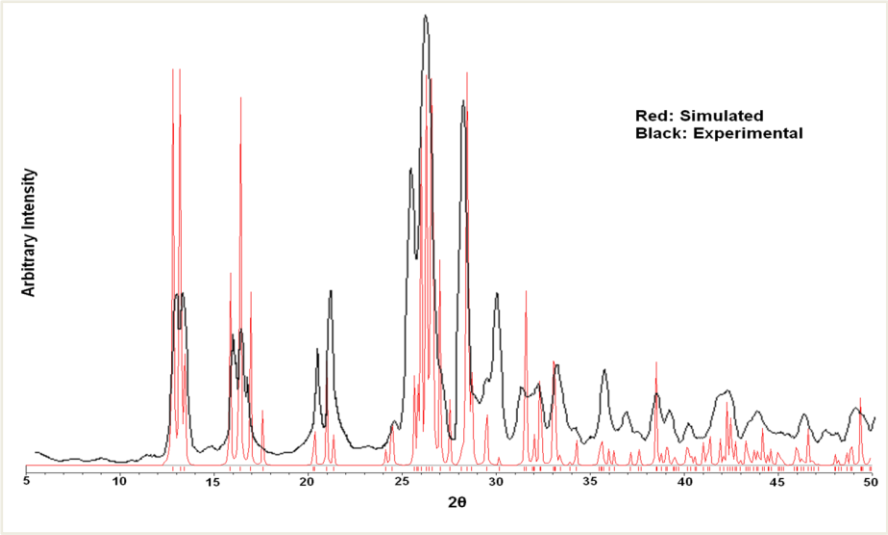
Appendix

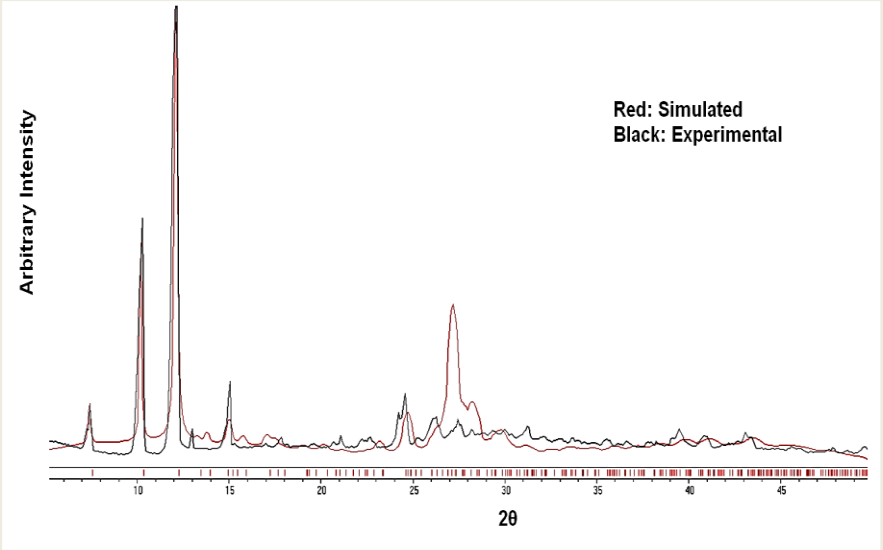
Table A.1 Single crystal X-ray data parameter of cocrystals **1-7**

Crystal data	**[1] Theo·Res·H_2O**	**[2] Theo·Phu·H_2O**	**[3] Theo·Orc·$2H_2O$**	**[4] Theo·2,6-DHBA·H_2O**
Formula unit	$C_7H_8N_4O_2$· $C_6H_6O_2$·H_2O	$C_7H_8N_4O_2$· $C_6H_6O_3$·H_2O	$C_7H_8N_4O_2$· $C_7H_8O_2$·$2H_2O$	$C_7H_9N_4O_2$· $C_7H_5O_4$·H_2O
Formula wt.	308.3	324.3	340.34	352.31
Crystal system	Monoclinic	Monoclinic	Orthorhombic	Monoclinic
T [K]	100	100	100	100
a [Å]	11.0728(4)	6.7236(3)	9.8095(15)	14.8098(5)
b [Å]	8.7248(4)	23.2123(9)	13.369(2)	6.6905(2)
c [Å]	14.6199(7)	9.2933(3)	23.858(4)	15.8509(6)
α [°]	90	90	90	90
β [°]	109.072(2)	98.822(2)	90	94.469(2)
γ [°]	90	90	90	90
Volume [$Å^3$]	1334.87(10)	1433.25(10)	3128.9(8)	1565.81(9)
Space group	*Cc*	$P2_1/c$	*Pbca*	$P2_1/c$
Z	4	4	8	4
D_{calc} [g cm^{-3}]	1.534	1.503,	1.445,	1.494,
μ (mm^{-1})	0.120	0.121	0.114	0.122
Reflns.	10271	20 611	6568	36 046,
collected	3196	7423	1602	6785
Unique observed	2751	4115	1358	3938
R1 [I > σ(I)],	0.0291	0.0617	0.0381,	0.0575
wR2	0.0849	0.1474	0.1076	0.1670
GOF	1.252	0.967	1.152	1.046
Instrument	Bruker APEX-II	Bruker APEX-II	Bruker APEX-II	Bruker APEX-II
X-ray	Mo k\α;λ=0.71073	Mo k\α; λ=0.71073	Mo k\α;λ=0.71073	Mo k\α; λ=0.71073
Refcode	WOCGON	WOCGUS	WOCHAZ	–

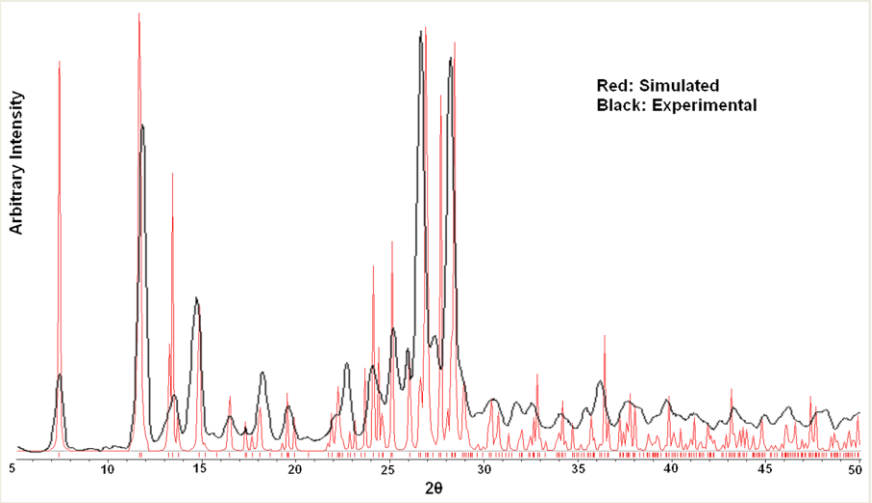
Crystal data	**[5] Theo·3,5-DHBA**	**[6] Theo·3,4-DHBA**	**[7] Theo·CA**
Formula unit	$C_7H_8N_4O_2·C_7H_6O_4$	$C_7H_8N_4O_2·C_7H_6O_4$	$C_7H_8N_4O_2·C_9H_8O_2$
Formula wt.	334.29	334.29	328.33
Crystal system	Triclinic	Triclinic	Orthorhombic
T [K]	296	296	296
a [Å]	7.3213(2)	8.0940(5)	7.2792(7)
b [Å]	8.0238(2)	8.5956(5)	8.7135(9)
c [Å]	12.6902(2)	11.5891(5)	24.272(2)
α [°]	81.6460(10)	103.168(3)	90
β [°]	85.6010(10)	105.023(5)	96.128(4)
γ [°]	82.1560(10)	105.320(4)	90
Volume [$Å^3$]	729.44(3)	712.05(7)	1530.7(3)
Space group	$P\bar{1}$	$P\bar{1}$	$P2_1/c$
Z	2	2	4
D_{calc} [g cm^{-3}]	1.522	1.559	1.425
μ (mm^{-1})	0.122	0.124	0.105
Reflns.	21 150	19 670	20 479
Collected	5826	5748	8056
Unique observed	4276	3652	4961
R1 [I > σ(I)]	0.0486	0.0753	0.0777
wR2	0.1381	0.2037	0.2043
GOF	1.073	1.082	0.998
Instrument	Bruker APEX-II	Bruker APEX-II	Bruker APEX-II
X-ray	Mo k\α; λ=0.71073	Mo k\α; λ=0.71073	Mo k\α; λ=0.71073
Refcode	WOCHIH	WOCHON	WOCHUT



(a) Cocrystal **1 [Theo•Res•H_2O]** (overlay only)

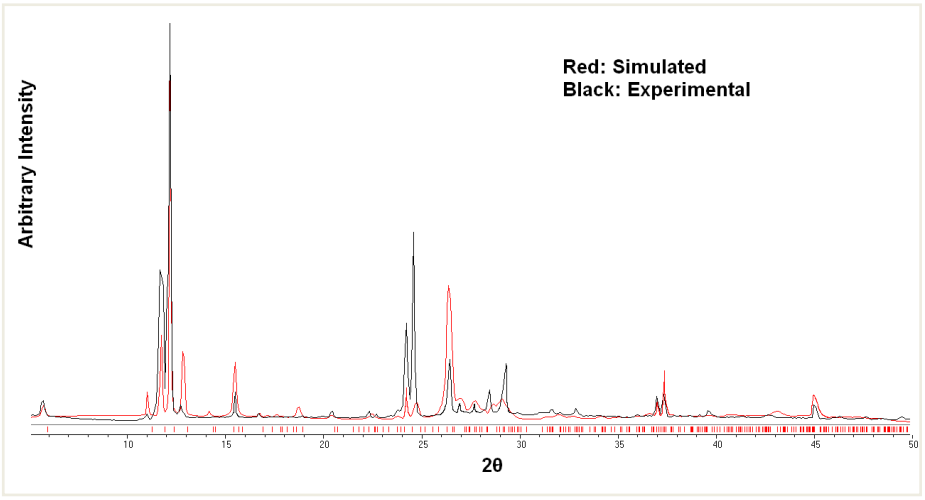


(b) Cocrystal **2 [Theo•Phu•H_2O]**

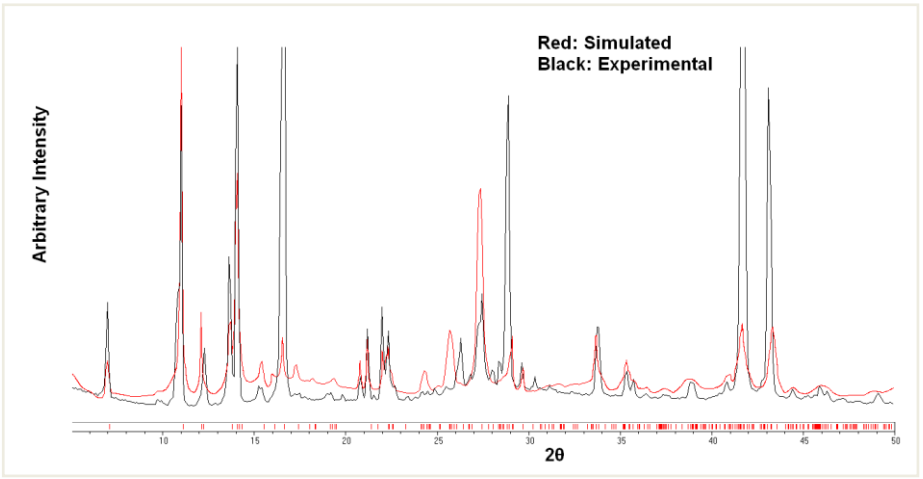


(c) Cocrystal **3 [Theo•Orc•2H_2O]** (overlay only)

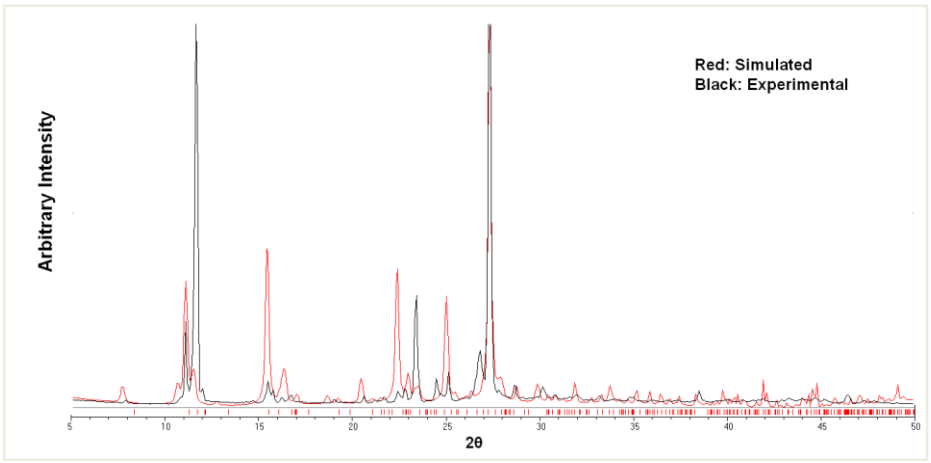
b



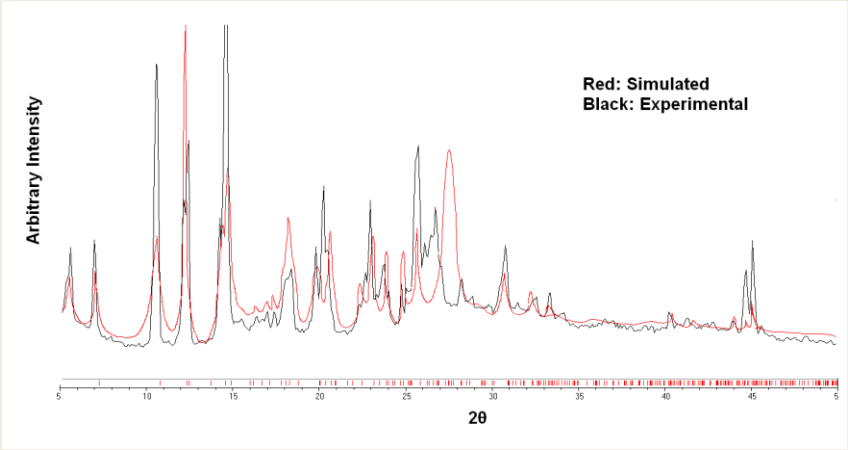
(d) Cocrystal **4 [Theo•2,6-DHBA•H_2O]**



(e) Cocrystal **5 [Theo•3,5-DHBA]**



(f) Cocrystal **6 [Theo•3,4-DHBA]**



(g) Cocrystal **7 [Theo•CA]**

Figure A.1 Powder X-ray diffraction of cocrystals **1-7** compared with simulated from corresponding crystal structure. Slight shifting of few peaks from the original crystal structure is due to the data collection temperature difference (Crystal structure at 100K, experimental PXRD at 298K for cocrystals **1** to **4**) which is not corrected during Reitveld refinement.

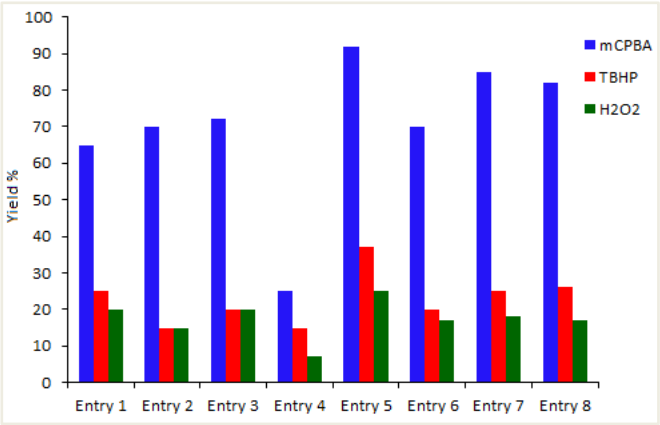
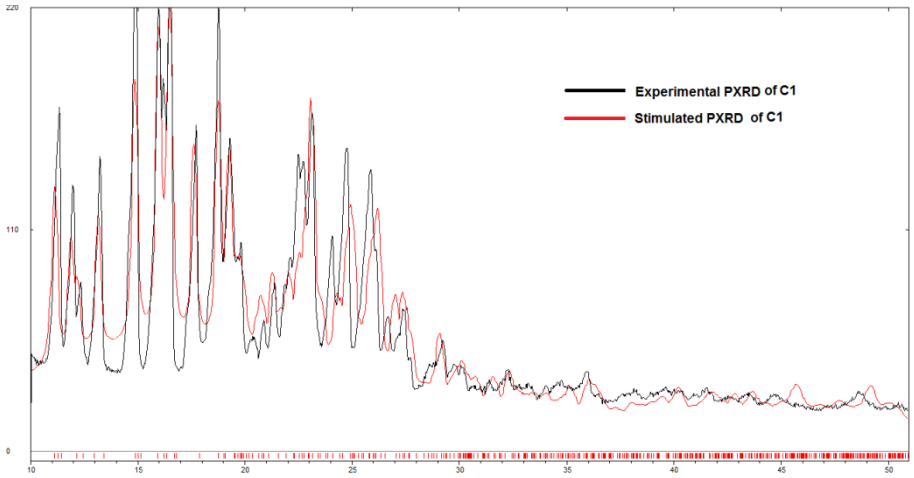


Figure A.2 Bar diagram showing yield % of pyridine *N*-oxides with respect to H_2O_2, *m*-CPBA and TBHP.

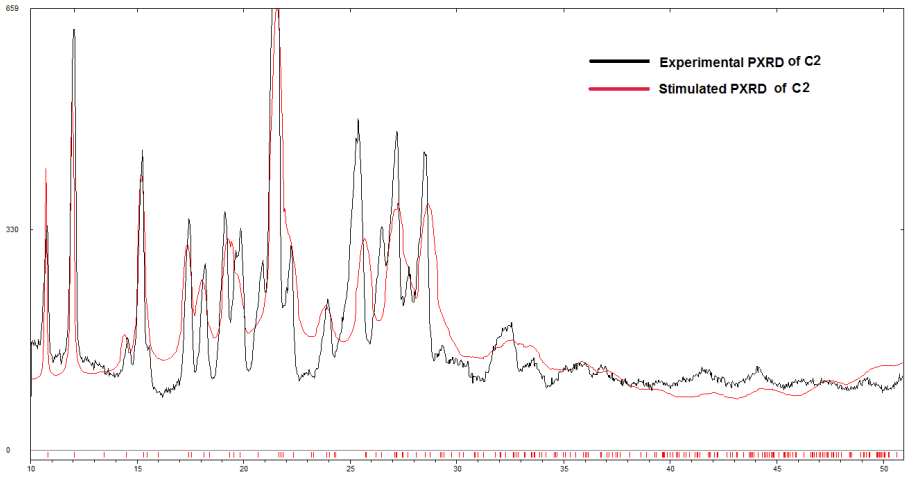
Table A.2 Single crystal X-ray data parameters of pyridine *N*-oxides and cocrystals **C1-C4**

Crystal data	**Entry 4** [Table E2]	**Entry 6** [Table E2]	**C1**	**C2**	**C3**	**C4**
Formula unit	$C_{13}H_{13}NO_3$	$C_{10}H_{12}N_2O_4$	$C_{58}H_{80}N_2O_6$	$C_{24}H_{22}N_4O_6$	$C_{15}H_{14}NO_5$	$C_{19}H_{17}N_5O_4S_2$
Formula weight (g mol^{-1})	231.24	224.22	901.24	462.46	288.27	443.50
Crystal system	Monoclinic	Orthorhombic	Monoclinic	Orthorhombic	Monoclinic	Monoclinic
T [K]	296	296	100	100	296	296
a [Å]	11.6691(9)	15.5890(13)	9.4702(2)	10.977(3)	10.1347(4)	10.5317(11)
b [Å]	6.8681(5)	5.2685(4)	15.5487(3)	12.112(4)	10.8799(5)	8.5508(8)
c [Å]	14.3968(9)	12.4962(10)	18.2269(4)	16.439(5)	12.0819(5)	21.750(2)

α [°]	90	90	90	90	90	90
β [°]	95.620(5)	90	102.0590(13)	90	101.789(2)	91.055(7)
γ [°]	90	90	90	90	90	90
Volume [Å^3]	1148.28(14)	1026.32(14)	2624.67(9)	2185.5(11)	1304.11(10)	1958.4(3)
Space group	*P*2$_1$/*n*	*Pbcn*	*P*2$_1$/*c*	*Pbca*	*P*2$_1$/*c*	*P*2$_1$/*n*
Z	4	4	2	4	4	4
D_{cal} [g cm^{-3}]	1.338	1.451	1.140	1.405	1.468	1.504
X-ray source	Mo, K(α)	Mo, K(α)	Mo, K(α)	Mo, K(α)	Mo, K(α)	Mo, K(α)
R_1, wR2	0.0524; 0.1293	0.0422; 0.1343	0.0435; 0.1113	0.0418; 0.1127	0.0527; 0.1347	0.0548; 0.1443
GOF	0.790	1.114	1.050	0.868	0.804	0.750
Instrument	Bruker APEX-II	Bruker APEX-II	Bruker APEX-II	Bruker APEX-II	Bruker APEX-II	Bruker APEX-II
Refcode	OXIDAC02	VAGQAW03	OXICUVO2	HUZCUA03	OXICIJ02	OXIDEG02

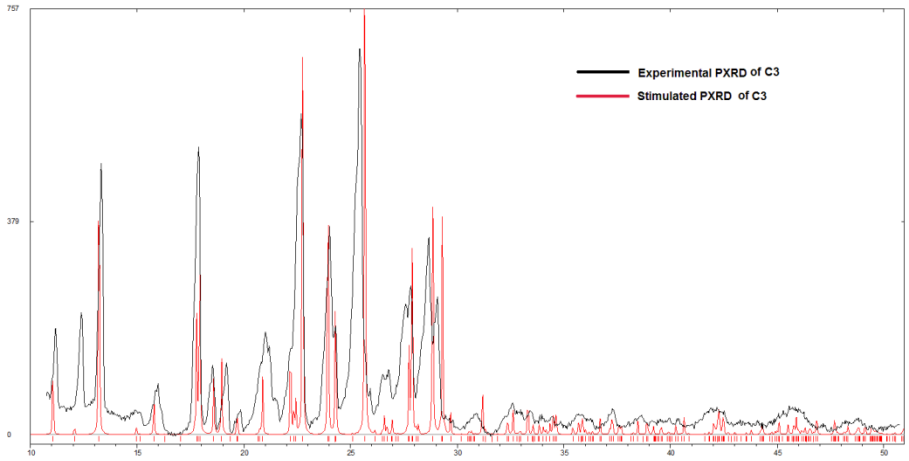


C1

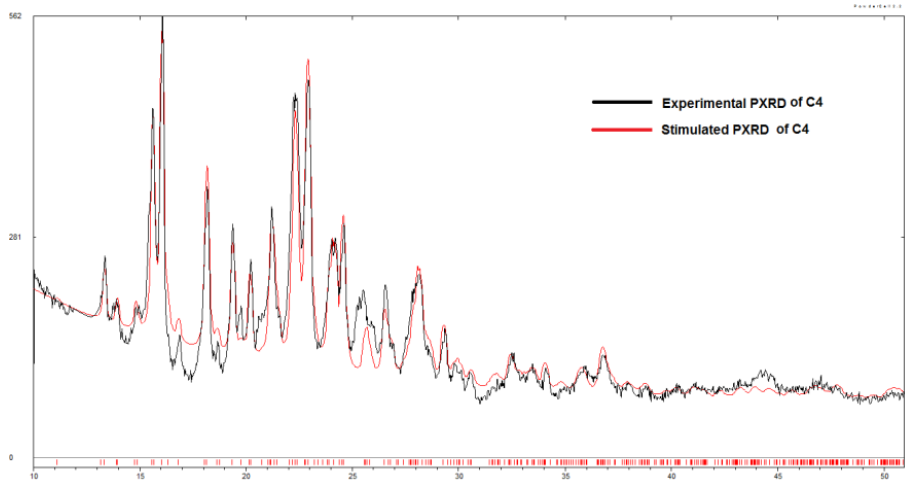


C2

e



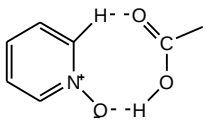
C3



C4

Figure A.3 Rietveld refinement of the experimental PXRD patterns with simulations from the individual crystal structures.

Table A.3 Cambridge Structural Database (CSD) Analysis for N-oxide cocrystals
Search Limits: Only organic and aromatic molecules, R factor less than 10% structures, no ions, no disordered and polymeric structures.

Hydrogen Bond Synthon	Reported Structure [CSD Refcode]	Hydrogen Bond Synthon	Reported Structure [CSD Refcode]
	CUZDAC; DAQZOL; DAQZUR; EQISIH; EQISON; FAFTAH; FOVPIQ; GAQVEA GAQVEA01; HOPKIH; HUZCUA; IWERUY; LICJUD; LIZVOH LIZWUO; NIMBAM		EDILAI; KAVFET ; LIZVIB; PYOTCA10 ROKQEN; TAWNEL TIXLAO; VARBOG WAJWAH; WAJWEL WOJHIM; HUWHAK

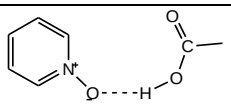
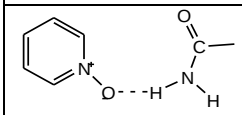
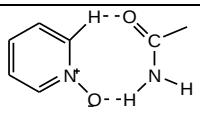
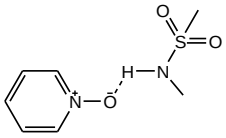
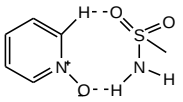
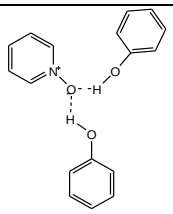
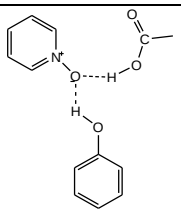
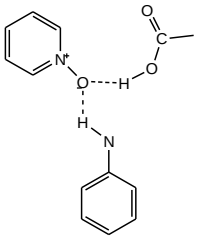
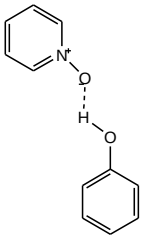
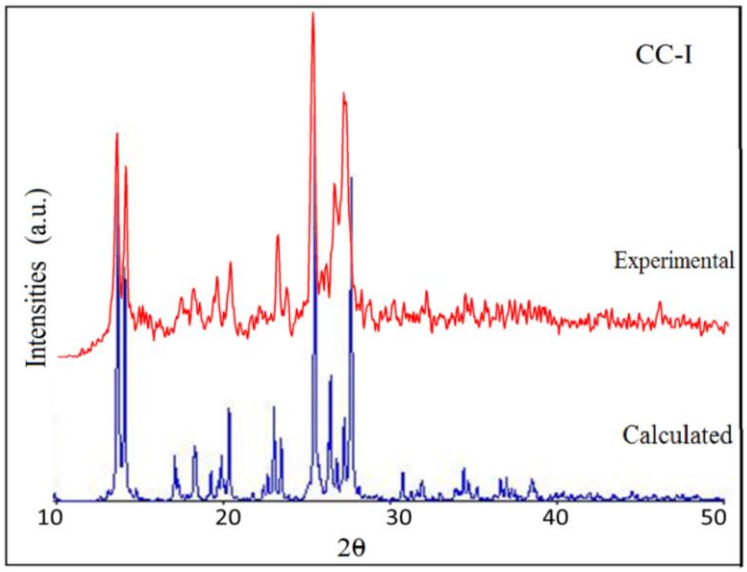
	PANRIH; PICFUM; RIYXUT; ROKQAJ RUJGUJ; SOPJEM WAJVUA; WOJGUX; WOJHAE; WOJHEJ; XONCIO		
	VIGGOI; VIGGUO; WOBQEK01; WOBQIO		Nil
	IWERAE; IWEREI		Nil
	LEQXAG; MOCNEY; PUYTAE; SIPSIU; SIPSOA; TIBZIO; YEXSEA; FAJZUO; RUWPEG		WAJXAI; HUWHAK
	SOJPEM; WAJWEL; HUZCUA		CIRNEY; DATQUL; DUZPEU; FAFTEL; HIDRIX; HINGUF; HOPKAZ; JUDNAX; LAPLEU; LIZVUN; LIZWAU; LIZWIC NELTIH; NILZOX NILZUD; QUMDIM NPOAPL; OWIYEZ PIFHAO; QUMDEZ RADHAH; RIDJOD RIDKUK; RIDLEV RIDPAV; RIDPEZ RIDQIE; SIPSEQ SUVZEO; TAZLOW TEFRUS; WAJVOU WAJVUA; WAJWAH WAJWIP; WAJWUB WIRWID; XIBGUL FAKBAX

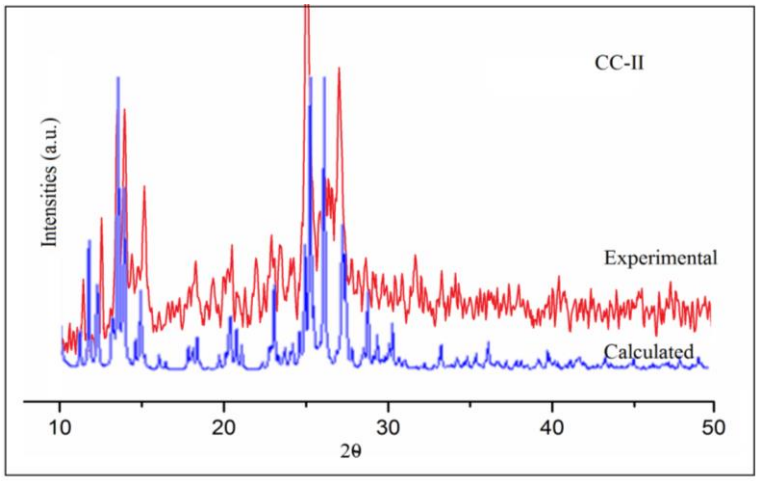
Table A.4 Single Crystal Data Parameter for THP Cocrystals [CC-I → CC-VI]

Crystal Data	**THP•*o*-ABA [2:3; CC-I]**	**THP•*o*-ABA•*i*BuOH [2:2:2; CC-II]**	**THP•*o*-ABA•H_2O [3:2:4; CC-III]**
Formula unit	$C_{35}H_{37}N_{11}O_{10}$	$C_{28}H_{30}N_{10}O_8$	$C_{35}H_{46}N_{14}O_{14}$
Formula wt.	771.76	634.62	886.86
Crystal system	Triclinic	Monoclinic	Triclinic
T [K]	100	100	100
a [Å]	7.0815(2)	18.6461(6)	11.0116(3)
b [Å]	13.2388(4)	7.5462(3)	13.3733(4)
c [Å]	20.0100(6)	25.8651(8)	15.8145(4)
α [°]	72.3800(10)	90	81.2280(10)
β [°]	83.0730(10)	108.326(2)	75.1310(10)
γ [°]	81.5490(10)	90	74.0320(10)
Volume [Å^3]	1762.75(9)	3454.8(2)	2155.61(10)
Space group	$P\bar{1}$	P_2/n	$P\bar{1}$
Z	2	4	2
D_{calc} [g cm^{-3}]	1.454	1.220	1.366
μ/mm^{-1}	0.110	0.092	0.108
Reflns. Collected	15338	22683	29227
Unique reflns.	4294	6833	8165
Observed reflns.	3690	4009	6901
R_1 [I>2σ(I)], wR_2	0.0353; 0.1015	0.0595; 0.1612	0.0499; 0.1574
GOF	1.116	1.066	1.126
Instrument	Bruker APEX-II	Bruker APEX-II	Bruker APEX-II
X-ray	MoK\α; λ=0.71073	MoK\α; λ=0.71073	MoK\α; λ=0.71073
Refcode.	WUTHEA	WUTHIE	WUTHOK
Others	-	PLATON-SQUEEZED	-

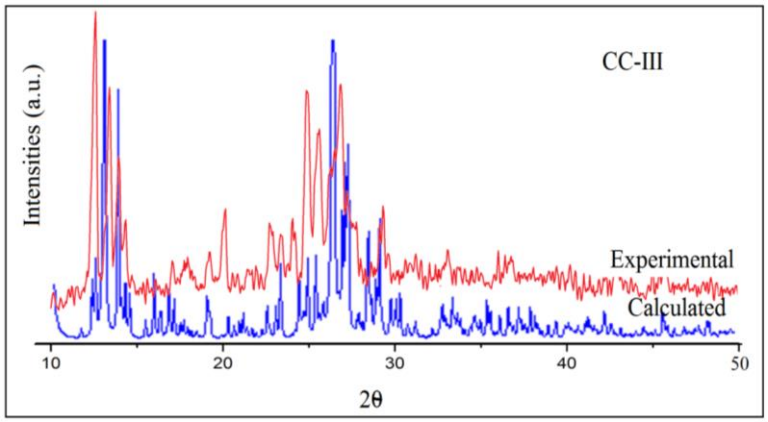
Crystal Data	THP•*o*-ABA•H_2O [2:1:4; **CC-IV**]	THP•*m*-ABA [1:1; **CC-V**]	THP•*p*-ABA [1:1; **CC-VI**]
Formula unit	$C_{21}H_{31}N_9O_{10}$	$C_{14}H_{15}N_5O_4$	$C_{14}H_{15}N_5O_4$
Formula wt.	569.55	317.31	317.31
Crystal system	Triclinic	Monoclinic	Triclinic
T [K]	100	100	100
a [Å]	10.0204(3)	7.5635(8)	6.8921(4)
b [Å]	10.8688(3)	14.2028(14)	8.5168(5)
c [Å]	13.2281(4)	13.7285(13)	13.0599(8)
α [°]	74.3760(10)	90	82.100(4)
β [°]	81.5940(10)	101.760(6)	89.216(3)
γ [°]	67.1680(10)	90	67.468(3)
Volume [Å^3]	1277.32(6)	1443.8(2)	700.72(7)
Space group	$P\bar{1}$	$P2_1/c$	$P\bar{1}$
Z	2	4	2
D_{calc} [g cm^{-3}]	1.481	1.460	1.504
μ/mm^{-1}	0.119	0.110	0.114
Reflns. Collected	40658	7811	11058
Unique reflns.	11461	2975	3131
Observed reflns.	8579	1236	2491
R_1 [I>2σ(I)], wR_2	0.0397; 0.1132	0.0581, 0.1251	0.0513; 0.1152
GOF	1.091	0.900	1.077
Instrument	Bruker APEX-II	Bruker APEX-II	Bruker APEX-II
X-ray	MoK\α; λ=0.71073	MoK\α; λ=0.71073	MoK\α; λ=0.71073
Refcode.	WUTHUQ	WUTJAY	HUMNEK01



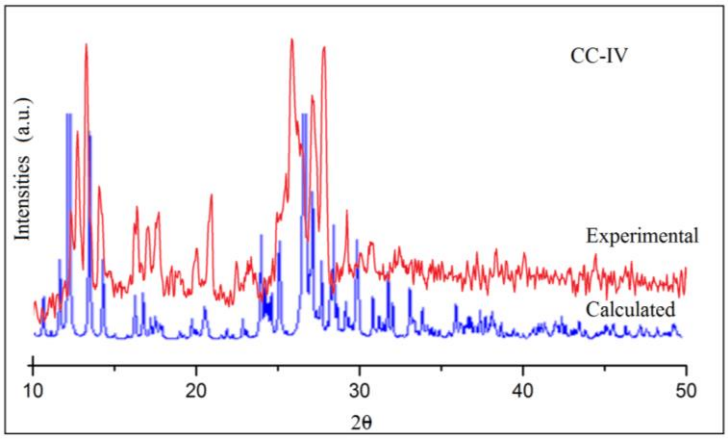
CC-I



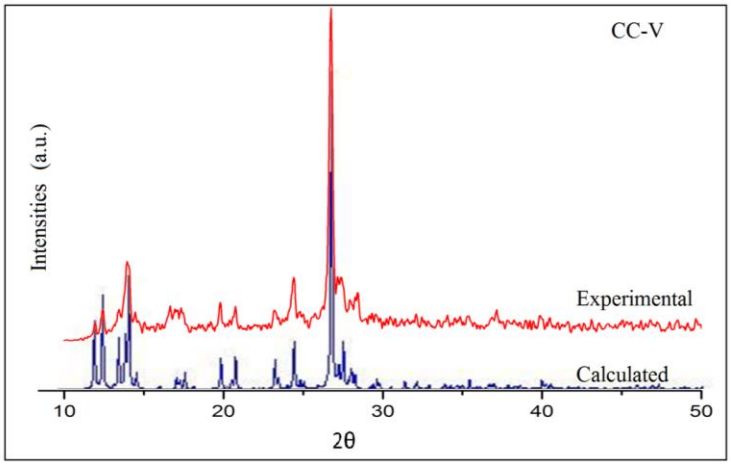
CC-II



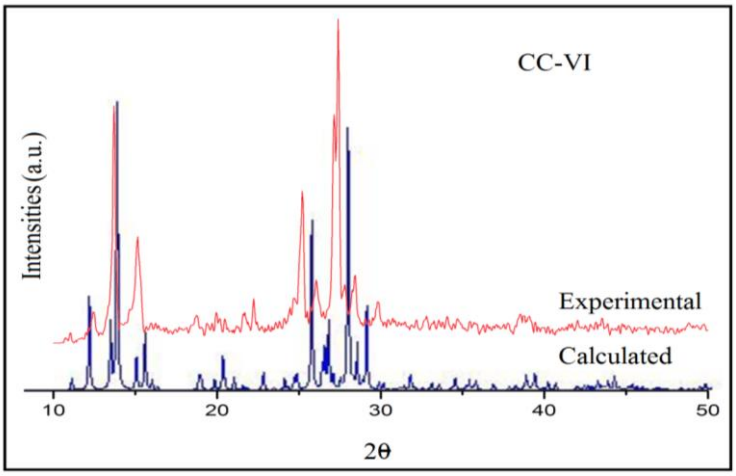
CC-III



CC-IV



CC-V



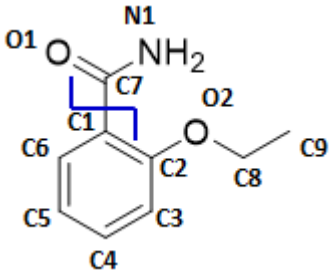
CC-VI

Figure A.4 Powder X-ray diffraction patterns of cocrystal materials compared with the simulated.

Table A.5 Crystallographic parameters of structures of cocrystals **1** to **4**

Crystal data	**1 [ZMD:2,5-DHBA]**	**2 [ZMD:2,6-DHBA]**	**3 [ZMD:3,4-DHBA]**	**4 [ZMD:3,5-DHBA:2H$_2$O]**
Formula unit	$C_{16}H_{17}NO_6$	$C_{16}H_{17}NO_6$	$C_{16}H_{17}NO_6$	$C_{30}H_{33}NO_{16}$
Formula weight ($gmol^{-1}$)	319.31	319.31	319.31	663.57
Crystal system	Triclinic	Monoclinic	Monoclinic	Triclinic
T [K]	296	100	100	296
a [Å]	8.0456 (3)	7.3291(3)	15.720(5)	11.278(11)
b [Å]	9.1098(4)	13.5985(5)	4.0408(12)	11.819(9)
c [Å]	22.6193(9)	14.7837(5)	23.577(7)	12.258(10)
α [°]	94.243	90	90	95.27
β [°]	91.501	95.57	92.55	102.49
γ [°]	113.843	90	90	100.87
Volume [$Å^3$]	1509.35(11)	1466.46 (10)	1496.2 (8)	1552 (2)
Space group	$P\bar{1}$	$P2_1/n$	$P2_1/n$	$P\bar{1}$
Z	4	4	4	2
D_{cal}[g/cm^3]	1.405	1.446	1.413	1.420
R_1, *w*R2	0.0490, 0.1383	0.0416, 0.1153	0.0859, 0.2317	0.0662, 0.1943
Instrument	Bruker Apex II	Bruker Apex II	Bruker Apex II	Bruker Apex II
Refcode	FENQEX	GEQXEH01	FENRIC	ODIDEN01

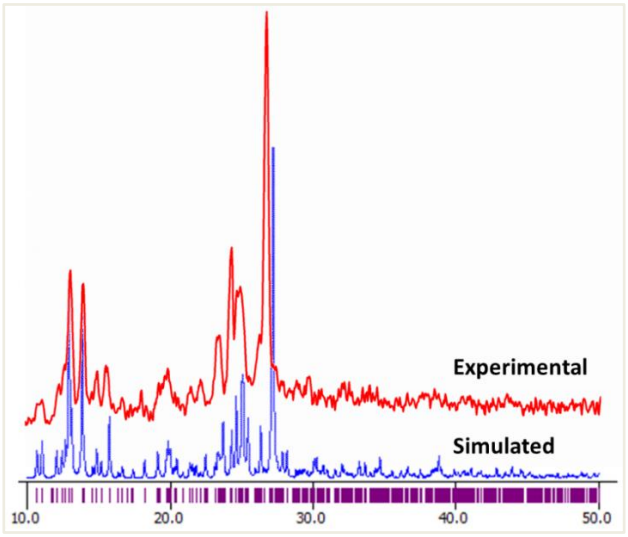
Table A.6 Dihedral angle (marked blue in the structure below) of the dangling amide group in ZMD systems reported in CSD and in our multicomponent systems.



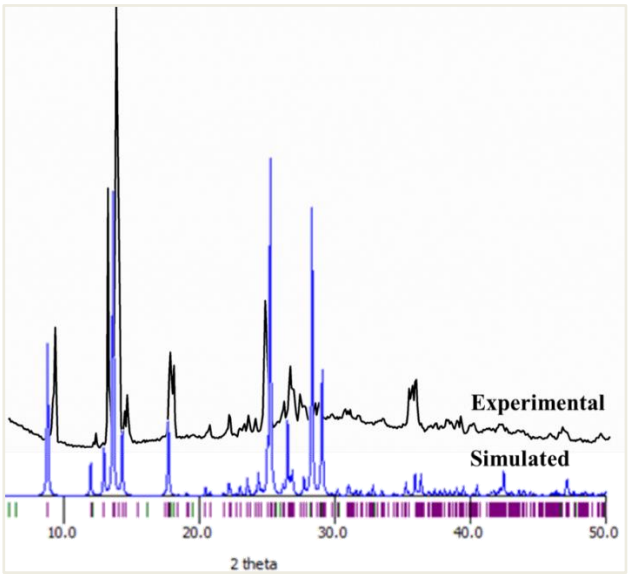
Refcode	**Dihedral angle**
GEQXEH	176
QULLUF	172, 171
QULLUF01	178
QULLUF02	179
REHSAA	176
REHSEE	179
REHSII	174
REHSOO	172, 176
REHSUU	178
REHTAB	175
VAKTOS	176
VAKTOS01	173
VUHFIO	175

VUHFIO01	179
WUZHOP	178
WUZHOP	165
WUZJEH	172
WUZKIM	175
ZIMBEE (HCL salt of ZMD)	177
ZIMBII (HBr salt of ZMD)	179
ZIMCAB (Perchlorate salt of ZMD)	173

This Work	
Cocrystal	Dihedral angle
1	172, 171
2	176
3	179
4	165



1



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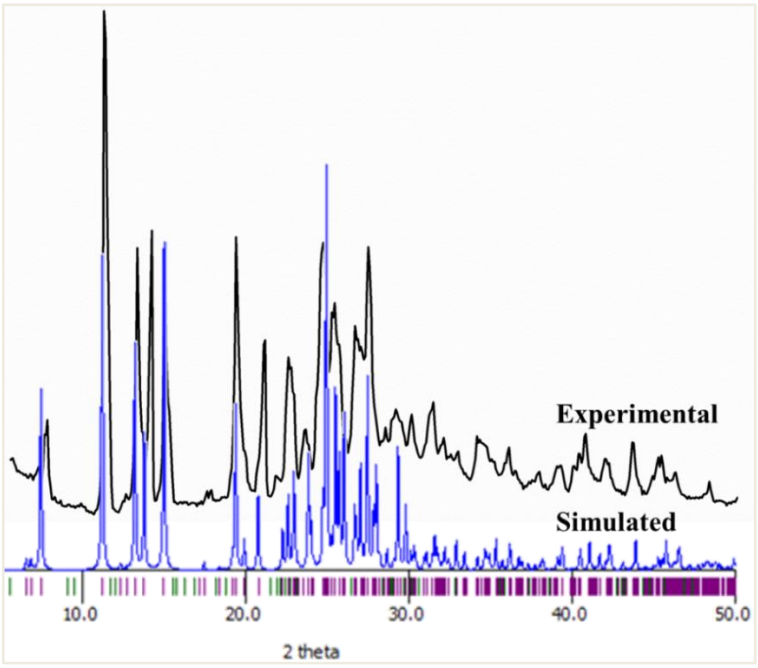

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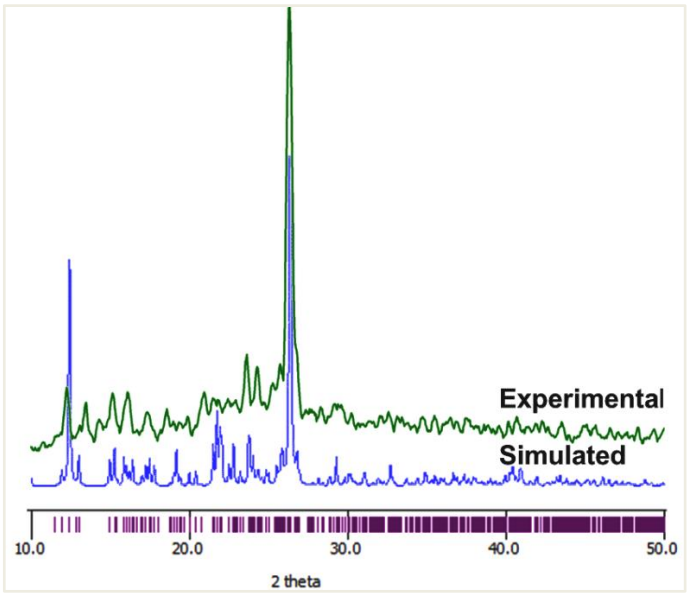
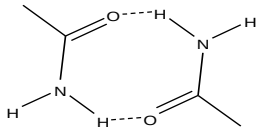
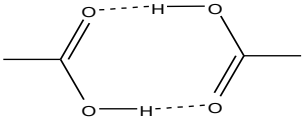
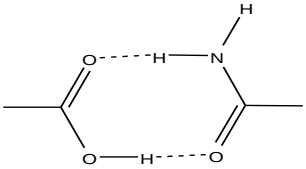


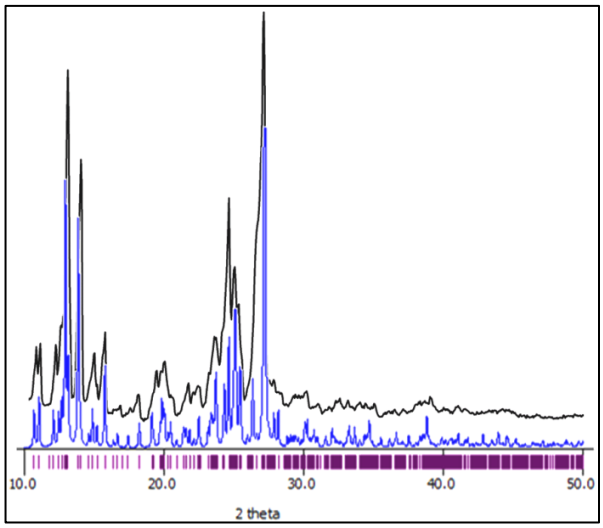
4

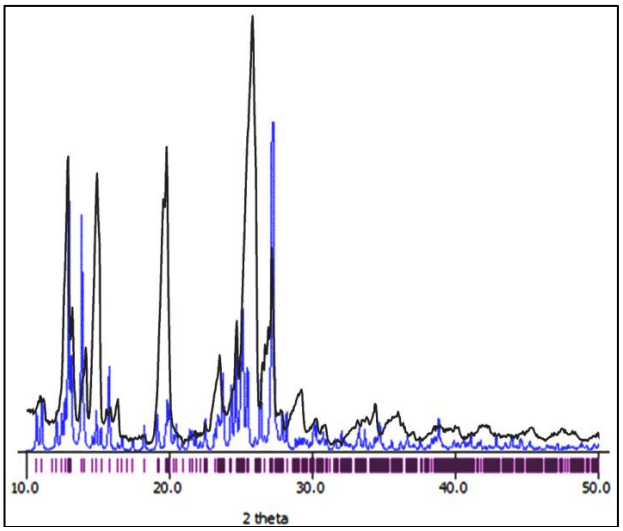
Figure A.5 Experimental PXRD pattern laid over simulated pattern from single crystal structure (**1** to **4**).

Table A.7 Cambridge Structural Database (CSD) analysis for various synthons.
Search Limits: Structures with R factor less than 10%, no ions, no disordered and polymeric structures.

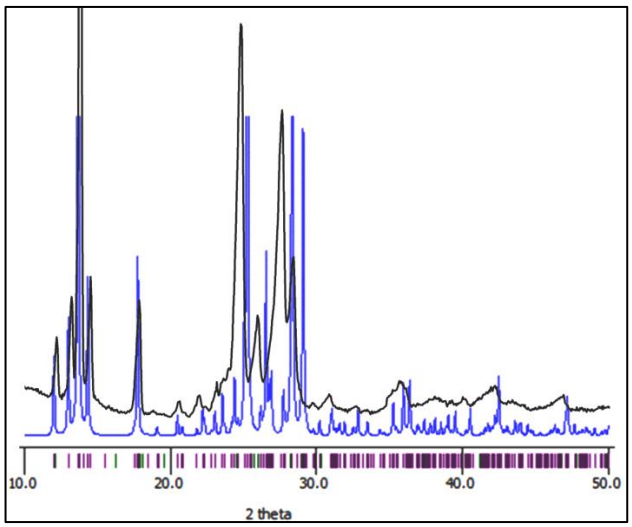
SYNTHON	REFCODE
 **Synthon I**	FURWOG, FURXIB, ULAWAF04, ULAWAF06, ABULIU, ACEROR, ACERUX, ACONIR, AJAKEB, ASAXOH, ASAXUN01, BICQAH, BOBRAN, BUDWEC, CACGUK, EBONUG, ERIWUY, EXAQIE, EXAQOK, ERIWUY, JILZOU, JOWZIG, JOWZIG01, KINTUY, KOVSAR, KOVSEV, LATTOR, LATBOZ, LATTOR01, LOFLID, LUNMAI, LUNMEM, LUNMUC, LUNNAJ, LATBOZ, LUNNUD01, LUNPEP, LUNNIR, LUNNOX, LUNNUD, MOXVIF01, MUDVUE, NUHYEU, NUKXUN01, NUKXUN02, NUKYOI, NUKZOJ, OCEBUV, PAMWUX, PEQBES, PIRNOV, PIRNOV01, PIRPEN, PIRPIR, PIRQEO, PIRQIS, PIRREP, PEFGEO01, REBXED, REBXIH, REBXON, ROLFUU, RONDEE, ULAWAF, ULAWEJ, ULAWOT, ULAWUZ, ULAXAG, UMUYUX, UMUZAE, UYOSUX, UYOTAE, UYOTEI, UYOTOS, UYOVAG, VEJXAJ02, XICRAE, XOGMUD, XOXHEY, XOZSOV, YAGGOE, ZOHXAX
 **Synthon II**	FOQRIO,LATBOZ,REBXED,REBXIH, XOXHEY, MOXVIF, MOXVIF01, MOXVOL, MOXXAZ, NUHYEU, PEFGEO01, PEFGEO02, ZOYCEX, ZOHXAX, ZOYCOH
 **Synthon III**	FURXUN, ACESOS, AJAKIF, AJAKUR, AJALEC, BIZTIP, BOBQUG, BUDZUV, BUFQAU, CUYXUQ, DAVPAS, DAVPEW, DINRUP01, EVETAB, EBOSIX01, ESATUN, ERIWUY, FOTFIF, FOTFOL, FOTFUR, FURAOX, GENLIV, GENLOB, GEQXIL, GESBAJ, GESBEN, GESBUD, GESCIS, GESCUE, GOGYUX, HIBGOP, HIQSEH, HIQMAX, HIQRIK, HIQSIL, HIQROQ, HIQRUW, HOGFIU, HOGFOA, HOGFUG, HOGGAN, HOGGOB, HOGGUH, JECZAS, KEMCEL, KEWNOQ, KINVAG, KODVAB,KOVSOF, LEZKEI, MECHAF, MIHXEG, MOXVAX, MOXVOL, MOXWAY, MOXXAZ, MUPNIV, MUPPAP, MUROXA02, NAXHOL, NEHPIZ01, NEMSUT, NEMTAA, NEMTEE, NUHXUJ, NUKYAU01, NUKYIC,NUKYUO, NUKZAV, NUKZID, NURFOW, OCIQAT, OFUYIZ, OPUSOI, OVEZUL, OVIBAX, OVIBEB, PEFGEO, PEFGEO03, PEFGIS, PILKOM, PILLAZ, PILLIH, PILLON, REBXUT, RINHUT, ROGKOO, RONDAA, RONRUJ, ROQLEQ, RUYHEZ01, SEZDIL, SLCADC01, SLCADC10, SOLBEC01, SUCTAN, SUCTIV, SUDDEC01, SUDFOO, TIPWIY, TOMWOJ, TONGOS, ULAXEK, UNEZIW, UNEZUI, UNIBIC, URISAQ, UROXAL, VAKTOR, VAKTOS, VEXLOA01, WANCUK, WEYFEN, WIXFAM, XAQPOV, XAQQIQ, XAQQOW, XAQRAJ, XAXPIV02, XAXPOB, XAXPUH, XEWTUO, XOGMIR, XOGNIS, XOGPAM, XOGPEQ, XORMUM, XOBCEX,XOBCIB, YASGEG, YASGIK, YASGOQ03, ZEBXOV, ZEBXUB,ZODWIY, ZOHWOK, ZOHWUQ, HABJIG, HABJUS, UROXAL02, VUTNAB, YUQQOS

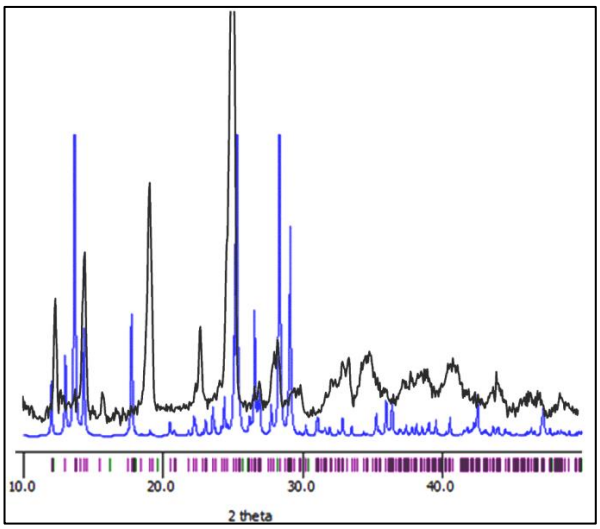
At pH 1.2 **At pH 7.4**





1





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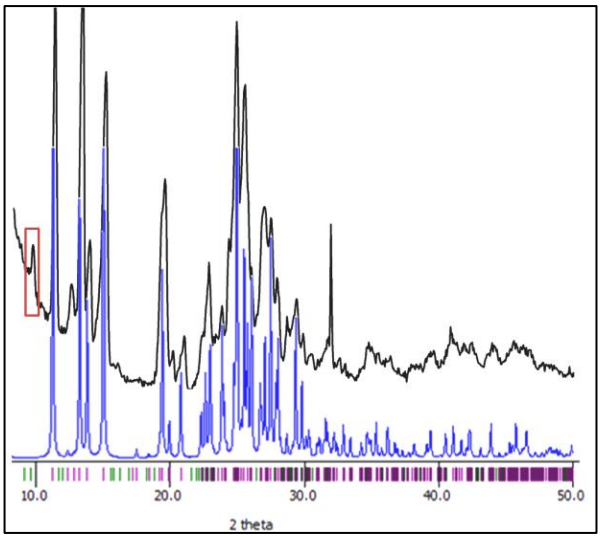
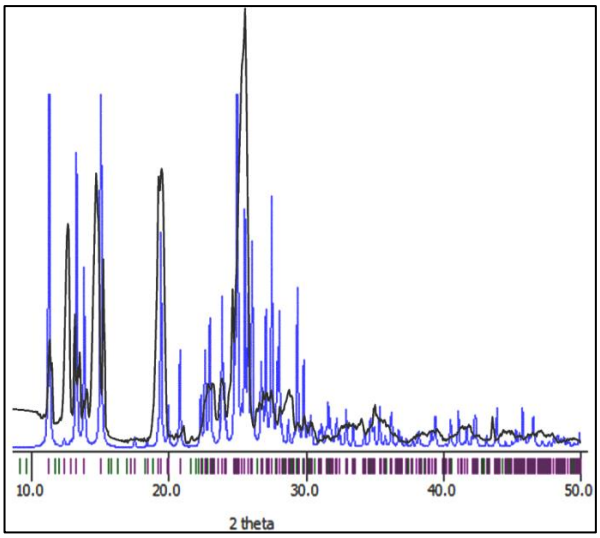
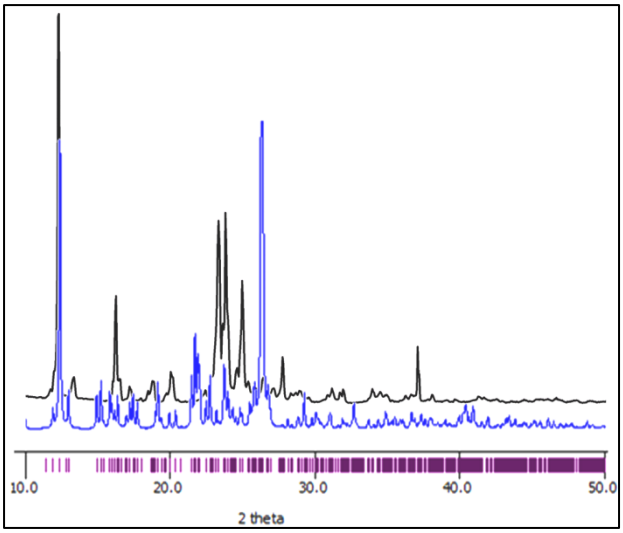
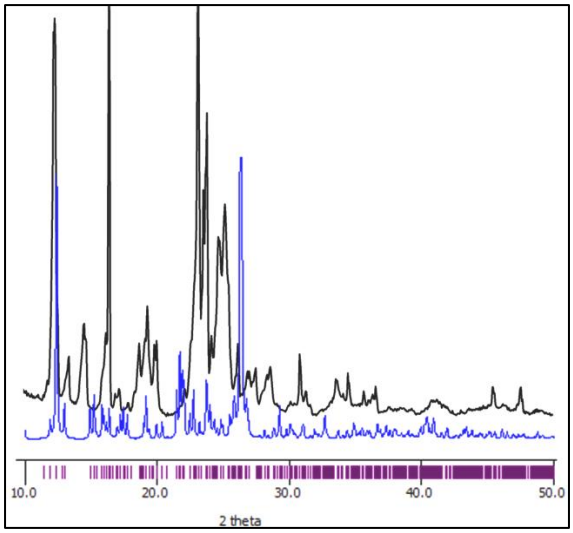




3

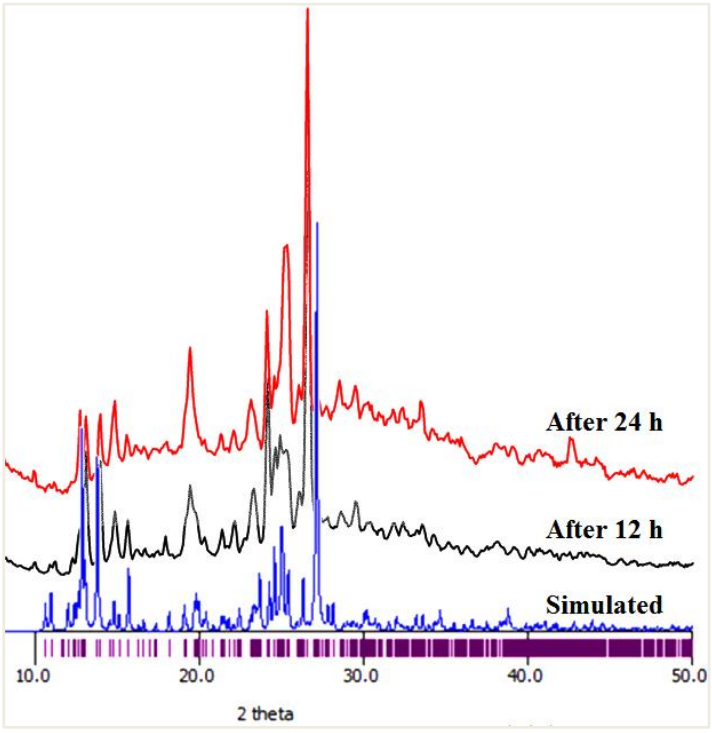
o



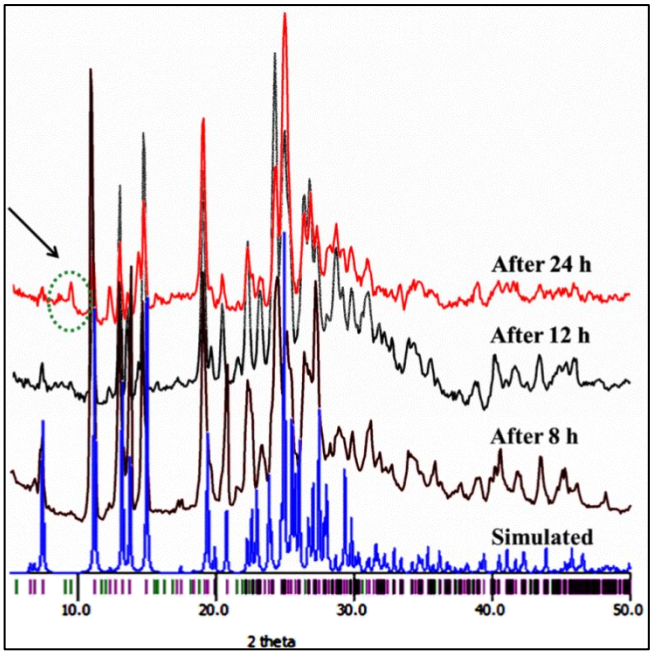


4

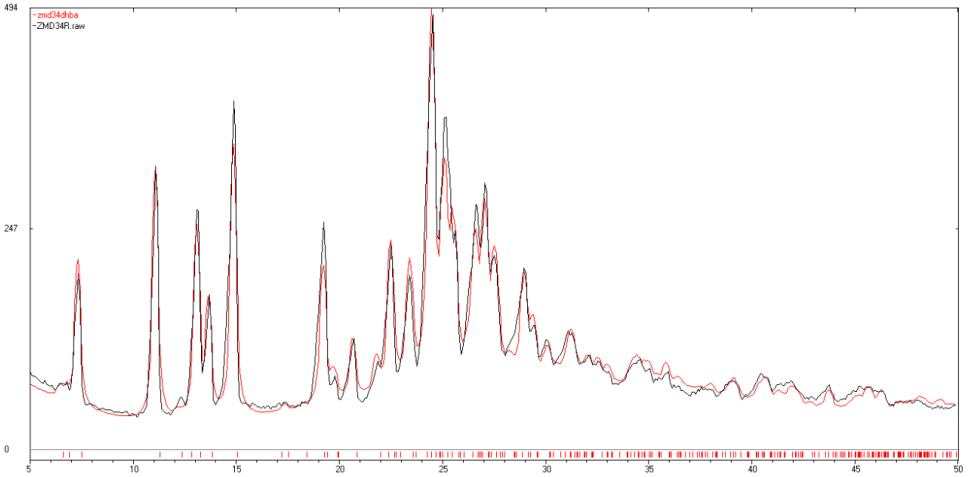
Figure A.6 Stack plots of PXRD pattern of simulated (blue) and slurry experiment (black) obtained after 12 h revealing the phase stability of cocrystals (**1** to **4**); however **4** transforms to it anhydrous form.



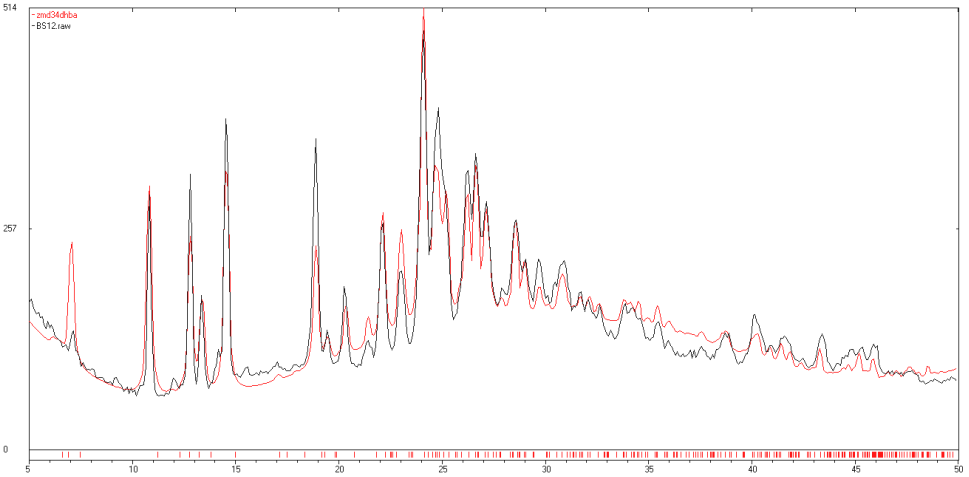
(a) Cocrystal 1



(b) Cocrystal 3

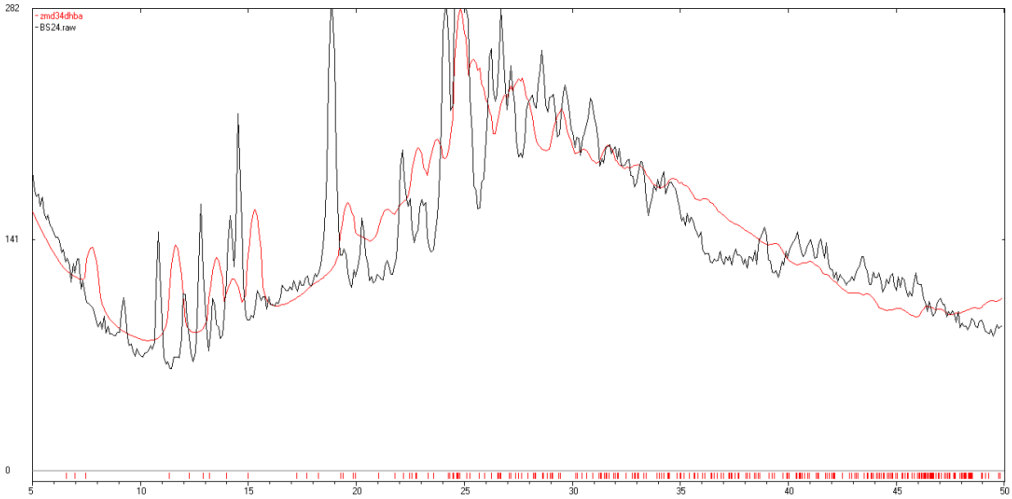


(c) Rietveld refinement for the slurry of cocrystal **3** after 8h indicates phase stability.



(d) Slurry of cocrystal **3** shows phase stability even after 12h.

q



(e) Cocrystal **3** has transformed after 24h into its possible hydrates formation

Figure A.7 Stack plots of PXRD pattern of slurry experiment of **1** (a) and **3** (b) attributing phase stability of materials in aqueous medium. Transformation of cocrystal **3** into possible hydrate formation monitored at 8h (c), 12h (d) and 24h (e) intervals.

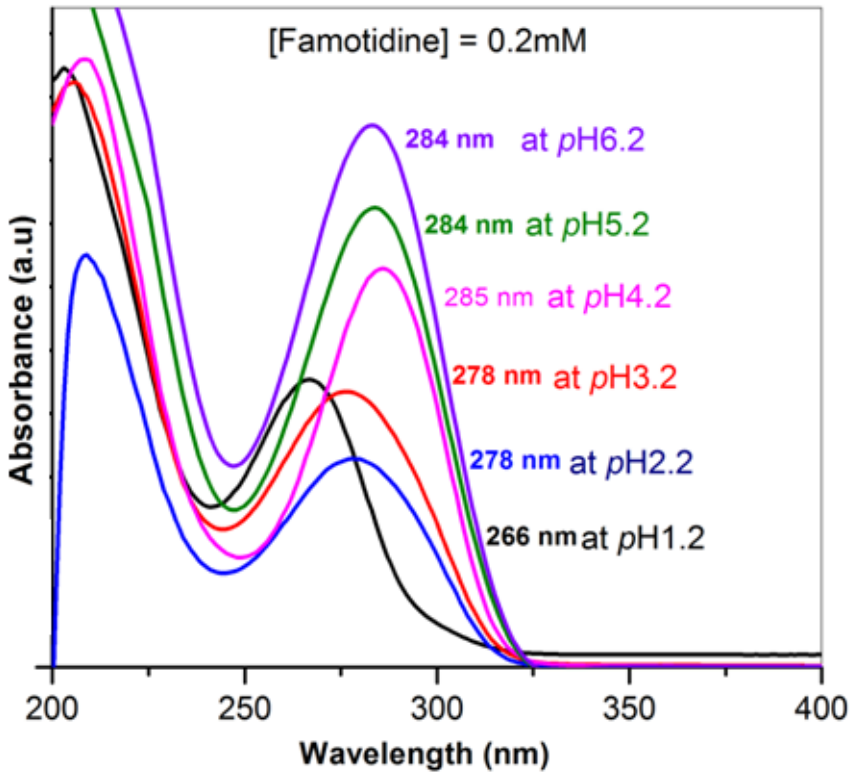


Figure A.8 UV-Visible spectrum of famotidine at different pH conditions.

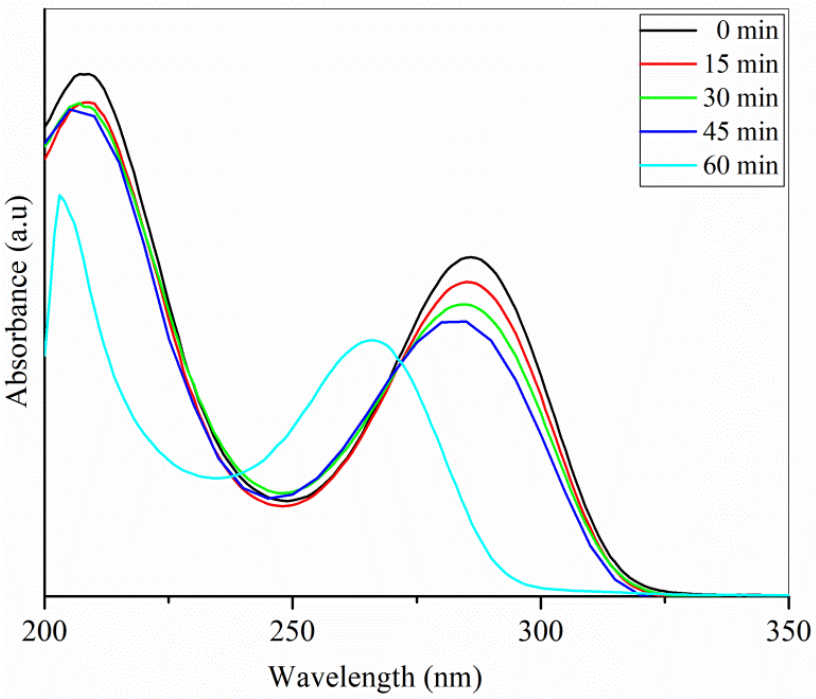
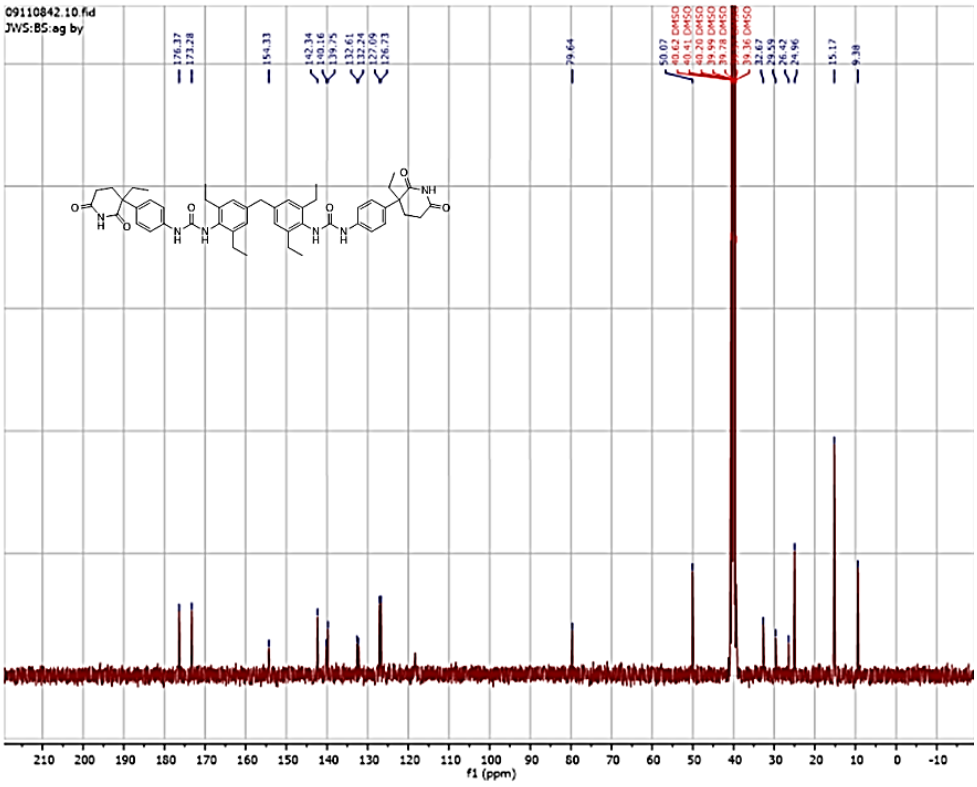


Figure A.9 Degradation of famotidine monitored by UV-Visible spectroscopy at different time.

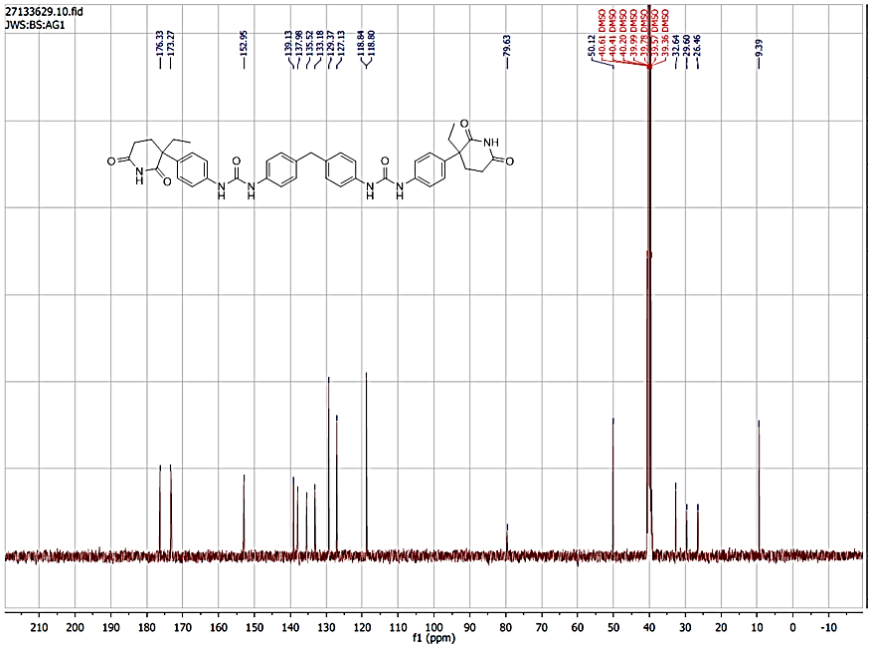
Table A.8 Crystallographic parameters of structures of cocrystals

Crystal data	**FAM.THP**	**FAM Form A**
Formula unit	C_{22} $H_{31}N_{15}$ O_6S_3	C_8 H_{15} N_7 O_2 S_3
Formula wt.	697.80	337.45
Crystal system	Triclinic	Monoclinic
T [K]	296	296
a [Å]	7.7722(6)	12.0082(4)
b [Å]	13.4252(10)	7.2103(4)
c [Å]	14.6013(11)	16.8488(8)
α [°]	98.375(4)	90
β [°]	92.445(5)	99.807(3)
γ [°]	93.659(5)	90
Volume [Å^3]	1502.1(2)	1437.50(12)
Space group	$P\bar{1}$	$P2_1/c$
Z	2	4
D_{calc} [g cm^{-3}]	1.543	1.559
μ (mm^{-1})	0.314	0.529
Reflns. collected	7611	3642
Unique observed	4555	2762

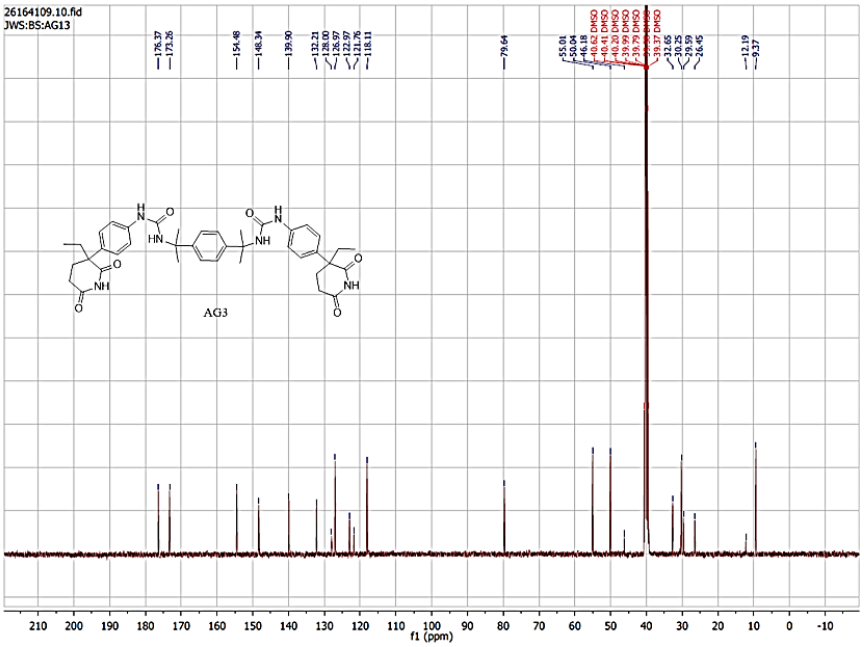
R1 [I > σ(I)]	0.0519	0.0390
wR2	0.1690	0.1320
Instrument	Bruker APEX-II	Bruker APEX-II
X-ray	Mok\α; λ=0.71073	Mok\α; λ=0.71073
CCDC no.	1891140	1891137



(a)

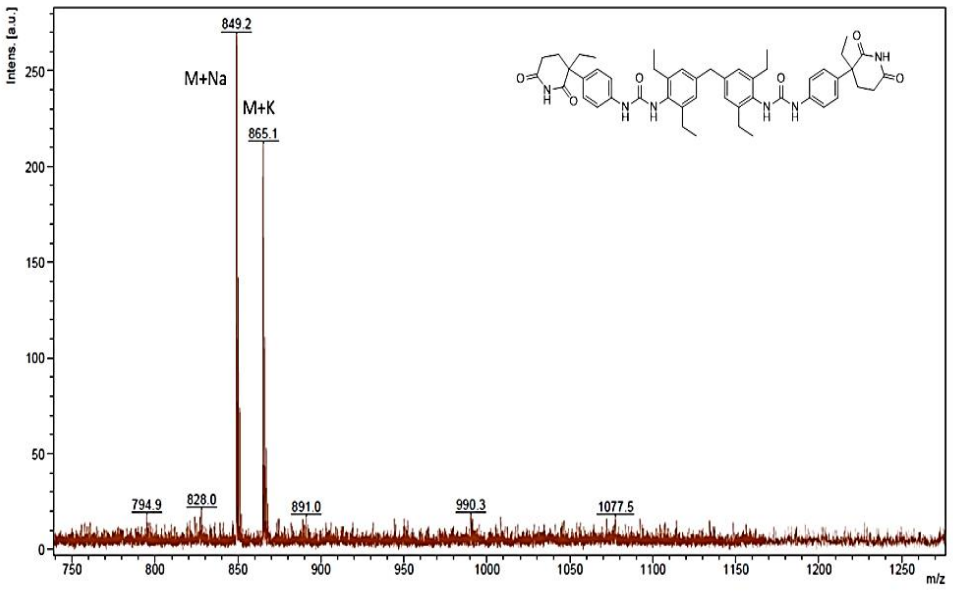


(b)

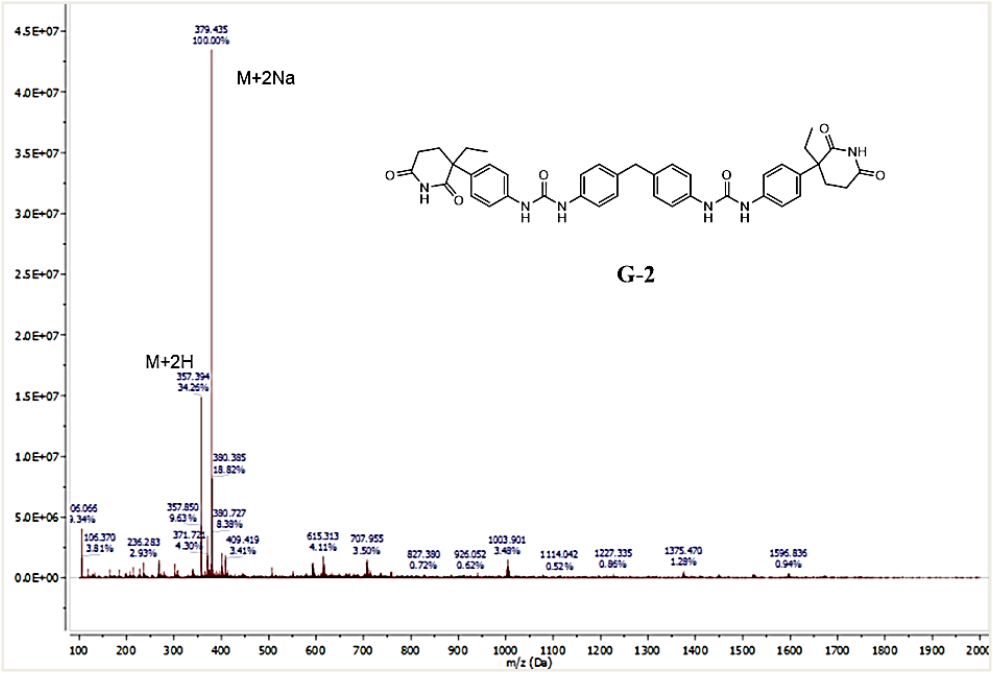


(c)

Figure A.10 ^{13}C spectra of gelators (a) G-1, (b) G-2 and (c) G-3. Extra peak appears at 79.6 is identified for residual $CHCl_3$.

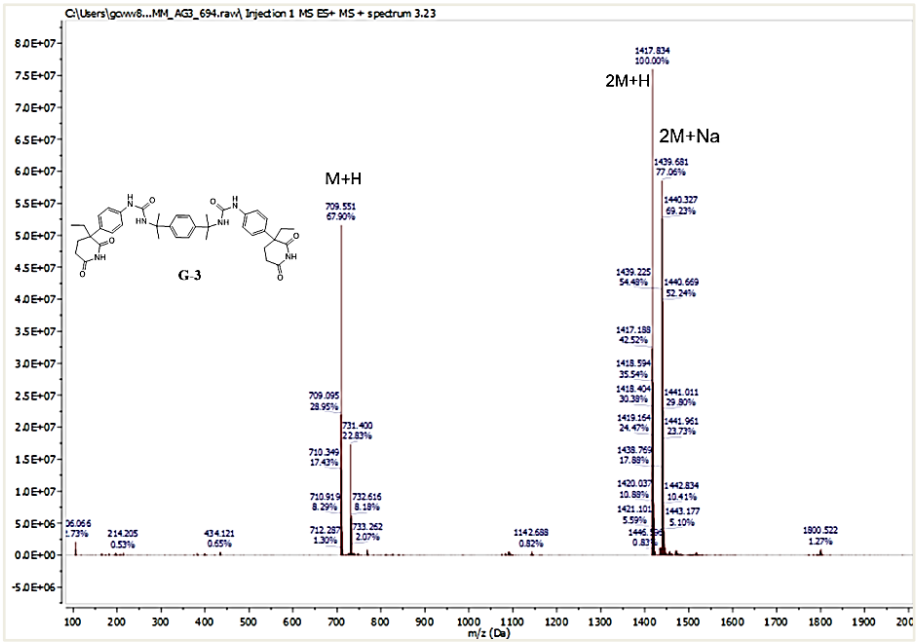

Intens. [a.u.]
849.2
M+Na
M+K
865.1
794.9
828.0
891.0
990.3
1077.5
m/z

(a)


379.435
100.00%
M+2Na
M+2H
357.394
34.26%
380.385
18.82%
357.850
9.63%
380.727
8.38%
615.313
4.11%
707.955
3.50%
827.390
0.72%
926.052
0.62%
1003.901
3.48%
1114.042
0.52%
1227.335
0.86%
1375.470
1.28%
1596.836
0.94%
m/z (Da)

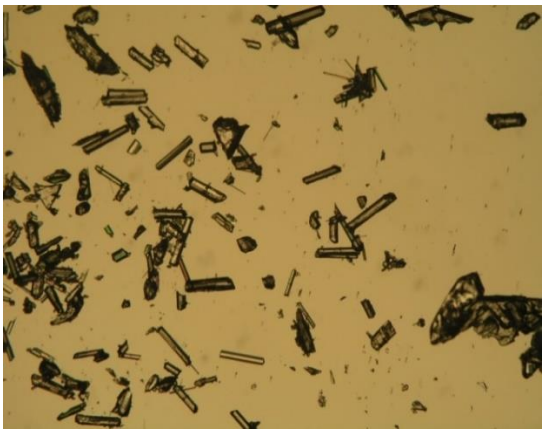
G-2

(b)

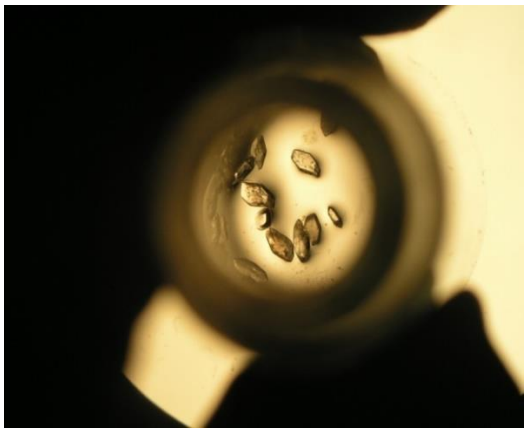


(c)

Figure A.11 Mass spectra of gelators (a) G-1, (b) G-2 and (c) G-3

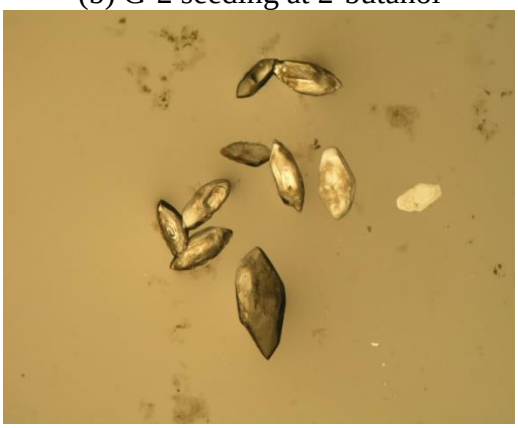


(a) 2-butanol



(b) G-2 seeding at 2-butanol

(c) methanol



(d) G-2 seeding at methanol

Figure A.12 Comparison of crystallization outcome of barbital from solution and seeding crystallization using the gelator G-2. Seeding crystallization resulted in Form III of barbital.

Research publications

1. Torres-moya, I., Saikia, B., Prieto, P., Carrillo, J. R., and Steed, J. W. High thermal stability, pH responsive organogels of 2H-benzo[d]1,2,3-triazole derivatives as pharmaceutical crystallization media. *CrystEngComm*, 2019.
2. Bora, P., Saikia, B., and Sarma, B. Regulation of π···π Stacking Interactions in Small Molecule Cocrystals and/or Salts for Physiochemical Property Modulation. *Crystal Growth and Design*, 18(3):1448-1458, 2018.
3. Khatioda, R., Talukdar, D., Saikia, B., Bania, K. K., and Sarma, B. Constructing two dimensional amide porous polymer to promote selective oxidation reactions. *Catalysis Science and Technology*, 7(14):3143-3150, 2017.
4. Khatioda, R., Saikia, B., Das, P. J., and Sarma, B. Solubility and: In vitro drug permeation behavior of ethenzamide cocrystals regulated in physiological pH environments. *CrystEngComm*, 19(46):6992-7000, 2017.
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8. Saikia B., Mulvee M., Torres-moya, I., Sarma, B., and Steed J. W. Controlling Concomitant Polymorphism of Drugs by Introducing Drug Mimetic Gelator as Nucleation Template. 2019, (Manuscript under preparation).
9. Saikia, B., Sultana M., and Sarma, B. Cocrystal Technology to Control the Degradation of Histamine H2-receptor Antagonist Drug Famotidine. 2019, (Manuscript under preparation).
10. Bora, P., Saikia, B., and Sarma, B. Design/Strategy to Nucleate Sulfathiazole Polymorphs on Heterogeneous Surfaces; 2019, (Manuscript Communicated).
11. B. Saikia, Khatioda, R., and B. Sarma, Control Bioavailability of Drug Propofol via Cocrystallization; 2019 (Manuscript under preparation).

Seminars/Conferences Attended

1. Poster presented entitled "Drug Mimetic Gelators in Nucleating Pure Drug Polymorphic Phases" at OrganiX-2018 an International Conference in Chemistry, Tezpur University, Assam, India, 20–21st December, 2018.
2. Poster presented entitled "Imide-Mimetic Supramolecular Gelators for Controlled Crystallizations of Pharmaceutical Polymorphs"; in the Sixth European Conference on Crystal Growth, Riviera Holiday Club, Varna, Bulgaria, 16–20th September, 2018.
3. Poster presented entitled "Solid Formulation of Liquid Drug Propofol via Cocrystallization"; at 24th Congress and General Assembly of the International Union of Crystallography, Hyderabad International Convention Centre, Hyderabad, India, 21–28th August, 2018.
4. Poster presented entitled "Predicting Bio- availability for Variable Stoichiometry Drug Cocrystals" at the National Symposium on Natural Products: Prospects & Perspectives; NEIST, Jorhat, Assam, India, 21−22nd March, 2016.
5. Poster presented entitled “Pharmacokinetic Property Enhancement for Ethenzamide Cocrystals” at National Symposium on Emerging Trends in Chemistry (ETC-2016), North Eastern Hill University (NEHU), Shillong, Meghalaya, India, 28−29th March, 2016.
6. Oral presentation entitled "Drug Bio-availability Prediction in Variable Stoichiometry Cocrystals of Theophylline and Aminobenzoic Acids" in Contemporary Developments in Chemical sciences, Tezpur University, Assam, India, 23−24th November, 2015.
7. Poster presented entitled “Variable Stoichiometry in the Cocrystallization of the Theophylline and Aminobenzoic Acids”, in the National Symposium on X–ray Diffraction and Recent Advances in Crystallography, Periyar University, Tamil Nadu, India, 27–28th February, 2015.
8. Poster presented entitled “Hydrogen Bond Synthons for Tactical Alteration of Drug Property”, in 8th Mid–Year Chemical Research Society of India (CRSI) National Symposium of Chemistry, NEIST, Jorhat, Assam, India, 10– 12th July, 2014.
9. Poster presented entitled “Stability, Solubility Modulation of drug Theophylline via Cocrystal Synthesis”; in Recent Advances in Chemical Research, Department of Chemistry (RACR–14), Rajiv Gandhi University, Arunachal Pradesh, India, 20–21th March, 2014.