J. Braz. Chem. Soc., Vol. 26, No. 5, S1-S3, 2015.
Printed in Brazil - ©2015 Sociedade Brasileira de Química
0103 - 5053 $6.00+0.00

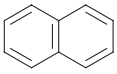
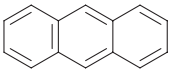
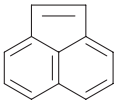
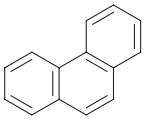
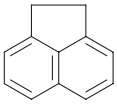
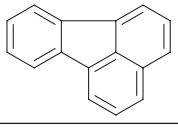
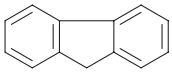
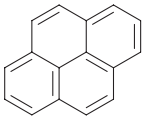
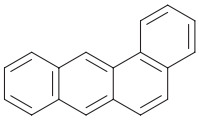
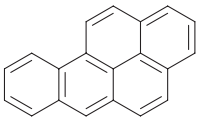
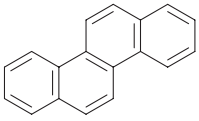
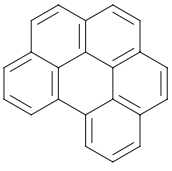
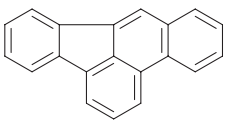
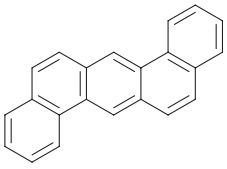
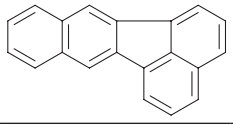
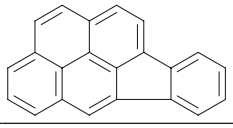
Supplementary Information

Determination of Polycyclic Aromatic Hydrocarbons in Groundwater Samples by Gas Chromatography-Mass Spectrometry After Pre-Concentration Using Cloud-Point Extraction with Surfactant Derivatization

Sarah A. R. Soares,[a,b] Cibele R. Costa,[b] Rennan G. O. Araujo,[a] Maria R. Zucchi,[c] Joil J. Celino[b] and Leonardo S. G. Teixeira*[*,a,d]

[a]Instituto de Química, [b]Instituto de Geociências, [c]Instituto de Física Nuclear and [d]Instituto Nacional de Ciência e Tecnologia de Energia e Ambiente (INCT E&A), Universidade Federal da Bahia, Campus Universitário de Ondina, 40170-115 Salvador-BA, Brazil

Table S1. Structure, formula and aqueous solubility at 25 °C of 16 priority PAH

HPA	Structure	Aqueous solubility / (mg L^{-1})	HPA	Structure	Aqueous solubility / (mg L^{-1})
Naphtalene		32	Anthracene		0.05-0.07
Acenaphtylene		3.93	Phenanthrene		1.0-1.3
Acenaphthene		3.4	Fluoranthene		0.26
Fluorene		1.9	Pyrene		0.14
Benzo (a) anthracene		0.01	Benzo (a) pyrene		0.0028
Chrysene		0.002	Benzo (g,h,i) perylene		0.0026
Benzo (b) fluoranthene		–	Dibenzo (a,h) anthracene		0.0005
Benzo (k) fluoranthene		–	Indeno (1,2,3-cd) pyrene		–

*e-mail: lsgt@ufba.br

Table S2. Matrix of 2^3 full factorial design, with triplicate of the center point[a]

Experiment	BSTFA volume / μL	Temperature / °C	time / min
1	+1 (150)	+1 (80)	+1 (60)
2	+1 (150)	+1 (80)	−1 (30)
3	+1 (150)	−1 (60)	+1 (60)
4	+1 (150)	−1 (60)	−1 (30)
5	−1 (100)	+1 (80)	+1 (60)
6	−1 (100)	+1 (80)	−1 (30)
7	−1 (100)	−1 (60)	+1 (60)
8	−1 (100)	−1 (60)	−1 (30)
9	0 (125)	0 (70)	0 (45)
10	0 (125)	0 (70)	0 (45)
11	0 (125)	0 (70)	0 (45)

[a]Real values are stated in parentheses.

Table S3. Response, in peak area for each analyte, and multiple responses obtained from 2^3 full factorial design applied to optimization of the surfactant derivatization reaction

Analyte	Experiment										
	1	2	3	4	5	6	7	8	9	10	11
Naphthalene	160113	120188	131225	93325	100709	94784	91464	86481	196634	173136	177607
Acenaphthylene	68148	44436	50220	32968	37806	34447	35235	30793	74192	63049	68949
Acenaphthene	52228	31008	38107	22269	25923	23996	24264	21758	54296	47010	46332
Fluorene	36521	24595	27146	17692	19845	19195	19459	16783	41134	38111	36966
Phenanthrene	21620	18072	17800	12393	13825	12963	13161	11771	25367	28731	23678
Anthracene	25345	19690	20311	12473	15554	14567	14803	12225	29053	30616	27262
Fluoranthene	10712	15300	12343	11376	11655	10704	11186	10421	16954	16983	17677
Pyrene	10270	13818	11815	11122	11452	11328	10910	10188	16501	16686	17146
Benzo (a) anthracene	6272	5318	5270	3551	4764	3984	4636	3718	7833	7092	7380
Chrysene	7487	6870	6483	4162	5785	5183	5478	4455	9703	9435	9328
Benzo (k) fluoranthene	5791	3736	4554	2335	3849	2669	3697	2563	6456	6097	5761
Benzo (b) fluoranthene	7590	4519	5916	3063	5061	3867	4962	3352	8647	8577	8002
Benzo (a) pyrene	5318	3617	4283	2138	3315	2252	3353	2095	6004	5501	5535
Benzo (g,h,i) perylene	4763	2788	3342	1476	2782	1762	2596	1774	4854	4606	4384
Indeno (1,2,3-cd) pyrene	1932	943	1257	576	909	829	1404	675	2033	2044	2261
Dibenzo (a,h) anthracene	6586	5046	5204	2329	4141	2905	3766	3195	7012	7149	7630
Multiple responses	13.3	10.0	10.7	6.7	8.7	7.4	8.5	6.8	15.5	14.9	14.8

Table S4. Results for determination of PAHs (μg L^{-1}) in ten groundwater samples by the proposed method

Analyte	Samples										Guiding values / (μg L^{-1})	
	1	2	3	4	5	6	7	8	9	10	CONAMA[31]	MS[32]
Naphtalene	< 0.12	< 0.12	< 0.12	< 0.12	< 0.12	< 0.12	< 0.12	< 0.12	< 0.12	< 0.12	–	–
Acenaphtylene	< 0.16	< 0.16	< 0.16	< 0.16	< 0.16	< 0.16	< 0.16	< 0.16	< 0.16	< 0.16	–	–
Acenaphthene	< 0.18	< 0.18	< 0.18	< 0.18	< 0.18	< 0.18	< 0.18	< 0.18	< 0.18	< 0.18	–	–
Fluorene	< 0.16	< 0.16	< 0.16	< 0.16	< 0.16	< 0.16	< 0.16	< 0.16	< 0.16	< 0.16	–	–
Phenanthrene	< 0.04	< 0.04	< 0.04	< 0.04	< 0.04	< 0.04	< 0.04	< 0.04	< 0.04	< 0.04	–	–
Anthracene	< 0.07	< 0.07	< 0.07	< 0.07	< 0.07	< 0.07	< 0.07	< 0.07	< 0.07	< 0.07	–	–
Fluoranthene	< 0.06	< 0.06	< 0.06	< 0.06	< 0.06	< 0.06	0.21 ± 0.01	< 0.06	< 0.06	< 0.06	–	–
Pyrene	< 0.09	< 0.09	< 0.09	< 0.09	< 0.09	< 0.09	0.71 ± 0.01	< 0.09	0.15 ± 0.01	< 0.09	–	–
Benzo (a) anthracene	< 0.11	< 0.11	< 0.11	< 0.11	< 0.11	< 0.11	< 0.11	< 0.11	< 0.11	< 0.11	–	–
Chrysene	< 0.07	< 0.07	< 0.07	< 0.07	< 0.07	< 0.07	< 0.07	< 0.07	< 0.07	< 0.07	0.15	–
Benzo (k) fluoranthene	< 0.08	< 0.08	< 0.08	< 0.08	< 0.08	< 0.08	< 0.08	< 0.08	< 0.08	< 0.08	0.15	–
Benzo (b) fluoranthene	< 0.08	< 0.08	< 0.08	< 0.08	< 0.08	< 0.08	< 0.08	< 0.08	< 0.08	< 0.08	0.15	–
Benzo (a) pyrene	< 0.07	< 0.07	< 0.07	< 0.07	< 0.07	< 0.07	< 0.07	< 0.07	< 0.07	< 0.07	0.15	0.7
Benzo (g,h,i) perylene	< 0.08	< 0.08	< 0.08	< 0.08	< 0.08	< 0.08	< 0.08	< 0.08	< 0.08	< 0.08	0.15	–
Indeno (1,2,3-cd) pyrene	< 0.06	< 0.06	< 0.06	< 0.06	< 0.06	< 0.06	0.09 ± 0.01	< 0.06	< 0.06	< 0.06	0.15	–
Dibenzo (a,h) anthracene	< 0.11	< 0.11	< 0.11	< 0.11	< 0.11	< 0.11	0.12 ± 0.01	< 0.11	< 0.11	< 0.11	–	–

CONAMA: Conselho Nacional do Meio Ambiente; MS: Ministério da Saúde (Ministry of Health); results expressed as mean ± standard deviation.