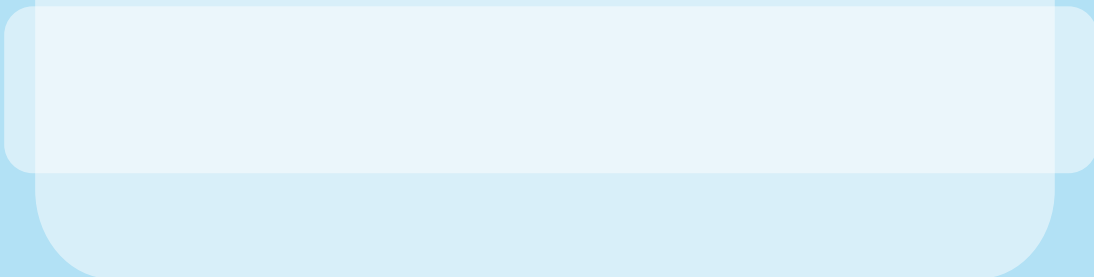


Jurnal Ilmiah
FARMASI

(Scientific Journal of Pharmacy)



JURNAL ILMIAH FARMASI
(SCIENTIFIC JOURNAL OF PHARMACY)

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Dekan Fakultas Matematika dan Ilmu Pengetahuan Alam
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**EKSPLORASI SIFAT FISIKOKIMIA 2-BENZILIDEN-SIKLOHEKSANA-1,3-DION
BERDASAR PERHITUNGAN KIMIA KUANTUM SEMIEMPIRIK**

Enade Perdana Istyastono

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ABSTRACT

Aromatic cyclic endione has been predicted qualitatively as anticancer agent. 2-Benzylidene-cyclohexane-1,3-dione is the simplest aromatic cyclic endione compound. Physicochemistry properties of 2-benzylidene-cyclohexane-1,3-dione have been explored. The properties were explored by semiempirical quantum-chemical calculations using the computational chemistry approach. Vibrations spectrum of 2-benzylidene-cyclohexane-1,3-dione has been used to determine the best semiempirical method. The AM1 semiempirical method was found to be the most appropriate method to describe the structure of 2-benzylidene-cyclohexane-1,3-dione and explore the physicochemistry properties.

Keywords : *anticancer, physicochemistry, semiempirical quantum-chemical calculation, 2-benzylidene-cyclohexane-1,3-dione.*