

Table S1 Analysis results for the prediction of the calibration set by PLS and SRACLS methods

Method				PLS								SRACLS							
ERG	MET	CAF	PAR	ERG		MET		CAF		PAR		ERG		MET		CAF		PAR	
True (ng mL ⁻¹)				Found	R%	Found	R%	Found	R%	Found	R%	Found	R%	Found	R%	Found	R%	Found	R%
0.50	2.50	25.00	165.00	0.52	104.33	2.43	97.38	24.98	99.91	166.65	101.00	-	-	2.42	96.86	25.04	100.17	167.00	101.21
0.50	2.00	20.00	195.00	0.53	105.51	1.99	99.68	20.29	101.47	195.12	100.06	-	-	1.86	92.82	20.98	104.90	197.68	101.38
0.40	2.00	30.00	145.00	0.52	129.54	2.00	99.81	30.34	101.14	144.57	99.71	-	-	2.09	104.33	30.31	101.03	143.68	99.09
0.40	3.00	22.50	195.00	0.51	126.81	2.97	99.16	22.77	101.22	187.34	96.07	-	-	2.89	96.21	22.96	102.06	186.84	95.82
0.60	2.25	30.00	165.00	0.50	83.51	2.28	101.53	30.12	100.41	164.96	99.97	-	-	2.32	103.28	30.26	100.85	163.85	99.30
0.45	3.00	25.00	145.00	0.53	116.98	2.98	99.26	25.13	100.53	143.13	98.71	-	-	3.02	100.83	24.65	98.58	142.46	98.25
0.60	2.50	22.50	145.00	0.54	90.57	2.51	100.33	22.49	99.94	146.12	100.77	-	-	2.53	101.07	22.22	98.77	146.98	101.37
0.50	2.25	22.50	180.00	0.52	104.79	2.26	100.59	22.74	101.05	179.83	99.91	-	-	2.19	97.28	23.03	102.35	181.03	100.57
0.45	2.25	27.50	195.00	0.50	111.06	2.25	100.18	27.18	98.82	191.74	98.33	-	-	2.20	97.60	27.69	100.68	191.26	98.08
0.45	2.75	30.00	180.00	0.48	107.18	2.75	100.16	30.02	100.08	180.73	100.40	-	-	2.75	100.02	30.24	100.78	179.11	99.51
0.55	3.00	27.50	165.00	0.50	91.32	2.99	99.82	27.31	99.30	165.06	100.03	-	-	3.01	100.49	27.15	98.71	163.89	99.33
0.60	2.75	25.00	195.00	0.50	83.22	2.80	101.77	24.63	98.52	195.64	100.33	-	-	2.71	98.49	24.96	99.83	195.74	100.38
0.55	2.50	30.00	195.00	0.48	87.05	2.53	101.38	30.12	100.41	197.74	101.41	-	-	2.49	99.57	30.69	102.29	196.69	100.87
0.50	3.00	30.00	130.00	0.51	101.90	3.01	100.48	30.15	100.49	131.41	101.09	-	-	3.15	104.98	29.49	98.30	129.32	99.48
0.60	3.00	20.00	180.00	0.52	87.18	3.01	100.46	19.82	99.12	181.88	101.05	-	-	2.93	97.62	19.85	99.25	183.13	101.74
0.60	2.00	27.50	130.00	0.53	88.73	2.03	101.26	27.08	98.46	129.42	99.56	-	-	2.17	108.51	26.75	97.26	129.36	99.51
0.40	2.75	20.00	165.00	0.52	129.91	2.74	99.80	20.23	101.17	167.78	101.69	-	-	2.69	97.89	20.26	101.32	169.09	102.48
0.55	2.00	25.00	180.00	0.50	90.66	1.98	99.13	24.76	99.05	180.13	100.07	-	-	1.92	96.07	25.16	100.63	180.94	100.52
0.40	2.50	27.50	180.00	0.46	116.21	2.45	97.87	27.55	100.19	181.44	100.80	-	-	2.41	96.48	27.88	101.37	180.78	100.43
0.50	2.75	27.50	145.00	0.48	95.16	2.71	98.48	27.37	99.53	144.81	99.87	-	-	2.78	101.19	27.07	98.43	143.56	99.01
0.55	2.75	22.50	130.00	0.50	90.54	2.78	100.91	22.34	99.30	130.97	100.75	-	-	2.84	103.42	21.82	96.98	131.22	100.94
0.55	2.25	20.00	145.00	0.49	89.67	2.25	99.83	19.82	99.11	144.77	99.84	-	-	2.25	99.95	19.61	98.03	146.22	100.84
0.45	2.00	22.50	165.00	0.46	101.24	2.01	100.68	22.47	99.85	166.05	100.63	-	-	1.97	98.35	22.69	100.86	166.98	101.20
0.40	2.25	25.00	130.00	0.45	113.33	2.23	99.29	25.13	100.51	126.95	97.65	-	-	2.35	104.34	24.69	98.76	126.09	96.99
0.45	2.50	20.00	130.00	0.44	98.71	2.53	101.09	20.15	100.75	130.75	100.58	-	-	2.57	102.77	19.67	98.37	131.41	101.09
Mean (%)				101.80		100.01		100.01		100.01		-		100.02		100.02		99.98	
S.D.				14.24		1.10		0.89		1.24		-		3.54		1.85		1.54	

Table S2 Analysis results for the prediction of the calibration set by MCR-ALS and SVR methods

Method				MCR-ALS										SVR					
ERG	MET	CAF	PAR	ERG		MET		CAF		PAR		ERG		MET		CAF		PAR	
	True (ng mL ⁻¹)			Found	R%	Found	R%	Found	R%	Found	R%	Found	R%	Found	R%	Found	R%	Found	R%
0.50	2.50	25.00	165.00	-	-	2.46	98.50	24.11	96.46	163.78	99.26	0.50	100.11	2.44	97.48	24.93	99.70	166.62	100.98
0.50	2.00	20.00	195.00	-	-	1.94	97.09	19.00	95.00	193.58	99.27	0.50	99.43	1.99	99.50	20.32	101.60	194.79	99.89
0.40	2.00	30.00	145.00	-	-	2.03	101.63	28.84	96.13	142.41	98.21	0.46	115.00	1.99	99.71	30.22	100.75	145.21	100.14
0.40	3.00	22.50	195.00	-	-	3.02	100.57	22.51	100.05	197.92	101.50	0.46	115.00	2.97	99.00	22.83	101.48	187.21	96.01
0.60	2.25	30.00	165.00	-	-	2.36	104.99	29.13	97.10	164.41	99.64	0.54	90.00	2.28	101.51	30.08	100.28	165.21	100.13
0.45	3.00	25.00	145.00	-	-	3.13	104.41	24.73	98.94	144.45	99.62	0.50	111.48	2.97	99.11	25.07	100.30	142.46	98.25
0.60	2.50	22.50	145.00	-	-	2.53	101.12	22.36	99.39	144.37	99.57	0.54	90.00	2.49	99.71	22.45	99.79	144.79	99.86
0.50	2.25	22.50	180.00	-	-	2.26	100.39	22.20	98.65	180.60	100.33	0.50	100.43	2.26	100.55	22.71	100.93	179.73	99.85
0.45	2.25	27.50	195.00	-	-	2.33	103.78	27.25	99.10	197.04	101.04	0.51	112.96	2.25	99.78	27.29	99.23	191.03	97.96
0.45	2.75	30.00	180.00	-	-	2.83	102.99	29.12	97.08	181.83	101.02	0.50	111.36	2.74	99.64	30.06	100.20	180.21	100.12
0.55	3.00	27.50	165.00	-	-	2.98	99.34	25.75	93.62	166.30	100.79	0.50	91.12	3.00	99.86	27.29	99.22	165.21	100.13
0.60	2.75	25.00	195.00	-	-	2.57	93.55	23.85	95.40	195.82	100.42	0.54	90.00	2.77	100.91	24.79	99.16	195.10	100.05
0.55	2.50	30.00	195.00	-	-	2.40	95.84	29.39	97.97	195.47	100.24	0.50	90.89	2.49	99.63	30.21	100.70	194.84	99.92
0.50	3.00	30.00	130.00	-	-	2.86	95.40	29.89	99.64	128.13	98.56	0.50	99.90	3.01	100.33	30.04	100.15	131.89	101.46
0.60	3.00	20.00	180.00	-	-	3.03	100.90	19.97	99.86	179.21	99.56	0.54	90.00	3.01	100.33	19.79	98.95	180.97	100.54
0.60	2.00	27.50	130.00	-	-	2.09	104.44	27.75	100.91	127.41	98.01	0.54	90.00	2.01	100.50	26.96	98.04	130.37	100.28
0.40	2.75	20.00	165.00	-	-	2.80	101.78	19.93	99.63	164.35	99.61	0.46	115.00	2.76	100.22	20.18	100.90	166.04	100.63
0.55	2.00	25.00	180.00	-	-	2.10	105.17	25.08	100.33	178.08	98.94	0.50	90.91	2.00	100.25	24.79	99.16	179.99	99.99
0.40	2.50	27.50	180.00	-	-	2.56	102.47	27.59	100.33	176.93	98.29	0.46	115.00	2.48	99.40	27.67	100.63	180.81	100.45
0.50	2.75	27.50	145.00	-	-	2.69	97.66	27.64	100.50	144.71	99.80	0.50	99.96	2.74	99.64	27.29	99.24	144.67	99.77
0.55	2.75	22.50	130.00	-	-	2.74	99.65	22.55	100.22	129.00	99.23	0.50	90.86	2.76	100.36	22.37	99.42	130.21	100.16
0.55	2.25	20.00	145.00	-	-	2.21	98.13	20.05	100.25	144.86	99.90	0.50	90.84	2.24	99.56	19.86	99.31	142.38	98.20
0.45	2.00	22.50	165.00	-	-	2.07	103.50	22.70	100.89	163.12	98.86	0.50	111.08	2.05	102.70	22.38	99.48	164.79	99.87
0.40	2.25	25.00	130.00	-	-	2.33	103.56	25.23	100.92	128.18	98.60	0.46	115.00	2.24	99.56	24.90	99.62	128.85	99.11
0.45	2.50	20.00	130.00	-	-	2.69	107.65	20.29	101.47	131.10	100.85	0.50	111.08	2.50	100.04	20.21	101.05	130.21	100.16
			Mean (%)	-	-	100.98		98.79		99.64		101.50		99.97		99.97		99.76	
			S.D.	-	-	3.47		2.13		0.96		10.52		0.94		0.88		1.12	

Table S3 Analysis results for the prediction of the calibration set by PC-ANN method

Method				PC-ANN							
ERG	MET	CAF	PAR	ERG		MET		CAF		PAR	
	True (ng mL ⁻¹)			Found	R%	Found	R%	Found	R%	Found	R%
0.50	2.50	25.00	165.00	0.50	100.25	2.44	97.72	24.76	99.02	163.85	99.30
0.50	2.00	20.00	195.00	0.51	101.61	1.94	97.19	20.09	100.47	190.25	97.56
0.40	2.00	30.00	145.00	0.42	104.31	2.03	101.35	29.61	98.70	144.37	99.56
0.40	3.00	22.50	195.00	0.42	103.83	2.94	97.84	22.48	99.92	183.32	94.01
0.60	2.25	30.00	165.00	0.59	98.17	2.23	99.19	29.89	99.64	164.35	99.61
0.45	3.00	25.00	145.00	0.43	96.17	2.97	99.16	25.21	100.84	140.56	96.94
0.60	2.50	22.50	145.00	0.62	102.52	2.44	97.70	22.34	99.29	142.53	98.29
0.50	2.25	22.50	180.00	0.48	95.21	2.19	97.45	22.70	100.90	176.03	97.80
0.45	2.25	27.50	195.00	0.47	103.36	2.14	95.27	27.12	98.63	189.59	97.23
0.45	2.75	30.00	180.00	0.48	107.04	2.67	97.01	28.84	96.13	179.83	99.90
0.55	3.00	27.50	165.00	0.51	93.08	2.97	98.87	27.51	100.05	163.12	98.86
0.60	2.75	25.00	195.00	0.58	96.85	2.73	99.34	24.78	99.10	192.27	98.60
0.55	2.50	30.00	195.00	0.51	93.04	2.41	96.26	29.18	97.27	196.65	100.85
0.50	3.00	30.00	130.00	0.50	100.86	2.98	99.27	29.82	99.39	131.06	100.82
0.60	3.00	20.00	180.00	0.62	103.96	2.92	97.21	19.93	99.65	176.69	98.16
0.60	2.00	27.50	130.00	0.60	99.25	2.03	101.50	27.33	99.38	128.22	98.63
0.40	2.75	20.00	165.00	0.40	101.25	2.74	99.64	19.62	98.08	163.29	98.96
0.55	2.00	25.00	180.00	0.53	96.69	1.95	97.62	24.41	97.62	177.63	98.69
0.40	2.50	27.50	180.00	0.45	112.45	2.44	97.57	27.23	99.03	180.22	100.12
0.50	2.75	27.50	145.00	0.51	102.51	2.81	102.33	26.94	97.97	144.03	99.33
0.55	2.75	22.50	130.00	0.57	104.33	2.78	101.04	22.52	100.09	128.39	98.76
0.55	2.25	20.00	145.00	0.54	98.32	2.27	101.02	20.05	100.24	141.40	97.52
0.45	2.00	22.50	165.00	0.45	100.83	2.02	100.79	21.79	96.83	163.88	99.32
0.40	2.25	25.00	130.00	0.40	100.71	2.30	102.42	24.96	99.86	126.49	97.30
0.45	2.50	20.00	130.00	0.48	105.60	2.51	100.24	20.00	99.99	128.57	98.90
			Mean (%)		100.89		99.00		99.12		98.60
			S.D.		4.45		1.95		1.23		1.42

