Electronic Supplementary Material (ESI) for Analytical Methods.

Supplemental Information

Targeted Analysis Data Processing:

Data was processed using LECO ChromaTOF BT software v5.40.12.0. The following parameters were used following optimization of the data processing method. Initial peak finding was accomplished using a signal-to-noise ratio of 20 and a minimum match of 500 required to combine slices. Analytes were quantitated using extracted ion chromatograms with a mass tolerance of 500 ppm.

Non-Targeted Analysis Data Processing:

Manufacturer guidelines were followed to import ChromaTOF BT data into ChromaTOF GC software v4.74.2.0 as .netCDF files. Parameters for basic peak finding and statistical compare were determined based on these guidelines. Initial peak finding was accomplished using a baseline offset of 1.0, no smoothing of data points, minimum signal-to-noise ratio of 200, and minimum match of 500 required to combine slices. Compound identification using the NIST MS Database (2014) required a minimum similarity match of 700. During the alignment process of statistical compare a second peak finding method is employed. Second peak finding was accomplished using a signal-to-noise ratio of 50. Alignment required a minimum match similarity of 600 for compounds. In order for aligned compounds to be retained within the final aligned peak table, compounds had to occur in at least 60% of samples within a class or within at least 60% of all samples.

SI Table 1. Standards used for method development and targeted analysis application. Standards used for method development are listed in red.

Compounds	Cas #	Manufacturer
1-methylnaphthalene	90-12-0	Chem Service
2,2',4,4',5,5'-Hexabromobiphenyl	59080-40-9	Restek
2,4'-Methoxychlor	30667-99-3	Restek
2,6-dimethylnaphthalene	581-42-0	Chem Service
2-methylnaphthalene	91-57-6	Chem Service
4,4'-Dichlorobenzophenone	90-98-2	Restek
4,4'-Methoxychlor olefin	2132-70-9	Restek
9,10-anthraquinone	84-65-1	Chem Service
Acetophenone	98-86-2	Restek
Aldrin	309-00-2	Restek
anthracene	120-12-7	Restek
BDE-100	189084-64-8	Restek
BDE-153	68631-49-2	Restek
BDE-47	5436-43-1	Restek
BDE-99	60348-60-9	Restek
benfluralin	1861-40-1	Chem Service

Compounds	Cas #	Manufacturer
benzophenone	119-61-9	Chem Service
caffeine	58-08-2	Restek
Celestolide	13171-00-1	TCI America
Chlorbenside	103-17-3	Restek
Chlorfenson (Ovex)	80-33-1	Restek
Chloroneb	2675-77-6	Restek
chlorpyrifos	2921-88-2	Restek
cis-Chlordane	5103-71-9	Restek
cis-Nonachlor	5103-73-1	Restek
cotinine	486-56-6	Restek
Dacthal	1861-32-1	Restek
Deet	134-62-3	Chem Service
DEHP Bis(2-ethylhexyl)phthalate	117-81-7	Restek
diazinon	333-41-5	Chem Service
dichlorvos	62-73-7	Chem Service
Dieldrin	60-57-1	Restek
diethyl phthalate	84-66-2	Chem Service
dl-camphor	76-22-2	Chem Service
Endosulfan ether	3369-52-6	Restek
Endosulfan I	959-98-8	Restek
Endosulfan II	33213-65-9	Restek
Endosulfan sulfate	1031-07-8	Restek
Endrin	72-20-8	Restek
Endrin aldehyde	7421-93-4	Restek
Endrin ketone	53494-70-5	Restek
Ethylan (Perthane)	72-56-0	Restek
Fenson	80-38-6	Restek
fluoranthene	206-44-0	Restek
Galaxolide	1222-05-5	TCI America
Heptachlor	76-44-8	Restek
Heptachlor epoxide	1024-57-3	Restek
Hexachlorobenzene	118-74-1	Restek
Indole	120-72-9	Chem Service
Isodrin	465-73-6	Restek
Isophorone	78-59-1	Chem Service
isoquinoline	119-65-3	Chem Service
menthol	1490-04-6	Chem Service
metalaxyl	57837-19-1	Chem Service
Methoxychlor	72-43-5	Restek
methyl salicylate	119-36-8	Chem Service
methyl triclosan	4640_01_1	Dr. Ehrenstorfer GmbH
Mirex	2385-85-5	Restek

Compounds	Cas #	Manufacturer
naphthalene	91-20-3	Restek
o,p'-DDD	53-19-0	Restek
o,p'-DDE	3424-82-6	Restek
o,p'-DDT	789-02-6	Restek
oxychlordane	27304-13-8	Chem Service
p,p'-DDD	72-54-8	Restek
p,p'-DDE	72-55-9	Restek
p,p'-DDT	50-29-3	Restek
Pentachloroanisole	1825-21-4	Restek
Pentachlorobenzene	608-93-5	Restek
Pentachlorothioanisole	1825-19-0	Restek
Phantolid	15323-35-0	Key Organics
Phenanthrene	85-01-8	Restek
pyrene	129-00-0	Restek
Tetradifon	116-29-0	Restek
Tonalid	21145-77-7	Key Organics
trans-Chlordane	5103-74-2	Restek
trans-Nonachlor	39765-80-5	Restek
Traseolide	68140-48-7	Chemcruz
tributoxyethyl phosphate	78-51-3	Chem Service
tributyl phosphate	126-73-8	Chem Service
triethyl citrate	77-93-0	Chem Service
Trifluralin	1582-09-8	Restek
triphenyl phosphate	115-86-6	Chem Service
tris(1,3-dichloroisopropyl)phosphate	13674-87-8	Restek
tris(2-chloroethyl)phosphate	115-96-8	Chem Service
α-HCH	319-84-6	Restek
β-HCH	319-85-7	Restek
γ-HCH	58-89-9	Restek
δ-HCH	319-86-8	Restek

SI Table 2. Polychlorinated biphenyl congeners used for method development and targeted analysis application. Congeners used in method development are listed in red.

PCB Congener	Cas #	Manufacturer
1	2051-60-7	AccuStandard
2	2051-61-8	AccuStandard
3	2051-62-9	AccuStandard
4	13029-08-8	AccuStandard
5	16605-91-7	AccuStandard
6	34883-39-1	AccuStandard
7	33284-50-3	AccuStandard
8	25569-80-6	AccuStandard
9	34883-43-7	AccuStandard
10	33146-45-1	AccuStandard
12	2974-92-7	AccuStandard
13	2974-90-5	AccuStandard
14	34883-41-5	AccuStandard
15	2050-68-2	AccuStandard
16	38444-73-4	AccuStandard
17	37680-66-3	AccuStandard
18	37680-65-2	AccuStandard
19	38444-78-9	AccuStandard
20	38444-84-7	AccuStandard
22	55712-37-3	AccuStandard
24	55702-45-9	AccuStandard
25	7012-37-5	AccuStandard
26	38444-81-4	AccuStandard
27	38444-76-7	AccuStandard
28	38444-85-8	AccuStandard
29	15862-07-4	AccuStandard
31	16606-02-3	AccuStandard
32	38444-77-8	AccuStandard
33	38444-86-9	AccuStandard
34	37680-68-5	AccuStandard
35	37680-69-6	AccuStandard
37	38444-90-5	AccuStandard
40	38444-93-8	AccuStandard
41	52663-59-9	AccuStandard
42	36559-22-5	AccuStandard
44	35693-99-3	AccuStandard
45	70362-45-7	AccuStandard
46	41464-47-5	AccuStandard
47	2437-79-8	AccuStandard
48	70362-47-9	AccuStandard
49	41464-40-8	AccuStandard
51	68194-04-7	AccuStandard
52	41464-39-5	AccuStandard
53	41464-41-9	AccuStandard
54	15968-05-5	AccuStandard
56	41464-46-4	AccuStandard
59	74472-33-6	AccuStandard
60	33025-41-1	AccuStandard
63	74472-34-7	AccuStandard
64	52663-58-8	AccuStandard
66	73557-53-8	AccuStandard
67	32690-93-0	AccuStandard
69	60233-24-1	AccuStandard
70	32598-11-1	AccuStandard
71	32598-10-0	AccuStandard
73	74338-23-1	AccuStandard
74	41464-43-1	AccuStandard
75	32598-12-2	AccuStandard
77	32598-13-3	AccuStandard
81	70362-50-4	AccuStandard
82	38380-01-7	AccuStandard
83	60145-20-2	AccuStandard
84	52663-60-2	AccuStandard
85	65510-45-4	AccuStandard
87	38380-02-8	AccuStandard
90	68194-07-0	AccuStandard
91	68194-05-8	AccuStandard
92	52663-61-3	AccuStandard
93	73575-56-1	AccuStandard
95	38379-99-6	AccuStandard
97	41464-51-1	AccuStandard
99	38380-03-9	AccuStandard
100	39485-83-1	AccuStandard
101	37680-73-2	AccuStandard
103	60145-21-3	AccuStandard
104	56558-16-8	AccuStandard
105	32598-14-4	AccuStandard
107	70424-68-9	AccuStandard

PCB Congener	Cas #	Manufacturer
110	52663-62-4	AccuStandard
114	74472-37-0	AccuStandard
115	74472-38-1	AccuStandard
117	68194-11-6	AccuStandard
118	31508-00-6	AccuStandard
119	56558-17-9	AccuStandard
122	76842-07-4	AccuStandard
123	65510-44-3	AccuStandard
124	70424-70-3	AccuStandard
128	38380-07-3	AccuStandard
129	55215-18-4	AccuStandard
130	52663-66-8	AccuStandard
131	61798-70-7	AccuStandard
132	38380-05-1	AccuStandard
134	52704-70-8	AccuStandard
135	52744-13-5	AccuStandard
136	38411-22-2	AccuStandard
137	35694-06-5	AccuStandard
138	68194-13-8	AccuStandard
141	52712-04-6	AccuStandard
144	68194-14-9	AccuStandard
146	51908-16-8	AccuStandard
147	35065-27-1	AccuStandard
149	38380-04-0	AccuStandard
151	52663-63-5	AccuStandard
153	52663-64-6	AccuStandard
154	60145-22-4	AccuStandard
156	38380-08-4	AccuStandard
157	69782-90-7	AccuStandard
158	74472-42-7	AccuStandard
163	74472-44-9	AccuStandard
164	74472-45-0	AccuStandard
165	74472-46-1	AccuStandard
167	52663-72-6	AccuStandard
170	35065-30-6	AccuStandard
171	52663-71-5	AccuStandard
172	52663-74-8	AccuStandard
173	35065-28-2	AccuStandard
174	52663-68-0	AccuStandard
175	40186-70-7	AccuStandard
176	52663-65-7	AccuStandard
177	38411-25-5	AccuStandard

PCB Congener	Cas #	Manufacturer
178	52663-67-9	AccuStandard
179	52663-70-4	AccuStandard
180	68194-16-1	AccuStandard
183	52663-69-1	AccuStandard
185	52712-05-7	AccuStandard
187	35065-29-3	AccuStandard
189	39635-31-9	AccuStandard
190	41411-64-7	AccuStandard
191	74472-50-7	AccuStandard
193	69782-91-8	AccuStandard
194	52663-75-9	AccuStandard
195	52663-76-0	AccuStandard
196	42740-50-1	AccuStandard
197	33091-17-7	AccuStandard
199	52663-78-2	AccuStandard
200	52663-73-7	AccuStandard
201	40186-71-8	AccuStandard
202	2136-99-4	AccuStandard
203	35694-08-7	AccuStandard
205	74472-53-0	AccuStandard
206	40186-72-9	AccuStandard
207	52663-79-3	AccuStandard
208	52663-77-1	AccuStandard
209	2051-24-3	AccuStandard

SI Table 3. Summary of recovery values using acetonitrile as the extraction solvent vs. ethyl acetate. Method detection limit (MDL) calculated using final optimization of method.

Analyte	Acetonitrile		Ethyl Acetate		
	Mean % Recovery	*Std. Error*	*Mean % Recovery*	*Std. Error*	*MDL (ng/g)*
BDE-47	10.67	0.83	16.76	1.98	0.04
BDE-99	6.11	0.74	7.37	1.37	0.22
BDE-100	4.24	1.76	7.33	1.79	0.31
BDE-153	0.00	N/A	41.42	2.12	2.17
2,2',4,4',5,5'-Hexabromobiphenyl	0.00	N/A	48.57	2.83	0.97
PCB 001	15.56	1.32	59.10	4.85	0.18
PCB 002	18.96	1.52	68.37	4.45	0.20
PCB 003	19.47	1.52	74.52	5.75	0.54
PCB 004	12.04	0.89	57.23	4.10	0.37
PCB 006	16.78	0.77	76.80	3.10	0.33
PCB 008	16.33	0.65	78.11	3.48	0.32
PCB 009	15.31	0.72	71.69	1.76	0.29
PCB 016	11.82	1.17	40.69	4.95	0.16
PCB 018	11.08	1.07	39.58	6.26	0.15
PCB 019	15.31	1.12	31.82	3.19	0.28
PCB 022	13.96	0.74	54.79	8.45	0.11
PCB 025	13.64	0.87	50.70	7.81	0.13
PCB 028	13.22	0.87	54.73	8.48	0.11
PCB 044	13.03	0.88	18.97	4.34	0.10
PCB 052	12.88	0.71	22.15	4.53	0.10
PCB 056	7.78	3.61	56.68	1.98	0.23
PCB 066	13.23	0.73	55.16	0.91	0.25
PCB 067	12.55	1.17	34.71	5.43	0.16
PCB 071	13.31	1.02	31.27	6.64	0.10
PCB 074	11.77	1.35	39.54	8.24	0.16
PCB 082	8.19	0.23	30.93	0.76	0.15
PCB 087	4.97	1.94	18.86	0.59	0.20
PCB 099	7.73	0.38	30.63	1.41	0.29
PCB 110	0.00	N/A	55.68	4.39	0.66
PCB 138	9.27	0.11	21.39	11.04	0.46
PCB 146	7.27	0.03	29.59	3.89	0.11
PCB 147	7.36	0.16	24.54	5.57	0.08
PCB 153	7.68	0.26	20.67	9.35	0.19
PCB 173	7.44	1.95	11.27	11.27	0.22
PCB 174	9.29	0.28	28.28	9.42	0.40
PCB 177	8.62	0.17	12.00	11.41	0.25
PCB 179	8.11	0.21	5.25	1.98	0.31

Analyte	Acetonitrile		Ethyl Acetate		
	Mean % Recovery	*Std. Error*	*Mean % Recovery*	*Std. Error*	*MDL (ng/g)*
PCB 180	5.17	2.72	35.37	1.29	0.06
PCB 194	3.88	2.03	78.10	1.35	0.08
PCB 195	5.85	1.97	71.56	8.35	0.26
PCB 199	8.04	0.50	60.75	1.11	0.11
PCB 203	6.24	0.29	66.44	2.72	0.11
PCB 206	4.67	0.48	87.21	1.39	0.10
α-HCH	15.81	0.84	60.72	9.06	0.64
β-HCH	23.95	1.37	74.31	10.07	0.40
γ-HCH	17.01	1.22	60.28	9.05	0.33
δ-HCH	14.46	1.43	70.55	9.26	0.18
p,p'-DDD	13.73	0.06	60.56	6.84	0.50
p,p'-DDE	7.67	0.41	76.73	7.19	0.52
p,p'-DDT	15.77	0.05	47.24	4.34	0.16
Aldrin	17.19	3.37	62.29	5.26	0.29
cis-Chlordane	2.46	2.46	65.52	3.94	0.45
Dieldrin	0.00	N/A	61.49	7.80	5.26
Endosulfan I	9.81	0.45	11.42	2.39	2.32
Endosulfan II	0.59	0.15	12.96	1.78	0.35
Endosulfan sulfate	7.36	4.00	38.69	2.79	0.57
Endrin	11.12	3.11	73.92	14.47	3.70
Endrin aldehyde	0.00	N/A	34.81	4.51	2.34
Endrin ketone	11.47	0.44	21.51	11.07	6.05
Heptachlor	14.43	0.63	65.50	6.35	0.32
Heptachlor epoxide	19.65	5.10	70.57	7.57	0.22
Methoxychlor	19.56	0.94	28.00	4.61	0.20
trans-Chlordane	1.55	0.15	11.99	3.23	0.91

SI Table 4. List of all 91 features included in multivariate analysis of YOY SMB samples. Named compounds were tentatively identified based on mass spectral match with NIST MS Database (2014) only. Compounds identified as significant features are listed in red.

Name	Mass	Avg t_{R1} (s)	StDev t_{R1}	Avg t_{R2} (s)	StDev t_{R2}	Match	Reverse	Probability
1,3-Oxathiolane, 2-acetyl-2-methyl-	103	2321.54	2.03	2.27	0.01	720	826	4393
11-(3,4-Dimethyl-5-pentyl-2-furyl)-dodecanoic acid, methyl ester	364	2607.60	1.23	2.37	0.01	736	869	9794
11-(3,4-Dimethyl-5-propyl-2-furyl)-undecanoic acid, methyl ester	307	2448.63	1.50	2.31	0.01	816	882	9720
13-Docosenamide, (Z)-	59	2852.40	1.23	2.80	0.01	855	866	9396
2,3,3,4,7-Pentamethyl-2,3-dihydro-benzofuran	175	1359.81	0.87	2.04	0.01	730	741	1636
2,4,4-Trimethyl-2-butenolide	111	1147.81	0.87	2.64	0.01	718	843	5002
2-Hexyldecanol	280	2204.00	1.46	1.72	0.10	718	770	2478
2-Piperidinone, 1-methyl-	113	939.06	2.25	2.54	0.01	859	872	8963
2-Pyrrolidinone, 1-methyl-	99	753.40	2.98	2.38	0.01	875	897	9342
2-Tetradecanone	58	1631.81	0.87	1.86	0.01	788	806	5305
3-Buten-2-one, 4-(6,6-dimethyl-1-cyclohexen-1-yl)-	59	1668.60	1.96	2.10	0.01	708	787	1896
4-(2,6,6-Trimethylcyclohexa-1,3-dienyl)but-3-en-2-one	175	1471.58	1.26	2.15	0.01	830	842	6690
4,7,10,13,16,19-Docosahexaenoic acid, methyl ester, (all-Z)-	79	2581.00	1.78	2.46	0.01	924	939	6582
7-Acetyl-6-ethyl-1,1,4,4-tetramethyltetralin	243	2119.76	0.97	2.19	0.01	727	771	8746
8-Hydroxyquinoline, 2-methylpropionate	145	2780.00	0.00	2.42	0.01	712	806	2872
9,12-Octadecadienoic acid (Z,Z)-, methyl ester	294	2231.58	1.84	2.10	0.12	892	900	3636
9-Octadecenamide, (Z)-	262	2478.12	3.20	2.53	0.32	723	766	2988
9-Octadecenoic acid (Z)-, 2,3-dihydroxypropyl ester	264	2759.27	3.93	2.84	0.04	724	795	8050
à-Hydroxyisobutyric acid, acetate	59	520.19	0.87	1.47	0.01	710	752	5046
Cholesta-3,5-diene	260	3182.67	3.60	2.44	0.03	772	824	2899
Cholesterol	276	3162.35	4.49	1.74	0.18	719	729	6634
Ethylparaben	121	1568.94	2.25	2.22	0.01	733	836	5738
Heptadecane, 2-methyl-	85	1715.71	4.83	1.71	0.08	780	847	2118
Indole	90	1160.38	1.20	2.72	0.01	936	944	6169
Methyl 3-hydroxyoctadecanoate	103	2873.78	2.05	2.61	0.01	736	817	4832
Myristic acid glycidyl ester	297	2623.50	1.41	2.34	0.01	760	835	8324
n-Hexadecanoic acid	60	2625.45	3.24	1.73	0.15	792	826	6135
Octacosane	351	2884.57	2.14	2.02	0.02	760	821	1415
Octadecanoic acid	330	2613.85	2.08	1.72	0.14	757	762	2383
Palmitinic acid	270	3084.42	3.75	1.53	0.04	836	842	6947
Pentadecanoic acid, methyl ester	74	1928.00	0.00	1.89	0.01	910	924	7007
Vitamin E	430	3145.26	1.91	3.00	0.02	863	906	4371
Analyte 29	71	535.81	0.87	1.62	0.01	N/A	N/A	N/A
Analyte 157	367	783.11	4.01	2.13	0.02	N/A	N/A	N/A

Name	Mass	Avg t_{R1} (s)	StDev t_{R1}	Avg t_{R2} (s)	StDev t_{R2}	Match	Reverse	Probability
Analyte 171	367	814.89	3.31	2.03	0.01	N/A	N/A	N/A
Analyte 219	441	897.41	3.14	2.68	0.02	N/A	N/A	N/A
Analyte 256	441	964.44	2.33	2.38	0.02	N/A	N/A	N/A
Analyte 266	441	989.20	1.93	2.30	0.02	N/A	N/A	N/A
Analyte 273	367	1000.33	1.15	1.68	0.02	N/A	N/A	N/A
Analyte 282	367	1019.71	1.07	1.65	0.01	N/A	N/A	N/A
Analyte 348	516	1116.71	2.11	2.72	0.02	N/A	N/A	N/A
Analyte 386	113	1175.58	1.26	2.71	0.01	N/A	N/A	N/A
Analyte 445	441	1246.13	2.56	1.73	0.01	N/A	N/A	N/A
Analyte 448	472	1251.81	0.87	1.47	0.01	N/A	N/A	N/A
Analyte 466	441	1276.24	2.22	1.69	0.01	N/A	N/A	N/A
Analyte 535	355	1371.56	1.29	1.75	0.01	N/A	N/A	N/A
Analyte 580	125	1443.80	0.89	3.03	0.01	N/A	N/A	N/A
Analyte 722	491	1616.00	0.00	1.44	0.01	N/A	N/A	N/A
Analyte 810	429	1754.53	4.26	1.77	0.12	N/A	N/A	N/A
Analyte 850	149	1824.60	1.96	2.27	0.01	N/A	N/A	N/A
Analyte 1210	321	2100.00	0.00	3.71	0.01	N/A	N/A	N/A
Analyte 1878	322	2340.71	1.57	2.28	0.01	N/A	N/A	N/A
Analyte 1938	176	2358.33	2.06	3.37	0.02	N/A	N/A	N/A
Analyte 1949	165	2363.50	2.48	3.10	0.01	N/A	N/A	N/A
Analyte 2110	336	2416.67	1.53	2.30	0.01	N/A	N/A	N/A
Analyte 2186	273	2444.00	2.67	1.62	0.01	N/A	N/A	N/A
Analyte 2252	266	2464.92	1.75	3.16	0.02	N/A	N/A	N/A
Analyte 2272	326	2472.00	1.57	2.07	0.01	N/A	N/A	N/A
Analyte 2307	527	2480.80	3.68	1.35	0.00	N/A	N/A	N/A
Analyte 2378	131	2504.00	3.58	2.08	0.05	N/A	N/A	N/A
Analyte 2383	215	2504.00	1.30	2.67	0.03	N/A	N/A	N/A
Analyte 2384	296	2504.29	1.07	2.71	0.01	N/A	N/A	N/A
Analyte 2666	393	2581.45	2.02	2.33	0.01	N/A	N/A	N/A
Analyte 2679	393	2587.00	1.85	2.12	0.01	N/A	N/A	N/A
Analyte 2683	103	2587.20	1.79	2.44	0.10	N/A	N/A	N/A
Analyte 2858	248	2629.00	3.10	2.48	0.03	N/A	N/A	N/A
Analyte 2951	191	2652.22	0.94	1.98	0.01	N/A	N/A	N/A
Analyte 3047	377	2671.11	3.33	0.07	0.02	N/A	N/A	N/A
Analyte 3065	300	2675.67	1.15	3.56	0.01	N/A	N/A	N/A
Analyte 3137	377	2692.00	2.83	3.92	0.03	N/A	N/A	N/A
Analyte 3240	464	2721.00	3.15	1.35	0.01	N/A	N/A	N/A

Name	Mass	Avg t_{R1} (s)	StDev t_{R1}	Avg t_{R2} (s)	StDev t_{R2}	Match	Reverse	Probability
Analyte 3361	476	2752.00	0.00	1.77	0.00	N/A	N/A	N/A
Analyte 3391	412	2762.00	2.19	2.35	0.02	N/A	N/A	N/A
Analyte 3393	215	2763.06	1.75	2.93	0.02	N/A	N/A	N/A
Analyte 3474	286	2780.29	2.92	1.75	0.01	N/A	N/A	N/A
Analyte 3495	103	2788.33	1.15	2.56	0.01	N/A	N/A	N/A
Analyte 3557	534	2808.00	0.00	1.76	0.01	N/A	N/A	N/A
Analyte 3562	131	2812.73	3.00	3.02	0.06	N/A	N/A	N/A
Analyte 3836	112	2894.91	1.87	1.83	0.03	N/A	N/A	N/A
Analyte 3871	331	2912.40	2.27	1.97	0.02	N/A	N/A	N/A
Analyte 3872	414	2909.25	2.82	2.10	0.16	N/A	N/A	N/A
Analyte 3977	398	2950.00	4.62	1.85	0.08	N/A	N/A	N/A
Analyte 3997	99	2959.11	1.76	1.76	0.00	N/A	N/A	N/A
Analyte 4031	476	2971.67	2.67	1.97	0.17	N/A	N/A	N/A
Analyte 4476	451	3155.00	2.83	2.18	0.01	N/A	N/A	N/A
Analyte 4556	429	3192.00	3.58	2.60	0.23	N/A	N/A	N/A
Analyte 4611	165	3224.33	2.06	3.75	0.05	N/A	N/A	N/A
Analyte 4732	579	3295.69	3.04	2.07	0.21	N/A	N/A	N/A
Analyte 4925	466	3428.62	3.95	2.06	0.05	N/A	N/A	N/A
Analyte 5317	430	3705.14	3.02	2.29	0.21	N/A	N/A	N/A
Analyte 5470	579	3816.57	4.43	1.82	0.18	N/A	N/A	N/A