

Drift Tube IMS Measured Collision cross sections ($^{DT}CCS_{N_2}$) for Xenobiotics

Polycyclic Aromatic Hydrocarbons (PAHs)

Compounds	Abbreviation	CAS	Formula	Exact Mass	[M+H] ⁺	Avg CCS	RSD%	[M] ⁺	Avg CCS	RSD%
Naphthalene	NAY	91-20-3	C10H8	128.0626	129.0704	120.28	0.32	128.0626	118.84	0.18
1-methylnaphthalene	1MA	90-12-0	C11H10	142.0782	143.0861	125.20	0.14	142.0782	123.49	0.14
2-methylnaphthalene	2MT	91-57-6	C11H10	142.0782	143.0861	124.57	0.11	142.0782	123.19	0.04
Acenaphthylene	ALE	208-96-8	C12H8	152.0626	153.0704	125.71	0.10	152.0626	124.80	0.04
Acenaphthene	ATC	83-32-9	C12H10	154.0782	155.0861	N/A	N/A	154.0782	128.5	0.11
1, 2-Dimethylnaphthalene	1DL	573-98-8	C12H12	156.0939	157.1017	130.93	0.35	156.0939	128.35	0.15
1,6-Dimethylnaphthalene	16D	575-43-9	C12H12	156.0939	157.1017	130.13	0.19	156.0939	127.82	0.10
2, 7-Dimethylnaphthalene	27D	582-16-1	C12H12	156.0939	157.1017	131.00	0.11	156.0939	N/A	N/A
Fluorene	FOR	86-73-7	C13H10	166.0782	167.0861	N/A	N/A	166.0782	130.9	0.12
2,3,4- Trimethylnaphthalene	TMN	2245-38-7	C13H14	170.1095	171.1174	N/A	N/A	170.1095	134.67	0.09
Anthracene	ACO	120-12-7	C14H10	178.0782	179.0861	N/A	N/A	178.0782	133.1	0.14
Perinaphthenon	PEN	548-39-0	C13H8O	180.0575	181.0653	134.59	0.55	180.0575	N/A	N/A
Acenaphthenequinone	AQL	82-86-0	C12H6O2	182.0368	183.0446	144.02	0.45	182.0368	N/A	N/A
Dibenzothiophene	DBT	132-65-0	C12 H8 S	184.0347	185.0425	N/A	N/A	184.0347	132.30	0.08
1-Methylphenanthrene	1ME	832-69-9	C15 H12	192.0939	193.1017	N/A	N/A	192.0939	137.83	0.08
2-Methylanthracene	2ME	613-12-7	C15H12	192.0939	193.1017	138.61	0.30	192.0939	137.27	0.28
9-Methylanthracene	9ME	779-02-2	C15H12	192.0939	193.1017	N/A	N/A	192.0939	136.43	0.06
Pyrene	PE5	129-00-0	C16H10	202.0782	203.0861	137.97	0.09	202.0782	137.50	0.19
Fluoranthene	FA	206-44-0	C16H10	202.0783	203.0861	138.84	0.00	202.0783	138.34	0.06
2, 3-Dimethylanthracene	23D	613-06-9	C16H14	206.1095	207.1174	146.15	0.09	206.1095	N/A	N/A
3,6-Dimethylphenanthrene	36T	1576-67-6	C16H14	206.1095	207.1174	145.58	0.06	206.1095	144.44	0.09
Anthraquinone	AQU	84-65-1	C14H8O2	208.0524	209.0603	141.89	0.13	208.0524	N/A	N/A
Triphenylene	TPE	127-59-4	C18H12	228.0939	229.1017	N/A	N/A	228.0939	144.81	0.03
Benzanthrone	BHR	82-05-3	C17H10O	230.0732	231.0810	145.71	0.07	230.0732	144.61	0.03
Pyrene-4,5 dione	PY4	6217-22-7	C16H8O2	232.0524	233.0603	144.30	0.03	232.0524	N/A	N/A
Benz(j)aceanthrylene	BJY	202-33-5	C20H12	252.0939	253.1017	155.08	0.03	252.0939	152.68	0.08
Benzo(b)fluoranthene	BBF	205-99-2	C20H12	252.0939	253.1017	N/A	N/A	252.0939	151.95	0.08
Benzo(k)fluoranthene	BKF	207-08-9	C20H12	252.0939	253.1017	154.36	0.53	252.0939	152.98	0.17
Benzo(a)Pyrene	BAP	50-32-8	C20H12	252.0939	253.1017	152.05	0.08	252.0939	151.24	0.11
5, 12-naphthacene quinone	5NA	1090-13-7	C18H10O2	258.0681	259.0759	157.54	0.88	258.0681	N/A	N/A
Benzo(g,h,i)perylene	BGI	191-24-2	C22H12	276.0939	277.1017	157.31	0.12	276.0939	155.83	0.11
Indeno(1,2,3-cd)pyrene	I12	193-39-5	C22H12	276.0939	277.1017	159.65	0.56	276.0939	158.15	0.19
Dibenzo(a,h)anthracene	DBA	53-70-3	C22 H14	278.1095	279.1174	164.07	0.04	278.1095	162.87	0.09
Coronene	CON	191-07-1	C24H12	300.0939	301.1017	N/A	N/A	300.0939	161.87	0.12
Dibenzo(a,h)pyrene	DAH	189-64-0	C24H14	302.1095	303.1174	166.49	0.10	302.1095	165.22	0.08
Dibenzochrysene	DBC	191-68-4	C26H16	302.1095	303.1174	166.69	0.05	302.1095	165.45	0.06

OH-PAHs

Compounds	Abbreviation	CAS	Formula	Exact Mass	[M-H] ⁻	Avg CCS	RSD%
1, 5 dihydroxynaphthalene	1DH	83-56-7	C10H8O2	160.0524	159.0446	133.63	0.35
2, 3-dihydroxynaphthalene	23A	92-44-4	C10H8O2	160.0524	159.0446	131.73	0.16
2, 6- dihydroxynaphthalene	26T	581-43-1	C10H8O2	160.0524	159.0446	137.47	0.41
12-Hydroxybenzo(a)pyrene	1AE	56892-33-2	C20H12O	268.0888	267.0810	163.10	0.06
7-hydroxybenzo(a)pyrene	7AR	37994-82-4	C20H12O	268.0888	267.0810	163.20	0.00
6-Hydroxychrysene		37515-51-8	C18H12O	244.0888	243.0810	157.83	0.07
1-Hydroxypyrene		5315-79-7	C16H10O	218.0732	217.0653	148.47	0.08

Polychlorinated biphenyl (PCBs)

Compound	Abbreviation	CAS number	Formula	Exact Mass	[M-Cl+O] ⁻	Avg CCS	RSD %
2,4,4'-Trichlorobiphenyl	PCB-28	7012-37-5	C12H7Cl3	255.9613	236.9874	149.67	0.14
2,4,5-Trichlorobiphenyl	PCB 29	15862-07-4	C12H7Cl3	255.9613	236.9874	150.67	0.17
2,4,6-Trichlorobiphenyl	PCB-30	35693-92-6	C12H7Cl3	255.9613	236.9874	150.10	0.12
2,2',5,5'-Tetrachlorobiphenyl	PCB-52	35693-99-3	C12H6Cl4	289.9224	270.9461	156.69	0.36
2,3',4',5'-Tetrachlorobiphenyl	PCB-70	32598-11-1	C12H6Cl4	289.9224	270.9484	155.63	0.15
3,3',4,4'-Tetrachlorobiphenyl	PCB-77	32598-13-3	C12H6Cl4	289.9224	270.9461	156.8	0.10
3,4,4',5'-Tetrachlorobiphenyl	PCB-81	70362-50-4	C12H6Cl4	289.9224	270.9484	158.57	0.07
2,2',4,5,5'-Pentachlorobiphenyl	PCB-101	37680-73-2	C12H5Cl5	323.8834	304.9061	162.55	0.07
2,2',4,5',6-Pentachlorobiphenyl	PCB-103	60145-21-3	C12H5Cl5	323.8834	304.9095	160.74	0.14
2,3,3',4,4'-Pentachlorobiphenyl	PCB-105	32598-14-4	C12H5Cl5	323.8834	304.9095	161.63	0.04
2,3,4,4',5-Pentachlorobiphenyl	PCB-114	74472-37-0	C12H5Cl5	323.8834	304.9095	162.13	0.04
3,3',4,4',5-Pentachlorobiphenyl	PCB-126	57465-28-8	C12H5Cl5	323.8834	304.9095	164.43	0.04
2,2',3,4,4',5-Hexachlorobiphenyl	PCB-138	35065-28-2	C12H4Cl6	357.8400	338.8661	167.98	0.12
2,3,3',4,4',5-Hexachlorobiphenyl	PCB-156	38380-08-4	C12H4Cl6	357.8444	338.8705	168.23	0.07
2,3',4,4',5,5'-Hexachlorobiphenyl	PCB-167	52663-72-6	C12H4Cl6	357.8444	338.8705	167.83	0.07
3,3',4,4',5,5'-Hexachlorobiphenyl	PCB-169	32774-16-6	C12H4Cl6	357.8444	338.8705	169.97	0.12
2,3,3',4,4',5,5'-Heptachlorobiphenyl	PCB-189	39635-31-9	C12H3Cl7	391.8054	372.8315	173.93	0.03
2,3,3',4,4',5,6-Heptachlorobiphenyl	PCB-190	41411-64-7	C12H3Cl7	391.8054	372.8315	173.33	0.07
2,3,3',4',5,5',6-Heptachlorobiphenyl	PCB-193	69782-91-8	C12H3Cl7	391.8054	372.8315	173.87	0.07
2,2',3,3',4,4',5,5'-Octachlorobiphenyl	PCB-194	35694-08-7	C12H2Cl8	425.7665	406.7925	180.33	0.03
2,2',3,3',4,4',5,6-Octachlorobiphenyl	PCB-195	52663-78-2	C12H2Cl8	425.7665	406.7925	178.03	0.03
2,2',3,3',5,5',6,6'-Octachlorobiphenyl	PCB-202	2136-99-4	C12H2Cl8	425.7665	406.7925	176.90	0.06
2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl	PCB-206	40186-72-9	C12H1Cl9	459.7275	440.7536	183.47	0.03
2,2',3,3',4,4',5,6,6'-Nonachlorobiphenyl	PCB-207	52663-79-3	C12H1Cl9	459.7275	440.7536	181.70	0.11
2,2',3,3',4,5,5',6,6'-Nonachlorobiphenyl	PCB-208	52663-77-1	C12H1Cl9	459.7275	440.7536	182.07	0.08
Decachlorobiphenyl	PCB 209	2051-24-3	C12Cl10	493.6800	474.7061	185.88	0.58

OH-PCBs

Compound	Abbreviation	CAS number	Formula	Exact Mass	[M-H] ⁻	Avg CCS	RSD %
4-Hydroxy-2-chlorobiphenyl	4-OH-PCB-001	23719-22-4	C12H9ClO	204.0342	203.0264	147.50	0.07
4-Hydroxy-3-chlorobiphenyl	4-OH-PCB-002	92-04-6	C12H9ClO	204.0342	203.0264	146.53	0.10
2-Hydroxy-5-chlorobiphenyl	6-OH-PCB-002	607-12-5	C12H9ClO	204.0342	203.0264	144.03	0.08
4-Hydroxy-4'-chlorobiphenyl	4'-OH-PCB-003	28034-99-3	C12H9ClO	204.0342	203.0264	148.3	0.38
2-Hydroxy-2',5'-dichlorobiphenyl	2'-OH-PCB-009	53905-30-9	C12H8Cl2O	237.9952	236.9874	151.6	0.43
3-Hydroxy-2',5'-dichlorobiphenyl	3'-OH-PCB-009	53905-29-6	C12H8Cl2O	237.9952	236.9874	155.4	0.04
4-Hydroxy-2',5'-dichlorobiphenyl	4'-OH-PCB-009	53905-28-5	C12H8Cl2O	237.9952	236.9874	153.13	0.08
4-Hydroxy-3,5-dichlorobiphenyl	4-OH-PCB-014	1137-59-3	C12H8Cl2O	237.9952	236.9874	151.5	0.10
4-Hydroxy-2,2',5'-trichlorobiphenyl	4'-OH-PCB-018	53905-33-2	C12H7Cl3O	271.9562	270.9484	158.9	0.06
4-Hydroxy-2',4',6'-trichlorobiphenyl	4'-OH-PCB-030	14962-28-8	C12H7Cl3O	271.9562	270.9484	159.83	0.04
4-Hydroxy-2,2',4',6'-tetrachlorobiphenyl	4'-OH-PCB-050	150304-08-8	C12H6Cl4O	305.9173	304.9095	163.2	0.04
4-Hydroxy-2',3',4',5'-tetrachlorobiphenyl	4'-OH-PCB-061	67651-34-7	C12H6Cl4O	305.9173	304.9095	163.67	0.04
4-Hydroxy-2',3',5',6'-tetrachlorobiphenyl	4'-OH-PCB-065	14962-32-4	C12H6Cl4O	305.9173	304.9095	163.97	0.19
2-Hydroxy-2',3',4',5,5'-pentachlorobiphenyl	6'-OH-PCB-106	67651-36-9	C12H5Cl5O	339.8783	338.8705	166.8	0.23
4-Hydroxy-2',3',3',4',5'-pentachlorobiphenyl	4'-OH-PCB-106	67651-35-8	C12H5Cl5O	339.8783	338.8705	170.0	0.09
4-Hydroxy-2',3,3',4',5,5'-hexachlorobiphenyl	4'-OH-PCB-159	158076-63-2	C12H4Cl6O	373.8393	372.8315	175.3	0.06
4-Hydroxy-2',3,3',3',4',5,5'-hexachlorobiphenyl	4'-OH-PCB-165	N/A	C12H4Cl6O	373.8393	372.8315	175.70	0.10
5-Hydroxy-2,2',3,4,4',5,5'-heptachlorobiphenyl	5-OH-PCB-138	N/A	C12H3Cl7O	373.8393	372.8315	174.6	0.03
4'-Hydroxy-2,2',3,3',4,4',5,5'-heptachlorobiphenyl	4'-OH-PCB-172	N/A	C12H3Cl7O	407.8004	406.7925	180.4	0.14
3'-Hydroxy-2,2',3,4,4',5,6'-heptachlorobiphenyl	3'-OH-PCB-182	N/A	C12H3Cl7O	407.8004	406.7925	178.6	0.29

Polybrominated diphenyl ethers (PBDEs)

Compound	Abbreviation	CAS number	Formula	Exact Mass	[M-Br+O] ⁻	Avg CCS	RSD %
2,2',4-Tribromodiphenyl ether	PBDE-017	147217-75-2	C12H7Br3O	403.8047	340.8813	160.63	0.07
2,2',4,4'-Tetrabromodiphenyl ether	PBDE-047	5436-43-1	C12H6Br4O	481.7152	418.7918	169.73	0.03
2,3',4,4'-Tetrabromodiphenyl ether	PBDE-066	189084-61-5	C12H6Br4O	481.7152	418.7918	170.30	0.10
3,3',4,4'-Tetrabromodiphenyl ether	PBDE-077	93703-48-1	C12H6Br4O	481.7152	418.7918	172.07	0.03
2,2',3,4,4'-Pentabromodiphenyl ether	PBDE-085	182346-21-0	C12H5Br5O	559.6257	496.7023	176.97	0.07
2,2',4,4',6-Pentabromodiphenyl ether	PBDE 100	189084-64-8	C12H5Br5O	559.6257	496.7023	175.37	0.03
2,3,4,5,6-Pentabromodiphenyl ether	PBDE-116	189084-65-9	C12H5Br5O	559.6257	496.7023	172.00	0.00
2,2',3,3',4,4'-Hexabromodiphenyl ether	PBDE-128	182677-28-7	C12H4Br6O	637.5362	574.6128	184.57	0.08
2,2',3,4,4',5'-Hexabromodiphenyl ether	PBDE-138	182677-30-1	C12H4Br6O	637.5362	574.6128	184.87	0.08
2,2',4,4',5,5'-Hexabromodiphenyl ether	PBDE-153	68631-49-2	C12H4Br6O	637.5362	574.6128	183.53	0.11
2,2',4,4',5,6'-Hexabromodiphenyl ether	PBDE 154	207122-15-4	C12H4Br6O	637.5362	574.6128	183.57	0.11
2,2',3,4,4',5'-Heptabromodiphenyl ether	PBDE-183	207122-16-5	C12H3Br7O	715.4467	652.523321	189.87	0.19
2,3,3',4,4',5,6-Heptabromodiphenyl ether	PBDE-190	189084-68-2	C12H3Br7O	715.4467	652.5233	191.03	0.03
2,2',3,4,4',5,5',6-Octabromodiphenyl ether	PBDE-203	337513-72-1	C12H2Br8O	793.3573	730.4338	195.70	0.05
2,2',3,3',4,4',5,5',6-Nonabromodiphenyl ether	PBDE-206	63387-28-0	C12H1Br9O	871.2678	808.3443	202.77	0.06
Decabromodiphenyl ether	PBDE-209	1163-19-5	C12Br10O	949.1783	886.2549	205.23	0.20

OH-PBDEs

Compound	Abbreviation	CAS number	Formula	Exact Mass	[M-H] ⁻	Avg CCS	RSD %
2'-Hydroxy-4-monobromodiphenyl ether	2'-OH-BDE-003	N/A	C12H9BrO2	263.9786	262.9708	152.97	0.10
3'-Hydroxy-2,4-dibromodiphenyl ether	3'-OH-BDE-007	N/A	C12H8Br2O2	341.8891	340.8813	164.60	0.16
4'-Hydroxy-2,2',4-tribromodiphenyl ether	4'-OH-BDE-017	N/A	C12H7Br3O2	419.7996	418.7917	169.87	0.12
2'-Hydroxy-2,4,4'-tribromodiphenyl ether	2'-OH-BDE-028	N/A	C12H7Br3O2	419.7996	418.7917	169.13	0.03
4-Hydroxy-2,2',3,4'-tetrabromodiphenyl ether	4-OH-BDE-042	N/A	C12H6Br4O2	497.7101	496.7022	176.90	0.10
3-Hydroxy-2,2',4,4'-tetrabromodiphenyl ether	3-OH-BDE-047	N/A	C12H6Br4O2	497.7101	496.7022	177.23	0.09
5-Hydroxy-2,2',4,4'-tetrabromodiphenyl ether	5-OH-BDE-047	N/A	C12H6Br4O2	497.7101	496.7022	177.53	0.12
6-Hydroxy-2,2',4,4'-tetrabromodiphenyl ether	6-OH-BDE-047	N/A	C12H6Br4O2	497.7101	496.7022	175.53	0.31
2'-Hydroxy-2,3',4,5'-tetrabromodiphenyl ether	2'-OH-BDE-068	N/A	C12H6Br4O2	497.7101	496.7022	176.07	0.14
6-Hydroxy-2,2',3,4,4'-pentabromodiphenyl ether	6-OH-BDE-085	N/A	C12H5Br5O2	575.6206	574.6127	183.53	0.08
5'-Hydroxy-2,2',4,4',5-pentabromodiphenyl ether	5'-OH-BDE-099	N/A	C12H5Br5O2	575.6206	574.6127	184.30	0.39
6'-Hydroxy-2,2',4,4',5-pentabromodiphenyl ether	6'-OH-BDE-099	N/A	C12H5Br5O2	575.6206	574.6127	183.27	0.06
3-Hydroxy-2,2',4,4',6-pentabromodiphenyl ether	3-OH-BDE-100	N/A	C12H5Br5O2	575.6206	574.6127	181.73	0.06
4'-Hydroxy-2,2',4,4',5-pentabromodiphenyl ether	4'-OH-BDE-101	N/A	C12H5Br5O2	575.6206	574.6127	185.40	0.25