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Article

Simultaneous multiplexed quantification of banned Sudan dyes using surface enhanced Raman scattering and chemometrics

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Supplementary Materials

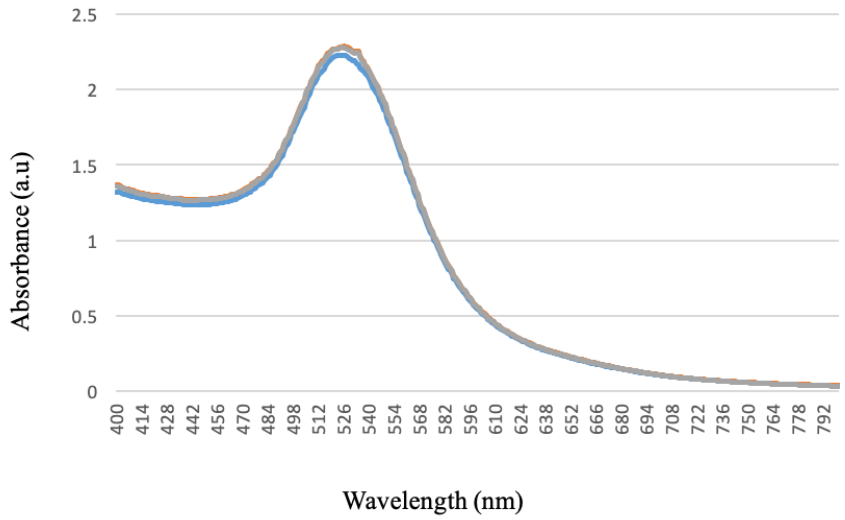

Figure S1: UV–Visible absorption spectra of the citrate reduced gold nanoparticles.

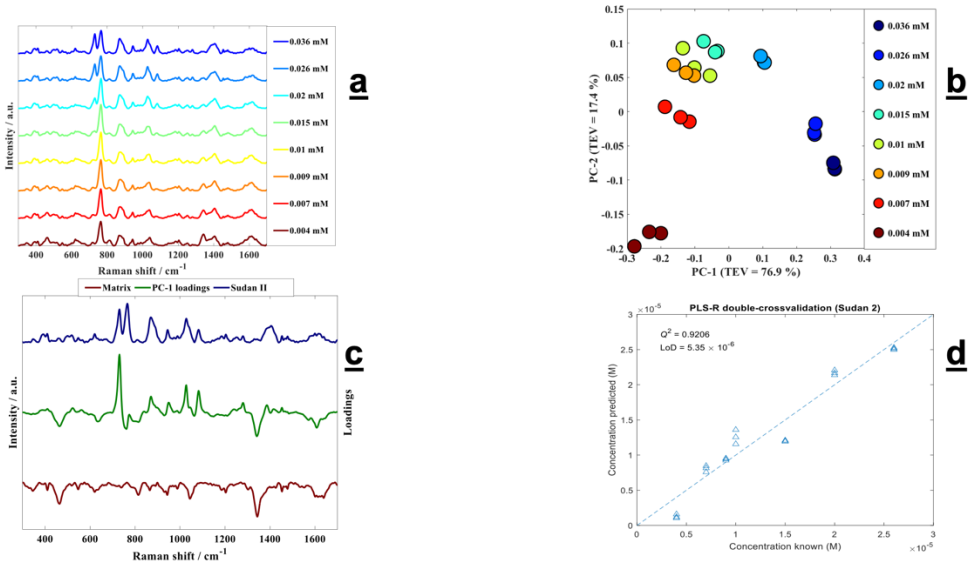

Figure S2: (a) SERS spectra of Sudan II shows different concentrations and spectra are offset for clarity; (b) PCA scores plot of Sudan II, the colours represent the concentrations, and the details are provided within the figure; (c) PC1 loadings plot (green), with Sudan II (blue) and matrix, aggregation agent (0.5M NaCl) and gold nanoparticles, (in brown and multiplied by -1 (i.e. inverted) for clarity); (d) PLS-R predictions of Sudan II, these models used double-cross validation.

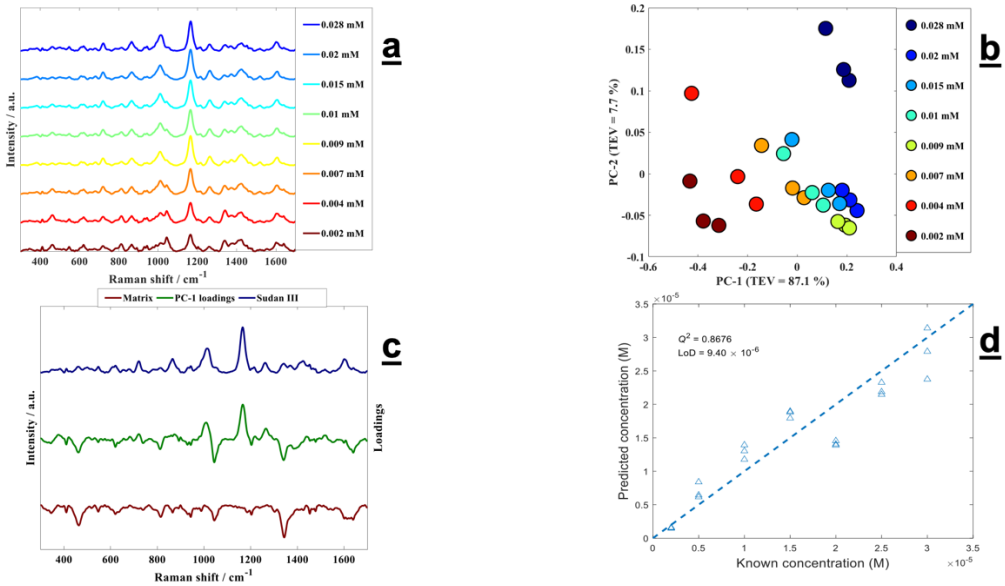

Figure S3: (a) SERS spectra of Sudan III shows different concentrations and spectra are offset for clarity; (b) PCA scores plot of Sudan III, the colours represent the concentrations, and the details are provided within the figure; (c) PC1 loadings plot (green), with Sudan III (blue) and matrix, aggregation agent (0.5M NaCl) and gold nanoparticles, (in brown and multiplied by -1 (i.e. inverted) for clarity); (d) PLS-R predictions of Sudan III, these models used double-cross validation.

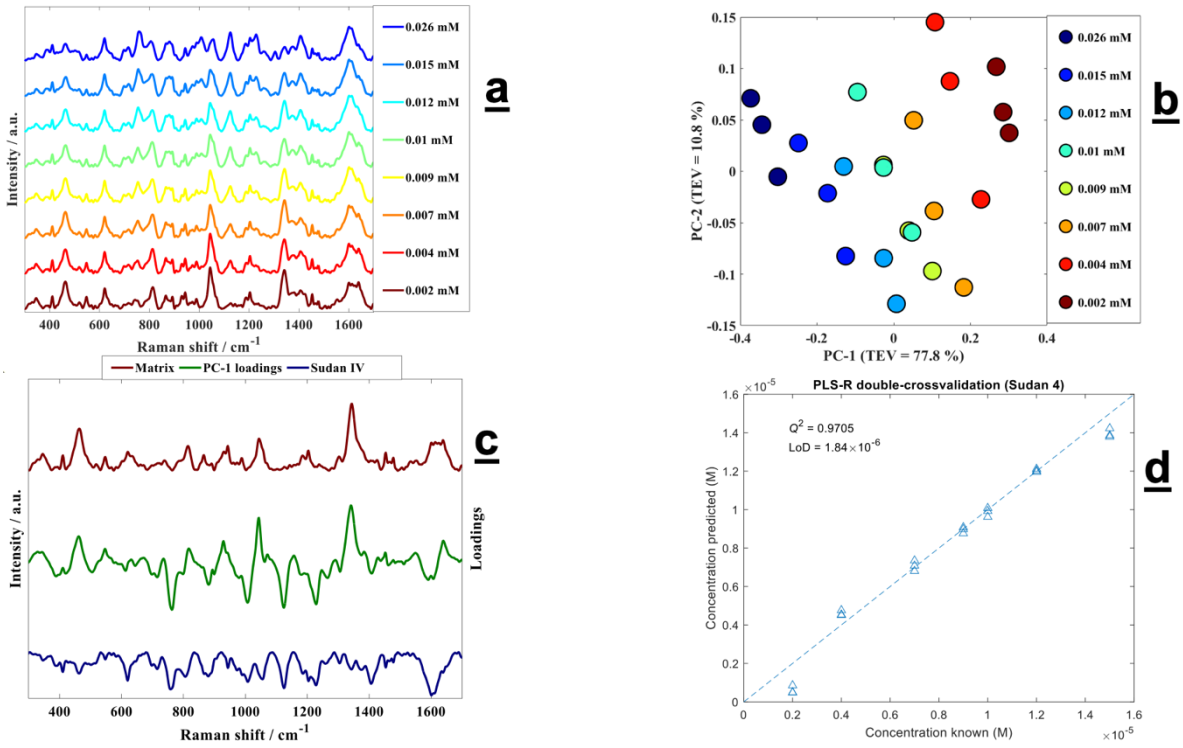

Figure S4: (a) SERS spectra of Sudan IV shows different concentrations and spectra are offset for clarity; (b) PCA scores plot of Sudan IV, the colours represent the concentrations, and the details are provided within the figure; (c) PC1 loadings plot (green), with Sudan IV (blue) and matrix, aggregation agent (0.5M NaCl) and gold nanoparticles, (in brown and multiplied by -1 (i.e. inverted) for clarity); (d) PLS-R predictions of Sudan IV, these models used double-cross validation**.**

Table S1: Latin Hypercubic Sampling of combination Sudan dyes I-IV

Sample	Sudan I	Sudan II	Sudan III	Sudan IV	Sample	Sudan I	Sudan II	Sudan III	Sudan IV
1	0	60	30	50	46	50	60	60	65
2	0	65	50	75	47	50	80	10	95
3	0	85	90	15	48	55	5	80	20
4	5	5	85	20	49	55	70	60	100
5	5	15	5	80	50	55	75	5	30
6	5	15	45	10	51	55	85	30	80
7	5	100	10	70	52	55	90	40	55
8	10	15	60	25	53	60	0	95	50
9	10	20	75	15	54	60	50	15	25
10	10	25	45	5	55	60	65	40	5
11	10	85	30	70	56	60	70	15	45
12	15	20	70	60	57	60	90	90	85
13	15	45	65	75	58	65	10	65	10
14	15	50	40	35	59	65	75	35	5
15	15	55	95	60	60	65	95	35	35

16	15	80	100	45	61	70	5	0	45
17	20	10	25	90	62	70	40	30	20
18	20	20	45	55	63	70	60	75	10
19	20	20	80	95	64	70	80	100	65
20	20	65	50	55	65	70	90	85	30
21	25	25	45	30	66	75	0	80	80
22	25	55	60	45	67	75	35	90	80
23	25	80	55	50	68	75	40	10	95
24	25	85	25	15	69	75	95	15	5
25	30	20	85	20	70	75	100	55	45
26	30	30	5	90	71	80	30	85	60
27	30	30	15	100	72	80	70	80	40
28	30	35	20	75	73	80	75	55	25
29	30	45	65	65	74	80	75	90	65
30	30	45	75	70	75	80	80	20	85
31	35	65	5	60	76	85	30	75	85
32	35	85	40	40	77	85	55	10	25
33	35	90	30	85	78	85	60	50	75
34	40	5	95	5	79	85	70	0	70
35	40	10	65	30	80	90	10	5	0
36	40	25	70	15	81	90	35	70	0
37	40	50	35	95	82	90	40	60	40
38	40	95	85	85	83	90	45	95	40
39	45	30	20	95	84	95	45	30	35
40	45	35	40	65	85	95	50	55	15
41	45	50	70	90	86	95	70	75	55
42	45	55	25	35	87	95	95	15	35
43	50	5	25	50	88	95	95	20	90
44	50	20	55	20	89	100	15	50	55
45	50	40	35	75	90	100	35	95	10

The values in the table are percentages that represent those of the different ranges from each of the dyes:

Sudan I is 0.048 – 0.002 mM

Sudan II: 0.036 – 0.004 mM

Sudan III: 0.028 – 0.002 mM

Sudan IV: 0.026 – 0.002 mM

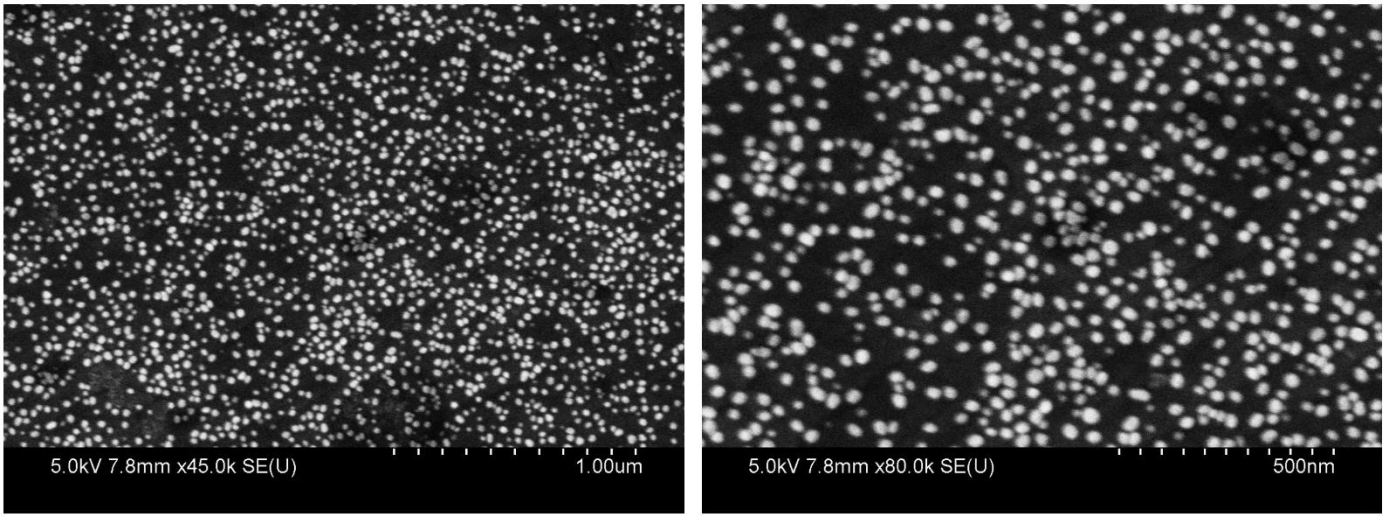

Figure S5: SEM micrographs acquired from gold nanoparticles bound to stainless steel substrate. The scale bars and magnification are inset in each of the images.

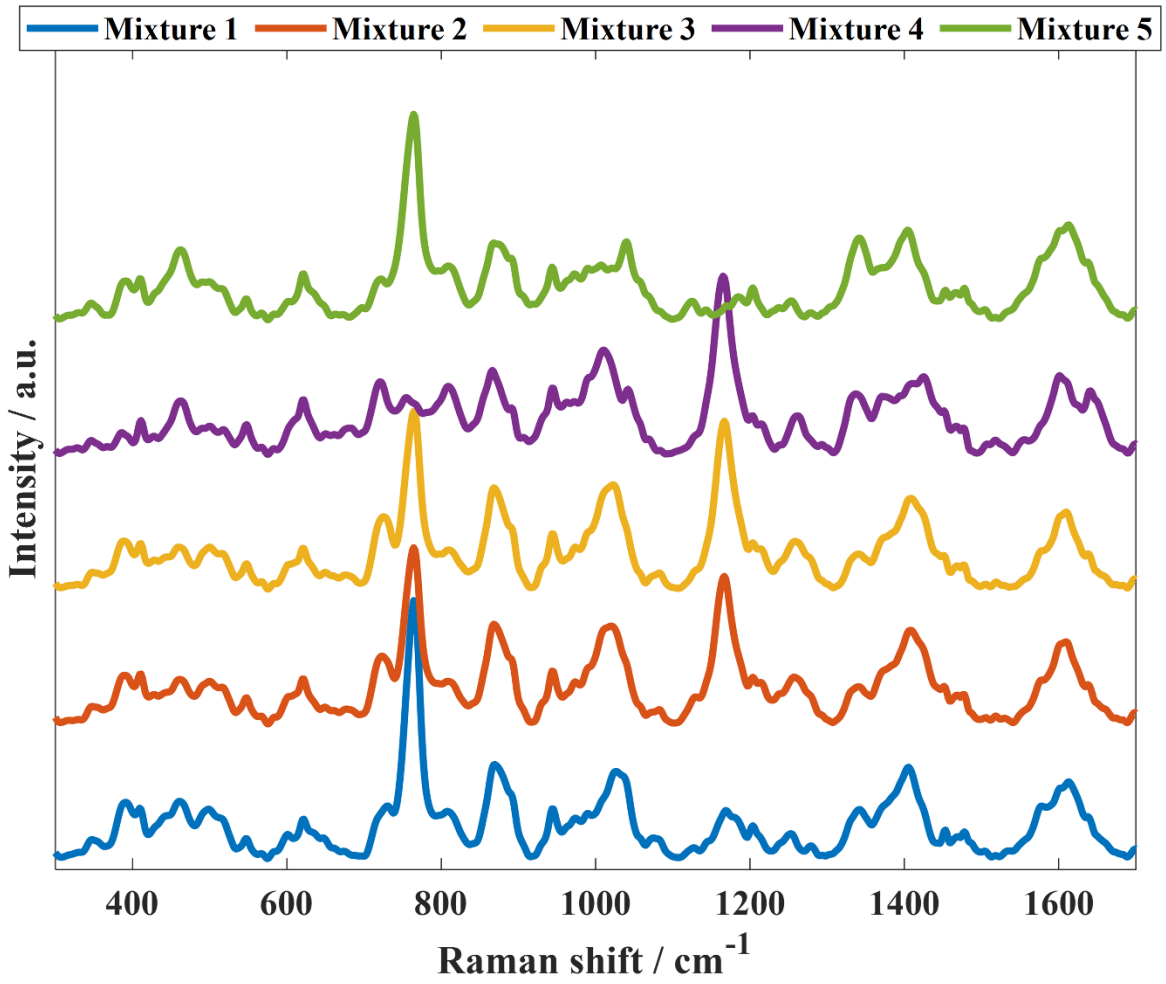

Figure S6: SERS spectra acquired from quadruplex mixtures. Mixture 1 (sample 1 in table S1); Mixture 2 (sample 2 in table S1); Mixture 3 (sample 3 in table S1); Mixture 4 (sample 4 in table S1); Mixture 5 (sample 5 in table S1).