

Model-based three way chemometric methods for quantitative analysis of linear alkyl benzene sulfonate and optical brightener in real samples using excitation–emission fluorescence data

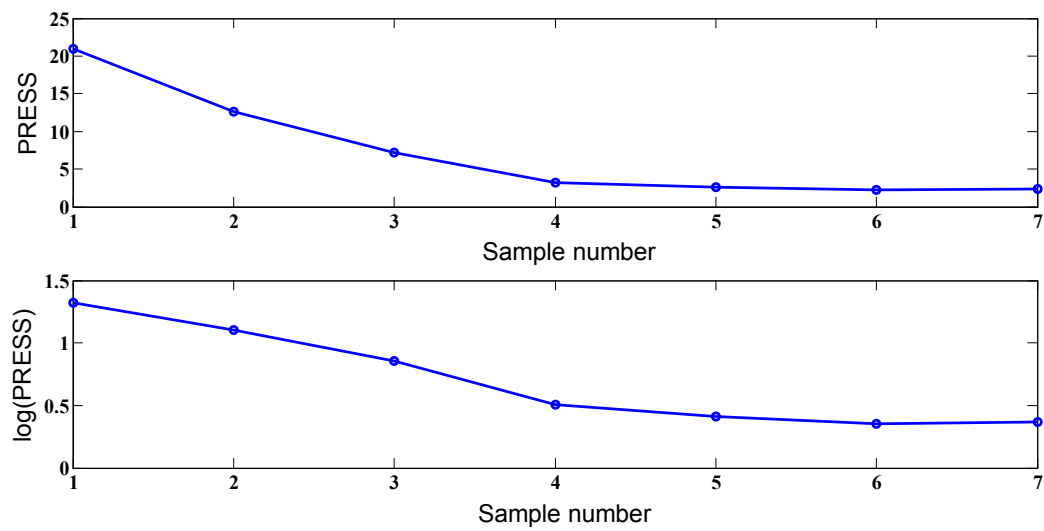
Saeed Masoum*, Saleheh Abbasi,

Department of Analytical Chemistry, Faculty of Chemistry, University of Kashan, Kashan, I.R. Iran

Corresponding author Tel.: +98 361 5912338; fax: +98 361 5912397.

E-mail address: masoum@kashanu.ac.ir (Saeed Masoum)

Supporting information



FigureS1. Number of estimated components by three-way cross validation

Table S1 Obtained coefficient of determination (R^2) from different three way chemometric methods

	Method	OB	LABS
Sample 1	PARAFAC	0.9930	0.9503
	APTLD	0.9397	0.9472
	SWATLD	0.9397	0.9472
	ATLD	0.9936	0.9489
Waste water	PARAFAC	0.9422	0.9520
	APTLD	0.9230	0.9481
	SWATLD	0.9230	0.9481
	ATLD	0.9340	0.9501
Soil	PARAFAC	0.9410	0.9452
	APTLD	0.9210	0.9490
	SWATLD	0.9210	0.9490
	ATLD	0.9344	0.9489

Table S2 Obtained results by three way methods for sample 1 at different component number for the determination of LABS

	N=4			N=5		
	Recovery (%)	Iteration number	Time (min)	Recovery (%)	Iteration number	Time (min)
PARAFAC	103.7	557	1.77	91.7	873	2.85
ATLD	96.5	24	0.08	97.8	55	0.18
SWATLD	96.2	73	0.23	97.0	94	0.31
APTLD	96.2	73	0.23	97.0	95	0.31

Table S3 Quantitative analysis of LABS in the three real laundry powder samples by different initial values

Sample	Method	Initial value (Best fitting model)	Iteration number	Time (min)	Initial value (DTLD)	Iteration number	Time (min)
Sample 1	PARAFAC	8.5 %	675	2.12	8.5%	380	1.19
	APTLD	8.0 %	110	0.34	8.0%	34	0.10
	SWATLD	8.0 %	110	0.34	8.1%	34	0.10
	ATLD	8.9%	39	0.1 2	9.0%	7	0.02
Sample 2	PARAFAC	8.5 %	559	1.76	8.5 %	126	0.40
	APTLD	6.5%	60	0.19	6.5%	46	0.14
	SWATLD	7.0%	60	0.19	7.0%	46	0.14
	ATLD	9.0%	21	0.07	9.0%	12	0.04

Table S4 Effect of penalty factors (p, q, r) on recoveries of LABS and iteration number in APTLD modeling

	N=4			N=5		
	Recoveries of LABS	Iteration number	Time (min)	Recoveries of LABS	Iteration number	Time (min)
$p=q=r=10^{-1}$	103.1	500	1.58	91.3	645	2.02
$p=q=r=10^{-6}$	104.9	505	1.59	93.4	650	2.04
$p=q=r=10^2$	105.8	450	1.42	95.0	587	1.84
$p=q=r=10^8$	96.2	262	0.82	98.7	285	0.90
$p=q=r=10^{10}$	96.2	210	0.66	97.0	245	0.77
$p=q=r=10^{15}$	96.2	198	0.62	97.0	205	0.65
$p=q=10^{15} \text{ } r=10^{10}$	96.2	197	0.62	97.0	220	0.69
$p=q=r=10^{20}$	96.2	73	0.23	97.0	105	0.33

Table S5 Influence of stop criteria on the performance of the four algorithms in the determination of LABS

	stop criteria= 10^{-4}			stop criteria= 10^{-6}			stop criteria= 10^{-9}		
	Recovery (%)	Iteration number	Tim (min)	Recovery (%)	Iteration number	Time (min)	Recovery (%)	Iteration number	Time (min)
PARAFAC	90.2	226	0.90	103.7	557	1.77	108.1	2050	6.50
ATLD	94.0	10	0.04	96.5	24	0.07	93.8	73	0.24
SWATLD	94.1	12	0.05	96.2	73	0.22	95.2	232	0.74
APTLD	94.3	12	0.05	96.2	73	0.22	95.2	232	0.74