## **Accepted Manuscript**

Presence of  $\pi...\pi$  and C-H... $\pi$  interactions in the new Schiff base 2-{(*E*)-[(3-*tert*-butyl-1-phenyl-1*H*-pyrazol-5-yl)imino]methyl}phenol: Experimental and DFT computational studies

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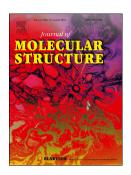
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#### ACCEPTED MANUSCRIPT

### **Graphical Abstract**

#### **HIGHLIGHTS**

- -The title compound was characterized by spectroscopic techniques such as elemental analysis, FT-IR, NMR, M.S., XRD and UV-Vis.
- -Quantum chemical calculations of compound  $\bf 3$ , using the DFT method, with the B3LYP functional and the 6-311++G(d,p) basis set, was performed.

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