

Tipe Koleksi: Indeks Artikel Jurnal

Eksplorasi sifat fisikokimia aspirin dengan pendekatan perhitungan kimia kuantum semiempirik

Enade Perdana Istyastono

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Abstrak

Acetyl salicylic acid (aspirin) has been known as anti-inflammatory agent since 1897 and still being used until now. The physicochemistry properties of aspirin have been explored by semiempirical quantum-chemical calculations using the computational chemistry approach. Electronic spectrum of aspirin has been used to determine the best semiempirical method. The MNDO semiempirical method was found to be the most appropriate method to describe the structure of aspirin and explore its physicochemistry properties.