

Publications

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- 1) **G.Morra**, M.Hodoscek, E.W.Knapp. Unfolding of the cold shock protein studied with biased molecular dynamics (2003). *Proteins*, 53, 597-606.
- 2) H.Hishikita, **G.Morra**, E.W.Knapp. Redox potential of quinones in photosynthetic reaction center from Rhodobacter sphaeroides: dependence on the protonation state of Glu-L212 and Asp-L213. (2003) *Biochemistry*, 42, 3882-3892.

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- 3) **G. Morra**, U. Koert, E.W. Knapp. Role of ions on structure and stability of a synthetic gramicidin ion channel in solution. A molecular dynamics study (2005). *J.Phys. Chem. B* 109, 10441-10444.
- 4) I. Merelli, **G. Morra**, D. D'Agostino, A. Clematis, L. Milanesi. High performance workflow implementation for protein surface characterization using grid technology (2005) *BMC Bioinformatics*.6 Suppl 4:S19.

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- 6) I. Merelli, **G. Morra**, L. Milanesi. Evaluation of a Grid based molecular dynamics approach for polypeptide simulations. (2006) *NanoBioscience –BioGrid special Issue*, 6, 229-234.

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- 7) **G. Morra**, M. Meli, G. Colombo. Molecular dynamics simulations of proteins and peptides: from folding to drug design. (2008) *Curr. Prot. Pep. Sci*, 9:181-96.
- 8) **G. Morra**, G. Colombo. The relationship between energy distribution and fold stability. Insights from molecular dynamics simulations of native and mutant proteins. (2008). *Proteins*, 72:660-72.
- 9) M.Meli, **G. Morra**, G. Colombo. Investigating the mechanism of peptide aggregation: Insights from mixed MonteCarlo-molecular dynamics simulations (2008) *Biophys. J.*, 94: 4414-26.
- 10) G. Colombo, **G. Morra**, M. Meli, G. Verkhivker. Understanding ligand-based modulation of the Hsp90 molecular chaperone dynamics at atomic resolution (2008). *Proc. Natl. Acad. Sci.*, 105:7976-7981.
- 11) A.Esteras-Chopo, **G. Morra**, E. Moroni, L.Serrano, M. Lopez de la Paz, G. Colombo. A Molecular Dynamics study of the interaction of D-peptide amyloid inhibitors with their target sequence reveals a potential inhibitory pharmacophore conformation (2008), *J. Mol. Biol.*, 383:266-80.

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- 12) **G. Morra**, G Verkhivker G. Colombo. Modeling signal propagation mechanisms and ligand based conformational dynamics of the Hsp90 molecular chaperone fulllength dimer.(2009) *PLoS Comput Biol.* 5, e1000323 .
- 13) G. Colombo, M. Meli, **G. Morra**, R. Gabizon, M. Gasset. Methionine sulfoxides on prion protein helix 3 switch on the alpha fold destabilization required for conversion. (2009) *PLoS One* 4, e4296.
- 14) G.M.Verkhivker, A. Dixit, **G. Morra**, G. Colombo. Structural and computational biology of the molecular chaperone Hsp90: from understanding molecular mechanisms to computer-based inhibitor design. (2009) *Curr. Top. Med. Chem.* , 9:1369-85.

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- 15) **G. Morra**, C. Baragli, G. Colombo. Selecting sequences that fold into a defined 3D structure: A new approach for protein design based on molecular dynamics and energetics. (2010) *Biophys. Chem.* 146: 76-84.
- 16) **G. Morra**, A. Genoni, M.A. Neves, K.M. Merz Jr, G. Colombo. Molecular recognition and drug-lead identification: What can molecular simulations tell us? (2010) *Curr. Med. Chem.* 17:25-41.

- 17) Mollapour M., Tsutsumi S., Donnelly AC, Beebe K., Tokita M.J., Lee S., **Morra G.**, Bourboulla D., Scroggins B.T., Colombo G., Blagg B.S., Panaretou B., Stetler-Stevenson W.G., Trepel JB., Piper PW, Prodromou C., Pearl L.H., Neckers L. Swe1/Wee1-dependent tyrosine phosphorylation of Hsp90 regulates distinct facets of chaperone function. (2010) *Mol. Cell*, 37,333-343
- 18) Scarabelli G, **Morra G**, Colombo G. Predicting interaction sites from the energetics of isolated proteins: A new approach to epitope mapping. (2010) *Biophys. J*, 98, 1966-1975
- 19) Genoni, A; **Morra, G**; Merz, KM, et al. Computational Study of the Resistance Shown by the Subtype B/HIV-1 Protease to Currently Known Inhibitors (2010) *Biochemistry* 9,4283-4295
- 20) **Morra, G**; Neves, MAC; Plescia, CJ, et al Dynamics-Based Discovery of Allosteric Inhibitors: Selection of New Ligands for the C-terminal Domain of Hsp90 (2010) *J Theor Chem Comput* , 2978-2989
- 21) Torella, R; Moroni, E; Caselle, M, et al. Investigating dynamic and energetic determinants of protein nucleic acid recognition: analysis of the zinc finger zif268-DNA complexes (2010) *BMC Struct Biol* 10, 42
- 22) **Morra G**, Genoni A., Colombo, G. Protein dynamics and drug design: the role of molecular simulations. Book Chapter, in *Protein, Protein Complexes: Analysis, Modeling and Drug Design*. 2009, 341-386, Imperial College Press. Editor Martin Zacharias. ISBN-10: 184816338X.
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- 23) Mollica L, **Morra G**, Colombo G, Musco G. HMGB1-Carbenoxolone Interactions: Dynamics Insights from Combined Nuclear Magnetic Resonance and Molecular Dynamics (2011) *Chem Asian J*. 2011 Feb 3. doi: 10.1002/asia.201000726