Supplementary Materials for

TD-DFT Monitoring of the Absorption Spectra of Polycyclic Aromatic Hydrocarbons over the Basque Country, Spain

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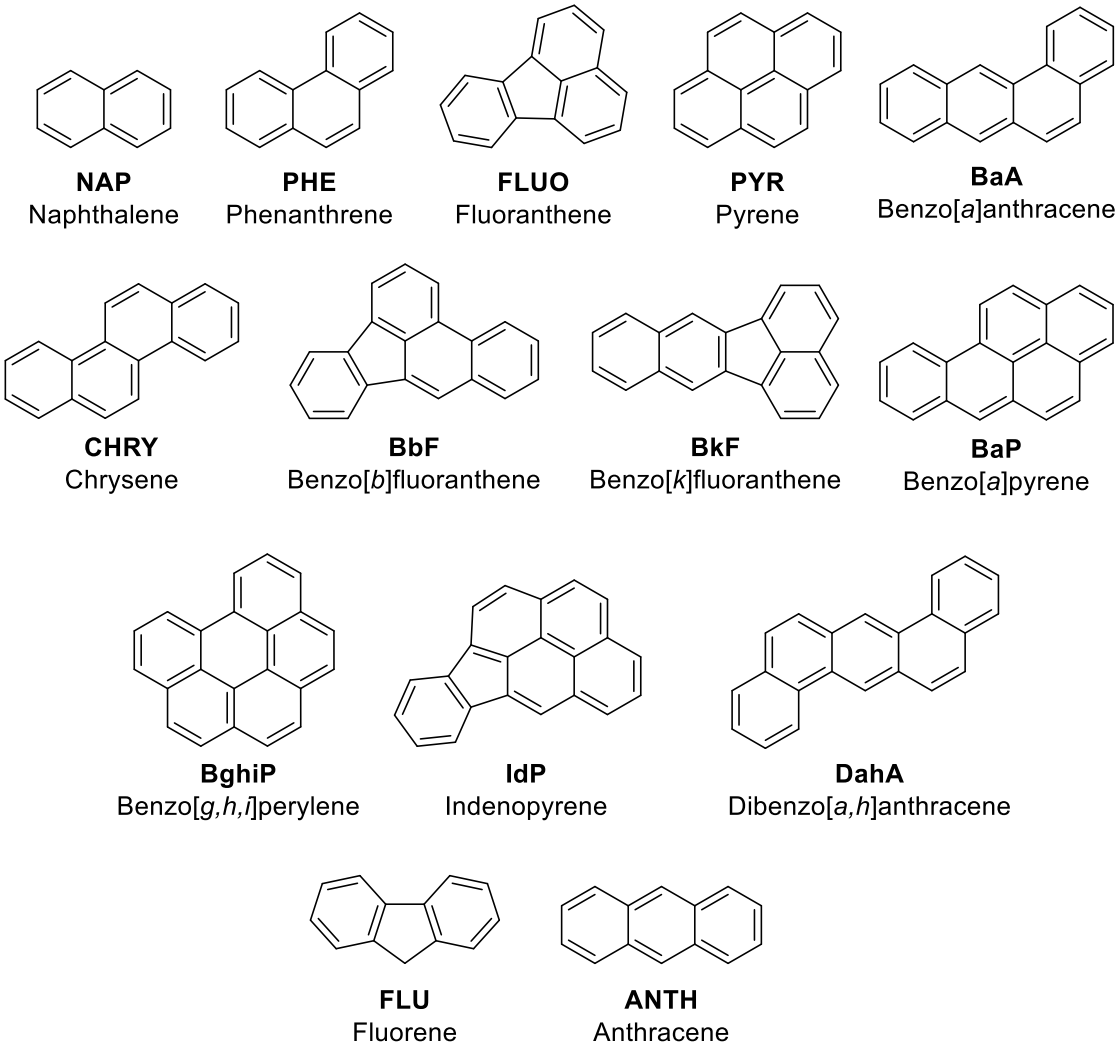

Figure S1. Chemical structures of the studied PAHs.

Figure S2. Map showing the location of the sampling sites.

Cartesian Coordinates:

ANTH (anthracene).

C	-2.21706	4.54539	0.
C	-3.46129	3.913	0.
C	-3.53424	2.52357	0.
C	-2.36307	1.76435	0.
C	-1.10325	2.38586	0.
C	-1.02924	3.79538	0.
C	0.23026	4.41765	0.
C	1.41768	3.6669	0.
C	1.34367	2.25738	0.
C	0.08416	1.63511	0.
C	2.67751	4.2884	0.
C	3.84867	3.52918	0.
C	3.77572	2.13975	0.
C	2.53148	1.50736	0.
H	-2.1806	5.63248	0.
H	-4.37191	4.50622	0.
H	-4.50198	2.02897	0.
H	-2.44065	0.67943	0.
H	0.28733	5.50449	0.
H	0.0271	0.54827	0.
H	2.75509	5.37332	0.
H	4.81641	4.02378	0.
H	4.68634	1.54652	0.
H	2.49502	0.42028	0.

Cartesian Coordinates:

BaA (benzo[*a*]anthracene).

C	-0.94337	3.44904	0.00172
C	-2.19643	2.85652	-0.01824
C	-2.29824	1.4686	-0.00998
C	-1.15133	0.65719	0.02124
C	0.14493	1.2346	0.04488
C	0.20561	2.65173	0.03184
C	1.29961	0.37021	0.08489
C	1.10908	-1.03311	0.10231
C	-0.18291	-1.56395	0.07175
C	-1.29676	-0.73133	0.03157
C	2.64349	0.8277	0.11313
C	2.20869	-1.90664	0.15408
C	3.52576	-1.43148	0.19104
C	3.74938	-0.04379	0.16692
C	5.07083	0.43569	0.2008
C	6.15166	-0.44617	0.26282
C	5.92685	-1.81854	0.2906
C	4.62147	-2.3091	0.25344
H	-0.85251	4.53208	-0.00458
H	-3.09319	3.46953	-0.03963
H	-3.28955	1.01985	-0.02572
H	1.16105	3.168	0.04778
H	-0.33943	-2.64063	0.08174
H	-2.28545	-1.18494	0.01142
H	2.84909	1.89461	0.09699
H	2.03623	-2.98163	0.17001
H	5.26784	1.50519	0.18105
H	7.16731	-0.06036	0.29071
H	6.7652	-2.50823	0.34137
H	4.46343	-3.385	0.27594

Cartesian Coordinates:

BaP (benzo[*a*]pyrene).

C	-0.6557	2.71807	1.12935
C	-1.88415	2.30101	0.60635
C	-2.04961	1.05128	-0.03578
C	-0.89831	0.22418	-0.129
C	0.35363	0.64534	0.40216
C	0.47105	1.90143	1.03468
C	1.70943	2.30786	1.55521
C	2.82716	1.4824	1.45395
C	2.71988	0.24113	0.83118
C	1.49399	-0.1889	0.30264
C	-0.98058	-1.03829	-0.75534
C	0.15686	-1.85185	-0.84572
C	1.37953	-1.43306	-0.3234
C	-3.29883	0.59064	-0.58512
C	-3.3506	-0.68078	-1.20772
C	-2.19951	-1.47066	-1.28317
C	-4.51092	1.32813	-0.55082
C	-5.7008	0.83805	-1.09865
C	-5.7212	-0.40946	-1.70154
C	-4.55243	-1.16293	-1.7549
H	-0.59411	3.69114	1.61163
H	-2.71941	2.98698	0.71513
H	1.81177	3.27375	2.04478
H	3.78175	1.80615	1.86019
H	3.60271	-0.39044	0.76097
H	0.10167	-2.8261	-1.32688
H	2.24163	-2.09016	-0.41129
H	-2.25304	-2.44602	-1.76442
H	-4.55188	2.31116	-0.09075
H	-6.60732	1.43569	-1.05093
H	-6.64122	-0.79765	-2.12956
H	-4.58671	-2.14045	-2.23212

Cartesian Coordinates:

BbF (benzo[*b*]fluoranthene).

C	0.06069	4.2435	0.
C	-1.02196	3.36479	0.
C	-0.82769	1.97495	0.
C	0.50531	1.44679	0.
C	1.57628	2.36589	0.
C	1.35718	3.74535	0.
C	-1.94753	1.11672	0.
C	-1.75204	-0.2506	0.
C	-0.46093	-0.75256	0.
C	0.69829	0.02427	0.
C	-2.67865	-1.3747	0.
C	-1.89377	-2.55921	0.
C	-0.49784	-2.14363	0.
C	0.68498	-2.85751	0.
C	1.88974	-2.14175	0.
C	1.90234	-0.72885	0.
C	-4.05989	-1.433	0.
C	-4.65995	-2.69633	0.
C	-3.88184	-3.87004	0.
C	-2.48475	-3.80893	0.
H	-0.1107	5.31675	0.
H	-2.02789	3.77988	0.
H	2.60513	2.01613	0.
H	2.20278	4.42834	0.
H	-2.95585	1.5194	0.
H	0.68897	-3.94198	0.
H	2.83397	-2.68231	0.
H	2.86481	-0.22447	0.
H	-4.66475	-0.53343	0.
H	-5.74497	-2.77539	0.
H	-4.37683	-4.83879	0.
H	-1.8909	-4.71583	0.

Cartesian Coordinates:

BkF (benzo[*k*]fluoranthene).

C	-1.44367	5.43667	0.
C	-0.05387	5.51011	0.
C	0.70788	4.34098	0.
C	0.09079	3.08143	0.
C	-1.33559	3.00396	0.
C	-2.07994	4.19356	0.
C	-1.97909	1.75207	0.
C	-1.2011	0.60909	0.
C	0.21676	0.68947	0.
C	0.86574	1.90946	0.
C	-1.54854	-0.80686	0.
C	-0.36538	-1.53233	0.
C	0.72481	-0.67508	0.
C	-2.75278	-1.4869	0.
C	-2.72833	-2.89426	0.
C	-1.51088	-3.61059	0.
C	-0.282	-2.92263	0.
C	1.02033	-3.4603	0.
C	2.14464	-2.60554	0.
C	2.00153	-1.20638	0.
H	-2.03516	6.34864	0.
H	0.44007	6.47838	0.
H	1.79269	4.42266	0.
H	-3.16732	4.1627	0.
H	-3.06155	1.67887	0.
H	1.94964	1.95351	0.
H	-3.69869	-0.95608	0.
H	-3.66734	-3.44421	0.
H	-1.52826	-4.69741	0.
H	1.16683	-4.53728	0.
H	3.14257	-3.03922	0.
H	2.8767	-0.56563	0.

Cartesian Coordinates:

BzP (benzo[*g*,*h*,*i*]perylene).

C	-0.42979	6.94421	-0.65787
C	-1.73097	6.48992	-0.30973
C	-1.98173	5.12183	-0.17874
C	-0.96456	4.2025	-0.38775
C	0.30861	4.64507	-0.74805
C	0.619	6.01895	-0.90327
C	-2.76071	7.41283	-0.09467
C	-2.52132	8.78083	-0.19745
C	-1.24519	9.25557	-0.51285
C	-0.19373	8.33588	-0.75314
C	1.91575	6.50682	-1.28402
C	2.14202	7.90622	-1.35457
C	1.09238	8.81626	-1.08314
C	-0.9976	10.63005	-0.59031
C	0.27625	11.10402	-0.89659
C	1.32473	10.2123	-1.14805
C	3.42159	8.41822	-1.70278
C	3.63582	9.80018	-1.74463
C	2.59956	10.68843	-1.46699
C	4.46546	7.54076	-2.00766
C	4.25897	6.17004	-1.96913
C	3.00933	5.66529	-1.60813
H	-2.97022	4.76091	0.0957
H	-1.15784	3.13936	-0.27163
H	1.066	3.8805	-0.89537
H	-3.76289	7.07458	0.15957
H	-3.3424	9.47236	-0.02206
H	-1.79456	11.34752	-0.40748
H	0.43964	12.17827	-0.943
H	4.61471	10.20129	-1.99834
H	2.79789	11.75686	-1.51004
H	5.44648	7.91857	-2.2861
H	5.06825	5.48923	-2.21985
H	2.90528	4.58429	-1.5984

Cartesian Coordinates:

CHR (chrysene).

C	-1.99357	2.52431	-0.0179
C	-3.22791	1.86583	-0.02941
C	-3.2716	0.48142	-0.0241
C	-2.08158	-0.23882	-0.00392
C	-0.83718	0.41568	0.01403
C	-0.75491	1.82807	0.00376
C	0.54561	2.46116	0.02111
C	1.73496	1.67723	0.07722
C	1.57913	0.27563	0.08085
C	0.32941	-0.34102	0.04484
C	0.70302	3.86217	-0.01658
C	1.95353	4.4782	0.00675
C	3.1185	3.72202	0.08328
C	3.03443	2.31042	0.12594
C	4.36292	4.37588	0.12038
C	5.55002	3.65622	0.21209
C	5.50358	2.273	0.26674
C	4.26992	1.61488	0.22202
H	-2.02338	3.60984	-0.01882
H	-4.14977	2.44138	-0.04084
H	-4.22554	-0.0382	-0.03306
H	-2.13202	-1.32585	0.00175
H	2.44078	-0.38492	0.1062
H	0.28595	-1.42817	0.04694
H	-0.15753	4.52239	-0.07161
H	1.99859	5.56471	-0.02941
H	4.41546	5.46213	0.08142
H	6.50367	4.17545	0.2441
H	6.42253	1.6981	0.34564
H	4.29709	0.53051	0.27341

Cartesian Coordinates:

DahA (dibenzo[*a*,*h*]anthracene).

C	0.232	7.10594	0.31711
C	-1.0548	6.50923	0.3871
C	-1.09268	5.09368	0.28923
C	0.06622	4.32116	0.1339
C	1.30729	4.93617	0.06817
C	1.38728	6.32144	0.15846
C	-2.21716	7.35894	0.55319
C	-2.03833	8.75454	0.65096
C	-0.75451	9.30174	0.57468
C	0.36295	8.49093	0.40817
C	-3.55925	6.90372	0.62913
C	-4.66722	7.76828	0.80059
C	-4.47759	9.1618	0.91217
C	-3.141	9.61443	0.82718
C	-5.96533	7.24683	0.86241
C	-7.07022	8.07958	1.03733
C	-6.91518	9.46207	1.16083
C	-5.61803	10.0304	1.10115
C	-8.04824	10.27644	1.34492
C	-7.93015	11.65747	1.47636
C	-6.67454	12.24135	1.42342
C	-5.54133	11.44169	1.23833
H	-6.56908	13.31838	1.52627
H	-4.58326	11.95253	1.20647
H	-8.81503	12.27172	1.62023
H	-9.04209	9.83499	1.38965
H	-8.0608	7.63081	1.07911
H	-6.13484	6.17579	0.77426
H	-3.76054	5.83765	0.55282
H	-2.93664	10.67939	0.89961
H	-0.60667	10.37718	0.64482
H	1.34303	8.96012	0.35366
H	2.36837	6.79015	0.10589
H	2.21093	4.34438	-0.05164
H	-0.00516	3.23856	0.06563
H	-2.03771	4.55986	0.33629

Cartesian Coordinates:

FLU (fluorene).

C	-0.10355	5.70967	-0.00793
C	-1.2921	4.76983	-0.00494
C	-0.85448	3.4272	-0.00165
C	0.59339	3.41014	-0.00176
C	1.06252	4.74208	-0.00513
C	-2.63882	5.09313	-0.00494
C	-3.56321	4.0467	-0.00159
C	-3.1346	2.70812	0.00152
C	-1.77232	2.39043	0.00149
C	2.41648	5.03356	-0.00536
C	3.31596	3.96565	-0.00213
C	2.85593	2.63754	0.00108
C	1.48655	2.35204	0.00126
H	-0.0962	6.32685	0.89516
H	-0.09642	6.32127	-0.91483
H	-2.96996	6.1261	-0.00729
H	-4.62803	4.26803	-0.00132
H	-3.87265	1.90938	0.00411
H	-1.45189	1.35439	0.00403
H	2.77187	6.05844	-0.00779
H	4.3857	4.16182	-0.00204
H	3.57496	1.82163	0.00358
H	1.1418	1.32383	0.00388

Cartesian Coordinates:

FLUO (fluoranthene).

C	-0.71519	4.15134	0.08114
C	-1.85666	3.34713	0.00205
C	-1.75329	1.94768	-0.12091
C	0.62182	2.11324	-0.09937
C	0.51713	3.52723	0.03454
C	-0.50578	1.31753	-0.17469
C	1.87455	4.05114	0.10651
C	2.74877	2.97756	0.01095
C	2.0423	1.79014	-0.11952
C	2.38827	5.32706	0.25074
C	3.78538	5.48583	0.29646
C	4.65629	4.37844	0.19499
C	4.13728	3.07729	0.04521
C	2.7395	0.60145	-0.23644
C	4.14558	0.64401	-0.21339
C	4.84344	1.86391	-0.07206
H	-0.80109	5.22755	0.17817
H	-2.84136	3.80815	0.03888
H	-2.65979	1.3485	-0.17365
H	-0.43282	0.24	-0.26771
H	1.73546	6.18953	0.33123
H	4.20515	6.48282	0.41408
H	5.73079	4.53665	0.23537
H	2.22136	-0.34531	-0.34457
H	4.70872	-0.28253	-0.30528
H	5.93013	1.86046	-0.05482

Cartesian Coordinates:

IdP (indeno[1,2,3-*cd*]pyrene).

C	-2.92899	3.44313	0.
C	-4.22888	2.88761	0.
C	-4.36319	1.51003	0.
C	-3.22128	0.72928	0.
C	-1.92976	1.23413	0.
C	-1.76229	2.62635	0.
C	-0.44259	3.10316	0.
C	0.64227	2.20774	0.
C	0.44255	0.80997	0.
C	-0.87304	0.31049	0.
C	-3.53564	-0.61852	0.
C	-2.50312	-1.54536	0.
C	-1.15577	-1.08928	0.
C	-0.06694	-1.97173	0.
C	1.24603	-1.48736	0.
C	1.49937	-0.11164	0.
C	-5.5061	0.608	0.
C	-4.99027	-0.72337	0.
C	-6.86645	0.85004	0.
C	-7.72339	-0.25452	0.
C	-7.21606	-1.56914	0.
C	-5.83821	-1.81436	0.
H	-2.82386	4.52647	0.
H	-5.09924	3.53516	0.
H	-0.24748	4.17279	0.
H	1.65265	2.61179	0.
H	-2.72433	-2.6082	0.
H	-0.23068	-3.047	0.
H	2.07848	-2.18718	0.
H	2.53003	0.23575	0.
H	-7.26168	1.85943	0.
H	-8.8	-0.09757	0.
H	-7.91027	-2.40693	0.
H	-5.45669	-2.82897	0.

Cartesian Coordinates:

NAP (naphthalene).

C	-6.29569	2.50665	0.2303
C	-7.28722	1.53441	0.0884
C	-6.93536	0.19173	-0.0144
C	-5.59098	-0.18212	0.02307
C	-4.58099	0.78343	0.16445
C	-4.93859	2.1475	0.27065
C	-3.22377	0.42447	0.2027
C	-2.23227	1.39669	0.34492
C	-2.58431	2.73905	0.45116
C	-3.92871	3.11286	0.41411
H	-6.59013	3.55063	0.3093
H	-8.33352	1.82676	0.05848
H	-7.70649	-0.5662	-0.12404
H	-5.33562	-1.2361	-0.05892
H	-2.92921	-0.61929	0.12137
H	-1.18585	1.10453	0.37275
H	-1.81329	3.4968	0.5628
H	-4.1842	4.16663	0.49844

Cartesian Coordinates:

PHE (phenanthrene).

C	-5.0144	4.27682	0.
C	-3.62266	4.2513	0.
C	-2.92819	3.03899	0.
C	-3.64271	1.81315	0.
C	-5.08376	1.83958	0.
C	-5.75285	3.0908	0.
C	-7.15703	3.15141	0.
C	-7.92684	1.99148	0.
C	-7.29956	0.7553	0.
C	-5.90317	0.68199	0.
C	-1.52273	3.04807	0.
C	-0.79598	1.86068	0.
C	-1.46817	0.64835	0.
C	-2.8663	0.62629	0.
H	-5.51739	5.24154	0.
H	-3.08463	5.19692	0.
H	-7.66613	4.11316	0.
H	-9.01136	2.05585	0.
H	-7.89059	-0.15677	0.
H	-5.46281	-0.31084	0.
H	-0.9787	3.99051	0.
H	0.29017	1.88525	0.
H	-0.91098	-0.28478	0.
H	-3.34278	-0.34972	0.

Cartesian Coordinates:

PYR (pyrene).

C	-0.73313	3.88562	0.
C	-1.80729	2.99194	0.
C	-1.58808	1.60773	0.
C	-0.26125	1.11829	0.
C	0.82805	2.02458	0.
C	0.58811	3.4183	0.
C	1.67695	4.3026	0.
C	2.98493	3.81907	0.
C	3.22248	2.44496	0.
C	2.15488	1.53513	0.
C	-0.02131	-0.27543	0.
C	1.29993	-0.74276	0.
C	2.37409	0.15093	0.
C	-2.65568	0.6979	0.
C	-2.41813	-0.6762	0.
C	-1.11015	-1.15973	0.
H	-0.93913	4.95365	0.
H	-2.82002	3.38877	0.
H	1.51318	5.37786	0.
H	3.82046	4.51423	0.
H	4.25002	2.08834	0.
H	1.50593	-1.81078	0.
H	3.38683	-0.2459	0.
H	-3.68322	1.05453	0.
H	-3.25366	-1.37136	0.
H	-0.94638	-2.23499	0.

Table S1 – Experimental mean concentration (in ng m^{-3}) of individual PAHs over Azpeitia, Urretxu, and Bilbao. [1,2]

PAHs	Azpeitia	Urretxu	Bilbao
BaA	0.05	0.05	0.22
BaP	0.05	0.05	0.22
BbF	0.14	0.13	0.69
BkF	0.05	0.05	0.23
BghiP	0.19	0.12	0.27
CHR	0.05	0.05	0.30
FLUO	0.05	0.05	0.34
IdP	0.05	0.05	0.24
NAP	0.05	0.05	n.d.
PHE	0.11	0.05	0.22
PYR	0.05	0.05	0.35
DahA	n.d.	n.d.	0.10
ANTH	n.d.	n.d.	0.06
FLU	n.d.	n.d.	0.09

Table S2 – Relative contribution (in %) of individual PAHs to the absorption intensity at ~380 nm, over Azpeitia, Urretxu, and Bilbao using BP86/6-31+G(d,p). Only the most relevant contributions are presented.

PAHs	Azpeitia	Urretxu	Bilbao
BbF	59	58	51
FLUO	16	17	21
IdP	11	10	7
PYR	7	8	14

Table S3 – Relative contribution (in %) of individual PAHs to the absorption intensity at ~425 nm, over Azpeitia, Urretxu, and Bilbao using BP86/6-31+G(d,p). Only the most relevant contributions are presented.

PAHs	Azpeitia	Urretxu	Bilbao
BaP	16	21	23
BkF	12	15	17
BghiP	60	49	30
IdP	8	10	16

Table S4 – Relative contribution (in %) of individual PAHs to the absorption intensity at ~345 nm, over Azpeitia, Urretxu, and Bilbao using PBE0/6-31G(d,p). Only the most relevant contributions are presented.

PAHs	Azpeitia	Urretxu	Bilbao
BbF	41	39	31
PYR	26	27	32
CHRY	16	16	15
FLUO	13	14	17

Table S5 – Relative contribution (in %) of individual PAHs to the absorption intensity at ~400 nm, over Azpeitia, Urretxu, and Bilbao using PBE0/6-31G(d,p). Only the most relevant contributions are presented.

PAHs	Azpeitia	Urretxu	Bilbao
BghiP	50	40	22
BbF	23	27	37
BkF	12	15	19
BaP	9	11	11

Table S6 – Relative contribution (in %) of individual PAHs to the absorption intensity at ~360 nm, over Azpeitia, Urretxu, and Bilbao using B3LYP/6-31+G(d,p). Only the most relevant contributions are presented.

PAHs	Azpeitia	Urretxu	Bilbao
BbF	49	47	42
PYR	23	24	28
FLUO	13	13	15
CHRY	10	10	10

Table S7 – Relative contribution (in %) of individual PAHs to the absorption intensity at ~410 nm, over Azpeitia, Urretxu, and Bilbao using B3LYP/6-31+G(d,p). Only the most relevant contributions are presented.

PAHs	Azpeitia	Urretxu	Bilbao
BghiP	64	53	34
BkF	15	20	27
BaP	15	19	23
BaA	4	6	7

Table S8 – Relative contribution (in %) of individual PAHs to the absorption intensity at ~325 nm, over Azpeitia, Urretxu, and Bilbao using wB97XD/6-31+G(d,p). Only the most relevant contributions are presented.

PAHs	Azpeitia	Urretxu	Bilbao
BbF	53	51	44
PYR	18	19	23
FLUO	14	14	16
CHRY	8	8	8

Table S9 – Relative contribution (in %) of individual PAHs to the absorption intensity at ~365 nm, over Azpeitia and Urretxu, and ~382 nm over Bilbao using wB97XD/6-31+G(d,p). Only the most relevant contributions are presented.

PAHs	Azpeitia	Urretxu	Bilbao
BghiP	75	65	21
BaP	9	11	53
BkF	8	12	1
BaA	6	8	2
IdP	3	4	19

Table S10 – Scope of the selected datasets.

Reference	Oleagoitia et al. [2]	Elorduy et al. [1]
PM fraction	PM2.5 (Fine fraction)	PM10 (Coarse fraction)
Available data (PAHs above DL)	BaA, BaP, BbF, BghiP, BkF, CHRY, FLUO, IcdP, NAP, PHEN, PYR (Median values)	ANTH, BaA, BaP, BbF, BghiP, BkF, CHRY, DahA, FLUO, FLU, IcdP, PHEN, PYR (Mean values)
Selected techniques	UHPLC + Fluorescence Detector	TD-GC/MS
Sampling Sites	Azpeitia (Azp) Urretxu (Urr)	Bilbao (Bil)
Type of Sampling Sites	Urban industrial	Urban
Sampling Period	Oct. 2011 – Oct. 2012	Jul. 2013, Sep. 2013 – Dec. 2013

Table S11 – Summary of the experimental datasets in which this is study was based. Results are presented in ng/m^3.

	Urretxu [2]	***Azpeitia*** [2]	***Bilbao*** [1]
ANTH	-	-	0.06
BaA	0.05	0.05	0.22
BaP	0.05	0.05	0.22
BbF	0.13	0.14	0.69
BkF	0.05	0.05	0.23
BghiP	0.12	0.19	0.27
CHRY	0.05	0.05	0.3
DahA	-	-	0.1
FLU	-	-	0.09
FLUO	0.05	0.05	0.34
IcdP	0.05	0.05	0.24
NAP	0.05	0.05	-
PHEN	0.05	0.11	0.22
PYR	0.05	0.05	0.35

References

[1] I. Elorduy, S. Elcoroaristizabal, N. Durana, J.A. Garcia, L. Alonso, Diurnal variation of particle-bound PAHs in an urban area of Spain using TD-GC/MS: Influence of meteorological parameters and emission sources, Atmospheric Environment 138 (2016) 87-98.

[2] M.B.Z. Oleagoitia, A.L. Manterola, J.I. Maurolagoitia, M.D.M.L. de Dicastillo, J. Alvarez, M.A. Barandiaran, A.I. Loibide, L. Santa-Marina, Polycyclic aromatic hydrocarbons (PAHs) in air associated with particles $PM_{2.5}$ in the Basque Country (Spain), Air Quality Atmosphere and Health 12(1) (2019) 107-114.