

Crystal structure, thermal crystal form transformation, desolvation process and desolvation kinetics of two novel solvates of ciclesonide

Table S1. Correlation Coefficients R^2 for HCC non-isothermal desolvation kinetics by the solid-state reaction rate model method.

Table S2. Correlation Coefficients R^2 for MC non-isothermal desolvation kinetics by the solid-state reaction rate model method.

Table S3. Correlation Coefficients for (a) HCC and (b) MC Isothermal Desolvation Kinetics by the solid-state reaction rate Model method.

Table S1. Correlation Coefficients R^2 for HCC non-isothermal desolvation kinetics by the solid-state reaction rate model method.

Model	1 K/min	2 K/min	5 K/min	10 K/min	20 K/min
P2	0.9828	0.9781	0.9817	0.956	0.9196
P3	0.9815	0.9766	0.9806	0.9533	0.9141
P4	0.9799	0.9748	0.9796	0.9504	0.908
A2	0.9499	0.9502	0.9918	0.9883	0.9793
A3	0.9416	0.9476	0.9915	0.9878	0.9783
A4	0.938	0.9447	0.9912	0.9873	0.9772
R2	0.9692	0.9688	0.9903	0.9768	0.9768
R3	0.9627	0.964	0.9916	0.9816	0.9656
D1	0.9848	0.9804	0.983	0.9597	0.927
D2	0.9765	0.9744	0.9881	0.9709	0.9463
D3	0.9639	0.965	0.9918	0.9821	0.9665
D4	0.9725	0.9714	0.9898	0.9752	0.9999
F0/R1	0.9842 ^b	0.9797 ^b	0.9826	0.9585	0.9002

F1	0.948	0.9527	0.9921 ^b	0.9888	0.9803
F2	0.8939	0.9094	0.9786	0.9922 ^b	0.9992 ^b
F3	0.8404	0.8654	0.954	0.9793	0.9948

^b Best fit model.

Table S2. Correlation Coefficients R² for MC non-isothermal desolvation kinetics by the solid-state reaction rate model method.

Model	1 K/min	2 K/min	5 K/min	20 K/min
P2	0.9649	0.9463	0.9724	0.9045
P3	0.9643	0.9453	0.9716	0.9001
P4	0.9637	0.9443	0.9706	0.8954
A2	0.9934	0.9878	0.998	0.9692
A3	0.9934	0.9877	0.998	0.9681
A4	0.9932	0.9875	0.9979	0.967
R2	0.9826	0.971	0.9893	0.9432
R3	0.987	0.9775	0.9931	0.9531
D1	0.9658	0.9478	0.9737	0.9106
D2	0.9767	0.9626	0.984	0.9315
D3	0.9871	0.9777	0.9932	0.953
D4	0.9807	0.9683	0.9877	0.9399
F0/R1	0.9655	0.9473	0.9733	0.9086
F1	0.9935	0.988	0.9881	0.9701
F2	0.9955 ^b	0.9994 ^b	0.9933 ^b	0.9968
F3	0.9818	0.9917	0.9726	0.9984 ^b

^b Best fit model.

Table S3. Correlaion Coefficients for (a) HCC and (b) MC Isothermal Desolvation Kinetics by the solid-state reaction rate Model method.

Model	HCC(a)				MC(b)	
	80°C	85°C	90°C	110°C	115°C	120°C
P2	0.8579	0.8616	0.9066	0.9611	0.9586	0.9325

P3	0.8289	0.8337	0.8835	0.9432	0.9404	0.9104
P4	0.8132	0.8186	0.8705	0.9327	0.9298	0.8979
A2 ^b	0.9743	0.9745	0.9862	0.9989	0.9993	0.9966
A3	0.9698	0.9525	0.9723	0.9985	0.9955	0.9865
A4	0.9695	0.9386	0.9626	0.9983	0.9905	0.9783
R2	0.9801	0.9802	0.9884	0.9981 ^b	0.9986 ^b	0.9996 ^b
R3	0.9910 ^b	0.9910 ^b	0.9933 ^b	0.9923	0.9935	0.9993
D1	0.9879	0.9875	0.9871	0.9858	0.9872	0.9964
D2	0.9992	0.9987	0.9869	0.9587	0.9621	0.9819
D3	0.9845	0.9852	0.9666	0.9011	0.9070	0.9378
D4	0.9977	0.9977	0.9825	0.9417	0.9460	0.9699
F0/R1	0.9247	0.9263	0.9552	0.9929	0.9914	0.9776
F1	0.9988	0.9996	0.9927	0.9678	0.9706	0.9856
F2	0.918	0.9229	0.9106	0.8060	0.8141	0.8498
F3	0.7619	0.7655	0.7599	0.6036	0.6166	0.659

^b Best fit model.