

Supporting Information

Halogen-bonded cocrystallization of racetam pharmaceuticals and perfluorinated iodobenzenes

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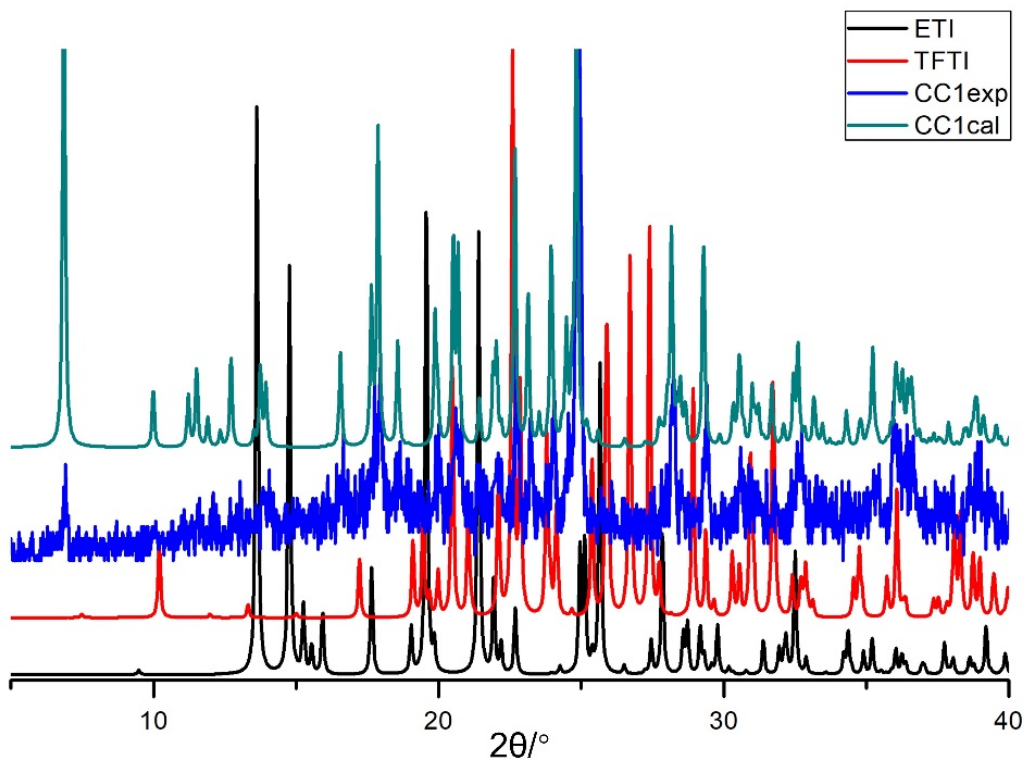


Figure S1. PXRD pattern of CC1. Black is ETI, red is TFTI, blue is experimental pattern of CC1 and green is simulated pattern of CC1.

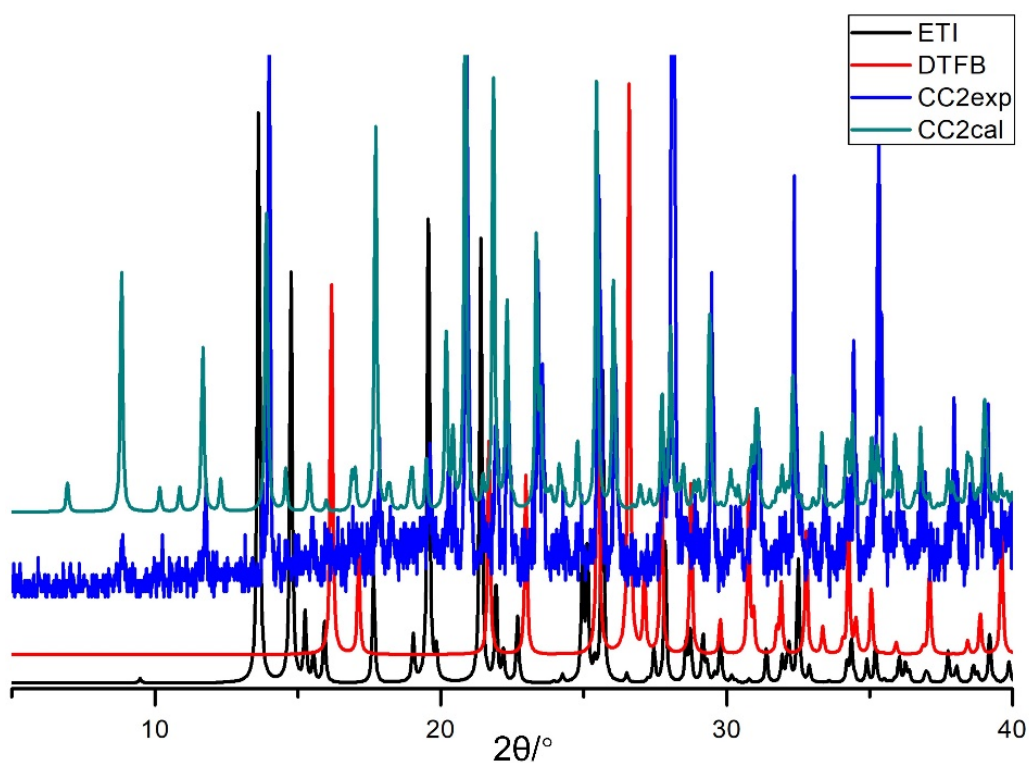


Figure S2. PXRD pattern of CC2. Black is ETI, red is DTFB, blue is experimental pattern of CC2 and green is simulated pattern of CC2.

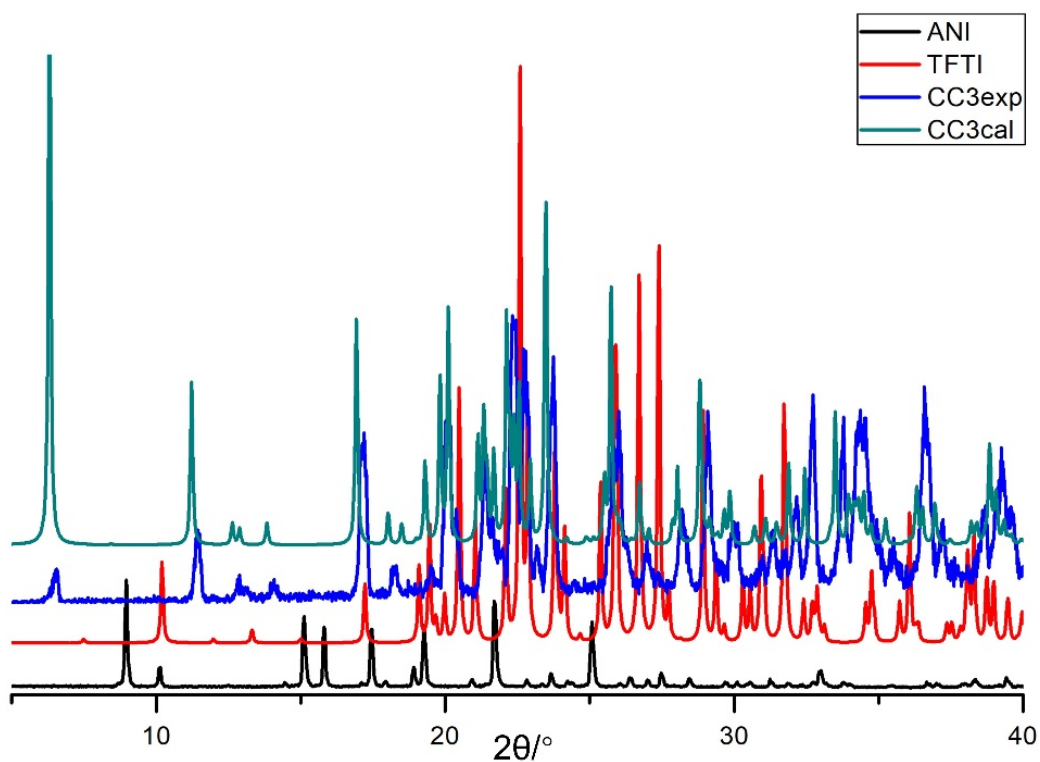


Figure S3. PXRD pattern of CC3. Black is ANI, red is TFTI, blue is experimental pattern of CC3 and green is simulated pattern of CC3.

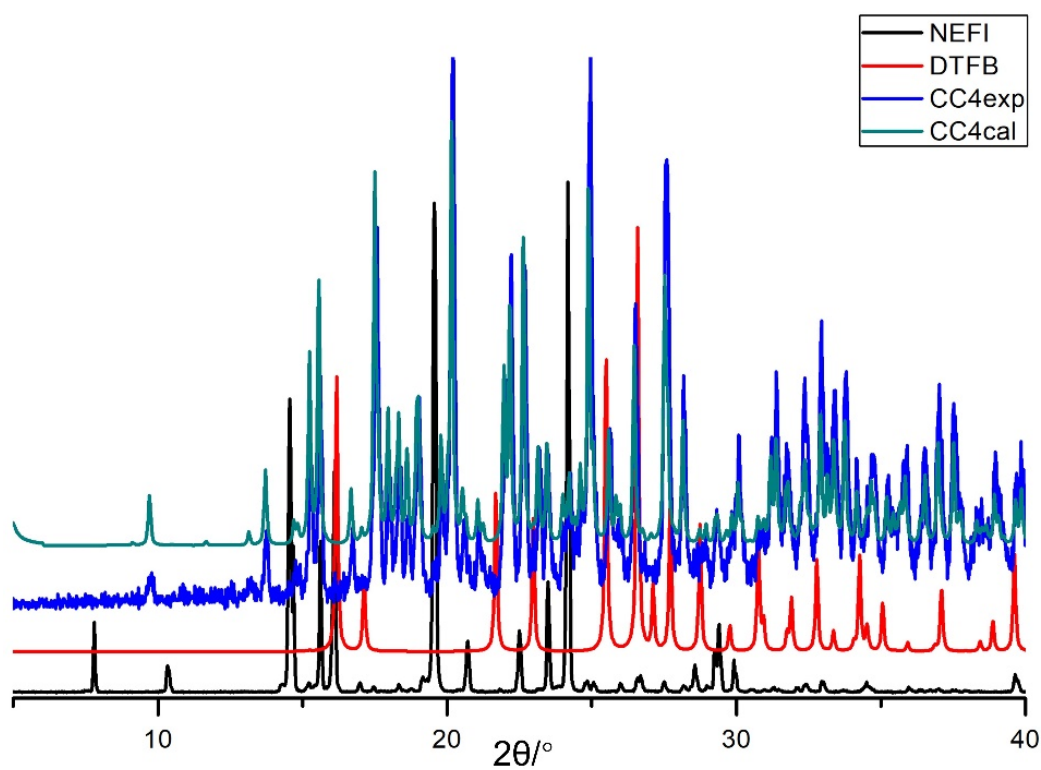


Figure S4. PXRD pattern of CC4. Black is NEFI, red is DTFB, blue is experimental pattern of CC4 and green is simulated pattern of CC4.

Table S1. Halogen bond details for CC1-CC4.

cocrystal	D...A	Acceptor specie	d(D...A)/ Å	$\angle(\text{C-D}\cdots\text{A})^\circ$
1	I3...O9	carbonyl oxygen	2.959	177.50
	I2...O3	carbonyl oxygen on the ring	3.035	166.53
2	I2...O9	carbonyl oxygen	3.043	172.80
	I3...O3	carbonyl oxygen on the ring	2.924	177.71
3	I1...O8	carbonyl oxygen	2.967	173.26
	I2...O3	carbonyl oxygen on the ring	2.951	173.91
4	I1...O3	carbonyl oxygen on the ring	2.842	177.55
	I2... π	benzene ring	4.231	

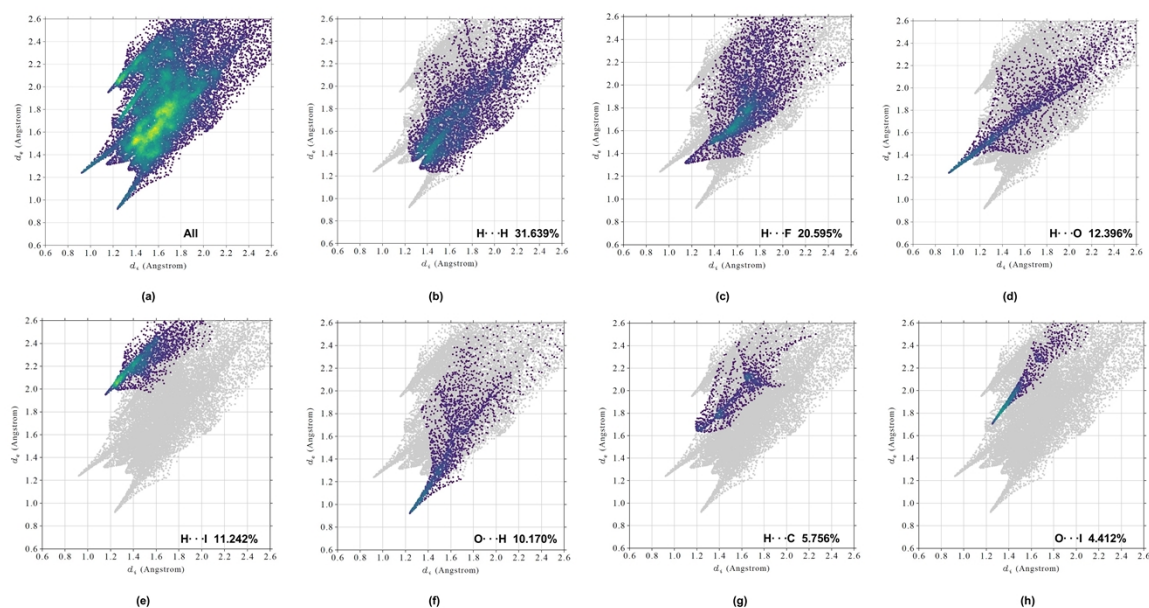
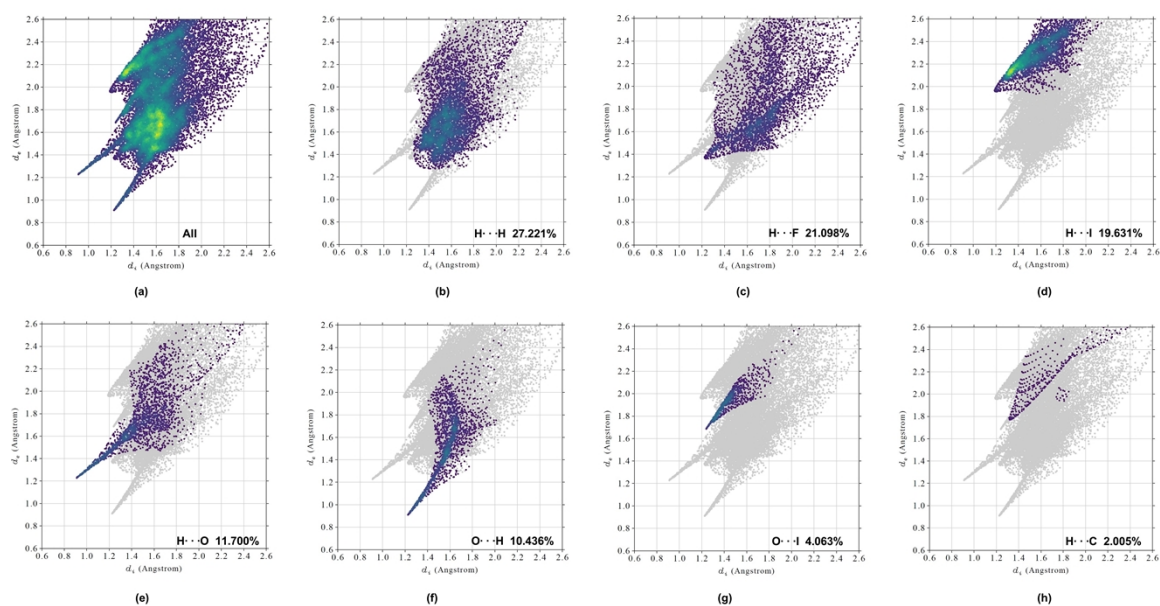
**Figure S5.** 2D fingerprint plots of CC1 according to d_{norm} value, Hirshfeld surface view about intermolecular interactions, and different features characteristic of some key intermolecular contacts, (a) all, (b) H...H, (c) H...F, (d) H...O, (e) H...I, (f) O...H, (g) H...C and (h) O...I.

Figure S6. 2D fingerprint plots of CC2 according to dnorm value, Hirshfeld surface view about intermolecular interactions, and different features characteristic of some key intermolecular contacts, (a) all, (b) H···H, (c) H···F, (d) H···I, (e) H···O, (f) O···H, (g) O···I and (h) H···C.

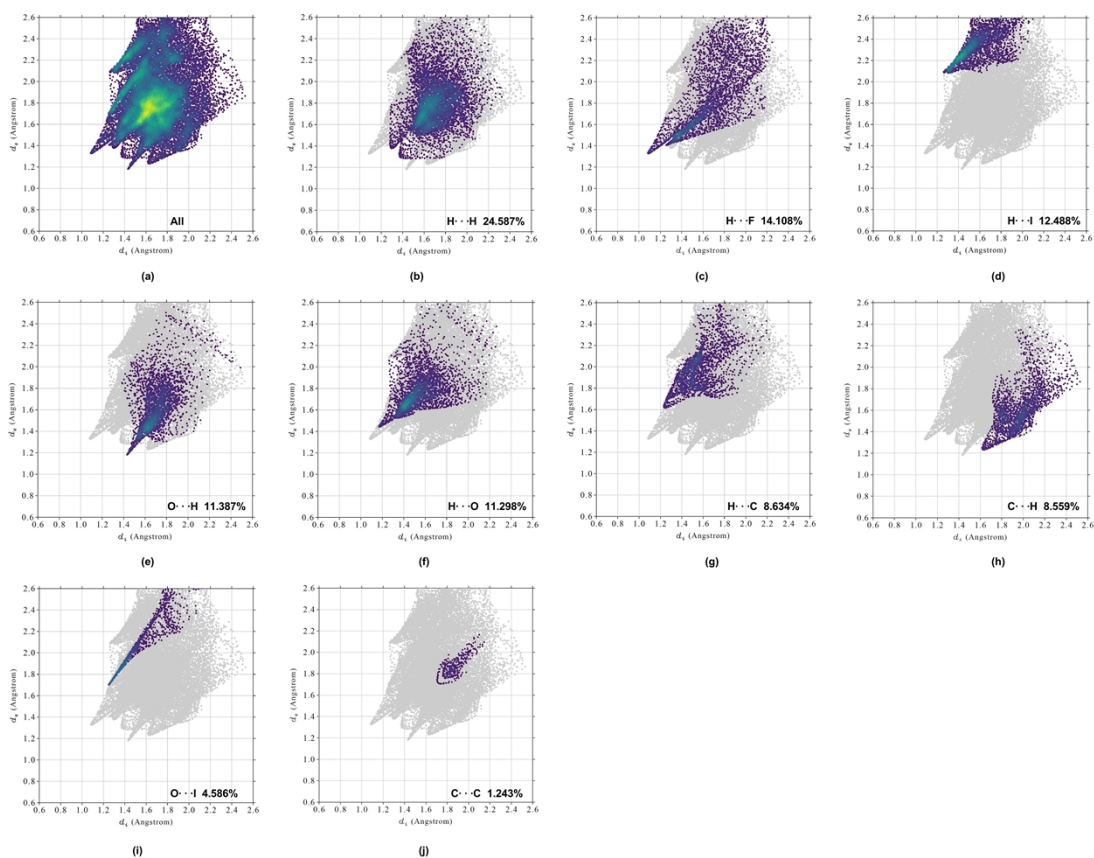


Figure S7. 2D fingerprint plots of CC3 according to dnorm value, Hirshfeld surface view about intermolecular interactions, and different features characteristic of some key intermolecular contacts, (a) all, (b) H···H, (c) H···F, (d) H···I, (e) O···H, (f) H···O, (g) H···C, (h) C···H, (i) O···I and (j) C···C.

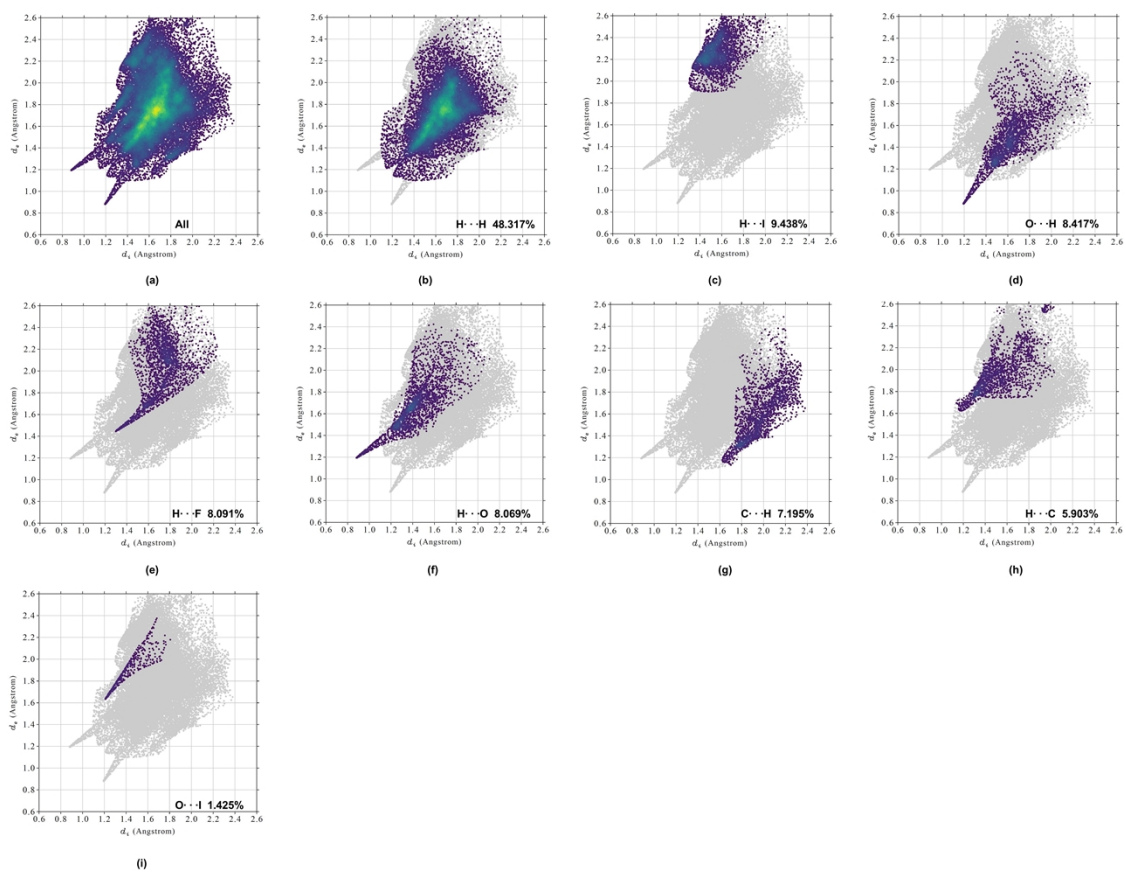


Figure S8. 2D fingerprint plots of CC4 according to d_{norm} value, Hirshfeld surface view about intermolecular interactions, and different features characteristic of some key intermolecular contacts, (a) all, (b) $H \cdots H$, (c) $H \cdots I$, (d) $O \cdots H$, (e) $H \cdots F$, (f) $H \cdots O$, (g) $C \cdots H$, (h) $H \cdots C$ and (i) $O \cdots I$.