Supplementary

A Fast and Robust Third-Order Multivariate Calibration Approach Coupled with Excitation–Emission Matrix Phosphorescence for the Quantification and Oxidation Kinetic Study of Fluorene in Wastewater Samples

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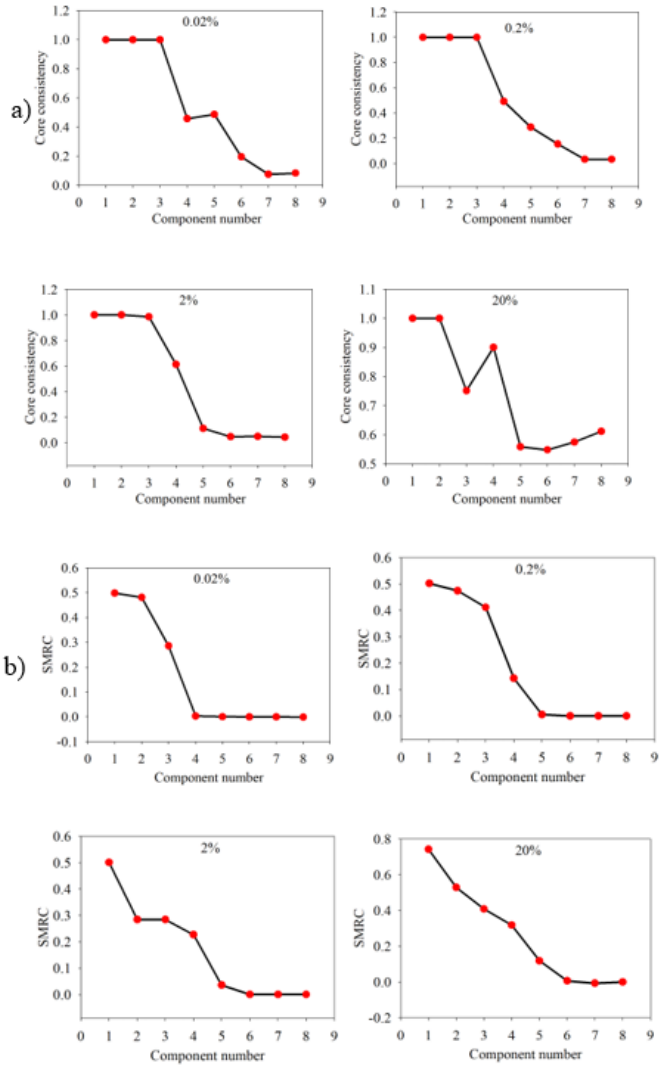

Figure S1. The results of 8 components for the simulated data with different homoscedastic noise levels using different methods, (**a**) CORCONDIA, (**b**) AWQLD-MCS. SMRC is the abbreviation of Sorted Mean Relative Concentration.

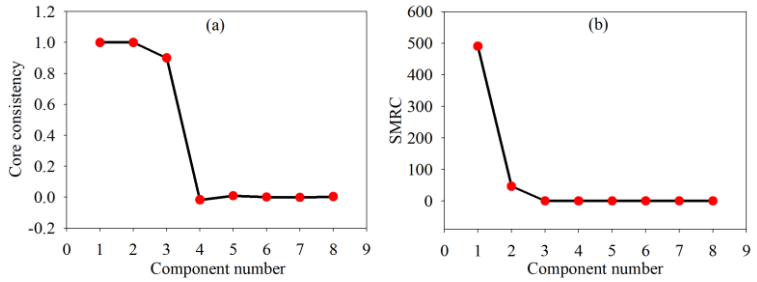

Figure S2. The results of 8 components for the first real four-way phosphorescence data using different methods, (**a**) CORCONDIA, (**b**) AWQLD-MCS.

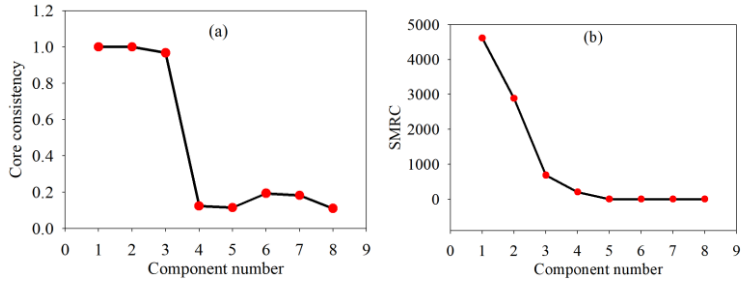

Figure S3. The results of 8 components for the second real four-way phosphorescence data using different methods, (**a**) CORCONDIA, (**b**) AWQLD-MCS.

Table S1. The convergence property of PARAFAC, AQLD and SWAQLD for simulated excitation-emission-kinetic four-way phosphorescence data with four levels of heteroscedastic noise.

$Noise_{heter}$ (%)	Iteration number (computation time (s))								
	PARAFAC			AQLD			SWAQLD		
	Min	Max	Average[a]	Min	Max	Average	Min	Max	Average
0.02	266(313.4)	2053(2411.0)	385(453.3)	5(0.4)	12(1.0)	6(0.5)	60(3.8)	212(14.0)	102(6.9)
0.2	226(321.8)	2108(3024.7)	352(557.4)	5(0.4)	10(0.9)	6(0.5)	59(3.7)	194(13.4)	89(6.2)
2	182(227.4)	877(1423.4)	279(399.0)	5(0.4)	11(0.8)	6(0.5)	47(4.2)	174(12.2)	75(5.7)
20	151(180.1)	3000[b](3583.0)	725.5(866.3)	5(0.4)	14(1.0)	6(0.5)	40(2.7)	159(11.3)	60(4.4)

[a] These values are average results for 100 runs with random initialization.

[b] PARAFAC did not converge within 3000 iterations for one time out of 100 runs (1/100).

Table S2. The influence of heteroscedastic noise levels on correlation coefficients, root-mean-square errors of prediction (RMSEPs) and k values predicted by PARAFAC, AQLD and SWAQLD, respectively, for simulated four-way data.

Modes		PARAFAC				AQLD				SWAQLD			
		0.02%	*0.2%*	*2%*	*20%*	*0.02%*	*0.2%*	*2%*	*20%*	*0.02%*	*0.2%*	*2%*	*20%*
A	a_1	1.0000[a]	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	a_2	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	a_3	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
B	b_1	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	b_2	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	b_3	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
C	c_1	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	c_2	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	c_3	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
D	d_1	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	d_2	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	d_3	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
RMSEP	Analyte 1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Analyte 2	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Predicted k^b		0.1000	0.1000	0.1000	0.1000	0.1000	0.1000	0.1000	0.1000	0.1000	0.1000	0.1000	0.1000

[a] All values in the first 12 rows of this table correspond to the correlation coefficient between the profiles predicted by the different methods and the reference profiles.

[b] The chosen constant rate of the analyte in the simulated data set is 0.1000.

Table S3. The influence of factor numbers (*N*) on correlation coefficients, RMSEPs and *k* values predicted by PARAFAC, AQLD and SWAQLD, respectively, for simulated four-way data with σ_{homo} = 2%.

Mode		PARAFAC			AQLD			SWAQLD		
		N=4	*N*=5	*N*=10	*N*=4	*N*=5	*N*=10	*N*=4	*N*=5	*N*=10
A	a_1	1.0000	1.0000	0.9833	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	a_2	1.0000	1.0000	0.9979	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	a_3	1.0000	0.9999	0.9999	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
B	b_1	1.0000	1.0000	0.9930	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	b_2	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	b_3	1.0000	1.0000	0.9881	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
C	c_1	1.0000	1.0000	0.9984	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	c_2	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	c3	1.0000	1.0000	0.9998	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
D	d_1	1.0000	1.0000	0.9841	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	d_2	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	d_3	1.0000	1.0000	0.9996	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
RMSEP	Analyte 1	0.0005	0.0005	**0.1001**	0.0007	0.0007	0.0007	0.0006	0.0006	0.0006
	Analyte 2	0.0006	0.0007	**0.0037**	0.0010	0.0009	0.0011	0.0003	0.0005	0.0007
Predicted *k*		0.1005	0.1002	**0.1884**	0.0940	0.0951	0.0943	0.1000	0.1000	0.1000

Table S4. The influence of factor numbers (*N*) on correlation coefficients, RMSEPs and *k* values predicted by PARAFAC, AQLD and SWAQLD, respectively, for simulated four-way data with σ_{heter} = 0.02%.

Mode		PARAFAC			AQLD			SWAQLD		
		N=3	*N*=4	*N*=10	*N*=3	*N*=4	*N*=10	*N*=3	*N*=4	*N*=10
A	a_1	1.0000	1.0000	0.9999	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	a_2	1.0000	1.0000	0.9968	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	a_3	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
B	b_1	1.0000	1.0000	0.9626	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	b_2	1.0000	1.0000	0.9986	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	b_3	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
C	c_1	1.0000	1.0000	0.9999	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	c_2	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	c3	1.0000	1.0000	0.9995	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
D	d_1	1.0000	1.0000	0.9677	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	d_2	1.0000	1.0000	0.9130	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	d_3	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
RMSEP	Analyte 1	0.0000	0.0000	**0.1444**	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Analyte 2	0.0000	0.0000	**0.2029**	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Predicted *k*		0.1000	0.1000	**0.1703**	0.1000	0.1000	0.1000	0.1000	0.1000	0.1000