

Analyte	Abbreviation	RT	Q1	Detection*
1-Nitronaphthalene	1-NNAP	12.12	173	P (86)
2-Nitronaphthalene	2-NNAP	12.62	173	P (43)
5-Nitroacenaphthene	5-NACE	17.52	199	n.d.
2-Nitrofluorene	2-NFLN	19.07	211	n.d.
9-Nitroanthracene	9-NANT	19.46	223	P (71)
9-Nitrophenanthrene	9-NPHE	20.64	223	n.d.
3-Nitrophenanthrene	3-NPHE	21.4	223	n.d.
2-Nitrofluoranthene	2-NFLT	25.75	247	P (71)
3-Nitrofluoranthene	3-NFLT	25.80	247	n.d.
1-Nitropyrene	1-NPYR	26.63	247	n.d.
2-Nitropyrene	2-NPYR	26.95	247	n.d.
7-Nitrobenz(a)anthracene	7-NBAA	29.41	273	n.d.
6-Nitrochrysene	6-NCHR	30.66	273	n.d.
1,3-Dinitropyrene	1,3-N ₂ PYR	31.8	292	n.d.
1,6-Dinitropyrene	1,6-N ₂ PYR	32.81	292	n.d.
1,8-Dinitropyrene	1,8-N ₂ PYR	33.54	292	n.d.
6-Nitrobenz(a)pyrene	6-NBAP	36.73	297	n.d.
1,4-Naphthoquinone	1,4-O ₂ NAP	10.18	158	A (14)
9-Fluorenone	9-OFLN	13.78	180	A (100) P (86)
9,10-Anthraquinone	9,10-O ₂ ANT	17.03	208	A (86) P (57)
2-Nitro-9-fluorenone	2-N-9-OFLN	20.54	225	n.d.
Benz(a)fluorenone	BaOFLN	22.88	230	A (29) P (100)
Benz(b)fluorenone	BbOFLN	23.82	230	P (86)
Benzanthrone	OBAT	25.07	230	A (29) B (43)
1,2-Benzanthraquinone	1,2-O ₂ BAA	26.46	258	A (71) B (100)
3-Nitrosalicylic acid	3-NSA	3.60	182	A (100) P (11)
5-Nitrosalicylic acid	5-NSA	5.07	182	A (100) P (11)
4-Nitrocatechol	4-NC	7.76	154	A (90) P (33)
4-nitroguaiacol	4-NG	8.29	168	A (50) P (22)
4-Methyl-5-nitrocatechol	4-M-5-NC	9.47	168	A (90) P (22)
4-Nitrophenol	4-NP	10.00	138	A (100) P (100)
2,4-Dinitrophenol	2,4-DNP	10.92	183	A (100) P (33)
3-Methyl-4-nitrophenol	3-M-4-NP	13.19	152	A (100) P (89)
3-Methyl-5-nitrocatechol	3-M-5-NC	14.01	168	A (100) P (22)
2-Methyl-4-nitrophenol	2-M-4-NP	16.72	152	A (100) P (89)
Dinitro-ortho-cresol	DNOC	17.05	197	A (100) P (78)