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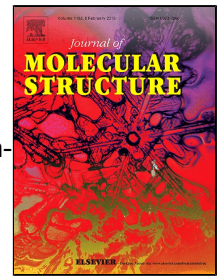

Carbonic anhydrase inhibition of Schiff base derivative of imino-methyl-naphthalen-2-ol: Synthesis, structure elucidation, molecular docking, dynamic simulation and density functional theory calculations

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Highlights

- Design and synthesis of Schiff base derivative
- Characterization by FT-IR, ^{1}H and ^{13}C NMR spectroscopy.
- Single crystal X-ray diffraction and NMR studies were performed.
- The synthetic compound was active against carbonic anhydrase II.
- Molecular docking and dynamic simulations studies were carried out.