An effective approach to the quantitative analysis of the skin-whitening agents in cosmetics with different substrates based on conventional UV-Vis determination

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Supplementary Information

The multi-resolution feature of TMs and formula derivation for *CORR* values

The function(4) in paper illustrates that the curve intensity is transformed into TMs by the normalized discrete Tchebichef polynomials of different degrees. The moments with low orders provide a global, general but coarse description about the curve, while with the increase of maximal moment orders, more and more detail information of the curve is included in the calculated moments[1]. This means that the original curve intensity $f(x)$, can be decomposed into different levels, and different image contents can be described using different moment orders. This ability can be known as 'multi-resolution capability'[2].

UV-Vis is based on the absorption of light frequencies in the ultraviolet to visible wavelength range (190-800 nm). Absorption emanating from electronic transitions from the electromagnetic radiation in the UV-Vis region corresponds and dependent on the chemical structure. When molecules absorb energy of external radiant and cause the electronic energy level transition, it must be accompanied by the transition of the vibration and rotational energy levels. Therefore, most of UV-Vis absorptions is broad band and used to the determination of single component. For the mixtures, the UV-Vis spectra usually contain the overlapping peaks and various interference signals. Here, the performance for the resolution of overlapping signals were illustrated by the calculation of the correlation coefficients between the 'added' and 'actual' TMs and quantitative determination of multiple overlapped five target compounds[2], where the 'actual' TMs correspond to the calculated TMs from the raw UV-Vis spectra of mixed standard sample (Fig. S1. *sn25*). Here, *sn*.25 is used as an example. The 'added' TMs correspond to the sum of the TMs

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obtained from the UV-Vis spectra (Fig. S1. cn^1~cn^5) of five pure compounds that weighted by their relative concentration (Ratio). If the overlapping signals are well resolved, the 'actual' TMs will be consistent with the 'added' ones, and high correlation coefficients between the 'actual' and 'added' TMs will be obtained. The correlation coefficients between the 'actual' and 'added' TMs are calculated as below:

$$CORR_{Sn}=corrcoef(TN_{Sn}, TN'_{Sn}) \quad (1)$$

where TN_{Sn} is the 'actual' TMs calculated based on the UV-Vis curve of *Sn*th sample, TN'_{Sn} is the 'added' TMs for *Sn*th sample, which can be calculated as follows:

$$TN'_{Sn} = \sum_{Sn=1}^{SN}\sum_{cn=1}^{CN} Ratio_{(Sn.cn)} TN^{cn} \quad (2)$$

where *SN* is the total number of the standard samples, *CN* is the total number of target components, TN^{cn} is the calculated TMs on the basis of raw UV-Vis spectra of the *cn*th single standard sample, while $Ratio_{(Sn,cn)}$ is the concentration ratio between the concentration of *cn*th target compound in the *Sn*th standard sample and in its corresponding single standard sample.

In our study, the *CORR* values all more than 0.9670 (Table S3). This suggests that the overlapping signals were well resolved by the TMs. The schematic diagram of calculation of 'actual' and 'added' TMs, and calculation of correlation coefficients between 'added' and 'actual' TMs are shown in Fig. S1.

Reference

[1] C.Y. Wee, R. Paramesran, R. Mukundan and X. Jiang, Image quality assessment by discrete orthogonal moments, Pattern Recognit., 2010, **43**, 4055-4068.
[2] B.Q. Li, X. Wang, M.L. Xu, H.L. Zhai, J. Chen and J.J. Liu, The multi-resolution capability of Tchebichef moments and its applications to the analysis of fluorescence excitation-emission spectra, Methods Appl. Fluoresc, 2017, **6**, 015008.

Table S1 The experimental and calculated concentrations (mg L^{-1}) of the five target compounds

Datasets	Sample No.	AR				NA				KA				HQ				PHE			
		Exp.	Cal.			Exp.	Cal.			Exp.	Cal.			Exp.	Cal.			Exp.	Cal.		
			PLS	MCR-ALS	TM		PLS	MCR-ALS	TM		PLS	MCR-ALS	TM		PLS	MCR-ALS	TM		PLS	MCR-ALS	TM
Calibration set	1	57.99	57.80	57.65	57.45	11.00	10.97	10.5	11.72	8.70	9.01	8.60	8.76	8.50	8.39	8.76	8.44	2.50	1.19	1.68	2.56
	2	53.99	53.98	53.89	54.82	8.50	8.48	8.79	8.13	5.50	5.37	5.39	5.46	4.50	4.47	4.37	4.61	5.80	6.32	5.97	5.81
	3	48.49	48.54	48.91	47.95	5.80	5.99	6.30	5.67	2.50	2.47	2.35	2.67	0.50	0.63	0.55	0.47	7.50	8.04	8.10	7.66
	4	38.99	39.36	39.85	39.52	3.20	3.17	2.94	2.90	11.50	11.31	11.28	11.14	9.00	8.54	8.40	8.84	9.50	9.62	9.80	9.36
	5	28.50	28.26	28.13	28.77	1.00	1.03	0.84	1.04	8.00	7.78	7.79	7.88	4.70	4.79	4.70	4.72	11.50	11.76	12.01	11.68
	6	26.50	26.23	25.54	25.38	12.00	11.95	12.08	11.91	4.70	4.68	4.85	4.67	0.80	0.83	0.73	0.77	13.50	13.65	13.28	13.39
	7	25.50	25.37	23.59	25.24	9.00	8.89	9.33	8.40	1.50	1.87	1.93	1.69	9.50	9.89	9.77	9.51	15.50	15.35	15.21	15.50
	8	24.00	24.18	25.28	23.45	6.70	6.40	6.21	6.59	10.00	10.16	10.10	10.18	5.00	4.89	4.72	5.10	20.00	20.18	20.56	19.93
	11	21.50	21.61	21.19	21.31	14.00	14.01	14.32	13.67	0.50	0.43	0.37	0.49	5.20	5.34	5.49	5.32	5.50	5.76	5.48	5.55
	12	20.50	20.63	20.21	20.30	9.70	9.69	9.40	9.54	9.00	9.22	9.29	9.10	1.50	1.84	1.85	1.51	7.00	6.58	6.58	6.72
	13	19.50	19.59	18.98	19.55	7.60	7.42	7.71	7.34	5.80	5.67	5.84	5.82	10.00	9.57	9.66	9.75	9.00	9.42	9.01	8.71
	14	18.50	18.59	18.85	18.46	4.60	4.44	4.27	4.54	3.00	3.23	3.05	3.35	5.50	5.38	5.68	5.47	11.00	11.11	11.47	11.21
	16	16.50	16.56	21.52	17.14	15.5	15.49	14.83	15.40	8.20	8.51	7.70	8.25	10.50	10.80	10.47	10.62	15.00	14.45	15.59	14.94
	17	15.50	15.50	14.70	16.23	10.50	11.26	11.74	11.16	5.00	4.12	4.38	4.33	5.80	5.87	5.76	5.82	19.00	19.26	18.79	18.99
	18	14.50	14.59	13.43	15.13	8.20	7.92	8.11	8.32	1.70	1.83	2.03	1.70	2.20	2.22	2.36	2.23	23.00	22.44	22.2	22.96
	19	13.50	13.35	13.01	13.82	5.50	5.71	5.81	5.58	10.50	10.71	10.94	10.76	11.00	11.32	11.39	11.25	1.00	1.62	1.32	1.17
	20	12.50	12.69	12.71	13.09	3.00	3.31	3.27	3.46	7.20	7.25	7.40	7.22	6.20	6.45	6.28	6.15	4.50	4.24	4.22	4.24
	23	9.80	9.35	9.14	9.77	8.70	8.33	8.15	8.63	9.50	9.30	9.51	9.29	6.50	6.16	6.11	6.41	10.50	10.92	10.64	10.95
	24	9.30	9.46	8.90	9.30	6.20	6.23	5.78	6.49	6.20	6.40	6.42	5.86	3.00	3.10	3.38	3.11	12.50	11.60	11.81	12.53
	25	8.70	8.45	7.53	8.11	3.50	3.50	3.54	3.54	3.20	3.37	3.32	3.36	13.00	13.03	13.31	13.06	14.5	14.00	14.2	14.43
	27	7.50	7.33	8.11	7.44	12.51	12.67	12.75	12.69	8.50	8.39	8.56	8.83	3.20	3.29	2.84	3.18	21.5	22.16	22.05	21.52
	28	7.00	7.27	7.36	7.27	9.40	9.26	9.70	9.09	5.20	4.68	4.83	5.00	14.00	13.90	13.79	14.03	0.85	1.67	1.13	0.84
	29	6.40	6.10	7.74	6.14	7.10	6.81	6.82	6.96	2.20	2.05	1.86	2.05	7.20	6.97	6.83	7.07	3.50	3.52	3.80	3.59

	31	5.50	5.38	4.61	5.18	1.80	2.06	2.03	2.07	7.50	7.60	7.70	7.72	15.00	15.27	15.36	15.12	8.00	7.49	7.48	7.77
	32	5.00	4.99	4.40	4.87	15.00	14.92	15.07	14.99	4.50	4.54	4.72	4.58	7.50	7.16	7.12	7.38	10.00	10.03	9.47	9.96
	33	4.50	4.81	5.19	4.89	10.00	10.16	9.63	10.21	1.00	1.35	0.99	1.03	3.90	3.67	4.06	3.91	12.00	11.45	12.05	11.94
	34	4.00	4.20	3.71	3.56	8.00	7.95	8.07	7.96	9.70	9.49	9.62	9.63	15.50	15.42	15.46	15.36	14.00	14.31	14.23	14.20
Predic tion	9	23.50	23.19	23.41	23.74	4.00	3.67	3.61	4.15	6.80	6.66	6.81	6.97	1.00	0.78	0.62	1.02	24.00	24.42	24.45	24.11
set	10	22.50	21.01	21.79	21.11	1.50	2.04	2.44	2.03	3.90	3.83	3.64	4.45	9.70	9.90	9.63	9.05	1.50	1.63	2.16	1.82
	15	17.50	17.19	17.20	18.19	2.00	2.15	1.54	2.41	12.5	12.95	13.06	12.76	1.70	1.84	1.85	1.86	13.00	12.88	13.2	13.08
	21	11.50	11.32	13.64	12.13	0.80	0.49	0.34	1.06	4.20	3.99	3.88	4.06	2.50	2.53	2.16	2.46	6.50	6.28	6.72	6.24
	22	10.50	10.88	10.91	10.54	11.50	11.46	11.83	11.24	0.80	0.53	0.46	0.80	12.00	12.06	12.09	12.32	8.50	8.89	8.58	8.27
	26	8.00	7.60	7.56	7.26	1.20	1.46	1.07	1.99	13.5	13.59	13.85	13.71	6.80	6.45	6.34	6.62	18.00	17.76	17.86	17.84
	30	6.00	5.83	8.49	6.98	4.20	4.24	3.32	4.39	11.00	11.74	11.71	11.38	3.50	3.39	2.94	3.58	6.00	5.41	5.56	5.23
	35	3.50	3.69	3.95	4.18	5.00	4.72	4.66	5.05	6.50	6.37	6.62	6.37	8.00	7.24	6.84	7.55	18.00	18.65	18.3	17.90
	36	2.50	2.98	4.11	3.13	2.60	2.00	1.19	2.62	3.50	3.68	3.42	3.23	4.20	3.55	3.54	4.10	20.5	19.22	19.85	19.54

Table S2 The performance of PLS, MCR-ALS and TM models for the five target components

Models	Chemicals	*LV*s	Calibration			Cross-validation		Prediction			Precision (RSD %)	
			R_c	R_{adj}	$RMSE_c$	$R_{loo\text{-}cv}$	$RMSE_{cv}$	R_p	$RMSE_p$	*CCC*	Intra-day variation	Inter-day variation
PLS	AR	7	0.9999	0.9998	0.2027	0.9996	0.4067	0.9985	0.5810	0.9967	0.79	3.27
	NA	6	0.9982	0.9981	0.2261	0.9965	0.3154	0.9942	0.3384	0.9940	0.30	0.36
	KA	6	0.9963	0.9961	0.2731	0.9924	0.3928	0.9986	0.3255	0.9971	0.22	0.70
	HQ	7	0.9985	0.9984	0.2317	0.9968	0.3316	0.9960	0.3728	0.9947	0.39	1.13
	PHE	6	0.9963	0.9961	0.5095	0.9906	0.8103	0.9970	0.5655	0.9969	0.36	0.55
MCR-ALS	AR	--	0.9965	0.9963	1.2362	0.9962	1.2963	0.9911	1.2697	0.9840	1.34	4.22
	NA	--	0.9943	0.9941	0.4047	0.9934	0.4359	0.9819	0.7057	0.9757	0.21	0.58
	KA	--	0.9966	0.9965	0.2616	0.9961	0.2822	0.9994	0.3727	0.9963	0.27	0.83
	HQ	--	0.9977	0.9976	0.2826	0.9974	0.3034	0.9946	0.5362	0.9892	0.25	0.65
	PHE	--	0.9973	0.9971	0.4361	0.9967	0.4821	0.9985	0.4028	0.9984	0.32	0.89
TM	AR	6	0.9995	0.9994	0.4739	0.9990	0.6790	0.9957	0.7641	0.9944	2.49	5.98
	NA	5	0.9969	0.9964	0.2968	0.9948	0.3876	0.9980	0.3746	0.9922	0.72	2.94
	KA	7	0.9976	0.9967	0.2208	0.9956	0.2976	0.9986	0.2780	0.9978	1.33	2.57
	HQ	7	0.9997	0.9995	0.1060	0.9990	0.1826	0.9971	0.2975	0.9965	0.76	1.07
	PHE	6	0.9996	0.9994	0.1646	0.9992	0.2357	0.9986	0.4468	0.9981	0.55	2.78

Table S3 The concentration of mixed standard samples and the relative concentration (proportions of the mixtures and single standard sample)

Sn.	AR		NA		KA		HQ		PHE		*CORR*
	Con.	Ratio*	Con.	Ratio*	Con.	Ratio*	Con.	Ratio*	Con.	Ratio*	
1(cn^1)	84.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	----
2(cn^2)	0.00	0.00	18.50	1.00	0.00	0.00	0.00	0.00	0.00	0.00	----
3(cn^3)	0.00	0.00	0.00	0.00	8.00	1.00	0.00	0.00	0.00	0.00	----
4(cn^4)	0.00	0.00	0.00	0.00	0.00	0.00	11.50	1.00	0.00	0.00	----
5(cn^5)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	35.50	1.00	----
1	57.99	0.69	11.00	0.59	8.70	1.09	8.50	0.74	2.50	0.07	0.9824
2	53.99	0.64	8.50	0.46	5.50	0.69	4.50	0.39	5.80	0.16	0.9940
3	48.49	0.58	5.80	0.31	2.50	0.31	0.50	0.04	7.50	0.21	0.9992
4	38.99	0.46	3.20	0.17	11.50	1.44	9.00	0.78	9.50	0.27	0.9905
5	28.50	0.34	1.00	0.05	8.00	1.00	4.70	0.41	11.50	0.32	0.9992
6	26.50	0.32	12.00	0.65	4.70	0.59	0.80	0.07	13.50	0.38	0.9944
7	25.50	0.30	9.00	0.49	1.50	0.19	9.50	0.83	15.50	0.44	0.9946
8	24.00	0.29	6.70	0.36	10.00	1.25	5.00	0.43	20.00	0.56	0.9820
9	23.50	0.28	4.00	0.22	6.80	0.85	1.00	0.09	24.00	0.68	0.9923
10	22.50	0.27	1.50	0.08	3.90	0.49	9.70	0.84	1.50	0.04	0.9996
11	21.50	0.26	14.00	0.76	0.50	0.06	5.20	0.45	5.50	0.15	0.9990
12	20.50	0.24	9.70	0.52	9.00	1.12	1.50	0.13	7.00	0.20	0.9969
13	19.50	0.23	7.60	0.41	5.80	0.72	10.00	0.87	9.00	0.25	0.9976
14	18.50	0.22	4.60	0.25	3.00	0.37	5.50	0.48	11.00	0.31	0.9997
15	17.50	0.21	2.00	0.11	12.50	1.56	1.70	0.15	13.00	0.37	0.9967
16	16.50	0.20	15.50	0.84	8.20	1.02	10.50	0.91	15.00	0.42	0.9670

17	15.50	0.18	10.50	0.57	5.00	0.62	5.80	0.50	19.00	0.54	0.9890
18	14.50	0.17	8.20	0.44	1.70	0.21	2.20	0.19	23.00	0.65	0.9954
19	13.50	0.16	5.50	0.30	10.50	1.31	11.00	0.96	1.00	0.03	0.9985
20	12.50	0.15	3.00	0.16	7.20	0.90	6.20	0.54	4.50	0.13	0.9999
21	11.50	0.14	0.80	0.04	4.20	0.52	2.50	0.22	6.50	0.18	0.9996
22	10.50	0.12	11.50	0.62	0.80	0.10	12.00	1.04	8.50	0.24	0.9984
23	9.80	0.12	8.70	0.47	9.50	1.19	6.50	0.57	10.50	0.30	0.9957
24	9.30	0.11	6.20	0.34	6.20	0.77	3.00	0.26	12.50	0.35	0.9993
25	8.70	0.10	3.50	0.19	3.20	0.40	13.00	1.13	14.50	0.41	0.9992
26	8.00	0.10	1.20	0.06	13.50	1.69	6.80	0.59	18.00	0.51	0.9924
27	7.50	0.09	12.51	0.68	8.50	1.06	3.20	0.28	21.50	0.61	0.9775
28	7.00	0.08	9.40	0.51	5.20	0.65	14.00	1.22	0.85	0.02	0.9992
29	6.40	0.08	7.10	0.38	2.20	0.27	7.20	0.63	3.50	0.10	0.9997
30	6.00	0.07	4.20	0.23	11.00	1.37	3.50	0.30	6.00	0.17	0.9993
31	5.50	0.07	1.80	0.10	7.50	0.94	15.00	1.30	8.00	0.23	0.9995
32	5.00	0.06	15.00	0.81	4.50	0.56	7.50	0.65	10.00	0.28	0.9952
33	4.50	0.05	10.00	0.54	1.00	0.12	3.90	0.34	12.00	0.34	0.9997
34	4.00	0.05	8.00	0.43	9.70	1.21	15.50	1.35	14.00	0.39	0.9882
35	3.50	0.04	5.00	0.27	6.50	0.81	8.00	0.70	18.00	0.51	0.9957
36	2.50	0.03	2.60	0.14	3.50	0.44	4.20	0.37	20.50	0.58	0.9997

*Ratio$_{(Sn,\ cn)}$ is the ratio between the concentration of the *cn*th target component in the *Sn*th standard sample and in its corresponding single standard sample

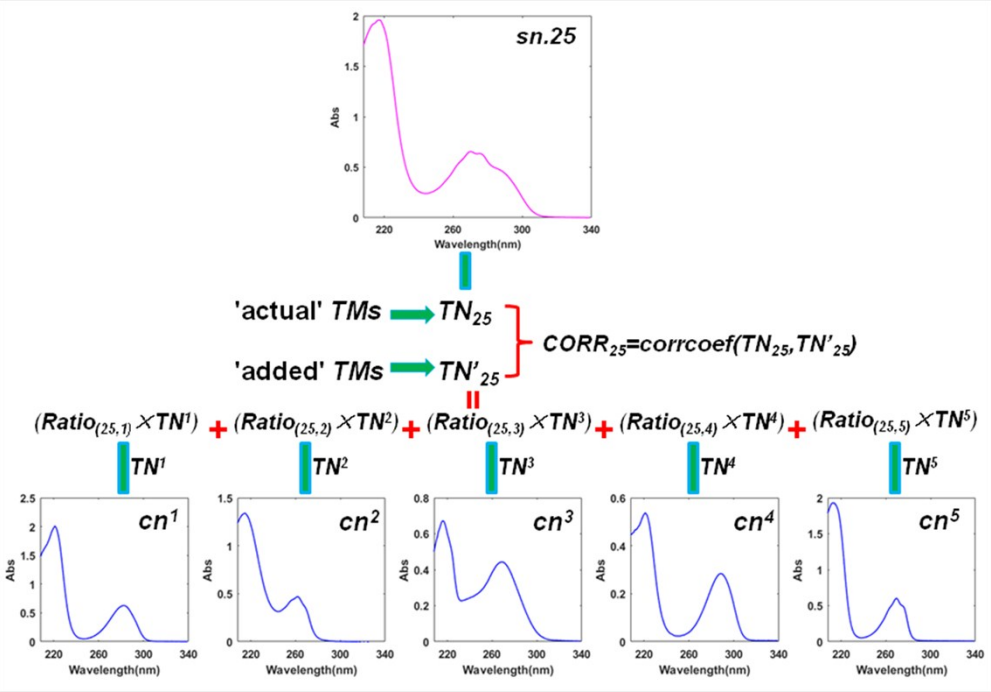

Fig.S1 The schematic diagram of calculation of 'actual' and 'added' TMs, and calculation of correlation coefficients between 'added' and 'actual' TMs.