

**Cerm Publications  
(December 2012)**

1. Banci, L. and Luchinat, C., Ivano Bertini 1940-2012., **Nat.Chem.Biol.**, 8, 807, 2012 (IF 14.690).
2. Pozzi, C., Ferrari, S., Cortesi, D., Luciani, R., Stroud, R. M., Catalano, A., Costi, M. P. Mangani, S., The structure of *Enterococcus faecalis* thymidylate synthase provides clues about folate bacterial metabolism, **Acta Crystallogr. D Biol.Crystallogr.**, 68, 1232-1241, 2012 (IF 12.619)
3. Banci, L., Bertini, I., Cantini, F., Kozyreva, T., Massagni, C., Palumaa, P., Rubino, J. T., and Zovo, K., Human SOD1 maturation through interaction with human CCS, **Proc.Natl.Acad.Sci.USA**, 109, 13555-13560, 2012 (IF 9.771).
4. Knight, M. J., Pell, A. J., Bertini, I., Felli, I. C., Gonnelli, L., Pierattelli, R., Hermann, T., Emsley, L., and Pintacuda, G., Structure and backbone dynamics of a microcrystalline metalloprotein by solid-state NMR, **Proc.Natl.Acad.Sci.USA**, 109, 11095-11100, 2012 (IF 9.771).
5. Tottey, S., Patterson, A. M., Banci, L., Bertini, I., Felli, I. C., Pavelkova, A., Dainty, S. J., Pernil, R., Waldron, K. J., Foster, A. W., and Robinson, N. J., Cyanobacterial metallochaperone inhibits deleterious side reactions of copper, **Proc.Natl.Acad.Sci.USA**, 109, 95-100, 2012 (IF 9.771).
6. Banci, L., Bertini, I., Blazevits, O., Calderone, V., Cantini, F., Mao, J., Trapananti, A., Vieru, M., Amori, I., Cozzolino, M., and Carri, M. T., Interaction of Cisplatin with Human Superoxide Dismutase, **J.Am.Chem.Soc.**, 134, 7009-7014, 2012 (IF 9.019).
7. Banci, L., Bertini, I., Calderone, V., Cefaro, C., Ciofi-Baffoni, S., Gallo, A., and Tokatlidis, K., An electron transfer path through an extended disulfide relay system: the case of the redox protein ALR, **J.Am.Chem.Soc.**, 134, 1442-1445, 2012 (IF 9.019).
8. Bertini, I., Lalli, D., Mangani, S., Pozzi, C., Rosa, C., Theil, E. C., and Turano, P., Structural insights into the ferroxidase site of ferritins from higher eukaryotes, **J.Am.Chem.Soc.**, 134, 6169-6176, 2012 (IF 9.019).
9. 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).
10. 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).
11. Knight, M. J., Felli, I. C., Pierattelli, R., Bertini, I., Emsley, L., Herrmann, T., and Pintacuda, G., Rapid measurement of pseudocontact shifts in metalloproteins by proton-detected solid-state NMR spectroscopy, **J.Am.Chem.Soc.**, 134, 14730-14733, 2012 (IF 9.019).
12. Bertini, I., Cacciatore, 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).
13. Holliday, G. L., Andreini, C., Fischer, C., Rahman, S. A., Almonacid, D. E., Williams, S. T., and Pearson, W. R., MACiE: exploring the diversity of biochemical reactions, **Nucleic Acids Res.**, 40, D783-D789, 2012 (IF 7.836).

14. Nagulapalli, M., Parigi, G., Yuan, J., Gsponer, J., Deraos, S., Bamm, V. V., Harauz, G., Matsoukas, J., de Planque, M.R., 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).
15. Rosato, A., Aramini, J. M., Arrowsmith, C., Bagaria, A., Baker, D., Cavalli, A., Doreleijers, J. F., Eletsky, A., Giachetti, A., Guerry, P., Gutmanas, A., Guntert, P., He, Y., Herrmann, T., Huang, Y. J., Jaravine, V., Jonker, H. R., Kennedy, M. A., Lange, O. F., Liu, G., Mallavin, T. E., Mani, R., Mao, B., Montelione, G. T., Nilges, M., Rossi, P., van der Schot, G., Schwalbe, H., Szyperski, T. A., Vendruscolo, M., Vernon, R., Vranken, W. F., de Vries, S., Vuister, G. W., Wu, B., Yang, Y., and Bonvin, A. M. J. J., Blind testing of routine, fully automated determination of protein structures from NMR data, **Structure**, 20, 227-236, 2012 (IF 6.337).
16. Kallergi, E., Andreadaki, M., Kritsiligkou, P., Katrakili, N., Pozidis, C., Tokatlidis, K., Banci, L., Bertini, I., Cefaro, C., Ciofi-Baffoni, S., Gajda, K., and Peruzzini, R., Targeting and maturation of Erv1/ALR in the mitochondrial intermembrane space, **ACS Chem Biol.**, 7, 707-714, 2012 (IF 5.838).
17. Caillet-Saguy, C., Piccioli, M., Turano, P., Lukat-Rodgers, G., Wolff, N., Rodgers, K., Izadi-Pruneyre, N., Delepierre, M., and Lecroisey, A., Heme carrier HasA: learning about the role of the iron axial ligands in the heme uptake and release processes, **J.Biol.Chem.**, 287, 26932-26943, 2012 (IF 5.328).
18. Gallo, A., Lo Sterzo, C., Mori, M., Di Matteo, A., Bertini, I., Banci, L., Brunori, M., and Federici, L., Structure of nucleophosmin DNA-binding domain and analysis of its complex with a G-quadruplex sequence from the c-MYC promoter, **J.Biol.Chem.**, 287, 26539-26548, 2012 (IF 5.328).
19. Mainz, A., Bardiaux, B., Kuppler, F., Multhaup, G., Felli, I. C., Pierattelli, R., and Reif, B., Structural and mechanistic implications of metal-binding in the small heat-shock protein  $\alpha$ B-crystallin, **J.Biol.Chem.**, 287, 1128-1138, 2012 (IF 5.328).
20. Banaszak, K., Martin-Diaconescu, V., Bellucci, M., Rypniewski, W. R., Maroney, M. J., and Ciurli, S., Crystallographic and X-ray absorption spectroscopic characterization of *Helicobacter pylori* UreE bound to Ni<sup>2+</sup> and Zn<sup>2+</sup> reveal a role for the disordered C-terminal arm in metal trafficking, **Biochem.J.**, 44, 1017-1026, 2012 (IF 5.016).
21. 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).
22. Andreini, C., Cavallaro, G., and Lorenzini, S., FindGeo: a tool for determining metal coordination geometry, **Bioinformatics**, 28, 1658-1660, 2012 (IF 4.877).
23. Maccaferri, S., Klinder, A., Cacciatore, 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).
24. Felli, I. C. and Pierattelli, R., Recent progress in NMR spectroscopy: towards the study of intrinsically disordered proteins of increasing size and complexity, **IUBMB Life**, 64, 473-481, 2012 (IF 4.251).

25. 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).
26. Real-Guerra, R., Staniscuaski, F., Zambelli, B., Musiani, F., Ciurli, S., and Carlini, C., Biochemical and structural studies on native and recombinant Glycine max UreG: a detailed characterization of a plant urease accessory protein, **Plant.Mol.Biol.**, 78, 461-475, 2012 (IF 4.150).
27. Monini, P., Cafaro, A., Srivastava, IK, Sharma, V. A., Andreini, C., Chiozzini, C., Ferrantelli, F., Cossut, M. R., Tripiciano, A., Nappi, F., Longo, O., Bellino, S., Picconi, O., Fanales-Belasio, E., Borsetti, A., Toschi, E., Schiavoni, I., Bacigalupo, I., Kan, E., Sernicola, L., Maggiorella, M. T., Montin, K., Porcu, M., Leone, P., Collacchi, B., Palladino, C., Ridolfi, B., Falchi, M., Macchia, I., Ulmer, J. B., Butto', S., Sgadari, C., Magnani, M., Federico, M. P., Titti, F., Banci, L., Dallochio, F., Rappuoli, R., Ensoli, F., Barnett, S. W., Garaci, E., and Ensoli, B., HIV-1 Tat Promotes Integrin-Mediated HIV Transmission to Dendritic Cells by Binding Env Spikes and Competes Neutralization by Anti-HIV Antibodies, **Plos ONE**, 7, e48781-, 2012 (IF 4.092).
28. Bermel, W., Bertini, I., Chill, J. H., Felli, I. C., Haba, N., Kumar, V. M. V., and Pierattelli, R., Exclusively heteronuclear <sup>13</sup>C-detected amino-acid-selective NMR experiments for the study of intrinsically disordered proteins (IDPs), **ChemBioChem**, 13, 2425-2432, 2012 (IF 3.944).
29. Zambelli, B., Cremades, N., Neyroz, P., Turano, P., Uversky, V. N., and Ciurli, S., Insights in the (un)structural organization of *Bacillus pasteurii* UreG, an intrinsically disordered GTPase enzyme, **Mol.Biosyst.**, 8, 220-228, 2012 (IF 3.825).
30. Bertini, I., Ferella, L., Luchinat, C., Parigi, G., Petoukhov, M. V., Ravera, E., and Rosato, A., MaxOcc: a web portal for Maximum Occurrence Analysis, **J.Biomol.NMR**, 53, 271-280, 2012 (IF 3.612).
31. Bermel, W., Bertini, I., Gonnelli, L., Felli, I. C., Kozminski, W., Piai, A., Pierattelli, R., and Stanek, J., Speeding up sequence specific assignment of IDPs, **J.Biomol.NMR**, 53, 293-301, 2012 (IF 3.612).
32. 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).
33. 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).
34. 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).
35. 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).
36. 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).

37. Veggi, D., Gentile, M., Cantini, F., Lo Surdo, P., Nardi-Dei, V., Seib, K., Pizza, M., Rappuoli, R., Banci, I., Savino, S., Scarselli, M., The factor H binding protein of *Neisseria meningitidis* interacts with xenosiderophores in vitro, **Biochemistry**, 51, 9384-9393, 2012 (IF 3.422)
38. Banci, L., Bertini, I., Ciofi-Baffoni, S., Jaiswal, D., Neri, S., Peruzzini, R., and Winkelmann, J., Structural characterization of CHCHD5 and CHCHD7: two atypical human twin CX(9)C proteins, **J.Struct.Biol.**, 180, 190-200, 2012 (IF 3.406).
39. Sgrignani, J., Dal Peraro, M., Carloni, P., Magistrato, A., Vila, A. J., and Pierattelli, R., On the active site of mononuclear B1 Metallo  $\beta$ -lactamases: a computational study, **J.Comp.Aided Mol.Design**, 26, 425-435, 2012 (IF 3.374).
40. Webber, A. L., Pell, A. J., Barbet-Massin, E., Knight, M. J., Bertini, I., Felli, I. C., Pierattelli, R., Emsley, L., Lesage, A., and Pintacuda, G., Combination of DQ and ZQ coherences for sensitive through-bond NMR correlation experiments in biosolids under ultra-fast MAS, **ChemPhysChem**, 13, 2405-2411, 2012 (IF 3.339).
41. Andreini, C. and Bertini, I., A bioinformatics view of zinc enzymes, **J.Inorg.Biochem.**, 111, 150-156, 2012 (IF 3.317).
42. Martin-Diaconescu, V., Bellucci, M., Musiani, F., Ciurli, S., and Maroney, M. J., Unraveling the *H. pylori* UreG zinc binding site using X-ray absorption spectroscopy (XAS) and structural modeling, **J.Biol.Inorg.Chem.**, 17, 353-361, 2012 (IF 3.287).
43. Sgrignani, J. and Pierattelli, R., Nuclear magnetic resonance signals chemical shifts and molecular simulations: a multidisciplinary approach to modeling copper protein structures, **J.Biol.Inorg.Chem.**, 17, 71-79, 2012 (IF 3.287).
44. Bertini, I., Calderone, V., Cerofolini, L., Fragai, M., Geraldès, 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).
45. Bergdale, T. E., Pinkelman, R. J., Hughes, S. R., Zambelli, B., Ciurli, S., and Bang, S. S., Engineered biosealant strains producing inorganic and organic biopolymers, **Journal of Biotechnology**, 161, 181-189, 2012 (IF 3.045).
46. Gladyshev, V. N., Kim, H-Y., Aachmann, F. L., Del Conte, R., and Dikiy, A., Structural and biochemical analysis of mammalian methionine sulfoxide reductase B2, **Proteins: Structure, Function, and Bioinformatics**, 79, 3123-3131, 2012 (IF 2.813).
47. 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).
48. 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).
49. Oakman, C., Tenori, L., Cappadona, S., Luchinat, C., Bertini, I., Di Leo, A., Targeting metabolomics in breast cancer, **Curr.Breast Cancer Reports**, 4, 249-256, 2012 (IF 2)

50. 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).
51. Jozefczuk, J., Kashofer, K., Ummanni, R., Henjes, F., Rehman, S., Geenen, S., Wruck, W., Regenbrecht, C., Daskalaki, A., Wierling, C., Turano, P., Bertini, I., Korf, U., Zatloukal, K., Westerhoff, H.V., Lehrach, H., Adjaye, J.A Systems Biology approach to deciphering the etiology of steatosis employing patient-derived dermal fibroblasts and iPS cells, **Front Physiol.** 3, 339, 2012