

Supporting Information

Diffusion- and Chemometric-Based Separation of Complex Electrochemical Signals that Originated from Multiple Redox-Active Molecules

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Table S1. Effective diffusion coefficients calculated for ascorbic acid (AA), clozapine (CLZ), ferricyanide (Ferri), L-homocysteine (HCy), and uric acid (UA) for different chitosan film thicknesses.

	Redox-active molecule	Thickness of the chitosan film (nm)					
		Bare	33.4	40.9	54.7	72	84.1
Effective diffusion coefficient [cm ² s ⁻¹]	AA	4.53×10 ⁻⁹ ± 3.43×10 ⁻¹³	4.87×10 ⁻⁹ ± 1.19×10 ⁻¹²	5.34×10 ⁻⁹ ± 4.12×10 ⁻¹³	4.05×10 ⁻⁹ ± 1.21×10 ⁻¹²	7.53×10 ⁻⁹ ± 3.13×10 ⁻¹²	3.56×10 ⁻⁹ ± 1.59×10 ⁻¹³
	CLZ	7.45×10 ⁻⁷ ± 4.22×10 ⁻¹⁰	3.26×10 ⁻⁷ ± 9.99×10 ⁻¹¹	4.61×10 ⁻⁸ ± 4.46×10 ⁻¹²	1.40×10 ⁻⁷ ± 4.96×10 ⁻¹¹	1.03×10 ⁻⁷ ± 7.11×10 ⁻¹¹	1.05×10 ⁻⁷ ± 1.96×10 ⁻¹¹
	Ferri	6.85×10 ⁻⁸ ± 6.49×10 ⁻⁹	1.27×10 ⁻⁷ ± 4.43×10 ⁻⁸	8.38×10 ⁻⁸ ± 1.17×10 ⁻⁸	5.80×10 ⁻⁸ ± 2.36×10 ⁻⁸	4.52×10 ⁻⁸ ± 1.68×10 ⁻⁸	5.93×10 ⁻⁸ ± 1.65×10 ⁻⁸
	HCy	3.01×10 ⁻⁹ ± 8.04×10 ⁻¹³	1.64×10 ⁻⁹ ± 9.09×10 ⁻¹³	1.50×10 ⁻⁹ ± 4.21×10 ⁻¹³	1.02×10 ⁻⁹ ± 7.79×10 ⁻¹³	5.63×10 ⁻¹⁰ ± 4.07×10 ⁻¹³	7.87×10 ⁻¹⁰ ± 4.87×10 ⁻¹³
	UA	2.08×10 ⁻⁹ ± 2.23×10 ⁻¹³	1.78×10 ⁻⁹ ± 3.78×10 ⁻¹³	3.32×10 ⁻⁹ ± 2.65×10 ⁻¹³	2.03×10 ⁻⁹ ± 4.55×10 ⁻¹³	3.30×10 ⁻⁹ ± 3.56×10 ⁻¹³	2.28×10 ⁻⁹ ± 3.58×10 ⁻¹³

Table S2. The composition of solutions used for the chemometric PLSR model training.

Solution number	Redox-active molecule concentration (μM)			
	CLZ	UA	HCy	AA
1	3.75	260	500	500
2	1	260	500	1000
3	3.75	140	300	1000
4	3.75	380	400	500
5	3.75	140	150	500
6	2.5	260	400	1000
7	1	500	500	1000
8	1	260	300	1000
9	1	500	400	1000
10	5	260	400	200
11	3.75	140	300	200
12	5	260	400	500
13	3.75	140	400	200
14	1	140	300	200
15	5	380	500	500
16	1	260	300	200
17	3.75	260	150	1000
18	5	260	300	0
19	3.75	140	300	0
20	2.5	140	400	500
21	1	260	300	500
22	3.75	380	300	1000

23	5	140	400	200
24	3.75	500	400	200
25	2.5	380	300	500
26	1	500	400	500
27	1	140	500	500
28	3.75	500	150	500
29	2.5	260	150	500
30	2.5	380	300	200
31	1	380	150	500
32	5	500	150	1000
33	3.75	380	400	1000
34	1	500	150	0
35	3.75	260	500	0
36	2.5	260	400	0
37	3.75	500	500	200
38	3.75	500	150	0
39	2.5	140	150	1000
40	1	140	500	0
41	3.75	380	500	0
42	2.5	380	500	1000
43	2.5	260	500	200
44	1	140	400	0
45	2.5	140	150	1000
46	2.5	380	500	0
47	2.5	260	150	200
48	1	380	150	200
49	5	500	500	200

50	2.5	500	500	200
51	5	500	300	500
52	5	380	400	1000
53	2.5	500	300	500
54	1	380	400	0
55	5	140	150	0
56	5	140	500	1000
57	2.5	500	400	0
58	5	260	150	0
59	2.5	500	300	0
60	5	500	300	1000
61	5	380	150	200
62	1	380	150	200
63	5	140	500	500
64	5	380	300	0

Table S3. The composition of solutions used for testing the trained chemometric PLSR model.

Solution number	Molecule concentration (μM)			
	CLZ	UA	HCy	AA
1	3.75	260	500	500
2	5	500	150	1000
3	3.75	500	400	200
4	1	140	500	1000
5	2.5	380	300	500
6	5	380	300	0
7	1	260	300	0
8	1	380	150	200
9	2.5	260	500	200
10	2.5	140	400	500
11	5	380	400	1000
12	5	260	300	0
13	3.75	260	300	0
14	2.5	380	300	200
15	3.75	380	500	0
16	5	260	150	1000
17	3.75	380	400	500
18	2.5	380	500	0
19	1	380	400	0
20	3.75	380	150	1000
21	5	380	150	0
22	5	260	150	500

23	3.75	140	150	200
24	5	260	400	500
25	5	500	150	1000
26	4.25	200	350	400
27	4.6	430	215	0
28	1.5	300	460	700
29	3.5	325	270	0
30	2	400	420	900
31	4.8	175	245	0

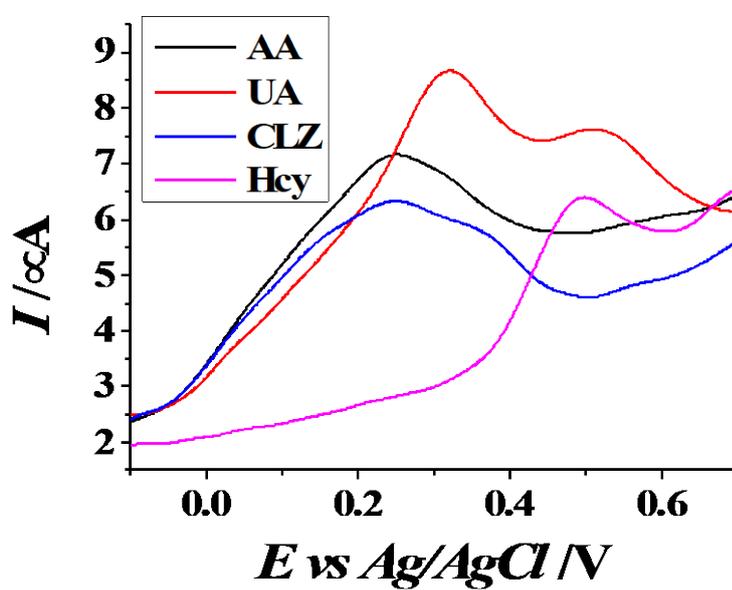


Figure S1. The electrochemical signatures measured from the same concentration of ascorbic acid (AA; black), uric acid (UA; red), clozapine (CLZ; blue), and L-homocysteine (Hcy; magenta) by using a gold bare electrode.

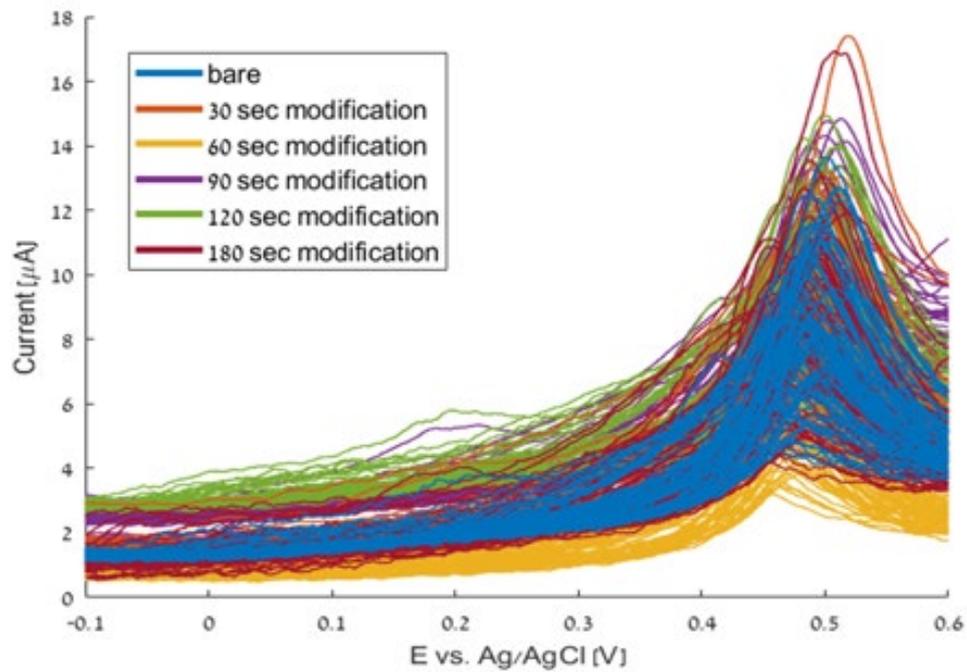


Figure S2. Example of the differential pulse voltammograms recorded from the different mixture solutions by using a bare electrode (blue) and electrodes modified with 30s- (orange), 60s- (yellow), 90s- (purple), 120s- (green), and 180s- (brown) chitosan electrodeposited electrodes.

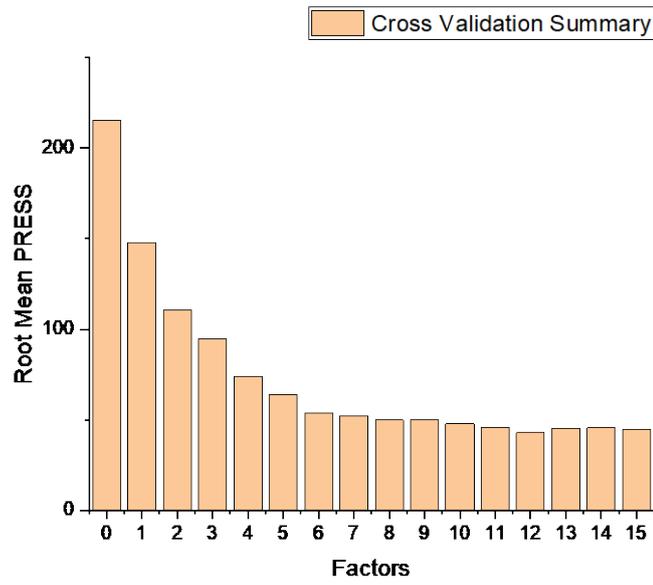


Figure S3. Root mean predicted residual error sum of squares (PRESS) calculated by a leave-one-out cross-validation.

Table S4. Explained X and Y variance.

Number of Factors	Variance Explained for X Effects (%)	Cumulative X Variance (%)	Variance Explained for Y Responses (%)	Cumulative Y Variance (%)
1	68.62809	68.62809	54.22085	54.22085
2	11.45509	80.08318	22.44814	76.66899
3	5.21964	85.30282	7.27516	83.94415
4	2.16823	87.47105	8.41452	92.35867
5	3.20797	90.67901	2.40783	94.7665
6	1.46711	92.14612	1.72614	96.49265
7	0.80359	92.94972	0.79287	97.28552
8	0.90078	93.85049	0.48951	97.77503
9	1.49947	95.34997	0.21606	97.99109
10	0.55315	95.90311	0.44503	98.43613
11	0.89668	96.79979	0.16075	98.59688
12	0.29571	97.0955	0.21004	98.80691