

Environmental Mass Spectrometry in the North American Great Lakes Fish Monitoring and Surveillance Program

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SI-1. Dual-column confirmation analyses were performed to provide two separate PCB analyses using two different column stationary phases (Agilent DB-XLB and Ultra II) and column lengths (60m and 25m). This allows for the unique determination, comparison, and confirmation of monitored compounds, and is a required element of many USEPA analytical methods. The lists of congeners for the two columns are as follows.

Primary column: PCB congeners analyzed with 25 m Ultra II

Assigned			Assigned			Assigned		
Peak #	# Cl	IUPAC #	Peak #	# Cl	IUPAC #	Peak #	# Cl	IUPAC #
1	1	1	35	4+4+4	41+64+71	69	6	137
2	1	3	36	5	96	70	6+7	130+176
3	2+2	4+10	37	4	40	71	6+6+6	138+163+164
4	2+2	7+9	38	4	67	72	6	158
5	2	6	39		OCS	73	6+7	129+178
6	2+2	5+8	40	4	74	74	6	166
7		HCB	41	4	70	75	7+7	182+187
8	2	14	42	4+5	66+95	76	7	183
9	3	19	43	5	91	77	6+6	128+167
10	3	30	44	4+4+5	56+60+92	78	7	185
11	2	11	45	5	84	79	7	174
12	2+2	12+13	46	5+5	89+101	80	7	177
13	3	18	47	5	99	81	6+7+8	156+171+202

14	2+3	15+17	48	5	119	82	6+7+8	157+173+201
15	3+3	24+27	49	5	83	83	7	172
16	3+3	16+32	50	5	97	84	8	197
17	3	34	51	5+5+5	87+115+117	85	7	180
18	3+4	29+54	52		p-p'-DDE	86	7	193
19	3	26	53	5	85	87	7	191
20	3	25	54	6	136	88	8	200
21	3	31	55	4+5	77+110+154	89		MIREX
22	3	28	56	5+6	82+151	90	7+7	170+190
23	3+3+4	20+33+53	57	5+6+6	124+135+144	91	8	198
24	4	51	58	5+6	109+147	92	8	199
25	3	22	59	5+6	123+149	93	8+8	196+203
26	4	45	60	5	118	94	7	189
27	4	46	61	6	134	95	8+9	195+208
28	4	52	62	5+6	114+133	96	9	207
29	4+4	43+49	63	5+6	122+131	97	8	194
30	4+4+4	47+48+75	64	6	146	98	8	205
31	4	65	65	6	153	99	9	206
32	3	35	66	5+6	105+132	100	10	209
33	4	44	67	6	141	101		PCT 5
34	3+4+4	37+42+59	68	7	179			

Confirmation analytical column: PCB congeners analyzed with 60m DB-XLB

Assigned			Assigned			Assigned		
Peak #	# Cl	IUPAC #	Peak #	# Cl	IUPAC #	Peak #	# Cl	IUPAC #
1	1	1	44	3	35	87	7	176
2	1	2	45	4	71	88	6	137
3	1	3	46	3+4	37+41	89	6	130
4	2+2	4+10	47	4	64	90	6	164
5	2	9	48	4+5	40+103	91	6	138
6	2	7	49	5	100	92	6	163
7	2	6	50	4	67	93	7	178
8	2	5	51	4+5	63+93	94	6	129
9	2	8	52	5	95	95	6	158
10		HCB	53	4	74	96	7	175
11	3	19	54	4	70	97	7	187
12	2	14	55	4+5	66+91	98	7	183
13	3	30	56	5	92	99	6+7	128+185
14	3	18	57	4+5	56+84	100	7	174
15	3	17	58	5+5	90+101	101	6	167
16	2	12	59	4	60	102	8	202
17	2+3	13+27	60	5	99	103	7	177
18	3	24	61	5+5	83+119	104	7+8	171+201
19	3	16	62	5	97	105	7	173
20	2	15	63	5	87	106	8	197
21	3	32	64		p-p' DDE	107	6	156
22	3+4	34+54	65	5+6	117+136	108	7	172
23	3	29	66	5+5+6	85+115+154	109	6	157
24	3	26	67	5	110	110	7	180
25	3	25	68	4	81	111	7	193
26	3	31	69	6	151	112	8	200
27	4	53	70	5	82	113	7	191
28	3	28	71	6	135	114	7	170
29	3+3	20+33	72	4+6	77+144	115	8	199
30	4	51	73	6	147	116	7	190

31	4	45	74	6	149	117		Mirex
32	3	22	75	5	124	118	8	196
33	4	46	76	5+5	109+123	119	8	203
34	4	73	77	6	134	120	9	208
35	4	69	78	5	118	121	7	189
36	4	52	79	6	131	122	8+9	195+207
37	4	48	80	5+6	122+165	123	8	194
38	4	49	81	6	146	124	8	205
39	4+5	47+104	82	5	114	125	9	206
40	4	75	83	6	153	126	10	209
41	4	44	84	6	132	127	5	PCT 5
42	4	59	85	7	179			
43	4	42	86	5+6	105+141			
