Appendix A

Table S1. Betacyanins (mg/g of extract) identified in every single run and the total betacyanin content.

Run	Peak 1		Peak 2		Peak 3		Peak 4		Peak 5		Peak 6		Peak 7		Total betacyanins	
	Betanin		Isobetanin		Gomphrenin I		(Iso)phyllocactin		17 decarboxy-betanin		Betanidin		Isobetanidin		mg/g	
	UAE	MAE	UAE	MAE	UAE	MAE	UAE	MAE	UAE	MAE	UAE	MAE	UAE	MAE	UAE	MAE
1	144.0	90.4	21.6	12.6	4.8	1.7	2.2	0.4	2.0	0.6	3.3	1.2	3.7	5.4	181.5	112.3
2	118.7	111.9	18.0	16.0	4.1	3.0	1.7	1.2	1.6	0.9	2.3	1.5	2.5	5.7	148.8	140.1
3	107.6	95.2	16.2	13.0	3.3	1.8	1.6	1.0	1.3	0.7	1.8	0.7	2.6	0.0	134.3	112.5
4	123.7	104.8	17.7	15.1	3.9	2.3	1.9	0.6	1.6	0.2	2.3	2.0	1.9	4.2	152.9	129.3
5	91.0	91.5	11.1	12.2	2.8	2.0	1.0	1.0	0.9	0.8	0.9	0.3	1.5	0.0	109.3	107.9
6	92.2	91.7	12.4	14.2	2.9	2.2	1.4	0.3	1.0	0.6	1.2	0.9	1.3	3.5	112.5	113.5
7	100.4	117.1	13.4	17.2	3.2	2.5	1.4	0.4	1.1	0.5	1.3	0.3	2.7	3.3	123.6	141.3
8	103.6	96.1	13.8	15.6	3.2	2.1	1.5	0.9	1.1	0.6	1.8	2.0	2.8	2.5	127.8	119.7
9	135.2	67.6	20.8	10.0	4.5	1.0	1.8	0.2	1.8	0.4	2.8	0.1	3.5	3.4	170.3	82.7
10	150.2	65.3	22.7	9.6	5.2	1.0	2.2	0.2	2.3	0.4	3.2	0.8	3.7	3.1	189.5	80.5
11	107.5	92.4	16.6	16.4	3.3	1.6	1.2	0.1	1.2	0.6	1.8	1.0	1.6	4.1	133.2	116.4
12	111.5	83.0	16.5	14.4	3.7	1.7	1.5	0.2	1.4	0.1	2.2	3.7	1.7	4.4	138.6	107.6
13	116.1	43.1	16.0	7.5	4.1	1.0	1.8	0.2	1.5	0.1	2.1	0.1	1.8	1.5	143.2	53.5
14	102.6	18.8	13.4	3.3	3.3	0.3	1.2	0.1	1.1	0.2	1.3	0.3	1.8	2.0	124.7	25.1
15	94.8	52.1	12.7	10.6	2.9	1.2	1.1	0.7	0.9	0.4	1.6	1.2	1.6	0.0	115.7	66.3
16	97.1	44.2	13.4	10.0	3.0	1.2	1.4	0.2	1.0	0.2	1.1	0.7	2.4	3.1	119.3	59.6
17	126.3	88.7	19.1	14.8	3.9	1.8	1.8	0.5	1.3	0.2	2.2	0.6	4.4	0.0	159.1	106.6
18	136.3	60.9	21.3	10.8	4.6	1.5	2.1	0.1	1.8	0.2	3.3	2.3	4.5	1.3	173.9	77.1
19	156.1	78.6	23.6	11.5	5.1	1.4	2.3	0.4	2.0	0.4	3.7	0.5	4.6	4.0	197.5	96.8

20	126.6	55.9	18.8	16.5	4.4	2.2	2.3	0.9	1.6	0.7	2.6	1.5	3.5	2.2	159.7	79.8
21	139.0	127.0	21.4	18.2	4.6	3.4	2.1	1.2	2.4	0.9	2.8	1.3	2.2	3.2	174.5	155.1
22	58.6	16.7	7.2	30.8	1.8	5.0	0.8	0.1	0.6	0.6	0.9	0.0	2.1	0.0	72.0	53.2
23	108.0	113.3	15.2	15.8	3.4	2.5	1.7	1.6	1.3	1.2	2.0	0.8	2.1	0.0	133.8	135.1
24	140.6	25.8	21.8	16.5	5.1	4.8	2.5	0.9	1.7	0.3	3.4	1.2	4.1	0.0	179.2	49.4
25	116.3	92.1	16.1	12.5	3.7	1.5	1.4	0.5	1.2	0.2	1.7	0.7	2.6	0.0	143.0	107.6
26	144.9	95.1	23.2	14.9	5.3	2.1	2.3	1.3	1.9	0.9	3.1	0.5	3.6	0.0	184.3	114.8
27	106.8	93.0	16.9	14.4	3.6	1.8	1.5	0.8	1.3	0.8	2.2	1.0	2.3	0.0	134.7	111.8
28	149.9	102.8	22.8	16.1	5.1	2.4	2.4	0.2	1.8	0.7	2.8	0.8	2.7	4.1	187.4	127.1
29	128.8	101.6	19.7	15.9	4.3	1.8	2.0	0.3	1.6	0.7	2.2	1.3	2.6	4.6	161.2	126.3
30	134.7	94.1	19.4	14.4	4.8	1.6	2.3	0.3	1.7	0.5	2.5	0.3	3.6	3.4	169.0	114.7
31	131.6	90.4	19.6	12.6	4.4	1.7	2.1	0.4	1.7	0.6	2.5	1.2	3.2	5.4	165.0	112.3

Table S2. Phenolic acids (mg/g of extract) identified in every single run and the total phenolic acid content.

Run	Peak 1		Peak 2		Peak 3		Peak 4		Total phenolic acids	
	Piscidic acid		3-*O*-Feruloylquinic acid		*cis*-Caffeic acid		Ferulic acid hexoside		mg/g	
	UAE	MAE	UAE	MAE	UAE	MAE	UAE	MAE	UAE	MAE
1	8.46	6.30	n/d	0.03	0.38	0.02	0.07	0.07	8.91	6.41
2	6.85	6.89	n/d	0.02	0.36	0.02	0.06	0.08	7.26	7.01
3	6.00	5.57	0.08	0.02	0.25	0.01	0.05	0.07	6.39	5.66
4	6.86	6.51	n/d	0.02	0.37	0.03	0.06	0.07	7.29	6.62
5	6.34	5.71	0.09	0.02	0.21	0.00	0.05	0.06	6.69	5.80
6	6.03	6.12	0.08	0.02	0.24	0.01	0.05	0.08	6.40	6.23
7	6.59	7.32	n/d	0.03	0.34	0.02	0.06	0.09	6.98	7.46
8	6.62	6.33	n/d	0.02	0.35	0.01	0.06	0.06	7.04	6.42
9	8.11	5.52	n/d	0.01	0.43	0.01	0.07	0.07	8.61	5.60
10	12.13	5.50	0.71	0.01	0.06	0.01	0.09	0.07	12.99	5.59
11	6.23	6.07	0.07	0.03	0.24	0.02	0.05	0.08	6.60	6.20
12	6.44	6.54	n/d	0.01	0.32	0.04	0.05	0.07	6.81	6.65
13	7.28	7.14	0.00	0.01	0.36	0.02	0.07	0.06	7.71	7.23
14	6.60	3.95	n/d	0.01	0.34	0.01	0.06	0.04	7.00	4.01
15	6.13	6.22	0.09	0.03	0.25	0.00	0.06	0.07	6.52	6.32
16	6.33	6.59	n/d	0.04	0.36	0.02	0.06	0.07	6.75	6.73
17	7.93	6.08	0.10	0.02	0.28	0.01	0.06	0.06	8.37	6.18
18	7.92	6.12	n/d	0.02	0.40	0.01	0.07	0.07	8.39	6.22
19	9.05	5.94	n/d	0.01	0.45	0.01	0.08	0.07	9.58	6.03
20	7.33	6.48	n/d	0.01	0.35	0.02	0.06	0.07	7.75	6.57

21	7.78	6.34	n/d	0.01	0.38	0.03	0.06	0.06	8.22	6.43
22	6.21	5.99	n/d	0.04	0.28	0.01	0.05	0.06	6.53	6.10
23	6.28	6.70	0.12	0.01	0.21	0.01	0.05	0.06	6.66	6.78
24	7.83	6.48	n/d	0.02	0.41	0.02	0.06	0.07	8.31	6.60
25	7.00	6.61	0.10	0.04	0.28	0.02	0.06	0.07	7.44	6.74
26	8.61	5.93	n/d	0.00	0.49	0.01	0.07	0.07	9.17	6.02
27	6.17	5.76	n/d	0.02	0.34	0.02	0.05	0.08	6.56	5.87
28	8.41	6.07	0.19	0.03	0.30	0.04	0.07	0.06	8.97	6.20
29	7.19	6.06	0.12	0.02	0.29	0.01	0.06	0.08	7.66	6.18
30	8.00	6.68	0.13	0.02	0.35	0.02	0.07	0.09	8.55	6.81
31	7.57	6.84	n/d	0.02	0.35	0.01	0.06	0.08	7.98	6.95

Table S3. Flavonoids (mg/g of extract) identified in every single run and the total flavonoid content.

Run	Peak 1		Peak 2		Peak 3		Peak 4		Peak 5		Peak 6		Peak 7		Peak 8		Total flavonoids	
	Isorhamnetin-*O*-hexoside-*O*-(di-deoxyhexosyl-hexoside)		Isorhamnetin-*O*-hexoside-(deoxyhexosyl-hexoside)		Apigenin-*O*-hexoside		Isorhamentin-dirutinoside		Isorhamentin-dirutinoside		Isorhamnetin-*O*-(di-deoxyhexosyl-hexoside)		Isorhamnetin-*O*-hexosyl-(deoxyhexosyl-hexoside)		Isorhamentin-O-(deoxyhexosyl-hexoside)		mg/g	
	UAE	MAE	UAE	MAE	UAE	MAE	UAE	MAE	UAE	MAE	UAE	MAE	UAE	MAE	UAE	MAE	UAE	MAE
1	0.38	0.23	0.09	0.06	0.31	0.29	0.11	0.08	0.03	0.03	0.13	0.14	0.08	0.10	0.00	0.02	1.13	0.94
2	0.34	0.29	0.03	0.10	0.30	0.35	0.09	0.09	0.02	0.03	0.11	0.18	0.06	0.09	0.01	0.03	0.95	1.16
3	0.22	0.22	0.04	0.04	0.25	0.25	0.08	0.06	0.02	0.02	0.10	0.13	0.06	0.06	0.00	0.01	0.77	0.80
4	0.31	0.20	0.03	0.03	0.24	0.26	0.09	0.07	0.02	0.03	0.10	0.11	0.06	0.06	0.02	0.01	0.88	0.76
5	0.25	0.23	0.03	0.07	0.20	0.18	0.09	0.02	0.02	0.02	0.08	0.13	0.05	0.06	0.01	0.03	0.73	0.72
6	0.30	0.24	0.05	0.10	0.28	0.36	0.10	0.09	0.03	0.04	0.11	0.16	0.07	0.09	0.01	0.03	0.96	1.09
7	0.31	0.28	0.06	0.09	0.31	0.35	0.10	0.10	0.02	0.04	0.10	0.16	0.06	0.09	0.01	0.02	0.96	1.13
8	0.29	0.22	0.03	0.08	0.27	0.29	0.08	0.07	0.02	0.03	0.11	0.13	0.06	0.06	0.01	0.01	0.88	0.89
9	0.35	0.20	0.06	0.05	0.37	0.30	0.09	0.07	0.03	0.03	0.14	0.15	0.09	0.09	0.01	0.02	1.14	0.90
10	0.55	0.20	0.28	0.05	0.59	0.29	0.19	0.07	0.07	0.03	0.23	0.15	0.13	0.09	0.02	0.01	2.06	0.88
11	0.21	0.28	0.07	0.09	0.25	0.31	0.07	0.08	0.02	0.03	0.09	0.15	0.06	0.08	0.00	0.02	0.79	1.02
12	0.31	0.21	0.04	0.08	0.27	0.27	0.09	0.07	0.02	0.03	0.09	0.12	0.06	0.06	0.00	0.01	0.89	0.86
13	0.35	0.29	0.06	0.12	0.34	0.26	0.12	0.01	0.03	0.05	0.14	0.19	0.08	0.10	0.01	0.02	1.13	1.03
14	0.30	0.13	0.05	0.02	0.30	0.15	0.09	0.05	0.02	0.01	0.11	0.07	0.07	0.04	0.02	0.00	0.96	0.47
15	0.29	0.24	0.03	0.06	0.24	0.31	0.08	0.09	0.02	0.03	0.10	0.14	0.06	0.07	0.01	0.02	0.83	0.93
16	0.32	0.23	0.05	0.06	0.29	0.30	0.10	0.07	0.02	0.03	0.10	0.14	0.06	0.08	0.01	0.02	0.95	0.91
17	0.23	0.24	0.10	0.06	0.31	0.27	0.08	0.06	0.03	0.03	0.13	0.13	0.06	0.06	0.01	0.02	0.96	0.87
18	0.37	0.22	0.06	0.09	0.37	0.31	0.12	0.07	0.03	0.04	0.15	0.13	0.09	0.07	0.01	0.01	1.21	0.94

19	0.40	0.25	0.05	0.06	0.41	0.33	0.13	0.08	0.04	0.02	0.15	0.15	0.09	0.08	0.01	0.01	1.28	0.99
20	0.34	0.26	0.04	0.11	0.30	0.29	0.13	0.08	0.02	0.03	0.12	0.13	0.07	0.06	0.01	0.02	1.02	0.99
21	0.32	0.21	0.05	0.06	0.35	0.29	0.08	0.07	0.03	0.03	0.13	0.12	0.07	0.07	0.01	0.01	1.03	0.86
22	0.21	0.20	0.03	0.04	0.19	0.25	0.04	0.05	0.03	0.02	0.09	0.12	0.04	0.06	0.01	0.01	0.64	0.76
23	0.27	0.13	0.04	0.07	0.24	0.27	0.08	0.07	0.02	0.03	0.09	0.13	0.05	0.06	0.01	0.01	0.81	0.78
24	0.37	0.26	0.05	0.06	0.35	0.30	0.12	0.07	0.04	0.03	0.13	0.13	0.08	0.06	0.01	0.02	1.15	0.93
25	0.32	0.28	0.05	0.08	0.28	0.33	0.11	0.07	0.02	0.03	0.11	0.16	0.08	0.08	0.02	0.02	0.99	1.04
26	0.38	0.20	0.06	0.04	0.38	0.30	0.11	0.08	0.03	0.03	0.14	0.14	0.09	0.06	0.01	0.02	1.21	0.87
27	0.30	0.20	0.05	0.08	0.31	0.30	0.09	0.07	0.02	0.03	0.11	0.15	0.07	0.08	0.01	0.02	0.96	0.93
28	0.41	0.24	0.05	0.10	0.36	0.23	0.12	0.01	0.03	0.03	0.13	0.14	0.08	0.08	0.01	0.03	1.20	0.86
29	0.31	0.20	0.06	0.07	0.30	0.29	0.10	0.08	0.02	0.03	0.12	0.14	0.07	0.07	0.01	0.02	0.98	0.90
30	0.24	0.27	0.10	0.07	0.29	0.36	0.10	0.09	0.03	0.02	0.12	0.17	0.06	0.08	0.01	0.04	0.95	1.09
31	0.30	0.29	0.07	0.07	0.32	0.34	0.10	0.10	0.04	0.03	0.13	0.16	0.07	0.08	0.01	0.02	1.03	1.08

Table S4. Colour coordinates acquired in the 31 runs for UAE and MAE. Terms used include: L*: lightness; a*: green-red colour component; b*: blue-yellow colour component and C: Chroma.

Run	Colour coordinates							
	*L**		*a**		*b**		Chroma	
	UAE	MAE	UAE	MAE	UAE	MAE	UAE	MAE
1	43.82	36.12	83.84	76.12	-22.35	-0.99	86.77	76.12
2	45.36	49.71	84.50	74.89	-23.90	26.47	87.82	79.43
3	47.39	46.89	85.33	78.96	-26.95	18.42	89.49	81.08
4	48.17	37.51	83.07	77.84	-24.19	-3.40	86.52	77.92
5	45.50	38.62	84.51	76.27	-22.47	4.67	87.44	76.41
6	47.70	50.57	85.37	74.00	-24.99	24.80	88.95	78.05
7	43.99	37.31	83.30	74.05	-21.97	11.04	86.15	74.87
8	46.60	38.17	86.48	76.71	-25.64	3.88	90.20	76.80
9	45.84	45.24	85.24	73.07	-23.82	25.69	88.51	77.46
10	45.60	36.20	84.99	75.34	-23.10	3.32	88.08	75.41
11	45.93	38.43	85.18	73.83	-24.28	8.39	88.57	75.01
12	48.44	40.32	86.35	75.52	-26.97	13.48	90.46	76.72
13	48.81	37.01	86.25	77.75	-27.53	0.38	90.54	77.75
14	55.56	34.01	76.34	72.32	-23.63	0.36	79.91	72.33
15	44.73	36.78	83.56	77.28	-22.94	-1.61	86.65	77.30
16	48.48	35.41	86.56	73.50	-27.00	5.64	90.67	73.72
17	44.76	35.11	84.74	73.47	-22.46	6.12	87.66	73.73
18	43.87	35.24	83.12	74.33	-21.03	1.23	85.74	74.34
19	43.14	41.82	83.22	76.36	-21.64	16.74	85.99	78.18
20	44.36	35.54	84.80	74.08	-21.43	5.65	87.47	74.30
21	45.24	34.86	84.83	74.35	-22.22	0.36	87.69	74.36
22	43.76	34.09	83.32	72.65	-20.83	1.82	85.89	72.67
23	48.05	36.70	85.75	75.18	-24.05	3.41	89.06	75.26
24	45.35	35.46	84.89	73.99	-21.61	4.10	87.60	74.10
25	47.51	36.19	85.71	72.86	-22.68	8.00	88.65	73.29
26	44.18	37.42	83.35	73.53	-20.70	8.36	85.88	74.00
27	44.96	36.78	84.71	77.95	-21.22	-5.64	87.32	78.16
28	44.50	34.71	84.58	73.31	-20.55	5.84	87.04	73.54
29	46.12	34.93	84.76	59.35	-23.37	26.34	87.93	64.99
30	43.67	35.31	83.03	75.06	-19.85	-0.79	85.37	75.07
31	44.40	35.39	83.24	74.07	-19.78	5.28	85.56	74.26

Figure S1. Total betacyanin content 3d response surface plots of UAE and MAE for the parametric responses. For representation purposes, the 2 variable which are not confronted, were positioned at the centre of their experimental domain.

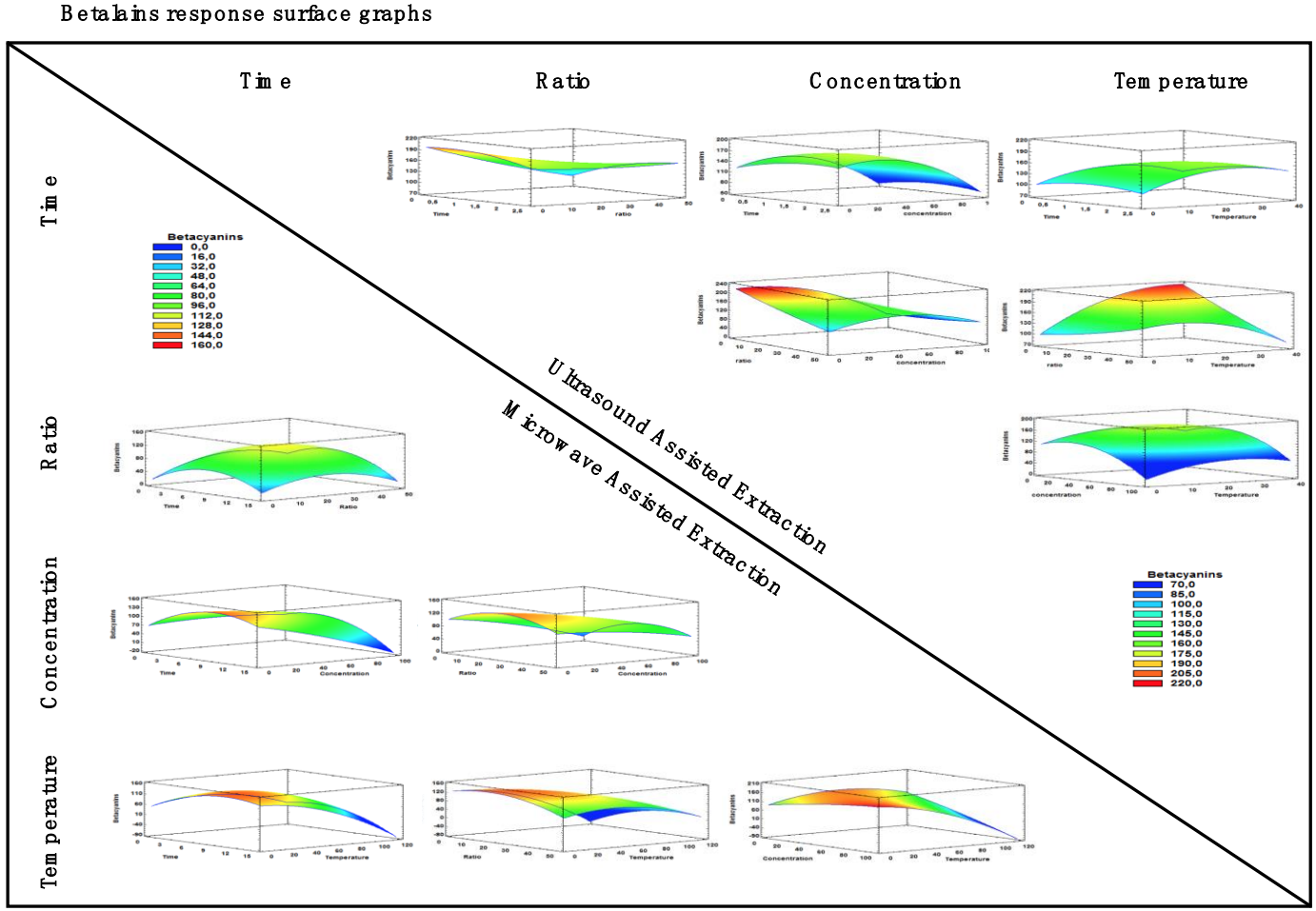

Figure S2. Total phenolic acid content 3d response surface plots of UAE and MAE for the parametric responses. For representation purposes, the 2 variable which are not confronted, were positioned at the centre of their experimental domain.

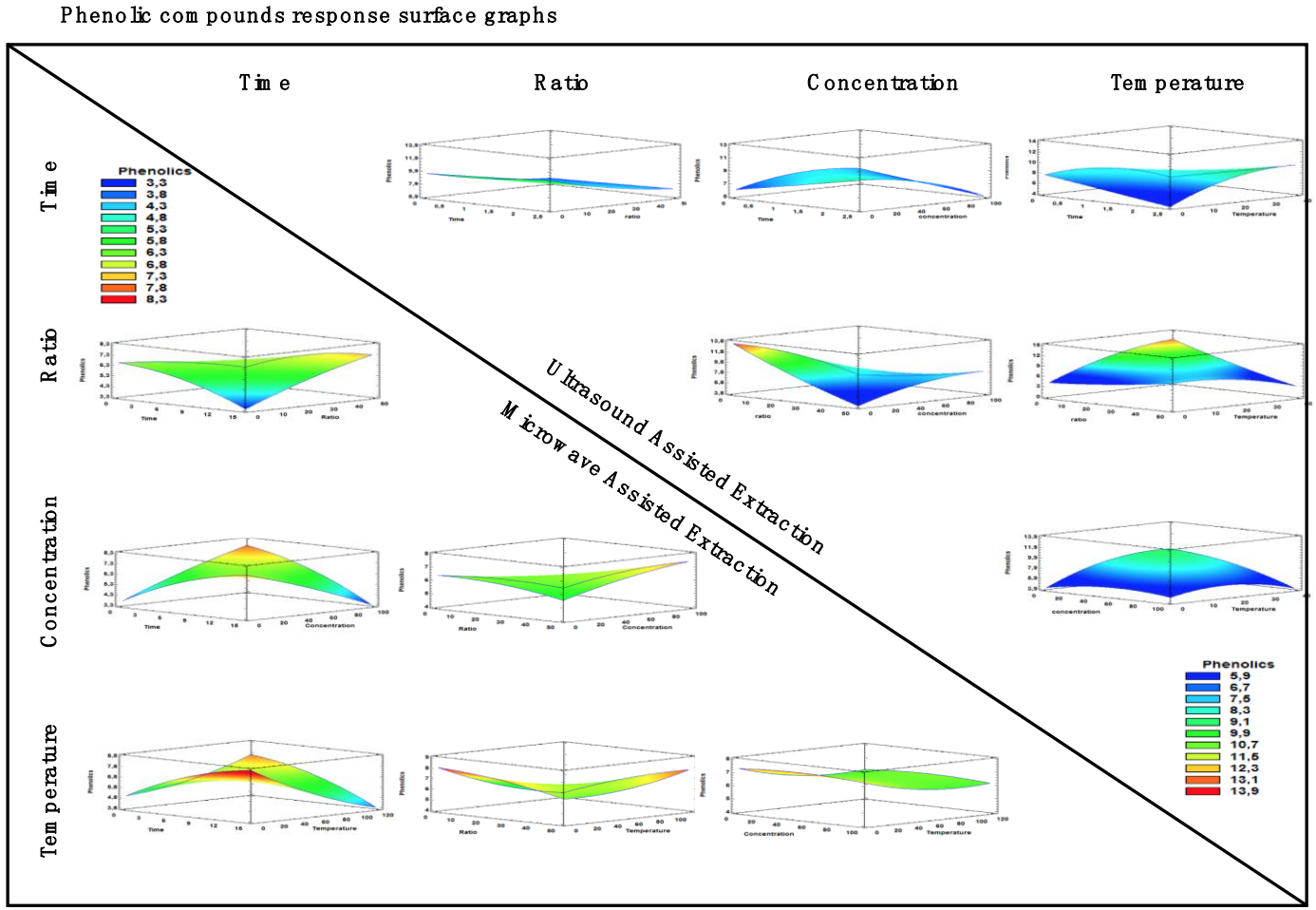

Figure S3. Total flavonoid content 3d response surface plots of UAE and MAE for the parametric responses. For representation purposes, the 2 variable which are not confronted, were positioned at the centre of their experimental domain.

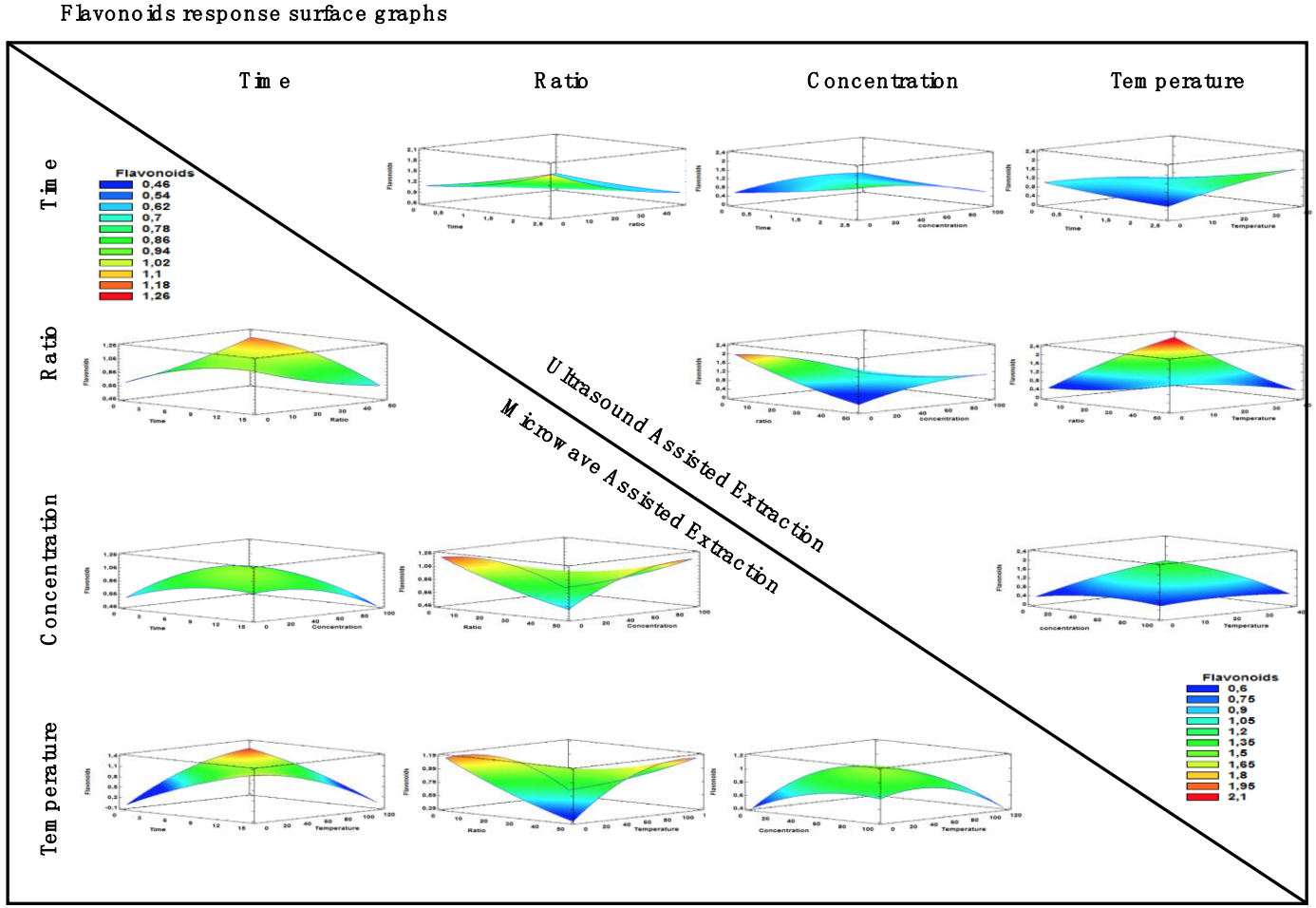

Figure S4. Antioxidant activity 3d response surface plots of UAE and MAE for the parametric responses. For representation purposes, the 2 variable which are not confronted, were positioned at the centre of their experimental domain.