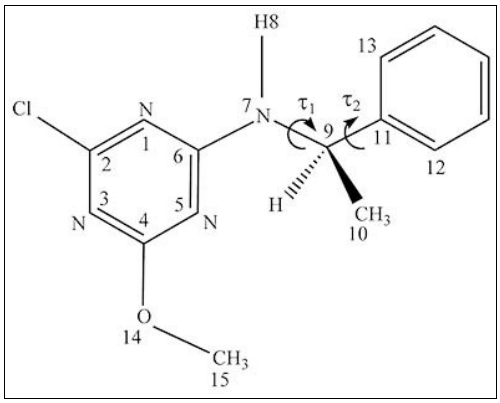
# Triazine

Triazine (2-chloro-4-methoxy-6-[(R)-1-phenylethylamino]-1,3,5-triazine) is a small molecule used as a chiral solvating agent in NMR spectroscopy studies. It is composed of 31 atoms, in a relatively simple structure made of two rigid disks connected by a bridge (see figure below).




*Triazine*

The different conformational positions that Triazine can assume are basically variations of τ1 and τ2, i.e. rotations around the two chemical links that connect N7, C9 and C11.

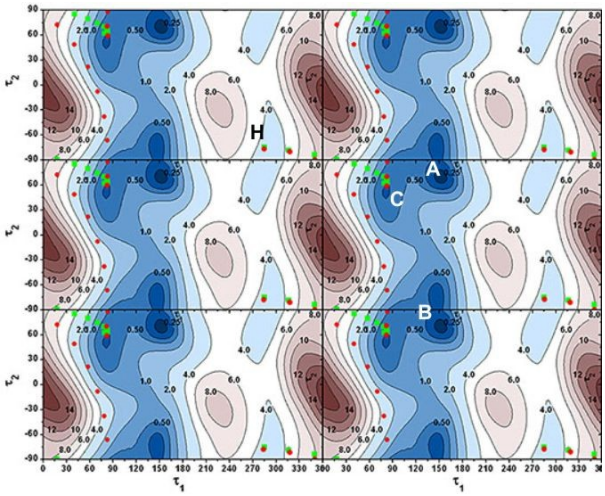
Triazine has been subject to dynamical simulation studies by Alagona et al (1), that have revealed the energy landscape for all possible conformations that it can assume. For this reason we chose it as the initial test molecule of our chemical Maya system.

The program used to import chemical data into Maya assigns every atom to a position. Atoms are linked through bones, which behave like chemical bonds, have fixed length, and are constrained by codified rules.

For each molecule, several positions can be imported, and assigned to different time points in the animation time (key-framed). The number of set positions imported and the time scale are decided by the operator.

For Triazine, we imported 4 conformers: the three minimal energy positions and one intermediate (H). We assigned the positions (in the order C-H-A-B) to 4 time points at 2 seconds intervals and let Maya interpolate transition conformers from one position to the others. One of the possible animations calculated can be seen in video. (A quite heavy version of high quality can be sent upon request).

Coordinates for all atoms in the intermediates positions calculated by Maya along two possible pathways between C and H were retrieved, fed back into pdb-like files and entered into Origin chemical software, allowing for physico-chemical evaluation of the path calculated by Maya. The positions of the paths are indicated in the Figure as dots on the Energy Landscape.




Note that the path labelled with red dots, which includes an almost 180° rotation of the phenyl ring, spans the energy field more than once. This is because the energy is calculated on a chemical basis, where Carbons 12 and 13 are equivalent; however, in a topological view, each of them has its own identity, and the landscape is in fact twice as large.

These results show that Maya can calculate paths avoiding the energy peaks, i.e. describing a movement that is chemically acceptable, flowing naturally in the 'valleys' of the landscape.

Further work is ongoing on different molecules.


1. Alagona, G., Ghio, C., Monti, S. (2006). A Test Case for Time-Dependent Density Functional Theory Calculations of Electronic Circular Dichroism: 2-Chloro-4-Methoxy-6-[(R)-1-Phenylethylamino]-1,3,5-Triazine (accepted).