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Supplement of

Polycyclic aromatic hydrocarbons (PAHs) and their alkylated, nitrated and oxygenated derivatives in the atmosphere over the Mediterranean and Middle East seas

Marco Wietzoreck et al.

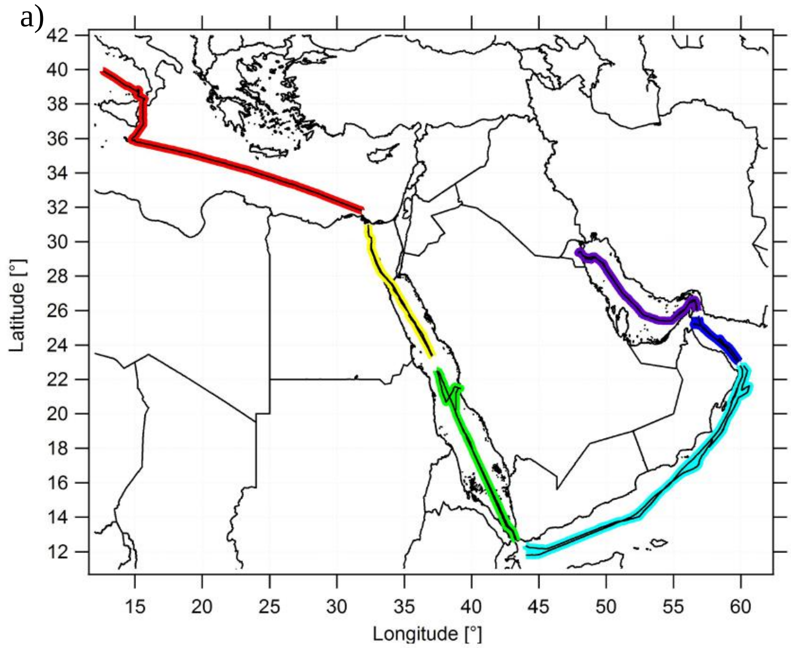
Correspondence to: Gerhard Lammel (g.lammel@mpic.de)

Content

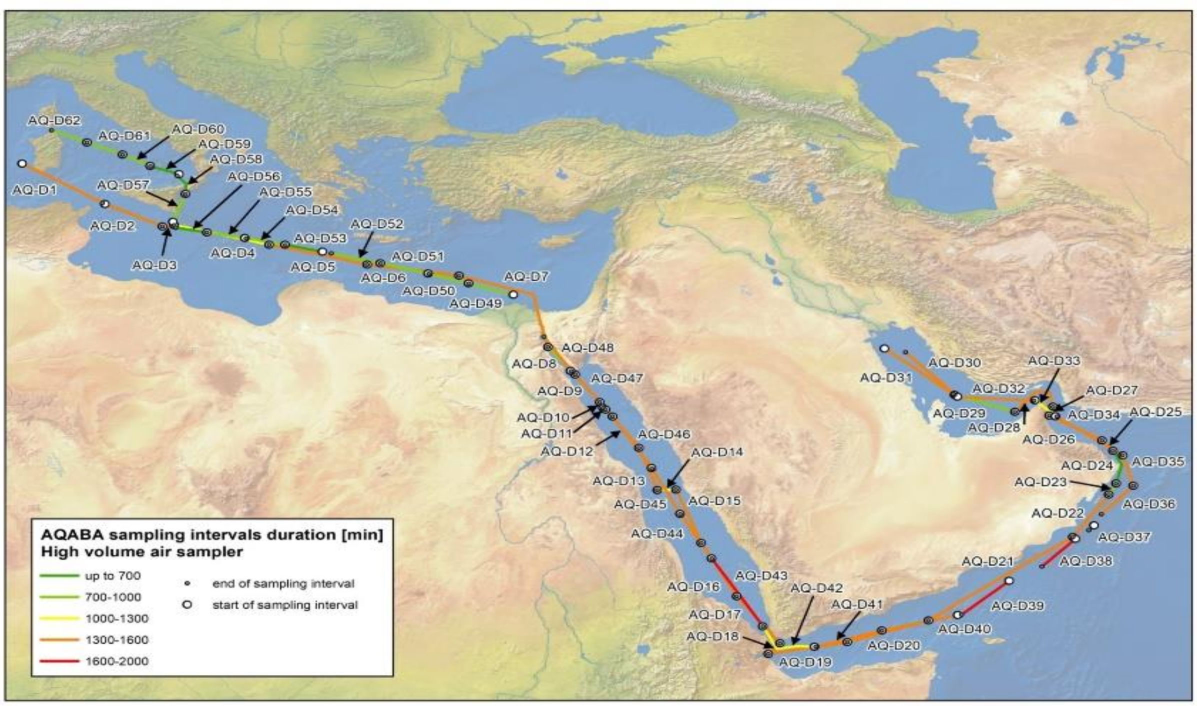
1 Methods

1.1 Sampling

a)



b)



c)

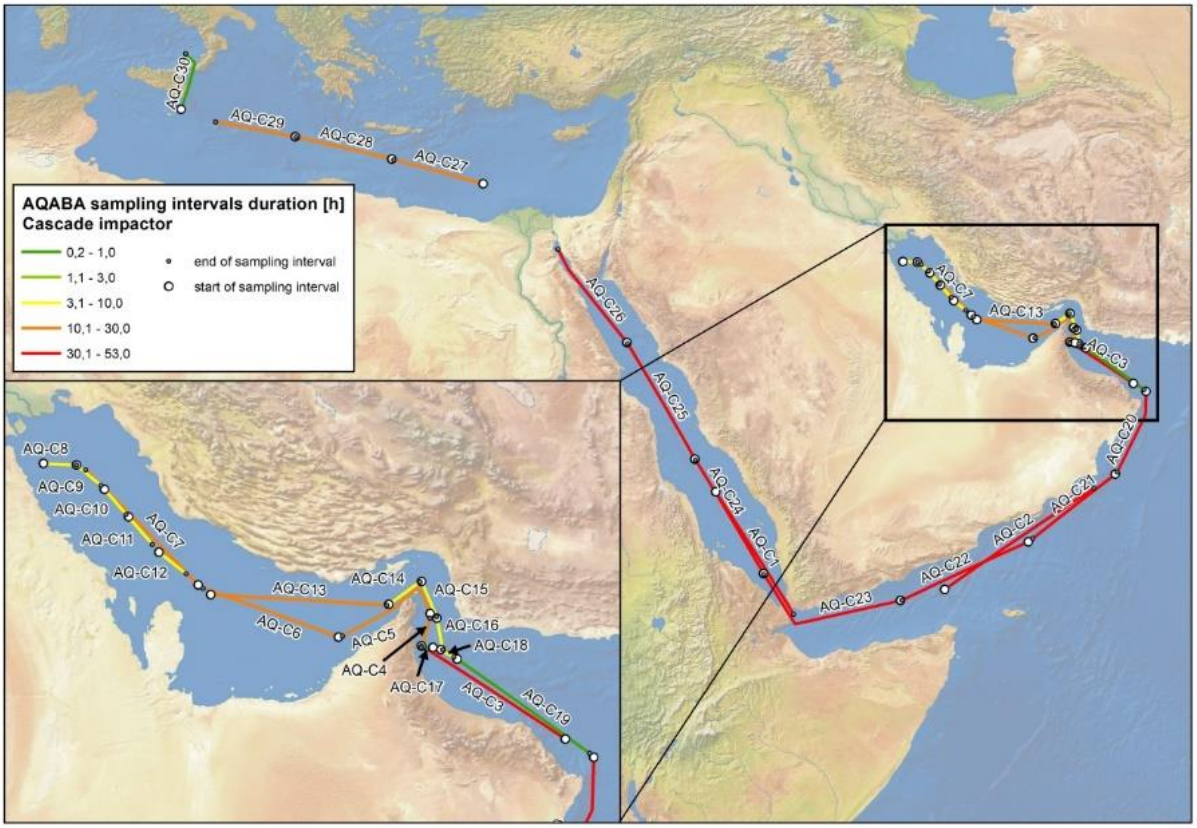


Figure S1. Overview of samples and sampling regions: (a) The ship cruise during both legs divided into six regions i.e. Mediterranean Sea (red), northern Red Sea (yellow), southern Red Sea (green), Arabian Sea (turquoise blue), Oman Gulf (blue) and Arabian Gulf (purple), taken from Tadic et al. (2020); (b) Digitel high volume air samples and (c) cascade impactor samples.

Table S1. Information about a) Digitel high-volume air samples, b) cascade impactor air samples and c) GMWL high volume air samples (MS: Mediterranean Sea; NRS: Northern Red Sea; SRS: Southern Red Sea; AS: Arabian Sea; OG: Gulf of Oman; AG: Arabian Gulf).

a)

Sample	Leg	Date (from)	Time (from) [CEST]	Date (to)	Time (to) [CEST]	GPS (from) N	E	GPS (to) N	E	Measured volume V_M [m³]	Sampling time [min]	Sampling distance [km]	Location
D1	1.	25.6.	20:00	26.6.	20:00	39.4110	7.8441	37.1900	11.6460	784	1440	436	MS
D2		26.6.	20:03	27.6.	20:03	37.1443	11.7618	35.8793	14.5000	795	1440	295	
D3		27.6.	20:05	28.6.	20:05	35.8793	14.5000	35.9497	15.0443	794	1440	52	
D4		28.6.	23:02	29.6.	20:04	35.9497	15.0443	34.8415	19.5523	695	1260	445	
D5		29.6.	20:06	30.6.	20:06	34.8415	19.5523	33.7255	24.1933	791	1440	458	
D6		30.6.	20:08	1.7.	20:08	33.7255	24.1933	33.1043	28.5567	812	1440	420	
D7		1.7.	20:10	2.7.	20:10	33.1043	28.5567	29.0867	32.7673	817	1440	596	
D8		4.7.	6:57	4.7.	18:57	29.0867	32.7673	27.5277	34.0502	402	720	210	NRS
D9		4.7.	18:59	5.7.	18:59	27.5277	34.0502	25.9717	35.2202	801	1440	204	
D10		5.7.	19:23	6.7.	18:53	25.9717	35.2202	25.6453	35.3770	784	1409	39	
D11		6.7.	18:55	7.7.	18:55	25.6453	35.3770	25.5470	35.4954	790	1440	16	
D12		7.7.	18:58	8.7.	18:58	25.5470	35.4954	23.3869	37.0715	794	1440	281	
D13		8.7.	19:00	9.7.	19:00	23.3869	37.0715	21.0164	37.9455	794	1440	274	
D14		9.7.	19:05	10.7.	12:05	21.0164	37.9455	21.0367	38.8356	568	1020	85	
D15		13.7.	18:39	14.7.	18:09	21.0367	38.8356	18.0332	40.0246	779	1410	349	SRS
D16		14.7.	18:13	15.7.	18:13	18.0332	40.0246	15.0308	41.7014	808	1440	367	
D17		15.7.	18:15	16.7.	18:15	15.0308	41.7014	12.3720	43.7483	803	1440	351	
D18		16.7.	18:18	17.7.	17:18	12.3720	43.7483	11.7775	43.2027	774	1380	83	AS
D19		17.7.	17:20	18.7.	17:20	11.7775	43.2027	12.4396	46.9400	796	1440	362	
D20		18.7.	17:22	19.7.	17:22	12.4396	46.9400	13.6648	50.7978	797	1440	390	

Sample	Leg	Date (from)	Time (from) [CEST]	Date (to)	Time (to) [CEST]	GPS (from) N	E	GPS (to) N	E	Measured volume V_M [m³]	Sampling time [min]	Sampling distance [km]	Loca-tion
D21		19.7.	17:26	20.7.	16:57	13.6648	50.7978	18.3700	57.6239	775	1410	830	
D22		21.7.	16:46	22.7.	16:46	18.3700	57.6239	20.7557	59.3353	809	1440	309	
D23		22.7.	16:57	23.7.	5:33	20.7557	59.3353	21.3861	59.6827	415	756	77	
D24		23.7.	5:37	23.7.	15:42	21.3861	59.6827	23.2304	59.5282	332	607	203	OG
D25		24.7.	16:10	25.7.	16:10	23.2304	59.5282	23.8155	59.0073	799	1440	81	
D26		25.7.	16:18	26.7.	16:18	23.8155	59.0073	25.2141	56.5100	805	1440	283	
D27		26.7.	16:32	27.7.	16:50	25.2141	56.5100	25.7168	56.6810	787	1413	58	
D28		27.7.	16:52	28.7.	16:52	25.7168	56.6810	25.4281	54.8918	817	1440	173	OG+AG
D29		28.7.	16:54	29.7.	17:01	25.4281	54.8918	26.3865	52.0304	499	864	292	AG
D30		29.7.	17:23	30.7.	17:23	26.3865	52.0304	28.7900	49.7010	825	1440	345	
D31		3.8.	17:10	4.8.	17:10	28.9927	48.6996	26.4322	51.9517	812	1441	418	
D32		4.8.	17:21	5.8.	17:20	26.2731	52.1573	26.0567	55.7913	807	1440	346	
D33		5.8.	17:40	6.8.	17:40	26.0756	55.8329	25.1666	56.8767	644	1155	141	AG+OG
D34		6.8.	17:42	7.8.	17:10	25.1700	56.8000	22.9889	59.9747	779	1408	385	OG
D35		7.8.	17:12	8.8.	16:12	22.9634	60.0008	21.2597	60.4880	742	1380	193	OG+AS
D36		8.8.	16:13	9.8.	16:13	21.2587	60.4874	19.6600	58.9770	789	1440	227	AS
D37		10.8.	10:08	10.8.	19:10	19.0221	58.6283	18.7540	58.3900	287	542	37	
D38	2.	11.8.	10:57	12.8.	20:01	18.2657	57.7522	16.7120	56.1640	1095	1984	228	
D39		13.8.	9:15	14.8.	15:55	15.8960	54.6114	14.0040	52.3650	1002	1840	298	
D40		14.8.	16:58	15.8.	16:58	13.9619	52.1715	13.0980	48.5870	793	1440	354	
D41		15.8.	16:59	16.8.	14:59	13.0980	48.5870	12.1754	45.4446	729	1321	315	
D42		16.8.	15:01	17.8.	8:26	12.1785	45.3979	13.3355	42.9452	577	1046	265	AS+SRS
D43		17.8.	8:59	18.8.	15:59	13.3344	42.9399	17.1423	40.5228	1036	1860	478	SRS
D44		18.8.	16:07	19.8.	16:47	17.1647	40.5099	19.6559	39.0315	822	1480	308	
D45		19.8.	16:51	20.8.	17:11	19.6672	39.0248	22.2321	37.6864	805	1460	309	SRS+NRS

Sample	Leg	Date (from)	Time (from) [CEST]	Date (to)	Time (to) [CEST]	GPS (from) N	E	GPS (to) N	E	Measured volume V_M [m³]	Sampling time [min]	Sampling distance [km]	Loca-tion
D46		20.8.	17:19	21.8.	17:39	22.2577	37.6721	25.1606	35.8253	807	1460	364	NRS
D47		21.8.	17:45	22.8.	17:45	25.1640	35.8230	27.7194	33.8617	788	1440	337	
D48		22.8.	17:49	23.8.	17:49	27.7194	33.8402	29.6664	32.5684	766	1390	246	
D49		25.8.	6:16	25.8.	17:56	32.0212	31.1175	32.6587	29.0216	382	700	211	MS
D50		25.8.	18:00	26.8.	5:49	32.6676	28.9995	33.2112	27.1166	387	710	189	
D51		26.8.	6:04	26.8.	17:54	33.2220	27.0848	33.7990	24.8300	388	710	223	
D52		26.8.	17:55	27.8.	5:58	33.7990	24.8260	34.3590	22.5030	390	720	229	
D53		27.8.	6:08	27.8.	18:08	34.4510	22.0770	34.8360	20.3220	327	600	172	
D54		27.8.	18:10	28.8.	5:50	34.8380	20.3110	35.2140	18.4550	380	700	181	
D55		28.8.	6:05	28.8.	18:05	35.2220	18.4070	35.5460	16.6030	395	720	175	
D56		28.8.	18:07	29.8.	5:07	35.5470	16.6000	35.7990	15.1150	364	660	144	
D57		29.8.	18:26	30.8.	6:26	36.1310	14.9850	37.6930	15.5790	393	720	181	
D58		30.8.	6:30	30.8.	17:48	37.7020	15.5790	38.7350	15.1990	370	679	119	
D59		30.8.	20:26	31.8.	6:27	38.8210	15.2770	39.2720	13.9380	327	600	137	
D60		31.8.	6:41	31.8.	18:41	39.2870	13.9100	39.9290	12.6160	391	720	142	
D61		31.8.	18:42	1.9.	6:42	39.9290	12.6160	40.6140	10.9285	393	720	177	
D62		1.9.	6:47	1.9.	18:47	40.6140	10.9285	41.2990	9.2410	397	720	177	

b)

Sample	Leg	Date (from)	Time (from) [CEST]	Date (to)	Time (to) [CEST]	GPS (from) N	E	GPS (to) N	E	Measured volume V_M [m³]	Sampling time [min]	Sampling distance [km]	Loca-tion
C1	1.	14.7.	16:57	16.7.	16:57	18.195	39.955	12.457	43.594	3265	720	2880	SRS
C2		19.7.	16:43	21.7.	16:43	13.618	50.646	18.364	57.617	3264	843	2880	AS
C3		24.7.	16:33	26.7.	16:33	23.2817	59.477	25.214	56.51	3265	353	2880	OG
C4		26.7.	17:24	27.7.	17:24	25.2140	56.5100	25.788	56.683	1634	65	1440	
C5		27.7.	18:07	28.7.	17:07	25.8859	56.6830	25.414	54.875	1565	179	1380	OG+AG
C6		28.7.	17:42	29.7.	17:42	25.3974	54.7936	26.411	51.995	1633	288	1440	AG
C7		29.7.	18:25	30.7.	18:25	26.4764	51.8983	28.861	49.571	1633	343	1440	
C8	2.	3.8.	17:15	3.8.	21:15	28.9927	48.6996	28.9646	49.3836	272	65	240	
C9		3.8.	21:35	4.8.	01:35	28.9646	49.3836	28.5397	49.8889	272	67	240	
C10		4.8.	01:50	4.8.	05:50	28.4588	49.9619	27.9373	50.4113	274	72	240	
C11		4.8.	06:21	4.8.	10:21	27.8865	50.456	27.3166	50.9476	272	78	240	
C12		4.8.	10:50	4.8.	14:50	27.1521	51.0884	26.7096	51.6455	272	72	240	
C13		4.8.	17:20	5.8.	17:20	26.2731	52.1573	26.0567	55.7913	1639	346	1440	
C14		5.8.	18:00	5.8.	22:00	26.0756	55.8329	26.5434	56.473	272	80	240	
C15		5.8.	22:55	6.8.	02:55	26.5498	56.5062	25.821	56.8161	280	85	240	OG
C16		6.8.	03:20	6.8.	07:20	25.7857	56.826	25.1382	56.9413	273	72	240	
C17		6.8.	07:40	6.8.	11:38	25.1349	56.9046	25.174	56.4922	272	39	240	
C18		6.8.	16:20	6.8.	20:20	25.1797	56.7423	24.9866	57.1796	273	47	240	
C19		6.8.	21:15	7.8.	17:17	24.942	57.2383	22.9889	59.9747	1369	337	1202	
C20		7.8.	17:40	9.8.	19:44	22.906	60.0624	19.1271	58.7116	3264	435	3004	AS
C21		10.8.	10:20	13.8.	07:27	19.0221	58.6283	16.006	54.765	3264	495	4147	
C22		13.8.	09:35	15.8.	15:35	15.852	54.5538	13.1192	48.6622	3604	635	3240	
C23		15.8.	16:50	17.8.	16:50	13.101	48.598	14.324	42.2126	3265	621	2880	AS+SRS
C24		17.8.	17:13	19.8.	17:13	14.3559	42.1942	19.6937	39.0091	3265	661	2880	SRS
C25		19.8.	17:33	21.8.	17:33	19.7215	38.9907	25.152	35.832	3264	668	2880	NRS

Sample	Leg	Date (from)	Time (from) [CEST]	Date (to)	Time (to) [CEST]	GPS (from) N	E	GPS (to) N	E	Measured volume V_M [m³]	Sampling time [min]	Sampling distance [km]	Loca-tion
C26		21.8.	17:57	23.8.	15:57	25.19	35.805	29.569	32.587	3128	571	2760	
C27		25.8.	17:34	26.8.	17:34	32.6345	29.0929	33.7758	24.9187	1632	416	1440	MS
C28		26.8.	17:52	27.8.	17:52	33.797	24.836	34.8299	20.355	1632	441	1440	
C29		27.8.	18:07	28.8.	18:07	34.836	20.319	35.547	16.599	1633	362	1440	
C30		29.8.	18:25	30.8.	17:48	36.131	14.985	38.735	15.199	1589	287	1403	

c)

Sample	Leg	Date (from)	Time (from) [CEST]	Date (to)	Time (to) [CEST]	GPS (from) N	E	GPS (to) N	E	Measured volume V_M [m³]	Sampling time [min]	Location
G1	1	25.06.2017	08:21	26.06.2017	06:52	No data	No data	38.225	9.401	709	1351	MS
G2		26.06.2017	08:14	27.06.2017	06:48	38.105	9.654	36.452	13.553	700	1354	MS
G3		27.06.2017	07:30	28.06.2017	06:44	36.406	13.675	35.879	14.501	720	1394	MS
G4		28.06.2017	07:29	29.06.2017	07:00	35.879	14.501	35.532	16.675	700	1411	MS
G5		29.06.2017	07:42	30.06.2017	06:54	35.497	16.824	34.363	21.593	733	1392	MS
G6		30.06.2017	07:29	01.07.2017	06:46	34.334	21.709	33.198	26.263	704	1397	MS
G7		01.07.2017	07:21	02.07.2017	06:56	33.167	26.383	32.319	30.378	725	1415	MS
G8		02.07.2017	07:34	03.07.2017	07:05	32.280	30.484	30.373	32.357	710	1411	NRS
G9		04.07.2017	07:43	05.07.2017	06:03	29.005	32.802	26.229	35.022	687	1340	NRS
G10		07.07.2017	11:17	08.07.2017	06:26	25.199	35.847	24.927	36.080	574	1152	NRS
G11		08.07.2017	06:56	09.07.2017	05:52	24.876	36.131	22.025	37.610	688	1377	NRS
G12		09.07.2017	06:19	10.07.2017	05:32	21.971	37.625	21.182	38.493	694	1391	NRS/SRS
G13		14.07.2017	05:34	15.07.2017	05:19	19.527	39.109	16.636	40.786	685	1429	SRS
G14		15.07.2017	05:49	16.07.2017	05:28	16.573	40.822	13.634	42.500	687	1424	SRS
G15		16.07.2017	07:47	17.07.2017	07:50	13.394	42.738	11.678	43.154	663	1326	SRS/AS
G16		19.07.2017	06:02	21.07.2017	04:57	13.086	48.956	17.085	56.037	1326	2817	AS
G17		21.07.2017	05:26	22.07.2017	04:59	17.135	56.104	20.012	59.022	714	1416	AS
G18		22.07.2017	05:24	22.07.2017	21:35	20.082	59.068	20.696	59.309	459	926	AS
G19		23.07.2017	04:03	23.07.2017	15:47	21.445	59.700	20.966	59.534	318	713	AS
G20		25.07.2017	09:29	26.07.2017	04:33	24.223	58.598	24.843	57.436	581	1151	OG
G21		26.07.2017	04:55	27.07.2017	05:35	24.878	57.390	25.224	56.499	691	1387	OG
G22		27.07.2017	05:56	28.07.2017	04:36	25.224	56.499	26.433	56.144	681	1363	OG
G23		29.07.2017	06:46	30.07.2017	04:24	25.648	53.110	27.354	50.895	652	1304	AG
G24		30.07.2017	04:50	31.07.2017	08:10	27.397	50.865	29.407	48.081	698	1395	AG

Sample	Leg	Date (from)	Time (from) [CEST]	Date (to)	Time (to) [CEST]	GPS (from) N	E	GPS (to) N	E	Measured volume V_M [m³]	Sampling time [min]	Location
G25	2	05.08.2017	05:15	06.08.2017	05:15	25.459	53.705	25.446	56.916	485	1012	AG
G26		06.08.2017	06:04	07.08.2017	05:15	25.312	56.949	24.170	58.495	450	931	OG
G27		07.08.2017	06:28	08.08.2017	05:03	24.082	58.683	21.606	60.115	664	1350	OG
G28		09.08.2017	05:32	10.08.2017	10:25	20.350	59.489	19.014	58.612	863	1726	AS
G29		10.08.2017	10:50	11.08.2017	08:38	19.041	58.636	18.103	57.658	677	1310	AS
G30		11.08.2017	11:02	13.08.2017	09:44	18.238	57.736	15.832	54.529	1428	2787	AS
G31		13.08.2017	10:22	14.08.2017	17:02	15.779	54.471	13.974	52.223	945	1830	AS
G32		14.08.2017	17:15	15.08.2017	09:12	13.968	52.195	13.429	49.657	490	957	AS
G33		16.08.2017	12:19	17.08.2017	06:48	12.228	45.788	13.029	43.163	557	1105	AS
G34		17.08.2017	07:47	18.08.2017	04:47	13.165	43.099	15.904	41.271	638	1266	SRS
G35		19.08.2017	06:12	20.08.2017	05:05	18.531	39.683	20.974	38.354	672	1367	SRS
G36		20.08.2017	05:26	21.08.2017	05:00	21.011	38.332	23.737	36.817	698	1407	NRS
G37		21.08.2017	05:39	22.08.2017	05:10	23.819	36.760	26.427	34.929	679	1404	NRS
G38		22.08.2017	05:50	23.08.2017	05:18	26.492	34.877	28.700	33.009	713	1403	NRS
G39		23.08.2017	05:52	23.08.2017	17:30	28.749	32.985	29.700	32.564	357	702	NRS
G40		25.08.2017	05:55	26.08.2017	05:15	32.007	31.164	33.177	27.224	732	1394	MS
G41		26.08.2017	05:49	27.08.2017	05:50	33.206	27.134	34.353	22.528	742	1436	MS
G42		27.08.2017	06:25	28.08.2017	05:53	34.381	22.413	35.215	18.447	725	1403	MS
G43		28.08.2017	06:30	29.08.2017	05:45	35.233	18.349	35.813	15.044	723	1389	MS

1.2 Chemicals and physico-chemical properties

Table S2. Physico-chemical properties of a) PAHs, b) OPAHs c) NPAHs taken from EPI-Suite (USEPA 2019); MW = Molecular weight, n.d. = not determined.

a)

Compound	Acro-nym	CAS #	MW [g mol^{-1}]	# of rings	log K_{ow}	Water solubility [mg L^{-1}]	Vapor pressure [Pa]	Subcooled liquid vapour pressure (P_L)[Pa]	Octanol–air partition coeffi-cient (K_{OA})	OH rate constant [cm^3 molec^{-1-} sec^{-1}]	Half-life (based on OH rate con-stant) [h]	Ozone rate constant [cm^3 molec^{-1-} sec^{-1-}]
Naphthalene	NAP	91-20-3	128.18	2	3.94	16.1	8.91E-01	4.14E+00	6.27	75.5 E-12	1.7	25.2 E-17
Acenaphthylene	ACY	208-96-8	152.20	3	3.92	3.9	2.87E-01	1.36E+00	6.31	66.9 E-12	1.92	
Acenaphthene	ACE	83-32-9	154.20	3	4.18	1.69	8.00E-02	6.18E-01	6.79	8.9 E-12	14.501	
Fluorene	FLN	86-73-7	166.23	3	4.46	1.15	1.61E-02	8.74E-02	7.57	13.0 E-12	9.873	
Phenanthrene	PHE	85-01-8	178.24	3	4.45	0.0434	8.71E-04	6.59E-02	7.55	40.0 E-12	3.209	
Anthracene	ANT	120-12-7	178.24	3	5.16	0.26	1.23E-03	8.10E-03	8.88	29.2 E-12	4.392	
Fluoranthene	FLT	206-44-0	202.26	4	4.88	0.135	6.00E-04	1.06E-02	8.80	50.0 E-12	2.567	
Pyrene	PYR	129-00-0	202.26	4	6.35	0.00848	0.000352	1.94E-03	8.70	41.7 E-12	3.078	
Retene	RET	483-65-8	234.34	3	5.77	0.03303	7.33E-06	5.18E-04	9.57	46.6 E-12	2.755	
Benzo(b)fluorene	BBN	243-17-4	216.28	4	5.52	0.04769	2.29E-05	4.66E-04	9.78	62.1 E-12	2.068	
Benzo(ghi)fluoranthene	BGF	203-12-3	226.28	5	5.70	0.03352	6.10E-05	1.06E-03	10.15	100.6 E-12	1.091	25.2 E-17
Cyclopenta(cd)pyrene	CCP	27208-37-3	226.28	5	5.70	0.03352	6.1E-005	0.00106	10.151	100.6 E-12	1.091	25.2 E-17
Benzo(a)anthracene	BAA	56-55-3	228.30	4	5.76	0.0094	2.80E-05	1.07E-04	9.07	50.0 E-12	2.567	
Triphenylene	TPH	217-59-4	228.30	4	5.49	0.0411	2.80E-06	1.47E-04	10.69	50.0 E-12	2.567	
Chrysene	CHR	218-01-9	228.30	4	5.81	0.002	8.31E-07	1.68E-04	9.48	50.0 E-12	2.567	
Benzo(b)fluoranthene	BBF	205-99-2	252.32	5	5.78	0.0015	6.67E-05	1.73E-03	10.35	18.6 E-12	6.918	
Benzo(j)fluoranthene	BJF	205-82-3	252.32	5	6.11	0.0025	3.50E-06	9.91E-05	10.59	53.6 E-12	2.394	
Benzo(k)fluoranthene	BKF	207-08-9	252.32	5	6.11	0.0008	1.29E-07	1.02E-05	10.73	53.6 E-12	2.394	
Benzo(e)pyrene	BEP	192-97-2	252.32	5	6.44	0.0063	7.60E-07	2.45E-05	11.35	50.0 E-12	2.567	
Benzo(a)pyrene	BAP	50-32-8	252.32	5	6.13	0.00162	7.32E-07	2.31E-05	10.86	50.0 E-12	2.567	

Compound	Acro-nym	CAS #	MW [g mol^{-1}]	# of rings	log K_{ow}	Water solubility [mg L^{-1}]	Vapor pressure [Pa]	Subcooled liquid vapour pressure (P_L)[Pa]	Octanol–air partition coeffi-cient (K_{OA})	OH rate constant [cm^3 molec^{-1-} sec^{-1}]	Half-life (based on OH rate con-stant) [h]	Ozone rate constant [cm^3 molec^{-1-} sec^{-1-}]
Perylene	PER	198-55-0	252.32	5	6.25	0.0004	7.00E-07	2.03E-04	10.08	50.0 E-12	2.567	
Indeno(123-cd)pyrene	INP	193-39-5	276.34	6	6.7	0.001176	4.24E-08	3.66E-06	12.37	50.0 E-12	2.567	
Dibenz(ah)anthracene	DBA	53-70-3	278.36	5	6.54	0.00103	1.27E-07	3.33E-05	11.78	50.0 E-12	2.567	
Dibenz(ac)anthracene	DCA	215-58-7	278.36	5	6.41	0.0016	1.33E-08	8.22E-07	11.11	50.0 E-12	2.567	
Benzo(ghi)perylene	BPE	191-24-2	276.34	6	6.63	0.00026	1.33E-08	4.24E-06	11.50	86.9 E-12	1.478	
Anthanthrene	ATT	191-26-4	276.34	6	7.04	0.001269	1.17E-07	8.11E-06	12.31	50.0 E-12	2.567	
Coronene	COR	191-07-1	300.36	7	7.64	0.00014	2.89E-10	3.46E-06	13.70	50.0 E-12	2.567	
Benzonaphtho-thiophene	BNT	239-35-0	234.32	4	5.34	0.06146	4.65E-05	8.42E-04	9.29	50.0 E-12	2.567	

b)

Compound	**Acronym**	**CAS #**	**MW [g mol^{-1}]**	**# of rings**	**log K_{ow}**	**Water solu-bility**	**Vapour pressure [Pa]**	**Sub-cooled liquid vapour pressure (P_L)[Pa]**	**Octanol–air partition coeffi-cient (K_{OA})**	**OH rate constant [cm^3 molec^{-1-} sec^{-1}]**	**Half-life (based on OH rate constant) [h]**	**Ozone rate constant [cm^3 molec^{-1-} sec^{-1-}]**
1,4-Naphthoquinone	1,4-O_2NAP	130-15-4	158.16	2	1.71 a	2417	2.25E-02	0.244	8.804	3.01E-12	42.71	1.75E-18
Naphthalene-1-aldehyde	1-(CHO)NAP	66-77-3	156.19	2	2.89	244.2	3.33E-01	0.397	7.161	2.78E-11	4.611	
9-Fluorenone	9-OFLN	486-25-9	180.21	3	3.58 [a]	3.74	7.63E-03	2.80E-02	8.138	6.18E-12	20.783	
9,10-Anthraquinone	9,10-O_2ANT	84-65-1	208.22	3	3.39 [a]	1.35[b]	1.55E-05	5.90E-03	9.407	1.50E-12	85.659	
1,4-Anthraquinone	1,4-O_2ANT	635-12-1	208.22	3	2.84	150.0	3.21E-04	3.95E-03	10.945	1.06E-11	12.160	1.75E-18
9,10-Phenanthroquinone	9,10-O_2PHE	84-11-7	208.22	3	2.52 [a]	7.5 [b]	1.14E-04	1.02E-02	9.477	6.18E-12	20.783	
11H-Benzo(a)fluoren-11-one	11-OBaFLN	479-79-8	230.27	4	4.73	0.22	5.16E-05	9.28E-04	10.298	1.80E-11	7.129	
11H-Benzo(b)fluoren-11-one	11-OBbFLN	3074-03-1	230.27	4	4.73	0.22	5.16E-05	9.28E-04	10.298	1.80E-11	7.129	
Benzanthrone (also called 7H-Benz(de) anthracene-7-one)	BAN	82-05-3	230.27	4	4.81 [a]	0.18	2.95E-05	9.28E-04	10.378	1.80E-11	7.129	
Benz(a)anthracene-7,12-dione	7,12-O_2BAA	2498-66-0	258.27	4	4.61	0.03	5.17E-06	1.59E-04	12.297	9.05E-12	14.185	
5,12-Naphthacenequinone	5,12-O_2NAC	1090-13-7	258.27	4	4.52	0.03	4.67E-06	1.59E-04	12.417	9.05E-12	14.185	

c)

Compound	Acronym	CAS #	MW [g mol^{-1}]	# of rings	log K_{ow}	Water solu-bility	Vapour pressure [Pa]	Sub-cooled liquid vapour pressure (P_L)[Pa]	Octanol–air partition coeffi-cient (K_{OA})	OH rate constant [cm^3 molec^{-1} sec^{-1}]	Half-life (based on OH rate constant) [h]	Ozone rate constant [cm^3 molec^{-1} sec^{-1}]
1-Nitronaphthalene	1-NNAP	86-57-7	173.17	2	3.19[a]	9.18[b]	6.40E-02	1.45E-01	7.31	2.70E-12	47.545	
2-Nitronaphthalene	2-NNAP	581-89-5	173.17	2	3.24[a]	9.24[b]	3.77E-02	1.23E-01	7.31	2.70E-12	47.545	
3-Nitroacenaphthene	3-NACE	3807-77-0	199.21	3	3.97	0.57	3.53E-03	2.97E-02	8.313	8.30E-12	15.457	
5-Nitroacenaphthene	5-NACE	602-87-9	199.21	3	3.85[a]	0.72	5.45E-03	2.97E-02	8.193	8.30E-12	15.457	1.07E-16
2-Nitrofluorene	2-NFLN	607-57-8	211.22	3	3.37	1.60	5.91E-04	1.32E-02	7.939	4.16E-12	30.828	1.45E-16
9-Nitroanthracene	9-NANT	602-60-8	223.23	3	4.78[a]	0.114[b]	1.60E-04	2.71E-03	9.861	5.00E-12	25.675	
9-Nitrophenanthrene	9-NPHE	954-46-1	223.23	3	4.16	0.29	1.80E-04	2.71E-03	9.241	1.62E-12	78.998	
3-Nitrophenanthrene	3-NPHE	17024-19-0	223.23	3	4.16	0.29	1.80E-04	2.71E-03	9.241	1.62E-12	78.998	
2-Nitrofluoranthene	2-NFLT	13177-29-2	247.26	4	4.29	2.12	3.93E-04	5.35E-03	8.517	2.13E-10	0.602	6.66E-16
1-Nitropyrene	1-NPYR	5522-43-0	247.26	4	5.06[a]	0.0118[b]	1.11E-05	2.35E-04	10.934	6.25E-12	20.54	
2-Nitropyrene	2-NPYR	789-07-1	247.26	4	4.75	0.07	7.36E-06	2.35E-04	10.624	6.25E-12	20.54	
7-Nitro-benzo(a)anthracene	7-NBAA	20268-51-3	273.29	4	5.34	0.02	1.01E-06	4.96E-05	11.432	6.25E-12	20.54	
6-Nitrochrysene	6-NCHR	7496-02-8	273.29	4	5.34	0.02	1.01E-06	4.96E-05	11.432	6.25E-12	20.54	
1,3-Dinitropyrene	1,3-N2PYR	75321-20-9	292.25	4	4.57	0.05	1.21E-07	9.70E-06	12.848	5.46E-13	470.136	
1,6-Dinitropyrene	1,6-N2PYR	42397-64-8	292.25	4	4.57	0.05	1.21E-07	9.70E-06	12.848	5.46E-13	470.136	
1,8-Dinitropyrene	1,8-N2PYR	42397-65-9	292.25	4	4.57	0.05	1.21E-07	9.70E-06	12.848	5.46E-13	470.136	
6-Nitro-benzo(a)pyrene	6-NBAP	63041-90-7	297.32	5	5.93	0.003	4.13E-08	4.01E-06	12.813	6.25E-12	20.54	

1.3 Analysis

Table S3. Gas chromatography mass spectrometry (GC-MS) parameters including retention times and mass-to-charge ratios (m/z) of a) PAHs analysis, b) NPAHs and OPAHs analysis and c) RPAHs analysis. SIM: Single ion monitoring; MRM: Multiple Reaction Monitoring

a)

Substance	Acronym	Quantifier SIM [m/z]	Qualifier SIM 1 [m/z]	Qualifier SIM 2 [m/z]	Retention time [min]
Naphthalene	NAP	128.0	129	126	9.167
Acenaphthylene	ACY	152.0	153	150	12.207
Acenaphthene	ACE	154.0	153	155	12.613
Fluorene	FLN	166.0	167	164	13.952
Phenanthrene	PHE	178.0	179	176	16.987
Anthracene	ANT	178.0	179	176	17.170
Fluoranthene	FLT	202.0	203	200	21.628
Pyrene	PYR	202.0	203	200	22.574
Retene	RET	219.0	234	205	23.950
Benzo(b)fluorene	BBN	216.0	215	217	24.369
Benzo(ghi)fluoranthene	BGF	226.0	235	232	27.047
Benzonaphthothiophene	BNT	234.0	227	224	27.222
Cyclopenta(cd)pyrene	CCP	228.0	227	224	27.953
Benzo(a)anthracene	BAA	226.0	229	226	28.056
Triphenylene	TPH	228.0	229	226	28.056
Chrysene	CHR	228.0	229	226	28.105
Benzo(b)fluoranthene	BBF	252.0	253	250	32.634
Benzo(j)fluoranthene	BJF	252.0	253	250	32.674
Benzo(k)fluoranthene	BKF	252.0	253	250	32.742
Benzo(e)pyrene	BEP	252.0	253	250	33.733
Benzo(a)pyrene	BAP	252.0	253	250	33.931
Perylene	PER	252.0	253	250	34.265
Indeno(123-cd)pyrene	INP	276.0	277	274	38.602
Dibenz(ah)anthracene	DBA	278.0	279	276	38.710
Dibenz(ac)anthracene	DCA	278.0	279	276	38.710
Benzo(ghi)perylene	BPE	276.0	277	274	39.848
Anthanthrene	ATT	276.0	277	274	40.510
Coronene	COR	300.0	301	298	49.473

b)

Substance	**Acronym**	**Group**	**Quantifier SRM transition [m/z]**	**Qualifier SRM transition [m/z]**	**Reten-tion time [min]**
1,4-Naphthoquinone	1,4-O_2NAP	OPAH	158 > 102	159 > 103	4.06
Naphthalene-1-aldehyde	1-(CHO)NAP	OPAH	156 > 128	157 > 128	5.33
1-Nitronaphthalene	1-NNAP	NPAH	174 > 127	173 > 145	6.01
2-Nitronaphthalene	2-NNAP	NPAH	173 > 127	174 > 127	6.37
9-Fluorenone	9-OFLN	OPAH	180 > 152	181 > 153	7.25
3-Nitroacenaphthene	3-NACE	NPAH	199 > 152	200 > 153	9.81
9,10-Anthraquinone	9,10-O_2ANT	OPAH	208 > 152	209 > 153	9.9
9,10-Phenanthrenequinone	9,10-O_2PHE	OPAH	180 > 152	209 > 153	10.01
5-Nitroacenaphthene	5-NACE	NPAH	199 > 169	199 > 152	10.34
1,4-Anthraquinone	1,4-O_2ANT	OPAH	208 > 152	209 > 153	10.83
2-Nitrofluorene	2-NFLN	NPAH	211 > 164	212 > 195	11.69
9-Nitroanthracene	9-NANT	NPAH	223 > 193	223 > 178	12.06
9-Nitrophenanthrene	9-NPHE	NPAH	223 > 167	223 > 178	13.11
3-Nitrophenanthrene	3-NPHE	NPAH	223 > 176	223 > 193	13.82
Benzo(a)fluoren-11-one	11-OBaFLN	OPAH	230 > 202	231 > 203	15.19
Benzo(b)fluoren-11-one	11-OBbFLN	OPAH	230 > 202	231 > 203	16.09
Benzanthrone	BAN	OPAH	230 > 202	231 > 203	17.28
2-Nitrofluoranthene	2-NFLT	NPAH	247 > 201	248 > 202	18.18
Benz(a)anthracene-7,12-dione	7,12-O_2BAA	OPAH	258 > 202	259 > 203	18.6
1-Nitropyrene	1-NPYR	NPAH	247 > 217	247 > 201	18.77
2-Nitropyrene	2-NPYR	NPAH	247 > 201	248 > 202	19.07
5,12-Naphthacenequinone	5,12-O_2NAC	OPAH	258 > 202	259 > 203	19.77
7-Nitrobenzo(a)anthracene	7-NBAA	NPAH	273 > 215	274 > 257	21.44
6-Nitrochrysene	6-NCHR	NPAH	273 > 215	274 > 226	22.65
1.3-Dinitropyrene	1,3-N_2PYR	NPAH	292 > 188	292 > 176	23.65
1.6-Dinitropyrene	1,6-N_2PYR	NPAH	292 > 176	292 > 232	24.4
1.8-Dinitropyrene	1,8-N_2PYR	NPAH	292 > 176	292 > 232	24.93
6-Nitrobenzo(a)pyrene	6-NBAP	NPAH	297 > 239	297 > 224	26.81

c)

Substance	**Acronym**	**Quantifier SIM (m/z)**	**Confirmation SIM (m/z)**	**Retention time [min]**
Phenanthrene	PHE	178 $[M]^+$	176 $[M\text{-}2H]^+$	12.82
1-Methylphenanthrene	1-MPHE	192 $[M]^+$	189 $[M\text{-}3H]^+$	14.77
2-Methylphenanthrene	2-MPHE	192 $[M]^+$	189 $[M\text{-}3H]^+$	14.87
3-Methylphenanthrene	3-MPHE	192 $[M]^+$	189 $[M\text{-}3H]^+$	15.18
4-Methylphenanthrene	4-MPHE	192 $[M]^+$	189 $[M\text{-}3H]^+$	15.28
3,6-Dimethylphenanthrene	3,6-M_2PHE	206 $[M]^+$	202 $[M\text{-}4H]^+$	16.37
2,6-Dimethylphenanthrene	2,6-M_2PHE	206 $[M]^+$	202 $[M\text{-}4H]^+$	16.71
2,7-Dimethylphenanthrene	2,7-M_2PHE	206 $[M]^+$	202 $[M\text{-}4H]^+$	16.83
1,3-/2,10-/3,9-/3,10-Dimethylphenanthrene	1,3-/2,10-/3,9-/1,10-M_2PHE	206 $[M]^+$	202 $[M\text{-}4H]^+$	16.92
1,6-/2,9-Dimethylphenanthrene	1,6-/2,9-M_2PHE	206 $[M]^+$	202 $[M\text{-}4H]^+$	17.13
1,7-Dimethylphenanthrene	1,7-M_2PHE	206 $[M]^+$	202 $[M\text{-}4H]^+$	17.26
2,3-Dimethylphenanthrene	2,3-M_2PHE	206 $[M]^+$	202 $[M\text{-}4H]^+$	17.36
1,9-/4,9-Dimethylphenanthrene	1,9-/4,9-M_2PHE	206 $[M]^+$	202 $[M\text{-}4H]^+$	17.50
1,8-Dimethylphenanthrene	1,8-M_2PHE	206 $[M]^+$	202 $[M\text{-}4H]^+$	18.06

1.4 Measurement of other supporting parameters

1.4.1 Meteorological data

The meteorological data such as GPS position and speed of the ship, wind direction and speed, temperature, humidity etc. was measured by a commercial weather station with GPS (STERELA METEO Neptune). The actinic flux was measured by a CCD spectral radiometer (Metcon 85237).

1.4.2 PM_{10} mass concentration

For PM concentration, QFFs were weighed before and after sampling using a laboratory balance following accommodation to a constant humidity and temperature.

1.4.3 Metals

- The content of transition metals (Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Mo, Cd) and Pb on baked QFFs was determined after microwave digestion (MWS 3+ Berghof, Eningen, Germany) of samples with concentrated nitric acid (4 mL, p.a., Merck, Darmstadt, Germany) and hydrogen peroxide (2 mL, p.a., Merck, Darmstadt, Germany) followed by inductively coupled plasma mass spectrometry (Agilent 7700x ICP-MS, Santa Clara, USA). The method was validated by analysis of samples spiked with known amount of analytes. Median recoveries for spiked samples were within the range 90–110 %. Relative standard deviations for replicate analyses of spiked samples were within single percentage points.

1.4.4 Elemental and organic carbon (EC/OC)

PM total elemental and organic carbon fraction concentrations were determined from punches of baked QFFs. C fractions were thermally desorbed from the filter medium under a He atmosphere followed by an oxidizing atmosphere using a OC-EC Aerosol Analyzer (Sunset Laboratory, Tigard, USA) with flame ionization detection (FID) measuring the CO_2 concentration. For heating ramps, the EUSAAR-2 protocol (Cavalli and Putaud, 2008) was followed.

1.5 Quality control

1.5.1 Filtering against contamination by the own ship exhaust

A stack contamination filter is available, which was based on wind direction and speed, particle number concentration (measured by condensation particle counter (CPC) and fast mobility particle sizer (FMPS)) and black carbon concentration (Aethalometer), WNC for short using measurement of the ship and from Celik et al. (2020). The advantage of that contamination filter compared to the filter applied by other studies of the campaign (Eger et al., 2019; Tadic et al, 2020) was that all of our samples are within the time period the filter can be applied. Moreover, the sampling inlet of the instrument for the parameters, which are crucial for the decision if there was a stack contamination or not, was closer to our air sampler than the inlets for the NO, O_3 and SO_2 measurement instruments used for the other stack contamination filter.

Nevertheless, it has to be considered that none of the instruments for the decision if there was a contamination by the own ship stack was exactly at the same location and same height as our air samplers. Thus, there is a chance that our sample is contaminated although it should not be the case according to the data of the stack contamination filter and vice versa. However, our approach, which will be discussed in the following, is rather rejecting false positive (samples treated as contaminated but are not) than false negative (samples are contaminated but treated as not contaminated). The difficulty in deciding for stack contamination of a sample is the fact that our instruments sampled on average for 12-24 hours. Since during this time period, the wind and the direction of the ship changed, another criterion was needed to decide if the total sample was contaminated by the ship stack or not. The first criterion was the usage of the percentage of the contaminated time from the total sampling time. Thus, the first criterion for rejecting a sample as "contaminated" was if more than 10 % of the total sampling time was classified as possibly contaminated based on the WNC filter.

However, since it does not only depend on the time of possible contamination but also on the intensity of contamination, we used another criterion. The photoelectric PAH sensor (EcoChem PAS2000, Ansyco, Karlsruhe, Germany) measured photoelectrons from PAHs on the surface of sub-micrometre particles (Niessner and Wilbring, 1989) with a time resolution of 10 s. Whenever the average PAH signal of sampling time marked as "possibly contaminated" by the WNC filter was more than 10 % higher than the PAH signal of the sampling time marked as "not contaminated", the sample was rejected. Based on this stack filtering process, we rejected 20 out of 62 Digitel high volume samples and 6 out of 30 impactor samples, especially from the first leg (see Table S4).

Table S4. Filtering for contamination from own stack of a) Digitel high-volume samples, b) cascade impactor samples and c) GMWL high volume samples.

a)

Sample	Possible contamination in % of sampling time	Percentage difference of average surface PAH of "possibly contaminated" and "not contaminated" sampling time [%]	Reject due to possible contamination?
D1	0.0	0.0	no
D2	4.9	21.4	yes
D3	21.2	1.4	yes
D4	0.0	0.0	no
D5	3.2	3.8	no
D6	4.6	8.2	no
D7	1.3	0.8	no
D8	53.2	1543	yes
D9	11.0	70.8	yes
D10	28.9	0.0	yes
D11	20.7	12.8	yes
D12	7.8	2.6	no
D13	0.0	0.0	no
D14	6.5	0.7	no
D15	7.2	0.2	no
D16	22.7	184	yes
D17	21.2	419	yes
D18	7.8	923	yes
D19	9.4	37.3	yes
D20	43.4	701	yes
D21	2.7	19.4	yes
D22	70.4	3797	yes
D23	51.8	3191	yes
D24	0.0	0.0	no
D25	6.8	0.1	no
D26	9.2	29.0	yes
D27	22.8	28.1	yes
D28	16.2	492	yes
D29	0.5	0.6	no
D30	0.0	0.0	no
D31	0.5	1.0	no
D32	0.2	1.0	no

Sample	Possible contamination in % of sampling time	Percentage difference of average surface PAH of "possibly contaminated" and "not contaminated" sampling time [%]	Reject due to possible contamination?
D33	0.8	0.3	no
D34	0.0	0.0	no
D35	1.4	0.3	no
D36	0.0	0.0	no
D37	26.6	340	yes
D38	12.5	325	yes
D39	0.0	0.0	no
D40	0.0	0.0	no
D41	0.0	0.0	no
D42	0.0	0.0	no
D43	0.0	0.0	no
D44	0.0	0.0	no
D45	0.0	0.0	no
D46	0.0	0.0	no
D47	0.0	0.0	no
D48	0.0	0.0	no
D49	2.6	0.1	no
D50	3.0	0.5	no
D51	0.0	0.0	no
D52	0.0	0.0	no
D53	0.0	0.0	no
D54	0.0	0.0	no
D55	0.0	0.0	no
D56	0.0	0.0	no
D57	0.0	0.0	no
D58	0.0	0.0	no
D59	1.1	1.7	no
D60	0.5	0.0	no
D61	8.5	0.0	no
D62	0.0	0.0	no

b)

Sample	Possible contamination in % of sampling time	Percentage difference of average surface PAH concentration of "possibly contaminated" and "not contaminated" sampling time [%]	Reject due to possible contamination?
C1	21.9	108	yes
C2	46.2	1774	yes
C3	7.9	15.1	yes
C4	22.4	28.1	yes
C5	17.0	507	yes
C6	0.3	0.6	no
C7	0.0	0.0	no
C8	0.0	0.0	no
C9	0.0	0.0	no
C10	0.0	0.0	no
C11	0.0	0.0	no
C12	0.0	0.0	no
C13	0.2	1.0	no
C14	0.0	0.0	no
C15	0.0	0.0	no
C16	0.0	0.0	no
C17	0.0	0.0	no
C18	0.0	0.0	no
C19	0.0	0.0	no
C20	0.6	0.1	no
C21	13.6	213	yes
C22	0.0	0.0	no
C23	0.0	0.0	no
C24	0.0	0.0	no
C25	0.0	0.0	no
C26	0.0	0.0	no
C27	1.5	0.3	no
C28	0.0	0.0	no
C29	0.0	0.0	no
C30	0.0	0.0	no

c)

Sample	Possible contamination in % of sampling time	Percentage difference of average surface PAH concentration of "possibly contaminated" and "not contaminated" sampling time [%]	Reject due to possible contamination?
G1	0.00	0.0	no
G2	0.00	0.0	no
G3	15.46	5.1	yes
G4	11.98	18.7	yes
G5	0.00	0.0	no
G6	3.97	4.7	no
G7	5.27	7.3	no
G8	3.37	24.1	yes
G9	35.93	931.9	yes
G10	0.17	0.8	no
G11	7.99	2.2	no
G12	4.74	0.4	no
G13	2.06	168.3	yes
G14	23.04	0.6	yes*
G15	24.73	1114.4	yes
G16	8.49	2191.5	yes
G17	83.00	2751.8	yes
G18	210.24	1210.5	yes
G19	0.00	0.0	no*[2]
G20	0.00	0.0	no
G21	17.23	40.5	yes
G22	33.02	453.9	yes
G23	0.00	0.0	no
G24	0.00	0.1	no
G25	0.00	0.0	no
G26	0.97	0.3	no
G27	0.00	0.0	no
G28	2.84	103.4	yes
G29	3.28	135.1	yes
G30	8.74	231.9	yes
G31	0.00	0.0	no
G32	0.00	0.0	no
G33	0.00	0.0	no
G34	0.00	0.0	no
G35	0.00	0.0	no
G36	0.00	0.0	no
G37	0.00	0.0	no
G38	0.00	0.0	no
G39	0.00	0.0	no
G40	22.27	0.2	no*

Sample	Possible contamination in % of sampling time	Percentage difference of average surface PAH concentration of "possibly contaminated" and "not contaminated" sampling time [%]	Reject due to possible contamination?
G41	0.00	0.0	no
G42	0.00	0.0	no
G43	0.00	0.0	no

1.5.2 Chemical analysis – quality control

Quantification of compounds was based on the calculation of relative response factors (RRF) to an internal standard (p-terphenyl for PAHs and PCB 121 for NPAHs and OPAHs). Each compound was identified by comparing retention time and the ion ratio between quantification and confirmation ion with reference standard mixtures.

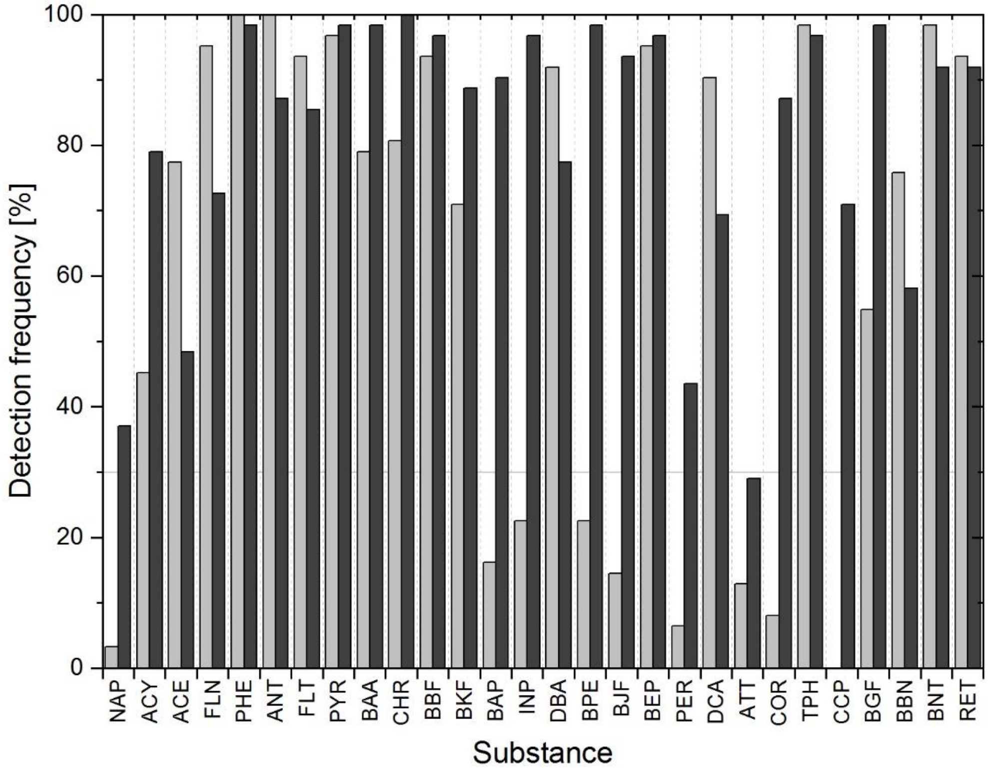
1.5.2.1 Recoveries and blank correction

The recoveries of the surrogate standards (deuterated PAHs and NPAHs) for gaseous (PUF) samples ranged 66-94 % (disregarded NAP-d8) and 41-74 %, respectively. For particulate samples (QFF, Digitel high-volume), the recoveries ranged 58-106 % and 46-114 %, respectively, and for size-segregated particulate (QFF, cascade impactor) samples, 52-93 % and 32-161 %, respectively. All results of this study were blank corrected (i.e., subtraction of the mean of 3 field blank values), but not recovery corrected. Laboratory solvent blanks were processed as one blank per max 20 samples but only the field blanks were used for blank subtraction.

The detection frequencies of substances from samples of the Digitel high volume are illustrated in Fig. S1. For calculating average values, values <LOQ of substances in one phase were replaced by blank corrected LOQ/2 if the substance specific detection frequency in one phase was >30 %. In case of a lower detection frequency of the substance in all samples was <30 %, the value 0 was used for further calculations. The same was done for the impactor samples. The detection frequency of each impactor stage was used individually. The results are shown in Table S5.

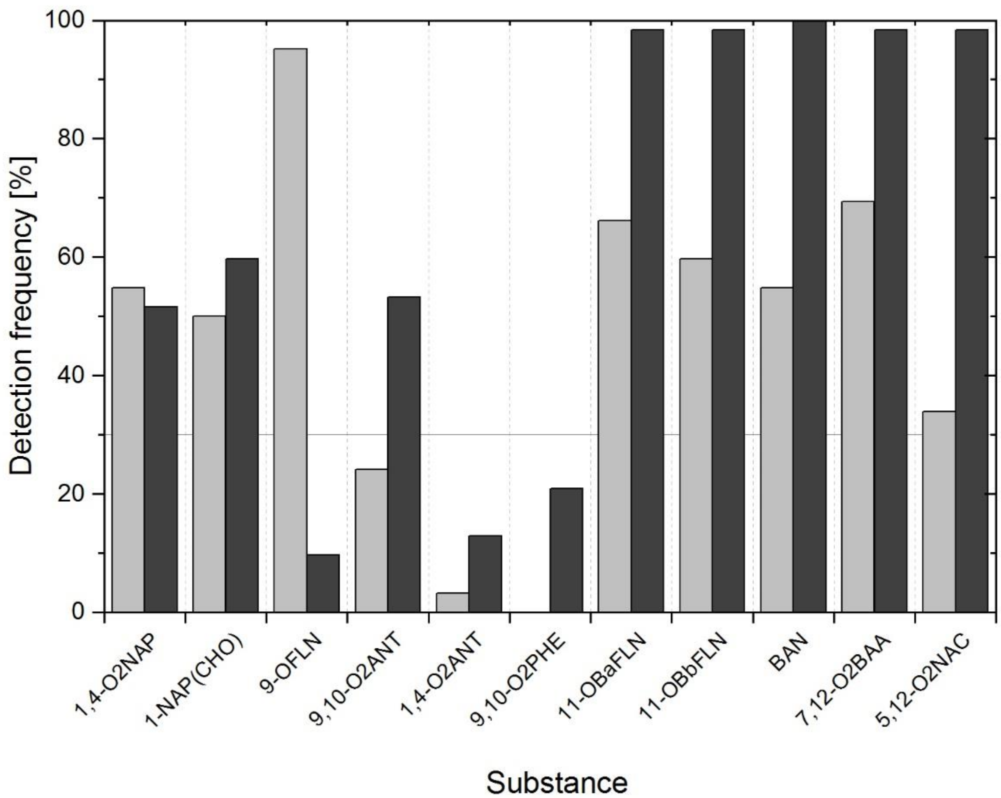
The recovery of the surrogate standard phenanthrene-d10 (Dr. Ehrenstorfer) for the PAHs and RPAHs from the second high volume sampler standard ranged 75-119 %. Blank sample media (3 QFFs, 3 PUFs) were analysed for the presence of target compounds. Blank concentrations ranged 0.03- 2.7 % of the target compounds. The samples were blank but not recovery corrected.

a)



Detection frequency [%]
0
20
40
60
80
100
NAP
ACY
ACE
FLN
PHE
ANT
FLT
PYR
BAA
CHR
BBF
BKF
BAP
INP
DBA
BPE
BJF
BEP
PER
DCA
ATT
COR
TPH
CCP
BGF
BBN
BNT
RET
Substance

b)



Detection frequency [%]
0
20
40
60
80
100
1,4-O2NAP
1-NAP(CHO)
9-OFLN
9,10-O2ANT
1,4-O2ANT
9,10-O2PHE
11-OBaFLN
11-OBbFLN
BAN
7,12-O2BAA
5,12-O2NAC
Substance

c)

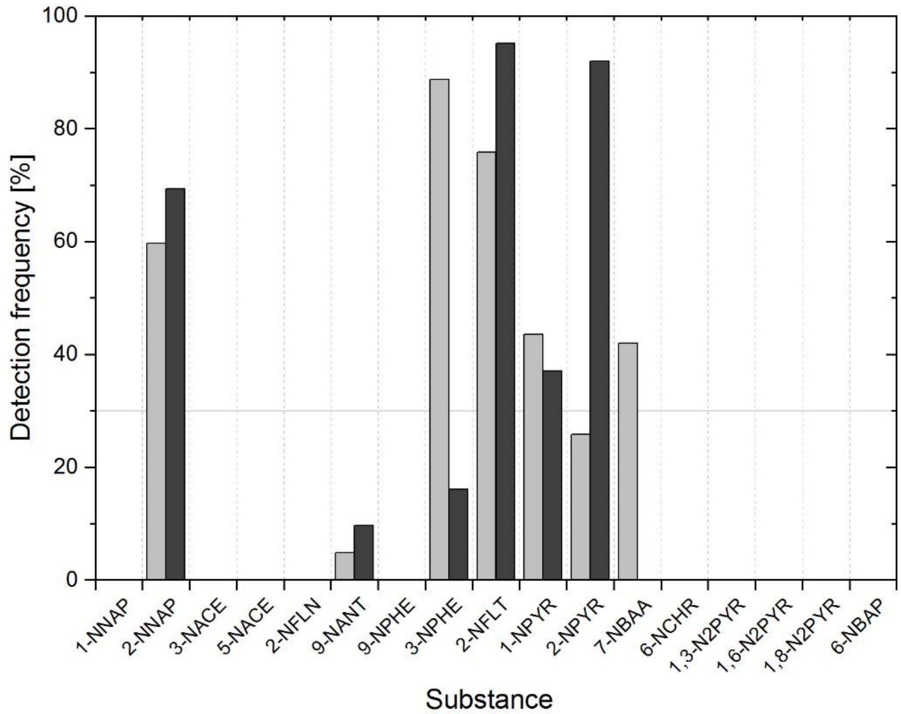


Figure S1. Detection frequency of a) PAHs, b) OPAHs and c) NPAHs in Digitel high volume samples (considering all samples) using the sum of the average of blanks and 3 × standard deviation of blanks as LOQ; Grey: Gas phase; Black: Particulate phase.

Table S5. Detection frequencies (in %) from impactor samples of a) PAHs, b) OPAHs and c) NPAHs.

a)

Substance	All stages	Stage A PM_{7-10}	Stage B PM_{3-7}	Stage C $PM_{1.5-3}$	Stage D $PM_{0.95-1.5}$	Stage E $PM_{0.49-0.95}$	Stage F $PM_{<0.49}$
ACY	**0**	0	0	0	0	0	0
ACE	**0**	0	0	0	0	0	0
FLN	**0**	0	0	0	0	0	0
PHE	**56**	57	60	53	63	60	40
ANT	**1**	0	0	0	0	0	7
FLT	**52**	20	37	47	53	60	93
PYR	**48**	20	33	50	53	57	73
BAA	**69**	53	63	63	67	90	80
CHR	**67**	30	57	63	67	83	100
BBF	**79**	47	60	73	93	100	100
BKF	**53**	13	33	47	63	73	87
BAP	**52**	20	50	47	63	70	63
INP	**65**	27	50	63	77	90	83
DBA	**22**	7	27	13	23	30	30
BPE	**77**	43	63	70	90	97	100
BJF	**61**	17	43	57	70	83	97
BEP	**71**	33	53	63	80	93	100
PER	**21**	3	13	7	23	27	53
DCA	**22**	10	27	13	20	27	33
ATT	**42**	30	43	33	50	53	40
COR	**45**	13	30	30	47	67	83
TPH	**52**	17	33	43	57	63	97
CCP	**5**	0	0	0	3	17	10
BGF	**59**	20	43	53	67	77	93
BBN	**13**	0	3	3	17	27	27
BNT	**61**	33	57	60	80	77	57
RET	**19**	0	3	3	3	3	100

b)

Substance	All stages	Stage A PM_{7-10}	Stage B PM_{3-7}	Stage C $PM_{1.5-3}$	Stage D $PM_{0.95-1.5}$	Stage E $PM_{0.49-0.95}$	Stage F $PM_{<0.49}$
1,4-O_2NAP	**1**	3	0	0	0	0	0
1-(CHO)NAP	**67**	67	67	67	67	67	67
9-OFLN	**17**	0	0	0	0	0	100
9,10-O_2ANT	**17**	0	0	0	0	0	100
1,4-O_2ANT	**0**	0	0	0	0	0	0
9,10-O_2PHE	**0**	0	0	0	0	0	0
11-OBaFLN	**44**	7	23	37	43	63	93
11-OBbFLN	**44**	7	20	33	43	63	100
BAN	**35**	7	7	10	33	53	100
7,12-O_2BAA	**63**	20	40	50	73	97	100
5,12-O_2NAC	**76**	37	53	70	100	100	97

c)

Substance	All stages	Stage A PM_{7-10}	Stage B PM_{3-7}	Stage C $PM_{1.5-3}$	Stage D $PM_{0.95-1.5}$	Stage E $PM_{0.49-0.95}$	Stage F $PM_{<0.49}$
1-NNAP	**1**	0	3	0	0	0	0
2-NNAP	**9**	0	0	0	0	0	53
3-NACE	**1**	0	0	0	0	0	7
5-NACE	**7**	0	0	0	3	0	40
2-NFLN	**0**	0	0	0	0	0	0
9-NANT	**1**	0	0	0	0	0	7
9-NPHE	**1**	3	0	0	0	0	0
3-NPHE	**4**	0	3	3	7	10	3
2-NFLT	**51**	10	27	40	53	83	93
1-NPYR	**45**	20	37	37	53	70	53
2-NPYR	**26**	3	7	17	23	40	63
7-NBAA	**17**	3	10	20	23	40	7
6-NCHR	**0**	0	0	0	0	0	0
1,3-N_2PYR	**0**	0	0	0	0	0	0
1,6-N_2PYR	**0**	0	0	0	0	0	0
1,8-N_2PYR	**0**	0	0	0	0	0	0
6-NBAP	**6**	0	3	3	10	10	10

1.5.2.2 Method uncertainty

The method uncertainty was determined by spiking PUFs with standard mix, followed by extraction and clean-up similar to the samples (DCM warm automated Soxhlet extraction, silica column clean-up). The data is listed in Table S6.

Table S6. Method uncertainty of a) PAHs, b) OPAHs and c) NPAHs.

a)

Substance	Relative standard deviation [%]	Extended uncertainty [%]
Acenaphthene	11.7	23.4
Acenaphthylene	11.4	22.8
Anthanthrene	13.1	26.1
Anthracene	14.2	28.3
Benz(a)anthracene	4.4	8.7
Benzo(a)pyrene	2.8	5.5
Benzo(b)fluoranthene	2.9	5.8
Benzo(b)fluorene	3.2	6.4
Benzo(e)pyrene	3.0	6.0
Benzo(ghi)fluoranthene	2.9	5.9
Benzo(ghi)perylene	3.4	6.8
Benzo(j)fluoranthene	3.3	6.6
Benzo(k)fluoranthene	2.9	5.9
Benzonaphtho-thiophene	3.4	6.9
Chrysene	2.4	4.8
Coronene	5.5	10.9
Cyclopenta(cd)pyrene	2.1	4.3
Dibenz(ah)anthracene	2.9	5.8
Dibenzo(ac)anthracene	3.1	6.2
Fluoranthene	10.3	20.6
Fluorene	11.8	23.5
Indeno(123-cd)pyrene	4.5	9.0
Naphthalene	13.9	27.8
Perylene	2.8	5.6
Phenantrene	11.1	22.1
Pyrene	5.3	10.7
Retene	5.3	10.5
Triphenylene	2.9	5.7

b)

Substance	Relative standard deviation [%]	Extended uncertainty [%]
1,4-O_2NAP	4.4	8.8
1-(CHO)NAP	7.9	15.9
9-OFLN	5.0	10.0
9,10-O_2ANT	2.4	4.7
1,4-O_2ANT	n.d.	n.d.
9,10-O_2PHE	n.d.	n.d.
11-OBaFLN	4.1	8.2
11-OBbFLN	4.4	8.8
BAN	5.4	10.7
7,12-O_2BAA	2.3	4.5
5,12-O_2NAC	7.6	15.2

n.d. = not determined

c)

Substance	Relative standard deviation [%]	Extended uncertainty [%]
1-NNAP	10.0	20.0
2-NNAP	8.6	17.1
3-NACE	13.5	27.1
5-NACE	8.9	17.8
2-NFLN	11.7	23.4
9-NANT	10.9	21.8
9-NPHE	11.1	22.2
3-NPHE	6.2	12.4
2-NFLT	7.1	14.2
1-NPYR	9.8	19.7
2-NPYR	6.4	12.8
7-NBAA	6.4	12.8
6-NCHR	7.3	14.6
1,3-N_2PYR	11.9	23.8
1,6-N_2PYR	4.9	9.8
1,8-N_2PYR	8.7	17.4
6-NBAP	8.5	16.9

1.5.2.3 Limits of quantification

For the evaluation, we used the maximum of two limits of quantification (LOQs). First, the instrumental LOQ (iLOQ), which is based on the limits in the analysis by the GC-MS and second the LOQ from field blanks (fbLOQ) including possible contamination during storage and transport of the samples and from the complete analytical method (extraction, clean-up and measurement). The fbLOQ was calculated from the average concentration of three field blanks (individual for different sampling media) plus 3 times the standard deviation of the concentration of these three field blanks.

The iLOQ of NPAHs and OPAHs was calculated based on the signal to noise ratio (S/N) for a specific compound and specific sample as the concentration which corresponds to S/N = 10:1. For PAHs, the iLOQ is calculated by extrapolation of S/N = 10:1 to the corresponding concentration, based on calibration standards. The LOQs can be found in Table S7.1 and S8 for the samples of the Digitel high volume sampler and Table S7.2 for the samples of the impactor sampler. The LOQ for all RPAHs was 0.05 pg m^{-3}.

Table S7.1. Limits of quantification (LOQ) including instrumental LOQs (iLOQs) and LOQs from field blanks (fbLOQs) from a) PAHs, b) OPAHs and c) NPAHs in ng sample^{-1} from the Digitel high-volume sampler.

a)

Substance	Acronym	iLOQ both phases	fbLOQ gas phase	fbLOQ particulate phase
Naphthalene	NAP	0.17	222.57	7.86
Acenaphthylene	ACY	0.12	5.22	0.24
Acenaphthene	ACE	0.14	17.23	0.20
Fluorene	FLN	0.10	30.21	1.70
Phenantrene	PHE	0.13	54.64	5.29
Anthracene	ANT	0.15	1.73	0.23
Fluoranthene	FLT	0.14	36.74	3.75
Pyrene	PYR	0.15	23.36	0.85
Benz(a)anthracene	BAA	0.15	1.79	0.15
Chrysene	CHR	0.14	4.78	0.28
Benzo(b)fluoranthene	BBF	0.33	1.17	0.33
Benzo(k)fluoranthene	BKF	0.39	0.39	0.39
Benzo(a)pyrene	BAP	0.53	0.53	0.53
Indeno(123-cd)pyrene	INP	0.31	0.31	0.31
Dibenz(ah)anthracene	DBA	0.25	3.29	0.25
Benzo(ghi)perylene	BPE	0.25	0.25	0.25
Benzo(j)fluoranthene	BJF	0.34	1.92	0.34
Benzo(e)pyrene	BEP	0.35	0.35	0.35
Perylene	PER	0.45	0.45	0.45
Dibenzo(ac)anthracene	DCA	0.25	3.06	0.25
Anthanthrene	ATT	0.29	1.14	0.29
Coronene	COR	0.42	0.42	0.42
Triphenylene	TPH	0.12	2.08	0.25
Cyclopenta(cd)pyrene	CCP	0.15	0.15	0.15
Benzo(ghi)fluoranthene	BGF	0.10	4.15	0.16
Benzo(b)fluorene	BBN	0.40	2.96	0.40
Retene	RET	0.34	4.49	0.34
Benzonaphtho-thiophene	BNT	0.12	0.35	0.12

b)

Substance	Average iLOQ gas phase	Standard deviation iLOQ gas phase	Average iLOQ particulate phase	Standard deviation iLOQ particulate phase	fbLOQ gas phase	fbLOQ particulate phase
1,4-O_2NAP	0.89	1.44	0.32	0.70	44.24	6.72
1-(CHO)NAP	1.96	4.14	0.42	0.38	16.25	1.80
9-OFLN	0.51	0.71	0.11	0.14	21.55	11.69
9,10-O_2ANT	0.80	1.52	0.14	0.21	72.76	10.33
1,4-O_2ANT	1.85	3.50	0.33	0.48	<iLOQ	<iLOQ
9,10-O_2PHE	5723	1317	54.7	144	<iLOQ	2.76
11-OBaFLN	0.85	1.91	0.48	1.44	5.96	0.58
11-OBbFLN	0.68	1.54	0.38	1.16	4.90	0.49
BAN	0.49	1.10	0.27	0.83	5.54	0.71
7,12-O_2BAA	0.34	1.15	0.32	0.80	2.96	0.32
5,12-O_2NAC	0.20	0.66	0.19	0.46	0.21	0.04

c)

Substance	Average iLOQ gas phase	Standard deviation iLOQ gas phase	Average iLOQ particulate phase	Standard deviation iLOQ particulate phase	fbLOQ gas phase	fbLOQ particulate phase
1-NNAP	2.45	4.17	0.45	0.21	<iLOQ	<iLOQ
2-NNAP	0.18	0.20	0.03	0.03	0.92	0.05
3-NACE	8.33	9.11	2.76	3.20	<iLOQ	<iLOQ
5-NACE	0.95	1.06	0.14	0.17	<iLOQ	<iLOQ
2-NFLN	0.07	0.18	0.01	0.01	<iLOQ	<iLOQ
9-NANT	5.69	8.96	0.21	0.32	2.67	0.04
9-NPHE	3.24	4.33	0.84	1.52	<iLOQ	<iLOQ
3-NPHE	0.54	0.83	0.09	0.14	0.15	<iLOQ
2-NFLT	0.03	0.06	0.03	0.09	0.19	0.02
1-NPYR	0.62	2.17	0.08	0.29	0.19	0.33
2-NPYR	0.02	0.04	0.02	0.06	0.02	0.004
7-NBAA	0.12	0.17	0.49	1.67	0.07	0
6-NCHR	0.07	0.11	0.30	1.01	<iLOQ	<iLOQ
1,3-N_2PYR	0.13	0.05	0.05	0.04	<iLOQ	<iLOQ
1,6-N_2PYR	0.29	0.23	0.28	0.33	<iLOQ	<iLOQ
1,8-N_2PYR	0.12	0.09	0.12	0.14	<iLOQ	<iLOQ
6-NBAP	0.27	0.23	0.34	0.69	<iLOQ	<iLOQ

Table S7.2. Limits of quantification (LOQ) including instrumental LOQs (iLOQs) and LOQ from field blanks (fbLOQs) from a) PAHs, b) OPAHs and c) NPAHs in ng sample^{-1} from the impactor sampler.

a)

Substance	Acronym	iLOQ	fbLOQ stages A-E ($PM_{0.49-10\ \mu m}$)	fbLOQ stage F ($PM_{<0.49\ \mu m}$)
Naphthalene	NAP	0.17	3.92	4.63
Acenaphthylene	ACY	0.12	0.94	1.73
Acenaphthene	ACE	0.14	2.59	10.22
Fluorene	FLN	0.10	2.93	4.46
Phenantrene	PHE	0.13	2.72	5.56
Anthracene	ANT	0.15	2.06	0.15
Fluoranthene	FLT	0.14	2.49	1.92
Pyrene	PYR	0.15	1.97	1.71
Benz(a)anthracene	BAA	0.15	<iLOQ	0.44
Chrysene	CHR	0.14	0.57	0.55
Benzo(b)fluoranthene	BBF	0.33	<iLOQ	<iLOQ
Benzo(k)fluoranthene	BKF	0.39	<iLOQ	<iLOQ
Benzo(a)pyrene	BAP	0.53	<iLOQ	<iLOQ
Indeno(123cd)pyrene	INP	0.31	<iLOQ	<iLOQ
Dibenz(ah)anthracene	DBA	0.25	<iLOQ	<iLOQ
Benzo(ghi)perylene	BPE	0.25	<iLOQ	<iLOQ
Benzo(j)fluoranthene	BJF	0.34	<iLOQ	<iLOQ
Benzo(e)pyrene	BEP	0.35	<iLOQ	<iLOQ
Perylene	PER	0.45	<iLOQ	<iLOQ
Dibenzo(ac)anthracene	DCA	0.25	<iLOQ	<iLOQ
Anthanthrene	ATT	0.29	<iLOQ	<iLOQ
Coronene	COR	0.42	<iLOQ	<iLOQ
Triphenylene	TPH	0.12	0.45	0.42
Cyclopenta(cd)pyrene	CCP	0.15	<iLOQ	<iLOQ
Benzo(ghi)fluoranthene	BGF	0.10	0.34	0.42
Benzo(b)fluorene	BBN	0.40	<iLOQ	<iLOQ
Retene	RET	0.34	1.64	0.34
Benzonaphtho-thiophene	BNT	0.12	<iLOQ	<iLOQ

b)

Substance	Average iLOQ	Standard deviation iLOQ	fbLOQ stages A-E ($PM_{0.49\text{-}10\ \mu m}$)	fbLOQ stage F ($PM_{<0.49\ \mu m}$)
1,4-O_2NAP	0.23	0.29	<iLOQ	<iLOQ
1-(CHO)NAP	0.16	0.20	<iLOQ	<iLOQ
9-OFLN	0.04	0.06	16.59	5.50
9,10-O_2ANT	0.16	0.66	36.10	3.43
1,4-O_2ANT	0.27	1.10	<iLOQ	<iLOQ
9,10-O_2PHE	688	3074	241	36.4
11-OBaFLN	0.22	1.32	0.40	0.32
11-OBbFLN	0.20	1.20	0.63	0.47
BAN	0.15	0.88	1.44	0.45
7,12-O_2BAA	0.11	0.46	0.39	0.23
5,12-O_2NAC	0.07	0.29	0.04	0.03

c)

Substance	Average iLOQ	Standard deviation iLOQ	fbLOQ stages A-E ($PM_{0.49\text{-}10\ \mu m}$)	fbLOQ stage F ($PM_{<0.49\ \mu m}$)
1-NNAP	0.09	0.08	<iLOQ	<iLOQ
2-NNAP	0.03	0.04	0.38	0.08
3-NACE	1.67	2.64	4.10	0.09
5-NACE	0.17	0.35	0.80	0.02
2-NFLN	0.01	0.02	0.02	0.00
9-NANT	0.16	0.43	1.45	0.04
9-NPHE	0.52	1.62	0.09	0.01
3-NPHE	0.08	0.17	0.05	0.00
2-NFLT	0.05	0.31	0.13	0.07
1-NPYR	0.33	1.50	0.15	0.07
2-NPYR	0.04	0.27	0.02	0.01
7-NBAA	0.69	3.27	0.04	0.04
6-NCHR	1.54	7.25	<iLOQ	<iLOQ
1,3-N_2PYR	5.15	7.34	3.70	0.00
1,6-N_2PYR	30.60	66.93	11.05	3.84
1,8-N_2PYR	36.68	80.24	13.39	3.01
6-NBAP	1.14	4.49	0.11	0.04

Table S8. Blank subtracted total LOQ (maximum of iLOQ and fbLOQ) of individual samples of a) 16 USEPA-prioritized PAHs, b) other PAHs, c) OPAHs and d) NPAHs in ng m^{-3}.

a)

Sample	ACY	ACE	FLN	PHE	ANT	FLT	PYR	BAA	CHR	BBF	BKF	BAP	INP	DBA	BPE
D1	3.2E-03	1.0E-02	1.7E-02	2.5E-02	1.0E-03	2.7E-02	1.8E-02	1.4E-03	3.3E-03	8.7E-04	9.9E-04	1.4E-03	7.8E-04	1.6E-03	6.5E-04
D2	3.2E-03	1.0E-02	1.7E-02	2.5E-02	9.9E-04	2.7E-02	1.8E-02	1.4E-03	3.3E-03	8.6E-04	9.8E-04	1.3E-03	7.7E-04	1.6E-03	6.4E-04
D3	3.2E-03	1.0E-02	1.7E-02	2.5E-02	1.0E-03	2.7E-02	1.8E-02	1.4E-03	3.3E-03	8.6E-04	9.8E-04	1.3E-03	7.7E-04	1.6E-03	6.4E-04
D4	3.6E-03	1.2E-02	1.9E-02	2.8E-02	1.1E-03	3.1E-02	2.0E-02	1.6E-03	3.8E-03	9.8E-04	1.1E-03	1.5E-03	8.8E-04	1.8E-03	7.3E-04
D5	3.2E-03	1.0E-02	1.7E-02	2.5E-02	1.0E-03	2.7E-02	1.8E-02	1.4E-03	3.3E-03	8.6E-04	9.8E-04	1.3E-03	7.7E-04	1.6E-03	6.4E-04
D6	3.1E-03	1.0E-02	1.6E-02	2.4E-02	9.7E-04	2.6E-02	1.7E-02	1.4E-03	3.2E-03	8.4E-04	9.6E-04	1.3E-03	7.5E-04	1.5E-03	6.2E-04
D7	3.1E-03	1.0E-02	1.6E-02	2.4E-02	9.7E-04	2.6E-02	1.7E-02	1.4E-03	3.2E-03	8.4E-04	9.5E-04	1.3E-03	7.5E-04	1.5E-03	6.2E-04
D8	6.3E-03	2.0E-02	3.3E-02	4.9E-02	2.0E-03	5.3E-02	3.5E-02	2.8E-03	6.5E-03	1.7E-03	1.9E-03	2.7E-03	1.5E-03	3.1E-03	1.3E-03
D9	3.2E-03	1.0E-02	1.7E-02	2.4E-02	9.9E-04	2.7E-02	1.8E-02	1.4E-03	3.3E-03	8.5E-04	9.7E-04	1.3E-03	7.6E-04	1.5E-03	6.3E-04
D10	3.2E-03	1.0E-02	1.7E-02	2.5E-02	1.0E-03	2.7E-02	1.8E-02	1.4E-03	3.3E-03	8.7E-04	9.9E-04	1.4E-03	7.8E-04	1.6E-03	6.5E-04
D11	3.2E-03	1.0E-02	1.7E-02	2.5E-02	1.0E-03	2.7E-02	1.8E-02	1.4E-03	3.3E-03	8.6E-04	9.8E-04	1.3E-03	7.7E-04	1.6E-03	6.4E-04
D12	3.2E-03	1.0E-02	1.7E-02	2.5E-02	1.0E-03	2.7E-02	1.8E-02	1.4E-03	3.3E-03	8.6E-04	9.8E-04	1.3E-03	7.7E-04	1.6E-03	6.4E-04
D13	3.2E-03	1.0E-02	1.7E-02	2.5E-02	1.0E-03	2.7E-02	1.8E-02	1.4E-03	3.3E-03	8.6E-04	9.8E-04	1.3E-03	7.7E-04	1.6E-03	6.4E-04
D14	4.4E-03	1.4E-02	2.3E-02	3.4E-02	1.4E-03	3.8E-02	2.5E-02	2.0E-03	4.6E-03	1.2E-03	1.4E-03	1.9E-03	1.1E-03	2.2E-03	8.9E-04
D15	3.2E-03	1.1E-02	1.7E-02	2.5E-02	1.0E-03	2.7E-02	1.8E-02	1.4E-03	3.3E-03	8.8E-04	1.0E-03	1.4E-03	7.8E-04	1.6E-03	6.5E-04
D16	3.1E-03	1.0E-02	1.6E-02	2.4E-02	9.8E-04	2.6E-02	1.7E-02	1.4E-03	3.2E-03	8.5E-04	9.6E-04	1.3E-03	7.6E-04	1.5E-03	6.3E-04
D17	3.1E-03	1.0E-02	1.7E-02	2.4E-02	9.9E-04	2.7E-02	1.7E-02	1.4E-03	3.2E-03	8.5E-04	9.7E-04	1.3E-03	7.6E-04	1.5E-03	6.3E-04
D18	3.3E-03	1.1E-02	1.7E-02	2.5E-02	1.0E-03	2.8E-02	1.8E-02	1.4E-03	3.4E-03	8.8E-04	1.0E-03	1.4E-03	7.9E-04	1.6E-03	6.5E-04
D19	3.2E-03	1.0E-02	1.7E-02	2.5E-02	9.9E-04	2.7E-02	1.8E-02	1.4E-03	3.3E-03	8.6E-04	9.7E-04	1.3E-03	7.7E-04	1.6E-03	6.4E-04
D20	3.2E-03	1.0E-02	1.7E-02	2.5E-02	9.9E-04	2.7E-02	1.8E-02	1.4E-03	3.3E-03	8.6E-04	9.7E-04	1.3E-03	7.6E-04	1.6E-03	6.3E-04
D21	3.3E-03	1.1E-02	1.7E-02	2.5E-02	1.0E-03	2.8E-02	1.8E-02	1.4E-03	3.4E-03	8.8E-04	1.0E-03	1.4E-03	7.9E-04	1.6E-03	6.5E-04
D22	3.1E-03	1.0E-02	1.6E-02	2.4E-02	9.8E-04	2.6E-02	1.7E-02	1.4E-03	3.2E-03	8.4E-04	9.6E-04	1.3E-03	7.5E-04	1.5E-03	6.3E-04
D23	6.1E-03	2.0E-02	3.2E-02	4.7E-02	1.9E-03	5.1E-02	3.4E-02	2.7E-03	6.3E-03	1.6E-03	1.9E-03	2.6E-03	1.5E-03	3.0E-03	1.2E-03
D24	7.6E-03	2.5E-02	4.0E-02	5.9E-02	2.4E-03	6.4E-02	4.2E-02	3.4E-03	7.9E-03	2.1E-03	2.3E-03	3.2E-03	1.8E-03	3.7E-03	1.5E-03
D25	3.2E-03	1.0E-02	1.7E-02	2.4E-02	9.9E-04	2.7E-02	1.8E-02	1.4E-03	3.3E-03	8.5E-04	9.7E-04	1.3E-03	7.6E-04	1.5E-03	6.3E-04
D26	3.1E-03	1.0E-02	1.6E-02	2.4E-02	9.8E-04	2.6E-02	1.7E-02	1.4E-03	3.2E-03	8.5E-04	9.6E-04	1.3E-03	7.6E-04	1.5E-03	6.3E-04
D27	3.2E-03	1.0E-02	1.7E-02	2.5E-02	1.0E-03	2.7E-02	1.8E-02	1.4E-03	3.3E-03	8.7E-04	9.9E-04	1.4E-03	7.7E-04	1.6E-03	6.4E-04

Sample	ACY	ACE	FLN	PHE	ANT	FLT	PYR	BAA	CHR	BBF	BKF	BAP	INP	DBA	BPE
D28	3.1E-03	1.0E-02	1.6E-02	2.4E-02	9.7E-04	2.6E-02	1.7E-02	1.4E-03	3.2E-03	8.4E-04	9.5E-04	1.3E-03	7.5E-04	1.5E-03	6.2E-04
D29	5.1E-03	1.6E-02	2.7E-02	3.9E-02	1.6E-03	4.3E-02	2.8E-02	2.2E-03	5.2E-03	1.4E-03	1.6E-03	2.1E-03	1.2E-03	2.5E-03	1.0E-03
D30	3.1E-03	1.0E-02	1.6E-02	2.4E-02	9.6E-04	2.6E-02	1.7E-02	1.4E-03	3.2E-03	8.3E-04	9.4E-04	1.3E-03	7.4E-04	1.5E-03	6.1E-04
D31	3.1E-03	1.0E-02	1.6E-02	2.4E-02	9.7E-04	2.6E-02	1.7E-02	1.4E-03	3.2E-03	8.4E-04	9.6E-04	1.3E-03	7.5E-04	1.5E-03	6.2E-04
D32	3.1E-03	1.0E-02	1.6E-02	2.4E-02	9.8E-04	2.6E-02	1.7E-02	1.4E-03	3.2E-03	8.5E-04	9.6E-04	1.3E-03	7.6E-04	1.5E-03	6.3E-04
D33	3.9E-03	1.3E-02	2.1E-02	3.0E-02	1.2E-03	3.3E-02	2.2E-02	1.7E-03	4.1E-03	1.1E-03	1.2E-03	1.7E-03	9.5E-04	1.9E-03	7.9E-04
D34	3.2E-03	1.1E-02	1.7E-02	2.5E-02	1.0E-03	2.7E-02	1.8E-02	1.4E-03	3.3E-03	8.8E-04	1.0E-03	1.4E-03	7.8E-04	1.6E-03	6.5E-04
D35	3.4E-03	1.1E-02	1.8E-02	2.6E-02	1.1E-03	2.9E-02	1.9E-02	1.5E-03	3.5E-03	9.2E-04	1.0E-03	1.4E-03	8.2E-04	1.7E-03	6.8E-04
D36	3.2E-03	1.0E-02	1.7E-02	2.5E-02	1.0E-03	2.7E-02	1.8E-02	1.4E-03	3.3E-03	8.7E-04	9.8E-04	1.4E-03	7.7E-04	1.6E-03	6.4E-04
D37	8.8E-03	2.9E-02	4.6E-02	6.8E-02	2.8E-03	7.4E-02	4.9E-02	3.9E-03	9.1E-03	2.4E-03	2.7E-03	3.7E-03	2.1E-03	4.3E-03	1.8E-03
D38	2.3E-03	7.5E-03	1.2E-02	1.8E-02	7.2E-04	1.9E-02	1.3E-02	1.0E-03	2.4E-03	6.2E-04	7.1E-04	9.7E-04	5.6E-04	1.1E-03	4.6E-04
D39	2.5E-03	8.2E-03	1.3E-02	2.0E-02	7.9E-04	2.1E-02	1.4E-02	1.1E-03	2.6E-03	6.8E-04	7.7E-04	1.1E-03	6.1E-04	1.2E-03	5.1E-04
D40	3.2E-03	1.0E-02	1.7E-02	2.5E-02	1.0E-03	2.7E-02	1.8E-02	1.4E-03	3.3E-03	8.6E-04	9.8E-04	1.3E-03	7.7E-04	1.6E-03	6.4E-04
D41	3.5E-03	1.1E-02	1.8E-02	2.7E-02	1.1E-03	2.9E-02	1.9E-02	1.5E-03	3.6E-03	9.4E-04	1.1E-03	1.5E-03	8.4E-04	1.7E-03	6.9E-04
D42	4.4E-03	1.4E-02	2.3E-02	3.4E-02	1.4E-03	3.7E-02	2.4E-02	1.9E-03	4.5E-03	1.2E-03	1.3E-03	1.8E-03	1.1E-03	2.1E-03	8.8E-04
D43	2.4E-03	7.9E-03	1.3E-02	1.9E-02	7.6E-04	2.1E-02	1.4E-02	1.1E-03	2.5E-03	6.6E-04	7.5E-04	1.0E-03	5.9E-04	1.2E-03	4.9E-04
D44	3.1E-03	1.0E-02	1.6E-02	2.4E-02	9.6E-04	2.6E-02	1.7E-02	1.4E-03	3.2E-03	8.3E-04	9.4E-04	1.3E-03	7.4E-04	1.5E-03	6.2E-04
D45	3.1E-03	1.0E-02	1.6E-02	2.4E-02	9.8E-04	2.6E-02	1.7E-02	1.4E-03	3.2E-03	8.5E-04	9.6E-04	1.3E-03	7.6E-04	1.5E-03	6.3E-04
D46	3.1E-03	1.0E-02	1.6E-02	2.4E-02	9.8E-04	2.6E-02	1.7E-02	1.4E-03	3.2E-03	8.5E-04	9.6E-04	1.3E-03	7.6E-04	1.5E-03	6.3E-04
D47	3.2E-03	1.0E-02	1.7E-02	2.5E-02	1.0E-03	2.7E-02	1.8E-02	1.4E-03	3.3E-03	8.7E-04	9.8E-04	1.4E-03	7.7E-04	1.6E-03	6.4E-04
D48	3.3E-03	1.1E-02	1.7E-02	2.6E-02	1.0E-03	2.8E-02	1.8E-02	1.5E-03	3.4E-03	8.9E-04	1.0E-03	1.4E-03	8.0E-04	1.6E-03	6.6E-04
D49	6.6E-03	2.1E-02	3.5E-02	5.1E-02	2.1E-03	5.6E-02	3.7E-02	2.9E-03	6.8E-03	1.8E-03	2.0E-03	2.8E-03	1.6E-03	3.2E-03	1.3E-03
D50	6.5E-03	2.1E-02	3.4E-02	5.1E-02	2.0E-03	5.5E-02	3.6E-02	2.9E-03	6.7E-03	1.8E-03	2.0E-03	2.8E-03	1.6E-03	3.2E-03	1.3E-03
D51	6.5E-03	2.1E-02	3.4E-02	5.0E-02	2.0E-03	5.5E-02	3.6E-02	2.9E-03	6.7E-03	1.8E-03	2.0E-03	2.7E-03	1.6E-03	3.2E-03	1.3E-03
D52	6.5E-03	2.1E-02	3.4E-02	5.0E-02	2.0E-03	5.5E-02	3.6E-02	2.9E-03	6.7E-03	1.8E-03	2.0E-03	2.7E-03	1.6E-03	3.2E-03	1.3E-03
D53	7.7E-03	2.5E-02	4.0E-02	6.0E-02	2.4E-03	6.5E-02	4.3E-02	3.4E-03	8.0E-03	2.1E-03	2.4E-03	3.3E-03	1.9E-03	3.8E-03	1.5E-03
D54	6.6E-03	2.2E-02	3.5E-02	5.1E-02	2.1E-03	5.6E-02	3.7E-02	2.9E-03	6.9E-03	1.8E-03	2.0E-03	2.8E-03	1.6E-03	3.3E-03	1.3E-03
D55	6.4E-03	2.1E-02	3.4E-02	5.0E-02	2.0E-03	5.4E-02	3.6E-02	2.8E-03	6.6E-03	1.7E-03	2.0E-03	2.7E-03	1.5E-03	3.1E-03	1.3E-03
D56	6.9E-03	2.3E-02	3.6E-02	5.4E-02	2.2E-03	5.9E-02	3.9E-02	3.1E-03	7.2E-03	1.9E-03	2.1E-03	2.9E-03	1.7E-03	3.4E-03	1.4E-03
D57	6.4E-03	2.1E-02	3.4E-02	5.0E-02	2.0E-03	5.4E-02	3.6E-02	2.8E-03	6.6E-03	1.7E-03	2.0E-03	2.7E-03	1.6E-03	3.2E-03	1.3E-03
D58	6.8E-03	2.2E-02	3.6E-02	5.3E-02	2.1E-03	5.8E-02	3.8E-02	3.0E-03	7.0E-03	1.8E-03	2.1E-03	2.9E-03	1.6E-03	3.3E-03	1.4E-03

Sample	ACY	ACE	FLN	PHE	ANT	FLT	PYR	BAA	CHR	BBF	BKF	BAP	INP	DBA	BPE
D59	7.7E-03	2.5E-02	4.1E-02	6.0E-02	2.4E-03	6.5E-02	4.3E-02	3.4E-03	8.0E-03	2.1E-03	2.4E-03	3.3E-03	1.9E-03	3.8E-03	1.5E-03
D60	6.5E-03	2.1E-02	3.4E-02	5.0E-02	2.0E-03	5.5E-02	3.6E-02	2.9E-03	6.7E-03	1.7E-03	2.0E-03	2.7E-03	1.6E-03	3.2E-03	1.3E-03
D61	6.4E-03	2.1E-02	3.4E-02	5.0E-02	2.0E-03	5.4E-02	3.6E-02	2.8E-03	6.6E-03	1.7E-03	2.0E-03	2.7E-03	1.6E-03	3.1E-03	1.3E-03
D62	6.4E-03	2.1E-02	3.3E-02	4.9E-02	2.0E-03	5.4E-02	3.5E-02	2.8E-03	6.6E-03	1.7E-03	2.0E-03	2.7E-03	1.5E-03	3.1E-03	1.3E-03

b)

Sample	BJF	BEP	PER	DCA	ATT	COR	TPH	CCP	BGF	BBN	BNT	RET
D1	2.3E-03	8.8E-04	1.1E-03	1.6E-03	1.0E-03	1.1E-03	1.2E-03	3.8E-04	3.1E-03	2.7E-03	3.1E-04	3.1E-03
D2	2.2E-03	8.7E-04	1.1E-03	1.6E-03	1.0E-03	1.1E-03	1.1E-03	3.8E-04	3.0E-03	2.7E-03	3.1E-04	3.1E-03
D3	2.2E-03	8.7E-04	1.1E-03	1.6E-03	1.0E-03	1.1E-03	1.1E-03	3.8E-04	3.0E-03	2.7E-03	3.1E-04	3.1E-03
D4	2.6E-03	9.9E-04	1.3E-03	1.8E-03	1.2E-03	1.2E-03	1.3E-03	4.3E-04	3.4E-03	3.1E-03	3.5E-04	3.6E-03
D5	2.2E-03	8.7E-04	1.1E-03	1.6E-03	1.0E-03	1.1E-03	1.2E-03	3.8E-04	3.0E-03	2.7E-03	3.1E-04	3.1E-03
D6	2.2E-03	8.5E-04	1.1E-03	1.6E-03	1.0E-03	1.0E-03	1.1E-03	3.7E-04	3.0E-03	2.6E-03	3.0E-04	3.0E-03
D7	2.2E-03	8.4E-04	1.1E-03	1.6E-03	9.9E-04	1.0E-03	1.1E-03	3.7E-04	2.9E-03	2.6E-03	3.0E-04	3.0E-03
D8	4.4E-03	1.7E-03	2.2E-03	3.2E-03	2.0E-03	2.1E-03	2.3E-03	7.5E-04	6.0E-03	5.3E-03	6.1E-04	6.1E-03
D9	2.2E-03	8.6E-04	1.1E-03	1.6E-03	1.0E-03	1.1E-03	1.1E-03	3.7E-04	3.0E-03	2.7E-03	3.0E-04	3.1E-03
D10	2.3E-03	8.8E-04	1.1E-03	1.6E-03	1.0E-03	1.1E-03	1.2E-03	3.8E-04	3.1E-03	2.7E-03	3.1E-04	3.1E-03
D11	2.2E-03	8.7E-04	1.1E-03	1.6E-03	1.0E-03	1.1E-03	1.2E-03	3.8E-04	3.0E-03	2.7E-03	3.1E-04	3.1E-03
D12	2.2E-03	8.7E-04	1.1E-03	1.6E-03	1.0E-03	1.1E-03	1.1E-03	3.8E-04	3.0E-03	2.7E-03	3.1E-04	3.1E-03
D13	2.2E-03	8.7E-04	1.1E-03	1.6E-03	1.0E-03	1.1E-03	1.1E-03	3.8E-04	3.0E-03	2.7E-03	3.1E-04	3.1E-03
D14	3.1E-03	1.2E-03	1.6E-03	2.2E-03	1.4E-03	1.5E-03	1.6E-03	5.3E-04	4.2E-03	3.7E-03	4.3E-04	4.3E-03
D15	2.3E-03	8.9E-04	1.2E-03	1.6E-03	1.0E-03	1.1E-03	1.2E-03	3.8E-04	3.1E-03	2.7E-03	3.1E-04	3.2E-03
D16	2.2E-03	8.5E-04	1.1E-03	1.6E-03	1.0E-03	1.0E-03	1.1E-03	3.7E-04	3.0E-03	2.6E-03	3.0E-04	3.1E-03
D17	2.2E-03	8.6E-04	1.1E-03	1.6E-03	1.0E-03	1.0E-03	1.1E-03	3.7E-04	3.0E-03	2.6E-03	3.0E-04	3.1E-03
D18	2.3E-03	8.9E-04	1.2E-03	1.6E-03	1.0E-03	1.1E-03	1.2E-03	3.9E-04	3.1E-03	2.7E-03	3.1E-04	3.2E-03

Sample	BJF	BEP	PER	DCA	ATT	COR	TPH	CCP	BGF	BBN	BNT	RET
D19	2.2E-03	8.7E-04	1.1E-03	1.6E-03	1.0E-03	1.1E-03	1.1E-03	3.8E-04	3.0E-03	2.7E-03	3.1E-04	3.1E-03
D20	2.2E-03	8.7E-04	1.1E-03	1.6E-03	1.0E-03	1.1E-03	1.1E-03	3.8E-04	3.0E-03	2.7E-03	3.1E-04	3.1E-03
D21	2.3E-03	8.9E-04	1.2E-03	1.6E-03	1.0E-03	1.1E-03	1.2E-03	3.9E-04	3.1E-03	2.7E-03	3.1E-04	3.2E-03
D22	2.2E-03	8.5E-04	1.1E-03	1.6E-03	1.0E-03	1.0E-03	1.1E-03	3.7E-04	3.0E-03	2.6E-03	3.0E-04	3.1E-03
D23	4.3E-03	1.7E-03	2.2E-03	3.1E-03	2.0E-03	2.0E-03	2.2E-03	7.2E-04	5.8E-03	5.1E-03	5.9E-04	6.0E-03
D24	5.3E-03	2.1E-03	2.7E-03	3.8E-03	2.4E-03	2.5E-03	2.7E-03	9.0E-04	7.2E-03	6.4E-03	7.3E-04	7.4E-03
D25	2.2E-03	8.6E-04	1.1E-03	1.6E-03	1.0E-03	1.1E-03	1.1E-03	3.8E-04	3.0E-03	2.7E-03	3.0E-04	3.1E-03
D26	2.2E-03	8.6E-04	1.1E-03	1.6E-03	1.0E-03	1.0E-03	1.1E-03	3.7E-04	3.0E-03	2.6E-03	3.0E-04	3.1E-03
D27	2.3E-03	8.8E-04	1.1E-03	1.6E-03	1.0E-03	1.1E-03	1.2E-03	3.8E-04	3.0E-03	2.7E-03	3.1E-04	3.1E-03
D28	2.2E-03	8.4E-04	1.1E-03	1.6E-03	9.9E-04	1.0E-03	1.1E-03	3.7E-04	2.9E-03	2.6E-03	3.0E-04	3.0E-03
D29	3.6E-03	1.4E-03	1.8E-03	2.5E-03	1.6E-03	1.7E-03	1.8E-03	6.0E-04	4.8E-03	4.3E-03	4.9E-04	4.9E-03
D30	2.2E-03	8.4E-04	1.1E-03	1.5E-03	9.8E-04	1.0E-03	1.1E-03	3.6E-04	2.9E-03	2.6E-03	2.9E-04	3.0E-03
D31	2.2E-03	8.5E-04	1.1E-03	1.6E-03	1.0E-03	1.0E-03	1.1E-03	3.7E-04	2.9E-03	2.6E-03	3.0E-04	3.0E-03
D32	2.2E-03	8.5E-04	1.1E-03	1.6E-03	1.0E-03	1.0E-03	1.1E-03	3.7E-04	3.0E-03	2.6E-03	3.0E-04	3.1E-03
D33	2.8E-03	1.1E-03	1.4E-03	2.0E-03	1.3E-03	1.3E-03	1.4E-03	4.7E-04	3.7E-03	3.3E-03	3.8E-04	3.8E-03
D34	2.3E-03	8.9E-04	1.2E-03	1.6E-03	1.0E-03	1.1E-03	1.2E-03	3.8E-04	3.1E-03	2.7E-03	3.1E-04	3.2E-03
D35	2.4E-03	9.3E-04	1.2E-03	1.7E-03	1.1E-03	1.1E-03	1.2E-03	4.0E-04	3.2E-03	2.9E-03	3.3E-04	3.3E-03
D36	2.2E-03	8.7E-04	1.1E-03	1.6E-03	1.0E-03	1.1E-03	1.2E-03	3.8E-04	3.0E-03	2.7E-03	3.1E-04	3.1E-03
D37	6.2E-03	2.4E-03	3.1E-03	4.4E-03	2.8E-03	2.9E-03	3.2E-03	1.0E-03	8.3E-03	7.4E-03	8.5E-04	8.6E-03
D38	1.6E-03	6.3E-04	8.2E-04	1.2E-03	7.4E-04	7.7E-04	8.3E-04	2.7E-04	2.2E-03	1.9E-03	2.2E-04	2.3E-03
D39	1.8E-03	6.9E-04	9.0E-04	1.3E-03	8.1E-04	8.4E-04	9.1E-04	3.0E-04	2.4E-03	2.1E-03	2.4E-04	2.5E-03
D40	2.2E-03	8.7E-04	1.1E-03	1.6E-03	1.0E-03	1.1E-03	1.1E-03	3.8E-04	3.0E-03	2.7E-03	3.1E-04	3.1E-03
D41	2.4E-03	9.5E-04	1.2E-03	1.7E-03	1.1E-03	1.2E-03	1.2E-03	4.1E-04	3.3E-03	2.9E-03	3.3E-04	3.4E-03
D42	3.1E-03	1.2E-03	1.6E-03	2.2E-03	1.4E-03	1.5E-03	1.6E-03	5.2E-04	4.2E-03	3.7E-03	4.2E-04	4.3E-03
D43	1.7E-03	6.7E-04	8.7E-04	1.2E-03	7.8E-04	8.1E-04	8.8E-04	2.9E-04	2.3E-03	2.0E-03	2.3E-04	2.4E-03

Sample	BJF	BEP	PER	DCA	ATT	COR	TPH	CCP	BGF	BBN	BNT	RET
D44	2.2E-03	8.4E-04	1.1E-03	1.5E-03	9.9E-04	1.0E-03	1.1E-03	3.7E-04	2.9E-03	2.6E-03	3.0E-04	3.0E-03
D45	2.2E-03	8.6E-04	1.1E-03	1.6E-03	1.0E-03	1.0E-03	1.1E-03	3.7E-04	3.0E-03	2.6E-03	3.0E-04	3.1E-03
D46	2.2E-03	8.5E-04	1.1E-03	1.6E-03	1.0E-03	1.0E-03	1.1E-03	3.7E-04	3.0E-03	2.6E-03	3.0E-04	3.1E-03
D47	2.3E-03	8.8E-04	1.1E-03	1.6E-03	1.0E-03	1.1E-03	1.2E-03	3.8E-04	3.0E-03	2.7E-03	3.1E-04	3.1E-03
D48	2.3E-03	9.0E-04	1.2E-03	1.7E-03	1.1E-03	1.1E-03	1.2E-03	3.9E-04	3.1E-03	2.8E-03	3.2E-04	3.2E-03
D49	4.6E-03	1.8E-03	2.4E-03	3.3E-03	2.1E-03	2.2E-03	2.4E-03	7.9E-04	6.3E-03	5.6E-03	6.4E-04	6.5E-03
D50	4.6E-03	1.8E-03	2.3E-03	3.3E-03	2.1E-03	2.2E-03	2.4E-03	7.8E-04	6.2E-03	5.5E-03	6.3E-04	6.4E-03
D51	4.6E-03	1.8E-03	2.3E-03	3.3E-03	2.1E-03	2.2E-03	2.3E-03	7.7E-04	6.2E-03	5.5E-03	6.3E-04	6.4E-03
D52	4.5E-03	1.8E-03	2.3E-03	3.2E-03	2.1E-03	2.2E-03	2.3E-03	7.7E-04	6.1E-03	5.4E-03	6.2E-04	6.3E-03
D53	5.4E-03	2.1E-03	2.7E-03	3.9E-03	2.5E-03	2.6E-03	2.8E-03	9.2E-04	7.3E-03	6.5E-03	7.4E-04	7.5E-03
D54	4.7E-03	1.8E-03	2.4E-03	3.3E-03	2.1E-03	2.2E-03	2.4E-03	7.9E-04	6.3E-03	5.6E-03	6.4E-04	6.5E-03
D55	4.5E-03	1.7E-03	2.3E-03	3.2E-03	2.1E-03	2.1E-03	2.3E-03	7.6E-04	6.1E-03	5.4E-03	6.2E-04	6.3E-03
D56	4.9E-03	1.9E-03	2.5E-03	3.5E-03	2.2E-03	2.3E-03	2.5E-03	8.2E-04	6.6E-03	5.8E-03	6.7E-04	6.8E-03
D57	4.5E-03	1.8E-03	2.3E-03	3.2E-03	2.1E-03	2.1E-03	2.3E-03	7.6E-04	6.1E-03	5.4E-03	6.2E-04	6.3E-03
D58	4.8E-03	1.9E-03	2.4E-03	3.4E-03	2.2E-03	2.3E-03	2.5E-03	8.1E-04	6.5E-03	5.7E-03	6.6E-04	6.7E-03
D59	5.4E-03	2.1E-03	2.7E-03	3.9E-03	2.5E-03	2.6E-03	2.8E-03	9.2E-04	7.3E-03	6.5E-03	7.5E-04	7.6E-03
D60	4.5E-03	1.8E-03	2.3E-03	3.2E-03	2.1E-03	2.2E-03	2.3E-03	7.7E-04	6.1E-03	5.4E-03	6.2E-04	6.3E-03
D61	4.5E-03	1.8E-03	2.3E-03	3.2E-03	2.1E-03	2.1E-03	2.3E-03	7.6E-04	6.1E-03	5.4E-03	6.2E-04	6.3E-03
D62	4.5E-03	1.7E-03	2.3E-03	3.2E-03	2.0E-03	2.1E-03	2.3E-03	7.6E-04	6.0E-03	5.3E-03	6.1E-04	6.2E-03

c)

Sample	1,4-O_2NAP	1-(CHO)NAP	9-OFLN	9,10-O_2ANT	1,4-O_2ANT	9,10-O_2PHE	11-OBaFLN	11-OBbFLN	BAN	7,12-O_2BAA	5,12-O_2NAC
D1	2.2E-02	1.2E-02	1.2E-02	5.9E-02	2.0E-03	1.9E-01	4.3E-03	3.2E-03	3.5E-03	3.1E-03	1.4E-03
D2	2.1E-02	1.1E-02	1.2E-02	5.9E-02	1.0E-03	3.8E-01	4.3E-03	3.2E-03	3.4E-03	3.1E-03	1.3E-03

Sample	1,4-O_2NAP	1-(CHO)NAP	9-OFLN	9,10-O_2ANT	1,4-O_2ANT	9,10-O_2PHE	11-OBaFLN	11-OBbFLN	BAN	7,12-O_2BAA	5,12-O_2NAC
D3	2.1E-02	1.1E-02	1.2E-02	5.9E-02	3.6E-03	1.2E+00	4.3E-03	3.2E-03	3.4E-03	3.1E-03	1.4E-03
D4	2.4E-02	1.3E-02	1.4E-02	6.7E-02	6.7E-04	1.2E-01	4.9E-03	3.6E-03	3.9E-03	3.5E-03	1.5E-03
D5	2.1E-02	1.1E-02	1.2E-02	5.9E-02	8.1E-04	1.3E-01	4.3E-03	3.2E-03	3.4E-03	3.1E-03	1.3E-03
D6	2.1E-02	1.1E-02	1.2E-02	5.7E-02	1.9E-03	1.2E-01	4.2E-03	3.1E-03	3.4E-03	3.0E-03	1.3E-03
D7	2.1E-02	1.1E-02	1.2E-02	5.7E-02	1.3E-03	2.0E-01	4.2E-03	3.1E-03	3.3E-03	3.0E-03	1.3E-03
D8	4.2E-02	2.2E-02	2.4E-02	1.2E-01	1.0E-02	5.4E+00	8.5E-03	6.3E-03	6.8E-03	6.1E-03	6.0E-03
D9	2.1E-02	1.1E-02	1.2E-02	5.8E-02	3.7E-03	5.1E-01	4.2E-03	3.2E-03	3.4E-03	3.1E-03	1.3E-03
D10	2.2E-02	1.2E-02	1.3E-02	5.9E-02	1.2E-03	2.7E-01	4.3E-03	3.2E-03	3.5E-03	3.1E-03	1.4E-03
D11	2.1E-02	1.1E-02	1.2E-02	5.9E-02	1.9E-03	1.7E-01	4.3E-03	3.2E-03	3.4E-03	3.1E-03	1.3E-03
D12	2.1E-02	1.1E-02	1.2E-02	5.9E-02	2.5E-03	2.9E-01	4.3E-03	3.2E-03	3.4E-03	3.1E-03	1.3E-03
D13	2.1E-02	1.1E-02	1.2E-02	5.9E-02	9.3E-04	1.9E-01	4.3E-03	3.2E-03	3.4E-03	3.1E-03	1.3E-03
D14	3.0E-02	1.6E-02	1.7E-02	8.2E-02	1.3E-03	2.0E-01	6.0E-03	4.4E-03	4.8E-03	4.3E-03	1.9E-03
D15	2.2E-02	1.2E-02	1.3E-02	6.0E-02	2.4E-03	1.8E-01	4.4E-03	3.2E-03	3.5E-03	3.2E-03	1.4E-03
D16	2.1E-02	1.1E-02	1.2E-02	5.8E-02	1.9E-03	1.0E+00	4.2E-03	3.1E-03	3.4E-03	3.0E-03	1.3E-03
D17	2.1E-02	1.1E-02	1.2E-02	5.8E-02	1.6E-03	4.6E-01	4.2E-03	3.1E-03	3.4E-03	3.1E-03	1.3E-03
D18	2.2E-02	1.2E-02	1.3E-02	6.0E-02	6.1E-03	4.6E+00	4.4E-03	3.3E-03	3.5E-03	3.2E-03	1.5E-03
D19	2.1E-02	1.1E-02	1.2E-02	5.9E-02	8.9E-04	6.6E-01	4.3E-03	3.2E-03	3.4E-03	3.1E-03	1.7E-03
D20	2.1E-02	1.1E-02	1.2E-02	5.8E-02	5.6E-03	1.0E+00	4.3E-03	3.2E-03	3.4E-03	3.1E-03	1.4E-03
D21	2.2E-02	1.2E-02	1.3E-02	6.0E-02	9.4E-04	1.6E-01	4.4E-03	3.3E-03	3.5E-03	3.2E-03	1.4E-03
D22	2.1E-02	1.1E-02	1.2E-02	5.8E-02	1.4E-02	6.7E+00	1.0E-02	7.8E-03	4.2E-03	3.0E-03	2.5E-03
D23	4.1E-02	5.2E-02	2.4E-02	1.1E-01	2.8E-02	1.9E+01	1.3E-02	9.9E-03	6.6E-03	1.9E-02	1.4E-02
D24	5.1E-02	2.7E-02	3.0E-02	1.4E-01	1.9E-03	5.3E-01	1.0E-02	7.6E-03	8.2E-03	7.4E-03	3.2E-03
D25	2.1E-02	1.1E-02	1.2E-02	5.8E-02	1.3E-03	2.6E+00	4.3E-03	3.2E-03	3.4E-03	3.1E-03	1.3E-03
D26	2.1E-02	1.1E-02	1.2E-02	5.8E-02	1.9E-03	1.5E+00	4.2E-03	3.1E-03	3.4E-03	3.1E-03	1.3E-03
D27	2.2E-02	1.1E-02	1.2E-02	5.9E-02	2.4E-03	9.2E-01	4.3E-03	3.2E-03	3.5E-03	3.1E-03	1.3E-03
D28	2.1E-02	1.1E-02	1.2E-02	5.7E-02	2.9E-02	2.2E+00	4.2E-03	3.1E-03	3.3E-03	3.0E-03	1.4E-03
D29	3.4E-02	1.8E-02	2.0E-02	9.3E-02	2.1E-03	1.5E-01	6.8E-03	5.1E-03	5.5E-03	4.9E-03	2.1E-03

Sample	1,4-O_2NAP	1-(CHO)NAP	9-OFLN	9,10-O_2ANT	1,4-O_2ANT	9,10-O_2PHE	11-OBaFLN	11-OBbFLN	BAN	7,12-O_2BAA	5,12-O_2NAC
D30	2.1E-02	1.1E-02	1.2E-02	5.6E-02	3.2E-03	1.4E-01	4.1E-03	3.1E-03	3.3E-03	3.0E-03	1.5E-03
D31	2.1E-02	1.1E-02	1.2E-02	5.7E-02	1.1E-03	3.6E-01	4.2E-03	3.1E-03	3.4E-03	3.0E-03	1.3E-03
D32	2.1E-02	1.1E-02	1.2E-02	5.8E-02	2.7E-03	3.6E-01	4.2E-03	3.1E-03	3.4E-03	3.0E-03	1.3E-03
D33	2.6E-02	1.4E-02	1.5E-02	7.2E-02	1.7E-03	3.2E-01	5.3E-03	3.9E-03	4.2E-03	3.8E-03	1.6E-03
D34	2.2E-02	1.2E-02	1.3E-02	6.0E-02	7.3E-04	1.1E-01	4.4E-03	3.2E-03	3.5E-03	3.2E-03	1.4E-03
D35	2.3E-02	1.2E-02	1.3E-02	6.3E-02	6.8E-04	9.5E-02	4.6E-03	3.4E-03	3.7E-03	3.3E-03	1.4E-03
D36	2.1E-02	1.1E-02	1.2E-02	5.9E-02	5.7E-04	7.6E-02	4.3E-03	3.2E-03	3.5E-03	3.1E-03	1.3E-03
D37	5.9E-02	3.1E-02	3.4E-02	1.6E-01	2.7E-03	4.1E-01	1.2E-02	8.8E-03	9.5E-03	8.6E-03	3.7E-03
D38	1.5E-02	8.3E-03	8.9E-03	4.3E-02	1.5E-03	3.1E-01	3.1E-03	2.3E-03	2.5E-03	2.2E-03	9.7E-04
D39	1.7E-02	9.0E-03	9.8E-03	4.6E-02	6.4E-04	8.4E-02	3.4E-03	2.5E-03	2.7E-03	2.5E-03	1.1E-03
D40	2.1E-02	1.1E-02	1.2E-02	5.9E-02	6.1E-04	6.5E-02	4.3E-03	3.2E-03	3.4E-03	3.1E-03	1.3E-03
D41	2.3E-02	1.2E-02	1.3E-02	6.4E-02	7.7E-04	9.2E-02	4.7E-03	3.5E-03	3.7E-03	3.4E-03	1.5E-03
D42	2.9E-02	1.6E-02	1.7E-02	8.1E-02	5.4E-04	9.0E-02	5.9E-03	4.4E-03	4.7E-03	4.3E-03	1.8E-03
D43	1.6E-02	8.7E-03	9.5E-03	4.5E-02	7.5E-04	1.0E-01	3.3E-03	2.4E-03	2.6E-03	2.4E-03	1.0E-03
D44	2.1E-02	1.1E-02	1.2E-02	5.7E-02	6.1E-04	1.3E-01	4.1E-03	3.1E-03	3.3E-03	3.0E-03	1.3E-03
D45	2.1E-02	1.1E-02	1.2E-02	5.8E-02	8.0E-04	6.5E-02	4.2E-03	3.1E-03	3.4E-03	3.1E-03	1.3E-03
D46	2.1E-02	1.1E-02	1.2E-02	5.8E-02	9.5E-04	1.8E-01	4.2E-03	3.1E-03	3.4E-03	3.0E-03	1.3E-03
D47	2.2E-02	1.1E-02	1.2E-02	5.9E-02	1.7E-03	2.1E-01	4.3E-03	3.2E-03	3.5E-03	3.1E-03	1.3E-03
D48	2.2E-02	1.2E-02	1.3E-02	6.1E-02	1.5E-03	1.6E-01	4.4E-03	3.3E-03	3.6E-03	3.2E-03	1.4E-03
D49	4.4E-02	2.4E-02	2.6E-02	1.2E-01	1.6E-03	2.7E-01	8.9E-03	6.6E-03	7.1E-03	6.4E-03	2.8E-03
D50	4.4E-02	2.3E-02	2.5E-02	1.2E-01	2.3E-03	2.1E-01	8.8E-03	6.5E-03	7.0E-03	6.4E-03	2.7E-03
D51	4.4E-02	2.3E-02	2.5E-02	1.2E-01	1.2E-03	1.0E-01	8.7E-03	6.5E-03	7.0E-03	6.3E-03	2.7E-03
D52	4.3E-02	2.3E-02	2.5E-02	1.2E-01	1.3E-03	1.9E-01	8.7E-03	6.5E-03	7.0E-03	6.3E-03	2.7E-03
D53	5.2E-02	2.8E-02	3.0E-02	1.4E-01	1.5E-03	6.1E-01	1.0E-02	7.7E-03	8.3E-03	7.5E-03	3.2E-03
D54	4.5E-02	2.4E-02	2.6E-02	1.2E-01	6.2E-03	5.7E-01	8.9E-03	6.6E-03	7.2E-03	6.5E-03	2.8E-03
D55	4.3E-02	2.3E-02	2.5E-02	1.2E-01	2.6E-03	2.5E-01	8.6E-03	6.4E-03	6.9E-03	6.2E-03	2.7E-03
D56	4.7E-02	2.5E-02	2.7E-02	1.3E-01	4.2E-03	2.3E-01	9.3E-03	6.9E-03	7.5E-03	6.8E-03	2.9E-03

Sample	1,4-O_2NAP	1-(CHO)NAP	9-OFLN	9,10-O_2ANT	1,4-O_2ANT	9,10-O_2PHE	11-OBaFLN	11-OBbFLN	BAN	7,12-O_2BAA	5,12-O_2NAC
D57	4.3E-02	2.3E-02	2.5E-02	1.2E-01	3.6E-03	6.4E-01	8.7E-03	6.4E-03	6.9E-03	6.3E-03	2.7E-03
D58	4.6E-02	2.4E-02	2.6E-02	1.3E-01	9.5E-03	4.2E-01	9.2E-03	6.8E-03	7.4E-03	6.6E-03	2.9E-03
D59	5.2E-02	2.8E-02	3.0E-02	1.4E-01	3.7E-03	3.9E-01	1.0E-02	7.7E-03	8.3E-03	7.5E-03	3.3E-03
D60	4.3E-02	2.3E-02	2.5E-02	1.2E-01	1.9E-03	3.3E-01	8.7E-03	6.5E-03	7.0E-03	6.3E-03	2.7E-03
D61	4.3E-02	2.3E-02	2.5E-02	1.2E-01	1.5E-03	3.9E-01	8.7E-03	6.4E-03	6.9E-03	6.3E-03	2.9E-03
D62	4.3E-02	2.3E-02	2.5E-02	1.2E-01	1.5E-03	4.0E+00	8.6E-03	6.4E-03	6.9E-03	6.2E-03	2.7E-03

c)

Sample	1-NNAP	2-NNAP	3-NACE	5-NACE	2-NFLN	9-NANT	9-NPHE	3-NPHE	2-NFLT	1-NPYR	2-NPYR	7-NBAA	6-NCHR	1,3-N_2PYR	1,6-N_2PYR	1,8-N_2PYR	6-NBAP
D1	2.4E-03	6.5E-04	1.0E-02	6.2E-04	4.8E-05	2.3E-03	1.9E-03	4.4E-04	5.6E-05	3.6E-04	1.9E-05	1.1E-04	8.3E-05	2.8E-04	6.4E-04	2.7E-04	5.8E-04
D2	4.5E-03	6.4E-04	1.1E-02	1.5E-03	6.1E-05	7.8E-03	4.4E-03	7.2E-04	5.5E-05	4.3E-04	1.8E-05	1.5E-04	1.2E-04	2.5E-04	6.4E-04	2.7E-04	4.8E-04
D3	4.9E-03	6.4E-04	2.7E-02	2.8E-03	1.2E-04	2.4E-02	1.7E-02	2.0E-03	5.5E-05	2.4E-03	5.9E-05	2.5E-04	1.8E-04	2.3E-04	7.2E-04	3.0E-04	6.1E-04
D4	2.2E-03	7.3E-04	8.4E-03	1.8E-03	3.1E-05	2.6E-03	2.4E-03	1.6E-04	6.3E-05	4.1E-04	2.1E-05	1.3E-04	7.8E-05	2.0E-04	4.7E-04	2.0E-04	4.0E-04
D5	2.5E-03	6.4E-04	9.5E-03	1.0E-03	3.7E-05	2.3E-03	2.4E-03	3.0E-04	5.5E-05	3.6E-04	1.3E-04	3.2E-04	2.3E-04	1.7E-04	4.7E-04	2.0E-04	3.9E-04
D6	1.6E-03	6.2E-04	7.5E-03	7.7E-04	3.8E-05	2.3E-03	1.4E-03	1.9E-04	5.4E-05	3.5E-04	1.8E-05	1.1E-04	7.6E-05	1.7E-04	5.2E-04	2.2E-04	3.4E-04
D7	1.8E-03	6.2E-04	8.9E-03	6.6E-04	3.6E-05	2.2E-03	2.2E-03	2.9E-04	5.4E-05	3.4E-04	1.8E-05	1.1E-04	7.5E-05	2.0E-04	4.7E-04	2.0E-04	5.1E-04
D8	6.4E-03	1.3E-03	4.9E-02	5.8E-03	3.2E-04	5.4E-02	2.4E-02	3.4E-03	1.8E-04	7.1E-03	3.6E-04	9.2E-04	6.2E-04	5.6E-04	1.7E-03	7.1E-04	1.4E-03
D9	3.1E-03	6.3E-04	1.7E-02	1.2E-03	5.8E-05	2.4E-03	2.7E-03	4.7E-04	5.5E-05	3.5E-04	1.8E-05	1.1E-04	8.5E-05	2.0E-04	5.0E-04	2.1E-04	1.1E-03
D10	2.9E-03	6.5E-04	1.2E-02	1.3E-03	5.4E-05	3.9E-03	2.5E-03	5.0E-04	5.6E-05	3.6E-04	1.9E-05	1.2E-04	1.0E-04	2.4E-04	5.7E-04	2.4E-04	7.0E-04
D11	2.2E-03	6.4E-04	9.9E-03	6.7E-04	4.0E-05	2.3E-03	2.9E-03	2.9E-04	5.5E-05	3.6E-04	1.9E-05	1.1E-04	8.7E-05	2.7E-04	6.3E-04	2.6E-04	9.8E-04
D12	4.7E-03	6.4E-04	1.2E-02	1.8E-03	5.5E-05	9.7E-03	9.8E-03	6.8E-04	5.5E-05	3.5E-04	1.8E-05	1.3E-04	1.1E-04	2.4E-04	6.6E-04	2.8E-04	5.7E-04
D13	1.6E-03	6.4E-04	1.2E-02	1.7E-03	6.6E-05	4.8E-03	4.6E-03	5.3E-04	5.5E-05	3.5E-04	1.8E-05	1.1E-04	8.1E-05	2.6E-04	5.9E-04	2.5E-04	4.5E-04
D14	2.0E-03	8.9E-04	1.0E-02	9.8E-04	5.5E-05	3.2E-03	2.6E-03	2.6E-04	7.7E-05	5.0E-04	2.6E-05	1.5E-04	9.6E-05	1.9E-04	5.6E-04	2.4E-04	4.4E-04
D15	1.5E-03	6.5E-04	1.0E-02	9.6E-04	4.5E-05	3.7E-03	2.8E-03	4.7E-04	5.6E-05	3.6E-04	1.9E-05	1.1E-04	6.9E-05	1.4E-04	4.7E-04	2.0E-04	4.0E-04
D16	2.0E-03	6.3E-04	2.7E-02	3.0E-03	1.2E-04	1.8E-02	1.1E-02	1.6E-03	5.4E-05	9.5E-04	1.8E-05	3.5E-04	2.4E-04	2.0E-04	5.1E-04	2.1E-04	5.5E-04
D17	2.9E-03	6.3E-04	2.7E-02	2.3E-03	1.1E-04	1.0E-02	6.3E-03	9.6E-04	5.5E-05	5.3E-04	1.8E-05	1.1E-04	9.8E-05	1.2E-04	5.0E-04	2.1E-04	4.1E-04

Sample	1-NNAP	2-NNAP	3-NACE	5-NACE	2-NFLN	9-NANT	9-NPHE	3-NPHE	2-NFLT	1-NPYR	2-NPYR	7-NBAA	6-NCHR	1,3-N_2PYR	1,6-N_2PYR	1,8-N_2PYR	6-NBAP
D18	4.1E-03	6.5E-04	2.6E-02	2.2E-03	2.0E-04	2.9E-02	1.8E-02	1.9E-03	5.7E-05	1.7E-03	1.9E-05	3.0E-04	2.1E-04	1.8E-04	6.7E-04	2.8E-04	5.5E-04
D19	1.7E-03	6.4E-04	1.0E-02	1.3E-03	4.4E-05	7.1E-03	3.4E-03	5.2E-04	5.5E-05	3.9E-04	1.8E-05	1.3E-04	1.1E-04	1.8E-04	4.3E-04	1.8E-04	4.4E-04
D20	7.1E-03	6.3E-04	1.6E-02	2.2E-03	1.5E-04	1.8E-02	1.2E-02	1.2E-03	5.5E-05	1.6E-03	1.8E-05	4.6E-04	3.1E-04	2.1E-04	5.5E-04	2.3E-04	5.2E-04
D21	2.2E-03	6.5E-04	6.2E-03	6.0E-04	2.9E-05	2.4E-03	1.7E-03	1.5E-04	5.6E-05	3.6E-04	1.9E-05	1.1E-04	6.6E-05	1.2E-04	3.9E-04	1.6E-04	3.1E-04
D22	3.6E-02	1.3E-03	5.6E-02	6.2E-03	1.2E-03	4.1E-02	2.0E-02	4.2E-03	5.4E-05	8.4E-03	1.1E-04	7.8E-04	5.0E-04	2.3E-04	1.1E-03	4.6E-04	1.0E-03
D23	4.7E-02	1.2E-03	1.3E-01	1.5E-02	2.5E-03	1.2E-01	5.0E-02	1.3E-02	5.4E-04	3.8E-02	5.9E-04	2.9E-03	1.8E-03	1.0E-03	4.8E-03	2.0E-03	4.4E-03
D24	3.2E-03	1.5E-03	1.8E-02	2.7E-03	9.0E-05	8.6E-03	7.1E-03	8.3E-04	1.3E-04	8.6E-04	4.4E-05	2.6E-04	1.8E-04	3.5E-04	1.1E-03	4.4E-04	9.1E-04
D25	3.2E-03	6.3E-04	1.3E-02	1.3E-03	6.3E-05	5.1E-03	4.0E-03	6.8E-04	5.5E-05	4.5E-04	1.8E-05	1.2E-04	1.0E-04	1.4E-04	4.3E-04	1.8E-04	3.7E-04
D26	2.4E-03	6.3E-04	1.9E-02	2.2E-03	1.2E-04	9.9E-03	1.1E-02	7.4E-04	5.4E-05	5.8E-04	5.6E-05	1.7E-04	1.3E-04	2.0E-04	5.5E-04	2.3E-04	5.3E-04
D27	2.1E-03	6.4E-04	2.6E-02	2.4E-03	2.2E-04	1.8E-02	9.6E-03	1.5E-03	5.6E-05	7.1E-04	1.9E-05	3.1E-04	2.2E-04	2.7E-04	7.1E-04	3.0E-04	7.9E-04
D28	4.6E-03	6.2E-04	3.0E-02	2.5E-03	2.0E-04	2.3E-02	1.2E-02	2.0E-03	5.4E-05	3.9E-03	5.2E-05	5.2E-04	3.5E-04	1.9E-04	6.4E-04	2.7E-04	5.6E-04
D29	2.0E-03	1.0E-03	9.7E-03	7.6E-04	4.9E-05	3.7E-03	1.8E-03	2.3E-04	8.8E-05	5.6E-04	2.9E-05	1.8E-04	9.6E-05	2.4E-04	6.5E-04	2.7E-04	6.2E-04
D30	2.5E-03	6.1E-04	1.4E-02	7.6E-04	4.4E-05	2.2E-03	2.2E-03	4.7E-04	5.3E-05	3.4E-04	1.8E-05	1.1E-04	7.6E-05	1.7E-04	5.6E-04	2.4E-04	3.8E-04
D31	1.6E-03	6.2E-04	2.2E-02	1.6E-03	8.7E-05	6.0E-03	9.3E-03	1.4E-03	5.4E-05	3.5E-04	1.8E-05	1.1E-04	8.9E-05	2.1E-04	6.3E-04	2.6E-04	4.8E-04
D32	4.0E-03	6.3E-04	1.5E-02	1.6E-03	5.5E-05	5.2E-03	3.3E-03	5.1E-04	5.4E-05	3.5E-04	1.8E-05	1.1E-04	8.0E-05	1.4E-04	5.1E-04	2.1E-04	3.1E-04
D33	5.0E-03	7.9E-04	1.4E-02	1.9E-03	5.3E-05	3.9E-03	4.2E-03	4.3E-04	6.8E-05	4.4E-04	2.3E-05	1.4E-04	1.0E-04	1.8E-04	5.7E-04	2.4E-04	5.6E-04
D34	2.0E-03	6.5E-04	7.4E-03	5.1E-04	3.1E-05	2.4E-03	1.4E-03	2.1E-04	5.6E-05	3.6E-04	1.9E-05	1.1E-04	8.9E-05	1.8E-04	4.4E-04	1.8E-04	5.0E-04
D35	3.3E-03	6.8E-04	7.1E-03	1.1E-03	3.2E-05	2.5E-03	2.1E-03	9.2E-04	5.9E-05	3.8E-04	2.0E-05	1.2E-04	7.2E-05	1.6E-04	4.4E-04	1.8E-04	4.5E-04
D36	1.6E-03	6.4E-04	5.9E-03	4.1E-04	2.4E-05	2.3E-03	8.0E-04	1.4E-04	5.5E-05	3.6E-04	1.9E-05	1.1E-04	6.6E-05	1.6E-04	4.5E-04	1.9E-04	4.1E-04
D37	5.3E-03	1.8E-03	2.2E-02	3.6E-03	9.5E-05	8.0E-03	7.0E-03	4.7E-04	1.5E-04	9.8E-04	5.1E-05	3.0E-04	1.8E-04	4.1E-04	1.1E-03	4.7E-04	1.1E-03
D38	4.1E-03	4.6E-04	1.1E-02	2.1E-03	1.0E-04	1.2E-02	5.6E-03	5.6E-04	4.0E-05	5.9E-04	1.3E-05	1.8E-04	1.3E-04	1.0E-04	3.8E-04	1.6E-04	5.5E-04
D39	1.8E-03	5.1E-04	5.2E-03	4.4E-04	2.0E-05	1.8E-03	8.4E-04	1.2E-04	4.4E-05	2.8E-04	1.5E-05	8.7E-05	5.6E-05	1.3E-04	3.3E-04	1.4E-04	3.0E-04
D40	2.3E-03	6.4E-04	7.0E-03	4.1E-04	2.8E-05	2.3E-03	7.6E-04	1.4E-04	5.5E-05	3.6E-04	1.8E-05	1.1E-04	7.5E-05	1.6E-04	4.8E-04	2.0E-04	3.2E-04
D41	2.3E-03	6.9E-04	7.2E-03	5.9E-04	3.0E-05	2.5E-03	1.4E-03	1.6E-04	6.0E-05	3.9E-04	2.0E-05	1.2E-04	7.4E-05	1.6E-04	4.5E-04	1.9E-04	4.5E-04
D42	1.8E-03	8.8E-04	6.9E-03	3.8E-04	2.8E-05	3.2E-03	6.9E-04	2.0E-04	7.6E-05	4.9E-04	2.5E-05	1.5E-04	9.4E-05	1.7E-04	4.9E-04	2.0E-04	3.7E-04
D43	1.8E-03	4.9E-04	6.7E-03	5.8E-04	2.9E-05	1.8E-03	6.7E-03	2.3E-04	4.2E-05	2.7E-04	1.4E-05	8.4E-05	6.1E-05	1.5E-04	3.6E-04	1.5E-04	3.2E-04
D44	1.4E-03	6.2E-04	5.9E-03	4.8E-04	3.1E-05	2.2E-03	8.2E-04	1.4E-04	5.3E-05	3.4E-04	1.8E-05	1.1E-04	7.1E-05	1.7E-04	4.5E-04	1.9E-04	5.1E-04

Sample	1-NNAP	2-NNAP	3-NACE	5-NACE	2-NFLN	9-NANT	9-NPHE	3-NPHE	2-NFLT	1-NPYR	2-NPYR	7-NBAA	6-NCHR	1,3-N_2PYR	1,6-N_2PYR	1,8-N_2PYR	6-NBAP
D45	1.3E-03	6.3E-04	5.8E-03	3.5E-04	2.8E-05	2.3E-03	6.4E-04	1.4E-04	5.4E-05	3.5E-04	1.8E-05	1.1E-04	6.2E-05	2.3E-04	4.8E-04	2.0E-04	4.6E-04
D46	2.1E-03	6.3E-04	6.4E-03	4.5E-04	2.7E-05	2.3E-03	8.0E-04	1.4E-04	5.4E-05	3.5E-04	1.8E-05	1.5E-04	1.2E-04	2.3E-04	6.0E-04	2.5E-04	1.0E-03
D47	2.6E-03	6.4E-04	7.8E-03	6.1E-04	4.2E-05	2.3E-03	1.3E-03	2.3E-04	5.6E-05	3.6E-04	1.9E-05	1.1E-04	7.9E-05	2.4E-04	5.9E-04	2.5E-04	4.6E-04
D48	3.7E-03	6.6E-04	1.1E-02	8.7E-04	9.7E-05	2.4E-03	1.6E-03	2.2E-04	5.7E-05	3.7E-04	1.9E-05	1.1E-04	8.1E-05	2.5E-04	6.5E-04	2.7E-04	4.9E-04
D49	3.9E-03	1.3E-03	1.3E-02	1.2E-03	5.4E-05	4.8E-03	3.5E-03	3.1E-04	1.1E-04	7.4E-04	3.8E-05	2.3E-04	1.4E-04	3.0E-04	8.9E-04	3.7E-04	6.5E-04
D50	5.6E-03	1.3E-03	1.3E-02	1.2E-03	5.0E-05	4.7E-03	2.4E-03	2.9E-04	1.1E-04	7.3E-04	3.8E-05	2.3E-04	1.8E-04	3.7E-04	1.1E-03	4.4E-04	7.1E-04
D51	3.1E-03	1.3E-03	1.0E-02	8.1E-04	5.7E-05	4.7E-03	1.7E-03	2.9E-04	1.1E-04	7.3E-04	3.8E-05	2.2E-04	1.8E-04	3.8E-04	1.1E-03	4.5E-04	7.2E-04
D52	4.8E-03	1.3E-03	1.0E-02	9.7E-04	4.6E-05	4.7E-03	1.7E-03	2.9E-04	1.1E-04	7.2E-04	3.8E-05	2.2E-04	1.8E-04	2.4E-04	7.1E-04	3.0E-04	6.7E-04
D53	3.9E-03	1.5E-03	1.1E-02	7.7E-04	5.0E-05	5.6E-03	1.6E-03	3.5E-04	1.3E-04	8.6E-04	4.5E-05	2.7E-04	2.1E-04	3.3E-04	1.0E-03	4.3E-04	8.1E-04
D54	6.1E-03	1.3E-03	1.4E-02	1.2E-03	5.2E-05	4.8E-03	2.1E-03	3.0E-04	1.2E-04	7.4E-04	4.8E-05	2.3E-04	1.6E-04	3.3E-04	1.1E-03	4.4E-04	8.5E-04
D55	9.4E-03	1.3E-03	1.7E-02	1.3E-03	6.3E-05	4.6E-03	2.6E-03	3.9E-04	1.1E-04	7.1E-04	3.7E-05	2.2E-04	1.8E-04	3.7E-04	9.9E-04	4.1E-04	9.1E-04
D56	3.3E-03	1.4E-03	1.2E-02	7.9E-04	7.5E-05	5.0E-03	1.7E-03	3.1E-04	1.2E-04	7.7E-04	4.0E-05	2.4E-04	1.4E-04	3.0E-04	9.1E-04	3.8E-04	7.4E-04
D57	3.7E-03	1.3E-03	1.5E-02	9.3E-04	6.3E-05	4.7E-03	1.8E-03	2.9E-04	1.1E-04	7.2E-04	3.7E-05	3.1E-04	2.5E-04	6.8E-04	1.3E-03	5.6E-04	1.1E-03
D58	6.6E-03	1.4E-03	2.3E-02	1.8E-03	1.2E-04	5.0E-03	2.8E-03	3.1E-04	1.2E-04	7.6E-04	4.0E-05	2.4E-04	1.7E-04	4.5E-04	1.1E-03	4.7E-04	7.8E-04
D59	5.8E-03	1.5E-03	1.9E-02	1.8E-03	7.2E-05	5.6E-03	3.2E-03	3.5E-04	1.3E-04	8.6E-04	4.5E-05	3.1E-04	2.6E-04	4.6E-04	1.1E-03	4.7E-04	9.6E-04
D60	4.7E-03	1.3E-03	1.1E-02	9.9E-04	6.4E-05	4.7E-03	1.7E-03	2.9E-04	1.1E-04	7.2E-04	3.7E-05	2.2E-04	1.5E-04	2.6E-04	7.7E-04	3.2E-04	6.1E-04
D61	5.5E-03	1.3E-03	1.6E-02	2.1E-03	9.0E-05	4.7E-03	3.4E-03	2.9E-04	1.1E-04	7.2E-04	3.7E-05	2.2E-04	1.3E-04	2.4E-04	7.0E-04	2.9E-04	6.4E-04
D62	4.8E-03	1.3E-03	1.4E-02	8.5E-04	5.0E-05	4.6E-03	1.7E-03	2.9E-04	1.1E-04	7.1E-04	3.7E-05	2.2E-04	1.2E-04	2.9E-04	8.9E-04	3.7E-04	6.6E-04

1.5.3 Aerosol source apportionment

Table S9. Summary of PMF diagnostics as values of objective function Q (USEPA, 2004), results of analysis methods displacement (DISP) and bootstrap (BS). PMF diagnostics are for a) modelled group 1 including sum of individual classes of organic pollutants as PCBs, HCHs, DDX, drins, PAHs, NPAHs and OPAHs – PMF results presented in SI and b) modelled group 2 including selected PAHs, OPAHs and NPAHs – PMF results presented in the main text.

a)

Diagnostic	Ship PM_{10}
Qexpected/theoretical	666
Qtrue	688
Qrobust	688
Species Q/Qexpected >2	–
DISP	0
BS mapping	81 - 99

b)

Diagnostic	Ship PM_{10}
Qexpected/theoretical	789
Qtrue	777
Qrobust	777
Species Q/Qexpected >2	Mn
DISP	0
BS mapping	72 - 100

2 Results

2.1 Concentrations

Table S10. Concentration of 16 USEPA-prioritized PAHs in high-volume samples (sum of gas and particulate phase) in ng m^{-3}. For calculation of the mean, values <LOQ were replaced by LOQ/2 if the detection frequency in all samples exceeded 30 %, else by 0. LOQ values given in Table S7. STD: Standard deviation.

a) in the Mediterranean Sea

Sample	Leg	ACY	ACE	FLN	PHE	ANT	FLT	PYR	BAA	CHR	BBF	BKF	BAP	INP	DBA	BPE	Σ_{15}PAHs
D1	1	1.7E-03	3.7E-02	9.0E-02	8.0E-01	6.0E-02	1.2E-01	8.2E-02	3.3E-03	2.6E-02	9.9E-03	2.2E-03	2.6E-03	3.6E-03	1.5E-02	3.9E-03	1.3E+00
D4		7.7E-03	2.2E-01	5.8E-01	1.3E+00	5.4E-02	4.2E-02	3.4E-02	1.2E-03	2.8E-03	2.5E-03	9.9E-04	1.4E-03	2.1E-03	1.4E-02	3.4E-03	2.3E+00
D5		2.6E-02	2.4E-01	4.7E-01	1.5E+00	1.0E-01	1.7E-01	1.5E-01	2.5E-03	1.4E-02	5.4E-03	1.2E-03	3.4E-04	9.2E-04	5.5E-03	1.2E-03	2.6E+00
D6		9.9E-03	2.0E-01	3.5E-01	1.1E+00	1.0E-01	1.4E-01	9.4E-02	2.4E-03	7.2E-03	5.6E-03	1.8E-03	2.2E-03	3.9E-03	1.8E-02	3.8E-03	2.0E+00
D7		1.7E-03	4.0E-02	2.7E-01	1.6E+00	1.7E-01	2.3E-01	1.9E-01	3.5E-03	1.3E-02	1.0E-02	3.3E-03	5.1E-03	6.8E-03	2.0E-02	7.0E-03	2.5E+00
D49	2	1.2E-02	6.0E-01	1.3E+00	2.2E+00	2.6E-01	2.3E-01	1.8E-01	7.7E-03	1.7E-02	2.0E-02	7.1E-03	1.1E-02	1.5E-02	2.1E-02	1.4E-02	4.7E+00
D50		2.1E-02	2.0E+00	4.0E+00	4.2E+00	4.9E-01	3.3E-01	1.9E-01	9.0E-03	1.7E-02	1.8E-02	6.8E-03	1.0E-02	1.2E-02	2.1E-02	1.1E-02	1.1E+01
D51		<6.5E-03	1.4E-01	2.8E-01	6.4E-01	8.2E-02	8.8E-02	8.2E-02	8.1E-03	1.4E-02	1.6E-02	5.8E-03	9.7E-03	1.1E-02	6.7E-03	1.1E-02	1.4E+00
D52		1.2E-02	1.4E+00	2.9E+00	2.5E+00	2.5E-01	1.8E-01	1.2E-01	5.3E-03	1.2E-02	1.3E-02	4.5E-03	7.4E-03	9.0E-03	4.2E-02	9.0E-03	7.5E+00
D53		4.0E-03	7.6E-02	3.4E-01	6.4E-01	8.1E-02	7.9E-02	8.5E-02	5.5E-03	8.7E-03	1.3E-02	4.7E-03	7.5E-03	9.1E-03	1.8E-02	8.9E-03	1.4E+00
D54		2.3E-02	3.2E+00	6.4E+00	6.0E+00	9.2E-01	4.6E-01	2.7E-01	3.5E-03	9.7E-03	1.1E-02	3.9E-03	5.5E-03	7.7E-03	1.5E-02	6.9E-03	1.7E+01
D55		<6.4E-03	8.1E-02	4.8E-01	2.4E+00	3.3E-01	2.4E-01	1.8E-01	3.4E-03	8.3E-03	1.2E-02	4.4E-03	6.8E-03	9.1E-03	2.3E-02	8.5E-03	3.8E+00
D56		<6.9E-03	<2.3E-02	4.9E-02	1.7E-01	1.1E-02	3.3E-02	2.4E-02	3.1E-03	7.4E-03	8.8E-03	3.3E-03	3.6E-03	7.1E-03	1.9E-02	6.3E-03	3.6E-01
D57		3.6E-03	2.5E-01	1.4E+00	1.3E+00	1.5E-01	1.8E-01	1.2E-01	8.5E-03	1.9E-02	2.9E-02	1.1E-02	1.6E-02	1.9E-02	5.6E-02	1.8E-02	3.5E+00
D58		4.1E-03	3.2E-01	7.0E-01	2.3E+00	2.1E-01	4.4E-01	2.8E-01	2.8E-02	5.5E-02	7.0E-02	2.4E-02	4.8E-02	6.4E-02	1.8E-02	6.0E-02	4.6E+00

Sam-ple	Leg	ACY	ACE	FLN	PHE	ANT	FLT	PYR	BAA	CHR	BBF	BKF	BAP	INP	DBA	BPE	Σ_{15}PAHs
D59		4.2E-03	2.6E-01	1.4E+00	1.3E+00	1.2E-01	1.2E-01	1.1E-01	3.4E-03	9.4E-03	1.1E-02	3.9E-03	5.0E-03	7.6E-03	9.0E-03	7.3E-03	3.4E+00
D60		3.5E-03	7.2E-01	7.7E-01	7.8E-01	9.9E-02	7.3E-02	5.2E-02	2.9E-03	8.3E-03	8.4E-03	3.5E-03	4.1E-03	6.3E-03	2.0E-03	5.9E-03	2.5E+00
D61		1.4E-02	7.6E-01	2.7E+00	3.8E+00	5.6E-01	3.9E-01	3.0E-01	1.1E-02	2.1E-02	1.4E-02	4.4E-03	4.4E-03	7.1E-03	1.7E-02	8.5E-03	8.6E+00
D62		3.5E-03	5.8E-02	1.3E-01	4.2E-01	4.5E-02	1.0E-01	7.2E-02	5.0E-03	2.1E-02	2.8E-02	1.0E-02	1.1E-02	1.4E-02	1.7E-02	1.2E-02	9.6E-01
Mean		**8.5E-03**	**5.6E-01**	**1.3E+00**	**1.8E+00**	**2.2E-01**	**1.9E-01**	**1.4E-01**	**6.2E-03**	**1.5E-02**	**1.6E-02**	**5.6E-03**	**8.5E-03**	**1.1E-02**	**1.9E-02**	**1.1E-02**	**4.3E+00**
STD		7.6E-03	8.1E-01	1.6E+00	1.5E+00	2.3E-01	1.3E-01	8.3E-02	5.9E-03	1.1E-02	1.5E-02	5.1E-03	1.0E-02	1.3E-02	1.2E-02	1.2E-02	4.2E+00
Median		4.1E-03	2.4E-01	5.8E-01	1.3E+00	1.2E-01	1.7E-01	1.2E-01	3.5E-03	1.3E-02	1.2E-02	4.4E-03	5.5E-03	7.7E-03	1.8E-02	8.5E-03	2.6E+00

b) in the Northern Red Sea

Sample	Leg	ACY	ACE	FLN	PHE	ANT	FLT	PYR	BAA	CHR	BBF	BKF	BAP	INP	DBA	BPE	Σ_{15}PAHs
D12	1	3.7E-02	4.7E-01	9.7E-01	4.1E+00	2.2E-01	3.9E-01	3.0E-01	7.0E-03	2.2E-02	1.7E-02	6.0E-03	1.0E-02	1.3E-02	2.1E-02	1.4E-02	6.6E+00
D13		2.6E-02	4.5E-01	1.1E+00	4.2E+00	3.8E-01	4.3E-01	3.5E-01	6.6E-03	2.3E-02	1.8E-02	5.8E-03	9.2E-03	1.3E-02	1.2E-02	1.3E-02	7.0E+00
D14		2.4E-03	2.6E-02	1.1E-01	1.5E+00	1.2E-01	1.4E-01	1.3E-01	5.7E-03	1.6E-02	1.6E-02	5.1E-03	6.5E-03	1.0E-02	1.4E-02	9.5E-03	2.2E+00
D45	2	1.7E-03	5.1E-03	1.9E-02	1.6E-01	1.9E-02	5.4E-02	4.7E-02	3.7E-03	7.9E-03	1.2E-02	4.1E-03	7.9E-03	1.0E-02	2.5E-02	1.0E-02	3.9E-01
D46		1.8E-03	2.7E-02	5.5E-02	2.5E-01	1.7E-02	5.6E-02	5.0E-02	5.2E-03	1.5E-02	1.4E-02	4.0E-03	7.6E-03	1.0E-02	2.1E-02	1.0E-02	5.4E-01
D47		4.5E-03	2.6E-02	6.6E-02	3.6E-01	2.3E-02	5.5E-02	5.8E-02	5.5E-03	1.6E-02	1.0E-02	3.2E-03	4.9E-03	7.5E-03	2.4E-02	7.4E-03	6.8E-01
D48		1.9E-03	5.4E-03	5.9E-02	3.5E-01	1.1E-02	6.3E-02	5.6E-02	6.3E-03	2.0E-02	1.5E-02	4.7E-03	3.5E-04	1.2E-02	3.3E-02	1.2E-02	6.5E-01
Mean		**1.1E-02**	**1.4E-01**	**3.4E-01**	**1.6E+00**	**1.1E-01**	**1.7E-01**	**1.4E-01**	**5.7E-03**	**1.7E-02**	**1.4E-02**	**4.7E-03**	**6.7E-03**	**1.1E-02**	**2.2E-02**	**1.1E-02**	**2.6E+00**
STD		1.5E-02	2.2E-01	4.8E-01	1.8E+00	1.4E-01	1.7E-01	1.3E-01	1.1E-03	5.0E-03	2.8E-03	1.0E-03	3.3E-03	2.0E-03	7.0E-03	2.3E-03	3.0E+00
Median		2.4E-03	2.6E-02	6.6E-02	3.6E-01	2.3E-02	6.3E-02	5.8E-02	5.7E-03	1.6E-02	1.5E-02	4.7E-03	7.6E-03	1.0E-02	2.1E-02	1.0E-02	6.8E-01

c) in the Southern Red Sea

Sample	Leg	ACY	ACE	FLN	PHE	ANT	FLT	PYR	BAA	CHR	BBF	BKF	BAP	INP	DBA	BPE	Σ_{15}PAHs
D15	1	1.7E-03	1.5E-02	6.3E-02	2.2E+00	1.1E-01	3.0E-01	2.3E-01	5.8E-03	2.0E-02	1.3E-02	3.7E-03	5.5E-03	8.5E-03	2.8E-02	8.3E-03	3.0E+00
D42	2	1.3E-02	7.2E-03	1.2E-02	6.0E-02	3.7E-03	1.8E-02	1.2E-02	9.7E-04	2.5E-03	5.9E-04	6.7E-04	4.6E-04	2.6E-04	2.1E-03	2.2E-04	1.4E-01
D43		1.3E-03	4.0E-03	1.7E-02	2.9E-01	1.8E-02	6.7E-02	6.4E-02	3.1E-03	6.8E-03	5.8E-03	2.3E-03	3.0E-03	4.6E-03	1.5E-02	4.7E-03	5.1E-01
D44		1.7E-03	5.1E-03	8.9E-03	1.4E-01	1.5E-02	5.1E-02	4.9E-02	4.6E-03	1.3E-02	1.6E-02	5.3E-03	1.1E-02	1.4E-02	2.1E-02	1.3E-02	3.7E-01
D45		1.7E-03	5.1E-03	1.9E-02	1.6E-01	1.9E-02	5.4E-02	4.7E-02	3.7E-03	7.9E-03	1.2E-02	4.1E-03	7.9E-03	1.0E-02	2.5E-02	1.0E-02	3.9E-01
Mean		**3.9E-03**	**7.3E-03**	**2.4E-02**	**5.7E-01**	**3.2E-02**	**9.7E-02**	**8.1E-02**	**3.6E-03**	**1.0E-02**	**9.4E-03**	**3.2E-03**	**5.5E-03**	**7.5E-03**	**1.8E-02**	**7.3E-03**	**8.9E-01**
STD		5.1E-03	4.6E-03	2.2E-02	9.2E-01	4.1E-02	1.1E-01	8.6E-02	1.8E-03	6.9E-03	6.2E-03	1.8E-03	4.0E-03	5.2E-03	1.0E-02	5.0E-03	1.2E+00
Median		1.7E-03	5.1E-03	1.7E-02	1.6E-01	1.8E-02	5.4E-02	4.9E-02	3.7E-03	7.9E-03	1.2E-02	3.7E-03	5.5E-03	8.5E-03	2.1E-02	8.3E-03	3.9E-01

d) in the Arabian Sea

Sample	Leg	ACY	ACE	FLN	PHE	ANT	FLT	PYR	BAA	CHR	BBF	BKF	BAP	INP	DBA	BPE	Σ_{15}PAHs
D35	2	1.7E-03	1.3E-01	1.9E-01	6.5E-01	7.3E-02	1.0E-01	1.5E-01	3.4E-03	5.2E-03	2.3E-03	5.2E-04	8.4E-04	1.3E-03	3.9E-03	1.5E-03	1.3E+00
D36		1.6E-03	2.1E-02	1.7E-02	1.1E-01	1.4E-02	1.5E-02	2.3E-02	1.6E-03	2.5E-03	1.6E-03	4.9E-04	1.0E-03	1.5E-03	1.7E-03	1.7E-03	2.1E-01
D39		1.3E-03	3.9E-02	3.6E-02	1.2E-01	1.4E-02	1.2E-02	2.9E-02	3.3E-03	5.5E-03	2.6E-03	5.8E-04	8.1E-04	1.2E-03	3.2E-03	1.4E-03	2.7E-01
D40		1.7E-03	5.3E-03	3.1E-02	5.2E-01	1.1E-01	9.1E-02	7.4E-02	5.4E-03	8.9E-03	4.9E-03	1.6E-03	1.5E-03	2.4E-03	8.2E-03	2.5E-03	8.7E-01
D41		1.7E-03	5.6E-03	2.6E-02	3.9E-01	3.2E-02	5.5E-02	5.9E-02	3.2E-03	8.2E-03	3.6E-03	1.2E-03	1.3E-03	2.1E-03	7.4E-03	2.3E-03	6.1E-01
D42		1.3E-02	7.2E-03	1.2E-02	6.0E-02	3.7E-03	1.8E-02	1.2E-02	9.7E-04	2.5E-03	5.9E-04	6.7E-04	4.6E-04	2.6E-04	2.1E-03	2.2E-04	1.4E-01
Mean		**3.5E-03**	**3.5E-02**	**5.2E-02**	**3.1E-01**	**4.1E-02**	**4.9E-02**	**5.9E-02**	**3.0E-03**	**5.5E-03**	**2.6E-03**	**8.5E-04**	**9.9E-04**	**1.5E-03**	**4.4E-03**	**1.6E-03**	**5.7E-01**
STD		4.7E-03	5.0E-02	6.9E-02	2.5E-01	4.1E-02	4.1E-02	5.2E-02	1.6E-03	2.7E-03	1.5E-03	4.5E-04	3.7E-04	7.4E-04	2.8E-03	8.2E-04	4.6E-01
Median		1.7E-03	1.4E-02	2.8E-02	2.6E-01	2.3E-02	3.6E-02	4.4E-02	3.3E-03	5.4E-03	2.4E-03	6.3E-04	9.2E-04	1.4E-03	3.5E-03	1.6E-03	4.4E-01

e) in the Gulf of Oman

Sample	Leg	ACY	ACE	FLN	PHE	ANT	FLT	PYR	BAA	CHR	BBF	BKF	BAP	INP	DBA	BPE	Σ_{15}PAHs
D24	1	3.8E-03	1.2E-02	2.0E-02	6.4E-01	5.6E-02	2.5E-01	5.5E-01	5.4E-02	7.5E-02	6.4E-03	2.8E-03	2.6E-03	2.8E-03	1.9E-03	3.4E-03	1.7E+00
D25		1.7E-03	7.2E-02	7.2E-02	1.1E+00	8.0E-02	2.4E-01	3.6E-01	2.8E-02	5.7E-02	5.6E-03	1.7E-03	8.3E-04	1.4E-03	1.0E-02	1.5E-03	2.0E+00
D33	2	4.3E-03	7.7E-02	9.0E-01	1.8E+00	1.6E-01	2.8E-01	3.4E-01	1.3E-02	2.6E-02	1.7E-02	4.7E-03	3.8E-03	1.0E-02	1.4E-02	1.1E-02	3.7E+00
D34		1.8E-03	1.5E-01	9.4E-02	3.1E-01	3.2E-02	4.9E-02	5.8E-02	5.8E-03	1.3E-02	4.4E-03	9.4E-04	3.4E-04	6.1E-04	5.8E-03	7.2E-04	7.3E-01
D35		1.7E-03	1.3E-01	1.9E-01	6.5E-01	7.3E-02	1.0E-01	1.5E-01	3.4E-03	5.2E-03	2.3E-03	5.2E-04	8.4E-04	1.3E-03	3.9E-03	1.5E-03	1.3E+00
Mean		**2.6E-03**	**9.0E-02**	**2.6E-01**	**9.0E-01**	**8.0E-02**	**1.9E-01**	**2.9E-01**	**2.1E-02**	**3.5E-02**	**7.1E-03**	**2.1E-03**	**1.7E-03**	**3.3E-03**	**7.2E-03**	**3.6E-03**	**1.9E+00**
STD		1.3E-03	5.6E-02	3.6E-01	5.9E-01	4.8E-02	1.0E-01	1.9E-01	2.1E-02	3.0E-02	5.7E-03	1.7E-03	1.5E-03	4.0E-03	4.9E-03	4.2E-03	1.1E+00
Median		1.8E-03	7.7E-02	9.4E-02	6.5E-01	7.3E-02	2.4E-01	3.4E-01	1.3E-02	2.6E-02	5.6E-03	1.7E-03	8.4E-04	1.4E-03	5.8E-03	1.5E-03	1.7E+00

f) in the Arabian Gulf

Sample	Leg	ACY	ACE	FLN	PHE	ANT	FLT	PYR	BAA	CHR	BBF	BKF	BAP	INP	DBA	BPE	Σ_{15}PAHs
D29	1	2.8E-03	8.2E-03	4.0E-02	9.6E-01	6.0E-02	1.6E-01	1.7E-01	5.8E-03	1.9E-02	1.6E-02	5.2E-03	5.7E-03	1.1E-02	5.3E-02	9.7E-03	1.5E+00
D30		2.0E-03	2.5E-02	5.5E-02	7.2E-01	6.6E-02	2.4E-01	1.9E-01	1.3E-02	2.9E-02	5.1E-02	1.5E-02	3.1E-02	4.6E-02	4.3E-02	4.4E-02	1.6E+00
D31	2	1.8E-03	1.1E-01	2.8E-01	1.7E+00	1.9E-01	3.9E-01	3.4E-01	6.3E-03	2.4E-02	1.6E-02	5.2E-03	6.2E-03	1.2E-02	3.1E-02	1.1E-02	3.2E+00
D32		1.7E-03	4.8E-02	1.3E-01	2.1E+00	2.9E-01	4.6E-01	3.5E-01	6.9E-03	1.8E-02	1.0E-02	2.8E-03	3.0E-03	5.2E-03	1.9E-03	5.8E-03	3.4E+00
D33		4.3E-03	7.7E-02	9.0E-01	1.8E+00	1.6E-01	2.8E-01	3.4E-01	1.3E-02	2.6E-02	1.7E-02	4.7E-03	3.8E-03	1.0E-02	1.4E-02	1.1E-02	3.7E+00
Mean		**2.5E-03**	**5.4E-02**	**2.8E-01**	**1.5E+00**	**1.5E-01**	**3.1E-01**	**2.8E-01**	**9.0E-03**	**2.3E-02**	**2.2E-02**	**6.5E-03**	**9.9E-03**	**1.7E-02**	**2.9E-02**	**1.6E-02**	**2.7E+00**
STD		1.1E-03	4.2E-02	3.6E-01	6.0E-01	9.4E-02	1.2E-01	9.0E-02	3.6E-03	4.4E-03	1.7E-02	4.8E-03	1.2E-02	1.7E-02	2.1E-02	1.6E-02	1.0E+00
Median		2.0E-03	4.8E-02	1.3E-01	1.7E+00	1.6E-01	2.8E-01	3.4E-01	6.9E-03	2.4E-02	1.6E-02	5.2E-03	5.7E-03	1.1E-02	3.1E-02	1.1E-02	3.2E+00

Table S11. Concentration of PAHs, additional to the 16 USEPA-prioritized PAHs, including one S-heterocycle in high-volume samples (sum of gas and particulate phase) in ng m^3. For calculation of the mean, values <LOQ were replaced by LOQ/2 if the detection frequency in all samples exceeded 30 %, else by 0. LOQ values given in Table S7. STD: Standard deviation.

a) in the Mediterranean Sea

Sample	Leg	BJF	BEP	PER	DCA	ATT	COR	TPH	CCP	BGF	BBN	BNT	Σ_{25}PAHs + BNT	RET*
D1		1.92E-03	4.73E-03	2.86E-04	1.09E-02	<LOQ	1.81E-03	1.78E-02	7.27E-04	8.25E-03	5.74E-03	6.88E-03	1.3E+00	1.4E-02
D4		1.24E-03	2.18E-03	3.23E-04	8.77E-03	<LOQ	1.07E-03	2.11E-03	4.75E-04	2.17E-03	1.53E-03	1.45E-03	2.3E+00	6.4E-03
D5	1	1.06E-03	1.92E-03	2.84E-04	4.71E-03	<LOQ	2.66E-04	9.74E-03	3.28E-04	6.00E-03	6.30E-03	6.91E-03	2.7E+00	2.0E-02
D6		2.19E-03	3.76E-03	2.77E-04	1.33E-02	<LOQ	1.83E-03	3.97E-03	5.23E-04	2.46E-03	4.26E-03	3.81E-03	2.0E+00	9.7E-03
D7		3.66E-03	6.88E-03	6.33E-04	1.68E-02	<LOQ	2.99E-03	7.90E-03	1.03E-03	6.01E-03	7.17E-03	6.28E-03	2.6E+00	2.0E-02
D49		7.93E-03	1.20E-02	5.88E-04	2.07E-02	<LOQ	4.77E-03	1.04E-02	2.05E-03	8.72E-03	3.88E-03	7.63E-03	4.9E+00	2.0E-02
D50		7.02E-03	1.13E-02	5.81E-04	1.59E-02	<LOQ	3.61E-03	7.27E-03	2.15E-03	7.84E-03	6.50E-03	5.78E-03	1.1E+01	1.3E-02
D51		4.46E-03	1.04E-02	2.18E-03	2.13E-03	<LOQ	2.45E-03	6.83E-03	1.22E-03	6.70E-03	3.39E-03	4.91E-03	1.4E+00	6.9E-03
D52		3.40E-03	8.21E-03	2.14E-03	2.99E-02	<LOQ	1.81E-03	8.64E-03	9.38E-04	5.54E-03	2.72E-03	5.74E-03	7.6E+00	9.1E-03
D53		2.87E-03	8.84E-03	2.61E-03	1.41E-02	1.80E-03	1.45E-03	5.13E-03	7.59E-04	5.62E-03	3.24E-03	5.37E-03	1.4E+00	5.0E-03
D54		5.31E-03	8.73E-03	5.90E-04	1.28E-02	<LOQ	2.15E-03	6.23E-03	8.96E-04	5.92E-03	6.81E-03	6.16E-03	1.7E+01	7.9E-03
D55	2	4.10E-03	8.04E-03	0.00E+00	2.23E-02	1.37E-03	2.06E-03	7.43E-03	1.05E-03	5.65E-03	2.69E-03	7.13E-03	3.8E+00	1.2E-02
D56		2.90E-03	6.20E-03	6.17E-04	2.09E-02	1.82E-03	1.51E-03	5.24E-03	6.15E-04	5.43E-03	2.92E-03	3.61E-03	4.1E-01	4.3E-03
D57		1.12E-02	1.94E-02	2.57E-03	3.57E-02	1.11E-03	4.48E-03	1.33E-02	2.50E-03	8.14E-03	4.44E-03	9.61E-03	3.7E+00	2.3E-02
D58		3.15E-02	4.50E-02	6.72E-03	1.23E-02	8.17E-03	2.32E-02	2.77E-02	1.72E-02	3.60E-02	1.90E-02	2.35E-02	4.9E+00	2.3E-01
D59		5.03E-03	7.59E-03	6.87E-04	9.33E-03	<LOQ	1.66E-03	6.06E-03	5.77E-04	5.74E-03	3.25E-03	5.17E-03	3.4E+00	1.6E-02
D60		3.85E-03	6.71E-03	5.74E-04	1.62E-03	<LOQ	1.48E-03	4.53E-03	5.86E-04	4.78E-03	2.72E-03	3.43E-03	2.6E+00	3.8E-03
D61		4.52E-03	9.81E-03	5.72E-04	1.12E-02	<LOQ	2.06E-03	1.03E-02	7.01E-04	1.31E-02	1.42E-02	7.68E-03	8.7E+00	2.1E-02
D62		1.08E-02	1.68E-02	5.65E-04	1.05E-02	<LOQ	2.65E-03	9.18E-03	8.11E-04	5.71E-03	5.48E-03	9.32E-03	1.0E+00	7.4E-03
Mean		**6.1E-03**	**1.0E-02**	**1.2E-03**	**1.4E-02**	**7.5E-04**	**3.3E-03**	**8.9E-03**	**1.9E-03**	**7.9E-03**	**5.6E-03**	**6.9E-03**	**4.4E+00**	**2.3E-02**
STD		6.8E-03	9.4E-03	1.6E-03	8.7E-03	1.9E-03	4.9E-03	5.8E-03	3.8E-03	7.2E-03	4.3E-03	4.5E-03	4.2E+00	**5.0E-02**
Median		4.1E-03	8.2E-03	5.9E-04	1.3E-02	<LOQ	2.1E-03	7.4E-03	8.1E-04	5.9E-03	4.3E-03	6.2E-03	2.7E+00	**1.2E-02**

*RET was measured in samples from the Digitel high-volume sampler but included into $\sum_{19}$RPAHs

b) in the Northern Red Sea

Sample	Leg	BJF	BEP	PER	DCA	ATT	COR	TPH	CCP	BGF	BBN	BNT	Σ_{25}PAHs + BNT	RET*
D12	1	6.86E-03	1.28E-02	1.05E-03	1.63E-02	1.23E-03	6.42E-03	1.16E-02	1.93E-03	8.66E-03	1.12E-02	1.11E-02	6.7E+00	4.5E-02
D13		7.29E-03	1.22E-02	9.55E-04	1.23E-02	8.53E-04	5.80E-03	1.37E-02	1.16E-03	9.84E-03	1.22E-02	1.19E-02	7.1E+00	4.0E-02
D14		5.18E-03	1.04E-02	3.95E-04	1.23E-02	<LOQ	4.22E-03	9.02E-03	7.58E-04	5.10E-03	6.83E-03	7.44E-03	2.2E+00	1.4E-02
D45	2	4.55E-03	8.60E-03	1.06E-03	1.68E-02	1.29E-03	3.69E-03	4.02E-03	8.84E-04	4.24E-03	1.95E-03	3.47E-03	4.4E-01	5.0E-03
D46		4.82E-03	9.13E-03	1.09E-03	1.84E-02	1.25E-03	3.90E-03	1.07E-02	1.06E-03	4.46E-03	4.75E-03	1.01E-02	6.1E-01	6.4E-03
D47		3.41E-03	7.09E-03	8.15E-04	1.45E-02	7.43E-04	3.58E-03	8.95E-03	8.28E-04	5.45E-03	5.05E-03	1.23E-02	7.4E-01	7.6E-03
D48		5.48E-03	1.07E-02	2.93E-04	2.65E-02	<LOQ	6.28E-03	1.37E-02	6.18E-04	6.81E-03	5.32E-03	1.74E-02	7.4E-01	8.6E-03
Mean		**5.4E-03**	**1.0E-02**	**8.1E-04**	**1.7E-02**	**7.7E-04**	**4.8E-03**	**1.0E-02**	**1.0E-03**	**6.4E-03**	**6.8E-03**	**1.1E-02**	**2.7E+00**	**1.8E-02**
STD		1.3E-03	2.0E-03	3.3E-04	4.9E-03	5.6E-04	1.3E-03	3.4E-03	4.3E-04	2.2E-03	3.7E-03	4.3E-03	3.0E+00	1.7E-02
Median		5.2E-03	1.0E-02	9.5E-04	1.6E-02	8.5E-04	4.2E-03	1.1E-02	8.8E-04	5.4E-03	5.3E-03	1.1E-02	7.4E-01	8.6E-03

c) in the Southern Red Sea

Sample	Leg	BJF	BEP	PER	DCA	ATT	COR	TPH	CCP	BGF	BBN	BNT	Σ_{25}PAHs + BNT	RET*
D15	1	4.12E-03	8.11E-03	6.19E-04	2.69E-02	6.14E-04	3.89E-03	1.33E-02	8.19E-04	1.00E-02	8.36E-03	1.18E-02	3.1E+00	3.4E-02
D42	2	2.96E-04	5.98E-04	3.89E-04	3.00E-03	1.56E-03	3.65E-04	7.89E-04	1.30E-04	2.19E-03	1.84E-03	2.11E-04	1.5E-01	2.6E-03
D43		1.93E-03	4.38E-03	5.11E-04	1.23E-02	1.41E-03	2.91E-03	4.19E-03	3.63E-04	2.70E-03	2.26E-03	3.33E-03	5.4E-01	9.0E-03
D44		6.13E-03	1.11E-02	1.33E-03	1.27E-02	5.40E-03	5.19E-03	5.43E-03	1.18E-03	5.32E-03	2.18E-03	4.59E-03	4.3E-01	6.2E-03
D45		4.55E-03	8.60E-03	1.06E-03	1.68E-02	1.29E-03	3.69E-03	4.02E-03	8.84E-04	4.24E-03	1.95E-03	3.47E-03	4.4E-01	5.0E-03
Mean		**3.4E-03**	**6.6E-03**	**7.8E-04**	**1.4E-02**	**2.1E-03**	**3.2E-03**	**5.5E-03**	**6.7E-04**	**4.9E-03**	**3.3E-03**	**4.7E-03**	**9.4E-01**	**1.1E-02**
STD		2.3E-03	4.1E-03	4.0E-04	8.7E-03	1.9E-03	1.8E-03	4.7E-03	4.2E-04	3.1E-03	2.8E-03	4.3E-03	1.2E+00	1.3E-02
Median		4.1E-03	8.1E-03	6.2E-04	1.3E-02	1.4E-03	3.7E-03	4.2E-03	8.2E-04	4.2E-03	2.2E-03	3.5E-03	4.4E-01	6.2E-03

d) in the Arabian Sea

Sample	Leg	BJF	BEP	PER	DCA	ATT	COR	TPH	CCP	BGF	BBN	BNT	Σ$_{25}$PAHs + BNT	RET*
D35	2	5.37E-04	1.56E-03	3.03E-04	2.70E-03	<LOQ	2.84E-04	3.98E-03	2.41E-04	3.72E-03	5.49E-03	3.37E-03	1.4E+00	4.0E-02
D36		5.75E-04	1.44E-03	2.85E-04	1.89E-03	<LOQ	2.67E-04	2.70E-03	9.51E-05	2.07E-03	1.35E-03	1.92E-03	2.3E-01	4.8E-03
D39		5.17E-04	1.92E-03	2.24E-04	3.36E-03	7.61E-04	9.18E-04	3.68E-03	7.49E-05	1.63E-03	2.75E-03	4.19E-03	2.9E-01	4.2E-03
D40		2.77E-03	3.01E-03	6.07E-04	6.48E-03	<LOQ	6.72E-04	4.53E-03	9.46E-05	2.29E-03	4.37E-03	4.54E-03	9.0E-01	6.9E-03
D41		2.54E-03	2.41E-03	3.08E-04	5.25E-03	<LOQ	7.40E-04	7.06E-03	1.03E-04	2.27E-03	3.35E-03	6.32E-03	6.4E-01	7.9E-03
D42		2.96E-04	5.98E-04	3.89E-04	3.00E-03	1.56E-03	3.65E-04	7.89E-04	1.30E-04	2.19E-03	1.84E-03	2.11E-04	1.5E-01	2.6E-03
Mean		**1.2E-03**	**1.8E-03**	**3.5E-04**	**3.8E-03**	**3.9E-04**	**5.4E-04**	**3.8E-03**	**1.2E-04**	**2.4E-03**	**3.2E-03**	**3.4E-03**	**5.9E-01**	**1.1E-02**
STD		1.1E-03	8.4E-04	1.4E-04	1.7E-03	6.5E-04	2.7E-04	2.1E-03	6.0E-05	7.1E-04	1.6E-03	2.1E-03	4.7E-01	1.4E-02
Median		5.6E-04	1.7E-03	3.1E-04	3.2E-03	<LOQ	5.2E-04	3.8E-03	9.9E-05	2.2E-03	3.0E-03	3.8E-03	4.6E-01	5.8E-03

e) in the Gulf of Oman

Sample	Leg	BJF	BEP	PER	DCA	ATT	COR	TPH	CCP	BGF	BBN	BNT	Σ$_{25}$PAHs + BNT	RET*
D24	1	5.15E-04	3.58E-03	6.77E-04	1.91E-03	<LOQ	6.34E-04	5.70E-02	2.26E-04	5.62E-02	7.51E-02	3.81E-02	1.9E+00	9.2E-02
D25		1.08E-03	2.94E-03	2.81E-04	6.21E-03	<LOQ	6.63E-04	4.20E-02	9.38E-05	2.90E-02	3.52E-02	2.72E-02	2.1E+00	6.0E-02
D33	2	4.87E-03	1.13E-02	3.49E-04	7.30E-03	<LOQ	5.08E-03	2.08E-02	6.44E-04	1.53E-02	1.96E-02	1.44E-02	3.8E+00	4.6E-02
D34		2.19E-04	2.98E-03	2.88E-04	4.22E-03	<LOQ	2.70E-04	9.80E-03	9.62E-05	1.60E-03	5.91E-03	1.10E-02	7.6E-01	1.3E-02
D35		5.37E-04	1.56E-03	3.03E-04	2.70E-03	<LOQ	2.84E-04	3.98E-03	2.41E-04	3.72E-03	5.49E-03	3.37E-03	1.4E+00	4.0E-02
Mean		**1.4E-03**	**4.5E-03**	**3.8E-04**	**4.5E-03**	**<LOQ**	**1.4E-03**	**2.7E-02**	**2.6E-04**	**2.1E-02**	**2.8E-02**	**1.9E-02**	**2.0E+00**	**5.0E-02**
STD		1.9E-03	3.9E-03	1.7E-04	2.3E-03	<LOQ	2.1E-03	2.2E-02	2.3E-04	2.2E-02	2.9E-02	1.4E-02	1.1E+00	2.9E-02
Median		5.4E-04	3.0E-03	3.0E-04	4.2E-03	<LOQ	6.3E-04	2.1E-02	2.3E-04	1.5E-02	2.0E-02	1.4E-02	1.9E+00	4.6E-02

f) in the Arabian Gulf

Sample	Leg	BJF	BEP	PER	DCA	ATT	COR	TPH	CCP	BGF	BBN	BNT	Σ_{25}PAHs + BNT	RET*
D29	1	5.85E-03	1.05E-02	4.50E-04	3.85E-02	1.50E-03	4.24E-03	1.05E-02	1.50E-04	5.77E-03	7.04E-03	1.23E-02	1.6E+00	2.6E-02
D30		2.04E-02	3.53E-02	3.51E-03	2.60E-02	5.57E-03	2.20E-02	1.58E-02	5.64E-03	1.15E-02	4.86E-03	2.36E-02	1.7E+00	1.7E-02
D31	2	6.10E-03	1.06E-02	2.76E-04	2.53E-02	<LOQ	5.74E-03	2.00E-02	6.17E-04	1.24E-02	1.07E-02	2.57E-02	3.3E+00	4.6E-02
D32		2.72E-03	5.92E-03	2.78E-04	1.69E-03	<LOQ	2.39E-03	1.37E-02	4.95E-04	8.86E-03	1.19E-02	1.40E-02	3.5E+00	3.3E-02
D33		4.87E-03	1.13E-02	0.00E+00	7.11E-03	<LOQ	5.08E-03	2.08E-02	6.44E-04	1.53E-02	1.96E-02	1.44E-02	3.8E+00	4.6E-02
Mean		**8.0E-03**	**1.5E-02**	**9.0E-04**	**2.0E-02**	**1.4E-03**	**7.9E-03**	**1.6E-02**	**1.5E-03**	**1.1E-02**	**1.1E-02**	**1.8E-02**	**2.8E+00**	**3.3E-02**
STD		7.1E-03	1.2E-02	1.5E-03	1.5E-02	2.4E-03	8.0E-03	4.3E-03	2.3E-03	3.6E-03	5.7E-03	6.2E-03	1.0E+00	1.3E-02
Median		5.8E-03	1.1E-02	2.8E-04	2.5E-02	<LOQ	5.1E-03	1.6E-02	6.2E-04	1.1E-02	1.1E-02	1.4E-02	3.3E+00	3.3E-02

Table S12. Concentration of OPAHs in high volume samples (sum of gas and particulate phase) in ng m³. For calculation of the mean, values <LOQ were replaced by LOQ/2 if the detection frequency in all samples exceeded 30 %, else by 0. LOQ values given in Table S7. STD: Standard deviation.

a) in the Mediterranean Sea

Sample	Leg	1,4-O_2NAP	1-(CHO)NAP	9-OFLN	9,10-O_2ANT	1,4-O_2ANT	9,10-O_2PHE	11-OBaFLN	11-OBbFLN	BAN	7,12-O_2BAA	5,12-O_2NAC	Σ_{11}OPAHs
D1	1	8.46E-02	3.85E-02	3.10E-02	6.92E-02	<LOQ	<LOQ	4.57E-02	4.73E-02	2.52E-02	3.98E-02	3.46E-03	3.8E-01
D4	1	<LOQ	2.61E-02	1.38E-02	<LOQ	<LOQ	<LOQ	3.32E-03	6.10E-03	6.75E-03	1.09E-02	1.68E-03	8.5E-02
D5	1	<LOQ	<LOQ	2.49E-02	9.21E-03	<LOQ	<LOQ	1.49E-02	1.33E-02	1.01E-02	1.47E-02	1.83E-03	1.1E-01
D6	1	<LOQ	1.90E-02	1.69E-02	1.02E-02	<LOQ	8.66E-03	9.57E-03	9.00E-03	1.12E-02	1.13E-02	1.36E-03	1.1E-01
D7	1	<LOQ	2.03E-02	2.66E-02	3.45E-03	<LOQ	<LOQ	1.28E-02	1.05E-02	1.09E-02	1.67E-02	1.78E-03	1.1E-01
D49	2	<LOQ	1.18E-02	2.23E-02	2.09E-02	<LOQ	<LOQ	8.23E-03	9.83E-03	1.37E-02	4.67E-03	1.46E-03	1.2E-01
D50	2	2.70E-02	2.70E-02	2.68E-02	4.07E-02	<LOQ	<LOQ	9.80E-03	1.12E-02	1.55E-02	5.35E-03	2.04E-03	1.7E-01
D51	2	4.17E-02	<LOQ	3.34E-02	1.88E-02	<LOQ	<LOQ	7.53E-03	8.23E-03	1.17E-02	4.15E-03	1.36E-03	1.4E-01
D52	2	<LOQ	<LOQ	1.87E-02	5.51E-02	<LOQ	<LOQ	7.54E-03	7.38E-03	1.05E-02	4.68E-03	1.26E-03	1.4E-01
D53	2	1.51E-01	1.58E-02	2.26E-02	2.54E-02	<LOQ	<LOQ	7.78E-03	8.28E-03	9.52E-03	4.77E-03	1.07E-03	2.5E-01
D54	2	2.34E-01	1.30E-02	4.70E-02	2.56E-01	<LOQ	<LOQ	8.32E-03	1.02E-02	1.16E-02	4.92E-03	1.41E-03	5.9E-01
D55	2	1.62E-01	1.31E-02	4.47E-02	1.47E-01	<LOQ	<LOQ	6.87E-03	1.04E-02	1.05E-02	7.02E-03	1.48E-03	4.0E-01
D56	2	1.24E-01	<LOQ	2.89E-02	1.31E-01	<LOQ	<LOQ	6.29E-03	6.64E-03	9.91E-03	3.98E-03	9.61E-04	3.2E-01
D57	2	4.30E-01	3.68E-02	9.66E-02	2.75E-01	<LOQ	<LOQ	1.57E-02	2.50E-02	2.43E-02	1.01E-02	4.25E-03	9.2E-01
D58	2	6.84E-01	1.38E-01	1.00E-01	3.08E-01	<LOQ	<LOQ	3.61E-02	5.18E-02	6.67E-02	2.28E-02	1.39E-02	1.4E+00
D59	2	1.79E-01	<LOQ	4.64E-02	1.62E-01	<LOQ	<LOQ	8.09E-03	8.79E-03	1.27E-02	5.32E-03	1.91E-03	4.4E-01
D60	2	1.75E-01	<LOQ	2.70E-02	1.23E-01	<LOQ	<LOQ	6.98E-03	7.57E-03	9.81E-03	4.09E-03	1.37E-03	3.7E-01
D61	2	4.59E-02	9.56E-02	2.65E-02	<LOQ	<LOQ	<LOQ	1.62E-02	1.36E-02	2.50E-02	6.73E-03	2.70E-03	2.4E-01
D62	2	2.14E-01	1.23E-02	3.29E-02	1.46E-01	<LOQ	<LOQ	1.93E-02	2.40E-02	2.13E-02	1.06E-02	3.90E-03	4.8E-01
Mean		**1.4E-01**	**2.8E-02**	**3.6E-02**	**9.5E-02**	<LOQ	**4.6E-04**	**1.3E-02**	**1.5E-02**	**1.7E-02**	**1.0E-02**	**2.6E-03**	**3.6E-01**
STD		1.7E-01	3.3E-02	2.4E-02	9.9E-02		2.0E-03	1.1E-02	1.3E-02	1.3E-02	8.8E-03	2.9E-03	3.3E-01
Median		8.5E-02	1.4E-02	2.7E-02	5.5E-02	<LOQ	<LOQ	8.3E-03	1.0E-02	1.2E-02	6.7E-03	1.7E-03	2.5E-01

b) in the Northern Red Sea

Sample	Leg	1,4-O_2NAP	1-(CHO)NAP	9-OFLN	9,10-O_2ANT	1,4-O_2ANT	9,10-O_2PHE	11-OBaFLN	11-OBbFLN	BAN	7,12-O_2BAA	5,12-O_2NAC	Σ_{11}OPAHs
D12	1	<LOQ	5.15E-02	5.36E-02	1.09E-02	<LOQ	9.48E-03	2.21E-02	1.36E-02	1.50E-02	1.56E-02	1.64E-03	2.0E-01
D13		<LOQ	3.46E-02	4.44E-02	<LOQ	<LOQ	1.37E-02	1.88E-02	1.06E-02	1.45E-02	1.34E-02	1.36E-03	1.7E-01
D14		3.01E-02	2.12E-02	1.75E-02	1.09E-02	2.45E-03	<LOQ	1.29E-02	9.97E-03	7.79E-03	8.00E-03	1.33E-03	1.2E-01
D45	2	3.85E-02	6.49E-03	6.72E-03	<LOQ	<LOQ	<LOQ	5.33E-03	4.73E-03	6.59E-03	4.34E-03	1.25E-03	7.7E-02
D46		7.41E-02	7.14E-03	1.18E-02	7.05E-02	<LOQ	<LOQ	8.51E-03	5.33E-03	1.06E-02	9.98E-03	1.76E-03	2.0E-01
D47		1.11E-01	3.73E-02	1.94E-02	7.75E-02	3.36E-04	<LOQ	1.09E-02	8.57E-03	1.38E-02	8.62E-03	1.89E-03	2.9E-01
D48		1.85E-01	6.72E-03	2.27E-02	7.22E-02	<LOQ	<LOQ	1.45E-02	1.23E-02	1.27E-02	1.09E-02	2.54E-03	3.4E-01
Mean		**6.6E-02**	**2.4E-02**	**2.5E-02**	**3.6E-02**	**4.0E-04**	**3.3E-03**	**1.3E-02**	**9.3E-03**	**1.2E-02**	**1.0E-02**	**1.7E-03**	**2.0E-01**
STD		6.4E-02	1.8E-02	1.7E-02	3.6E-02	9.1E-04	5.8E-03	5.8E-03	3.3E-03	3.3E-03	3.7E-03	4.5E-04	9.1E-02
Median		3.8E-02	2.1E-02	1.9E-02	1.1E-02	<LOQ	<LOQ	1.3E-02	1.0E-02	1.3E-02	1.0E-02	1.6E-03	2.0E-01

c) in the Southern Red Sea

Sample	Leg	1,4-O_2NAP	1-(CHO)NAP	9-OFLN	9,10-O_2ANT	1,4-O_2ANT	9,10-O_2PHE	11-OBaFLN	11-OBbFLN	BAN	7,12-O_2BAA	5,12-O_2NAC	Σ_{11}OPAHs
D15	1	<LOQ	<LOQ	3.36E-02	<LOQ	<LOQ	<LOQ	1.41E-02	9.99E-03	8.92E-03	1.38E-02	1.02E-03	1.0E-01
D42	2	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	2.84E-03	<LOQ	1.16E-04	3.9E-02
D43		2.64E-02	5.44E-03	1.71E-02	5.46E-02	<LOQ	<LOQ	4.77E-03	2.98E-03	4.85E-03	4.29E-03	6.33E-04	1.2E-01
D44		4.92E-02	7.37E-03	9.49E-03	<LOQ	<LOQ	<LOQ	6.38E-03	6.75E-03	1.15E-02	6.58E-03	1.76E-03	1.0E-01
D45		3.85E-02	6.49E-03	6.72E-03	<LOQ	<LOQ	<LOQ	5.33E-03	4.73E-03	6.59E-03	4.34E-03	1.25E-03	7.7E-02
Mean		**2.8E-02**	**6.6E-03**	**1.4E-02**	**1.4E-02**	<LOQ	<LOQ	**6.7E-03**	**5.3E-03**	**6.9E-03**	**6.0E-03**	**9.6E-04**	**8.8E-02**
STD		1.6E-02	1.0E-03	1.2E-02	2.3E-02			4.3E-03	3.1E-03	3.4E-03	4.8E-03	6.2E-04	3.2E-02
Median		2.6E-02	6.5E-03	9.5E-03	3.6E-03	<LOQ	<LOQ	5.3E-03	4.7E-03	6.6E-03	4.3E-03	1.0E-03	1.0E-01

d) in the Arabian Sea

Sample	Leg	1,4-O_2NAP	1-(CHO)NAP	9-OFLN	9,10-O_2ANT	1,4-O_2ANT	9,10-O_2PHE	11-OBaFLN	11-OBbFLN	BAN	7,12-O_2BAA	5,12-O_2NAC	Σ_{11}OPAHs
D35	2	1.27E-02	1.48E-02	1.03E-02	<LOQ	<LOQ	<LOQ	3.06E-03	3.16E-03	3.53E-03	1.66E-03	2.68E-04	5.3E-02
D36		1.51E-02	7.48E-03	<LOQ	<LOQ	<LOQ	<LOQ	3.12E-03	2.88E-03	3.09E-03	1.21E-03	3.11E-04	3.9E-02
D39		1.18E-02	5.27E-03	<LOQ	<LOQ	<LOQ	<LOQ	2.55E-03	2.36E-03	5.22E-03	3.17E-03	4.94E-04	3.5E-02
D40		1.51E-02	7.12E-03	1.03E-02	<LOQ	<LOQ	<LOQ	3.12E-03	2.92E-03	3.66E-03	4.32E-03	3.98E-04	5.0E-02
D41		3.35E-02	7.93E-03	7.99E-03	<LOQ	<LOQ	<LOQ	3.04E-03	3.50E-03	4.73E-03	4.84E-03	7.66E-04	7.0E-02
D42		<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	2.84E-03	<LOQ	1.16E-04	3.9E-02
Mean		**1.7E-02**	**8.4E-03**	**5.8E-03**	**3.7E-03**	<LOQ	<LOQ	**3.0E-03**	**2.8E-03**	**3.8E-03**	**2.7E-03**	**3.9E-04**	**4.8E-02**
STD		8.1E-03	3.3E-03	4.2E-03	6.7E-04			2.2E-04	4.9E-04	9.4E-04	1.7E-03	2.2E-04	1.3E-02
Median		1.5E-02	7.7E-03	5.3E-03	3.7E-03	<LOQ	<LOQ	3.0E-03	2.9E-03	3.6E-03	2.4E-03	3.5E-04	4.5E-02

e) in the Gulf of Oman

Sample	Leg	1,4-O_2NAP	1-(CHO)NAP	9-OFLN	9,10-O_2ANT	1,4-O_2ANT	9,10-O_2PHE	11-OBaFLN	11-OBbFLN	BAN	7,12-O_2BAA	5,12-O_2NAC	Σ_{11}OPAHs
D24	1	<LOQ	1.47E-02	1.33E-02	<LOQ	<LOQ	1.20E-01	7.24E-02	4.80E-02	4.73E-02	9.79E-03	1.65E-03	3.6E-01
D25		<LOQ	7.04E-03	1.92E-02	1.05E-02	<LOQ	3.51E-02	4.15E-02	3.32E-02	3.41E-02	1.68E-02	1.58E-03	2.1E-01
D33	2	1.46E-02	1.51E-02	2.32E-02	<LOQ	<LOQ	<LOQ	1.38E-02	1.63E-02	2.33E-02	1.15E-02	2.42E-03	1.2E-01
D34		1.40E-02	7.10E-03	4.29E-03	<LOQ	<LOQ	<LOQ	6.04E-03	4.78E-03	6.86E-03	7.18E-03	8.00E-04	5.5E-02
D35		1.27E-02	1.48E-02	1.03E-02	<LOQ	<LOQ	<LOQ	3.06E-03	3.16E-03	3.53E-03	1.66E-03	2.68E-04	5.3E-02
Mean		**1.5E-02**	**1.2E-02**	**1.4E-02**	**6.2E-03**	<LOQ	**3.1E-02**	**2.7E-02**	**2.1E-02**	**2.3E-02**	**9.4E-03**	**1.3E-03**	**1.6E-01**
STD		5.8E-03	4.3E-03	7.4E-03	3.1E-03		5.2E-02	2.9E-02	1.9E-02	1.8E-02	5.6E-03	8.3E-04	1.3E-01
Median		1.4E-02	1.5E-02	1.3E-02	4.4E-03	<LOQ	<LOQ	1.4E-02	1.6E-02	2.3E-02	9.8E-03	1.6E-03	1.2E-01

f) in the Arabian Gulf

Sample	Leg	1,4-O_2NAP	1-(CHO)NAP	9-OFLN	9,10-O_2ANT	1,4-O_2ANT	9,10-O_2PHE	11-OBaFLN	11-OBbFLN	BAN	7,12-O_2BAA	5,12-O_2NAC	Σ_{11}OPAHs
D29	1	7.84E-02	9.05E-03	1.34E-02	<LOQ	<LOQ	<LOQ	9.52E-03	6.38E-03	1.05E-02	5.35E-03	8.91E-04	1.4E-01
D30		1.59E-01	6.81E-03	3.35E-02	8.77E-02	<LOQ	1.11E-02	1.52E-02	1.01E-02	1.81E-02	1.98E-02	3.00E-03	3.6E-01
D31	2	1.41E-02	1.31E-02	3.71E-02	8.21E-03	<LOQ	<LOQ	2.04E-02	1.28E-02	1.21E-02	1.06E-02	9.56E-04	1.3E-01
D32		5.40E-02	6.16E-03	3.74E-02	1.03E-02	<LOQ	<LOQ	1.35E-02	8.70E-03	8.38E-03	9.26E-03	9.68E-04	1.5E-01
D33		2.63E-03	1.46E-02	2.32E-02	<LOQ	<LOQ	<LOQ	1.38E-02	1.63E-02	2.33E-02	1.15E-02	2.37E-03	1.1E-01
Mean		**6.2E-02**	**1.0E-02**	**2.9E-02**	**2.2E-02**	<LOQ	**2.2E-03**	**1.4E-02**	**1.1E-02**	**1.4E-02**	**1.1E-02**	**1.6E-03**	**1.8E-01**
STD		6.2E-02	3.8E-03	1.0E-02	3.7E-02		5.0E-03	3.9E-03	3.8E-03	6.1E-03	5.3E-03	9.8E-04	1.1E-01
Median		5.4E-02	9.1E-03	3.3E-02	8.2E-03	<LOQ	<LOQ	1.4E-02	1.0E-02	1.2E-02	1.1E-02	9.7E-04	1.4E-01

Table S13. Concentration of NPAHs in high volume samples (sum of gas and particulate phase) in ng m³. For calculation of the mean, values <LOQ were replaced by LOQ/2 if the detection frequency in all samples exceeded 30 %, else by 0. LOQ values given in Table S7. STD: Standard deviation.

a) in the Mediterranean Sea

Sample	Leg	2-NNAP	9-NANT	3-NPHE	2-NFLT	1-NPYR	2-NPYR	7-NBAA	Σ_{17}NPAHs
D1	1	3.58E-03	3.50E-03	1.43E-03	7.68E-03	5.19E-04	1.86E-04	5.57E-05	1.7E-02
D4		9.98E-04	<LOQ	2.05E-04	3.41E-04	<LOQ	5.47E-05	<LOQ	1.8E-03
D5		<LOQ	<LOQ	7.09E-04	8.82E-04	<LOQ	1.73E-05	<LOQ	2.2E-03
D6		7.48E-04	<LOQ	2.89E-04	5.17E-04	5.30E-04	5.67E-05	5.01E-05	2.2E-03
D7		1.09E-03	<LOQ	5.68E-04	2.29E-04	2.41E-04	5.99E-05	6.93E-05	2.3E-03
D49	2	7.07E-04	<LOQ	6.25E-04	4.32E-04	7.4E-04	4.89E-05	<LOQ	2.2E-03
D50		7.09E-04	<LOQ	2.24E-04	2.16E-04	<LOQ	3.02E-05	<LOQ	1.6E-03
D51		<LOQ	<LOQ	1.38E-04	2.24E-04	<LOQ	<LOQ	<LOQ	1.4E-03
D52		6.90E-04	<LOQ	1.79E-04	3.13E-04	<LOQ	<LOQ	<LOQ	1.6E-03
D53		8.41E-04	<LOQ	<LOQ	2.09E-04	<LOQ	2.65E-05	<LOQ	1.6E-03
D54		7.16E-04	7.21E-04	<LOQ	2.71E-04	4.92E-04	3.33E-05	<LOQ	2.3E-03
D55		1.27E-03	<LOQ	2.73E-04	6.36E-04	5.25E-04	2.96E-05	<LOQ	2.8E-03
D56		7.20E-04	<LOQ	2.33E-04	3.43E-04	<LOQ	1.83E-05	<LOQ	1.8E-03
D57		1.46E-03	3.39E-04	4.04E-04	1.40E-03	9.38E-04	<LOQ	<LOQ	4.7E-03
D58		2.99E-02	1.33E-03	1.14E-02	2.97E-03	<LOQ	5.51E-04	<LOQ	4.7E-02
D59		<LOQ	<LOQ	6.57E-04	6.18E-04	<LOQ	2.96E-05	<LOQ	2.6E-03
D60		6.78E-04	<LOQ	3.11E-04	7.26E-05	<LOQ	1.71E-05	<LOQ	1.5E-03
D61		<LOQ	<LOQ	3.84E-04	9.00E-05	4.74E-04	<LOQ	<LOQ	1.7E-03
D62		6.88E-04	<LOQ	3.64E-04	1.67E-04	<LOQ	4.20E-05	<LOQ	1.7E-03
Mean		**2.5E-03**	**3.1E-04**	**9.7E-04**	**9.3E-04**	**4.2E-04**	**6.9E-05**	**5.6E-05**	**5.2E-03**
STD		6.7E-03	8.4E-04	2.5E-03	1.8E-03	1.6E-04	1.2E-04	2.2E-05	1.1E-02
Median		7.2E-04	<LOQ	3.1E-04	3.4E-04	<LOQ	3.0E-05	<LOQ	2.2E-03

b) in the Northern Red Sea

Sample	Leg	2-NNAP	9-NANT	3-NPHE	2-NFLT	1-NPYR	2-NPYR	7-NBAA	Σ_{17}NPAHs
D12	1	1.82E-03	<LOQ	9.22E-04	9.11E-04	3.31E-04	1.22E-04	<LOQ	4.1E-03
D13		1.41E-03	<LOQ	6.61E-04	2.38E-04	<LOQ	5.12E-05	6.88E-05	2.6E-03
D14		1.77E-03	<LOQ	2.60E-04	5.26E-04	<LOQ	7.74E-05	<LOQ	2.9E-03
D45	2	3.34E-04	<LOQ	<LOQ	1.81E-04	<LOQ	2.07E-05	<LOQ	8.4E-04
D46		1.31E-03	4.65E-03	2.63E-04	3.84E-04	<LOQ	2.81E-05	3.22E-04	7.1E-03
D47		2.64E-03	<LOQ	<LOQ	3.18E-04	3.07E-04	2.75E-05	1.39E-04	3.8E-03
D48		5.48E-03	2.29E-03	7.06E-04	9.13E-04	4.93E-04	6.88E-05	2.92E-04	1.0E-02
Mean		**2.1E-03**	**9.9E-04**	**4.6E-04**	**5.0E-04**	**2.7E-04**	**5.7E-05**	**1.3E-04**	**4.5E-03**
STD		1.6E-03	1.8E-03	3.0E-04	3.0E-04	1.2E-04	3.6E-05	1.3E-04	3.2E-03
Median		1.8E-03	0.0E+00	3.3E-04	3.8E-04	<LOQ	5.1E-05	6.9E-05	3.8E-03

c) in the Southern Red Sea

Sample	Leg	2-NNAP	9-NANT	3-NPHE	2-NFLT	1-NPYR	2-NPYR	7-NBAA	Σ_{17}NPAHs
D15	1	2.31E-03	<LOQ	9.95E-04	9.66E-04	<LOQ	3.04E-05	5.47E-05	4.5E-03
D42	2	<LOQ	<LOQ	<LOQ	4.91E-05	<LOQ	4.62E-06	<LOQ	8.1E-04
D43		6.88E-04	<LOQ	1.91E-04	1.68E-04	<LOQ	1.61E-05	<LOQ	1.2E-03
D44		3.62E-04	<LOQ	1.77E-04	2.52E-04	<LOQ	3.12E-05	<LOQ	1.0E-03
D45		3.34E-04	<LOQ	1.05E-04	1.81E-04	<LOQ	2.07E-05	<LOQ	8.4E-04
Mean		**8.3E-04**	<LOQ	**3.0E-04**	**3.2E-04**	**1.8E-04**	**2.1E-05**	**2.9E-05**	**1.7E-03**
STD		8.4E-04		3.9E-04	3.7E-04	3.9E-05	1.1E-05	1.5E-05	1.6E-03
Median		4.4E-04	<LOQ	1.8E-04	1.8E-04	<LOQ	2.1E-05	<LOQ	1.0E-03

d) in the Arabian Sea

Sample	Leg	2-NNAP	9-NANT	3-NPHE	2-NFLT	1-NPYR	2-NPYR	7-NBAA	Σ_{17}NPAHs
D35	2	3.60E-04	<LOQ	<LOQ	7.62E-05	2.98E-04	3.60E-06	<LOQ	1.2E-03
D36		3.32E-04	<LOQ	8.32E-05	7.14E-05	<LOQ	8.45E-06	<LOQ	7.0E-04
D39		2.92E-04	<LOQ	1.28E-04	1.11E-04	<LOQ	7.65E-06	9.25E-05	7.7E-04
D40		3.87E-04	<LOQ	3.29E-05	3.95E-05	3.95E-04	3.36E-06	5.76E-05	9.2E-04
D41		4.03E-04	<LOQ	1.13E-04	1.29E-04	3.09E-04	3.66E-06	<LOQ	9.8E-04
D42		<LOQ	<LOQ	<LOQ	4.91E-05	<LOQ	4.62E-06	<LOQ	8.1E-04
Mean		**3.7E-04**	<LOQ	**1.4E-04**	**7.9E-05**	**2.6E-04**	**5.2E-06**	**4.2E-05**	**8.9E-04**
STD		5.2E-05		1.4E-04	3.5E-05	9.3E-05	2.2E-06	2.8E-05	1.7E-04
Median		3.7E-04	<LOQ	9.8E-05	7.4E-05	2.7E-04	4.1E-06	<LOQ	8.6E-04

e) in the Gulf of Oman

Sample	Leg	2-NNAP	9-NANT	3-NPHE	2-NFLT	1-NPYR	2-NPYR	7-NBAA	Σ_{17}NPAHs
D24	1	<LOQ	<LOQ	1.98E-03	1.13E-04	<LOQ	2.01E-05	5.39E-05	3.4E-03
D25		2.12E-03	<LOQ	1.83E-03	3.14E-04	9.05E-04	7.38E-05	2.74E-05	5.3E-03
D33	2	3.63E-03	<LOQ	1.87E-03	5.34E-04	4.23E-03	6.32E-05	2.06E-04	1.1E-02
D34		<LOQ	<LOQ	3.36E-04	1.58E-04	4.15E-04	5.99E-06	2.54E-04	1.5E-03
D35		3.60E-04	<LOQ	<LOQ	7.62E-05	2.98E-04	3.60E-06	<LOQ	1.2E-03
Mean		**1.4E-03**	<LOQ	**1.3E-03**	**2.4E-04**	**1.3E-03**	**3.3E-05**	**1.1E-04**	**4.4E-03**
STD		1.4E-03		8.3E-04	1.9E-04	1.7E-03	3.3E-05	1.1E-04	3.8E-03
Median		7.6E-04	<LOQ	1.8E-03	1.6E-04	4.3E-04	2.0E-05	5.4E-05	3.4E-03

f) in the Arabian Gulf

Sample	Leg	2-NNAP	9-NANT	3-NPHE	2-NFLT	1-NPYR	2-NPYR	7-NBAA	Σ_{17}NPAHs
D29	1	6.29E-04	<LOQ	2.36E-04	1.33E-04	2.82E-04	3.14E-05	<LOQ	1.3E-03
D30		5.92E-03	<LOQ	1.24E-03	2.15E-03	8.48E-04	1.61E-04	<LOQ	1.0E-02
D31	2	1.86E-03	<LOQ	1.57E-03	4.79E-04	2.09E-03	3.53E-05	<LOQ	6.1E-03
D32		1.94E-03	<LOQ	8.02E-04	1.10E-03	9.89E-04	4.05E-05	9.75E-05	5.0E-03
D33		3.63E-03	<LOQ	1.87E-03	5.34E-04	4.23E-03	6.32E-05	2.06E-04	1.1E-02
Mean		**2.8E-03**	<LOQ	**1.1E-03**	**8.8E-04**	**1.7E-03**	**6.6E-05**	**7.7E-05**	**6.6E-03**
STD		2.0E-03		6.4E-04	7.9E-04	1.6E-03	5.4E-05	7.9E-05	3.9E-03
Median		1.9E-03	<LOQ	1.2E-03	5.3E-04	9.9E-04	4.0E-05	<LOQ	6.1E-03

Table S14. Total concentration (sum of gas and particulate phase) of RPAHs and PHE in high volume samples (sum of gas and particulate phase) in ng m³ (only samples filtered for stack contamination). STD: Standard deviation.

Sample	1-MPHE	2-MPHE	3-MPHE	4-MPHE	3,6-M_2PHE	2,6-M_2PHE	2,7-M_2PHE	1,3-/2,10-/3,9-/1,10-M_2PHE	1,6-/2,9-M_2PHE	1,7-M_2PHE	2,3-M_2PHE	1,9-/4,9-M_2PHE	1,8-M_2PHE	PHE	ΣMPHE/PHE	1,7-M_2PHE/(1,7-M_2PHE+2,6-M_2PHE)
G1	0.111	0.178	0.092	0.101	0.006	0.023	0.029	0.026	0.072	0.039	0.035	0.026	0.006	0.751	0.64	0.62
G2	0.09	0.114	0.057	0.053	0.005	0.019	0.025	0.017	0.045	0.023	0.017	0.017	0.003	0.437	0.72	0.54
G5	0.066	0.088	0.044	0.042	0.003	0.007	0.016	0.011	0.032	0.017	0.015	0.012	0.003	0.389	0.61	0.70
G6	0.214	0.254	0.169	0.133	0.012	0.028	0.053	0.035	0.124	0.06	0.046	0.041	0.009	0.768	1.00	0.68
G7	0.493	0.688	0.37	0.371	0.044	0.14	0.203	0.146	0.442	0.215	0.143	0.131	0.025	1.113	1.73	0.61
G10	0.075	0.105	0.054	0.05	0.004	0.013	0.02	0.01	0.039	0.02	0.015	0.013	0.003	0.469	0.61	0.61
G11	0.475	0.614	0.403	0.336	0.035	0.09	0.169	0.107	0.409	0.189	0.127	0.134	0.028	0.544	3.36	0.68
G20	0.179	0.245	0.144	0.129	0.013	0.033	0.059	0.038	0.126	0.064	0.044	0.042	0.009	0.59	1.18	0.66
G24	0.192	0.264	0.163	0.154	0.013	0.029	0.051	0.036	0.132	0.069	0.056	0.044	0.009	0.573	1.35	0.70
G25	0.134	0.209	0.119	0.113	0.012	0.033	0.044	0.035	0.1	0.058	0.051	0.044	0.009	0.47	1.22	0.64
G27	0.074	0.098	0.052	0.047	0.004	0.01	0.019	0.014	0.043	0.024	0.018	0.017	0.003	0.267	1.02	0.71
G32	0.048	0.065	0.036	0.034	0.003	0.011	0.015	0.011	0.032	0.017	0.012	0.01	0.002	0.231	0.79	0.61
G33	0.145	0.205	0.098	0.099	0.009	0.028	0.043	0.035	0.082	0.045	0.041	0.031	0.007	0.568	0.96	0.62
G34	0.073	0.105	0.053	0.054	0.006	0.012	0.019	0.014	0.043	0.023	0.021	0.015	0.004	0.249	1.14	0.65
G35	0.077	0.133	0.058	0.073	0.009	0.023	0.031	0.025	0.061	0.038	0.037	0.028	0.004	0.237	1.44	0.62
G36	0.084	0.123	0.057	0.059	0.007	0.023	0.032	0.025	0.059	0.031	0.025	0.022	0.005	0.245	1.32	0.57
G37	0.055	0.081	0.037	0.04	0.004	0.013	0.019	0.016	0.037	0.022	0.019	0.017	0.003	0.221	0.96	0.62
G40	0.036	0.045	0.028	0.025	0.002	0.004	0.008	0.006	0.021	0.019	0.009	0.012	0.001	0.205	0.65	0.81

Sample	1-MPHE	2-MPHE	3-MPHE	4-MPHE	3,6-M_2PHE	2,6-M_2PHE	2,7-M_2PHE	1,3-/2,10-/3,9-/1,10-M_2PHE	1,6-/2,9-M_2PHE	1,7-M_2PHE	2,3-M_2PHE	1,9-/4,9-M_2PHE	1,8-M_2PHE	PHE	ΣMPHE/PHE	1,7-M_2PHE/(1,7-M_2PHE+2,6-M_2PHE)
G41	0.037	0.059	0.025	0.026	0.003	0.009	0.014	0.012	0.024	0.012	0.011	0.01	0.002	0.055	2.65	0.58
G42	0.026	0.05	0.019	0.022	0.002	0.006	0.009	0.008	0.018	0.01	0.009	0.007	0.001	0.147	0.79	0.61
G43	0.047	0.066	0.031	0.031	0.003	0.006	0.011	0.008	0.023	0.012	0.011	0.009	0.002	0.267	0.65	0.65
Mean	**0.130**	**0.180**	**0.100**	**0.095**	**0.009**	**0.027**	**0.042**	**0.030**	**0.094**	**0.048**	**0.036**	**0.032**	**0.007**	**0.419**	**1.18**	**0.64**
STD	0.129	0.171	0.105	0.095	0.011	0.032	0.050	0.034	0.116	0.054	0.036	0.035	0.007	0.253	0.67	0.057
Median	0.077	0.114	0.057	0.054	0.006	0.019	0.025	0.017	0.045	0.024	0.021	0.017	0.004	0.389	1.00	0.62

Table S15. Particulate mass (PM), elemental carbon (EC) and organic carbon (OC) concentration in Digitel high volume samples.

Sample	PM [µg m^{-3}]	EC [µg m^{-3}]	OC [µg m^{-3}]
D1	13.07	0.18	1.27
D4	24.04	0.12	1.09
D5	16.38	0.16	0.90
D6	30.80	0.21	1.17
D7	30.95	0.19	1.59
D12	34.93	0.45	2.11
D13	25.88	0.37	1.22
D14	16.10	0.30	0.87
D15	85.19	0.34	1.77
D24	62.38	<LOQ	1.27
D25	101.21	1.92	0.94
D29	80.84	1.13	0.93
D30	77.60	1.55	2.35
D31	79.37	1.00	1.25
D32	89.02	0.81	1.44
D33	58.65	0.72	1.64
D34	70.82	<LOQ	1.36
D35	19.48	<LOQ	0.71
D36	52.22	0.12	1.90
D39	43.22	<LOQ	1.71
D40	55.44	<LOQ	1.66
D41	37.36	<LOQ	1.22
D42	18.02	<LOQ	<LOQ
D43	73.55	0.33	0.84
D44	60.31	0.36	0.99

Sample	PM [µg m^{-3}]	EC [µg m^{-3}]	OC [µg m^{-3}]
D45	39.61	0.38	1.37
D46	37.66	0.38	1.42
D47	32.54	0.30	1.30
D48	124.37	0.24	2.39
D49	42.53	0.21	1.85
D50	53.66	0.17	1.75
D51	36.94	<LOQ	1.71
D52	25.89	<LOQ	1.23
D53	42.48	0.20	2.30
D54	33.53	0.33	3.46
D55	50.43	0.24	2.49
D56	19.23	0.35	1.82
D57	11.59	0.24	3.50
D58	54.59	0.51	3.76
D59	25.72	0.25	3.19
D60	29.56	0.25	2.36
D61	63.53	0.32	2.31
D62	9.57	<LOQ	0.60

2.2 Back trajectories

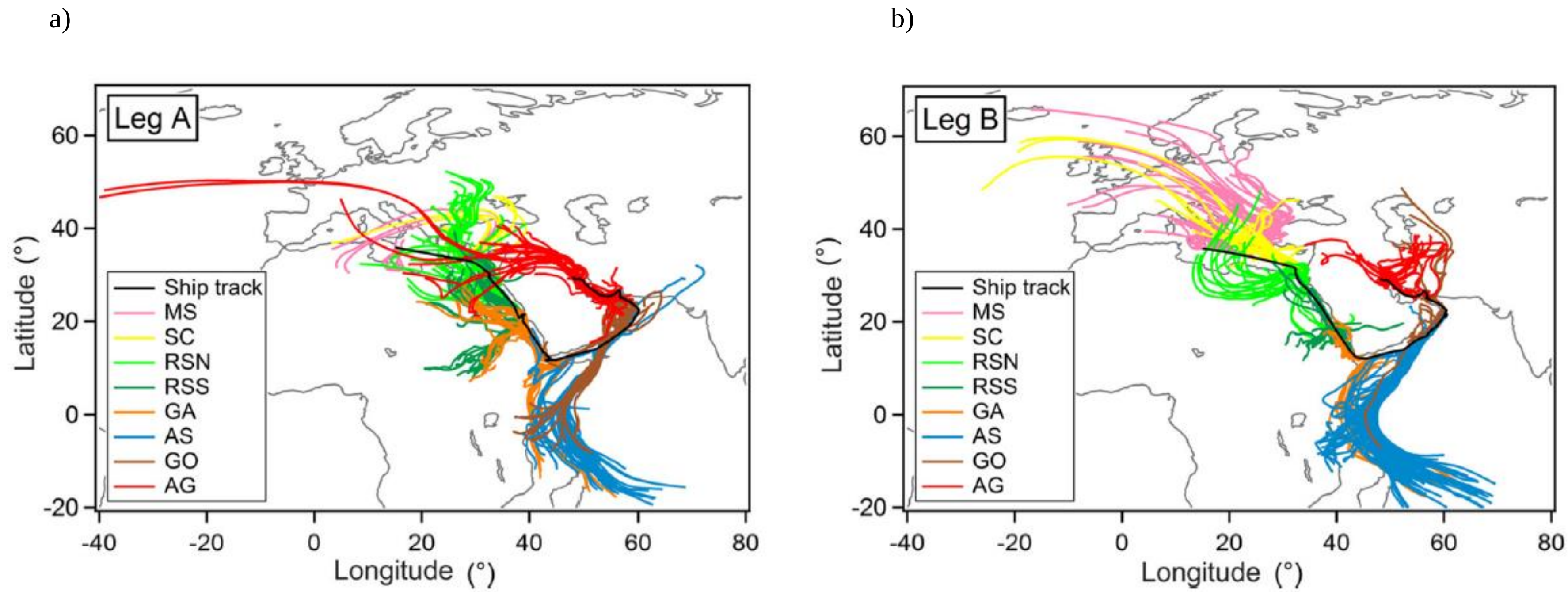
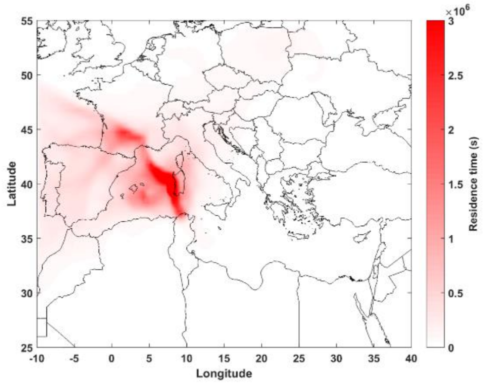


Figure S2. Summary of air mass back trajectories (4 days on an hourly time grid, HYSPLIT model, NOAA) during the AQABA ship campaign, taken from Bourtsoukidis et al. (2019), a) 1. leg; b) 2. leg (MS: Mediterranean Sea; SC: Suez canal; RSN: Northern Red Sea; RSS: Southern Red Sea; GA: Gulf of Aden; AS: Arabian Sea; OG: Gulf of Oman; AG: Arabian Gulf).

Residence time distributions of air mass histories:

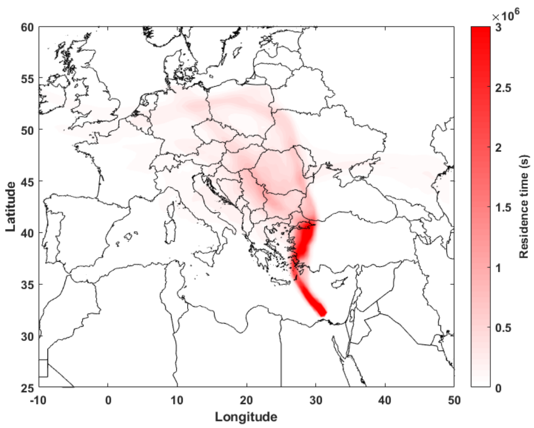
a) Mediterranean Sea:

1. Leg:

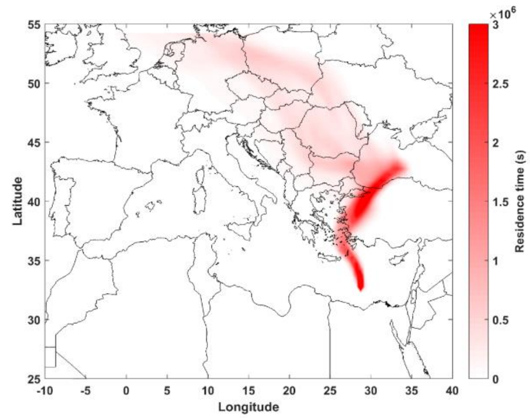


25.-26.06. (D1)

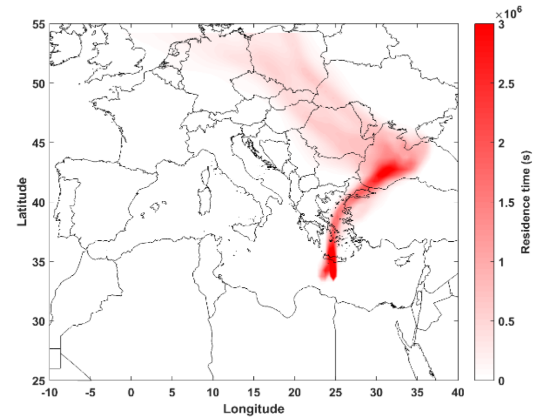
2. Leg:



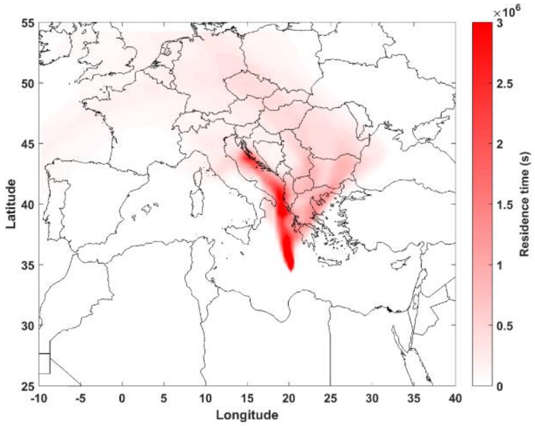
25.08. (D49)



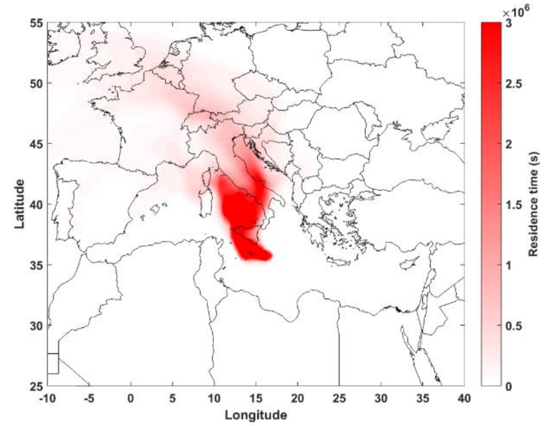
25.-26.08. (D49-51, C27)



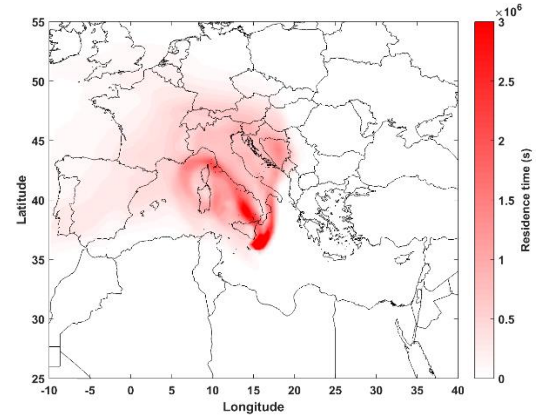
26.-27.08. (D52-53; C28)



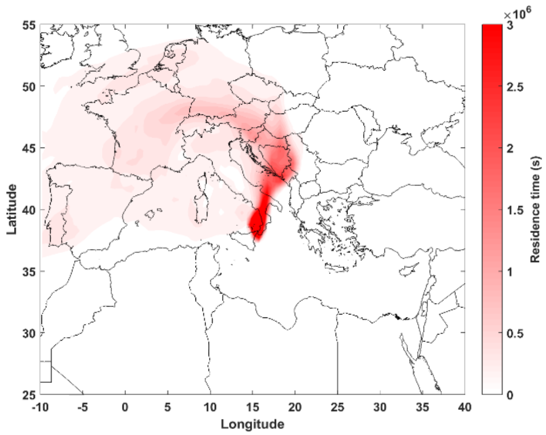
27.-28.08. (D54-55, C29)



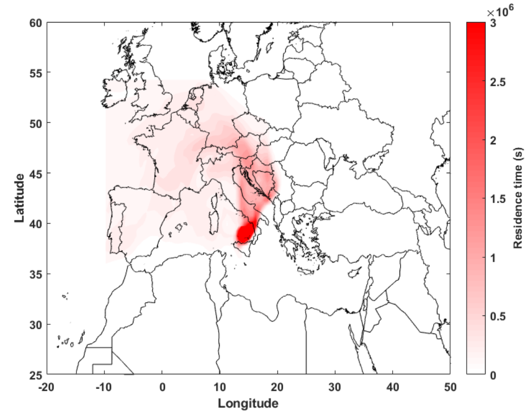
28.-29.08. (D56)



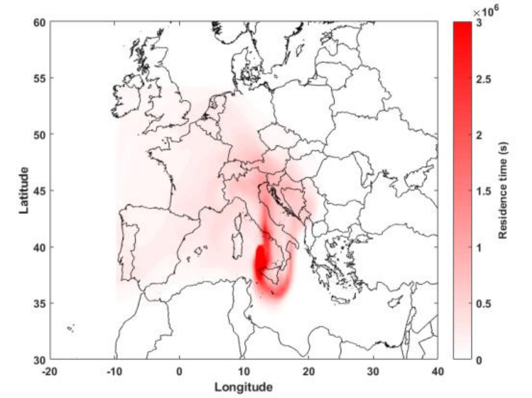
29.-30.08. (D55-58; C30)



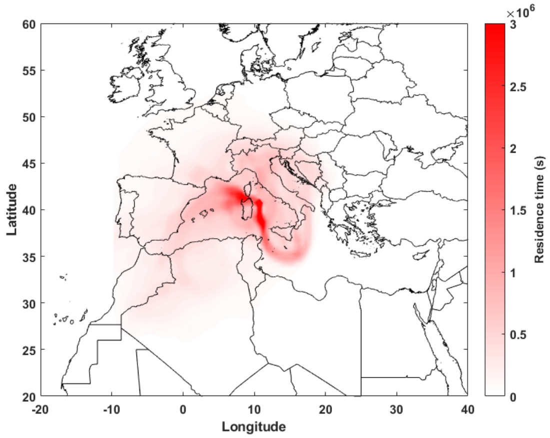
30.-31.08. (D59-60)



31.08. (D60)



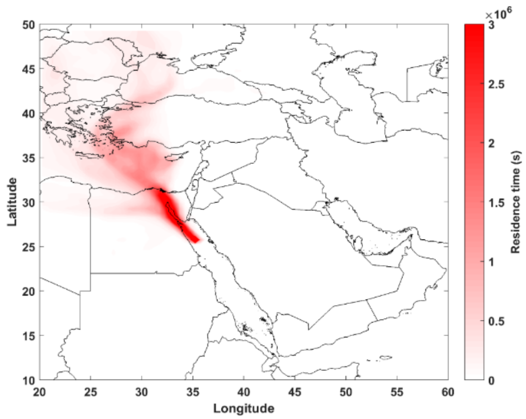
31.08.-01.09. (D61)



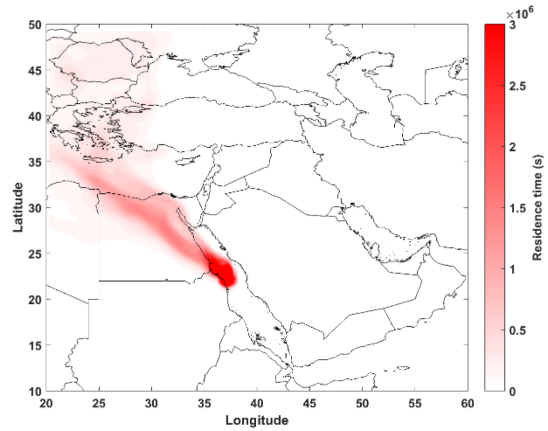
01.09. (D62)

b) Northern Red Sea:

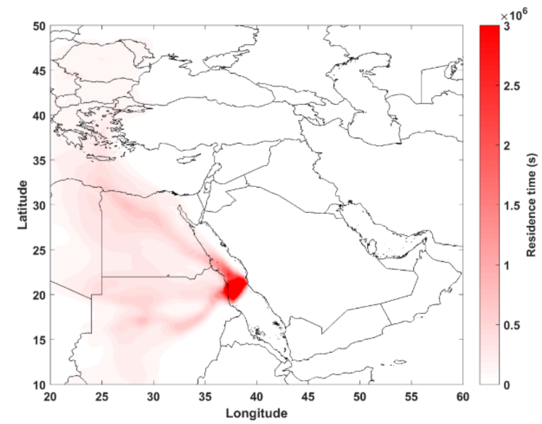
1. Leg:



07.-08.07. (D12)

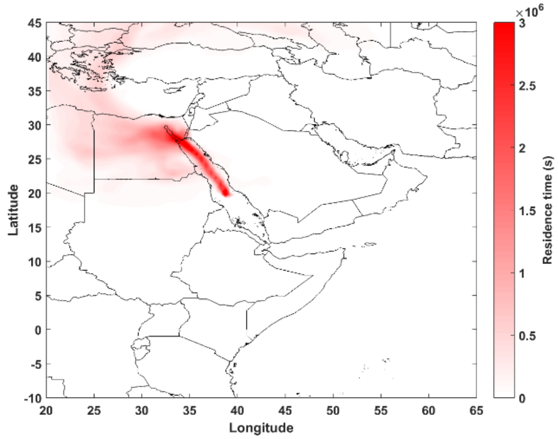


08.-09.07. (D13)

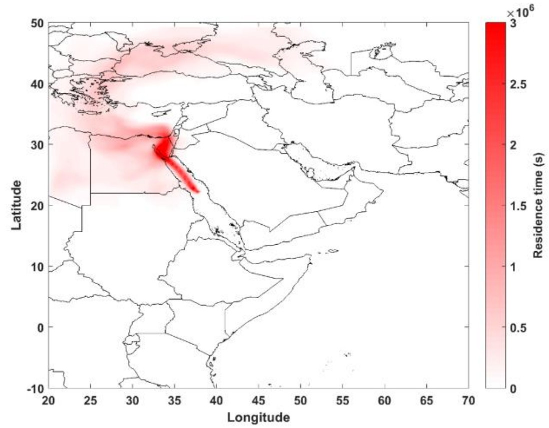


09.-10.07. (D14)

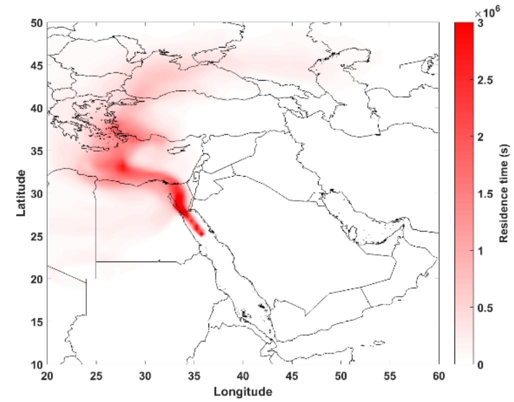
2. Leg:



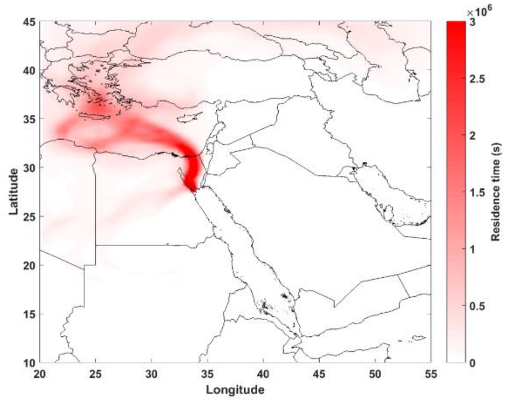
19.-20.08. (D45, C25)



20.-21.08. (D46, C25)



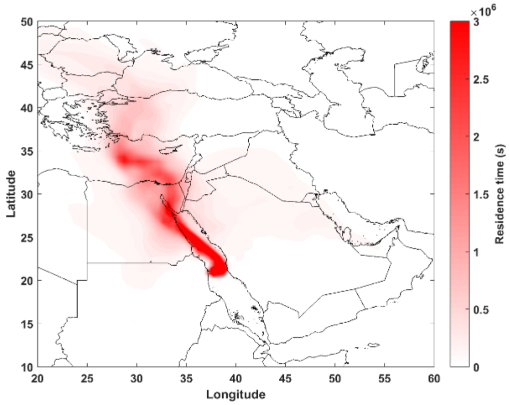
21.-22.08. (D47; C26)



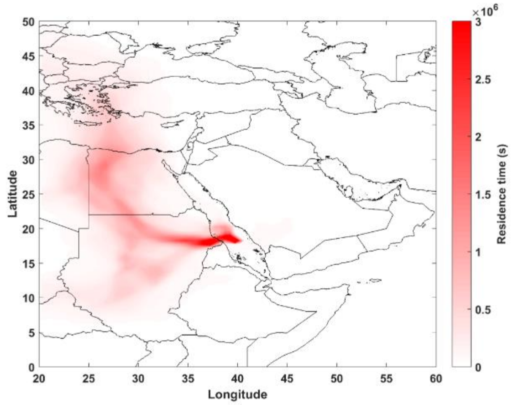
22.-23.08. (D48, C26)

c) Southern Red Sea

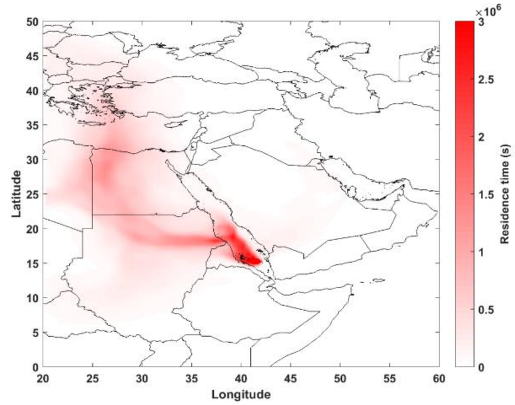
1. Leg:



13.-14.07. (D15)

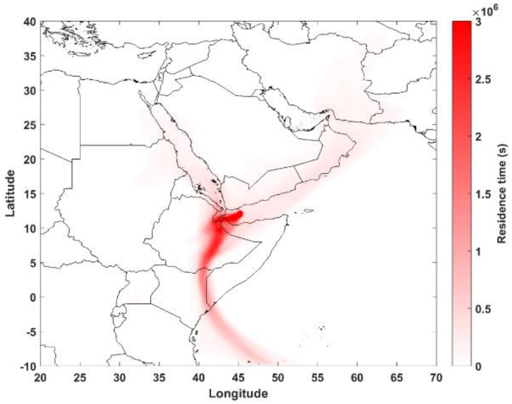


14.-15.07. (D16; C1)

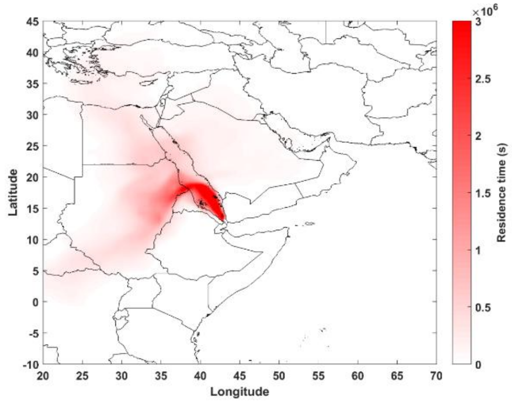


15.-16.07. (D17; C1)

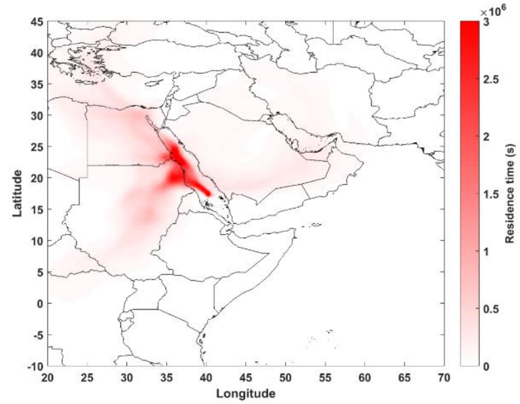
2.Leg:



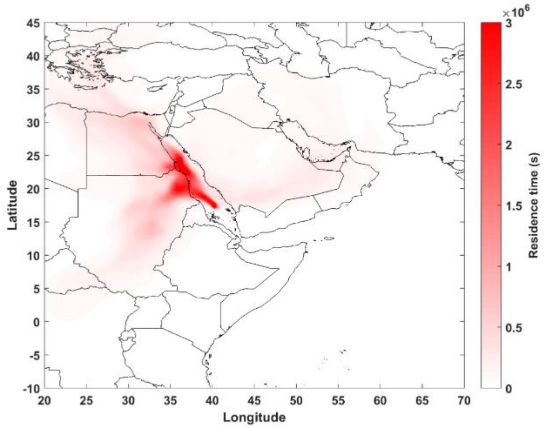
16.-17.08. (D42, C23)



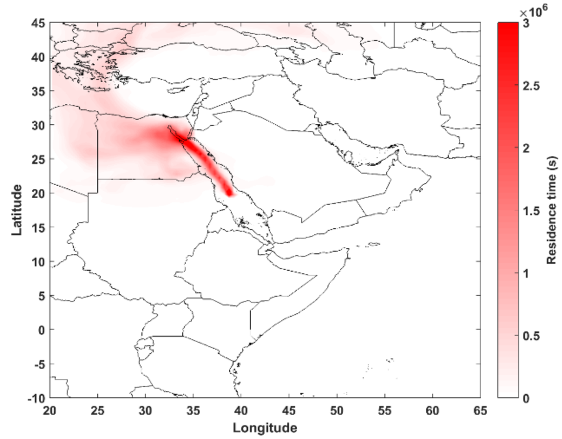
17.-18.08. (D43, C24)



18.-19.08. (D44; C24)



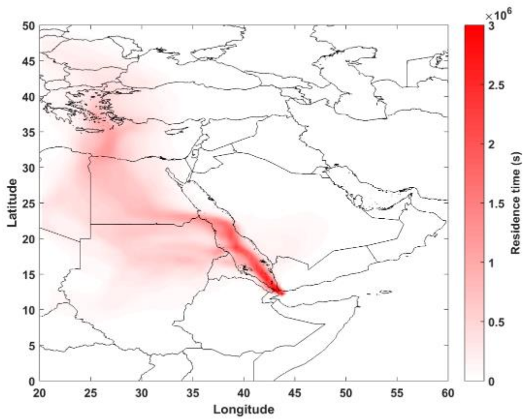
18.-19.08. (D44, C24)



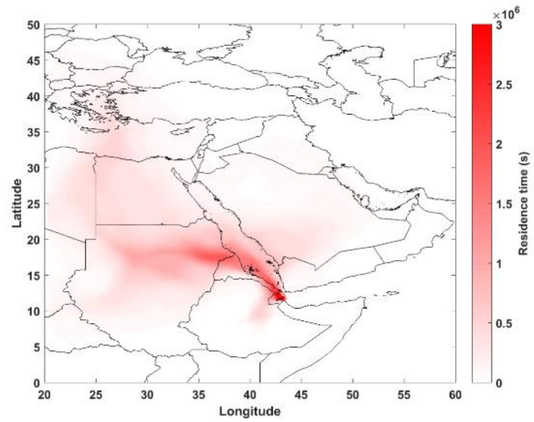
19.-20.08. (D45, C25)

d) Arabian Sea

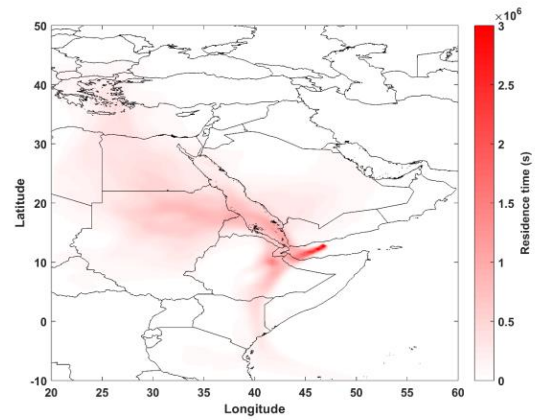
1. Leg:



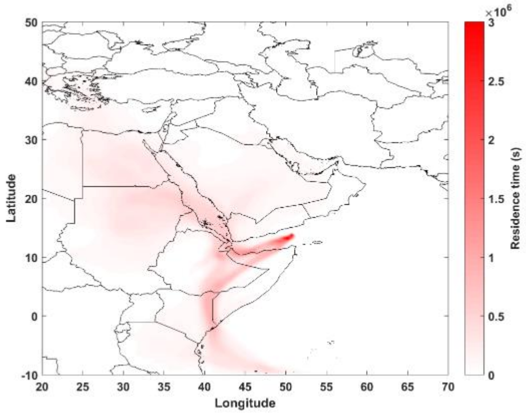
16.-17.07. (D18)

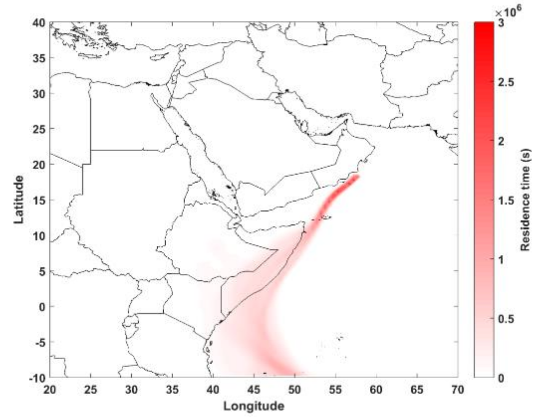


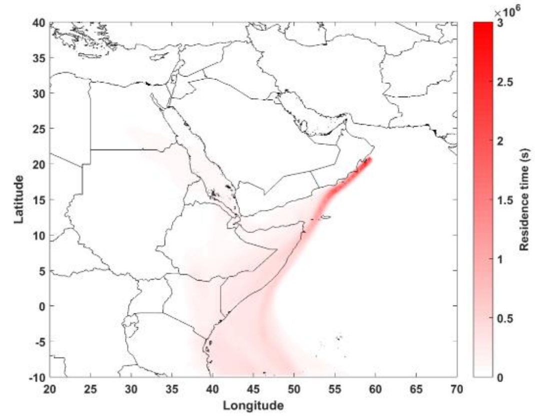
17.-18.07. (D19)



18.-19.07. (D20)





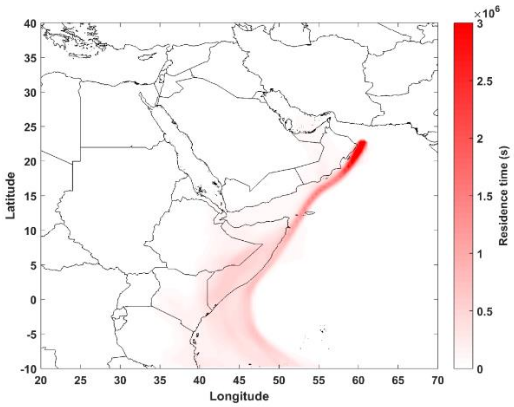


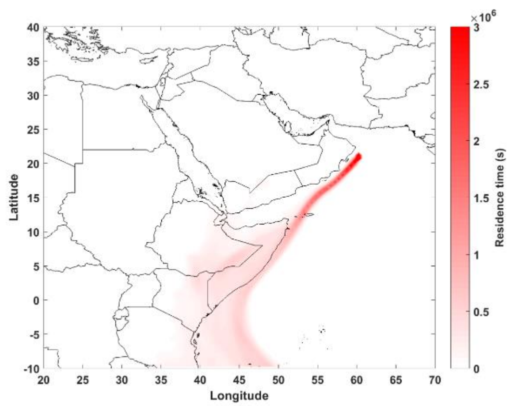
19.-20.07. (D21, C2)

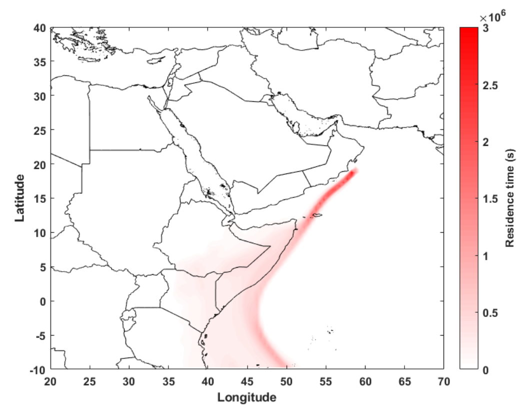
21.-22.07. (D22)

22.-23.07. (D23; D24)

2.Leg:



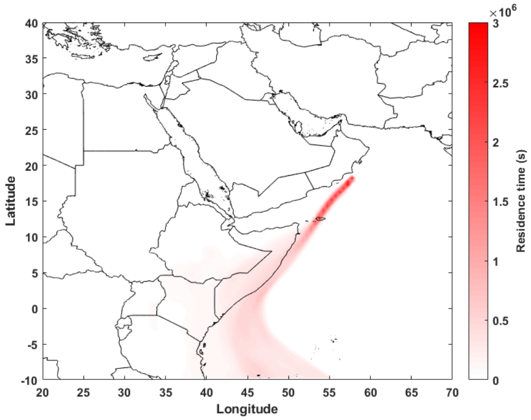




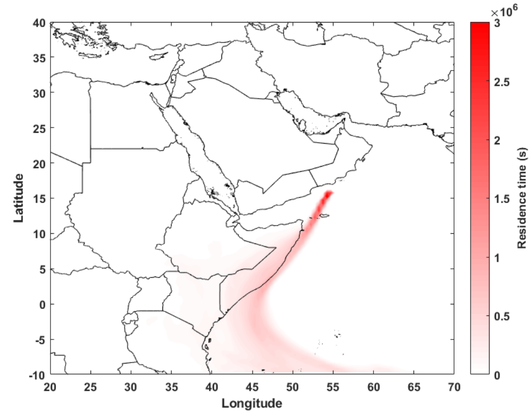
07.-08.08. (D35; C20)

08.-09.08. (D36, C20)

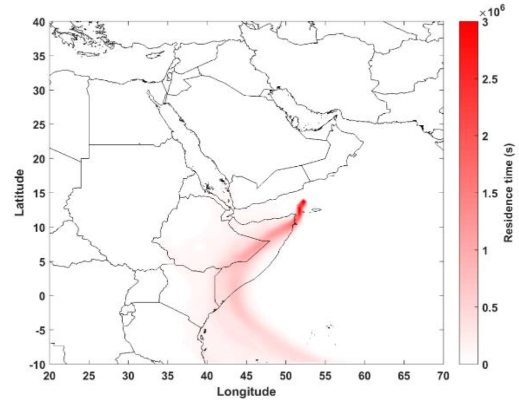
10.08. (D37)



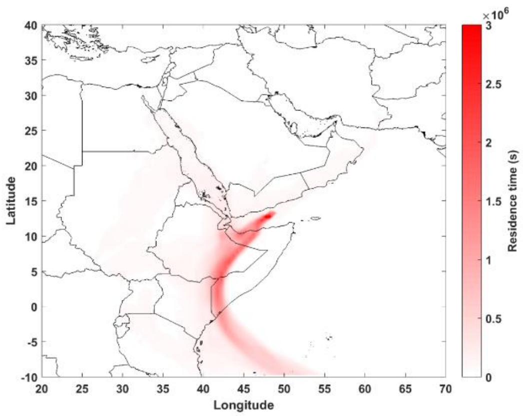
11.-12.08. (D38; C21)



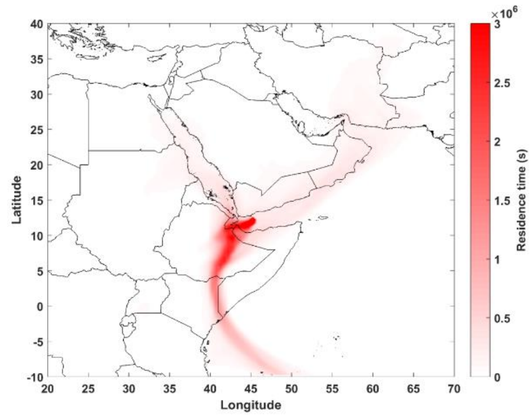
13.-14.08. (D39, C22)



14.-15.08. (D40)



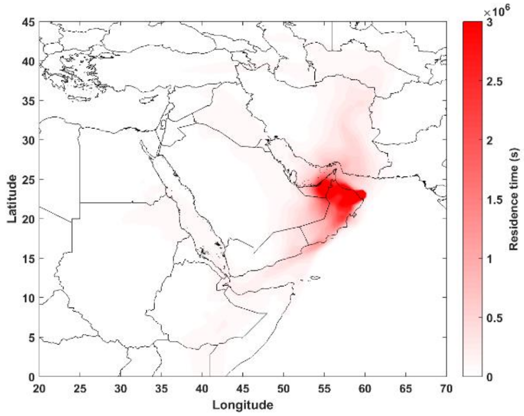
15.-16.08. (D41; C23)



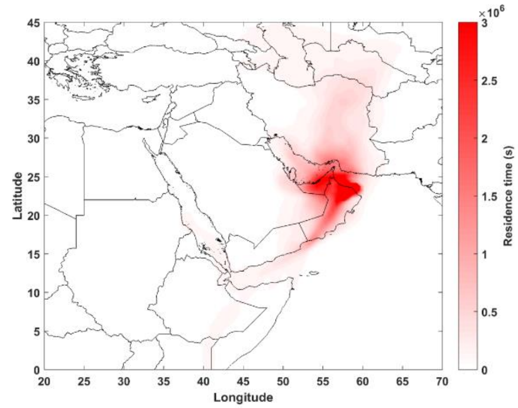
16.-17.08. (D42, C23)

e) Gulf of Oman

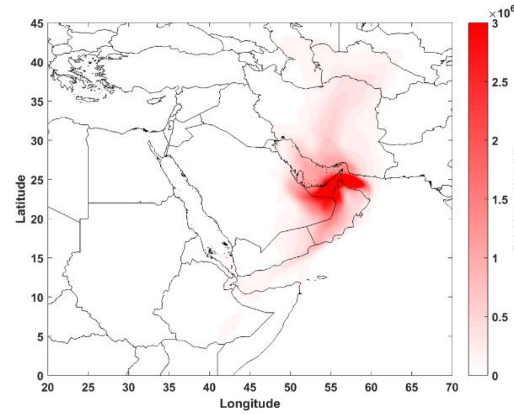
1. Leg:



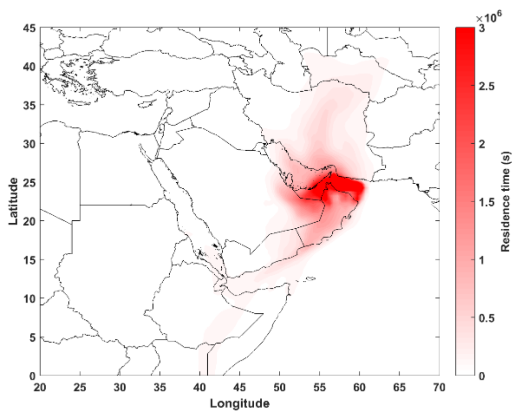
24-25.07. (D25, C3)



25.-26.07. (D26, C3)

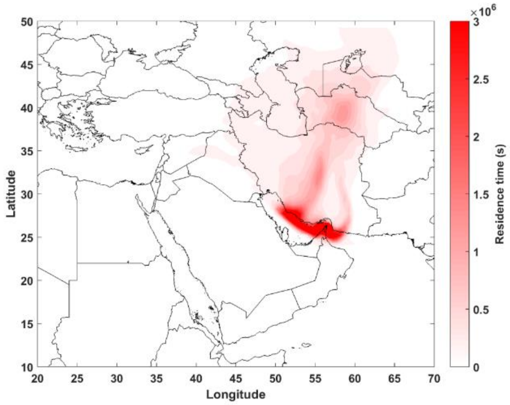


26.-27.07. (D27; C4)

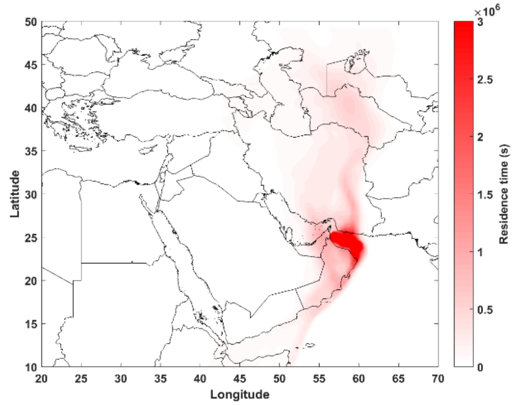


27-28.07. (D28, C5)

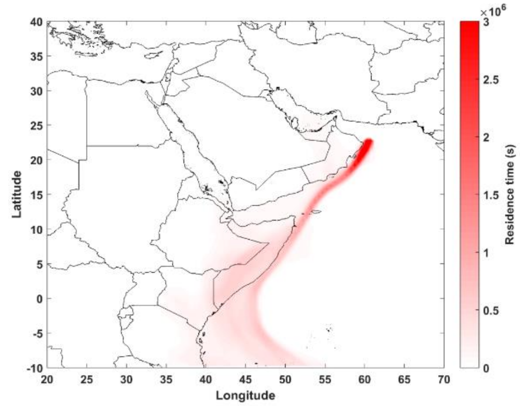
2. Leg:



05.-06.08. (D33; C14-17)



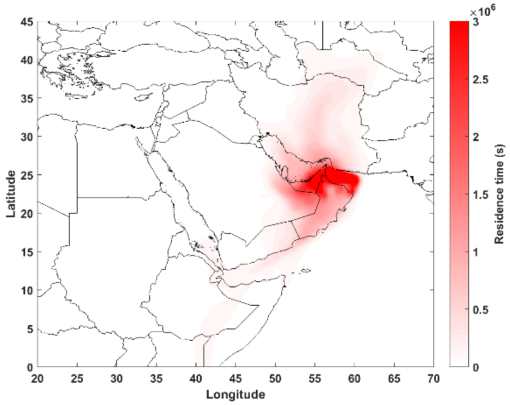
06.-07.08. (D34, C18-19)



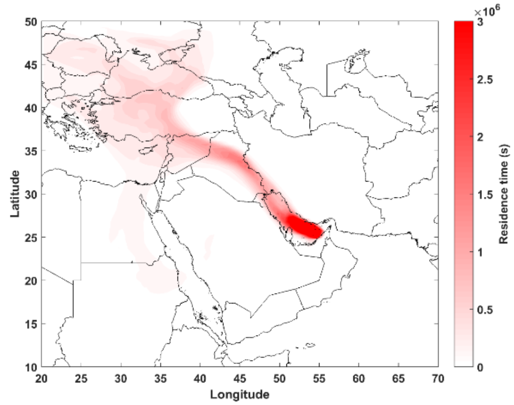
07.-08.08. (D35; C20)

f) Arabian Gulf

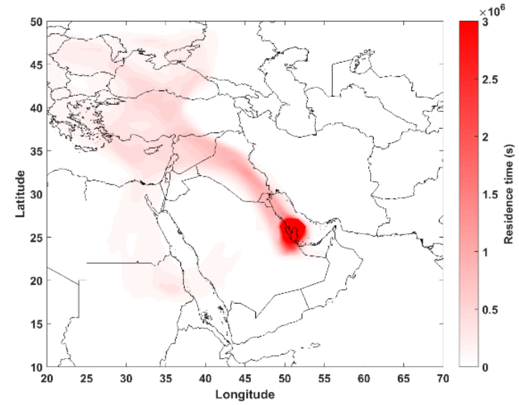
1. Leg:



27-28.07. (D28, C5)

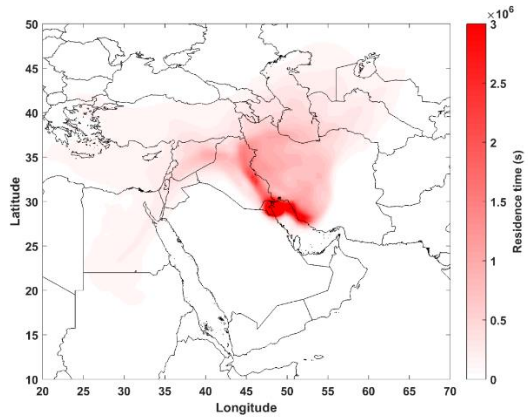


28.-29.07. (D29, C6)

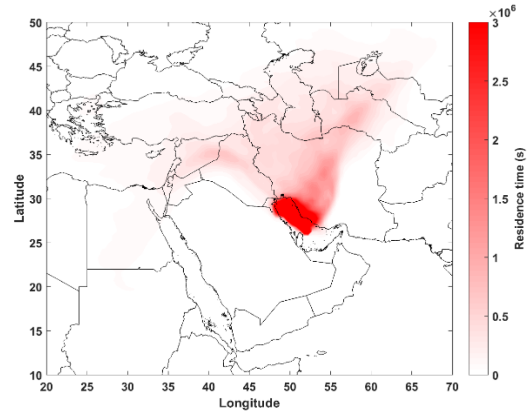


29.-30.07. (D30; C7)

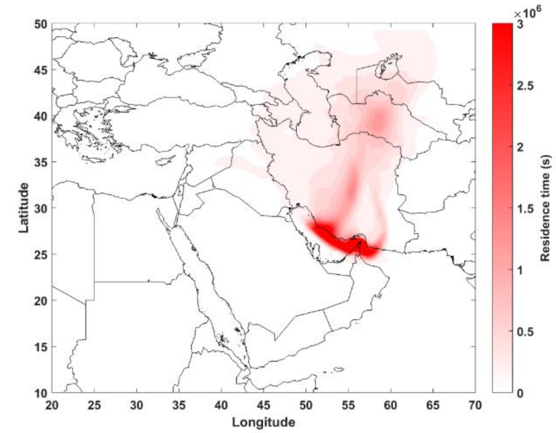
2. Leg:



03.-04.08. (D31, C8-C12)



04.-05.08. (D32, C13)



05.-06.08. (D33; C14-17)

Figure S3. Distribution of residence times of air masses received at specified dates using FLEXPART Lagrangian particle dispersion model, with ECMWF meteorological data ordered by sea regions and legs: a) Mediterranean Sea, b) Northern Red Sea, c) Southern Red Sea, d) Arabian Sea, e) Gulf of Oman, f) Arabian Gulf. All particles were followed for 10 days backward in time.

2.3 Composition pattern

Table S16. Relative contribution (in %) of individual compounds to the sum of the concentration of all compounds from the same class, a) PAHs, b) OPAHs, c) NPAHs

a)

Sample	ACY	ACE	FLN	PHE	ANT	FLT	PYR	BAA	CHR	BBF	BKF	BAP	INP	DBA	BPE
D1	0.1	2.9	7.0	62.2	4.7	9.4	6.4	0.3	2.0	0.8	0.2	0.2	0.3	1.1	0.3
D4	0.3	9.3	25.1	58.1	2.3	1.8	1.5	0.0	0.1	0.1	0.0	0.1	0.1	0.6	0.1
D5	1.0	9.0	17.6	54.4	3.8	6.5	5.6	0.1	0.5	0.2	0.0	0.0	0.0	0.2	0.0
D6	0.5	9.9	17.5	53.0	4.9	6.8	4.7	0.1	0.4	0.3	0.1	0.1	0.2	0.9	0.2
D7	0.1	1.6	10.6	61.6	6.5	9.2	7.4	0.1	0.5	0.4	0.1	0.2	0.3	0.8	0.3
D12	0.6	7.2	14.7	62.4	3.3	5.9	4.6	0.1	0.3	0.3	0.1	0.2	0.2	0.3	0.2
D13	0.4	6.4	15.6	59.8	5.4	6.2	5.0	0.1	0.3	0.3	0.1	0.1	0.2	0.2	0.2
D14	0.1	1.2	4.9	72.1	5.6	6.7	6.2	0.3	0.8	0.8	0.2	0.3	0.5	0.7	0.4
D15	0.1	0.5	2.1	72.7	3.4	9.8	7.6	0.2	0.7	0.4	0.1	0.2	0.3	0.9	0.3
D24	0.2	0.7	1.1	33.8	2.9	13.1	29.0	2.8	4.0	0.3	0.1	0.1	0.1	0.1	0.2
D25	0.1	3.4	3.4	50.2	3.8	11.4	16.7	1.3	2.7	0.3	0.1	0.0	0.1	0.5	0.1
D29	0.2	0.5	2.6	62.0	3.8	10.5	11.1	0.4	1.2	1.0	0.3	0.4	0.7	3.4	0.6
D30	0.1	1.7	3.8	49.7	4.5	16.6	12.8	0.9	2.0	3.5	1.0	2.1	3.2	3.0	3.1
D31	0.1	3.5	8.7	54.6	5.8	12.4	10.7	0.2	0.7	0.5	0.2	0.2	0.4	1.0	0.3
D32	0.1	1.4	3.6	60.9	8.4	13.4	10.2	0.2	0.5	0.3	0.1	0.1	0.2	0.1	0.2
D33	0.1	2.1	24.0	49.2	4.3	7.6	9.1	0.3	0.7	0.5	0.1	0.1	0.3	0.4	0.3
D34	0.2	20.4	12.4	40.6	4.2	6.4	7.7	0.8	1.8	0.6	0.1	0.0	0.1	0.8	0.1
D35	0.1	10.0	14.3	48.8	5.4	7.7	11.5	0.3	0.4	0.2	0.0	0.1	0.1	0.3	0.1
D36	0.8	10.3	8.3	52.6	6.6	7.1	11.3	0.8	1.2	0.8	0.2	0.5	0.7	0.8	0.8
D39	0.5	14.1	13.2	42.9	5.3	4.3	10.6	1.2	2.0	0.9	0.2	0.3	0.5	1.2	0.5
D40	0.2	0.6	3.5	59.6	12.5	10.5	8.5	0.6	1.0	0.6	0.2	0.2	0.3	0.9	0.3
D41	0.3	0.9	4.2	64.7	5.2	8.9	9.6	0.5	1.4	0.6	0.2	0.2	0.3	1.2	0.4

Sample	ACY	ACE	FLN	PHE	ANT	FLT	PYR	BAA	CHR	BBF	BKF	BAP	INP	DBA	BPE
D42	9.5	5.3	8.9	43.6	2.7	13.5	9.1	0.7	1.8	0.4	0.5	0.3	0.2	1.5	0.2
D43	0.3	0.8	3.3	57.5	3.6	13.3	12.8	0.6	1.4	1.2	0.5	0.6	0.9	3.1	0.9
D44	0.5	1.6	2.8	43.8	4.5	15.8	15.4	1.4	4.0	5.1	1.7	3.3	4.3	6.5	4.1
D45	0.5	1.4	5.3	44.6	5.4	15.0	13.1	1.0	2.2	3.3	1.1	2.2	2.9	7.0	2.8
D46	0.3	5.1	10.4	46.8	3.2	10.7	9.5	1.0	2.9	2.6	0.8	1.4	1.9	4.0	1.9
D47	0.7	3.8	9.7	53.5	3.5	8.1	8.6	0.8	2.4	1.5	0.5	0.7	1.1	3.6	1.1
D48	0.3	0.8	9.2	53.7	1.7	9.8	8.7	1.0	3.1	2.3	0.7	0.1	1.9	5.1	1.9
D49	0.2	12.5	26.1	45.6	5.4	4.9	3.8	0.2	0.4	0.4	0.1	0.2	0.3	0.4	0.3
D50	0.2	17.7	35.6	37.0	4.4	2.9	1.7	0.1	0.2	0.2	0.1	0.1	0.1	0.2	0.1
D51	0.2	10.2	20.1	47.1	6.0	6.5	6.0	0.6	1.0	1.2	0.4	0.7	0.8	0.5	0.8
D52	0.2	18.5	39.3	33.1	3.4	2.4	1.6	0.1	0.2	0.2	0.1	0.1	0.1	0.6	0.1
D53	0.3	5.6	25.1	46.7	5.9	5.7	6.2	0.4	0.6	0.9	0.3	0.5	0.7	1.3	0.6
D54	0.1	18.3	36.9	34.9	5.3	2.7	1.6	0.0	0.1	0.1	0.0	0.0	0.0	0.1	0.0
D55	0.1	2.1	12.9	63.0	8.9	6.3	4.8	0.1	0.2	0.3	0.1	0.2	0.2	0.6	0.2
D56	1.0	3.1	13.4	46.3	3.0	9.0	6.7	0.9	2.0	2.4	0.9	1.0	2.0	5.3	1.7
D57	0.1	7.2	39.1	37.1	4.2	5.1	3.5	0.2	0.5	0.8	0.3	0.5	0.5	1.6	0.5
D58	0.1	7.2	15.5	51.2	4.8	9.8	6.3	0.6	1.2	1.6	0.5	1.1	1.4	0.4	1.3
D59	0.1	7.7	40.7	39.9	3.6	3.6	3.3	0.1	0.3	0.3	0.1	0.1	0.2	0.3	0.2
D60	0.1	28.6	30.8	30.9	3.9	2.9	2.1	0.1	0.3	0.3	0.1	0.2	0.2	0.1	0.2
D61	0.2	8.8	31.1	44.5	6.5	4.5	3.5	0.1	0.2	0.2	0.1	0.1	0.1	0.2	0.1
D62	0.4	6.9	15.6	50.1	5.3	12.2	8.5	0.6	2.5	3.3	1.2	1.3	1.7	2.0	1.4

Sample	BJF	BEP	PER	DCA	ATT	COR	TPH	CCP	BGF	BBN	BNT
D1	0.15	0.37	0.02	0.85	0.00	0.14	1.39	0.06	0.64	0.45	0.54
D4	0.05	0.09	0.01	0.38	0.00	0.05	0.09	0.02	0.09	0.07	0.06
D5	0.04	0.07	0.01	0.18	0.00	0.01	0.36	0.01	0.22	0.24	0.26
D6	0.11	0.19	0.01	0.66	0.00	0.09	0.20	0.03	0.12	0.21	0.19
D7	0.14	0.27	0.02	0.66	0.00	0.12	0.31	0.04	0.23	0.28	0.25
D12	0.10	0.19	0.02	0.25	0.02	0.10	0.18	0.03	0.13	0.17	0.17
D13	0.10	0.17	0.01	0.18	0.01	0.08	0.20	0.02	0.14	0.17	0.17
D14	0.24	0.49	0.02	0.58	0.00	0.20	0.42	0.04	0.24	0.32	0.35
D15	0.13	0.27	0.02	0.88	0.02	0.13	0.43	0.03	0.33	0.27	0.39
D24	0.03	0.19	0.04	0.10	0.00	0.03	3.01	0.01	2.97	3.97	2.02
D25	0.05	0.14	0.01	0.29	0.00	0.03	1.97	0.00	1.36	1.66	1.28
D29	0.38	0.67	0.03	2.48	0.10	0.27	0.68	0.01	0.37	0.45	0.79
D30	1.40	2.43	0.24	1.79	0.38	1.51	1.09	0.39	0.79	0.33	1.62
D31	0.19	0.33	0.01	0.80	0.00	0.18	0.63	0.02	0.39	0.34	0.81
D32	0.08	0.17	0.01	0.05	0.00	0.07	0.40	0.01	0.26	0.35	0.41
D33	0.13	0.30	0.01	0.20	0.00	0.14	0.56	0.02	0.41	0.53	0.39
D34	0.03	0.39	0.04	0.56	0.00	0.04	1.30	0.01	0.21	0.78	1.46
D35	0.04	0.12	0.02	0.20	0.00	0.02	0.30	0.02	0.28	0.41	0.25
D35	0.04	0.12	0.02	0.20	0.00	0.02	0.30	0.02	0.28	0.41	0.25
D36	0.28	0.69	0.14	0.91	0.00	0.13	1.31	0.05	1.00	0.65	0.93
D39	0.19	0.70	0.08	1.23	0.28	0.34	1.35	0.03	0.60	1.01	1.53
D40	0.32	0.35	0.07	0.75	0.00	0.08	0.52	0.01	0.26	0.50	0.52
D41	0.42	0.39	0.05	0.86	0.00	0.12	1.16	0.02	0.37	0.55	1.04
D42	0.22	0.44	0.28	2.19	1.14	0.27	0.58	0.09	1.60	1.34	0.15
D43	0.39	0.88	0.10	2.46	0.28	0.58	0.84	0.07	0.54	0.45	0.67
D44	1.91	3.47	0.41	3.96	1.68	1.62	1.69	0.37	1.66	0.68	1.43
D45	1.27	2.39	0.30	4.67	0.36	1.03	1.12	0.25	1.18	0.54	0.97
D46	0.92	1.74	0.21	3.50	0.24	0.74	2.03	0.20	0.85	0.90	1.92

Sample	BJF	BEP	PER	DCA	ATT	COR	TPH	CCP	BGF	BBN	BNT
D47	0.50	1.04	0.12	2.13	0.11	0.53	1.32	0.12	0.80	0.74	1.82
D48	0.85	1.66	0.05	4.12	0.00	0.98	2.13	0.10	1.06	0.83	2.70
D49	0.16	0.25	0.01	0.43	0.00	0.10	0.22	0.04	0.18	0.08	0.16
D50	0.06	0.10	0.01	0.14	0.00	0.03	0.06	0.02	0.07	0.06	0.05
D51	0.33	0.76	0.16	0.16	0.00	0.18	0.50	0.09	0.49	0.25	0.36
D52	0.05	0.11	0.03	0.40	0.00	0.02	0.12	0.01	0.07	0.04	0.08
D53	0.21	0.64	0.19	1.03	0.13	0.11	0.37	0.06	0.41	0.24	0.39
D54	0.03	0.05	0.00	0.07	0.00	0.01	0.04	0.01	0.03	0.04	0.04
D55	0.11	0.21	0.00	0.59	0.04	0.05	0.20	0.03	0.15	0.07	0.19
D56	0.80	1.71	0.17	5.77	0.50	0.42	1.45	0.17	1.50	0.80	1.00
D57	0.32	0.56	0.07	1.02	0.03	0.13	0.38	0.07	0.23	0.13	0.27
D58	0.70	1.00	0.15	0.27	0.18	0.52	0.62	0.38	0.80	0.42	0.52
D59	0.15	0.23	0.02	0.28	0.00	0.05	0.18	0.02	0.17	0.10	0.15
D60	0.15	0.27	0.02	0.06	0.00	0.06	0.18	0.02	0.19	0.11	0.14
D61	0.05	0.11	0.01	0.13	0.00	0.02	0.12	0.01	0.15	0.16	0.09
D62	1.28	1.99	0.07	1.24	0.00	0.31	1.09	0.10	0.68	0.65	1.10

b)

Sample	1,4-O_2NAP	1-(CHO)NAP	9-OFLN	9,10-O_2ANT	1,4-O_2ANT	9,10-O_2PHE	11-OBaFLN	11-OBbFLN	BAN	7,12-O_2BAA	5,12-O_2NAC
D1	22.0	10.0	8.0	18.0	0	0	11.9	12.3	6.5	10.3	0.9
D4	14.4	30.8	16.3	4.8	0	0	3.9	7.2	8.0	12.8	2.0
D5	10.2	5.4	23.6	8.7	0	0	14.1	12.6	9.6	13.9	1.7
D6	9.7	17.6	15.7	9.5	0	8.0	8.9	8.4	10.4	10.5	1.3
D7	9.1	17.9	23.4	3.0	0	0	11.3	9.2	9.6	14.7	1.6
D12	5.2	25.3	26.2	5.3	0	4.6	10.8	6.7	7.4	7.6	0.8
D13	6.5	20.9	26.8	2.1	0	8.3	11.4	6.4	8.8	8.1	0.8
D14	24.7	17.3	14.3	8.9	2.0	0	10.5	8.2	6.4	6.5	1.1
D15	10.7	5.7	33.0	3.6	0	0	13.9	9.8	8.8	13.6	1.0
D24	7.1	4.1	3.7	2.3	0	33.3	20.0	13.3	13.1	2.7	0.5
D25	5.1	3.4	9.2	5.0	0	16.7	19.8	15.8	16.3	8.0	0.8
D29	56.3	6.5	9.6	4.1	0	0	6.8	4.6	7.6	3.8	0.6
D30	43.6	1.9	9.2	24.1	0	3.1	4.2	2.8	5.0	5.4	0.8
D31	10.9	10.2	28.7	6.4	0	0	15.7	9.9	9.3	8.2	0.7
D32	36.3	4.1	25.1	6.9	0	0	9.1	5.9	5.6	6.2	0.7
D33	11.7	12.1	18.6	3.5	0	0	11.1	13.1	18.7	9.2	1.9
D34	25.6	13.0	7.8	6.6	0	0	11.0	8.7	12.5	13.1	1.5
D35	23.9	27.7	19.4	7.1	0	0	5.7	5.9	6.6	3.1	0.5
D36	39.0	19.4	4.8	9.3	0	0	8.1	7.5	8.0	3.1	0.8
D39	33.6	15.0	4.2	8.0	0	0	7.2	6.7	14.9	9.0	1.4
D40	29.8	14.1	20.4	7.0	0	0	6.2	5.8	7.2	8.6	0.8
D41	47.8	11.3	11.4	5.5	0	0	4.3	5.0	6.7	6.9	1.1
D42	37.7	20.1	6.6	12.5	0	0	7.6	5.6	7.3	2.3	0.3
D43	21.8	4.5	14.1	45.1	0	0	3.9	2.5	4.0	3.5	0.5
D44	48.0	7.2	9.3	3.3	0	0	6.2	6.6	11.3	6.4	1.7

Sample	1,4-O_2NAP	1-(CHO)NAP	9-OFLN	9,10-O_2ANT	1,4-O_2ANT	9,10-O_2PHE	11-OBaFLN	11-OBbFLN	BAN	7,12-O_2BAA	5,12-O_2NAC
D45	49.7	8.4	8.7	4.5	0	0	6.9	6.1	8.5	5.6	1.6
D46	37.1	3.6	5.9	35.3	0	0	4.3	2.7	5.3	5.0	0.9
D47	38.4	12.9	6.7	26.8	0.1	0	3.8	3.0	4.8	3.0	0.7
D48	54.6	2.0	6.7	21.2	0	0	4.3	3.6	3.7	3.2	0.7
D49	19.3	10.3	19.4	18.1	0	0	7.1	8.5	11.9	4.1	1.3
D50	16.3	16.3	16.2	24.6	0	0	5.9	6.7	9.4	3.2	1.2
D51	30.1	8.4	24.1	13.6	0	0	5.4	5.9	8.5	3.0	1.0
D52	15.7	8.4	13.5	39.8	0	0	5.4	5.3	7.6	3.4	0.9
D53	61.3	6.4	9.2	10.3	0	0	3.2	3.4	3.9	1.9	0.4
D54	39.9	2.2	8.0	43.6	0	0	1.4	1.7	2.0	0.8	0.2
D55	40.2	3.3	11.1	36.5	0	0	1.7	2.6	2.6	1.7	0.4
D56	38.3	3.8	8.9	40.4	0	0	1.9	2.0	3.1	1.2	0.3
D57	46.9	4.0	10.5	30.0	0	0	1.7	2.7	2.7	1.1	0.5
D58	48.1	9.7	7.0	21.7	0	0	2.5	3.6	4.7	1.6	1.0
D59	40.9	3.2	10.6	37.0	0	0	1.8	2.0	2.9	1.2	0.4
D60	47.7	3.2	7.4	33.6	0	0	1.9	2.1	2.7	1.1	0.4
D61	19.2	39.9	11.1	3.0	0	0	6.8	5.7	10.5	2.8	1.1
D62	44.1	2.5	6.8	30.2	0	0	4.0	5.0	4.4	2.2	0.8

c)

Sample	Region & leg	2-NNAP	9-NANT	3-NPHE	2-NFLT	1-NPYR	2-NPYR	7-NBAA
D1	MS1	**21.1**	**20.6**	**8.4**	**45.3**	**3.1**	**1.1**	**0.3**
D4	MS1	**54.6**	**0.0**	**11.2**	**18.7**	**11.1**	**3.0**	**1.4**
D5	MS1	**14.3**	**0.0**	**31.7**	**39.4**	**8.0**	**0.8**	**5.8**
D6	MS1	**34.1**	**0.0**	**13.2**	**23.6**	**24.2**	**2.6**	**2.3**
D7	MS1	**48.2**	**0.0**	**25.2**	**10.1**	**10.7**	**2.7**	**3.1**
D12	NRS1	**44.0**	**0.0**	**22.3**	**22.0**	**8.0**	**2.9**	**0.8**
D13	NRS1	**54.1**	**0.0**	**25.4**	**9.1**	**6.8**	**2.0**	**2.6**
D14	NRS1	**60.7**	**0.0**	**8.9**	**18.1**	**8.5**	**2.7**	**1.1**
D15	SRS1	**51.0**	**0.0**	**21.9**	**21.3**	**4.0**	**0.7**	**1.2**
D24	OG1	**22.7**	**0.0**	**58.9**	**3.4**	**12.8**	**0.6**	**1.6**
D25	OG1	**40.2**	**0.0**	**34.7**	**6.0**	**17.2**	**1.4**	**0.5**
D29	AG1	**46.7**	**0.0**	**17.5**	**9.9**	**21.0**	**2.3**	**2.7**
D30	AG1	**57.3**	**0.0**	**12.0**	**20.7**	**8.2**	**1.6**	**0.2**
D31	AG2	**30.7**	**0.0**	**25.9**	**7.9**	**34.5**	**0.6**	**0.4**
D32	AG2	**39.0**	**0.0**	**16.2**	**22.1**	**19.9**	**0.8**	**2.0**
D33	AG2, OG2	**34.5**	**0.0**	**17.7**	**5.1**	**40.2**	**0.6**	**2.0**
D34	OG2	**21.8**	**0.0**	**22.5**	**10.6**	**27.8**	**0.4**	**17.0**
D35	OG2, AS2	**30.6**	**0.0**	**35.3**	**6.5**	**25.3**	**0.3**	**2.0**
D36	AS2	**47.7**	**0.0**	**11.9**	**10.3**	**25.6**	**1.2**	**3.3**
D39	AS2	**37.8**	**0.0**	**16.6**	**14.4**	**18.2**	**1.0**	**12.0**
D40	AS2	**42.3**	**0.0**	**3.6**	**4.3**	**43.1**	**0.4**	**6.3**
D41	AS2	**41.0**	**0.0**	**11.5**	**13.1**	**31.4**	**0.4**	**2.5**
D42	AS2, SRS2	**54.0**	**0.0**	**5.6**	**6.0**	**30.0**	**0.6**	**3.8**
D43	SRS2	**56.6**	**0.0**	**15.7**	**13.8**	**11.2**	**1.3**	**1.4**
D44	SRS2	**35.6**	**0.0**	**17.5**	**24.8**	**16.9**	**3.1**	**2.1**

Sample	Region & leg	2-NNAP	9-NANT	3-NPHE	2-NFLT	1-NPYR	2-NPYR	7-NBAA
D45	SRS2, NRS2	**39.9**	**0.0**	**12.5**	**21.6**	**20.9**	**2.5**	**2.7**
D46	NRS2	**18.3**	**65.2**	**3.7**	**5.4**	**2.4**	**0.4**	**4.5**
D47	NRS2	**70.1**	**0.0**	**8.8**	**8.5**	**8.2**	**0.7**	**3.7**
D48	NRS2	**53.5**	**22.4**	**6.9**	**8.9**	**4.8**	**0.7**	**2.9**
D49	MS2	**31.7**	**0.0**	**28.0**	**19.4**	**16.6**	**2.2**	**2.1**
D50	MS2	**44.6**	**0.0**	**14.1**	**13.6**	**22.9**	**1.9**	**2.9**
D51	MS2	**45.4**	**0.0**	**9.6**	**15.6**	**25.3**	**0.8**	**3.2**
D52	MS2	**43.2**	**0.0**	**11.2**	**19.6**	**22.6**	**0.5**	**2.9**
D53	MS2	**51.2**	**0.0**	**4.9**	**12.8**	**26.2**	**1.6**	**3.3**
D54	MS2	**30.5**	**30.7**	**2.9**	**11.5**	**21.0**	**1.4**	**2.0**
D55	MS2	**45.8**	**0.0**	**9.8**	**22.9**	**18.9**	**1.1**	**1.6**
D56	MS2	**41.1**	**0.0**	**13.3**	**19.6**	**22.1**	**1.0**	**2.8**
D57	MS2	**31.0**	**7.2**	**8.6**	**29.7**	**20.0**	**1.5**	**1.9**
D58	MS2	**64.2**	**2.9**	**24.4**	**6.4**	**0.8**	**1.2**	**0.1**
D59	MS2	**29.9**	**0.0**	**25.4**	**23.9**	**16.7**	**1.1**	**2.9**
D60	MS2	**45.7**	**0.0**	**21.0**	**4.9**	**24.3**	**1.1**	**3.1**
D61	MS2	**39.0**	**0.0**	**23.2**	**5.4**	**28.7**	**0.9**	**2.8**
D62	MS2	**41.4**	**0.0**	**21.9**	**10.1**	**21.4**	**2.5**	**2.7**

2.4 Source apportionment

2.4.1 Identification of PMF factors

Six factors of anthropogenic sources with 54 % and 48 % contribution to PM10 were identified based on two subsets of species (groups 1 and 2, respectively; Figs. 4, S4).

The first factor, desert dust, was associated with high concentration of the Earth's crust elements (Ti, Mn, Fe, Co, Cr) and endosulfan sulfate (Figs. 4 and S4) a banned insecticide's metabolite still used in many countries despite the high toxicity to humans and its persistence in the environment (US EPA, 2002; Tuduri et al., 2006). The factor contributed to PM_{10} by 44 % and 48 % in the first and the second subset of species input, respectively (Fig. S4).

The second factor (the third factor in PMF group 2), fresh ship emissions, dominated by EC, OC, PAHS, OPAHs and NPAHs (Yu et al., 2004; Gregoris et al., 2016; Merico et al., 2017; Zhao et al., 2019, 2020) and contributed by 18 % and 15% to PM10. Fresh ship emissions represent the main source of PAHs as well as their nitrated and oxygenated derivatives in this campaign. The peaks in the factor time series correspond primarily to the stock emissions of the research vessel. The factor shows strong correlation with NO and SO2 (Pearson correlation coefficient r = 0.83/67 and 0.69/61), gases heavily emitted from ship engines (Agrawal et al., 2008a, b) since around 15% of global anthropogenic NOx and 5 – 8 % of global SOx emissions are attributable to oceangoing ships (Eyring et al., 2005; Corbett et al., 2007).

The third factor (the second factor in PMF group 2) assigned as aged ship emissions contained primarily , Zn, Pb, Cd (Isakson et al., 2001; Viana et al., 2014) and also PAHs and their nitrated and oxygenated derivatives (Zhao et al., 2019, 2020). Diesel PM emitted by ship engines is a mixture of different kinds of particles with size spanning from few nanometers to several microns (di Natale and Carotenuto, 2015). The factor shows moderate to strong correlation with SO_2, CH_4, CO and O_3 (Pearson correlation coefficient r = 0.60/57, 0.59/66, 0.63/62 and 0.56/60) and a contribution of 17% and 26% to PM_{10} in PMF group 1 and 2, respectively.

The forth factor was ascribed to continental pollution, which is characterized by a strong contribution of OC, Ni, PAHs, OPAHs, PCBs and several pesticide/insecticides (HCH, DDX and drins). Several studies showed that these substances can come from continental pollution

(Menichini et al., 2007). The factor contributed by 16 and 6% to PM10. The air masses of continental origin represent the second most important source of PAHs and OPAHs (Gevao et al., 2006; Romagnoli et al., 2016, 2019; Merico et al., 2017; Rhusdi et al., 2017; Javed et al., 2019).

The fifth factor (the sixth factor in PMF group 2), residual oil combustion, was represented by V, Ni and Mo i.e., markers for fuel oil/pet-coke combustion, petrochemical sources, or industrial emissions (Querol et al., 2002; Alleman et al., 2010). However, the calculated Ni/V ratio of 0.3 corresponds to the petro-chemical industry, mainly at the coasts (Alleman et al., 2010). The factor residual oil combustion moderately correlates with NO_2, SO_2 and CO (Pearson correlation coefficients r = 0.71/70; 0.38/56; 0.38/46). The factor contributed by 3% and 1% to PM_{10} (Fig. S4).

Last factor (the fifth in PMF group 2) ascribed as sea salt dominated by Na^+ (Pey et al., 2013; Chembari et al., 2014; Bove et al., 2016). The factor contributed by 2% and 4% to PM_{10} (Fig. S4). Considering the data coverage of only around 65 % of the sampling time, the contribution of sea salt to PM might be higher than based on the PMF output.

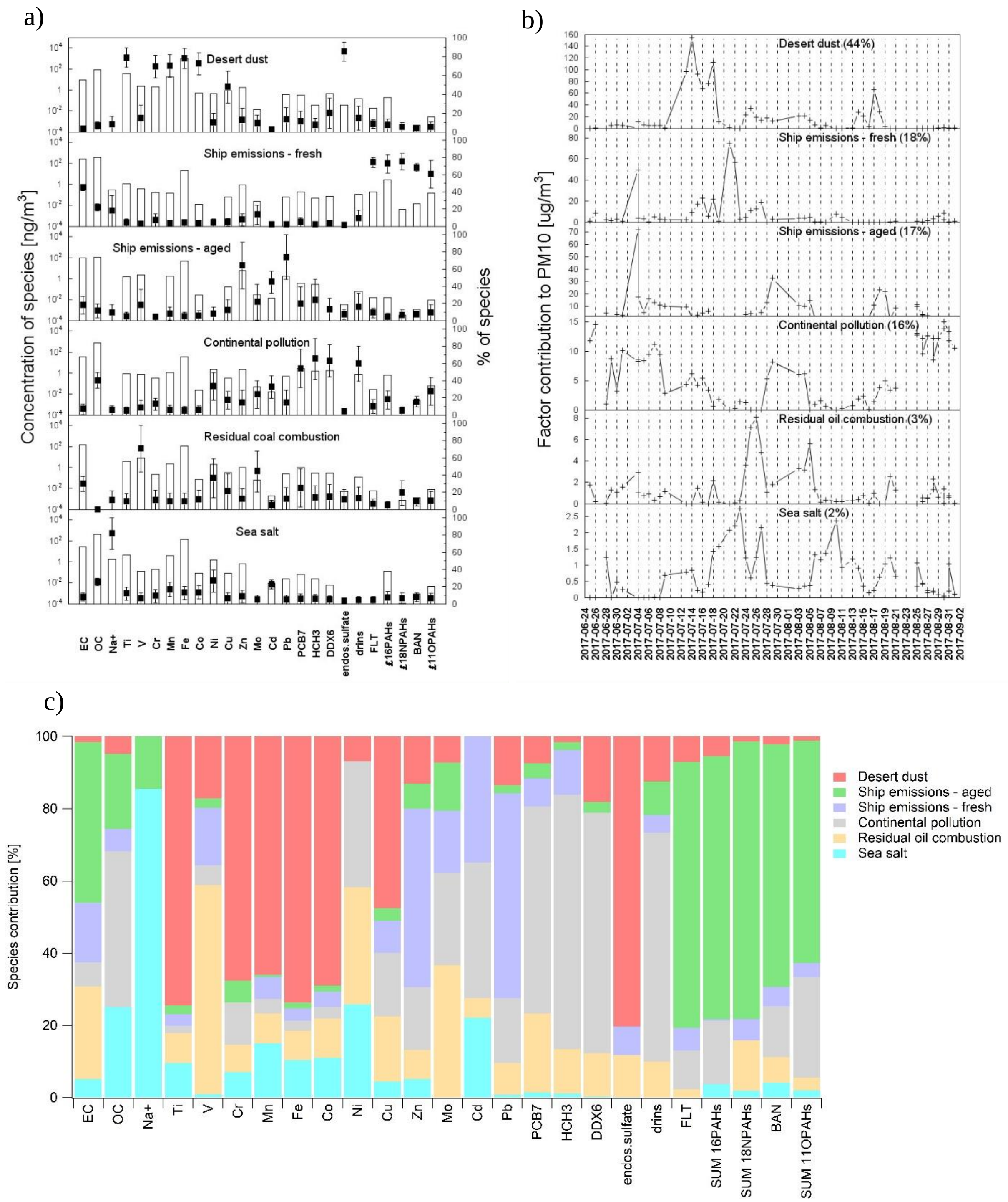


Figure S4. PMF group 1: a) Factor profiles (Bars: Concentration of the species, black squares: Percentage of the species explained, box: Displacement (DISP) average, whiskers: DISP max and DISP min), b) time series of factor contributions to sample composition with their relative contributions and c) relative contribution of the five factors resolved by PMF to the concentration of each substance in PMF group 1.

2.4.2 Influence of ship emissions

Table S17. Relative concentration of target compounds in samples strongly influenced by own ship emissions (see Table S4 and Fig. S4) compared to average concentration of samples not influences by own ship emissions in the same region for a) PAHs, b) OPAHs and c) NPAHs.

a)

Substance	D16;17 compared to average of Southern Red Sea	D20;22;23;37;38 compared to average of Arabian Sea	D28 compared to average of Oman and Arabian Gulf
ACY	56.7	16.1	4.6
ACE	59.4	2.4	1.7
FLN	37.8	22.0	1.4
PHE	7.4	30.8	3.4
ANT	10.4	20.2	3.2
FLT	5.9	23.0	3.2
PYR	9.9	38.7	4.6
BAA	10.8	69.8	7.4
CHR	5.7	42.8	4.8
BBF	2.1	52.5	3.4
BKF	1.8	48.6	3.0
BAP	1.5	54.9	1.2
INP	1.5	58.4	2.2
DBA	0.4	2.0	0.8
BPE	1.9	84.1	3.5
BJF	2.5	48.7	4.3
BEP	2.2	55.4	3.9
PER	1.2	25.5	1.3
DCA	0.4	2.0	1.0
ATT	0.3	0.0	0.0
COR	1.5	42.3	2.7
TPH	7.7	45.7	4.8
CCP	0.5	1.1	0.1
BGF	4.7	61.2	4.8
BBN	17.4	63.7	5.5
BNT	7.7	30.5	3.5
RET	9.1	19.0	3.9

b)

Substance	D16;17 compared to average of Southern Red Sea	D20;22;23;37;38 compared to average of Arabian Sea	D28 compared to average of Oman and Arabian Gulf
1,4-O_2NAP	2.3	31.9	1.6
1-(CHO)NAP	21.2	46.7	4.5
9-OFLN	5.3	28.9	3.7
9,10-O_2ANT	3.1	8.1	1.3
1,4-O_2ANT	a	a	a
9,10-O_2PHE	a	a	6.2
11-OBaFLN	9.1	66.2	4.5
11-OBbFLN	7.4	42.0	4.9
BAN	7.9	31.2	4.8
7,12-O_2BAA	5.2	16.0	5.4
5,12-O_2NAC	12.1	25.7	12.3
Σ_{11}OPAHs	6.5	34.4	3.8

a: Quantified in contaminated samples but not possible to calculate ratio because <LOQ in stack filtered regional averages

c)

Substance	D16;17 compared to average of Southern Red Sea	D20;22;23;37;38 compared to average of Arabian Sea	D28 compared to average of Oman and Arabian Gulf
2-NNAP	4.0	27.9	2.6
3-NPHE	6.5	23.0	2.7
2-NFLT	1.0	5.6	0.9
1-NPYR	17.7	53.4	3.1
2-NPYR	11.5	64.9	7.8
7-NBAA	4.8	12.2	2.4
Σ_{17}NPAHs	5.5	32.1	2.6

Table S18. Number of bypassing ships (n) influencing a) Digitel and b) impactor samples, based on ship counts based on same analysis as done in Celik et al. (2020).

a)

Sample	Amount of ship plumes	Sample	Amount of ship plumes	Sample	Amount of ship plumes
D1	0	**D22**	1	**D43**	9
D2	0	**D23**	1	**D44**	8
D3	0	**D24**	0	**D45**	2
D4	0	**D25**	41	**D46**	24
D5	0	**D26**	26	**D47**	24
D6	6	**D27**	0	**D48**	25
D7	31	**D28**	37	**D49**	2
D8	1	**D29**	28	**D50**	2
D9	3	**D30**	14	**D51**	1
D10	9	**D31**	4	**D52**	3
D11	8	**D32**	41	**D53**	6
D12	17	**D33**	35	**D54**	15
D13	28	**D34**	34	**D55**	4
D14	9	**D35**	11	**D56**	2
D15	19	**D36**	4	**D57**	10
D16	4	**D37**	0	**D58**	4
D17	25	**D38**	12	**D59**	1
D18	16	**D39**	21	**D60**	3
D19	0	**D40**	0	**D61**	0
D20	12	**D41**	21	**D62**	6
D21	18	**D42**	24		

b)

Sample	Amount of ship plumes	Sample	Amount of ship plumes
C1	29	**C16**	5
C2	19	**C17**	2
C3	67	**C18**	7
C4	0	**C19**	30
C5	37	**C20**	14
C6	29	**C21**	18
C7	10	**C22**	31
C8	0	**C23**	52
C9	0	**C24**	4
C10	0	**C25**	26
C11	0	**C26**	41
C12	1	**C27**	3
C13	41	**C28**	8
C14	1	**C29**	19
C15	4	**C30**	14

2.4.3 Source attribution by application of diagnostic ratios

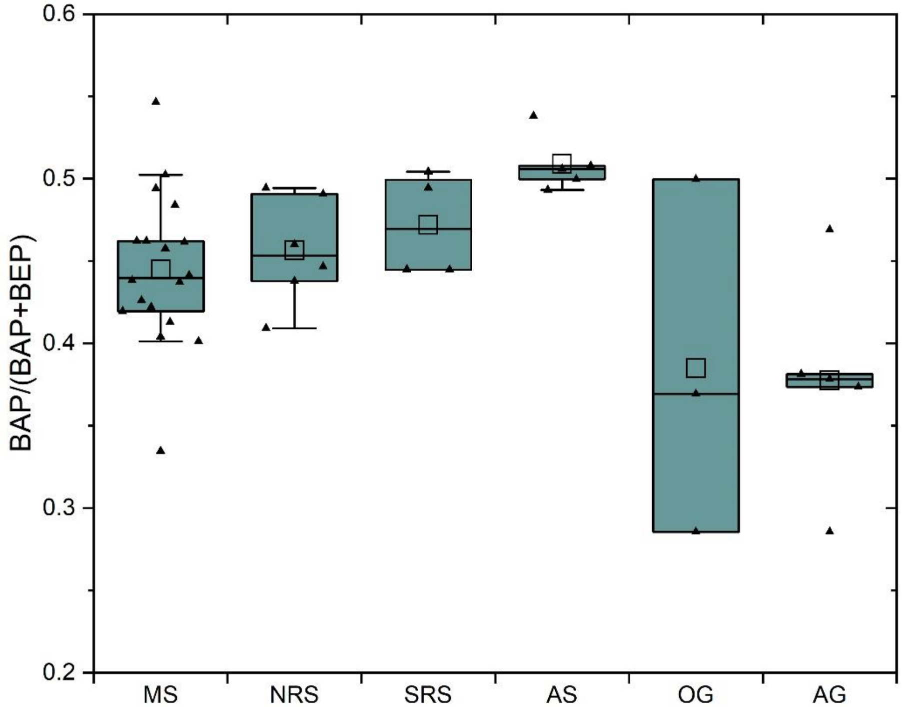


Figure S5. Box-Whisker plot of the ratios of the particulate concentrations of BAP/(BAP+BEP) across sea regions (without samples with BAP or BEP <LOQ; MS: Mediterranean Sea; NRS: Northern Red Sea; SRS: Southern Red Sea; AS: Arabian Sea; OG: Gulf of Oman; AG: Arabian Gulf; Empty square: Mean value; Filled, grey triangles: Measurement points; Box with additional borders: Interquartile range (IQR) bound by the 75th and 25th percentile and range of 1.5 IQR; Horizontal line: Median).

2.4.4 Source attribution by principal component analysis (PCA)

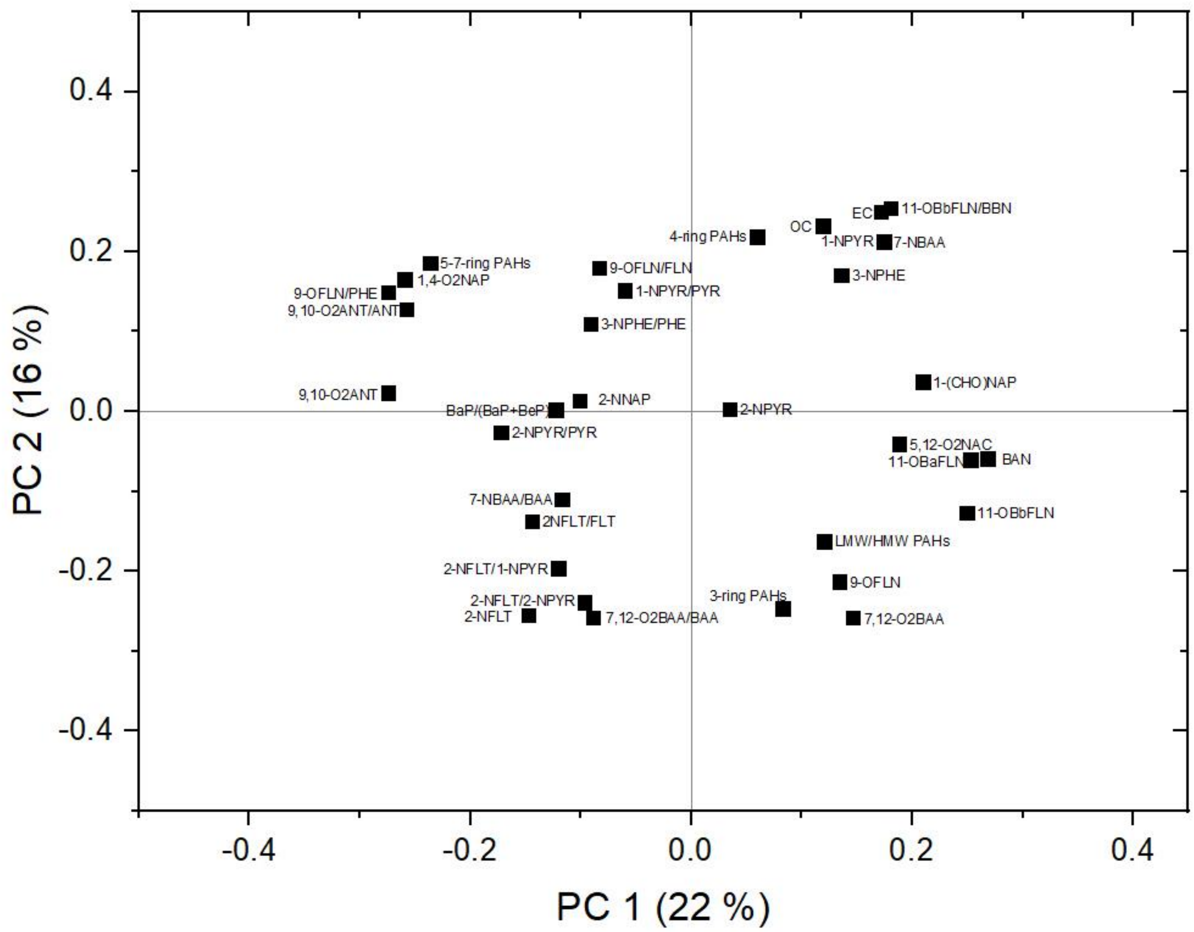
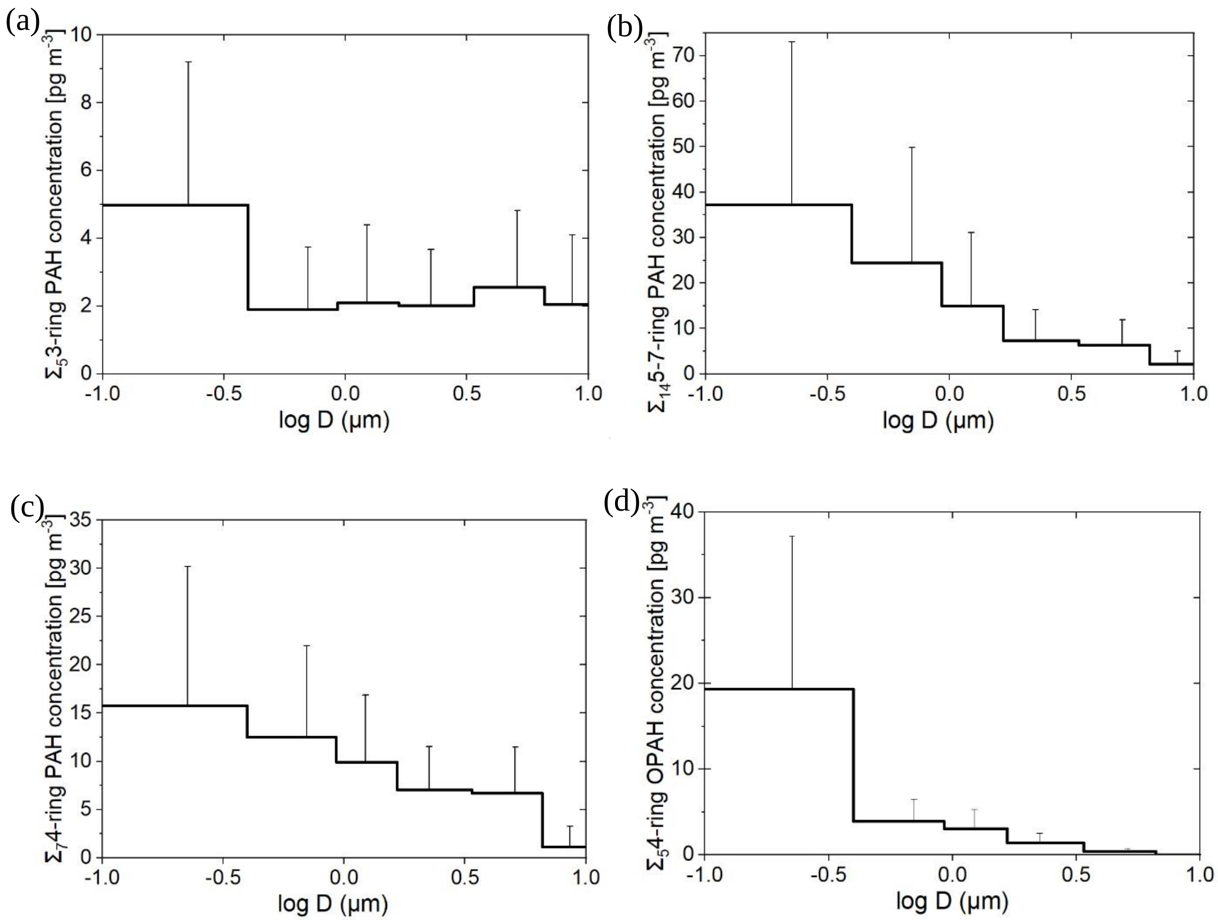


Figure S6. Principal component scores of individual PACs, groups of PACs and ratios thereof (PCA). Individual PACs' concentrations were normalized to the mass fraction in the substance class.

2.5 Mass size distributions



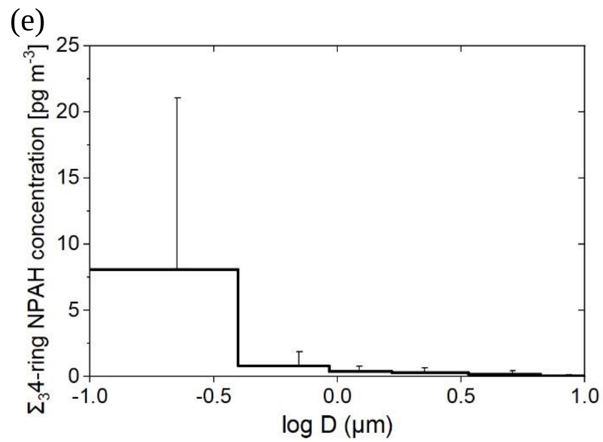


Fig. S7: Campaign average mass size distributions (MSDs) of a) $\sum_5$3-ring PAHs, b) $\sum_{14}$5-7-ring PAHs, c) $\sum_7$4-ring PAHs, d) $\sum_5$4-ring OPAHs, e) $\sum_3$4-ring NPAHs.

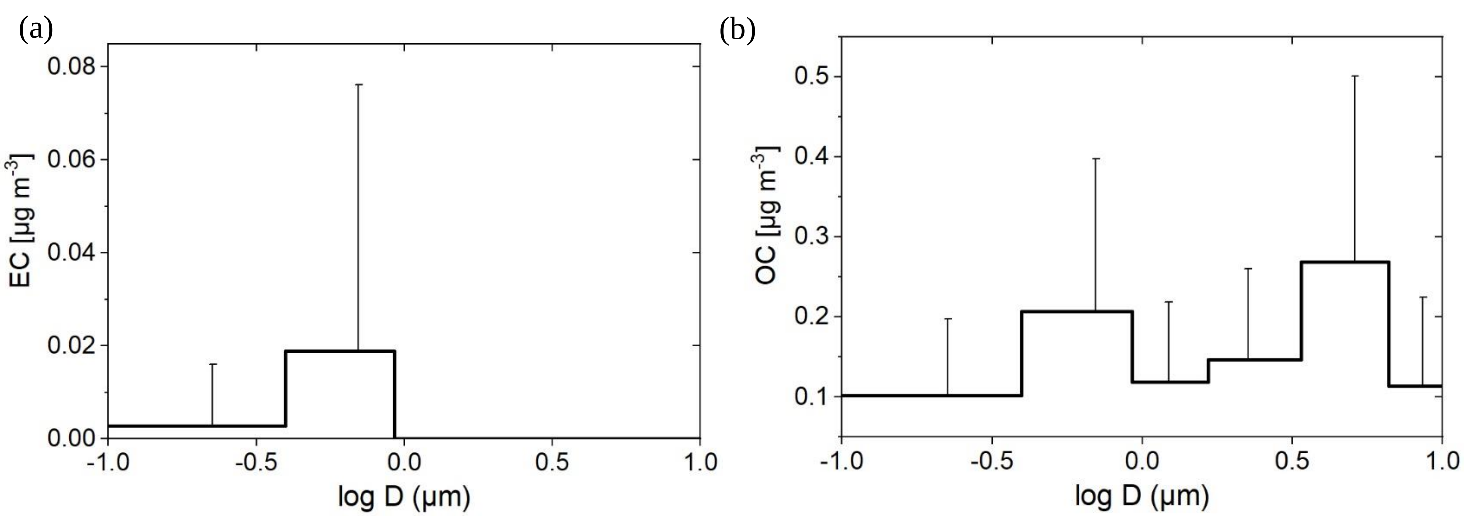


Fig. S8: Campaign average mass size distributions (MSDs) of (a) EC and (b) OC during the campaign; including standard deviation as error bars

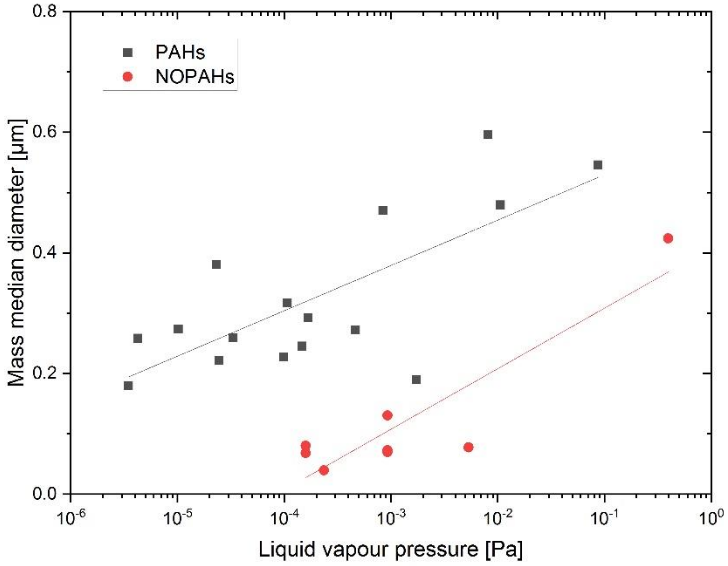
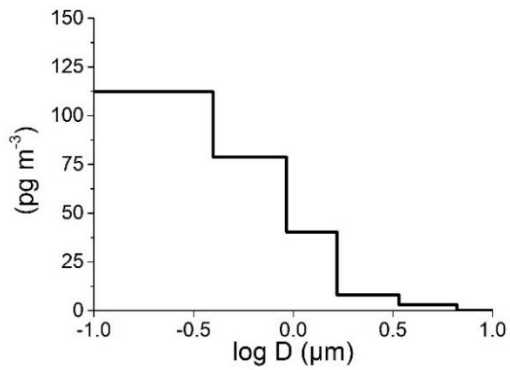
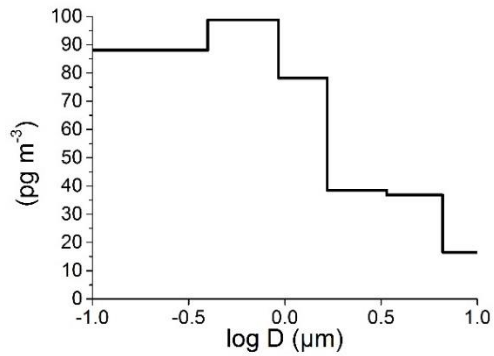
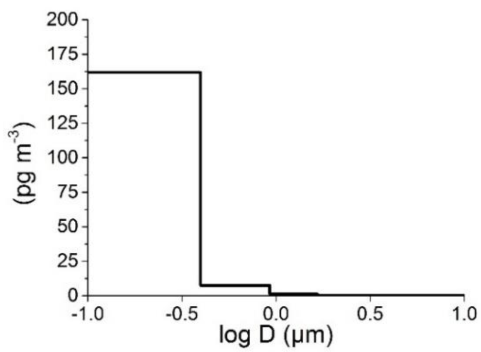
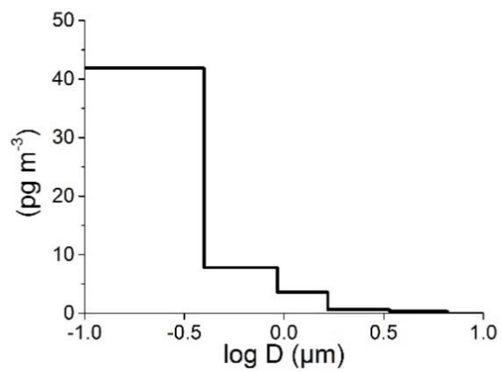


Fig. S9: Mass median diameter (MMD) of PACs in dependence of their subcooled liquid vapour pressure (only considered compounds with a detection frequency >30 %).

Substances	Sample C8 (03.08.), mostly fresh aerosol	Sample C7 (29.-30.07.), mostly aged aerosol
$\sum_{26}$PAHs		
$\sum_{11}$OPAHs		

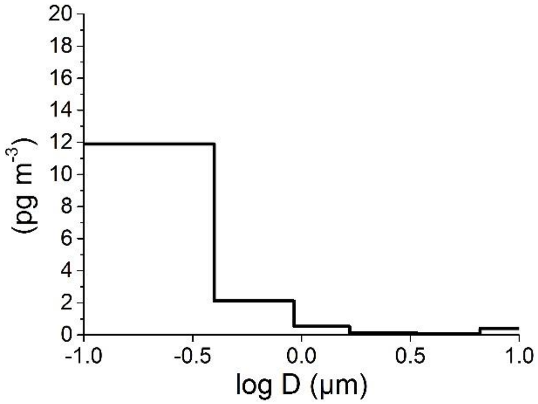
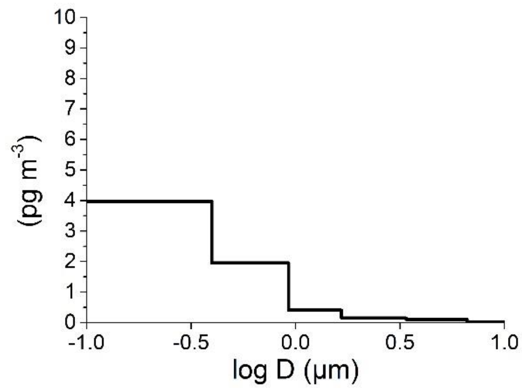
Substances	Sample C8 (03.08.), mostly fresh aerosol	Sample C7 (29.-30.07.), mostly aged aerosol
$\sum_{17}$NPAHs		

Fig. S10: Exemplary mass size distributions (MSDs) for fresh (1st column) and aged (2nd column) aerosols, respectively.

Table S19. Campaign average mass median diameter (MMD) (calculated from campaign average concentrations) of a) PAHs, b) OPAHs and c) NPAHs. (n.d.: not determined since not detected in particulate phase)

a)

Substance	MMD average (from average concentrations)	Detection frequency all stages (only filtered) [%]
ACY	n.d.	0
ACE	n.d.	0
FLN	n.d.	0
PHE	0.55	48
ANT	0.02	1
FLT	0.60	49
PYR	0.48	44
BAA	0.32	65
CHR	0.29	62
BBF	0.19	75
BKF	0.27	49
BAP	0.38	48
DBA	0.26	60
INP	0.43	15
BPE	0.26	74
BJF	0.23	58
BEP	0.22	66
PER	0.08	20
DCA	0.12	14
ATT	1.00	33
COR	0.18	38
TPH	0.25	46
CCP	0.12	6
BGF	0.27	54
BBN	0.12	10
BNT	0.47	56
RET	0.02	19

b)

Substance	MMD average (from average concentrations)	Detection frequency all stages (only filtered) [%]
1,4-O2NAP	8.49	1
1-(CHO)NAP	0.42	63
9-OFLN	0.02	17
9,10-O2ANT	0.02	17
1,4-O2ANT	n.d.	0
9,10-O2PHE	n.d.	0
11-OBaFLN	0.13	37
11-OBbFLN	0.07	36
BAN	0.07	27
7,12-O2BAA	0.07	57
5,12-O2NAC	0.08	72

c)

Substance	MMD average (from average concentrations)	Detection frequency all stages (only filtered) [%]
1-NNAP	4.65	1
2-NNAP	0.02	8
3-NACE	0.02	1
5-NACE	0.02	8
2-NFLN	n.d.	0
9-NANT	0.02	1
9-NPHE	n.d.	0
3-NPHE	0.06	3
2-NFLT	0.08	47
1-NPYR	0.04	35
2-NPYR	0.05	17
7-NBAA	0.05	10
6-NCHR	n.d.	0
1,3-N2PYR	n.d.	0
1,6-N2PYR	n.d.	0
1,8-N2PYR	n.d.	0
6-NBAP	0.03	3

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