

Table S1

The chromatographic data regions for modeling by MCR-ALS

Analyte	Retention time	Time region	Wavelength range	Factors *
	Scan No.(min)	Scan No. (min)	Scan No. (min)	
CBZ	618 (4.1)	4.08-4.17(610-627)	236-400(24-106)	3/3
DIC	784 (5.2)	5.14-5.29(773-796)	242-400(27-106)	3/2

*Number of MCR-ALS factors in influent and effluent

Table S2

The BBD design and its response values

Std	Run	Block	Factor 1 A:sorbent	Factor 2 B:desorb vol	Factor 3 C:desorb ratio	Response 1 R1	Response 2 R2	Response 3 R3	Response 4 R4	Response 5 R5	Response 6 R6	Response 7 R7
3	1	Block 1	25.00	3.00	0.00	61.36	228	61.8	831	204	34.3	0.677133
12	2	Block 1	40.00	3.00	1.00	98.1	311.6	89.2	1051.4	264.7	59.7	0.976802
13	3	Block 1	40.00	2.00	0.00	82.5	265.2	75.2	856.9	248.5	56.4	0.850646
6	4	Block 1	55.00	2.00	-1.00	66.5	245	68.3	816.7	188.5	44	0.724421
7	5	Block 1	25.00	2.00	1.00	62.7	218.1	55.9	671.7	193.7	29.4	0.618657
11	6	Block 1	40.00	1.00	1.00	71.6	238.7	67.3	959.3	238.8	44.6	0.780074
17	7	Block 1	40.00	2.00	0.00	91.7	272.6	69.8	977.6	243	57.1	0.876619
10	8	Block 1	40.00	3.00	-1.00	81.8	294.7	84.8	998.1	259.8	50.4	0.894501
8	9	Block 1	55.00	2.00	1.00	71.7	256.4	71.4	907.6	197.7	51.5	0.784198
15	10	Block 1	40.00	2.00	0.00	89.4	276.4	72.8	1017.8	239.6	53.6	0.875667
1	11	Block 1	25.00	1.00	0.00	59.1	204.3	52.3	714.5	187.9	18.7	0.55865
4	12	Block 1	55.00	3.00	0.00	78.6	269.1	78.2	1210.4	226.8	52.1	0.876551
2	13	Block 1	55.00	1.00	0.00	62.2	231.7	64.4	789.9	171.9	42.5	0.684319
16	14	Block 1	40.00	2.00	0.00	86.7	267.8	75.8	1003.3	245	56.8	0.882116
5	15	Block 1	25.00	2.00	-1.00	56.4	210.2	53.8	765.5	186.3	27.6	0.603132
9	16	Block 1	40.00	1.00	-1.00	70.9	228.7	65.1	824.2	228.5	40.8	0.733326
14	17	Block 1	40.00	2.00	0.00	88.4	269.7	74.2	986.5	248.3	58.5	0.886706