

Supplementary Materials

Deep eutectic solvent-based emulsification liquid-liquid microextraction coupled with gas chromatography for the determination of thiophenols in water samples

Shirin Babaei, Ali Daneshfar*, Reza Sahraei

Tel/fax: +98-843-2227022

E-mail: daneshfara@yahoo.com; a.daneshfar@mail.ilam.ac.ir

Department of Chemistry, Faculty of Science, Ilam University, Ilam, 69315-516, Iran

Table of contents in Supporting Information:

1. Figure (S1). ^{13}C -NMR spectrum of DES.

2. Figure (S2). Pareto chart for the Box-Behnken. The vertical line in the chart defines the 95% confidence level.

3. Figure (S3). 3D plots of significant factors: X_1 : volume of acetone (μL), X_2 : volume of DES (μL), X_3 : ultrasonic time (min), X_4 : pH.

4. Table S1 Factors, actual and coded levels used in Box-Behnken for extraction of Thiophenols.

5. Table S2 ANOVA results obtained by Box-Behnken.

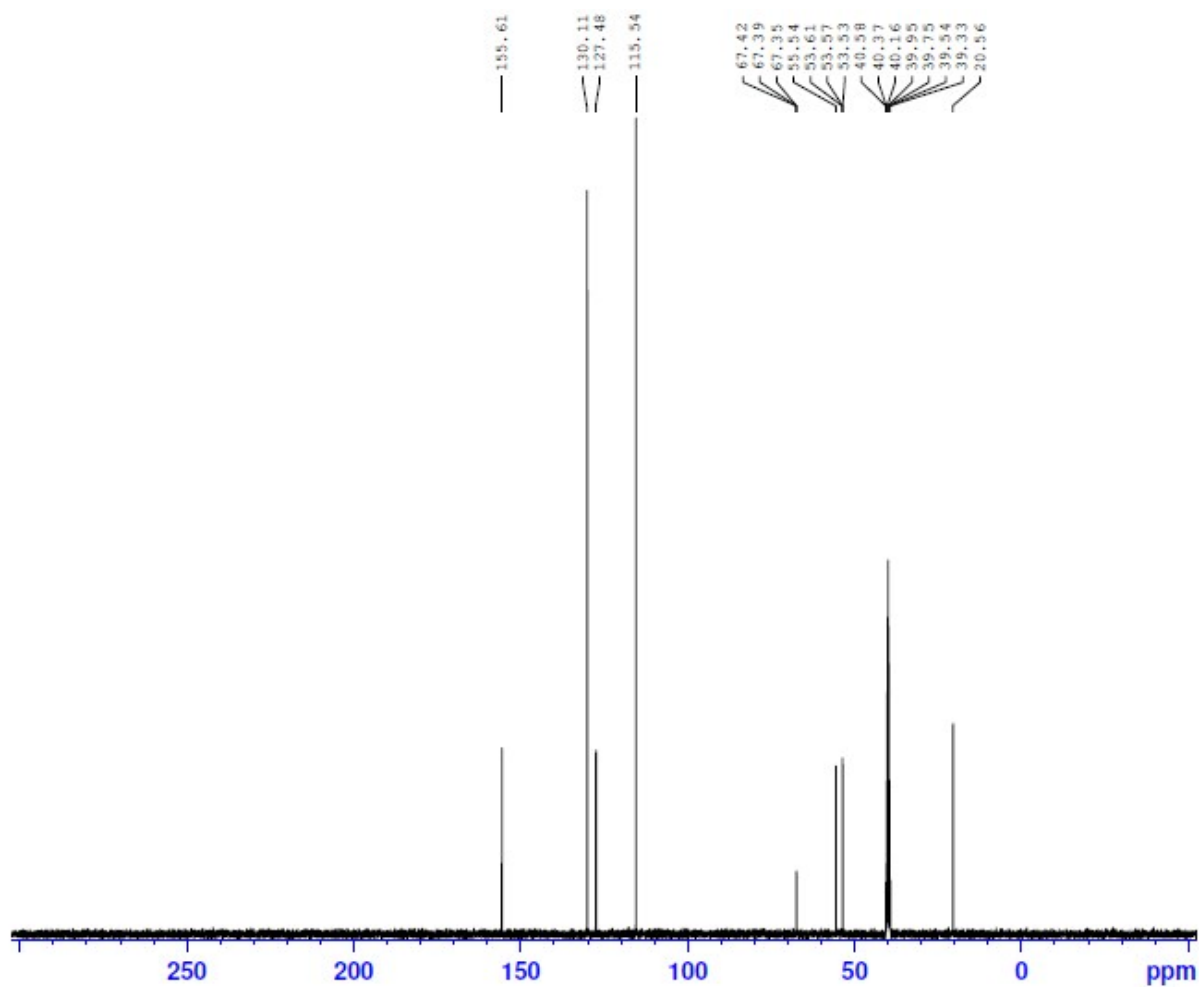
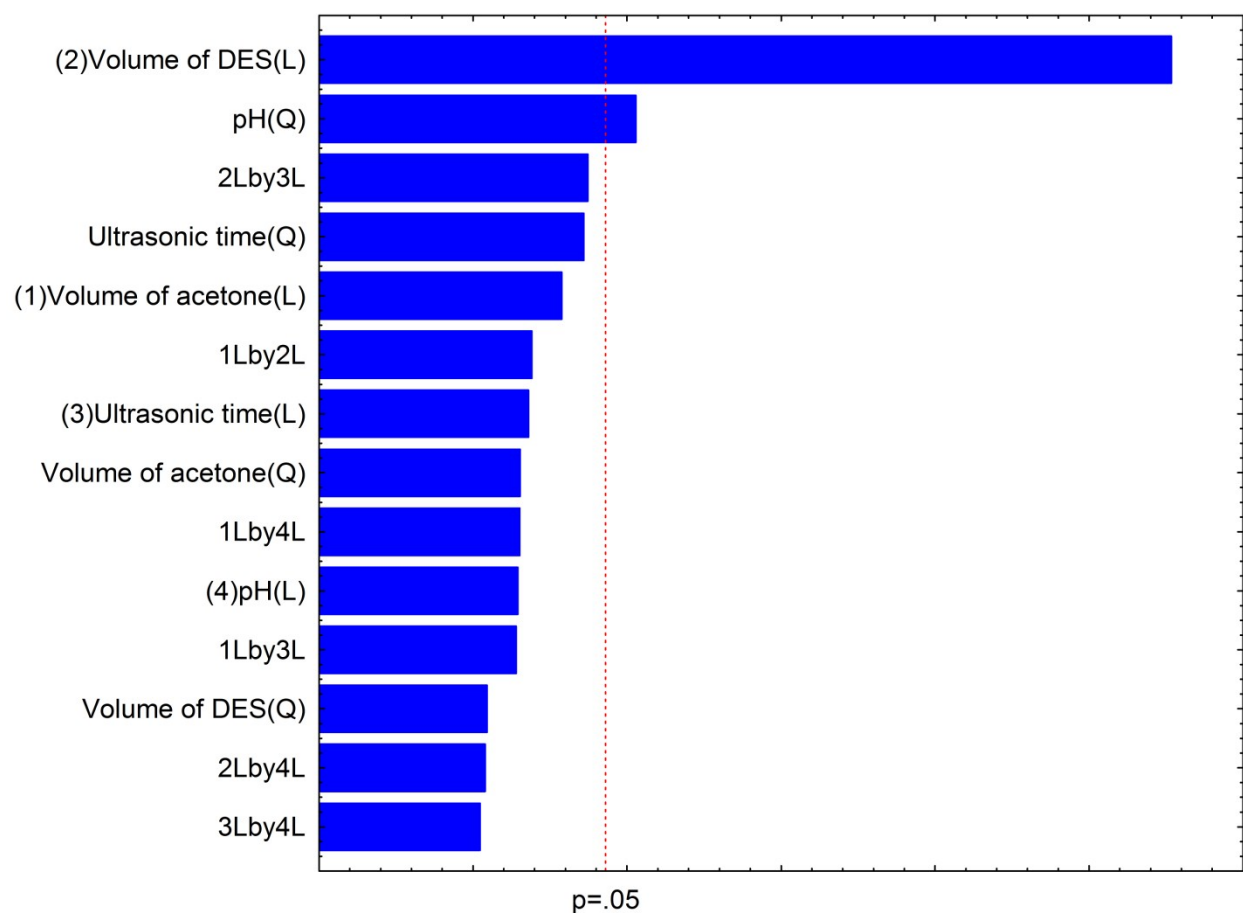
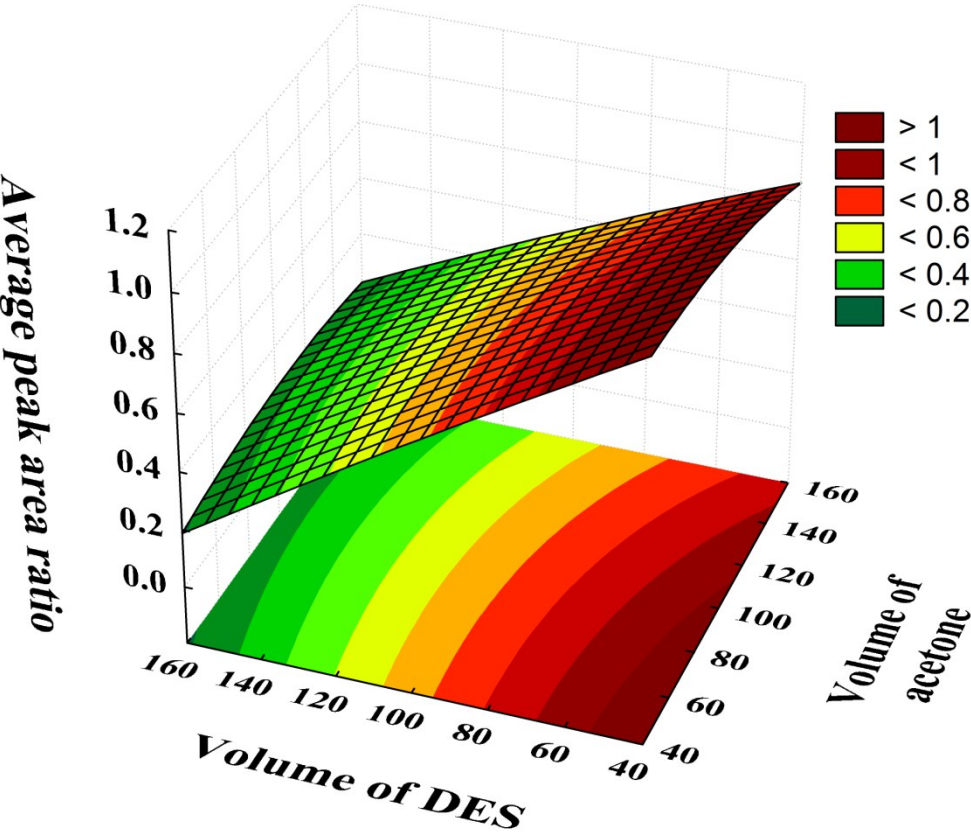


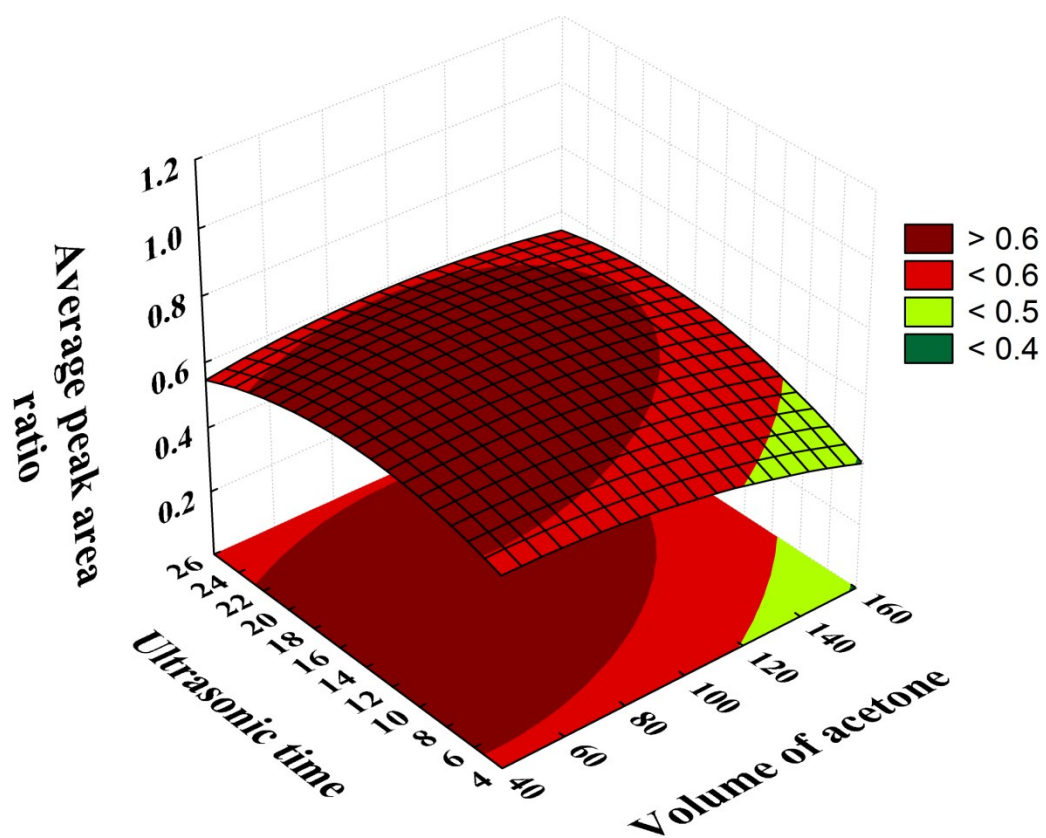
Figure (S1)



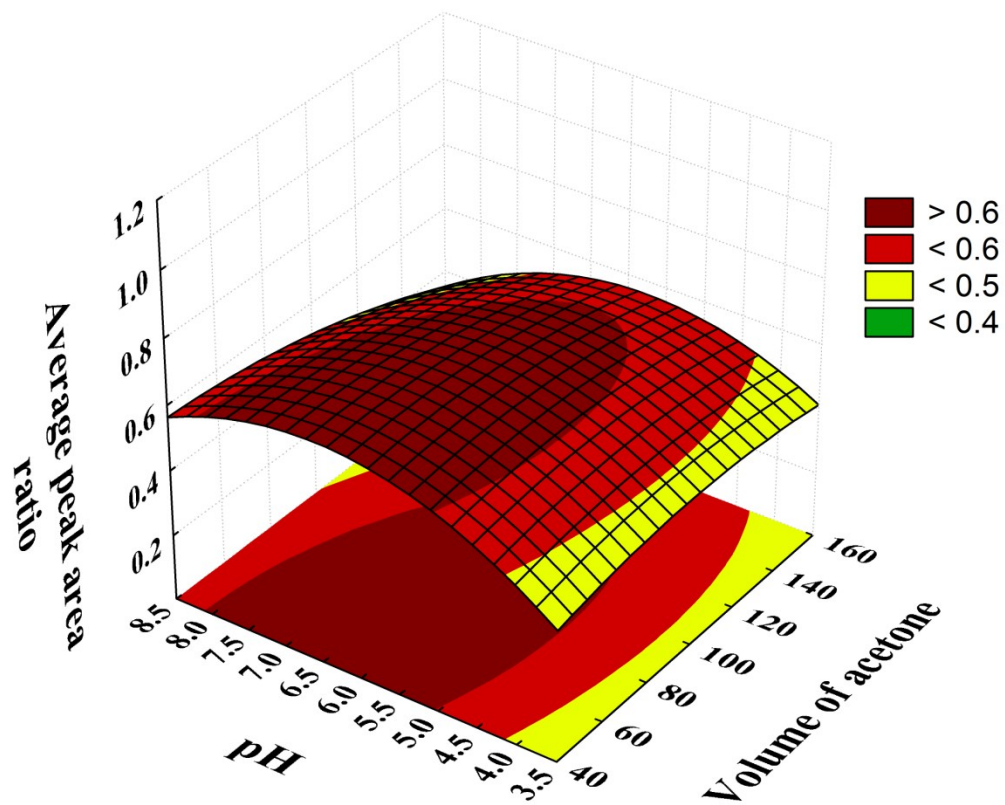
p=.05
Standardized Effect Estimate (Absolute Value)

Figure (S2)





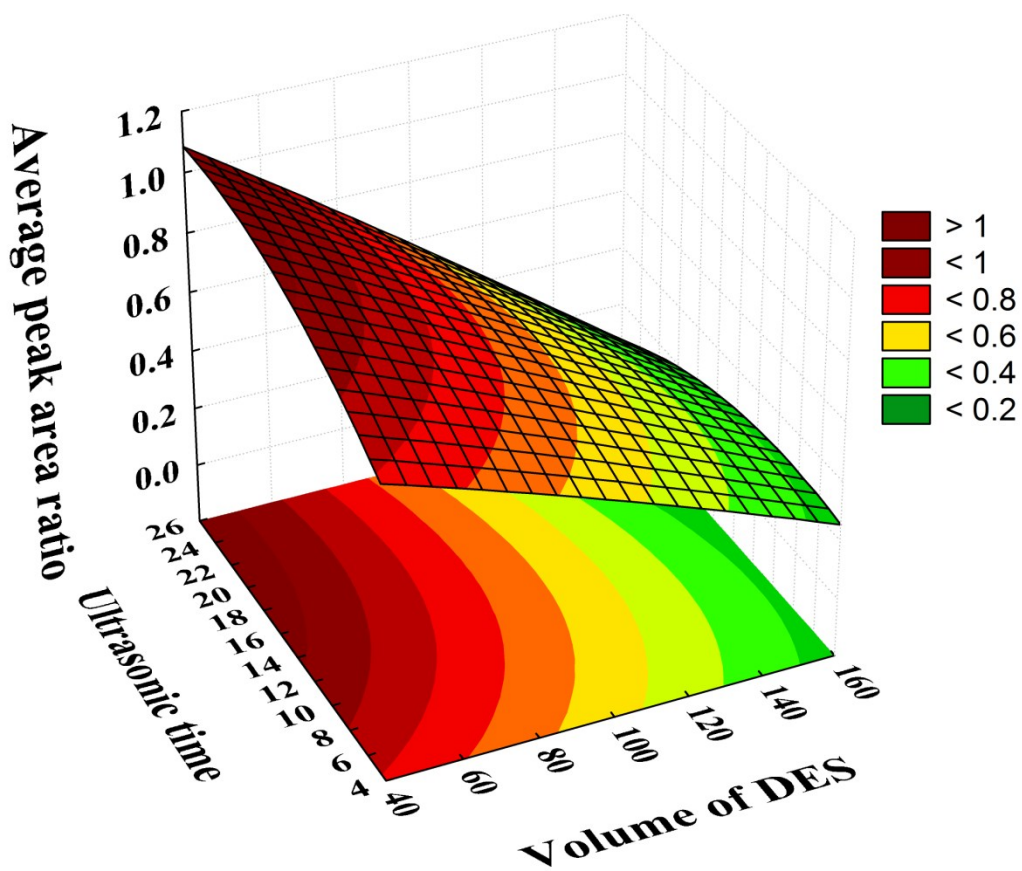
29
30
31
32



33

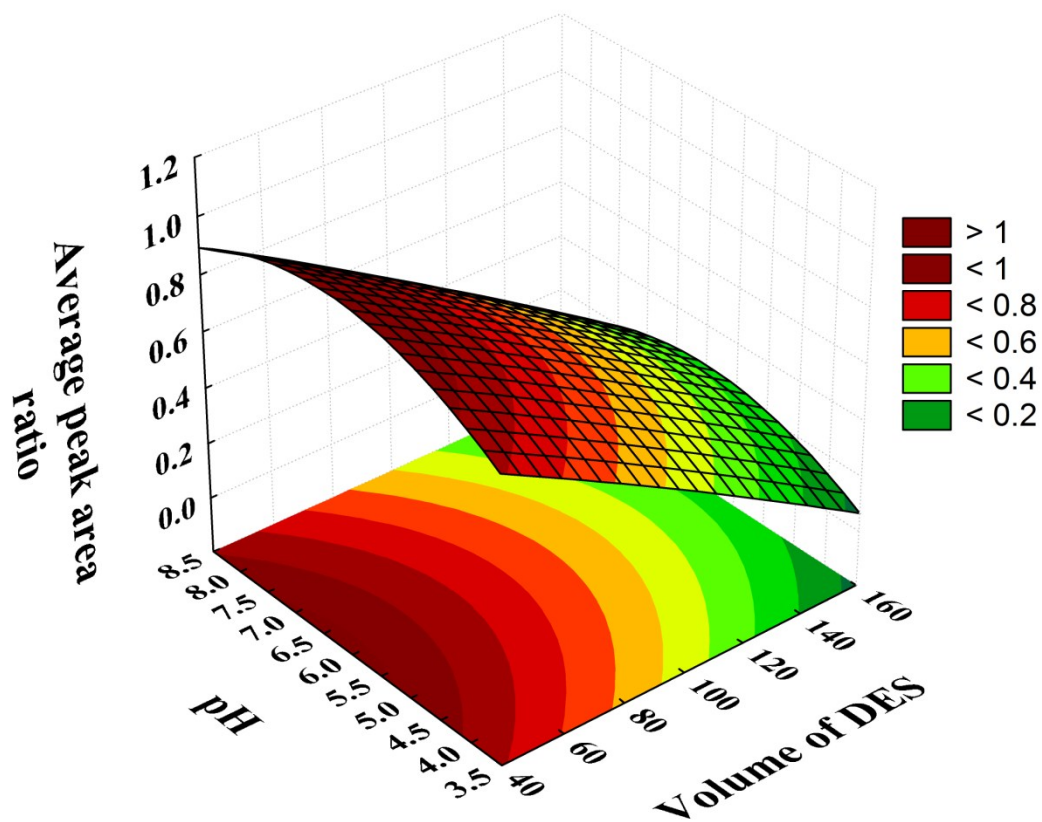
34

35



36

37



38

39

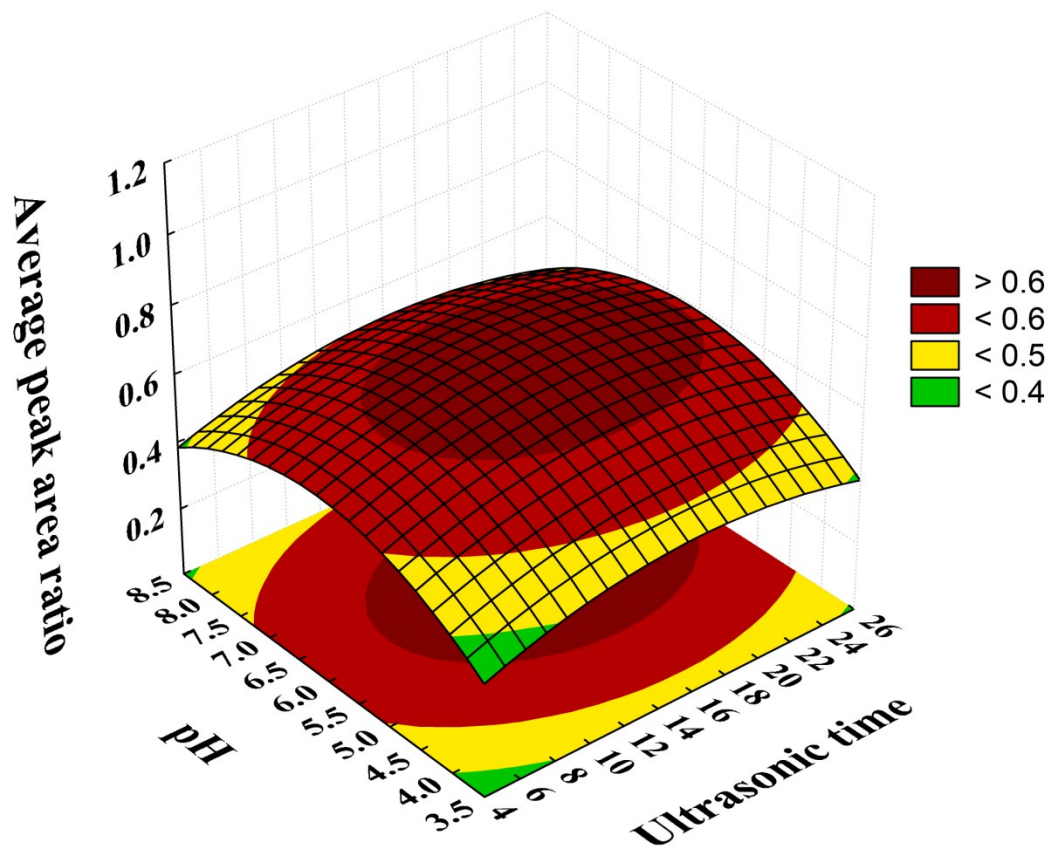


Figure (S3)

43 **Table S1** Actual and coded values of factors used in Box-Behnken for the extraction of Thiophenols.

Factors	Levels				
	Low (-1)	Central (0)	High (+1)		
(X ₁) Volume of acetone (μL)	50	100	150		
(X ₂) Volume of DES (μL)	50	100	150		
(X ₃) Ultrasonic time (min)	5	15	25		
(X ₄) pH	4	6	8		
Run	X ₁	X ₂	X ₃	X ₄	P ^a
1	-1	-1	0	0	1.025
2	+1	-1	0	0	0.83
3	-1	+1	0	0	0.401
4	+1	+1	0	0	0.394
5	0	0	-1	-1	0.52
6	0	0	+1	-1	0.511
7	0	0	-1	+1	0.508
8	0	0	+1	+1	0.521
9 CP	0	0	0	0	0.627
10	-1	0	0	-1	0.514
11	+1	0	0	-1	0.42
12	-1	0	0	+1	0.639
13	+1	0	0	+1	0.395
14	0	-1	-1	0	0.713
15	0	+1	-1	0	0.219
16	0	-1	+1	0	1.067
17	0	+1	+1	0	0.205
18 CP	0	0	0	0	0.626
19	-1	0	-1	0	0.544
20	+1	0	-1	0	0.499
21	-1	0	+1	0	0.458
22	+1	0	+1	0	0.551
23	0	-1	0	-1	0.818
24	0	+1	0	-1	0.107
25	0	-1	0	+1	0.912
26	0	+1	0	+1	0.162
27 CP	0	0	0	0	0.712

44 ^aAverage peak area ratio

45 **Table S2** ANOVA results obtained by Box-Behnken.

Factors	Sum of Square (SS)	Degree of Freedom (DF)	Mean Square (MS)	F-value	p-Value
X ₁ (L+Q)	0.025834	2	0.012917	5.3004	0.158720
X ₂ (L+Q)	1.253097	2	0.626548	257.0982	0.003874
X ₃ (L+Q)	0.039544	2	0.019772	8.1132	0.109731
X ₄ (L+Q)	0.073327	2	0.036664	15.0446	0.062326
X ₁ X ₂	0.008836	1	0.008836	3.6258	0.197197
X ₁ X ₃	0.004761	1	0.004761	1.9536	0.297052
X ₁ X ₄	0.005625	1	0.005625	2.3082	0.268040
X ₂ X ₃	0.033856	1	0.033856	13.8925	0.065038
X ₂ X ₄	0.000380	1	0.000380	0.1560	0.730983
X ₃ X ₄	0.000132	1	0.000132	0.0543	0.837467
Lack of Fit	0.095611	10	0.009561	3.9233	0.220110
Pure Error	0.004874	2	0.002437		
Total SS	1.526883	26			
R-squared	93.4				
R-adjusted	85.7				

46

47