Chem Sci J 2018, Volume 9
DOI: 10.4172/2150-3494-C2-021

8th European Chemistry Congress

June 21-23, 2018 | Paris, France

Synthesis and conformational study of a new N Ferrocenyl indolone

Francisco Xavier Domínguez Villa
Universidad Nacional Autónoma de México, Mexico

Ferrocene derivatives have been of great interest in medicinal chemistry in the las two decades due to their diverse biological activities. The antimalarial Ferroquine and anticancer Ferrocifen have been widely studied since their discovery in the 90s. In the other hand, 4-indolones are an interesting class of compounds sinthetized by Ávila and coworkers that represent versatil precursos of molecules with biological activity, cytotoxic principally. In this work we present the synthesis of a N-ferrocenyl-4-indolone using as a starting material 5,5-dimethyl-1,3-cyclohexanodione and the subsequent Paal Knorr reaction using mild conditions to obtain the target compound in high yield (74%). Knowig the conformation of minimal energy is interesting due to the biological activity is determined by conformational changes between a drug and its receptor. So we also present its conformational study both in gas phase (theoretical calculations) and in solution (NOESY experiments). A rotation scan of ferrocenic fragment was carried out and the conformations of minnimal energy were determined, these strcutures were useful to find the most stable conformer using Density Functional Theory by the M062X method. The results show that in this reaction two atropoismers could be formed, however, under this conditions only one of them is obtained. The NOESY experiments were used to find what conformer is produced, and the interactions betweeen the ferrocenic protons and the protons of indolone were analysed and correlated with the structure of minnimal energy obtained from the teoretical caclulations.

fx.dominguezvilla@gmail.com