, C. and Xia, Z., Paramagnetism and dynamic properties of electrons and nuclei, **Coord.Chem.Rev.**, 120, 281-307, 1992
183. Luchinat, C., Ciurli, S., and Capozzi, F., Towards an understanding of the electronic structure of Fe<sub>4</sub>S<sub>4</sub> high-potential iron-sulfur proteins, in: Perspectives in coordination chemistry, Williams, A. F., Floriani, C., and Merbach, A. E., 245, <[05] Date, primary>
182. Luchinat, C., Capozzi, F., Vittori Antisari, L., Ciavatta, C., and Sequi, P., Evaluation of systematic exploitation of tolerance with respect to a declared nutrient content in the production of fertilizers, **Fert.Research**, 32, 45-53, 1992
181. Bertini, I., Capozzi, F., Ciurli, S., Luchinat, C., Messori, L., and Piccioli, M., Identification of the iron ions of HiPIP from *Chromatium vinosum* within the protein frame through 2D NMR experiments, **J.Am.Chem.Soc.**, 114, 3332-3340, 1992
180. Bertini, I. and Luchinat, C., Synthetic nickel-containing heterometal cubane-type clusters with NiFe<sub>3</sub>Q<sub>4</sub> cores (Q=S,Se), **Chem.Tracts**, 4, 269-271, 1992
179. Bertini, I. and Luchinat, C., NMR of paramagnetic substances in solution, in: Physical methods for chemists, Drago, R. S., 500, <[05] Date, primary>
178. Bertini, I., Capozzi, F., Luchinat, C., Piccioli, M., and Vicens Oliver, M., NMR is a unique and necessary step in the investigation of iron-sulfur proteins: the HiPIP from *R. gelatinosus* as an example, **Inorg.Chim.Acta**, 198-200, 483-491, 1992
177. Bertini, I., Luchinat, C., Ming, L.-J., Piccioli, M., Sola, M., and Valentine, J. S., Two-dimensional 1H-NMR studies of the paramagnetic metalloenzyme copper-nickel superoxide dismutase, **Inorg.Chem.**, 31, 4433-4435, 1992
176. Bertini, I., Luchinat, C., and Xia, Z., Electron relaxation of titanium(III) hexaaqua complex detected by solvent water 1H-NMRD spectroscopy, **Inorg.Chem.**, 31, 3152-3154, 1992
175. Bertini, I., Luchinat, C., Pierattelli, R., and Vila, A. J., The interaction of acetate and formate with cobalt carbonic anhydrase. An NMR study, **Eur.J.Biochem.**, 208, 607-615, 1992
174. Bertini, I., Luchinat, C., and Xia, Z., Solvent water 1H NMRD study of oxovanadium(IV) aquaion, **J.Magn.Reson.**, 99, 235-246, 1992
173. Bertini, I., Briganti, F., Luchinat, C., Messori, L., Monnanni, R., Scozzafava, A., and Vallini, G., 1H NMR studies on partially and fully reduced 2(4Fe-4S) ferredoxin from *Clostridium pasteurianum*, **Eur.J.Biochem.**, 204, 831-839, 1992
172. Bertini, I., Luchinat, C., Pierattelli, R., and Vila, A. J., A multinuclear ligand NMR investigation of cyanide, cyanate and thiocyanate binding to zinc and cobalt carbonic anhydrase, **Inorg.Chem.**, 31, 3975-3979, 1992
171. Banci, L., Dugad, L. B., La Mar, G. N., Keating, K. A., Luchinat, C., and Pierattelli, R., 1H Nuclear Magnetic Resonance investigation of cobalt(II) substituted carbonic anhydrase, **Biophys.J.**, 63, 530-543, 1992
170. Banci, L., Bertini, I., Capozzi, F., and Luchinat, C., The electron-nucleus coupling: a breakthrough in the investigation of paramagnetic metalloproteins, **Int.J.Quantum Chem.**, 42, 1383-1396, 1992
169. Banci, L., Bertini, I., Carloni, P., Luchinat, C., and Orioli, P. L., Molecular dynamics simulations on HiPIP from *Chromatium vinosum* and comparison with NMR data, **J.Am.Chem.Soc.**, 114, 10683-10689, 1992
168. Azab, H. A., Banci, L., Borsari, M., Luchinat, C., Sola, M., and Viezzoli, M. S., Redox chemistry of superoxide dismutase. Cyclic voltammetry of wild-type enzymes and mutants on functionally relevant residues, **Inorg.Chem.**, 31, 4649-4655, 1992
- 1991**
167. Frega, N., Bocci, F., Capozzi, F., Luchinat, C., Capella, P., and Lercker, G., A new lipid component identified in avocado pear by GC-MS and NMR spectroscopies, **Chem.Phys.Lipids**, 60, 133-142, 1991
166. Bertini, I., Capozzi, F., Luchinat, C., Piccioli, M., and Viezzoli, M. S., Assignment of active site protons in the 1H NMR spectrum of reduced human Cu<sub>2</sub>Zn superoxide dismutase, **Eur.J.Biochem.**, 197, 691-697, 1991
165. Bertini, I., Banci, L., Luchinat, C., and Sola, M., The interaction of inhibitors with carbonic anhydrase, in: Carbonic Anhydrase, Botre', F. and Storey, B. T., 86, <[05] Date, primary>
164. Bertini, I., Capozzi, F., Luchinat, C., and Turano, P., Applications of COSY to paramagnetic heme-containing systems, **J.Magn.Reson.**, 95, 244-252, 1991
163. Bertini, I., Capozzi, F., and Luchinat, C., Water proton relaxation rate enhancements as a function of magnetic field strength and nature and size of paramagnetic solutes, **Magn.Res.Imaging**, 9, 849-853, 1991
162. Bertini, I., Luchinat, C., Piccioli, M., Vicens Oliver, M., and Viezzoli, M. S., 1H NMR investigation of reduced copper-cobalt superoxide dismutase, **Eur.Biophys.J.**, 20, 269-279, 1991
161. Bertini, I., Briganti, F., Luchinat, C., Scozzafava, A., and Sola, M., 1H NMR spectroscopy and the electronic structure of the high potential iron-sulfur protein from *Chromatium vinosum*, **J.Am.Chem.Soc.**, 113, 1237-1245, 1991
160. Bertini, I., Briganti, F., Luchinat, C., Messori, L., Monnanni, R., Scozzafava, A., and Vallini, G., 2D 1H NMR studies of oxidized ferredoxin from *Clostridium pasteurianum*, **FEBS Lett.**, 289, 253-256, 1991
159. Bertini, I., Lepori, A., Luchinat, C., and Turano, P., Role of Arg-143 in human Cu<sub>2</sub>Zn<sub>2</sub>SOD studied through anion binding, **Inorg.Chem.**, 30, 3363-3364, 1991
158. Banci, L., Bertini, I., Briganti, F., Luchinat, C., Scozzafava, A., and Vicens Oliver, M., 1H NMR spectra of oxidized high-potential iron-sulfur protein (HiPIP) from *Rhodocyclus gelatinosus*. A model for oxidized HiPIPs, **Inorg.Chem.**, 30, 4517-4524, 1991

157. Banci, L., Bertini, I., Luchinat, C., and Piccioli, M., Frontiers in NMR of paramagnetic molecules: 1H NOE and related experiments, in: NMR and biomolecular structure, Bertini, I., Molinari, H., and Niccolai, N., 31, <[05] Date, primary>
156. Banci, L., Bertini, I., Cabelli, D. E., Hallewell, R. A., Luchinat, C., and Viezzoli, M. S., Advances in understanding of the structure-function relationship in Cu,Zn superoxide dismutase, **Free Radical Res.Comms.**, 12-13, 239-251, 1991
155. Banci, L., Bertini, I., Briganti, F., Luchinat, C., Scozzafava, A., and Vicens Oliver, M., 1H NOE studies of oxidized high potential iron sulfur protein II from *Ectothiorhodospira halophila*, **Inorg.Chim.Acta**, 180, 171-175, 1991
154. Banci, L., Bertini, I., Briganti, F., and Luchinat, C., The electronic structure of paramagnetic polynuclear metal clusters in proteins studied through 1H NMR spectroscopy, **New J.Chem.**, 15, 467-477, 1991
153. Banci, L., Bertini, I., Briganti, F., Luchinat, C., and Scozzafava, A., Iron-sulfur proteins: an insight into their electronic structure through 1H NMR spectroscopy, in: Chemistry and properties of biomolecular systems, Rizzarelli, E. and Theophanides, T., 73, <[05] Date, primary>
152. Banci, L., Bertini, I., and Luchinat, C., Nuclear and electron relaxation. The magnetic nucleus-unpaired electron coupling in solution, 1991

## 1990

151. Luchinat, C., Monnanni, R., and Sola, M., 13C and 1H NMR studies of imidazole binding to native and cobalt(II)-substituted human carbonic anhydrase I, **Inorg.Chim.Acta**, 177, 133-139, 1990
150. Luchinat, C., Steuernagel, S., and Turano, P., Application of 2D-NMR techniques to paramagnetic systems, **Inorg.Chem.**, 29, 4351-4353, 1990
149. Bertini, I., Briganti, F., and Luchinat, C., Double exchange versus J-inequality in Fe<sub>3</sub>S<sub>4</sub>O clusters, **Inorg.Chim.Acta**, 175, 9-10, 1990
148. Bertini, I., Briganti, F., Luchinat, C., and Scozzafava, A., 1H NMR studies of the oxidized and partially reduced 2(4Fe-4S) ferredoxin from *Clostridium pasteurianum*, **Inorg.Chem.**, 29, 1874-1880, 1990
147. Bertini, I., Luchinat, C., Monnanni, R., Moratal Mascarell, J. M., Donaire, A., and Auld, D. S., Azide and chloride binding to carboxypeptidase A in the presence of L-phenylalanine, **J.Inorg.Biochem.**, 39, 9-16, 1990
146. Bertini, I., Luchinat, C., and Vasavada, K. V., The effect of magnetic anisotropy on the longitudinal nuclear relaxation time in paramagnetic systems, **J.Magn.Reson.**, 89, 243-254, 1990
145. Bertini, I., Luchinat, C., Rosi, M., Sgamellotti, A., and Tarantelli, F., pKa of zinc-bound water and nucleophilicity of hydroxo-containing species. Ab initio calculations on models for zinc-enzymes, **Inorg.Chem.**, 29, 1460-1463, 1990
144. Bertini, I., Luchinat, C., Banci, L., and Viezzoli, M. S., 1H NMR and relaxometry of copper-containing dimers in proteins, **Biol.Met.**, 3, 146-150, 1990
143. Bertini, I., Banci, L., Luchinat, C., and Piccioli, M., Spectroscopic studies on Cu<sub>2</sub>Zn<sub>2</sub>SOD: a continuous advancement of investigation tools, **Coord.Chem.Rev.**, 100, 67-103, 1990
142. Banci, L., Bertini, I., Luchinat, C., Donaire, A., Martinez, M.-J., and Moratal Mascarell, J. M., The factors governing the coordination number in the anion derivatives of carbonic anhydrase, **Comments Inorg.Chem.**, 9, 245-261, 1990
141. Banci, L., Bertini, I., Luchinat, C., and Moratal Mascarell, J. M., The mechanism of action of carbonic anhydrase, in: Enzymatic and model carboxylation and reduction reactions for carbon dioxide utilization, Aresta, M. and Schloss, J. V., 181, <[05] Date, primary>
140. Banci, L., Bertini, I., and Luchinat, C., The 1H NMR parameters of magnetically coupled dimers - The Fe<sub>2</sub>S<sub>2</sub> proteins as an example, **Struct.Bonding**, 72, 113-135, 1990
139. Banci, L., Bencini, A., Bertini, I., Luchinat, C., and Viezzoli, M. S., The angular overlap analysis of the spectroscopic parameters of copper zinc SOD and its mutants. Dedicated to Prof. Angelo Mangini, **Gazz.Chim.Ital.**, 120, 179-185, 1990
138. Banci, L., Bertini, I., Luchinat, C., and Piccioli, M., Transient versus steady state NOE in paramagnetic molecules. Cu<sub>2</sub>Co<sub>2</sub>SOD as an example, **FEBS Lett.**, 272, 175-180, 1990
137. Banci, L., Bencini, A., Bertini, I., Luchinat, C., and Piccioli, M., 1H NOE and ligand field studies of copper-cobalt superoxide dismutase with anions, **Inorg.Chem.**, 29, 4867-4873, 1990
136. Banci, L., Bertini, I., Cabelli, D., Hallewell, R. A., Luchinat, C., and Viezzoli, M. S., Investigation of copper-zinc superoxide dismutase Ser-137 and Ala-137 mutants, **Inorg.Chem.**, 29, 2398-2403, 1990
135. Banci, L., Bertini, I., Luchinat, C., and Viezzoli, M. S., A comment on the 1H NMR spectra of cobalt(II) substituted superoxide dismutases with histidines deuterated in e1-position, **Inorg.Chem.**, 29, 1438-1440, 1990

## 1989

134. Bertini, I., Luchinat, C., Viezzoli, M. S., and Wang, Y., Active-site modification of SOD by H<sub>2</sub>O<sub>2</sub> studied through 1H NMR of the cobalt(II)-derivative, **Arch.Biochem.Biophys.**, 269, 586-594, 1989
133. Bertini, I., Banci, L., and Luchinat, C., 1H NMR of paramagnetic metalloproteins, in: Nuclear Magnetic Resonance, Part B, Oppenheimer, N. J. and James, T. L., 246, <[05] Date, primary>
132. Bertini, I., Luchinat, C., Brown III, R. D., and Koenig, S. H., Relaxation of the electronic spin moment of copper(II)-macromolecular complexes in solution, **J.Am.Chem.Soc.**, 111, 3532-3536, 1989
131. Bertini, I., Banci, L., Luchinat, C., Bielski, B. H. J., Cabelli, D., Mullenbach, G. T., and Hallewell, R. A., An investigation of a human erythrocyte SOD modified at the position 137, **J.Am.Chem.Soc.**, 111, 714-719, 1989
130. Bertini, I., Luchinat, C., Viezzoli, M. S., Banci, L., Koenig, S. H., Leung, H. T., and Coleman, J. E., Copper(II) as a probe of the active centers of alkaline phosphatase, **Inorg.Chem.**, 28, 352-358, 1989
129. Bertini, I., Luchinat, C., Messori, L., and Vasak, M., Proton NMR spectra of the Co<sub>4</sub>S<sub>11</sub> cluster in metallothioneins: a theoretical model, **J.Am.Chem.Soc.**, 111, 7300-7303, 1989
128. Bertini, I., Luchinat, C., Messori, L., and Vasak, M., Proton NMR studies on the cobalt(II)-metallothionein system in solution, **J.Am.Chem.Soc.**, 111, 7296-7300, 1989
127. Banci, L., Bertini, I., Luchinat, C., Monnanni, R., and Moratal Mascarell, J. M., 1H NMR spectra of cobalt(II)-substituted carbonic anhydrase isoenzymes, **Gazz.Chim.Ital.**, 119, 23-29, 1989
126. Banci, L., Bertini, I., Luchinat, C., Piccioli, M., Scozzafava, A., and Turano, P., 1H NOE studies on dicopper(II) dicobalt(II) superoxide

dismutase, **Inorg.Chem.**, 28, 4650-4656, 1989

125. Banci, L., Bertini, I., Luchinat, C., and Scozzafava, A., Cyanide and azide behave in a similar fashion versus cuprozinc superoxide dismutase, **J.Biol.Chem.**, 264, 9742-9744, 1989

124. Banci, L., Bertini, I., Luchinat, C., Scozzafava, A., and Turano, P., Binding of fluoride to copper zinc superoxide dismutase, **Inorg.Chem.**, 28, 2377-2381, 1989

123. Banci, L., Bertini, I., Hallewell, R. A., Luchinat, C., and Viezzoli, M. S., Water in the active cavity of copper/zinc superoxide dismutase. A water 1H-nuclear-magnetic-relaxation-dispersion study, **Eur.J.Biochem.**, 184, 125-129, 1989

## 1988

122. Ming, L.-J., Banci, L., Luchinat, C., Bertini, I., and Valentine, J. S., Characterization of copper-nickel and silver-nickel bovine superoxide dismutase by 1H NMR spectroscopy, **Inorg.Chem.**, 27, 4458-4463, 1988

121. Ming, L.-J., Banci, L., Luchinat, C., Bertini, I., and Valentine, J. S., NMR study of cobalt(II)-substituted yeast and human copper-zinc superoxide dismutase, **Inorg.Chem.**, 27, 728-733, 1988

120. Luchinat, C., Monnanni, R., Roelens, S., Vallee, B. L., and Auld, D. S., <sup>13</sup>C NMR studies of D- and L-phenylalanine binding to cobalt(II) carboxypeptidase A, **J.Inorg.Biochem.**, 32, 1-6, 1988

119. Bicknell, R., Schaeffer, A., Bertini, I., Luchinat, C., Auld, D. S., and Vallee, B. L., The interaction of anions with the active site of carboxypeptidase A, **Biochemistry**, 27, 1050-1057, 1988

118. Bertini, I., Hirose, J., Kozlowski, H., Luchinat, C., Messori, L., and Scozzafava, A., Effect of nonsynergistic anions on copper transferrin, **Inorg.Chem.**, 27, 1081-1086, 1988

117. Bertini, I., Hayashi, T., Kuroda, Y., Luchinat, C., and Tabushi, I., 1H NMR characterization of the system cobalt(II) bis (histamino)-B-cyclodextrin-imidazole, **Gazz.Chim.Ital.**, 118, 777-781, 1988

116. Bertini, I., Luchinat, C., and Messori, L., The role of aminoacidic residues inside the active sites of metalloproteins, **J.Pure Appl.Chem.**, 60, 1261-1261, 1988

115. Bertini, I., Hirose, J., Luchinat, C., Messori, L., Piccioli, M., and Scozzafava, A., Kinetic studies on metal removal from transferrins by pyrophosphate, **Inorg.Chem.**, 27, 2405-2409, 1988

114. Bertini, I., Banci, L., and Luchinat, C., NMR of paramagnetic systems: magnetically coupled dimetallic systems. Cu<sub>2</sub>Co<sub>2</sub>-superoxide dismutase as an example, in: Metal clusters in proteins, Que, L., Jr., 70, <[05] Date, primary>

113. Bertini, I., Banci, L., Brown III, R. D., Koenig, S. H., and Luchinat, C., Electronic relaxation of a copper(II) dimer in a macromolecular complex as evaluated from solvent proton relaxation, **Inorg.Chem.**, 27, 951-953, 1988

112. Bertini, I., Luchinat, C., Messori, L., Monnanni, R., Auld, D. S., and Riordan, J. F., 1H NMR spectroscopic characterization of binary and ternary complexes of cobalt(II) carboxypeptidase A with inhibitors, **Biochemistry**, 27, 8318-8325, 1988

111. Bertini, I., Banci, L., Luchinat, C., and Hallewell, R. A., The exploration of the active-site cavity of copper-zinc superoxide dismutase, in: Annals of the New York academy of sciences, Blanch, H. W. and Klibanov, A. M., 37, <[05] Date, primary>

110. Banci, L., Bertini, I., Luchinat, C., Viezzoli, M. S., and Wang, Y., Characterization of Cu<sub>2</sub>Co<sub>2</sub>- and Co<sub>2</sub>Co<sub>2</sub>-alkaline phosphatase complexes at acidic pH, **Inorg.Chem.**, 27, 1442-1446, 1988

109. Banci, L., Bertini, I., Luchinat, C., and Hallewell, R. A., An investigation of superoxide dismutase Lys-143, Ile-143, and Glu-143 mutants: Cu<sub>2</sub>Co<sub>2</sub>SOD derivatives, **J.Am.Chem.Soc.**, 110, 3629-3633, 1988

108. Banci, L., Bertini, I., Luchinat, C., Monnanni, R., and Scozzafava, A., Water 1H nuclear magnetic relaxation dispersion (NMRD) of Cu<sub>2</sub>Zn<sub>2</sub> SOD with some anions and 1H NMR spectra of Cu<sub>2</sub>Co<sub>2</sub>SOD in the presence of CN<sup>-</sup>, **Inorg.Chem.**, 27, 107-109, 1988

107. Banci, L., Bertini, I., Luchinat, C., Viezzoli, M. S., and Wang, Y., The cobalt(II)-alkaline phosphatase system at alkaline pH, **J.Biol.Chem.**, 263, 11263-11268, 1988

## 1987

106. Mota De Freitas, D., Luchinat, C., Banci, L., Bertini, I., and Valentine, J. S., 31P NMR study of the interaction of inorganic phosphate with bovine copper-zinc superoxide dismutase, **Inorg.Chem.**, 26, 2788-2791, 1987

105. Luchinat, C. and Roelens, S., Group 14 organometallic reagents. 4. Stereodynamics of substituted dioxastannolanes. Carbon-13 and Tin-119 NMR studies, **J.Org.Chem.**, 25, 4444-4449, 1987

104. Bertini, I., Luchinat, C., Owens, C., and Drago, R. S., NMR Proton Relaxation in Bimetallic Complexes Containing Co(II), **J.Am.Chem.Soc.**, 109, 5208-5212, 1987

103. Bertini, I., Lanini, G., Luchinat, C., Haas, C., Maret, W., and Zeppezauer, M., The influence of anions and inhibitors on the catalytic metal ion in Co(II)-substituted horse liver alcohol dehydrogenase, **Eur.Biophys.J.**, 14, 431-439, 1987

102. Bertini, I., Luchinat, C., and Messori, L., Nuclear relaxation in NMR of paramagnetic systems, in: Metal ions in biological systems, vol. 21. Applications of nuclear magnetic resonance to paramagnetic species, Sigel, H., 47, <[05] Date, primary>

101. Bertini, I., Luchinat, C., Monnanni, R., Roelens, S., and Moratal Mascarell, J. M., Interaction of CO<sub>2</sub> and copper(II) carbonic anhydrase, **J.Am.Chem.Soc.**, 109, 7855-7856, 1987

100. Bertini, I., Luchinat, C., and Monnanni, R., The enzyme carbonic anhydrase, in: Carbon dioxide as a source of carbon, Aresta, M. and Forti, G., 139, <[05] Date, primary>

99. Bertini, I., Viezzoli, M. S., Luchinat, C., Stafford, E., Cardin, A. D., Behnke, W. D., Bhattacharyya, L., and Brewer, C., Circular dichroism and 1H NMR studies of Co<sup>2+</sup> and Ni<sup>2+</sup> substituted concanavalin A and the Lentil and Pea Lectins, **J.Biol.Chem.**, 262, 16984-16994, 1987

98. Banci, L., Bertini, I., Gallori, E., Luchinat, C., Paoletti, F., Polsinelli, M., and Viezzoli, M. S., A spectroscopic investigation of cobalt(II) substituted alkaline phosphatase, **J.Inorg.Biochem.**, 30, 77-85, 1987

97. Banci, L., Bertini, I., Luchinat, C., Monnanni, R., and Scozzafava, A., Characterization of the cobalt(II)-substituted superoxide dismutase-phosphate system, **Inorg.Chem.**, 26, 153-156, 1987

96. Banci, L., Bertini, I., Luchinat, C., and Scozzafava, A., Nuclear relaxation in the magnetic coupled system Cu<sub>2</sub> Co<sub>2</sub>SOD. histidine-44 is detached upon anion binding, **J.Am.Chem.Soc.**, 109, 2328-2334, 1987

## 1986

95. Vasak, M., in: Zinc Enzymes, Bertini, I., Luchinat, C., Maret, W., and Zeppenauer, M., 595, <[05] Date, primary>
94. Rosi, M., Sgamellotti, A., Tarantelli, F., Bertini, I., and Luchinat, C., Ab initio calculations of the Cu<sup>2+</sup>-O<sub>2</sub><sup>-</sup> interaction as a model for the mechanism of copper-zinc superoxide dismutase, **Inorg.Chem.**, 25, 1005-1008, 1986
93. Owens, C., Drago, R. S., Bertini, I., Luchinat, C., and Banci, L., NMR proton relaxation in bimetallic complexes of zinc(II), nickel(II), and copper(II), **J.Am.Chem.Soc.**, 108, 3298-3303, 1986
92. Luchinat, C. and Roelens, S., Enantiomeric purity determination of 1,2-diols through NMR spectroscopy without chiral auxiliaries, **J.Am.Chem.Soc.**, 108, 4873-4878, 1986
91. Bertini, I., Luchinat, C., Messori, L., Monnanni, R., and Scozzafava, A., The metal binding properties of ovotransferrin: an investigation of cobalt(II) derivatives, **J.Biol.Chem.**, 261, 1139-1146, 1986
90. Bertini, I., Briganti, F., and Luchinat, C., Solvent proton nuclear magnetic relaxation dispersion (NMRD) in solutions of paramagnetic macromolecules, in: Advances in magnetic resonance techniques in systems of high molecular complexity, Niccolai, N. and Valensin, G., 165, <[05] Date, primary>
89. Bertini, I., Luchinat, C., and Viezzoli, M. S., Metal substitution as a tool for the investigation of zinc proteins, in: Zinc Enzymes, Bertini, I., Luchinat, C., Maret, W., and Zepezauer, M., 27, <[05] Date, primary>
88. Bertini, I., Luchinat, C., Messori, L., Scozzafava, A., Pellacani, G. C., and Sola, M., <sup>13</sup>C NMR study of the synergistic anion in transferrins, **Inorg.Chem.**, 25, 1782-1786, 1986
87. Bertini, I. and Luchinat, C., NMR of paramagnetic molecules in biological systems, Benjamin/Cummings Pub., 1986
86. Bertini, I., Dei, A., Luchinat, C., and Monnanni, R., Anion binding properties of cobalt(II)-substituted carbonic anhydrases, in: *Zinc enzymes*, Bertini, I., Luchinat, C., Maret, W., and Zepezauer, M., 371, Birkhäuser, 1986
85. Bertini, I. and Luchinat, C., NMR studies on copper(II) containing biological molecules, in: *Biological and Inorganic Copper Chemistry*, Karlin, K. D. and Zubieta, J., 23, 1986
84. Banci, L., Bertini, I., and Luchinat, C., Electron relaxation, **Magn.Reson.Rev.**, 11, 1-40, 1986
83. Banci, L., Bertini, I., Luchinat, C., Monnanni, R., Scozzafava, A., and Salvato, B., A spectroscopic investigation of Co<sub>2</sub>Zn<sup>2-</sup> and Co<sub>2</sub>Co<sup>2-</sup> superoxide dismutase, **Gazz.Chim.Ital.**, 116, 51-54, 1986
82. Banci, L., Bertini, I., Briganti, F., and Luchinat, C., The electron-nucleus dipolar coupling in slow rotating systems. 4. The effect of zero-field splitting and hyperfine coupling when S = 5/2 and I = 5/2, **J.Magn.Reson.**, 66, 58-65, 1986
81. Bertini, I., Luchinat, C., Maret, M., Zepezauer, M., Zinc Enzymes, Birkhäuser, 1986

## 1985

80. Rosi, M., Sgamellotti, A., Tarantelli, F., Bertini, I., and Luchinat, C., A theoretical investigation of the copper-superoxide system. A model for the mechanism of copper-zinc superoxide dismutase, **Inorg.Chim.Acta**, 107, L21-L22, 1985
79. Bertini, I. and Luchinat, C., High spin cobalt(II) as a probe for the investigation of metalloproteins, **Adv.Inorg.Biochem.**, 6, 71-111, 1985
78. Bertini, I., Briganti, F., Koenig, S. H., and Luchinat, C., Magnetic relaxation of solvent protons by Cu<sup>2+</sup>- and VO<sub>2</sub><sup>+</sup>- substituted transferrin: theoretical analysis and biochemical implications, **Biochemistry**, 24, 6287-6290, 1985
77. Bertini, I., Dei, A., Luchinat, C., and Monnanni, R., Acid-base properties of cobalt(II)-substituted carbonic anhydrases, **Inorg.Chem.**, 24, 301-303, 1985
76. Bertini, I., Luchinat, C., Mancini, M., and Spina, G., The dipolar coupling between unpaired electrons and resonating nuclei, in: *Magneto-structural correlations in exchange-coupled systems*, Gatteschi, D., Kahn, O., and Willett, R. D., 421 Kluwer Academic Publishers, 1985
75. Bertini, I., Luchinat, C., and Messori, L., Spectral characterization of vanadium-transferrin systems, **J.Inorg.Biochem.**, 25, 57-60, 1985
74. Bertini, I. and Luchinat, C., Metal ions in biochemistry, in: *Structure and motion: membranes, nucleic acids and proteins*, Clementi, E. and et al., 293, Adenine Press, 1985
73. Bertini, I., Briganti, F., Luchinat, C., Mancini, M., and Spina, G., The electron nucleus dipolar coupling in slow rotating systems (2): the effect of g anisotropy and hyperfine coupling when S=1/2 and I=3/2, **J.Magn.Reson.**, 63, 41-55, 1985
72. Bertini, I., Luchinat, C., and Monnanni, R., Zinc enzymes, **J.Chem.Educ.**, 62, 924-927, 1985
71. Bertini, I., Lanini, G., Luchinat, C., Messori, L., Monnanni, R., and Scozzafava, A., Investigation of Cu<sub>2</sub>Co<sub>2</sub>SOD and its anion derivatives. <sup>1</sup>H NMR and electronic spectra, **J.Am.Chem.Soc.**, 107, 4391-4396, 1985
70. Bertini, I., Luchinat, C., and Kowalewski, J., Nuclear spin relaxation in paramagnetic (S>1/2) systems. A comparison of two new theoretical approaches, **J.Magn.Reson.**, 62, 235-241, 1985
69. Bertini, I., Lanini, G., Luchinat, C., and Monnanni, R., Investigation of cobalt(II) substituted carboxypeptidase A interacting with azide and cyanate ions, **Inorg.Chim.Acta**, 107, 153-157, 1985
68. Bertini, I., Lanini, G., Luchinat, C., Mancini, M., and Spina, G., The electron-nucleus dipolar coupling in slow rotating systems. 3. The effect of isotropic exchange coupling of the electron spin with a second paramagnetic center, **J.Magn.Reson.**, 63, 56-63, 1985
67. Bertini, I., Luchinat, C., and Monnanni, R., Evidence of the breaking of the copper-imidazolate bridge in copper/cobalt-substituted superoxide dismutase upon reduction of the copper(II) centers, **J.Am.Chem.Soc.**, 107, 2178-2179, 1985
66. Banci, L., Bertini, I., and Luchinat, C., Solvent <sup>1</sup>H NMRD of copper(II) complexes, **Chem.Phys.Lett.**, 118, 345-347, 1985
65. Banci, L., Bertini, I., and Luchinat, C., <sup>1</sup>H NMRD studies of solutions of paramagnetic metal ions in ethyleneglycol, **Inorg.Chim.Acta**, 100, 173-181, 1985
64. Banci, L., Bertini, I., and Luchinat, C., Lanthanide ions as NMR probes, in: *Rare Earths Spectroscopy*, Trebiatowska, B. J., Legendziewicz, J., and Streck, W., 80, World Scientific Publishing, 1985

## 1984

63. Bertini, I., Lanini, G., and Luchinat, C., <sup>1</sup>H NMR spectra of reduced spinach ferredoxin, **Inorg.Chem.**, 23, 2729-2730, 1984

62. Bertini, I., Lanini, G., and Luchinat, C., A water 1H and 17O N.M.R. study on PHG-modified SOD, **Inorg.Chim.Acta**, 93, 51-53, 1984
61. Bertini, I., Gerber, M., Lanini, G., Luchinat, C., Maret, W., Rawer, S., and Zeppezauer, M., 1H NMR investigation of the active site of cobalt(II)-substituted liver alcohol dehydrogenase, **J.Am.Chem.Soc.**, 106, 1826-1830, 1984
60. Bertini, I., Luchinat, C., Mancini, M., and Spina, G., The electron-nucleus dipolar coupling. The effect of zero-field splitting of an S=3/2 manifold, **J.Magn.Reson.**, 59, 213-222, 1984
59. Bertini, I., Luchinat, C., and Monnanni, R., Carbonic anhydrase: a zinc enzyme investigated through cobalt(II) substitution: a comparison among various isoenzymes, *Rend.Acc.Lincei (Rome)*, 41-54, 1984
58. Bertini, I., Borghi, E., Luchinat, C., and Scozzafava, A., Multinuclear NMR investigation of the metal binding sites of transferrins, **J.Mol.Struct.**, 113, 191-200, 1984
57. Bertini, I., Luchinat, C., Messori, L., and Scozzafava, A., Cobalt(II) as an NMR probe for the investigation of the coordination sites of conalbumin, **Eur.J.Biochem.**, 141, 375-378, 1984
56. Bertini, I., Luchinat, C., Monnanni, R., Scozzafava, A., and Borghi, E., Investigation of zinc-deprived bovine superoxide dismutase, **Inorg.Chim.Acta**, 91, 109-111, 1984
55. Bertini, I., Lanini, G., and Luchinat, C., Differences between high activity bovine carbonic anhydrase B and low activity human carbonic anhydrase B monitored through metal substitution, **J.Mol.Catal.**, 23, 133-144, 1984
54. Bertini, I. and Luchinat, C., The structure of cobalt(II)-substituted carbonic anhydrase and its implications for the catalytic mechanism of the enzyme, **Ann.N.Y.Acad.Sci.**, 429, 89-98, 1984
53. Bertini, I., Lanini, G., Luchinat, C., and Raciti, A., Are there other acidic groups capable of affecting the electronic spectra of cobalt(II) substituted carbonic anhydrase?, **Inorg.Chim.Acta**, 91, 173-177, 1984

### 1983

52. Koenig, S. H., Brown III, R. D., Bertini, I., and Luchinat, C., Water exchange at the active site of carbonic anhydrase. A synthesis of the OH- and H<sub>2</sub>O-models, **Biophys.J.**, 41, 179-187, 1983
51. Bertini, I., The coordination properties of the active site of zinc enzymes, in: *The coordination chemistry of metalloenzymes*, Bertini, I., Drago, R. S., and Luchinat, C., 1, <[05] Date, primary>
50. Bertini, I., Lanini, G., and Luchinat, C., 1H NMR relaxation rate and coordination number in high spin cobalt(II) complexes, **Inorg.Chim.Acta**, 80, 123-126, 1983
49. Bertini, I., Luchinat, C., and Scozzafava, A., A comment on anion binding to superoxide dismutase, in: *The coordination chemistry of metalloenzymes*, Bertini, I., Drago, R. S., and Luchinat, C., 155-158 Springer, 1983
48. Bertini, I. and Luchinat, C., An insight on the active site of zinc enzymes through metal substitution, in: *Metal ions in biological systems*, Sigel, H., 101, M. Dekker, 1983
47. Bertini, I. and Luchinat, C., Cobalt(II) as a probe of the structure and function of carbonic anhydrase, **Acc.Chem.Res.**, 16, 272-279, 1983
46. Bertini, I., Canti, G., Luchinat, C., and Borghi, E., Investigation of the system copper(II) carbonic anhydrase and HCO<sub>3</sub><sup>-</sup>/CO<sub>2</sub>, **J.Inorg.Biochem.**, 18, 221-229, 1983
45. Bertini, I., Lanini, G., and Luchinat, C., Equilibrium species in cobalt(II) carbonic anhydrase, *J.Am.Chem.Soc.*, 105, 5116-5118, 1983
44. Bertini, I., Luchinat, C., Scozzafava, A., Maldotti, A., and Traverso, O., Investigation of the copper-magnesium-alkaline phosphatase system, **Inorg.Chim.Acta**, 78, 19-22, 1983
43. Bertini, I., Luchinat, C., and Messori, L., 205TI as an NMR probe for the investigation of transferrin, **J.Am.Chem.Soc.**, 105, 1347-1350, 1983
42. Bertini, I., Lanini, G., Luchinat, C., and Monnanni, R., Spectroscopic studies on cobalt(II) carboxypeptidase A, in: *The coordination chemistry of metalloenzymes*, Bertini, I., Drago, R. S., and Luchinat, C., 93-97, Springer, 1983
41. Bertini, I., Drago, R.S., Luchinat, C., *The Coordination Chemistry of Metalloenzymes*, Springer 1983 DOI <https://doi.org/10.1007/978-94-009-7049-6>

### 1982

40. Bertini, I., Luchinat, C., Monnanni, R., and Scozzafava, A., Different behavior of sulfonamides with respect to copper- substituted bovine and human carbonic anhydrases, **J.Inorg.Biochem.**, 16, 155-160, 1982
39. Bertini, I., Canti, G., and Luchinat, C., 1H NMR study of cobalt(II)-substituted carboxypeptidase A, **J.Am.Chem.Soc.**, 104, 4943-4946, 1982
38. Bertini, I., Canti, G., Luchinat, C., and Messori, L., 1H NMR detection of CoOH<sub>2</sub> <-> CoOH interconversions in high- spin cobalt(II) complexes, **Inorg.Chem.**, 21, 3426-3429, 1982
37. Bertini, I., Canti, G., and Luchinat, C., Preparation and characterization of the vanadium(III) derivative of transferrin, **Inorg.Chim.Acta**, 67, L21-L23, 1982
36. Bertini, I., Borghi, E., Luchinat, C., and Monnanni, R., Nickel carbonic anhydrase: a re-examination of the electronic spectra with the help of CD spectra, **Inorg.Chim.Acta**, 67, 99-102, 1982
35. Bertini, I., Luchinat, C., and Scozzafava, A., Carbonic anhydrase: an insight into the zinc binding site and into the active cavity through metal substitution, **Struct.Bonding**, 48, 45-92, 1982

### 1981

34. Bertini, I., Canti, G., and Luchinat, C., Water in the coordination sphere of metalcarbonic anhydrases: a solvent proton longitudinal relaxation study at several frequencies, **Inorg.Chim.Acta**, 56, 99-107, 1981
33. Bertini, I., Canti, G., Luchinat, C., and Mani, F., 1H NMR spectra of the coordination sphere of cobalt- substituted carbonic anhydrase, **J.Am.Chem.Soc.**, 103, 7784-7788, 1981
32. Bertini, I., Canti, G., Luchinat, C., and Mani, F., pH-dependent properties of a CoN<sub>4</sub>(OH<sub>2</sub>) chromophore: a spectroscopic model of cobalt carbonic anhydrase, **Inorg.Chem.**, 20, 1670-1673, 1981

31. Bertini, I., Borghi, E., Luchinat, C., and Scozzafava, A., 2. Binding sites of anions in superoxide dismutase, **J.Am.Chem.Soc.**, 103, 7779-7783, 1981
30. Bertini, I., Canti, G., and Luchinat, C., 17O NMR investigation of copper(II) substituted carbonic anhydrases, **Inorg.Chim.Acta**, 56, 1-4, 1981
29. Bertini, I., Luchinat, C., and Messori, L., A water 17O NMR study of the pH dependent properties of superoxide dismutase, **Biochem.Biophys.Res.Comm.**, 101, 577-583, 1981
28. Bertini, I., Luchinat, C., and Borghi, E., A fourier-transform NMR investigation of [(C4H9)4Z][MP(C6H5)3I3](Z = N,P; M = Co,Ni), **Inorg.Chem.**, 20, 303-306, 1981
27. Bencini, A., Bertini, I., Canti, G., Gatteschi, D., and Luchinat, C., The EPR spectra of the inhibitor derivatives of cobalt carbonic anhydrase, **J.Inorg.Biochem.**, 14, 81-93, 1981
26. Alberti, G., Bertini, I., Luchinat, C., and Scozzafava, A., A new class of inhibitors capable of binding both the acidic and alkaline forms of carbonic anhydrase, **Biochim.Biophys.Acta**, 668, 16-26, 1981

#### 1980

25. Bertini, I., Luchinat, C., and Scozzafava, A., Superoxide dismutase-thiocyanate: a study of the binding sites of anions to copper(II) in superoxide dismutase, **J.Am.Chem.Soc.**, 102, 7349-7353, 1980
24. Bertini, I., Canti, G., Luchinat, C., and Mani, F., The complex cation [Co(tris(3,5-dimethyl-1-pyrazolylmethyl)amine) H2O]2+: a model for metalloenzymes containing bivalent zinc(II) chromophores with a water molecule in the coordination sphere, **Inorg.Chim.Acta**, 46, L91-L92, 1980
23. Bertini, I., Luchinat, C., and Scozzafava, A., The acid-base equilibria of carbonic anhydrase, **Inorg.Chim.Acta**, 46, 85-89, 1980
22. Bertini, I., Luchinat, C., Mani, F., and Scozzafava, A., Adducts of bis(N-substituted ethylenediamine)copper(II) complexes with hexacyanoferrate(III), **Inorg.Chem.**, 19, 1333-1336, 1980
21. Bertini, I., Luchinat, C., and Scozzafava, A., Some structural aspects of carbonic anhydrase, in: *Biophysics and physiology of carbon dioxide*, Bauer, C., Gros, G., and Bartels, H., 151-153, 1980
20. Bertini, I., Canti, G., Luchinat, C., and Romanelli, P., Cyanometallates and cobalt(II) bovine carbonic anhydrase B. Five coordination with dicyanoaurate(I), **Inorg.Chim.Acta**, 46, 211-214, 1980

#### 1979

19. Bertini, I., Luchinat, C., and Scozzafava, A., 31P NMR spectra of paramagnetic MBr2(OPPh3)2 complexes. A breakdown in the validity of the Solomon-Bloembergen equations, **Inorg.Nucl.Chem.Letters**, 15, 89-91, 1979
18. Bertini, I., Borghi, E., Canti, G., and Luchinat, C., Investigation of the system cobalt(II) bovine carbonic anhydrase B-trichloroacetaldehyde, **J.Inorg.Biochem.**, 11, 49-56, 1979
17. Bertini, I., Canti, G., Luchinat, C., and Scozzafava, A., Characterization of oxovanadium(IV) substituted bovine carbonic anhydrase B, **Inorg.Chim.Acta**, 36, 9-12, 1979
16. Bertini, I., Borghi, E., and Luchinat, C., Investigation of the system CO2-HCO3<sup>-</sup> in the presence of copper(II) bovine carbonic anhydrase B, **J.Am.Chem.Soc.**, 101, 7069-7071, 1979
15. Barzi, D., Bertini, I., Luchinat, C., and Scozzafava, A., The electronic spectra of cobalt(II) bovine carbonic anhydrase, **Inorg.Chim.Acta**, 36, L431-L432, 1979

#### 1978

14. Bertini, I., Luchinat, C., and Scozzafava, A., A 31P NMR study of phosphate in presence of cobalt(II)- and copper(II)- substituted bovine carbonic anhydrase B, **FEBS Lett.**, 93, 251-254, 1978
13. Bertini, I., Luchinat, C., and Scozzafava, A., Binding affinity of bicarboxylate ions for cobalt(II) bovine carbonic anhydrase, **Bioinorg.Chem.**, 9, 93-100, 1978
12. Bertini, I., Luchinat, C., and Scozzafava, A., Evidence of exchangeable protons in the acidic form of manganese(II) bovine carbonic anhydrase B, **FEBS Lett.**, 87, 92-94, 1978
11. Bertini, I., Borghi, E., and Luchinat, C., Characterization of nickel(II) bovine carbonic anhydrase and its inhibitor derivatives, **Bioinorg.Chem.**, 9, 495-504, 1978
10. Bertini, I., Canti, G., Luchinat, C., and Scozzafava, A., Spectroscopic investigation of copper(II) bovine carbonic anhydrase and its inhibitor derivatives, **J.Chem.Soc.Dalton Trans.**, 1269-1273, 1978
9. Bertini, I., Canti, G., Luchinat, C., and Scozzafava, A., Characterization of cobalt(II) bovine carbonic anhydrase and of its derivatives, **J.Am.Chem.Soc.**, 100, 4873-4877, 1978

#### 1977

8. Bertini, I., Luchinat, C., and Scozzafava, A., Carbon-13 longitudinal relaxation times of acetate ion in the presence of metal-substituted bovine carbonic anhydrase, **J.Chem.Soc.Dalton Trans.**, 1962-1965, 1977
7. Bertini, I., Canti, G., Luchinat, C., and Scozzafava, A., Evidence of exchangeable protons in the donor groups of the acidic form of cobalt bovine carbonic anhydrase B, **Biochem.Biophys.Res.Comm.**, 78, 158-160, 1977
6. Bertini, I., Canti, G., Luchinat, C., and Scozzafava, A., Proton relaxation of water solutions containing copper carbonic anhydrase, **Inorg.Chim.Acta**, 23, L15-L16, 1977
5. Bertini, I., Luchinat, C., and Scozzafava, A., Stereochemistry of cobalt(II) in cobalt bovine carbonic anhydrase and its derivatives, **Inorg.Chim.Acta**, 22, L23-L24, 1977
4. Bertini, I., Luchinat, C., and Scozzafava, A., Interaction of cobalt(II) bovine carbonic anhydrase with aniline, benzoate and anthranilate, **J.Am.Chem.Soc.**, 99, 581-584, 1977
3. Bertini, I., Luchinat, C., and Scozzafava, A., Interactions between  $\alpha$ -Amino acids and cobalt(II) bovine carbonic anhydrase, **Bioinorg.Chem.**, 7, 225-231, 1977



1976

2. Bertini, I., Luchinat, C., and Scozzafava, A., Interaction of cobalt bovine carbonic anhydrase with the acetate ion, **Biochim.Biophys.Acta**, 452, 239-244, 1976

1. Bertini, I., Luchinat, C., and Scozzafava, A., <sup>13</sup>C NMR spectra of hexakis pyridine-N-oxide cobalt(II) and nickel(II) complexes, **Inorg.Chim.Acta**, 19, 201-202, 1976