LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091124\
Data File : BF139335.D
Acq On : 11 Sep 2024 19:34
Operator : RC/JU
Sample : P3929-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BIN-2

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139335.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	10	18	25	rBV	1201773	1851606	71.05%	9.994%
2	5.104	503	512	522	rBV	81438	127707	4.90%	0.689%
3	5.504	574	580	585	rBV	1230731	1632779	62.66%	8.813%
4	6.510	744	751	756	rBV	1157544	1605655	61.62%	8.667%
5	6.881	809	814	819	rVB	371708	462677	17.75%	2.497%
6	7.445	903	910	915	rBV	796288	1032037	39.60%	5.571%
7	7.698	948	953	957	rBV	31616	38120	1.46%	0.206%
8	8.163	1027	1032	1037	rBV	639220	792529	30.41%	4.278%
9	9.239	1209	1215	1220	rBV	2121344	2605942	100.00%	14.066%
10	9.916	1325	1330	1334	rBV	412526	512044	19.65%	2.764%
11	10.628	1444	1451	1458	rVB	101574	126889	4.87%	0.685%
12	10.704	1458	1464	1469	rBV	669839	841093	32.28%	4.540%
13	11.404	1577	1583	1591	rBV2	508520	842366	32.32%	4.547%
14	11.475	1591	1595	1599	rBV	28843	36419	1.40%	0.197%
15	11.633	1616	1622	1629	rBV	18790	34225	1.31%	0.185%
16	11.928	1663	1672	1679	rVV	360543	566583	21.74%	3.058%
17	12.016	1683	1687	1695	rVB	47693	92545	3.55%	0.500%
18	12.204	1714	1719	1720	rBV	18834	26222	1.01%	0.142%
19	12.222	1720	1722	1726	rVB	25510	27284	1.05%	0.147%
20	12.451	1757	1761	1765	rBV	20405	28501	1.09%	0.154%
21	12.539	1772	1776	1781	rVB	18337	26349	1.01%	0.142%
22	12.616	1784	1789	1798	rBV	334116	449476	17.25%	2.426%
23	12.710	1802	1805	1813	rBV2	46393	80989	3.11%	0.437%
24	12.845	1821	1828	1833	rBV	273777	408276	15.67%	2.204%
25	12.986	1844	1852	1859	rVB	1313945	1748973	67.11%	9.440%
26	13.063	1859	1865	1869	rBV3	29194	54763	2.10%	0.296%
27	13.169	1875	1883	1887	rVB2	46173	93447	3.59%	0.504%
28	13.233	1887	1894	1897	rBV3	32924	62069	2.38%	0.335%
29	13.275	1897	1901	1904	rVB2	28711	36717	1.41%	0.198%
30	13.674	1965	1969	1974	rVB	19648	29822	1.14%	0.161%
31	13.786	1984	1988	1991	rBV2	22080	34223	1.31%	0.185%
32	13.886	2001	2005	2015	rVB3	73443	125155	4.80%	0.676%
33	14.039	2024	2031	2043	rBV2	312981	594688	22.82%	3.210%
34	14.433	2093	2098	2100	rBV2	28472	48338	1.85%	0.261%
35	14.521	2109	2113	2116	rBV5	37826	70703	2.71%	0.382%
36	14.674	2135	2139	2143	rBV2	37493	58005	2.23%	0.313%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091124\
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Acq On : 11 Sep 2024 19:34
Operator : RC/JU
Sample : P3929-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BIN-2

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.898	2173	2177	2184	rVB	115693	161883	6.21%	0.874%
38	15.080	2203	2208	2218	rVB	121013	277002	10.63%	1.495%
39	15.163	2218	2222	2225	rBV2	35772	51429	1.97%	0.278%
40	15.386	2256	2260	2266	rVB	63455	95782	3.68%	0.517%
41	15.451	2266	2271	2276	rVV	75671	117359	4.50%	0.633%
42	15.516	2276	2282	2294	rVB	240490	436343	16.74%	2.355%
43	15.998	2359	2364	2368	rBV	21360	33893	1.30%	0.183%
44	16.810	2496	2502	2512	rVB9	13787	30306	1.16%	0.164%
45	16.980	2526	2531	2538	rBV2	18408	42374	1.63%	0.229%
46	17.427	2602	2607	2622	rVB	30128	74896	2.87%	0.404%

Sum of corrected areas: 18526483

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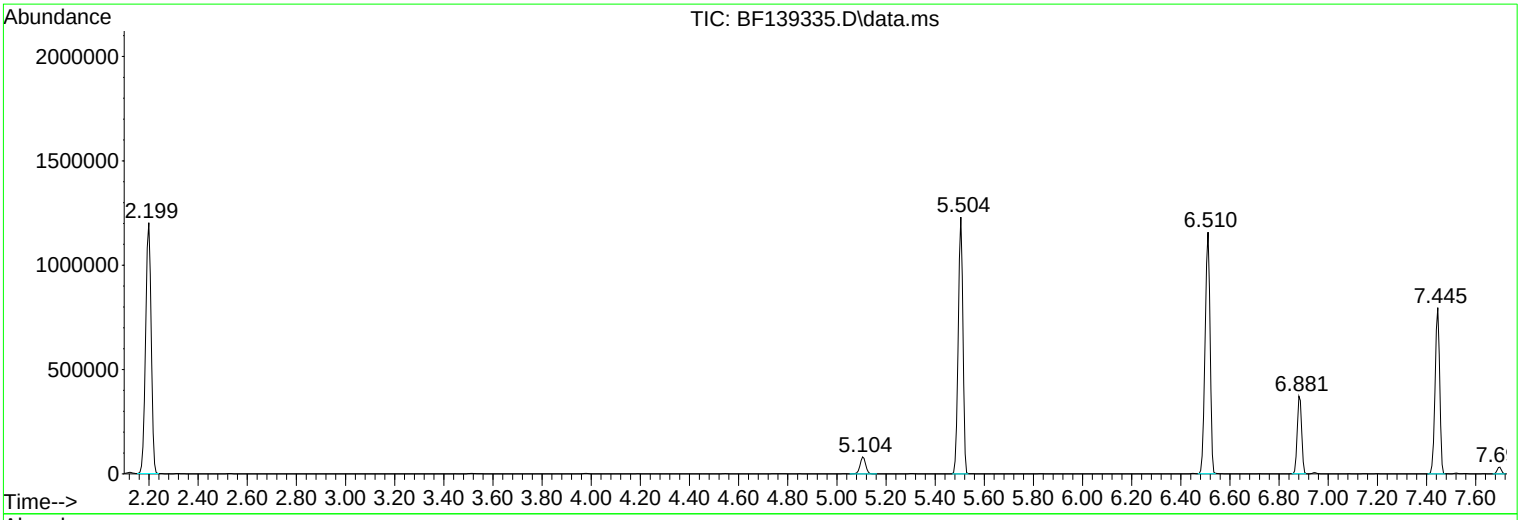
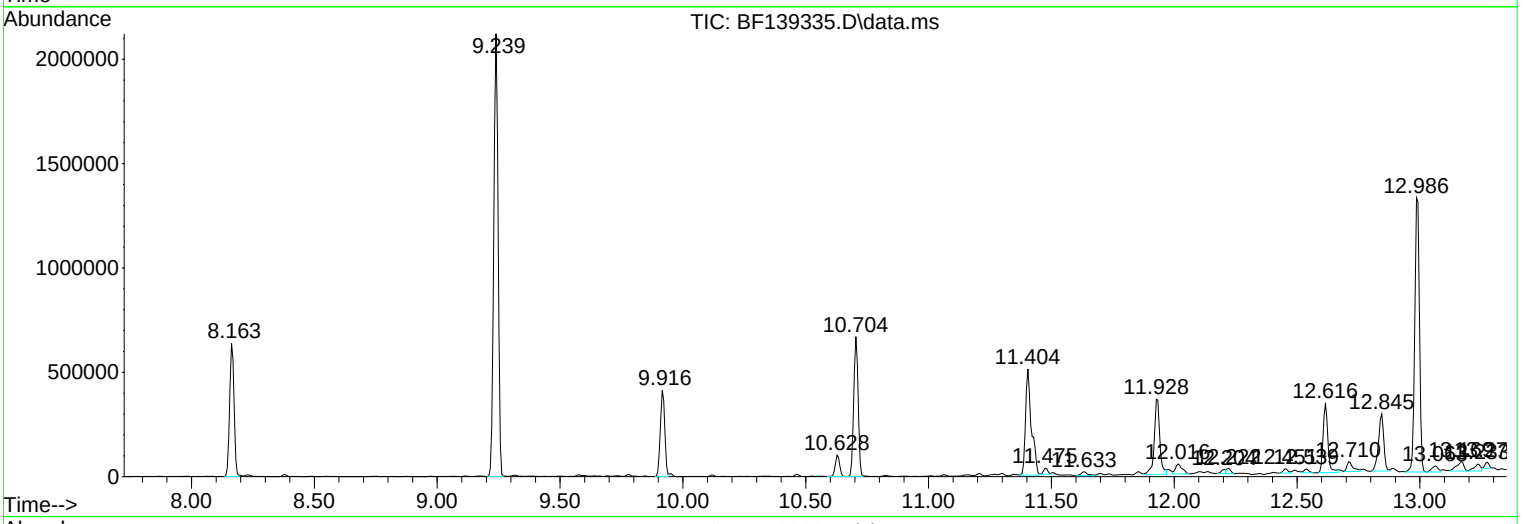
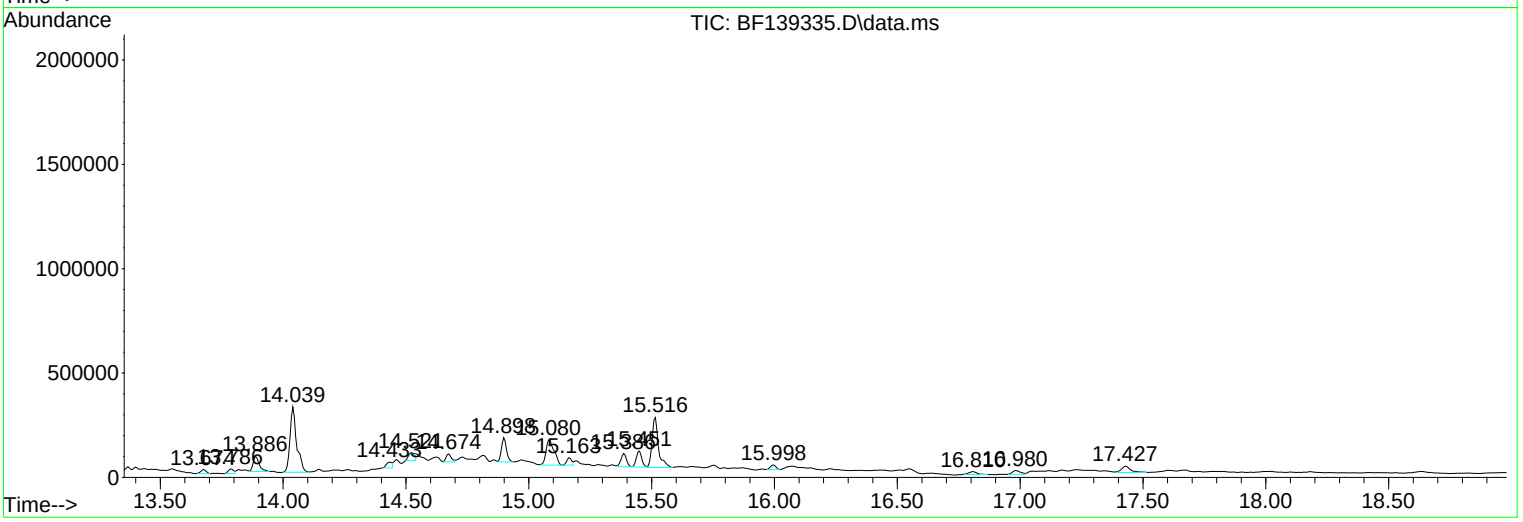
ClientSampleId :
BIN-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091124\
Data File : BF139335.D
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Operator : RC/JU
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

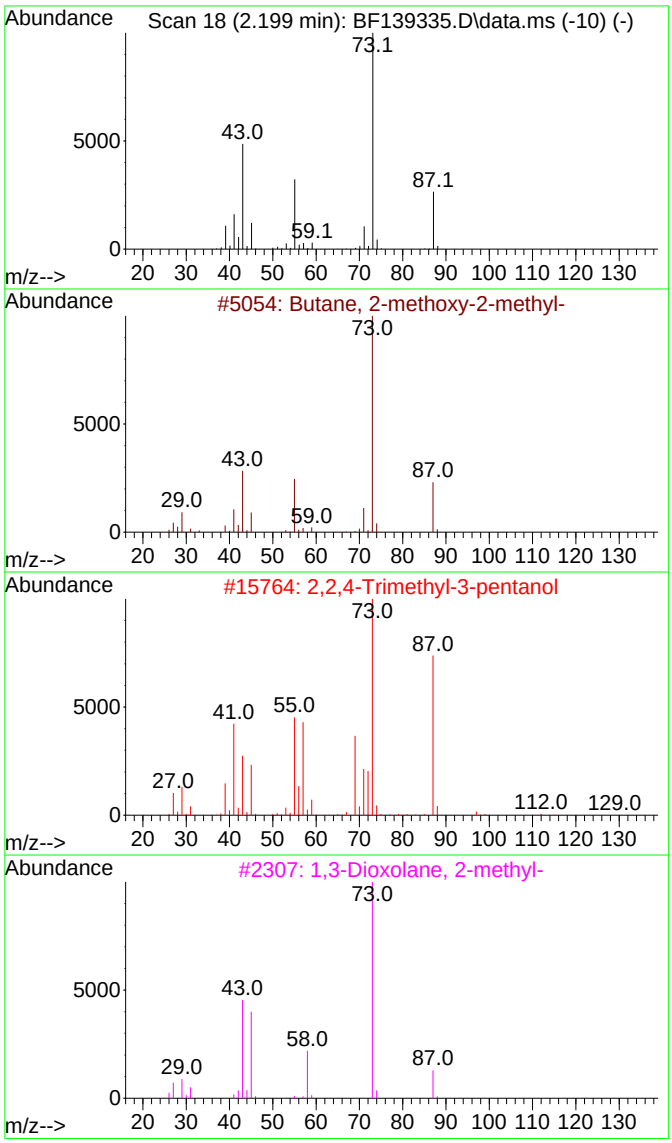
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

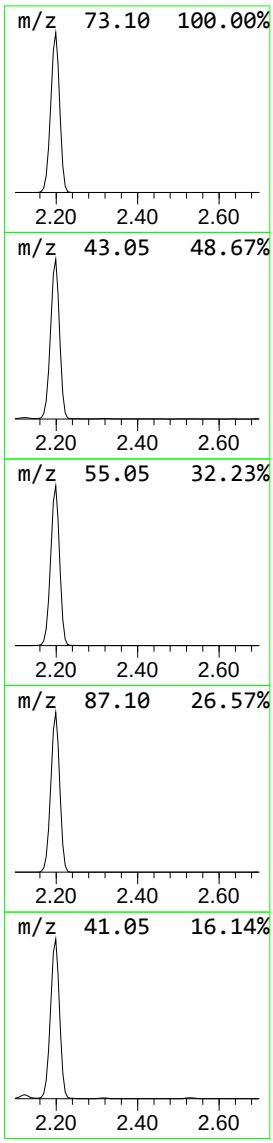
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	80.04 ng	1851610	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





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Data File : BF139335.D
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Operator : RC/JU
Sample : P3929-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BIN-2

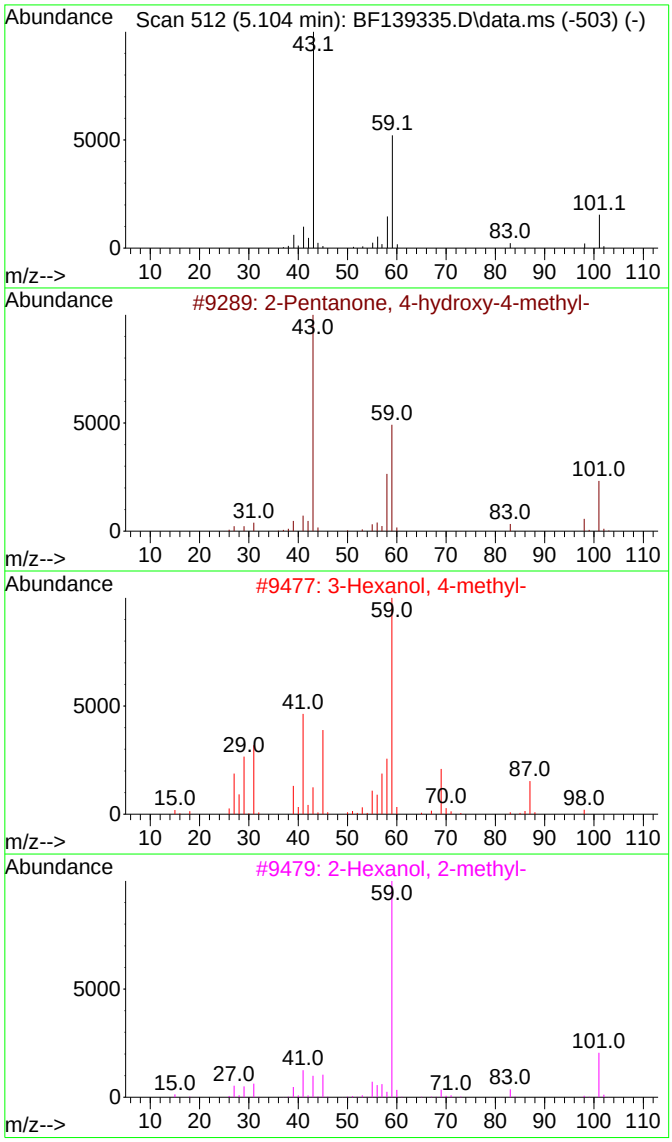
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

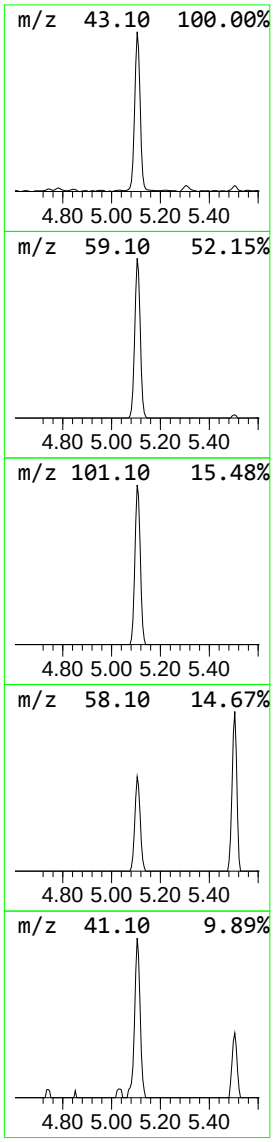
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	5.52 ng	127707	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091124\
Data File : BF139335.D
Acq On : 11 Sep 2024 19:34
Operator : RC/JU
Sample : P3929-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BIN-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

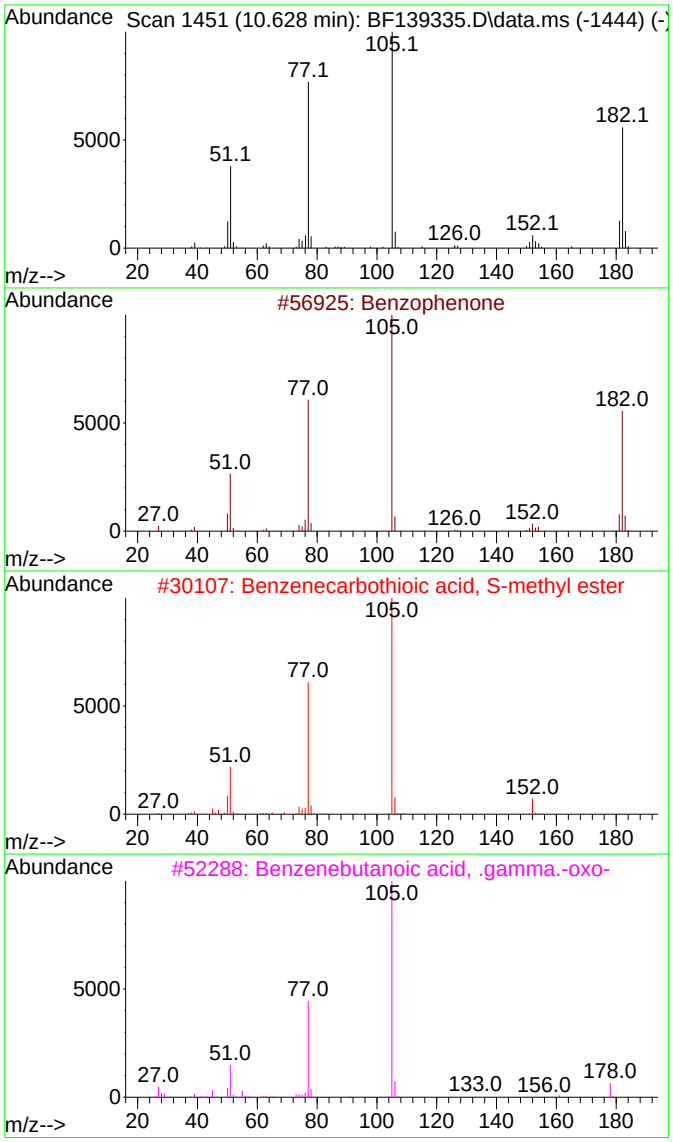
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

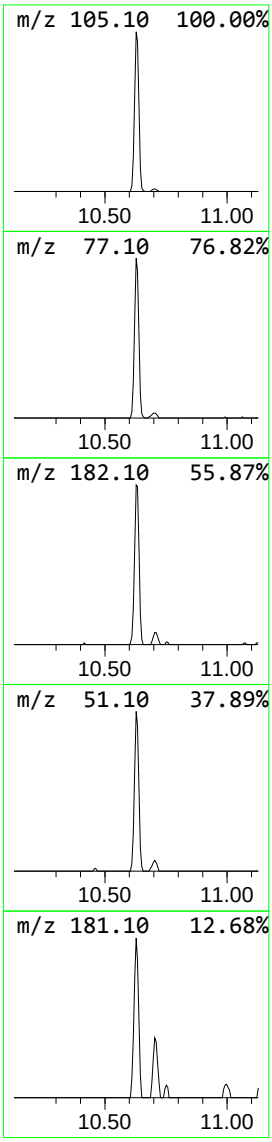
****

Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.628	4.96 ng	126889	Acenaphthene-d10	9.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	62
3	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	53
4	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	53
5	1,2,4-Triazine-3,5(2H,4H)-dione,...	249	C10H7N3O3S	024168-34-1	53





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Misc :
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Instrument :
BNA_F
ClientSampleId :
BIN-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

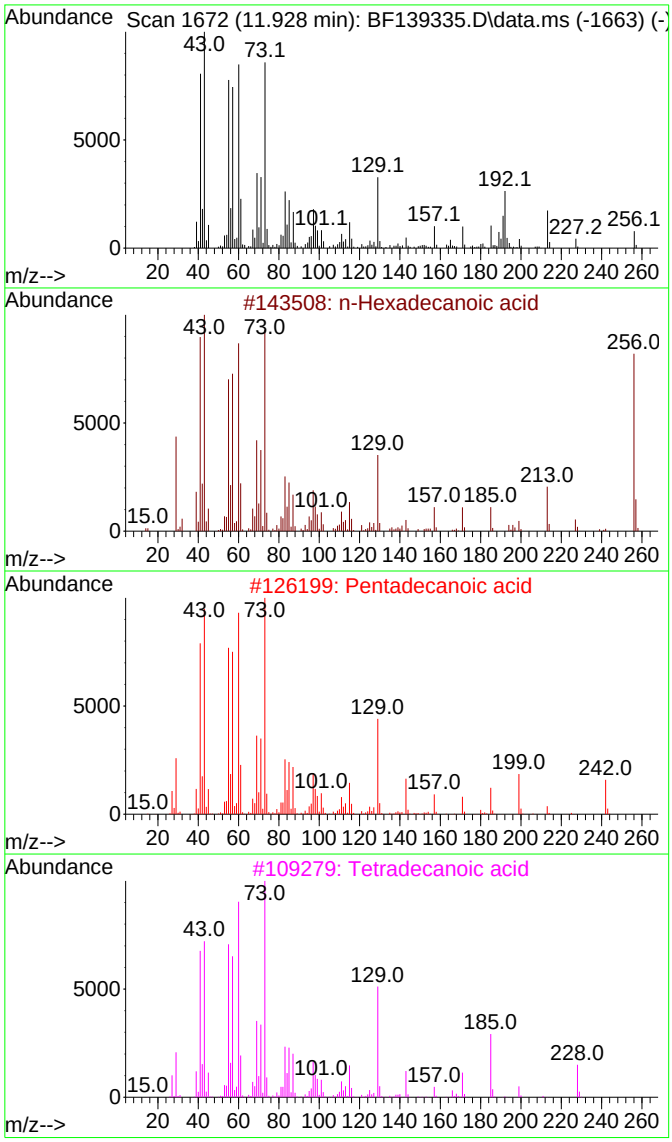
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

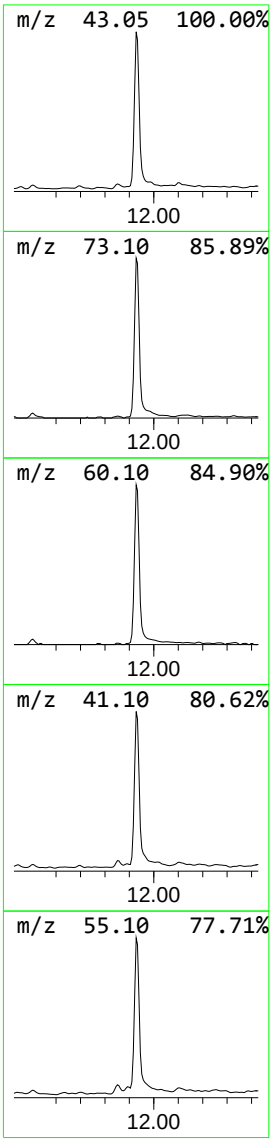
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.928	13.45 ng	566583	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	52





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Data File : BF139335.D
Acq On : 11 Sep 2024 19:34
Operator : RC/JU
Sample : P3929-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

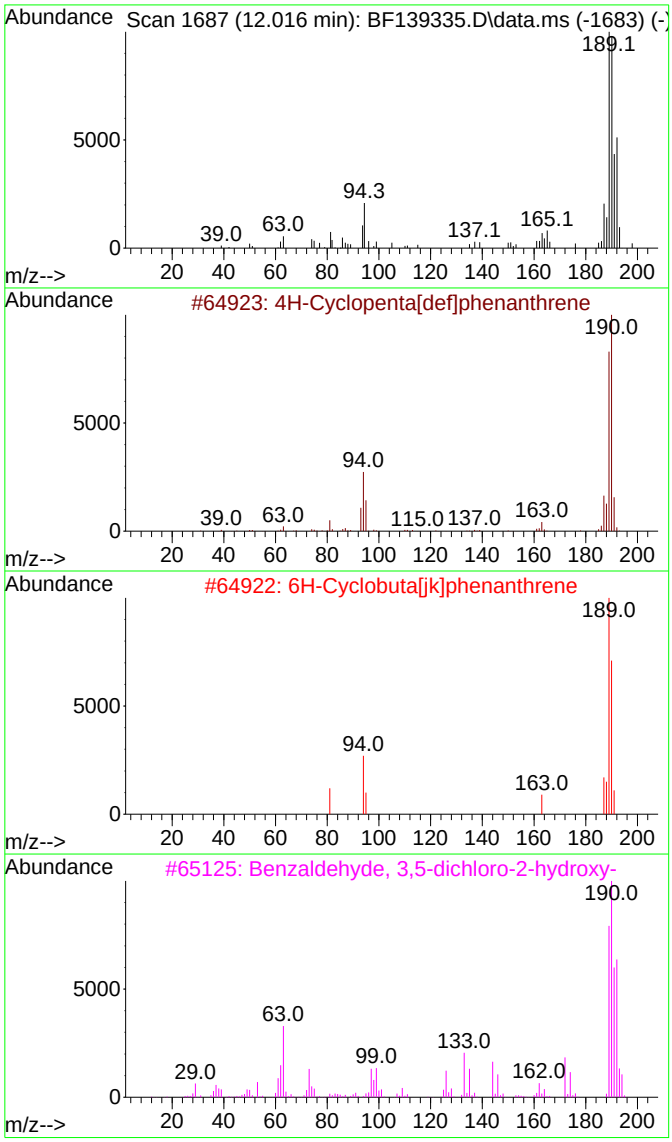
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

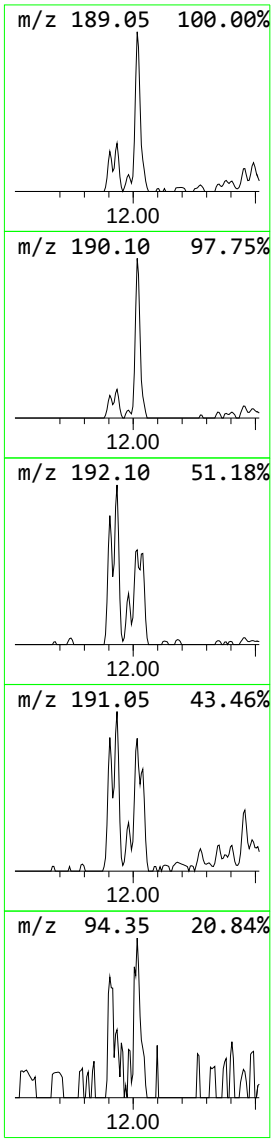
****

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.016	2.20 ng	92545	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	53
3	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	50
4	Methyl diselenide	190	C2H6Se2	007101-31-7	38
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	22





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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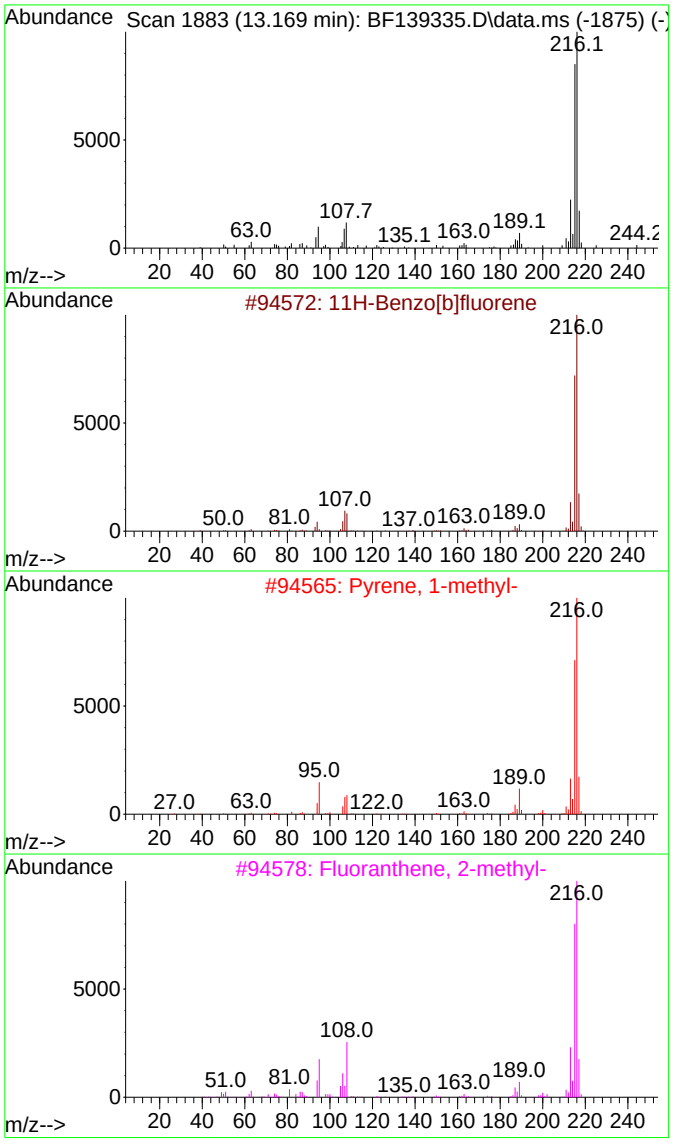
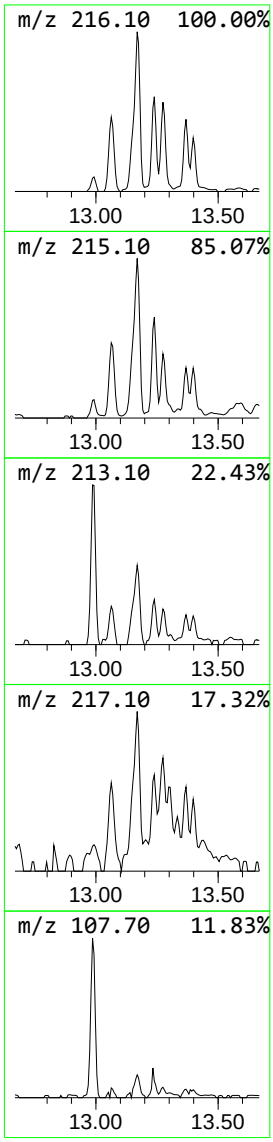
Peak Number 6 11H-Benzo[b]fluorene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.169	3.14 ng	93447	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	94
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	94
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	91
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	91
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	72





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Data File : BF139335.D
Acq On : 11 Sep 2024 19:34
Operator : RC/JU
Sample : P3929-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BIN-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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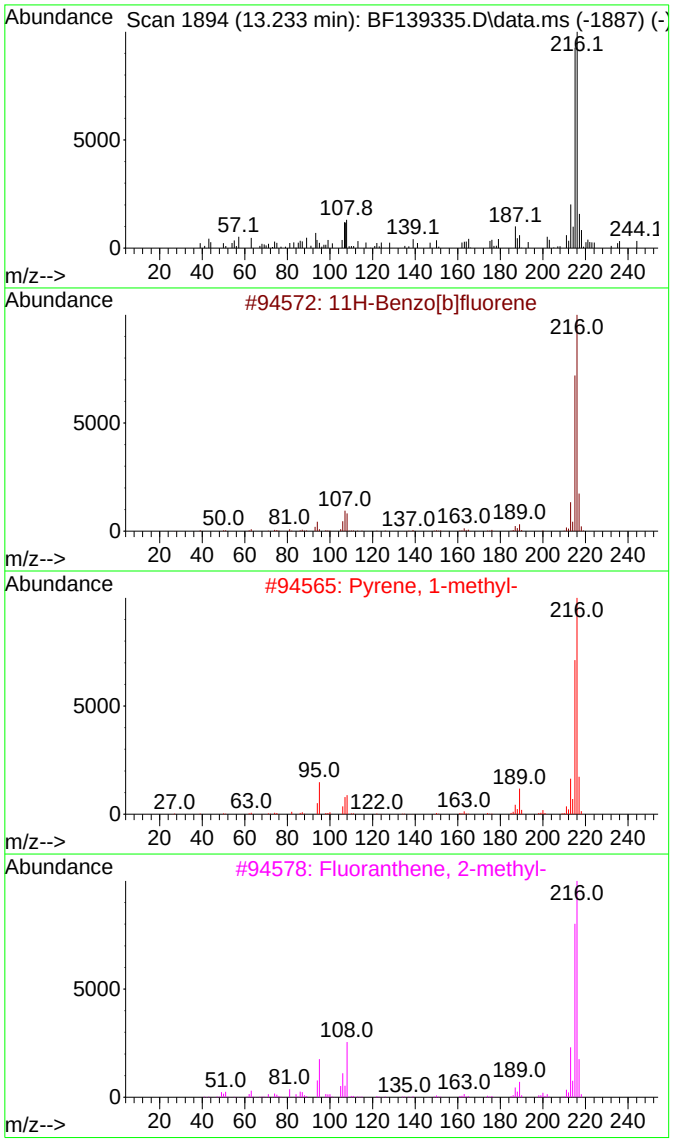
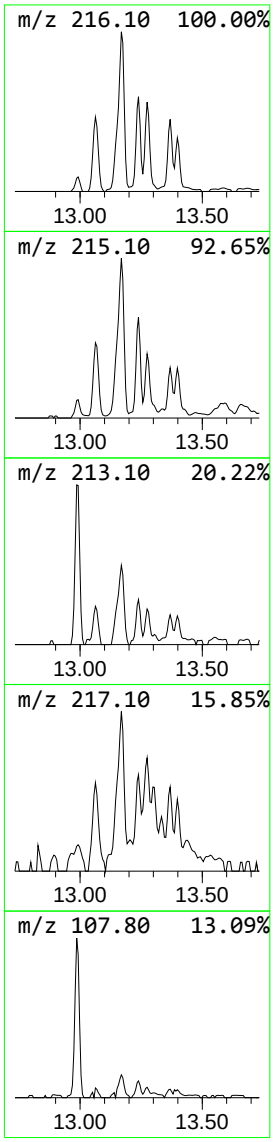
Peak Number 7 Pyrene, 1-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.233	2.09 ng	62069	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	90
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	68
4	6H-Thiazolo[5,4-e]indole, 2,7,8-...	216	C12H12N2S	1000338-32-0	64
5	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091124\
Data File : BF139335.D
Acq On : 11 Sep 2024 19:34
Operator : RC/JU
Sample : P3929-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BIN-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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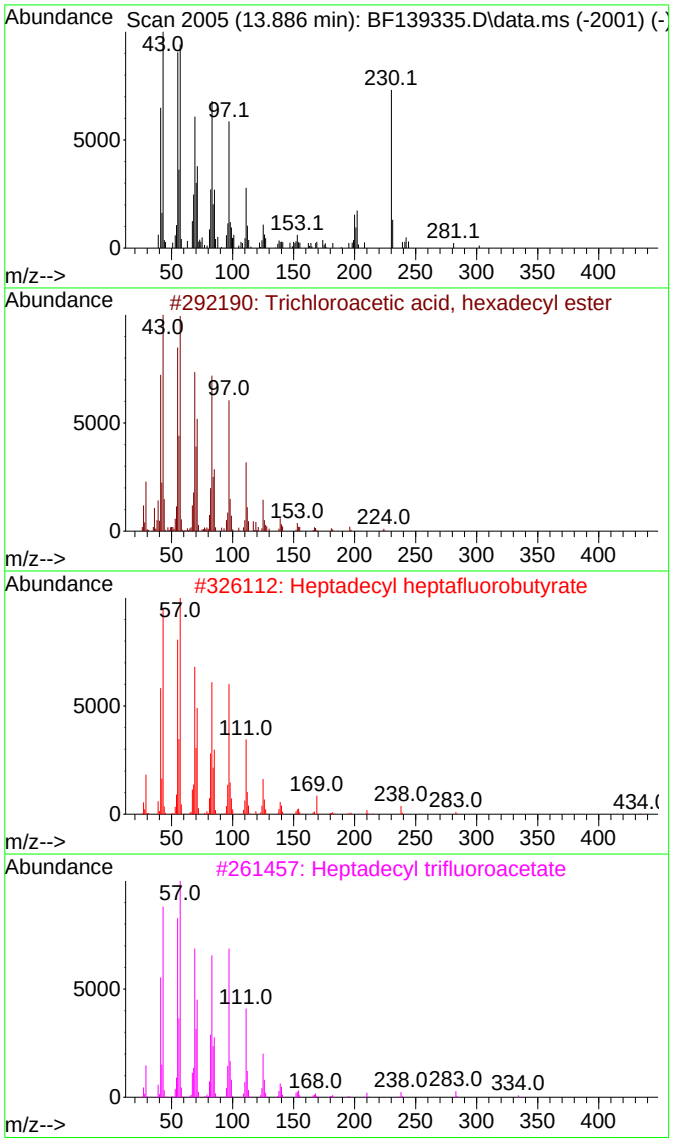
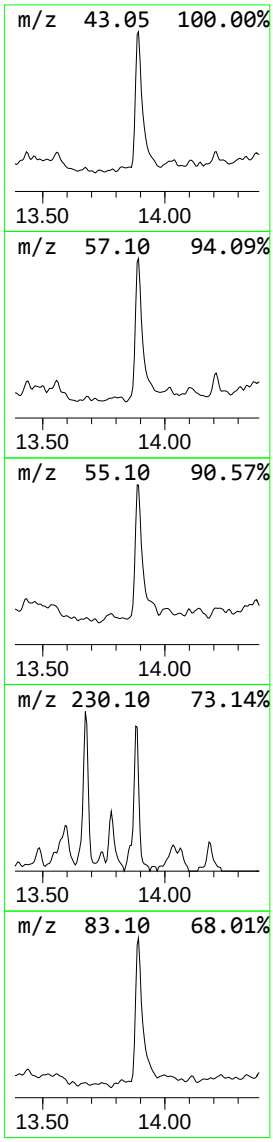
Peak Number 8 Trichloroacetic acid, hexad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	4.21 ng	125155	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	64
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	64
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	64
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	64
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	50





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Acq On : 11 Sep 2024 19:34
Operator : RC/JU
Sample : P3929-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BIN-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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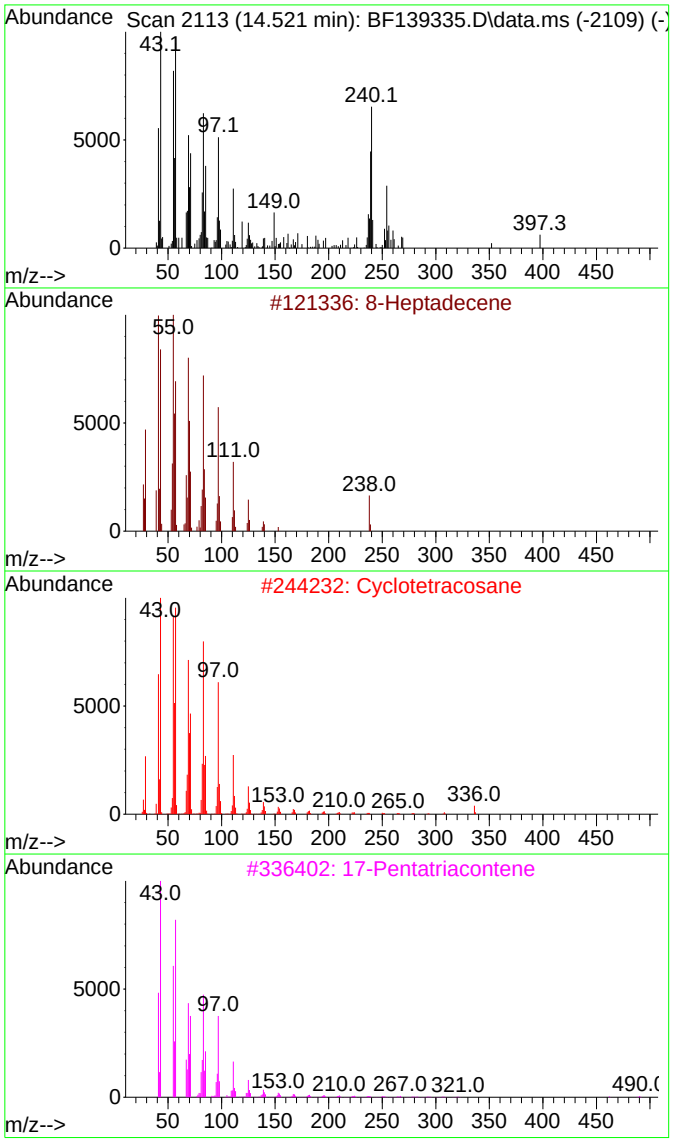
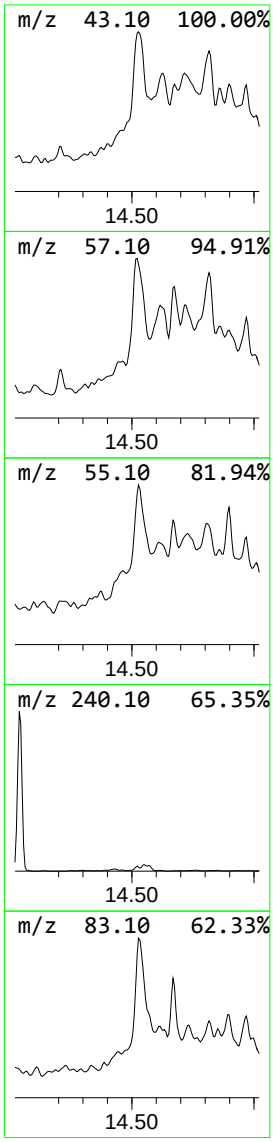
Peak Number 9 8-Heptadecene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.522	2.38 ng	70703	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	8-Heptadecene	238	C17H34	002579-04-6	60
2	Cyclotetracosane	336	C24H48	000297-03-0	55
3	17-Pentatriacontene	491	C35H70	006971-40-0	55
4	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	55
5	1-Heptacosanol	396	C27H56O	002004-39-9	55





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BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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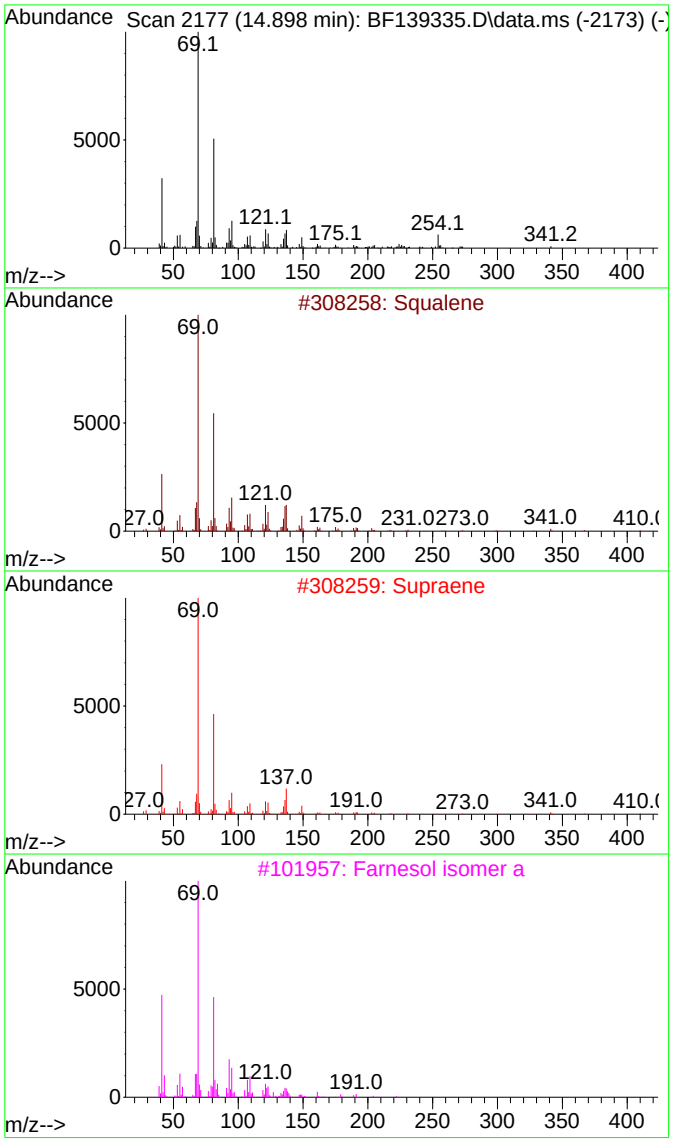
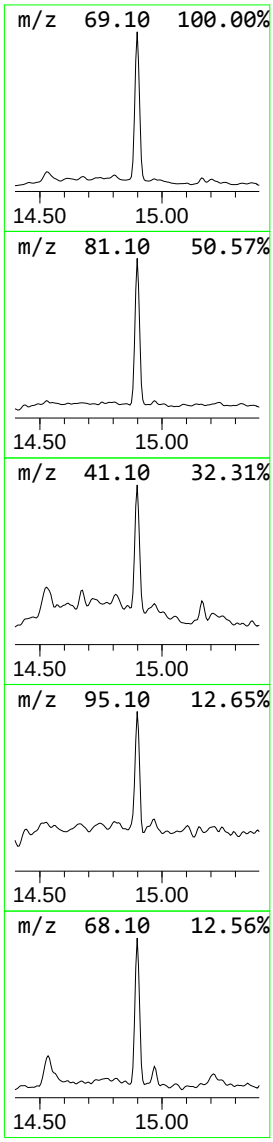
Peak Number 10 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.898	7.42 ng	161883	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	87
3	Farnesol isomer a	222	C15H26O	1000108-92-4	87
4	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	78
5	(3E,7E)-4,8,12-Trimethyltrideca-...	218	C16H26	062235-06-7	68





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Data File : BF139335.D
Acq On : 11 Sep 2024 19:34
Operator : RC/JU
Sample : P3929-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BIN-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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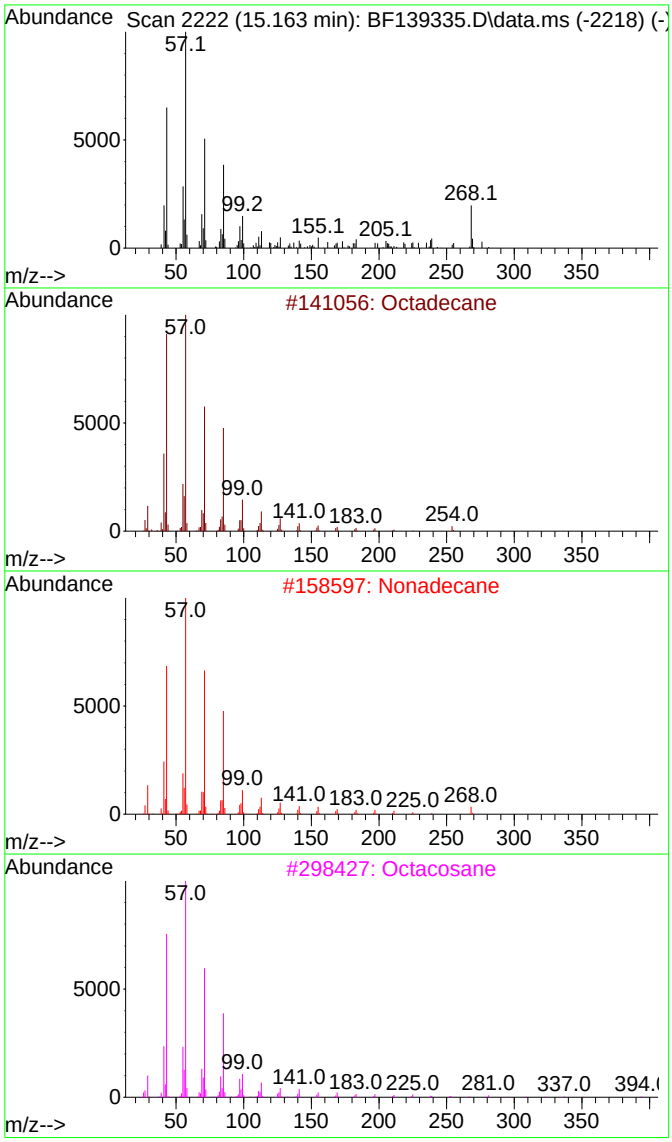
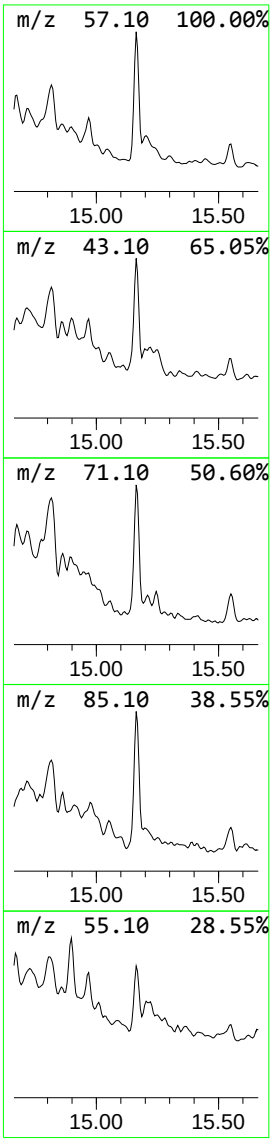
Peak Number 11 Octadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.163	2.36 ng	51429	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	93
2	Nonadecane	268	C19H40	000629-92-5	91
3	Octacosane	394	C28H58	000630-02-4	76
4	Hexacosane	366	C26H54	000630-01-3	76
5	Heneicosane	296	C21H44	000629-94-7	76





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Data File : BF139335.D
Acq On : 11 Sep 2024 19:34
Operator : RC/JU
Sample : P3929-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BIN-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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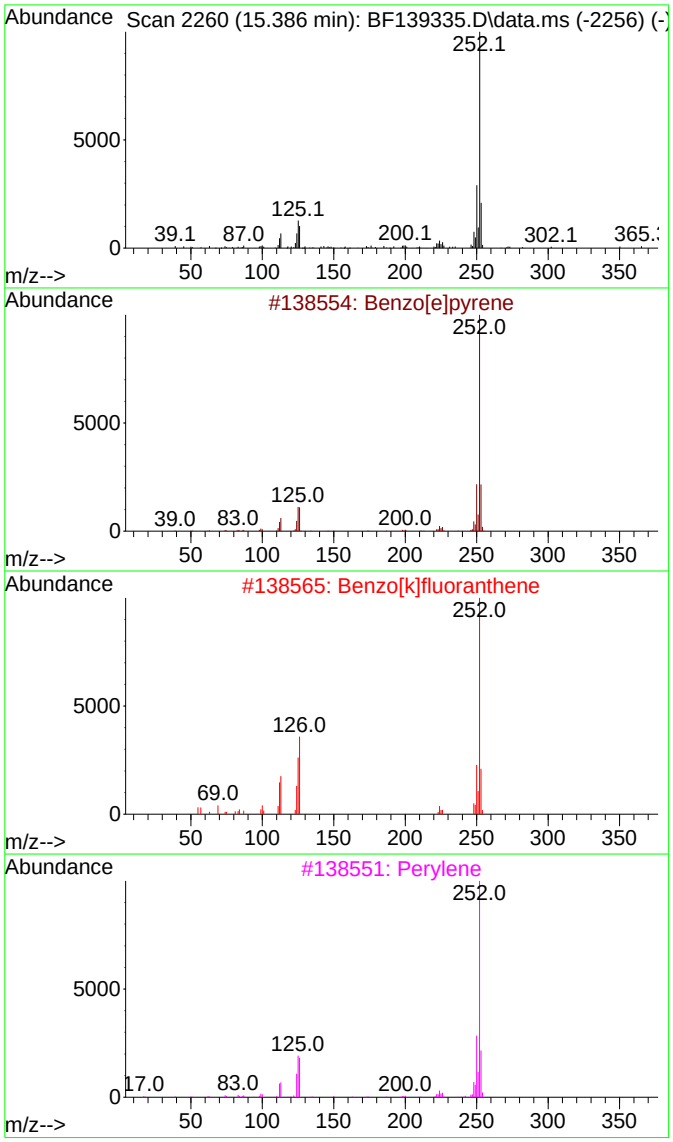
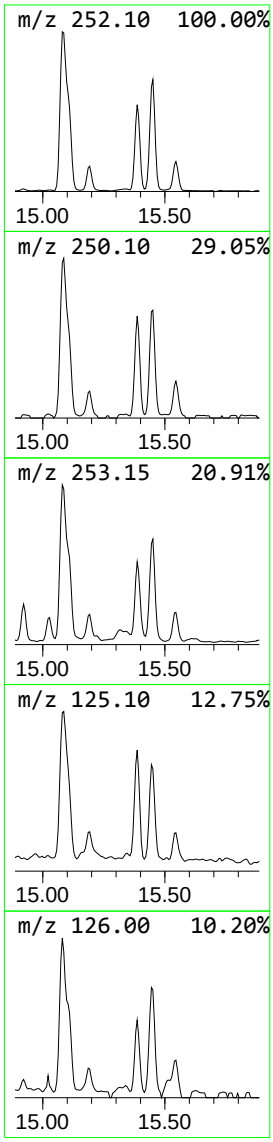
Peak Number 12 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.386	4.39 ng	95782	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
3	Perylene	252	C20H12	000198-55-0	95
4	Benzo[a]pyrene	252	C20H12	000050-32-8	90
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90





Tentatively Identified Compound (LSC) summary

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Data File : BF139335.D
Acq On : 11 Sep 2024 19:34
Operator : RC/JU
Sample : P3929-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BIN-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.199	80.0	ng	1851610	1	6.881	462677	20.0
2-Pentanone, 4-...	5.104	5.5	ng	127707	1	6.881	462677	20.0
Benzophenone	10.628	5.0	ng	126889	3	9.916	512044	20.0
n-Hexadecanoic ...	11.928	13.4	ng	566583	4	11.404	842366	20.0
4H-Cyclopenta[d...	12.016	2.2	ng	92545	4	11.404	842366	20.0
11H-Benzo[b]flu...	13.169	3.1	ng	93447	5	14.039	594688	20.0
Pyrene, 1-methyl-	13.233	2.1	ng	62069	5	14.039	594688	20.0
Trichloroacetic...	13.886	4.2	ng	125155	5	14.039	594688	20.0
8-Heptadecene	14.522	2.4	ng	70703	5	14.039	594688	20.0
Squalene	14.898	7.4	ng	161883	6	15.515	436343	20.0
Octadecane	15.163	2.4	ng	51429	6	15.515	436343	20.0
Benzo[e]pyrene	15.386	4.4	ng	95782	6	15.515	436343	20.0