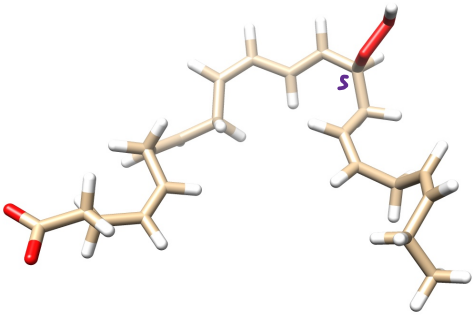
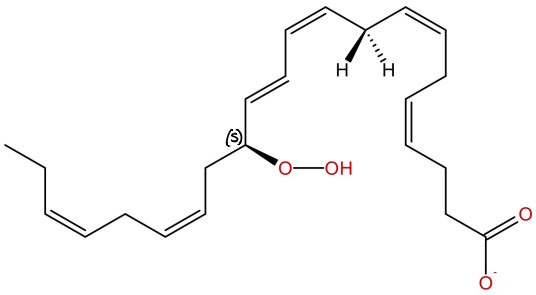
4B. 1-7/10/18 week

4B.1. 2/10/18

Epoxidation from 14S-DHA (continuation I)



Representation of generated 14S-HpDHA



2D representation of 14S-HpDHA

14S-HpDHA

Charge = -1 Multiplicity = 1 N° atoms = 57 { 22C, 4O, 31H

ANTECHAMBER PROTOCOL:

1. The initial structure has been built and the bonds modified in order to obtain a logical (in terms of valence, GaussView considers strange bonds) structure.
2. > antechamber -i 14S-DHA.mol2 -fi mol2 -o 14S-HpDHA_gaussian.com -fo gcrt -gv 1 -ge 14S-HpDHA_gaussian.gesp.

   A Gaussian input file has been obtained. It optimises the structure and calculates RESP chgs
3. The Gaussian input has been modified: %nproc=32 has been added and charge has been changed from 0 to 1. Calculation has been sent to picard (w 8h 46')
4. Once Gaussian calculation has finished, the calculated ESP charges have to be transformed in order to be readable by antechamber.

   > espgen -i 14S-HpDHA_gaussian.gesp -o 14S-HpDHA_gaussian.esp

5. From Gaussian output and ESP charges, parameters have been obtained:

>antechamber -i *_gaussian.log -fi gout -o 14S-HpDHA_gaussian.ac -fo ac -c esp -cf *_gaussian.esp

6. frcmod has been generated including all parameters (for the whole molecule)

>parmchk2 -i *.ac -o 14S-HpDHA.frcmod -a Y -w Y

7. Mol2 including charges can be now created:

>antechamber -i 14S-HpDHA_gaussian.ac -fi ac -o 14S-HpDHA_ac.mol2 -fo mol2

TLEAP PROTOCOL:

1. Generate de pdb that includes both protein and HpDHA. Delete all waters (the original pdb was solvated.)
2. Modify the pdb: remove the CONNECT section and change the keyword UNK to HPD of the 14S-HpDHA atoms.
3. Modify the .mol2 from antechamber: change the keyword MOL to HPD both in MOLECULE and SUBSTRUCTURE sections.
4. Change active center residues (their three-letters code) to the one used in tleap.
5. Modify the leap_script.in so it gets in accordance to the new system (change .mol2 of the substrate, the .frcmod...).
6. Run the script:

>tleap -f leap_script.in

The program says that some atom types from HpDHA can't be understood. It generates the pdb of the non-solvated system.