† Electronic Supplementary Information

A novel approach to design Febuxostat-Salicylic acid eutectic system: evaluation and characterization

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Overlay of PXRD of FXT_form Q and residue obtained after dissolution study is shown in Fig. S1. Optimized structure of FXT is shown in Fig. S2. Optimized structure of SAA is shown in Fig. S3. Schematic presentation of FXT, SAA and FXT-SAA eutectic system is shown in Fig. S4. Potential energy surface scan with varying dihedral angle of FXT-SAA eutectic system is shown in Fig. S5. Comparison of the observed and simulated (scaled) Raman spectra of monomer, dimer of SAA, FXT and FXT-SAA eutectic system, in the region 100-1100 cm^{-1}, 1100-1800 cm^{-1}, 2150-2350 cm^{-1}, and 2700-3200 cm^{-1} is shown in Fig. S6. Comparison of the observed and simulated (scaled) IR spectra of monomer, dimer of SAA, FXT and FXT-SAA eutectic system in the region 100-1100 cm^{-1}, 1100-1800 cm^{-1}, 2200-2450 cm^{-1}, and 2400-4000 cm^{-1} is shown in Fig. S7. Comparison of the observed and simulated (scaled) Raman spectra of monomer and dimer of FXT in the region 200-1000 cm^{-1}, 1000-1800 cm^{-1}, and 1800-3800 cm^{-1} is shown in Fig. S8. Comparison of the observed and simulated (scaled) IR spectra of monomer and dimer of FXT in the region 100-1000 cm^{-1}, 1000-1800 cm^{-1}, and 2100-3800 cm^{-1} is shown in Fig. S9. Comparison of the observed and simulated (scaled) Raman spectra of monomer and dimer of SAA in the region 100-1000 cm^{-1}, 1000-1800 cm^{-1}, and 2700-3700 cm^{-1} is shown in Fig. S10. Comparison of the observed and simulated (scaled) IR spectra of monomer and dimer of SAA in the region 200-1000 cm^{-1}, 1000-1800 cm^{-1}, and 2800-3700 cm^{-1} is shown in Fig. S11. Molecular electrostatic potential (MEP) surface shaped by mapping of total density over electrostatic potential in the gas phase for the monomer of FXT is shown in Fig. S12. Molecular electrostatic potential (MEP) surface shaped by mapping of total density over electrostatic potential in the gas phase for the monomer of SAA is shown in Fig. S13. Molecular electrostatic potential (MEP) surface shaped by mapping of total density over electrostatic potential in the gas phase for the dimer of FXT is shown in Fig. S14. Molecular electrostatic potential (MEP) surface shaped by mapping of total density over electrostatic potential in the gas phase for the dimer of SAA is shown in Fig. S15. Different models of FXT-SAA eutectic system and their energies are shown in Table S1.

Part I. FIGURES

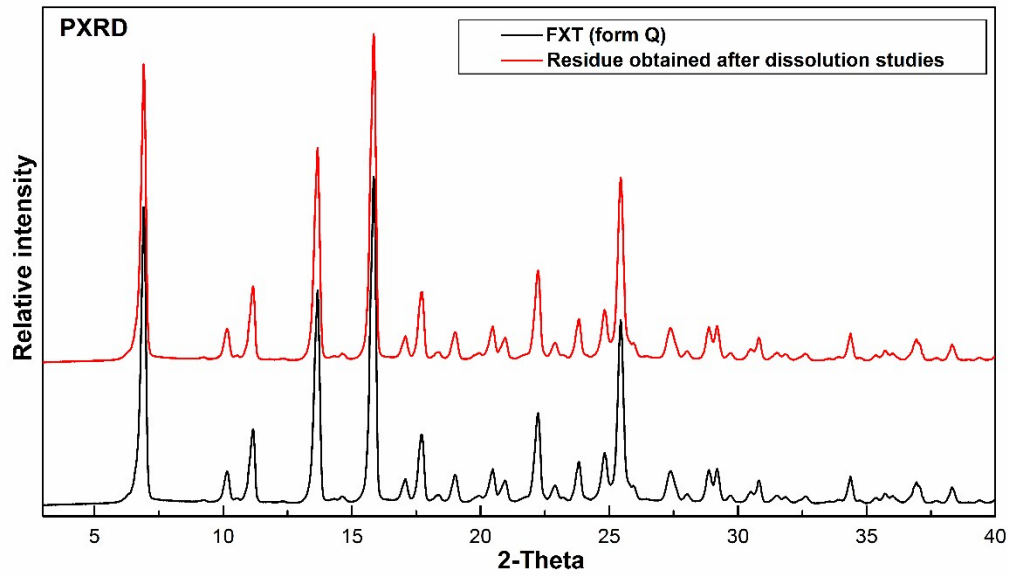

Fig. S1 Overlay of PXRD of FXT_form Q and residue obtained after dissolution study.

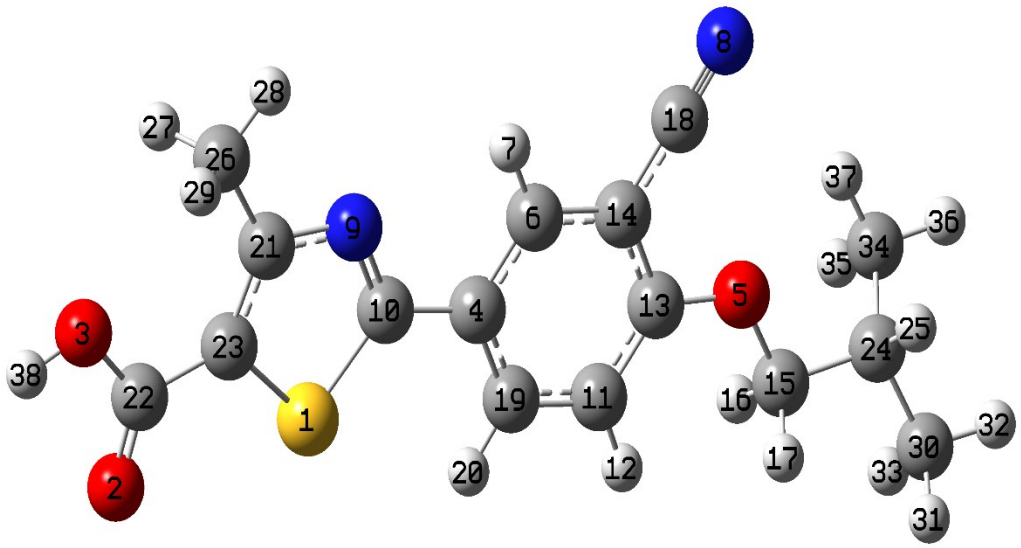

Fig. S2 Optimized structure of FXT.

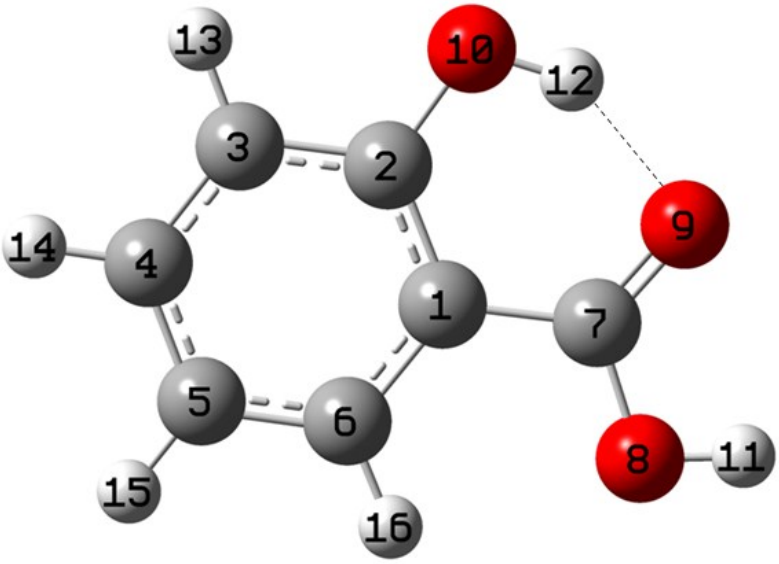

Fig. S3 Optimized structure of SAA.

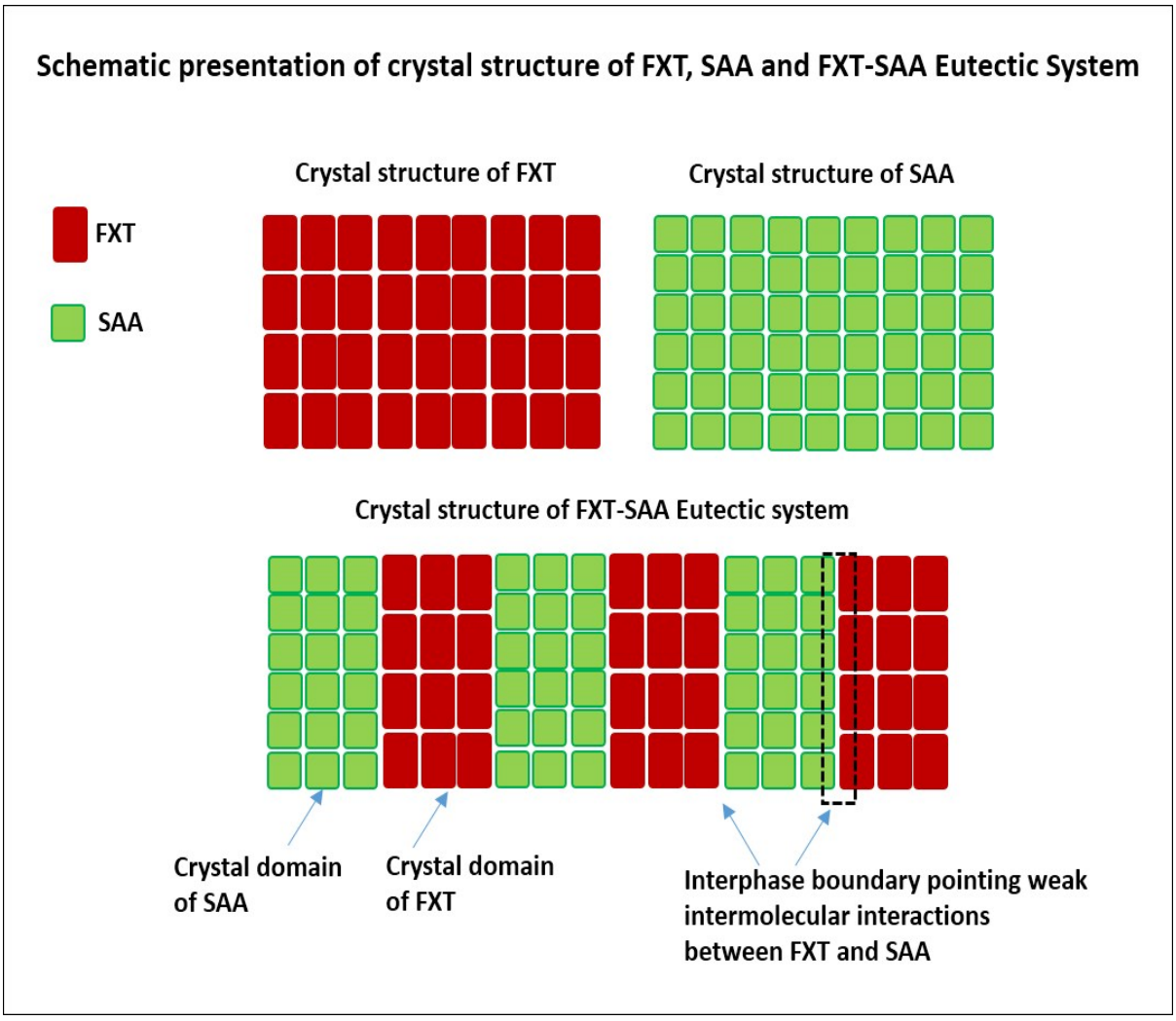

Fig. S4 Schematic presentation of FXT, SAA and FXT-SAA eutectic system.

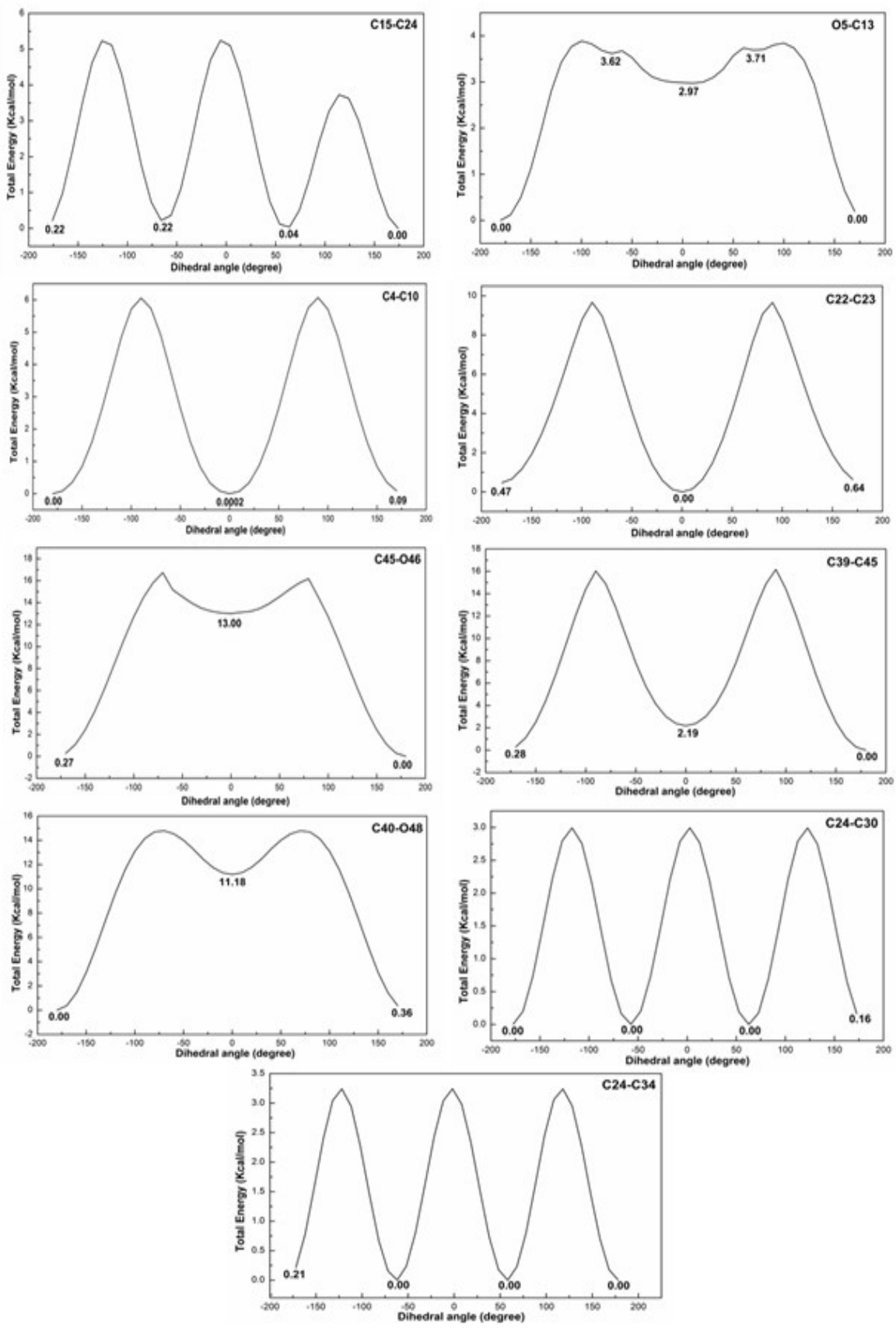

Fig. S5 Potential energy surface scan with varying dihedral angle of FXT-SAA eutectic system.

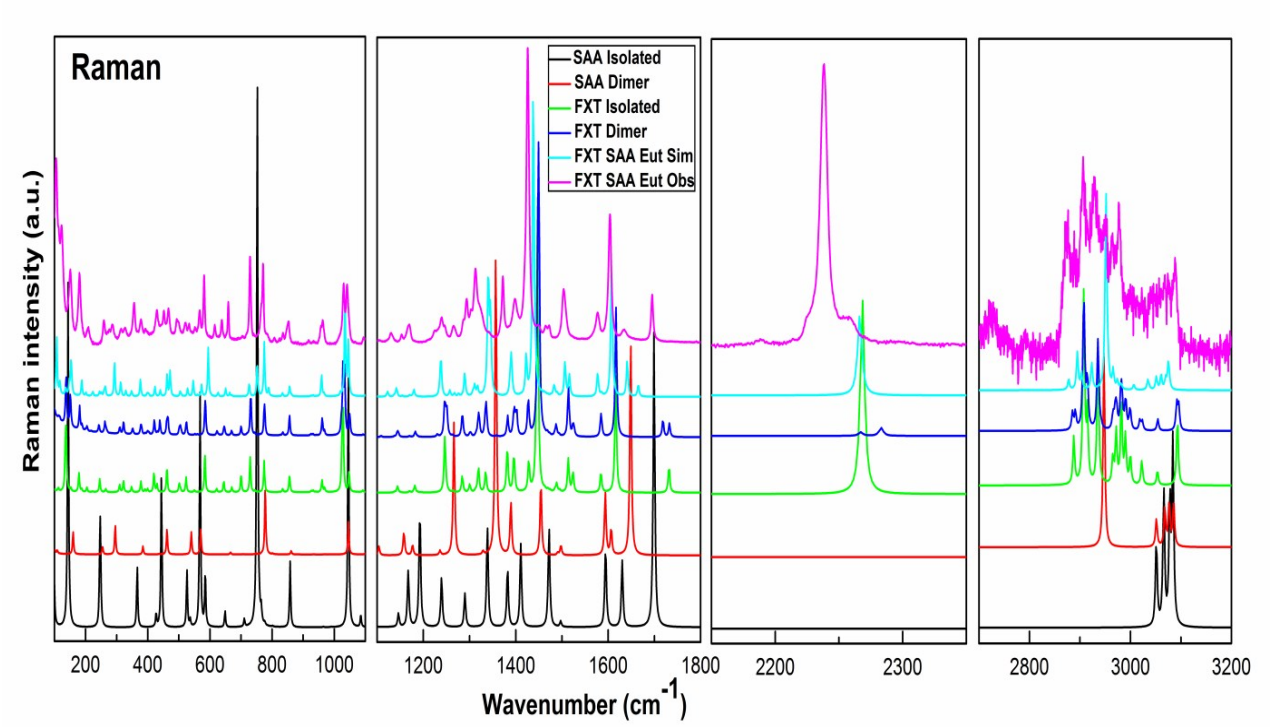

Fig. S6 Comparison of the observed and simulated (scaled) Raman spectra of monomer, dimer of SAA, FXT and FXT-SAA eutectic system, in the region 100-1100 cm^{-1}, 1100-1800 cm^{-1}, 2150-2350 cm^{-1}, and 2700-3200 cm^{-1}.

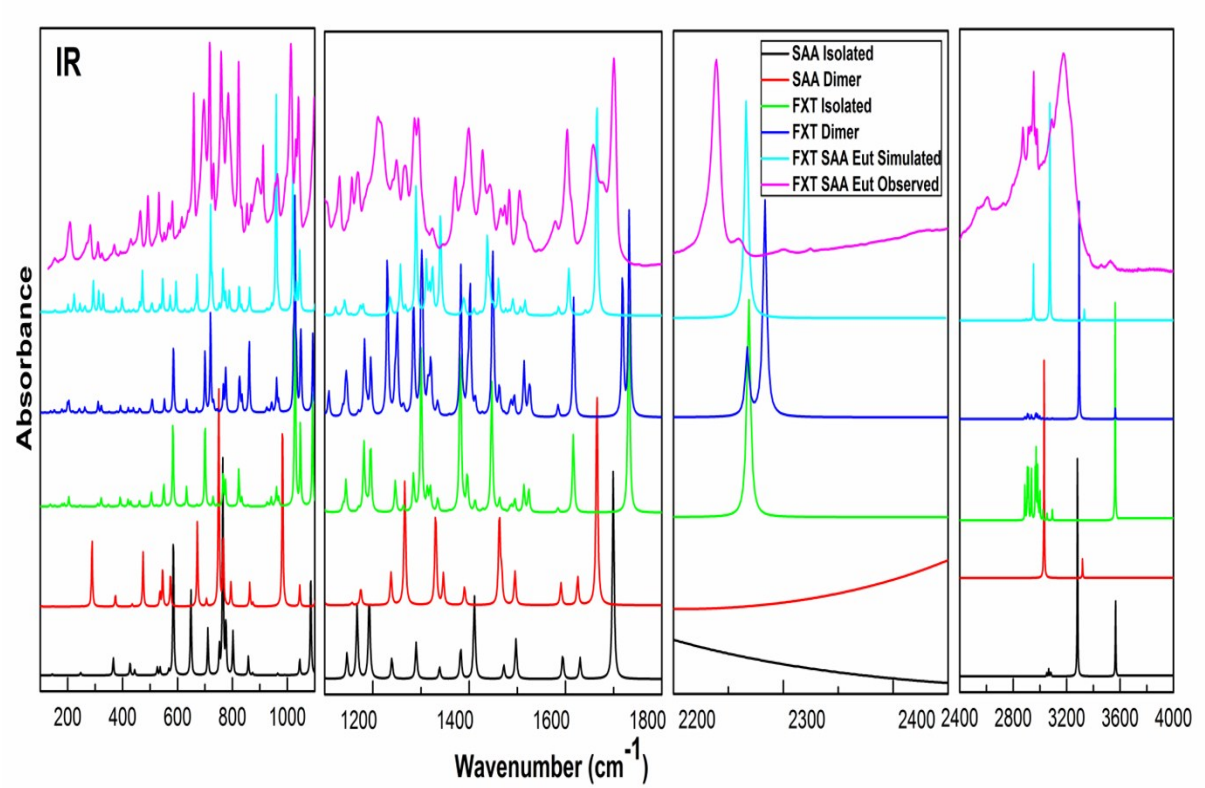

Fig. S7 Comparison of the observed and simulated (scaled) IR spectra of monomer, dimer of SAA, FXT and FXT-SAA eutectic system, in the region 100-1100 cm^{-1}, 1100-1800 cm^{-1}, 2200-2450 cm^{-1}, and 2400-4000 cm^{-1}.

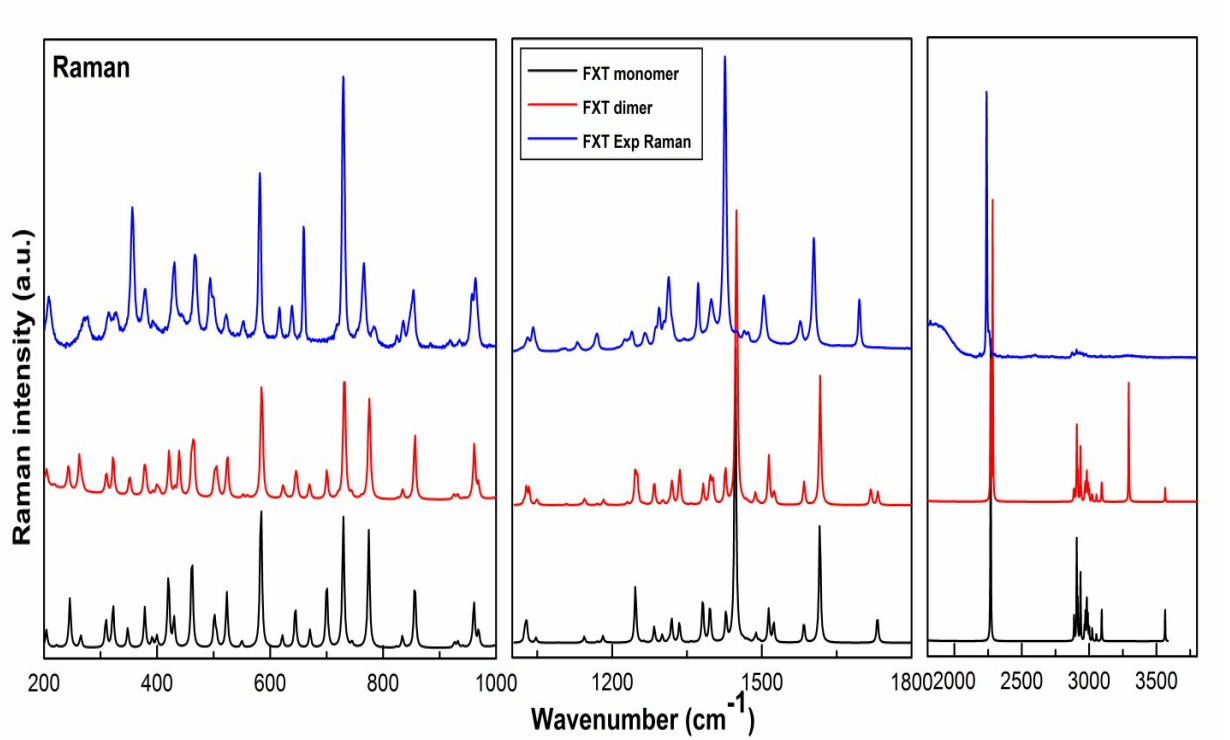

Fig. S8 Comparison of the observed and simulated (scaled) Raman spectra of monomer and dimer of FXT in the region 200-1000 cm^{-1}, 1000-1800 cm^{-1}, and 1800-3800 cm^{-1}.

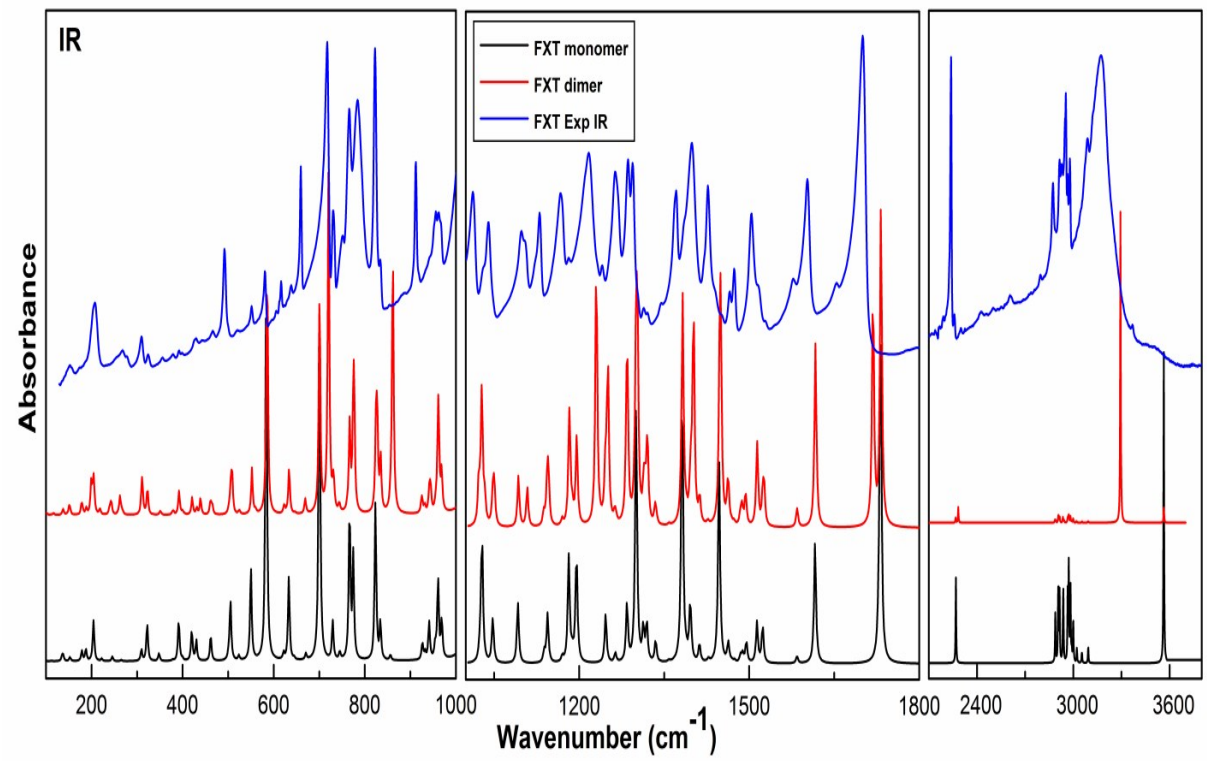

Fig. S9 Comparison of the observed and simulated (scaled) IR spectra of monomer and dimer of FXT in the region 100-1000 cm^{-1}, 1000-1800 cm^{-1}, and 2100-3800 cm^{-1}.

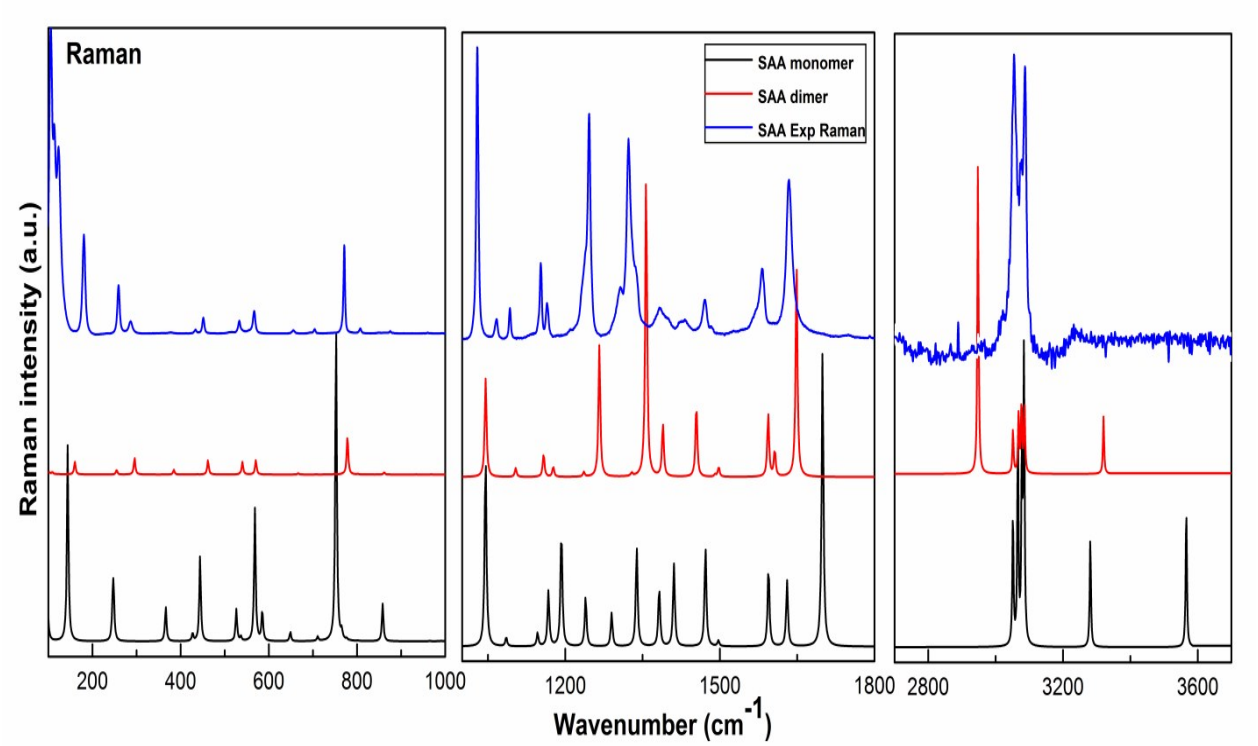

Fig. S10 Comparison of the observed and simulated (scaled) Raman spectra of monomer and dimer of SAA in the region 100-1000 cm^{-1}, 1000-1800 cm^{-1}, and 2700-3700 cm^{-1}.

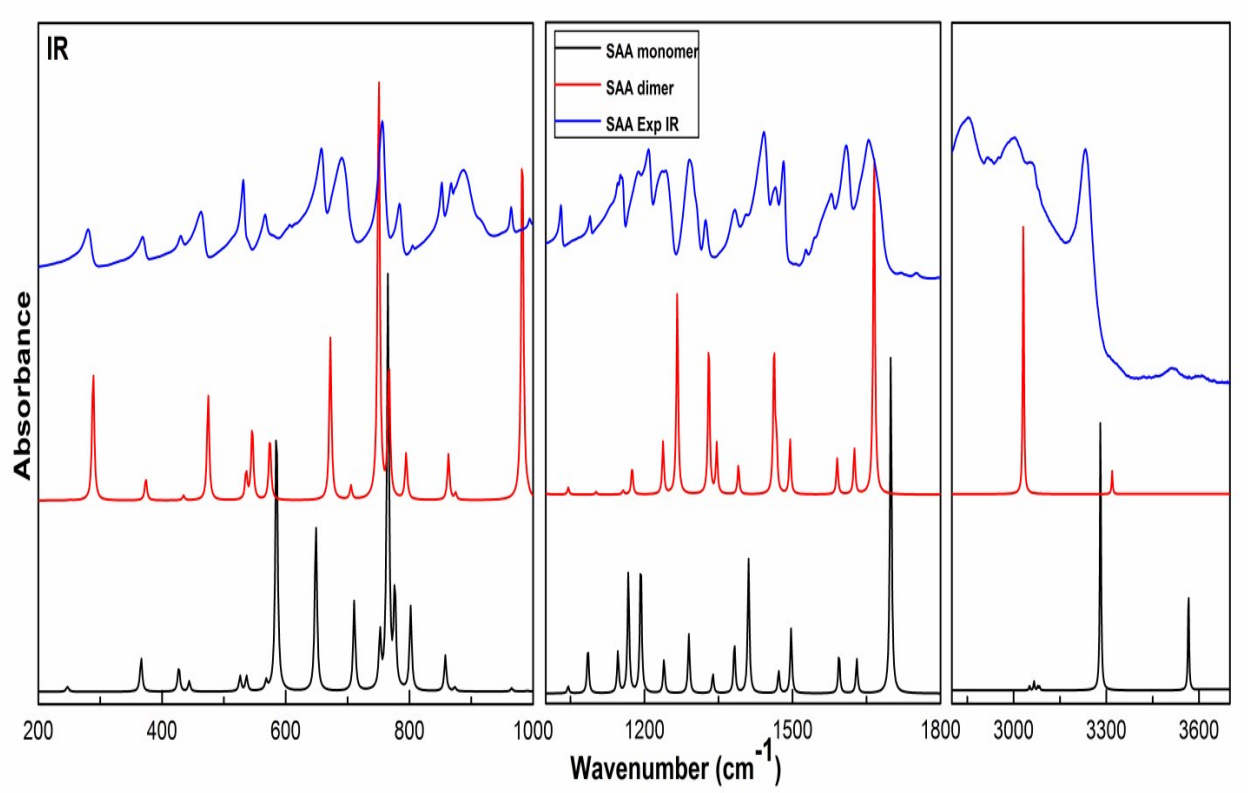

Fig. S11 Comparison of the observed and simulated (scaled) IR spectra of monomer and dimer of SAA in the region 200-1000 cm^{-1}, 1000-1800 cm^{-1}, and 2800-3700 cm^{-1}.

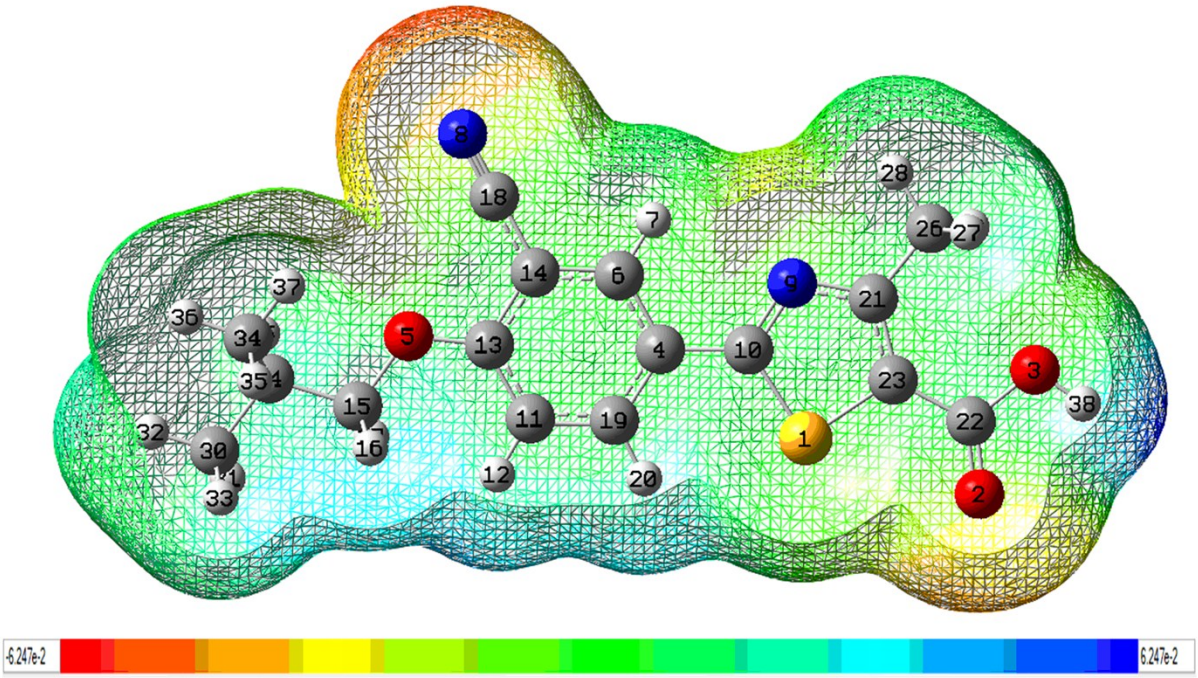

Fig. S12 Molecular electrostatic potential (MEP) surface shaped by mapping of total density over electrostatic potential in the gas phase for the monomer of FXT.

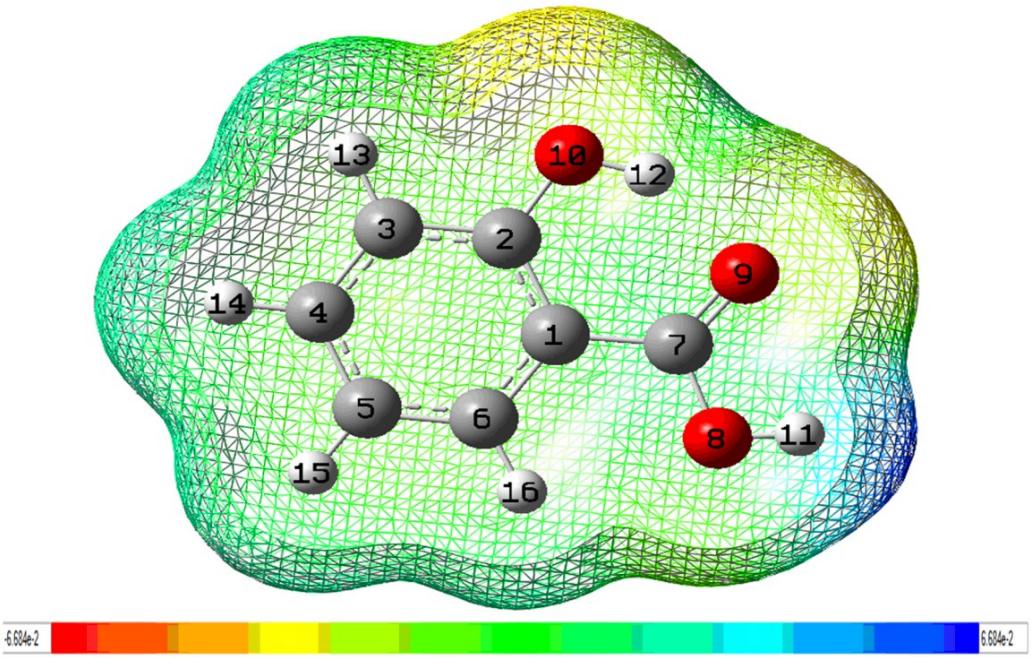

Fig. S13 Molecular electrostatic potential (MEP) surface shaped by mapping of total density over electrostatic potential in the gas phase for the monomer of SAA.

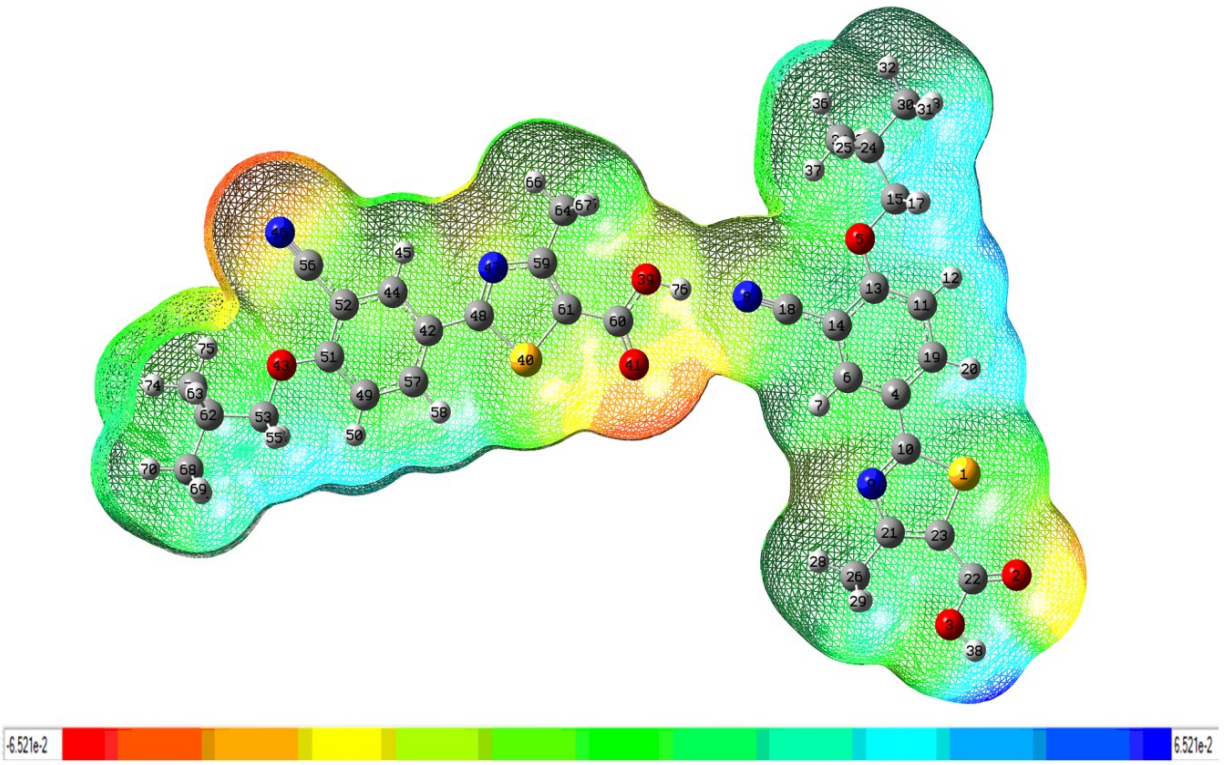

Fig. S14 Molecular electrostatic potential (MEP) surface shaped by mapping of total density over electrostatic potential in the gas phase for the dimer of FXT.

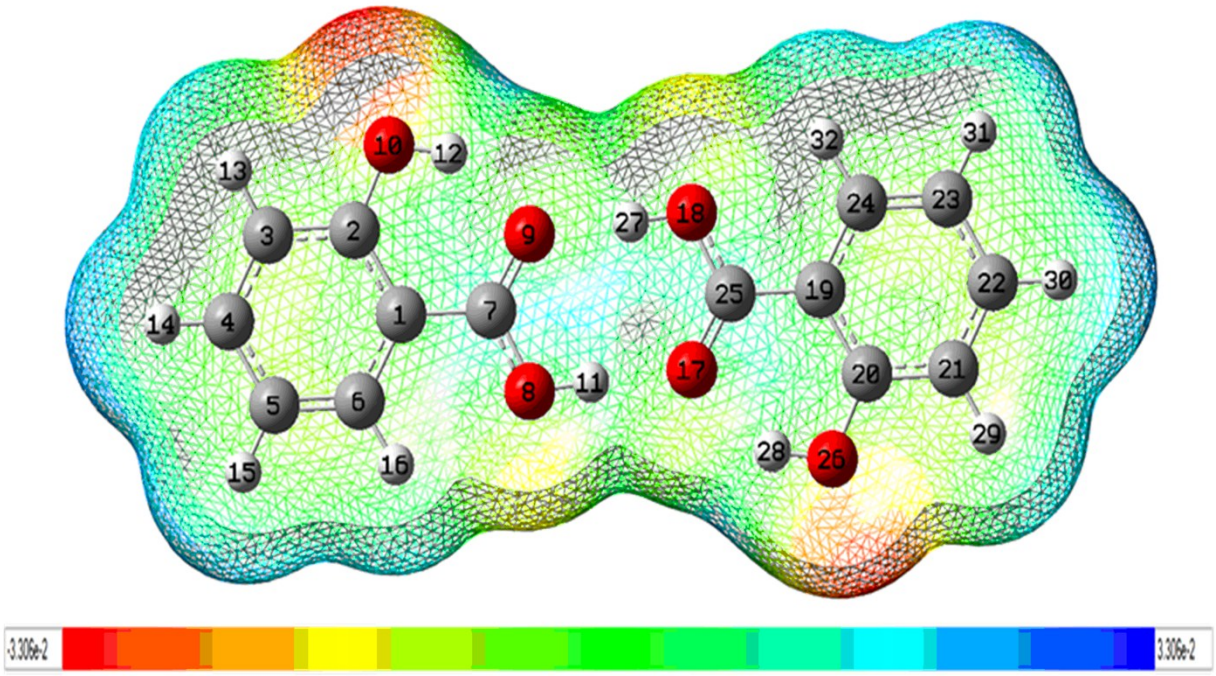

Fig. S15 Molecular electrostatic potential (MEP) surface shaped by mapping of total density over electrostatic potential in the gas phase for the dimer of SAA.

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Part II. TABLES

Table S1 Different models of FXT-SAA eutectic system and their energies.

Models	Energy	
	Hartree	**Kcal/mol**
1	-1849.23791	0.00
2	-1849.22502	-8.091
3	-1849.22413	-8.646
4	-1849.22409	-8.673
5	-1849.22400	-8.727
6	-1849.22163	-10.217
7	-1849.21957	-11.505