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.


Horta BAC, Merz PT, Fuchs PFJ, Dolenc J, Riniker S, Hünenberger PH.

Dolenc J, Meier BH, Rusu VH, van Gunsteren WF.

Dolenc J, Renn O.

2015

Torbeev V, Ebert MO, Dolenc J, Hilvert, D.

2014

Bachmann SJ, Lin Z, Stafforst T, van Gunsteren WF, Dolenc J.
On the sensitivity of peptide nucleic acid duplex formation and crystal dissolution to a
variation of force-field parameters.


**2013**

Pechlaner M, Sigel RKO, van Gunsteren WF, Dolenc J.
Structure and conformational dynamics of the domain 5 RNA hairpin of a bacterial group II intron revealed by solution NMR and molecular dynamics simulations.


Bachmann SJ, Dolenc J, van Gunsteren WF.
On the use of one-step perturbation to investigate the dependence of different properties of liquid water upon a variation of model parameters from a single simulation.


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


Choutko A, Eichenberger AP, van Gunsteren WF, Dolenc J.
Exploration of swapping enzymatic function between two proteins: a simulation study of chorismate mutase and isochorismate pyruvate lyase.


Meier K, Choutko A, Dolenc J, Eichenberger AP, Riniker S, van Gunsteren WF.
Multi-resolution simulation of biomolecular systems: a review of methodological issues.


**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.


Validation of the GROMOS 54A7 force field regarding mixed α/β peptide molecules.

Allison J, Hertig S, Missimer JH, Smith L, Steinmetz MO, Dolenc J. 
Probing the structure and dynamics of proteins by combining molecular dynamics 
simulations and experimental NMR data. 

Hansen N, Dolenc J, Knecht M, Riniker S, van Gunsteren WF. 
Assessment of enveloping distribution sampling to calculate relative free enthalpies of 
binding for eight netropsin-DNA duplex complexes in aqueous solution. 

van Gunsteren WF, Dolenc J. 
Thirty-five years of biomolecular simulation: development of methodology, force fields, 
software. 

2011

Dolenc J, Riniker S, Gaspari R, Daura X, van Gunsteren WF. 
Free energy calculations offer insights into the influence of receptor flexibility on ligand-
receptor binding affinities. 

Eichenberger AP, Allison JR, Dolenc J, Geerke DP, Horta BAC, Meier K, Oostenbrink C, 
Schmid N, Steiner D, Wang D, van Gunsteren WF. 
The GROMOS++ software for the analysis of biomolecular simulation trajectories. 

Schmid N, Allison JR, Dolenc J, Eichenberger AP, Kunz APE, van Gunsteren WF. 
Biomolecular structure refinement using the GROMOS simulation software. 

2010

Dolenc J, Missimer JH, Steinmetz MO, van Gunsteren WF. 
Methods of NMR structure refinement: molecular dynamics simulations improve the 
agreement with measured NMR data of a C-terminal peptide of GCN4-p1. 
*J. Biomol. NMR.* 2010; 47:221-235.

Missimer JH, Dolenc J, Steinmetz MO, van Gunsteren WF. 
Exploring the trigger sequence of the GCN4 coiled-coil: Biased molecular dynamics 
resolves apparent inconsistencies in NMR measurements. 
2008

Dolenc J, Baron R, Missimer JH, Steinmetz MO, van Gunsteren WF.
Exploring the conserved water site and hydration of a coiled-coil trimerisation motif: A
MD simulaton study.

van Gunsteren WF, Dolenc J.
Biomolecular simulation: historical picture and future perspectives.

van Gunsteren WF, Dolenc J, Mark AE.
Molecular simulation as an aid to experimentalists.

2006

Vlachy N, Dolenc J, Jerman B, Kogej K.
Influence of stereoregularity of the polymer chain on interactions with surfactants:
binding of cetylpyridinium chloride by isotactic and atactic poly(methacrylic acid).

Dolenc J, Baron R, Oostenbrink C, Koller J, van Gunsteren WF.
Configuratonal entropy change of netropsin and distamycin upon DNA minor-groove
binding.
Biophys. J. 2006; 91:1460-1470.

Dolenc J, Koller J.
An improved semiempirical MO PM3 method for hydrogen bonded systems.

2005

Dolenc J, Borštnik U, Hodošček M, Koller J, Janežič D.
An ab inito QM/MM study of the conformational stability of the complexes formed by
netropsin and DNA. The importance of van der Waals interactions and hydrogen
bonding.

Dolenc J, Oostenbrink C, Koller J, van Gunsteren WF.
Molecular dynamics simulations and free energy calculations of netropsin and distamycin
binding to an AAAAA DNA binding site.