

Electronic Structure, Vibrational (FT-IR and FT-Raman), UV–Vis and NMR analysis of 5-(4-(2-(5-ethylpyridin-2-yl) ethoxy) benzyl) thiazolidine-2,4-dione by Quantum Chemical method

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Highlights

- Electronic structure and spectroscopic analysis on structural confirmation of pioglitazone were made using DFT methods
- Complete vibrational assignments were theoretically made and compared with experimental data
- The NBO, ^1H and ^{13}C NMR analysis were made and results interpreted
- MEP and HOMO – LUMO were discussed

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