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CRYSTAL ENGINEERING  
MATERIALS

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**Supporting information for article:**

**Supramolecular networks and Hirshfeld surfaces of oxydiacetic acid  
and iminodiacetic acid salts**

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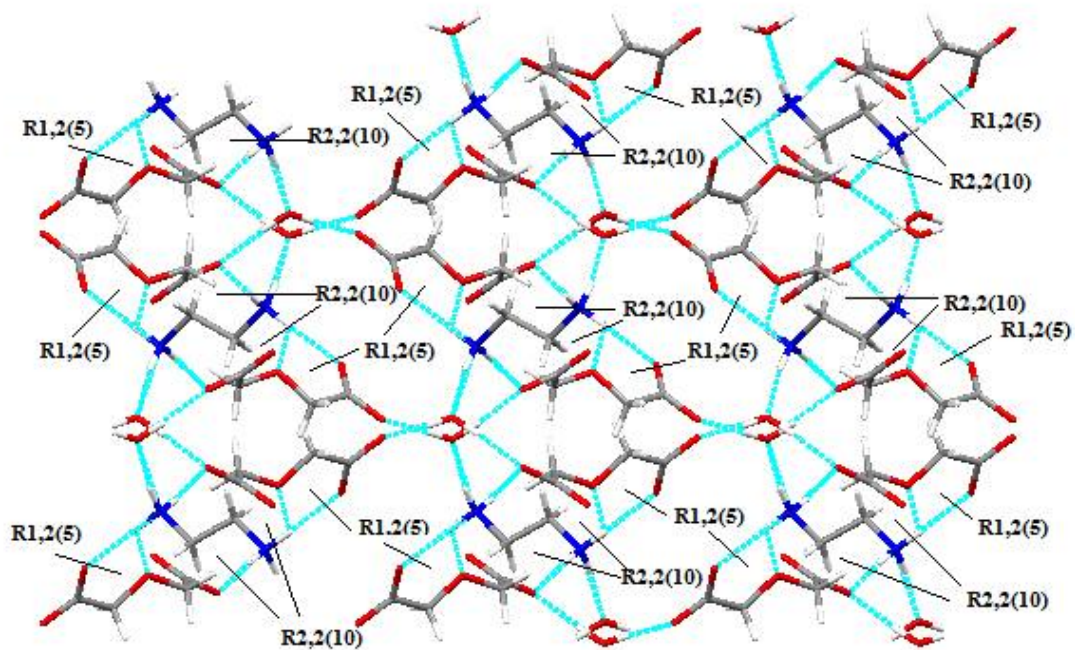


Fig.S1. Ring motifs formed by N(1) hydrogen atoms in Odaen (interaction of water cluster also included)

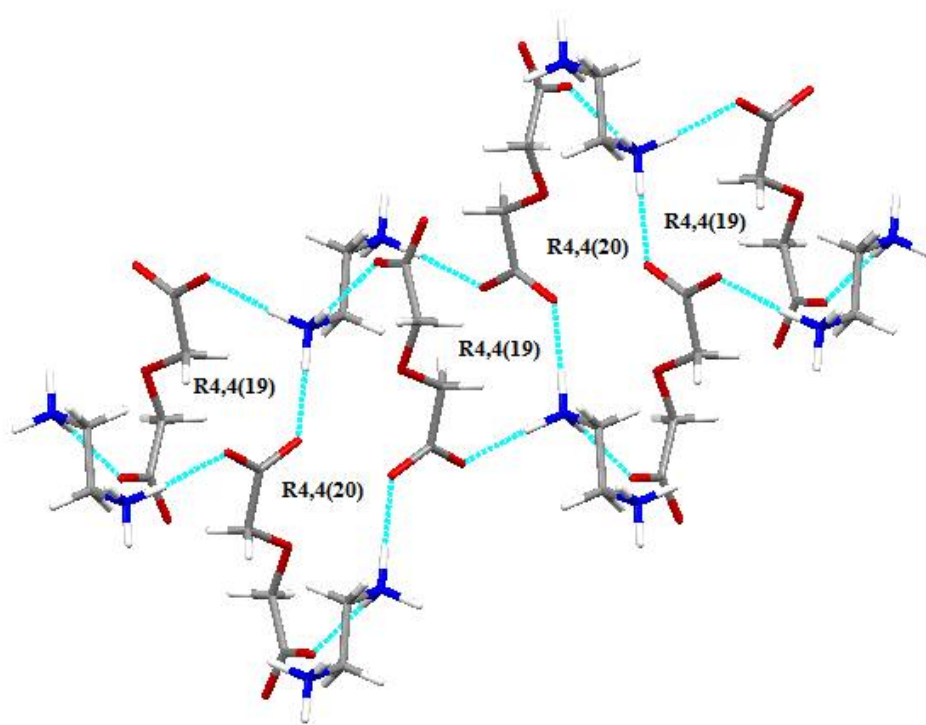
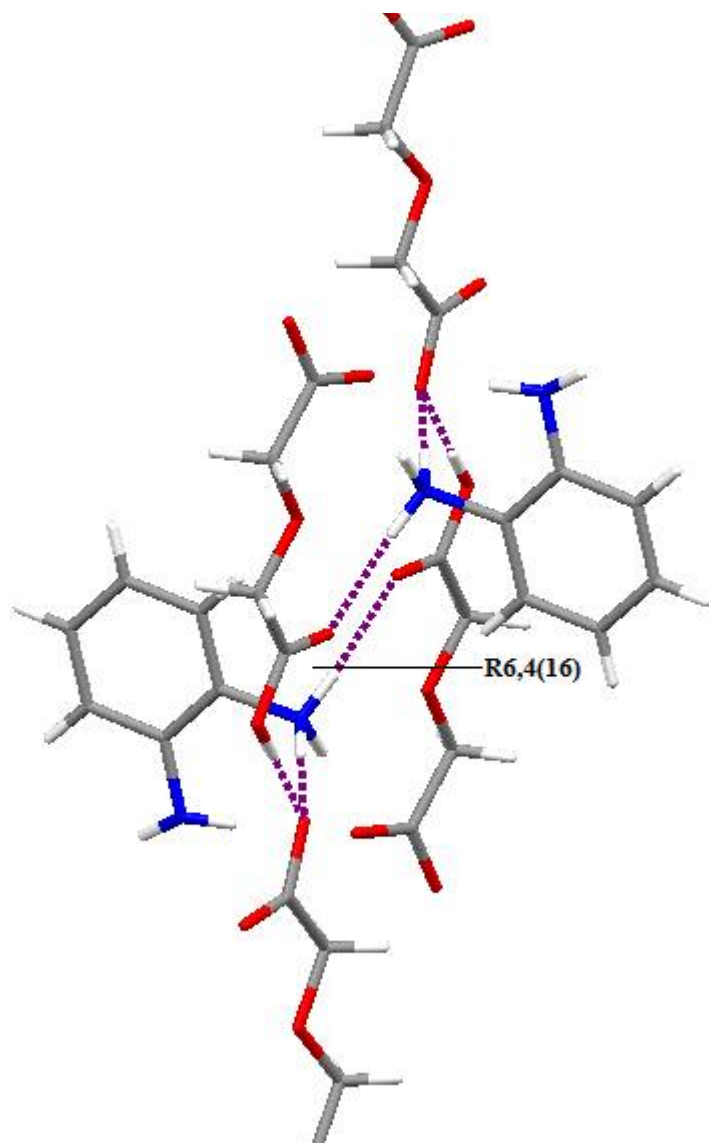


Fig.S2. Ring motifs formed by N(2) hydrogen atoms in Odaen



**Fig.S3.** Ring motif formed by the interaction between the hydrogen atoms of N(1)-H<sub>3</sub><sup>+</sup> cations, carboxylic proton O(1)-H and carboxylate oxygen atoms O(2) and O(7) [N(1)-H(1A)...O(7), N(1)-H(1C)...O(2) and O(1)-H(1A)...O(7)] in Odaophen

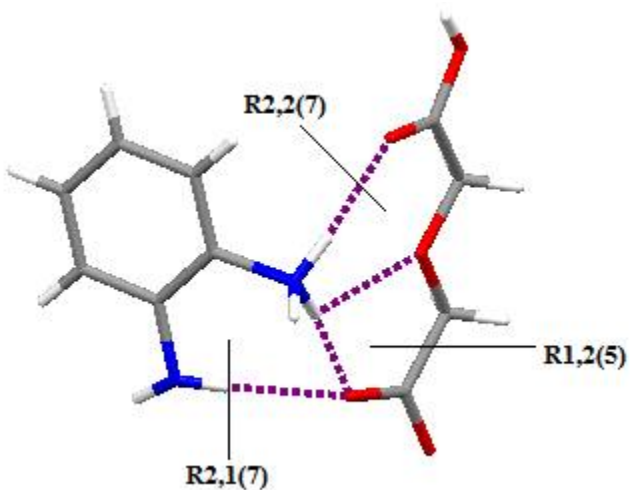


Fig.S4. Ring motifs formed by the interaction between hydrogen atoms of N(1)-H<sub>3</sub><sup>+</sup> cations, N(2)-H<sub>2</sub> amino group of o-phen moiety and carboxylate oxygen atoms O(2), O(3) and O(4) of Oda moiety [N(1)-H(1C)...O(2) and N(1)-H(1B)...O(3) form R<sub>2</sub><sup>2</sup>(7) motif, N(1)-H(1B)...O(3) and N(1)-H(1B)...O(4) form bifurcated ring R<sub>1</sub><sup>2</sup>(5) and N(1)-H(1B)...O(4) and N(2)-H(2B)...O(4) form R<sub>2</sub><sup>2</sup>(7)]

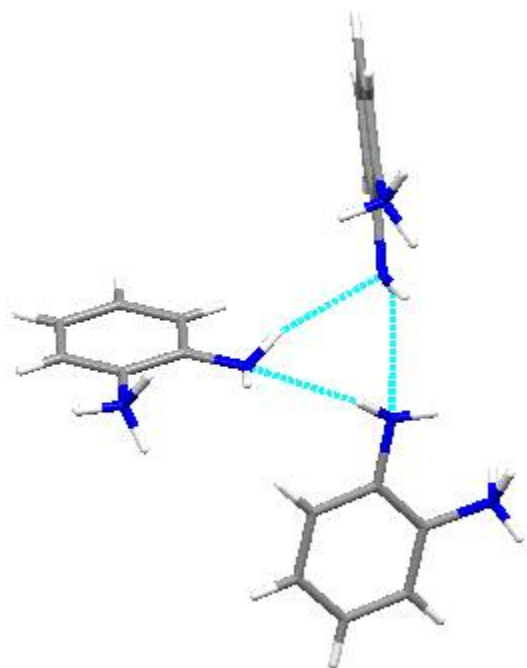
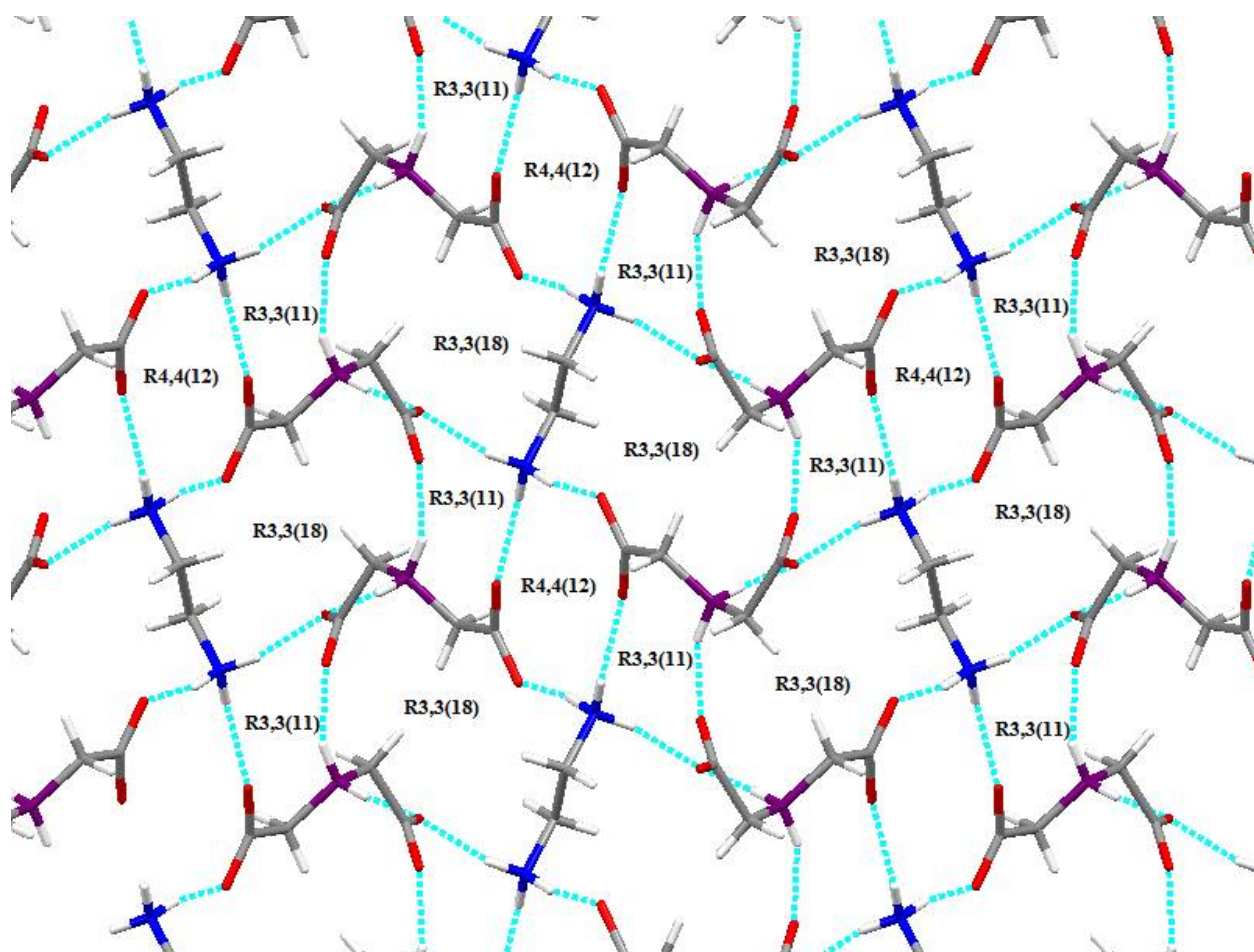
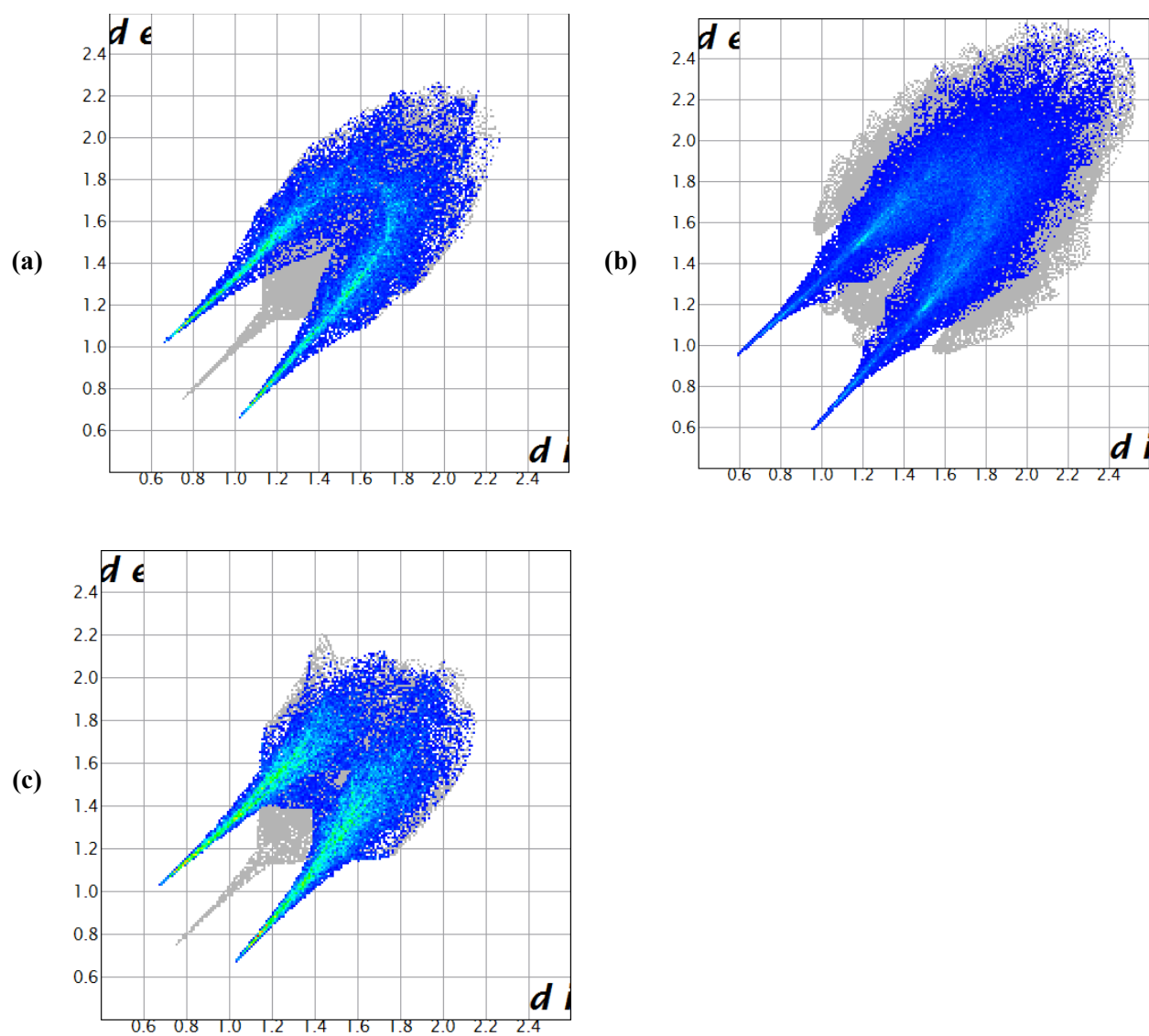


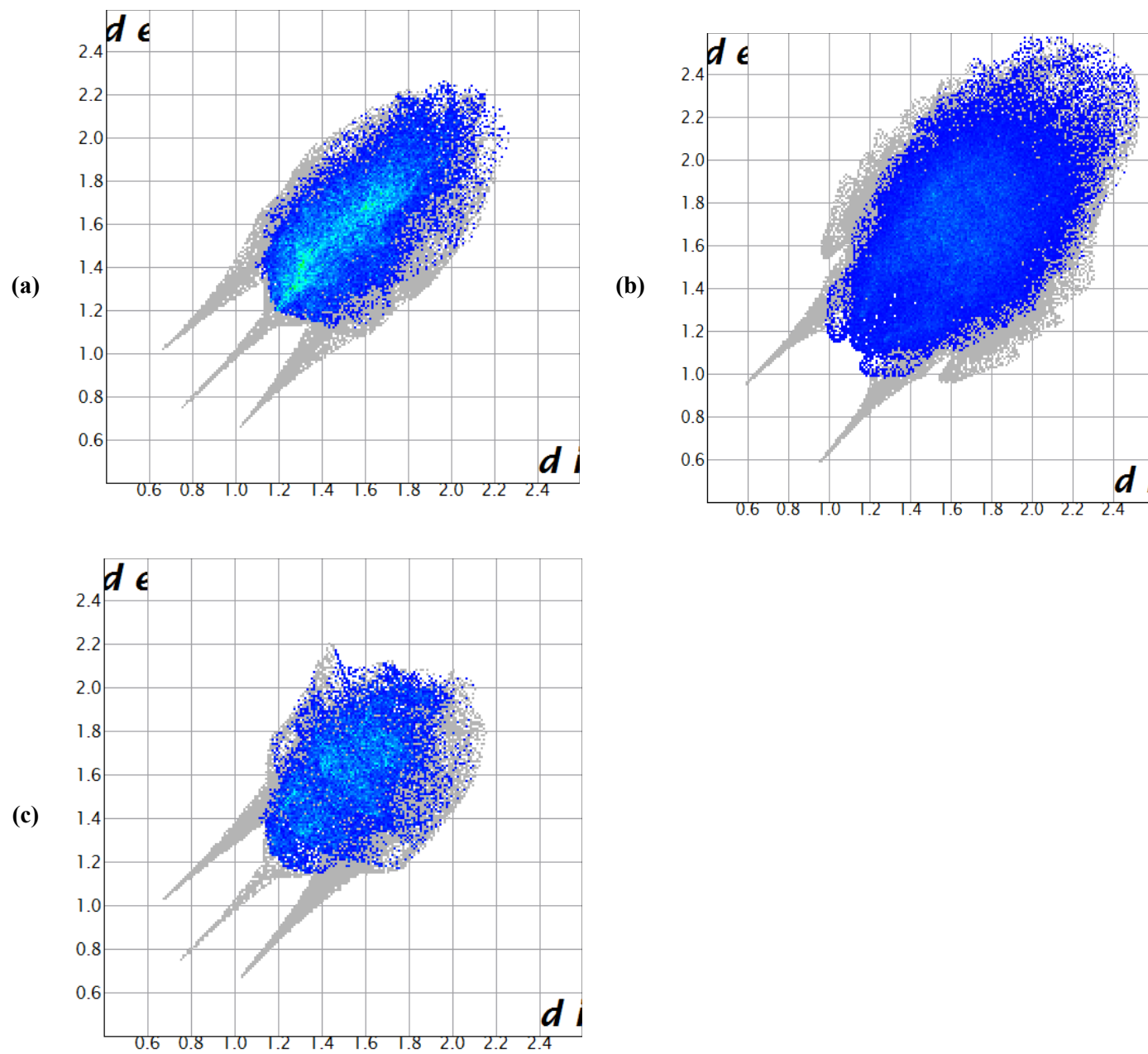
Fig.S5. N-H...N interactions in Odaophen between the amino groups (-NH<sub>2</sub>) of o-phen moieties [N(2)-H(2A)...N(3), N(3)-H(3B)...N(5) and N(5)-H(5B)...N(2)]



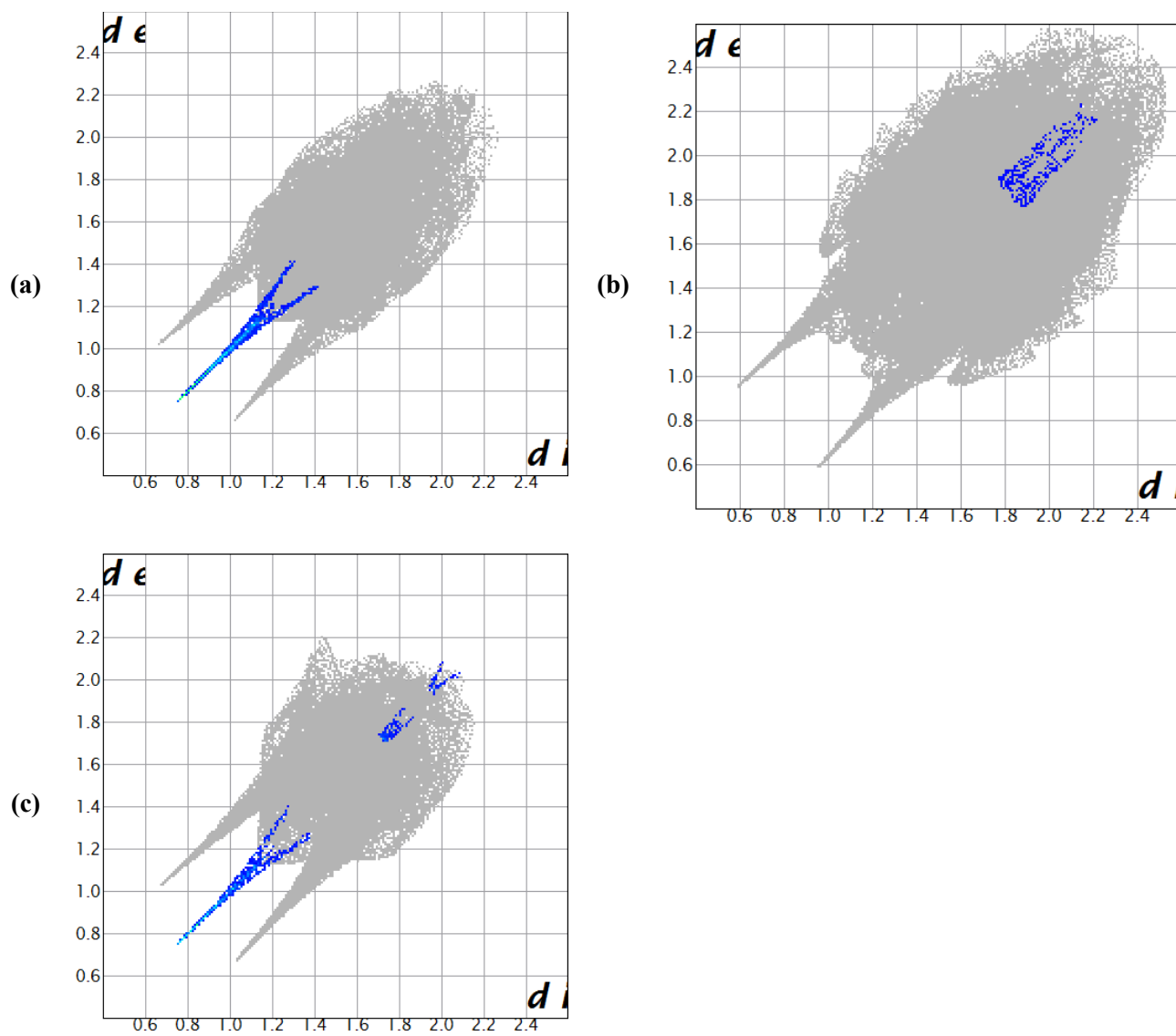
**Fig.S6.** Ring motifs in Idaen formed by the interaction of hydrogen atom of  $-\text{NH}_2^+$  cation in Ida moiety and  $-\text{NH}_3^+$  cation of en moiety between the carboxylate oxygen atoms of Ida moiety. (nitrogen atom of Ida moiety is highlighted by purple colour)



**Fig. S7. Fingerprint plot of O...H/H...O interactions of (a) Odaen (48.0%) (b) Odaophen (40.8%) (c) Idaen(64.2%)**



**Fig. S8. Fingerprint plot H...H interactions of (a) Odaen (43.3%) (b) Odaophen (33.3%) (c) Idaen(28.5%)**



**Fig. S9. Fingerprint plot of C...C contacts of (a) Odaen (2.3%) (b) Odaophen (0.2%) (c) Idaen(1.8%)**



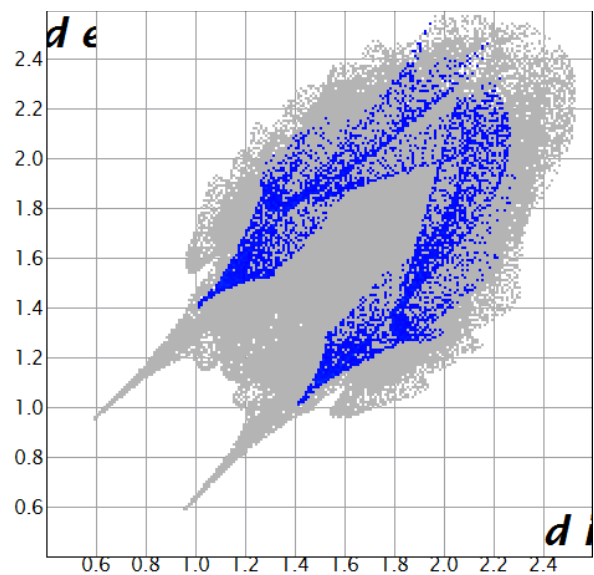
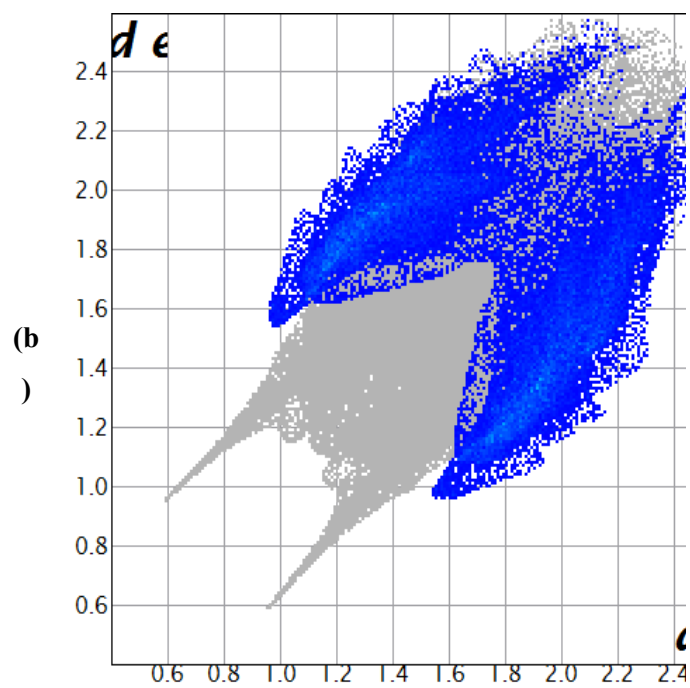
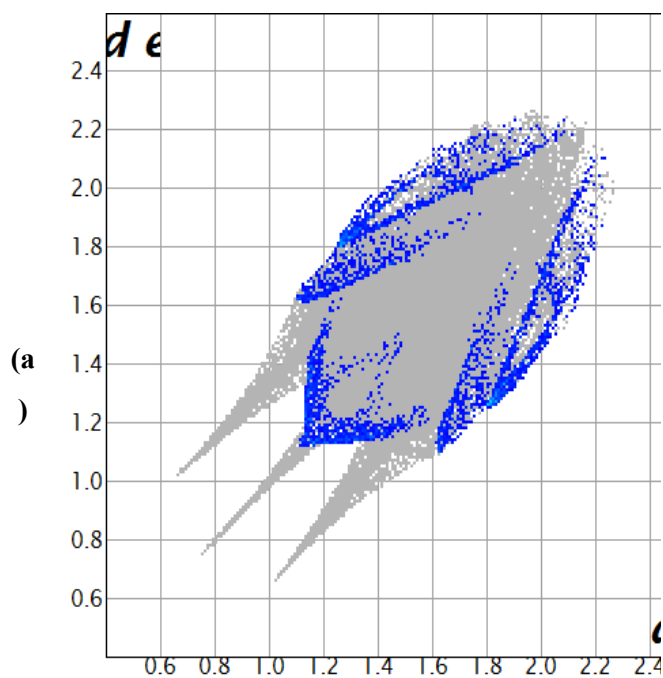
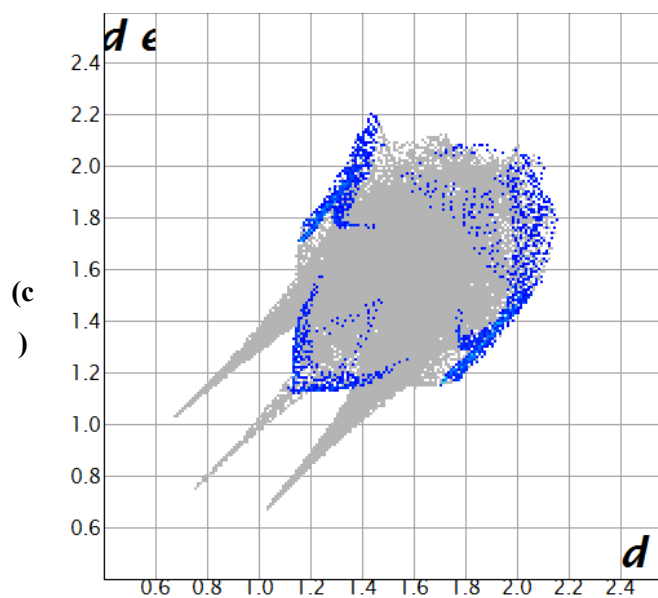
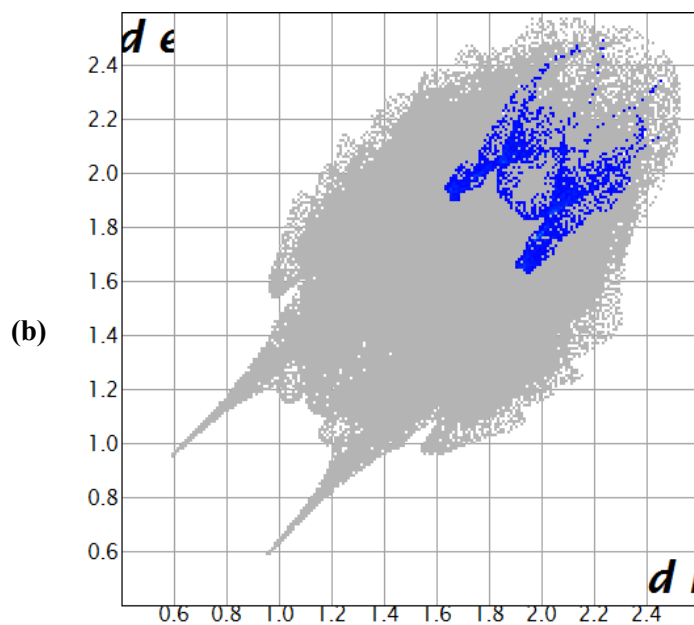
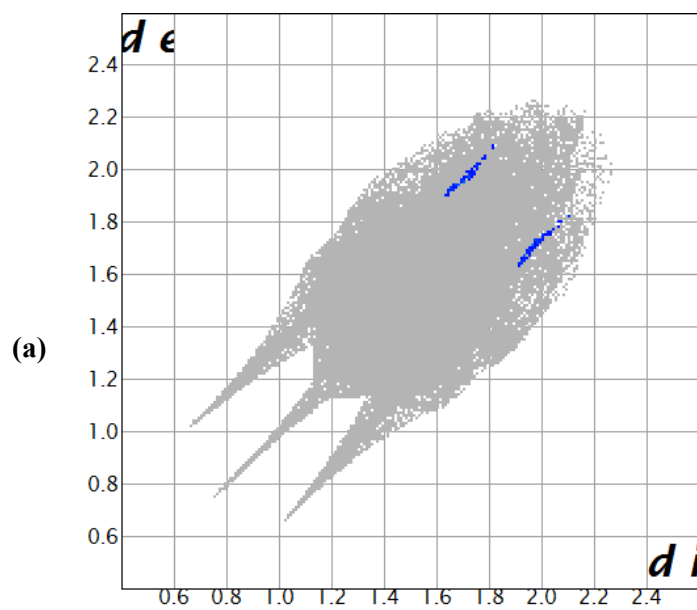


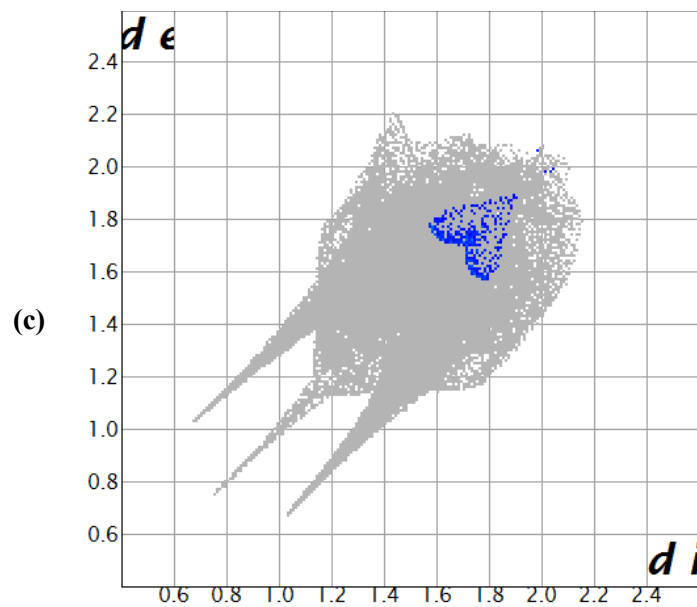
Fig. S10. Fingerprint plot of N-H...N contacts in Odaophen (2.6%)



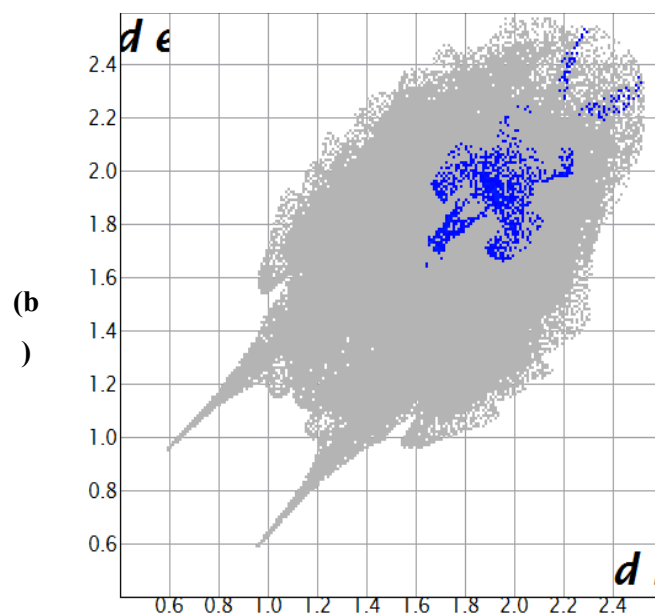
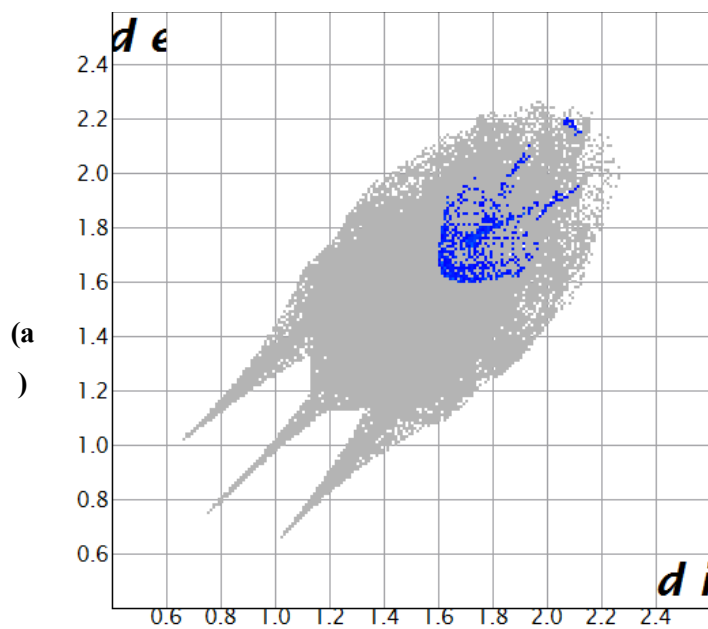


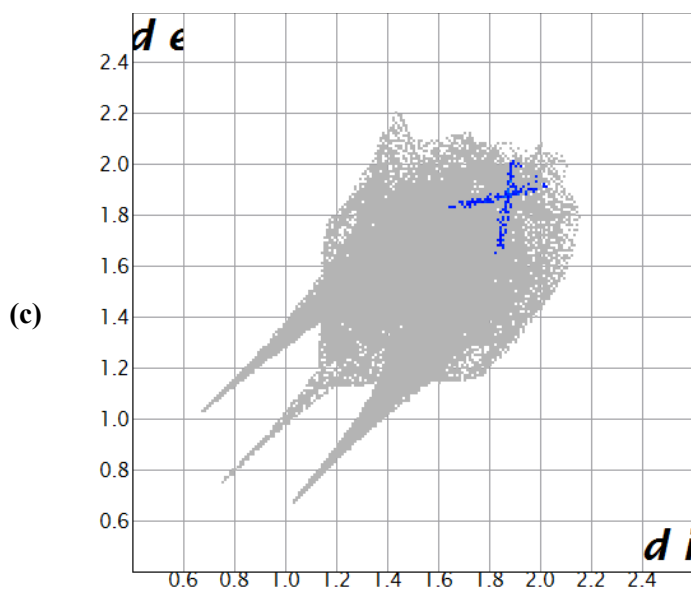
**Fig. S11. Fingerprint plot of C...H/H...C contacts of (a) Odaen (4.9%) (b) Odaophen (21.1%) (c) Idaen(4.3%)**



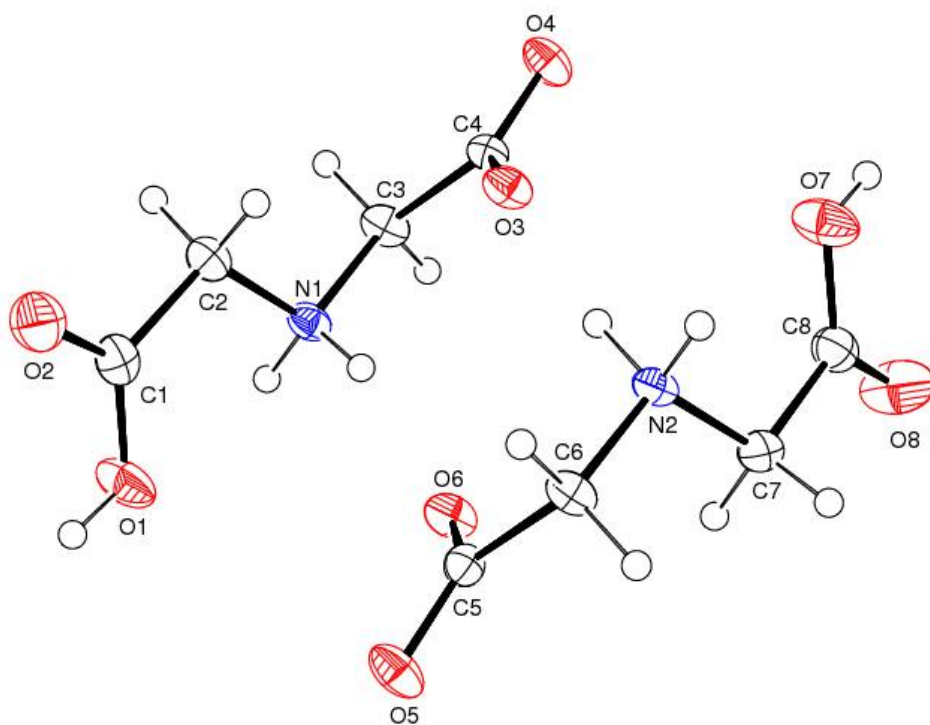


**Fig. S12. Fingerprint plot of C...O/O...C contacts of (a) Odaen (0.2%) (b) Odaophen (1.3%) (c) Idaen(0.8%)**

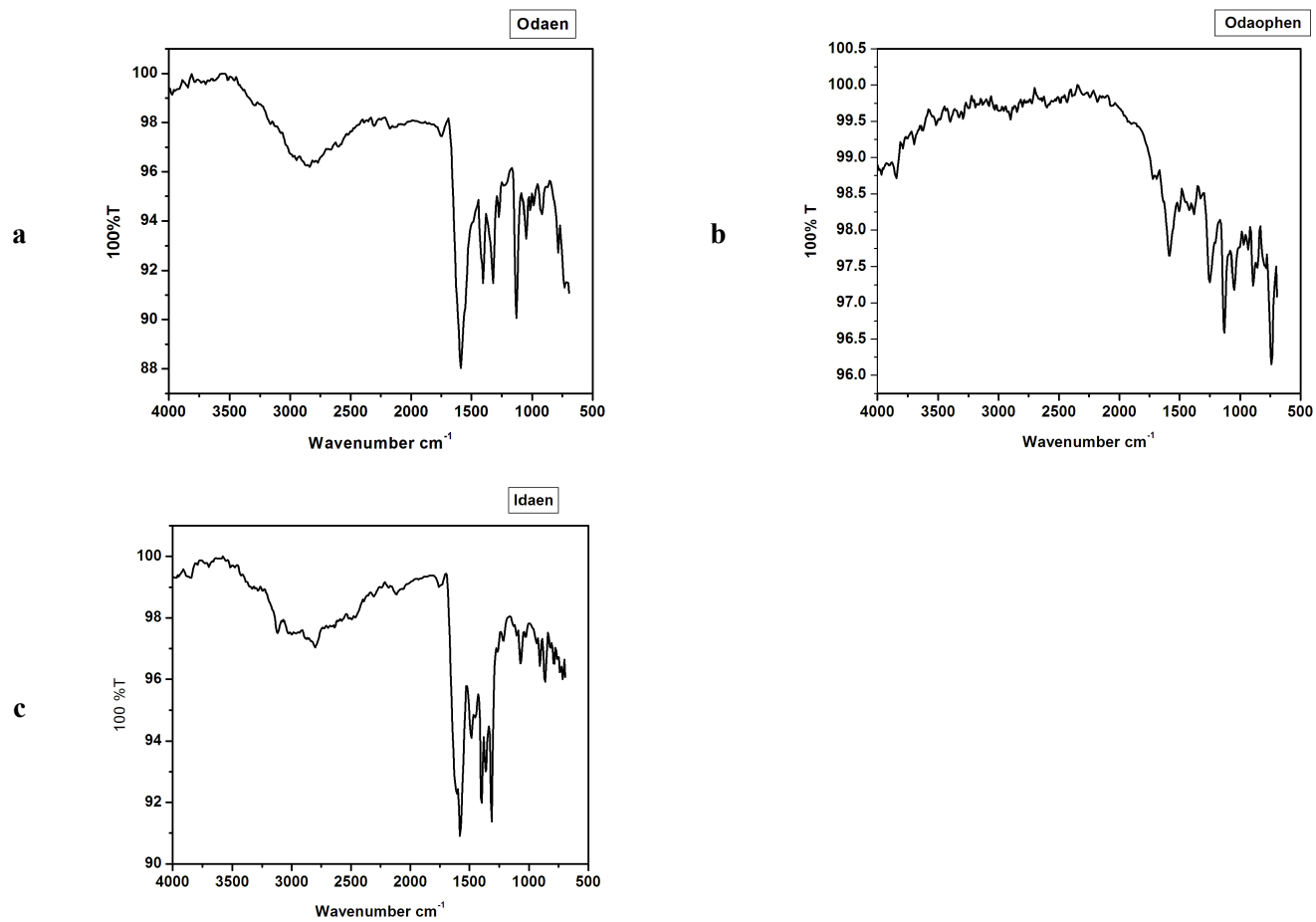




**Fig. S13. Fingerprint plot of O...O interactions of (a) Odaen (1.1%) (b) Odaophen (0.7%) (c) Idaen(0.4%)**



**Fig. S14. ORTEP diagram of Ida Zwitterion displacement ellipsoids drawn at 40% probability level**



**Fig. S15.** ATR spectrum of (a) Odaen (b) Odaophen (c) Idaen