Novel pharmaceutical salts of the Albendazole

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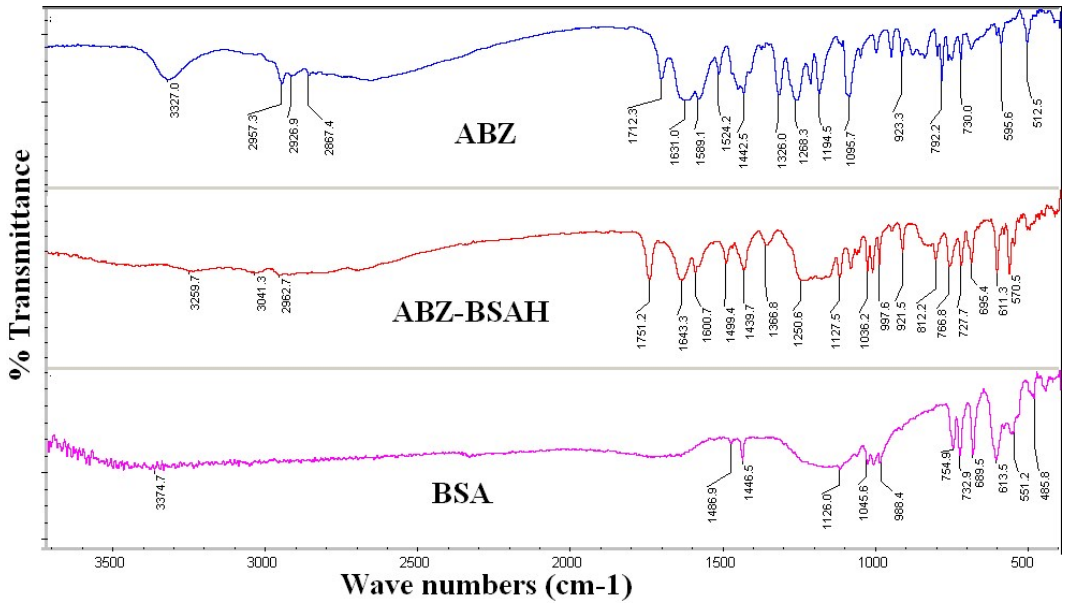
Table S1 Hydrogen bond parameters of the slats and salt hydrates in this study.

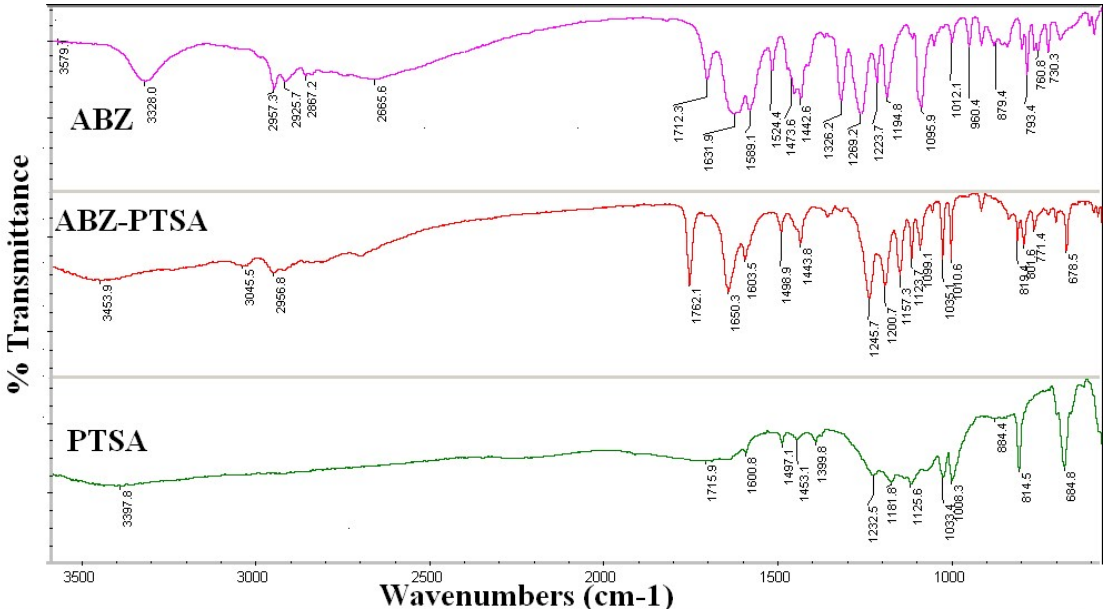
Name	Interaction	H···A /Å	D···A /Å	∠D–H···A /º	Symmetry code
ABZ–BSA (2:2)	N1–H1···O6	1.91	2.7647(2)	174	1-x,2-y,1-z
	N2–H2···O1	2.19	2.6908(2)	117	Intramolecular
	N2–H2···O7	2.08	2.8244(2)	145	1-x,1-y,1-z
	N3–H3···O5	1.91	2.7578(2)	169	1-x,2-y,1-z
	N4–H4A···O9	1.90	2.7601(2)	175	x,1+y,z
	N5–H5···O3	2.22	2.7110(2)	117	Intramolecular
	N5–H5···O8	2.09	2.8384(2)	146	1+x,y,z
	N6–H6A···O10	1.91	2.7532(2)	166	1-x,2-y,1-z
ABZ–BSAH (1:1:1)	N1–H1A···O6	1.84	2.687(4)	169	-x,1-y,1-z
	N2–H2A···O1	2.23	2.723(4)	117	Intramolecular
	N2–H2A···O5	2.08	2.808(4)	143	1-x,-y,1-z
	N3–H3A···O3	1.94	2.798(4)	173	-x,1-y,1-z
	O6–H6A···O4	1.86	2.686(6)	162	1-x,1-y,1-z
	O6–H6B···O3	2.18	2.834(4)	134	----[a]
	C18–H18···O5	2.52	2.894(5)	104	Intramolecular
	C18–H18···O1	2.59	3.439(5)	152	1-x,-y,1-z
ABZ–PTSA (1:1)	N1–H1A···O4	1.93	2.763(5)	163	1/2-x,1/2+y,3/2-z
	N2–H2A···O1	2.25	2.746(6)	116	Intramolecular
	N2–H2A···O5	2.06	2.820(5)	146	-x,-y,1-z
	N3–H3A···O3	1.86	2.703(5)	164	1/2-x,1/2+y,3/2-z
	C10–H10B···O3	2.49	3.309(9)	142	x,1+y,z
	C12–H12A···S1	2.69	3.137(12)	109	Intramolecular
	C18–H18···O5	2.50	2.878(7)	104	Intramolecular
ABZ–PTSAH (1:1:1)	N1–H1A···O6	1.79	2.665(4)	174	----[a]
	N2–H2A···O1	2.15	2.717(3)	115	Intramolecular
	N2–H2A···O5	1.94	2.790(4)	142	-x,1-y,1-z
	N3–H3A···O4	2.06	2.865(4)	175	1-x,-y,1-z
	O6–H6A···O3	1.95	2.678(4)	141	----[a]
	O6–H6B···O4	2.01	2.747(3)	145	1-x,-y,1-z
	C18–H18···O5	2.55	2.915(4)	103	Intramolecular
ABZ–2,6-DHBA (2:2)	N1–H1A···O5	1.67	2.703(4)	177	1-x,1-y,1-z
	N2–H2A···O3	2.27	2.703(4)	119	Intramolecular
	N2–H2A···O9	2.07	2.820(4)	148	3/2-x,1/2+y,1/2-z
	N3–H3A···O6	1.78	2.640(4)	170	1-x,1-y,1-z

	N4–H4A···O1	2.31	2.744(5)	111	Intramolecular
	N4–H4A···O3	2.01	2.839(4)	158	3/2-x,-1/2+y,1/2-z
	N5–H5A···O11	1.84	2.694(4)	177	1-x,-y,-z
	N6–H6A···O12	1.72	2.6784)	168	1-x,-y,-z
	O7–H7A···O5	1.76	2.583(4)	150	Intramolecular
	O7–H7A···O1	2.60	3.071(4)	113	3/2-x,1/2+y,1/2-z
	O8–H8A···O6	1.75	2.534(4)	150	Intramolecular
	O9–H9A···O11	1.75	2.544(4)	146	Intramolecular
	O10–H10A···O12	1.64	2.543(4)	162	Intramolecular
ABZ–OAH (1:1:1)	N1–H1A···O4	1.90	2.671(4)	171	-1+x,y,z
	N2–H2A···O1	2.22	2.710(4)	124	Intramolecular
	N2–H2A···O5	2.18	2.786(4)	139	1/2+x,1/2-y,1/2+z
	N3–H3A···O3	1.77	2.689(4)	174	-1+x,y,z
	O6–H6A···O7	1.79	2.603(4)	175	-1+x,y,z
	O7–H7A···O4	2.04	2.827(4)	147	----[a]
	O7–H7A···O6	2.56	3.251(4)	135	----[a]
	O7–H7B···O1	2.09	2.859(4)	154	1/2+x,1/2-y,-1/2+z
	C3–H4···O3	2.37	3.312(4)	169	1/2+x,1/2-y,1/2+z
ABZ–2,6-DHBA (2:2)	N1–H1A···O5	1.67	2.703(4)	177	1-x,1-y,1-z
	N2–H2A···O3	2.27	2.703(4)	119	Intramolecular
	N2–H2A···O9	2.07	2.820(4)	148	3/2-x,1/2+y,1/2-z
	N3–H3A···O6	1.78	2.640(4)	170	1-x,1-y,1-z
	N4–H4A···O1	2.31	2.744(5)	111	Intramolecular
	N4–H4A···O3	2.01	2.839(4)	158	3/2-x,-1/2+y,1/2-z
	N5–H5A···O11	1.84	2.694(4)	177	1-x,-y,-z
	N6–H6A···O12	1.72	2.6784)	168	1-x,-y,-z
	O7–H7A···O5	1.76	2.583(4)	150	Intramolecular
	O7–H7A···O1	2.60	3.071(4)	113	3/2-x,1/2+y,1/2-z
	O8–H8A···O6	1.75	2.534(4)	150	Intramolecular
	O9–H9A···O11	1.75	2.544(4)	146	Intramolecular
	O10–H10A···O12	1.64	2.543(4)	162	Intramolecular

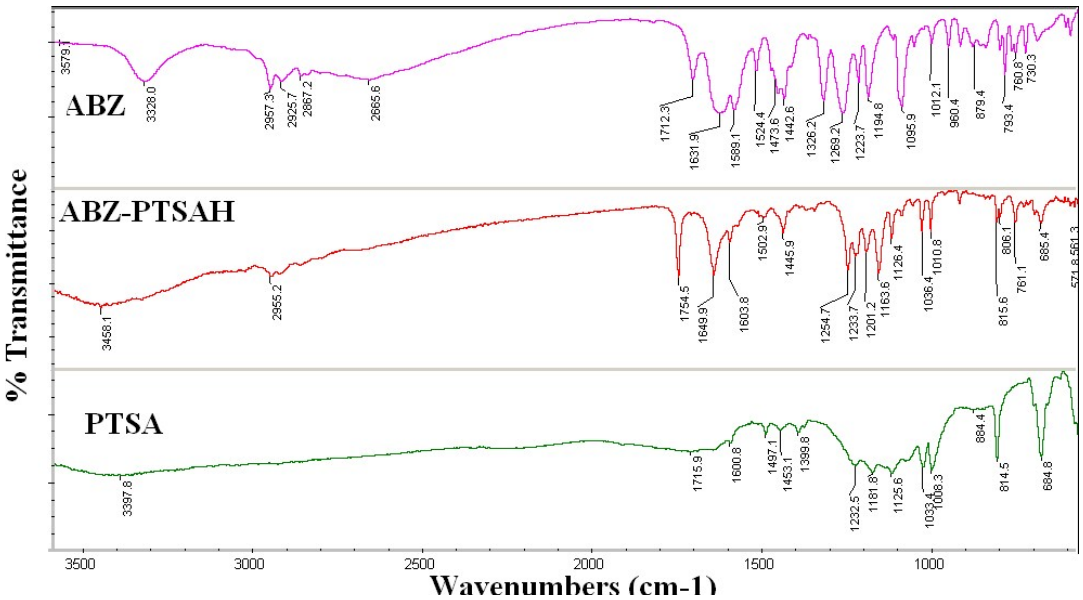
[a] Symmetrically Independent molecules.



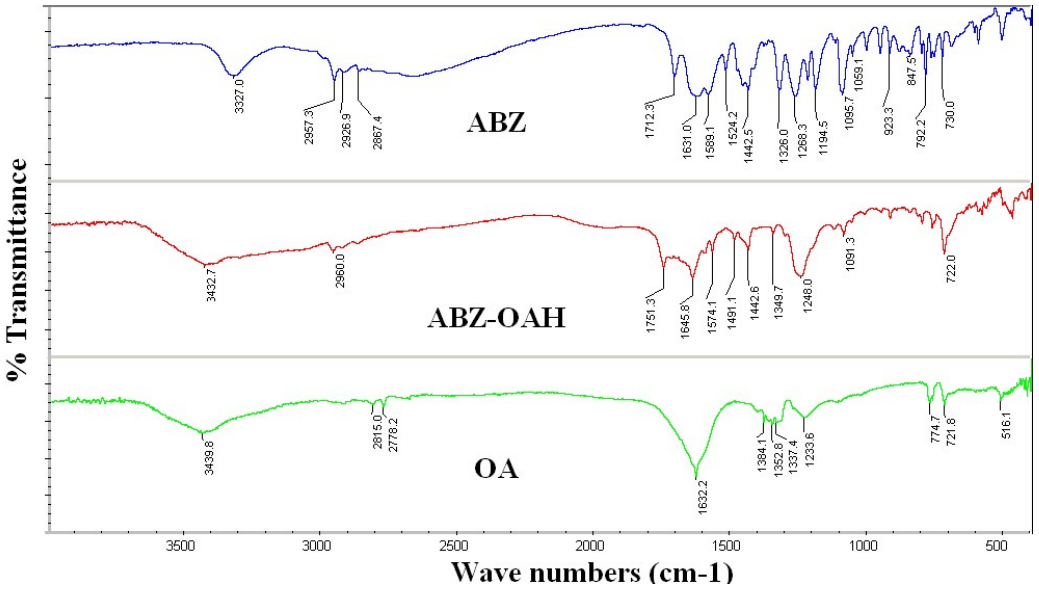
(a)


ABZ
ABZ-PTSA
PTSA
% Transmittance
Wavenumbers (cm-1)
3500
3000
2500
2000
1500
1000

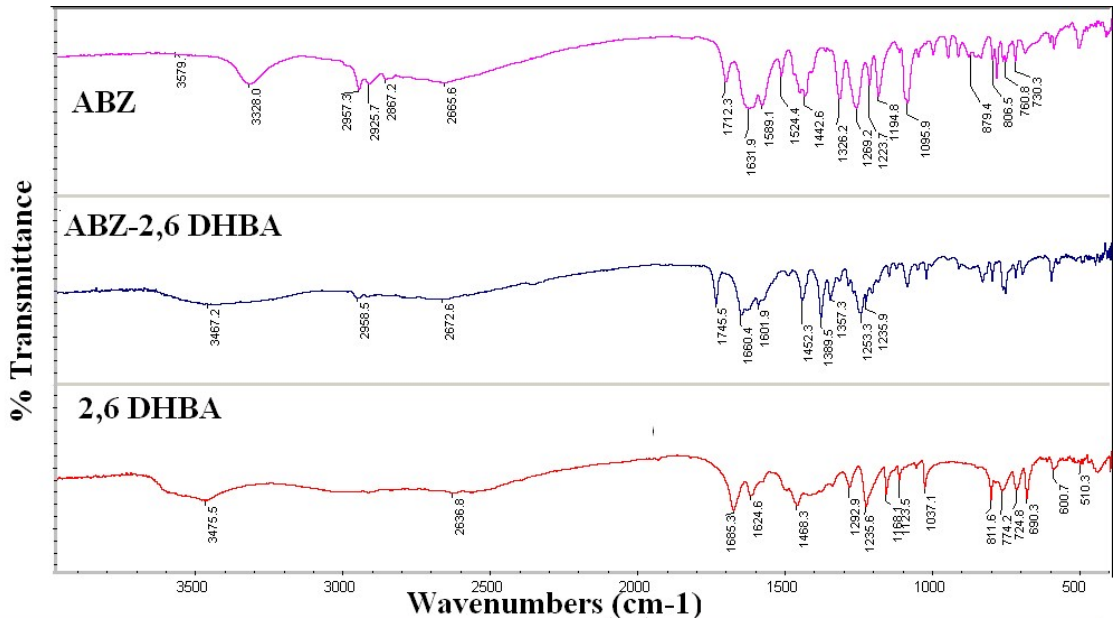
(b)


ABZ
ABZ-PTSAH
PTSA
% Transmittance
Wavenumbers (cm-1)
3500
3000
2500
2000
1500
1000

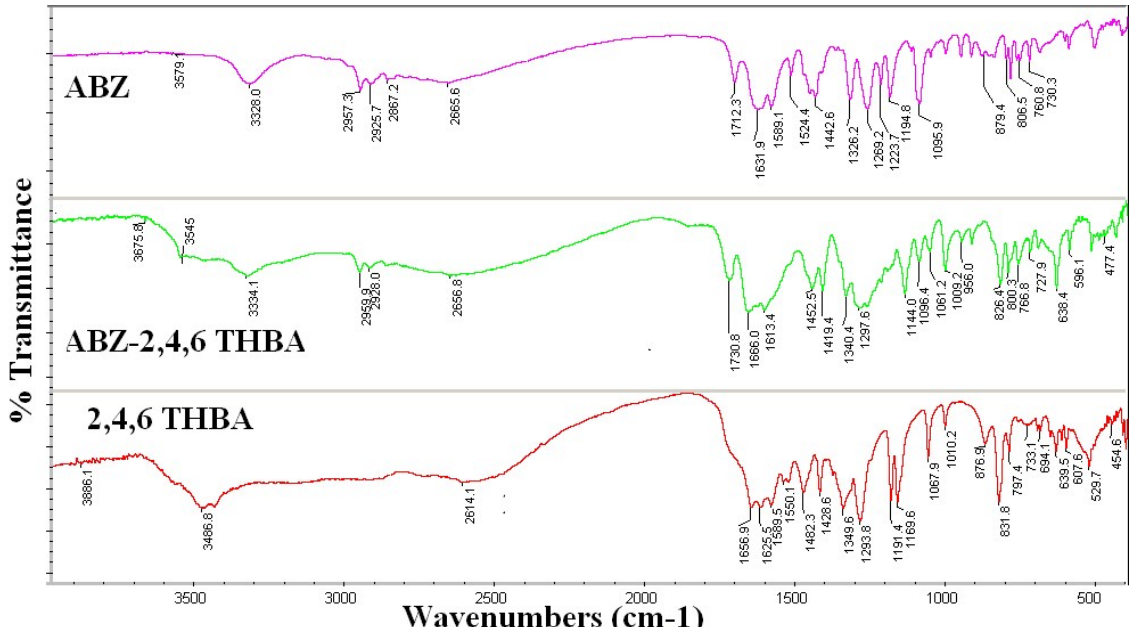
(c)


% Transmittance
ABZ
3327.0
2957.3
2926.9
2867.4
1712.3
1631.0
1589.1
1524.2
1442.5
1326.0
1268.3
1194.5
1095.7
1059.1
923.3
847.5
792.2
730.0
ABZ-OAH
3432.7
2960.0
1751.3
1645.8
1574.1
1491.1
1442.6
1349.7
1248.0
1091.3
722.0
OA
3439.8
2815.0
2778.2
1632.2
1384.1
1352.8
1337.4
1233.6
774.7
721.8
516.1
3500
3000
2500
2000
1500
1000
500
Wave numbers (cm-1)

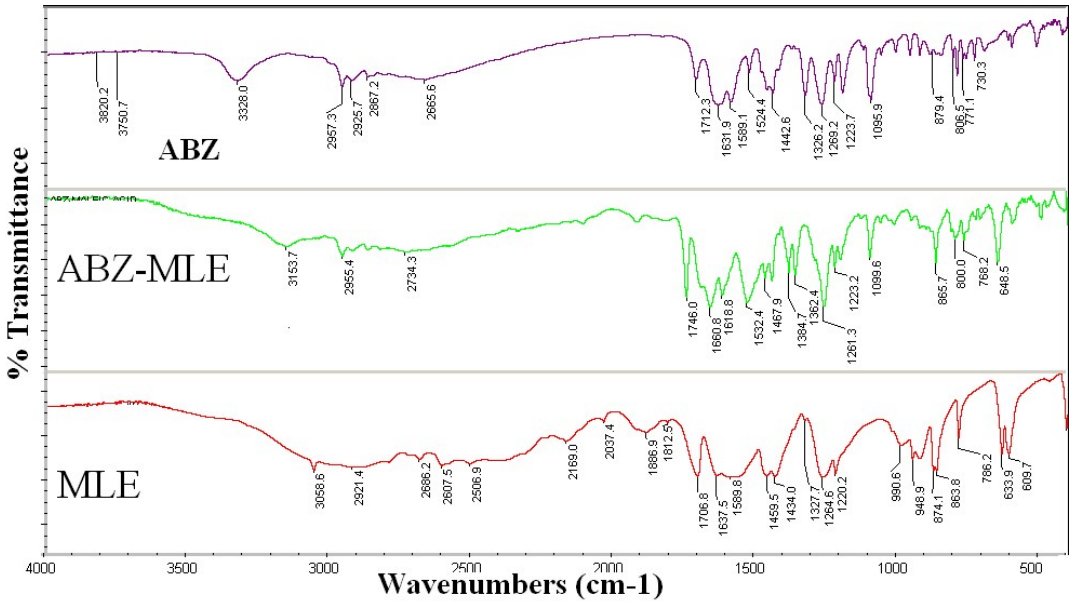
(d)


% Transmittance
ABZ
3579
3328.0
2957.3
2925.7
2867.2
2665.6
1712.3
1631.9
1589.1
1524.4
1442.6
1326.2
1269.2
1223.7
1194.8
1095.9
879.4
806.5
760.8
730.3
ABZ-2,6 DHBA
3467.2
2958.5
2672.6
1745.5
1660.4
1601.9
1452.3
1389.5
1357.3
1253.3
1235.9
2,6 DHBA
3475.5
2636.8
1685.3
1624.6
1468.3
1292.9
1235.6
1168.1
1123.5
1037.1
811.6
774.2
724.8
690.3
600.7
510.3
3500
3000
2500
2000
1500
1000
500
Wavenumbers (cm-1)

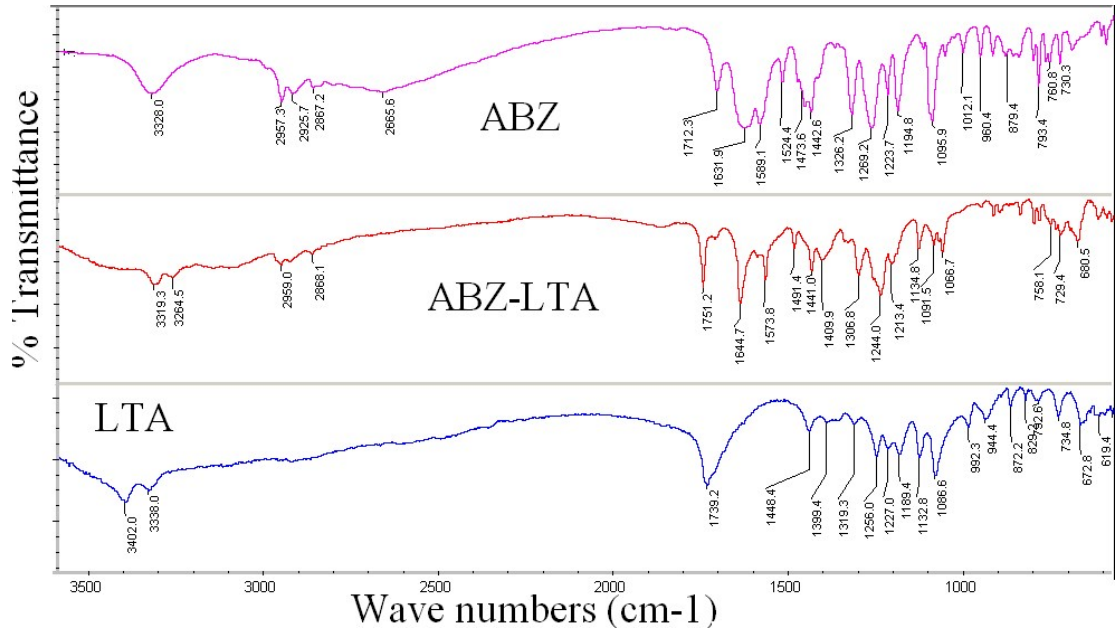
(e)


ABZ
ABZ-2,4,6 THBA
2,4,6 THBA
% Transmittance
Wavenumbers (cm-1)

(f)

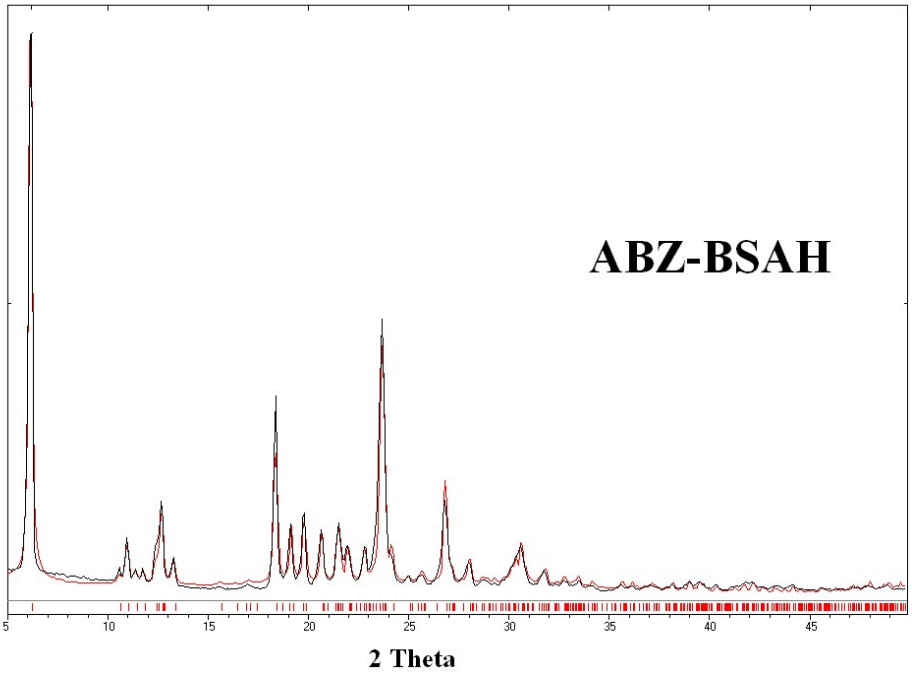

ABZ
ABZ-MLE
MLE
% Transmittance
Wavenumbers (cm-1)

(g)

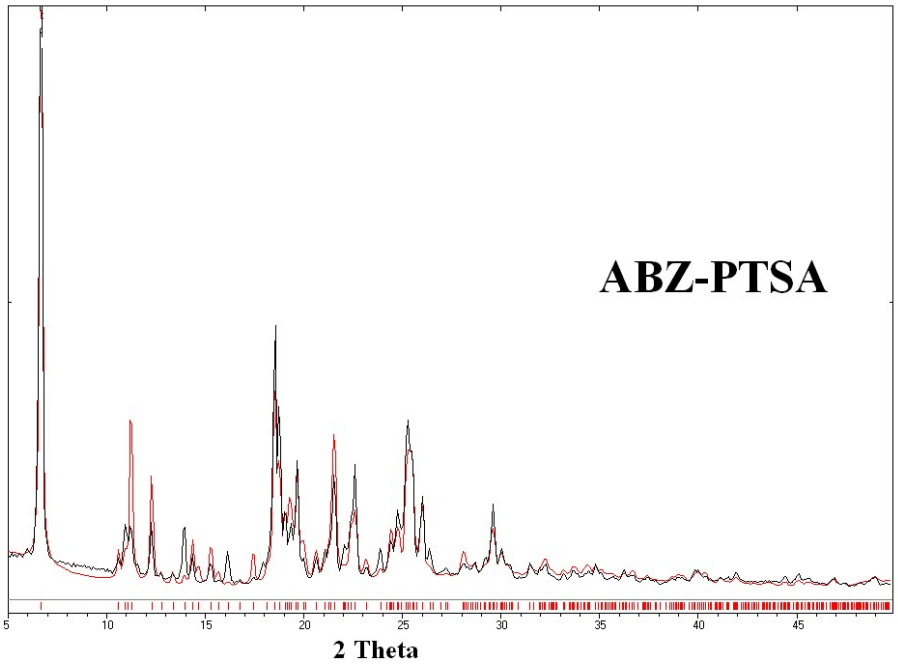


(h)

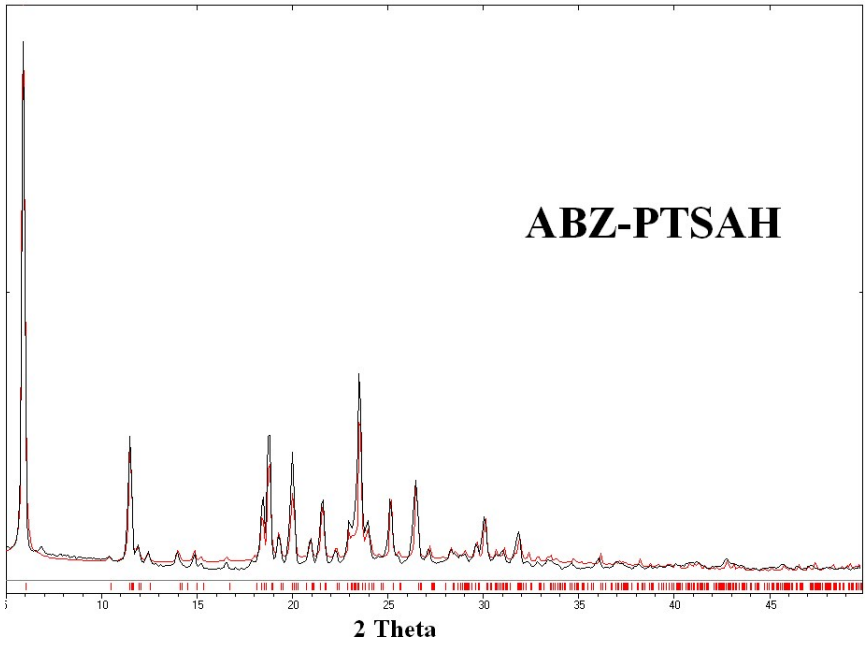
Fig. S1 FT-IR spectra comparison of the binary adducts (a), ABZ–BSAH, (b) ABZ–PTSA, (c) ABZ–PTSAH, (d) ABZ–OAH, (e) ABZ–2,6-DHBA, (f) ABZ–2,4,6-THBA, (g) ABZ–MLE, (h) ABZ–LTA along with its starting materials ABZ and coformers in this study.



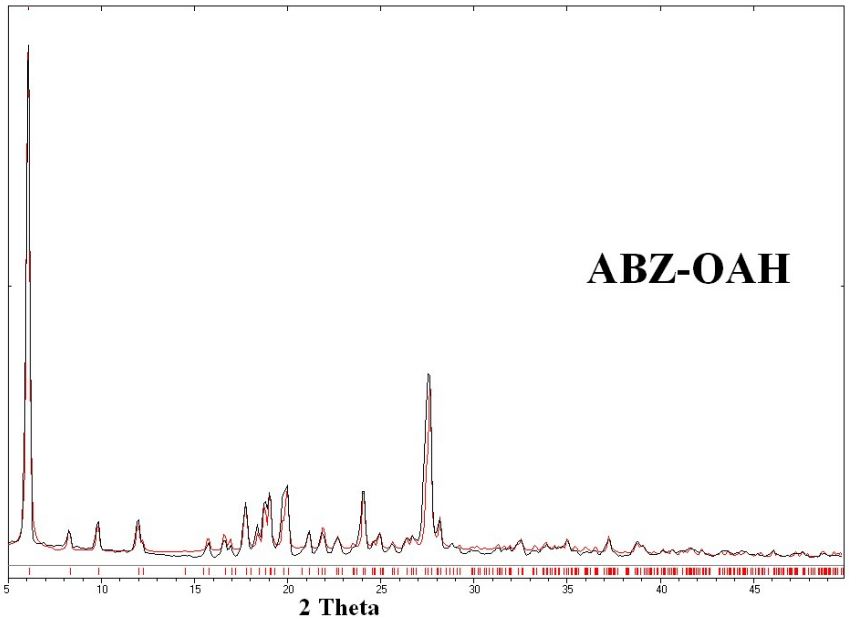
(a)


ABZ-PTSA
5
10
15
20
25
30
35
40
45
2 Theta

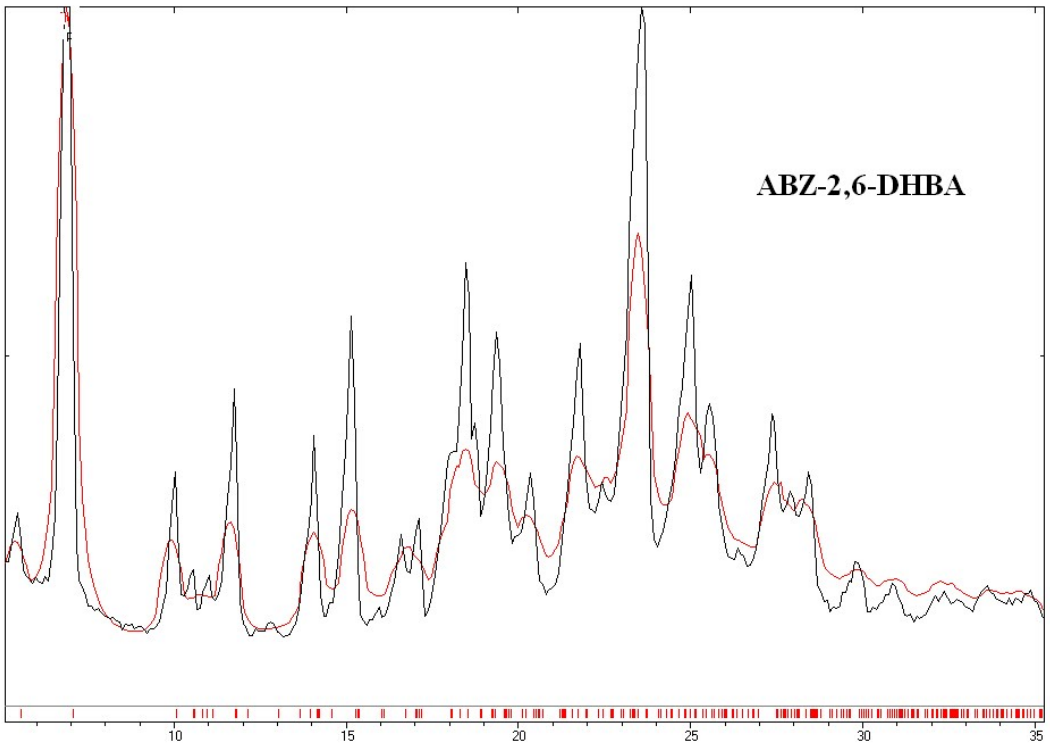
(b)


ABZ-PTSAH
10
15
20
25
30
35
40
45
2 Theta

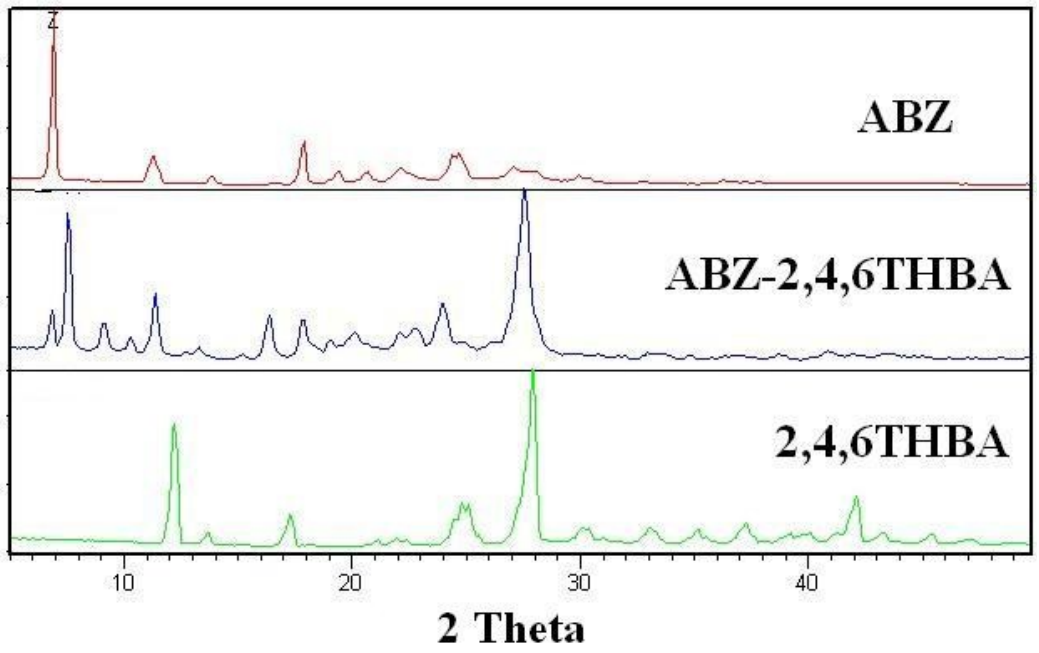
(c)


ABZ-OAH
5
10
15
20
25
30
35
40
45
2 Theta

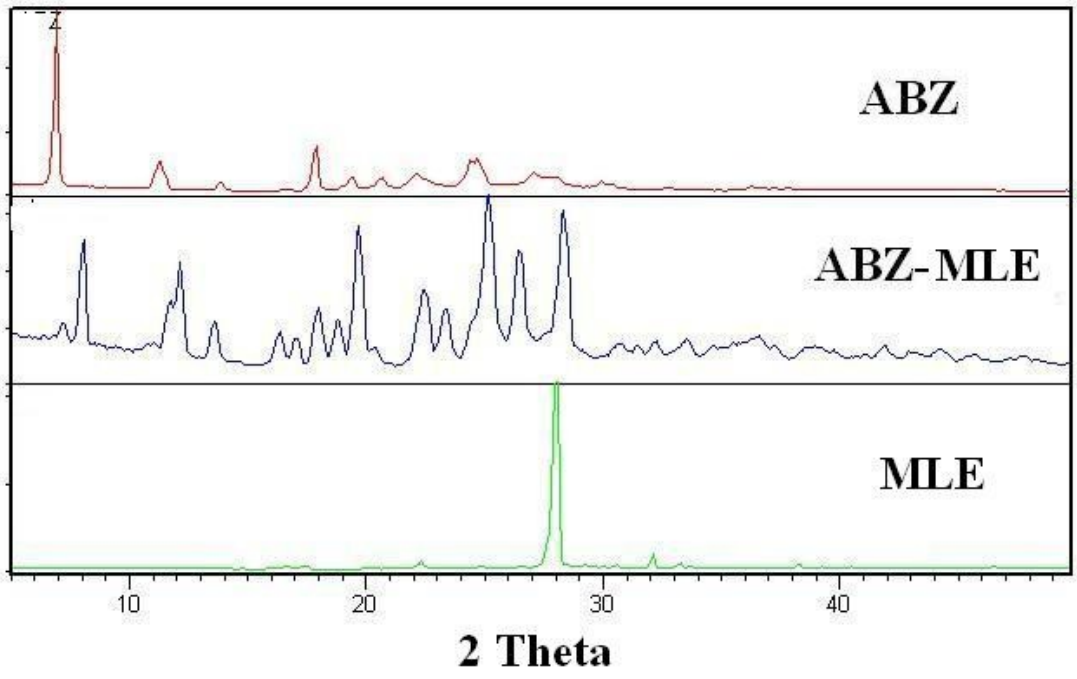
(d)


ABZ-2,6-DHBA
10
15
20
25
30
35

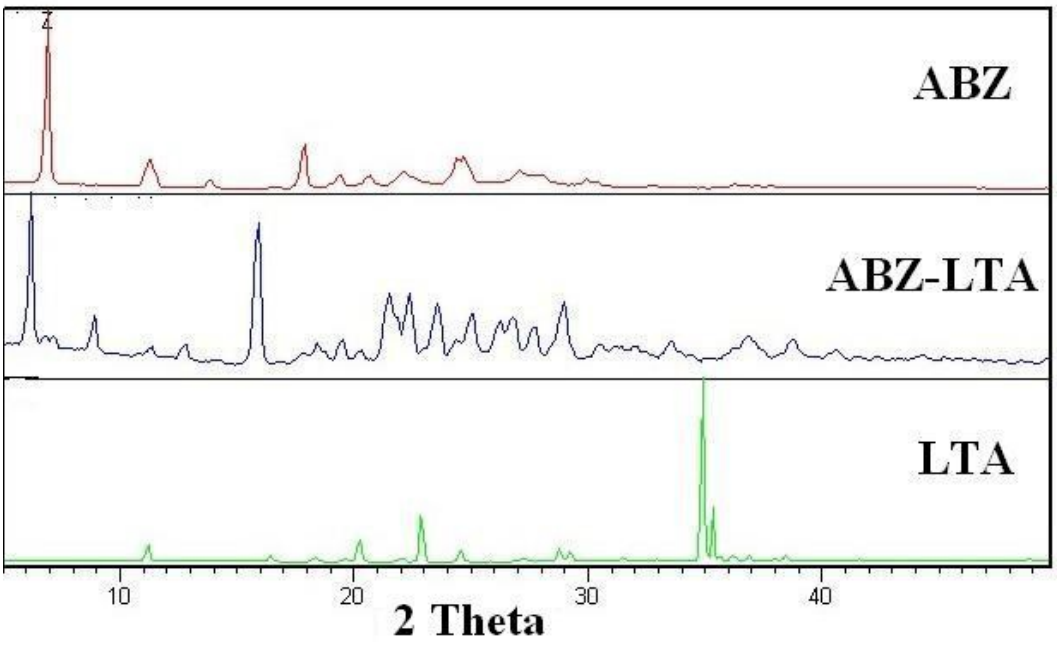
(e)


ABZ
ABZ-2,4,6THBA
2,4,6THBA
10
20
30
40
2 Theta

(f)

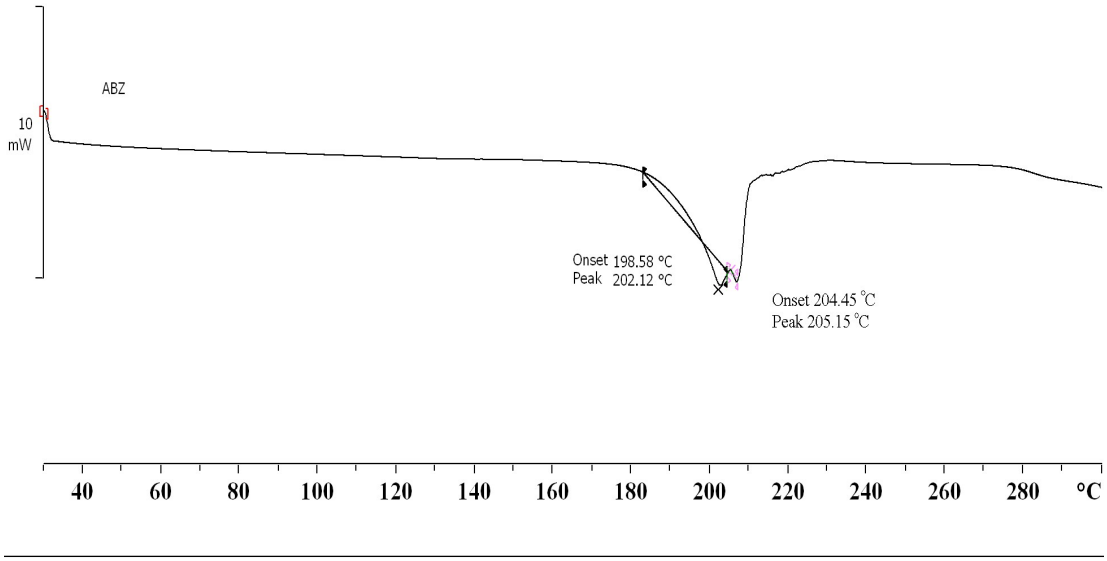

ABZ
ABZ-MLE
MLE
10
20
30
40
2 Theta

(g)

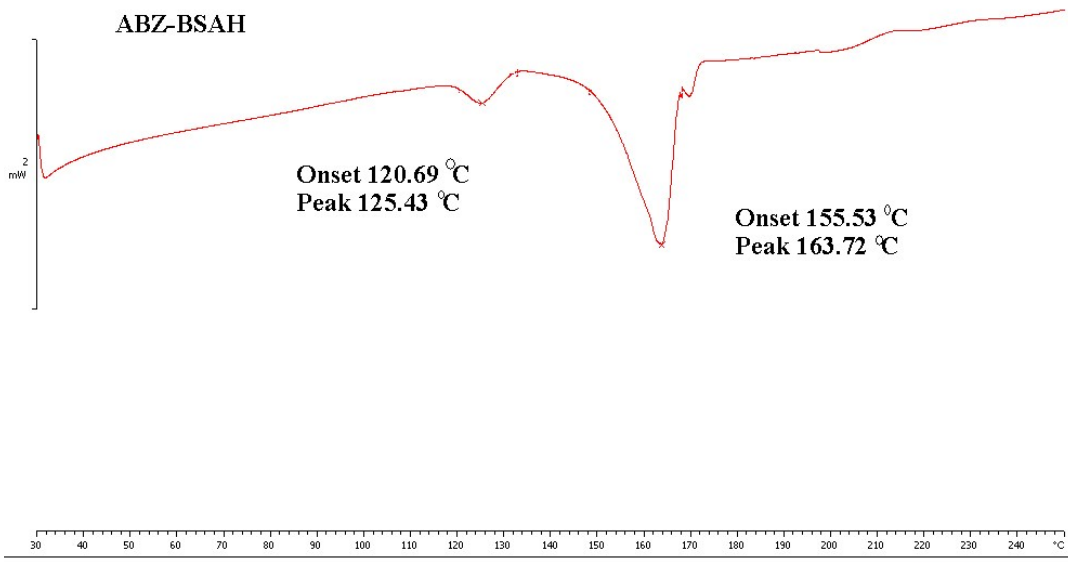


(h)

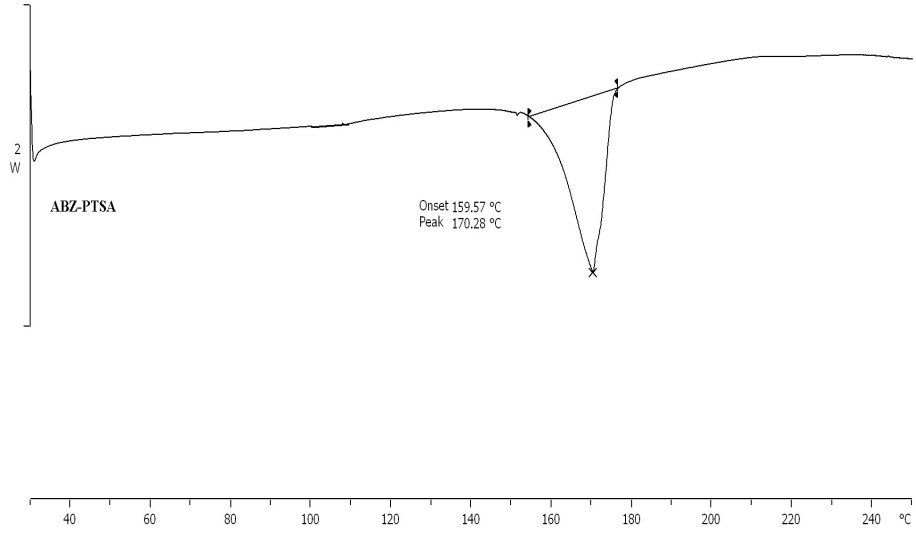
Fig. S2 (a), (b), (c), (d) and (e) PXRD overlay pattern of the grinded materials with single X-ray diffraction patterns of the ABZ–BSAH, ABZ–PTSA, ABZ–PTSAH, ABZ–OAH, and ABZ–2,6-DHBA. Good matching of the both indicates the material purity. Red color is the single crystal X-Ray pattern and black one is grinded materials. (f), (g) and (h) PXRD comparison of the ground material diffraction patterns of the ABZ–2,4,6-THBA, ABZ–MLE and ABZ–LTA along with their starting materials, unique new diffracted 2 theta values allow us to confirm new solid phase.



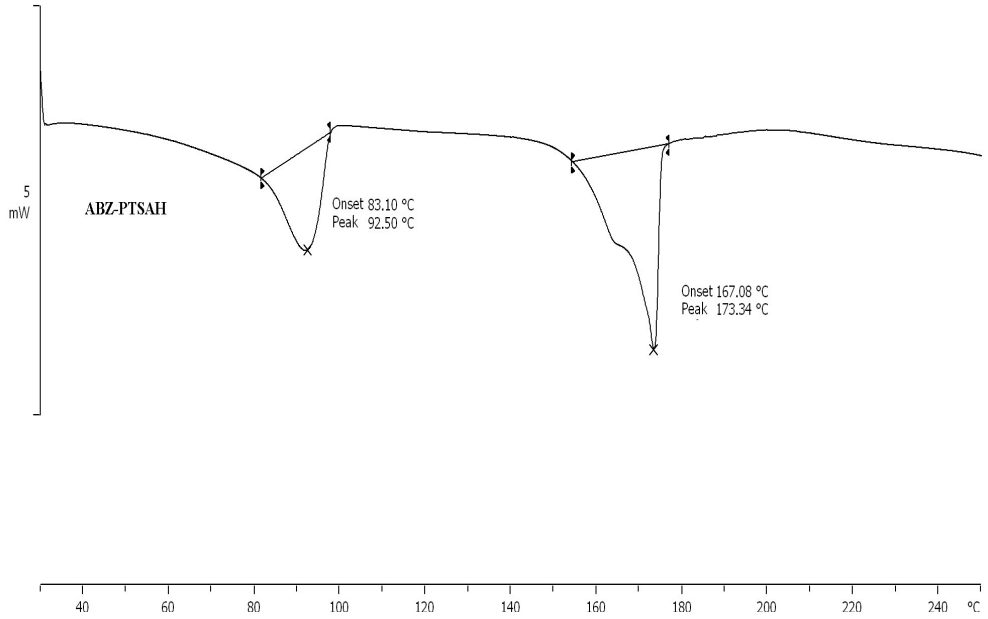
(a)


ABZ-BSAH
2
mW
Onset 120.69 °C
Peak 125.43 °C
Onset 155.53 °C
Peak 163.72 °C
30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 °C

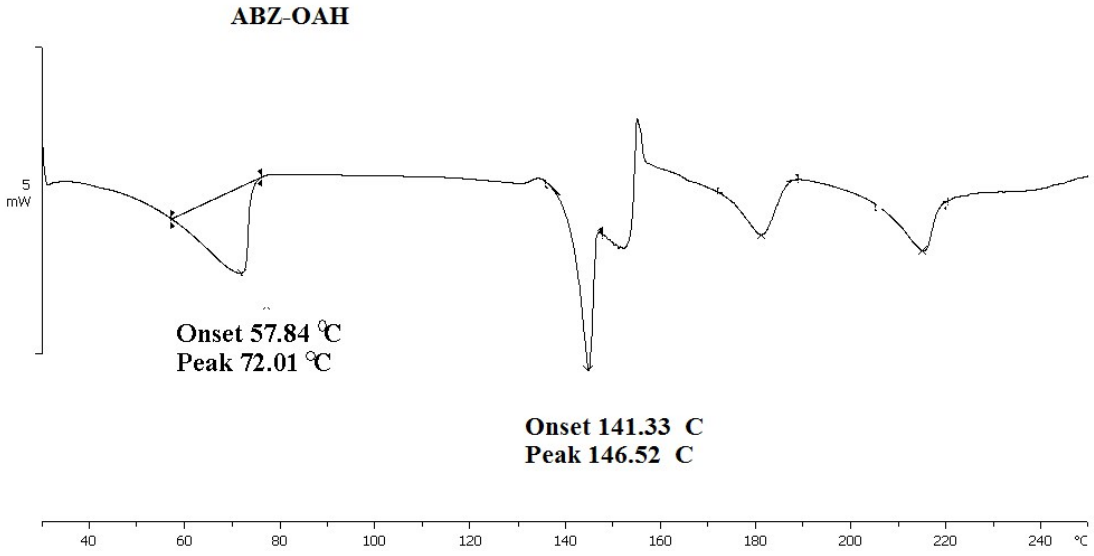
(b)


2
W
ABZ-PTSA
Onset 159.57 °C
Peak 170.28 °C
40 60 80 100 120 140 160 180 200 220 240 °C

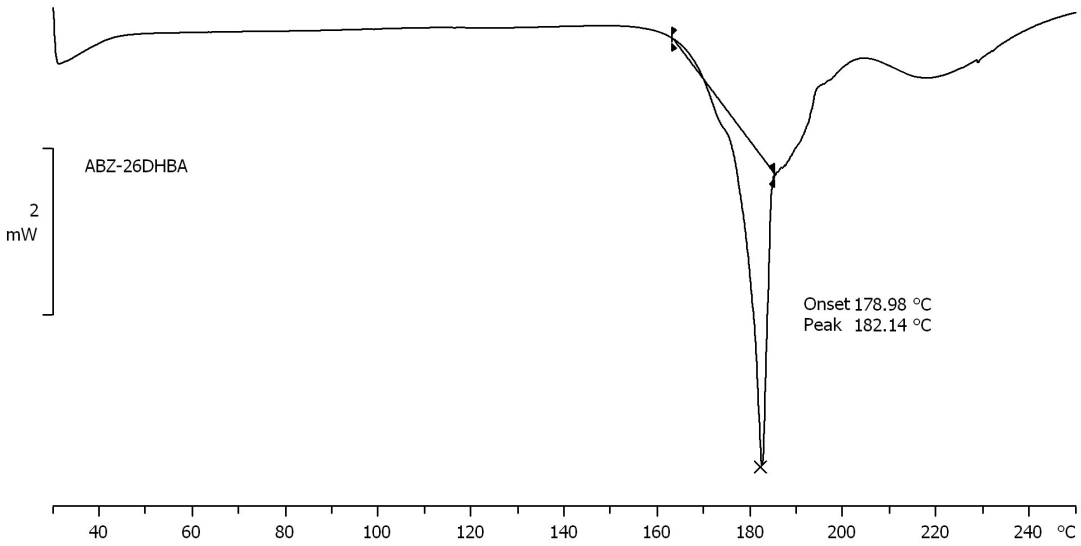
(c)


5
mW
ABZ-PTSAH
Onset 83.10 °C
Peak 92.50 °C
Onset 167.08 °C
Peak 173.34 °C
40
60
80
100
120
140
160
180
200
220
240
°C

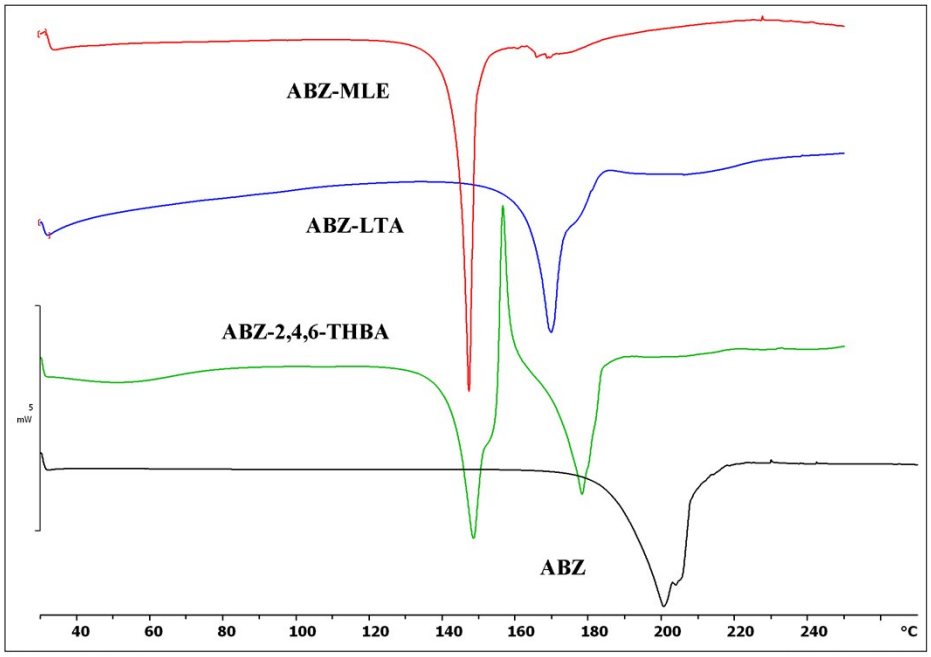
(d)


ABZ-OAH
5
mW
Onset 57.84 °C
Peak 72.01 °C
Onset 141.33 C
Peak 146.52 C
40
60
80
100
120
140
160
180
200
220
240
°C

(e)



(f)



(g)

Fig. S3 (a) DSC endotherm of ABZ. DSC endotherm of grinded materials (b) ABZ–BSAH, (c) ABZ–PTSA, (d) ABZ–PTSAH, (e) ABZ–OAH, (f) ABZ–2,6DHBA, (g) ABZ–MLE, ABZ–LTA, ABZ–2,4,6-THBA.