

**Synthesis, antimicrobial and computational studies of natural products derivatives of tricarbonyl (2-methoxycyclohexadienyl)iron tetrafluoroborate salt: An alternative route to natural products modification.**

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**Abstract:** Biologically active natural products addition to [(1-5-η-2-MeOC<sub>6</sub>H<sub>6</sub>) Fe(CO)<sub>3</sub>][BF<sub>4</sub>] has resulted in its 1,3-diene substituted derivatives. The subsequent removal of the tricarbonyliron moiety of these derivatives through demetallation with trimethylamine-N-oxide (Me<sub>3</sub>NO), gave new organic compounds with enhanced antimicrobial properties as supported by quantum descriptors and QSAR measurements.

**Keywords:** Natural products, Tricarbonyl(2-methoxycyclohexadienyl)iron, Trimethylamine-N-oxide, Antimicrobial, computational studies.