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Abinitio Quantum Mechanic Calculations of New Models of 6-Methoxy Substituted Naphthalene Derivatives[#]

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Abstract: The 6- methoxy -2-alkyl naphthalene derivatives Naproxen, Nabumetone are analgesic and non steroidal anti-inflammatory drugs of the arylalkanoic acids family. It is they are used to relieve pain or inflammation caused by arthritis. In an effort to increase affinity and selectivity at receptor side. Nitric oxide (NO) is an important biological messenger involved in a variety of physiological processes .New series of 6-methoxy -2- naphthyl derivatives were synthesized and identified their structures using FTIR spectrophotometer and ^{1}H NMR and ^{13}C NMR techniques .A new chemical entity with analgesic activity will introduced exhibiting (COX inhibiting nitric oxide donors, CINODs) may increase analgesic activity. Molecular modelling calculations (MM) showed the compound with lowest strain energy (S.E) is the more stable form , as well as application of Lipinski s rule for calculated drugs , and expected acts as nitric oxide donors.

Keywords: *Nitric oxide, NSAIDs, CINODs, analgesic activity, strain energy.*

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