Electronic Supplementary Information

Color tuning of active pharmaceutical ingredient through cocrystallization: A case study of metronidazole–pyrogallol cocrystal

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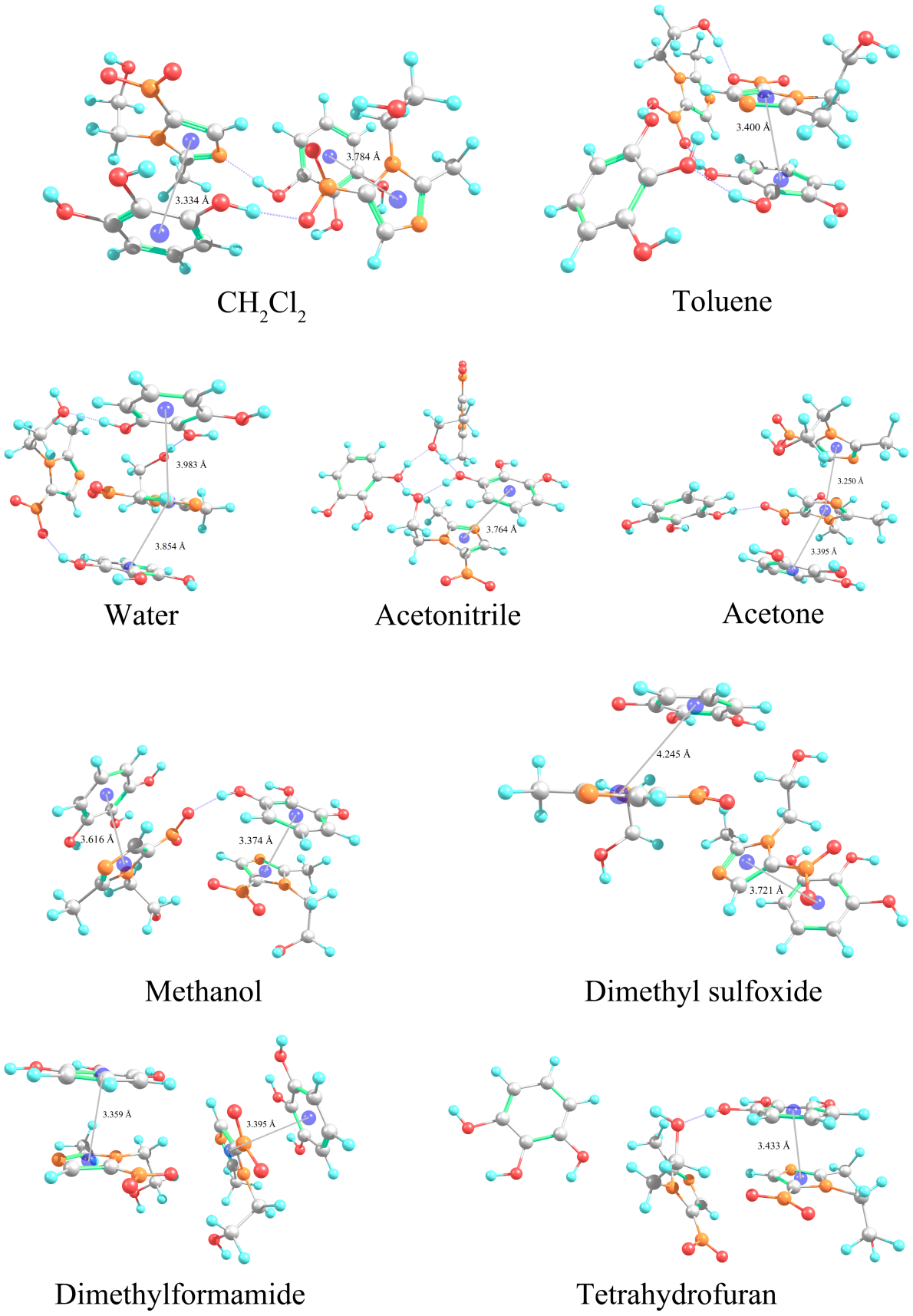

Fig. S1. The lowest-energy geometries of **MNZ–GA** clusters in solvents. The distance between the two rings is given.

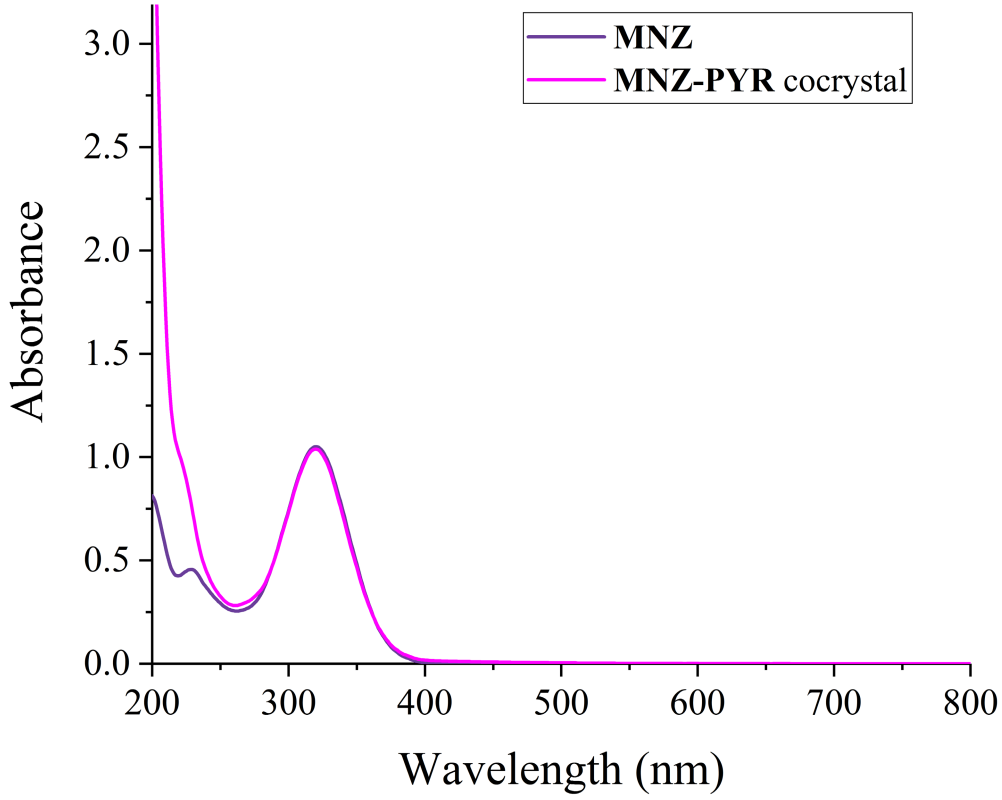

Fig. S2. The UV–vis absorption spectra of **MNZ** and **MNZ–GA** cocrystal in water. The concentration is 100 μM.

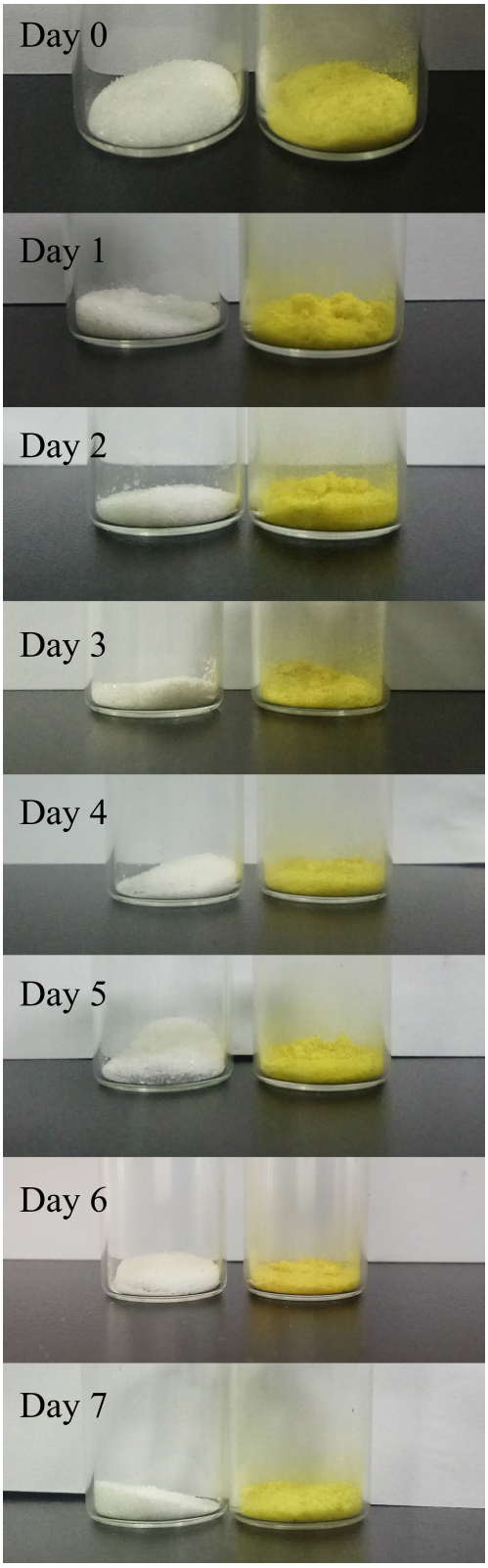

Fig. S3. The appearance of **MNZ** and **MNZ–PYR** cocrystal at accelerated condition (40 °C/75% relative humidity). The powder of **MNZ** and **MNZ–PYR** cocrystal were placed in open vessels and kept in a closed screw cap reagent bottle. The temperature was controlled by an oven and the relative humidity was achieved by placing a tray of saturated NaCl solution in the closed bottle.

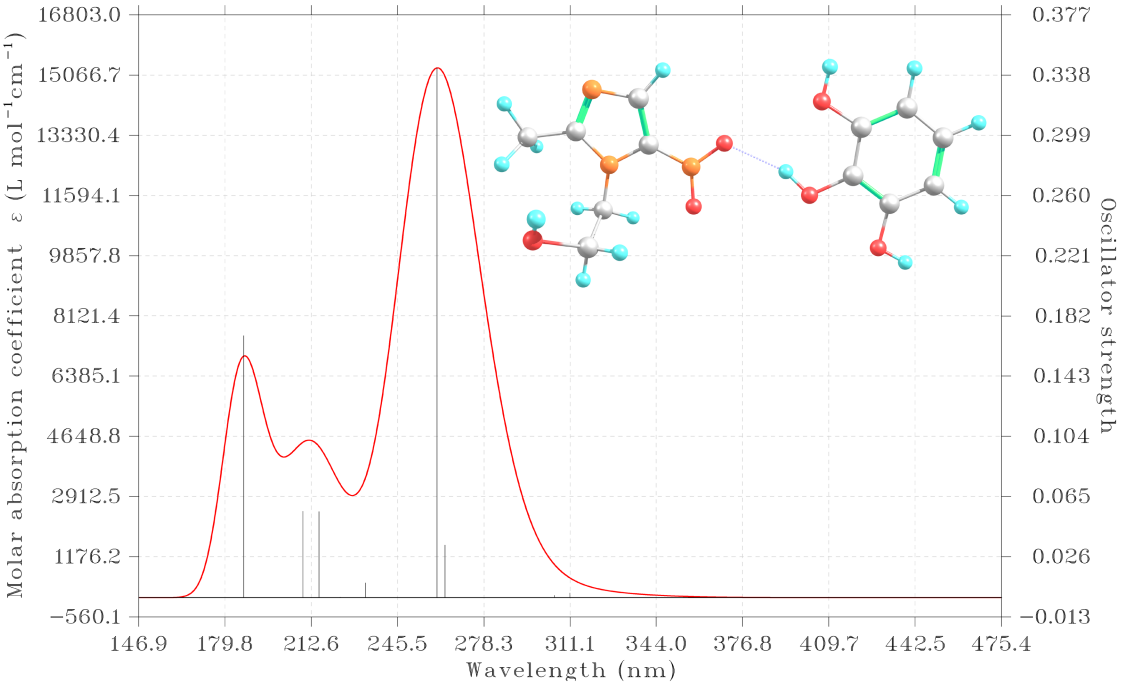

Fig. S4. Simulated absorption spectrum of **MNZ–PYR** cluster through the –OH of **PYR** and –NO_2 of **MNZ**.

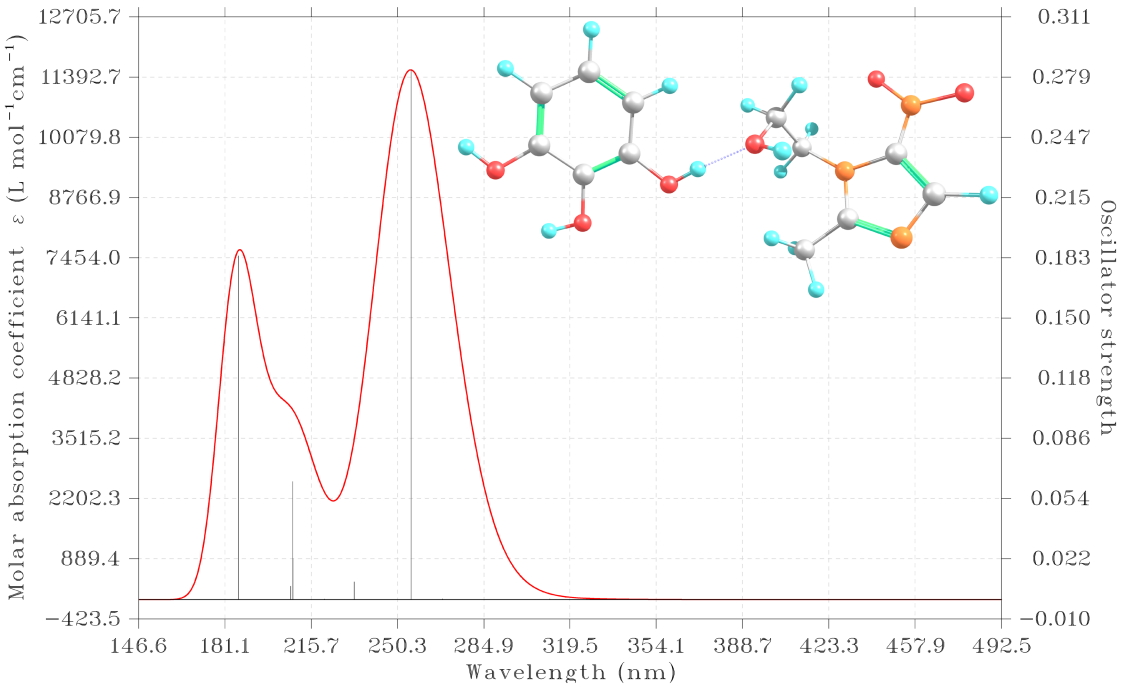

Fig. S5. Simulated absorption spectrum of **MNZ–PYR** cluster through the –OH of **PYR** and –OH of **MNZ**.

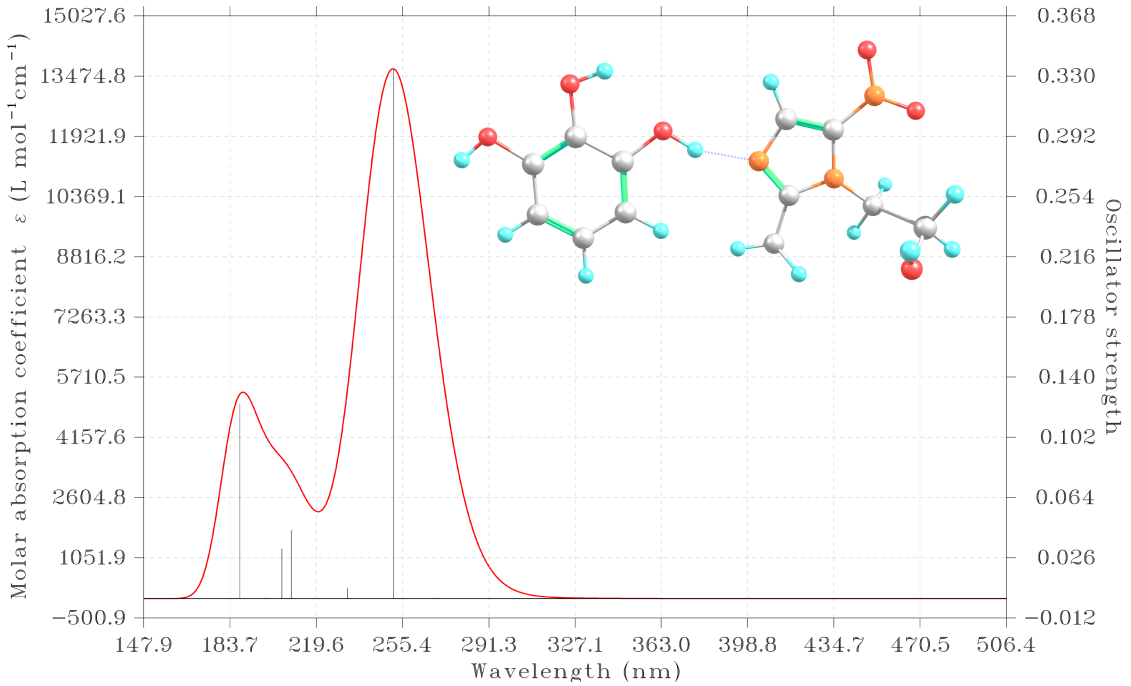

Fig. S6. Simulated absorption spectrum of **MNZ–PYR** cluster through the O–H···$N_{heterocycle}$ synthon.

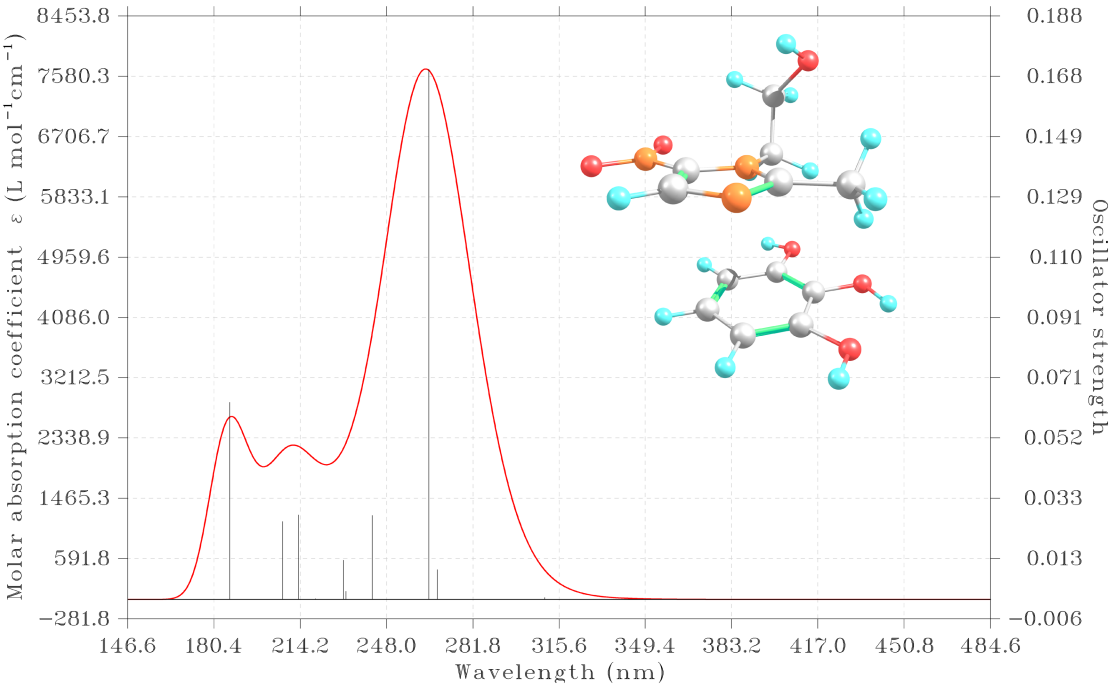

Fig. S7. Simulated absorption spectrum of **MNZ–PYR** cluster through π–π stacking interaction.

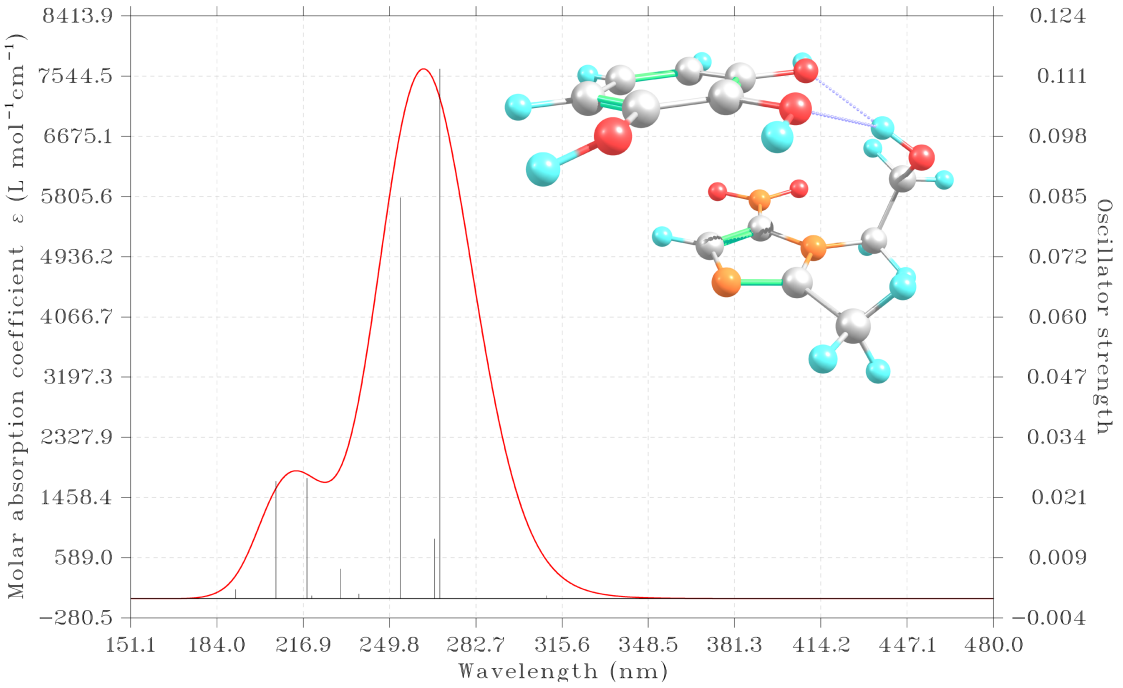

Fig. S8. Simulated absorption spectrum of **MNZ–PYR** cluster through π–π stacking interaction and O–H···O hydrogen bonding.

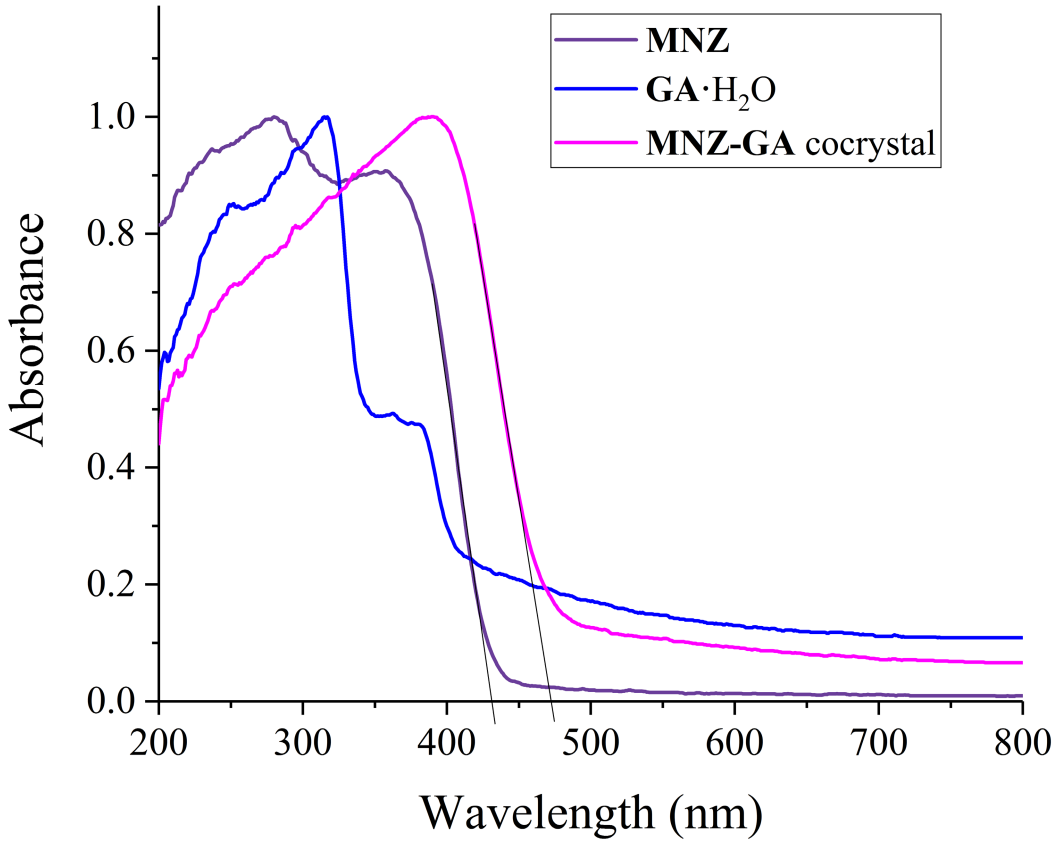

Fig. S9. Normalized solid-state UV–vis spectra of **MNZ**, **GA**·H_2O, and **MNZ–GA** cocrystal.

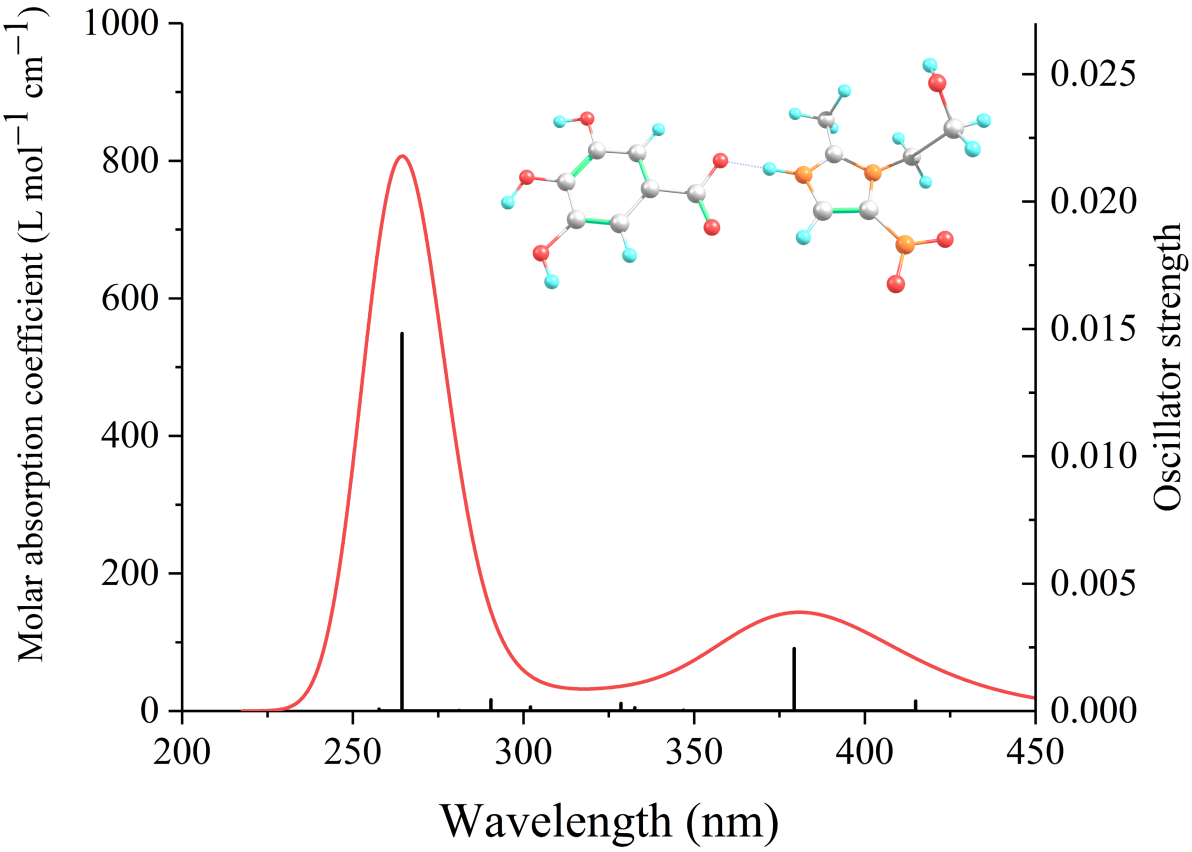

Fig. S10. Simulated absorption spectra of **MNZ–GA** cluster due to the excited-state proton transfer process within O–H···$N_{heterocycle}$ synthon. Inset shows the first singlet excited state optimized structure of **MNZ–GA** cluster.