

# Determining the Roles of Auxiliary Structures of Dynemicin A in Bergman Cyclization

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Dynemicin A has the potential for novel cancer treatments. Eneidyne within the molecule are converted, via Bergman Cyclization, into para-benzyne, a diradical responsible for destroying cancer cells. However, the enediyne typically associated with Bergman Cyclization is also accompanied by more complex auxiliary structures within Dynemicin A. This study seeks to investigate the role these structures have in the Bergman Cyclization of Dynemicin A. The activation barriers and reaction energies are calculated for various structures using density functional theory with a 6-31G\* basis set and a B3LYP functional.

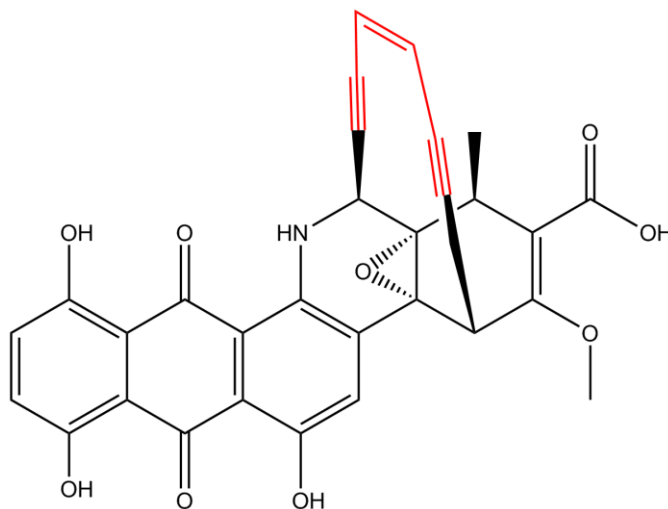


Figure 1. Chemical Structure of Dynemicin A (Enediyne Shown in Red)