

Mechanism of solvent-mediated polymorphic transformation to prepare axitinib form XLI controlled by water activity

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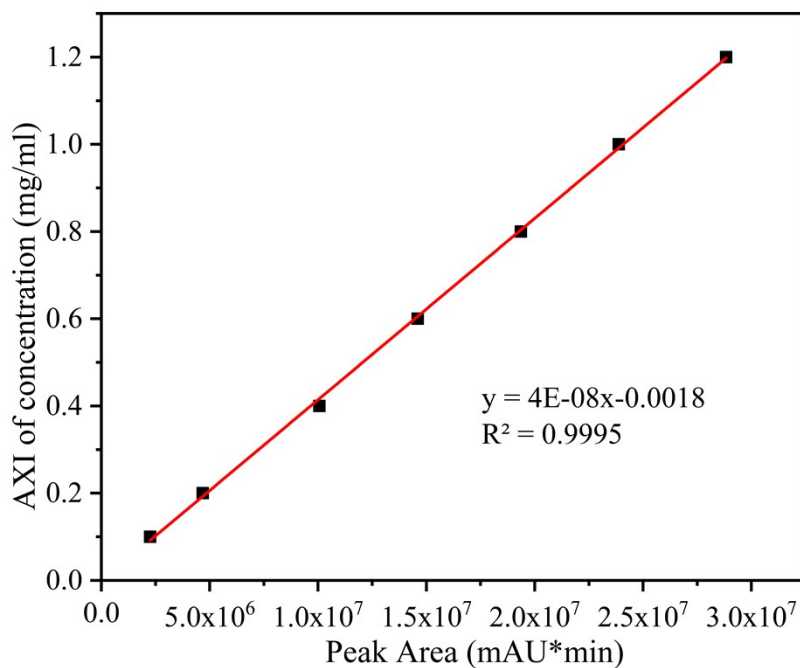
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Table S1 Experimental conditions for the SMPT process of solvated S_{DMF}

Volume fraction of water (V _W)	Volume fraction of methanol (V _M)	Molar fraction of water (X _W)	water activity(α_w)
0.00	1	0	0
0.05	0.95	0.106	0.167
0.10	0.90	0.200	0.294
0.15	0.85	0.284	0.394
0.20	0.80	0.360	0.475
0.25	0.75	0.429	0.540
0.30	0.70	0.491	0.595
0.35	0.65	0.548	0.641
0.40	0.60	0.600	0.682
0.50	0.50	0.692	0.751
0.60	0.40	0.771	0.809
0.7	0.30	0.840	0.861
0.8	0.20	0.900	0.909
0.9	0.10	0.953	0.955
1.00	0.00	1	1

Table S2 Details of experimental conditions for the S_{DMF} solvate transformation

Number	Methanol:Water (v:v)	Solid content/g	Temperature/ K	Agitation speed/rpm
1	0:10	1.6	333.15	300
2	1:9	1.6	333.15	300
3	3:7	1.6	333.15	300
4	5:5	1.6	333.15	300
5	1:9	0.4	333.15	300
6	1:9	0.8	333.15	300
7	1:9	2.4	333.15	300
8	2:8	1.6	333.15	300
9	2:8	1.6	323.15	300
10	2:8	1.6	313.15	300

**Figure S1.** The standard curve of HPLC for AXI

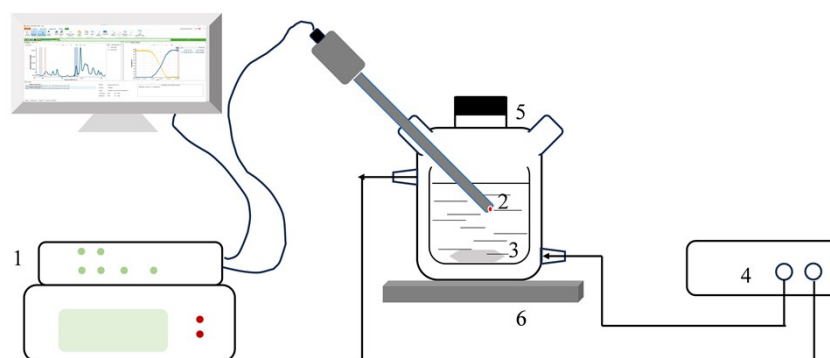


Figure S2. Diagram of the experimental setup for solvent-mediated polymorphic transformation. 1- Raman laser transmitter; 2- Raman probe; 3- Magneton; 4-Constant temperature water-bathing; 5- 100ml crystallizer; 6- Magnetic stirring

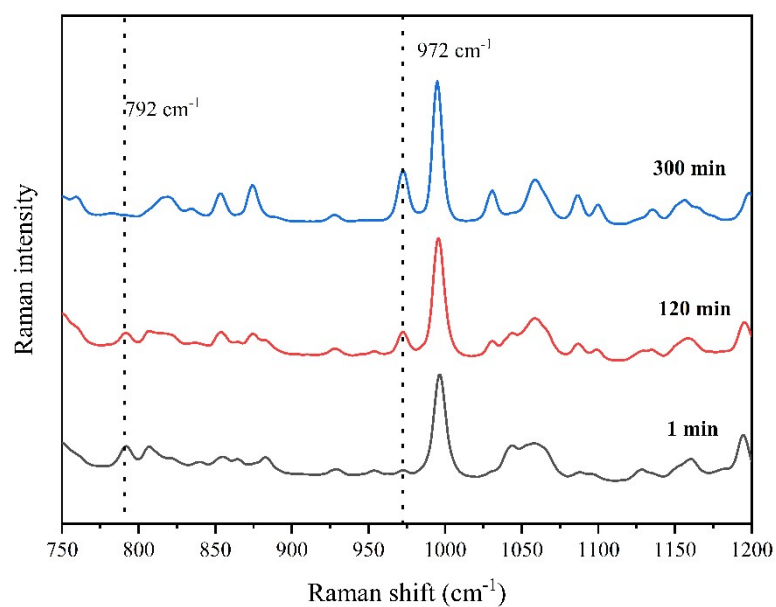


Figure S3. Raman spectra of intermittent sampling during solution-mediated