

SUPPLEMENTARY DATA

Organic salts of *p*-coumaric acid and *trans*-ferulic acid with aminopicolines

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HYDROGEN BOND DATA

Table S1. Geometrical data for hydrogen bonds of salt 1.

	D-H (Å)	H...A (Å)	D...A (Å)	<DHA (°)	Symmetry operation
N1-H4...O2	0.95	1.71	2.662(2)	173.5	
N2-H9A...O1	0.92	1.98	2.893(3)	171.6	
O3-H1...O1	0.89	1.79	2.671(2)	169.6	$x^{-1/2}, y, -z+3/2$
N2-H9B...O2	0.82	2.60	3.365(2)	156.3	$x+1/2, -y+1/2, -z+1$

Table S2. Geometrical data for hydrogen bonds of salt 2.

	D-H (Å)	H...A (Å)	D...A (Å)	<DHA (°)	Symmetry operation
N1-H4...O1	0.88	1.87	2.741(3)	169	
N2-H9A...O2	0.93	1.92	2.822(4)	165.7	
N3-H14...O4	0.95	1.82	2.753(3)	165.5	
N4-H16A...O5	1.00	1.76	2.758(3)	172.3	
N5-H19...O7	0.97	1.80	2.722(2)	159.4	
N6-H24A...O8	0.87	2.00	2.845(3)	163.5	
N7-H29...O10	0.97	1.81	2.793(3)	158.6	
N8-H31...O11	0.93	1.87	2.793(3)	167.7	
N2-H9B...O4	0.94	2.05	2.941(3)	156.1	
N4-H16B...O7	0.99	1.90	2.861(3)	162.7	
N6-H24B...O10	0.92	2.06	2.898(3)	151.8	
O3-H1...O8	0.92	1.77	2.668(3)	165.1	$-x, y-1/2, 1-z$
O9-H9...O2	0.90	1.72	2.621(3)	175.8	$1-x, 1/2+y, 1-z$
N8-H31B...O1	0.96	1.97	2.894(3)	161.0	$x, y, 1+z$
O6-H10...O5	0.96	1.71	2.666(3)	171.1	$-x, 1/2+y, 1-z$
O12-H25...O11	0.89	1.73	2.606(3)	169.1	$1-x, y-1/2, 2-z$

Table S3. Geometrical data for hydrogen bonds of salt **3**.

	D-H (Å)	H...A (Å)	D...A (Å)	<DHA (°)	Symmetry operation
N1-H1...O2	0.90(3)	1.75 (3)	2.647(3)	172(3)	
N2-H3A...O1	1.05(3)	1.85(3)	2.904(3)	175(2)	
O6-H13...O2	0.97(4)	1.75(4)	2.661(2)	156(4)	
O6-H13...O2	0.95(4)	1.64(4)	2.589(3)	174(3)	
N2-H3B...O4	0.91	2.10(4)	2.964(3)	156(3)	$x-1/2, y+5/2, z-1/2$
O5-H9B...O1	0.92(4)	1.84(4)	2.745(3)	169(3)	$-x, -y+2, -z$
O5-H9A...O6	0.64(4)	2.16(4)	2.789(3)	170(5)	$x, y-1, z$
C12-H12...O3	0.95	3.28	3.447(3)	92.2	$-x, -y+3, -z$

TORSION ANGLES

Table S4. Torsion angles of salts **1**, **2** and **3**.

	1	2	3
Torsion angle	(°)	(°)	(°)
τ_1 (C2-C1-C7-C8)	12.8	14.4	0.2
τ'_1 (C17-C16-C22-C23)	-	0.5	-
τ''_1 (C32-C31-C37-C38)	-	2.7	-
τ'''_1 (C47-C46-C52-C53)	-	4.6	-
τ_2 (C7-C8-C9-O1)	10.1	12.8	4.9
τ'_2 (C22-C23-C24-O4)	-	26.7	-
τ''_2 (C37-C38-C39-O7)	-	9.1	-
τ'''_2 (C52-C53-C54-O10)	-	5.1	-

HIRSHFELD SURFACE ANALYSIS

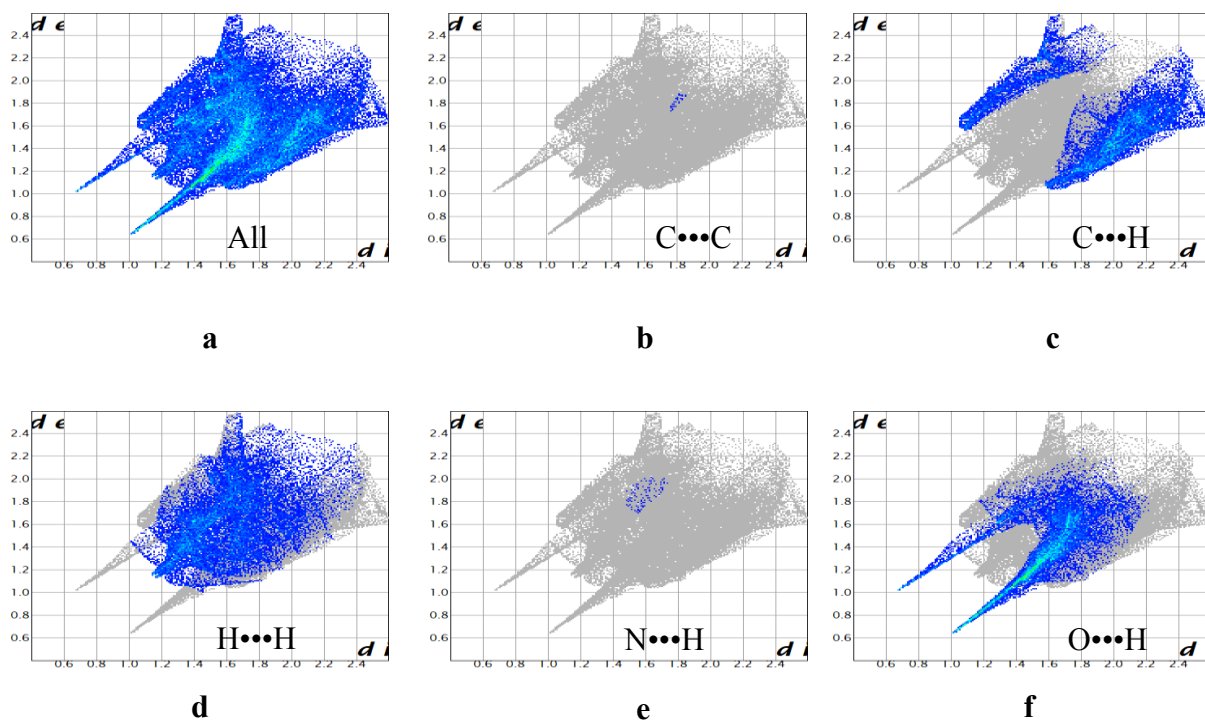


Figure S1. Fingerprint plot of p CA in salt 1.

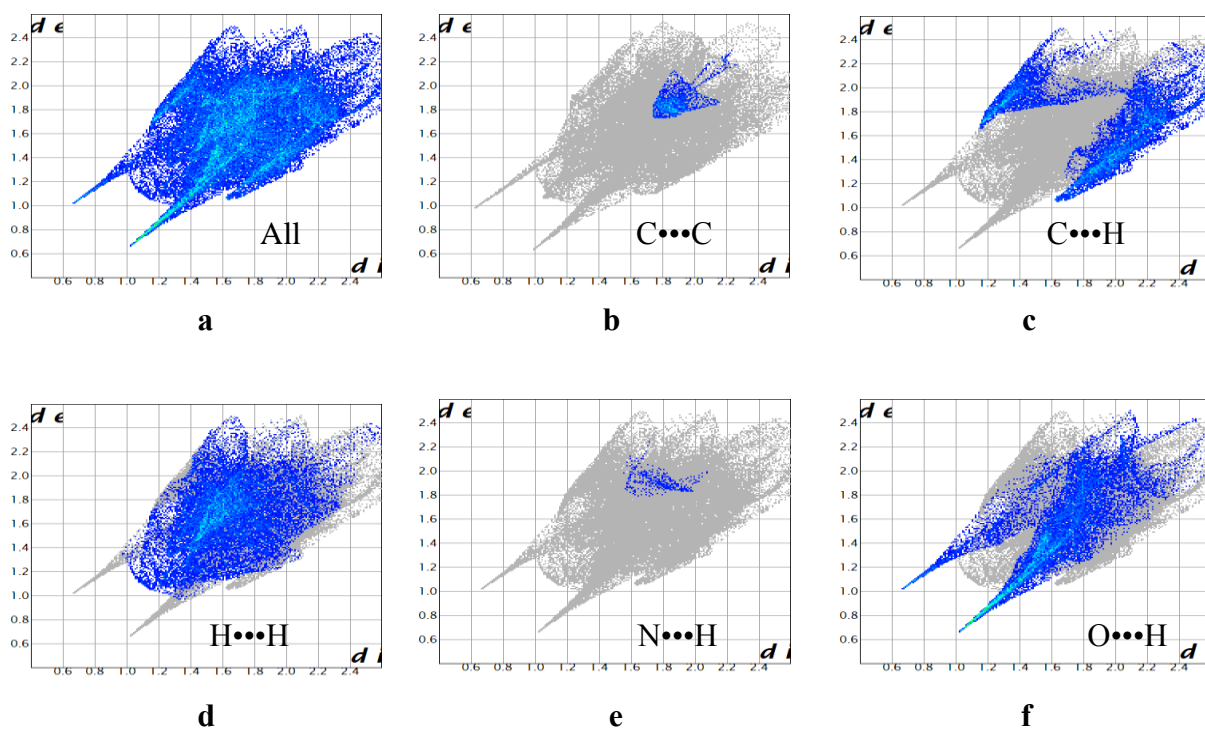


Figure S2 Fingerprint plot of p CA in salt 2.

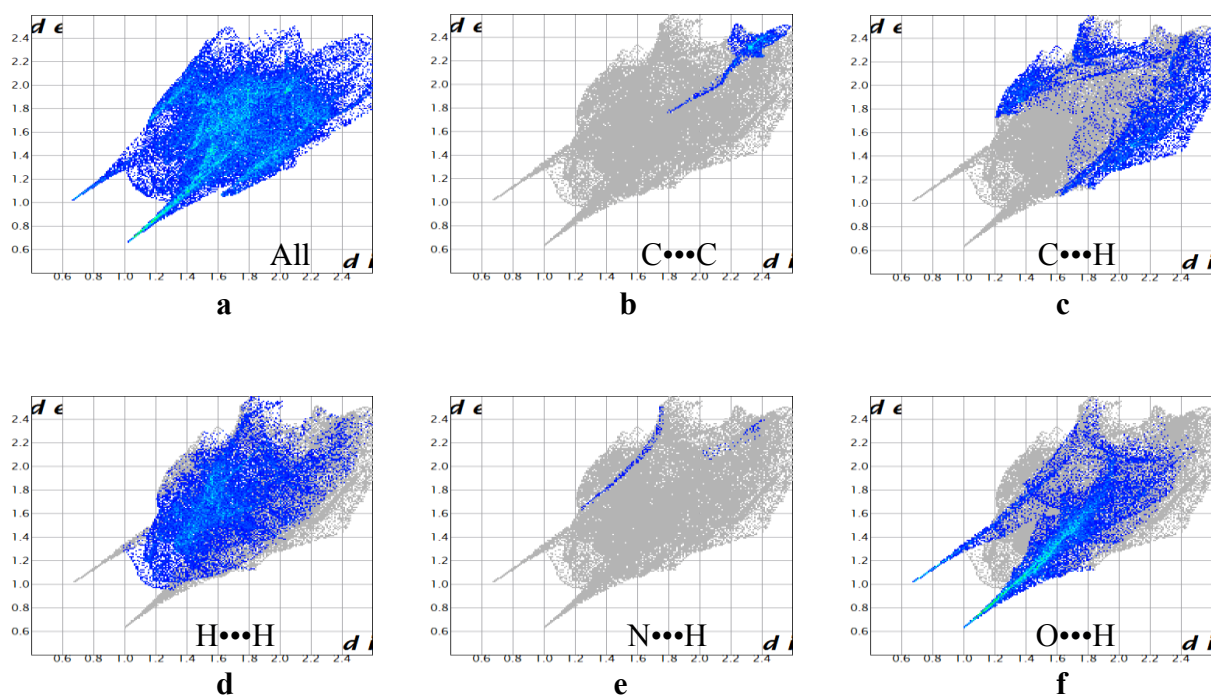


Figure S3. Fingerprint plot of pCA' in salt 2.

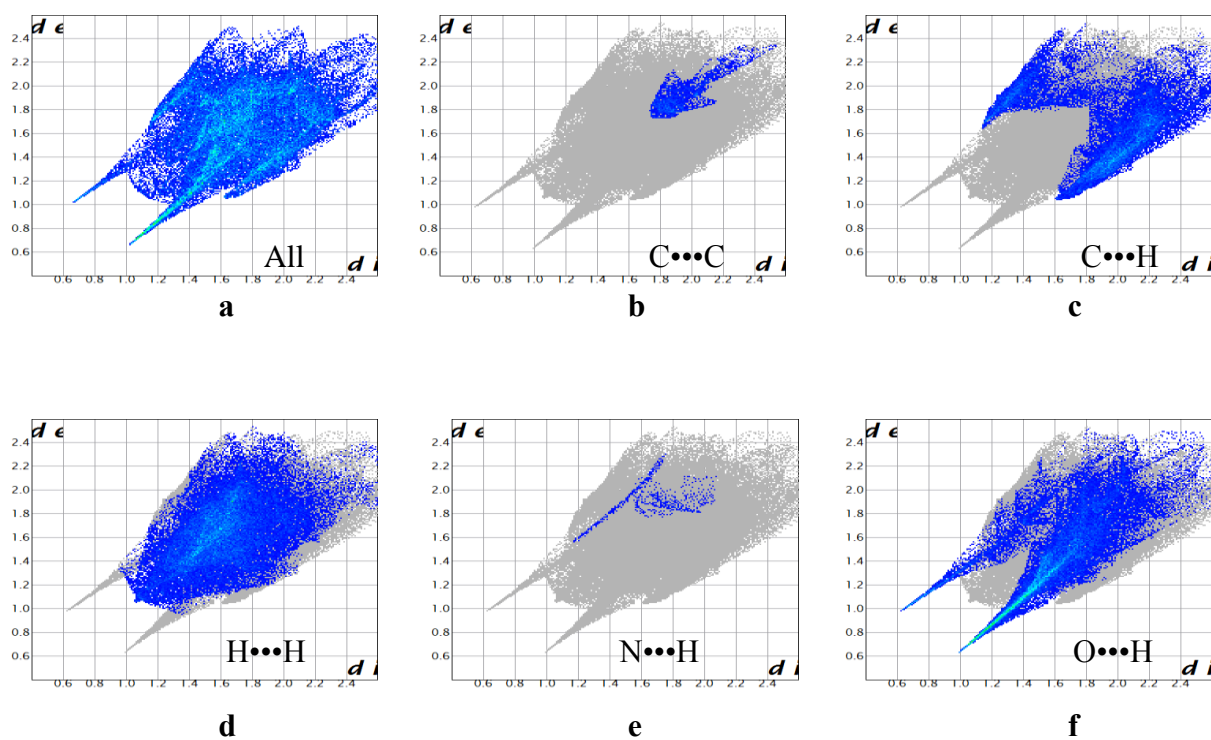


Figure S4. Fingerprint plot of pCA'' in salt 2.

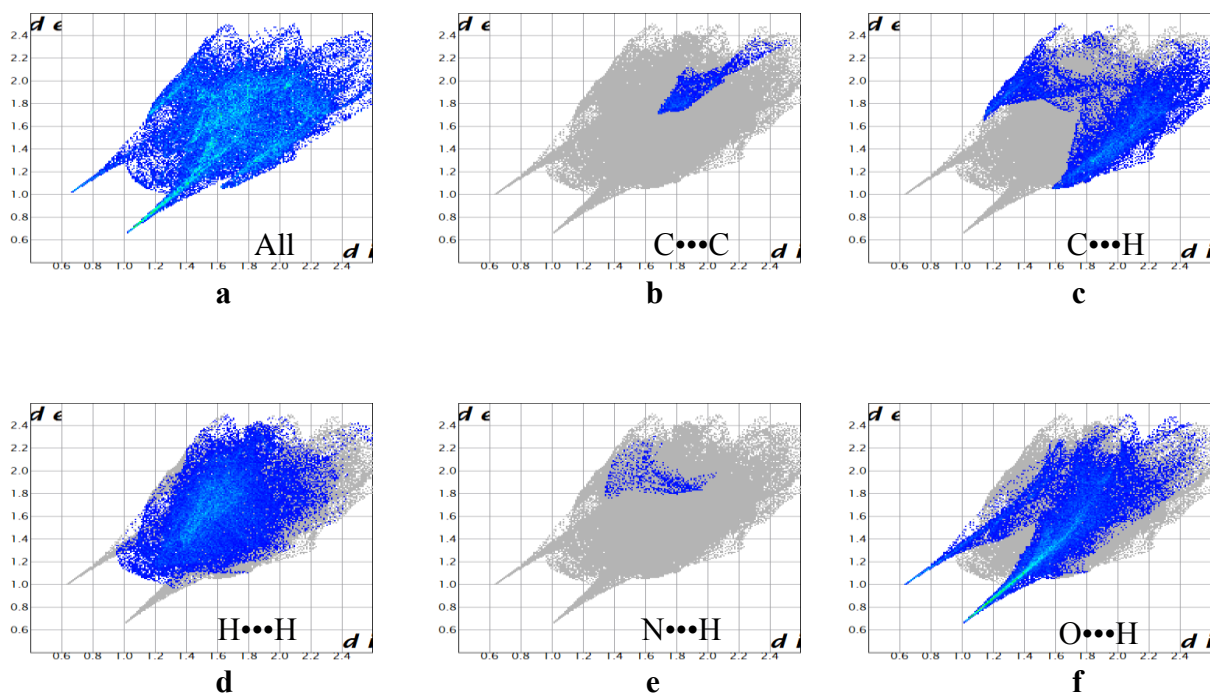


Figure S5. Fingerprint plot of pCA''' in salt 2.

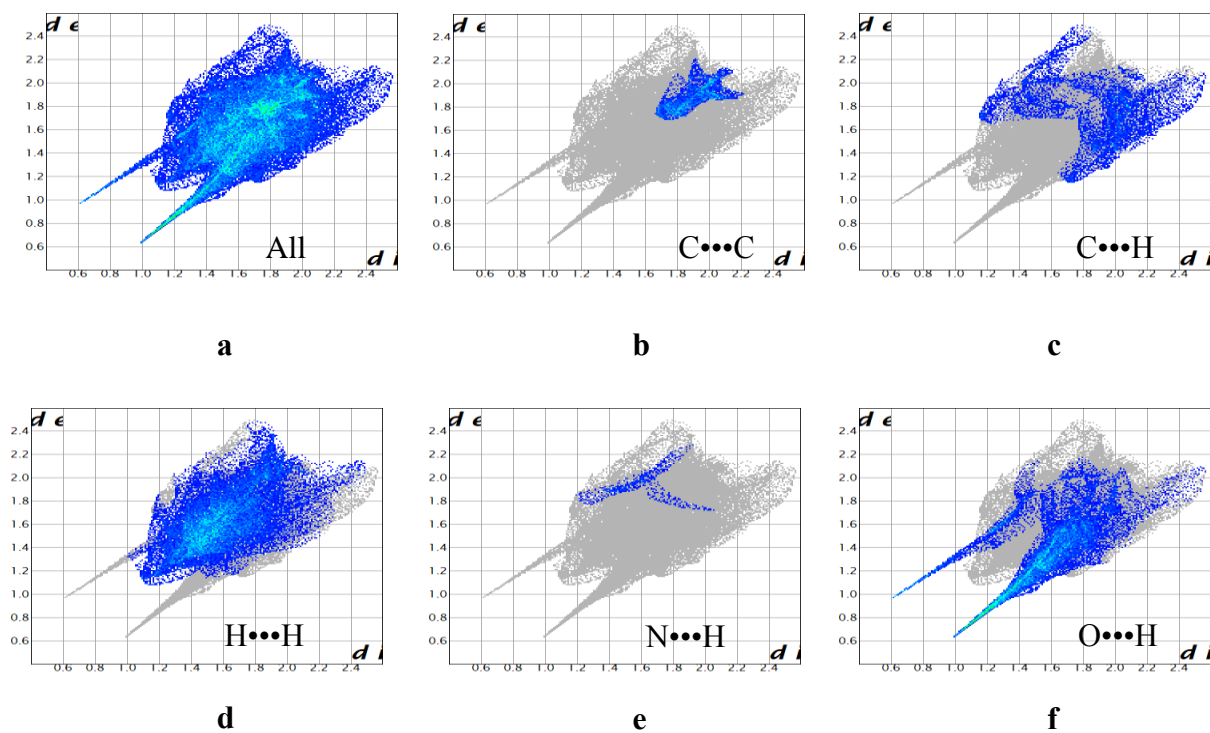


Figure S6. Fingerprint plot of TFA in salt 3.

Table S5. Quantitative summary of the various interactions of *p*CA and TFA salts.

Salt		C...C (%)	C...H (%)	H...H (%)	N...H (%)	O...H (%)
1		0.1	29.6	38.3	0.2	30.1
2	<i>p</i> CA	1.7	25.2	38.9	0.7	30.8
	<i>p</i> CA'	3.4	22.7	38.4	0.5	31.6
	<i>p</i> CA''	2.8	23.3	40	0.7	30.7
	<i>p</i> CA'''	2.5	21.9	39.6	0.8	32.1
3		7.5	13.5	45.1	1.3	29.5

GRINDING EXPERIMENTS

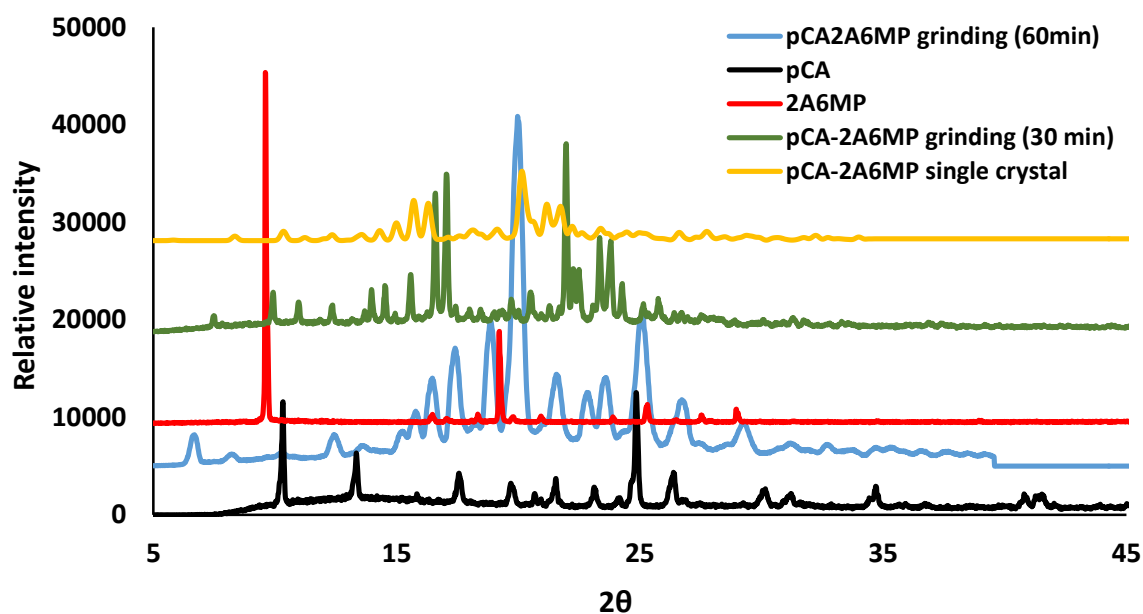


Figure S7. PXRD analyses of *p*CA and 2A6MP grinding (60 min) (blue), *p*CA (black), 2A6MP (red), *p*CA2A6MP grinding (30 min) (green) and the calculated pattern (yellow).

FTIR SPECTRA

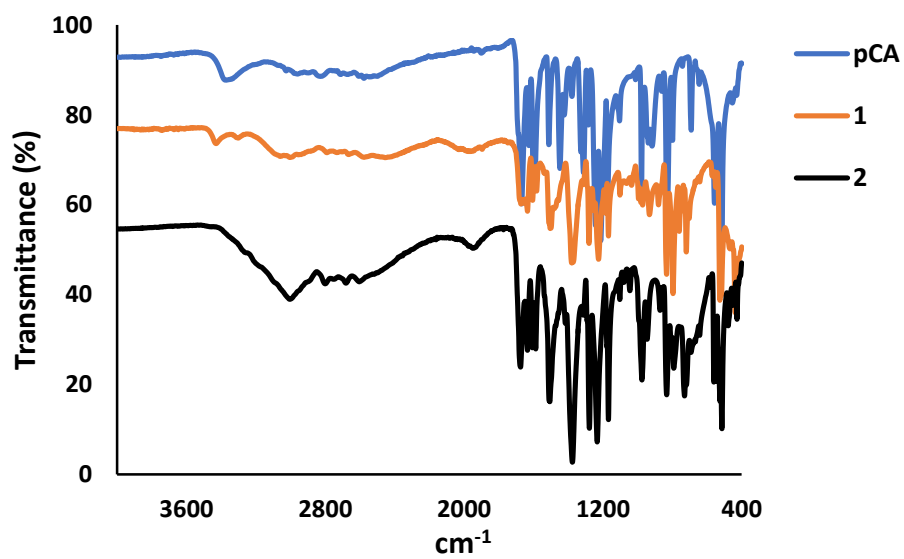


Figure S8. FTIR spectra of *p*CA (blue), salt 1 (orange) and salt 2 (black).

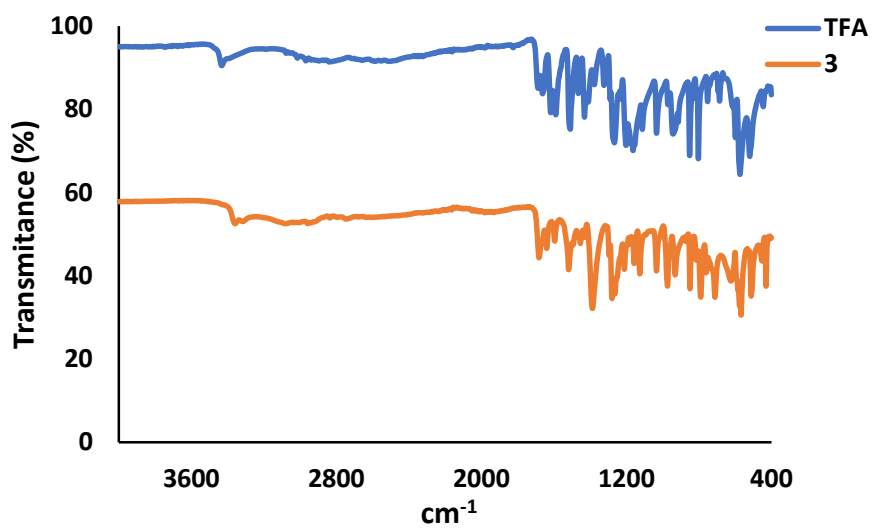


Figure S9. FTIR spectra of TFA (blue) and salt 3 (orange).