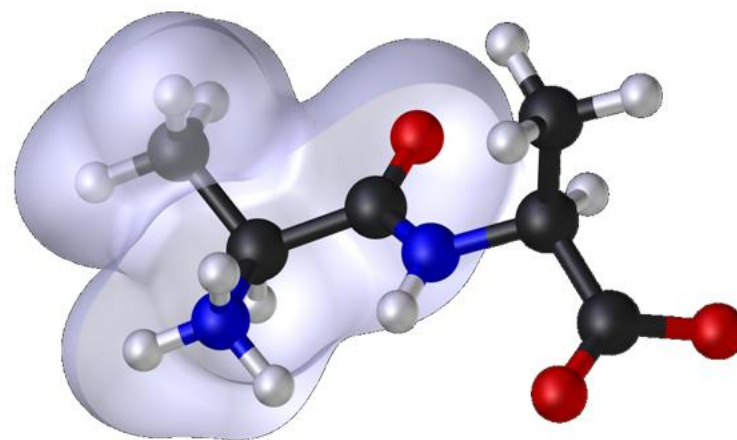


Why do computational chemistry?



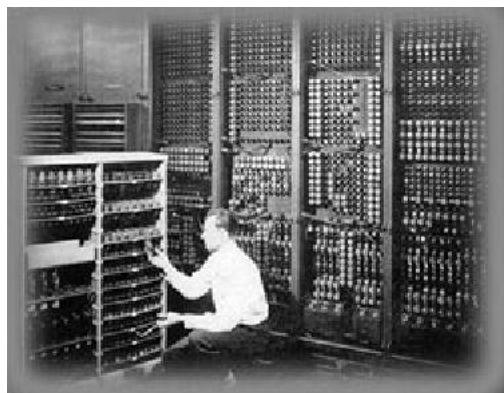
Lab work vs *in silico*



VS



Evolution of computational chemistry



1 The accelerating pace of change ...



2 ... and exponential growth in computing power ...

Computer technology, shown here climbing dramatically by powers of 10, is now progressing more each hour than it did in its entire first 90 years

COMPUTER RANKINGS

By calculations per second per \$1,000



Analytical engine
Never fully built, Charles Babbage's invention was designed to solve computational and logical problems



Colossus
The electronic computer, with 1,500 vacuum tubes, helped the British crack German codes during WW II

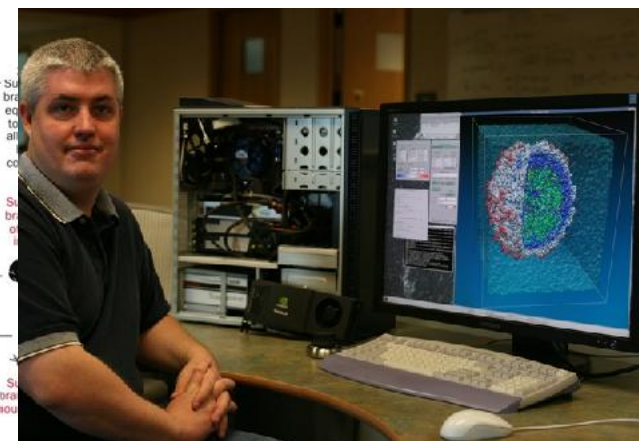
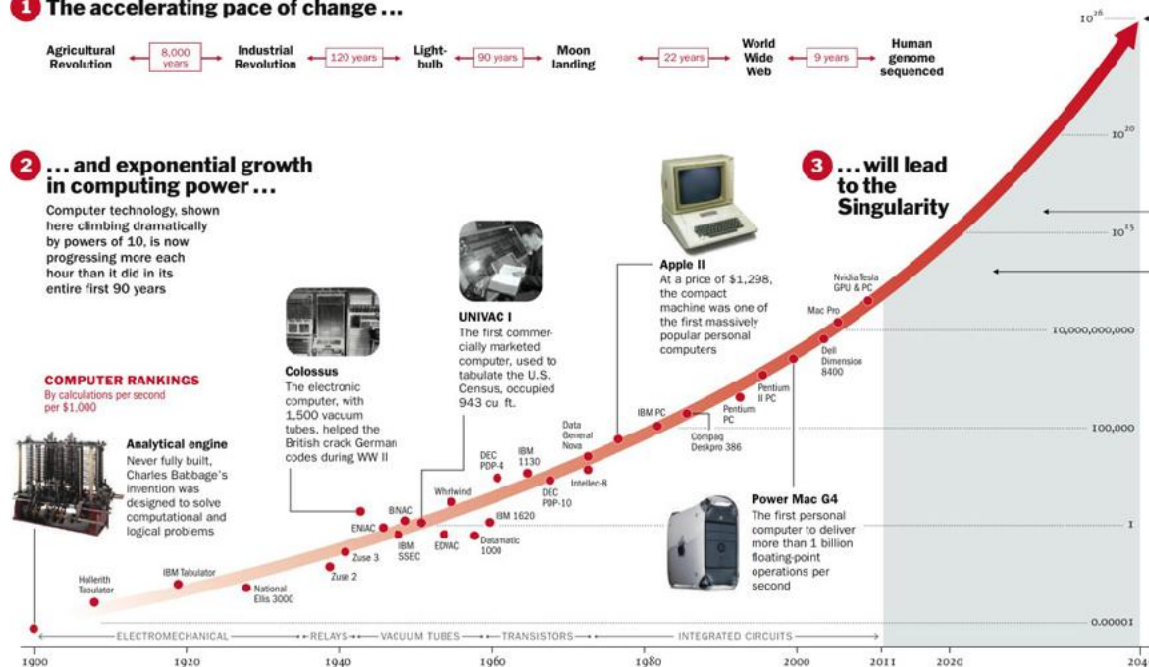


UNIVAC I
The first commercially marketed computer, used to tabulate the U.S. Census, occupied 943 cu. ft.

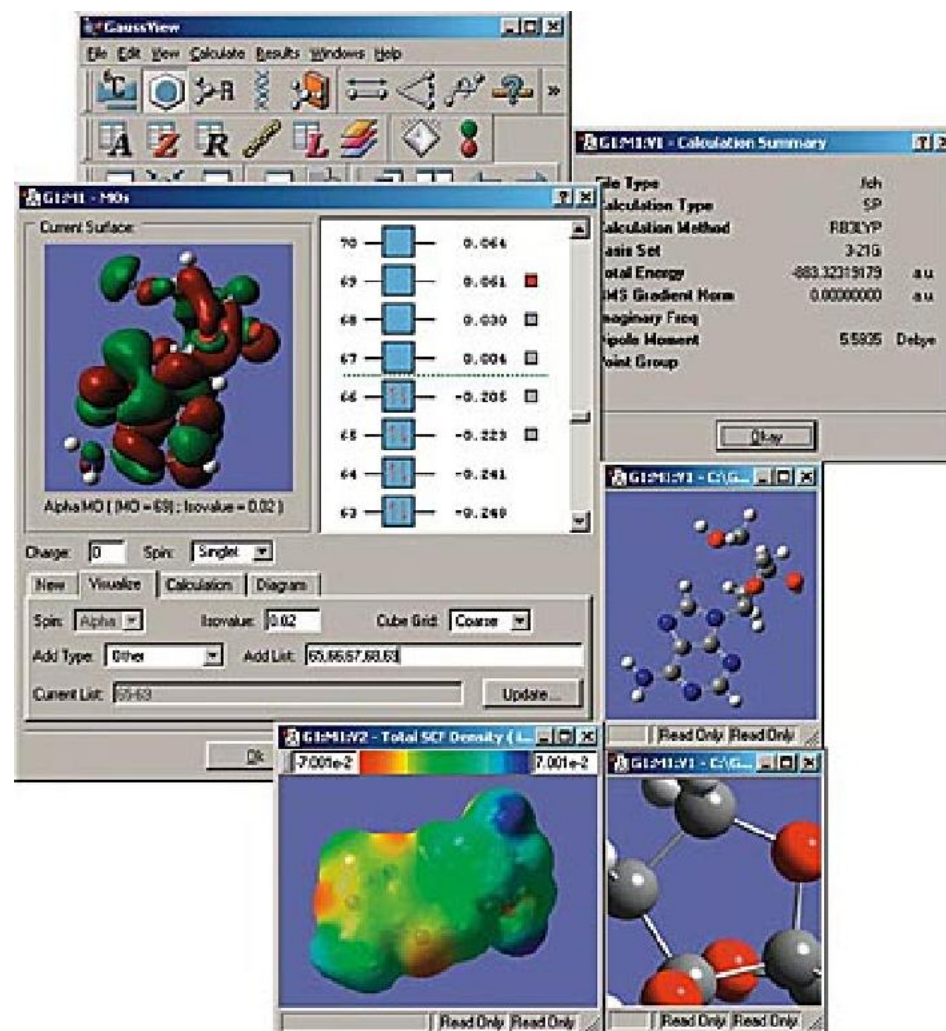
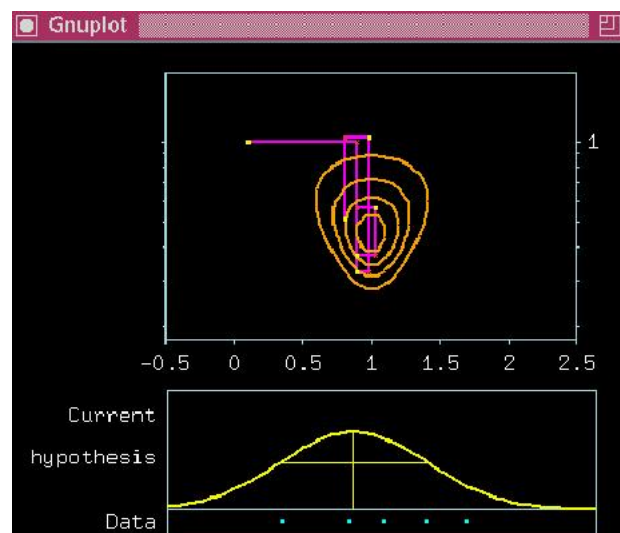
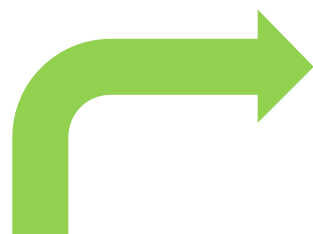


Apple II
At a price of \$1,298, the compact machine was one of the first massively popular personal computers

3 ... will lead to the Singularity



Evolution of computational chemistry



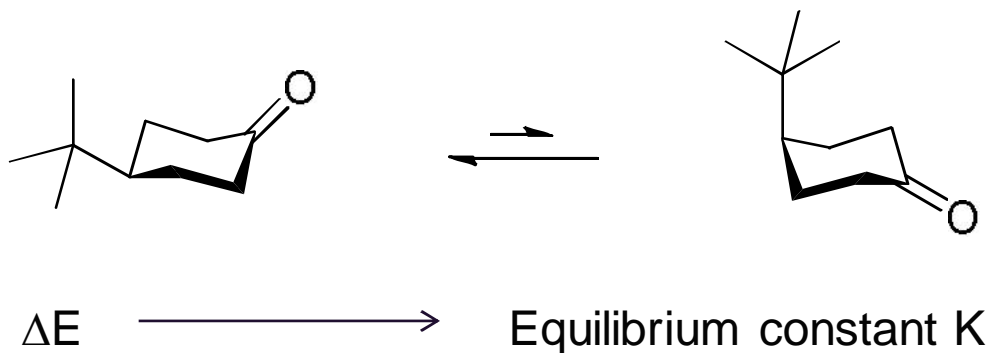
What computational chemistry brings

Computational chemistry can

- Explains chemical behaviours which might not be obvious to our chemical intuition.
- Predicts chemical behaviours from molecular properties and stability to reactivity and selectivity.
- Give us direct access to species which are not possible to observe with any physical or chemical techniques, i.e. transition states.

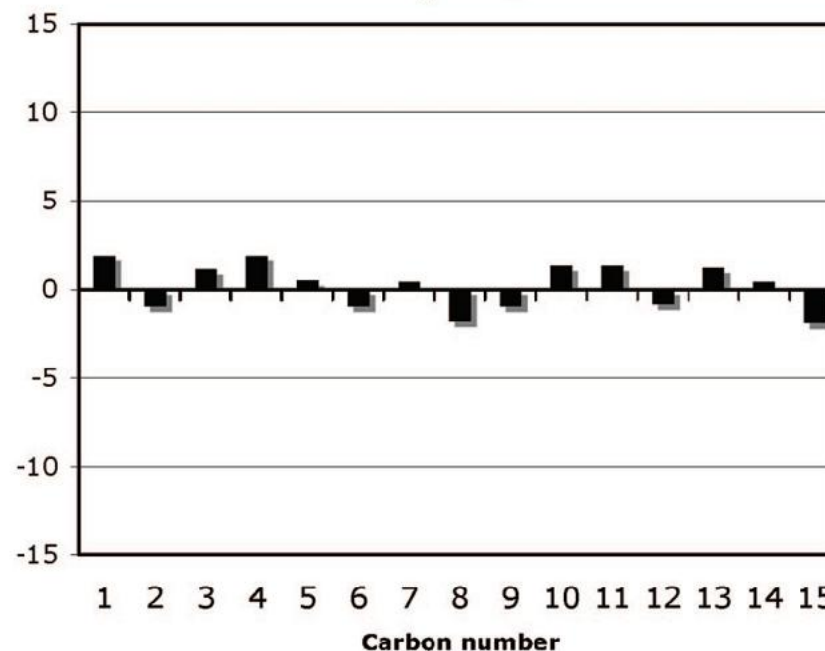
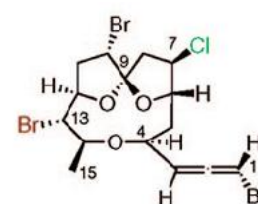
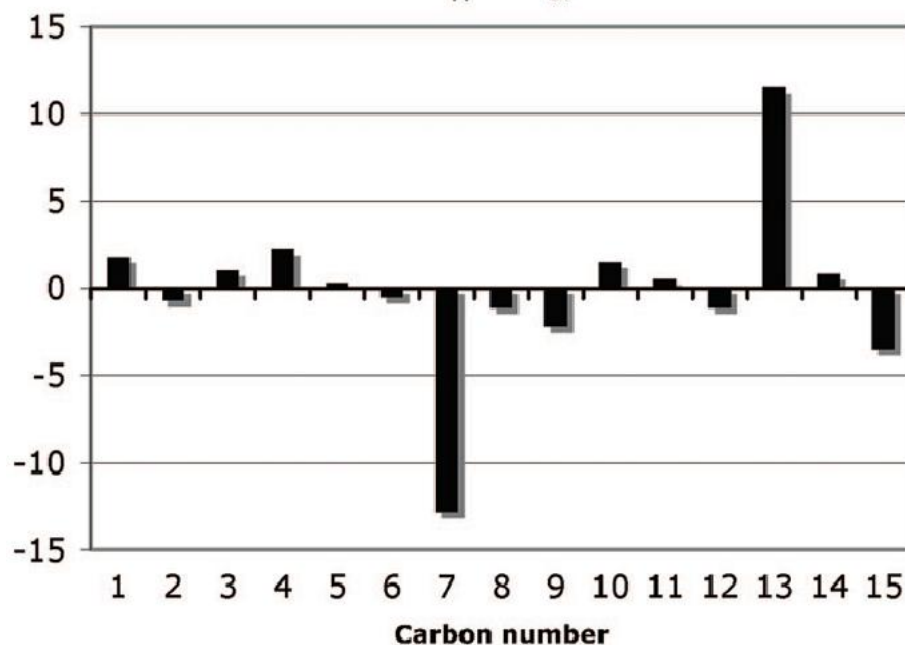
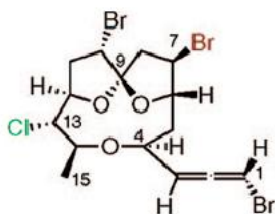
Some examples

- Energy minimisation and molecule visualisation, leading to insights about reactivity and stereocontrol.
- Comparison of energies of isomers of starting material/product can help understand and predict reaction outcomes.



Some examples

- Spectroscopic prediction can help assignment of complex molecules.

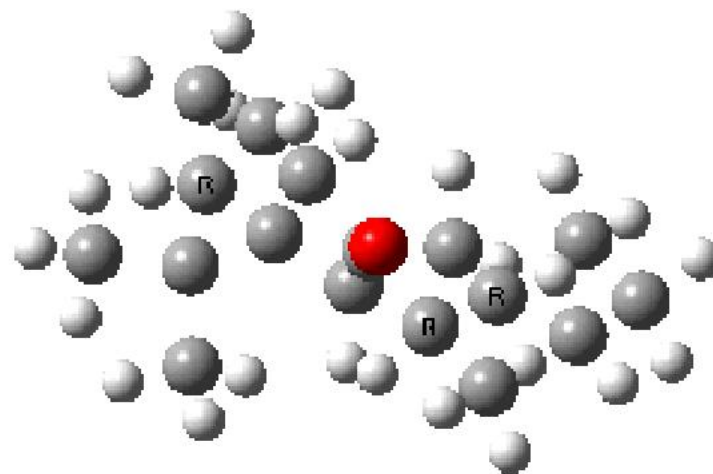
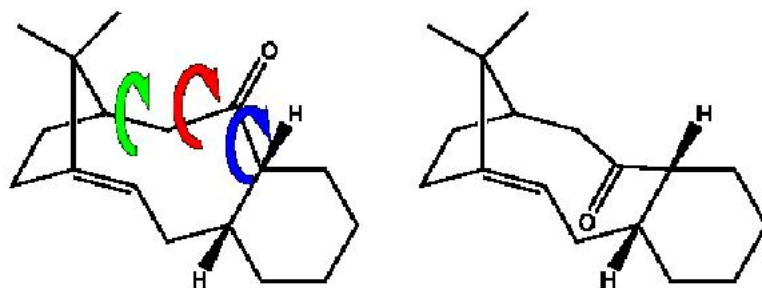


Some examples

- Molecular orbital calculations allow determination of their energy levels and visualisation of key orbitals to improve our understanding of bonding and reactivity (HOMO and LUMO).

<http://www.chemtube3d.com/Cycloaddition2.html>

- Transition state modelling



The course structure

- Module 1: Structure and Spectroscopy
 - Problems
 - Mini project
- Module 2: Bonding
 - Problems
 - Mini project
- Module 3: Transition States and Reactivity
 - Problems