Electronic Supplementary Material (ESI) for Journal of Environmental Monitoring

Supplementary information

Table S1. Optimum values selected for the variables involved in the extraction procedure.

Table S2. Results obtained for the classification of the identified compounds according to the main chemical group present in the molecule.

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Figure S1. Sampling device. DMA, differential mobility analyzer; FH, Filter holder; HVS, high voltage supply; IS, ionization source; R, restrictor; and VS, vacuum system.

Figure S2. Average maximum and minimum values for the classification of the Fg-Id compounds as a function of the main chemical group present in the molecule. A, Classification in terms of number of compounds; B, Classification in terms of relative peak area.

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Table S1. Optimum values selected for the variables of the extraction procedure.

Variable	First design	Second design	Optimum
Probe position (cm)	0–2		2
Amplitude (%)**	10–50		50
Duty Cycle (%)	10–50		50
Flow-rate (ml/min)	0.25–1		1
Extraction time (min)	5–15	15–25	30*
Extractant composition (% acetone v/v)	0–50	50–75	50

* Calculated using a univariate approach

**Of the applied power (100 W) of the converter

Table S2. Classification of the identified compounds according to the main chemical group and the specific element present in the molecule. Number of compounds and ∑NRF calculated per sample. 21 samples analyzed (9, TSP; 6, 50 nm particles; and 6, 30 nm particles). Relative peak area expressed as m^{-3}.

			Number of compounds			∑NRF		
			Average	Min	Max	Average	Min	Max
Hydrocarbons	Alkanes	TSP	15	12	24	12.0	4.6	27.5
		50 nm	7	5	9	10.0	4.1	22.5
		30 nm	18	15	21	95.0	24.5	245.0
	Cyclo alkanes	TSP	9	7	14	3.5	1.1	8.5
		50 nm	10	7	13	20.0	5.5	55.0
		30 nm	10	8	14	80.0	8.0	750.0
	Alkenes	TSP	47	42	52	28.0	10.5	75.0
		50 nm	52	50	56	195.0	70.0	950.0
		30 nm	63	54	67	650.0	85.0	1600.0
	Cyclo alkenes	TSP	9	8	11	3.8	0.7	10.0
		50 nm	9	7	10	11.0	2.5	28.0
		30 nm	8	5	9	185.0	3.0	50.0
	Aromatic compounds	TSP	9	7	11	2.5	0.7	6.5
		50 nm	11	9	14	21.0	4.6	46.0
		30 nm	5	4	6	11.5	1.1	34.5
Halogenated compounds	F	TSP	9	7	11	34.5	1.9	215.0
		50-nm	9	8	10	13.5	3.0	34.5
		30-nm	16	14	17	190.0	19.5	600.0
	Cl	TSP	6	5	6	6.0	0.8	39.0
		50-nm	7	5	11	60.0	6.5	185.0
		30-nm	14	13	14	345.0	20.0	800.0
	Br	TSP	8	7	9	18.0	1.2	145.0
		50-nm	6	4	7	14.5	1.7	41.0
		30-nm	10	8	12	65.0	4.3	280.0
	I	TSP	4	2	6	2.7	0.8	17.5
		50-nm	2	1	2	15.0	1.0	80.0
		30-nm	3	3	3	13.0	4.1	48.5

Table S2. Cont.

			Number of compounds			∑NRF		
			Average	Min	Max	Average	Min	Max
Nitrogen compounds	Amino acids	TSP	21	18	29	12.5	1.8	40.5
		50 nm	16	13	22	75.0	14.0	550.0
		30 nm	30	26	33	420.0	80.0	850.0
	Nitro compounds	TSP	3	2	4	0.9	0.1	3.2
		50 nm	7	6	9	9.5	3.2	28.5
		30 nm	4	3	5	2.9	0.9	9.0
	Amine	TSP	3	2	4	2.1	0.1	14.0
		50 nm	5	4	6	12.0	3.1	35.0
		30 nm	8	7	8	90.0	6.0	305.0
	Amides	TSP	5	5	8	2.4	0.3	11.5
		50 nm	3	3	4	6.0	1.1	23.5
		30 nm	10	7	15	90.0	7.5	440.0
	Nitriles	TSP	3	3	4	1.1	0.3	2.1
		50 nm	7	6	7	28.5	2.5	230.0
		30 nm	6	6	7	55.0	3.6	300.0
	Imides	TSP	9	6	14	0.5	1.6	14.5
		50 nm	5	4	7	10.5	1.7	36.0
		30 nm	12	10	15	270.0	28.5	750.0
	Urea derivatives	TSP	1	1	1	0.8	0.1	2.5
		50 nm	1	1	1	3.1	0.1	11.0
		30 nm	1	1	1	3.1	0.1	13.0
	Amino acids N-derivatives	TSP	13	9	18	6.5	1.7	22.5
		50 nm	11	10	13	15.5	2.8	32.5
		30 nm	10	9	12	145.0	11.5	455.0
	Glycosamines	TSP	1	1	2	3.4	0.2	30.5
		50 nm	2	1	2	1.6	0.5	2.8
		30 nm	0	0	1	0.1	-	0.7
	Hetero N compounds	TSP	0	0	1	0.1	-	1.0
		50 nm	1	1	1	5.5	0.4	30.0
		30 nm	4	3	4	3.1	1.4	7.0
Sulphur compounds	Sulfonamide	TSP	2	1	2	13.0	0.3	47.5
		50 nm	1	0	2	2.6	-	9.5
		30 nm	1	0	1	0.1	-	0.7
	Sulfonic compounds	TSP	1	1	2	0.4	0.0	2.2
		50 nm	0	0	0	0.0	0.0	0.0
		30 nm	0	0	0	0.0	0.0	0.0
	Thio compounds	TSP	5	4	9	6.1	1.8	20.0
		50 nm	3	2	5	2.7	0.6	6.5
		30 nm	3	2	6	2.7	0.7	9.1

Table S2. Cont.

			Number of compounds			∑NRF		
			Average	Min	Max	Average	Min	Max
Carboxyl Compounds	Acids	TSP	48	43	56	95.0	13.5	285.0
		50 nm	35	30	39	135.0	31.5	330.0
		30 nm	20	17	25	60.0	24.5	130.0
	Hydroxy acids	TSP	19	17	24	16.5	4.8	60.0
		50 nm	15	14	17	60.0	14.0	295.0
		30 nm	5	4	5	0.5	2.0	7.5
	Keto-acids	TSP	6	5	7	44.0	0.6	180.0
		50 nm	8	6	8	49.0	7.0	290.0
		30 nm	2	2	2	30.5	2.3	155.0
	Ester	TSP	46	35	60	5.0	10.0	245.0
		50 nm	60	53	69	230.0	55.0	700.0
		30 nm	40	36	46	155.0	55.0	400.0
	Anhydrides	TSP	0	0	0	-	-	-
		50 nm	1	1	2	2.8	-	16.5
		30 nm	0	0	0	-	-	-
Hydroxyl compounds	Alcohols	TSP	86	77	104	60.0	11.0	250.0
		50 nm	81	76	88	330.0	70.0	1200.0
		30 nm	79	75	88	455.0	170.0	1000.0
	Polyols	TSP	4	4	5	5.5	1.2	12.5
		50 nm	4	3	5	6.5	2.7	15.5
		30 nm	3	3	3	9.0	1.0	25.5
	Ethers	TSP	1	1	1	1.7	0.0	13.0
		50 nm	2	1	2	11.5	0.3	95.0
		30 nm	1	0	3	4.6	-	44.5
Carbonyl compounds	Ketones	TSP	33	24	47	460.0	200.0	1000.0
		50 nm	37	32	41	240.0	115.0	600.0
		30 nm	43	37	53	2100.0	550.0	4200.0
	Aldehydes	TSP	16	13	19	14.0	4.9	41.5
		50 nm	12	10	13	19.0	4.5	43.5
		30 nm	15	13	18	60.0	9.5	255.0

Table S3. Detailed comparison of the different size aerosol particles collected simultaneously according to the main chemical group and the specific element present in the molecule. Number of compounds and ∑NRF calculated per sample. 10 samples analyzed (5, TSP and 5, 50 nm particles). Relative peak area expressed as m^{-3}.

			Number of compounds			∑NRF		
			Average	Min	Max	Average	Min	Max
Hydrocarbon	Alkanes	50-nm	7	5	9	1.3	0.4	2.3
		TSP	18	13	24	2.8	0.5	5.4
	Cyclo alkanes	50-nm	10	7	13	2.5	0.6	5.5
		TSP	10	9	14	0.6	0.1	0.9
	Alkenes	50-nm	53	51	56	17.2	7.7	26.3
		TSP	49	46	52	3.5	1.1	7.3
	Cyclo alkenes	50-nm	9	8	10	1.5	0.3	2.8
		TSP	10	9	11	0.4	0.1	1.0
	Aromatic compounds	50-nm	10	9	12	2.3	0.6	4.5
		TSP	10	9	11	0.3	0.1	0.7
Halogenated compounds	F	50-nm	8	8	9	2.0	0.5	3.4
		TSP	10	7	11	2.1	0.7	6.1
	Cl	50-nm	8	5	11	6.6	0.8	18.4
		TSP	6	5	6	1.1	0.1	3.9
	Br	50-nm	6	4	7	1.7	0.2	4.1
		TSP	9	8	9	1.0	0.1	2.4
	I	50-nm	2	1	2	2.5	0.4	8.2
		TSP	5	3	6	0.5	0.1	1.8
Nitrogen compounds	Amino acids	50-nm	16	13	22	5.1	1.9	9.6
		TSP	22	18	29	1.5	0.2	4.1
	Nitro compounds	50-nm	7	6	9	1.2	0.3	2.8
		TSP	3	2	4	0.1	0.0	0.3
	Amines	50-nm	5	5	5	1.7	0.5	3.5
		TSP	3	3	4	0.4	0.1	1.4
	Amides	50-nm	3	3	4	0.9	0.1	2.4
		TSP	6	5	7	0.2	0.1	0.5
	Nitriles	50-nm	7	6	7	1.4	0.3	2.4
		TSP	3	3	4	0.1	0.1	0.2
	Imides	50-nm	5	4	6	1.1	0.2	2.5
		TSP	11	8	14	0.6	0.2	1.4
	Urea derivatives	50-nm	1	1	1	0.5	0.1	1.1
		TSP	1	1	1	0.1	0.1	0.2
	Amino acids	50-nm	11	10	11	1.9	0.3	3.3
	N derivatives	TSP	15	12	18	0.8	0.3	2.3
	Glycosamines	50-nm	2	2	2	0.2	0.1	0.3
		TSP	2	1	2	0.6	0.1	3.0
	Hetero	50-nm	1	1	1	0.5	0.1	3.0
	N compounds	TSP	1	0	1	0.0	-	0.1

Table S3. Cont.

			Number of compounds			∑NRF		
			Average	Min	Max	Average	Min	Max
Sulphur compounds	Sulfonamides	50-nm	1	1	2	0.5	0.1	1.0
		TSP	2	1	2	1.9	-	3.3
	Sulfonic compounds	50-nm	0	0	0	-	-	-
		TSP	1	1	2	0.1	0.1	0.1
	Thio compounds	50-nm	3	2	4	0.5	0.1	1.6
		TSP	5	4	7	0.7	0.2	1.5
Carboxyl compounds	Acids	50-nm	34	32	37	19.5	3.3	32.8
		TSP	51	47	56	12.1	1.4	26.2
	Hydroxy acids	50-nm	16	15	17	4.2	1.7	8.0
		TSP	21	17	24	2.6	0.5	6.0
	Keto-acids	50-nm	8	8	8	4.0	1.0	8.9
		TSP	6	6	7	7.5	0.1	15.8
	Ester	50-nm	58	53	65	33.3	5.6	69.1
		TSP	51	44	60	12.6	1.1	39.2
	Anhydrides	50-nm	1	1	2	0.5	0.2	1.7
		TSP	0	0	0	-	-	-
Hydroxyl compounds	Alcohols	50-nm	79	76	86	43.2	7.5	120.9
		TSP	91	83	104	8.9	1.2	24.8
	Polyols	50-nm	3	3	3	0.9	0.4	1.6
		TSP	4	4	5	0.6	0.1	1.2
	Ethers	50-nm	2	2	2	2.0	0.1	9.5
		TSP	1	1	1	0.4	0.1	1.3
Carbonyl compounds	Ketones	50-nm	35	32	40	17.9	11.3	25.0
		TSP	39	33	47	70.6	34.4	120.8
	Aldehydes	50-nm	12	11	13	2.4	0.6	4.3
		TSP	17	15	19	1.7	0.5	3.0

Figure S1. Sampling device. DMA, differential mobility analyzer; FH, Filter holder; HVS, high voltage supply; IS, ionization source; R, restrictor; and VS, vacuum system.

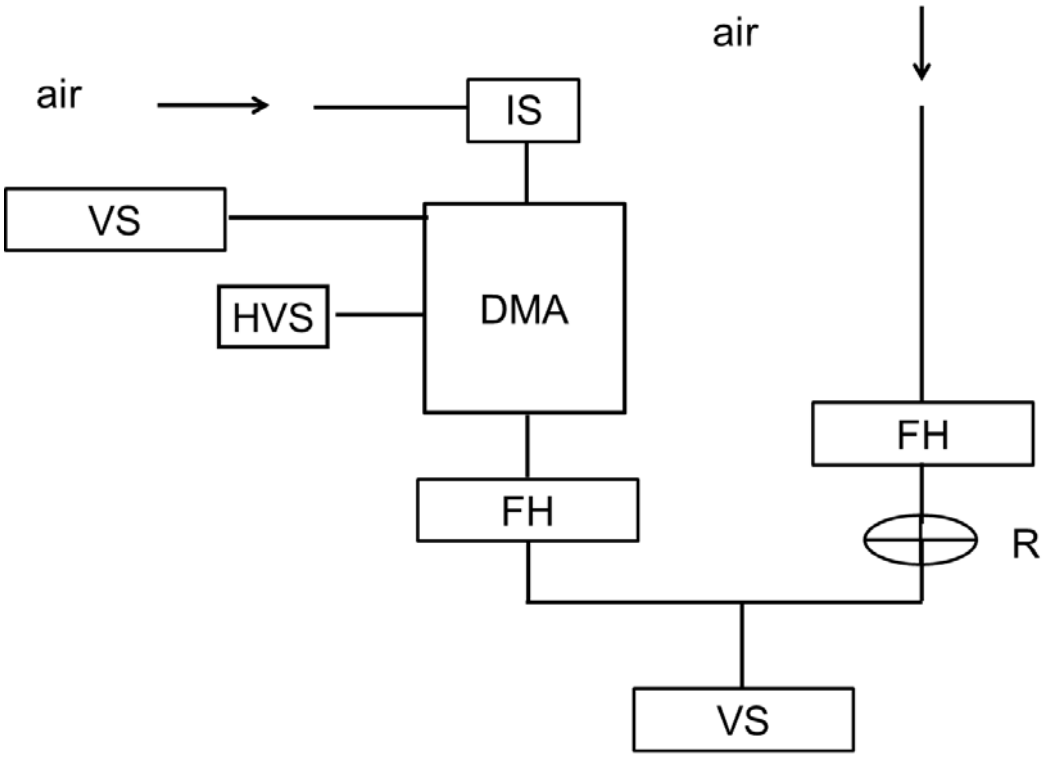
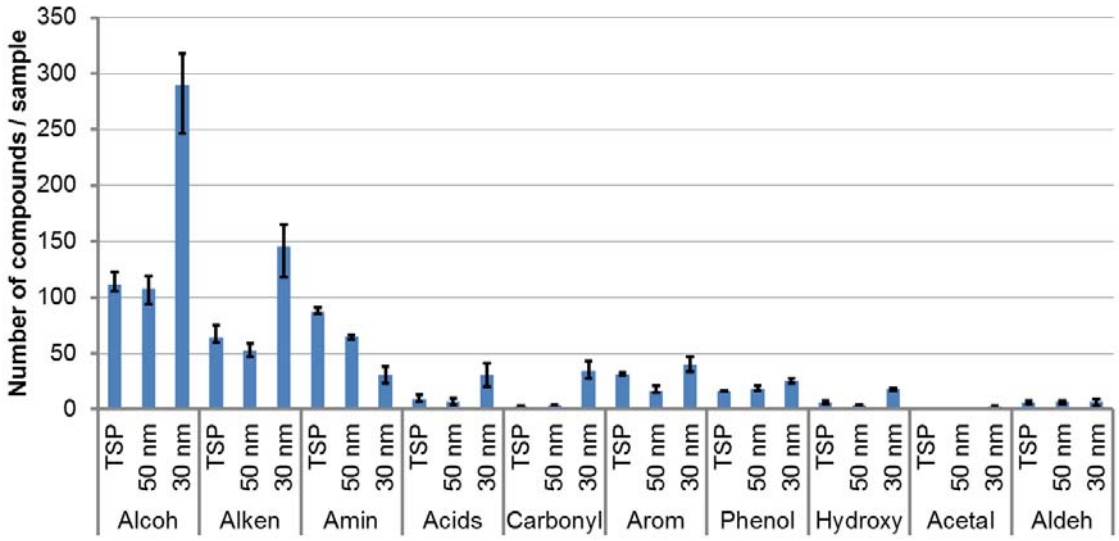


Figure S2. Average maximum and minimum values for the classification of the Fg-Id compounds as a function of the main chemical group present in the molecule. **A**, Classification in terms of number of compounds; **B**, Classification in terms of relative peak area.

A



B