

1: Noto R, Santangelo MG, Levantino M, Cupane A, Mangione MR, Parisi D, Ricagno S, Bolognesi M, Manno M, Martorana V. Functional and dysfunctional conformers of human neuroserpin characterized by optical spectroscopies and Molecular Dynamics. *Biochim Biophys Acta*. 2014 Nov 6;1854(2):110-117. doi: 10.1016/j.bbapap.2014.10.002. [Epub ahead of print] PubMed PMID: 25450507.

2: DiFrancesco JC, Novara F, Zuffardi O, Forlino A, Gioia R, Cossu F, Bolognesi M, Andreoni S, Saracchi E, Frigeni B, Stellato T, Tolnay M, Winkler DT, Remida P, Isimbaldi G, Ferrarese C. TREX1 C-terminal frameshift mutations in the systemic variant of retinal vasculopathy with cerebral leukodystrophy. *Neurol Sci*. 2014 Sep 12. [Epub ahead of print] PubMed PMID: 25213617.

3: Haas J, Frese KS, Peil B, Kloos W, Keller A, Nietsch R, Feng Z, Müller S, Kayvanpour E, Vogel B, Sedaghat-Hamedani F, Lim WK, Zhao X, Fradkin D, Köhler D, Fischer S, Franke J, Marquart S, Barb I, Li DT, Amr A, Ehlermann P, Mereles D, Weis T, Hassel S, Kremer A, King V, Wirsz E, Isnard R, Komajda M, Serio A, Grasso M, Syrris P, Wicks E, Plagnol V, Lopes L, Gadgaard T, Eiskjær H, Jørgensen M, Garcia-Giustiniani D, Ortiz-Genga M, Crespo-Leiro MG, Deprez RH, Christiaans I, van Rijsingen IA, Wilde AA, Waldenstrom A, Bolognesi M, Bellazzi R, Mörner S, Bermejo JL, Monserrat L, Villard E, Mogensen J, Pinto YM, Charron P, Elliott P, Arbustini E, Katus HA, Meder B. Atlas of the clinical genetics of human dilated cardiomyopathy. *Eur Heart J*. 2014 Aug 27. pii: ehu301. [Epub ahead of print] PubMed PMID: 25163546.

4: Barbet-Massin E, Pell AJ, Retel JS, Andreas LB, Jaudzems K, Franks WT, Nieuwkoop AJ, Hiller M, Higman V, Guerry P, Bertarello A, Knight MJ, Felletti M, Le Marchand T, Kotelovica S, Akopjana I, Tars K, Stoppini M, Bellotti V, Bolognesi M, Ricagno S, Chou JJ, Griffin RG, Oschkinat H, Lesage A, Emsley L, Herrmann T, Pintacuda G. Rapid proton-detected NMR assignment for proteins with fast magic angle spinning. *J Am Chem Soc*. 2014 Sep 3;136(35):12489-97. doi: 10.1021/ja507382j. Epub 2014 Aug 18. PubMed PMID: 25102442; PubMed Central PMCID: PMC4156866.

5: de Rosa M, Bemporad F, Pellegrino S, Chiti F, Bolognesi M, Ricagno S. Edge strand engineering prevents native-like aggregation in *Sulfolobus solfataricus* acylphosphatase. *FEBS J.* 2014 Sep;281(18):4072-84. doi: 10.1111/febs.12861. Epub 2014 Jun 13. PubMed PMID: 24893801.

6: Ascenzi P, Leboffe L, Pesce A, Ciaccio C, Sbardella D, Bolognesi M, Coletta M. Nitrite-reductase and peroxynitrite isomerization activities of *Methanosarcina acetivorans* protoglobin. *PLoS One.* 2014 May 14;9(5):e95391. doi: 10.1371/journal.pone.0095391. eCollection 2014. PubMed PMID: 24827820; PubMed Central PMCID: PMC4020757.

7: Lolicato M, Bucchi A, Arrigoni C, Zucca S, Nardini M, Schroeder I, Simmons K, Aquila M, DiFrancesco D, Bolognesi M, Schwede F, Kashin D, Fishwick CW, Johnson AP, Thiel G, Moroni A. Cyclic dinucleotides bind the C-linker of HCN4 to control channel cAMP responsiveness. *Nat Chem Biol.* 2014 Jun;10(6):457-62. doi: 10.1038/nchembio.1521. Epub 2014 Apr 28. Erratum in: *Nat Chem Biol.* 2014 Aug;10(8):692. PubMed PMID: 24776929.

8: Lassaux P, Conchillo-Solé O, Manjasetty BA, Yero D, Perletti L, Belrhali H, Daura X, Gourlay LJ, Bolognesi M. Redefining the PF06864 Pfam family based on *Burkholderia pseudomallei* PilO2(Bp) S-SAD crystal structure. *PLoS One.* 2014 Apr 11;9(4):e94981. doi: 10.1371/journal.pone.0094981. eCollection 2014. PubMed PMID: 24728008; PubMed Central PMCID: PMC3984277.

9: DiFrancesco JC, Sestini R, Cossu F, Bolognesi M, Sala E, Mariani S, Saracchi E, Papi L, Ferrarese C. Novel neurofibromatosis type 2 mutation presenting with status epilepticus. *Epileptic Disord.* 2014 Mar;16(1):132-7. doi: 10.1684/epd.2014.0647. PubMed PMID: 24667735.

10: Croci R, Tarantino D, Milani M, Pezzullo M, Rohayem J, Bolognesi M, Mastrangelo E. PPNDS inhibits murine Norovirus RNA-dependent RNA-polymerase mimicking two RNA stacking bases. *FEBS Lett.* 2014 May 2;588(9):1720-5. doi: 10.1016/j.febslet.2014.03.021. Epub 2014 Mar 18. PubMed PMID: 24657439.

11: Croci R, Pezzullo M, Tarantino D, Milani M, Tsay SC, Sureshbabu R, Tsai YJ,

Mastrangelo E, Rohayem J, Bolognesi M, Hwu JR. Structural bases of norovirus RNA dependent RNA polymerase inhibition by novel suramin-related compounds. PLoS One. 2014 Mar 12;9(3):e91765. doi: 10.1371/journal.pone.0091765. eCollection 2014. PubMed PMID: 24622391; PubMed Central PMCID: PMC3951423.

12: Mastrangelo E, Mazzitelli S, Fabbri J, Rohayem J, Ruokolainen J, Nykänen A, Milani M, Pezzullo M, Nastruzzi C, Bolognesi M. Delivery of Suramin as an Antiviral Agent through Liposomal Systems. ChemMedChem. 2014 May;9(5):933-9. doi: 10.1002/cmdc.201300563. Epub 2014 Mar 11. PubMed PMID: 24616282.

13: Halabelian L, Ricagno S, Giorgetti S, Santambrogio C, Barbiroli A, Pellegrino S, Achour A, Grandori R, Marchese L, Raimondi S, Mangione PP, Esposito G, Al-Shawi R, Simons JP, Speck I, Stoppini M, Bolognesi M, Bellotti V. Class I major histocompatibility complex, the trojan horse for secretion of amyloidogenic  $\beta$ 2-microglobulin. J Biol Chem. 2014 Feb 7;289(6):3318-27. doi: 10.1074/jbc.M113.524157. Epub 2013 Dec 13. PubMed PMID: 24338476; PubMed Central PMCID: PMC3916536.

14: Tarantino D, Pezzullo M, Mastrangelo E, Croci R, Rohayem J, Robel I, Bolognesi M, Milani M. Naphthalene-sulfonate inhibitors of human norovirus RNA-dependent RNA-polymerase. Antiviral Res. 2014 Feb;102:23-8. doi: 10.1016/j.antiviral.2013.11.016. Epub 2013 Dec 4. PubMed PMID: 24316032.

15: Pesce A, Bolognesi M, Nardini M. Protoglobin: structure and ligand-binding properties. Adv Microb Physiol. 2013;63:79-96. doi: 10.1016/B978-0-12-407693-8.00003-0. Review. PubMed PMID: 24054795.

16: Pesce A, Bolognesi M, Nardini M. The diversity of 2/2 (truncated) globins. Adv Microb Physiol. 2013;63:49-78. doi: 10.1016/B978-0-12-407693-8.00002-9. Review. PubMed PMID: 24054794.

17: Gourlay LJ, Peri C, Ferrer-Navarro M, Conchillo-Solé O, Gori A, Rinchai D, Thomas RJ, Champion OL, Mitchell SL, Kewcharoenwong C, Nithichanon A, Lassaux P, Perletti L, Longhi R, Lertmemongkolchai G, Titball RW, Daura X, Colombo G, Bolognesi M. Exploiting the Burkholderia pseudomallei acute phase antigen BPSL2765 for structure-based epitope discovery/design in structural vaccinology.

Chem Biol. 2013 Sep 19;20(9):1147-56. doi:  
10.1016/j.chembiol.2013.07.010. Epub  
2013 Aug 29. PubMed PMID: 23993463.

18: Pesce A, Tilleman L, Donn  J, Aste E, Ascenzi P, Ciaccio C, Coletta M, Moens L, Viappiani C, Dewilde S, Bolognesi M, Nardini M. Structure and haem-distal site plasticity in Methanosarcina acetivorans protoglobin. PLoS One. 2013 Jun 12;8(6):e66144. doi: 10.1371/journal.pone.0066144. Print 2013. PubMed PMID: 23776624; PubMed Central PMCID: PMC3680402.

19: Colanzi A, Grimaldi G, Catara G, Valente C, Cericola C, Liberali P, Ronci M, Lalioti VS, Bruno A, Beccari AR, Urbani A, De Flora A, Nardini M, Bolognesi M, Luini A, Corda D. Molecular mechanism and functional role of brefeldin A-mediated ADP-ribosylation of CtBP1/BARS. Proc Natl Acad Sci U S A. 2013 Jun 11;110(24):9794-9. doi: 10.1073/pnas.1222413110. Epub 2013 May 28. PubMed PMID: 23716697; PubMed Central PMCID: PMC3683763.

20: Besio R, Gioia R, Cossu F, Monzani E, Nicolis S, Cucca L, Profumo A, Casella L, Tenni R, Bolognesi M, Rossi A, Forlino A. Kinetic and structural evidences on human prolidase pathological mutants suggest strategies for enzyme functional rescue. PLoS One. 2013;8(3):e58792. doi: 10.1371/journal.pone.0058792. Epub 2013 Mar 13. PubMed PMID: 23516557; PubMed Central PMCID: PMC3596340.

21: Ciaccio C, Pesce A, Tundo GR, Tilleman L, Bertolacci L, Dewilde S, Moens L, Ascenzi P, Bolognesi M, Nardini M, Coletta M. Functional and structural roles of the N-terminal extension in Methanosarcina acetivorans protoglobin. Biochim Biophys Acta. 2013 Sep;1834(9):1813-23. doi: 10.1016/j.bbapap.2013.02.026. Epub 2013 Feb 26. PubMed PMID: 23485914.

22: Ascenzi P, Marino M, Polticelli F, Coletta M, Gioia M, Marini S, Pesce A, Nardini M, Bolognesi M, Reeder BJ, Wilson MT. Non-covalent and covalent modifications modulate the reactivity of monomeric mammalian globins. Biochim Biophys Acta. 2013 Sep;1834(9):1750-6. doi: 10.1016/j.bbapap.2013.02.012. Epub 2013 Feb 14. PubMed PMID: 23416443.

- 23: Nardini M, Gnesutta N, Donati G, Gatta R, Forni C, Fossati A, Vonrhein C, Moras D, Romier C, Bolognesi M, Mantovani R. Sequence-specific transcription factor NF-Y displays histone-like DNA binding and H2B-like ubiquitination. *Cell*. 2013 Jan 17;152(1-2):132-43. doi: 10.1016/j.cell.2012.11.047. PubMed PMID: 23332751.
- 24: Bucci A, Baruscotti M, Nardini M, Barbuti A, Micheloni S, Bolognesi M, DiFrancesco D. Identification of the molecular site of ivabradine binding to HCN4 channels. *PLoS One*. 2013;8(1):e53132. doi: 10.1371/journal.pone.0053132. Epub 2013 Jan 4. PubMed PMID: 23308150; PubMed Central PMCID: PMC3537762.
- 25: Gabba M, Abbruzzetti S, Spyarakis F, Forti F, Bruno S, Mozzarelli A, Luque FJ, Viappiani C, Cozzini P, Nardini M, Germani F, Bolognesi M, Moens L, Dewilde S. CO rebinding kinetics and molecular dynamics simulations highlight dynamic regulation of internal cavities in human cytoglobin. *PLoS One*. 2013;8(1):e49770. doi: 10.1371/journal.pone.0049770. Epub 2013 Jan 4. PubMed PMID: 23308092; PubMed Central PMCID: PMC3537629.
- 26: Villa R, Martorana AM, Okuda S, Gourlay LJ, Nardini M, Sperandeo P, Dehò G, Bolognesi M, Kahne D, Polissi A. The Escherichia coli Lpt transenvelope protein complex for lipopolysaccharide export is assembled via conserved structurally homologous domains. *J Bacteriol*. 2013 Mar;195(5):1100-8. doi: 10.1128/JB.02057-12. Epub 2013 Jan 4. PubMed PMID: 23292770; PubMed Central PMCID: PMC3571315.
- 27: Ascenzi P, Pesce A, Nardini M, Bolognesi M, Ciaccio C, Coletta M, Dewilde S. Reductive nitrosylation of Methanosarcina acetivorans protoglobin: a comparative study. *Biochem Biophys Res Commun*. 2013 Jan 25;430(4):1301-5. doi: 10.1016/j.bbrc.2012.11.122. Epub 2012 Dec 19. PubMed PMID: 23261459.
- 28: Cossu F, Milani M, Vachette P, Malvezzi F, Grassi S, Lecis D, Delia D, Drago C, Seneci P, Bolognesi M, Mastrangelo E. Structural insight into apoptosis proteins recognition by a potent divalent smac-mimetic. *PLoS One*. 2012;7(11):e49527. doi: 10.1371/journal.pone.0049527. Epub 2012 Nov 15. PubMed

PMID: 23166698; PubMed Central PMCID: PMC3499469.

29: Lassaux P, Peri C, Ferrer-Navarro M, Gourlay LJ, Gori A, Conchillo-Solé O, Rinchai D, Lertmemongkolchai G, Longhi R, Daura X, Colombo G, Bolognesi M. A structure-based strategy for epitope discovery in *Burkholderia pseudomallei* OppA antigen. *Structure*. 2013 Jan 8;21(1):167-75. doi: 10.1016/j.str.2012.10.005. Epub 2012 Nov 15. PubMed PMID: 23159127.

30: Lecis D, Mastrangelo E, Belvisi L, Bolognesi M, Civera M, Cossu F, De Cesare M, Delia D, Drago C, Manenti G, Manzoni L, Milani M, Moroni E, Perego P, Potenza D, Rizzo V, Scavullo C, Scolastico C, Servida F, Vasile F, Seneci P. Dimeric Smac mimetics/IAP inhibitors as in vivo-active pro-apoptotic agents. Part II: Structural and biological characterization. *Bioorg Med Chem*. 2012 Nov 15;20(22):6709-23. doi: 10.1016/j.bmc.2012.09.041. Epub 2012 Sep 24. PubMed PMID: 23062821.

31: Narula N, Favalli V, Tarantino P, Grasso M, Pilotto A, Bellazzi R, Serio A, Gambarin FI, Charron P, Meder B, Pinto Y, Elliott PM, Mogensen J, Bolognesi M, Bollati M, Arbustini E. Quantitative expression of the mutated lamin A/C gene in patients with cardiomyopathy. *J Am Coll Cardiol*. 2012 Nov 6;60(19):1916-20. doi: 10.1016/j.jacc.2012.05.059. Epub 2012 Oct 10. PubMed PMID: 23062543.

32: Germani F, Pesce A, Venturini A, Moens L, Bolognesi M, Dewilde S, Nardini M. High Resolution Crystal Structures of the *Cerebratulus lacteus* Mini-Hb in the Unligated and Carbomonoxy States. *Int J Mol Sci*. 2012;13(7):8025-37. doi: 10.3390/ijms13078025. Epub 2012 Jun 28. PubMed PMID: 22942687; PubMed Central PMCID: PMC3430218.

33: Salter MD, Blouin GC, Soman J, Singleton EW, Dewilde S, Moens L, Pesce A, Nardini M, Bolognesi M, Olson JS. Determination of ligand pathways in globins: apolar tunnels versus polar gates. *J Biol Chem*. 2012 Sep 28;287(40):33163-78. Epub 2012 Aug 1. PubMed PMID: 22859299; PubMed Central PMCID: PMC3460423.

34: Valleix S, Gillmore JD, Bridoux F, Mangione PP, Dogan A, Nedelec B, Boimard

M, Touchard G, Goujon JM, Lacombe C, Lozeron P, Adams D, Lacroix C, Maisonobe T, Planté-Bordeneuve V, Vrana JA, Theis JD, Giorgetti S, Porcari R, Ricagno S, Bolognesi M, Stoppini M, Delpech M, Pepys MB, Hawkins PN, Bellotti V. Hereditary systemic amyloidosis due to Asp76Asn variant  $\beta$ 2-microglobulin. *N Engl J Med*. 2012 Jun 14;366(24):2276-83. doi: 10.1056/NEJMoal201356. PubMed PMID: 22693999.

35: Mastrangelo E, Pezzullo M, De Burghgraeve T, Kaptein S, Pastorino B, Dallmeier K, de Lamballerie X, Neyts J, Hanson AM, Frick DN, Bolognesi M, Milani M. Ivermectin is a potent inhibitor of flavivirus replication specifically targeting NS3 helicase activity: new prospects for an old drug. *J Antimicrob Chemother*. 2012 Aug;67(8):1884-94. doi: 10.1093/jac/dks147. Epub 2012 Apr 25. PubMed PMID: 22535622; PubMed Central PMCID: PMC3888155.

36: Ami D, Ricagno S, Bolognesi M, Bellotti V, Doglia SM, Natalello A. Structure, stability, and aggregation of  $\beta$ -2 microglobulin mutants: insights from a Fourier transform infrared study in solution and in the crystalline state. *Biophys J*. 2012 Apr 4;102(7):1676-84. doi: 10.1016/j.bpj.2012.02.045. Epub 2012 Apr 3. PubMed PMID: 22500768; PubMed Central PMCID: PMC3318121.

37: Abbruzzetti S, Tilleman L, Bruno S, Viappiani C, Desmet F, Van Doorslaer S, Coletta M, Ciaccio C, Ascenzi P, Nardini M, Bolognesi M, Moens L, Dewilde S. Ligation tunes protein reactivity in an ancient haemoglobin: kinetic evidence for an allosteric mechanism in *Methanosarcina acetivorans* protoglobin. *PLoS One*. 2012;7(3):e33614. doi: 10.1371/journal.pone.0033614. Epub 2012 Mar 27. PubMed PMID: 22479420; PubMed Central PMCID: PMC3313925.

38: Mastrangelo E, Pezzullo M, Tarantino D, Petazzi R, Germani F, Kramer D, Robel I, Rohayem J, Bolognesi M, Milani M. Structure-based inhibition of Norovirus RNA-dependent RNA polymerases. *J Mol Biol*. 2012 Jun 8;419(3-4):198-210. doi: 10.1016/j.jmb.2012.03.008. Epub 2012 Mar 21. PubMed PMID: 22446684.

39: Noto R, Santangelo MG, Ricagno S, Mangione MR, Levantino M, Pezzullo M,

Martorana V, Cupane A, Bolognesi M, Manno M. The tempered polymerization of human neuroserpin. PLoS One. 2012;7(3):e32444. doi: 10.1371/journal.pone.0032444. Epub 2012 Mar 6. PubMed PMID: 22412873; PubMed Central PMCID: PMC3295756.

40: Colombo M, de Rosa M, Bellotti V, Ricagno S, Bolognesi M. A recurrent D-strand association interface is observed in  $\beta$ -2 microglobulin oligomers. FEBS J. 2012 Mar;279(6):1131-43. doi: 10.1111/j.1742-4658.2012.08510.x. Epub 2012 Feb 23. PubMed PMID: 22289140.

41: Bollati M, Barbiroli A, Favalli V, Arbustini E, Charron P, Bolognesi M. Structures of the lamin A/C R335W and E347K mutants: implications for dilated cardiomyopathies. Biochem Biophys Res Commun. 2012 Feb 10;418(2):217-21. doi: 10.1016/j.bbrc.2011.12.136. Epub 2012 Jan 10. PubMed PMID: 22266370.

42: Mastrangelo E, Bolognesi M, Milani M. Flaviviral helicase: insights into the mechanism of action of a motor protein. Biochem Biophys Res Commun. 2012 Jan 6;417(1):84-7. doi: 10.1016/j.bbrc.2011.11.060. Epub 2011 Nov 19. PubMed PMID: 22138238.

43: Santangelo MG, Noto R, Levantino M, Cupane A, Ricagno S, Pezzullo M, Bolognesi M, Mangione MR, Martorana V, Manno M. On the molecular structure of human neuroserpin polymers. Proteins. 2012 Jan;80(1):8-13. doi: 10.1002/prot.23197. Epub 2011 Nov 9. PubMed PMID: 22072549.

44: Lolicato M, Nardini M, Gazzarrini S, Möller S, Bertinetti D, Herberg FW, Bolognesi M, Martin H, Fasolini M, Bertrand JA, Arrigoni C, Thiel G, Moroni A. Tetramerization dynamics of C-terminal domain underlies isoform-specific cAMP gating in hyperpolarization-activated cyclic nucleotide-gated channels. J Biol Chem. 2011 Dec 30;286(52):44811-20. doi: 10.1074/jbc.M111.297606. Epub 2011 Oct 17. PubMed PMID: 22006928; PubMed Central PMCID: PMC3247997.

45: Forti F, Boechi L, Bikiel D, Martí MA, Nardini M, Bolognesi M, Viappiani C, Estrin D, Luque FJ. Ligand migration in Methanosarcina acetivorans protoglobin: effects of ligand binding and dimeric assembly. J Phys Chem B. 2011 Nov 24;115(46):13771-80. doi: 10.1021/jp208562b. Epub 2011 Oct 31. PubMed PMID:



21985496.

46: Santambrogio C, Ricagno S, Sobott F, Colombo M, Bolognesi M, Grandori R.

Characterization of  $\beta$ 2-microglobulin conformational intermediates associated to different fibrillation conditions. *J Mass Spectrom.* 2011 Aug;46(8):734-41. doi: 10.1002/jms.1946. PubMed PMID: 21766392.

47: Milani M, Ciriello F, Baroni S, Pandini V, Canevari G, Bolognesi M, Aliverti

A. FAD-binding site and NADP reactivity in human renalase: a new enzyme involved in blood pressure regulation. *J Mol Biol.* 2011 Aug 12;411(2):463-73. doi: 10.1016/j.jmb.2011.06.010. Epub 2011 Jun 14. PubMed PMID: 21699903.

48: Raimondi S, Barbarini N, Mangione P, Esposito G, Ricagno S, Bolognesi M,

Zorzoli I, Marchese L, Soria C, Bellazzi R, Monti M, Stoppini M, Stefanelli M, Magni P, Bellotti V. The two tryptophans of  $\beta$ 2-microglobulin have distinct roles in function and folding and might represent two independent responses to evolutionary pressure. *BMC Evol Biol.* 2011 Jun 10;11:159. doi: 10.1186/1471-2148-11-159. PubMed PMID: 21663612; PubMed Central PMCID: PMC3124429.

49: Pesce A, Tilleman L, Dewilde S, Ascenzi P, Coletta M, Ciaccio C, Bruno S,

Moens L, Bolognesi M, Nardini M. Structural heterogeneity and ligand gating in ferric Methanosarcina acetivorans protoglobin mutants. *IUBMB Life.* 2011 May;63(5):287-94. doi: 10.1002/iub.484. Review. PubMed PMID: 21618401.

50: Nuccitelli A, Cozzi R, Gourlay LJ, Donnarumma D, Necchi F, Norais N, Telford

JL, Rappuoli R, Bolognesi M, Maione D, Grandi G, Rinaudo CD. Structure-based approach to rationally design a chimeric protein for an effective vaccine against Group B Streptococcus infections. *Proc Natl Acad Sci U S A.* 2011 Jun 21;108(25):10278-83. doi: 10.1073/pnas.1106590108. Epub 2011 May 18. PubMed PMID: 21593422; PubMed Central PMCID: PMC3121859.

51: Azinas S, Colombo M, Barbiroli A, Santambrogio C, Giorgetti S, Raimondi S,

Bonomi F, Grandori R, Bellotti V, Ricagno S, Bolognesi M. D-strand perturbation and amyloid propensity in beta-2 microglobulin. *FEBS J.* 2011 Jul;278(13):2349-58. doi: 10.1111/j.1742-4658.2011.08157.x. Epub 2011 May 31. PubMed PMID: 21569201.

52: Colombo M, Ricagno S, Barbiroli A, Santambrogio C, Giorgetti S, Raimondi S, Bonomi F, Grandori R, Bellotti V, Bolognesi M. The effects of an ideal beta-turn on beta-2 microglobulin fold stability. *J Biochem.* 2011 Jul;150(1):39-47. doi: 10.1093/jb/mvr034. Epub 2011 Mar 11. PubMed PMID: 21398368.

53: Pesce A, Nardini M, Dewilde S, Capece L, Martí MA, Congia S, Salter MD, Blouin GC, Estrin DA, Ascenzi P, Moens L, Bolognesi M, Olson JS. Ligand migration in the apolar tunnel of *Cerebratulus lacteus* mini-hemoglobin. *J Biol Chem.* 2011 Feb 18;286(7):5347-58. doi: 10.1074/jbc.M110.169045. Epub 2010 Dec 7. PubMed PMID: 21147768; PubMed Central PMCID: PMC3037647.

54: Ricagno S, Pezzullo M, Barbiroli A, Manno M, Levantino M, Santangelo MG, Bonomi F, Bolognesi M. Two latent and two hyperstable polymeric forms of human neuroserpin. *Biophys J.* 2010 Nov 17;99(10):3402-11. doi: 10.1016/j.bpj.2010.09.021. PubMed PMID: 21081089; PubMed Central PMCID: PMC2980742.

55: Pesce A, Nardini M, Labarre M, Richard C, Wittenberg JB, Wittenberg BA, Guertin M, Bolognesi M. Structural characterization of a group II 2/2 hemoglobin from the plant pathogen *Agrobacterium tumefaciens*. *Biochim Biophys Acta.* 2011 Jun;1814(6):810-6. doi: 10.1016/j.bbapap.2010.11.001. Epub 2010 Nov 9. PubMed PMID: 21070893.

56: Gourlay LJ, Sommaruga S, Nardini M, Sperandeo P, Dehò G, Polissi A, Bolognesi M. Probing the active site of the sugar isomerase domain from *E. coli* arabinose-5-phosphate isomerase via X-ray crystallography. *Protein Sci.* 2010 Dec;19(12):2430-9. doi: 10.1002/pro.525. PubMed PMID: 20954237; PubMed Central PMCID: PMC3009410.

57: Cossu F, Malvezzi F, Canevari G, Mastrangelo E, Lecis D, Delia D, Seneci P, Scolastico C, Bolognesi M, Milani M. Recognition of Smac-mimetic compounds by the BIR domain of cIAP1. *Protein Sci.* 2010 Dec;19(12):2418-29. doi: 10.1002/pro.523. PubMed PMID: 20954235; PubMed Central PMCID: PMC3009409.

58: Santambrogio C, Ricagno S, Colombo M, Barbiroli A, Bonomi F, Bellotti V, Bolognesi M, Grandori R. DE-loop mutations affect beta2 microglobulin stability, oligomerization, and the low-pH unfolded form. *Protein Sci.* 2010 Jul;19(7):1386-94. doi: 10.1002/pro.419. PubMed PMID: 20506535; PubMed Central PMCID: PMC2974830.

59: Geuens E, Hoogewijs D, Nardini M, Vinck E, Pesce A, Kiger L, Fago A, Tilleman L, De Henau S, Marden MC, Weber RE, Van Doorslaer S, Vanfleteren J, Moens L, Bolognesi M, Dewilde S. Globin-like proteins in *Caenorhabditis elegans*: in vivo localization, ligand binding and structural properties. *BMC Biochem.* 2010 Apr 2;11:17. doi: 10.1186/1471-2091-11-17. PubMed PMID: 20361867; PubMed Central PMCID: PMC2867796.

60: Barbet-Massin E, Ricagno S, Lewandowski JR, Giorgetti S, Bellotti V, Bolognesi M, Emsley L, Pintacuda G. Fibrillar vs crystalline full-length beta-2-microglobulin studied by high-resolution solid-state NMR spectroscopy. *J Am Chem Soc.* 2010 Apr 28;132(16):5556-7. doi: 10.1021/ja1002839. PubMed PMID: 20356307.

61: Bollati M, Alvarez K, Assenberg R, Baronti C, Canard B, Cook S, Coutard B, Decroly E, de Lamballerie X, Gould EA, Grard G, Grimes JM, Hilgenfeld R, Jansson AM, Malet H, Mancini EJ, Mastrangelo E, Mattevi A, Milani M, Moureau G, Neyts J, Owens RJ, Ren J, Selisko B, Speroni S, Steuber H, Stuart DI, Unge T, Bolognesi M. Structure and functionality in flavivirus NS-proteins: perspectives for drug design. *Antiviral Res.* 2010 Aug;87(2):125-48. doi: 10.1016/j.antiviral.2009.11.009. Epub 2009 Nov 27. Review. PubMed PMID: 19945487; PubMed Central PMCID: PMC3918146.

62: Gourlay LJ, Colombo G, Soriani M, Grandi G, Daura X, Bolognesi M. Why is a protective antigen protective? *Hum Vaccin.* 2009 Dec;5(12):872-5. Epub 2009 Dec 1. Review. PubMed PMID: 19786841.

63: Crobu D, Canevari G, Milani M, Pandini V, Vanoni MA, Bolognesi M, Zanetti G, Aliverti A. *Plasmodium falciparum* ferredoxin-NADP+ reductase His286 plays a dual

role in NADP(H) binding and catalysis. *Biochemistry*. 2009 Oct 13;48(40):9525-33.  
doi: 10.1021/bi9013209. PubMed PMID: 19736991.

64: Seneci P, Bianchi A, Battaglia C, Belvisi L, Bolognesi M, Caprini A, Cossu F, Franco Ed, Matteo Md, Delia D, Drago C, Khaled A, Lecis D, Manzoni L, Marizzoni M, Mastrangelo E, Milani M, Motto I, Moroni E, Potenza D, Rizzo V, Servida F, Turlizzi E, Varrone M, Vasile F, Scolastico C. Rational design, synthesis and characterization of potent, non-peptidic Smac mimics/XIAP inhibitors as proapoptotic agents for cancer therapy. *Bioorg Med Chem*. 2009 Aug 15;17(16):5834-56. doi: 10.1016/j.bmc.2009.07.009. Epub 2009 Jul 10. PubMed PMID: 19620011.

65: Milani M, Mastrangelo E, Bollati M, Selisko B, Decroly E, Bouvet M, Canard B, Bolognesi M. Flaviviral methyltransferase/RNA interaction: structural basis for enzyme inhibition. *Antiviral Res*. 2009 Jul;83(1):28-34. doi: 10.1016/j.antiviral.2009.03.001. Epub 2009 Mar 14. PubMed PMID: 19501254.

66: Cossu F, Milani M, Mastrangelo E, Vachette P, Servida F, Lecis D, Canevari G, Delia D, Drago C, Rizzo V, Manzoni L, Seneci P, Scolastico C, Bolognesi M. Structural basis for bivalent Smac-mimetics recognition in the IAP protein family. *J Mol Biol*. 2009 Sep 25;392(3):630-44. doi: 10.1016/j.jmb.2009.04.033. Epub 2009 Apr 22. PubMed PMID: 19393243.

67: Nardini M, Valente C, Ricagno S, Luini A, Corda D, Bolognesi M. CtBP1/BARS Gly172-->Glu mutant structure: impairing NAD(H)-binding and dimerization. *Biochem Biophys Res Commun*. 2009 Mar 27;381(1):70-4. doi: 10.1016/j.bbrc.2009.02.010. Epub 2009 Feb 10. PubMed PMID: 19351597.

68: Gourlay LJ, Santi I, Pezzicoli A, Grandi G, Soriani M, Bolognesi M. Group B streptococcus pullulanase crystal structures in the context of a novel strategy for vaccine development. *J Bacteriol*. 2009 Jun;191(11):3544-52. doi: 10.1128/JB.01755-08. Epub 2009 Mar 27. PubMed PMID: 19329633; PubMed Central PMCID: PMC2681907.

69: Ricagno S, Raimondi S, Giorgetti S, Bellotti V, Bolognesi M. Human beta-2

microglobulin W60V mutant structure: Implications for stability and amyloid aggregation. *Biochem Biophys Res Commun.* 2009 Mar 13;380(3):543-7. doi: 10.1016/j.bbrc.2009.01.116. Epub 2009 Jan 25. PubMed PMID: 19284997.

70: Bollati M, Milani M, Mastrangelo E, de Lamballerie X, Canard B, Bolognesi M.  
Crystal structure of a methyltransferase from a no-known-vector Flavivirus.  
*Biochem Biophys Res Commun.* 2009 Apr 24;382(1):200-4. doi: 10.1016/j.bbrc.2009.03.008. Epub 2009 Mar 9. PubMed PMID: 19275894.

71: Ricagno S, Caccia S, Sorrentino G, Antonini G, Bolognesi M. Human neuroserpin: structure and time-dependent inhibition. *J Mol Biol.* 2009 Apr 24;388(1):109-21. doi: 10.1016/j.jmb.2009.02.056. Epub 2009 Mar 2. PubMed PMID: 19265707.

72: Pesce A, Thijs L, Nardini M, Desmet F, Sisinni L, Gourlay L, Bolli A, Coletta M, Van Doorslaer S, Wan X, Alam M, Ascenzi P, Moens L, Bolognesi M, Dewilde S.  
HisE11 and HisF8 provide bis-histidyl heme hexa-coordination in the globin domain of *Geobacter sulfurreducens* globin-coupled sensor. *J Mol Biol.* 2009 Feb 13;386(1):246-60. doi: 10.1016/j.jmb.2008.12.023. Epub 2008 Dec 16. PubMed PMID: 19109973.

73: Bolognesi M, Smith JL. Proteins: ever larger, stranger and more dynamic. *Curr Opin Struct Biol.* 2008 Dec;18(6):690-2. doi: 10.1016/j.sbi.2008.11.003. Epub 2008 Nov 27. PubMed PMID: 19041238.

74: Cossu F, Mastrangelo E, Milani M, Sorrentino G, Lecis D, Delia D, Manzoni L, Seneci P, Scolastico C, Bolognesi M. Designing Smac-mimetics as antagonists of XIAP, cIAP1, and cIAP2. *Biochem Biophys Res Commun.* 2009 Jan 9;378(2):162-7. doi: 10.1016/j.bbrc.2008.10.139. Epub 2008 Nov 4. PubMed PMID: 18992220.

75: Bollati M, Milani M, Mastrangelo E, Ricagno S, Tedeschi G, Nonnis S, Decroly E, Selisko B, de Lamballerie X, Coutard B, Canard B, Bolognesi M.  
Recognition of RNA cap in the Wesselsbron virus NS5 methyltransferase domain: implications for RNA-capping mechanisms in Flavivirus. *J Mol Biol.* 2009 Jan 9;385(1):140-52. doi: 10.1016/j.jmb.2008.10.028. Epub 2008 Oct 19. PubMed PMID: 18976670.

76: Mastrangelo E, Cossu F, Milani M, Sorrentino G, Lecis D, Delia D, Manzoni L, Drago C, Seneci P, Scolastico C, Rizzo V, Bolognesi M. Targeting the X-linked inhibitor of apoptosis protein through 4-substituted azabicyclo[5.3.0]alkane smac mimetics. Structure, activity, and recognition principles. *J Mol Biol.* 2008 Dec 19;384(3):673-89. doi: 10.1016/j.jmb.2008.09.064. Epub 2008 Oct 7. PubMed PMID: 18851976.

77: Salter MD, Nienhaus K, Nienhaus GU, Dewilde S, Moens L, Pesce A, Nardini M, Bolognesi M, Olson JS. The apolar channel in *Cerebratulus lacteus* hemoglobin is the route for O<sub>2</sub> entry and exit. *J Biol Chem.* 2008 Dec 19;283(51):35689-702. doi: 10.1074/jbc.M805727200. Epub 2008 Oct 7. PubMed PMID: 18840607; PubMed Central PMCID: PMC2602902.

78: Ricagno S, Colombo M, de Rosa M, Sangiovanni E, Giorgetti S, Raimondi S, Bellotti V, Bolognesi M. DE loop mutations affect beta2-microglobulin stability and amyloid aggregation. *Biochem Biophys Res Commun.* 2008 Dec 5;377(1):146-50. doi: 10.1016/j.bbrc.2008.09.108. Epub 2008 Oct 1. PubMed PMID: 18835253.

79: Ouellet YH, Daigle R, Lagüe P, Dantsker D, Milani M, Bolognesi M, Friedman JM, Guertin M. Ligand binding to truncated hemoglobin N from *Mycobacterium tuberculosis* is strongly modulated by the interplay between the distal heme pocket residues and internal water. *J Biol Chem.* 2008 Oct 3;283(40):27270-8. doi: 10.1074/jbc.M804215200. Epub 2008 Aug 2. PubMed PMID: 18676995; PubMed Central PMCID: PMC2556007.

80: Dewilde S, Ioaniteanu AI, Kiger L, Gilany K, Marden MC, Van Doorslaer S, Vercruysse J, Pesce A, Nardini M, Bolognesi M, Moens L. The hemoglobins of the trematodes *Fasciola hepatica* and *Paramphistomum epiclitum*: a molecular biological, physico-chemical, kinetic, and vaccination study. *Protein Sci.* 2008 Oct;17(10):1653-62. doi: 10.1110/ps.036558.108. Epub 2008 Jul 11. PubMed PMID: 18621914; PubMed Central PMCID: PMC2548365.

- 81: Boechi L, Martí MA, Milani M, Bolognesi M, Luque FJ, Estrin DA. Structural determinants of ligand migration in Mycobacterium tuberculosis truncated hemoglobin O. *Proteins*. 2008 Nov 1;73(2):372-9. doi: 10.1002/prot.22072. PubMed PMID: 18433052.
- 82: Esposito G, Ricagno S, Corazza A, Rennella E, Gümral D, Mimmi MC, Betto E, Pucillo CE, Fogolari F, Viglino P, Raimondi S, Giorgetti S, Bolognesi B, Merlini G, Stoppini M, Bolognesi M, Bellotti V. The controlling roles of Trp60 and Trp95 in beta2-microglobulin function, folding and amyloid aggregation properties. *J Mol Biol*. 2008 May 9;378(4):887-97. doi: 10.1016/j.jmb.2008.03.002. Epub 2008 Mar 8. PubMed PMID: 18395224.
- 83: Milani M, Nardini M, Pesce A, Mastrangelo E, Bolognesi M. Hemoprotein time-resolved X-ray crystallography. *IUBMB Life*. 2008 Mar;60(3):154-8. doi: 10.1002/iub.23. Review. PubMed PMID: 18380006.
- 84: Dewilde S, Mees K, Kiger L, Lechauve C, Marden MC, Pesce A, Bolognesi M, Moens L. Expression, purification, and crystallization of neuro- and cytoglobin. *Methods Enzymol*. 2008;436:341-57. doi: 10.1016/S0076-6879(08)36019-4. PubMed PMID: 18237642.
- 85: Pesce A, Milani M, Nardini M, Bolognesi M. Mapping heme-ligand tunnels in group I truncated(2/2) hemoglobins. *Methods Enzymol*. 2008;436:303-15. doi: 10.1016/S0076-6879(08)36017-0. PubMed PMID: 18237640.
- 86: Bolli A, Ciaccio C, Coletta M, Nardini M, Bolognesi M, Pesce A, Guertin M, Visca P, Ascenzi P. Ferrous Campylobacter jejuni truncated hemoglobin P displays an extremely high reactivity for cyanide - a comparative study. *FEBS J*. 2008 Feb;275(4):633-45. doi: 10.1111/j.1742-4658.2007.06223.x. Epub 2008 Jan 10. PubMed PMID: 18190529.
- 87: Nardini M, Pesce A, Thijs L, Saito JA, Dewilde S, Alam M, Ascenzi P, Coletta M, Ciaccio C, Moens L, Bolognesi M. Archaeal protoglobin structure indicates new ligand diffusion paths and modulation of haem-reactivity. *EMBO Rep*. 2008

Feb;9(2):157-63. doi: 10.1038/sj.embor.7401153. Epub 2008 Jan 11. PubMed  
PMID:  
18188182; PubMed Central PMCID: PMC2246406.

88: Ascenzi P, Bocedi A, Heptonstall J, Capobianchi MR, Di Caro A, Mastrangelo E, Bolognesi M, Ippolito G. Ebolavirus and Marburgvirus: insight the Filoviridae family. Mol Aspects Med. 2008 Jun;29(3):151-85. Epub 2007 Oct 22. Review. PubMed  
PMID: 18063023.

89: Spallarossa A, Cesarini S, Ranise A, Ponassi M, Unge T, Bolognesi M. Crystal structures of HIV-1 reverse transcriptase complexes with thiocarbamate non-nucleoside inhibitors. Biochem Biophys Res Commun. 2008 Jan 25;365(4):764-70. Epub 2007 Nov 21. PubMed PMID: 18035053.

90: Nadra AD, Martí MA, Pesce A, Bolognesi M, Estrin DA. Exploring the molecular basis of heme coordination in human neuroglobin. Proteins. 2008 May 1;71(2):695-705. PubMed PMID: 17975837.

91: Ouellet H, Milani M, LaBarre M, Bolognesi M, Couture M, Guertin M. The roles of Tyr(CD1) and Trp(G8) in Mycobacterium tuberculosis truncated hemoglobin O in ligand binding and on the heme distal site architecture. Biochemistry. 2007 Oct 16;46(41):11440-50. Epub 2007 Sep 22. PubMed PMID: 17887774.

92: Pesce A, Nardini M, Milani M, Bolognesi M. Protein structure in the truncated (2/2) hemoglobin family. IUBMB Life. 2007 Aug-Sep;59(8-9):535-41. PubMed PMID: 17701548.

93: Mastrangelo E, Milani M, Bollati M, Selisko B, Peyrane F, Pandini V, Sorrentino G, Canard B, Konarev PV, Svergun DI, de Lamballerie X, Coutard B, Khromykh AA, Bolognesi M. Crystal structure and activity of Kunjin virus NS3 helicase; protease and helicase domain assembly in the full length NS3 protein. J Mol Biol. 2007 Sep 14;372(2):444-55. Epub 2007 Jun 27. PubMed PMID: 17658551.

94: Ricagno S, de Rosa M, Aliverti A, Zanetti G, Bolognesi M. The crystal structure of FdxA, a 7Fe ferredoxin from Mycobacterium smegmatis. Biochem Biophys Res Commun. 2007 Aug 17;360(1):97-102. Epub 2007 Jun 12. Erratum in: Biochem



Biophys Res Commun. 2008 Jan 25;365(4):890. PubMed PMID: 17577575.

95: Nardini M, Pesce A, Milani M, Bolognesi M. Protein fold and structure in the truncated (2/2) globin family. Gene. 2007 Aug 15;398(1-2):2-11. Epub 2007 Apr 29. Review. PubMed PMID: 17532150.

96: Ascenzi P, Bolognesi M, Milani M, Guertin M, Visca P. Mycobacterial truncated hemoglobins: from genes to functions. Gene. 2007 Aug 15;398(1-2):42-51. Epub 2007 Apr 29. Review. PubMed PMID: 17532149.

97: Mastrangelo E, Bollati M, Milani M, Selisko B, Peyrane F, Canard B, Grard G, de Lamballerie X, Bolognesi M. Structural bases for substrate recognition and activity in Meaban virus nucleoside-2'-O-methyltransferase. Protein Sci. 2007 Jun;16(6):1133-45. Epub 2007 May 1. PubMed PMID: 17473012; PubMed Central PMCID: PMC2206675.

98: Ascenzi P, Bolognesi M, Visca P. \*NO dissociation represents the rate limiting step for O<sub>2</sub>-mediated oxidation of ferrous nitrosylated Mycobacterium leprae truncated hemoglobin O. Biochem Biophys Res Commun. 2007 Jun 8;357(3):809-14. Epub 2007 Apr 13. PubMed PMID: 17451651.

99: Milani M, Balconi E, Aliverti A, Mastrangelo E, Seeber F, Bolognesi M, Zanetti G. Ferredoxin-NADP<sup>+</sup> reductase from Plasmodium falciparum undergoes NADP<sup>+</sup>-dependent dimerization and inactivation: functional and crystallographic analysis. J Mol Biol. 2007 Mar 23;367(2):501-13. Epub 2007 Jan 9. PubMed PMID: 17258767.

100: Ascenzi P, Bocedi A, Antonini G, Bolognesi M, Fasano M. Reductive nitrosylation and peroxynitrite-mediated oxidation of heme-hemopexin. FEBS J. 2007 Jan;274(2):551-62. PubMed PMID: 17229156.

101: Nardini M, Pesce A, Labarre M, Richard C, Bolli A, Ascenzi P, Guertin M, Bolognesi M. Structural determinants in the group III truncated hemoglobin from Campylobacter jejuni. J Biol Chem. 2006 Dec 8;281(49):37803-12. Epub 2006 Oct 5. PubMed PMID: 17023416.

102: Mastrangelo E, Bollati M, Milani M, Brisbarre N, de Lamballerie X, Coutard B, Canard B, Khromykh A, Bolognesi M. Preliminary crystallographic characterization of an RNA helicase from Kunjin virus. *Acta Crystallogr Sect F Struct Biol Cryst Commun.* 2006 Sep 1;62(Pt 9):876-9. Epub 2006 Aug 11. PubMed PMID: 16946468; PubMed Central PMCID: PMC2242862.

103: Quinlan KG, Verger A, Kwok A, Lee SH, Perdomo J, Nardini M, Bolognesi M, Crossley M. Role of the C-terminal binding protein PXDLS motif binding cleft in protein interactions and transcriptional repression. *Mol Cell Biol.* 2006 Nov;26(21):8202-13. Epub 2006 Aug 28. PubMed PMID: 16940173; PubMed Central PMCID: PMC1636740.

104: Quinlan KG, Nardini M, Verger A, Francescato P, Yaswen P, Corda D, Bolognesi M, Crossley M. Specific recognition of ZNF217 and other zinc finger proteins at a surface groove of C-terminal binding proteins. *Mol Cell Biol.* 2006 Nov;26(21):8159-72. Epub 2006 Aug 28. PubMed PMID: 16940172; PubMed Central PMCID: PMC1636751.

105: de Sanctis D, Ascenzi P, Bocedi A, Dewilde S, Burmester T, Hankeln T, Moens L, Bolognesi M. Cyanide binding and heme cavity conformational transitions in *Drosophila melanogaster* hexacoordinate hemoglobin. *Biochemistry.* 2006 Aug 22;45(33):10054-61. PubMed PMID: 16906763.

106: Mastrangelo E, Bollati M, Milani M, de Lamballerie X, Brisbarre N, Dalle K, Lantez V, Egloff MP, Coutard B, Canard B, Gould E, Forrester N, Bolognesi M. Preliminary characterization of (nucleoside-2'-O-)-methyltransferase crystals from Meaban and Yokose flaviviruses. *Acta Crystallogr Sect F Struct Biol Cryst Commun.* 2006 Aug 1;62(Pt 8):768-70. Epub 2006 Jul 24. Erratum in: *Acta Crystallogr Sect F Struct Biol Cryst Commun.* 2007 Mar 1;63(Pt 3):252. de Lamballeire, Xavier [corrected de Lamballerie, Xavier]; Brisbare, Nadège [corrected to Brisbarre, Nadège]. PubMed PMID: 16880552; PubMed Central PMCID: PMC2242907.

107: Ouellet Y, Milani M, Couture M, Bolognesi M, Guertin M. Ligand interactions in the distal heme pocket of *Mycobacterium tuberculosis* truncated hemoglobin N:

roles of TyrB10 and GlnE11 residues. *Biochemistry*. 2006 Jul 25;45(29):8770-81. PubMed PMID: 16846220.

108: Bidon-Chanal A, Martí MA, Crespo A, Milani M, Orozco M, Bolognesi M, Luque FJ, Estrin DA. Ligand-induced dynamical regulation of NO conversion in *Mycobacterium tuberculosis* truncated hemoglobin-N. *Proteins*. 2006 Aug 1;64(2):457-64. PubMed PMID: 16688782.

109: Nardini M, Svergun D, Konarev PV, Spanò S, Fasano M, Bracco C, Pesce A, Donadini A, Cericola C, Secundo F, Luini A, Corda D, Bolognesi M. The C-terminal domain of the transcriptional corepressor CtBP is intrinsically unstructured. *Protein Sci*. 2006 May;15(5):1042-50. Epub 2006 Apr 5. PubMed PMID: 16597837; PubMed Central PMCID: PMC2242513.

110: Zuccotti S, Rosano C, Bemporad F, Stefani M, Bolognesi M. Preliminary characterization of two different crystal forms of acylphosphatase from the hyperthermophile archaeon *Sulfolobus solfataricus*. *Acta Crystallogr Sect F Struct Biol Cryst Commun*. 2005 Jan 1;61(Pt 1):144-6. Epub 2004 Dec 24. PubMed PMID: 16508117; PubMed Central PMCID: PMC1952370.

111: Martí MA, Bikiel DE, Crespo A, Nardini M, Bolognesi M, Estrin DA. Two distinct heme distal site states define *Cerebratulus lacteus* mini-hemoglobin oxygen affinity. *Proteins*. 2006 Mar 15;62(3):641-8. PubMed PMID: 16432879.

112: Ascenzi P, Bocedi A, Bolognesi M, Fabozzi G, Milani M, Visca P. Nitric oxide scavenging by *Mycobacterium leprae* GlbO involves the formation of the ferric heme-bound peroxynitrite intermediate. *Biochem Biophys Res Commun*. 2006 Jan 6;339(1):450-6. Epub 2005 Nov 14. PubMed PMID: 16307730.

113: Rosano C, Zuccotti S, Sturla L, Fruscione F, Tonetti M, Bolognesi M. Quaternary assembly and crystal structure of GDP-D-mannose 4,6 dehydratase from *Paramecium bursaria* Chlorella virus. *Biochem Biophys Res Commun*. 2006 Jan 6;339(1):191-5. Epub 2005 Nov 10. PubMed PMID: 16297878.

114: Corazza A, Rosano C, Pagano K, Alverdi V, Esposito G, Capanni C, Bemporad F,

Plakoutsi G, Stefani M, Chiti F, Zuccotti S, Bolognesi M, Viglino P. Structure, conformational stability, and enzymatic properties of acylphosphatase from the hyperthermophile *Sulfolobus solfataricus*. *Proteins*. 2006 Jan 1;62(1):64-79. PubMed PMID: 16287076.

115: Pesce A, Nardini M, Dewilde S, Hoogewijs D, Ascenzi P, Moens L, Bolognesi M. Modulation of oxygen binding to insect hemoglobins: the structure of hemoglobin from the botfly *Gasterophilus intestinalis*. *Protein Sci*. 2005 Dec;14(12):3057-63. Epub 2005 Oct 31. PubMed PMID: 16260762; PubMed Central PMCID: PMC2253232.

116: Milani M, Leoni L, Rampioni G, Zennaro E, Ascenzi P, Bolognesi M. An active-like structure in the unphosphorylated StyR response regulator suggests a phosphorylation-dependent allosteric activation mechanism. *Structure*. 2005 Sep;13(9):1289-97. PubMed PMID: 16154086.

117: Rosano C, Zuccotti S, Bolognesi M. The three-dimensional structure of beta2 microglobulin: results from X-ray crystallography. *Biochim Biophys Acta*. 2005 Nov 10;1753(1):85-91. Epub 2005 Jul 27. Review. PubMed PMID: 16084780.

118: Ascenzi P, Gallina C, Bolognesi M. Thrombin inhibition by the highly selective 'reversible suicide substrate' N-ethoxycarbonyl-D-phenylalanyl-L-prolyl-alpha-azalysine p-nitrophenyl ester. *Protein Pept Lett*. 2005 Jul;12(5):433-8. Review. PubMed PMID: 16029155.

119: de Sanctis D, Dewilde S, Vonnrhein C, Pesce A, Moens L, Ascenzi P, Hankeln T, Burmester T, Ponassi M, Nardini M, Bolognesi M. Bishistidyl heme hexacoordination, a key structural property in *Drosophila melanogaster* hemoglobin. *J Biol Chem*. 2005 Jul 22;280(29):27222-9. Epub 2005 May 24. PubMed PMID: 15917230.

120: de Sanctis D, Pesce A, Nardini M, Bolognesi M, Bocedi A, Ascenzi P. Structure-function relationships in the growing hexa-coordinate hemoglobin sub-family. *IUBMB Life*. 2004 Nov-Dec;56(11-12):643-51. Review. Erratum in: *IUBMB Life*. 2005 Jun;57(6):459-60. PubMed PMID: 15844231.

121: Pesce A, De Sanctis D, Nardini M, Dewilde S, Moens L, Hankeln T, Burmester

T, Ascenzi P, Bolognesi M. Reversible hexa- to penta-coordination of the heme Fe atom modulates ligand binding properties of neuroglobin and cytoglobin. IUBMB Life. 2004 Nov-Dec;56(11-12):657-64. Review. PubMed PMID: 15804829.

122: Hankeln T, Ebner B, Fuchs C, Gerlach F, Haberkamp M, Laufs TL, Roesner A, Schmidt M, Weich B, Wystub S, Saaler-Reinhardt S, Reuss S, Bolognesi M, De Sanctis D, Marden MC, Kiger L, Moens L, Dewilde S, Nevo E, Avivi A, Weber RE, Fago A, Burmester T. Neuroglobin and cytoglobin in search of their role in the vertebrate globin family. J Inorg Biochem. 2005 Jan;99(1):110-9. Review. PubMed PMID: 15598495.

123: Milani M, Pesce A, Nardini M, Ouellet H, Ouellet Y, Dewilde S, Bocedi A, Ascenzi P, Guertin M, Moens L, Friedman JM, Wittenberg JB, Bolognesi M. Structural bases for heme binding and diatomic ligand recognition in truncated hemoglobins. J Inorg Biochem. 2005 Jan;99(1):97-109. Review. PubMed PMID: 15598494.

124: Ascenzi P, Bocedi A, Leoni L, Visca P, Zennaro E, Milani M, Bolognesi M. CO sniffing through heme-based sensor proteins. IUBMB Life. 2004 Jun;56(6):309-15. Review. PubMed PMID: 15370879.

125: Relini A, Rolandi R, Bolognesi M, Aboudan M, Merlini G, Bellotti V, Gliozzi A. Ultrastructural organization of ex vivo amyloid fibrils formed by the apolipoprotein A-I Leu174Ser variant: an atomic force microscopy study. Biochim Biophys Acta. 2004 Sep 6;1690(1):33-41. PubMed PMID: 15337168.

126: Ascenzi P, Bocedi A, de Sanctis D, Pesce A, Bolognesi M, Marden MC, Dewilde S, Moens L, Hankeln T, Burmester T. Neuroglobin and cytoglobin: Two new entries in the hemoglobin superfamily\*. Biochem Mol Biol Educ. 2004 Sep;32(5):305-13. doi: 10.1002/bmb.2004.494032050386. PubMed PMID: 21706744.

127: Dantsker D, Samuni U, Ouellet Y, Wittenberg BA, Wittenberg JB, Milani M, Bolognesi M, Guertin M, Friedman JM. Viscosity-dependent relaxation significantly modulates the kinetics of CO recombination in the truncated hemoglobin TrHbN from

Mycobacterium tuberculosis. J Biol Chem. 2004 Sep 10;279(37):38844-53.  
Epub 2004  
Jul 1. PubMed PMID: 15234986.

128: Rosano C, Zuccotti S, Cobucci-Ponzano B, Mazzone M, Rossi M, Moracci M,  
Petoukhov MV, Svergun DI, Bolognesi M. Structural characterization of the  
nonameric assembly of an Archaeal alpha-L-fucosidase by synchrotron small  
angle  
X-ray scattering. Biochem Biophys Res Commun. 2004 Jul 16;320(1):176-82.  
PubMed  
PMID: 15207718.

129: Pesce A, Nardini M, Ascenzi P, Geuens E, Dewilde S, Moens L,  
Bolognesi M,  
Riggs AF, Hale A, Deng P, Nienhaus GU, Olson JS, Nienhaus K. Thr-E11  
regulates O2  
affinity in Cerebratulus lacteus mini-hemoglobin. J Biol Chem. 2004 Aug  
6;279(32):33662-72. Epub 2004 May 25. Erratum in: J Biol Chem. 2004  
Sep;279(39):41258. PubMed PMID: 15161908.

130: Zuccotti S, Rosano C, Ramazzotti M, Degl'Innocenti D, Stefani M,  
Manao G,  
Bolognesi M. Three-dimensional structural characterization of a novel  
Drosophila  
melanogaster acylphosphatase. Acta Crystallogr D Biol Crystallogr. 2004  
Jun;60(Pt  
6):1177-9. Epub 2004 May 21. PubMed PMID: 15159593.

131: Milani M, Ouellet Y, Ouellet H, Guertin M, Boffi A, Antonini G,  
Bocedi A,  
Mattu M, Bolognesi M, Ascenzi P. Cyanide binding to truncated  
hemoglobins: a  
crystallographic and kinetic study. Biochemistry. 2004 May  
11;43(18):5213-21.  
PubMed PMID: 15122887.

132: Nardini M, Mazzocco M, Massaro A, Maffei M, Vergano A, Donadini A,  
Scartezzini P, Bolognesi M. Crystal structure of the glutaredoxin-like  
protein  
SH3BGRL3 at 1.6 Angstrom resolution. Biochem Biophys Res Commun. 2004 May  
28;318(2):470-6. PubMed PMID: 15120624.

133: Relini A, Torrassa S, Rolandi R, Gliozzi A, Rosano C, Canale C,  
Bolognesi M,  
Plakoutsi G, Bucciantini M, Chiti F, Stefani M. Monitoring the process of  
HypF  
fibrillization and liposome permeabilization by protofibrils. J Mol Biol.  
2004  
May 14;338(5):943-57. PubMed PMID: 15111058.

134: de Sanctis D, Dewilde S, Pesce A, Moens L, Ascenzi P, Hankeln T,  
Burmester

T, Bolognesi M. Crystal structure of cytoglobin: the fourth globin type discovered in man displays heme hexa-coordination. *J Mol Biol.* 2004 Feb 27;336(4):917-27. PubMed PMID: 15095869.

135: de Sanctis D, Dewilde S, Pesce A, Moens L, Ascenzi P, Hankeln T, Burmester T, Bolognesi M. Mapping protein matrix cavities in human cytoglobin through Xe atom binding. *Biochem Biophys Res Commun.* 2004 Apr 16;316(4):1217-21. PubMed PMID: 15044115.

136: Pesce A, Dewilde S, Nardini M, Moens L, Ascenzi P, Hankeln T, Burmester T, Bolognesi M. The human brain hexacoordinated neuroglobin three-dimensional structure. *Micron.* 2004;35(1-2):63-5. PubMed PMID: 15036293.

137: Hamdane D, Kiger L, Dewilde S, Green BN, Pesce A, Uzan J, Burmester T, Hankeln T, Bolognesi M, Moens L, Marden MC. Coupling of the heme and an internal disulfide bond in human neuroglobin. *Micron.* 2004;35(1-2):59-62. PubMed PMID: 15036292.

138: Milani M, Pesce A, Ouellet Y, Dewilde S, Friedman J, Ascenzi P, Guertin M, Bolognesi M. Heme-ligand tunneling in group I truncated hemoglobins. *J Biol Chem.* 2004 May 14;279(20):21520-5. Epub 2004 Mar 11. PubMed PMID: 15016811.

139: Milani M, Pesce A, Ouellet H, Guertin M, Bolognesi M. Truncated hemoglobins and nitric oxide action. *IUBMB Life.* 2003 Oct-Nov;55(10-11):623-7. Review. PubMed PMID: 14711009.

140: Spallarossa A, Forlani F, Carpen A, Armirotti A, Pagani S, Bolognesi M, Bordo D. The "rhodanese" fold and catalytic mechanism of 3-mercaptopyruvate sulfurtransferases: crystal structure of SseA from *Escherichia coli*. *J Mol Biol.* 2004 Jan 9;335(2):583-93. PubMed PMID: 14672665.

141: Ponassi M, Cantoni C, Biassoni R, Conte R, Spallarossa A, Moretta A, Moretta L, Bolognesi M, Bordo D. Expression and crystallographic characterization of the extracellular domain of human natural killer cell triggering receptor NKp46. *Acta*

Crystallogr D Biol Crystallogr. 2003 Dec;59(Pt 12):2259-61. Epub 2003 Nov 27.  
PubMed PMID: 14646088.

142: Roncone R, Monzani E, Murtas M, Battaini G, Pennati A, Sanangelantoni AM, Zuccotti S, Bolognesi M, Casella L. Engineering peroxidase activity in myoglobin: the haem cavity structure and peroxide activation in the T67R/S92D mutant and its derivative reconstituted with protohaemin-1-histidine. Biochem J. 2004 Feb 1;377(Pt 3):717-24. PubMed PMID: 14563209; PubMed Central PMCID: PMC1223899.

143: Hamdane D, Kiger L, Dewilde S, Green BN, Pesce A, Uzan J, Burmester T, Hankeln T, Bolognesi M, Moens L, Marden MC. The redox state of the cell regulates the ligand binding affinity of human neuroglobin and cytoglobin. J Biol Chem. 2003 Dec 19;278(51):51713-21. Epub 2003 Oct 6. PubMed PMID: 14530264.

144: Pesce A, Dewilde S, Nardini M, Moens L, Ascenzi P, Hankeln T, Burmester T, Bolognesi M. Human brain neuroglobin structure reveals a distinct mode of controlling oxygen affinity. Structure. 2003 Sep;11(9):1087-95. PubMed PMID: 12962627.

145: Ponassi M, Cantoni C, Biassoni R, Conte R, Spallarossa A, Pesce A, Moretta A, Moretta L, Bolognesi M, Bordo D. Structure of the human NK cell triggering receptor Nkp46 ectodomain. Biochem Biophys Res Commun. 2003 Sep 19;309(2):317-23. PubMed PMID: 12951052.

146: de Sanctis D, Dewilde S, Pesce A, Ascenzi P, Burmester T, Hankeln T, Moens L, Bolognesi M. New insight into the haemoglobin superfamily: preliminary crystallographic characterization of human cytoglobin. Acta Crystallogr D Biol Crystallogr. 2003 Jul;59(Pt 7):1285-7. Epub 2003 Jun 27. PubMed PMID: 12832788.

147: Zuccotti S, Rosano C, Mangione P, Bellotti V, Bolognesi M. Preliminary crystallographic characterization of the human beta2 microglobulin His31Tyr mutant in a tetrameric assembly. Acta Crystallogr D Biol Crystallogr. 2003 Jul;59(Pt 7):1270-2. Epub 2003 Jun 27. PubMed PMID: 12832782.



148: Spallarossa A, Forlani F, Pagani S, Salvati L, Visca P, Ascenzi P, Bolognesi M, Bordo D. Inhibition of *Azotobacter vinelandii* rhodanese by NO-donors. *Biochem Biophys Res Commun.* 2003 Jul 11;306(4):1002-7. PubMed PMID: 12821142.

149: Nardini M, Spanò S, Cericola C, Pesce A, Massaro A, Millo E, Luini A, Corda D, Bolognesi M. CtBP/BARS: a dual-function protein involved in transcription co-repression and Golgi membrane fission. *EMBO J.* 2003 Jun 16;22(12):3122-30. PubMed PMID: 12805226; PubMed Central PMCID: PMC162135.

150: Cantoni C, Ponassi M, Biassoni R, Conte R, Spallarossa A, Moretta A, Moretta L, Bolognesi M, Bordo D. The three-dimensional structure of the human NK cell receptor NKp44, a triggering partner in natural cytotoxicity. *Structure.* 2003 Jun;11(6):725-34. PubMed PMID: 12791260.

151: Ascenzi P, Bocedi A, Bolognesi M, Spallarossa A, Coletta M, De Cristofaro R, Menegatti E. The bovine basic pancreatic trypsin inhibitor (Kunitz inhibitor): a milestone protein. *Curr Protein Pept Sci.* 2003 Jun;4(3):231-51. Review. PubMed PMID: 12769721.

152: Milani M, Savard PY, Ouellet H, Ascenzi P, Guertin M, Bolognesi M. A TyrCD1/TrpG8 hydrogen bond network and a TyrB10TyrCD1 covalent link shape the heme distal site of *Mycobacterium tuberculosis* hemoglobin O. *Proc Natl Acad Sci U S A.* 2003 May 13;100(10):5766-71. Epub 2003 Apr 28. PubMed PMID: 12719529; PubMed Central PMCID: PMC156275.

153: Spallarossa A, Carpen A, Forlani F, Pagani S, Bolognesi M, Bordo D. SseA, a 3-mercaptopyruvate sulfurtransferase from *Escherichia coli*: crystallization and preliminary crystallographic data. *Acta Crystallogr D Biol Crystallogr.* 2003 Jan;59(Pt 1):168-70. Epub 2002 Dec 19. PubMed PMID: 12499560.

154: Visca P, Fabozzi G, Milani M, Bolognesi M, Ascenzi P. Nitric oxide and *Mycobacterium leprae* pathogenicity. *IUBMB Life.* 2002 Sep;54(3):95-9. Review. PubMed PMID: 12489635.

155: Pesce A, Bolognesi M, Bocedi A, Ascenzi P, Dewilde S, Moens L, Hankeln T, Burmester T. Neuroglobin and cytoglobin. Fresh blood for the vertebrate globin family. *EMBO Rep.* 2002 Dec;3(12):1146-51. Review. PubMed PMID: 12475928; PubMed Central PMCID: PMC1308314.

156: Kitadokoro K, Ponassi M, Galli G, Petracca R, Falugi F, Grandi G, Bolognesi M. Subunit association and conformational flexibility in the head subdomain of human CD81 large extracellular loop. *Biol Chem.* 2002 Sep;383(9):1447-52. PubMed PMID: 12437138.

157: Ascenzi P, Visca P, Ippolito G, Spallarossa A, Bolognesi M, Montecucco C. Anthrax toxin: a tripartite lethal combination. *FEBS Lett.* 2002 Nov 20;531(3):384-8. Review. PubMed PMID: 12435580.

158: Pesce A, Nardini M, Dewilde S, Ascenzi P, Burmester T, Hankeln T, Moens L, Bolognesi M. Human neuroglobin: crystals and preliminary X-ray diffraction analysis. *Acta Crystallogr D Biol Crystallogr.* 2002 Oct;58(Pt 10 Pt 2):1848-50. Epub 2002 Sep 28. PubMed PMID: 12351835.

159: Cantoni C, Ponassi M, Biassoni R, Conte R, Spallarossa A, Moretta A, Moretta L, Bolognesi M, Bordo D. Crystallization and preliminary crystallographic characterization of the extracellular Ig-like domain of human natural killer cell activating receptor NKp44. *Acta Crystallogr D Biol Crystallogr.* 2002 Oct;58(Pt 10 Pt 2):1843-5. Epub 2002 Sep 28. PubMed PMID: 12351833.

160: Rosano C, Zuccotti S, Bucciantini M, Stefani M, Ramponi G, Bolognesi M. Crystal structure and anion binding in the prokaryotic hydrogenase maturation factor HypF acylphosphatase-like domain. *J Mol Biol.* 2002 Aug 30;321(5):785-96. PubMed PMID: 12206761.

161: Visca P, Fabozzi G, Petrucca A, Ciaccio C, Coletta M, De Sanctis G, Bolognesi M, Milani M, Ascenzi P. The truncated hemoglobin from *Mycobacterium leprae*. *Biochem Biophys Res Commun.* 2002 Jun 28;294(5):1064-70. PubMed PMID: 12074585.

162: Nardini M, Spanò S, Cericola C, Pesce A, Damonte G, Luini A, Corda D, Bolognesi M. Crystallization and preliminary X-ray diffraction analysis of brefeldin A-ADP ribosylated substrate (BARS). *Acta Crystallogr D Biol Crystallogr*. 2002 Jun;58(Pt 6 Pt 2):1068-70. Epub 2002 May 29. PubMed PMID: 12037320.

163: Salvati L, Bolognesi M, Ascenzi P. Does inhibition of Trypanosoma cruzi key enzymes affect parasite life cycle and geographic distribution? *IUBMB Life*. 2002 Jan;53(1):45-7. Review. PubMed PMID: 12018407.

164: Pesce A, Nardini M, Dewilde S, Geuens E, Yamauchi K, Ascenzi P, Riggs AF, Moens L, Bolognesi M. The 109 residue nerve tissue minihemoglobin from *Cerebratulus lacteus* highlights striking structural plasticity of the alpha-helical globin fold. *Structure*. 2002 May;10(5):725-35. PubMed PMID: 12015154.

165: Seri M, Savino M, Bordo D, Cusano R, Rocca B, Meloni I, Di Bari F, Koivisto PA, Bolognesi M, Ghiggeri GM, Landolfi R, Balduini CL, Zelante L, Ravazzolo R, Renieri A, Savoia A. Epstein syndrome: another renal disorder with mutations in the nonmuscle myosin heavy chain 9 gene. *Hum Genet*. 2002 Feb;110(2):182-6. Epub 2001 Dec 14. PubMed PMID: 11935325.

166: Milani M, Pesce A, Dewilde S, Ascenzi P, Moens L, Bolognesi M. Structural plasticity in the eight-helix fold of a trematode haemoglobin. *Acta Crystallogr D Biol Crystallogr*. 2002 Apr;58(Pt 4):719-22. Epub 2002 Mar 22. PubMed PMID: 11914507.

167: Rosano C, Zuccotti S, Stefani M, Bucciantini M, Ramponi G, Bolognesi M. Crystallization and preliminary X-ray characterization of the acylphosphatase-like domain from the *Escherichia coli* hydrogenase maturation factor HypF. *Acta Crystallogr D Biol Crystallogr*. 2002 Mar;58(Pt 3):524-5. Epub 2002 Feb 21. PubMed PMID: 11856843.

168: Wittenberg JB, Bolognesi M, Wittenberg BA, Guertin M. Truncated hemoglobins: a new family of hemoglobins widely distributed in bacteria, unicellular

eukaryotes, and plants. *J Biol Chem.* 2002 Jan 11;277(2):871-4. Epub 2001 Nov 5.  
Review. PubMed PMID: 11696555.