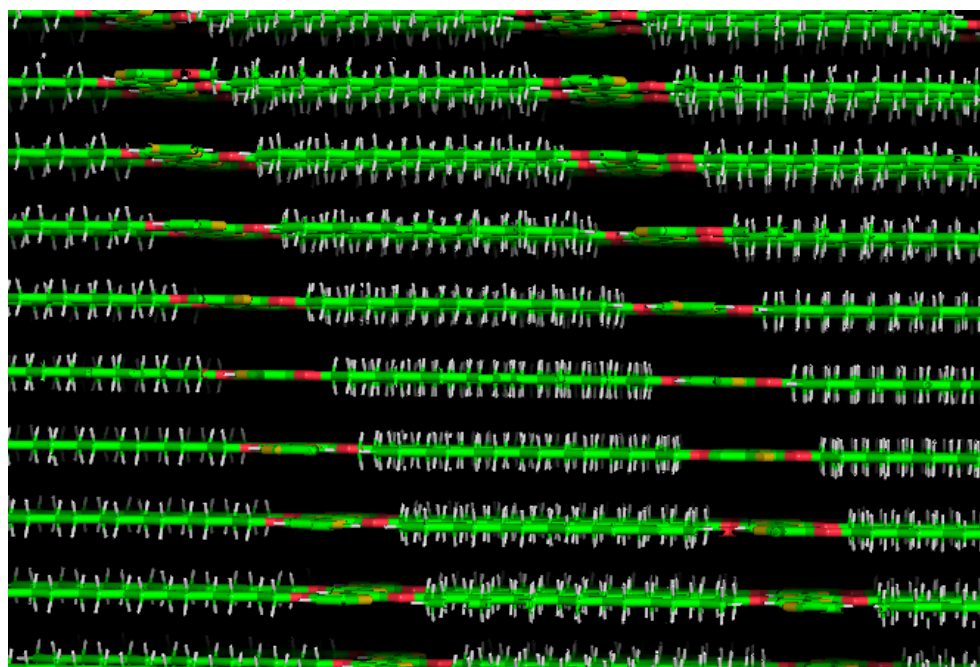


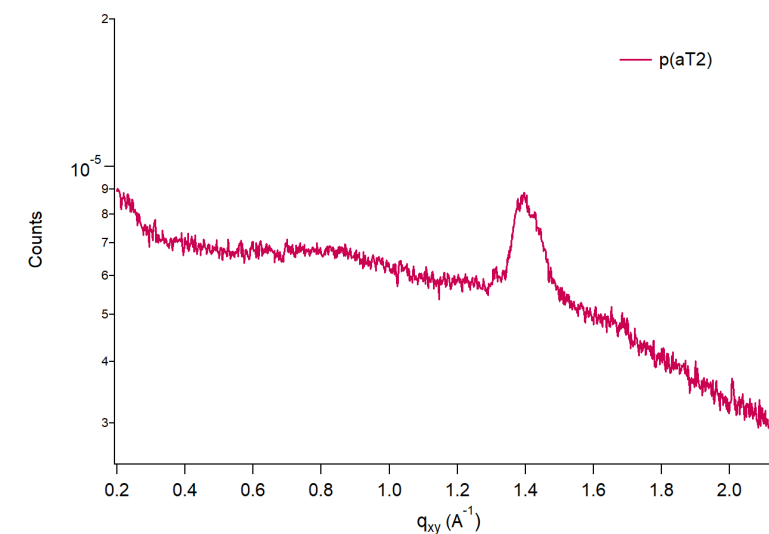
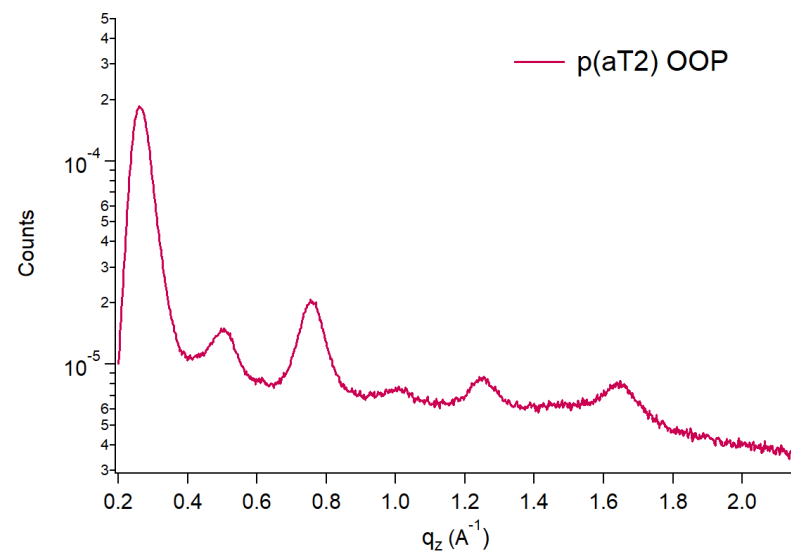
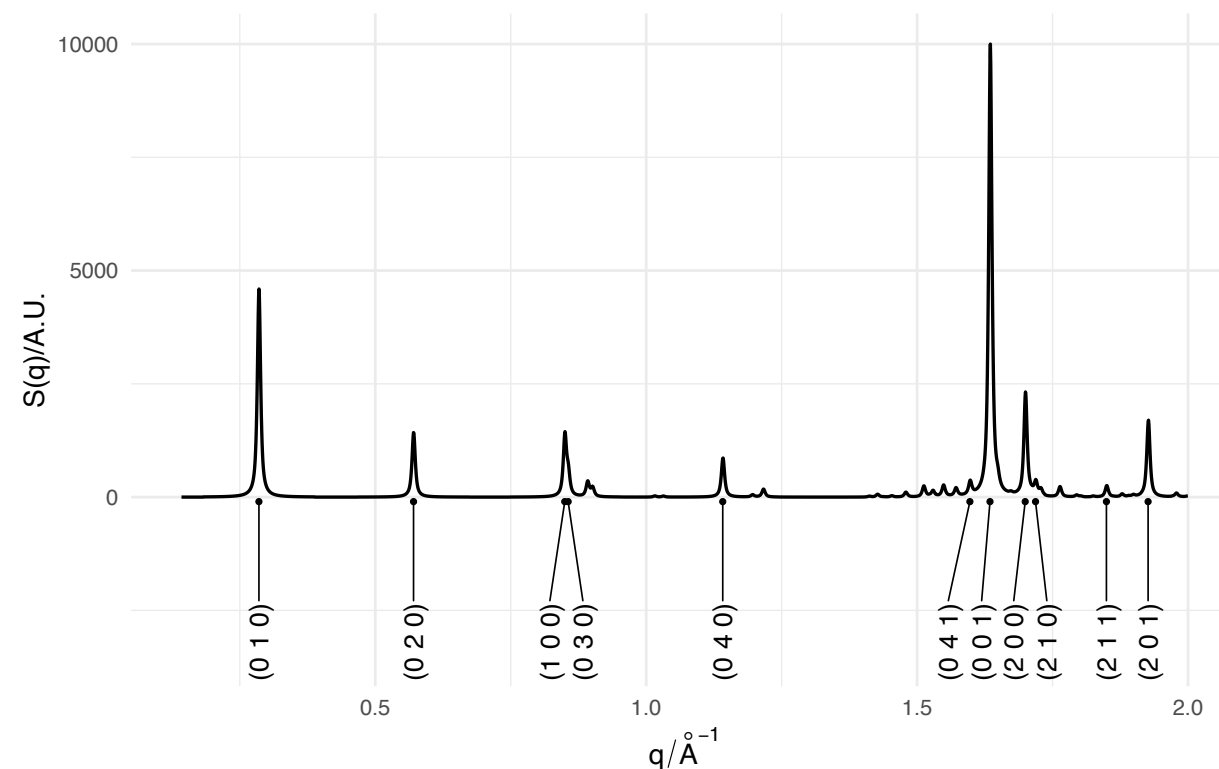
Testing alkylated crystal structure

Initial structure - inspired by monomer structure



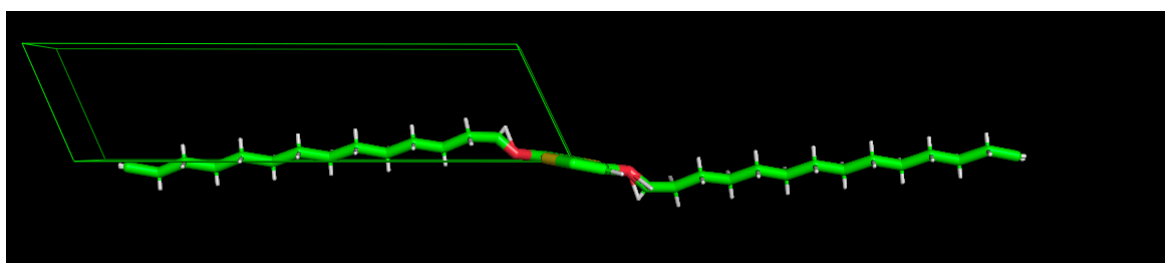
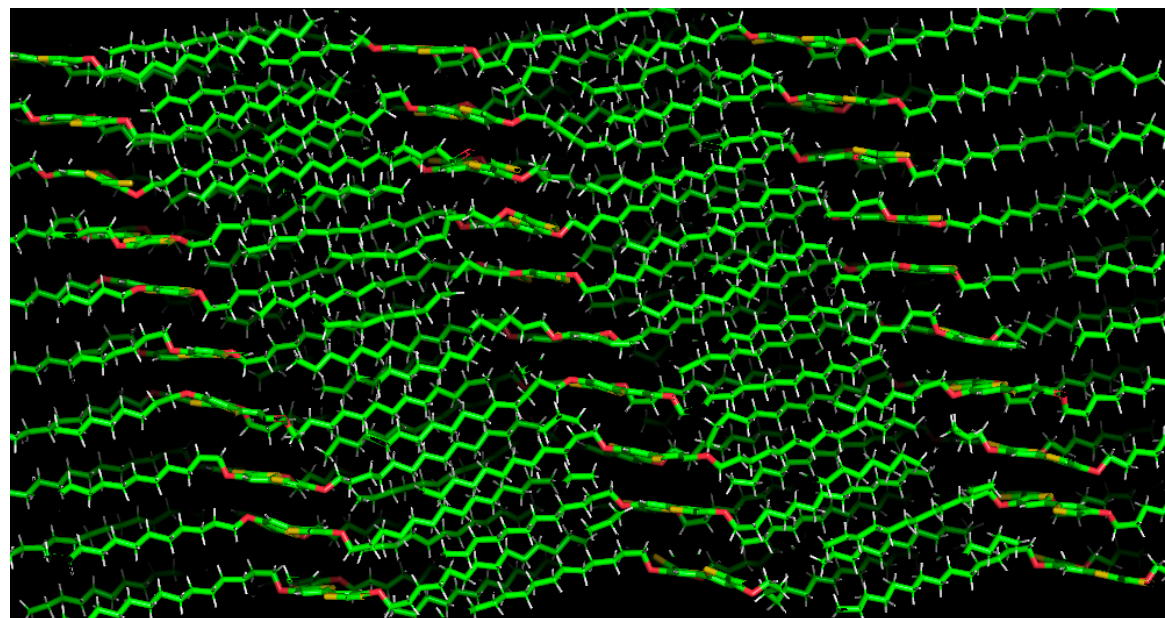
a = 7.95
b = 24.150
c = 4.4700
alpha = 65.78
beta = 68.47
gamma = 80.52

- straight side chains
- Unit cell angles chosen to replicate the pi-pi stacking as seen in the monomer structure

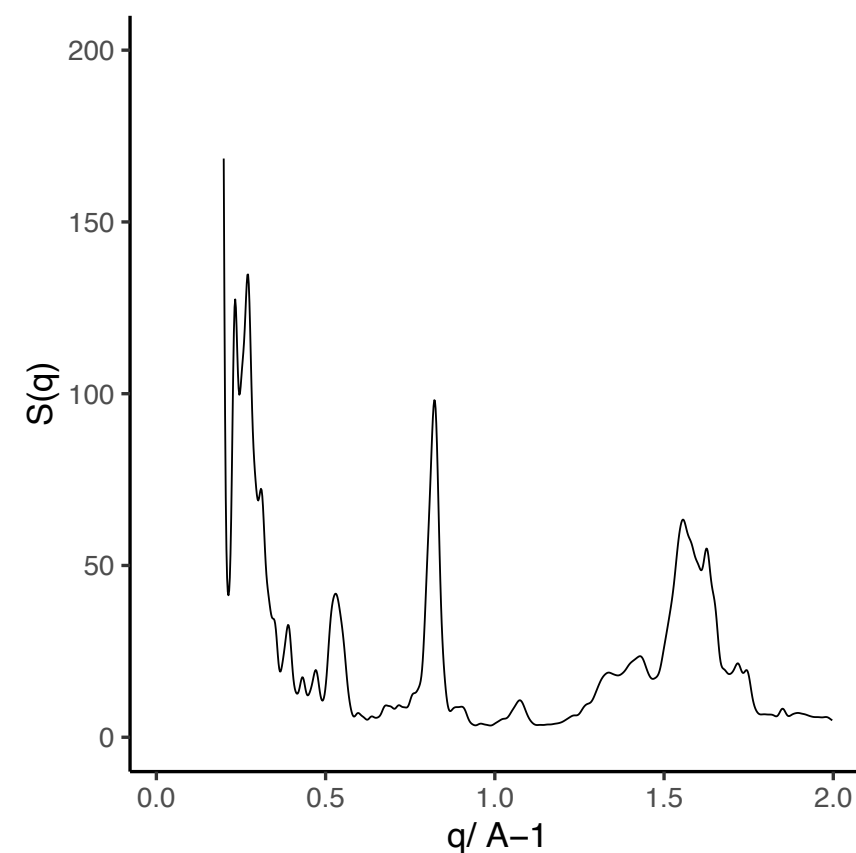
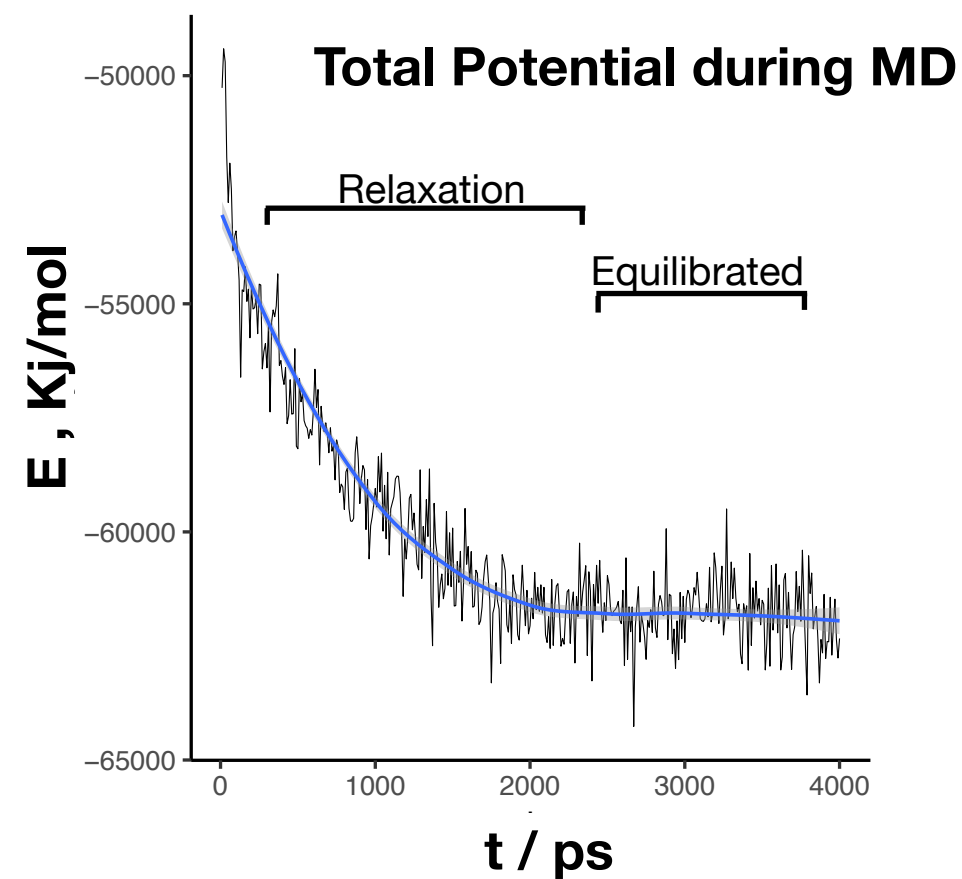


pre-MD spectra (top) calculated from Mercury strongly agrees with measurements from Camilla and Alex (bottom)

After MD



$a = 7.67$
 $b = 21.85$
 $c = 5.84$
 $\alpha = 65.27$
 $\beta = 79.60$
 $\gamma = 92.02$



**Very strong agreement in the peaks
from MD and from Alex and Camilla!**