



STRUCTURAL SCIENCE
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Supporting information for article:

Synthesis, crystal growth, characterization and DFT investigation of nonlinear optically active cuminaldehyde derivative hydrazone

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Supplementary information contains FT-IR, UV-Vis, GC-mass, LC-mass, elemental analysis and packing projection and crystal packing diagram along a, b and c axis and molecular electrostatic potential surface.

Figure S1 FT-IR spectrum of IBIHM (a) Experimental and (b) theoretical.

Figure S2 TG-DTA spectrum of IBIHM.

Figure S3 UV-vis spectrum of IBIHM.

Figure S4 GC-mass spectrum of IBIHM.

Figure S5 LC-mass spectrum of IBIHM.

Figure S6 Elemental analysis spectrum of IBIHM.

Figure S7 Packing projections of N-H...O bonding interactions of IBIHM.

Figure S8 Packing projections of N...H bonding interactions of IBIHM.

Figure S9 Packing projections of O...H bonding interactions of IBIHM.

Figure S10 Crystal packing showing hydrogen bonding interactions along 'a' axis

Figure S11 Crystal packing showing hydrogen bonding interactions along 'b' axis.

Figure S12 Crystal packing showing hydrogen bonding interactions along 'c' axis.

Figure S13 Molecular surfaces of IBIHM (a) MEP (b) contour MEP (c) ESP.

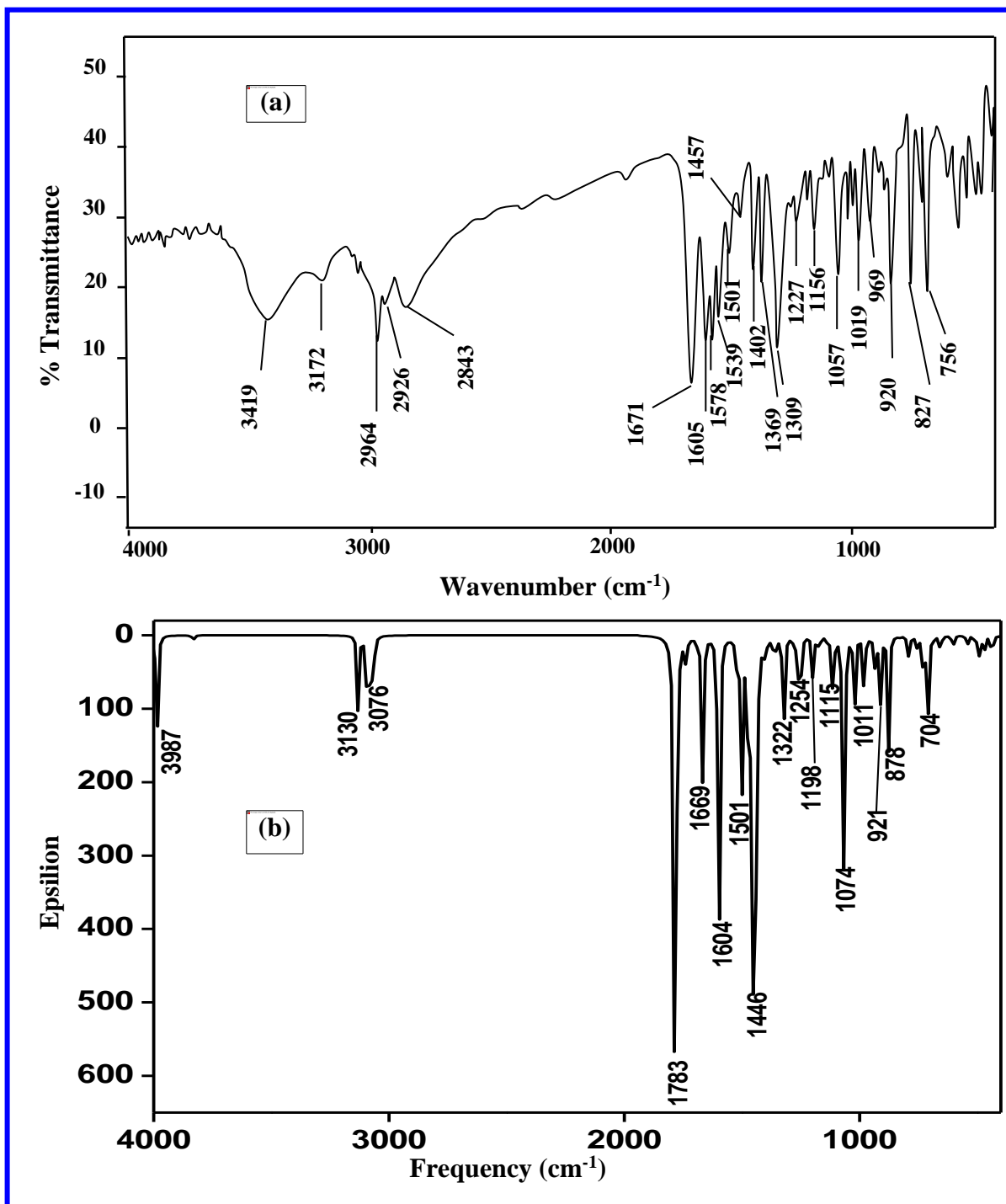


Figure. S1

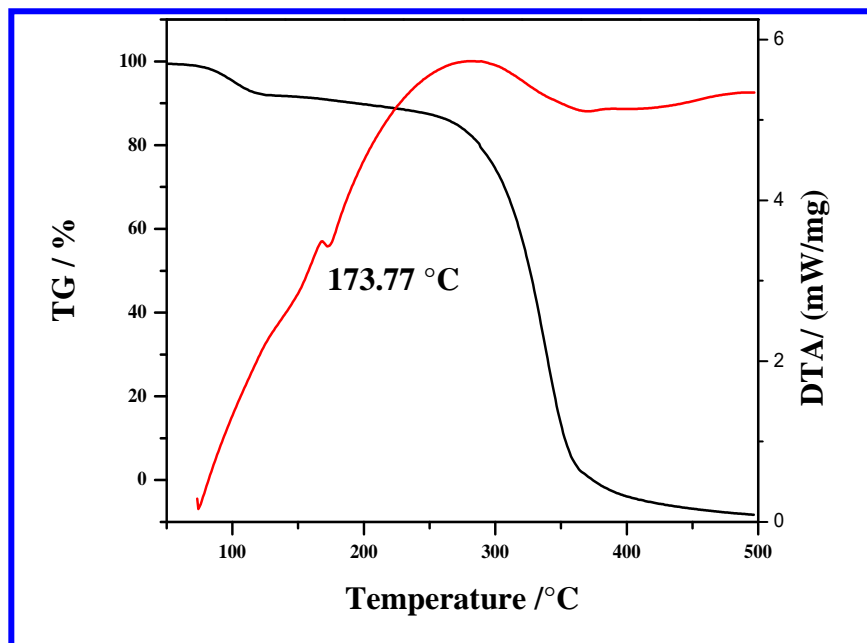


Figure. S2

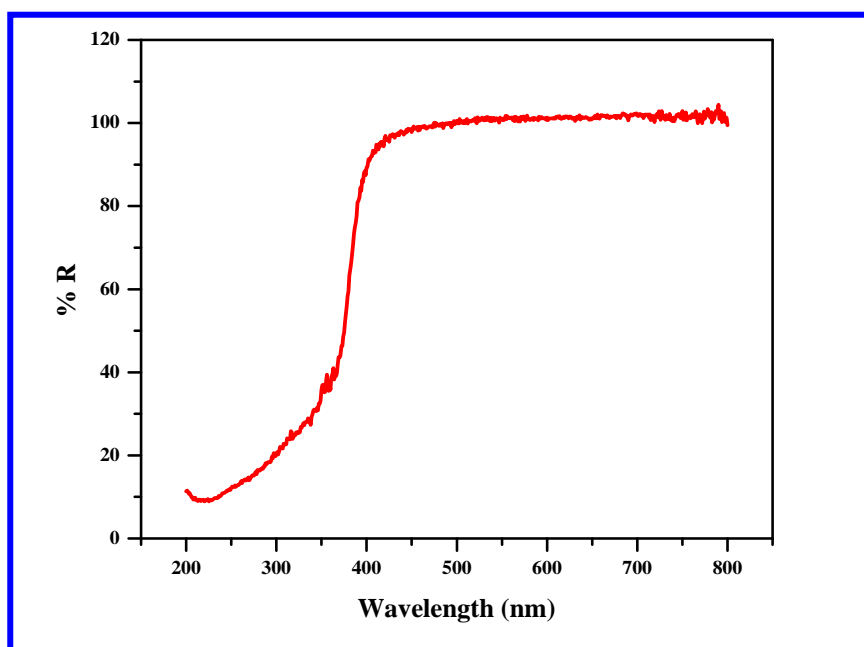


Figure. S3

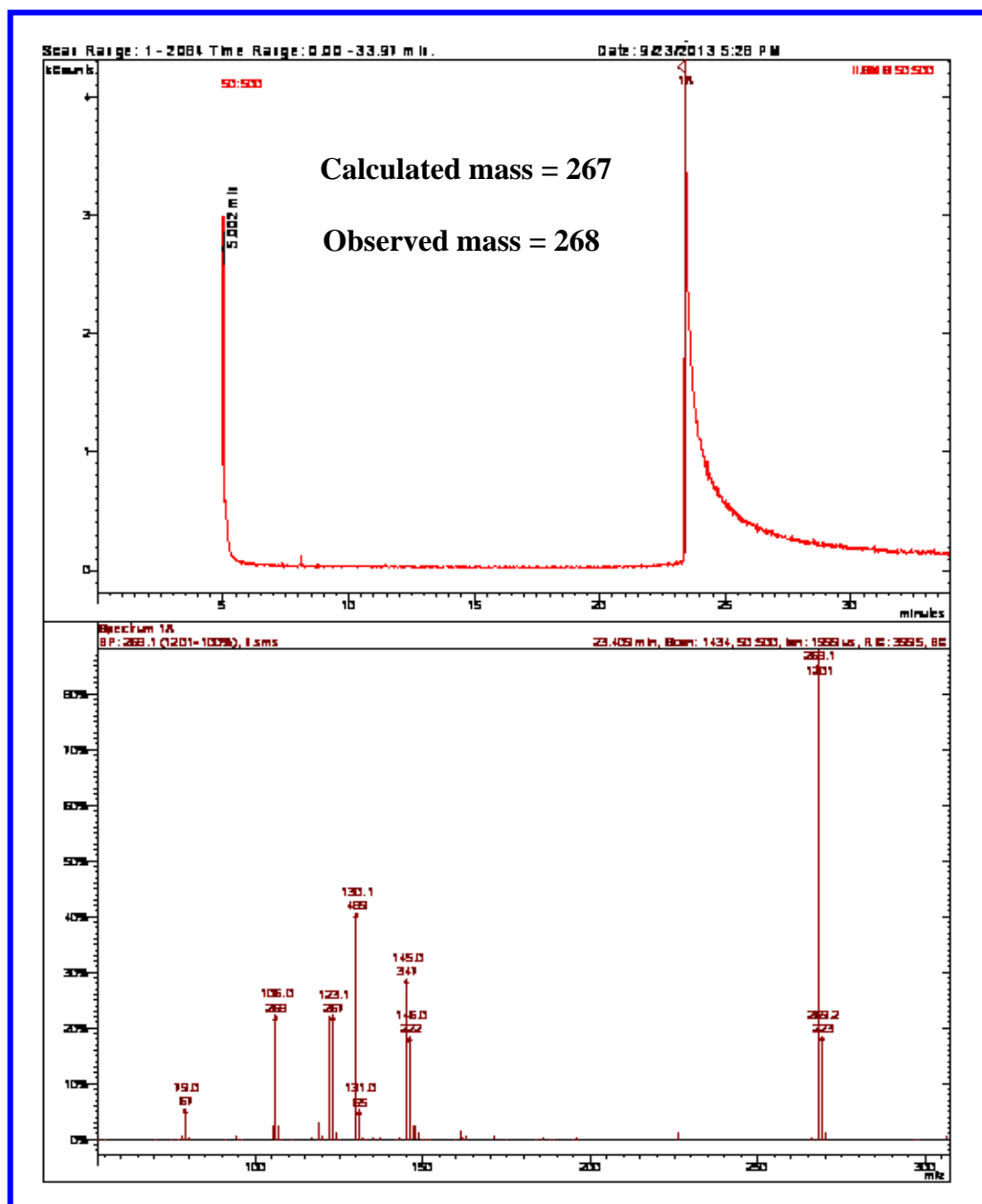


Figure. S4

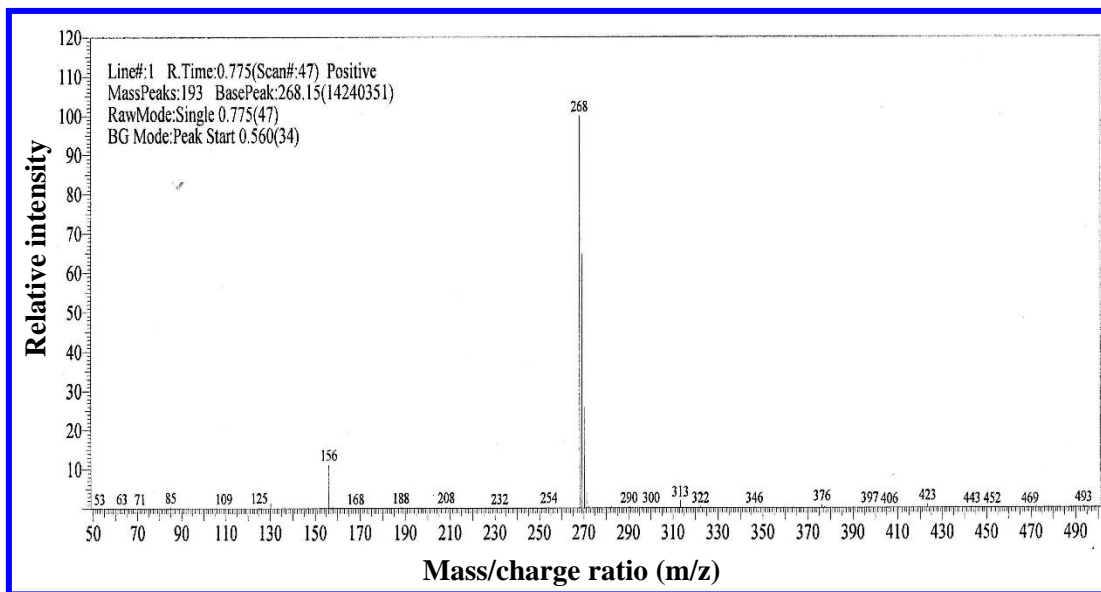


Figure. S5

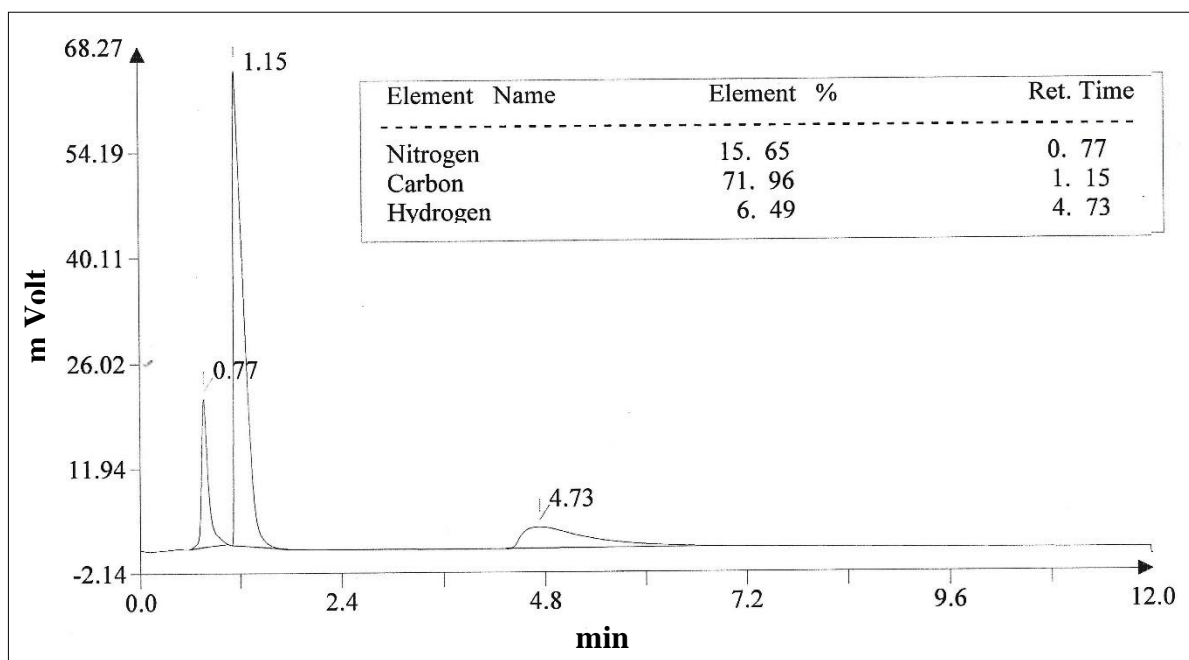
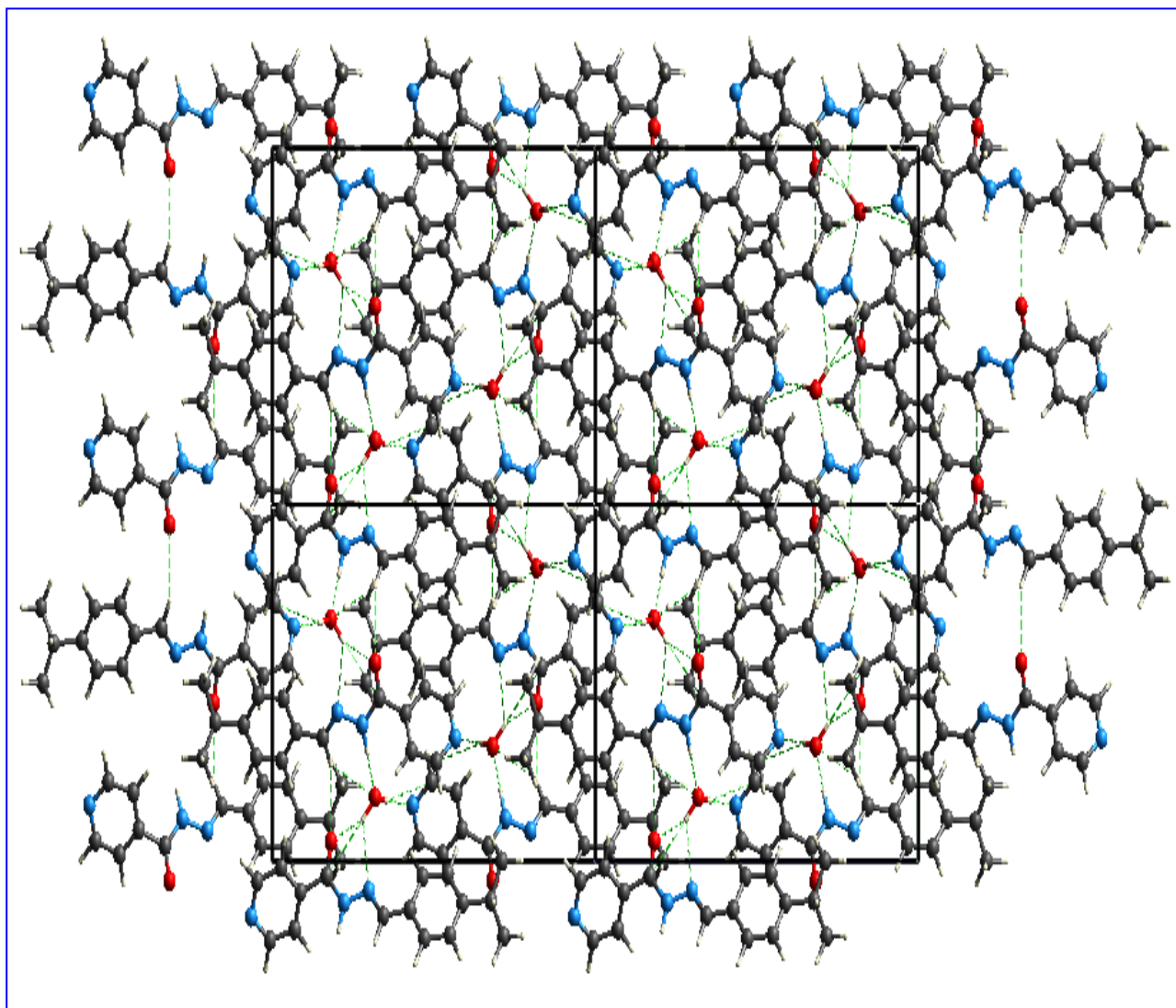


Figure. S6

**Figure. S7**

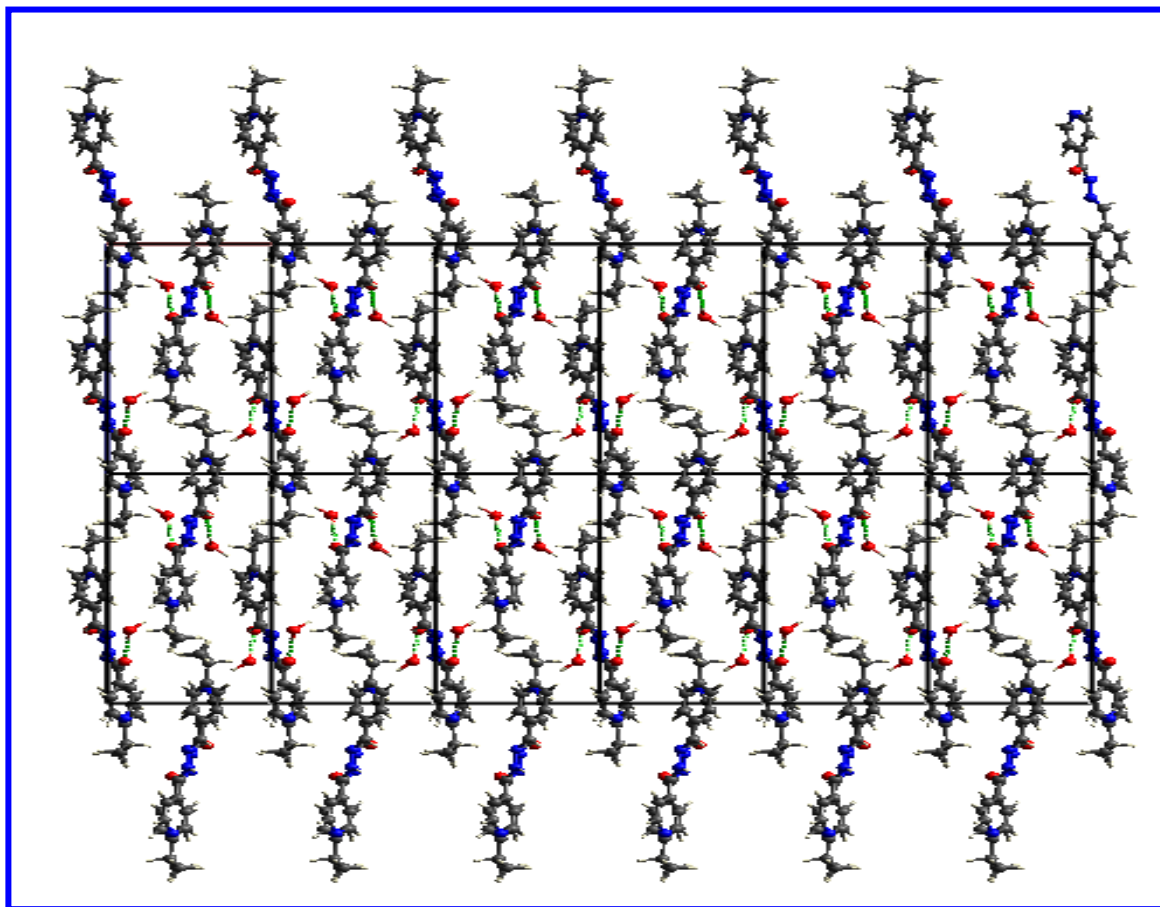


Figure. S8

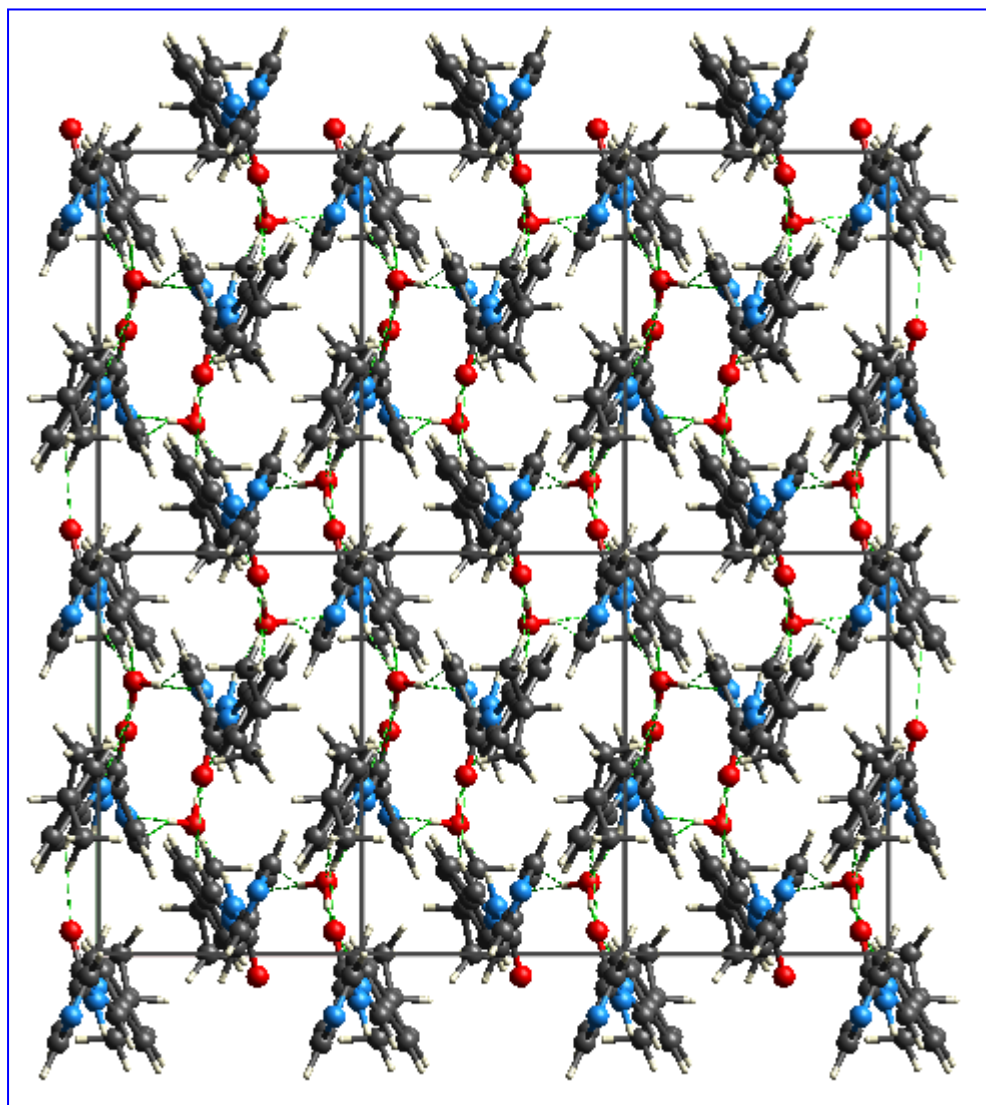


Figure. S9

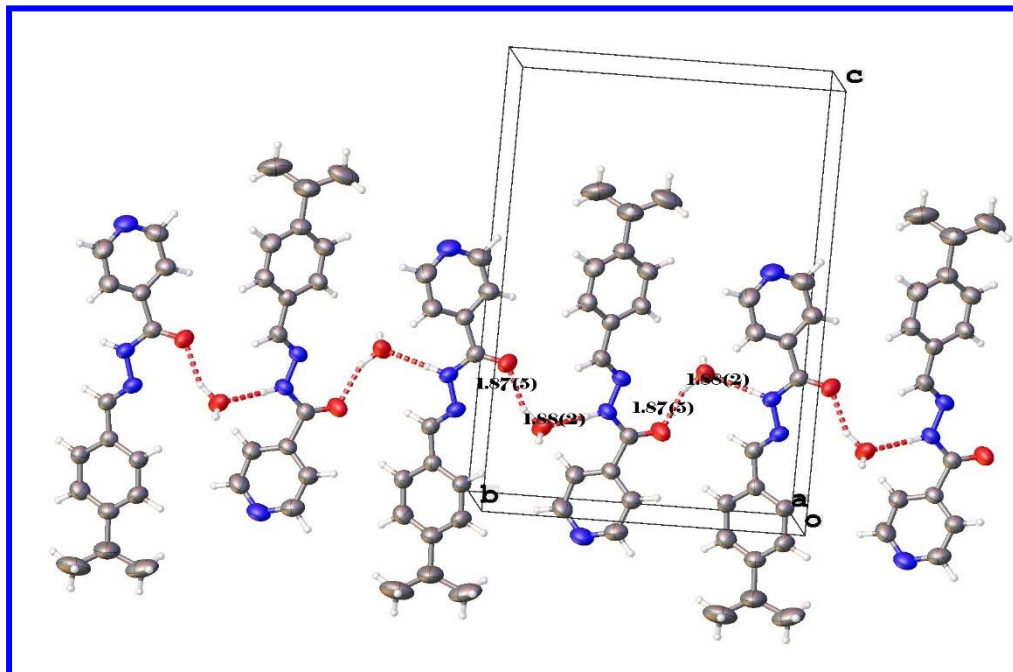


Figure. S10

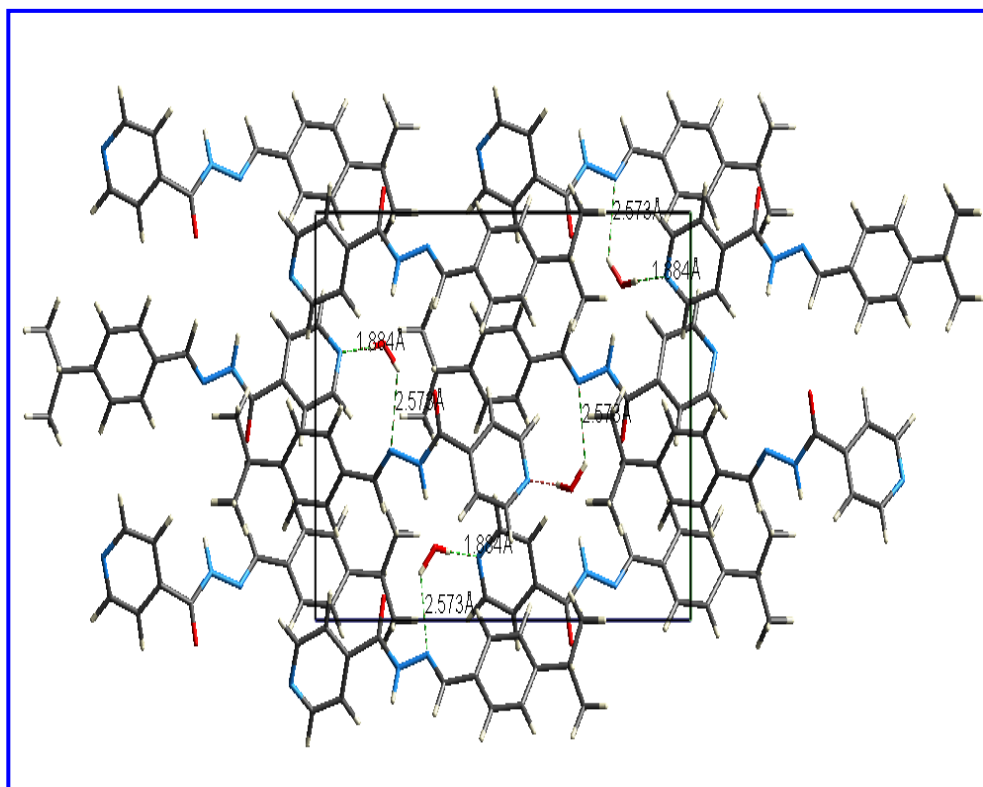
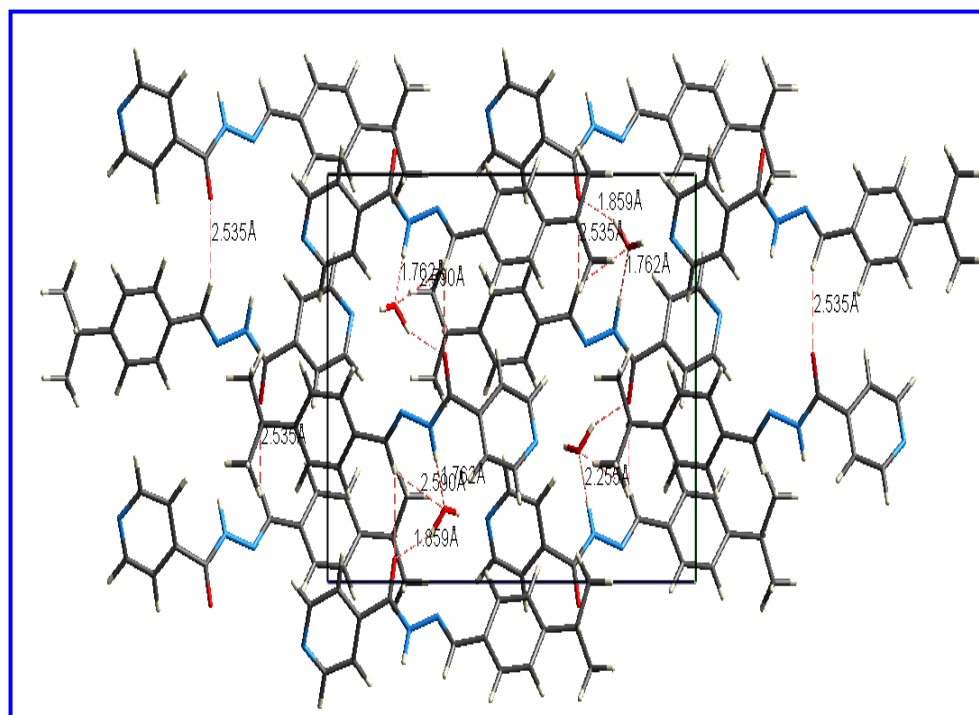


Figure. S11

**Figure. S12**

