

Antibiotic property interpretation of Metronidazole; Spectroscopic and computational validation

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Abstract

In this attempt, the biological and drug importance of Metronidazole was studied by interpreting physico-chemical, structural and biological properties using FT-Raman, FT-IR, NMR and UV-Visible spectral datum along with computational results. The geometry optimization was made on molecular structure to calibrate stabilized structure to expose its definite physico-chemical property. The chemical mechanism for generating drug process by the physical injection of ethylhydroxy, methyl and nitro groups over imidazole base was evaluated. The molecular charge population delocalization per substituent was monitored and purpose of electron cloud accumulation on different entities was justified. The drug likeness score and bioavailability was tested on parametric values of molecule obtained from HyperChem and Osiris results and enzymatic target investigation made on theoretical results. The vibrational characteristics of every bonded element was evaluated and studied and patrician chemical energy over the bonds and their influences were tested. The chemical patrician potential was calculated by observing chemical shift of various core and allied carbon fragments and parallel the chemical reaction path mechanism to restore chemical kinetics to enable antimicrobial activity on the Metronidazole. The doubly degenerate interaction orbitals were viewed and the transitions assigned to facilitate the drug activity were studied. The toxicity profile was evaluated by opting enantiomer and validated by simulating VCD spectrograph.

Speaker Publications:

- 1 “Activity and safety of nivolumab, an anti-PD-1 immune checkpoint inhibitor, for patients with advanced, refractory squamous non-small-cell lung cancer (CheckMate 063): a phase 2, single-arm trial”; The Lancet, Volume 16, Issue 3, March 2015, Pages 257-265
2. “Adsorption of dye from aqueous solution by cashew nut shell: Studies on equilibrium isotherm, kinetics and thermodynamics of interactions”; Desalination, Volume 261, Issues 1–2, 15 October 2010, Pages 52-60
3. “ Nivolumab plus Ipilimumab in Lung Cancer with a High Tumor Mutational Burden: Journal of medicine

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Biography:

S Ramalingam completed education in Department of Physics, Jamal Mohamed College, Tiruchirappalli, Tamilnadu, India.