Supplementary

S1 Crystal Structures Experimental Conditions

Table S1 Experimental details

	(izact+C6)	(izact+C7)	(izact+C8)	(izact+C9)	(izact+C10)
Chemical formula	$(C_9H_{11}N_3O)\cdot(C_3H_5O_2)$	$2(C_9H_{11}N_3O)\cdot(C_7H_{12}O_4)$	$(C_9H_{11}N_3O)\cdot(C_4H_7O_2)$	$(C_9H_{11}N_3O)\cdot(C_4H_8O_2)$	$2(C_9H_{11}N_3O)\cdot(C_{10}H_{18}O_4)$
M_r	250.28	514.58	264.3	271.32	556.66
Crystal system, space group	Monoclinic, $P2_1/c$	Monoclinic, $C2/c$	Monoclinic, $P2_1/c$	Monoclinic, $C2/c$	Triclinic, $P1$
Temperature (K)	173	173	173	173	173
a, b, c (Å)	19.0668 (10), 8.1886 (4), 8.0487 (4)	47.130 (4), 5.0755 (4), 23.567 (2)	19.888 (4), 8.2744 (15), 8.3942 (15)	22.0145 (19), 16.7461 (15), 7.9045 (6)	7.9554 (4), 13.7715 (8), 14.6005 (8)
α, β, γ (°)	90, 91.561 (3), 90	90, 111.352 (2), 90	90, 96.316 (6), 90	90, 100.476 (3), 90	72.874 (3), 75.014 (3), 84.453 (3)
V (Å^3)	1256.18 (11)	5250.6 (8)	1373.0 (4)	2865.5 (4)	1476.32 (14)
Z	4	8	4	8	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.10	0.10	0.09	0.09	0.09
Crystal size (mm)	0.55 × 0.20 × 0.15	0.46 × 0.24 × 0.08	0.34 × 0.15 × 0.08	0.38 × 0.20 × 0.05	0.36 × 0.22 × 0.14
F(000)	532	2192	564	1160	596
2Θ range for data collection (°)	2.137 - 27.997	2.726 - 28.000	2.060 - 28.345	2.887 - 28.279	1.504 - 28.317
Reflections collected	11423	50090	27737	54106	54935
Independent reflns	3034 [R_{int} = 0.0321]	6309 [R_{int} = 0.0389]	3282 [R_{int} = 0.1042]	3570 [R_{int} = 0.1327]	7371 [R_{int} = 0.0882]
Goodness-of-fit on F^2	1.044	1.182	1.032	1.031	1.027
final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0465$, $wR_2 = 0.1097$	$R_1 = 0.0829$, $wR_2 = 0.1916$	$R_1 = 0.0664$, $wR_2 = 0.1659$	$R_1 = 0.0506$, $wR_2 = 0.1077$	$R_1 = 0.0528$, $wR_2 = 0.1317$
final R indexes [all data]	$R_1 = 0.0701$, $wR_2 = 0.1225$	$R_1 = 0.1011$, $wR_2 = 0.1988$	$R_1 = 0.1118$, $wR_2 = 0.1913$	$R_1 = 0.1070$, $wR_2 = 0.1354$	$R_1 = 0.0783$, $wR_2 = 0.1490$

S2 Hydrogen Bond Tables

Table S2 Hydrogen-bond geometry (Å, º) for (izact+C6)

D—H$\cdots A$	D—H	H$\cdots A$	$D \cdots A$	D—H$\cdots A$
N1—H1$\cdots$N3^i	0.88 (2)	2.56 (2)	3.1789 (19)	128.7 (17)
N1—H1$\cdots$O1^i	0.88 (2)	2.65 (2)	3.515 (2)	169.3 (18)
O2—H2$A\cdots$N2	0.89 (2)	1.82 (2)	2.7069 (17)	175 (2)

Symmetry codes: (i) x, $-y+1/2$, $z+1/2$.

Table S3 Hydrogen-bond geometry (Å, º) for (izact+C7)

D—H$\cdots A$	D—H	H$\cdots A$	$D \cdots A$	D—H$\cdots A$
N1B—H1$B\cdots$O1B^i	0.88	2.18	3.030 (4)	162
N1A—H1$A\cdots$O1A^i	0.88	2.16	3.016 (4)	163
O2—H2$\cdots$N2A	0.84	1.79	2.620 (4)	170
O4—H4$\cdots$N2B	0.84	1.82	2.635 (4)	164

Symmetry code: (i) x, $y-1$, z.

Table S4 Hydrogen-bond geometry (Å, º) for (izact+C8)

D—H$\cdots A$	D—H	H$\cdots A$	$D \cdots A$	D—H$\cdots A$
O2—H2$B\cdots$N1	0.84	1.87	2.686 (3)	163

Table S5 Hydrogen-bond geometry (Å, º) for (izact+C9)

D—H$\cdots A$	D—H	H$\cdots A$	$D \cdots A$	D—H$\cdots A$
N2—H2$A\cdots$N3^i	0.89 (3)	2.30 (3)	3.054 (2)	142 (2)
N2—H2$A\cdots$O1^i	0.89 (3)	2.60 (3)	3.403 (2)	150 (2)
O2—H2$B\cdots$N1	0.99 (3)	1.71 (3)	2.690 (2)	174 (3)

Symmetry codes: (i) x, $-y+1$, $z+1/2$.

Table S6 Hydrogen-bond geometry (Å, º) for (izact+C10)

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···N6^i	0.88 (2)	2.35 (2)	3.088 (2)	141.8 (18)
N2—H2B···O6^i	0.88 (2)	2.60 (2)	3.384 (2)	149.2 (17)
O2—H2···N1	0.96 (3)	1.80 (3)	2.706 (2)	156 (3)
O4—H4···N4	0.94 (3)	1.74 (3)	2.6770 (18)	176 (3)
N5—H5A···N3^{ii}	0.84 (2)	2.31 (2)	3.0476 (19)	147.4 (19)

Symmetry codes: (i) −x+1, −y+1, −z+1; (ii) −x+2, −y+1, −z+1.

S2 PXRD Patterns
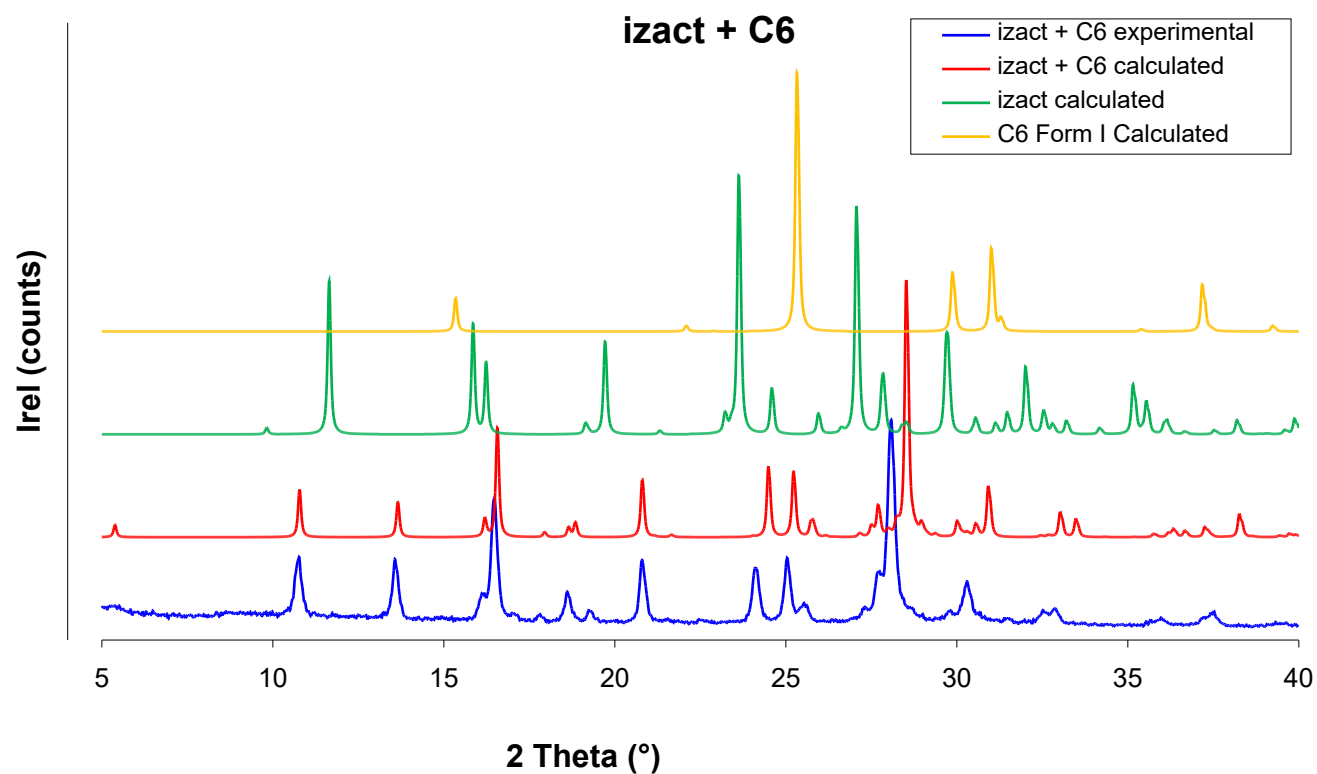
Figure S1 Powder patterns for the experimental and calculated patterns of the cocrystal of izact + C6, together with the calculated patterns of its coformers in their pure form.
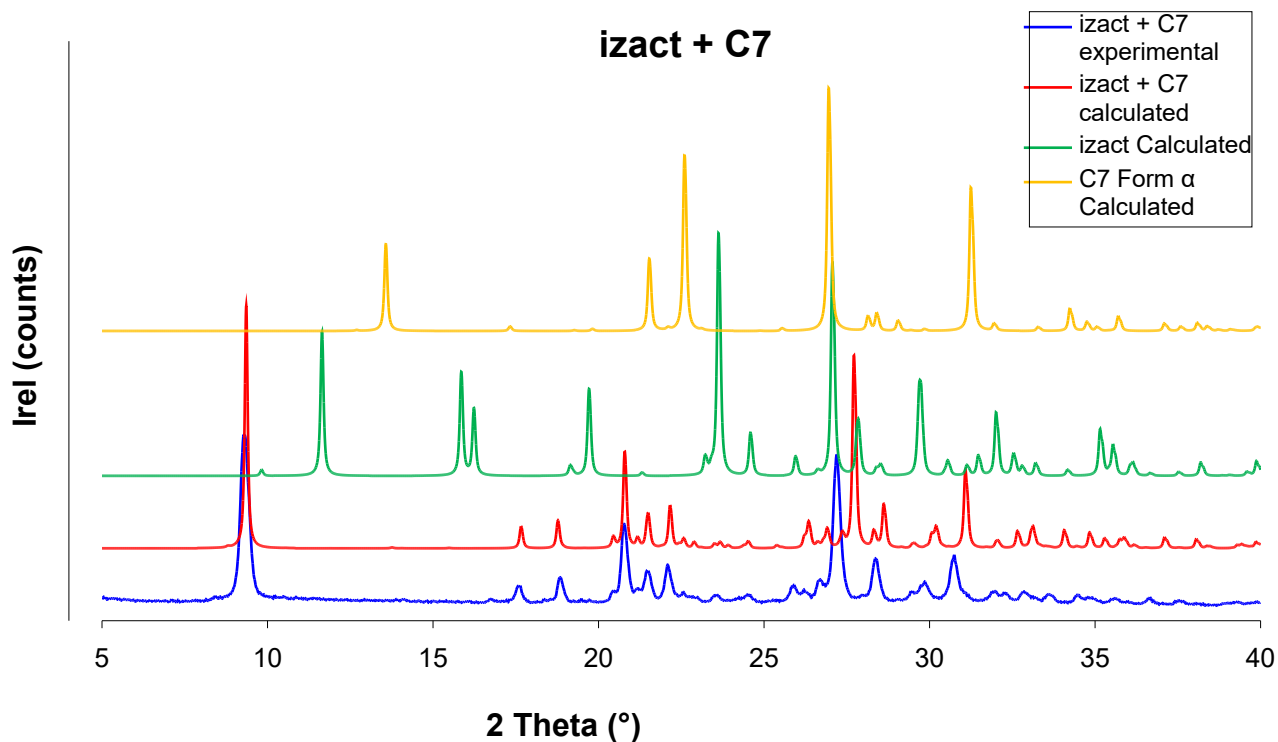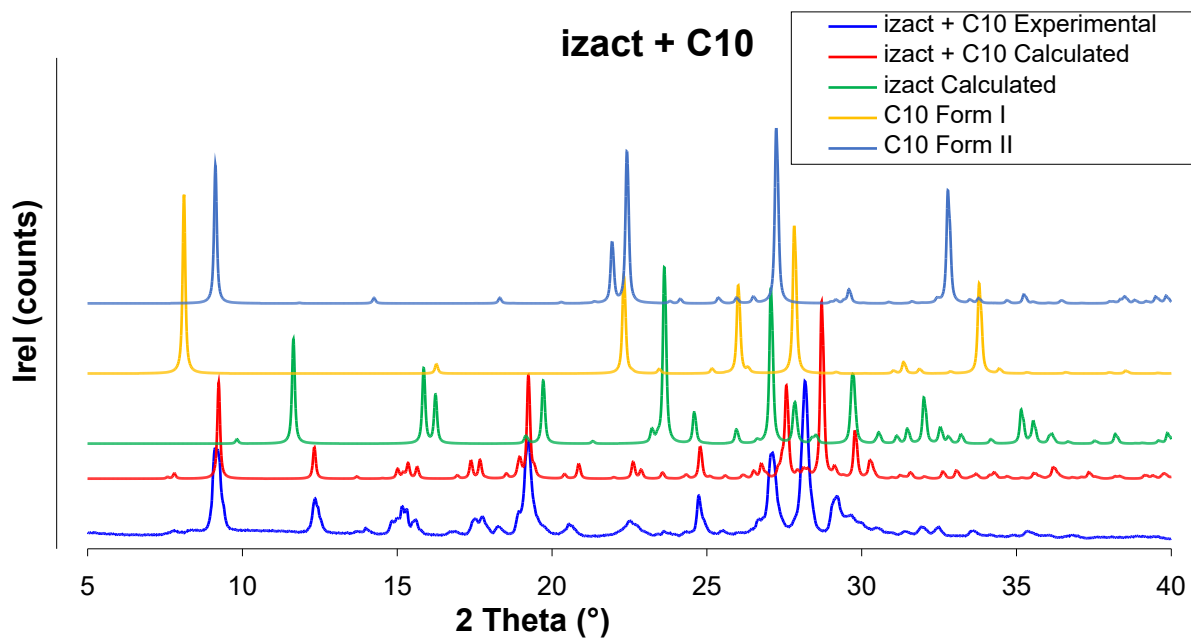
Figure S2 Powder patterns for the experimental and calculated patterns of the cocrystal of izact + C7, together with the calculated patterns of its coformers in their pure form.
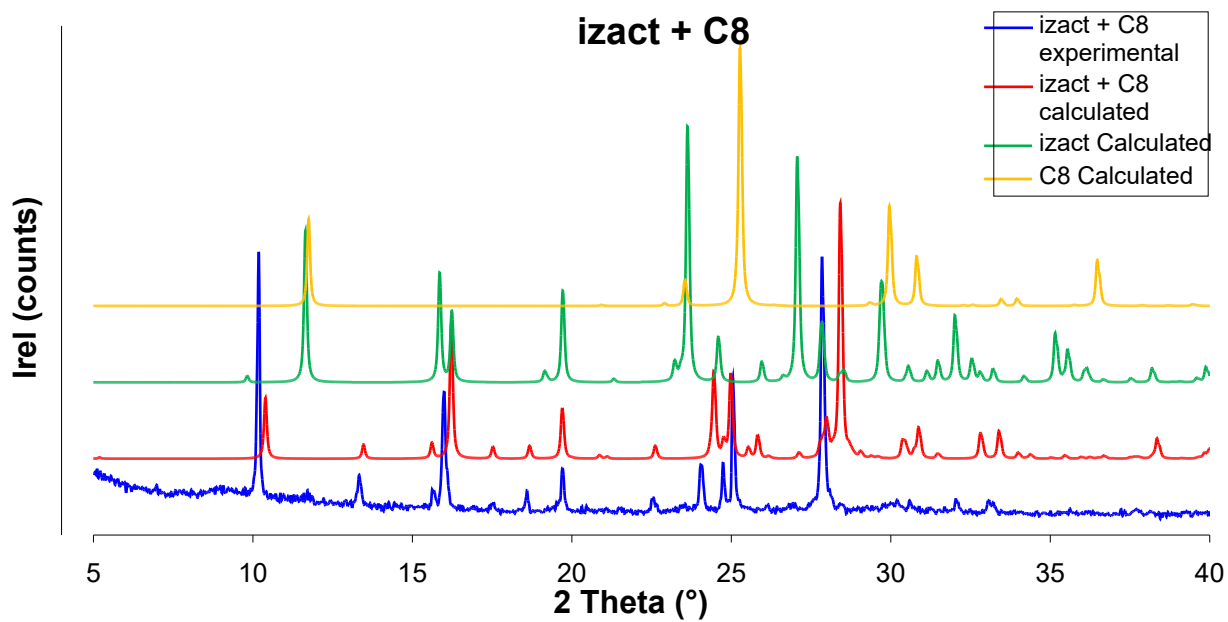
**Figure S3** Powder patterns for the experimental and calculated patterns of the cocrystal of izact + C8, together with the calculated patterns of its coformers in their pure form.
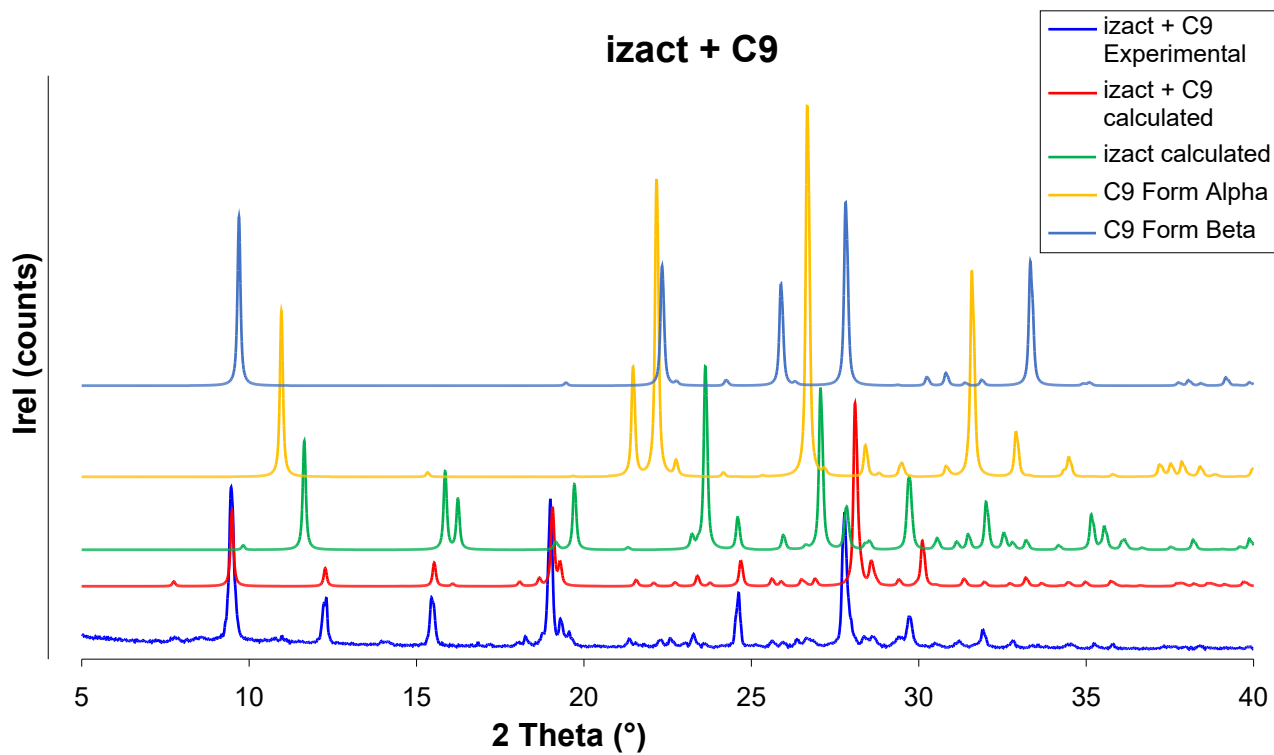
Figure S4 Powder patterns for the experimental and calculated patterns of the cocrystal of izact + C9, together with the calculated patterns of its coformers in their pure form.

Figure S5 Powder patterns for the experimental and calculated patterns of the cocrystal of izact + C7, together with the calculated patterns of its coformers in their pure form.

S3 DSC Analysis
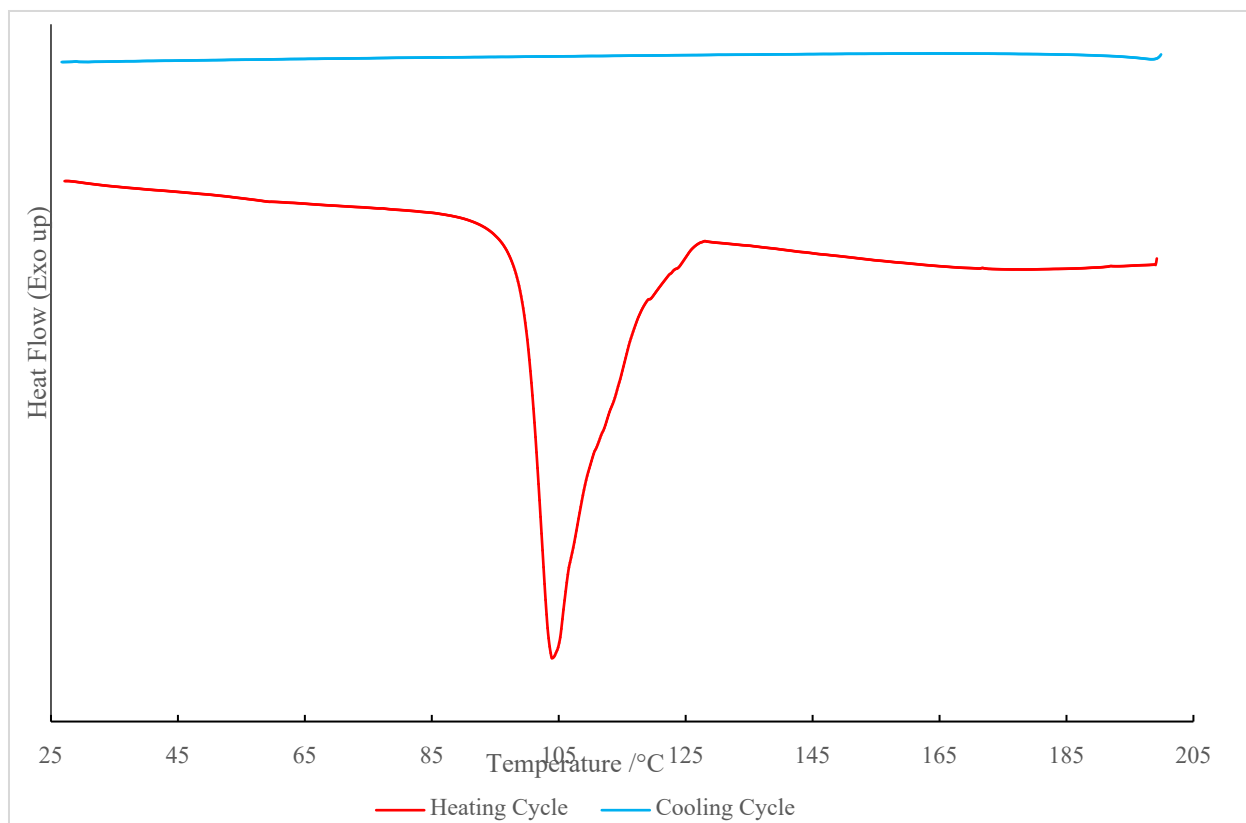
Figure S6 DSC curve of **izact + C6**
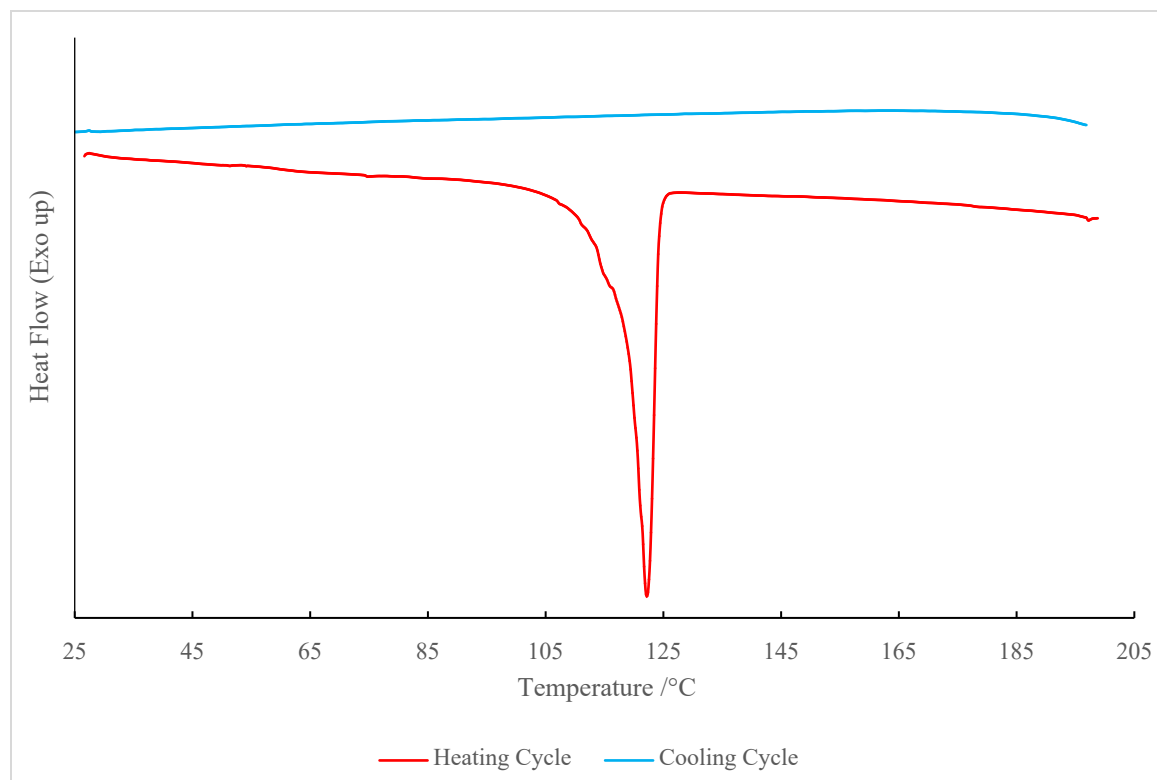
Figure S7 DSC curve of **izact + C7**
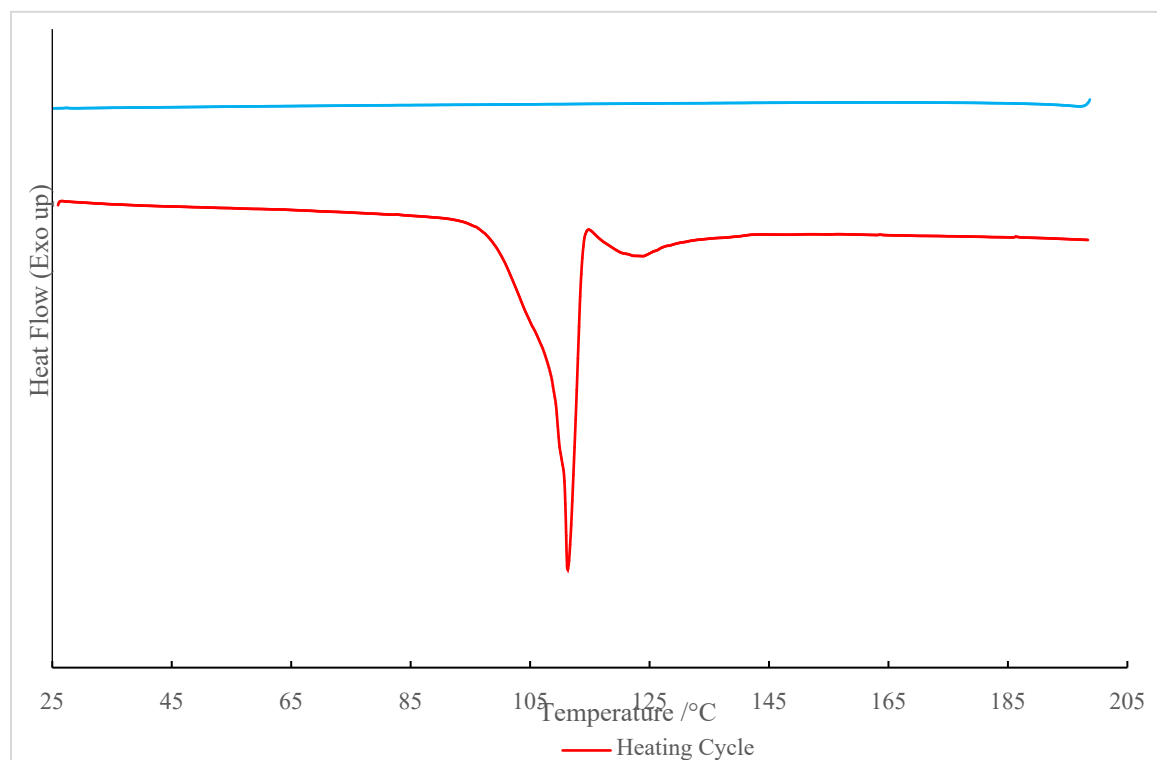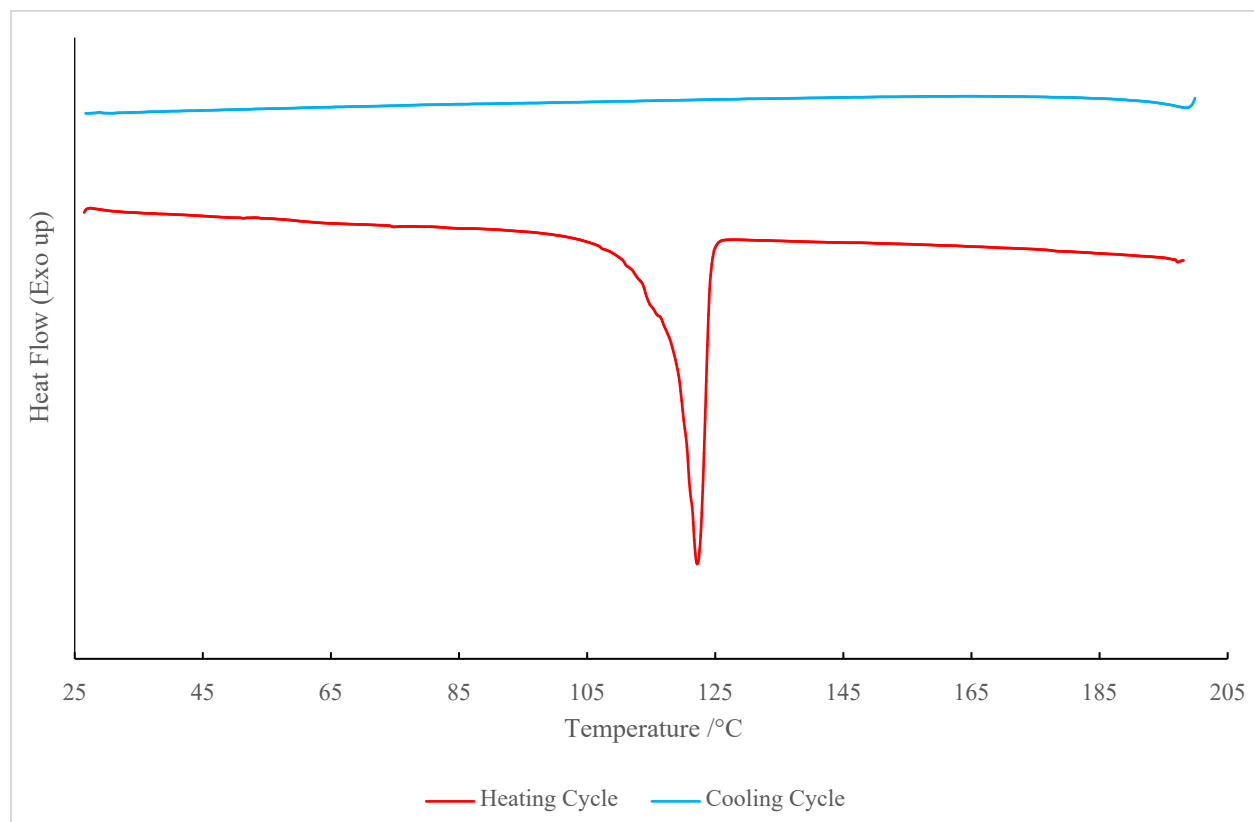

Figure S8 DSC curve of **izact + C8**

Figure S9 DSC curve of **izact + C9**
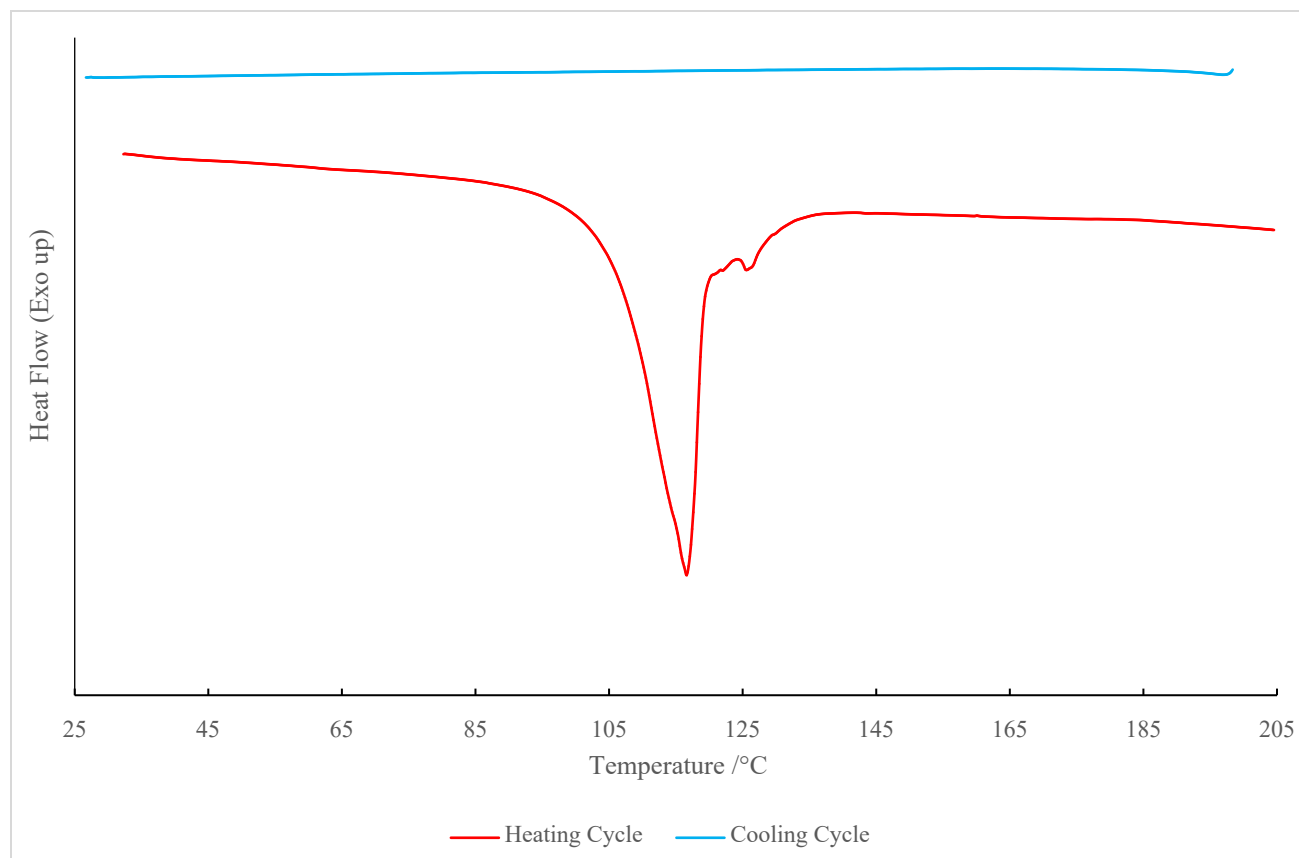
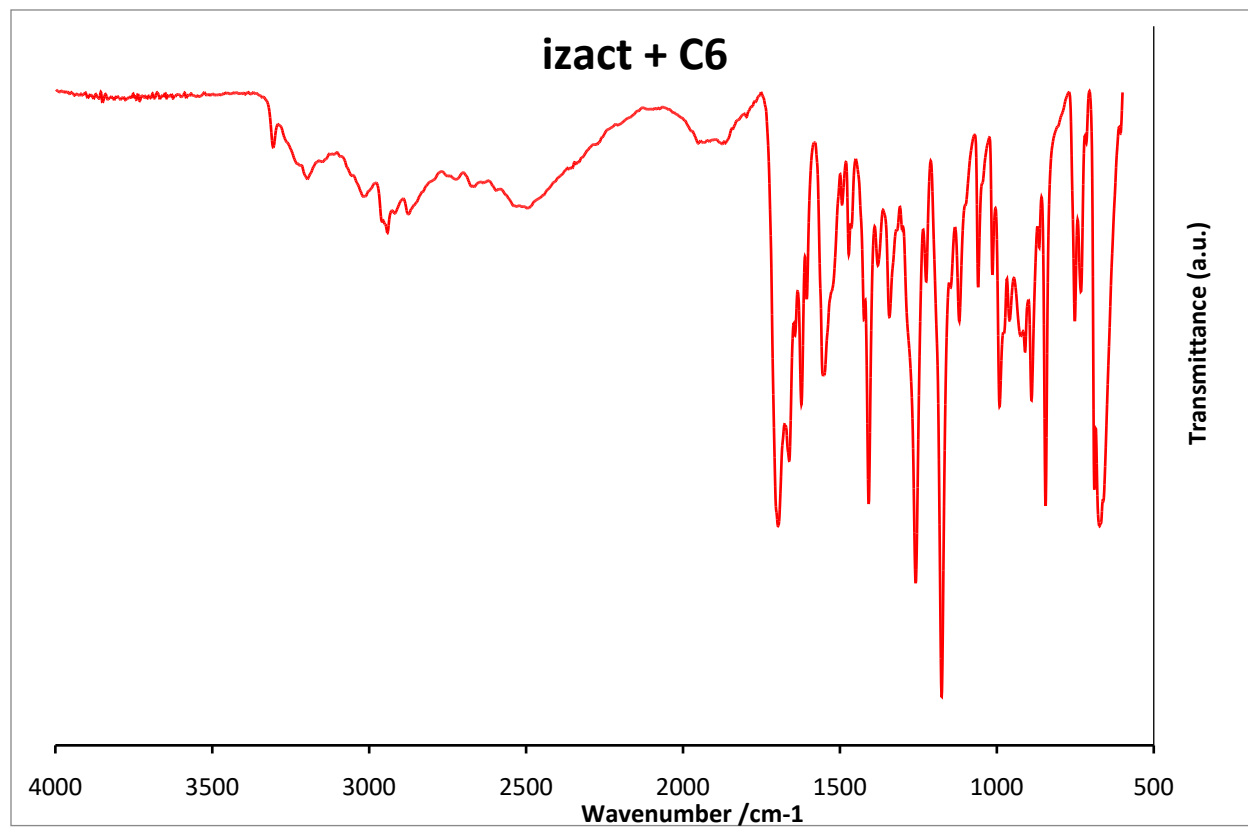**Figure S10** DSC curve of **izact + C10**

FTIR

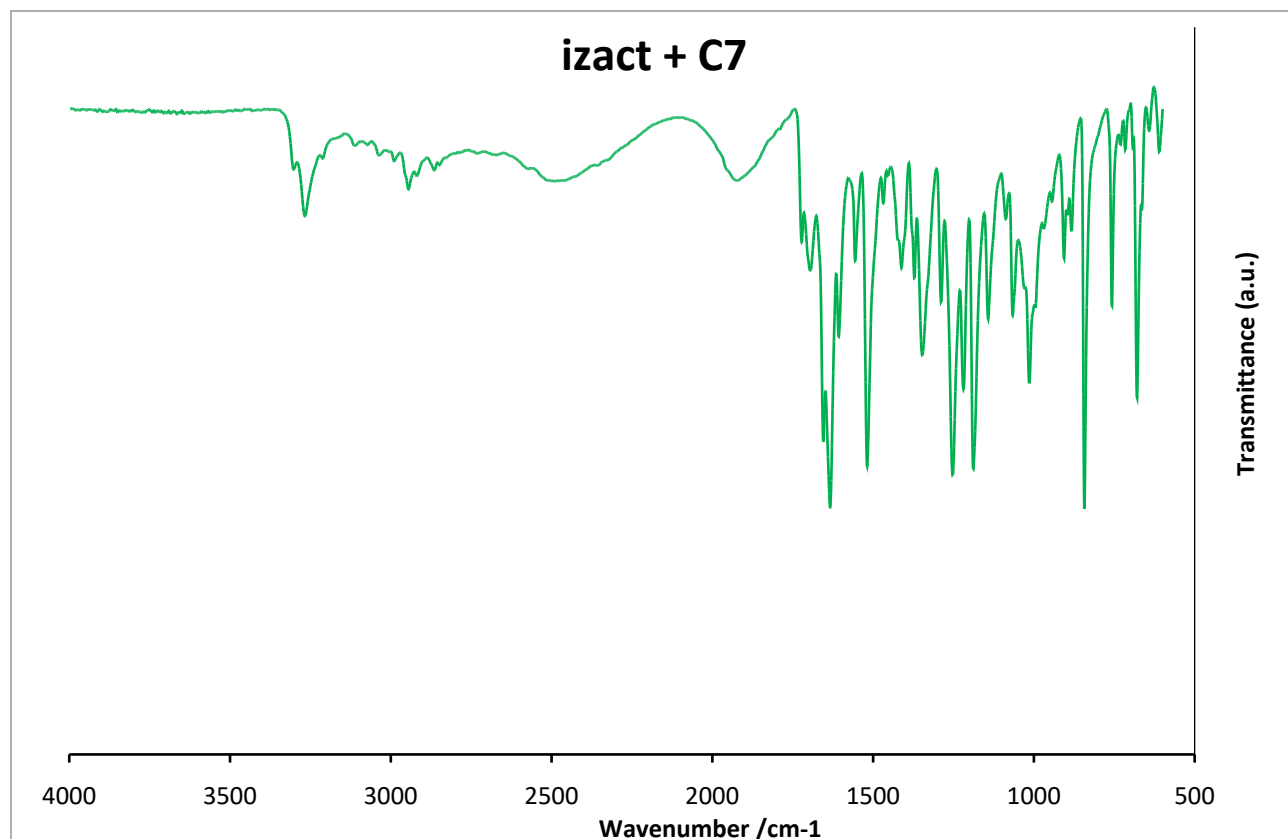
Figure S11 FTIR Spectra of izact + C6.

Figure S12 FTIR Spectra of izact + C7.
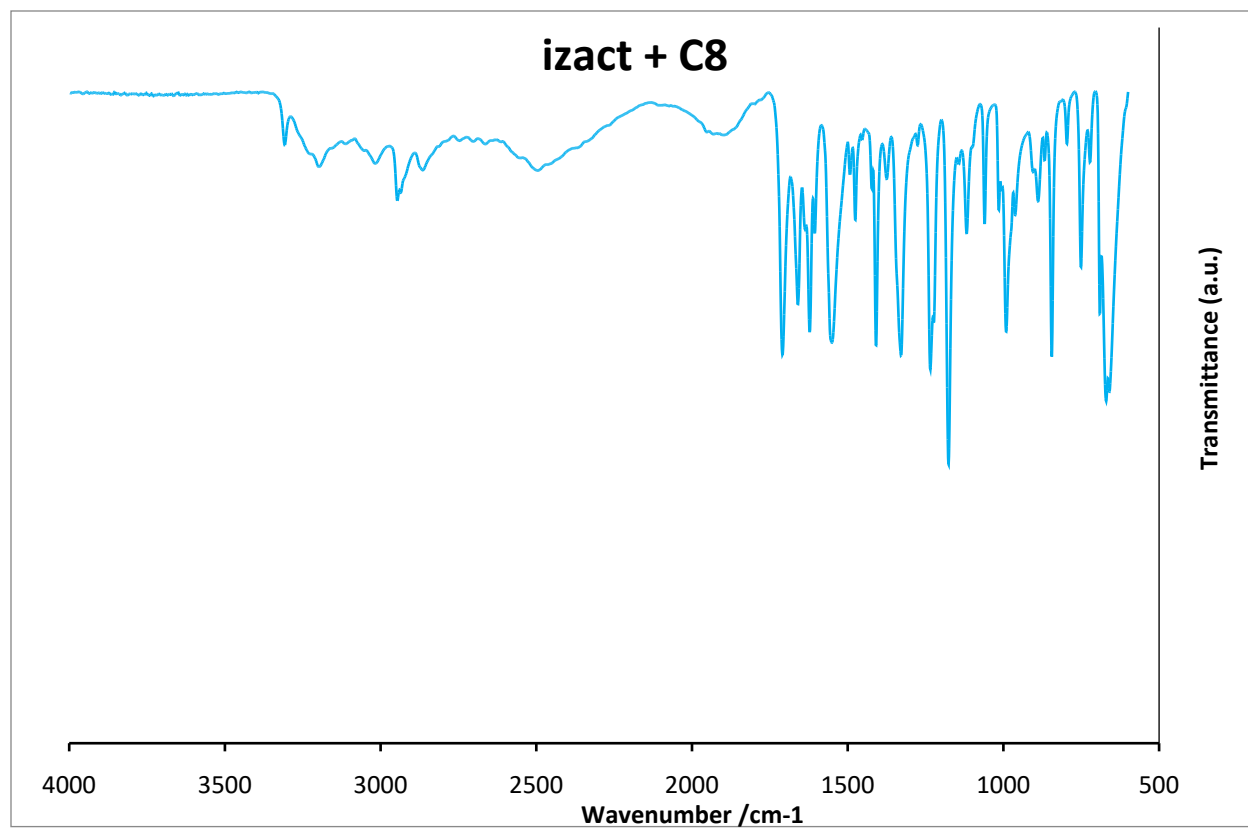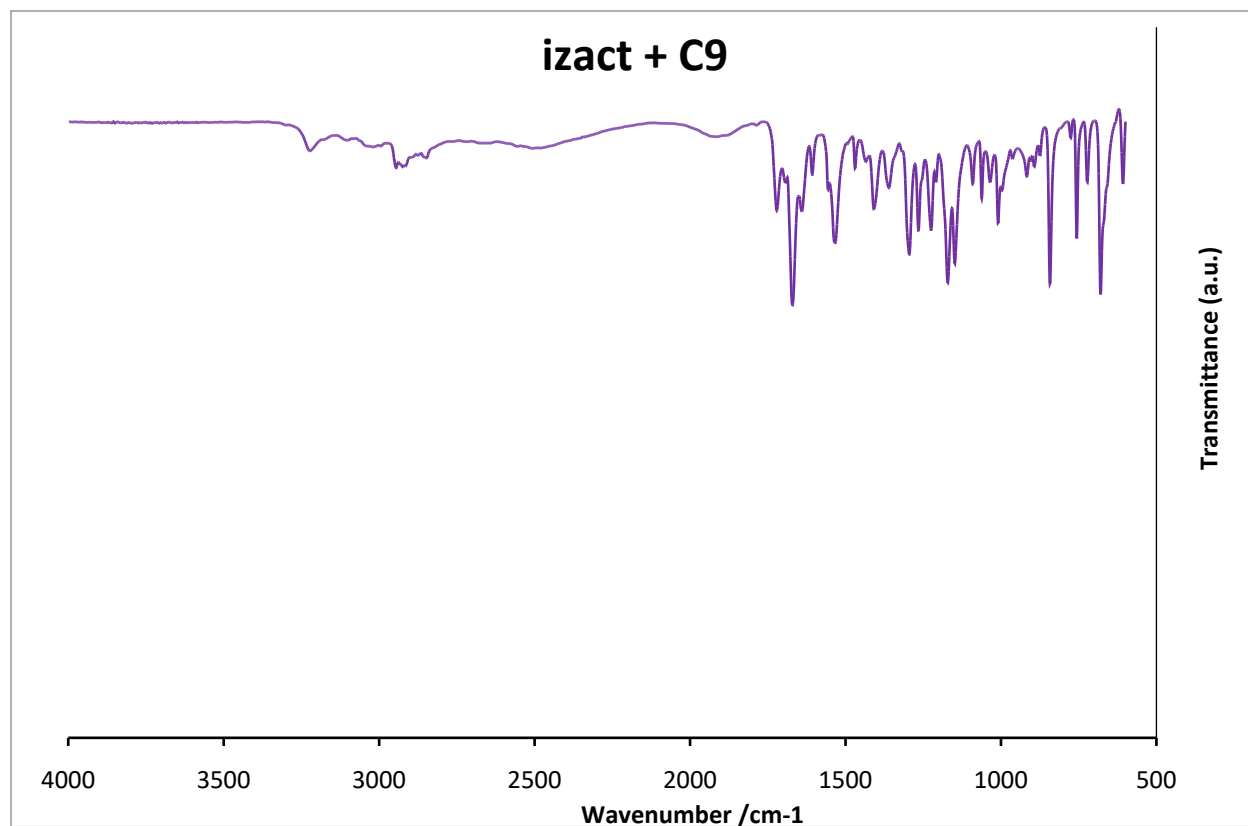
Figure S13 FTIR Spectra of izact + C8.
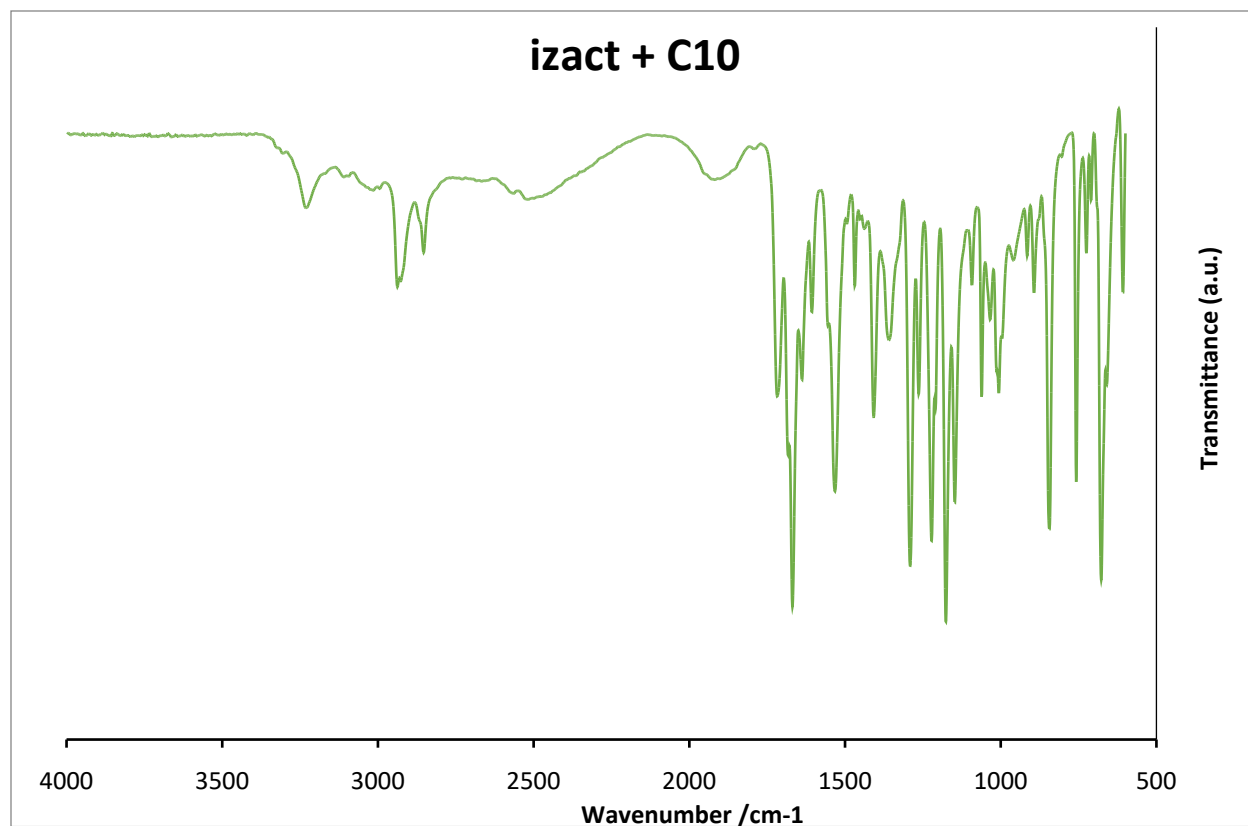
Figure S14 FTIR Spectra of izact + C9.

Figure S15 FTIR Spectra of izact + C10.

Table S7 Some FTIR assignments for the cocrystals of izact with dicarboxylic acids.

Solid form	ν (-C=O)	ν (-NH-)	ν (-OH)
izact + C6	1697.19	3196.66	2941.77
izact + C7	1633.75	3267.29	2944.95
izact + C8	1709.44	3307.85	2946.19
izact + C9	1670.66	3222.19	2945.48
izact + C10	1668.81	3231.23	2937.37