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Supporting Information

Pharmaceutical salt and salt hydrates of vortioxetine with sulfonic acid to ameliorate the solubility and hygroscopicity through charge-assisted hydrogen bond assembly

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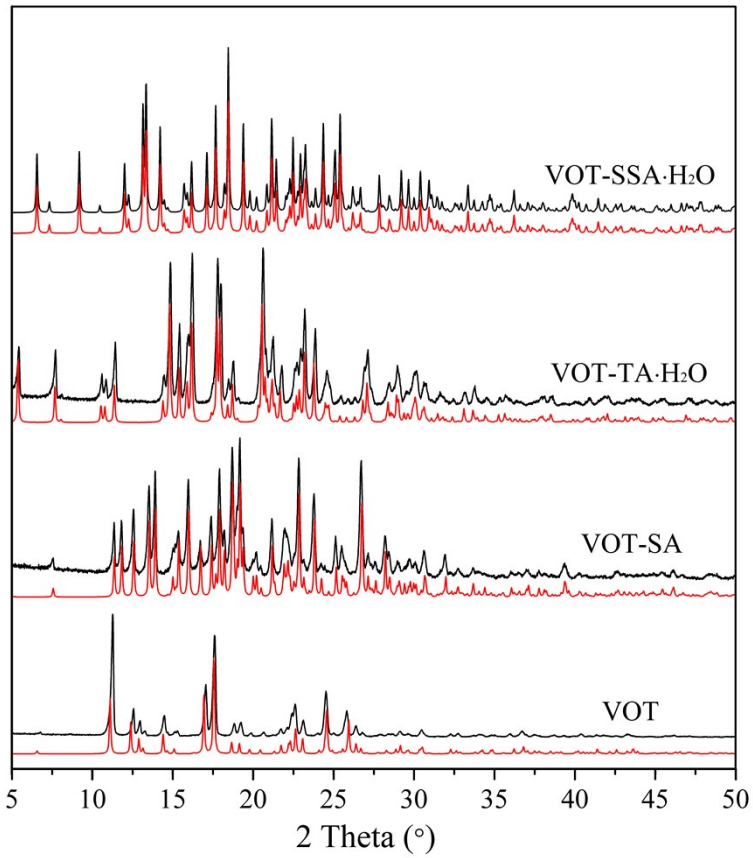

Fig. S1 Overlay of experimental (black) PXRD patterns and the simulated (red) PXRD patterns generated from the single crystal diffraction data.

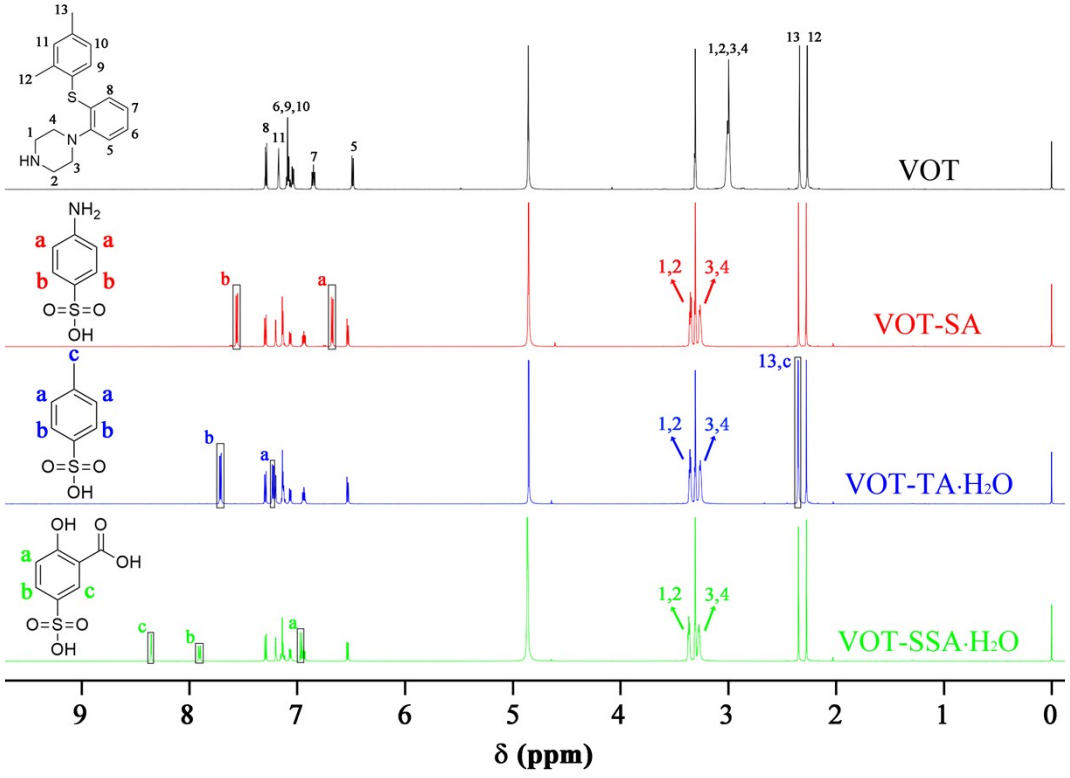

Fig. S2 The ^{1}H-NMR spectra of the VOT and its salts.

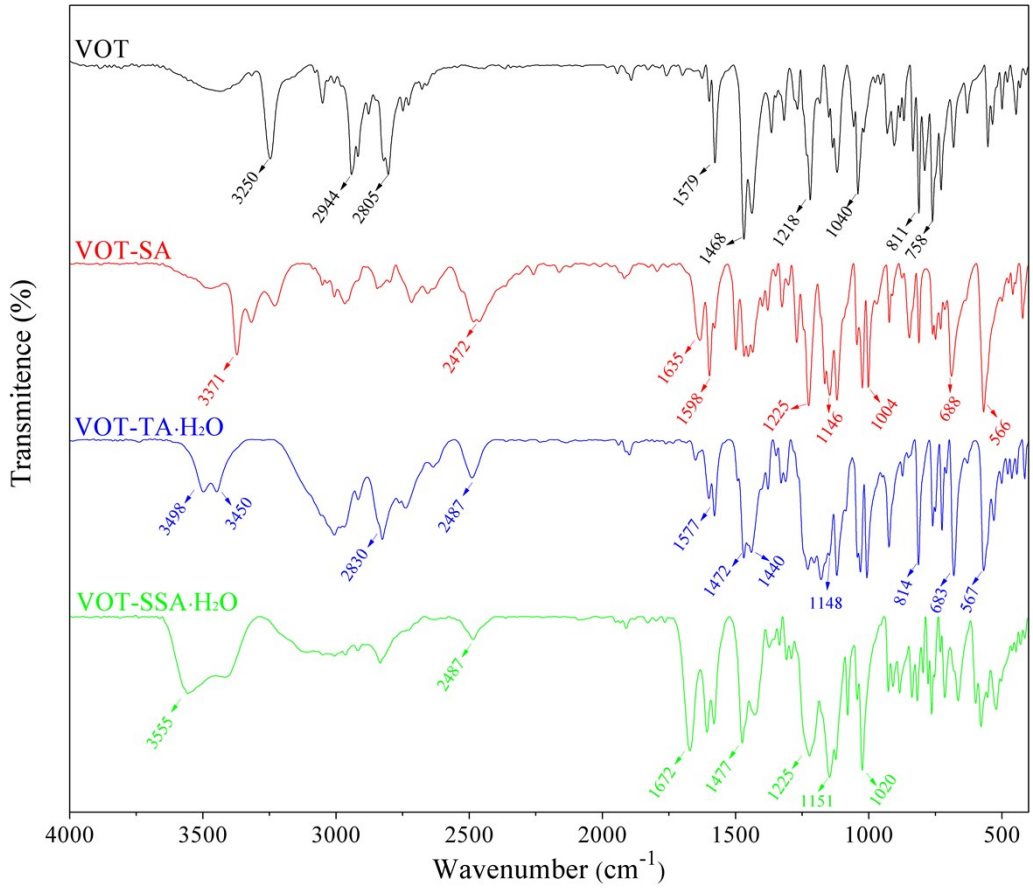

Fig. S3 The FT-IR spectrum of the VOT and its salts.

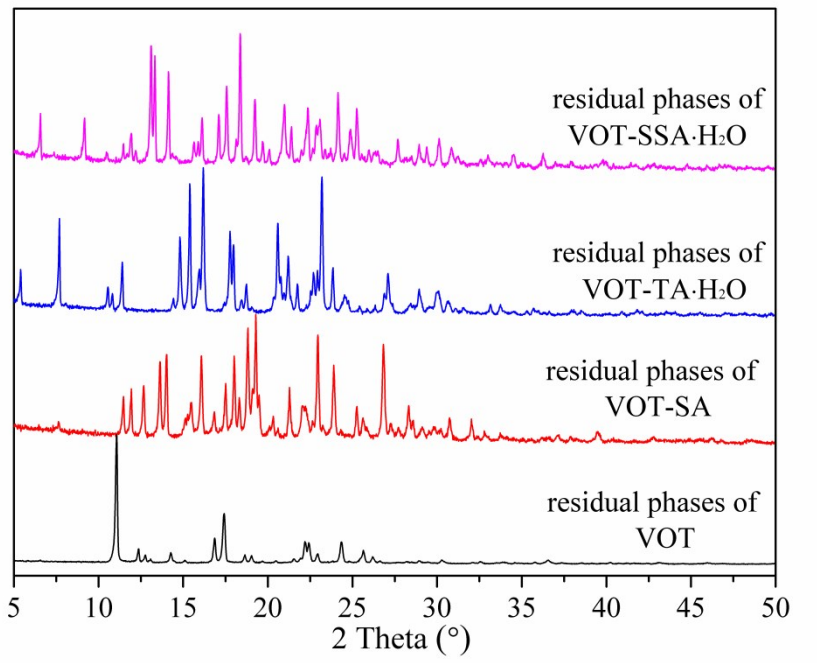

Fig. S4 The PXRD patterns of the residual phases after solubility experiments for VOT and its salts.

Table S1 The hydrogen bond metrics of VOT salts.

D-H···A	d(D-H)(Å)	d(H···A)(Å)	d(D···A)(Å)	∠DHA(°)	symmetry code
			VOT-SA		
N1B-H1BC···O3B	0.97	1.76	2.730(12)	177.5	
N1B-H1BD···N3B	0.97	1.91	2.881(14)	175.6	[x+1/2, -y+1/2, z]
N3A-H3AC···O1A	1.06(10)	2.12(11)	3.074(14)	149(8)	[x+1/2, -y+1/2, z]
N3A-H3AD···O1B	0.81(10)	2.49(10)	3.215(13)	150(9)	[x, y+1, z]
N3B-H3BC···O2A	0.98(12)	2.24(12)	3.199(13)	165(10)	
N3B-H3BD···O2B	1.02(10)	2.15(10)	3.017(13)	142(7)	[x-1/2, -y-1/2, z]
N1A-H1AC···N3A	0.97(3)	1.97(4)	2.923(15)	167(12)	[x-1/2, -y+3/2, z]
N1A-H1AD···O3A	0.97(3)	1.8(2)	2.674(13)	156(46)	
			VOT-TA·H_2O		
N1-H1C···O2	0.91(3)	2.01(3)	2.837(3)	151(2)	[x-1/2, -y-1/2, z-1/2]
N1-H1D···O3	0.86(3)	2.01(3)	2.861(3)	171(2)	[-x+2, -y, -z]
O4-H4C···O3	0.88(4)	2.00(4)	2.870(3)	170(3)	[-x+2, -y, -z]
O4-H4D···O1	0.79(3)	2.00(3)	2.782(3)	170(3)	[-x+2, -y+1, -z]
			VOT-TA		
N1A-H1AC···O1B	0.97	2.10	2.928(10)	142.3	[x+1, y, z]
N1A-H1AC···O3B	0.97	2.27	3.078(10)	139.8	[x+1, y, z]
N1A-H1AD···O1A	0.97	1.85	2.810(10)	170.2	
N1B-H1BC···O3B	0.97	1.82	2.784(9)	175.0	
N1B-H1BD···O2A	0.97	2.56	3.265(11)	129.5	
N1B-H1BD···O3A	0.97	1.87	2.789(10)	156.7	
			VOT-SSA·H_2O		
N2-H2C···O5	0.84(2)	2.16(3)	2.877(2)	143(2)	[x, y+1, z]
N2-H2C···O7	0.84(2)	2.51(2)	3.033(2)	121.5(19)	[-x+1, -y+2, -z+2]
N2-H2D···O7	0.90(2)	1.96(2)	2.845(2)	169(2)	
O1-H1···O4	0.88(3)	1.75(3)	2.6155(19)	166(3)	[-x, -y+1, -z+2]
O3-H3···O2	0.87(3)	1.87(3)	2.641(2)	148(2)	
O3-H3···O6	0.87(3)	2.57(2)	3.016(2)	113(2)	[-x+1, -y+1, -z+2]
O7-H7A···O4	0.84(3)	2.45(3)	3.105(2)	135(2)	[x+1, y+1, z]
O7-H7A···O6	0.84(3)	2.56(3)	3.374(2)	162(2)	[x+1, y+1, z]
O7-H7B···O6	0.83(3)	2.04(3)	2.861(2)	169(3)	[-x+1, -y+1, -z+2]