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supplementary

COMF: Comprehensive Model-Fitting Method for Simulating Isothermal and Single-Step Solid-State Reactions

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In every case we have fitted the conversion fraction with polynomials of the form:

$$P_n(t) = \sum_{i=0}^{n} a_i t^i \tag{S1}$$

These polynomials were used instead of the experimental data when the reaction speed was fitted.

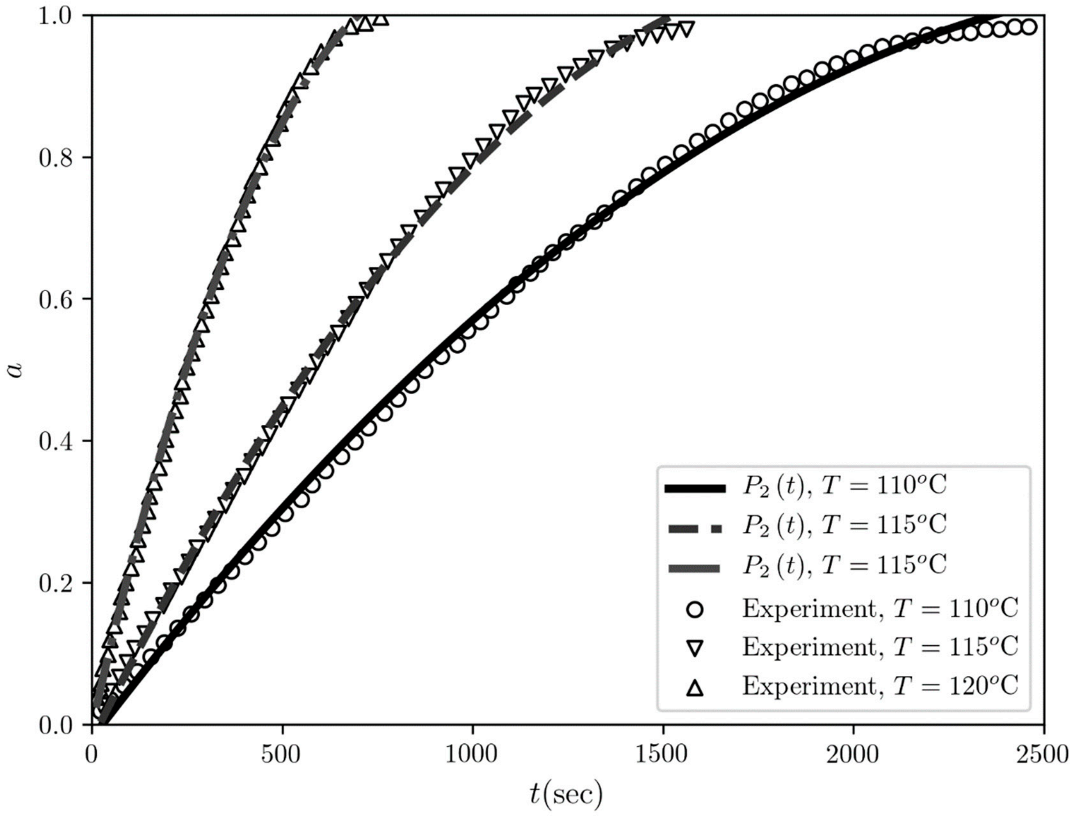

Figure S1. The experimentally measured conversion fractions along with the corresponding polynomial fits used instead of the experimental data for fitting the reaction speed in the case of the desolvation of methanol solvates of ciclesonide. All the polynomials are of 2nd degree.

Table S1. The coefficients for the polynomial fit of the conversion fraction at each temperature in the case of the desolvation of methanol solvates of ciclesonide.

Polynomial Coefficients	$T=110^{o}C$	$T=115^{o}C$	$T=120^{o}C$
a_0	$-1.1621\cdot10^{-7}$	$-2.6357\cdot10^{-7}$	$-1.3448\cdot10^{-6}$
a_1	$7.0594\cdot10^{-4}$	$1.0720\cdot10^{-3}$	$2.3754\cdot10^{-3}$
a_2	$-2.0015\cdot10^{-2}$	$-2.2583\cdot10^{-2}$	$-4.1471\cdot10^{-3}$

Table S2. The calculated determination coefficients and Euclidean distances calculated via the COMF method for all the tested models in the case of the desolvation of methanol solvates of ciclesonide at 110 °C.The superscript b indicates the BCM in each case.

Model	R_g^2	R_a^2	R_f^2	$d\left(R_a^2,R_g^2,R_f^2\right)$
A2	0.9663	0.9652	−0.2621	1.2630
A3	0.6500	0.8667	−5.3148	6.3259
A4	−0.0077	0.7778	−15.8244	16.8560
D1	0.9535	0.9189	−2656.3573	2657.3573
D2	0.8987	0.8552	−4874.1900	4875.1900
D3	0.7661	−6.3536	−1198.9002	1199.9228
D4	0.8597	0.9158	−1340.0000	1336.2892
F0	0.9431	0.9431	−0.1080	1.1109
F1	0.8758	0.9544	0.2561	0.7556
F2	0.4596	0.8303	−3.0535	4.0929
F3	0.2749	0.7098	−3.5093	4.5764
P2	0.3069	0.3848	−8.1151	9.1621
P3	−0.9637	−0.2200	−21.8074	22.9243
P4	−2.8404	−0.7092	−41.3798	42.5877
R2	0.9945*b*	0.9958*b*	0.9425*b*	0.0579*b*
R3	0.9743	0.9859	0.7867	0.2153

Table S3. The Arrhenius rate constants for each model calculated by fitting the conversion fraction itself and the integral reaction rate in the case of the desolvation of methanol solvates of ciclesonide at 110 °C.

Model	k_a	k_g
A2	0.0543	0.0513
A3	0.0548	0.0453
A4	0.0556	0.0428
D1	0.0223	0.0242
D2	0.0216	0.0203
D3	0.0017	0.0097
D4	0.0056	0.0058
F0	0.0287	0.0287
F1	0.0564	0.0793
F2	0.0973	0.5973
F3	0.1000	10.0000
P2	0.0291	0.0321
P3	0.0282	0.0334
P4	0.0275	0.0342
R2	0.0211	0.0218
R3	0.0155	0.0173

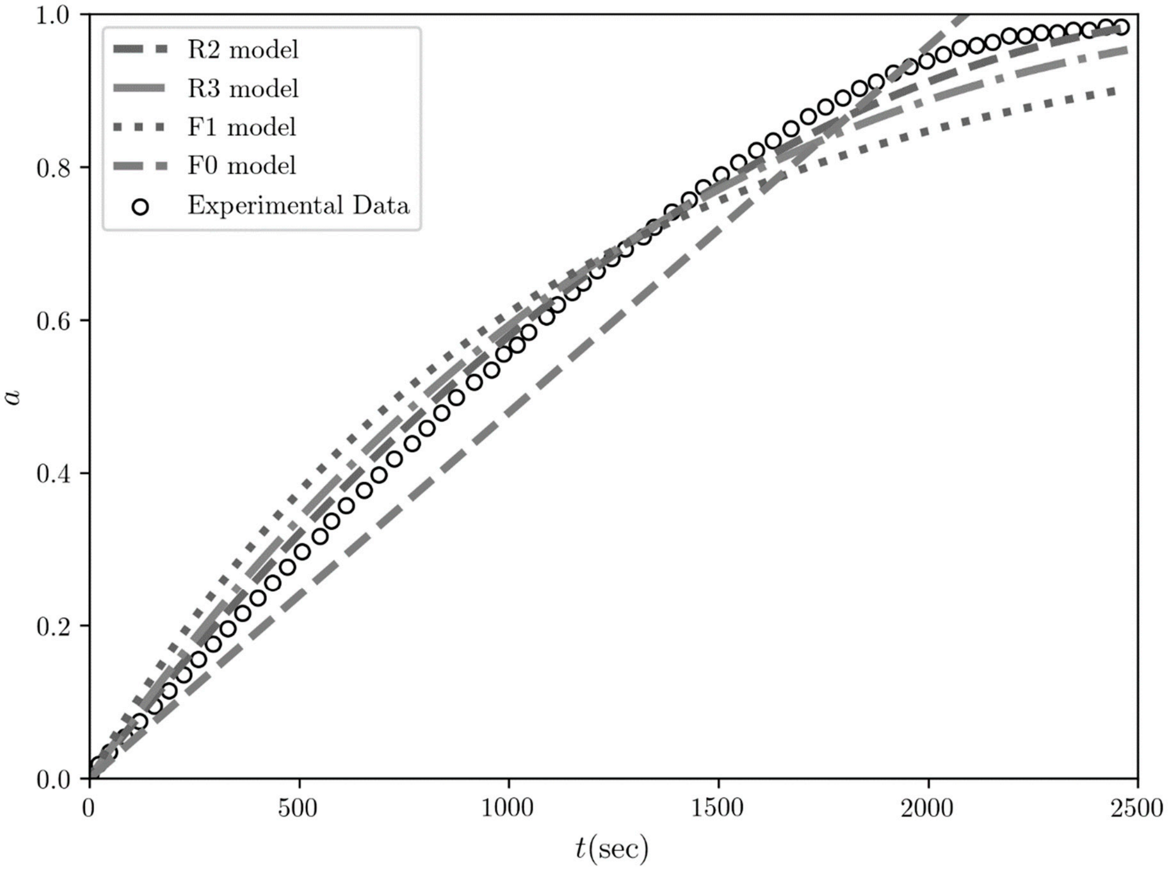

Figure S2. The conversion fraction time evolution regarding the desolvation of methanol solvates of ciclesonide at 110 °C for the first four highly ranked solid-state reaction kinetics models.

Table S4. The calculated determination coefficients and Euclidean distances calculated via the COMF method for all the tested models in the case of the desolvation of methanol solvates of ciclesonide at 115 °C. The superscript b indicates the BCM in each case.

Model	R_g^2	R_a^2	R_f^2	$d\left(R_a^2, R_g^2, R_f^2\right)$
A2	0.9509	0.9565	−0.4502	1.4517
A3	0.5279	0.8349	−6.5056	7.5223
A4	−0.3367	0.7256	−19.1669	20.2130
D1	0.9407	0.8979	−378.3201	379.3201
D2	0.8807	0.8453	−537.5531	538.5531
D3	0.7495	0.9408	−175.7421	176.7423
D4	0.8416	0.9016	−164.6580	165.6581
F0	0.9526	0.9526	−0.1453	1.1473
F1	0.8807	0.9528	0.1453	0.8642
F2	0.4551	0.7748	−1.6390	2.7041
F3	0.2457	0.4806	−2.9279	4.0333
P2	0.2194	0.3723	−9.5523	10.5997
P3	−1.3835	−0.2603	−25.5092	26.6460
P4	−3.8410	−0.7606	−48.0887	49.3583
R2	0.9942*b*	0.9950*b*	0.9103*b*	0.0900*b*
R3	0.9739	0.9846	0.7194	0.2822

Table S5. The Arrhenius rate constants for each model calculated by fitting the conversion fraction itself and the integral reaction rate in the case of the desolvation of methanol solvates of ciclesonide at 115 °C.

Model	k_a	k_g
A2	0.0839	0.0785
A3	0.0855	0.0713
A4	0.0873	0.0682
D1	0.0327	0.0364
D2	0.0274	0.0296
D3	0.0025	0.0133
D4	0.0045	0.0082
F0	0.0450	0.0450
F1	0.0830	0.1124
F2	0.1000	0.6496
F3	0.1000	9.4716
P2	0.0462	0.0517
P3	0.0447	0.0545
P4	0.0435	0.0560
R2	0.0319	0.0330
R3	0.0233	0.0258

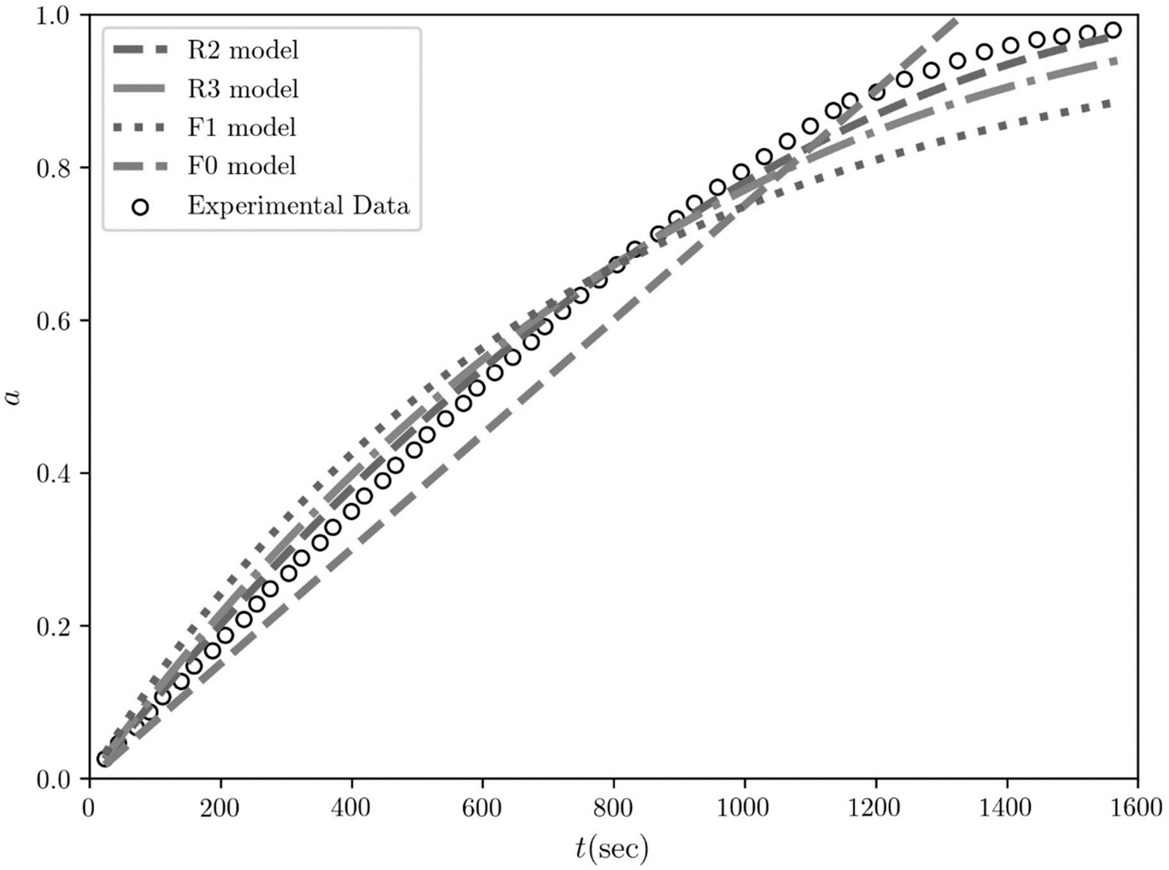

Figure S3. The conversion fraction time evolution regarding the desolvation of methanol solvates of ciclesonide at 115 °C for the first four highly ranked solid-state reaction kinetics models.

Table S6. The calculated determination coefficients and Euclidean distances calculated via the COMF method for all the tested models in the case of the desolvation of methanol solvates of ciclesonide at 120 °C. The superscript b indicates the BCM in each case.

Model	R_g^2	R_a^2	R_f^2	$d\left(R_a^2, R_g^2, R_f^2\right)$
A2	0.9354	−0.0817	−0.1841	1.6051
A3	0.4642	−0.5713	0.1377	1.8707
A4	−0.5245	−0.9191	−0.8163	3.0505
D1	0.9480	0.9109	−19.4976	20.4978
D2	0.8833	0.8500	−37.7209	38.7214
D3	0.6947	0.9507	−9.2607	10.2653
D4	0.8325	0.8972	−6.5939	7.5965
F0	0.9259	0.9254	−0.2159	1.2204
F1	0.8080	0.5234	−1.1662	2.2263
F2	0.1893	0.0965	−2.9477	4.1302
F3	−0.0189	−0.2355	−3.9523	5.2048
P2	−0.0057	0.1717	−8.5505	9.6390
P3	−1.9851	−0.6183	−22.7878	24.0289
P4	−5.0014	−1.2256	−41.3065	42.7880
R2	0.9964*b*	0.9981*b*	0.9569*b*	0.0433*b*
R3	0.9693	0.9908	0.8091	0.1936

Table S7. The Arrhenius rate constants for each model calculated by fitting the conversion fraction itself and the integral reaction rate in the case of the desolvation of methanol solvates of ciclesonide at 120 °C.

Model	k_a	k_g
A2	0.1000	0.1803
A3	0.1000	0.1630
A4	0.1000	0.1561
D1	0.0724	0.0804
D2	0.0329	0.0655
D3	0.0056	0.0311
D4	0.0164	0.0184
F0	0.1000	0.1011
F1	0.1000	0.2669
F2	0.1000	3.5759
F3	0.1000	10.0000
P2	0.1000	0.1172
P3	0.0965	0.1240
P4	0.0924	0.1277
R2	0.0722	0.0743
R3	0.0526	0.0584

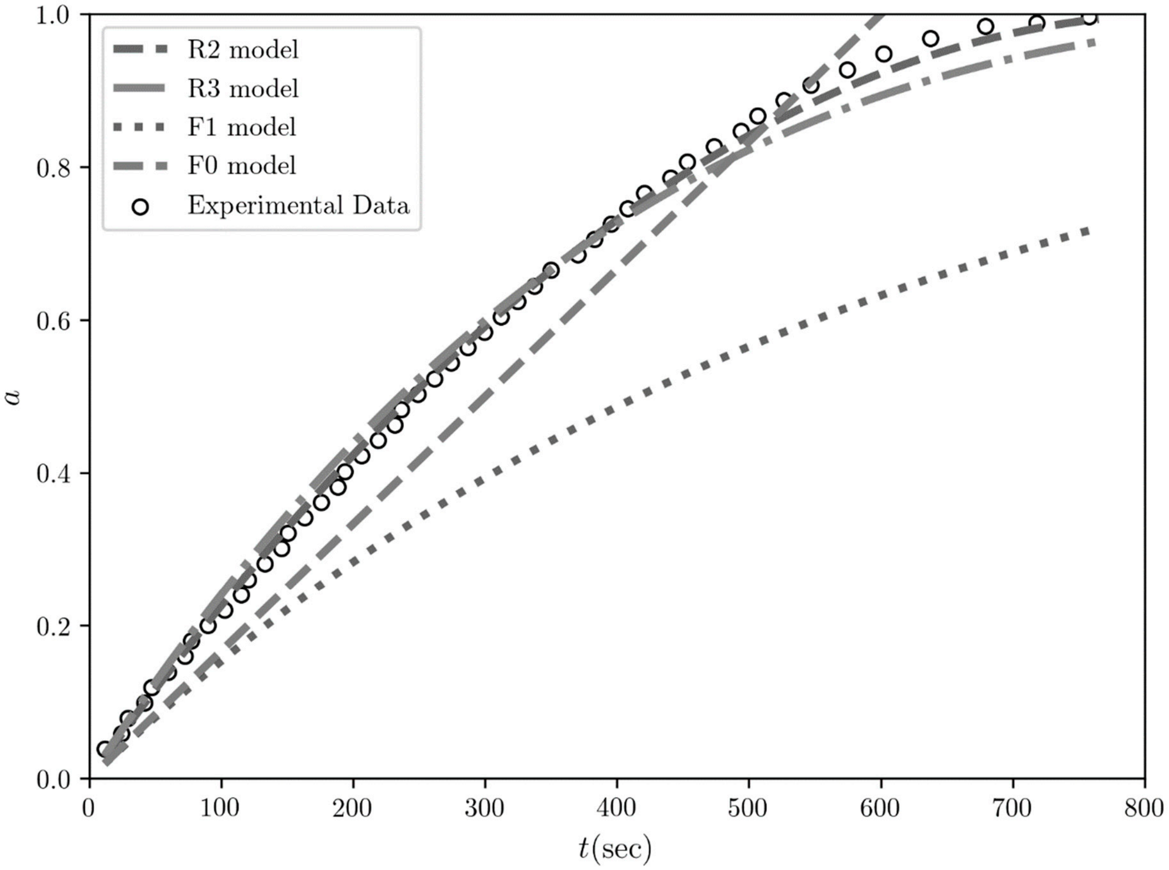

Figure S4. The conversion fraction time evolution regarding the desolvation of methanol solvates of ciclesonide at 120 °C for the first four highly ranked solid-state reaction kinetics models.

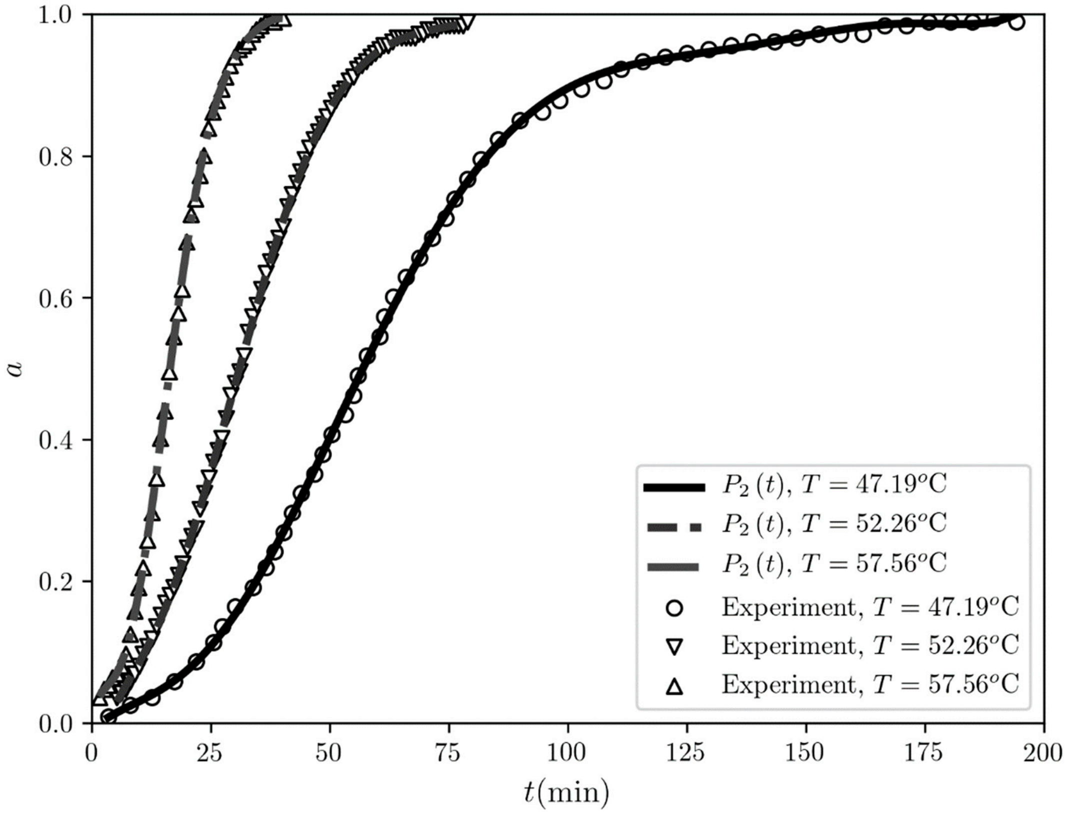

Figure S5. The experimentally measured conversion fractions along with the corresponding polynomial fits used instead of the experimental data for fitting the reaction speed in the case of the desolvation of tetrahydrofuran solvates of sulfameter. All the polynomials are of 7th degree.

Table S8. The coefficients for the polynomial fit of the conversion fraction at each temperature in the case of the desolvation of methanol solvates of ciclesonide.

Polynomial Coefficients	$T = 47.19^{o} C$	$T = 52.26^{o} C$	$T = 57.56^{o} C$
a_0	$1.0987 \cdot 10^{-4}$	$6.3735 \cdot 10^{-13}$	$1.3135 \cdot 10^{-10}$
a_1	$-7.9100 \cdot 10^{-12}$	$-2.5992 \cdot 10^{-10}$	$-2.5449 \cdot 10^{-8}$
a_2	$2.2119 \cdot 10^{-9}$	$4.1580 \cdot 10^{-8}$	$1.9370 \cdot 10^{-6}$
a_3	$-2.9522 \cdot 10^{-7}$	$-3.2409 \cdot 10^{-6}$	$-7.2071 \cdot 10^{-5}$
a_4	$1.7970 \cdot 10^{-5}$	$1.2179 \cdot 10^{-4}$	$1.2907 \cdot 10^{-3}$
a_5	$-3.4394 \cdot 10^{-4}$	$-1.8681 \cdot 10^{-3}$	$-8.7771 \cdot 10^{-3}$
a_6	$5.8830 \cdot 10^{-3}$	$2.3970 \cdot 10^{-2}$	$3.2466 \cdot 10^{-2}$
a_7	$-9.4793 \cdot 10^{-3}$	$-6.0624 \cdot 10^{-2}$	$2.1170 \cdot 10^{-3}$

Table S9. The calculated determination coefficients and Euclidean distances calculated via the COMF method for all the tested models in the case of the desolvation of tetrahydrofuran solvates of sulfameter at 47.19 °C. The superscript b indicates the BCM in each case.

Model	R_g^2	R_a^2	R_f^2	$d\left(R_a^2, R_g^2, R_f^2\right)$
A2	0.9553	0.9967*b*	0.9270*b*	0.0857*b*

A3	0.6763	0.9790	0.5410	0.5621
A4	0.1205	0.9401	−0.7909	1.9961
D1	0.8885	0.8255	−9160.9528	9161.9528
D2	0.9002	0.8617	−8125.0876	8126.0876
D3	0.8565	0.8571	−4022.1314	4023.1314
D4	0.8964	0.9662	−3899.1707	3900.1707
F0	0.7936	0.7936	−0.1113	1.1490
F1	0.9214	0.8803	0.2260	0.7872
F2	0.4338	0.7173	−1.0845	2.1785
F3	0.1598	0.5753	−4.7483	5.8249
P2	0.1407	−0.0355	−2.2815	3.5467
P3	−1.0664	−0.7823	−5.6033	7.1450
P4	−2.8235	−1.3013	−10.1701	12.0286
R2	0.9401	0.9426	0.5417	0.4658
R3	0.9575*b*	0.9261	0.4676	0.5392

Table S10. The Arrhenius rate constants for each model calculated by fitting the conversion fraction itself and the integral reaction rate in the case of the desolvation of tetrahydrofuran solvates of sulfameter at 47.19 °C.

Model	k_a	k_g
A2	0.0147	0.0129
A3	0.0152	0.0110
A4	0.0155	0.0102
D1	0.0056	0.0061
D2	0.0065	0.0054
D3	0.0004	0.0029
D4	0.0001	0.0016
F0	0.0068	0.0068
F1	0.0143	0.0225
F2	0.0241	0.2965
F3	0.0415	10.0000
P2	0.0065	0.0074
P3	0.0061	0.0077
P4	0.0059	0.0078
R2	0.0055	0.0055
R3	0.0040	0.0045

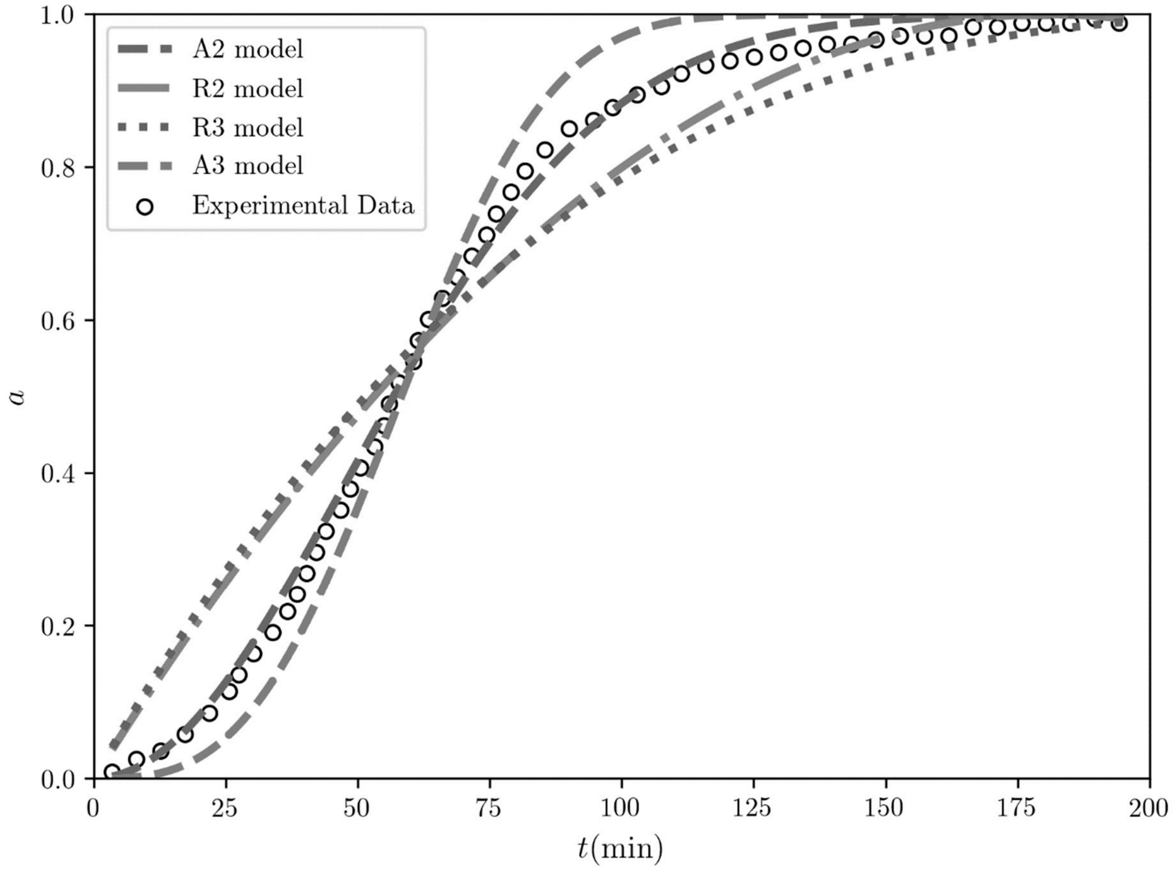

Figure S6. The conversion fraction time evolution regarding the desolvation of tetrahydrofuran solvates of sulfameter at 47.19 °C for the first four highly ranked solid-state reaction kinetics models.

Table S11. The calculated determination coefficients and Euclidean distances calculated via the COMF method for all the tested models in the case of the desolvation of tetrahydrofuran solvates of sulfameter at 52.26 °C. The superscript b indicates the BCM in each case.

Model	R_g^2	R_a^2	R_f^2	$d\left(R_a^2, R_g^2, R_f^2\right)$
A2	0.9959*b*	0.9985*b*	0.9577*b*	0.0425*b*
A3	0.8679	0.9738	0.4973	0.5204
A4	0.4977	0.9268	−1.3271	2.3818
D1	0.8960	0.7999	−11.8994	12.9013
D2	0.8626	0.8128	−22.0115	23.0127
D3	0.7720	0.8528	−5.2232	6.2292
D4	0.8378	0.8935	−4.8977	5.9009
F0	0.9332	0.9332	−0.0617	1.0659
F1	0.8600	0.8581	−0.0250	1.0442
F2	0.4895	0.6862	−1.7469	2.8115
F3	0.2741	0.5423	−5.8877	6.9410
P2	0.5970	0.5014	−3.3463	4.3934
P3	−0.2562	−0.0695	−9.2313	10.3635
P4	−1.6323	−0.5617	−17.5611	18.8118
R2	0.9560	0.9373	0.5021	0.5037
R3	0.9384	0.9136	0.3569	0.6517

Table S12. The Arrhenius rate constants for each model calculated by fitting the conversion fraction itself and the integral reaction rate in the case of the desolvation of tetrahydrofuran solvates of sulfameter at 52.26 °C.

Model	k_a	k_g
A2	0.0275	0.0276
A3	0.0277	0.0239
A4	0.0281	0.0224
D1	0.0116	0.0131
D2	0.0178	0.0114
D3	0.0009	0.0057
D4	0.0036	0.0033
F0	0.0150	0.0150
F1	0.0283	0.0454
F2	0.0473	0.4026
F3	0.0805	9.5222
P2	0.0153	0.0165
P3	0.0148	0.0172
P4	0.0144	0.0175
R2	0.0108	0.0118
R3	0.0079	0.0095

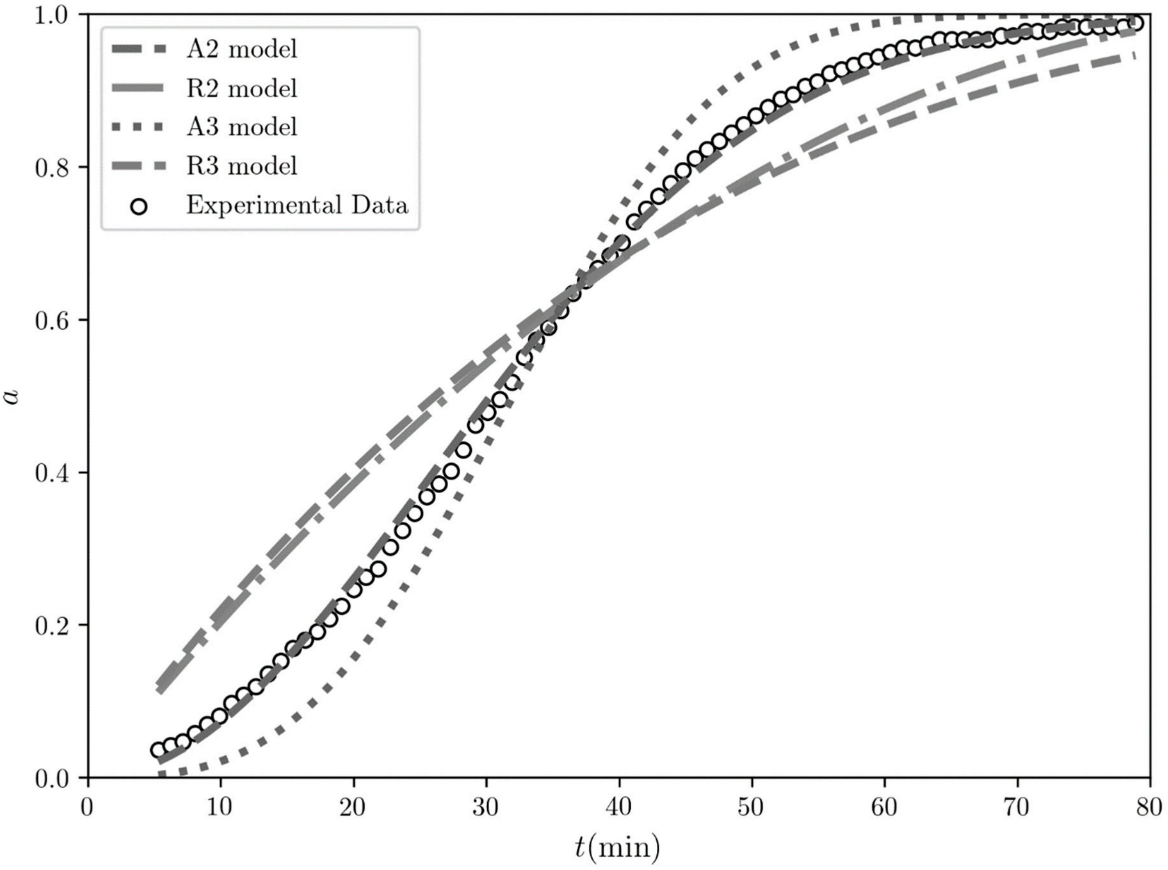

Figure S7. The conversion fraction time evolution regarding the desolvation of tetrahydrofuran solvates of sulfameter at 52.26 °C for the first four highly ranked solid-state reaction kinetics models.

Table S13. The calculated determination coefficients and Euclidean distances calculated via the COMF method for all the tested models in the case of the desolvation of tetrahydrofuran solvates of sulfameter at 57.56 °C. The superscript b indicates the BCM in each case.

Model	R_g^2	R_a^2	R_f^2	$d\left(R_a^2, R_g^2, R_f^2\right)$
A2	0.9911*b*	0.9939*b*	0.8523*b*	0.1481*b*
A3	0.9278	0.9880	0.7385	0.2715
A4	0.6554	0.9559	−0.3584	1.4021
D1	0.8881	0.7826	−16.0762	17.0779
D2	0.8531	0.8125	−25.9141	26.9151
D3	0.7416	0.8357	−7.0684	8.0742
D4	0.8247	0.8854	−6.7801	7.7830
F0	0.9401	0.9401	−0.0606	1.0640
F1	0.8139	0.8460	−0.4283	1.4485
F2	0.3395	0.6898	−2.3316	3.4106
F3	−0.0405	0.5265	−3.1658	4.3198
P2	0.7272	0.6257	−2.4013	3.4327
P3	0.0984	0.1650	−6.9422	8.0367
P4	−0.9619	−0.2420	−13.4196	14.6054
R2	0.9466	0.9226	0.1843	0.8211
R3	0.9224	0.8987	0.0044	1.0037

Table S14. The Arrhenius rate constants for each model calculated by fitting the conversion fraction itself and the integral reaction rate in the case of the desolvation of tetrahydrofuran solvates of sulfameter at 57.56 °C.

Model	k_a	k_g
A2	0.0521	0.0553
A3	0.0525	0.0474
A4	0.0532	0.0441
D1	0.0220	0.0256
D2	0.0277	0.0224
D3	0.0017	0.0120
D4	0.0061	0.0065
F0	0.0291	0.0291
F1	0.0532	0.0949
F2	0.0867	1.3829
F3	0.1000	10.0000
P2	0.0298	0.0321
P3	0.0289	0.0334
P4	0.0282	0.0342
R2	0.0205	0.0232
R3	0.0150	0.0190

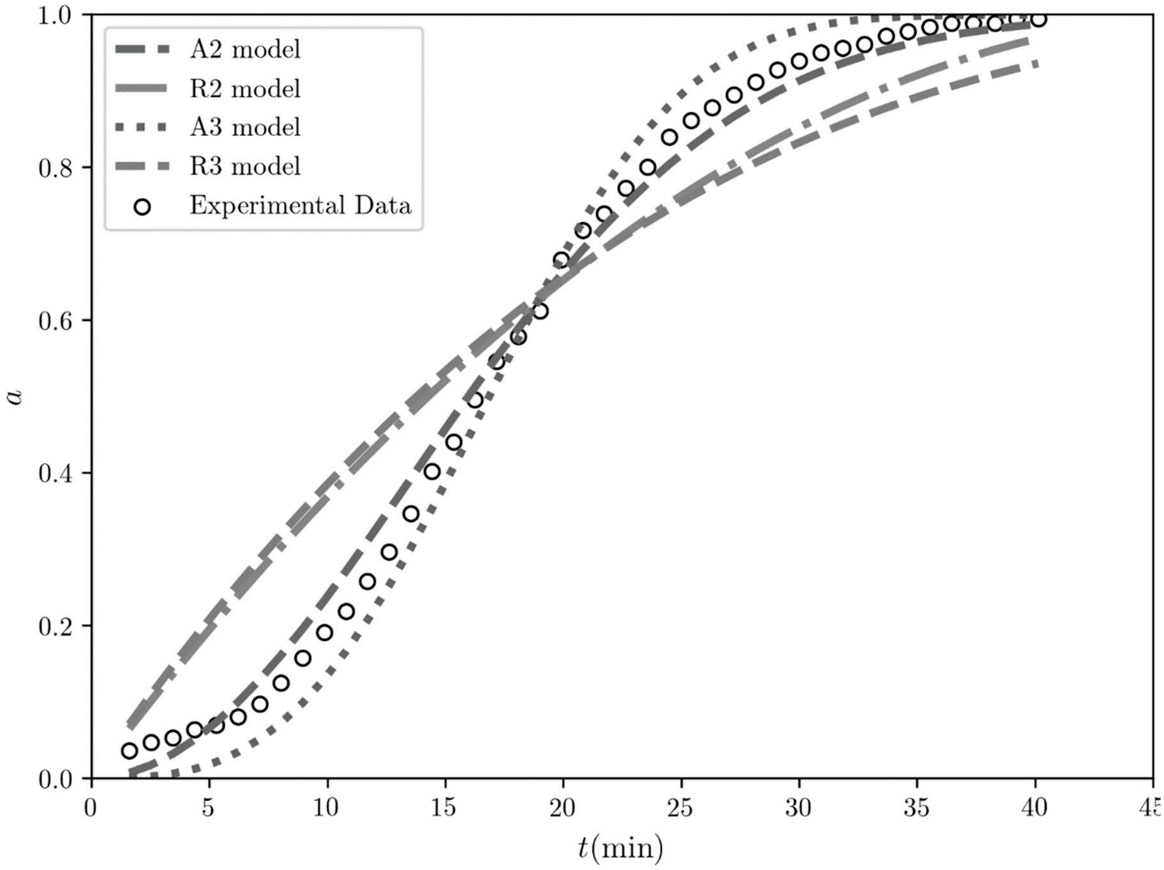

Figure S8. The conversion fraction time evolution regarding the desolvation of tetrahydrofuran solvates of sulfameter at 57.56 °C for the first four highly ranked solid-state reaction kinetics models.