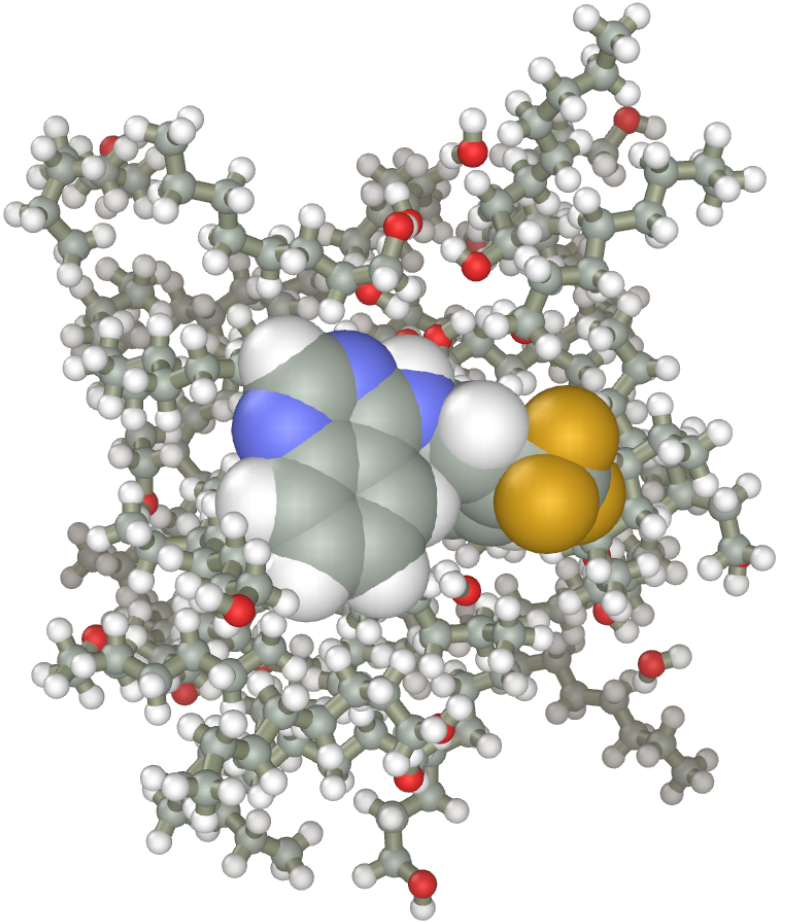

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Метод

Molecular Dynamics in new more robust Expanded Ensembles algorithm (article in preparation) by alchemical coordinate

Calculation solvation free energy difference in water and in aqueous octanol.

Tools

Abalone FF generator [1]

NWChem [2]

Abalone II for GPU accelerated MD calculations [3]

Force field

AMBER/OPLS like force field with combining rules from the article [4]

Preliminary model with automatic FF generator

Manual editing

F parameters from article [4]

Results

LogP RMSD 0.74, MAE 0.67

Problems

Small model: 32 octanol and 12 water molecules.
Error in logP for benzylamine: 32 mol -0.31, 64 mol +0.17

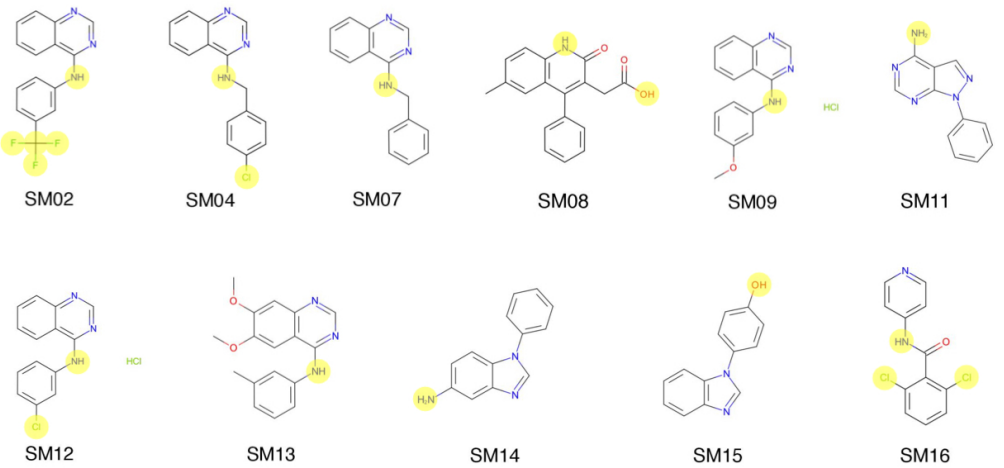
Insufficient calculation time: from 10 to 40 passes

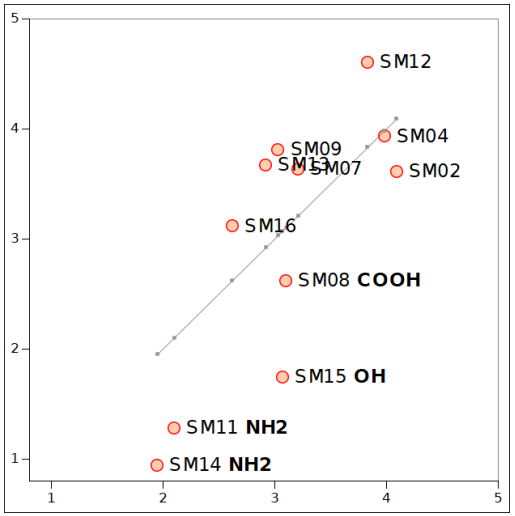
For further consideration

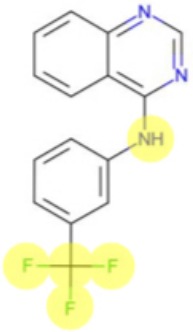
Model size

Hydrogen bond parameters

Systematic procedure for FF development







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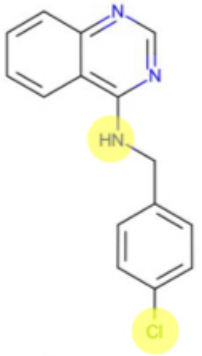

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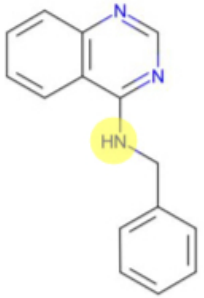

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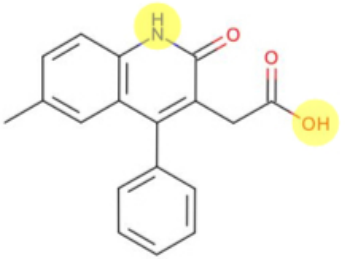

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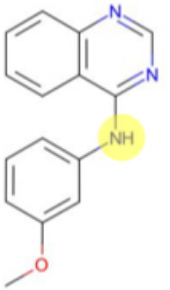
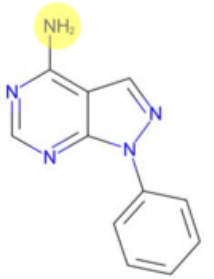


SM09

HCl



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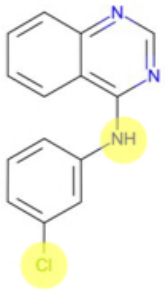
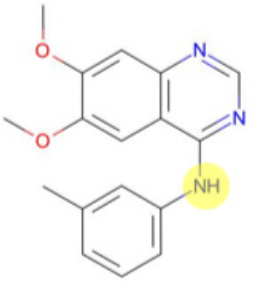


SM12

HCl



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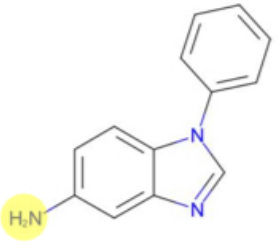

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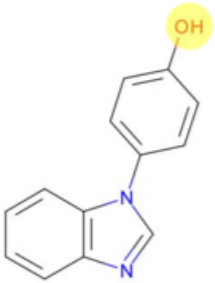

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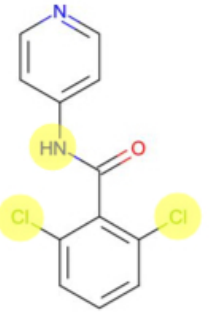

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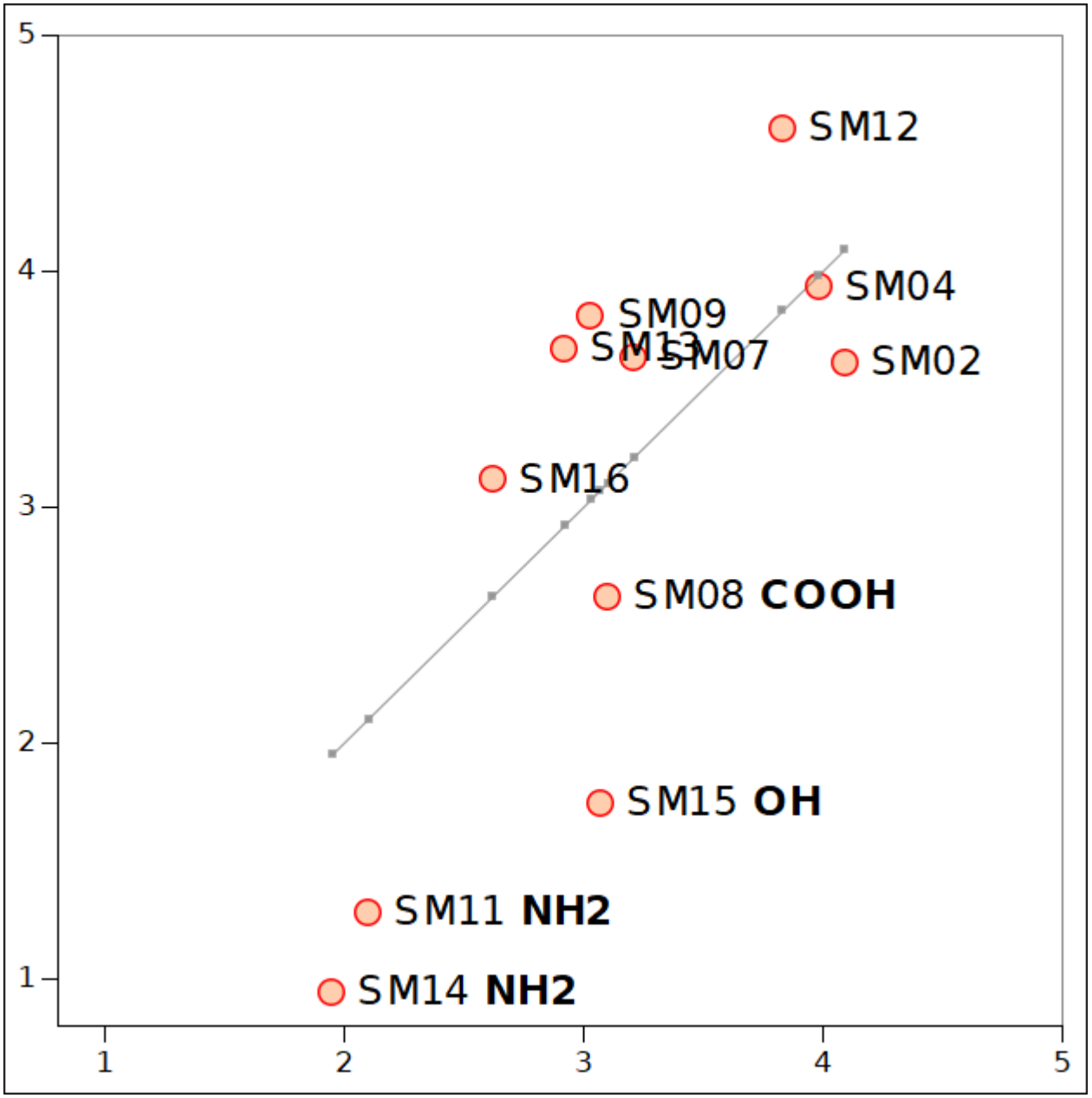

LogP RMSD 0.74, MAE 0.67

Rreferences

- [1] http://www.biomolecular-modeling.com/FF/index.html
- [2] http://www.nwchem-sw.org/index.php/Main_Page
- [3] http://www.biomolecular-modeling.com/Abalone/index.html
- [4] Alexei M. Nikitin, Yury V. Milchevskiy and Alexander P. Lyubartsev AMBER-ii: New Combining Rules and Force Field for Perfluoroalkanes. J. Phys. Chem. B, 2015, 119 (46), pp 14563–14573 DOI 10.1021/acs.jpcb.5b07233