Supporting information

Solubility modeling, solution thermodynamics and preferential solvation of hymecromone in binary solvent mixtures of *N*,*N*-dimethylformamide + (methanol, ethanol and *n*-propanol)

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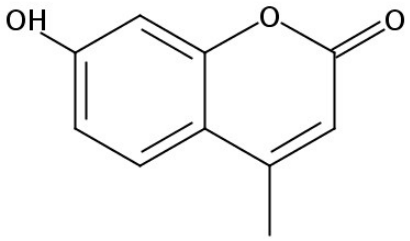

Fig. S1. Chemical structure of hymecromone.

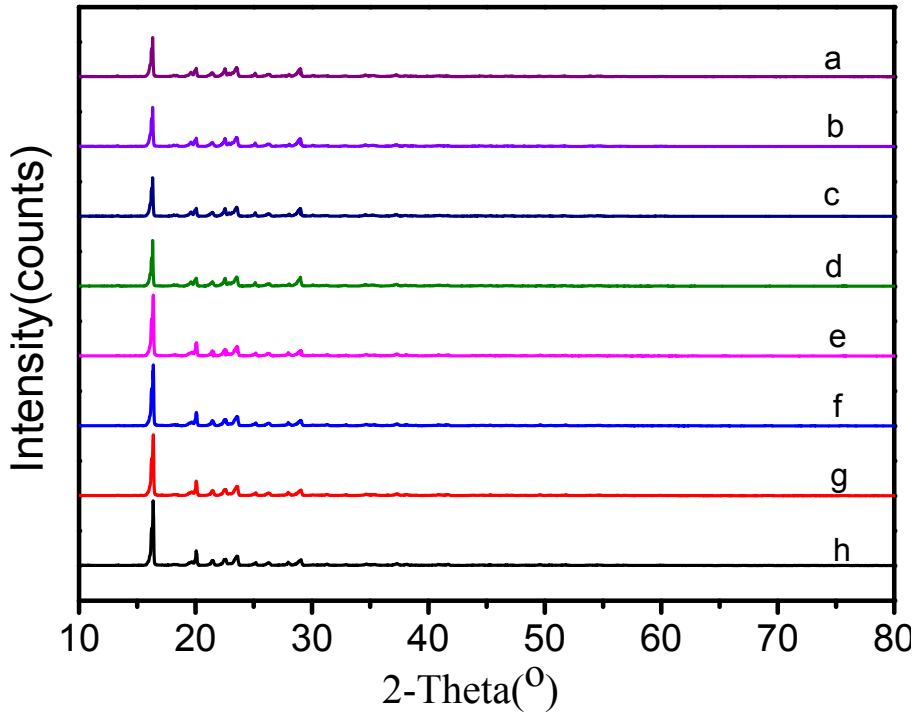

Fig. S2. XRD patterns of hymecromone: (a) raw material; (b) crystallized in neat methanol; (c) crystallized in neat ethanol; (d) crystallized in neat *n*-propanol; (e) crystallized in neat DMF; (f) crystallized in DMF + methanol mixture; (g) crystallized in DMF + ethanol mixture; (h) crystallized in DMF + *n*-propanol mixture.

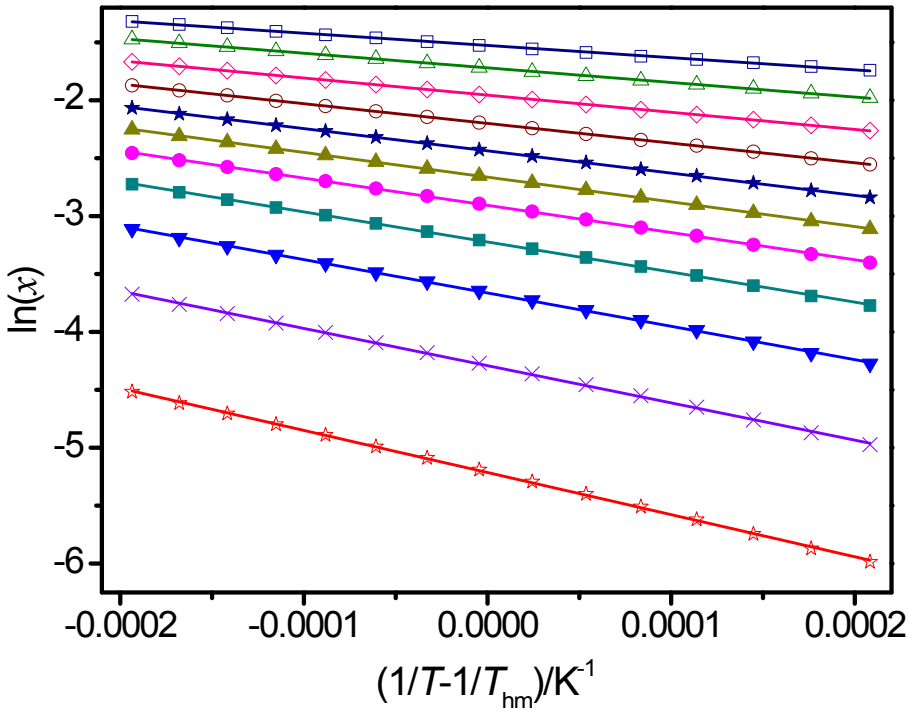

Fig. S3. Van't Hoff plots of the mole fraction solubility (ln(x)) of hymecromone in DMF (w) + methanol (1-w) mixed solutions versus (1/T-1/T_{hm}) with a straight line to correlate the data: ☆, w=0; ×, w=0.0999; ▼, w=0.1997; ■, w=0.2996; ●, w=0.3995; ▲, w=0.4968; ★, w=0.5940; ○, w=0.6969; ◇, w=0.7998; △, w=0.8999; □, w=1.

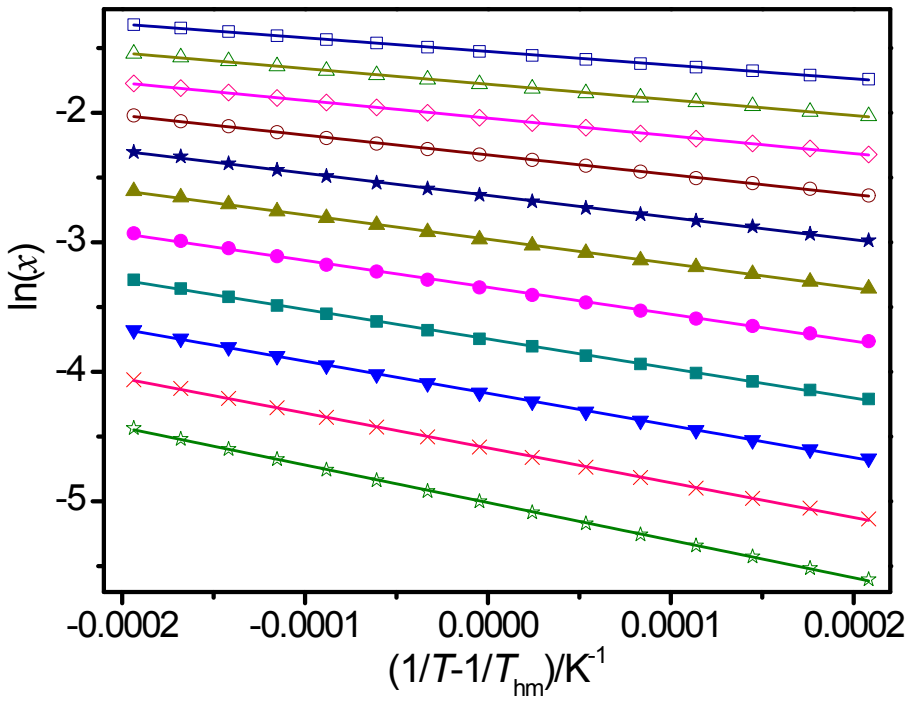

Fig. S4. Van't Hoff plots of the mole fraction solubility (ln(x)) of hymecromone in DMF (w) + ethanol (1-w) mixed solutions versus ($1/T$-$1/T_{hm}$) with a straight line to correlate the data: ☆, w=0; ×, w=0.0999; ▼, w=0.1999; ■, w=0.3001; ●, w=0.4002; ▲, w=0.4999; ★, w=0.5997; ○, w=6998; ◇, w=0.8000; △, w=0.9000; □, w=1.

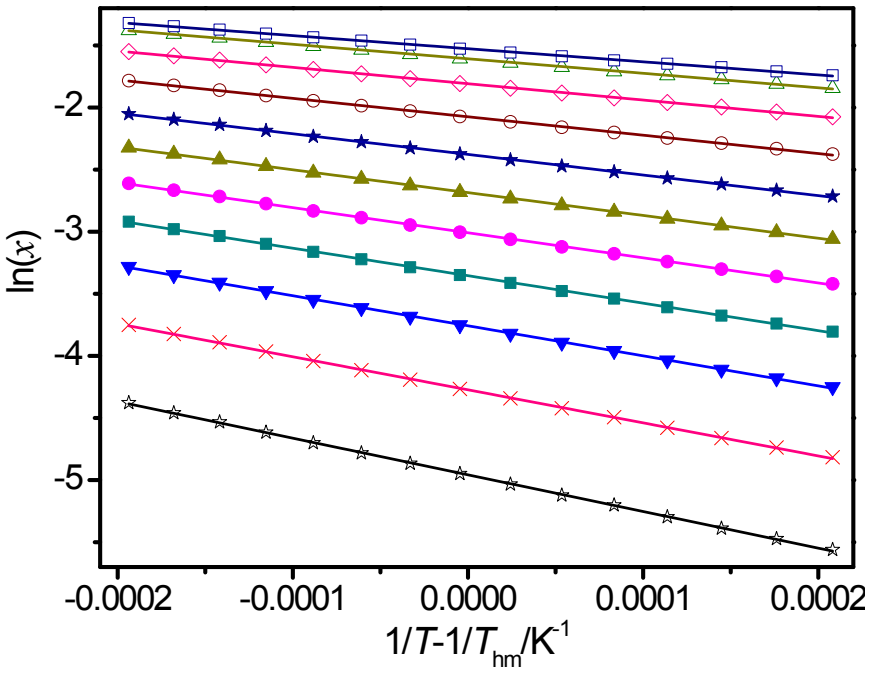

Fig. S5. Van't Hoff plots of the mole fraction solubility (ln(x)) of hymecromone in DMF (w) + n-propanol (1-w) mixed solutions versus ($1/T$-$1/T_{hm}$) with a straight line to correlate the data: ☆, w=0; ×, w=0.0999; ▼, w=0.1997; ■, w=0.2995; ●, w=0.3993; ▲, w=0.5001; ★, w=0.6008; ○, w=0.6999; ◇, w=0.7990; △, w=0.8995; □, w=1.

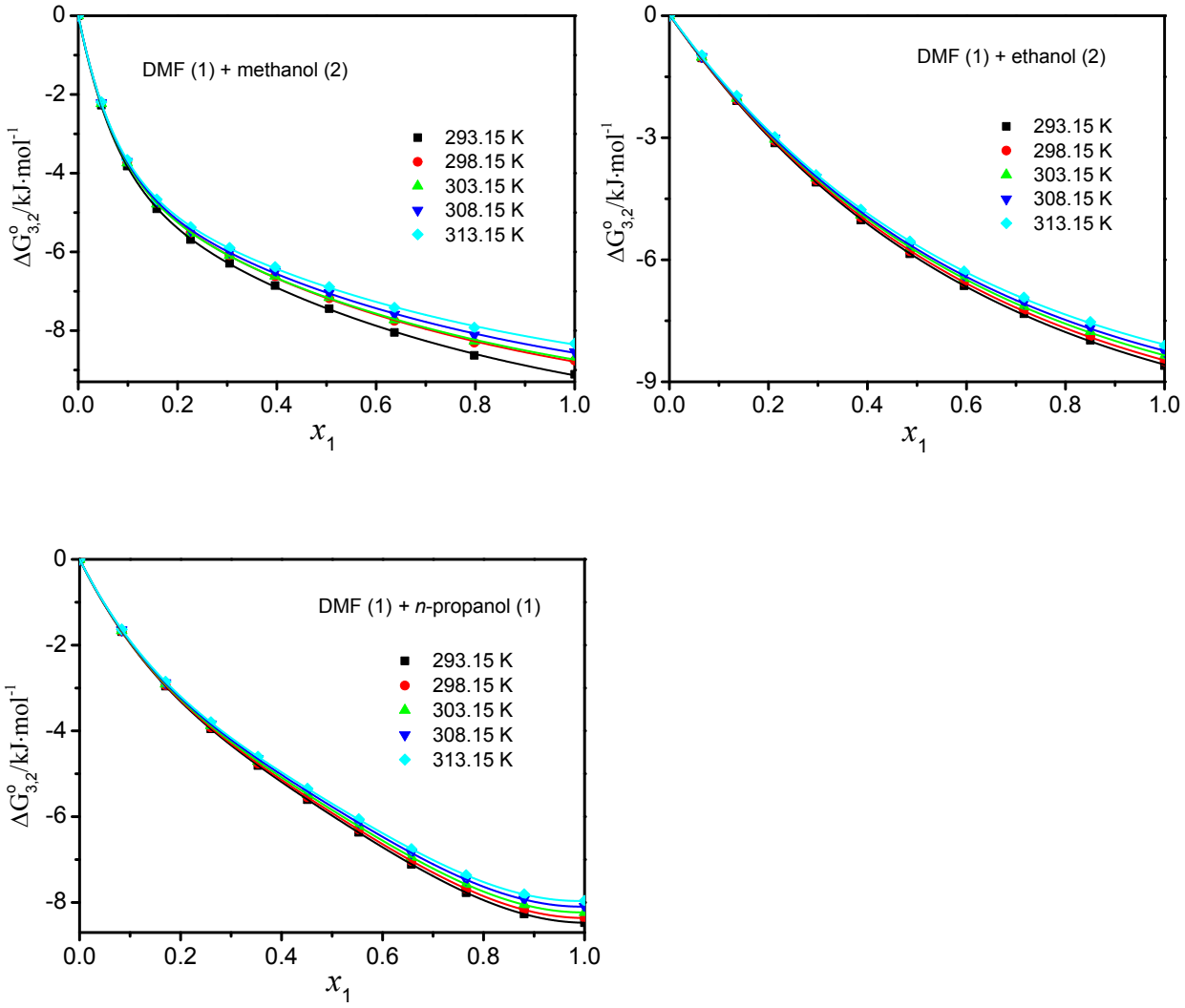

Fig. S6. Gibbs energy of transfer (kJ·mol^{-1}) of hymecromone (3) from neat alcohol (2) to DMF (1) + methanol (2), DMF (1) + ethanol (2) and DMF (1) + *n*-propanol (2) mixtures at several temperatures.

Table S1 Experimental mole fraction solubility ($x^{e}_{T,w} \cdot 10^{2}$) of hymecromone in mixed solvent of DMF (*w*) + methanol (1-*w*) with various mass fractions within the temperature range from *T*/K = (278.15 to 313.15) under *p*=101.1 kPa.[a]

T/K	*w*											x^{idl}
	0	0.0999	0.1997	0.2996	0.3995	0.4968	0.5940	0.6969	0.7998	0.8999	1	
278.15	0.2513	0.6918	1.393	2.299	3.329	4.451	5.849	7.776	10.41	13.82	17.55	2.159
280.65	0.2822	0.7663	1.526	2.496	3.585	4.759	6.210	8.196	10.90	14.36	18.11	2.311
283.15	0.3199	0.8563	1.685	2.730	3.886	5.118	6.628	8.678	11.45	14.97	18.73	2.472
285.65	0.3627	0.9565	1.860	2.980	4.202	5.488	7.048	9.149	11.96	15.51	19.25	2.642
288.15	0.4052	1.055	2.029	3.221	4.506	5.843	7.453	9.606	12.47	16.05	19.79	2.823
290.65	0.4517	1.161	2.212	3.483	4.836	6.232	7.899	10.12	13.05	16.69	20.45	3.015
293.15	0.5024	1.275	2.406	3.757	5.179	6.631	8.353	10.63	13.62	17.31	21.08	3.217
295.65	0.5575	1.398	2.612	4.047	5.540	7.050	8.828	11.16	14.22	17.95	21.74	3.432
298.15	0.6170	1.530	2.832	4.355	5.922	7.493	9.330	11.73	14.85	18.65	22.46	3.658
300.65	0.6805	1.669	3.063	4.675	6.318	7.951	9.847	12.31	15.50	19.36	23.20	3.898
303.15	0.7524	1.823	3.314	5.018	6.734	8.422	10.37	12.88	16.12	20.00	23.82	4.151
305.65	0.8248	1.977	3.565	5.361	7.152	8.899	10.90	13.47	16.77	20.70	24.54	4.418
308.15	0.9050	2.147	3.840	5.736	7.608	9.419	11.48	14.12	17.48	21.48	25.34	4.700
310.65	0.9900	2.324	4.123	6.115	8.064	9.931	12.04	14.73	18.15	22.18	26.04	4.998
313.15	1.092	2.535	4.455	6.556	8.585	10.51	12.67	15.40	18.86	22.90	26.73	5.312

[a] Standard uncertainties *u* are $u(T) = 0.02$ K, $u(p) = 0.45$ kPa; Relative standard uncertainty u_r is $u_r(x) = 0.026$.

Solvent mixtures were prepared by mixing different masses of the solvents with relative standard uncertainty $u_r(w) = 0.0002$. *w* represents the mass fraction of DMF in mixed solvents of DMF + methanol.

Table S2 Experimental mole fraction solubility ($x^{e}_{T,w} \cdot 10^{2}$) of hymecromone in mixed solvent of DMF (*w*) + ethanol (1-*w*) with various mass fractions within the temperature range from *T*/K = (278.15 to 313.15) under *p*=101.1 kPa.[a]

T/K	*w*											x^{idl}
	0	0.0999	0.1999	0.3001	0.4002	0.4999	0.5997	0.6998	0.8000	0.9000	1	
278.15	0.3689	0.5885	0.9381	1.485	2.321	3.484	5.051	7.149	9.809	13.19	17.55	2.159
280.65	0.4022	0.6397	1.007	1.592	2.466	3.673	5.310	7.526	10.28	13.64	18.11	2.311
283.15	0.4400	0.6893	1.081	1.701	2.609	3.898	5.626	7.861	10.68	14.26	18.73	2.472
285.65	0.4787	0.746	1.168	1.815	2.763	4.111	5.877	8.173	11.08	14.70	19.25	2.642
288.15	0.5213	0.8101	1.256	1.946	2.938	4.333	6.181	8.589	11.53	15.23	19.79	2.823
290.65	0.5678	0.8772	1.347	2.075	3.129	4.590	6.488	8.993	12.06	15.75	20.45	3.015
293.15	0.6184	0.9456	1.457	2.231	3.316	4.857	6.825	9.411	12.50	16.32	21.08	3.217
295.65	0.6736	1.025	1.560	2.363	3.515	5.093	7.178	9.804	13.03	16.89	21.74	3.432
298.15	0.7290	1.108	1.678	2.525	3.730	5.387	7.539	10.23	13.53	17.50	22.46	3.658
300.65	0.7926	1.196	1.797	2.702	3.974	5.695	7.876	10.67	14.11	18.11	23.20	3.898
303.15	0.8599	1.289	1.925	2.867	4.186	6.005	8.299	11.14	14.65	18.72	23.82	4.151
305.65	0.9328	1.388	2.070	3.056	4.471	6.321	8.706	11.65	15.17	19.39	24.54	4.418
308.15	1.009	1.492	2.216	3.268	4.758	6.678	9.150	12.20	15.83	20.17	25.34	4.7
310.65	1.090	1.611	2.367	3.483	5.034	7.046	9.655	12.68	16.38	20.77	26.04	4.998
313.15	1.186	1.723	2.526	3.727	5.338	7.395	9.991	13.26	16.98	21.37	26.73	5.312

[a] Standard uncertainties *u* are $u(T)$ = 0.02 K, $u(p)$ = 0.45 kPa; Relative standard uncertainty u_r is $u_r(x)$ = 0.026.

Solvent mixtures were prepared by mixing different masses of the solvents with relative standard uncertainty $u_r(w)$ = 0.0002. *w* represents the mass fraction of DMF in mixed solvents of DMF + ethanol.

Table S3 Experimental mole fraction solubility ($x^{e}_{T,w} \cdot 10^{2}$) of hymecromone in mixed solvent of DMF (*w*) + *n*-propanol (1-*w*) with various mass fractions within the temperature range from *T*/K = (278.15 to 313.15) under *p*=101.1 kPa.[a]

T/K	*w*											x^{idl}
	0	0.0999	0.1997	0.2995	0.3993	0.5001	0.6008	0.6999	0.7990	0.8995	1	
278.15	0.3847	0.8102	1.426	2.227	3.272	4.695	6.623	9.301	12.56	15.82	17.55	2.159
280.65	0.4202	0.8761	1.531	2.376	3.472	4.955	6.953	9.714	13.05	16.37	18.11	2.311
283.15	0.457	0.9454	1.641	2.533	3.683	5.229	7.303	10.16	13.59	16.98	18.73	2.472
285.65	0.5007	1.027	1.768	2.709	3.913	5.522	7.666	10.59	14.09	17.52	19.25	2.642
288.15	0.5509	1.118	1.909	2.905	4.168	5.842	8.059	11.07	14.63	18.09	19.79	2.823
290.65	0.5965	1.202	2.040	3.087	4.408	6.151	8.447	11.55	15.21	18.74	20.45	3.015
293.15	0.6516	1.301	2.192	3.298	4.682	6.496	8.873	12.06	15.81	19.39	21.08	3.217
295.65	0.7092	1.404	2.348	3.512	4.960	6.847	9.306	12.59	16.42	20.06	21.74	3.432
298.15	0.7704	1.513	2.514	3.740	5.254	7.218	9.764	13.15	17.07	20.78	22.46	3.658
300.65	0.8376	1.633	2.696	3.988	5.574	7.618	10.26	13.74	17.76	21.53	23.20	3.898
303.15	0.9089	1.757	2.881	4.235	5.887	8.004	10.72	14.29	18.38	22.18	23.82	4.151
305.65	0.9895	1.898	3.090	4.516	6.242	8.440	11.24	14.91	19.09	22.93	24.54	4.418
308.15	1.075	2.045	3.308	4.808	6.612	8.897	11.80	15.57	19.84	23.74	25.34	4.700
310.65	1.157	2.185	3.514	5.081	6.956	9.318	12.30	16.17	20.52	24.47	26.04	4.998
313.15	1.255	2.351	3.755	5.397	7.348	9.790	12.86	16.81	21.23	25.20	26.73	5.312

[a] Standard uncertainties *u* are $u(T)$ = 0.02 K, $u(p)$ = 0.45 kPa; Relative standard uncertainty u_r is $u_r(x)$ = 0.026. Solvent mixtures were prepared by mixing different masses of the solvents with relative standard uncertainty $u_r(w)$ = 0.0002. *w* represents the mass fraction of DMF in mixed solvents of DMF + *n*-propanol.

Table S4 Values of parameters obtained using solubility models.

	Jouyban−Acree		van't Hoff−Jouyban−Acree		Apelblat− Jouyban−Acree	
	parameter	value	parameter	value	parameter	value
DMF + methanol						
	J_0	825.55	A_1	2.067	A_1	-29.85
	J_1	775.63	B_1	-1061.0	B_1	351.80
	J_2	576.2	A_2	6.953	C_1	4.770
			B_2	-3591.8	A_2	70.48
			J_0	824.46	B_2	-6425.9
			J_1	772.97	C_2	-9.48
			J_2	573.49	J_0	822.6
					J_1	774.0
					J_2	568.85
$RAD \cdot 10^2$		0.09		0.38		0.21
$RMSD \cdot 10^4$		0.15		3.07		2.25
DMF + ethanol						
	J_0	343.13	A_1	2.067	A_1	-29.85
	J_1	-49.57	B_1	-1061.0	B_1	351.80
	J_2	-107.21	A_2	4.925	C_1	4.770
			B_2	-2933.5	A_2	-63.24
			J_0	344.05	B_2	101.10
			J_1	-48.56	C_2	10.18
			J_2	-104.91	J_0	330.94
					J_1	-68.08
					J_2	-137.68
$RAD \cdot 10^2$		0.21		0.51		0.43
$RMSD \cdot 10^4$		2.00		4.21		2.94
DMF + n-propanol						
	J_0	657.28	A_1	2.067	A_1	-29.85
	J_1	165.53	B_1	-1061.0	B_1	351.80
	J_2	510.50	A_2	5.123	C_1	4.770
			B_2	-2976.6	A_2	-44.72
			J_0	657.83	B_2	-757.50
			J_1	165.32	C_2	7.440
			J_2	516.8	J_0	659.05
					J_1	171.95
					J_2	519.80
$RAD \cdot 10^2$		0.13		0.40		0.23
$RMSD \cdot 10^4$		1.77		4.42		2.81

Table S5 Standard enthalpy change of hymecromone in mixed solvents of DMF (*w*) + methanol (1-*w*), DMF (*w*) + ethanol (1-*w*) and DMF (*w*) + *n*-propanol (1-*w*).

DMF (*w*) + methanol (1-*w*)		DMF (*w*) + ethanol (1-*w*)		DMF (*w*) + *n*-propanol (1-*w*)	
w	ΔH^{o}_{sol} / kJ · mol^{-1}	*w*	ΔH^{o}_{sol} / kJ · mol^{-1}	*w*	ΔH^{o}_{sol} / kJ · mol^{-1}
0	30.24	0	24.13	0	24.54
0.0999	26.73	0.0999	22.34	0.0999	22.13
0.1997	23.95	0.1999	20.64	0.1997	20.11
0.2996	21.59	0.3001	18.94	0.2995	18.40
0.3995	19.54	0.4002	17.28	0.3993	16.82
0.4968	17.73	0.4999	15.63	0.5001	15.28
0.5940	15.97	0.5997	14.22	0.6008	13.81
0.6969	14.14	0.6998	12.70	0.6999	12.32
0.7998	12.31	0.8000	11.36	0.7990	10.94
0.8999	10.49	0.9000	10.05	0.8995	9.709
1	8.774	1	8.774	1	8.774

Table S6 Activity coefficients (γ_3) of hymecromone in DMF (1) + methanol (2) mixtures at several temperatures.

T/K	*w*										
	0	0.0999	0.1997	0.2996	0.3995	0.4968	0.5940	0.6969	0.7998	0.8999	1
278.15	8.591	3.121	1.550	0.939	0.649	0.485	0.369	0.278	0.207	0.156	0.123
280.65	8.188	3.015	1.514	0.926	0.645	0.486	0.372	0.282	0.212	0.161	0.128
283.15	7.726	2.886	1.467	0.905	0.636	0.483	0.373	0.285	0.216	0.165	0.132
285.65	7.285	2.763	1.421	0.887	0.629	0.481	0.375	0.289	0.221	0.170	0.137
288.15	6.967	2.676	1.391	0.876	0.627	0.483	0.379	0.294	0.226	0.176	0.143
290.65	6.674	2.597	1.363	0.866	0.623	0.484	0.382	0.298	0.231	0.181	0.147
293.15	6.404	2.523	1.337	0.856	0.621	0.485	0.385	0.303	0.236	0.186	0.153
295.65	6.155	2.455	1.314	0.848	0.619	0.487	0.389	0.307	0.241	0.191	0.158
298.15	5.929	2.391	1.292	0.840	0.618	0.488	0.392	0.312	0.246	0.196	0.163
300.65	5.728	2.335	1.273	0.834	0.617	0.490	0.396	0.317	0.251	0.201	0.168
303.15	5.517	2.277	1.253	0.827	0.616	0.493	0.400	0.322	0.258	0.208	0.174
305.65	5.357	2.235	1.239	0.824	0.618	0.496	0.405	0.328	0.263	0.213	0.180
308.15	5.194	2.189	1.224	0.819	0.618	0.499	0.409	0.333	0.269	0.219	0.185
310.65	5.048	2.151	1.212	0.817	0.620	0.503	0.415	0.339	0.275	0.225	0.192
313.15	4.864	2.095	1.192	0.810	0.619	0.505	0.419	0.345	0.282	0.232	0.199

Table S7 Activity coefficients (γ_3) of hymecromone in DMF (1) + ethanol (2) mixtures at several temperatures.

T/K	*w*										
	0	0.0999	0.1999	0.3001	0.4002	0.4999	0.5997	0.6998	0.8000	0.9000	1
278.15	5.852	3.668	2.301	1.454	0.930	0.620	0.427	0.302	0.220	0.164	0.123
280.65	5.745	3.612	2.295	1.451	0.937	0.629	0.435	0.307	0.225	0.169	0.128
283.15	5.617	3.586	2.286	1.453	0.947	0.634	0.439	0.314	0.231	0.173	0.132
285.65	5.520	3.542	2.262	1.456	0.956	0.643	0.450	0.323	0.238	0.180	0.137
288.15	5.416	3.485	2.248	1.451	0.961	0.652	0.457	0.329	0.245	0.185	0.143
290.65	5.309	3.437	2.238	1.453	0.963	0.657	0.465	0.335	0.250	0.191	0.147
293.15	5.203	3.402	2.208	1.442	0.970	0.662	0.471	0.342	0.257	0.197	0.153
295.65	5.094	3.348	2.200	1.452	0.976	0.674	0.478	0.350	0.263	0.203	0.158
298.15	5.018	3.302	2.180	1.449	0.981	0.679	0.485	0.358	0.270	0.209	0.163
300.65	4.918	3.259	2.169	1.443	0.981	0.684	0.495	0.365	0.276	0.215	0.168
303.15	4.827	3.220	2.156	1.448	0.992	0.691	0.500	0.373	0.283	0.222	0.174
305.65	4.736	3.183	2.134	1.446	0.988	0.699	0.507	0.379	0.291	0.228	0.180
308.15	4.658	3.150	2.121	1.438	0.988	0.704	0.514	0.385	0.297	0.233	0.185
310.65	4.585	3.102	2.111	1.435	0.993	0.709	0.518	0.394	0.305	0.241	0.192
313.15	4.479	3.083	2.103	1.425	0.995	0.718	0.532	0.401	0.313	0.249	0.199

Table S8 Activity coefficients (γ_3) of hymecromone in DMF (1) + *n*-propanol (2) mixtures at several temperatures.

T/K	*w*										
	0	0.0999	0.1997	0.2995	0.3993	0.5001	0.6008	0.6999	0.7990	0.8995	1
278.15	5.612	2.665	1.514	0.969	0.660	0.460	0.326	0.232	0.172	0.136	0.123
280.65	5.499	2.637	1.509	0.973	0.666	0.466	0.332	0.238	0.177	0.141	0.128
283.15	5.409	2.614	1.506	0.976	0.671	0.473	0.338	0.243	0.182	0.146	0.132
285.65	5.277	2.573	1.495	0.975	0.675	0.479	0.345	0.250	0.188	0.151	0.137
288.15	5.125	2.525	1.479	0.972	0.677	0.483	0.350	0.255	0.193	0.156	0.143
290.65	5.054	2.508	1.478	0.977	0.684	0.490	0.357	0.261	0.198	0.161	0.147
293.15	4.937	2.473	1.468	0.976	0.687	0.495	0.363	0.267	0.203	0.166	0.153
295.65	4.839	2.444	1.461	0.977	0.692	0.501	0.369	0.273	0.209	0.171	0.158
298.15	4.749	2.418	1.455	0.978	0.696	0.507	0.375	0.278	0.214	0.176	0.163
300.65	4.654	2.387	1.446	0.977	0.699	0.512	0.380	0.284	0.219	0.181	0.168
303.15	4.567	2.362	1.441	0.980	0.705	0.519	0.387	0.290	0.226	0.187	0.174
305.65	4.465	2.328	1.43	0.978	0.708	0.523	0.393	0.296	0.231	0.193	0.180
308.15	4.372	2.298	1.421	0.978	0.711	0.528	0.398	0.302	0.237	0.198	0.185
310.65	4.320	2.287	1.422	0.984	0.718	0.536	0.406	0.309	0.244	0.204	0.192
313.15	4.232	2.259	1.415	0.984	0.723	0.543	0.413	0.316	0.250	0.211	0.199

Table S9 Gibbs energy of transfer (kJ·mol^{-1}) of hymecromone (3) from neat methanol (2) or ethanol (2) to DMF (1) + methanol (2) and DMF (1) + ethanol (2) mixtures at several temperatures.

DMF (1) + methanol (2)						DMF (1) + ethanol (2)					
x_1[a]	293.15 K	298.15 K	303.15 K	308.15 K	313.15 K	x_1[a]	293.15 K	298.15 K	303.15 K	308.15 K	313.15 K
0	0	0	0	0	0	0	0	0	0	0	0
0.04640	-2.272	-2.213	-2.232	-2.213	-2.193	0.06538	-1.038	-1.038	-1.020	-1.002	-0.972
0.09860	-3.819	-3.714	-3.738	-3.703	-3.661	0.1361	-2.090	-2.067	-2.031	-2.016	-1.968
0.1579	-4.906	-4.763	-4.784	-4.731	-4.666	0.2128	-3.129	-3.079	-3.035	-3.011	-2.981
0.2258	-5.688	-5.512	-5.525	-5.454	-5.368	0.2961	-4.095	-4.047	-3.989	-3.973	-3.916
0.3021	-6.290	-6.085	-6.089	-6.002	-5.895	0.3865	-5.025	-4.958	-4.898	-4.842	-4.765
0.3907	-6.853	-6.620	-6.613	-6.508	-6.382	0.4857	-5.854	-5.791	-5.714	-5.649	-5.548
0.5020	-7.441	-7.178	-7.160	-7.039	-6.890	0.5950	-6.637	-6.548	-6.456	-6.386	-6.285
0.6365	-8.045	-7.753	-7.725	-7.586	-7.418	0.7160	-7.329	-7.241	-7.146	-7.053	-6.929
0.7976	-8.629	-8.308	-8.269	-8.114	-7.923	0.8501	-7.979	-7.878	-7.764	-7.674	-7.528
1	-9.109	-8.761	-8.709	-8.537	-8.326	1	-8.602	-8.497	-8.371	-8.258	-8.111

[a] x_1 is the mole fraction of DMF (1) in the DMF (1) + methanol (ethanol) (2) mixtures free of hymecromone (3).

Table S10 Gibbs energy of transfer (kJ·mol^{-1}) of hymecromone (3) from neat *n*-propanol (2) to DMF (1) + *n*-propanol (2) mixtures at several temperatures.

ethyl acetate (1) + *n*-propanol (2)					
x_1[a]	293.15 K	298.15 K	303.15 K	308.15 K	313.15 K
0	0	0	0	0	0
0.08358	-1.684	-1.674	-1.661	-1.648	-1.634
0.1702	-2.955	-2.933	-2.907	-2.880	-2.853
0.2600	-3.951	-3.918	-3.878	-3.838	-3.798
0.3533	-4.805	-4.760	-4.708	-4.654	-4.601
0.4512	-5.603	-5.547	-5.483	-5.414	-5.348
0.5529	-6.363	-6.296	-6.219	-6.138	-6.058
0.6571	-7.111	-7.034	-6.944	-6.848	-6.756
0.7656	-7.771	-7.681	-7.578	-7.469	-7.364
0.8803	-8.268	-8.169	-8.052	-7.929	-7.810
1	-8.472	-8.361	-8.231	-8.096	-7.963

[a] x_1 is the mole fraction of DMF (1) in the DMF (1) + *n*-propanol (2) mixtures free of hymecromone (3).

Table S11 Coefficients of Eqs. (36) and (37) ($kJ \cdot mol^{-1}$) applied to Gibbs energy of transfer of hymecromone (3) from neat methanol (ethanol and *n*-propanol) (2) to DMF(1) + methanol (2), DMF (1) + ethanol (2) and DMF (1) + *n*-propanol mixtures at several temperatures.

Coefficient	DMF (1) + methanol (2)					DMF (1) + ethanol (2)				
	293.15 K	298.15 K	303.15 K	308.15 K	313.15 K	293.15 K	298.15 K	303.15 K	308.15 K	313.15 K
A_0	-10.795	-10.364	-10.273	-10.056	-9.7766	-10.623	-10.501	-10.332	-10.141	-9.9158
A_1	3.9983	6.4564	6.3186	3.9485	3.9249	5.3243	5.2607	5.1788	5.0848	4.9760
t_1	0.07394	0.70913	0.70722	0.07343	0.0731	0.60614	0.60746	0.60473	0.59683	0.59072
A_2	6.8031	3.9141	3.9610	6.1146	5.8584	5.3243	5.2607	5.1788	5.0848	4.9760
t_2	0.70851	0.0738	0.07352	0.70876	0.70667	0.60614	0.60746	0.60473	0.59683	0.59072

Coefficient	DMF (1) + *n*-propanol (2)				
	293.15 K	298.15 K	303.15 K	308.15 K	313.15 K
a	3.005×10^{-4}	1.745×10^{-4}	1.148×10^{-4}	1.339×10^{-4}	2.093×10^{-4}
b	-23.725	-23.605	-23.448	-23.295	-23.124
c	48.326	48.408	48.437	48.4862	48.386
d	-72.766	-73.029	-73.290	-73.503	-73.346
e	53.165	53.429	53.799	54.052	53.891
f	-13.472	-13.565	-13.728	-13.835	-13.770

Table S12 *D* values (kJ·mol^{-1}) of hymecromone (3) from neat methanol (2) or ethanol (2) to DMF (1) + methanol (2) and DMF (1) + ethanol (2) mixtures at several temperatures.

	DMF (1) + methanol (2)					DMF (1) + ethanol (2)				
x_1[a]	293.15 K	298.15 K	303.15 K	308.15 K	313.15 K	293.15 K	298.15 K	303.15 K	308.15 K	313.15 K
0	-63.68	-62.14	-62.81	-62.40	-61.98	-17.57	-17.32	-17.13	-17.13	-16.85
0.05	-36.45	-35.42	-35.62	-35.26	-34.82	-16.18	-15.95	-15.77	-15.77	-15.48
0.10	-22.32	-21.59	-21.58	-21.27	-20.87	-14.90	-14.69	-14.52	-14.52	-14.22
0.15	-14.88	-14.32	-14.23	-13.95	-13.60	-13.72	-13.53	-13.37	-13.37	-13.07
0.20	-10.86	-10.40	-10.28	-10.04	-9.728	-12.63	-12.46	-12.31	-12.31	-12.01
0.25	-8.586	-8.192	-8.071	-7.849	-7.576	-11.63	-11.48	-11.33	-11.33	-11.03
0.30	-7.223	-6.874	-6.756	-6.554	-6.309	-10.71	-10.57	-10.43	-10.43	-10.14
0.35	-6.335	-6.020	-5.908	-5.723	-5.499	-9.862	-9.735	-9.602	-9.602	-9.316
0.40	-5.702	-5.414	-5.309	-5.138	-4.933	-9.081	-8.966	-8.840	-8.840	-8.560
0.45	-5.211	-4.946	-4.847	-4.689	-4.499	-8.362	-8.257	-8.138	-8.138	-7.865
0.50	-4.804	-4.559	-4.466	-4.320	-4.143	-7.700	-7.605	-7.492	-7.492	-7.227
0.55	-4.450	-4.223	-4.135	-4.001	-3.836	-7.090	-7.004	-6.898	-6.898	-6.640
0.60	-4.133	-3.922	-3.840	-3.715	-3.561	-6.529	-6.451	-6.350	-6.350	-6.101
0.65	-3.845	-3.649	-3.572	-3.456	-3.312	-6.012	-5.941	-5.846	-5.846	-5.606
0.70	-3.579	-3.397	-3.324	-3.217	-3.082	-5.536	-5.471	-5.382	-5.382	-5.151
0.75	-3.334	-3.164	-3.096	-2.996	-2.870	-5.097	-5.039	-4.955	-4.955	-4.733
0.80	-3.106	-2.948	-2.884	-2.791	-2.673	-4.694	-4.641	-4.562	-4.562	-4.349
0.85	-2.893	-2.747	-2.686	-2.601	-2.490	-4.322	-4.274	-4.200	-4.200	-3.996
0.90	-2.696	-2.559	-2.503	-2.423	-2.320	-3.980	-3.937	-3.867	-3.867	-3.672
0.95	-2.512	-2.385	-2.332	-2.258	-2.161	-3.665	-3.625	-3.560	-3.560	-3.374
1	-2.341	-2.223	-2.173	-2.104	-2.014	-3.375	-3.339	-3.277	-3.277	-3.100

[a] x_1 is the mole fraction of DMF (1) in the DMF (1) + methanol (ethanol) (2) mixtures free of hymecromone (3).

Table S13 *D* values (kJ·mol^{-1}) of hymecromone (3) from neat *n*-propanol (2) to DMF (1) + *n*-propanol (2) mixtures at several temperatures.

x_1[a]	DMF (1) + *n*-propanol (2)				
	293.15 K	298.15 K	303.15 K	308.15 K	313.15 K
0	-23.72	-23.61	-23.45	-23.29	-23.13
0.05	-19.41	-19.29	-19.13	-18.97	-18.81
0.10	-16.04	-15.91	-15.75	-15.59	-15.44
0.15	-13.45	-13.32	-13.17	-13.02	-12.87
0.20	-11.53	-11.40	-11.26	-11.10	-10.96
0.25	-10.15	-10.02	-9.878	-9.729	-9.584
0.30	-9.180	-9.057	-8.920	-8.775	-8.633
0.35	-8.531	-8.414	-8.279	-8.138	-7.999
0.40	-8.106	-7.993	-7.862	-7.723	-7.587
0.45	-7.820	-7.711	-7.582	-7.447	-7.314
0.50	-7.600	-7.495	-7.368	-7.234	-7.104
0.55	-7.384	-7.280	-7.155	-7.023	-6.895
0.60	-7.116	-7.013	-6.890	-6.759	-6.634
0.65	-6.755	-6.651	-6.529	-6.400	-6.277
0.70	-6.266	-6.162	-6.041	-5.914	-5.792
0.75	-5.627	-5.522	-5.403	-5.277	-5.158
0.80	-4.824	-4.720	-4.602	-4.479	-4.362
0.85	-3.854	-3.753	-3.638	-3.519	-3.403
0.90	-2.725	-2.630	-2.517	-2.405	-2.290
0.95	-1.453	-1.369	-1.260	-1.156	-1.042
1	-0.066	7.635×10^{-4}	0.1040	0.1980	0.3110

[a] x_1 is the mole fraction of DMF (1) in the DMF (1) + *n*-propanol (2) mixtures free of hymecromone (3).

Table S14 $G_{1,3}$ and $G_{2,3}$ values ($cm^3 \cdot mol^{-1}$) for hymecromone (3) in DMF (1) + methanol (2) mixtures at several temperatures.

x_1[a]	$G_{1,3}$					$G_{2,3}$				
	293.15 K	298.15 K	303.15 K	308.15 K	313.15 K	293.15 K	298.15 K	303.15 K	308.15 K	313.15 K
0	-1188	-1145	-1151	-1134	-1117	-130.5	-130.5	-130.4	-130.4	-130.3
0.05	-683.7	-659.0	-659.4	-648.5	-636.9	-184.6	-182.1	-182.0	-180.9	-179.6
0.10	-440.5	-425.2	-423.7	-416.3	-408.1	-194.8	-191.6	-191.1	-189.5	-187.7
0.15	-319.7	-309.4	-307.5	-302.2	-296.1	-193.2	-189.7	-188.9	-187.1	-185.0
0.20	-257.0	-249.5	-247.6	-243.5	-238.9	-190.1	-186.6	-185.6	-183.6	-181.3
0.25	-222.1	-216.4	-214.7	-211.5	-207.8	-188.3	-184.7	-183.5	-181.4	-179.1
0.30	-201.1	-196.5	-195.0	-192.4	-189.4	-188.0	-184.2	-182.9	-180.7	-178.3
0.35	-187.1	-183.4	-182.1	-179.9	-177.5	-188.5	-184.7	-183.3	-181.0	-178.5
0.40	-177.0	-173.9	-172.8	-171.0	-169.0	-189.6	-185.7	-184.2	-181.9	-179.2
0.45	-169.2	-166.6	-165.7	-164.2	-162.5	-190.9	-186.9	-185.3	-182.9	-180.2
0.50	-162.9	-160.7	-160.0	-158.7	-157.2	-192.2	-188.1	-186.5	-184.0	-181.2
0.55	-157.6	-155.8	-155.2	-154.1	-152.9	-193.4	-189.2	-187.6	-185.1	-182.2
0.60	-153.1	-151.6	-151.1	-150.2	-149.2	-194.6	-190.3	-188.6	-186.1	-183.2
0.65	-149.3	-148.0	-147.6	-146.8	-146.0	-195.6	-191.3	-189.6	-187.0	-184.0
0.70	-145.9	-144.9	-144.5	-143.9	-143.2	-196.6	-192.2	-190.5	-187.9	-184.9
0.75	-142.9	-142.1	-141.8	-141.3	-140.8	-197.7	-193.2	-191.5	-188.8	-185.8
0.80	-140.3	-139.7	-139.4	-139.1	-138.6	-198.8	-194.3	-192.5	-189.8	-186.7
0.85	-137.9	-137.5	-137.3	-137.0	-136.7	-200.1	-195.5	-193.7	-191.0	-187.8
0.90	-135.8	-135.5	-135.4	-135.2	-135.0	-201.7	-197.0	-195.1	-192.4	-189.1
0.95	-133.8	-133.7	-133.6	-133.5	-133.4	-203.6	-198.8	-196.8	-194.0	-190.7
1	-132.0	-131.9	-131.9	-131.9	-131.9	-206.0	-201.0	-199.0	-196.1	-192.7

[a] x_1 is the mole fraction of ethyl acetate in the DMF (1) + methanol (2) mixtures.

Table S15 $G_{1,3}$ and $G_{2,3}$ values ($cm^3 \cdot mol^{-1}$) for hymecromone (3) in DMF (1) + ethanol (2) mixtures at several temperatures.

x_1[a]	$G_{1,3}$					$G_{2,3}$				
	293.15 K	298.15 K	303.15 K	308.15 K	313.15 K	293.15 K	298.15 K	303.15 K	308.15 K	313.15 K
0	-551.1	-540.4	-531.3	-527.0	-516.4	-130.8	-130.7	-130.7	-130.6	-130.6
0.05	-503.6	-492.6	-483.0	-478.1	-467.1	-156.5	-155.7	-155.0	-154.6	-153.8
0.10	-456.6	-446.1	-436.9	-431.8	-421.2	-178.3	-176.7	-175.3	-174.5	-173.0
0.15	-412.2	-402.7	-394.3	-389.6	-379.6	-196.0	-193.8	-191.8	-190.6	-188.3
0.20	-371.8	-363.6	-356.1	-352.0	-342.9	-210.0	-207.2	-204.7	-203.3	-200.3
0.25	-335.8	-328.9	-322.5	-318.9	-310.8	-220.7	-217.6	-214.7	-213.1	-209.5
0.30	-304.4	-298.7	-293.2	-290.2	-283.1	-228.7	-225.4	-222.3	-220.6	-216.5
0.35	-277.2	-272.5	-267.9	-265.5	-259.2	-234.6	-231.2	-228.0	-226.2	-221.7
0.40	-253.7	-249.9	-246.2	-244.2	-238.7	-238.8	-235.4	-232.0	-230.2	-225.4
0.45	-233.6	-230.5	-227.4	-225.8	-221.1	-241.6	-238.3	-234.9	-233.1	-228.0
0.50	-216.3	-213.8	-211.3	-210.0	-206.0	-243.5	-240.2	-236.8	-235.0	-229.7
0.55	-201.4	-199.5	-197.4	-196.4	-193.0	-244.5	-241.3	-237.9	-236.2	-230.7
0.60	-188.6	-187.1	-185.4	-184.6	-181.7	-245.0	-241.8	-238.4	-236.8	-231.1
0.65	-177.6	-176.3	-175.0	-174.3	-172.0	-244.9	-241.8	-238.5	-236.9	-231.1
0.70	-168.0	-167.0	-166.0	-165.5	-163.6	-244.5	-241.5	-238.1	-236.6	-230.7
0.75	-159.7	-159.0	-158.1	-157.8	-156.3	-243.7	-240.8	-237.4	-236.0	-230.0
0.80	-152.5	-152.0	-151.4	-151.1	-149.9	-242.8	-239.9	-236.5	-235.1	-229.0
0.85	-146.3	-145.9	-145.5	-145.3	-144.4	-241.7	-238.9	-235.5	-234.2	-228.0
0.90	-140.9	-140.6	-140.3	-140.2	-139.7	-240.5	-237.8	-234.5	-233.2	-227.0
0.95	-136.1	-136.0	-135.9	-135.8	-135.5	-239.5	-236.9	-233.7	-232.4	-226.0
1	-132.0	-131.9	-131.9	-131.9	-131.9	-238.6	-236.2	-233.1	-231.9	-225.4

[a] x_1 is the mole fraction of ethyl acetate in the DMF (1) + ethanol (2) mixtures.

Table S16 $G_{1,3}$ and $G_{2,3}$ values ($cm^3 \cdot mol^{-1}$) for hymecromone (3) in DMF (1) + *n*-propanol (2) mixtures at several temperatures.

x_1[a]	$G_{1,3}$					$G_{2,3}$				
	293.15 K	298.15 K	303.15 K	308.15 K	313.15 K	293.15 K	298.15 K	303.15 K	308.15 K	313.15 K
0	-858.8	-846.8	-833.8	-821.0	-808.8	-131.1	-131.0	-131.0	-130.9	-130.9
0.05	-708.5	-695.0	-681.2	-667.8	-655.1	-161.9	-161.1	-160.3	-159.6	-159.0
0.10	-586.7	-573.6	-560.5	-547.9	-536.0	-182.5	-181.0	-179.5	-178.1	-176.8
0.15	-491.3	-479.4	-467.8	-456.5	-446.0	-195.8	-193.7	-191.6	-189.6	-187.7
0.20	-418.7	-408.3	-398.3	-388.6	-379.5	-204.5	-201.8	-199.3	-196.8	-194.5
0.25	-364.4	-355.6	-347.1	-338.8	-331.1	-210.7	-207.7	-204.8	-202.0	-199.4
0.30	-324.2	-316.8	-309.5	-302.5	-296.0	-216.0	-212.7	-209.5	-206.5	-203.6
0.35	-294.1	-287.9	-281.7	-275.8	-270.2	-221.3	-217.9	-214.4	-211.2	-208.1
0.40	-270.9	-265.7	-260.5	-255.4	-250.7	-227.0	-223.5	-219.9	-216.4	-213.1
0.45	-252.1	-247.8	-243.3	-239.0	-235.0	-233.2	-229.5	-225.8	-222.1	-218.7
0.50	-236.0	-232.4	-228.6	-225.0	-221.6	-239.4	-235.6	-231.8	-228.0	-224.4
0.55	-221.4	-218.4	-215.3	-212.2	-209.3	-245.1	-241.3	-237.3	-233.4	-229.7
0.60	-207.6	-205.1	-202.5	-200.0	-197.6	-249.7	-245.8	-241.8	-237.8	-234.0
0.65	-194.3	-192.3	-190.1	-188.0	-186.1	-252.3	-248.4	-244.3	-240.2	-236.4
0.70	-181.4	-179.7	-178.0	-176.4	-174.8	-252.1	-248.1	-244.0	-239.9	-236.1
0.75	-169.1	-167.8	-166.4	-165.1	-163.9	-248.2	-244.2	-240.1	-236.0	-232.1
0.80	-157.6	-156.7	-155.7	-154.7	-153.8	-239.5	-235.6	-231.5	-227.4	-223.6
0.85	-147.6	-147.0	-146.3	-145.6	-144.9	-224.9	-221.2	-217.2	-213.3	-209.6
0.90	-139.5	-139.1	-138.7	-138.3	-137.9	-203.4	-200.0	-196.2	-192.5	-188.9
0.95	-134.0	-133.9	-133.7	-133.5	-133.3	-173.6	-170.7	-167.2	-163.8	-160.3
1	-132.0	-131.9	-131.9	-131.9	-131.9	-134.0	-131.9	-128.7	-125.8	-122.5

[a] x_1 is the mole fraction of DMF (1) in the DMF (1) + *n*-propanol (2) mixtures.

Table S17 Correlation volume and $\delta x_{1,3}$ values for hymecromone (3) in DMF (1) + methanol (2) mixtures at several temperatures.

x_1[a]	V_{cor} ($cm^3 \cdot mol^{-1}$)					100 $\delta x_{1,3}$				
	293.15 K	298.15 K	303.15 K	308.15 K	313.15 K	293.15 K	298.15 K	303.15 K	308.15 K	313.15 K
0	1101	1101	1109	1113	1117	0	0	0	0	0
0.05	1114	1115	1123	1128	1132	-2.621	-2.492	-2.472	-2.405	-2.335
0.10	1144	1145	1154	1158	1163	-2.391	-2.261	-2.228	-2.158	-2.080
0.15	1177	1178	1186	1191	1196	-1.673	-1.574	-1.543	-1.487	-1.425
0.20	1209	1210	1218	1223	1228	-1.064	-0.997	-0.973	-0.934	-0.890
0.25	1240	1241	1250	1254	1259	-0.607	-0.567	-0.552	-0.529	-0.503
0.30	1271	1271	1280	1285	1289	-0.255	-0.238	-0.232	-0.223	-0.212
0.35	1301	1301	1310	1315	1320	0.029	0.027	0.024	0.022	0.020
0.40	1331	1331	1340	1345	1349	0.264	0.245	0.235	0.223	0.209
0.45	1360	1360	1370	1374	1379	0.455	0.423	0.407	0.386	0.364
0.50	1390	1389	1399	1404	1408	0.604	0.562	0.541	0.514	0.484
0.55	1418	1418	1428	1433	1437	0.712	0.662	0.638	0.606	0.571
0.60	1447	1447	1457	1461	1466	0.778	0.724	0.698	0.664	0.626
0.65	1475	1475	1485	1490	1495	0.805	0.750	0.723	0.688	0.648
0.70	1503	1503	1513	1518	1523	0.794	0.740	0.713	0.679	0.640
0.75	1531	1530	1541	1546	1551	0.748	0.697	0.671	0.639	0.603
0.80	1558	1557	1568	1573	1578	0.666	0.621	0.599	0.570	0.538
0.85	1585	1584	1595	1601	1606	0.552	0.514	0.496	0.473	0.446
0.90	1611	1611	1622	1627	1633	0.404	0.376	0.363	0.346	0.326
0.95	1638	1637	1649	1654	1660	0.221	0.206	0.199	0.189	0.179
1	1664	1663	1675	1680	1686	0	0	0	0	0

[a] x_1 is the mole fraction of DMF in the DMF (1) + methanol (2) mixtures.

Table S18 Correlation volume and $\delta x_{1,3}$ values for hymecromone (3) in DMF (1) + ethanol (2) mixtures at several temperatures.

x_1[a]	V_{cor} ($cm^3 \cdot mol^{-1}$)					100 $\delta x_{1,3}$				
	293.15 K	298.15 K	303.15 K	308.15 K	313.15 K	293.15 K	298.15 K	303.15 K	308.15 K	313.15 K
0	1386	1391	1396	1401	1406	0	0	0	0	0
0.05	1396	1401	1406	1411	1417	-1.349	-1.302	-1.262	-1.238	-1.193
0.10	1408	1413	1418	1424	1429	-2.084	-2.005	-1.935	-1.893	-1.815
0.15	1421	1426	1432	1437	1442	-2.312	-2.218	-2.135	-2.086	-1.991
0.20	1435	1440	1446	1451	1457	-2.171	-2.082	-2.001	-1.952	-1.858
0.25	1450	1455	1461	1466	1472	-1.799	-1.725	-1.658	-1.618	-1.535
0.30	1465	1470	1476	1481	1487	-1.310	-1.258	-1.209	-1.180	-1.118
0.35	1480	1485	1491	1496	1502	-0.787	-0.757	-0.728	-0.712	-0.674
0.40	1495	1500	1506	1511	1517	-0.286	-0.277	-0.267	-0.262	-0.249
0.45	1510	1515	1521	1526	1532	0.157	0.150	0.144	0.139	0.130
0.50	1525	1530	1536	1541	1547	0.525	0.506	0.486	0.475	0.446
0.55	1540	1545	1550	1556	1561	0.809	0.781	0.752	0.736	0.692
0.60	1554	1559	1565	1570	1576	1.007	0.974	0.938	0.919	0.863
0.65	1568	1574	1579	1584	1590	1.121	1.084	1.045	1.025	0.962
0.70	1582	1588	1593	1599	1604	1.154	1.118	1.078	1.058	0.992
0.75	1596	1601	1607	1612	1618	1.113	1.078	1.040	1.022	0.957
0.80	1610	1615	1621	1626	1632	1.003	0.973	0.939	0.922	0.863
0.85	1623	1629	1634	1640	1645	0.831	0.807	0.779	0.765	0.716
0.90	1637	1642	1648	1653	1659	0.604	0.586	0.566	0.557	0.520
0.95	1650	1656	1661	1667	1673	0.325	0.316	0.306	0.301	0.281
1	1663	1669	1675	1680	1686	0	0	0	0	0

[a] x_1 is the mole fraction of DMF in the DMF (1) + ethanol (2) mixtures.

Table S19 Correlation volume and $\delta x_{1,3}$ values for hymecromone (3) in DMF (1) + *n*-propanol (2) mixtures at several temperatures.

x_1[a]	V_{cor} ($cm^3 \cdot mol^{-1}$)					100 $\delta x_{1,3}$				
	293.15 K	298.15 K	303.15 K	308.15 K	313.15 K	293.15 K	298.15 K	303.15 K	308.15 K	313.15 K
0	1631	1636	1642	1648	1653	0	0	0	0	0
0.05	1631	1637	1642	1648	1654	-1.800	-1.750	-1.699	-1.650	-1.603
0.10	1632	1637	1643	1649	1655	-2.582	-2.493	-2.406	-2.321	-2.242
0.15	1633	1638	1644	1650	1656	-2.705	-2.599	-2.496	-2.397	-2.304
0.20	1634	1639	1645	1651	1657	-2.472	-2.367	-2.265	-2.168	-2.077
0.25	1635	1640	1646	1652	1658	-2.080	-1.988	-1.898	-1.813	-1.733
0.30	1636	1642	1647	1653	1659	-1.638	-1.564	-1.492	-1.423	-1.359
0.35	1638	1643	1649	1655	1661	-1.191	-1.137	-1.085	-1.035	-0.988
0.40	1639	1645	1650	1656	1662	-0.755	-0.722	-0.689	-0.657	-0.628
0.45	1641	1646	1652	1658	1664	-0.335	-0.321	-0.307	-0.293	-0.281
0.50	1643	1648	1654	1660	1666	0.059	0.057	0.055	0.052	0.049
0.55	1645	1650	1656	1662	1668	0.415	0.399	0.382	0.365	0.349
0.60	1646	1652	1658	1664	1670	0.710	0.682	0.654	0.626	0.600
0.65	1649	1654	1660	1666	1672	0.920	0.885	0.849	0.813	0.780
0.70	1651	1656	1662	1668	1674	1.026	0.986	0.946	0.906	0.869
0.75	1653	1658	1664	1670	1676	1.013	0.974	0.933	0.893	0.856
0.80	1655	1660	1666	1672	1678	0.884	0.848	0.811	0.774	0.740
0.85	1657	1662	1668	1674	1680	0.658	0.629	0.599	0.569	0.540
0.90	1659	1665	1670	1676	1682	0.380	0.361	0.339	0.319	0.298
0.95	1661	1667	1672	1678	1684	0.123	0.114	0.104	0.093	0.083
1	1664	1669	1675	1680	1686	0	0	0	0	0

[a] x_1 is the mole fraction of DMF (1) in the DMF (1) + *n*-propanol (2) mixtures.