Supplementary information for:

Structure-making solvation of ferulic acid across protic and aprotic solvents: viscosity experiments, simulations, and implications for antioxidant function

Renato Tomaš[a], Olivera Politeo[a], Milan Vraneš[b], Moez Guettari[c], Safija Herenda[d], Martina Požar[e*]

[a]Faculty of Chemistry and Technology, University of Split, Ruđera Boškovića 35, HR-21000 Split, Croatia

[b]Faculty of Sciences, University of Novi Sad, Trg Dositeja Obradovića 3, 21000 Novi Sad, Serbia

[c]University of Tunis, Preparatory Institute for Engineering studies of Tunis. Materials and Fluids Laboratory. Tunisia.

[d]Faculty of Science, University of Sarajevo, Zmaja od Bosne 35, 71 000 Sarajevo, Bosnia and Herzegovina

[e]Faculty of Science, University of Split, Ruđera Boškovića 33, HR-21000 Split, Croatia

*Corresponding author E-mail address: marpoz@pmfst.hr

1. Density and viscosity data

Table S1. Density, ρ and viscosity, η data for ferulic acid in MeOH at different concentrations and temperatures

273.15 K						
c / mol dm^{-3}	$c^{1/2}$ / (mol dm^{-3})$^{1/2}$	m / mol kg^{-1}	ρ / g cm^{-3}	η / mPa s	η_r	η_r -1
0	0	0	0.81040	0.7166		0
0.00809	0.08994	0.01000	0.81106	0.7250	1.0117	0.0117
0.02185	0.14782	0.02703	0.81243	0.7348	1.0254	0.0254
0.04357	0.20873	0.05406	0.81444	0.7493	1.0456	0.0456
0.08108	0.28475	0.10118	0.81706	0.7764	1.0834	0.0834
0.15881	0.39851	0.20002	0.82480	0.8328	1.1622	0.1622
0.22480	0.47413	0.28522	0.83180	0.8893	1.2410	0.2410
0.31299	0.55946	0.40275	0.83791	0.9626	1.3433	0.3433
0.36707	0.60586	0.47670	0.84131	1.0088	1.4078	0.4078
0.46024	0.67841	0.60548	0.84950	1.1092	1.5479	0.5479
0.52111	0.72188	0.69198	0.85426	1.1786	1.6447	0.6447
278.15 K						
0	0	0	0.80585	0.6692		0
0.00805	0.08972	0.01000	0.80675	0.6767	1.0112	0.0112
0.02173	0.14741	0.02703	0.80809	0.6852	1.0239	0.0239
0.04337	0.20825	0.05406	0.81060	0.7018	1.0487	0.0487
0.08061	0.28392	0.10118	0.81235	0.7190	1.0744	0.0744
0.15791	0.39738	0.20002	0.82011	0.7715	1.1529	0.1529
0.22351	0.47277	0.28522	0.82705	0.8259	1.2342	0.2342
0.31123	0.55788	0.40275	0.83320	0.8895	1.3292	0.3292
0.36502	0.60417	0.47670	0.83661	0.9306	1.3906	0.3906
0.45768	0.67652	0.60548	0.84477	1.0222	1.5275	0.5275
0.51826	0.71990	0.69198	0.84958	1.0842	1.6201	0.6201
283.15 K						
0	0	0	0.80089	0.6261		0
0.00800	0.08944	0.01000	0.80158	0.6315	1.0086	0.0086
0.02159	0.14693	0.02703	0.80291	0.6378	1.0187	0.0187
0.04306	0.20751	0.05406	0.80490	0.6498	1.0379	0.0379
0.08014	0.28309	0.10118	0.80764	0.6746	1.0775	0.0775
0.15696	0.39618	0.20002	0.81521	0.7179	1.1466	0.1466
0.22217	0.47135	0.28522	0.82210	0.7631	1.2188	0.2188
0.30941	0.55625	0.40275	0.82833	0.8227	1.3140	0.3140
0.36292	0.60243	0.47670	0.83180	0.8590	1.3720	0.3720
0.45513	0.67463	0.60548	0.84006	0.9398	1.5010	0.5010
0.51541	0.71792	0.69198	0.84491	0.9952	1.5895	0.5895
288.15 K						
0	0	0	0.79627	0.5833		0
0.00795	0.08916	0.01000	0.79686	0.5879	1.0079	0.0079
0.02146	0.14650	0.02703	0.79815	0.5938	1.0180	0.0180
0.04281	0.20690	0.05406	0.80016	0.6045	1.0363	0.0363
0.07968	0.28227	0.10118	0.80294	0.6260	1.0732	0.0732
0.15607	0.39506	0.20002	0.81058	0.6655	1.1409	0.1409
0.22094	0.47004	0.28522	0.81754	0.7061	1.2105	0.2105
0.30770	0.55471	0.40275	0.82376	0.7595	1.3021	0.3021
0.36091	0.60076	0.47670	0.82719	0.7923	1.3583	0.3583
0.45262	0.67277	0.60548	0.83543	0.8642	1.4816	0.4816
0.51255	0.71593	0.69198	0.84023	0.9136	1.5663	0.5663

Table S1. (continued)

293.15 K						
c / mol dm^{-3}	$c^{1/2}$ / (mol dm^{-3})$^{1/2}$	m / mol kg^{-1}	ρ / g cm^{-3}	η / mPa s	h_r	h_r -1
0	0	0	0.79140	0.5477		0
0.00791	0.08894	0.01000	0.79206	0.5531	1.0099	0.0099
0.02133	0.14606	0.02703	0.79338	0.5571	1.0172	0.0172
0.04255	0.20628	0.05406	0.79539	0.5666	1.0345	0.0345
0.07921	0.28144	0.10118	0.79823	0.5918	1.0805	0.0805
0.15511	0.39384	0.20002	0.80560	0.6208	1.1335	0.1135
0.21966	0.46868	0.28522	0.81279	0.6550	1.1959	0.1959
0.30589	0.55308	0.40275	0.81891	0.7041	1.2856	0.2856
0.35886	0.59905	0.47670	0.82249	0.7320	1.3365	0.3365
0.45011	0.67090	0.60548	0.83080	0.7966	1.4544	0.4544
0.50970	0.71393	0.69198	0.83556	0.8411	1.5357	0.5357
298.15 K						
0	0	0	0.78660	0.5098		0
0.00786	0.08866	0.01000	0.78730	0.5139	1.0080	0.0080
0.02121	0.14562	0.02703	0.78862	0.5182	1.0165	0.0165
0.04230	0.20567	0.05406	0.79065	0.5268	1.0333	0.0333
0.07874	0.28061	0.10118	0.79352	0.5458	1.0706	0.0706
0.15425	0.39274	0.20002	0.80111	0.5757	1.1293	0.1293
0.21838	0.46731	0.28522	0.80805	0.6082	1.1930	0.1930
0.30417	0.55152	0.40275	0.81430	0.6514	1.2778	0.2778
0.35682	0.59734	0.47670	0.81780	0.6772	1.3284	0.3284
0.44754	0.66899	0.60548	0.82606	0.7360	1.4437	0.4437
0.50685	0.71193	0.69198	0.83088	0.7764	1.5230	0.5230
303.15 K						
0	0	0	0.78180	0.4769		0
0.00781	0.08837	0.01000	0.78253	0.4803	1.0071	0.0071
0.02108	0.14518	0.02703	0.78386	0.4845	1.0159	0.0159
0.04204	0.20504	0.05406	0.78588	0.4922	1.0321	0.0321
0.07827	0.27977	0.10118	0.78881	0.5078	1.0648	0.0648
0.15333	0.39158	0.20002	0.79637	0.5364	1.1248	0.1248
0.21709	0.46593	0.28522	0.80330	0.5661	1.1870	0.1870
0.30242	0.54993	0.40275	0.80962	0.6049	1.2684	0.2684
0.35476	0.59561	0.47670	0.81308	0.6289	1.3187	0.3187
0.44500	0.66709	0.60548	0.82137	0.6818	1.4296	0.4296
0.50399	0.70992	0.69198	0.82620	0.7182	1.5060	0.5060
308.15 K						
0	0	0	0.77712	0.4482		0
0.00776	0.08809	0.01000	0.77781	0.4514	1.0069	0.0069
0.02095	0.14474	0.02703	0.77911	0.4552	1.0156	0.0156
0.04179	0.20443	0.05406	0.78115	0.4624	1.0317	0.0317
0.07781	0.27894	0.10118	0.78410	0.4780	1.0665	0.0665
0.15243	0.39043	0.20002	0.79169	0.5030	1.1223	0.1223
0.21585	0.46460	0.28522	0.79871	0.5286	1.1794	0.1794
0.30069	0.54836	0.40275	0.80499	0.5647	1.2599	0.2599
0.35270	0.59389	0.47670	0.80837	0.5867	1.3090	0.3090
0.44247	0.66519	0.60548	0.81670	0.6326	1.4114	0.4114
0.50115	0.70792	0.69198	0.82154	0.6643	1.4822	0.4822

Table S1. (continued)

313.15 K						
c / mol dm^{-3}	$c^{1/2}$ / (mol dm^{-3})$^{1/2}$	m / mol kg^{-1}	ρ / g cm^{-3}	η / mPa s	h_r	h_r -1
0		0	0.77090	0.4225		0
0.00770	0.08775	0.01000	0.77189	0.4252	1.0064	0.0064
0.02079	0.14419	0.02703	0.77322	0.4289	1.0151	0.0151
0.04148	0.20368	0.05406	0.77543	0.4353	1.0303	0.0303
0.07734	0.27810	0.10118	0.77939	0.4482	1.0608	0.0608
0.15147	0.38919	0.20002	0.78669	0.4721	1.1174	0.1174
0.21452	0.46317	0.28522	0.79379	0.4960	1.1740	0.1740
0.29901	0.54682	0.40275	0.80049	0.5287	1.2514	0.2514
0.35066	0.59217	0.47670	0.80370	0.5492	1.2999	0.2999
0.44000	0.66333	0.60548	0.81214	0.5915	1.4000	0.4000
0.49808	0.70574	0.69198	0.81650	0.6208	1.4693	0.4693
318.15 K						
0	0	0	0.76661	0.3995		0
0.00766	0.08752	0.01000	0.76783	0.4017	1.0055	0.0055
0.02068	0.14379	0.02703	0.76893	0.4053	1.0145	0.0145
0.04126	0.20312	0.05406	0.77122	0.4112	1.0293	0.0293
0.07706	0.27760	0.10118	0.77660	0.4223	1.0571	0.0571
0.15073	0.38824	0.20002	0.78285	0.4443	1.1121	0.1121
0.21326	0.46180	0.28522	0.78910	0.4646	1.1630	0.1630
0.29773	0.54565	0.40275	0.79706	0.4947	1.2383	0.2383
0.34940	0.59110	0.47670	0.80081	0.5142	1.2871	0.2871
0.43830	0.66204	0.60548	0.80900	0.5499	1.3765	0.3765
0.49642	0.70457	0.69198	0.81379	0.5750	1.4393	0.4393
323.15 K						
0	0	0	0.76177	0.3804		0
0.00762	0.08729	0.01000	0.76305	0.3820	1.0042	0.0042
0.02055	0.14334	0.02703	0.76411	0.3850	1.0121	0.0121
0.04100	0.20249	0.05406	0.76641	0.3909	1.0276	0.0276
0.07661	0.27679	0.10118	0.77208	0.4000	1.0515	0.0515
0.14982	0.38707	0.20002	0.77813	0.4211	1.1070	0.1070
0.21196	0.46039	0.28522	0.78429	0.4398	1.1562	0.1562
0.29600	0.54406	0.40275	0.79243	0.4668	1.2271	0.2271
0.34740	0.58940	0.47670	0.79621	0.4854	1.2760	0.2760
0.43584	0.66018	0.60548	0.80446	0.5162	1.3570	0.3570
0.49368	0.70263	0.69198	0.80930	0.5400	1.4196	0.4196

Table S2. Density, ρ and viscosity, η data for ferulic acid in EtOH at different concentrations and temperatures

273.15 K						
c / mol dm^{-3}	$c^{1/2}$ / (mol dm^{-3})$^{1/2}$	m / mol kg^{-1}	ρ / g cm^{-3}	η / mPa s	η_r	η_r -1
0	0	0	0.80863	1.7891		0
0.00870	0.09327	0.01077	0.80946	1.8156	1.0148	0.0148
0.08274	0.28765	0.10346	0.81584	1.9595	1.0952	0.0952
0.12713	0.35655	0.15992	0.81965	2.0560	1.1492	0.1492
0.15372	0.39207	0.19404	0.82205	2.1180	1.1838	0.1838
0.19616	0.44290	0.24909	0.82560	2.2153	1.2382	0.2382
0.23952	0.48941	0.30601	0.82923	2.3199	1.2967	0.2967
0.27320	0.52269	0.35065	0.83218	2.4098	1.3469	0.3469
0.30692	0.55401	0.39580	0.83505	2.4994	1.3970	0.3970
0.34718	0.58922	0.45028	0.83845	2.6135	1.4608	0.4608
0.37663	0.61370	0.49052	0.84095	2.7008	1.5096	0.5096
278.15 K						
0	0	0	0.80429	1.6238		0
0.00865	0.09302	0.01077	0.80510	1.6459	1.0136	0.0136
0.08231	0.28690	0.10346	0.81157	1.7727	1.0917	0.0917
0.12647	0.35563	0.15992	0.81542	1.8573	1.1438	0.1438
0.15294	0.39108	0.19404	0.81790	1.9114	1.1771	0.1771
0.19515	0.44176	0.24909	0.82135	1.9958	1.2291	0.2291
0.23826	0.48812	0.30601	0.82488	2.0864	1.2849	0.2849
0.27179	0.52134	0.35065	0.82789	2.1647	1.3331	0.3331
0.30532	0.55256	0.39580	0.83068	2.2421	1.3808	0.3808
0.34537	0.58768	0.45028	0.83408	2.3412	1.4418	0.4418
0.37467	0.61210	0.49052	0.83658	2.4169	1.4884	0.4884
283.15 K						
0	0	0	0.79994	1.4684		0
0.00860	0.09276	0.01077	0.80061	1.4864	1.0123	0.0123
0.08186	0.28610	0.10346	0.80707	1.5965	1.0872	0.0872
0.12578	0.35466	0.15992	0.81095	1.6704	1.1376	0.1376
0.15206	0.38995	0.19404	0.81320	1.7169	1.1692	0.1692
0.19407	0.44054	0.24909	0.81682	1.7884	1.2179	0.2179
0.23698	0.48681	0.30601	0.82045	1.8641	1.2695	0.2695
0.27031	0.51991	0.35065	0.82337	1.9334	1.3167	0.3167
0.30368	0.55107	0.39580	0.82623	2.0000	1.3620	0.3620
0.34352	0.58611	0.45028	0.82961	2.0847	1.4197	0.4197
0.37267	0.61046	0.49052	0.83210	2.1499	1.4641	0.4641
288.15 K						
0	0	0	0.79560	1.3293		0
0.00856	0.09252	0.01077	0.79639	1.3435	1.0107	0.0107
0.08141	0.28533	0.10346	0.80269	1.4396	1.0830	0.0830
0.12509	0.35368	0.15992	0.80650	1.5033	1.1309	0.1309
0.15124	0.38890	0.19404	0.80882	1.5437	1.1613	0.1613
0.19302	0.43935	0.24909	0.81240	1.6050	1.2074	0.2074
0.23570	0.48549	0.30601	0.81602	1.6705	1.2567	0.2567
0.26887	0.51853	0.35065	0.81899	1.7297	1.3012	0.3012
0.30211	0.54964	0.39580	0.82194	1.7861	1.3436	0.3436
0.34174	0.58459	0.45028	0.82532	1.8592	1.3986	0.3986
0.37076	0.60890	0.49052	0.82784	1.9153	1.4408	0.4408

Table S2. (continued)

293.15 K						
c / mol dm^{-3}	$c^{1/2}$ / (mol dm^{-3})$^{1/2}$	m / mol kg^{-1}	ρ / g cm^{-3}	η / mPa s	η_r	η_r -1
0	0	0	0.79123	1.2044		0
0.00851	0.09226	0.01077	0.79204	1.2165	1.0100	0.0100
0.08098	0.28457	0.10346	0.79842	1.3006	1.0799	0.0799
0.12443	0.35275	0.15992	0.80224	1.3562	1.1260	0.1260
0.15045	0.38788	0.19404	0.80459	1.3912	1.1551	0.1551
0.19202	0.43820	0.24909	0.80816	1.4444	1.1993	0.1993
0.23449	0.48424	0.30601	0.81180	1.5006	1.2459	0.2459
0.26747	0.51717	0.35065	0.81472	1.5518	1.2884	0.2884
0.30050	0.54818	0.39580	0.81757	1.6004	1.3288	0.3288
0.33994	0.58305	0.45028	0.82097	1.6631	1.3809	0.3809
0.36880	0.60729	0.49052	0.82347	1.7112	1.4208	0.4208
298.15 K						
0	0	0	0.78690	1.0935		0
0.00847	0.09201	0.01077	0.78770	1.1031	1.0088	0.0088
0.08054	0.28379	0.10346	0.79406	1.1777	1.0770	0.0770
0.12376	0.35179	0.15992	0.79791	1.2265	1.1216	0.1216
0.14963	0.38682	0.19404	0.80018	1.2571	1.1496	0.1496
0.19098	0.43701	0.24909	0.80378	1.3027	1.1913	0.1913
0.23323	0.48293	0.30601	0.80744	1.3523	1.2367	0.2367
0.26604	0.51579	0.35065	0.81035	1.3956	1.2763	0.2763
0.29889	0.54671	0.39580	0.81320	1.4350	1.3123	0.3123
0.33814	0.58150	0.45028	0.81661	1.4913	1.3638	0.3638
0.36685	0.60568	0.49052	0.81911	1.5336	1.4025	0.4025
303.15 K						
0	0	0	0.78260	0.9951		0
0.00842	0.09175	0.01077	0.78334	1.0016	1.0065	0.0065
0.08010	0.28302	0.10346	0.78975	1.0685	1.0738	0.0738
0.12309	0.35084	0.15992	0.79360	1.1111	1.1166	0.1166
0.14883	0.38578	0.19404	0.79589	1.1386	1.1442	0.1442
0.18995	0.43583	0.24909	0.79946	1.1782	1.1840	0.1840
0.23197	0.48163	0.30601	0.80308	1.2188	1.2248	0.2248
0.26461	0.51440	0.35065	0.80600	1.2587	1.2649	0.2649
0.29729	0.54524	0.39580	0.80883	1.2966	1.3030	0.3030
0.33632	0.57993	0.45028	0.81223	1.3411	1.3477	0.3477
0.36488	0.60405	0.49052	0.81472	1.3758	1.3826	0.3826
308.15 K						
0	0	0	0.77823	0.9086		0
0.00837	0.09150	0.01077	0.77898	0.9154	1.0075	0.0075
0.07965	0.28223	0.10346	0.78535	0.9725	1.0703	0.0703
0.12240	0.34986	0.15992	0.78918	1.0093	1.1108	0.1108
0.14800	0.38471	0.19404	0.79146	1.0333	1.1372	0.1372
0.18891	0.43464	0.24909	0.79509	1.0690	1.1765	0.1765
0.23073	0.48035	0.30601	0.79881	1.1067	1.2180	0.2180
0.26318	0.51301	0.35065	0.80166	1.1413	1.2561	0.2561
0.29570	0.54378	0.39580	0.80451	1.1752	1.2934	0.2934
0.33454	0.57840	0.45028	0.80793	1.2161	1.3384	0.3384
0.36296	0.60246	0.49052	0.81042	1.2478	1.3733	0.3733

Table S2. (continued)

313.15 K						
c / mol dm^{-3}	$c^{1/2}$ / (mol dm^{-3})$^{1/2}$	m / mol kg^{-1}	ρ / g cm^{-3}	η / mPa s	η_r	η_r -1
0		0	0.77261	0.8811		0
0.00831	0.09118	0.01077	0.77351	0.8896	1.0096	0.0096
0.07910	0.28124	0.10346	0.77986	0.9585	1.0878	0.0878
0.12156	0.34865	0.15992	0.78371	0.9970	1.1315	0.1315
0.14700	0.38340	0.19404	0.78610	1.0180	1.1554	0.1554
0.18761	0.43314	0.24909	0.78963	1.0504	1.1921	0.1921
0.22911	0.47866	0.30601	0.79320	1.0812	1.2271	0.2271
0.26140	0.51127	0.35065	0.79622	1.1032	1.2521	0.2521
0.29371	0.54195	0.39580	0.79911	1.1234	1.2750	0.2750
0.33230	0.57645	0.45028	0.80251	1.1454	1.3000	0.3000
0.36054	0.60045	0.49052	0.80503	1.1599	1.3164	0.3164
318.15 K						
0	0	0	0.76811	0.8351		0
0.00826	0.09091	0.01077	0.76900	0.8430	1.0095	0.0095
0.07864	0.28043	0.10346	0.77540	0.9129	1.0932	0.0932
0.12086	0.34765	0.15992	0.77922	0.9495	1.1370	0.1370
0.14616	0.38230	0.19404	0.78161	0.9705	1.1621	0.1621
0.18657	0.43194	0.24909	0.78523	1.0000	1.1975	0.1975
0.22787	0.47735	0.30601	0.78888	1.0283	1.2313	0.2313
0.25994	0.50984	0.35065	0.79179	1.0467	1.2534	0.2534
0.29206	0.54043	0.39580	0.79462	1.0639	1.2740	0.2740
0.33043	0.57483	0.45028	0.79800	1.0808	1.2942	0.2942
0.35853	0.59877	0.49052	0.80054	1.0900	1.3052	0.3052
323.15 K						
0	0	0	0.76360	0.8040		0
0.00822	0.09065	0.01077	0.76452	0.8138	1.0122	0.0122
0.07818	0.27961	0.10346	0.77088	0.8840	1.0995	0.0995
0.12016	0.34664	0.15992	0.77472	0.9232	1.1483	0.1483
0.14533	0.38122	0.19404	0.77719	0.9432	1.1731	0.1731
0.18547	0.43066	0.24909	0.78060	0.9725	1.2096	0.2096
0.22652	0.47594	0.30601	0.78422	0.9984	1.2418	0.2418
0.25845	0.50838	0.35065	0.78725	1.0154	1.2629	0.2629
0.29041	0.53889	0.39580	0.79011	1.0295	1.2805	0.2805
0.32858	0.57322	0.45028	0.79352	1.0430	1.2973	0.2973
0.35652	0.59709	0.49052	0.79605	1.0500	1.3060	0.3060

Table S3. Density, ρ and viscosity, η data for ferulic acid in 2-PrOH at different concentrations and temperatures

273.15 K						
c / mol dm^{-3}	$c^{1/2}$ / (mol dm^{-3})$^{1/2}$	m / mol kg^{-1}	ρ / g cm^{-3}	η / mPa s	η_r	η_r -1
0	0	0	0.80240	4.5890		0
0.01053	0.10260	0.01314	0.80324	4.6357	1.0102	0.0102
0.07969	0.28229	0.10037	0.80943	5.0127	1.0923	0.0923
0.11805	0.34358	0.14946	0.81275	5.2435	1.1426	0.1426
0.14913	0.38618	0.18956	0.81570	5.4440	1.1863	0.1863
0.19466	0.44120	0.24898	0.81962	5.7538	1.2538	0.2538
0.23181	0.48147	0.29800	0.82290	6.0214	1.3121	0.3121
0.25863	0.50856	0.33371	0.82525	6.2390	1.3596	0.3596
0.30267	0.55015	0.39296	0.82900	6.5970	1.4376	0.4376
0.34463	0.58705	0.45000	0.83276	6.9648	1.5177	0.5177
0.38426	0.61989	0.50454	0.83622	7.3333	1.5980	0.5980
278.15 K						
0	0	0	0.79814	3.9450		0
0.01047	0.10233	0.01314	0.79900	3.9814	1.0092	0.0092
0.07927	0.28155	0.10037	0.80519	4.3069	1.0917	0.0917
0.11743	0.34268	0.14946	0.80848	4.5000	1.1407	0.1407
0.14837	0.38519	0.18956	0.81151	4.6697	1.1837	0.1837
0.19366	0.44006	0.24898	0.81540	4.9260	1.2487	0.2487
0.23059	0.48020	0.29800	0.81858	5.1500	1.3054	0.3054
0.25737	0.50731	0.33371	0.82120	5.3198	1.3485	0.3485
0.30121	0.54882	0.39296	0.82500	5.6121	1.4226	0.4226
0.34299	0.58566	0.45000	0.82881	5.9090	1.4978	0.4978
0.38247	0.61844	0.50454	0.83233	6.2047	1.5728	0.5728
283.15 K						
0	0	0	0.79379	3.3658		0
0.01042	0.10206	0.01314	0.79469	3.3850	1.0057	0.0057
0.07885	0.28080	0.10037	0.80088	3.6385	1.0810	0.0810
0.11680	0.34177	0.14946	0.80419	3.7975	1.1283	0.1283
0.14758	0.38416	0.18956	0.80719	3.9306	1.1678	0.1678
0.19261	0.43887	0.24898	0.81100	4.1438	1.2311	0.2311
0.22933	0.47889	0.29800	0.81411	4.3220	1.2841	0.2841
0.25596	0.50592	0.33371	0.81670	4.4899	1.3340	0.3340
0.29954	0.54731	0.39296	0.82044	4.7388	1.4079	0.4079
0.34100	0.58395	0.45000	0.82400	5.0022	1.4862	0.4862
0.38023	0.61663	0.50454	0.82745	5.2711	1.5661	0.5661
288.15 K						
0	0	0	0.78963	2.8607		0
0.01036	0.10179	0.01314	0.79051	2.8778	1.0060	0.0060
0.07843	0.28006	0.10037	0.79666	3.0878	1.0794	0.0794
0.11617	0.34084	0.14946	0.79985	3.2119	1.1228	0.1228
0.14680	0.38314	0.18956	0.80292	3.3274	1.1631	0.1631
0.19160	0.43772	0.24898	0.80673	3.4942	1.2214	0.2214
0.22817	0.47767	0.29800	0.80998	3.6387	1.2720	0.2720
0.25457	0.50455	0.33371	0.81228	3.7622	1.3151	0.3151
0.29798	0.54587	0.39296	0.81615	3.9588	1.3839	0.3839
0.33925	0.58245	0.45000	0.81977	4.1600	1.4542	0.4542
0.37823	0.61500	0.50454	0.82310	4.3666	1.5264	0.5264

Table S3. (continued)

293.15 K						
c / mol dm^{-3}	$c^{1/2}$ / (mol dm^{-3})$^{1/2}$	m / mol kg^{-1}	ρ / g cm^{-3}	η / mPa s	η_r	η_r -1
0	0	0	0.78540	2.4343		0
0.01031	0.10152	0.01314	0.78632	2.4563	1.0090	0.0090
0.07800	0.27929	0.10037	0.79230	2.6224	1.0773	0.0773
0.11556	0.33994	0.14946	0.79562	2.7305	1.1217	0.1217
0.14603	0.38213	0.18956	0.79870	2.8169	1.1572	0.1572
0.19058	0.43655	0.24898	0.80243	2.9599	1.2159	0.2159
0.22696	0.47640	0.29800	0.80567	3.0746	1.2630	0.2630
0.25327	0.50326	0.33371	0.80814	3.1928	1.3116	0.3116
0.29656	0.54457	0.39296	0.81226	3.3545	1.3780	0.3780
0.33775	0.58116	0.45000	0.81614	3.5293	1.4498	0.4498
0.37674	0.61379	0.50454	0.81985	3.7060	1.5224	0.5224
298.15 K						
0	0	0	0.78118	2.0800		0
0.01025	0.10124	0.01314	0.78203	2.1062	1.0126	0.0126
0.07758	0.27854	0.10037	0.78805	2.2447	1.0792	0.0792
0.11495	0.33904	0.14946	0.79140	2.3334	1.1218	0.1218
0.14524	0.38110	0.18956	0.79439	2.4043	1.1559	0.1559
0.18956	0.43539	0.24898	0.79817	2.5190	1.2111	0.2111
0.22575	0.47514	0.29800	0.80140	2.6110	1.2553	0.2553
0.25195	0.50194	0.33371	0.80391	2.7000	1.2981	0.2981
0.29499	0.54313	0.39296	0.80796	2.8244	1.3579	0.3579
0.33597	0.57963	0.45000	0.81185	2.9570	1.4216	0.4216
0.37476	0.61218	0.50454	0.81555	3.0891	1.4851	0.4851
303.15 K						
0	0	0	0.77688	1.7934		0
0.01019	0.10097	0.01314	0.77778	1.8146	1.0118	0.0118
0.07716	0.27778	0.10037	0.78377	1.9320	1.0773	0.0773
0.11432	0.33811	0.14946	0.78706	2.0026	1.1166	0.1166
0.14447	0.38010	0.18956	0.79021	2.0617	1.1496	0.1496
0.18854	0.43421	0.24898	0.79387	2.1483	1.1979	0.1979
0.22453	0.47385	0.29800	0.79706	2.2160	1.2356	0.2356
0.25059	0.50059	0.33371	0.79959	2.2822	1.2726	0.2726
0.29340	0.54166	0.39296	0.80360	2.3700	1.3215	0.3215
0.33417	0.57808	0.45000	0.80750	2.4619	1.3728	0.3728
0.37277	0.61055	0.50454	0.81121	2.5511	1.4225	0.4225
308.15 K						
0	0	0	0.77262	1.5670		0
0.01014	0.10069	0.01314	0.77354	1.5812	1.0091	0.0091
0.07674	0.27702	0.10037	0.77949	1.6839	1.0746	0.0746
0.11370	0.33719	0.14946	0.78280	1.7448	1.1135	0.1135
0.14368	0.37905	0.18956	0.78586	1.7953	1.1457	0.1457
0.18752	0.43304	0.24898	0.78958	1.8735	1.1956	0.1956
0.22332	0.47257	0.29800	0.79276	1.9400	1.2380	0.2380
0.24925	0.49925	0.33371	0.79531	1.9906	1.2703	0.2703
0.29184	0.54023	0.39296	0.79935	2.0755	1.3245	0.3245
0.33242	0.57656	0.45000	0.80325	2.1607	1.3789	0.3789
0.37082	0.60895	0.50454	0.80697	2.2444	1.4323	0.4323

Table S3. (continued)

313.15 K						
c / mol dm^{-3}	$c^{1/2}$ / (mol dm^{-3})$^{1/2}$	m / mol kg^{-1}	ρ / g cm^{-3}	η / mPa s	η_r	η_r -1
0	0	0	0.76644	1.3732		0
0.01006	0.10029	0.01314	0.76743	1.3858	1.0092	0.0092
0.07614	0.27594	0.10037	0.77341	1.4859	1.0821	0.0821
0.11283	0.33590	0.14946	0.77682	1.5635	1.1386	0.1386
0.14255	0.37756	0.18956	0.77971	1.6200	1.1797	0.1797
0.18610	0.43140	0.24898	0.78360	1.7377	1.2654	0.2654
0.22167	0.47082	0.29800	0.78692	1.8455	1.3439	0.3439
0.24738	0.49737	0.33371	0.78933	1.9280	1.4040	0.4040
0.28969	0.53822	0.39296	0.79344	2.0800	1.5147	0.5147
0.32983	0.57431	0.45000	0.79700	2.2422	1.6328	0.6328
0.36813	0.60673	0.50454	0.80111	2.4125	1.7568	0.7568
318.15 K						
0	0	0	0.76191	1.2863		0
0.01000	0.10000	0.01314	0.76292	1.3050	1.0145	0.0145
0.07570	0.27513	0.10037	0.76890	1.4289	1.1109	0.1109
0.11218	0.33493	0.14946	0.77233	1.4900	1.1584	0.1584
0.14173	0.37648	0.18956	0.77522	1.5470	1.2027	0.2027
0.18501	0.43013	0.24898	0.77900	1.6153	1.2558	0.2558
0.22040	0.46947	0.29800	0.78240	1.6701	1.2984	0.2984
0.24596	0.49594	0.33371	0.78481	1.7080	1.3278	0.3278
0.28802	0.53668	0.39296	0.78888	1.7669	1.3736	0.3736
0.32808	0.57279	0.45000	0.79278	1.8200	1.4149	0.4149
0.36608	0.60505	0.50454	0.79666	1.8666	1.4511	0.4511
323.15 K						
0	0	0	0.75742	1.2692		0
0.00994	0.09970	0.01314	0.75847	1.2900	1.0164	0.0164
0.07526	0.27433	0.10037	0.76440	1.4299	1.1266	0.1266
0.11152	0.33395	0.14946	0.76781	1.4935	1.1767	0.1767
0.14091	0.37538	0.18956	0.77070	1.5642	1.2324	0.2324
0.18394	0.42888	0.24898	0.77450	1.6325	1.2862	0.2862
0.21914	0.46812	0.29800	0.77791	1.6900	1.3315	0.3315
0.24445	0.49442	0.33371	0.78000	1.7285	1.3619	0.3619
0.28631	0.53508	0.39296	0.78419	1.7888	1.4094	0.4094
0.32620	0.57114	0.45000	0.78822	1.8400	1.4497	0.4497
0.36388	0.60323	0.50454	0.79188	1.8811	1.4821	0.4821

Table S4. Density, ρ and viscosity, η data for ferulic acid in THF at different concentrations and temperatures

273.15 K						
c / mol dm^{-3}	$c^{1/2}$ / (mol dm^{-3})$^{1/2}$	m / mol kg^{-1}	ρ / g cm^{-3}	η / mPa s	η_r	η_r -1
0	0	0	0.90959	0.5390		0
0.01815	0.13472	0.02000	0.91100	0.5495	1.0195	0.0195
0.08508	0.29168	0.09463	0.91555	0.5924	1.0991	0.0991
0.13168	0.36287	0.14745	0.91860	0.6240	1.1577	0.1577
0.17009	0.41242	0.19144	0.92150	0.6509	1.2076	0.2076
0.21158	0.45998	0.23961	0.92409	0.6847	1.2703	0.2703
0.26203	0.51189	0.29881	0.92780	0.7251	1.3453	0.3453
0.29618	0.54423	0.33947	0.93000	0.7593	1.4087	0.4087
0.33016	0.57459	0.38020	0.93249	0.7864	1.4590	0.4590
0.40530	0.63663	0.47186	0.93764	0.8591	1.5939	0.5939
0.46399	0.68117	0.54454	0.94218	0.9215	1.7096	0.7096
278.15 K						
0	0	0	0.90409	0.5127		0
0.01804	0.13432	0.02000	0.90554	0.5223	1.0187	0.0187
0.08457	0.29080	0.09463	0.91006	0.5618	1.0958	0.0958
0.13089	0.36179	0.14745	0.91311	0.5912	1.1531	0.1531
0.16908	0.41119	0.19144	0.91604	0.6157	1.2009	0.2009
0.21032	0.45861	0.23961	0.91860	0.6467	1.2614	0.2614
0.26046	0.51035	0.29881	0.92222	0.6837	1.3335	0.3335
0.29448	0.54266	0.33947	0.92464	0.7152	1.3950	0.3950
0.32825	0.57293	0.38020	0.92710	0.7400	1.4433	0.4433
0.40297	0.63480	0.47186	0.93226	0.8066	1.5732	0.5732
0.46129	0.67918	0.54454	0.93669	0.8637	1.6846	0.6846
283.15 K						
0	0	0	0.89858	0.4888		0
0.01793	0.13390	0.02000	0.90000	0.4975	1.0178	0.0178
0.08406	0.28992	0.09463	0.90458	0.5333	1.0910	0.0910
0.13011	0.36071	0.14745	0.90769	0.5600	1.1457	0.1457
0.16807	0.40997	0.19144	0.91057	0.5831	1.1929	0.1929
0.20910	0.45728	0.23961	0.91329	0.6111	1.2502	0.2502
0.25897	0.50889	0.29881	0.91697	0.6448	1.3191	0.3191
0.29276	0.54107	0.33947	0.91925	0.6738	1.3785	0.3785
0.32633	0.57125	0.38020	0.92168	0.6963	1.4245	0.4245
0.40065	0.63297	0.47186	0.92688	0.7570	1.5487	0.5487
0.45875	0.67731	0.54454	0.93154	0.8090	1.6551	0.6551
288.15 K						
0	0	0	0.89308	0.4661		0
0.01782	0.13350	0.02000	0.89455	0.4738	1.0165	0.0165
0.08354	0.28903	0.09463	0.89900	0.5061	1.0858	0.0858
0.12933	0.35962	0.14745	0.90222	0.5313	1.1399	0.1399
0.16706	0.40873	0.19144	0.90509	0.5520	1.1843	0.1843
0.20784	0.45590	0.23961	0.90777	0.5776	1.2392	0.2392
0.25744	0.50739	0.29881	0.91155	0.6086	1.3057	0.3057
0.29104	0.53948	0.33947	0.91386	0.6353	1.3630	0.3630
0.32442	0.56958	0.38020	0.91629	0.6556	1.4066	0.4066
0.39832	0.63113	0.47186	0.92150	0.7113	1.5261	0.5261
0.45602	0.67530	0.54454	0.92600	0.7599	1.6303	0.6303

Table S4. (continued)

293.15 K						
c / mol dm^{-3}	$c^{1/2}$ / (mol dm^{-3})$^{1/2}$	m / mol kg^{-1}	ρ / g cm^{-3}	η / mPa s	η_r	η_r -1
0	0	0	0.88759	0.4435		0
0.01771	0.13308	0.02000	0.88900	0.4508	1.0165	0.0165
0.08304	0.28816	0.09463	0.89363	0.4808	1.0841	0.0841
0.12855	0.35854	0.14745	0.89679	0.5040	1.1364	0.1364
0.16606	0.40750	0.19144	0.89966	0.5232	1.1797	0.1797
0.20660	0.45453	0.23961	0.90235	0.5466	1.2325	0.2325
0.25591	0.50587	0.29881	0.90612	0.5750	1.2965	0.2965
0.28934	0.53790	0.33947	0.90850	0.5999	1.3526	0.3526
0.32251	0.56790	0.38020	0.91088	0.6184	1.3944	0.3944
0.39599	0.62928	0.47186	0.91611	0.6695	1.5096	0.5096
0.45351	0.67343	0.54454	0.92090	0.7133	1.6083	0.6083
298.15 K						
0	0	0	0.88211	0.4227		0
0.01760	0.13267	0.02000	0.88355	0.4290	1.0149	0.0149
0.08253	0.28728	0.09463	0.88815	0.4573	1.0819	0.0819
0.12776	0.35744	0.14745	0.89130	0.4788	1.1327	0.1327
0.16505	0.40626	0.19144	0.89420	0.4965	1.1746	0.1746
0.20537	0.45318	0.23961	0.89699	0.5190	1.2278	0.2278
0.25438	0.50436	0.29881	0.90071	0.5447	1.2886	0.2886
0.28761	0.53629	0.33947	0.90308	0.5675	1.3426	0.3426
0.32060	0.56622	0.38020	0.90550	0.5844	1.3825	0.3825
0.39367	0.62743	0.47186	0.91073	0.6314	1.4937	0.4937
0.45088	0.67147	0.54454	0.91555	0.6711	1.5877	0.5877
303.15 K						
0	0	0	0.87660	0.4038		0
0.01749	0.13226	0.02000	0.87801	0.4099	1.0151	0.0151
0.08202	0.28640	0.09463	0.88270	0.4356	1.0788	0.0788
0.12700	0.35637	0.14745	0.88599	0.4555	1.1280	0.1280
0.16406	0.40504	0.19144	0.88881	0.4720	1.1689	0.1689
0.20410	0.45178	0.23961	0.89144	0.4929	1.2207	0.2207
0.25285	0.50284	0.29881	0.89529	0.5166	1.2793	0.2793
0.28589	0.53469	0.33947	0.89769	0.5378	1.3318	0.3318
0.31865	0.56450	0.38020	0.90000	0.5533	1.3702	0.3702
0.39134	0.62557	0.47186	0.90535	0.5965	1.4772	0.4772
0.44815	0.66944	0.54454	0.91000	0.6333	1.5684	0.5684
308.15 K						
0	0	0	0.87111	0.3860		0
0.01739	0.13185	0.02000	0.87266	0.3919	1.0153	0.0153
0.08151	0.28550	0.09463	0.87719	0.4156	1.0767	0.0767
0.12620	0.35525	0.14745	0.88040	0.4344	1.1254	0.1254
0.16304	0.40379	0.19144	0.88333	0.4496	1.1648	0.1648
0.20286	0.45040	0.23961	0.88600	0.4684	1.2135	0.2135
0.25132	0.50132	0.29881	0.88986	0.4908	1.2715	0.2715
0.28418	0.53308	0.33947	0.89230	0.5108	1.3233	0.3233
0.31677	0.56282	0.38020	0.89468	0.5245	1.3588	0.3588
0.38903	0.62372	0.47186	0.90000	0.5647	1.4630	0.4630
0.44568	0.66759	0.54454	0.90500	0.5999	1.5541	0.5541

Table S4. (continued)

313.15 K						
c / mol dm^{-3}	$c^{1/2}$ / (mol dm^{-3})$^{1/2}$	m / mol kg^{-1}	ρ / g cm^{-3}	η / mPa s	η_r	η_r -1
0	0	0	0.86560	0.3700		0
0.01727	0.13143	0.02000	0.86700	0.3749	1.0132	0.0132
0.08098	0.28457	0.09463	0.87151	0.3964	1.0714	0.0714
0.12538	0.35409	0.14745	0.87469	0.4150	1.1216	0.1216
0.16197	0.40246	0.19144	0.87752	0.4301	1.1624	0.1624
0.20151	0.44889	0.23961	0.88010	0.4477	1.2100	0.2100
0.24961	0.49961	0.29881	0.88380	0.4666	1.2611	0.2611
0.28219	0.53121	0.33947	0.88605	0.4882	1.3195	0.3195
0.31460	0.56089	0.38020	0.88855	0.5000	1.3514	0.3514
0.38629	0.62152	0.47186	0.89366	0.5377	1.4532	0.4532
0.44229	0.66505	0.54454	0.89811	0.5700	1.5405	0.5405
318.15 K						
0	0	0	0.86015	0.3551		0
0.01717	0.13102	0.02000	0.86171	0.3596	1.0127	0.0127
0.08047	0.28367	0.09463	0.86600	0.3799	1.0698	0.0698
0.12458	0.35296	0.14745	0.86909	0.3977	1.1200	0.1200
0.16095	0.40119	0.19144	0.87200	0.4119	1.1600	0.1600
0.20026	0.44750	0.23961	0.87466	0.4281	1.2056	0.2056
0.24806	0.49806	0.29881	0.87833	0.4466	1.2577	0.2577
0.28042	0.52955	0.33947	0.88050	0.4674	1.3162	0.3162
0.31264	0.55914	0.38020	0.88300	0.4788	1.3484	0.3484
0.38389	0.61959	0.47186	0.88811	0.5136	1.4464	0.4464
0.43957	0.66300	0.54454	0.89259	0.5444	1.5331	0.5331
323.15 K						
0	0	0	0.85462	0.3413		0
0.01705	0.13059	0.02000	0.85600	0.3456	1.0126	0.0126
0.07996	0.28278	0.09463	0.86055	0.3650	1.0694	0.0694
0.12375	0.35178	0.14745	0.86329	0.3824	1.1204	0.1204
0.15995	0.39993	0.19144	0.86655	0.3960	1.1603	0.1603
0.19899	0.44608	0.23961	0.86911	0.4111	1.2045	0.2045
0.24651	0.49650	0.29881	0.87285	0.4290	1.2570	0.2570
0.27867	0.52789	0.33947	0.87500	0.4499	1.3182	0.3182
0.31071	0.55741	0.38020	0.87756	0.4600	1.3478	0.3478
0.38152	0.61768	0.47186	0.88264	0.4933	1.4454	0.4454
0.43720	0.66121	0.54454	0.88777	0.5239	1.5350	0.5350

Table S5. Density, ρ and viscosity, η data for ferulic acid in DMSO at different concentrations and temperatures

293.15 K						
c / mol dm^{-3}	$c^{1/2}$ / (mol dm^{-3})$^{1/2}$	m / mol kg^{-1}	ρ / g cm^{-3}	η / mPa s	η_r	η_r -1
0	0	0	1.10040	2.2379		0
0.01777	0.13330	0.01619	1.10101	2.2725	1.0155	0.0155
0.10911	0.33032	0.10075	1.10415	2.4755	1.1062	0.1062
0.16243	0.40302	0.15117	1.10600	2.6109	1.1667	0.1667
0.20577	0.45362	0.19276	1.10746	2.7222	1.2164	0.2164
0.25550	0.50547	0.24115	1.10910	2.8689	1.2820	0.2820
0.30674	0.55384	0.29179	1.11080	3.0300	1.3539	0.3539
0.36557	0.60462	0.35093	1.11269	3.2182	1.4380	0.4380
0.42250	0.65000	0.40924	1.11444	3.4200	1.5282	0.5282
0.47193	0.68697	0.46071	1.11600	3.6000	1.6087	0.6087
0.50935	0.71369	0.50019	1.11722	3.7502	1.6758	0.6758
298.15 K						
0	0	0	1.09539	2.0300		0
0.01769	0.13300	0.01619	1.09600	2.0609	1.0152	0.0152
0.10861	0.32956	0.10075	1.09910	2.2383	1.1026	0.1026
0.16168	0.40209	0.15117	1.10089	2.3555	1.1603	0.1603
0.20481	0.45256	0.19276	1.10229	2.4579	1.2108	0.2108
0.25432	0.50430	0.24115	1.10400	2.5800	1.2709	0.2709
0.30532	0.55256	0.29179	1.10566	2.7184	1.3391	0.3391
0.36395	0.60328	0.35093	1.10777	2.8852	1.4213	0.4213
0.42066	0.64858	0.40924	1.10958	3.0638	1.5093	0.5093
0.46992	0.68551	0.46071	1.11125	3.2212	1.5868	0.5868
0.50728	0.71224	0.50019	1.11268	3.3515	1.6510	0.6510
303.15 K						
0	0	0	1.09031	1.8429		0
0.01761	0.13269	0.01619	1.09099	1.8699	1.0147	0.0147
0.10811	0.32880	0.10075	1.09402	2.0250	1.0988	0.0988
0.16081	0.40101	0.15117	1.09499	2.1277	1.1545	0.1545
0.20387	0.45151	0.19276	1.09720	2.2170	1.2030	0.2030
0.25316	0.50315	0.24115	1.09894	2.3266	1.2625	0.2625
0.30395	0.55132	0.29179	1.10070	2.4431	1.3257	0.3257
0.36234	0.60195	0.35093	1.10288	2.5888	1.4047	0.4047
0.41878	0.64713	0.40924	1.10462	2.7419	1.4878	0.4878
0.46780	0.68396	0.46071	1.10623	2.8772	1.5612	0.5612
0.50484	0.71052	0.50019	1.10733	2.9900	1.6224	0.6224
308.15 K						
0	0	0	1.08525	1.6809		0
0.01752	0.13238	0.01619	1.08585	1.7049	1.0143	0.0143
0.10761	0.32804	0.10075	1.08899	1.8422	1.0960	0.0960
0.16015	0.40019	0.15117	1.09050	1.9333	1.1502	0.1502
0.20294	0.45049	0.19276	1.09222	2.0111	1.1964	0.1964
0.25201	0.50201	0.24115	1.09399	2.1033	1.2513	0.2513
0.30258	0.55007	0.29179	1.09572	2.2089	1.3141	0.3141
0.36066	0.60055	0.35093	1.09777	2.3326	1.3877	0.3877
0.41694	0.64571	0.40924	1.09977	2.4697	1.4693	0.4693
0.46567	0.68240	0.46071	1.10120	2.5870	1.5391	0.5391
0.50266	0.70899	0.50019	1.10255	2.6888	1.5996	0.5996

Table S5. (continued)

313.15 K						
c / mol dm^{-3}	$c^{1/2}$ / (mol dm^{-3})$^{1/2}$	m / mol kg^{-1}	ρ / g cm^{-3}	η / mPa s	η_r	η_r -1
0	0	0	1.08021	1.5413		0
0.01744	0.13208	0.01619	1.08089	1.5655	1.0157	0.0157
0.10712	0.32729	0.10075	1.08400	1.6846	1.0930	0.0930
0.15947	0.39934	0.15117	1.08588	1.7599	1.1418	0.1418
0.20204	0.44948	0.19276	1.08735	1.8376	1.1922	0.1922
0.25087	0.50086	0.24115	1.08900	1.9070	1.2373	0.2373
0.30120	0.54882	0.29179	1.09075	1.9799	1.2846	0.2846
0.35903	0.59919	0.35093	1.09281	2.1111	1.3697	0.3697
0.41505	0.64424	0.40924	1.09479	2.2383	1.4522	0.4522
0.46364	0.68091	0.46071	1.09639	2.3409	1.5188	0.5188
0.50048	0.70745	0.50019	1.09777	2.4298	1.5765	0.5765
318.15 K						
0	0	0	1.07520	1.4244		0
0.01736	0.13177	0.01619	1.07577	1.4429	1.0130	0.0130
0.10661	0.32651	0.10075	1.07885	1.5509	1.0888	0.0888
0.15871	0.39838	0.15117	1.08070	1.6158	1.1344	0.1344
0.20112	0.44846	0.19276	1.08240	1.6846	1.1827	0.1827
0.24972	0.49972	0.24115	1.08402	1.7470	1.2265	0.2265
0.29981	0.54755	0.29179	1.08572	1.8125	1.2725	0.2725
0.35741	0.59784	0.35093	1.08788	1.9292	1.3544	0.3544
0.41320	0.64280	0.40924	1.08990	2.0398	1.4320	0.4320
0.46162	0.67943	0.46071	1.09161	2.1301	1.4954	0.4954
0.49820	0.70584	0.50019	1.09277	2.2075	1.5498	0.5498
323.15 K						
0	0	0	1.07062	1.2156		0
0.01729	0.13149	0.01619	1.07129	1.2444	1.0237	0.0237
0.10617	0.32584	0.10075	1.07444	1.3779	1.1335	0.1335
0.15803	0.39753	0.15117	1.07609	1.4730	1.2117	0.2117
0.20022	0.44746	0.19276	1.07760	1.5777	1.2979	0.2979
0.24869	0.49869	0.24115	1.07955	1.6200	1.3327	0.3327
0.29846	0.54631	0.29179	1.08080	1.6944	1.3939	0.3939
0.35592	0.59659	0.35093	1.08333	1.7998	1.4806	0.4806
0.41176	0.64168	0.40924	1.08611	1.8633	1.5328	0.5328
0.45967	0.67799	0.46071	1.08700	2.0000	1.6453	0.6453
0.49643	0.70458	0.50019	1.08888	2.0200	1.6617	0.6617

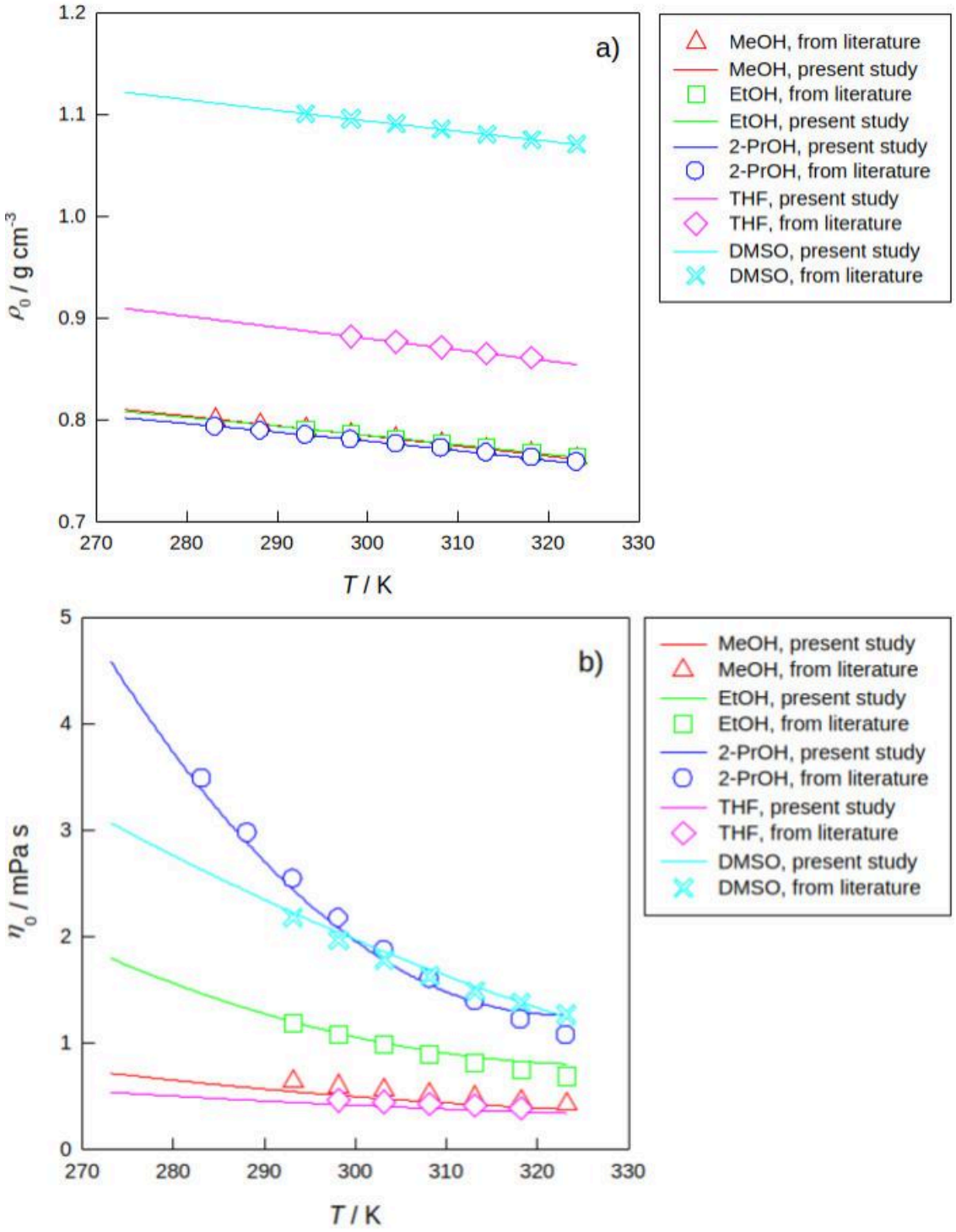

Figure S1. Comparison of our density (a) and viscosity date (b) of the investigated solvents with the literature (density: MeOH [1], EtOH [2], 2-PrOH [3], THF [4], DMSO [5], viscosity: MeOH [2], EtOH [2], 2-PrOH [3], THF [4], DMSO [5]). Full curves are polynomial fits from present study (see Tables S1–S5) while symbols represent literature data. In both cases density and viscosity of the solvents are given as a function of the temperature.

2. Simulation data

Pair correlation functions

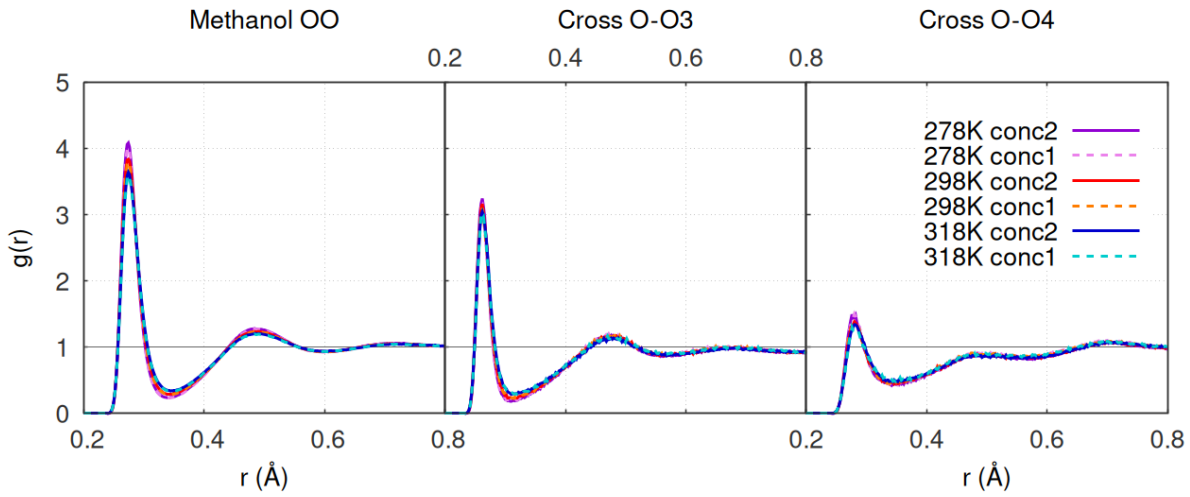

Figure S2. The pair correlation functions for the OO sites in: methanol (left), methanol O - FA O3 (center) and methanol O - FA O4 (right), for 3 temperatures (278 K - purple tones, 298 K - red tones, 318 K - blue tones) and 2 mole fractions (x(FA) = 0.01274 as conc1 and x(FA) = 0.02169 as conc2).

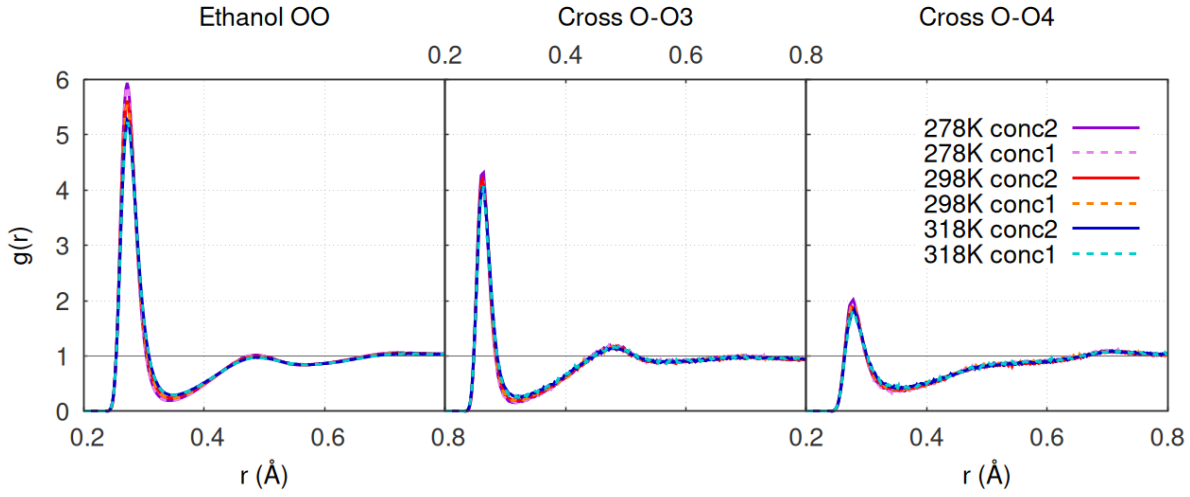

Figure S3. The pair correlation functions for the OO sites in: ethanol (left), ethanol O - FA O3 (center) and ethanol O - FA O4 (right), for 3 temperatures (278 K - purple tones, 298 K - red tones, 318 K - blue tones) and 2 mole fractions (x(FA) = 0.01134 as conc1 and x(FA) = 0.0221 as conc2).

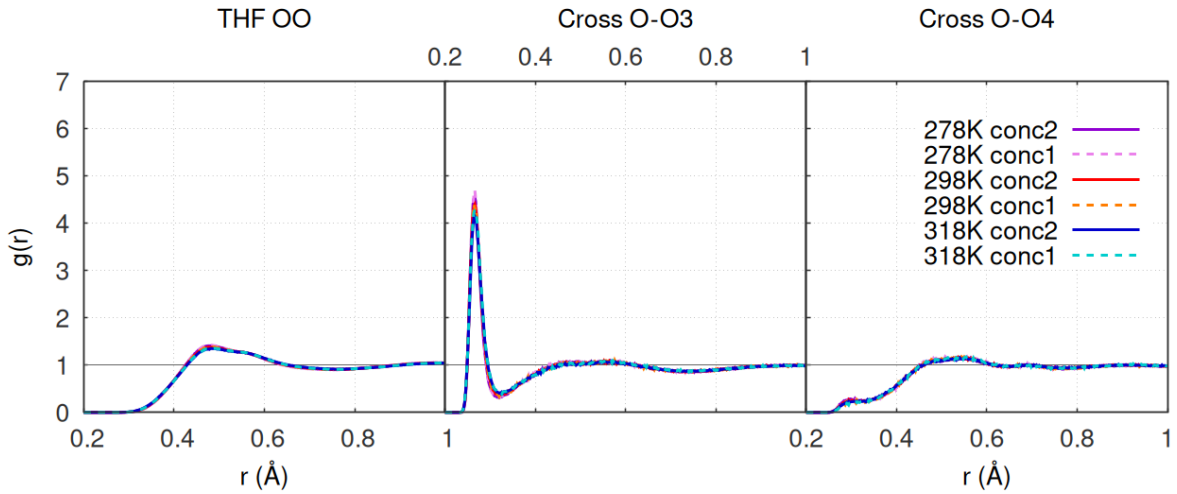

Figure S4. The pair correlation functions for the OO sites in: THF (left), THF O - FA O3 (center) and THF O - FA O4 (right), for 3 temperatures (278 K - purple tones, 298 K - red tones, 318 K - blue tones) and 2 mole fractions (x(FA) = 0.01698 as conc1 and x(FA) = 0.03778 as conc2).

Coordination numbers

Table S6. Coordination numbers for the first neighbors in MeOH - FA, EtOH - FA and THF - FA, calculated from the pair correlation functions presented in Figures S1, S2 and S3.

n(r)	**278 K**			**298 K**			**318 K**		
MeOH - FA									
	OO	**O3O**	**O4O**	**OO**	**O3O**	**O4O**	**OO**	**O3O**	**O4O**
xFA = 0.01274	1.980	0.016	0.015	1.979	0.017	0.015	1.952	0.017	0.014
xFA = 0.02169	1.951	0.028	0.024	1.940	0.029	0.025	1.922	0.028	0.022
EtOH - FA									
	OO	**O3O**	**O4O**	**OO**	**O3O**	**O4O**	**OO**	**O3O**	**O4O**
xFA = 0.01134	1.969	0.013	0.010	1.965	0.013	0.011	1.957	0.013	0.010
xFA = 0.0221	1.932	0.025	0.021	1.926	0.025	0.020	1.923	0.026	0.020
THF - FA									
	OO	**O3O**	**O4O**	**OO**	**O3O**	**O4O**	**OO**	**O3O**	**O4O**
xFA = 0.01698	12.165	0.017	0.001	12.018	0.017	0.001	11.764	0.017	0.001
xFA = 0.03778	11.841	0.036	0.003	11.607	0.036	0.003	11.368	0.036	0.002

Cluster probability distributions

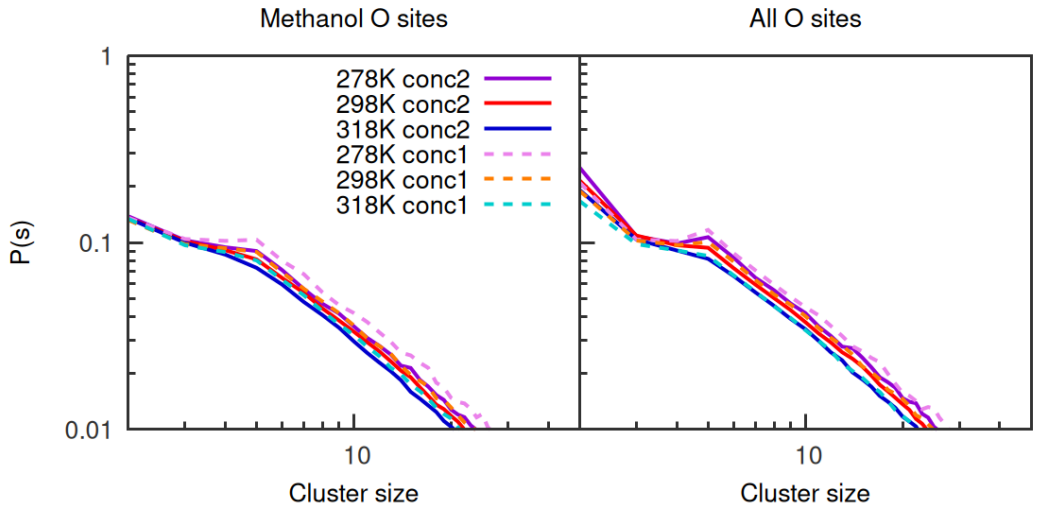

Figure S5. The cluster distribution probabilities for O sites in methanol (left panel) and all O sites in the binary mixture (right panel) for 3 temperatures (278 K - purple tones, 298 K - red tones, 318 K - blue tones) and 2 mole fractions (x(FA) = 0.01274 as conc1 and x(FA) = 0.02169 as conc2).

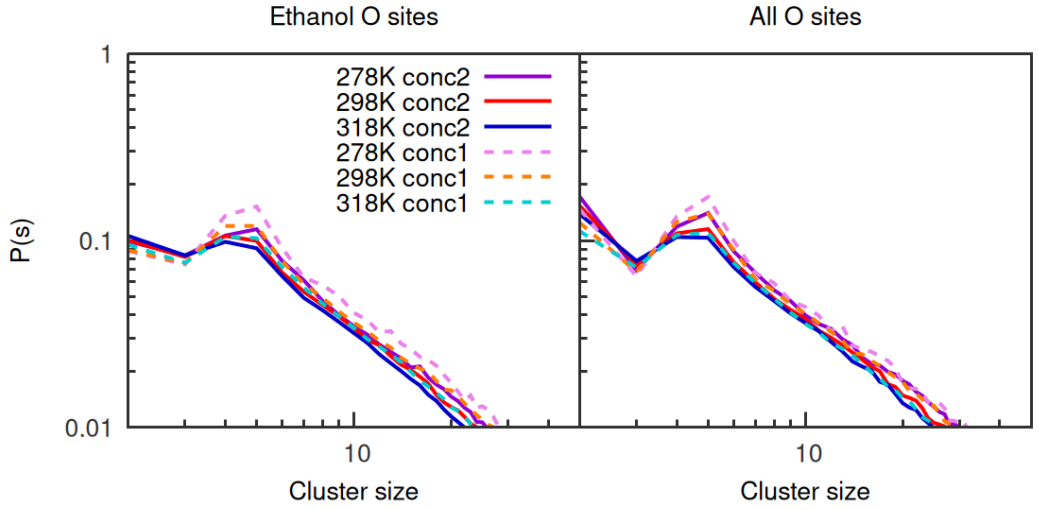

Figure S6. The cluster distribution probabilities for O sites in ethanol (left panel) and all O sites in the binary mixture (right panel) for 3 temperatures (278 K - purple tones, 298 K - red tones, 318 K - blue tones) and 2 mole fractions (x(FA) = 0.01134 as conc1 and x(FA) = 0.0221 as conc2).

Hydrogen bond autocorrelation functions

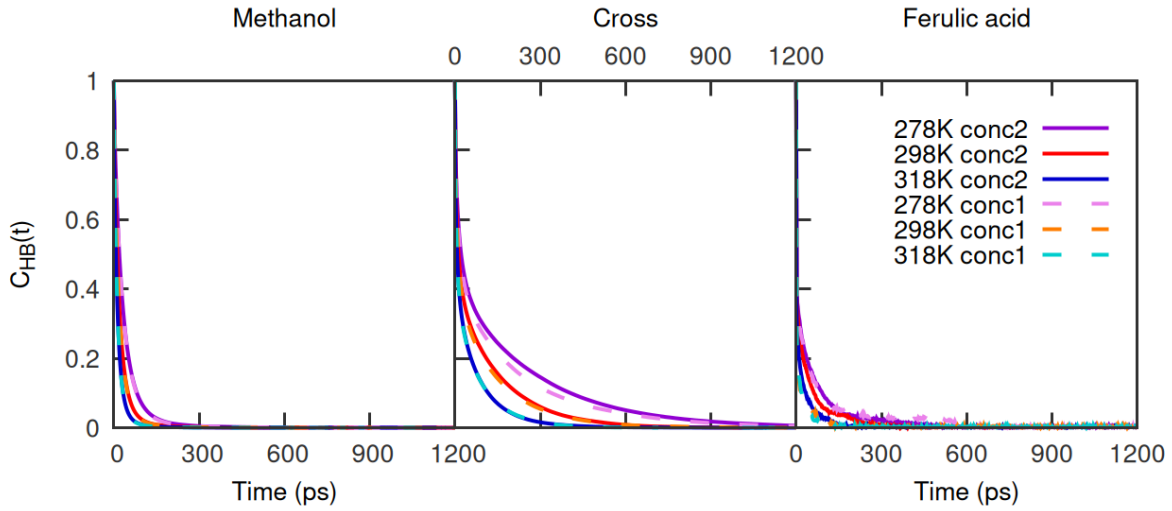

Figure S7. The continuous hydrogen bond autocorrelation functions C(t) for: methanol (left), methanol - FA (center) and FA (right), for 3 temperatures (278 K - purple tones, 298 K - red tones, 318 K - blue tones) and 2 mole fractions (x(FA) = 0.01274 as conc1 and x(FA) = 0.02169 as conc2).

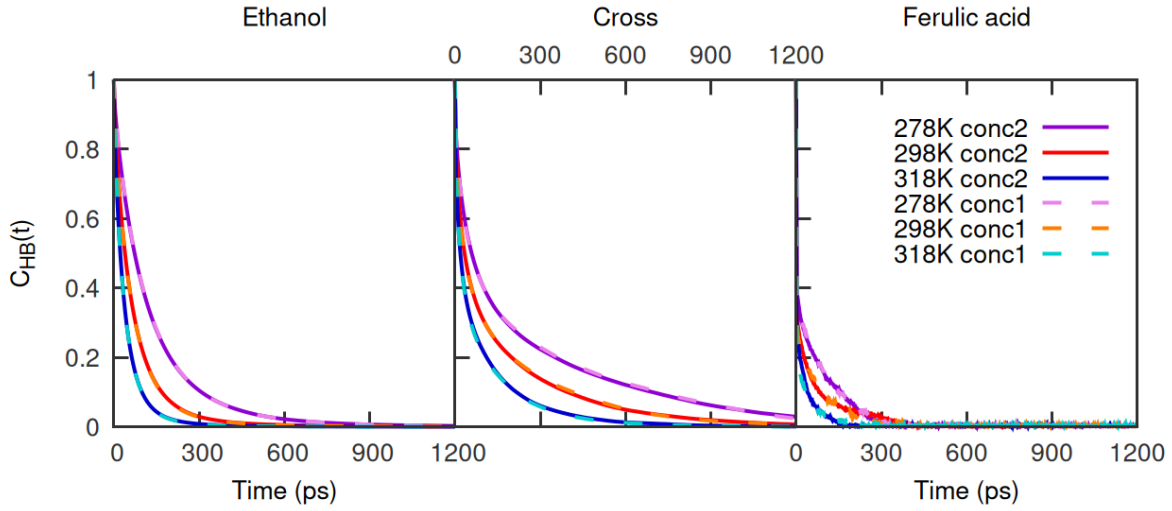

Figure S8. The continuous hydrogen bond autocorrelation functions C(t) for: ethanol (left), ethanol - FA (center) and FA (right), for 3 temperatures (278 K - purple tones, 298 K - red tones, 318 K - blue tones) and 2 mole fractions (x(FA) = 0.01134 as conc1 and x(FA) = 0.0221 as conc2).

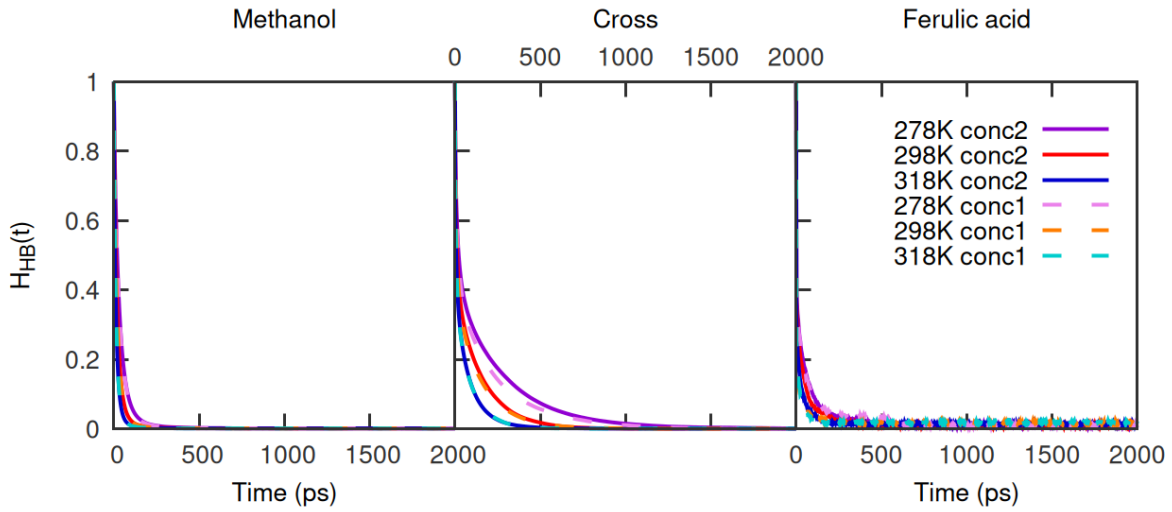

Figure S9. The intermittent hydrogen bond autocorrelation functions H(t) for: methanol (left), methanol - FA (center) and FA (right), for 3 temperatures (278 K - purple tones, 298 K - red tones, 318 K - blue tones) and 2 mole fractions (x(FA) = 0.01274 as conc1 and x(FA) = 0.02169 as conc2).

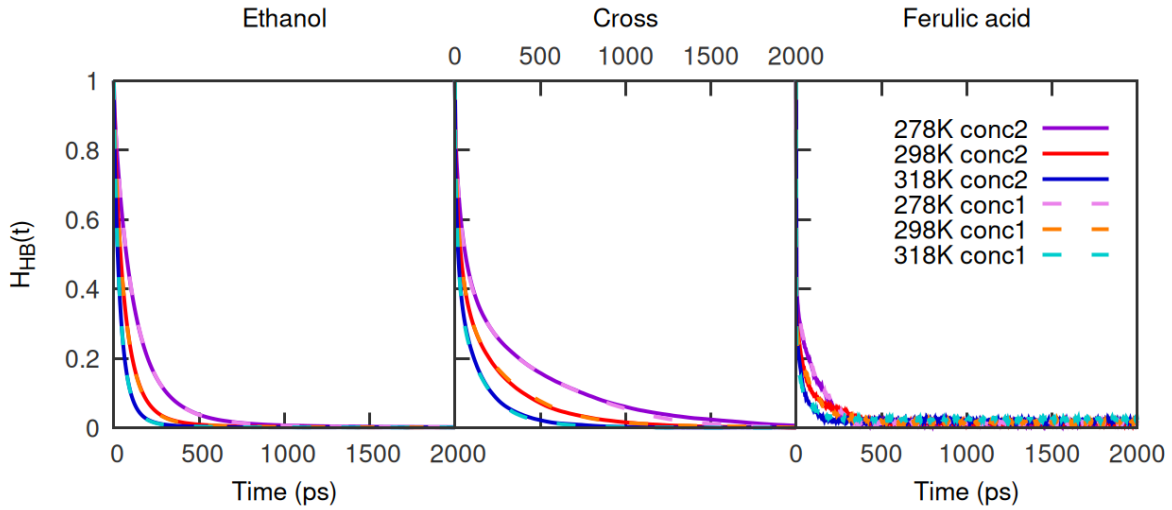

Figure S10. The intermittent hydrogen bond autocorrelation functions H(t) for: ethanol (left), ethanol - FA (center) and FA (right), for 3 temperatures (278 K - purple tones, 298 K - red tones, 318 K - blue tones) and 2 mole fractions (x(FA) = 0.01134 as conc1 and x(FA) = 0.0221 as conc2).

Hydrogen bond lifetimes

Table S7. Continuous hydrogen-bond lifetimes τ_{HB}^{cont} calculated from the autocorrelation function in Figures S6 and S7 for the MeOH - FA and EtOH - FA binary mixtures, respectively.

τ_{HB}^{cont} [ps]	**278 K**			**298 K**			**318 K**		
MeOH - FA									
	MeOH	**Cross**	**FA**	**MeOH**	**Cross**	**FA**	**MeOH**	**Cross**	**FA**
xFA = 0.01274	33.58	107.51	35.03	20.62	64.05	8.32	13.53	37.36	6.73
xFA = 0.02169	34.34	124.38	31.44	21.15	68.12	21.71	13.85	38.09	11.61
EtOH - FA									
	EtOH	**Cross**	**FA**	**EtOH**	**Cross**	**FA**	**EtOH**	**Cross**	**FA**
xFA = 0.01134	126.50	208.33	39.57	69.27	129.02	26.29	40.87	70.42	11.75
xFA = 0.0221	125.94	205.75	40.16	70.04	127.63	29.27	41.22	73.47	13.61

Table S8. Intermittent hydrogen-bond lifetimes τ_{HB}^{int} calculated from the autocorrelation function in Figures S8 and S9 for the MeOH - FA and EtOH - FA binary mixtures, respectively.

τ_{HB}^{int} [ps]	**278 K**			**298 K**			**318 K**		
MeOH - FA									
	MeOH	**Cross**	**FA**	**MeOH**	**Cross**	**FA**	**MeOH**	**Cross**	**FA**
xFA = 0.01274	35.86	108.98	57.86	22.88	64.51	49.71	15.77	38.41	53.02
xFA = 0.02169	36.63	129.00	50.75	23.46	68.73	46.05	16.05	38.95	45.92
EtOH - FA									
	EtOH	**Cross**	**FA**	**EtOH**	**Cross**	**FA**	**EtOH**	**Cross**	**FA**
xFA =	130.74	222.08	74.87	71.75	134.62	67.38	43.06	70.90	71.81

0.01134									
xFA = 0.0221	131.42	233.79	67.49	72.76	131.73	64.70	43.64	74.51	62.65

REFERENCES

1 A. Valtz, C. Coquelet and D. Richon, *Thermochim. Acta*, 2005, **428**, 185–191.
2 M. S. Alam, B. Ashokkumar and A. Mohammed Siddiq, *J. Mol. Liq.*, 2018, **251**, 458–469.
3 A. Ibrahim, C. Coquelet, A. Valtz and F. Espitalier, *Fluid Phase Equilib.*, 2025, **589**, 114254.
4 B. B. Dhaduk, Ch. B. Patel, and P. H. Parsania, *Russ. J. Phys. Chem. A*, 2017, **91**, 2495–2502.
5 M. S. Alam, B. Ashokkumar and A. M. Siddiq, *J. Mol. Liq.*, 2019, **281**, 584–597.