

Supporting information

Separation of natural compounds using DES-based biphasic systems
and centrifugal partition chromatography.

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Experimental binodal data

Heptane + 1-Butanol + EG					
100 w_{EG}	100 $w_{heptane}$	100 w_{EG}	100 $w_{heptane}$	100 w_{EG}	100 $w_{heptane}$
13.200	56.956	20.594	43.990	29.085	30.575
13.555	56.177	20.909	43.474	29.681	29.733
13.982	55.346	21.292	42.756	30.213	28.951
14.399	54.650	21.551	42.396	30.785	28.261
14.793	53.911	21.936	41.630	31.358	27.451
15.127	53.394	22.262	41.227	32.096	26.568
15.453	52.793	22.661	40.426	33.161	24.963
15.763	52.233	23.032	39.836	34.157	23.841
16.212	51.293	23.361	39.324	35.249	22.664
16.512	50.960	23.663	38.910	36.636	20.997
16.911	50.116	24.011	38.365	37.799	19.741
17.240	49.652	24.333	37.821	39.023	18.632
17.567	49.048	24.730	37.176	40.184	17.511
17.909	48.509	25.141	36.514	41.761	16.052
18.248	47.898	25.608	35.770	43.749	14.282
18.566	47.373	26.001	35.222	46.253	12.331
18.952	46.659	26.454	34.405	49.683	10.071
19.318	46.046	27.007	33.637	52.165	8.706
19.697	45.376	27.522	32.838	55.676	6.829
19.986	44.978	28.008	32.103	59.894	5.383
20.332	44.369	28.570	31.344		

Table S1: Experimental percentage weight fraction data for the clear points of the system composed of EG + 1-Butanol + Heptane

Heptane + 1-Butanol + ChClLevA 1:2					
100 $w_{ChClLevA}$	100 $w_{heptane}$	100 $w_{ChClLevA}$	100 $w_{heptane}$	100 $w_{ChClLevA}$	100 $w_{heptane}$
15.456	47.038	41.293	17.815	50.587	11.337
19.208	40.476	43.667	16.117	53.447	8.968
28.186	30.490	44.200	14.744	54.219	10.360
37.150	22.568	46.688	13.734	57.459	6.955
39.329	19.094	48.728	12.927		
39.508	20.173	48.954	12.385		

Table S2: Experimental percentage weight fraction data for the clear points of the system composed of ChClLevA 1:2 + 1-Butanol + Heptane

Heptane + 1-Butanol + ChClLevA 1:3					
$100 w_{ChClLevA}$	$100 w_{heptane}$	$100 w_{ChClLevA}$	$100 w_{heptane}$	$100 w_{ChClLevA}$	$100 w_{heptane}$
10.721	46.778	35.899	23.480	50.557	12.133
14.936	42.705	36.223	23.032	52.994	10.640
18.882	38.956	37.297	21.568	53.020	10.652
20.353	37.497	37.304	22.235	53.764	10.036
22.172	35.918	38.648	21.028	54.658	9.486
23.360	34.591	39.988	19.900	56.677	8.739
24.685	33.315	41.100	18.919	58.362	8.121
25.912	31.764	42.748	17.606	59.785	7.259
28.205	29.427	44.650	16.055	54.658	9.486
31.242	26.933	47.086	14.342	56.677	8.739
32.947	25.327	48.455	13.151	58.362	8.121
34.868	23.609	48.669	13.251	59.785	7.259

Table S3: Experimental percentage weight fraction data for the clear points of the system composed of ChClLevA 1:3 + 1-Butanol + Heptane

Heptane + 1-Butanol + LevA					
$100 w_{LevA}$	$100 w_{heptane}$	$100 w_{LevA}$	$100 w_{heptane}$	$100 w_{LevA}$	$100 w_{heptane}$
15.595	60.414	26.963	41.762	42.484	21.584
16.749	58.209	28.345	39.410	44.373	19.904
17.842	56.225	29.813	37.158	45.555	19.089
19.263	53.594	30.925	35.625	46.734	17.722
21.108	50.356	32.550	33.122	48.220	16.539
21.798	49.749	35.195	29.642	50.240	15.065
23.471	46.893	36.692	27.788	52.574	13.067
24.824	44.762	38.776	25.048	58.183	10.433
26.173	42.738	40.867	23.145	61.881	7.898

Table S4: Experimental percentage weight fraction data for the clear points of the system composed of LevA + 1-Butanol + Heptane

Heptane + Ethyl acetate + LevA					
100 w_{EG}	100 $w_{heptane}$	100 w_{EG}	100 $w_{heptane}$	100 w_{EG}	100 $w_{heptane}$
8.341	54.781	24.844	31.384	33.681	22.052
10.480	50.243	25.238	30.771	34.304	21.469
12.182	47.189	25.985	30.070	34.865	21.050
13.803	44.869	26.631	29.396	35.220	20.711
14.931	43.324	26.905	28.936	35.772	20.291
16.101	41.837	27.532	28.416	36.237	19.831
16.972	40.657	27.884	27.915	36.688	19.458
17.555	39.963	28.522	27.368	37.175	19.032
18.362	38.934	28.817	26.899	37.685	18.636
19.311	37.766	29.445	26.320	38.037	18.159
20.070	36.915	29.821	25.699	38.920	17.562
21.013	35.778	30.676	25.109	39.521	17.055
21.731	34.932	30.838	24.650	40.231	16.340
22.265	34.223	31.544	24.089	41.466	15.450
23.337	33.044	32.053	23.627	43.162	14.643
23.672	32.673	32.499	23.181	43.960	14.059
24.309	31.949	32.846	22.659		

Table S5: Experimental percentage weight fraction data for the clear points of the system composed of LevA + Ethyl acetate + Heptane

Heptane + Ethyl acetate + Thy:LevA 1:2					
100 w_{EG}	100 $w_{heptane}$	100 w_{EG}	100 $w_{heptane}$	100 w_{EG}	100 $w_{heptane}$
18.384	49.131	27.352	41.044	42.810	30.580
19.204	49.484	28.753	40.373	44.536	29.433
19.979	48.188	30.236	38.765	45.929	28.616
20.517	48.152	31.997	37.580	47.913	26.737
21.154	47.187	35.082	35.249	52.485	22.556
22.049	45.897	36.966	34.677	57.012	20.306
23.583	44.128	39.480	32.555	62.764	16.912
25.533	42.320	40.825	32.141		

Table S6: Experimental percentage weight fraction data for the clear points of the system composed of Thy:LevA 1:2 + Ethyl acetate + Heptane

Heptane + Ethyl acetate + Thy:LevA 1:1					
100 w_{EG}	100 $w_{heptane}$	100 w_{EG}	100 $w_{heptane}$	100 w_{EG}	100 $w_{heptane}$
31.543	48.720	38.310	44.909	47.424	40.011
32.072	48.346	38.803	44.686	48.633	39.234
32.616	48.138	39.339	44.397	49.887	38.426
33.202	47.724	39.795	44.196	51.167	37.648
33.793	47.465	40.329	43.934	52.631	36.693
34.314	47.165	40.869	43.610	53.808	36.120
34.695	46.990	41.293	43.489	55.328	34.984
35.382	46.511	42.061	42.992	56.728	34.248
35.904	46.152	42.715	42.767	58.326	33.090
36.467	45.887	43.437	42.276	59.723	32.264
36.963	45.575	44.359	41.763	60.793	31.666
37.372	45.373	45.294	41.236		
37.814	45.128	46.368	40.599		

Table S7: Experimental percentage weight fraction data for the clear points of the system composed of Thy:LevA 1:1 + Ethyl acetate + Heptane

Heptane + 1-Butanol + Thy:LevA 1:1					
100 w_{EG}	100 $w_{heptane}$	100 w_{EG}	100 $w_{heptane}$	100 w_{EG}	100 $w_{heptane}$
2.882	93.101	27.008	63.548	39.416	51.401
7.634	84.636	28.856	61.657	44.607	46.155
21.066	69.090	30.439	60.182	55.946	34.648
23.186	67.061	33.368	56.964		
25.401	64.943	36.332	54.191		

Table S8: Experimental percentage weight fraction data for the clear points of the system composed of Thy:LevA 1:1 + 1-Butanol + Heptane

Experimental determination of phases composition

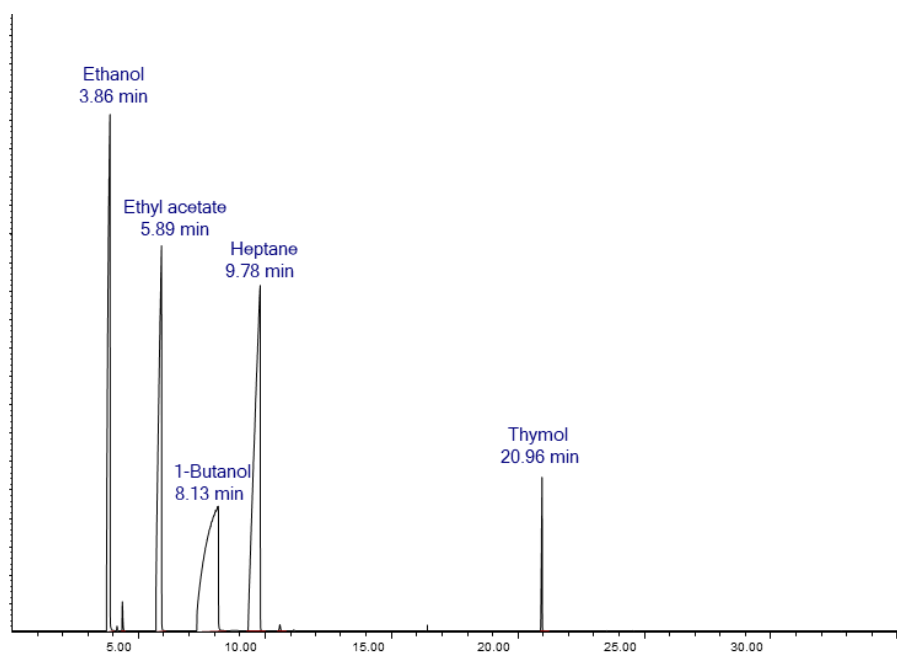


Figure S1: GC-FID chromatogram of the solvents used in biphasic systems

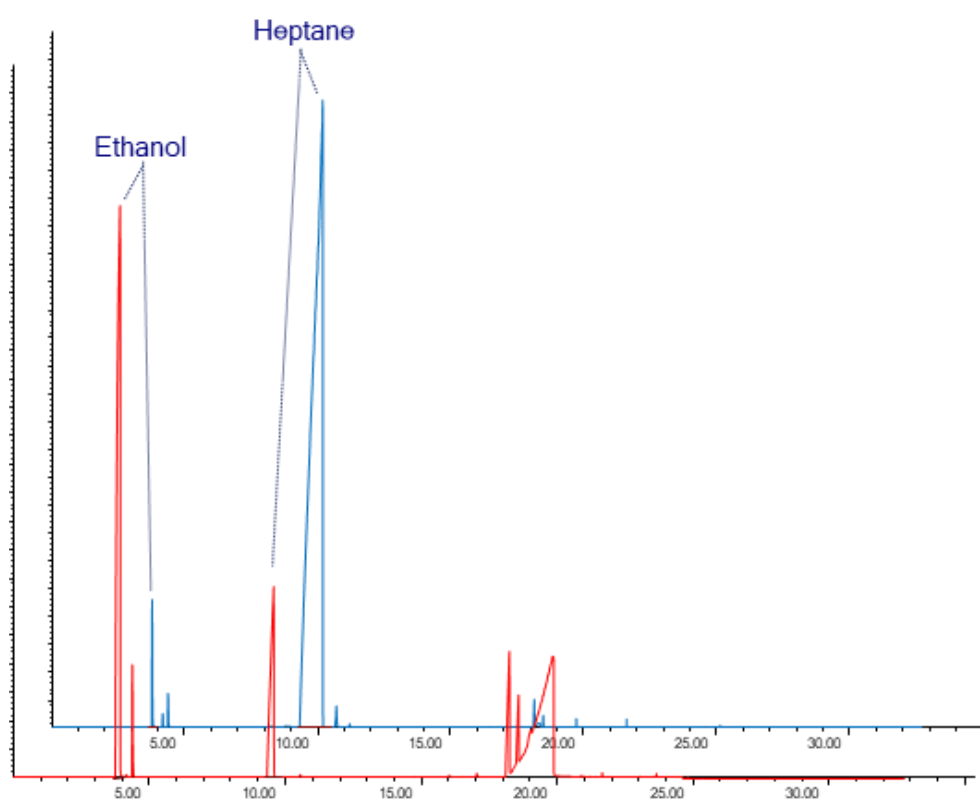


Figure S2: Example of GC-FID chromatogram of the solvents used for determination of phases compositions. Upper phase (in blue) and lower phase (in red) of the biphasic system Heptane/Ethanol/LevA (37.5/25/37.5). Time and response offset for legibility.

Separation of natural compounds using CPC

Fraction No.	Retention time (min)	m _{Apigenin} (mg)	m _{Coumarin} (mg)	m _{β-Ionone} (mg)	m _{α-Tocopherol} (mg)
10	6.67	0.000	0.000	0.000	0.000
20	13.33	0.000	0.000	0.000	0.000
28	18.67	0.000	0.000	0.000	0.000
30	20.00	0.000	0.000	0.000	0.000
32	21.33	0.007	0.000	0.000	0.000
33	22.00	0.016	0.000	0.000	0.000
34	22.67	0.033	0.000	0.000	0.000
35	23.33	0.045	0.000	0.000	0.000
36	24.00	0.059	0.000	0.000	0.000
37	24.67	0.063	0.000	0.000	0.000
38	25.33	0.064	0.000	0.000	0.000
39	26.00	0.056	0.003	0.000	0.000
40	26.67	0.051	0.014	0.000	0.000
41	27.33	0.042	0.035	0.000	0.000
42	28.00	0.035	0.073	0.000	0.000
43	28.67	0.026	0.137	0.000	0.000
44	29.33	0.023	0.196	0.000	0.000
45	30.00	0.016	0.277	0.000	0.000
46	30.67	0.014	0.319	0.000	0.000
47	31.33	0.011	0.394	0.000	0.000
48	32.00	0.010	0.414	0.000	0.000
49	32.67	0.008	0.408	0.000	0.000
50	33.33	0.006	0.408	0.000	0.000
51	34.00	0.006	0.367	0.000	0.000
52	34.67	0.006	0.311	0.000	0.000
53	35.33	0.005	0.284	0.000	0.000
54	36.00	0.004	0.238	0.000	0.000
55	36.67	0.003	0.190	0.000	0.000
56	37.33	0.003	0.161	0.000	0.000
57	38.00	0.003	0.133	0.000	0.000
58	38.67	0.003	0.112	0.000	0.000
59	39.33	0.003	0.097	0.000	0.000
60	40.00	0.003	0.078	0.000	0.000
61	40.67	0.002	0.070	0.000	0.000
62	41.33	0.003	0.056	0.000	0.000
63	42.00	0.003	0.050	0.000	0.000
64	42.67	0.002	0.036	0.000	0.000
66	44.00	0.002	0.027	0.000	0.000
68	45.33	0.001	0.022	0.000	0.000
70	46.67	0.001	0.006	0.000	0.000
72	48.00	0.000	0.000	0.000	0.000
82	54.67	0.000	0.000	0.000	0.000
83	55.33	0.000	0.000	0.000	0.015

84	56.00	0.000	0.000	0.004	0.160
85	56.67	0.000	0.000	0.004	0.299
86	57.33	0.000	0.000	0.003	0.511
87	58.00	0.000	0.000	0.005	0.609
88	58.67	0.000	0.000	0.014	0.460
89	59.33	0.000	0.000	0.023	0.171
90	60.00	0.000	0.000	0.028	0.103
92	61.33	0.000	0.000	0.087	0.003
93	62.00	0.000	0.000	0.127	0.004
94	62.67	0.000	0.000	0.200	0.005
95	63.33	0.000	0.000	0.262	0.000
96	64.00	0.000	0.000	0.329	0.000
97	64.67	0.000	0.000	0.395	0.000
98	65.33	0.000	0.000	0.316	0.000
99	66.00	0.000	0.000	0.215	0.000
100	66.67	0.000	0.000	0.151	0.000
101	67.33	0.000	0.000	0.101	0.000
102	68.00	0.000	0.000	0.041	0.000
103	68.67	0.000	0.000	0.020	0.000
105	70.00	0.000	0.000	0.000	0.000
112	74.67	0.000	0.000	0.000	0.003
114	76.00	0.000	0.000	0.000	0.006
116	77.33	0.000	0.000	0.000	0.000
119	79.33	0.000	0.000	0.000	0.002
123	82.00	0.000	0.000	0.000	0.000
125	83.33	0.000	0.000	0.000	0.001

Table S9 –Mass of apigenin, coumarin, β -ionone and α -tocopherol in the different fractions obtained during CPC experiment in dual elution mode.

Fraction No.	Retention time (min)	m _{Apigenin} (mg)	m _{Coumarin} (mg)	m _{β-Ionone} (mg)	m _{α-Tocopherol} (mg)
11	7,33	0,000	0,000	0,001	0,000
12	8,00	0,000	0,000	0,000	0,003
13	8,67	0,000	0,000	0,001	0,010
14	9,33	0,000	0,000	0,000	0,110
15	10,00	0,000	0,000	0,000	0,412
16	10,67	0,000	0,000	0,000	0,789
17	11,33	0,000	0,000	0,001	0,750
18	12,00	0,000	0,000	0,000	0,591
19	12,67	0,000	0,000	0,002	0,398
20	13,33	0,000	0,000	0,005	0,180
21	14,00	0,000	0,000	0,026	0,077
22	14,67	0,000	0,000	0,060	0,033
23	15,33	0,000	0,000	0,114	0,023
24	16,00	0,000	0,000	0,175	0,012
25	16,67	0,000	0,000	0,229	0,004
26	17,33	0,000	0,000	0,244	0,000
27	18,00	0,000	0,000	0,230	0,000
28	18,67	0,000	0,000	0,180	0,000
29	19,33	0,000	0,000	0,141	0,000
30	20,00	0,000	0,000	0,106	0,000
31	20,67	0,000	0,000	0,075	0,000
32	21,33	0,000	0,000	0,046	0,000
33	22,00	0,000	0,000	0,034	0,000
34	22,67	0,000	0,000	0,023	0,000
35	23,33	0,000	0,000	0,019	0,000
36	24,00	0,000	0,000	0,012	0,000
37	24,67	0,000	0,000	0,012	0,000
38	25,33	0,000	0,000	0,008	0,000
39	26,00	0,000	0,000	0,007	0,000
40	26,67	0,000	0,000	0,006	0,000
41	27,33	0,000	0,000	0,008	0,000
43	28,67	0,000	0,000	0,003	0,000
45	30,00	0,000	0,000	0,000	0,000
60	40,00	0,000	0,000	0,000	0,000
75	50,00	0,000	0,000	0,000	0,000
82	54,67	0,000	0,000	0,000	0,000
95	63,33	0,000	0,000	0,000	0,000
110	73,33	0,000	0,000	0,000	0,000
115	76,67	0,000	0,000	0,000	0,000
117	78,00	0,000	0,000	0,000	0,000
119	79,33	0,000	0,000	0,000	0,000
120	80,00	0,000	0,000	0,000	0,000
121	80,67	0,000	0,001	0,000	0,000
122	81,33	0,000	0,003	0,000	0,000
123	82,00	0,000	0,008	0,000	0,000

124	82,67	0,000	0,007	0,000	0,000
125	83,33	0,000	0,011	0,000	0,000
126	84,00	0,000	0,018	0,000	0,000
127	84,67	0,000	0,028	0,000	0,000
128	85,33	0,000	0,042	0,000	0,000
129	86,00	0,000	0,056	0,000	0,000
130	86,67	0,000	0,072	0,000	0,000
131	87,33	0,000	0,088	0,000	0,000
132	88,00	0,000	0,097	0,000	0,000
133	88,67	0,000	0,108	0,000	0,000
134	89,33	0,000	0,118	0,000	0,000
135	90,00	0,000	0,116	0,000	0,000
136	90,67	0,000	0,123	0,000	0,000
137	91,33	0,000	0,123	0,000	0,000
138	92,00	0,000	0,109	0,000	0,000
139	92,67	0,000	0,098	0,000	0,000
140	93,33	0,000	0,090	0,000	0,000
141	94,00	0,000	0,081	0,000	0,000
142	94,67	0,000	0,070	0,000	0,000
143	95,33	0,000	0,061	0,000	0,000
144	96,00	0,000	0,051	0,000	0,000
145	96,67	0,000	0,046	0,000	0,000
146	97,33	0,000	0,039	0,000	0,000
147	98,00	0,000	0,032	0,000	0,000
148	98,67	0,000	0,027	0,000	0,000
149	99,33	0,000	0,023	0,000	0,000
150	100,00	0,000	0,020	0,000	0,000
151	100,67	0,003	0,016	0,000	0,000
152	101,33	0,002	0,017	0,000	0,000
153	102,00	0,006	0,014	0,000	0,000
154	102,67	0,012	0,012	0,000	0,000
155	103,33	0,017	0,011	0,000	0,000
156	104,00	0,024	0,009	0,000	0,000
157	104,67	0,035	0,009	0,000	0,000
158	105,33	0,042	0,008	0,000	0,000
159	106,00	0,054	0,007	0,000	0,000
160	106,67	0,060	0,006	0,000	0,000
161	107,33	0,065	0,006	0,000	0,000
162	108,00	0,070	0,005	0,000	0,000
163	108,67	0,070	0,005	0,000	0,000
164	109,33	0,061	0,005	0,000	0,000
165	110,00	0,057	0,004	0,000	0,000
166	110,67	0,049	0,003	0,000	0,000
167	111,33	0,033	0,003	0,000	0,000
168	112,00	0,030	0,003	0,000	0,000
169	112,67	0,024	0,002	0,000	0,000
170	113,33	0,019	0,001	0,000	0,000
171	114,00	0,017	0,001	0,000	0,000

172	114,67	0,014	0,001	0,000	0,000
173	115,33	0,011	0,001	0,000	0,000
174	116,00	0,009	0,001	0,000	0,000
175	116,67	0,006	0,000	0,000	0,000
176	117,33	0,006	0,000	0,000	0,000
177	118,00	0,006	0,000	0,000	0,000
178	118,67	0,004	0,000	0,000	0,000
179	119,33	0,004	0,000	0,000	0,000
180	120,00	0,003	0,000	0,000	0,000
181	120,67	0,003	0,000	0,000	0,000
182	121,33	0,002	0,000	0,000	0,000
183	122,00	0,002	0,000	0,000	0,000
184	122,67	0,003	0,000	0,000	0,000
185	123,33	0,002	0,000	0,000	0,000
186	124,00	0,002	0,000	0,000	0,000
187	124,67	0,002	0,000	0,000	0,000

Table S10 –Mass of apigenin, coumarin, β -ionone and α -tocopherol in the different fractions obtained during CPC experiment in elution/extrusion mode.