Synthesis, Characterization and Theoretical Calculation of 2-(2-hydroxy-4-methoxybenzylideneamino)-6-methyl (and ethyl)-4,5,6,7-tetrahydrobenzo[β]thiophene-3-carbonitriles as Potent Bioactive Molecules

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Heterocyclic thiophenes bonded to imine group are a kind of important structures which usually show diverse pharmacological profiles with antimicrobial, anticonvulsant, anti-inflammatory activities and agrochemical applications. S-heterocyclic core is present in many natural products, several of which show antifungal, antiamoebic, antitumor, anticoagulant and antithrombotic activities. Chemical modification and structure–activity relationship (SAR) studies of thiophene derivatives have yielded several inhibitors with improved potency.

Fig. 1. HOMO and LUMO shapes for 2-(2-hydroxy-4-methoxybenzylideneamino)-6-methyl-4,5,6,7-tetrahydrobenzo[β]thiophene-3-carbonitrile

In this work, heterocyclic thiophenes bonded to imine group were synthesized and characterized by elemental analyses, FT-IR, 1H-NMR and 13C-NMR techniques. Gaussian 09 software was used to obtain the most stable conformer of the compounds with DFT/B3LYP/6-311G (d,p) method. The physico-chemical parameters (binding energy, heat of formation etc.) and electronic parameters (HOMO, LUMO etc.) were calculated by using QSAR models in Hyperchem 8 to correlate the structure activity relation (SAR) for further approach.

References
3) Bello Forero, J.S.; Carvalho, E.M., Jones Junior, J.; Silva, F.M., Heterocyclic Lett. 2011, 1, 61