Electronic Supplementary Information

Fast identification and quantification of BTEX by Raman spectrometry and chemometrics

Jonathan Moreau and Emmanuel Rinnert

IFREMER, Laboratoire Détection, Capteurs et Mesures, CS10070, 29280 Plouzané, France.

Tables S-1 and S-2 exhibit the actual concentrations of each BTEX in all the samples for Raman measurements. Samples 55 to 72 were used to determine spectral uncertainty and to check sample preparation uncertainty.

Figure S-1 shows the comparison between the previous concentrations and those calculated by the data processing (SIMPLISMA 1 way from chart 1 in the article) for each BTEX.

Figure S-2 displays a 3D bar graph representing the concentrations of the last samples (table S-2) obtained thanks to the data processing.

Table S-1. Experiment plan, part 1. Concentration values in g/L (± 5 %).

S. n°	B.	T.	E.	o-X.	m-X.	p-X.	S. n°	B.	T.	E.	o-X.	m-X.	p-X.
01	153	142	143	147	143	141	**26**	14	0	0	541	264	56
02	287	19	38	77	151	297	**27**	439	430.3	0	0	0	0
03	288	299	19	39	75	148	**28**	438	0	432	0	0	0
04	287	149	301	19	38	74	**29**	432	0	0	444	0	0
05	283	75	150	309	19	37	**30**	438	0	0	0	433	0
06	78	75	601	39	38	37	**31**	441	0	0	0	0	426
07	24	599	75	19	38	111	**32**	863	11	0	0	0	0
08	287	150	301	19	38	74	**33**	863	0	11	0	0	0
09	794	22	45	0	0	11	**34**	863	0	0	11	0	0
10	370	0	376	39	11	74	**35**	863	0	0	0	11	0
11	422	11	0	386	19	37	**36**	836	0	0	0	0	11
12	115	150	150	155	151	148	**37**	840	0	0	11	11	11.2
13	836	7.4	7.4	7.4	7.4	7.3	**38**	433	0	0	386	38	19
14	829	38	7.4	0	0	0	**39**	8.3	0	214	220	215	211
15	710	0	0	116	11	37	**40**	188	0	601	11	23	44
16	142	374	188	97	45	22	**41**	188	0	601	46	11	22
17	1.7	172	173	178	173	171	**42**	65	0	601	155	38	11
18	10	299	368	39	113	37	**43**	4.8	0	11	711	76	74
19	1.7	0	38	232	262	371	**44**	9.6	0	19	97	56	682
20	14	0	0	541	264	56	**45**	115	150	150	155	151	148
21	115	150	150	155	151	148	**46**	874	0	0	0	0	0
22	115	150	150	155	151	148	**47**	0	865	0	0	0	0
23	115	150	150	155	151	148	**48**	0	0	867	0	0	0
24	115	150	150	155	151	148	**49**	0	0	0	879	0	0
25	115	150	150	155	151	148	**50**	0	0	0	0	868	0
							51	0	0	0	0	0	861

S. n°: Sample n°, B.: Benzene, T.: Toluene, E.: Ethylbenzene, o-X.: ortho-Xylene, m-X.: meta-Xylene, p-X.: para-Xylene, Chlf: Chloroform.

Table S-2. Experiment plan, part 2. Concentration values in g/L (± 5 %).

S. n°	B.	T.	E.	o-X.	m-X.	p-X.	Chlf	S. n°	B.	T.	E.	o-X.	m-X.	p-X.
51b	0	0	0	0	0	0	$1.49_{10}{}^{6}$	**63**	288	19	38	77	151	297
52	393	433	41	0	0	2.2	0	**64**	1.7	0	38	232	262	371
53	153	151	108	0	22	431	0	**65**	1.7	0	38	232	262	371
54	437	0	0	308	109	22	0	**66**	1.7	0	38	232	262	371
51c	140	138	139	141	139	137	60	**67**	1.7	0	38	232	262	371
51d	109	108	108	110	109	108	393	**68**	1.7	0	38	232	262	371
55	288	19	38	77	151	297	0	**69**	1.7	0	38	232	262	371
56	288	19	38	77	151	297	0	**70**	1.7	0	38	232	262	371
57	288	19	38	77	151	297	0	**71**	1.7	0	38	232	262	371
58	288	19	38	77	151	297	0	**72**	1.7	0	38	232	262	371
59	288	19	38	77	151	297	0							
60	288	19	38	77	151	297	0							
61	288	19	38	77	151	297	0							
62	288	19	38	77	151	297	0							

S. n°: Sample n°, B.: Benzene, T.: Toluene, E.: Ethylbenzene, o-X.: ortho-Xylene, m-X.: meta-Xylene, p-X.: para-Xylene, Chlf: Chloroform.

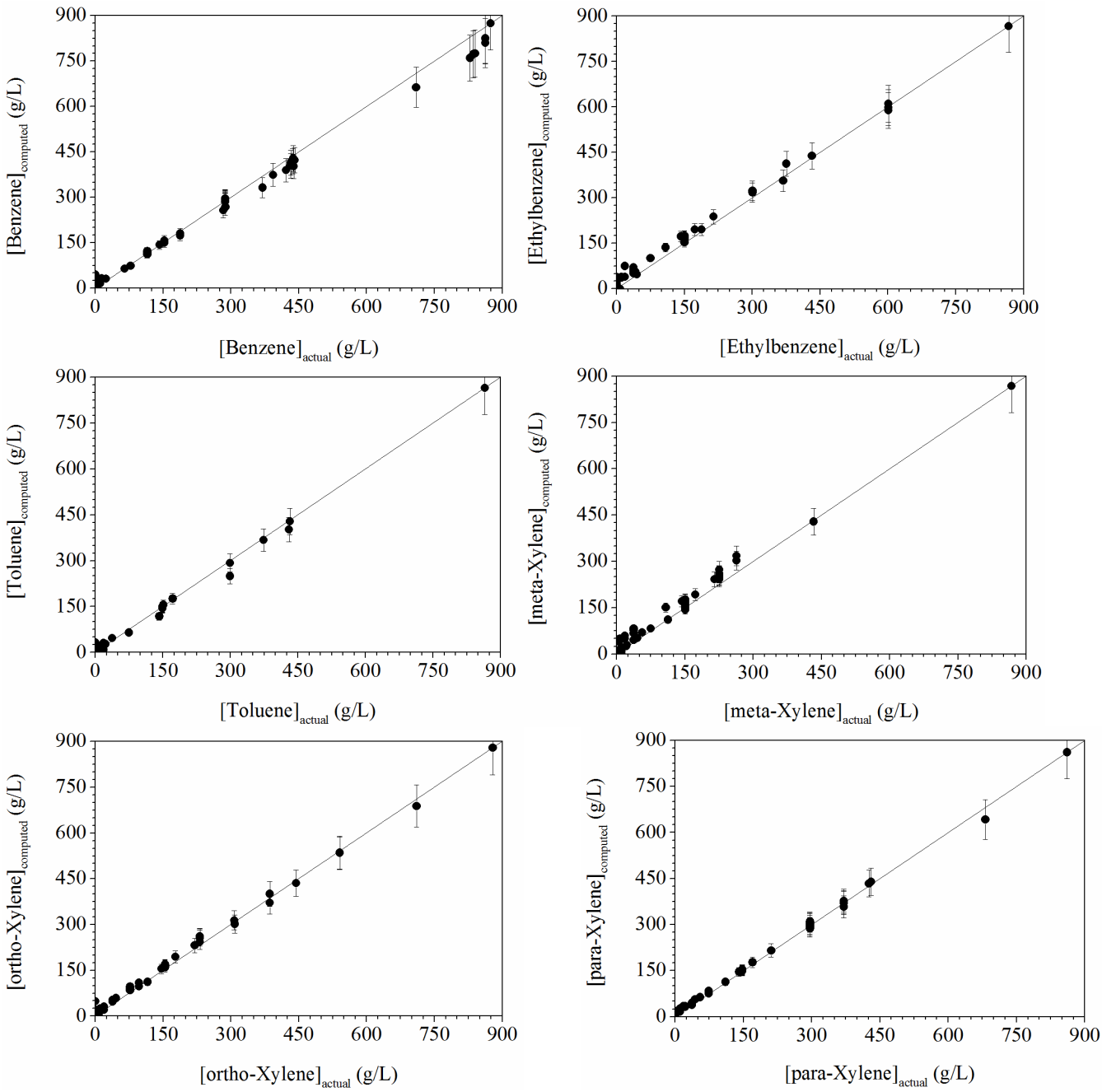

Figure S-2. Plots of computed vs actual concentrations of BTEX compounds in different mixtures using resolved spectra calculated by SIMPLISMA.

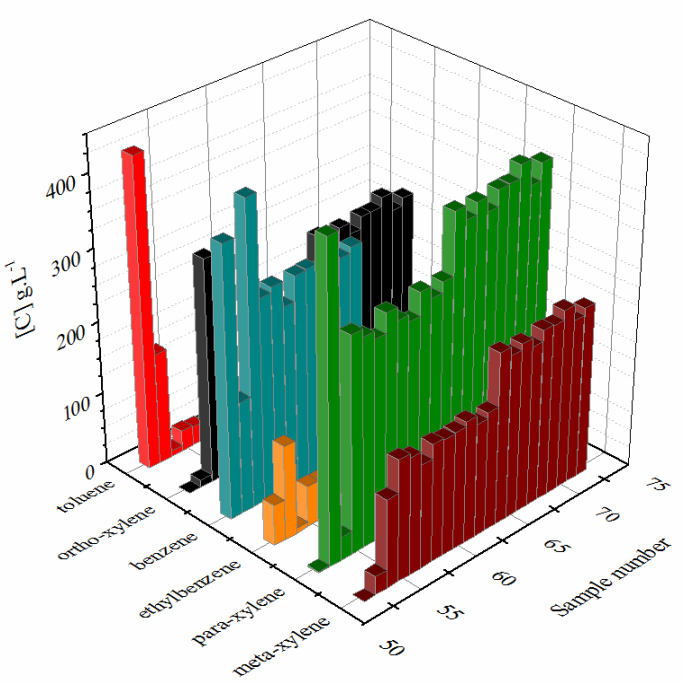

Figure S-3. Graphical results of the data processing showing the concentration of each BTEX compound from sample 52 to 72.