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Lista publikacji

z dnia 31 października 2013

Publikacje w czasopismach

1. Sieradzan A.K., Liwo A., Hansmann U.H.E, 2012, ***Folding and Self-Assembly of a Small Protein Complex***, J. Chem. Theory Comput., 8 (9): 3416-3422
2. Sieradzan A. K., Scheraga H. A., Liwo A., 2012, ***Determination of Effective Potentials for the Stretching of Ca ...Ca Virtual Bonds in Polypeptide Chains for Coarse-Grained Simulations of Proteins from ab Initio Energy Surfaces of N-Methylacetamide and N-Acetylpyrrolidine*** J. Chem. Theory Comput., 8(4):1334-1343
3. Łęgowska A, Lesner A, Bulak E, Jaśkiewicz A, Sieradzan A, Cydzik M, Stefanowicz P, Szewczuk Z, Rolka K., 2010, ***Inhibitory activity of double-sequence analogues of trypsin inhibitor SFTI-1 from sunflower seeds: an example of peptide splicing.*** FEBS J. 277(10):2351-9.
4. Sieradzan A.K., Hansmann U.H.E., Scheraga H.A., Liwo A., 2012, ***Extension of UNRES force field to treat polypeptide chains with D-aminoacid residues*** J. Chem. Theory Comput., 8 (11):4746–4757
5. He Y., Mozolewska M.A., Krupa P., Sieradzan A.K., Wirecki T.K., Liwo A., Kachlishvili K., Rackovsky S., Jagieła D., Ślusarz R., Czaplewski R.C., Ołdziej S., Scheraga H.A., 2013 ***Lessons from application of the UNRES force field to predictions of structures of CASP10 targets*** Proc. Natl. Acad. Sci. USA, 110(37):14936-14941
6. Krupa P., Sieradzan A.K., Rackovsky S., Baranowski M., Ołdziej S., Scheraga H.A., Liwo A., Czaplewski C., 2013, ***Improvement of the Treatment of Loop Structures in the UNRES Force Field by Inclusion of Coupling between Backbone- and Side-Chain-Local Conformational States.*** J. Chem. Theory Comput., 9(10): 4620–4632