

Supporting Information

Solubility Enhancement of Hydrophobic Compounds in Aqueous Solutions Using Biobased Solvents as Hydrotropes

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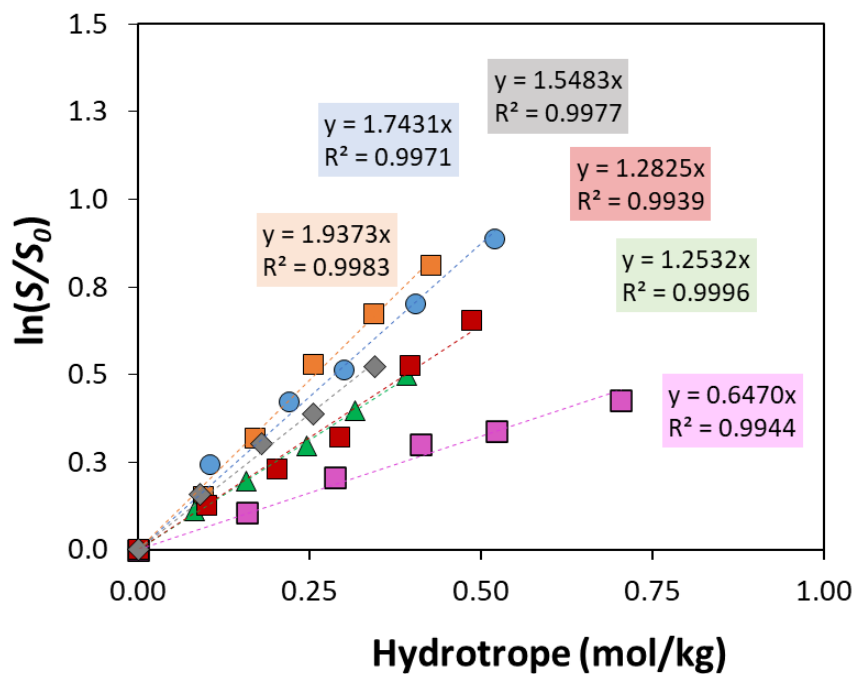


Figure S1. Setschenow constant for ferulic acid in aqueous solutions of biobased solvents:
(■) 1,6-hexanediol, (●) GVL, (◆) ethyl lactate, (■) 1,5-pentanediol, (▲) cyrene and
(■) 1,2-propanediol.

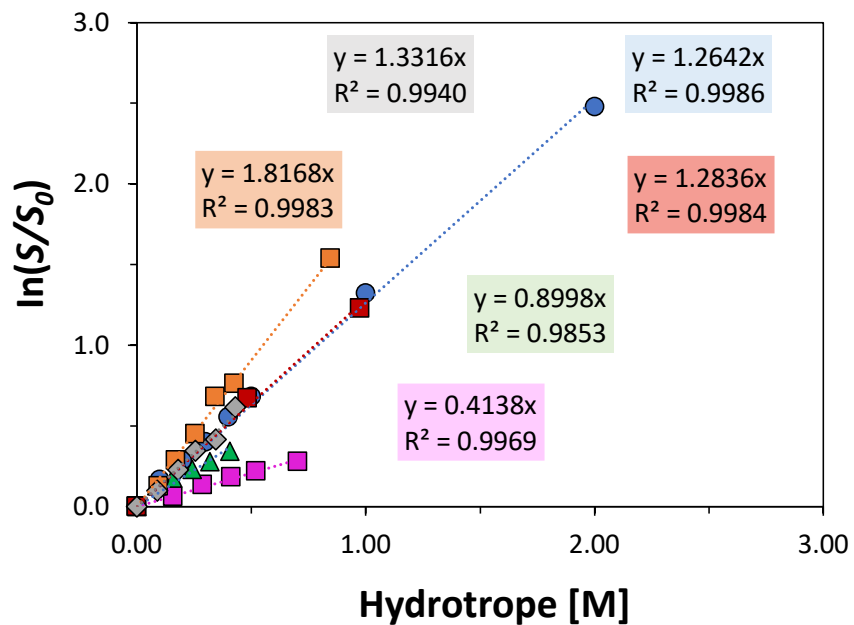


Figure S2. Setschenow constant for syringic acid in aqueous solutions of biobased solvents:
 (■) 1,6-hexanediol, (◆) ethyl lactate, (●) GVL, (■) 1,5-pentanediol, (▲) cyrene and
 (■) 1,2-propanediol.

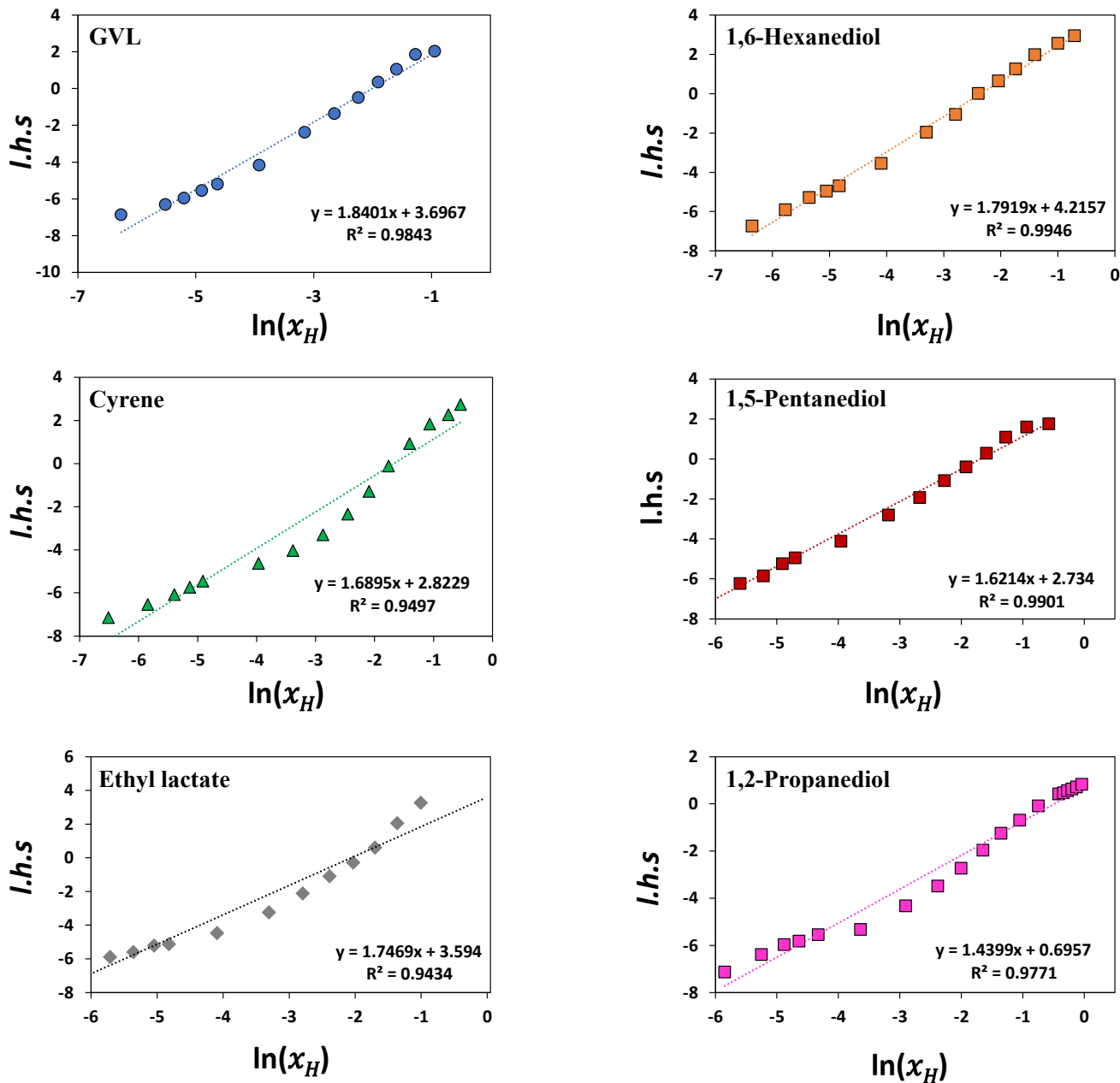


Figure S3. Representation of the linearized plot of the cooperative model of ferulic acid in the presence of aqueous solutions of biobased solvents. The y-axis is the left-hand side (*l.h.s.*) of Equation 3 as a function of the natural logarithm of hydrotrope mole fraction in the water/hydrotrope/solute at 303.15 K.

Dashed lines corresponds to the best fitting obtained using the method of least squares.

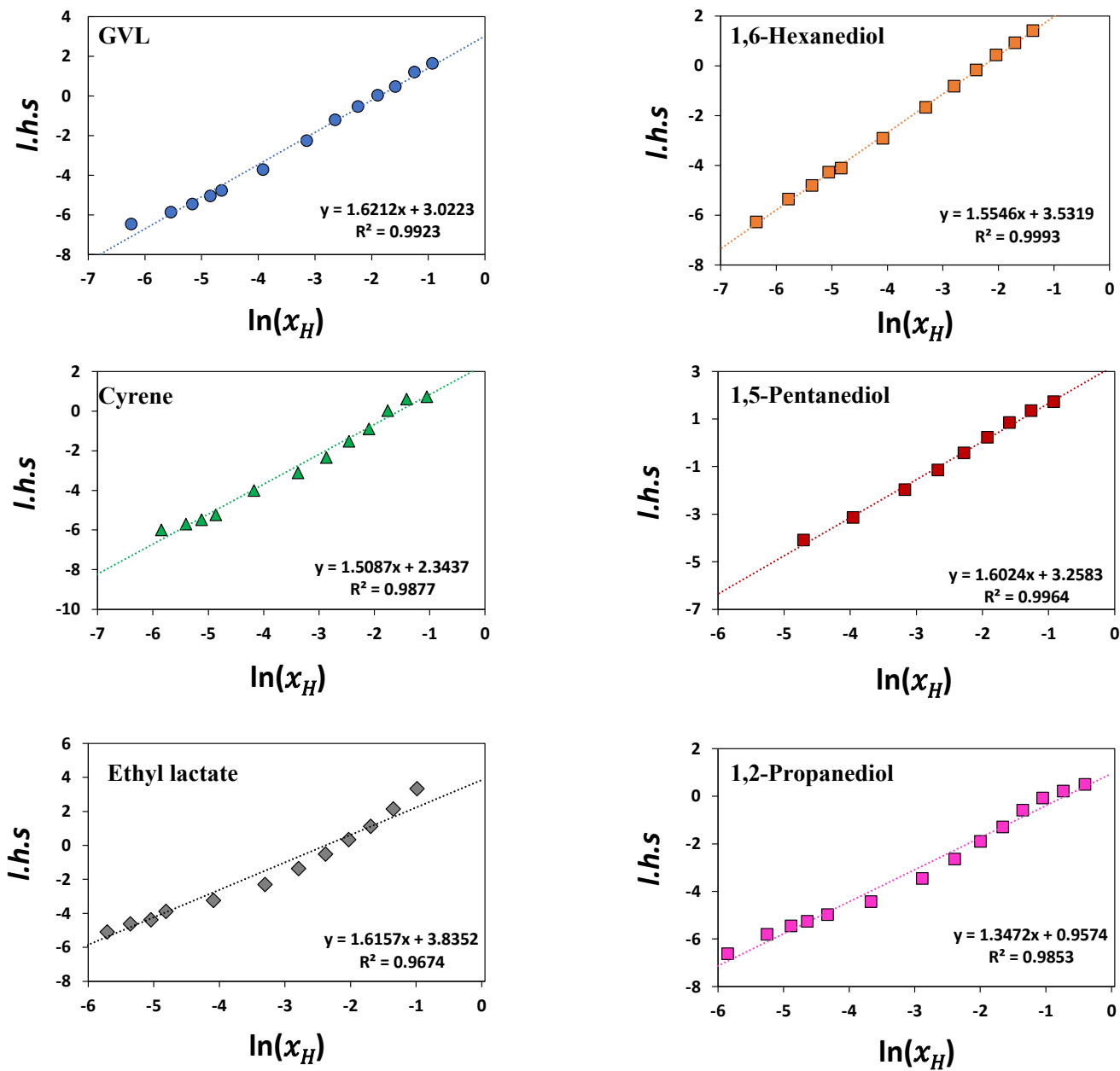


Figure S4. Representation of the linearized plot of the cooperative model of syringic acid in the presence of aqueous solutions of biobased solvents. The y-axis is the left-hand side (*l.h.s.*) of Equation 3 as a function of the natural logarithm of hydrotrope mole fraction in the water/hydrotrope/solute at 303.15 K. Dashed lines corresponds to the best fitting obtained using the method of least squares.

Tables

Table S1. Solubility (*S*) of ferulic acid in aqueous solutions of biobased solvents.

1,6-Hexanediol		Ethyl lactate		GVL		1,5-Pentanediol		Cyrene		1,2-Propanediol	
wt %	S (g/L)	wt %	S (g/L)	wt %	S (g/L) ¹	wt %	S (g/L)	wt %	S (g/L)	wt %	S (g/L)
0.00	0.83 ± 0.05	0.00	0.83 ± 0.05	0.00	0.83 ± 0.05	0.00	0.83 ± 0.05	0.00	0.83 ± 0.05	0.00	0.83 ± 0.05
1.13	0.97 ± 0.01	1.06	1.0 ± 0.1	1.05	1.06 ± 0.07	1.04	0.95 ± 0.04	1.05	0.93 ± 0.07	1.21	0.93 ± 0.01
2.00	1.15 ± 0.01	2.13	1.1 ± 0.2	2.21	1.23 ± 0.06	2.11	1.05 ± 0.01	2.02	1.01 ± 0.01	2.18	1.02 ± 0.05
3.02	1.41 ± 0.08	3.01	1.2 ± 0.2	3.01	1.39 ± 0.04	3.05	1.15 ± 0.01	3.15	1.12 ± 0.03	3.13	1.1 ± 0.2
4.05	1.6 ± 0.1	4.08	1.4 ± 0.1	4.04	1.68 ± 0.02	4.12	1.41 ± 0.01	4.05	1.2 ± 0.1	3.97	1.17 ± 0.03
5.04	1.9 ± 0.1	5.07	1.5 ± 0.2	5.21	2.03 ± 0.08	5.05	1.60 ± 0.05	5.01	1.4 ± 0.1	5.35	1.3 ± 0.2
10.01	4.03 ± 0.08	10.02	2.0 ± 0.4	10.14	4.18 ± 0.04	10.17	2.59 ± 0.06	12.07	2.05 ± 0.06	10.25	1.4 ± 0.1
20.09	15.0 ± 0.3	19.99	5 ± 1	20.00	19 ± 2	20.02	7.1 ± 0.1	20.02	3.01 ± 0.09	19.74	2.3 ± 0.2
30.09	30.6 ± 0.5	29.97	12 ± 2	29.96	45 ± 2	30.08	14.8 ± 0.3	29.92	5.3 ± 0.5	30.14	4.3 ± 0.2
40.09	59 ± 3	40.03	27.3 ± 0.2	40.27	84.2 ± 0.4	40.08	28.6 ± 0.8	40.13	11.8 ± 0.7	39.81	7.8 ± 0.3
49.98	77 ± 1	50.00	46.4 ± 0.8	50.09	130 ± 2	50.01	45 ± 1	50.15	28.0 ± 0.8	50.39	14.9 ± 0.4
58.88	91 ± 2	59.93	69.4 ± 0.5	59.82	163.7 ± 0.2	60.16	64 ± 1	60.04	60 ± 2	59.75	26 ± 1
68.94	103 ± 3	70.00	95 ± 2	70.04	192 ± 2	69.81	83 ± 4	70.44	91 ± 2	69.90	39.1 ± 0.5
80.28	109 ± 2	79.96	103 ± 2	79.82	196 ± 1	79.73	92.7 ± 0.4	79.82	109 ± 6	79.73	56 ± 1
87.52	111 ± 3	90.01	93 ± 2	89.93	191 ± 1	89.12	95 ± 1	87.58	114 ± 6	89.89	70 ± 1
nd	nd	91.99	90 ± 2	91.96	188 ± 2	91.86	92 ± 1	92.00	118.5 ± 0.1	92.02	71.6 ± 0.4
nd	nd	94.00	84 ± 3	93.69	183 ± 7	93.87	90 ± 2	94.05	113 ± 2	93.94	73.9 ± 0.8
nd	nd	95.99	83 ± 1	95.91	163 ± 4	95.80	88 ± 1	95.88	98.9 ± 0.8	95.85	75.9 ± 0.3
nd	nd	97.86	75 ± 2	97.82	140.6 ± 0.5	97.78	86 ± 1	98.03	74 ± 1	97.77	78.1 ± 0.5
nd	nd	100.00	69.3 ± 0.7	100.00	111 ± 3	100.00	84 ± 4	100.00	50 ± 2	100.00	81.2 ± 0.9

Table S2. Solubility (*S*) of syringic acid in aqueous solutions of biobased solvents. Data measured in this work or taken from the literature (blue data).^{1,2}

1,6-Hexanediol		Ethyl lactate		GVL		1,5-Pentanediol		Cyrene		1,2-Propanediol	
wt %	S (g/L)	wt %	S (g/L)	wt %	S (g/L) ¹	wt %	S (g/L)	wt %	S (g/L)	wt %	S (g/L)
0.00	1.48 ± 0.03	0.00	1.48 ± 0.03	0.00	1.48 ± 0.03	0.00	1.48 ± 0.03	0.00	1.48 ± 0.03	0.00	1.48 ± 0.03
1.13	1.68 ± 0.07	1.06	1.63 ± 0.04	1.07	1.7 ± 0.2	5.03	2.9 ± 0.1	1.13	1.69 ± 0.07	1.21	1.58 ± 0.07
2.00	1.97 ± 0.04	2.13	1.86 ± 0.02	2.15	2.0 ± 0.1	10.16	5.06 ± 0.06	2.02	1.77 ± 0.04	2.18	1.69 ± 0.03
3.02	2.3 ± 0.1	3.01	2.1 ± 0.2	3.10	2.2 ± 0.3	20.21	11.96 ± 0.03	3.11	1.86 ± 0.04	3.13	1.78 ± 0.02
4.05	2.92 ± 0.32	4.08	2.25 ± 0.04	4.22	2.6 ± 0.3	30.11	22.2 ± 0.2	4.08	1.96 ± 0.04	3.97	1.84 ± 0.05
5.04	3.2 ± 0.4	5.07	2.7 ± 0.1	5.13	2.9 ± 0.2	39.99	35.6 ± 0.8	5.22	2.09 ± 0.06	5.35	1.96 ± 0.09
10.15	6.89 ± 0.06	10.02	3.82 ± 0.01	10.15	5.5 ± 0.5	49.97	49.48 ± 0.07	10.00	3.52 ± 0.04	10.03	2.30 ± 0.05
20.02	18.0 ± 0.1	19.99	7.1 ± 0.4	20.06	17.6 ± 0.7	60.04	62.1 ± 0.2	20.00	6.3 ± 0.2	20.03	3.63 ± 0.03
30.05	33.5 ± 0.6	29.97	14.2 ± 0.3	30.03	41 ± 1	70.01	70.1 ± 0.4	30.00	11.55 ± 0.06	29.97	6.14 ± 0.04
39.82	49.4 ± 0.2	40.03	25 ± 1	40.13	64 ± 6	79.89	74.9 ± 0.5	40.00	22.03 ± 0.08	40.00	10.53 ± 0.06
49.84	65.0 ± 0.3	50.00	38 ± 1	50.11	88.7 ± 0.6	89.95	64 ± 2	50.00	34.8 ± 0.2	50.02	16.58 ± 0.01
59.99	76.4 ± 0.9	59.93	48.2 ± 0.8	59.72	107 ± 1	100.00	47.2 ± 0.6	60.00	59 ± 1	59.85	26.5 ± 0.4
69.55	86 ± 2	70.00	57 ± 1	70.26	133.5 ± 0.3	---	---	70.00	76 ± 1	69.83	35.2 ± 0.8
79.87	79.7 ± 0.2	79.96	61 ± 1	79.73	145.4 ± 0.5	---	---	79.82	78 ± 2	79.91	40.3 ± 0.4
89.34	65.7 ± 0.2	90.01	49 ± 2	89.32	126.0 ± 0.4	---	---	87.58	74 ± 4	89.96	45 ± 2
---	---	91.99	45 ± 1	91.96	116 ± 4	---	---	92.00	70.9 ± 0.3	92.02	44.1 ± 0.8
---	---	94.00	42 ± 1	93.58	104 ± 2	---	---	94.05	65 ± 1	93.94	44.3 ± 0.6
---	---	95.99	32.1 ± 0.3	95.91	91 ± 1	---	---	95.88	54.1 ± 0.6	94.21	44.2 ± 0.4
---	---	97.86	29 ± 1	97.82	72.4 ± 0.6	---	---	98.03	39.0 ± 0.8	97.77	44.5 ± 0.7
---	---	100.00	25.8 ± 0.5	100.00	46.9 ± 0.6	---	---	100.00	21.7 ± 0.2	100.00	42.8 ± 0.8

Table S3. Initial pH of biobased solvents at different concentrations.

1,6-Hexanediol				Ethyl lactate			GVL			1,5-Pentanediol			Cyrene			1,2-Propanediol							
wt %		pH		wt %	pH		wt %	pH		wt %	pH		wt %	pH		wt %	pH						
0.00	5.65	±	0.01	0.00	5.65	0.01	0.00	5.65	±	0.01	0.00	5.65	±	0.01	0.00	6.11	±	0.01	0.00	5.65	±	0.01	
1.13	6.24	±	0.01	1.06	3.07	0.03	1.05	3.85	±	0.01	1.04	5.96	±	0.01	1.05	4.28	±	0.01	1.21	6.05	±	0.01	
2.00	5.65	±	0.03	2.13	2.93	0.01	2.21	3.59	±	0.03	2.11	5.94	±	0.01	2.02	4.02	±	0.01	2.18	6.01	±	0.03	
3.02	5.70	±	0.01	3.01	2.82	0.01	3.01	3.52	±	0.01	3.05	5.91	±	0.03	3.15	3.99	±	0.01	3.13	5.98	±	0.01	
4.05	5.43	±	0.01	4.08	2.77	0.01	4.04	3.41	±	0.01	4.12	6.02	±	0.01	4.05	3.78	±	0.01	3.97	5.95	±	0.01	
5.04	5.37	±	0.01	5.07	2.72	0.02	5.21	3.37	±	0.01	5.05	5.95	±	0.02	5.01	3.71	±	0.03	5.35	5.94	±	0.01	
10.01	5.06	±	0.01	10.02	2.60	0.01	10.14	3.24	±	0.01	10.17	5.85	±	0.01	12.07	3.44	±	0.01	10.25	6.00	±	0.01	
20.09	5.35	±	0.03	19.99	2.47	0.03	20.00	3.16	±	0.01	20.02	5.79	±	0.01	20.02	3.22	±	0.03	19.74	5.98	±	0.01	
30.09	5.40	±	0.01	29.97	2.44	0.01	29.96	3.22	±	0.02	30.08	5.73	±	0.02	29.92	3.10	±	0.01	30.14	5.93	±	0.01	
40.09	5.57	±	0.01	40.03	2.41	0.01	40.27	3.37	±	0.01	40.08	5.72	±	0.01	40.13	3.01	±	0.02	39.81	5.81	±	0.01	
49.98	5.63	±	0.01	50.00	2.44	0.02	50.09	3.52	±	0.03	50.01	5.66	±	0.03	50.15	2.96	±	0.01	50.39	5.73	±	0.02	
58.88	5.90	±	0.01	59.93	2.37	0.01	59.82	3.65	±	0.01	60.16	5.63	±	0.02	60.04	2.89	±	0.01	59.75	5.68	±	0.01	
68.94	6.81	±	0.01	70.00	2.39	0.01	70.04	3.91	±	0.02	69.81	5.55	±	0.01	70.44	2.77	±	0.01	69.90	5.57	±	0.01	
80.28	6.68	±	0.01	79.96	2.31	0.02	79.82	4.21	±	0.01	79.73	5.49	±	0.03	79.82	2.63	±	0.01	79.73	5.34	±	0.0	
87.52	nd			90.01	nd			89.93	nd			89.12	nd			87.58	nd			89.89	nd		
---	---			91.99	nd			91.96	nd			91.86	nd			92.00	nd			92.02	nd		
---	---			94.00	nd			93.69	nd			93.87	nd			94.05	nd			93.94	nd		
---	---			95.99	nd			95.91	nd			95.80	nd			95.88	nd			95.85	nd		
---	---			97.86	nd			97.82	nd			97.78	nd			98.03	nd			97.77	nd		
---	---			100.00	nd			100.00	nd			100.00	nd			100.00	nd			100.00	nd		

nd - no data

Table S4. pH of aqueous solutions of biobased solvents after saturation with ferulic acid.

1,6-Hexanediol		Ethyl lactate		GVL		1,5-Pentanediol		Cyrene		1,2-Propanediol	
wt %	pH	wt %	pH	wt %	pH	wt %	pH	wt %	pH	wt %	pH
0.00	3.47 ± 0.01	0.00	3.47 ± 0.01	0.00	3.47 ± 0.01	0.00	3.47 ± 0.01	0.00	3.47 ± 0.01	0.00	3.47 ± 0.01
1.13	3.46 ± 0.01	1.06	2.44 ± 0.01	1.05	3.31 ± 0.10	1.04	3.44 ± 0.07	1.05	3.38 ± 0.01	1.21	3.56 ± 0.01
2.00	3.46 ± 0.01	2.13	2.22 ± 0.01	2.21	3.20 ± 0.01	2.11	3.46 ± 0.04	2.02	3.33 ± 0.01	2.18	3.55 ± 0.01
3.02	3.48 ± 0.01	3.01	2.12 ± 0.02	3.01	3.15 ± 0.03	3.05	3.42 ± 0.01	3.15	3.30 ± 0.01	3.13	3.54 ± 0.01
4.05	3.46 ± 0.01	4.08	2.03 ± 0.01	4.04	3.08 ± 0.03	4.12	3.41 ± 0.03	4.05	3.23 ± 0.01	3.97	3.53 ± 0.01
5.04	3.43 ± 0.01	5.07	1.98 ± 0.01	5.21	3.03 ± 0.02	5.05	3.40 ± 0.02	5.01	3.19 ± 0.01	5.35	3.52 ± 0.01
10.01	3.34 ± 0.01	10.02	1.81 ± 0.04	10.14	2.89 ± 0.01	10.17	3.31 ± 0.01	12.07	2.99 ± 0.03	10.25	3.49 ± 0.03
20.09	3.20 ± 0.01	19.99	1.64 ± 0.03	20.00	2.78 ± 0.03	20.02	3.20 ± 0.03	20.02	2.81 ± 0.01	19.74	3.41 ± 0.01
30.09	3.15 ± 0.01	29.97	1.31 ± 0.04	29.96	2.75 ± 0.01	30.08	3.17 ± 0.01	29.92	2.68 ± 0.01	30.14	3.34 ± 0.01
40.09	3.17 ± 0.01	40.03	1.23 ± 0.03	40.27	2.74 ± 0.01	40.08	3.11 ± 0.01	40.13	2.53 ± 0.01	39.81	3.30 ± 0.01
49.98	3.21 ± 0.02	50.00	1.19 ± 0.03	50.09	2.70 ± 0.01	50.01	3.22 ± 0.04	50.15	2.44 ± 0.01	50.39	3.28 ± 0.01
58.88	3.34 ± 0.01	59.93	1.16 ± 0.02	59.82	2.64 ± 0.04	60.16	3.28 ± 0.03	60.04	2.30 ± 0.01	59.75	3.25 ± 0.02
68.94	3.44 ± 0.04	70.00	1.19 ± 0.01	70.04	2.57 ± 0.01	69.81	3.40 ± 0.04	70.44	2.23 ± 0.01	69.90	3.22 ± 0.01
80.28	3.75 ± 0.01	79.96	1.24 ± 0.01	79.82	2.35 ± 0.03	79.73	3.70 ± 0.04	79.82	2.11 ± 0.01	79.73	3.19 ± 0.01
87.52	nd	90.01	nd	89.93	nd	89.12	nd	87.58	nd	89.89	nd
---	---	91.99	nd	91.96	nd	91.86	nd	92.00	nd	92.02	nd
---	---	94.00	nd	93.69	nd	93.87	nd	94.05	nd	93.94	nd
---	---	95.99	nd	95.91	nd	95.80	nd	95.88	nd	95.85	nd
---	---	97.86	nd	97.82	nd	97.78	nd	98.03	nd	97.77	nd
---	---	100.00	nd	100.00	nd	100.00	nd	100.00	nd	100.00	nd

nd - no data

Table S5. pH of aqueous solutions of biobased solvents after saturation with syringic acid.

1,6-Hexanediol		Ethyl lactate		GVL		1,5-Pentanediol		Cyrene		1,2-Propanediol	
wt %	pH			wt %	pH	wt %	pH	wt %	pH	wt %	pH
0.00	3.62 ± 0.02	0.00	3.62 ± 0.02	0.00	3.62 ± 0.02	0.00	3.62 ± 0.02	0.00	3.62 ± 3.62	0.00	3.62 ± 0.02
1.13	3.31 ± 0.01	1.06	2.72 ± 0.02	1.07	3.18 ± 0.02	---	---	1.13	3.33 ± 0.04	1.21	3.60 ± 0.02
2.00	3.29 ± 0.01	2.13	2.50 ± 0.01	2.15	3.07 ± 0.01	---	---	2.02	3.22 ± 0.01	2.18	3.37 ± 0.01
3.02	3.25 ± 0.02	3.01	2.39 ± 0.01	3.10	2.93 ± 0.01	---	---	3.11	3.21 ± 0.01	3.13	3.31 ± 0.01
4.05	3.24 ± 0.02	4.08	1.94 ± 0.01	4.22	2.94 ± 0.03	---	---	4.08	3.15 ± 0.02	3.97	3.26 ± 0.03
5.04	3.19 ± 0.01	5.07	1.86 ± 0.01	5.13	2.93 ± 0.01	---	---	5.22	3.11 ± 0.01	5.35	3.27 ± 0.01
---	---	10.02	1.68 ± 0.01	10.15	2.84 ± 0.02	---	---	---	---	---	---
---	---	19.99	1.51 ± 0.01	20.06	2.74 ± 0.01	---	---	---	---	---	---
---	---	29.97	1.46 ± 0.01	30.03	2.70 ± 0.01	---	---	---	---	---	---
---	---	40.03	1.43 ± 0.01	40.13	2.66 ± 0.01	---	---	---	---	---	---
---	---	50.00	1.43 ± 0.01	50.11	2.68 ± 0.02	---	---	---	---	---	---
---	---	59.93	1.50 ± 0.01	59.72	2.62 ± 0.01	---	---	---	---	---	---
---	---	70.00	1.51 ± 0.02	70.26	2.79 ± 0.03	---	---	---	---	---	---
---	---	79.96	1.46 ± 0.01	79.73	2.74 ± 0.04	---	---	79.82	2.56 ± 0.02	---	---
---	---	90.01	nd	89.32	nd	---	---	87.58	nd	---	---
---	---	91.99	nd	91.96	nd	---	---	92.00	nd	---	---
---	---	94.00	nd	93.58	nd	---	---	94.05	nd	---	---
---	---	95.99	nd	95.91	nd	---	---	95.88	nd	---	---
---	---	97.86	nd	97.82	nd	---	---	98.03	nd	---	---
---	---	100.00	nd	100.00	nd	---	---	100.00	nd	---	---

nd - no data

Table S6. Parameters acquire from the cooperative model of hydrotropy by using the experimental data collect in this work.

		Shimuzu					
		1,6-Hexanediol	Ethyl lactate	GVL	1,5-Pentanediol	Cyrene	1,2-Propanediol
Syringic acid	m	1.555	1.616	1.621	1.602	1.509	1.347
	b	3.532	3.835	3.022	3.258	2.344	0.957
	R ²	0.999	42.83	0.992	0.996	0.988	0.985
	S/S _{0max}	71.658	0.967	116.849	59.378	78.192	48.429
Ferulic acid	m	1.792	1.747	1.840	1.621	1.689	1.440
	b	4.216	3.594	3.697	2.734	2.823	0.696
	R ²	0.995	0.943	0.984	0.990	0.950	0.977
	S/S _{0max}	140.431	128.106	266.043	133.481	151.329	139.506

References

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