

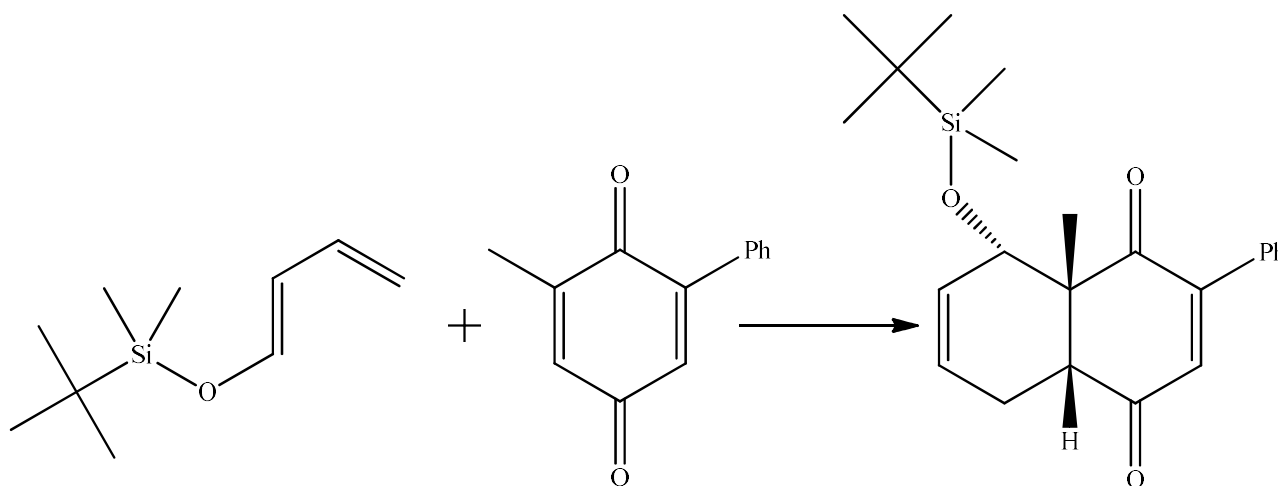
# Reaction Energetics & Diels-Alder Reaction Profiles for Enediones and Decalines by Means of DFT

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The original goal of our study was an energy comparison between isomers of several forskolin derivatives. Relative stabilities of decalines and related enediones were assessed with respect to *cis/trans* isomerism at the ring junction as well as with respect to axial/equatorial position of *tert*-butylsilyloxy substituent.

A comparison with experiment motivated us to perform a reaction path analysis for enedione synthesis from *cis*-(*tert*-butyldimethylsilyloxy)buta-1,3-diene with *p*-benzoquinone, which has been substituted by methyl and phenyl/naphthyl groups in the positions 2 and 5, respectively. Our results demonstrate that all energy barriers are quite close to each other (it is about 19–23 kcal mol<sup>-1</sup>). The mechanism of the substituted *p*-benzoquinone addition to butadiene appears to be a non-concerted one.

All calculations were performed by means of density functional theory (DFT) employing the B3LYP/6-31G\* implementation along with the SMD implicit solvation model of toluene and tetrahydrofuran.



**Figure 1:** Example of the synthesis within Diels-Alder reaction.