A Study of the Flexibility of Calicheamicin γ_1 and Esperamicin A_1

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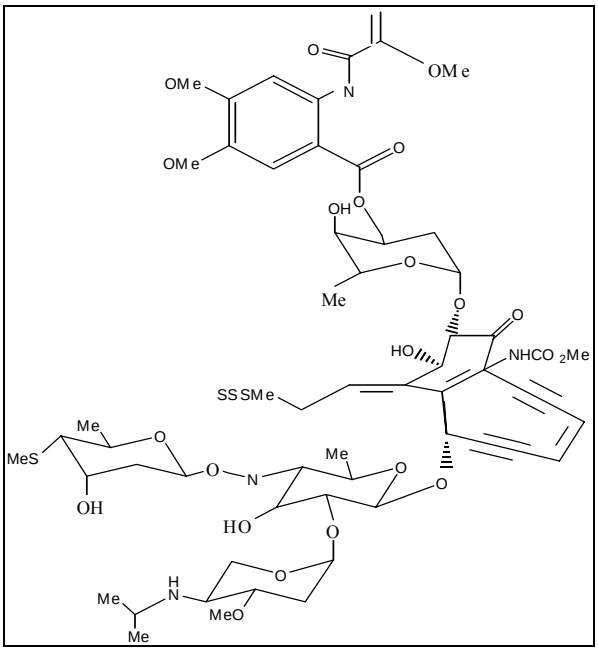
The aim of this study is to understand the behaviour of the anti-cancer drugs Calicheamicin γ_1 and Esperamicin A_1 in aqueous solution. In order to achieve this, the flexibility of the molecules must be investigated.



Esperamicin A_1

In this project the flexibility of the aforementioned drugs was investigated using molecular modeling. Molecular behavior was determined using the LM:MC conformational search algorithm to search exhaustively the potential energy surface generated using the new OPLS2005 force field along with the GBSA continuum solvent model for water. This allowed the identification of the global minimum energy structure along with all low energy, accessible conformations for Calicheamicin γ_1 and Esperamicin A_1.