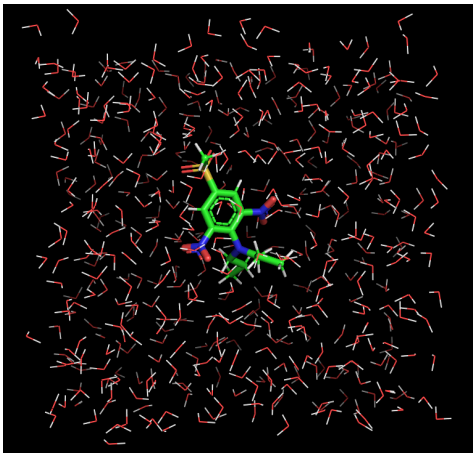
Barbara Morales - Simulations Log

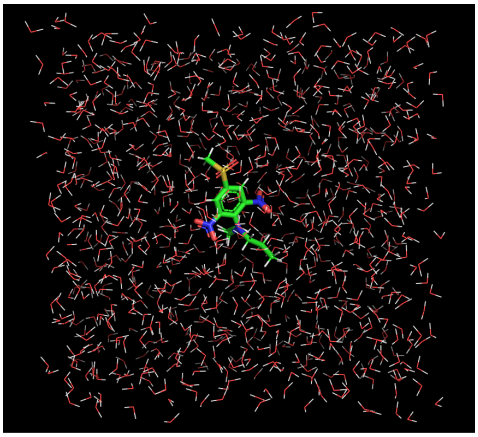
Experiments/Simulations Log

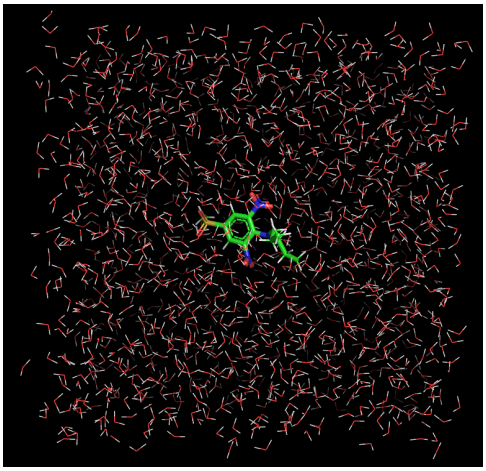
08/29/2024

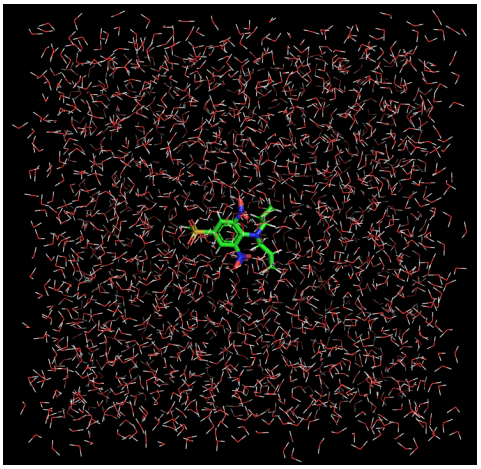
- SFEs - **Test water models**
  - Molecule CC(C)C
  - System size: 1000 total (999 waters)
  - Experiment: 9.6232 +/- 0.8368000000000001 kJ/mol
  - **Tip3p**
    - Calculation: 10.6933196676346 +/- 0.2286284239107238 kJ/mol
    - # states solvent 1: 23
    - # states solvent 2: 2
    - Wall time: 03:18:26
  - **Tip3p-fb**
    - Calculation: 12.1794553081268 +/- 0.22931099803079408 kJ/mol
    - # states solvent 1: 23
    - # states solvent 2: 2
    - Wall time: 03:18:45
  - Tip4p-ew
    - Pending: ERROR - yank.pipeline - Atom number mismatch: solvent_1.xml has 4010 atoms; solvent_1.pdb has 3011 atoms.
    - Calculation:
    - # states solvent 1:
    - # states solvent 2:
    - Wall time:
  - Tip4p-fb
    - Pending: ERROR - yank.pipeline - Atom number mismatch: solvent_1.xml has 4010 atoms; solvent_1.pdb has 3011 atoms.
    - Calculation:
    - # states solvent 1:
    - # states solvent 2:
    - Wall time:
  - **OPC3**
    - Calculation: 11.566535903612137 +/- 0.252.78288110814788 kJ/mol
    - # states solvent 1: 23
    - # states solvent 2: 2
    - Wall time: 03:15:29

    - OPC
        - Pending: ERROR - yank.pipeline - Atom number mismatch: solvent_1.xml has 4010 atoms; solvent_1.pdb has 3011 atoms.
        - Calculation:
        - # states solvent 1:
        - # states solvent 2:
        - Wall time:
    - Gopal
        - Pending: ERROR - yank.pipeline - Atom number mismatch: solvent_1.xml has 4010 atoms; solvent_1.pdb has 3011 atoms.
        - Calculation:
        - # states solvent 1:
        - # states solvent 2:
        - Wall time:

- SFEs - **Test box size**
    - CCCN(CCC)c1c([N+](=O)[O-])cc(S(C)(=O)=O)cc1[N+](=O)[O-] box size
        - Experiment: -33.38832 +/- 8.07512 kJ/mol
        - 500
            - 
            - Calculated: -56.30199980990216 +/- 0.3238062362782637 kJ/mol
            - # of states solvent 1: 52
            - # of states solvent 2: 5
            - Wall time: 07:17:15

- 1000
  - 
  - Calculated: -56.73590447773604 +/- 0.3280576327668656 kJ/mol
  - # of states solvent 1: 52
  - # of states solvent 1: 5
  - Wall time: 07:52:49

- 1500
  - 
  - Calculated: -55.75292687091854 +/- 0.31635809320505626 kJ/mol
  - # of states solvent 1: 53
  - # of states solvent 2: 5
  - Wall time: 08:52:34

        - 2000
            - 
            - Calculated: -55.92478472792014 +/- 346.9515666545986 kJ/mol
            - # of states solvent 1: 52
            - # of states solvent 2: 5
            - Wall time: 09:01:28

08/28/2024

- SFEs
    - Test different water models with small molecule
        - Molecule CC(C)C
        - System size: 1000 total (999 waters)
        - Running:
            - Tip3p
            - Tip3p-fb
            - Tip4p-ew
            - Tip4p-fb
            - OPC3
            - OPC
            - gopal
    - Test different box sizes with large molecule
        - Molecule: CCCN(CCC)c1c([N+](=O)[O-])cc(S(C)(=O)=O)cc1[N+](=O)[O-]
        - Water model: tip3p
        - Running:
            - 500
            - 1000
            - 1500
            - 2000
    - To-do:
        - Test with hexane to check for phase separation