Supplementary material

Simultaneous detection of food dyes from different samples in a 96-well plate by spectrophotometry

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Table S1 ε data of six synthetic dyes obtained at the group I wavelengths

dye	ε_{425}	ε_{480}	ε_{496}	ε_{508}	ε_{520}	ε_{626}
TA	0.0361	0.0116	0.0027	0.0006	0.0001	0
SY	0.0149	0.0334	0.0312	0.0279	0.0176	0
AR	0.0101	0.0274	0.0313	0.0293	0.0259	0
PO	0.0061	0.0177	0.0212	0.0220	0.0207	0
AM	0.0054	0.0153	0.0199	0.0224	0.0236	0.0001
BB	0.0027	0.0003	0.0007	0.0011	0.0019	0.0640

Table S2 ε data of six synthetic dyes obtained at the group II wavelengths

dye	ε_{425}	ε_{478}	ε_{525}	ε_{331}	ε_{555}	ε_{626}
TA	0.0361	0.0133	0.0001	0.0044	0	0
SY	0.0149	0.0332	0.012	0.0072	0.0005	0
AR	0.0101	0.0263	0.0246	0.0078	0.0114	0
PO	0.0061	0.0171	0.0195	0.0113	0.0085	0
AM	0.0054	0.0146	0.0235	0.0096	0.0161	0.0001
BB	0.0027	0.0003	0.0024	0.0021	0.0077	0.064

Table S3 ε data of six synthetic dyes obtained at the group III wavelengths

dye	ε_{383}	ε_{466}	ε_{534}	ε_{331}	ε_{558}	ε_{638}
TA	0.0246	0.0213	0	0.0044	0	0
SY	0.0105	0.0297	0.005	0.0072	0.0003	0
AR	0.0065	0.0206	0.022	0.0078	0.0096	0
PO	0.0036	0.0134	0.017	0.0113	0.0072	0
AM	0.0045	0.0110	0.022	0.0096	0.0149	0
BB	0.0041	0.0002	0.003	0.0021	0.0088	0.0552

Table S4 The contents of the mixture solutions, the unit of the concentrations in the table is μg·mL^{-1}.

No.	C_{TA}	C_{SY}	C_{AR}	C_{PO}	C_{AM}	C_{BB}
1	4	4	4	4	4	4
2	5	5	5	5	5	5
3	7	7	7	7	7	7
4	8	8	8	8	8	8
5	10	10	10	10	10	10
6	12	12	12	12	12	12
7	13	13	13	13	13	13
8	14	14	14	14	14	14
9	15	15	15	15	15	15
10	16	16	16	16	16	16
11	20	20	20	20	20	20
12	5	10	15	20	25	30
13	10	5	25	30	20	15
14	15	20	5	25	30	10
15	20	15	30	5	10	25
16	25	30	10	15	5	20
17	30	25	20	10	15	5

Table S5 Dye concentrations (μg·mL^{-1}) in mixture samples No. 1–17 predicted by equation group (4)

Sample	C_{TA}	C_{SY}	C_{AR}	C_{PO}	C_{AM}	C_{BB}
1	4.42(4)	2.13(4)	-0.62(4)	20.68(4)	-2.86(4)	4.19(4)
2	5.45(5)	2.66(5)	-0.9(5)	25.88(5)	-3.75(5)	5.19(5)
3	7.52(7)	4.33(7)	-0.05(7)	31.06(7)	-2.71(7)	7.27(7)
4	8.61(8)	4.88(8)	0.4(8)	34.95(8)	-3.11(8)	8.29(8)
5	10.7(10)	6.81(10)	1.81(10)	38.03(10)	-1.01(10)	10.39(10)
6	12.85(12)	8.15(12)	2.43(12)	45.57(12)	-1.66(12)	12.42(12)
7	13.85(13)	8.79(13)	3.35(13)	47.74(13)	-1.51(13)	13.4(13)
8	14.86(14)	10.17(14)	4.97(14)	45.22(14)	1.9(14)	14.48(14)
9	15.9(15)	10.85(15)	5.98(15)	47.51(15)	1.98(15)	15.49(15)
10	16.81(16)	12.45(16)	6.45(16)	46.48(16)	4.79(16)	16.52(16)
11	20.86(20)	17.07(20)	11.64(20)	44.33(20)	12.49(20)	20.57(20)
12	5.04(5)	7.82(10)	8.09(15)	38.80(20)	19.00(25)	30.13(30)
13	10.41(10)	0.56(5)	14.53(25)	66.07(30)	5.26(20)	15.49(15)
14	14.76(15)	19.35(20)	1.88(5)	35.41(25)	25.82(30)	10.23(10)
15	19.29(20)	17.26(15)	28.57(30)	-11.81(5)	29.32(10)	25.48(25)
16	24.29(25)	33.45(30)	10.55(10)	-4.68(15)	22.35(5)	20.48(20)
17	29.34(30)	29.97(25)	21.38(20)	-22.06(10)	42.31(15)	5.26(5)

Table S6 Dye concentrations (μg·mL^{-1}) in mixture samples No. 1–17 predicted by equations group (5).

Sample	C_{TA}	C_{SY}	C_{AR}	C_{PO}	C_{AM}	C_{BB}
1	4.37(4)	0.25(4)	10.1(4)	6.35(4)	-1.18(4)	4.19(4)
2	5.36(5)	0.74(5)	11.7(5)	7.71(5)	-0.85(5)	5.19(5)
3	7.45(7)	1.47(7)	15.87(7)	10.26(7)	-0.61(7)	7.27(7)
4	8.52(8)	1.86(8)	17.81(8)	11.86(8)	-0.59(8)	8.28(8)
5	10.65(10)	3(10)	21.24(10)	14.32(10)	0.29(10)	10.39(10)
6	12.73(12)	4.43(12)	24.01(12)	16.74(12)	1.63(12)	12.41(12)
7	13.72(13)	5.07(13)	25.36(13)	17.87(13)	2.16(13)	13.4(13)
8	14.83(14)	5.55(14)	27.5(14)	18.98(14)	2.39(14)	14.48(14)
9	15.83(15)	6.61(15)	28.24(15)	20.11(15)	3.52(15)	15.49(15)
10	16.81(16)	7.46(16)	29.39(16)	21.13(16)	4.28(16)	16.52(16)
11	20.98(20)	11.27(20)	33.64(20)	25.14(20)	8.21(20)	20.58(20)
12	4.46(5)	12.72(10)	9.93(15)	18.64(20)	28.32(25)	29.61(30)
13	9.84(10)	2.87(5)	26.99(25)	31.73(30)	17.74(20)	14.97(15)
14	13.74(15)	32.77(20)	-14.08(5)	18.90(25)	45.33(30)	9.71(10)
15	19.74(20)	12.56(15)	32.68(30)	6.28(5)	7.91(10)	24.95(25)
16	24.12(25)	37.93(30)	-1.50(10)	11.19(15)	14.23(5)	19.95(20)
17	29.79(30)	28.07(25)	14.71(20)	8.71(10)	19.24(15)	4.74(5)

Table S7 Dye concentrations (μg·mL^{-1}) in mixture samples No. 1–17 predicted by equations group (6).

Sample	C_{TA}	C_{SY}	C_{AR}	C_{PO}	C_{AM}	C_{BB}
1	4.45(4)	1.79(4)	7.73(4)	4.81(4)	1.37(4)	4.17(4)
2	5.46(5)	2.37(5)	9.12(5)	6.1(5)	1.88(5)	5.15(5)
3	7.56(7)	3.64(7)	12.45(7)	8.08(7)	3.07(7)	7.21(7)
4	8.64(8)	4.31(8)	13.89(8)	9.33(8)	3.68(8)	8.21(8)
5	10.7(10)	5.83(10)	16.73(10)	11.55(10)	5.07(10)	10.33(10)
6	12.81(12)	7.35(12)	19.36(12)	13.9(12)	6.55(12)	12.31(12)
7	13.77(13)	8.04(13)	20.63(13)	15(13)	7.15(13)	13.3(13)
8	14.81(14)	9.05(14)	22(14)	15.6(14)	8.25(14)	14.37(14)
9	15.79(15)	9.99(15)	22.88(15)	16.9(15)	9.15(15)	15.37(15)
10	16.69(16)	10.96(16)	23.94(16)	17.79(16)	10.1(16)	16.39(16)
11	20.79(20)	14.65(20)	28.18(20)	22.03(20)	13.9(20)	20.44(20)
12	4.34(5)	11.46(10)	11.95(15)	19.48(20)	26.50(25)	29.65(30)
13	9.96(10)	3.86(5)	25.81(25)	30.99(30)	18.90(20)	15.03(15)
14	12.91(15)	27.02(20)	-5.72(5)	22.96(25)	37.59(30)	9.77(10)
15	19.68(20)	13.97(15)	31.01(30)	5.38(5)	9.45(10)	24.99(25)
16	23.61(25)	34.62(30)	3.22(10)	13.51(15)	9.87(5)	20.02(20)
17	29.31(30)	27.07(25)	16.34(20)	9.45(10)	17.81(15)	4.80(5)

Note: The data in brackets are the spiked concentrations of the dyes in the mixtures. The highlight indicated that the predicted result is within 80%-120% of the spiked value.

Table S8-1 ε data of TA, SY and PO corresponding to the selected wavelengths for equation (7) and (8)

dye	ε matrix for equation (7)			ε matrix for equation (8)		
	ε_{425}	ε_{480}	ε_{508}	ε_{401}	ε_{476}	ε_{551}
TA	0.0233	0.0072	0.0004	0.0202	0.0092	0
SY	0.0125	0.0285	0.0237	0.011	0.0282	0.001
PO	0.0054	0.0157	0.0195	0.004	0.0146	0.009

Table S8-2 ε data of TA, AM and BB corresponding to the selected wavelengths for equation (9) and (10)

dye	ε matrix for equation (9)			ε matrix for equation (10)		
	ε_{425}	ε_{520}	ε_{626}	ε_{390}	ε_{520}	ε_{626}
TA	0.0269	0	0	0.0203	0	0
AM	0.0048	0.0212	0	0.004	0.0212	0
BB	0.0025	0.0018	0.0614	0.0047	0.0018	0.0614

Table S8-3 ε data of TA, AR and BB corresponding to the selected wavelengths for equation (11) and (12)

dye	ε matrix for equation (11)			ε matrix for equation (12)		
	ε_{425}	ε_{496}	ε_{626}	ε_{390}	ε_{501}	ε_{626}
TA	0.0269	0.0019	0	0.0203	0.001	0
AR	0.0089	0.0277	0	0.0065	0.0272	0
BB	0.0025	0.0006	0.0614	0.0047	0.0018	0.0614

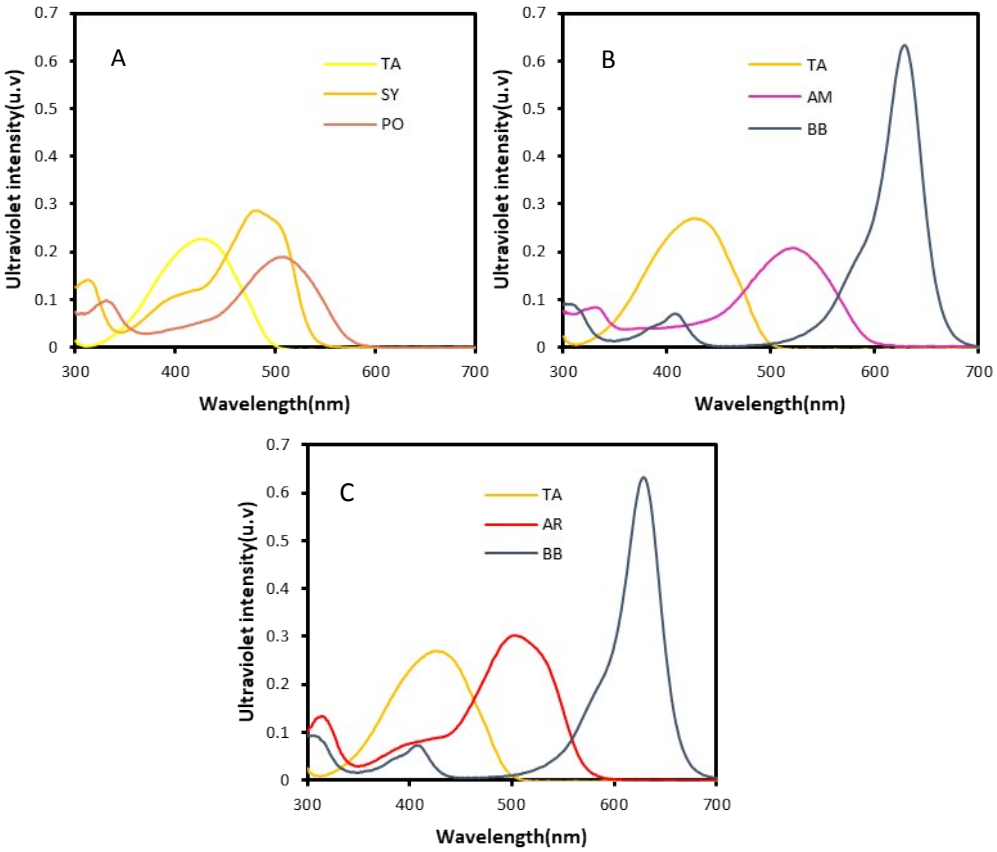

Figure S1. Spectra of food dyes tartrazine (TA), sunset yellow (SY), allura red (AR), ponceau 4R (PO), amaranth (AM), and bright blue (BB) classed in three groups: A) yellow orange, B) red purple and C) blue green.

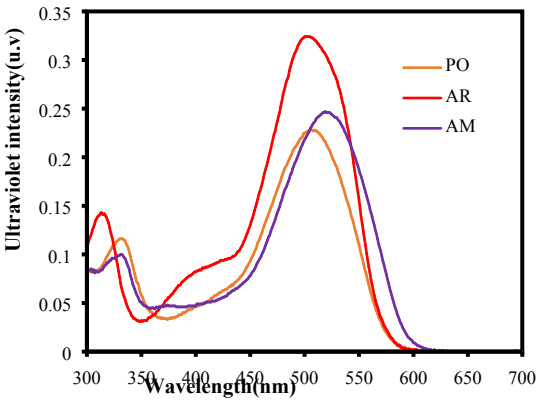

Figure S2. Spectra of three highly overlapped red dyes, ponceau 4R (PO), allura red (AR) and amaranth (AM)