

# Supplementary Information

## HPLC/DAD Determination of Rosmarinic Acid in *Salvia officinalis*: Sample Preparation Optimization by Factorial Design

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**Table S1.** Comparison of <sup>1</sup>H and <sup>13</sup>C NMR data of isolated of RA with those of the literature

H / C	<sup>1</sup> H NMR δ / ppm (multiplicity, J / Hz)		<sup>13</sup> C NMR δ / ppm	
	Literature <sup>1</sup> (acetone- <i>d</i> <sub>6</sub> , 220 MHz)	Experimental (CD <sub>3</sub> OD, 200 MHz)	Literature <sup>2</sup> (D <sub>2</sub> O, 15 MHz)	Experimental (CD <sub>3</sub> OD, 50 MHz)
1	-		126.5	127.9
1'	-		129.9	126.3
2	7.09 (d, 2)	7.05 (d, 2)	113.6	113.0
2'	6.79 (d, 2)	6.79 (d, 2)	117.1	116.2
3	-		143.7	145.4
3'	-		143.7	144.7
4	-		146.7	148.3
4'	-		142.4	143.9
5	6.79 (d, 8)	6.74 (d, 8)	115.9	115.1
5'	6.69 (d, 8)	6.63 (d, 8)	115.9	114.9
6	6.96 (dd, 2; 8)	6.98 (dd, 2; 8)	122.4	121.8
6'	6.60 (dd, 2; 8)	6.59 (dd, 2; 8)	121.8	120.4
7	7.50 (d, 16)	7.55 (d, 16)	145.8	146.3
7' (2 H)	3.03 (2 q, 5; 8;14)	3.04 (2 q, 5; 8;14)	36.8	36.5
8	6.23 (d, 16)	6.27 (d, 16)	115.0	113.8
8'	5.17 (dd, 5; 8)	5.18 (dd, 5; 8)	76.2	73.3
9	-		168.6	167.1
9'	-		177.2	180.5

### Reference

1. Kelley, C. J.; Mahajan, J. R.; Brooks, L. C.; Neubert, L. A.; Breneman, W. R.; Carmack, M.; *J. Org. Chem.* **1975**, *40*, 1804.
2. Kelley, C. J.; Harruff, R. C.; Carmack, M.; *J. Org. Chem.* **1976**, *41*, 449.

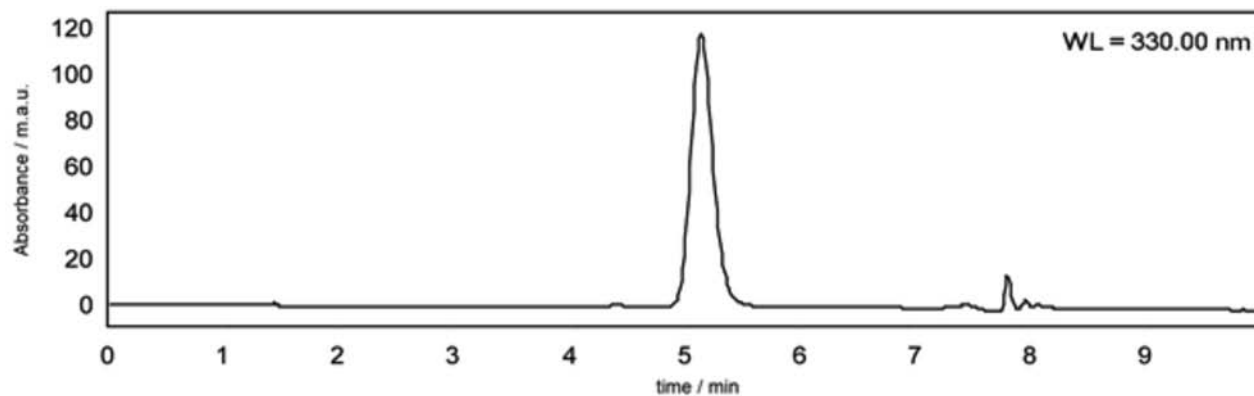


Figure S1. Chromatogram of RA isolated from *S. officinalis*.

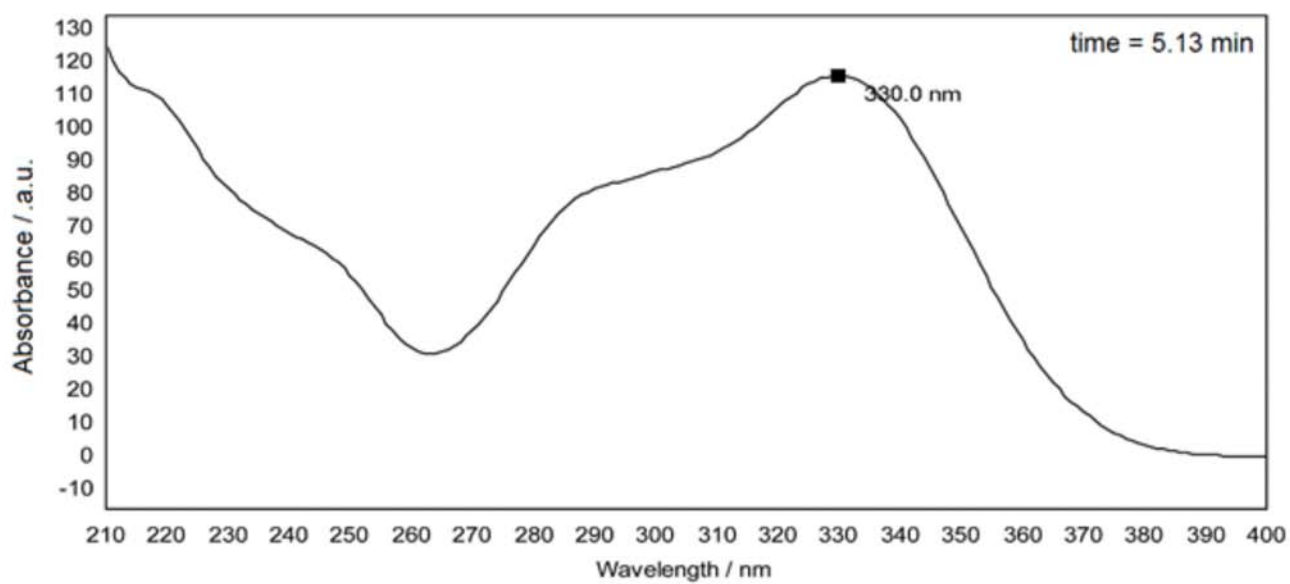


Figure S2. DAD UV spectrum of RA.

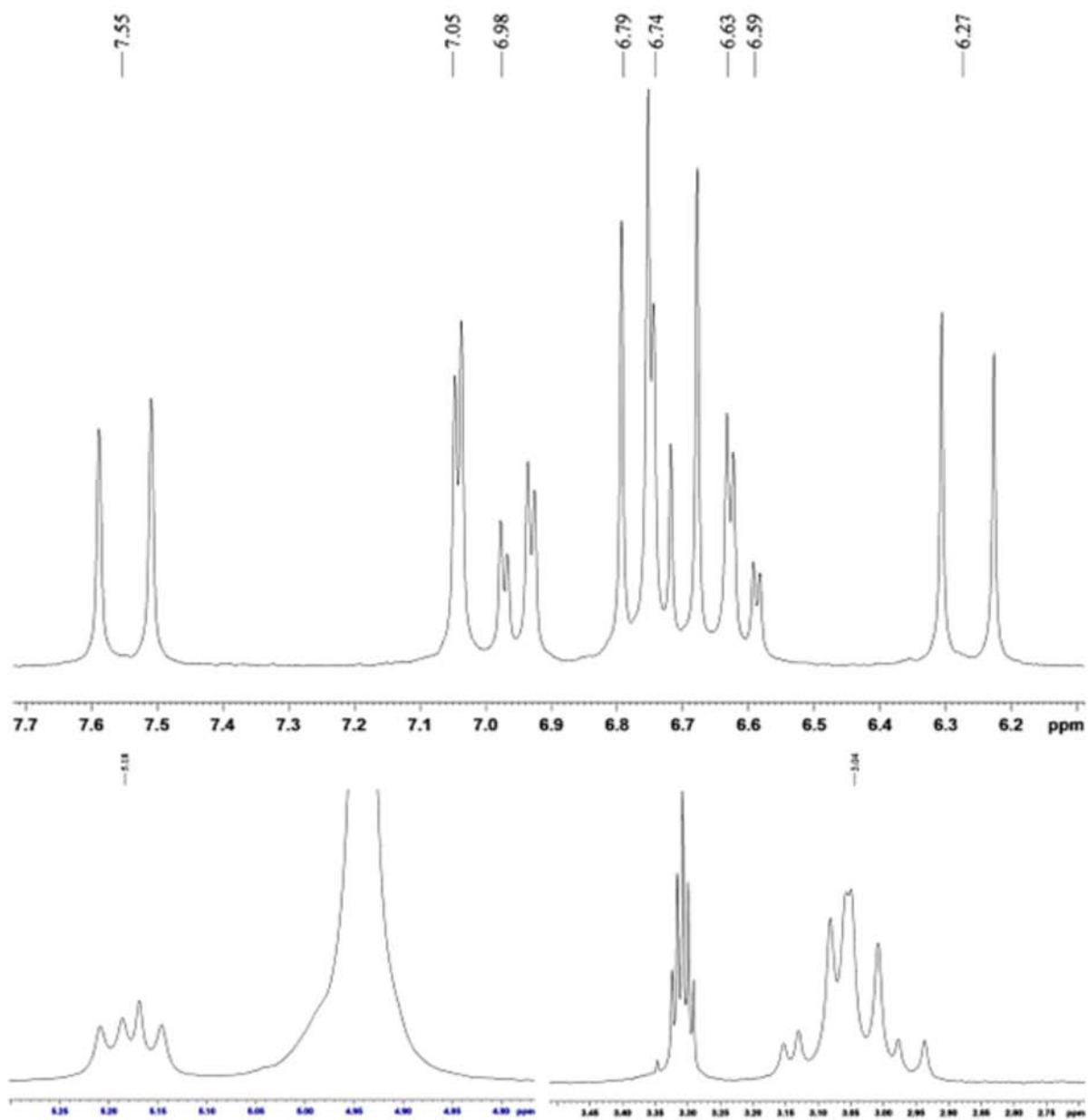


Figure S3. Expanded  $^1\text{H}$  NMR spectra (200 MHz,  $\text{CD}_3\text{OD}$ ) of RA.

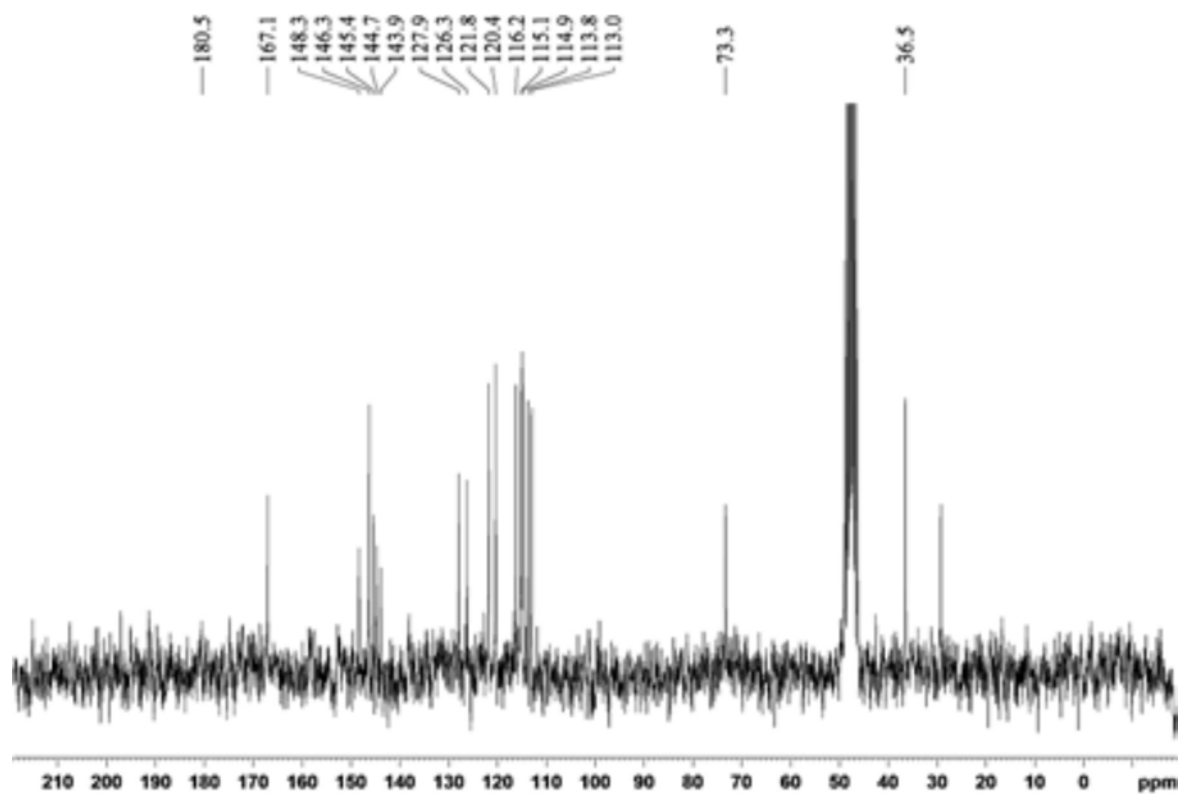


Figure S4.  $^{13}\text{C}$  NMR spectrum (50 MHz,  $\text{CD}_3\text{OD}$ ) of RA.

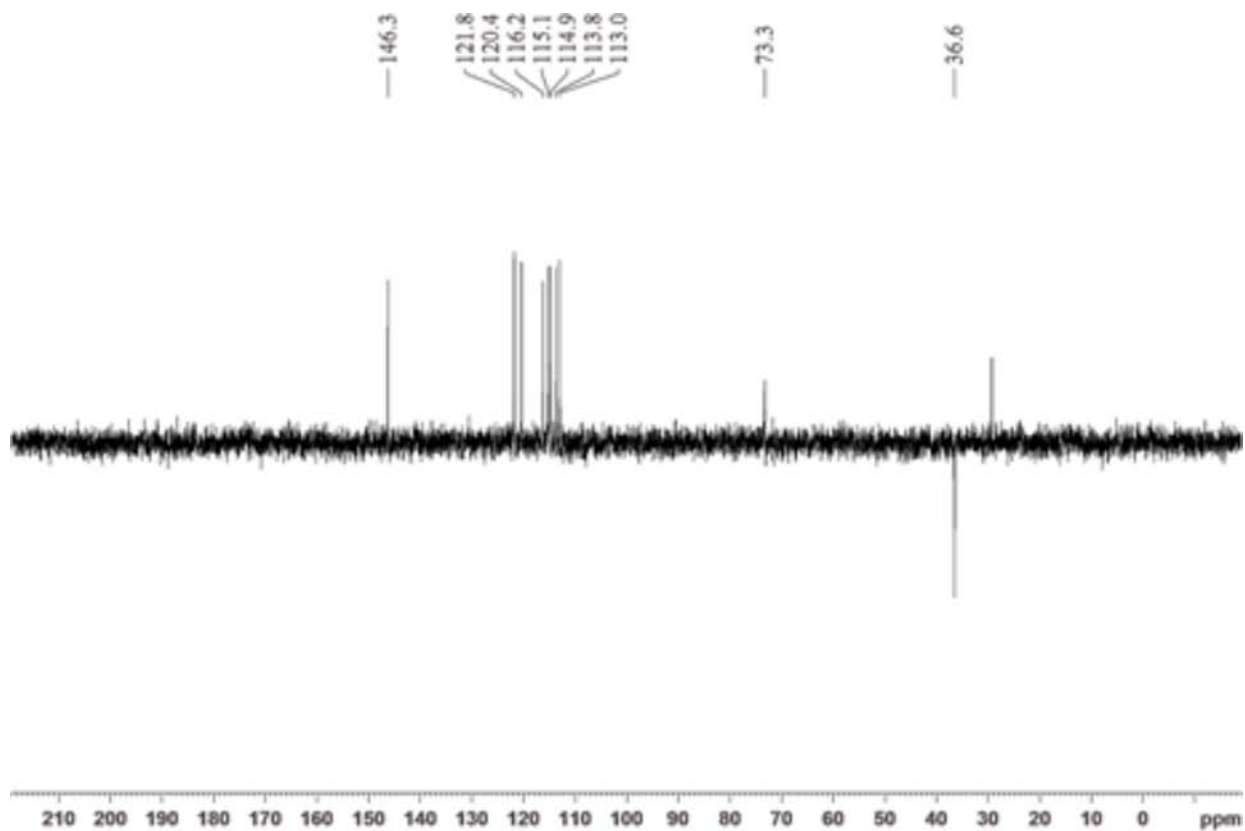
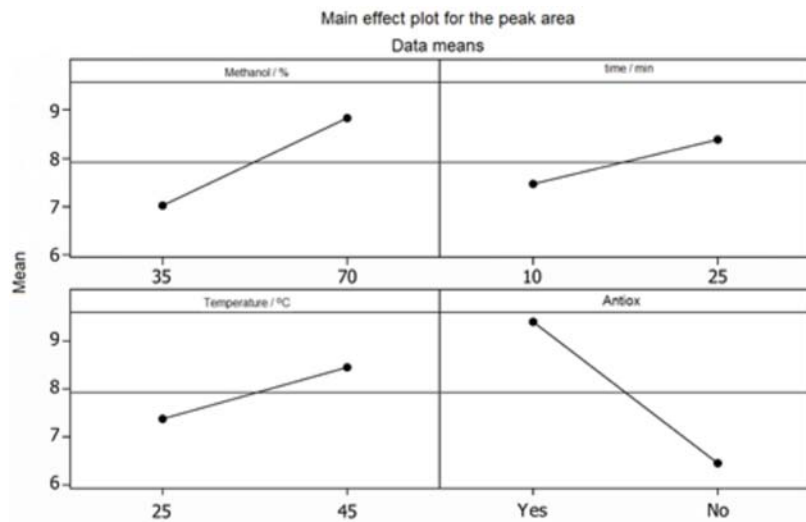
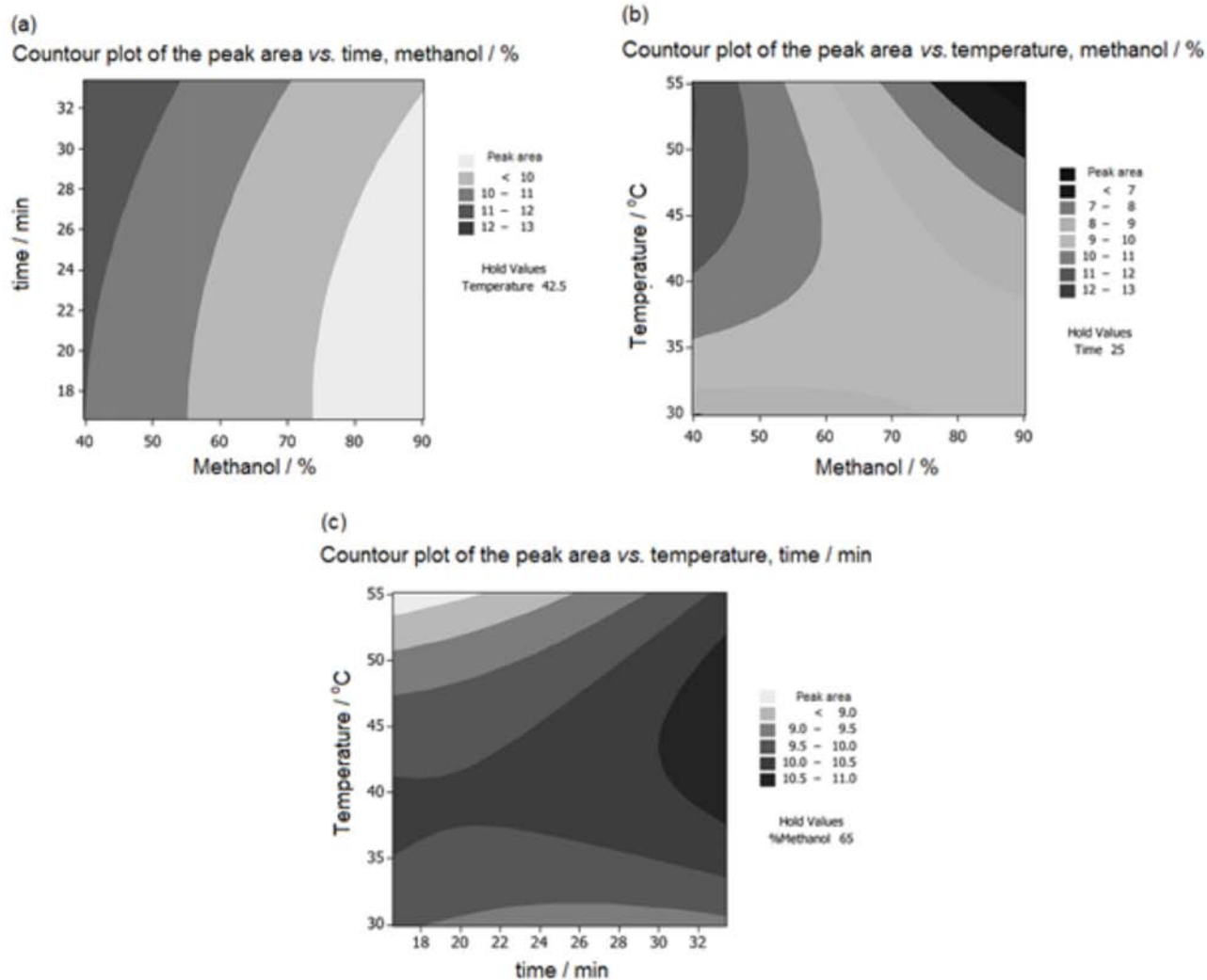


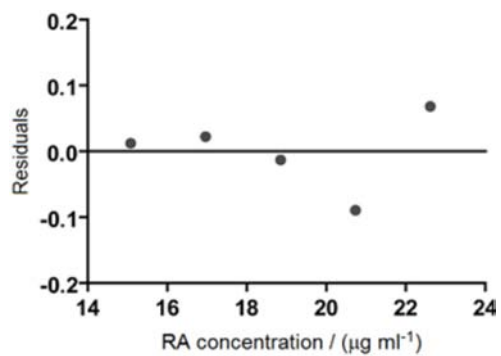
Figure S5.  $^{13}\text{C}$  NMR DEPT 135 spectrum (50 MHz,  $\text{CD}_3\text{OD}$ ) of RA.



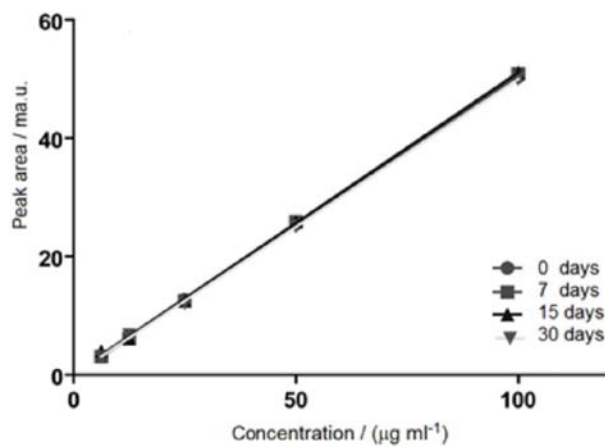
**Figure S6.** Main effect plot for the screening of parameters for extraction of RA from *S. officinalis*. Measured response was peak area.



**Figure S7.** Contour maps for the initial optimization of factors for RA extraction from *S. officinalis*. All extractions were carried out in the presence of antioxidants.



**Figure S8.** Residual plots of the linear regression for RA calibration.



**Figure S9.** Stability of calibration solutions of RA: solutions were stored at 4 °C between injections.