Supplementary Materials

Screening terpene-based eutectic solvents for bisphenol A extraction from plastic-packed dairy products and water storage tanks: COSMO-RS and quantum chemistry calculations

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Table S1 CCD matrix and responses.

Run order	X_1	X_2	X_3	ER%
1	130	4	138	25
2	100	5	125	52
3	70	4	112	60
4	100	3	125	29
5	100	5	125	54
6	70	6	112	54
7	150	5	125	37
8	70	4	138	31
9	130	6	138	37
10	70	6	138	46
11	100	5	125	53
12	100	5	100	72
13	130	4	112	54
14	100	7	125	49
15	100	5	150	26
16	50	5	125	49
17	100	5	125	45
18	130	6	112	48

Table S2 ANOVA results of the CCD.

Source	F-value	p-value	
Model	15.30	0.0004	Significant
X_1	8.84	0.0178	
X_2	10.25	0.0126	
X_3	94.48	< 0.0001	
X_1X_2	0.061	0.8111	
X_1X_3	0.061	0.8111	
X_2X_3	10.31	0.0124	
X_1^2	5.39	0.0487	
X_2^2	11.15	0.0102	
X_3^2	0.34	0.5754	
Lack of Fit	1.17	0.4786	Not significant
R^2	0.9554		
Adjusted R^2	0.9311		
Predicted R^2	0.8507		
C.V. %	8.26		
Adeq Precision	20.263		

Table S3 Relative recoveries of BPA in spiked dairy products and water samples.

Sample	Concentration (μg/L, n=3)	Added (μg/L)	Found (μg/L, n=3)	Relative Recovery (%)
Water (Garden House, Plastic tank, Summer season, Exposed to sunlight)	67.2 ± 3.5	10	78.1 ± 4.2	109
Water (Apartment, Plastic tank, Summer season, In the shadow)	11.5 ± 0.6	20	32.1 ± 2.3	103
Milk	n.d.	50	47.5 ± 3.1	95
Coffee milk	n.d.	100	103.9 ± 6.4	104
Yogurt	n.d.	120	115.6 ± 8.5	96

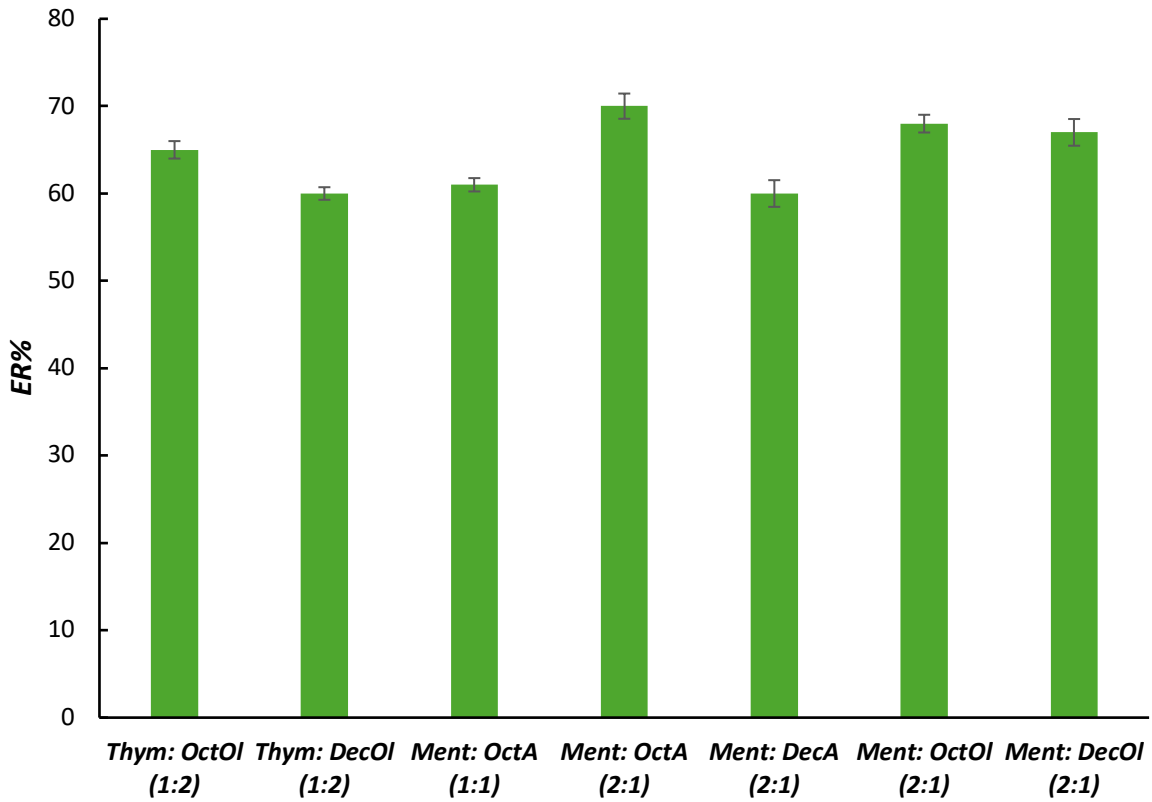
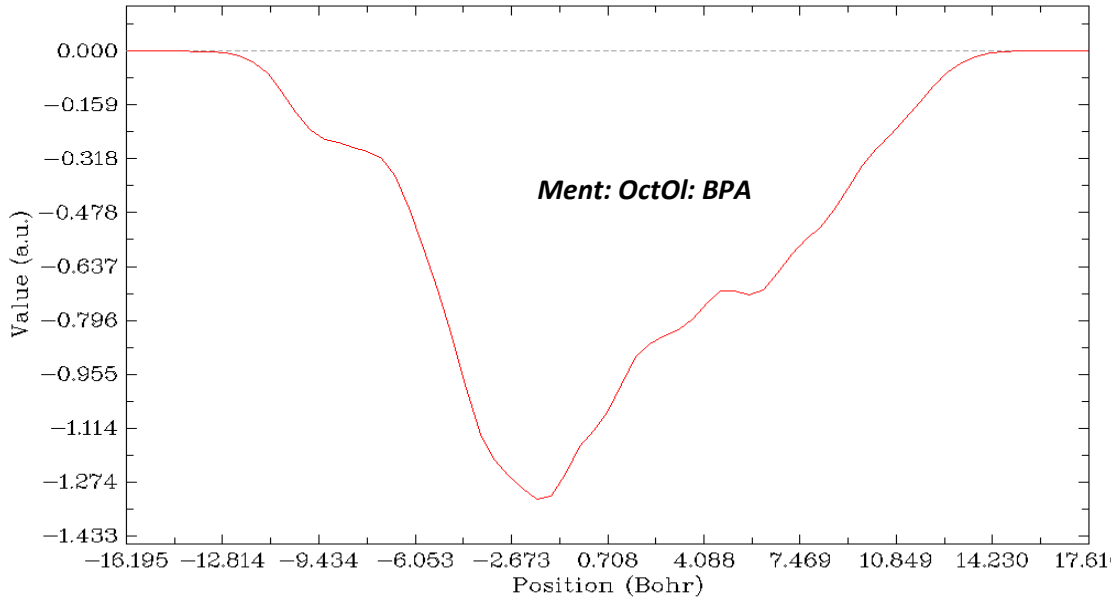
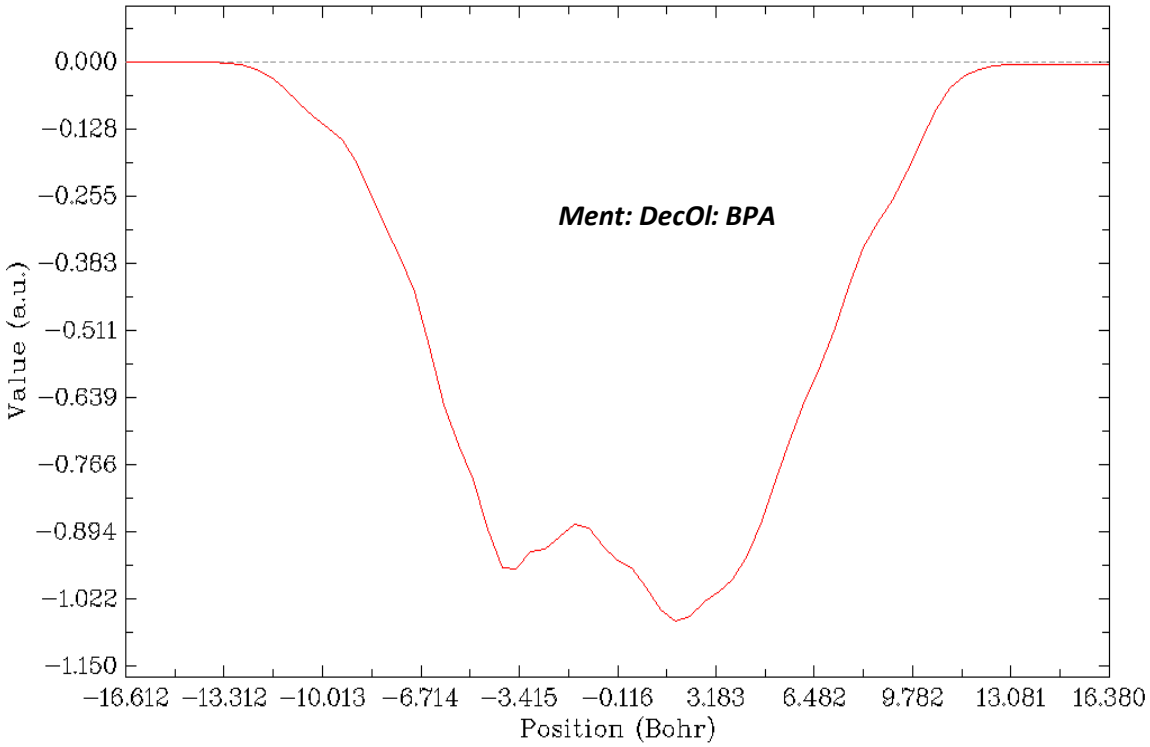
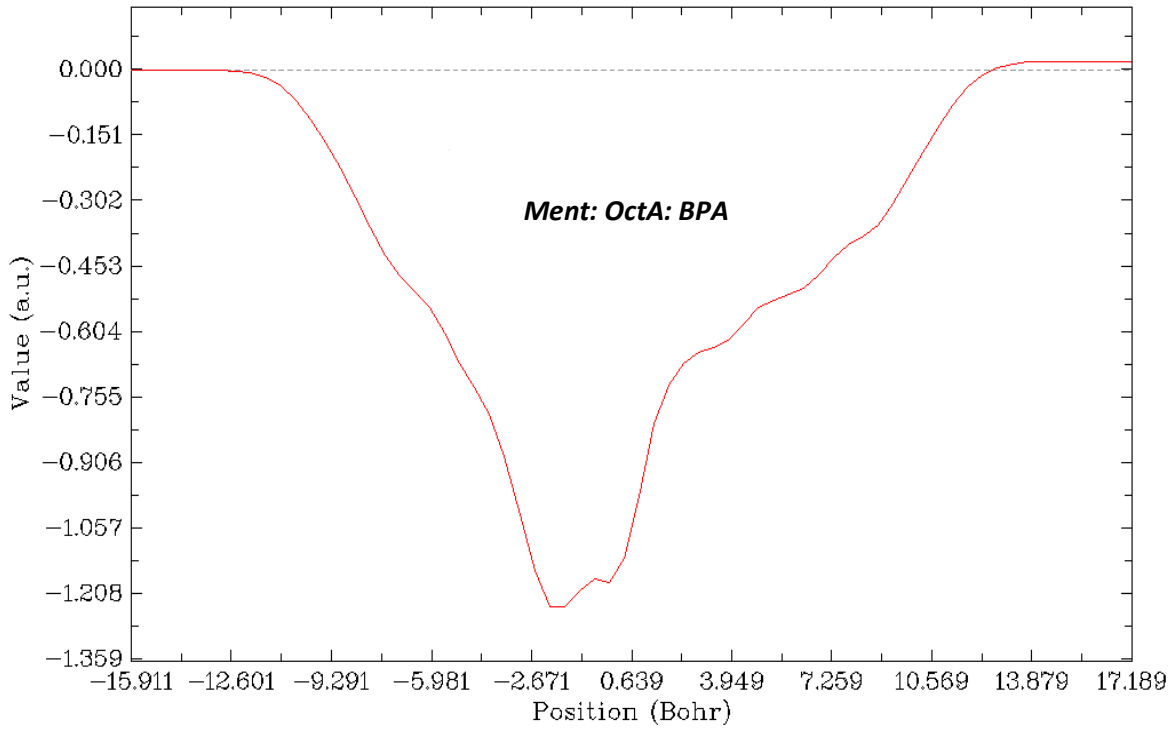


Fig. S1. Extraction efficiency of different HESs using VA-LLME for BPA.


Ment: OctOl: BPA
Value (a.u.)
0.000
−0.159
−0.318
−0.478
−0.637
−0.796
−0.955
−1.114
−1.274
−1.433
−16.195 −12.814 −9.434 −6.053 −2.673 0.708 4.088 7.469 10.849 14.230
Position (Bohr)


Ment: DecOl: BPA
Value (a.u.)
0.000
−0.128
−0.255
−0.383
−0.511
−0.639
−0.766
−0.894
−1.022
−1.150
−16.612 −13.312 −10.013 −6.714 −3.415 −0.116 3.183 6.482 9.782 13.081 16.380
Position (Bohr)



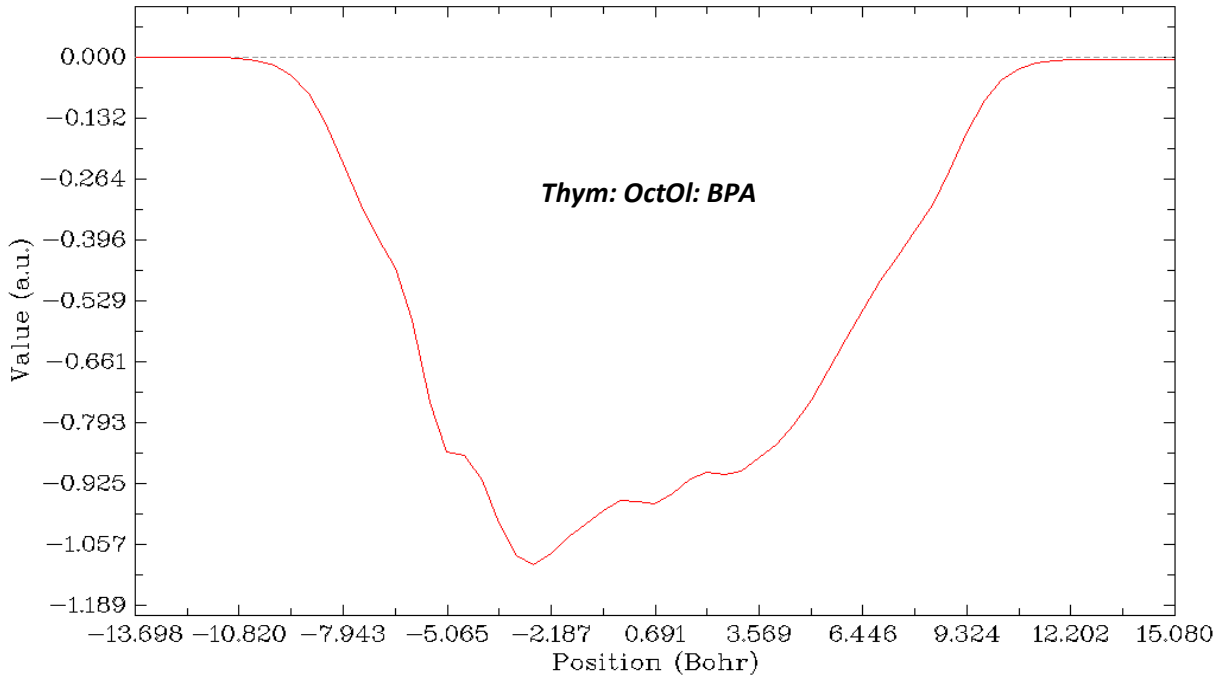
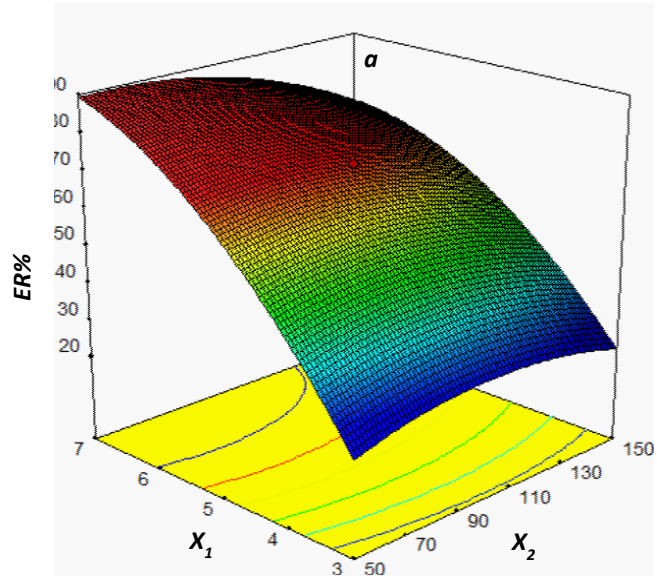
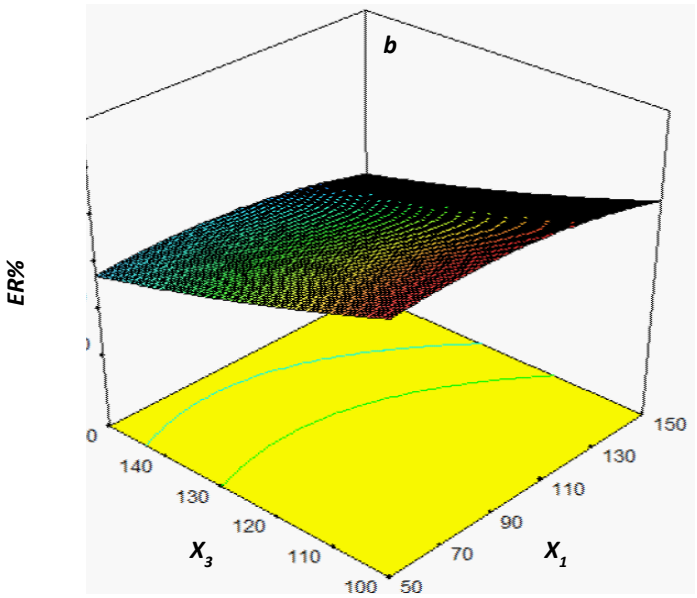


Fig. S2 CD curves of the HES: BPA complexes generated by quantum mechanical chemistry.


a
ER%
70
60
50
40
30
20
7
6
5
4
3
X1
50
70
90
110
130
150
X2


b
ER%
0
140
130
120
110
100
X3
50
70
90
110
130
150
X1

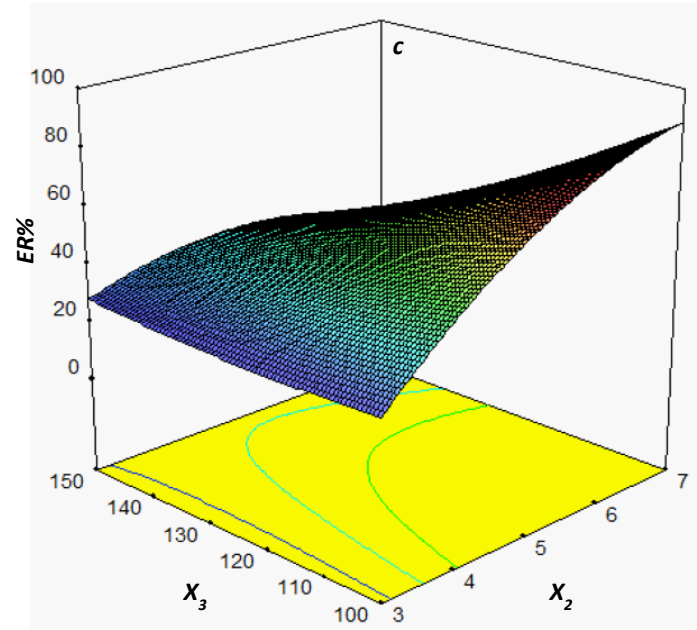

c
ER%
100
80
60
40
20
0
150
140
130
120
110
100
X3
3
4
5
6
7
X2

Fig. S3 Response surface plots illustrating the combined effects of variables on BPA extraction efficiency: (a) HES volume (X_1) and KOH concentration (X_2), (b) HES volume and HCl volume (X_3), (c) KOH concentration and HCl volume.