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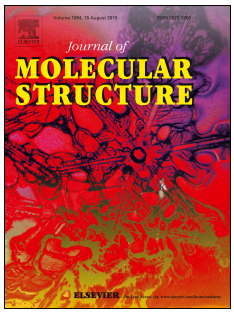

Investigation of potential anti-malarial lead candidate 2-(4-fluorobenzylthio)-5-(5-bromothiophen-2-yl)-1,3,4-oxadiazole: Insights from crystal structure, DFT, QTAIM and hybrid QM/MM binding energy analysis

Lamya H. Al-Wahaibi, Nandakumar Santhosh Kumar, Ali A. El-Emam, Natarajan S. Venkataramanan, Hazem A. Ghabbour, Abdul-Malek S. Al-Tamimi, Judith Percino, Subbiah Thamotharan

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GRAPHICAL ABSTRACT