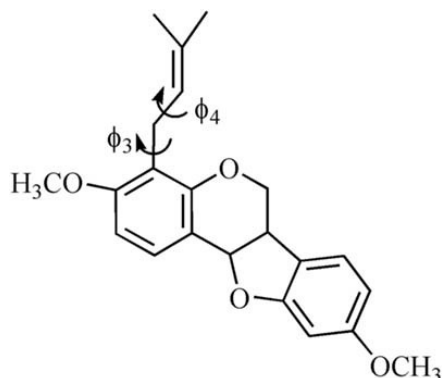


Bitucarpin A

Bitucarpin A, a plant chemical, was used as an example of movement calculated by Maya.



We imported into Maya the positions corresponding to 4 'low sites' in the energy map, and let Maya interpolate between them. The animation, rendered as blobby particles (see video) with surface displacement, shows the entire molecule and the part most active in the movement, as calculated by Alagona et al. (Alagona, G., Ghio, C. and Monti, S. B3LYP/6-31G* conformational landscape in vacuo of

some pterocarpan stereoisomers with biological activity. *Phys. Chem. Chem. Phys.*, 2004, 6, 2849-2857).

Intermediate positions were plotted on the energy map, and reveal that the path calculated by Maya is entirely consistent with the energy landscape.

