Table 1. Thermal data as well as the constants which are needed to calculate the activities of different solid forms[1-3]

Solid form	(kJ/mol)$\Delta_{fus}H_m$	(K)T_{fus}	$q\ (J/(K\ mol))$	$r\ (J/(K^2 mol))$
m-ABA, form I	35.51	445.19	146.5	-0.3502
m-ABA, form II	26.74	451.13	128.1	-0.3090
m-HBA, form I	35.83	474.23	160.1	-0.421
m-HBA, form II	32.68	467.49	149.8	-0.393
Etiracetam, form I	31.98	385.44	56.1104	0.715
Etiracetam, form II	31.16	392.39	68.87682	0.562

Table 2. Activity coefficients of m-ABA in two solvents along the two solubility curves

	acetonitrile				**ethyl acetate**			
***T*/K**	$x_{m-ABA,I}$	$\gamma_{m-ABA,I}$	$x_{m-ABA,II}$	$\gamma_{m-ABA,II}$	$x_{m-ABA,I}$	$\gamma_{m-ABA,I}$	$x_{m-ABA,II}$	$\gamma_{m-ABA,II}$
273.15	-	-	-	-	-	-	0.0123	5.51
278.15	-	-	0.0042	17.29	-	-	0.0134	5.43
283.15	0.0016	15.88	0.005	15.60	0.0043	5.92	0.0152	5.12
288.15	0.0018	15.94	0.006	13.97	0.0049	5.86	0.0168	5.00
293.15	0.0021	15.43	0.007	12.87	0.0056	5.78	0.0187	4.83
298.15	0.0028	13.07	0.0081	11.96	0.0067	5.46	0.0211	4.60
303.15	0.0034	12.12	-	-	0.0083	4.97	0.0229	4.55
308.15	0.0045	10.31	-	-	0.0097	4.77	-	-
313.15	0.0056	9.32	-	-	0.0117	4.46	-	-
318.15	0.0067	8.78	-	-	0.0136	4.32	-	-
323.15	0.0083	7.96	-	-	0.0165	4.00	-	-

Table 3. Activity coefficients of m-HBA in acetonitrile or ethyl acetate along the two solubility curves

	acetonitrile				**ethyl acetate**			
***T*/K**	$x_{m-HBA,I}$	$\gamma_{m-HBA,I}$	$x_{m-HBA,II}$	$\gamma_{m-HBA,II}$	$x_{m-HBA,I}$	$\gamma_{m-HBA,I}$	$x_{m-HBA,II}$	$\gamma_{m-HBA,II}$
283.15	0.0071	3.75	0.0090	4.34	0.0396	0.67	0.0517	0.75
288.15	0.0082	3.57	0.0103	4.12	0.0431	0.68	0.0550	0.77
293.15	0.0096	3.37	0.0119	3.88	0.0468	0.69	0.0591	0.78
298.15	0.0111	3.20	0.0139	3.64	0.0507	0.70	0.0642	0.79
303.15	0.0132	2.97	0.0161	3.42	0.0556	0.70	0.0693	0.80
308.15	0.0154	2.80	0.0189	3.18	0.0602	0.72	0.0753	0.80
313.15	0.0179	2.65	0.0219	3.00	0.0658	0.72	0.0814	0.81
318.15	0.0201	2.59	0.0255	2.81	0.0717	0.73	0.0885	0.81
323.15	0.0231	2.48	0.0294	2.66	0.0773	0.74	0.0958	0.82

Table 4. Activity coefficients of m-HBA in acetic acid or acetone along the two solubility curves

	acetic acid				**acetone**			
***T*/K**	$x_{m-HBA,I}$	$\gamma_{m-HBA,I}$	$x_{m-HBA,II}$	$\gamma_{m-HBA,II}$	$x_{m-HBA,I}$	$\gamma_{m-HBA,I}$	$x_{m-HBA,II}$	$\gamma_{m-HBA,II}$
283.15	0.0220	1.21	0.0291	1.34	0.1006	0.27	0.1188	0.33
288.15	0.0244	1.20	0.0311	1.36	0.1058	0.28	0.1240	0.34
293.15	0.0273	1.19	0.0341	1.36	0.1117	0.29	0.1298	0.36
298.15	0.0303	1.18	0.0375	1.35	0.1173	0.30	0.1369	0.37
303.15	0.0335	1.17	0.0415	1.33	0.1241	0.32	0.1446	0.38
308.15	0.0376	1.15	0.0459	1.31	0.1309	0.33	0.1527	0.39
313.15	0.0415	1.14	0.0511	1.29	0.1386	0.34	0.1608	0.41
318.15	0.0462	1.13	0.0561	1.28	0.1451	0.36	0.1702	0.42
323.15	0.0512	1.12	0.0614	1.27	0.1532	0.37	0.1815	0.43

Table 5. Activity coefficients of m-HBA in water or 1-propanol along the two solubility curves

	water				1-propanol			
***T*/K**	$x_{m-HBA,I}$	$\gamma_{m-HBA,I}$	$x_{m-HBA,II}$	$\gamma_{m-HBA,II}$	$x_{m-HBA,I}$	$\gamma_{m-HBA,I}$	$x_{m-HBA,II}$	$\gamma_{m-HBA,II}$
283.15	0.0005	51.12	0.0007	53.13	0.0880	0.30	0.0997	0.39
288.15	0.0006	45.78	0.0009	46.98	0.0914	0.32	0.1051	0.40
293.15	0.0008	40.74	0.0011	43.19	0.0956	0.34	0.1091	0.42
298.15	0.0010	36.08	0.0014	37.29	0.1009	0.35	-	-
303.15	0.0012	32.29	0.0017	33.06	0.1073	0.37	-	-
308.15	0.0015	28.42	0.0020	29.47	0.1127	0.38	-	-
313.15	0.0019	24.90	0.0027	24.62	0.1191	0.40	-	-
318.15	0.0023	22.28	0.0031	23.03	0.1258	0.41	-	-
323.15	0.0029	19.48	0.0039	19.88	0.1330	0.43	-	-

Table 6. Activity coefficients of etiracetam in methanol along the two solubility curves

***T*/K**	$x_{Etiracetam,I}$	$\gamma_{Etiracetam,I}$	$x_{Etiracetam,II}$	$\gamma_{Etiracetam,II}$
263.15	0.0227	1.02	0.0322	0.81
269.15	0.0322	0.88	-	-
270.15	-	-	0.0371	0.87
270.65	0.0346	0.86	0.0397	0.83
273.15	0.0356	0.91	0.0397	0.89
273.65	0.0371	0.89	0.0423	0.85
277.15	0.0423	0.88	0.0477	0.84
283.15	0.0529	0.86	0.0561	0.86
283.65	0.0532	0.87	0.0561	0.87
287.15	0.0590	0.89	0.0651	0.83
293.15	0.0743	0.86	0.0780	0.83
303.15	0.1023	0.87	0.0995	0.88

Table 7. Fitting of activity coefficients from the solubility curve of each form of polymorphic compounds. $\%AARD_{I}^{NRTL}$ *and* $\%AARD_{I}^{Wilson}$: fitting NRTL and Wilson respectively to the activity coefficients along the solubility curve of the more stable form; $\%AARD_{II}^{NRTL}$ *and* $\%AARD_{II}^{Wilson}$: fitting NRTL and Wilson respectively to the activity coefficients along the solubility curve of the less stable form

Solute	**Solvent**	Deviation of fitting models to the activity coefficients along the solubility curve of the stable form		Deviation of fitting models to the activity coefficients along the solubility curve of the metastable form	
		$\%AARD_{I}^{NRTL}$	$\%AARD_{I}^{Wilson}$	$\%AARD_{II}^{NRTL}$	$\%AARD_{II}^{Wilson}$
m-ABA	Acetonitrile	2.35	2.13	0.62	0.57
	Ethyl acetate	1.26	3.92	0.58	0.73
m-HBA	Acetonitrile	0.69	0.73	0.19	0.22
	Ethyl acetate	0.18	0.26	0.19	0.42
	Acetic acid	0.17	1.45	0.41	0.58
	Acetone	0.26	0.28	0.61	0.54
	Water	1.97	0.36	0.73	0.98
	1-Propanol	0.33	0.43	-	-
Etiracetam	Methanol	2.80	2.11	2.20	2.13

Table 8. Prediction of the activity coefficients along the solubility curve of the less stable polymorph and simultaneous fitting of the activity coefficients along both solubility curves. ($\%AARD_{II}^{NRTL}$ *and* $\%AARD_{II}^{Wilson}$: deviations in prediction of the activity coefficients using respectively NRTL and Wilson; $\%AARD_{I,II}^{NRTL}$ *and* $\%AARD_{I,II}^{Wilson}$: deviations in fitting NRTL and Wilson respectively to the activity coefficients along both solubility curves)

Solute	**Solvent**	Deviations of models in prediction of activity coefficients from the metastable form solubility data		Deviations of models in simultaneous fitting of activity coefficients from the solubility curves of both forms	
		$\%AARD_{II}^{NRTL}$	$\%AARD_{II}^{Wilson}$	$\%AARD_{I,II}^{NRTL}$	$\%AARD_{I,II}^{Wilson}$
m-ABA	Acetonitrile	38.07	36.02	3.40	9.12
	Ethyl acetate	28.68	1.78	3.81	2.62
m-HBA	Acetonitrile	19.55	21.72	2.72	7.86
	Ethyl acetate	14.99	9.90	0.90	4.87
	Acetic acid	14.33	11.73	6.06	6.20
	Acetone	11.20	11.65	6.08	5.25
	Water	3.96	10.63	6.43	4.80
	1-Propanol	20.63	16.80	2.60	4.52
Etiracetam	Methanol	4.12	4.34	2.83	2.86

References:

1. M. Svärd, F. L. Nordström, T. Jasnobulka and Å. C. Rasmuson, *Cryst. Growth Des.* 2010, **10**, 195.
2. M. Svärd and Å. C. Rasmuson, *Cryst. Growth Des.* 2013, **12**, 1140.
3. C. Herman, T. Leyssens, V. Vermylen, V. Halloin and B. Haut, *J. Chem. Thermody.* 2011, **43**, 677.