### Imperial College London

# Department of Chemistry Third Year Advanced Practical Organic Chemistry

### Experiments 8 & 9

# Computer Assisted Molecular Modelling and Medchem Homology Modelling

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## INTRODUCTION TO COMPUTATIONAL TECHNIQUES FOR ORGANIC CHEMISTRY

There are two experiments. You will be allocated *ONE* of these experiments to complete:

#### **EXPERIMENT 8:**

### COMPUTER ASSISTED MOLECULAR MODELLING

Details of this experiment can be found on the departmental web site at the following URL: <a href="http://www.ch.ic.ac.uk/local/organic/t5.html">http://www.ch.ic.ac.uk/local/organic/t5.html</a>

OR

#### **EXPERIMENT 9:**

### MEDCHEM HOMOLOGY MODELLING

Details of this experiment can be found on the departmental web site at the following URL: <a href="http://www.ch.ic.ac.uk/local/organic/9">http://www.ch.ic.ac.uk/local/organic/9</a> medchem.html

For either experiment you must submit your report by e-mail (e.g. as a Microsoft Word attachment) to: **organic-3@ic.ac.uk** 

### When doing so, please follow some simple guidelines:

- 1. Use Microsoft Word only
- **2.** Give files appropriate extensions (i.e. .doc). This prevents confusion when the files may travel through a Windows system.
- **3.** Try to send just one file. If not possible, create an archive first (ZIP, or use Dropstuff on a Mac).
- **4.** Give the file a name which includes your own name (i.e. don't call it report.doc)