Electronic Supporting Information for

Ciprofloxacin salts of benzene mono/di-carboxylate: Crystal structures and the improvement of solubility

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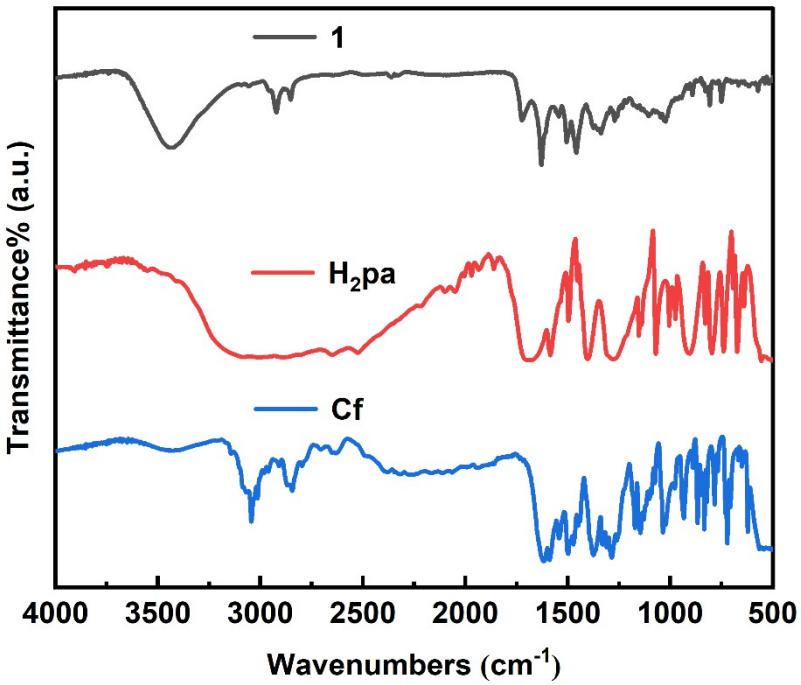
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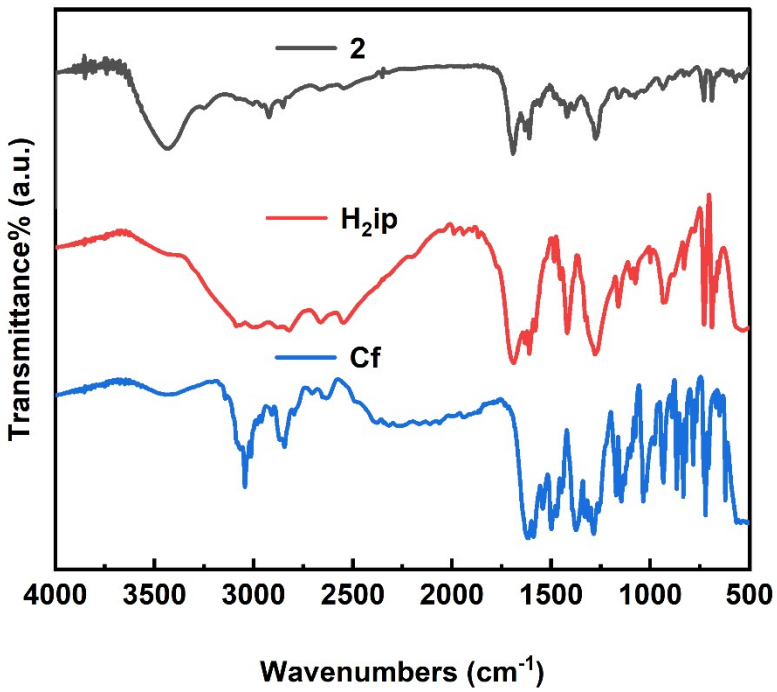
Wavenumbers (cm-1)

(a)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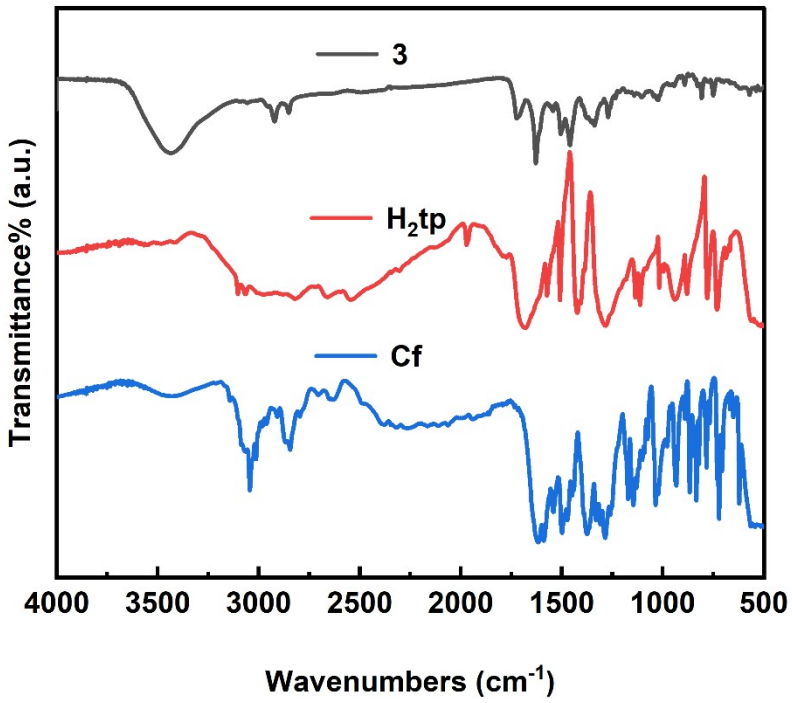
(b)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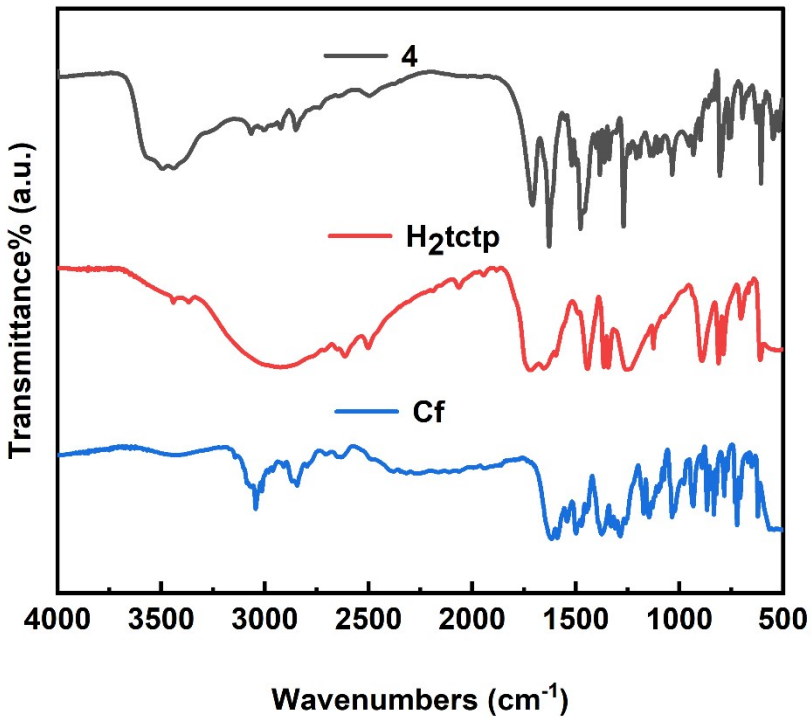
(c)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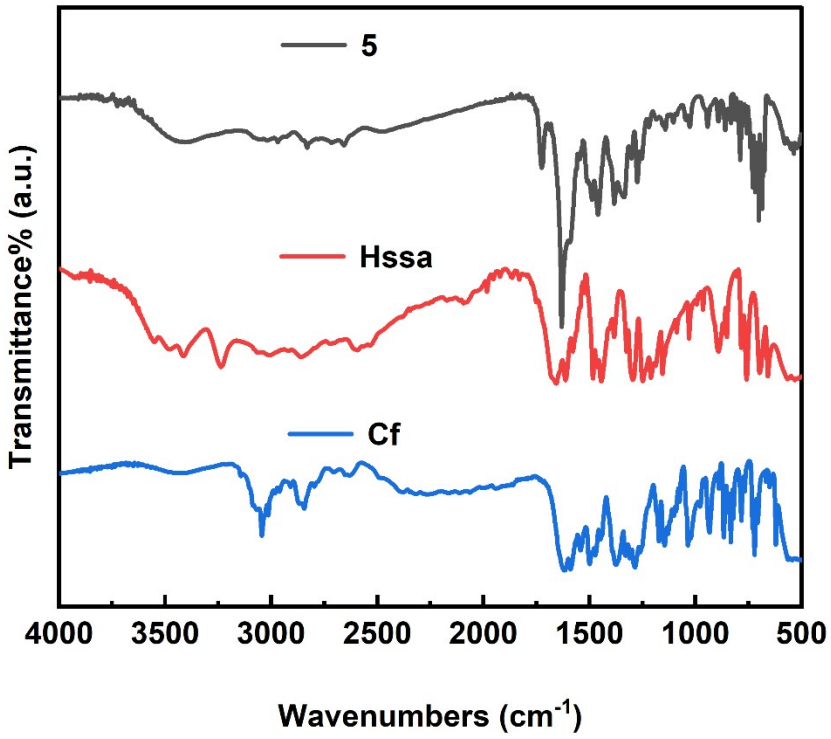
(d)



(e)

Fig. S1 Infrared spectra of Cf, coformers, and **1**-**5** (a-e)

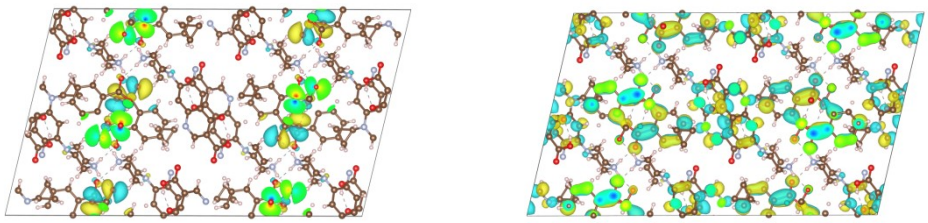


Fig. S2 HOMO (left) and LUMO (right) for **1**

Fig. S3 HOMO (left) and LUMO (right) for **2**

Fig. S4 HOMO (left) and LUMO (right) for **3**

Fig. S5 HOMO (left) and LUMO (right) for **4**

Fig. S6 HOMO (left) and LUMO (right) for **5**

Table S1. Crystal data and structural refinement parameters of salts **1-5**

Salt	**1**	**2**	**3**	**4**	**5**
Empirical formula	$C_{25}H_{24}FN_3O_7$	$C_{84}H_{94}F_4N_{12}O_{25}$	$C_{21}H_{27}N_3O_8F$	$C_{29}H_{21}N_3O_9FCl_6$	$C_{69}H_{70}F_2N_6O_{23}$
Moiety formula	$C_{17}H_{19}FN_3O_3$, $C_8H_5O_4$	$4(C_{17}H_{19}FN_3O_3)$, $2(C_8H_4O_4)$, $5(H_2O)$	$C_{17}H_{19}FN_3O_3$, $0.5(C_8H_4O_4)$, $3(H_2O)$	$C_{17}H_{19}FN_3O_3$, $C_8H_2Cl_4O_4$, $0.5(C_8Cl_4O_4)$	$2(C_{17}H_{19}FN_3O_3)$, $3(C_7H_6O_3)$, $2(C_7H_5O_3)$, $2(H_2O)$
Formula weight	497.47	1747.71	468.45	787.19	1389.31
Crystal size (mm^3)	0.26×0.21×0.20	0.20 × 0.19 × 0.16	0.22×0.18×0.15	0.28×0.22×0.20	0.22×0.18×0.16
Crystal system	Monoclinic	Triclinic	Triclinic	Triclinic	Triclinic
Space group	*C2/c*	*P*-1	*P*-1	*P*-1	*P*-1
a (Å)	32.213(12)	10.5368(12)	7.311(2)	9.2235(8)	9.194(3)
b (Å)	7.738(2)	13.7042(16)	11.567(4)	11.3207(10)	12.720(4)
c (Å)	19.107(6)	15.0079(17)	13.026(4)	15.6694(14)	14.712(5)

α (°)	90	84.737(2)	95.552(8)	89.989(2)	82.783(9)
β (°)	103.238(10)	86.232(2)	98.490(8)	75.496(2)	77.177(9)
γ (°)	90	69.254(2)	92.972(8)	85.944(2)	76.989(9)
V (Å^3)	4636(3)	2016.8(4)	1082.0(6)	1579.8(2)	1629.4(10)
Z	8	1	2	2	1
ρ_{calc} *(g·cm^{-3})*	1.425	1.439	1.438	1.655	1.416
μ *(mm^{-1})*	0.110	0.113	0.116	0.610	0.111
F (000)	2080	918	494	798	728
Reflection collected	11880	14122	6128	10976	9181
Reflection unique	4079	9715	3786	7598	5695
Parameters	327	580	308	436	488
R_{int}	0.1012	0.0219	0.0351	0.0168	0.0291
$R^a/R_w{}^b$	0.1017/0.2705	0.0610/0.1871	0.0589/0.1741	0.0409/0.1204	0.0816/0.2455
Goodness-of-fit (GOF)^c	1.060	1.054	1.024	1.060	0.994
Δρ (max/min) (e Å^{-3})	0.682/-0.407	0.488/-0.355	0.411/-0.450	0.437/-0.380	0.730/-0.414

$^aR = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$; $^bR_w = [\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma w(F_o^2)^2]^{1/2}$. GOF = $\{\sum [w(F_o^2 - F_c^2)^2]/(n - p)]\}^{1/2}$

Table S2. Hydrogen bond geometry for salts **1-5**.

Salt	D—H···A	D—H /Å	H···A / Å	D···A / Å	D—H···A/ Deg
1	O1—H1···O3	0.82	1.77	2.525 (6)	152
	N1—H1A···O4^{i}	0.89	1.85	2.726 (7)	167
	N1—H1B···O7^{ii}	0.89	1.91	2.762 (7)	161
	O5—H5···O6	0.82	1.61	2.387 (7)	157
2	O2—H2···O1	0.82	1.80	2.558(2)	154
	N1—H1A···O10	0.89	1.98	2.848(3)	164
	N1—H1B···O8^{i}	0.89	1.85	2.635(2)	147
	O6—H6A···O4	0.82	1.75	2.517(2)	155
	N4—H4C···O12^{ii}	0.89	1.96	2.831(3)	165
	N4—H4D···O10^{iii}	0.89	1.96	2.815(2)	161
	C20—H20···F2	0.97	2.17	2.837(3)	125
	O11—H11A···O9^{iv}	0.85	1.97	2.817(4)	179
	O11A—H11C···O9^{iv}	0.85	1.96	2.808(16)	174
	O12—H12A···O7^{v}	0.82	2.06	2.877(3)	174
	O12—H12B···O7^{i}	0.82	2.08	2.840(3)	153

	O13—H13A···O10	0.82	1.91	2.662(5)	151
	O13—H13B···O10^{vi}	0.86	1.96	2.774(5)	156
3	C3—H3A···F1	0.97	2.17	2.864(5)	127
	N1—H1C···O8^{i}	0.89	1.94	2.821(5)	170
	N1—H1D···O4^{ii}	0.89	1.80	2.656(4)	162
	O2—H2···O1	0.82	1.77	2.529(4)	153
	O6—H6A···O5	0.85	1.91	2.742(4)	166
	O7—H7A···O8^{iii}	0.85	1.95	2.769(4)	160
	O7—H7B···O4^{iv}	0.85	1.98	2.830(5)	176
	O8—H8A···O6	0.85	1.92	2.736(5)	161
	O8—H8B···O7^{v}	0.85	2.36	2.887(6)	121
4	N1—H1C···O9^{i}	0.89	1.96	2.794 (3)	155
	N1—H1D···O4^{iii}	0.89	1.87	2.755 (3)	177
	O2—H2···O1	0.82	1.69	2.455 (3)	155
	O5—H5···O8	0.82	1.67	2.464 (2)	162
	O7—H7A···O3^{ii}	0.82	1.75	2.575 (3)	178
5	O10—H10B···O5^{i}	0.82	2.04	2.826 (5)	161
	O10—H10A···O1^{ii}	0.82	1.99	2.789 (5)	166
	O9—H9···O7	0.82	1.83	2.574 (4)	150
	O8—H8···O10	0.82	1.76	2.571 (4)	168
	O6—H6···O5	0.82	1.88	2.587 (1)	144
	O2—H2···O7^{ii}	0.82	2.46	2.871 (5)	112
	O2—H2···O1	0.82	1.82	2.567 (4)	150
	N1—H1B···O4^{iii}	0.89	1.86	2.740 (3)	170
	N1—H1A···O3^{iv}	0.89	1.85	2.742 (1)	179

Symmetry codes for **1**: (i) −*x*+1/2, *y*+1/2, −*z*+1/2; (ii) −*x*+1/2, −*y*+1/2, −*z*+1. For **2**: (i) *x*−1, *y*, *z*; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*, *y*, *z*+1; (iv) −*x*+1, −*y*+1, −*z*; (v) −*x*+2, −*y*+1, −*z*; (vi) −*x*+1, −*y*+2, −*z*. For **3**: (i) −*x*, −*y*+2, −*z*+1; (ii) −*x*, −*y*+2, −*z*+1; (iii) *x*, *y*−1, *z*; (iv) −*x*, −*y*+1, −*z*; (v) −*x*+1, −*y*+1, −*z*. For **4**: (i) *x*+1, *y*, *z*; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) −*x*+2, −*y*+1, −*z*. For **5**: (i) −*x*, −*y*+1, −*z*+1; (ii) −*x*, −*y*+1, −*z*+1; (iii) −*x*, −*y*, −*z*+1; (iv) *x*+1, *y*−1, *z*.