Simulation Details Report

System Details

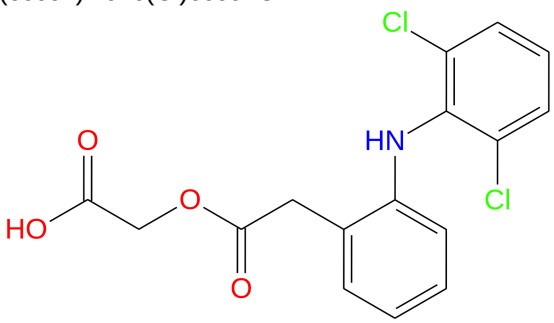
Jobname: multistage_simulation_Aceclofenac_soluplus_1_8_5
Entry title: disordered_system_ds_all_components_amorphous

Ensemble	Force Field	Temp. [K]	Sim Time [ns]	Num. Atoms	Num. Mols	Mol Weight [au]	Charge
NPT	S-OPLS	300.0	100.102	23698	54	156896.566	0

Molecule(s) Details

Molecule **1**:

SMILES	O=C(O)COC(=O)Cc1c(cccc1)Nc2c(Cl)cccc2Cl
Molecular formula	C16H13Cl2NO4
Number of molecules	53
Number of atoms	36 (total), 23 (heavy)
Molecular weight	354.192
Charge	0
Number of rot. bonds	8



Molecule **2**:

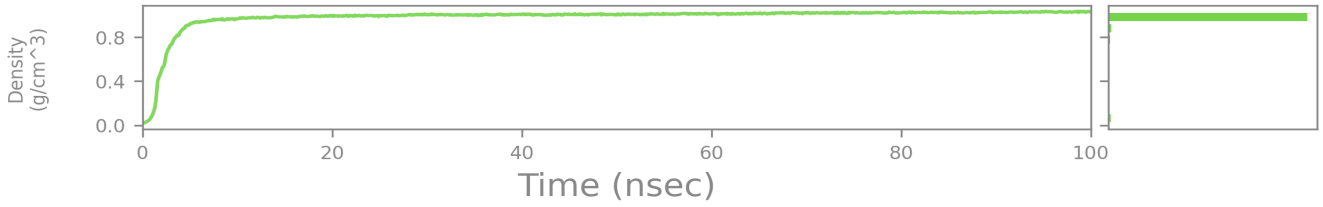
SMILES	Not generated for Molecule 54
Molecular formula	C7326H12012N606O1846
Number of molecules	1
Number of atoms	21790 (total), 9778 (heavy)
Molecular weight	138124.373
Charge	0
Number of rot. bonds	More than 100

Molecule too big to render in 2D.

Bulk Properties

	Volume Angstrom^3	Density g/cm^3	Cohesive E kcal/mol	Solubility Parameter MPa^(1/2)	Solubility Parameter Vdw MPa^(1/2)	Solubility Parameter Ele MPa^(1/2)	Heat of Vap. kcal/mol	Specific Heat Capacity (Cp) J / (g * K)
Average:	253949.13	1.03	46.26	8.27	7.05	4.32	46.85	4.38
Stdev:	913.051	0.004	0.344	0.038	0.037	0.047	0.344	N/A

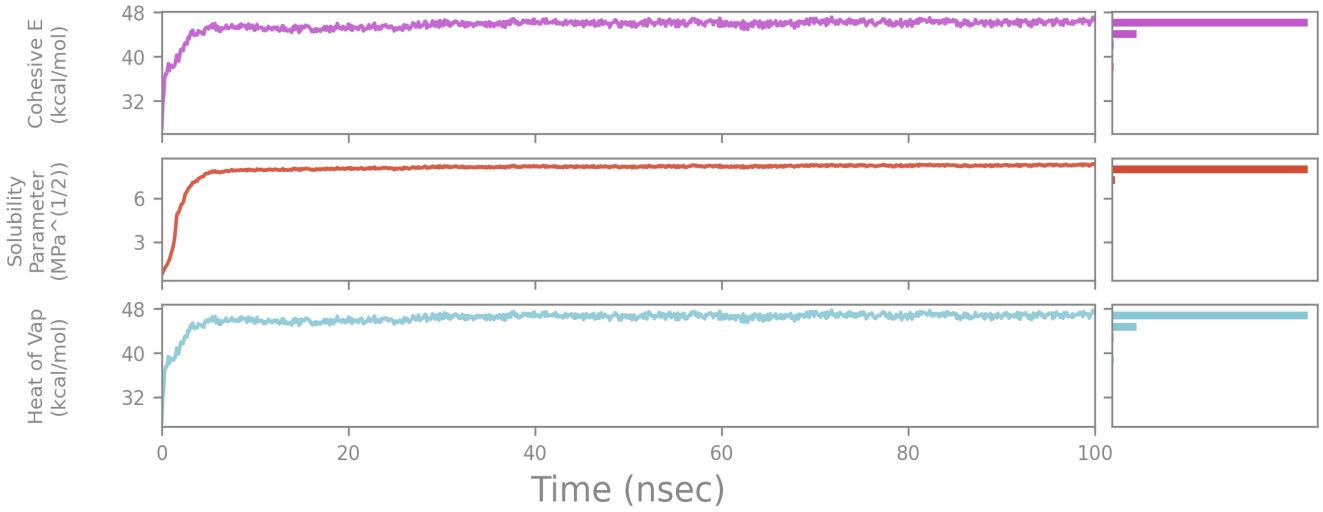
Note: *Statistics reported are for the final 20% of the simulation.*



Density is a fundamental structural parameter that can be compared directly to experiment. Density (ρ) is defined as mass, *m*, per unit volume:

$$\rho = m/V$$

Density is expressed in g/cm^3, and is computed for each frame over the course of the trajectory. Inspection of the convergence of density gives important feedback on the degree of system convergence. With the OPLS force fields, the fully equilibrated density can be computed to within 3% of experimental values.



The heat of vaporization and Hildebrand solubility parameter are closely related properties. The solubility parameter is useful for estimating the miscibility of various components being considered for applications requiring multicomponent mixtures. The solubility parameter (δ) for a pure liquid is defined as

$$\delta = [(\Delta H_v - RT)/V_m]^{1/2}$$

where ΔH_v is the heat of vaporization and V_m is the molar volume. *RT* is the ideal gas PV term. The heat of vaporization, ΔH_v, is measured in *kcal/mol* and is calculated from the energy of periodic unit cell minus the sum of the *N* individual molecules, E_i, averaged over the MD trajectory.

$$\Delta H_{vap} = \langle |E_{cell} - \sum_{i=1}^{N} E_i| \rangle + RT$$