Supporting Information

Investigations on the Solubility of Vortioxetine Based on X-ray Structural Data and Crystal Contacts

Contents:

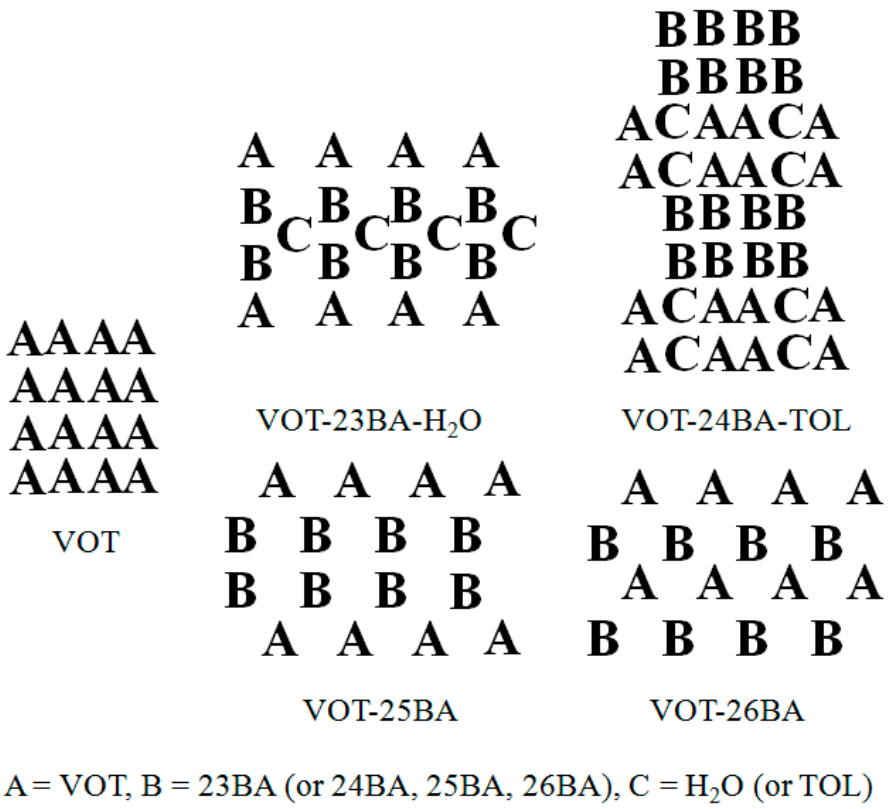

Figure S1. The different space stacked structure of VOT, VOT-23BA-H_2O, VOT-24BA-TOL, VOT-25BA and VOT-26BA salts.

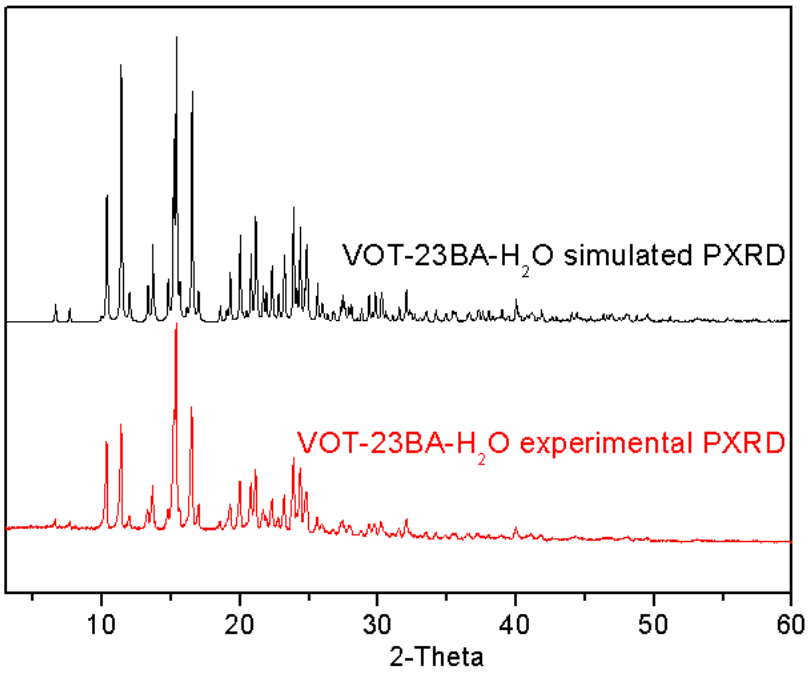

Figure S2. Experimental (red) and simulated (black) PXRD patterns for VOT-23BA-H_2O salt.

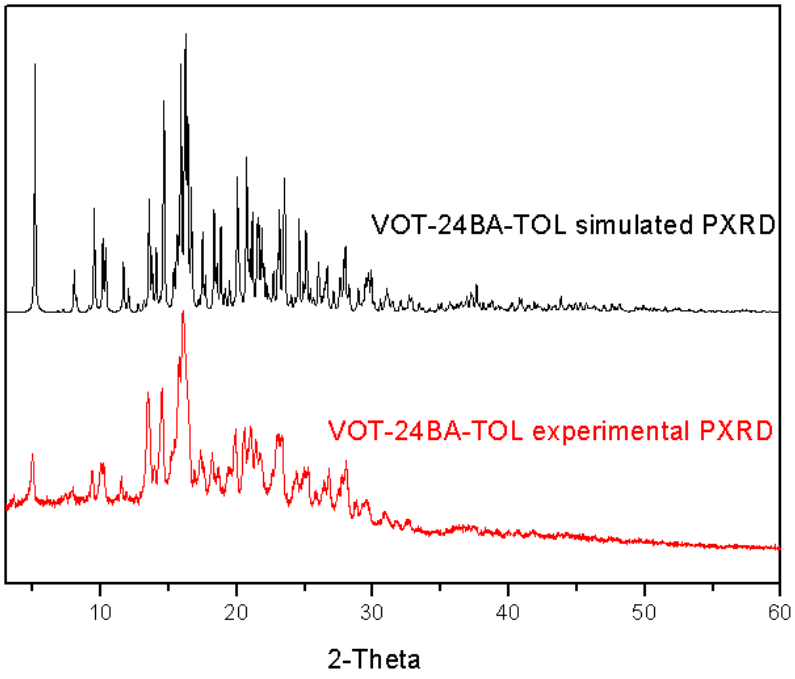

Figure S3. Experimental (red) and simulated (black) PXRD patterns for VOT-24BA-TOL salt.

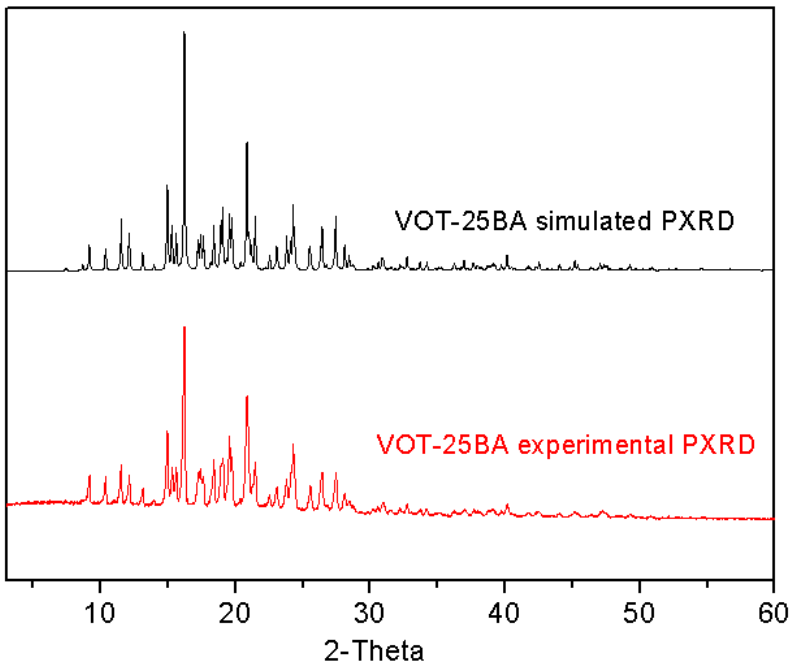

Figure S4. Experimental (red) and simulated (black) PXRD patterns for VOT-25BA salt.

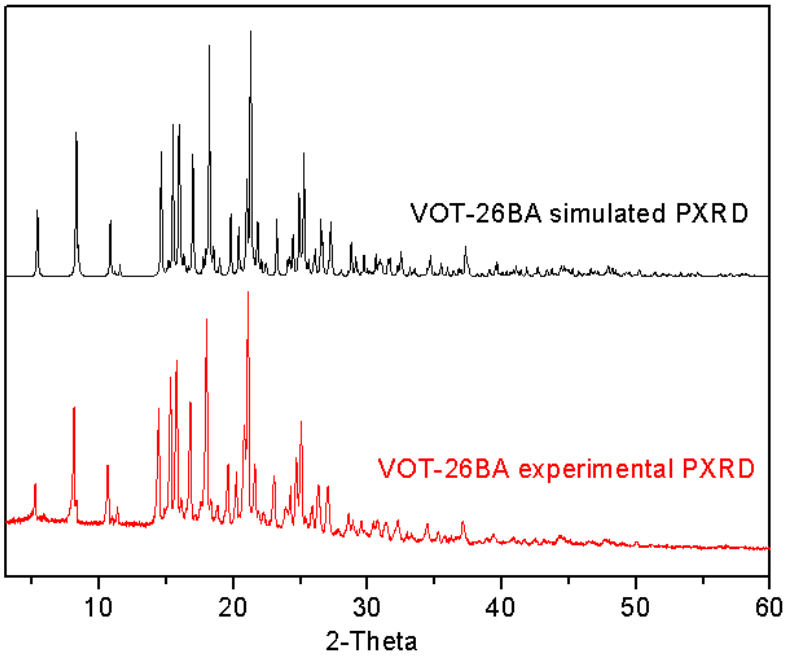

Figure S5. Experimental (red) and simulated (black) PXRD patterns for VOT-26BA salt.

Table S1. The major PXRD peaks (2θ) for VOT, VOT-23BA-H_2O, VOT-24BA-TOL, VOT-25BA and VOT-26BA salts.

Number	2θ (VOT)	2θ (VOT-23BA-H_2O)	2θ (VOT-24BA-TOL)	2θ (VOT-25BA)	2θ (VOT-26BA)
1	11.60	6.64	5.18	9.18	5.24
2	12.34	7.68	8.06	10.40	8.12
3	12.80	10.36	9.56	11.50	10.62
4	14.32	11.40	10.18	12.14	11.34
5	15.12	12.00	11.70	13.14	14.42
6	16.84	13.34	12.06	14.96	15.30
7	17.40	13.68	13.58	15.32	15.76
8	18.62	15.38	14.46	15.62	16.78
9	19.64	16.52	16.08	16.18	17.98
10	20.48	17.00	17.28	17.28	18.80
11	21.50	18.58	18.22	18.42	19.60
12	22.48	19.30	19.92	19.06	20.22
13	22.96	20.02	20.58	19.58	21.10
14	24.38	20.80	20.98	20.86	21.60
15	25.66	21.14	21.40	21.46	23.04
16	26.18	21.70	22.98	24.32	23.90
17		22.32			24.24
18		22.80			24.70
19		23.24			25.04
20		23.88			25.88
21		24.36			26.34
22		24.82			

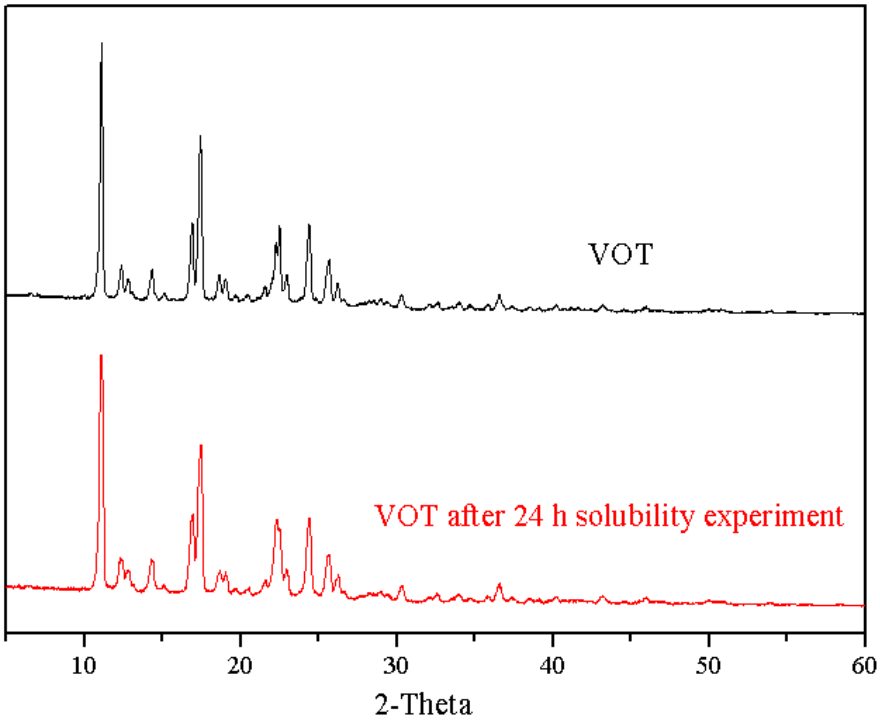

Figure S6. PXRD analysis of the residual materials of VOT after 24h solubility in aqueous medium.

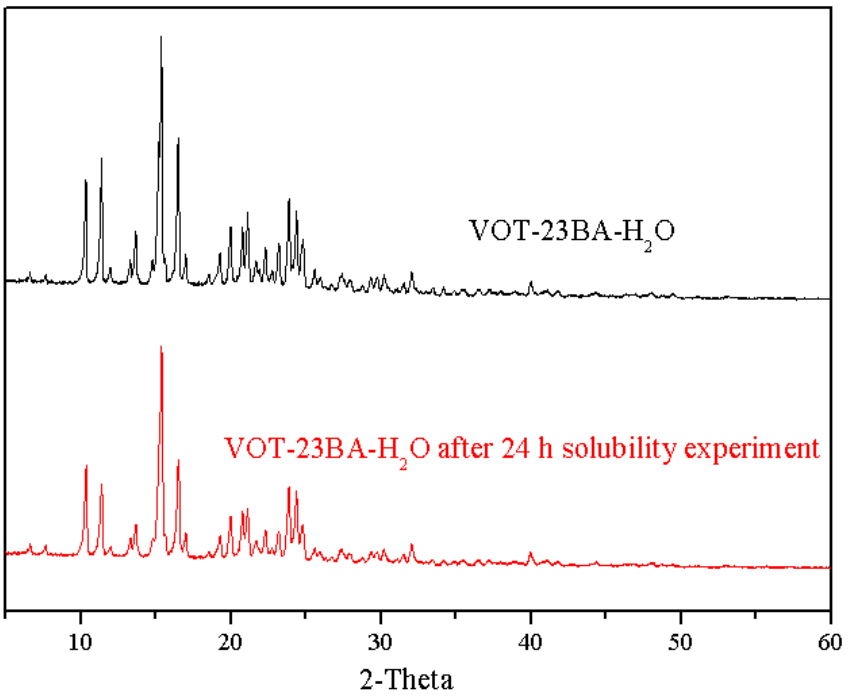

Figure S7. PXRD analysis of the residual materials of VOT-23BA-H_2O after 24h solubility in aqueous medium.

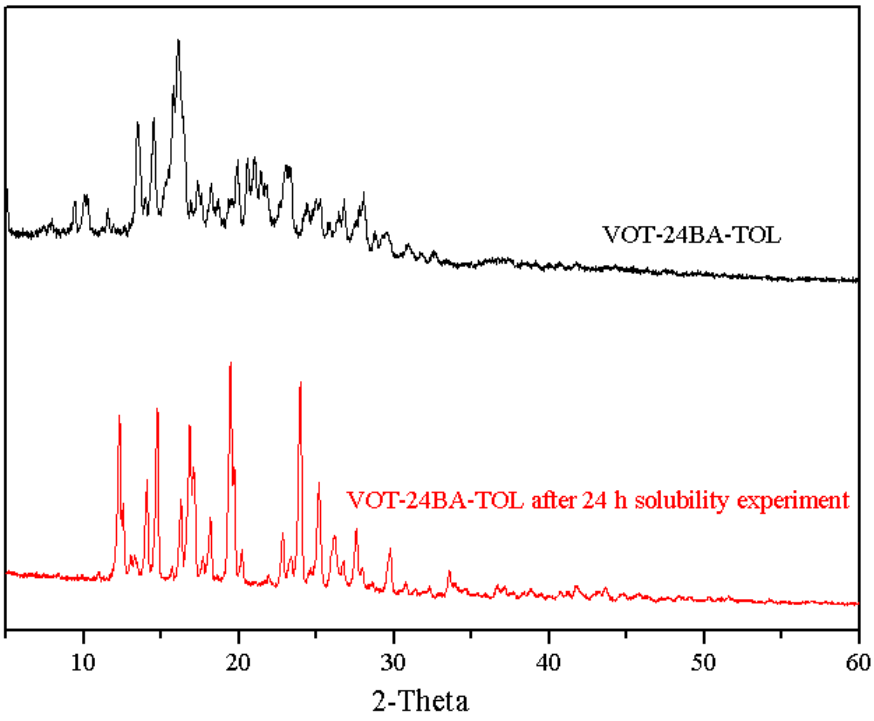

Figure S8. PXRD analysis of the residual materials of VOT-24BA-TOL after 24h solubility in aqueous medium.

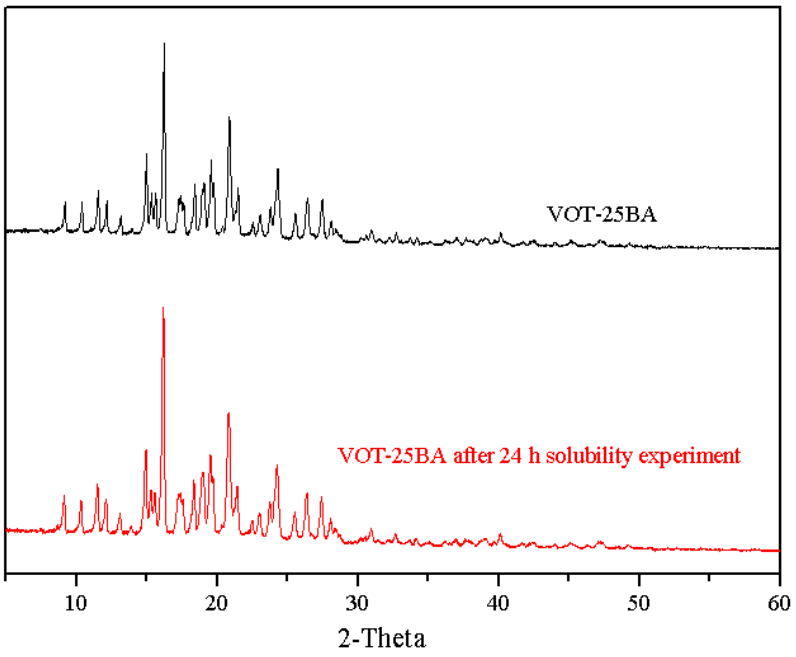

Figure S9. PXRD analysis of the residual materials of VOT-25BA after 24h solubility in aqueous medium.

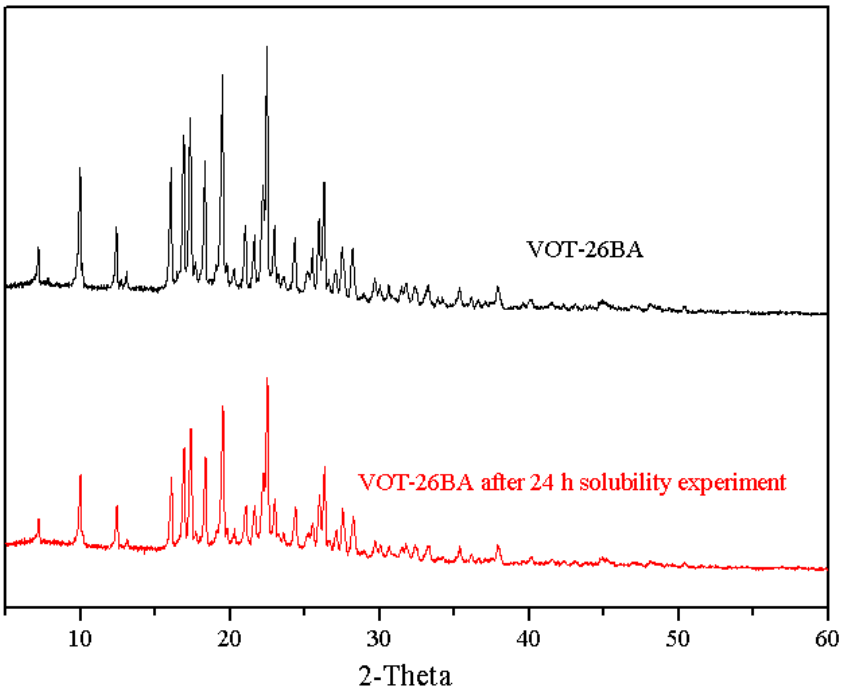

Figure S10. PXRD analysis of the residual materials of VOT-26BA after 24h solubility in aqueous medium.

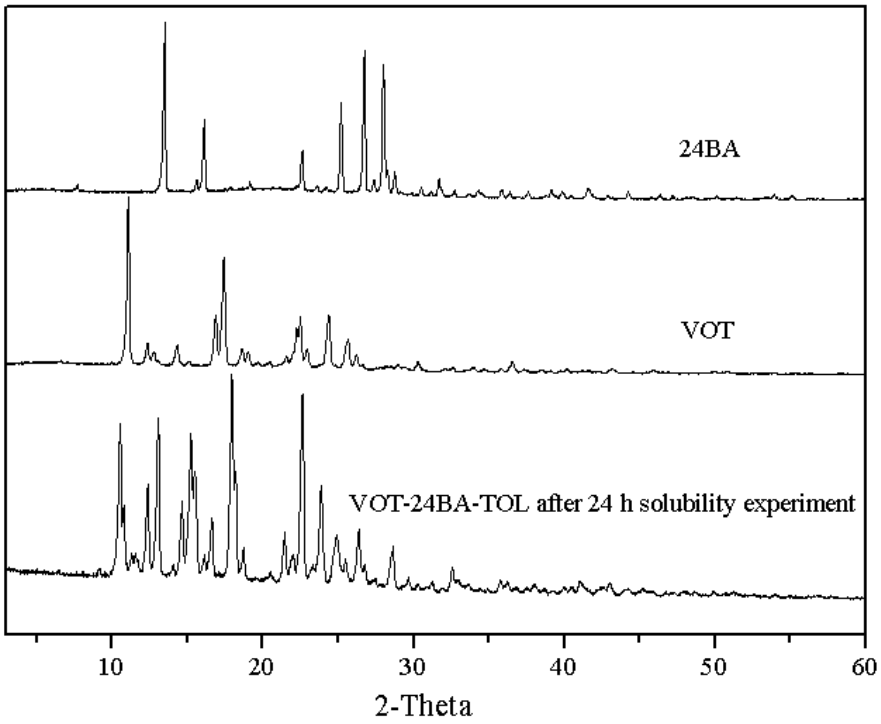

Figure S11. The comparison diagram of the residual materials of VOT-24BA-TOL after 24h solubility with the patterns of former compounds (VOT and 24BA).

Table S2. The major PXRD peaks (2θ) for the residual materials of VOT-24BA-TOL, VOT and 24BA.

Number	2θ (VOT)	2θ (24BA)	2θ (the residual materials of VOT-24BA-TOL)
1	11.60	7.70	12.28
2	12.34	13.50	14.04
3	12.80	16.12	14.70
4	14.32	22.62	16.22
5	15.12	25.22	16.82
6	16.84	26.76	17.08
7	17.40	27.96	18.16
8	18.62	28.78	19.42
9	19.64		20.18
10	20.48		22.82
11	21.50		23.94
12	22.48		25.18
13	22.96		26.14
14	24.38		27.58
15	25.66		29.70
16	26.18		