List of Publications
Dr. Jožica Dolenc

2016

van Gunsteren WF, Allison JR, Daura X, Dolenc J, Hansen N, Mark AE, Oostenbrink C, Rusu VH, Smith LJ.
Deriving structural information from experimentally measured data on biomolecules.
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Smith LJ, Rought Whitta G, Dolenc J, Wang D, van Gunsteren WF.
A molecular dynamics simulation investigation of the relative stability of the cyclic peptide octreotide and its deprotonated and its (CF_3)-Trp substituted analogs in different solvents.
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Horta BAC, Merz PT, Fuchs PFJ, Dolenc J, Riniker S, Hünenberger PH.
A GROMOS-compatible force field for small organic molecules in the condensed phase: the 2016H66 parameter set.
J. Chem. Theory Comput. 2016; 12: 3825-3850.

Dolenc J, Meier BH, Rusu VH, van Gunsteren WF.
Investigation of the structural preference and flexibility of the loop residues in amyloid fibrils of the HET-s prion.
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Dolenc J, Renn O.
Vermittlung von Informatonskompetenz à la carte im Informationszentrum Chemie | Biologie | Pharmazie der ETH Zürich.
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2015

Torbeev V, Ebert MO, Dolenc J, Hilvert, D.
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J. Am. Chem. Soc. 2015; 137:2524-2535.

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Bachmann SJ, Lin Z, Stafforst T, van Gunsteren WF, Dolenc J.
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Mol. Phys. 2013; 111:2334-2344.

Wang D, Böckmann A, Dolenc J, Meier BH, van Gunsteren WF.
On the behavior of water at subfreezing temperatures in a protein crystal: evidence of higher mobility than in bulk water
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Exploration of swapping enzymatic function between two proteins: a simulation study of chorismate mutase and isochorismate pyruvate lyase.
Protein Sci. 2013; 22:809-822.

Meier K, Choutko A, Dolenc J, Eichenberger AP, Riniker S, van Gunsteren WF.
Multi-resolution simulation of biomolecular systems: a review of methodological issues.
Angew. Chem. Int. Ed. 2013; 52:2820-2834.

2012

Missimer JH, Steinmetz MO, van Gunsteren WF, Dolenc J.
Influence of 63Ser phosphorylation and dephosphorylation on the structure of the stathmin helical nucleation sequence: A molecular dynamics study.
Biochemistry. 2012; 51:8455-8463.

Wang D, Freitag F, Gattin Z, Haberkern H, Jaun B, Siwko M, Vyas R, van Gunsteren WF, Dolenc J.
Validation of the GROMOS 54A7 force field regarding mixed α/β peptide molecules.
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van Gunsteren WF, Dolenc J.
Thirty-five years of biomolecular simulation: development of methodology, force fields, software.
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J. Biomol. NMR 2011; 51:265-281.

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