Multivariate image analysis-thin layer chromatography (MIA-TLC) for simultaneous determination of co-eluting components

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Table S1 Calibration Set Composition

MY (ng)	BG (ng)	CR (ng)
169	524	344
169	279	191
113	279	478
113	977	268
214	349	478
146	977	344
214	524	268
169	349	268
146	349	402
146	698	478
191	977	402
214	698	344
191	524	478
169	977	478
214	977	191
214	279	402
113	698	191
191	279	344
113	524	402
169	698	402
191	698	268

191	349	191
146	279	268
113	349	344
146	524	191

Table S2 Prediction Set Composition

MY (ng)	BG (ng)	CR (ng)
135	838	325
158	454	287
180	838	382
203	628	325
180	558	440
158	838	440

Table S3 Calibration set composition for nifedipine (NIF) and photodegrated product of nifedipine (P-NIF) (detection with UV=254 nm).

Sample no	NIF (μg)	P-NIF (μg)
1	4.8	6.0
2	6.5	2.5
3	6.5	4.8
4	3.1	3.6
5	1.4	4.8
6	3.1	2.5
7	1.4	6.0
8	4.8	4.8

9	4.8	2.5
10	6.5	3.6
11	1.4	3.6
12	1.4	2.5
13	3.1	6.0
14	4.8	3.6
15	6.5	6.0
16	3.1	4.8

Table S4 Prediction set composition, the predicted values obtained by the proposed PLS model and corresponding errors of prediction (REP)

No	Actual		Predicted (µg)		REP (%)	
	NIF	*P-NIF*	*NIF*	*P-NIF*	*NIF*	*P-NIF*
1	1.60	2.70	1.52	2.81	-5.00	4.07
2	2.20	4.00	2.13	3.87	-3.18	-3.25
3	4.50	4.30	4.20	4.70	-6.67	9.30
4	5.30	5.00	5.65	5.19	6.60	3.80
5	4.00	5.10	4.30	5.40	7.50	5.88
6	3.40	3.00	3.60	2.80	5.88	-6.67
7	2.90	5.50	2.82	5.90	-2.76	7.27
8	4.90	3.80	4.60	4.40	-6.12	15.79
9	6.20	2.30	5.80	2.51	-6.45	9.13
10	2.50	3.40	2.70	3.70	8.00	8.82

a

b

c
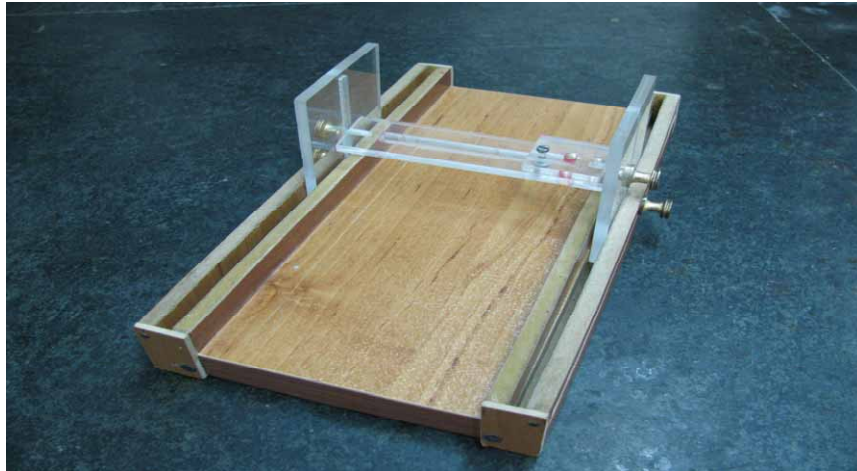
Figure S1. Photographs of the constructed imaging cabinet (a and b) and the spotting tool (c)

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                    ┌─────────────────────────────────────┐
                    │  Data matrix of TLC chromatograms   │
                    └─────────────────────────────────────┘
                                     │
                          ┌─────────────────────┐
                          │ Retention correction │
                          └─────────────────────┘
                                     │
                             ┌──────────────┐
                             │ Solvent line │
                             └──────────────┘
                                     │
                          ┌────────────────────┐
                          │ Variable selection │
                          └────────────────────┘
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Type of unfolding

| Sum of columns (SC) | Sum of rows (SR) | Simple unfolding (SU) | Sum of columns (SC) | Sum of rows (SR) | Simple unfolding (SU) | Sum of columns (SC) | Sum of rows (SR) | Simple unfolding (SU) | Sum of columns (SC) | Sum of rows (SR) | Simple unfolding (SU) |

Total range (TR) — Input data — Original matrix (OM) / Principal components (PC)

Selected variables (SV) — Input data — Original matrix (OM) / Principal components (PC)
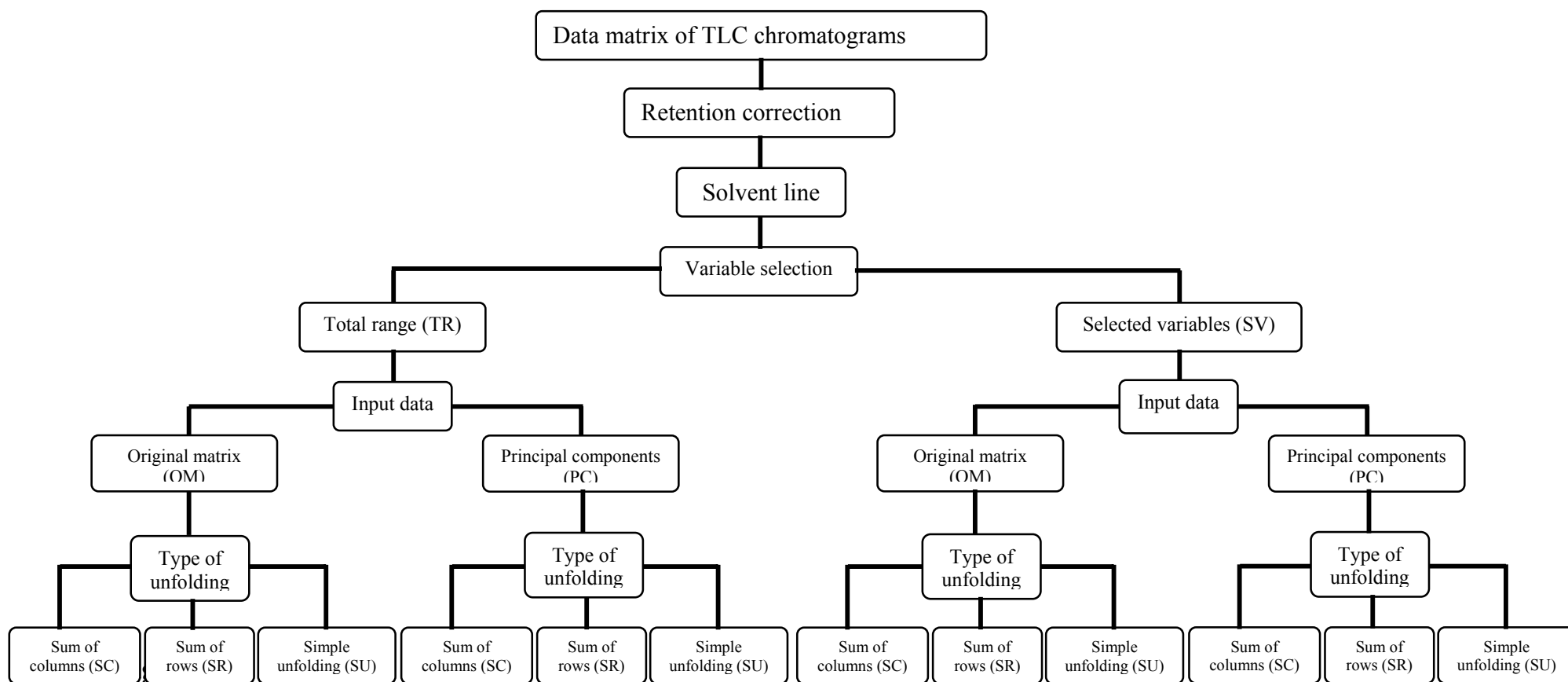
Figure S2. Schematic diagram of the data preparation for multivariate calibration
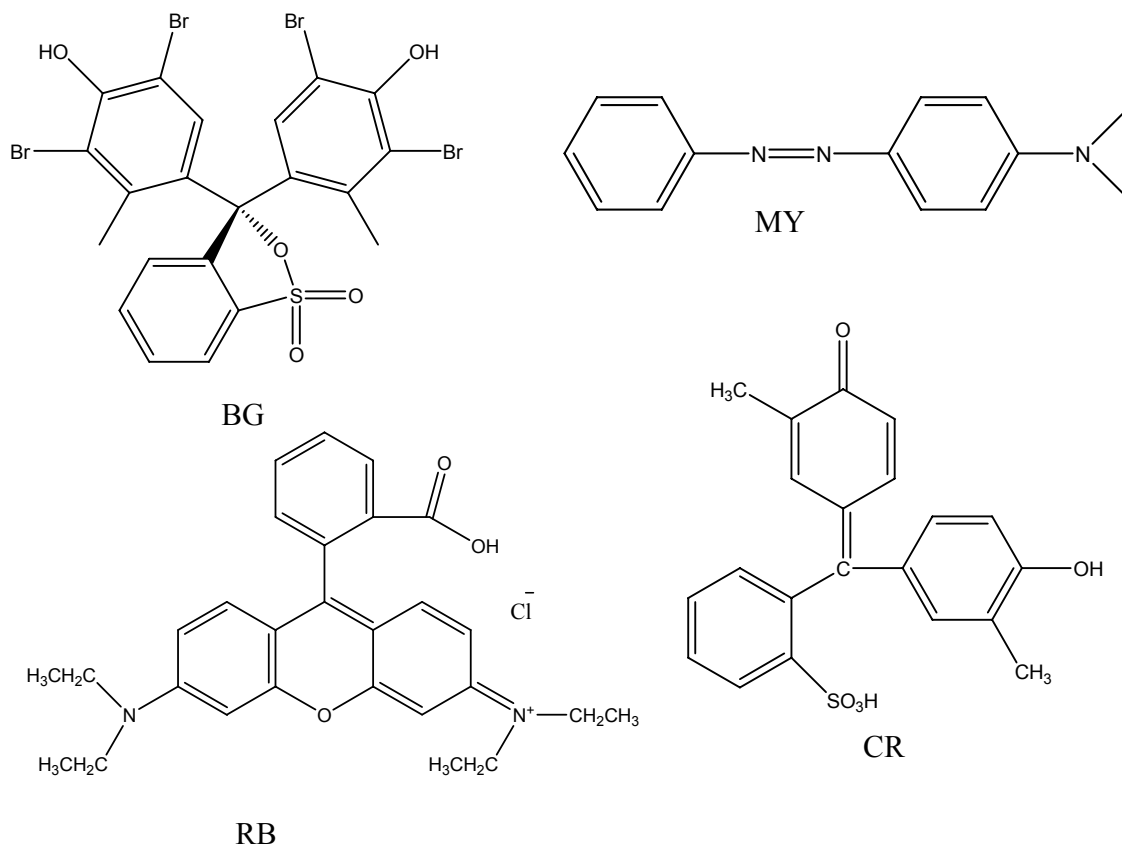
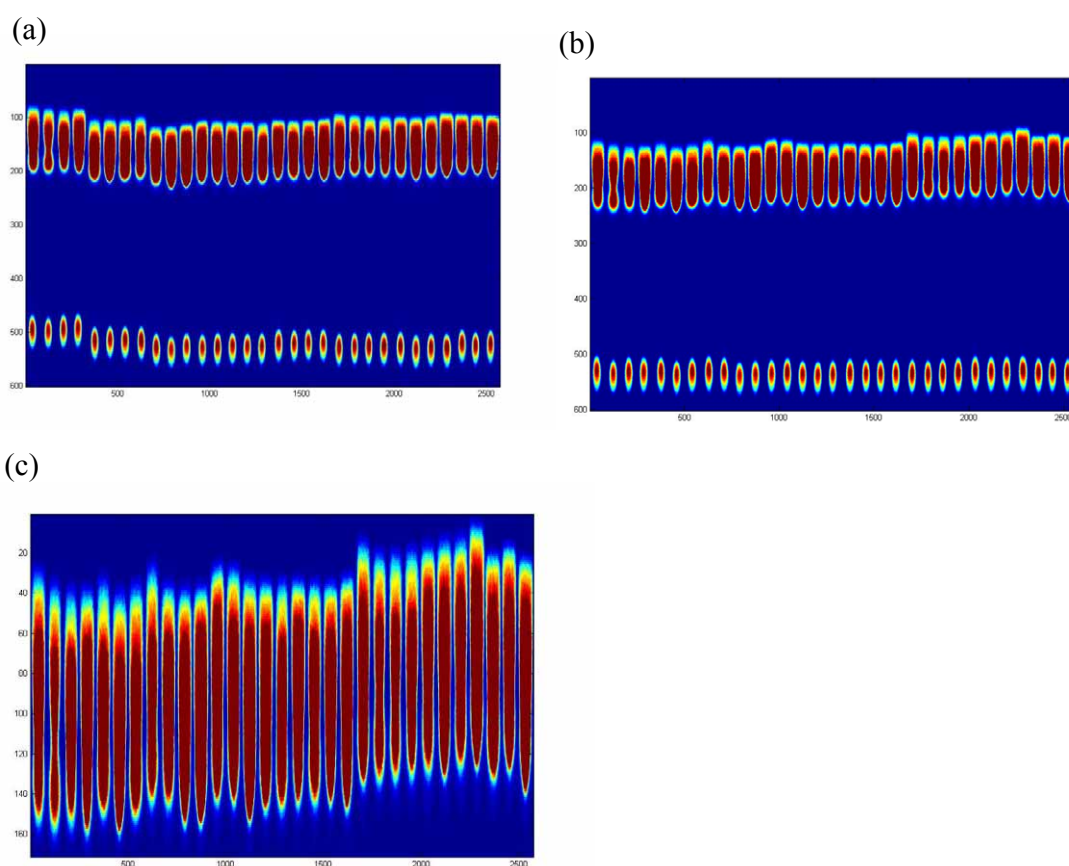**Fig. S3.** Chemical structure of the indicators used in this study.

Fig. S4. Two-dimensional image of the TLC sheets (cut digitally beside each others) after development of different calibration and prediction sets: (a) before internal standard correction, (b) after internal standard correction and (c) after removing redundant parts.