Lab0:

Introduction – brief summary and reason for project

Procedure – what steps did you actually perform and in what order

Methods – kinds of calculations, programs used, level of theory, any assumptions or approximation such as quantities varied, restraints and constraints, special program options

Results – data obtained, usually in tables and plots

Analysis – explain your result

**Tinker-FFE version 8.10.1 Results**

I downloaded from Pubchem but the structure from Cactus has tiny bit higher energy

Analyze ibuprofen before Minimization:
Analysis Types [E]
Total Potential Energy : 21.0277 Kcal/mole

Analyze ibuprofen after Minimization:
Analysis Types [E]
Total Potential Energy : 12.2922 Kcal/mole

Running spacefill (FFE-Tinker version 8.10.1) on minimized energy structure. Realized that for *Probe Radius in Angstroms (Leave blank for van der Waals Area and Volume)* this needs to be added to work for (2) and (3) below.

**(1) Van der Waals Area and Volume: works WITHOUT & WITH probe radii**

```
$ ~/tools/Tinker-FFE/tinker/bin/spacefill ~/tools/Tinker-FFE/NIHdownloads/ibuprofen.xyz $(echo 1
N) -k ~/tools/Tinker-FFE/NIHdownloads/ibuprofen.key # $(echo <my_in1> <my_in2> …) does same as
stdin

Van der Waals Surface Area and Volume :
Total Area :             240.174 Square Angstroms
Total Volume :           232.243 Cubic Angstroms

$ ~/tools/Tinker-FFE/tinker/bin/spacefill ~/tools/Tinker-FFE/NIHdownloads/ibuprofen.xyz $(echo 1
1.4 N) -k ~/tools/Tinker-FFE/NIHdownloads/ibuprofen.key

Van der Waals Surface Area and Volume :
Total Area :             240.174 Square Angstroms
Total Volume :           232.243 Cubic Angstroms
```

**(2) Accessible Area and Excluded Volume: works only WITH probe radii**

```
# this will ask to input the Probe Radius anyway and in FFE it just stalls at “Enter a Value for
the Probe Radius [1.4 Ang] :”
$ ~/tools/Tinker-FFE/tinker/bin/spacefill ~/tools/Tinker-FFE/NIHdownloads/ibuprofen.xyz $(echo 2
N) -k ~/tools/Tinker-FFE/NIHdownloads/ibuprofen.key

# this works
$ ~/tools/Tinker-FFE/tinker/bin/spacefill ~/tools/Tinker-FFE/NIHdownloads/ibuprofen.xyz $(echo 2
1.4 N) -k ~/tools/Tinker-FFE/NIHdownloads/ibuprofen.key

Accessible Surface Area and Excluded Volume :
Total Area :             428.639 Square Angstroms
Total Volume :           693.930 Cubic Angstroms
```

**(3) Contact-Reentrant Area and Volume: works only WITH probe radii**

```
# this will ask to input the Probe Radius anyway and in FFE it just stalls at “Enter a Value for
the Probe Radius [1.4 Ang] :”
$ ~/tools/Tinker-FFE/tinker/bin/spacefill ~/tools/Tinker-FFE/NIHdownloads/ibuprofen.xyz $(echo 3
N) -k ~/tools/Tinker-FFE/NIHdownloads/ibuprofen.key

# this works
$ ~/tools/Tinker-FFE/tinker/bin/spacefill ~/tools/Tinker-FFE/NIHdownloads/ibuprofen.xyz $(echo 3
1.4 N) -k ~/tools/Tinker-FFE/NIHdownloads/ibuprofen.key

Contact-Reentrant Surface Area and Volume :
Total Area :             229.593 Square Angstroms
Total Volume :           238.914 Cubic Angstroms
```

## Conclusions:

Contact-Reentrant Area much closer to VDW surface area/volume than SASA, makes sense.