

Publications

- 1) Schirò A, Carlon A, Parigi G, Murshudov G, **Calderone C**, Ravera E, Luchinat C. (2020).
On the complementarity of X-ray and NMR data.
J Struct Biol X 4 DOI: 10.1016/j.yjsbx.2020.100019 IF= 3.754
- 2) Vourloumis D, Tsoukalidou S, Kakou M, Mavridis I, Koumantou D, Calderone V, Fragai M, Stratikos E, Papakyriakou A. (2019).
Exploration of zinc-binding groups for the design of inhibitors for the Oxytocinase Subfamily of M1 Aminopeptidases.
Bioorg & Med Chem 27(24):115177 DOI: 10.1016/j.bmc.2019.115177 IF= 2.802
- 3) Cerofolini L, Fragai M, Ravera E, Diebolder CA, Renault L and **Calderone V**. (2019).
Integrative Approaches in Structural Biology: A More Complete Picture from the Combination of Individual Techniques.
Biomolecules 9(8), 370 DOI: 10.3390/biom9080370 IF= 4.694
- 4) Gourdoupsis S, Nasta V, Ciofi-Baffoni S, Banci L. and **Calderone V**. (2019).
In-house high energy remote SAD-phasing using the magic triangle: how to tackle the P1 low symmetry using multiple orientations on the same human IBA57 crystal to increase multiplicity.
Acta Cryst Sect D 75: 317–324 DOI: 10.1107/S2059798319000214 IF=3.099
- 5) Cerofolini L, Giuntini S, Carlon A, Ravera E, Calderone V, Fragai M, Parigi G, Luchinat C. (2019).
Characterization of PEGylated asparaginase: new opportunities from NMR analysis of large pegylated therapeutics.
Chem Eur J 25: 1–9 DOI: 10.1002/chem.201804488 IF= 5.160
- 6) Silva JM, Giuntini S, Cerofolini L, Geraldes CFGC, Macedo AL, Ravera E, Fragai M, Luchinat C, **Calderone V**. (2019).
Non crystallographic symmetry in proteins: Jahn-Teller-like and butterfly-like effects?
J Biol Inorg Chem 24: 91–101 DOI: 10.1007/s00775-018-1630-0 IF= 2.952
- 7) **Calderone V**, Fragai M and Luchinat C. (2019)
Reviewing the crystal structure of S100Z and other members of the S100 family: implications in calcium-regulated quaternary structure.
In CW Heizmann (Ed.) Calcium-Binding Proteins of the EF-hand Superfamily: from Basics to Medical Applications.
Methods Mol Biol. 1929:487-499
Springer Protocols, Humana Press DOI: 10.1007/978-1-4939-9030-6_30 IF= 1.090
- 8) Silva JM, Cerofolini L, Giuntini S, Calderone V, Geraldes CFGC, Macedo AL, Parigi G, Fragai M, Ravera E, Luchinat C. (2018).
Metal centers in biomolecular solid-state NMR.
J Struct Biol pii: S1047-8477(18)30313-7 DOI: 10.1016/j.jsb.2018.11.013 IF= 3.433
- 9) Cantini F, Calderone V, Di Cesare Mannelli L, Korsak M, Gonnelli L, Francesconi O, Ghelardini C, Banci L, and Nativi C. (2018).
Interaction of half oxa-/half cis-platin complex with human superoxide dismutase and induced reduction of neurotoxicity.
ACS Med. Chem. Lett. 9: 1094–1098. DOI: 10.1021/acsmedchemlett.8b00199 IF= 3.794
- 10) Gourdoupsis S, Nasta V, Calderone V, Ciofi-Baffoni S, Banci L. (2018).
IBA57 recruits ISCA2 to form a [2Fe-2S] cluster-mediated complex.
J Am Chem Soc. 140(43):14401-14412 DOI: 10.1021/jacs.8b09061 IF= 14.350
- 11) **Calderone V**, Fragai M, Luchinat C. (2018).
When molecular replacement has no trivial solution: The importance of model editing in human S100Z X-ray structure solution.
Inorg Chim Acta 470: 402-406. DOI: 10.1016/j.ica.2017.06.055 IF= 2.002
- 12) Fragai M, Comito G, Di Cesare Mannelli L, Galdani R, Calderone V, Louka A, Richichi B, Francesconi O, Angeli A, Nocentini A, Gratteri P, Chiarugi P, Ghelardini C, Tadini-Buoninsegni F, Supuran CT, Nativi, C. (2017).
Lipoyl-Homotaurine Derivative (ADM-12) Reverts Oxaliplatin-Induced Neuropathy and Reduces Cancer Cells Malignancy by Inhibiting Carbonic Anhydrase IX (CAIX).
J Med Chem 60(21): 9003-9011. DOI: 10.1021/acs.jmedchem.7b01237 IF= 4.898
- 13) **Calderone V**, Fragai M, Gallo G, Luchinat C. (2017).
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(4):519-526. DOI: 10.1007/s00775-017-1437-4 IF= 2.545
- 14) Chakrabarti VS, Mikolajczyk M, Boscaro F, **Calderone V.** (2014).
 Human Ind1 expression causes over-expression of E. coli beta-lactamase ampicillin resistance protein.
Protein Expr Purif 104C: 26-33. DOI: 10.1016/j.pep.2014.09.005 IF= 1.345
 - 15) Rinaldelli M, Ravera E, Calderone V, Parigi G, Murshudov GN, Luchinat C. (2014).
 Simultaneous use of solution NMR and X-ray data in REFMAC5 for joint refinement/detection of structural differences.
Acta Crystallogr D Biol Crystallogr. 70(4): 958-967. DOI: 10.1107/S1399004713034160 IF= 14.103
 - 16) Mori M, Massaro A, Calderone V, Fragai M, Luchinat C and Mordini A. (2013).
 Discovery of a New Class of Potent MMP Inhibitors by Structure-Based Optimization of the Arylsulfonamide Scaffold.
ACS Med Chem Lett 4: 565-569. DOI: 10.1021/ml300446a IF= 3.311
 - 17) Belviso BD, Caliendo R, Siliqi D, Calderone V, Arnesano F, Natile G. (2013).
 Structure of matrix metalloproteinase-3 with a platinum-based inhibitor.
Chem Commun (Camb). 49(48):5492-5494. DOI: 10.1039/c3cc41278d IF= 6.169
 - 18) Banci L, Bertini I, Calderone V, Ciofi-Baffoni S, Giachetti A, Jaiswal D, Mikolajczyk M, Piccioli M, Winkelmann J. (2013).
 Molecular view of an electron transfer process essential for iron-sulfur protein biogenesis.
Proc Natl Acad Sci U S A 110(18):7136-7141. DOI: 10.1073/pnas.1302378110 IF= 9.432
 - 19) Udi Y, Fragai M, Grossman M, Mitternacht S, Arad-Yellin R, Calderone V, Melikian M, Toccafondi M, Berezovsky IN, Luchinat C, Sagi I. (2013).
 Unraveling Hidden Regulatory Sites in Structurally Homologous Metalloproteases.
J Mol Biol 425(13):2330-2346. DOI: 10.1016/j.jmb.2013.04.009 IF= 3.871
 - 20) Czarny B, Stura EA, Devel L, Vera L, Cassar-Lajeunesse E, Beau F, Calderone V, Fragai M, Luchinat C, Dive V. (2013).
 Molecular determinants of a selective matrix metalloprotease-12 inhibitor: insights from crystallography and thermodynamic studies.
J Med Chem. 56(3):1149-59. DOI: 10.1021/jm301574d IF= 4.898
 - 21) Banci L, Bertini I, Blaževič O, Calderone V, Cantini F, Mao J, Trapananti A, Vieru M, Amori I, Cozzolino M, Carrì MT. (2012).
 Interaction of cisplatin with human superoxide dismutase
J Am Chem Soc 134 (16): 7009-7014. DOI: 10.1021/ja211591n IF= 9.019
 - 22) Banci L, Bertini I, Calderone V, Cefaro C, Ciofi-Baffoni S, Gallo A, Tokatlidis K. (2012).
 An Electron-Transfer Path through an Extended Disulfide Relay System: The Case of the Redox Protein ALR.
J Am Chem Soc 134(3):1442-1445. DOI: 10.1021/ja209881f IF= 9.019
 - 23) Bertini I, Calderone V., Cerofolini L, Fragai M, Geraldès CF, Hermann P, Luchinat C, Parigi G, Teixeira JM. (2012).
 The catalytic domain of MMP-1 studied through tagged lanthanides.
FEBS Lett. 586 (5): 557-567. DOI: 10.1016/j.febslet.2011.09.020 IF= 3.601
 - 24) Docquier J-D, Benvenuti M, Calderone V, Rossolini GM, Mangani S. (2011).
 Structure of the extended-spectrum β -lactamase TEM-72 inhibited by citrate.
Acta Crystallogr Sect F 67(3):303-306. DOI: 10.1107/S1744309110054680 IF= 0.563
 - 25) Banci L, Bertini I, Calderone V, Cefaro C, Ciofi-Baffoni S, Gallo A, Kallergi E, Lionaki E, Pozidis C, Tokatlidis K. (2011).
 Molecular recognition and substrate mimicry drive the electron-transfer process between MIA40 and ALR.
Proc Natl Acad Sci U S A. 108(12):4811-4816. DOI: 10.1073/pnas.1014542108 IF= 9.432
 - 26) Babini E, Bertini I, Borsi V, Calderone V, Hu X, Luchinat C, Parigi G. (2010).
 Structural characterization of human S100A16, a low-affinity calcium binder.
J Biol Inorg Chem 16(2):243-56. DOI: 10.1007/s00775-010-0721-3 IF= 3.415
 - 27) Attolino E, Calderone V, Dragoni E, Fragai M, Richichi B, Luchinat C, Nativi C. (2010).
 Structure-based approach to nanomolar, water soluble matrix metalloproteinases inhibitors (MMPi).
Eur J Med Chem. 45(12):5919-25 DOI: 10.1016/j.ejmech.2010.09.057 IF= 3.269

- 28) Docquier JD, Benvenuti M, Calderone V, Stoczko M, Mencias N, Rossolini GM, Mangani S. (2010). High-Resolution Crystal Structure of the Subclass B3 BJP-1 Metallo- β -lactamase: Rational Basis for Substrate Specificity and Interaction with Sulfonamides. *Antimicrob Agents Chemother.* 54(10):4343-4351. DOI: 10.1128/AAC.00409-10 IF= 4.802
- 29) Borsi V, Calderone V, Fragai M, Luchinat C and Sarti N. (2010). Entropic Contribution to the Linking Coefficient in Fragment Based Drug Design: A Case Study. *J Med Chem.* 53(10):4285-9. DOI:10.1021/jm901723z IF= 4.898
- 30) Docquier JD, Benvenuti M, Calderone V, Giuliani F, Kapetis D, De Luca F, Rossolini GM, Mangani S. (2010). Crystal Structure of the Narrow-Spectrum OXA-46 Class D β -lactamase: Relationship between Active Site Lysine Carbamylation and Inhibition by Polycarboxylates. *Antimicrob Agents Chemother.* 54(5):2167-2174. DOI: 10.1128/AAC.01517-09 IF= 4.802
- 31) Bertini I, Calderone V, Fragai M, Luchinat C, Talluri E. (2009). Structural basis of serine/threonine phosphatase inhibition by the archetypal small molecules cantharidin and norcantharidin. *J Med Chem* 52(15):4838-43. DOI: 10.1021/jm900610k IF= 4.898
- 32) Docquier JD, Calderone V, De Luca F, Benvenuti M, Giuliani F, Bellucci L, Tafi A, Nordmann P, Botta M, Rossolini GM, Mangani S. (2009). Crystal structure of the OXA-48 β -lactamase reveals mechanistic diversity among class D carbapenemases. *Chem Biol* 16(5):540-7. DOI: 10.1016/j.chembiol.2009.04.010 IF= 6.523
- 33) Banci L, Bertini I, Calderone V, Della-Malva N, Felli IC, Neri S, Pavelkova A, Rosato A. (2009). Copper(I)-mediated protein-protein interactions result from suboptimal interaction surfaces. *Biochem J* 422(1):37-42. DOI: 10.1042/BJ20090422 IF= 5.155
- 34) Banci L, Bertini I, Boca M, Calderone V, Cantini F, Girotto S, Vieru M. (2009). Structural and dynamic aspects related to oligomerization of apo SOD1 and its mutants. *Proc Natl Acad Sci U S A.* 106(17):6980-6985. DOI: 10.1073/pnas.0809845106 IF= 9.432
- 35) Dragoni E, Calderone V, Fragai M, Jaiswal R, Luchinat C, Nativi C. (2009). Biotin-tagged probes for MMP expression and activation: design, synthesis, and binding properties. *Bioconjug Chem* 20(4):719-727. DOI: 10.1021/bc8003827 IF= 4.350
- 36) Bertini I, Calderone V, Fragai M, Jaiswal R, Luchinat C, Melikian M, Mylonas E, Svergun DI. (2008). Evidence of reciprocal reorientation of the catalytic and hemopexin-like domains of full-length MMP-12. *J Am Chem Soc* 130(22):7011-7021. DOI: 10.1021/ja710491y IF= 8.580
- 37) Bertini I and Calderone V. (2007) A Structural Model of the CorA Translocation Cycle: Divalent Cation Specificity and Mg²⁺ Homeostasis. *ChemTracts Inorganic Chemistry* 20(2): 43-51
- 38) Bertini I, Calderone V, Fragai M, Giachetti A, Loconte M, Luchinat C, Maletta M, Nativi C, Kwon Joo Y. (2007). Exploring the Subtleties of Drug-Receptor Interactions: the Case of Matrix Metalloproteinases. *J Am Chem Soc* 129(9):2466-2475. DOI: 10.1021/ja065156z IF= 8.580
- 39) Bertini I, Calderone V, Fragai M, Luchinat C, Maletta M, Kwon Joo Y. (2006). Snapshots of the Reaction Mechanism of Matrix Metalloproteinases. *Angew Chem Int Ed Engl* 45(47):7952-7955. DOI: 10.1002/anie.200603100 IF= 11.829
- 40) Mannino C, Nievo M, Machetti F, Papakyriakou A, Calderone V, Fragai M and Guarna A. (2006). Synthesis of bicyclic molecular scaffolds (BTAA): An investigation towards new selective MMP-12 inhibitors. *Bioorg Med Chem* 14(22):7392-403. DOI: 10.1016/j.bmc.2006.07.028 IF= 2.822
- 41) Banci L, Bertini I, Calderone V, Ciofi-Baffoni S, Mangani S, Martinelli M, Palumaa P, Wang S. (2006). A hint for the function of human Sco1 from different structures. *Proc Natl Acad Sci U S A* 103(23):8595-8600. DOI: 10.1073/pnas.0601375103 IF= 9.432
- 42) **Calderone V**, Fragai M, Luchinat C, Nativi C, Richichi B and Roelens S. (2006). A High-Affinity Carbohydrate-Containing Inhibitor of Matrix Metalloproteinases *Chem Med Chem* 1: 598-601. DOI: 10.1002/cmdc.200600020 IF= 3.232
- 43) **Calderone V**, Casini A, Mangani S, Messori L and Orioli PL. (2006). Structural investigation of cisplatin-protein interactions: selective platination of His 19 in cuprozinic superoxide dismutase *Angew Chem Int Ed Engl* 45(8):1267-1269. DOI: 10.1002/anie.200502599 IF=

- 44) **Calderone V**, Forleo C, Benvenuti M, Thaller MC, Rossolini GM and Mangani S. (2005).
A structure-based proposal for the catalytic mechanism of the bacterial acid phosphatase AphA of the DDDD family from crystallographic data.
J Mol Biol 355(4): 708-721. DOI: 10.1016/j.jmb.2005.10.068 IF= 3.871
- 45) Banci L, Benvenuti M, Bertini I, Cabelli DE, Calderone V, Fantoni A, Mangani S, Migliardi M, Viezzoli MS. (2005).
From an inactive prokaryotic SOD homolog to an active protein through site directed mutagenesis
J Am Chem Soc 127(38):13287-13292. DOI: 10.1021/ja052790o IF= 8.580
- 46) Banci L, Bertini I, Calderone V, Cramaro F, Del Conte R, Fantoni A, Mangani S, Quattrone A, Viezzoli MS. (2005).
A prokaryotic superoxide dismutase paralog lacking two Cu ligands: From largely unstructured in solution to ordered in the crystal.
Proc Natl Acad Sci U S A 102(21):7541-7546. DOI: 10.1073/pnas.0502450102 IF= 9.432
- 47) Bertini I, Calderone V, Cosenza M, Fragai M, Lee Y-M, Luchinat C, Mangani S, Terni B and Turano P. (2005).
Conformational variability of MMPs: beyond a single 3D structure.
Proc Natl Acad Sci U S A 102(15):5334-5339. DOI: 10.1073/pnas.0407106102 IF= 9.432
- 48) Lunelli M, Di Paolo ML, Biadene M, Calderone V, Battistutta R, Scarpa M, Rigo A and Zanotti G. (2005).
Crystal Structure of Amine Oxidase from Bovine Serum
J Mol Biol 346(4):991-1004. DOI: 10.1016/j.jmb.2004.12.038 IF= 3.871
- 49) **Calderone V**, Dolderer B, Hartmann H-J, Echner H, Luchinat C, Del Bianco C, Mangani S, Weser U. (2005).
The crystal structure of yeast copper thionein: the solution of a long-lasting enigma.
Proc Natl Acad Sci U S A 102(1):51-6. DOI: 10.1073/pnas.0408254101 IF= 9.432
- 50) **Calderone V**. (2004).
Practical aspects of the integration of different software in protein structure solution.
Acta Cryst D60 :2150-2155. DOI: 10.1107/S0907444904019055 IF= 2.257
- 51) Bertini I, Calderone V, Fragai M, Luchinat C, Mangani S and Terni B. (2004).
Crystal structure of the catalytic domain of human matrix metalloproteinase 10.
J Mol Biol 336(3): 707-716. DOI: 10.1016/j.jmb.2003.12.033 IF= 3.871
- 52) **Calderone V**, Forleo C, Benvenuti M, Thaller MC, Rossolini GM and Mangani S. (2004).
The first structure of a bacterial class B acid phosphatase reveals further structural heterogeneity among phosphatases members of the haloacid dehydrogenase fold.
J Mol Biol 335(3): 761-773. DOI: 10.1016/j.jmb.2003.10.050 IF= 3.871
- 53) Arnesano F, Banci L, Benvenuti M, Bertini I, Calderone V, Mangani S, Viezzoli MS. (2003).
The evolutionarily conserved trimeric structure of CutA1 proteins suggests a role in signal transduction.
J Biol Chem 278(46): 45999-46006. DOI: 10.1074/jbc.M304398200 IF= 5.328
- 54) Bertini I, Calderone V, Fragai M, Luchinat C, Mangani S and Terni B. (2003).
X-ray structures of binary enzyme-product and ternary enzyme-product-inhibitor complexes of MMP.
Angew Chem Int Ed Engl 42(23): 2673-2676. DOI: 10.1002/anie.200350957 IF= 11.829
- 55) Forleo C, Benvenuti M, Calderone V, Schippa S, Docquier JD, Thaller MC, Rossolini GM and Mangani S. (2003).
Expression, purification, crystallization and preliminary X-ray characterization of the class B acid phosphatase (AphA) from *Escherichia coli*.
Acta Cryst D59(6):1058-1060. DOI: 10.1107/S0907444903006826 IF= 2.257
- 56) **Calderone V**, Trabucco M, Vujcic A, Battistutta R, Giacometti, GM, Andreucci F, Barbato R Zanotti G. (2003).
Crystal structure of the PsbQ protein of photosystem II from higher plants.
EMBO Rep 4(9): 900-905. DOI: 10.1038/sj.embor.embor923 IF= 6.907
- 57) **Calderone V**, Berni R and Zanotti G. (2003).
High-resolution structures of retinol-binding protein in complex with retinol: pH-induced protein structural changes in the crystal state.
J Mol Biol 329(4):841-850. DOI: 10.1016/S0022-2836(03)00468-6 IF= 3.871
- 58) **Calderone V**, Di Paolo ML, Trabucco M, Biadene M, Rigo A and Zanotti G. (2003).
Crystallization and preliminary X-ray data of amine oxidase from bovine serum.
Acta Cryst D59(4): 727-729. DOI: 10.1107/S0907444903002117 IF= 2.257

- 59) Folli C, Calderone V, Ramazzina I, Zanotti G and Berni R. (2002).
Ligand binding and structural analysis of a human putative cellular retinol-binding protein.
J Biol Chem 277 (44): 41970-41977. DOI: 10.1074/jbc.M207124200 IF= 5.328
- 60) **Calderone V**, Folli C, Marchesani A, Berni R and Zanotti G. (2002).
Identification and structural analysis of a zebrafish apo and holo cellular retinol-binding protein.
J Mol Biol 321: 527-535. DOI: 10.1016/S0022-2836(02)00628-9 IF= 3.871
- 61) **Calderone V**, Negro A, Trabucco M, Menin V and Zanotti G. (2002).
Cloning of human 3-hydroxyanthranilic acid dioxygenase in E.coli:characterisation of the purified enzyme and its in vitro inhibition by Zn⁺⁺.
Bioch Bioph Acta 1596/2: 283-292. DOI: 10.1016/S0167-4838(02)00216-9 IF= 2.958
- 62) Zanotti G, Calderone V, Beda M, Berni R. (2001).
Structure of chicken plasma retinol-binding protein.
Bioch. Bioph. Acta 1550: 64-69. DOI: 10.1016/S0167-4838(01)00268-0 IF= 2.958
- 63) Folli C, Calderone V, Ottonello S, Bolchi A, Zanotti G, Stoppini M and Berni R. (2001).
Identification, retinoid binding and X-ray analysis of a human retinol-binding protein.
Proc Natl Acad Sci USA 98 (7): 3710-3715. DOI: 10.1073/pnas.061455898 IF= 9.432
- 64) **Calderone V**, Chevrier B, Van Zandt M, Lamour V, Howard E, Poterszman A, Barth P, Mitschler A, Jianhui L, Dvornik DM, Klebe G, Kraemer O, Moorman AR, Moras D & Podjarny A. (2000).
The structure of human aldose reductase bound to the inhibitor IDD384.
*Acta Cryst D*56: 536-540. DOI: 10.1107/S0907444900002341 IF= 2.257
- 65) Giuffrida MG, Cavaletto M, Giunta C, Neuteboom B, Cantisani A, Napolitano L Calderone V, Godovac-Zimmerman J and Conti A. (1997).
The unusual aminoacid triplet Asn-Ile-Cys is a glycosylation consensus site in human a-lactalbumin.
Journal of Protein Chemistry 16: 747-753. DOI: 10.1023/a:1026359715821 IF= 1.304
- 66) **Calderone V**, Giuffrida MG, Viterbo D, Napolitano L, Fortunato D, Conti A and Acharya KR. (1996).
Amino acid sequence and crystal structure of buffalo alpha-lactalbumin.
FEBS Letters 394: 91-95 (front cover). DOI: 10.1016/0014-5793(96)00933-7 IF= 3.541
- 67) Bertino E, Prandi GM, Fabris C, Cavaletto M, Di Martino S, Cardaropoli S, Calderone V and Conti A. (1996).
Human milk proteins may interfere in ELISA measurements of bovine beta-lactoglobulin in human milk.
Acta Paediatrica Scandinavica 85: 543-549. DOI: 10.1111/j.1651-2227.1996.tb14083.x IF= 1.768
- 68) Cavaletto M, Cantisani AM, Napolitano L, Giuffrida MG, Calderone V, Fabris C, Bertino E, Prandi MG and Conti A. (1994).
Comparative study of casein content in human colostrum and milk.
Milchwissenschaft 49: 303-305. IF= 0.406
- 69) Bertino E, Prandi GM, Nicocia M, Cavaletto M, Di Martino S, Cardaropoli S, Calderone V, Conti A, Fabris C. (1994).
Rivalutazione del passaggio della beta-lattoglobulina bovina nel latte umano.
Italian Journal of Paediatrics 20: 107-113. IF= 0.101
- 70) Bertino E, Bagna R, Soldi A, Prandi GM, Cavaletto M, Conti A, Cantisani AM, Napolitano L, Giuffrida MG, Calderone V and Fabris C. (1993).
Assenza della caseina nel colostro umano.
Italian Journal of Paediatrics 19: 423. IF= 0.101