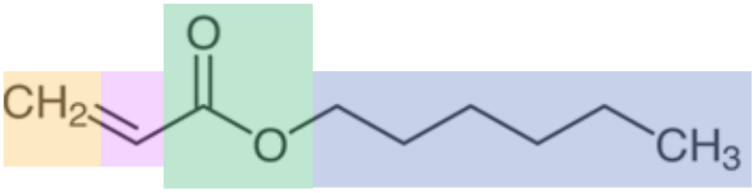
Section 1: Atom Identities

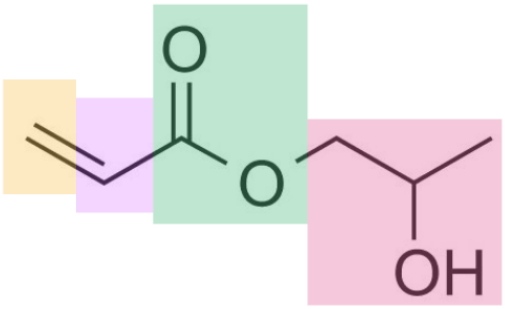
Hexyl acrylate (HA) atom identities for OPLS, labeled by color:




```
C  opls_143   12.01100  ; alkene C (H2-C=)
H  opls_144    1.00800  ; alkene H (H-C=)
H  opls_144    1.00800  ; alkene H (H-C=)

C  opls_142   12.01100  ; alkene C (RH-C=)
H  opls_144    1.00800  ; alkene H (H-C=)

C  opls_465   12.01100  ; AA C:   esters for R-C=O,O
O  opls_466   15.99940  ; AA =O:  esters
O  opls_467   15.99940  ; AA -OR: ester
```

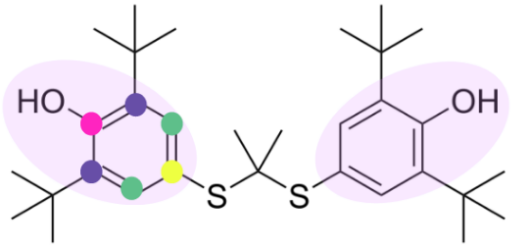
```
C opls_182  12.01100  ; C(H2OR): ethyl  ether
H opls_185   1.00800  ; H(COR): alpha H ether
H  opls_185   1.00800; H(COR): alpha H ether

C opls_136   12.01100  ; alkane CH2
H opls_140    1.00800  ; alkane H
H opls_140    1.00800  ; alkane H

C opls_136   12.01100  ; alkane CH2
H opls_140    1.00800  ; alkane H
H opls_140    1.00800  ; alkane H

C opls_136   12.01100  ; alkane CH2
H opls_140    1.00800  ; alkane H
H opls_140    1.00800  ; alkane H

C opls_136   12.01100  ; alkane CH2
H opls_140    1.00800  ; alkane H
H opls_140    1.00800  ; alkane H

C opls_135   12.01100  ; alkane CH3
H opls_140    1.00800  ; alkane H
H opls_140    1.00800  ; alkane H
H opls_140    1.00800  ; alkane H
```

Hydroxypropyl acrylate (HPA) atom identities for OPLS, labeled by color




```
H  opls_144    1.00800  ; alkene H (H-C=)
H  opls_144    1.00800  ; alkene H (H-C=)
C  opls_143   12.01100  ; alkene C (H2-C=)

C opls_142   12.01100  ; alkene C (RH-C=)
H  opls_144    1.00800  ; alkene H (H-C=)

C opls_465   12.01100  ; AA C:   esters for R-C=O,O
O  opls_466   15.99940  ; AA =O:  esters
O  opls_467   15.99940  ; AA -OR: ester

C opls_136   12.01100  ; alkane CH2
H opls_140    1.00800  ; alkane H
H opls_140    1.00800  ; alkane H

C opls_158   12.01100  ; all-atom C: CH, alcohols
O opls_078   15.99940  ; O   ALCOHOLS   JPC,90,1276 (1986)
H opls_155    1.00800  ; all-atom H(O): mono alcohols

C  opls_135   12.01100  ; alkane CH3
H  opls_140    1.00800  ; alkane H
H  opls_140    1.00800  ; alkane H
H  opls_140    1.00800  ; alkane H
```

Probucol (PBL) atom identities for OPLS, labeled by color

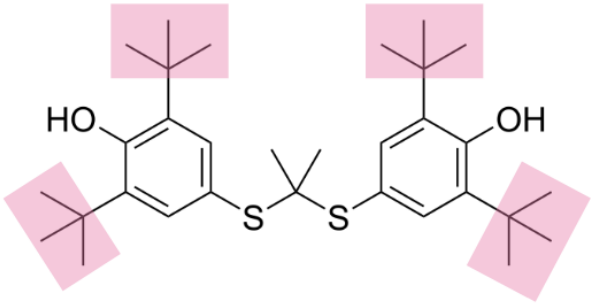


C opls_166 12.01100 ; C(OH) phenol
O opls_167 15.99940 ; O phenol C
H opls_168 1.00800 ; H phenol H

C opls_516 12.01100 ; all-atom C: C, t-butyl benzene

C opls_145 12.01100 ; Benzene C
H opls_146 1.00800 ; Benzene H - 12 site.

C opls_735 12.01100 ; C(S) thiophenol

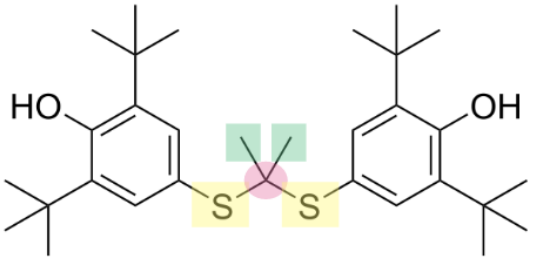


Center C opls_516

Terminal C1, opls_516
H opls_140 1.00800 ; alkane H
H opls_140 1.00800 ; alkane H
H opls_140 1.00800 ; alkane H

Terminal C2 opls_516
H opls_140 1.00800 ; alkane H
H opls_140 1.00800 ; alkane H
H opls_140 1.00800 ; alkane H

Terminal C3 opls_516
H opls_140 1.00800 ; alkane H
H opls_140 1.00800 ; alkane H
H opls_140 1.00800 ; alkane H



S opls_084 32.06000 ; S IN RSR, JPC,90,6379 (1986)

C opls_216 12.01100 ; all-atom C: C, disulfides

C opls_135 12.01100 ; alkane CH3
H opls_140 1.00800 ; alkane H
H opls_140 1.00800 ; alkane H
H opls_140 1.00800 ; alkane H

Section 2: GROMACS command lines and argument descriptions

Line

```
gmx insert-molecules -f PBL.gro -ci PBL.gro -nmol 10 -try 30 -box 4 4 4 -rot xyz -o 10PBL.gro
```

Description of each argument

-f = coordinate file to insert the molecule(s) into
-ci = coordinates (ie structure file) of the molecule you wish to insert
-nmol = how many copies you would like to add
-try = how many configurations you would like GROMACS to try to make all of your molecules fit
-box= place all molecules in a Z nm x Z nm x Z nm box where Z=your size of interest
-rot xyz = gives GROMACS position to rotate your molecule(s) to make them fit better
-o = output, provide the name and file type you wish to produce by this command

Line

```
 gmx solvate -cp new_withbox.gro -cs tip3p.gro -o new_withsolv.gro -p topol.top
```

Description of each new argument

-cp = coordinates of protein (in this case your 'protein' is your complete system's .gro file
-cs = coordinates of solvent, we selected the tip3p model for water.
-p = parameter file (topol.top) that you wish to add a solvent line to

Line

```
gmx grompp -f minim.mdp -c new_withsolv.gro -p topol.top -o em.tpr
```

Description of each new argument

grompp = preprocessing step, checks to make sure your system looks okay before you do an MD run
-f = file that contains the MD parameters for this step
-c = coordinate file of the system you are preforming the run on
-p = parameter file (topol.top) you want to update
-o = output file, the name before .tpr has to match the name you will use in the next step.

Line

```
gmx mdrun -deffnm em
```

Description of each new argument

mdrun = you are performing a molecular dynamics run
-deffnm = the name of your -o file previously, all output files from this MD step will have the same name (with different file types)

Line

```
gmx grompp -f nvt.mdp -c em.gro -r em.gro -p topol.top -o nvt.tpr
```

Description of each new argument

-r = using the coordinates of the previous step as restraints on for this step

Line

```
gmx grompp -f npt.mdp -c nvt.gro -r nvt.gro -t nvt.cpt -p topol.top -o npt.tpr
```

Description of each new argument

-t = continue the trajectory from previous step

Line

```
gmx mdrun -deffnm npt
```

Line

```
gmx grompp -f md.mdp -c npt.gro -t npt.cpt -p topol.top -o md_0_1.tpr
```

Line

```
gmx mdrun -deffnm md_0_1
```

Section 3: Necessary files

In the working directory, the following files are needed:

- Minim.mdp (parameters for minimization)
- NVT.mdp (parameters for NVT equilibration)
- NPT.md (parameters for NPT equilibration)
- MD.mdp (parameters for MD production)
- Structure files (HPA.gro, HXA.gro, PBL.gro)
- Topology file, modified for each system with forcefield-compatible atom identities (see topol.top)

GROMACS & OPLS references:

W.L. Jorgensen, D.S. Maxwell, and J. Tirado-Rives, “Development and testing of the oPLS all-atom force field on conformational energetics and properties of organic liquids,” *J. Am. Chem. Soc.*, 118 11225–11236 (1996)

M.J. Robertson, J. Tirado-Rives, and W.L. Jorgensen, “Improved peptide and protein torsional energetics with the oPLS-aA force field,” *J. Chem. Theory Comput.*, 11 3499–3509 (2015).

H. Bekker, H.J.C. Berendsen, E.J. Dijkstra, S. Achterop, R. van Drunen, D. van der Spoel, A. Sijbers, and H. Keegstra *et al.*, “Gromacs: A parallel computer for molecular dynamics simulations”; pp. 252–256 in *Physics computing 92*. Edited by R.A. de Groot and J. Nadrchal. World Scientific, Singapore, 1993.

S. Pronk, S. Páll, R. Schulz, P. Larsson, P. Bjelkmar, R. Apostolov, M.R. Shirts, and J.C. Smith *et al.*, “GROMACS 4.5: A high-throughput and highly parallel open source molecular simulation toolkit,” *Bioinformatics*, 29 [7] 845–854 (2013)

M.J. Abraham, T. Murtola, R. Schulz, S. Páll, J.C. Smith, B. Hess, and E. Lindahl, “GROMACS: High performance molecular simulations through multi-level parallelism from laptops to supercomputers,” *SoftwareX*, 1–2 19–25 (2015).