1 - Introduction
A group of amine-oxides was selected as being of interest for the following reasons:
- They form monolayers, bilayers and micelles just as lipids do
- Surfaces made from such molecules are protein resistant, making these molecules biocompatible.
- They could be potential drug delivery systems, since molecules contained within would be protected.

2 – Single Molecule Studies
0.5 ns equilibration, 1 ns simulation. NPT ensemble.

- Molecules 2 and 5 curl to reduce hydrophobic surface area
- Molecules 1, 4 and 3 curl, then uncurl and chains compress instead

2.1 Solvation distance for oxide 1
![Graph showing solvation distance](image)

2.2 Solvation distances (distribution of water as function of distance) differ only slightly between oxide 3 and the other molecules – the nitrogen atoms have different constraints.

2.3 Average Hydrogen bonding during simulation is similar for most molecules, but not oxide 3: less affinity at oxide site so water moves to carbonyl.

<table>
<thead>
<tr>
<th></th>
<th>Oxide 1</th>
<th>Oxide 2</th>
<th>Oxide 3</th>
<th>Oxide 4</th>
<th>Oxide 5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carboxyl O</td>
<td>0.999</td>
<td>0.991</td>
<td>1.172</td>
<td>1.011</td>
<td>0.954</td>
</tr>
<tr>
<td>Oxide O'</td>
<td>2.073</td>
<td>2.227</td>
<td>1.970</td>
<td>2.145</td>
<td>2.251</td>
</tr>
</tbody>
</table>

3 – Multiple Molecule Studies
Same conditions as for single molecules, using N = 2, 4 and 8, spaced 4 Å apart.
Still 0.5 ns equilibration and 1 ns simulation.
Aggregation not always seen in this length of simulation.
In N = 8 studies a single, but disordered, mass of molecules formed.

4 – Conclusions and Further Work

**Aggregation was seen** in these simulations, as was normal amphiphilic behaviour in single molecules.
Formation into any kind of micelle was not seen.

Simulations using **many more molecules** may show better formation of structures.
Simulations using molecules **bound to a surface** (Au or Si) should also be attempted.

5 - References