LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120123\
Data File : BF136364.D
Acq On : 02 Dec 2023 06:48
Operator : CG\JU
Sample : 05521-04
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-2-COMP

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-BF112723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136364.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.910	305	310	315	rVB2	14953	22261	1.22%	0.141%
2	5.046	497	503	508	rVB	30102	39277	2.15%	0.250%
3	5.440	566	570	573	rBV	2015159	1827451	100.00%	11.609%
4	6.440	735	740	743	rBV	1877217	1648174	90.19%	10.470%
5	6.640	771	774	782	rBV3	12936	23918	1.31%	0.152%
6	6.804	799	802	806	rVB	892709	703264	38.48%	4.468%
7	6.957	825	828	831	rBV2	41707	35342	1.93%	0.225%
8	7.363	893	897	900	rBV	1242151	1057949	57.89%	6.721%
9	7.828	973	976	981	rVB	49620	37307	2.04%	0.237%
10	8.081	1015	1019	1023	rBV	961884	786777	43.05%	4.998%
11	9.157	1198	1202	1205	rBV	1973073	1598905	87.49%	10.157%
12	9.281	1220	1223	1227	rVB	26400	25444	1.39%	0.162%
13	9.492	1256	1259	1263	rBV2	57217	52184	2.86%	0.332%
14	9.545	1264	1268	1270	rVV2	31248	24519	1.34%	0.156%
15	9.686	1288	1292	1296	rBV3	36602	33650	1.84%	0.214%
16	9.839	1310	1318	1321	rBV	834287	776887	42.51%	4.935%
17	9.886	1321	1326	1329	rVB2	35306	36706	2.01%	0.233%
18	10.628	1448	1452	1463	rBV	933476	796068	43.56%	5.057%
19	10.880	1492	1495	1503	rVB4	15039	21351	1.17%	0.136%
20	11.280	1560	1563	1567	rBV4	22971	26409	1.45%	0.168%
21	11.327	1567	1571	1574	rVV	749612	663549	36.31%	4.215%
22	11.351	1574	1575	1580	rVV	71380	55748	3.05%	0.354%
23	11.392	1580	1582	1587	rVB3	14033	21282	1.16%	0.135%
24	11.798	1645	1651	1654	rBV3	26711	38485	2.11%	0.244%
25	11.869	1659	1663	1673	rVB2	242259	257180	14.07%	1.634%
26	12.122	1703	1706	1710	rBV3	30326	36975	2.02%	0.235%
27	12.469	1763	1765	1771	rVB4	16804	19241	1.05%	0.122%
28	12.545	1774	1778	1782	rBV	197815	204299	11.18%	1.298%
29	12.592	1784	1786	1792	rVV6	27800	40418	2.21%	0.257%
30	12.657	1794	1797	1807	rVB3	55862	68264	3.74%	0.434%
31	12.774	1810	1817	1821	rBV	168003	182279	9.97%	1.158%
32	12.927	1839	1843	1846	rBV	1984169	1608933	88.04%	10.221%
33	12.998	1850	1855	1860	rBV6	14571	21196	1.16%	0.135%
34	13.104	1871	1873	1877	rVB2	22110	23546	1.29%	0.150%
35	13.169	1877	1884	1887	rBV3	27739	40393	2.21%	0.257%
36	13.210	1887	1891	1894	rBV2	26634	29620	1.62%	0.188%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120123\
Data File : BF136364.D
Acq On : 02 Dec 2023 06:48
Operator : CG\JU
Sample : 05521-04
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-2-COMP

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-BF112723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.416	1923	1926	1931	rVB7	17414	22811	1.25%	0.145%
38	13.621	1958	1961	1969	rVB3	21697	33139	1.81%	0.211%
39	13.727	1975	1979	1982	rBV4	17292	23921	1.31%	0.152%
40	13.839	1997	1998	2003	rVB	37374	27828	1.52%	0.177%
41	13.916	2006	2011	2016	rVV7	39979	108721	5.95%	0.691%
42	13.980	2017	2022	2025	rVV	802369	876332	47.95%	5.567%
43	14.004	2025	2026	2033	rVB	106539	100315	5.49%	0.637%
44	14.468	2101	2105	2107	rVB	62381	61678	3.38%	0.392%
45	14.857	2168	2171	2177	rVB2	38387	49097	2.69%	0.312%
46	14.927	2180	2183	2190	rVB	101963	112109	6.13%	0.712%
47	15.027	2197	2200	2204	rBV	82140	117351	6.42%	0.745%
48	15.127	2213	2217	2224	rVB2	123165	163722	8.96%	1.040%
49	15.339	2249	2253	2259	rVB	55329	84077	4.60%	0.534%
50	15.398	2259	2263	2269	rVB	60491	75640	4.14%	0.481%
51	15.468	2270	2275	2281	rBV	427643	529536	28.98%	3.364%
52	15.733	2316	2320	2324	rBV2	32524	49849	2.73%	0.317%
53	15.974	2356	2361	2370	rBV	205840	353855	19.36%	2.248%
54	17.339	2589	2593	2599	rVB9	34052	66200	3.62%	0.421%

Sum of corrected areas: 15741432

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120123\
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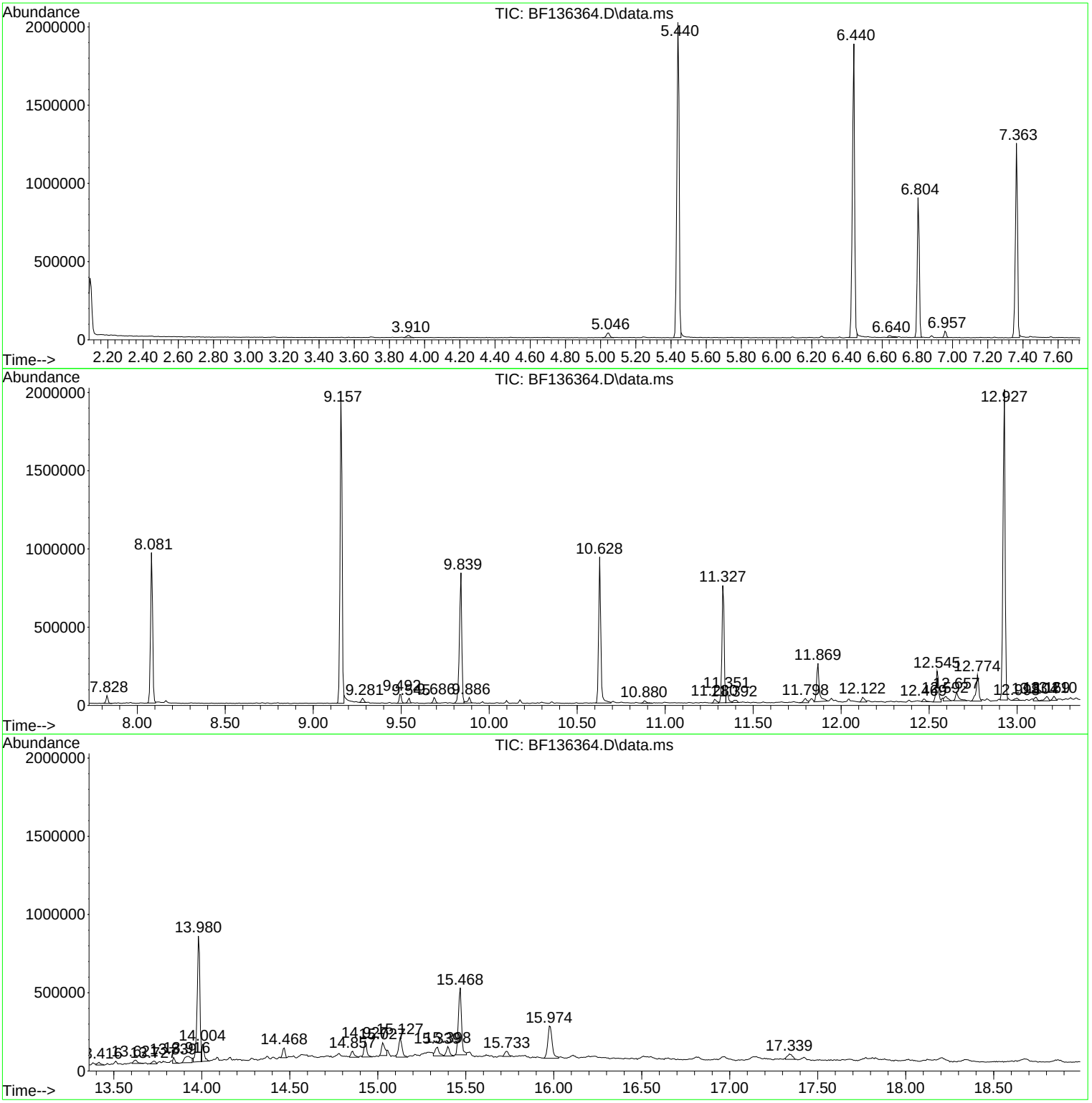
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-2-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.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\BF120123\
Data File : BF136364.D
Acq On : 02 Dec 2023 06:48
Operator : CG\JU
Sample : 05521-04
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.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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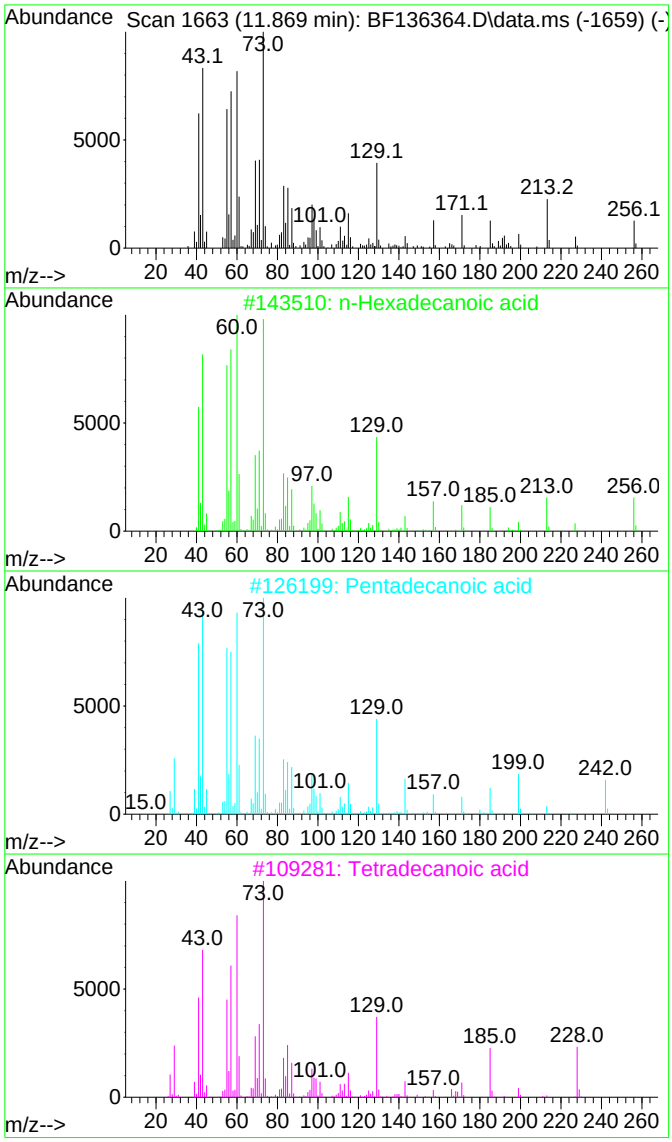
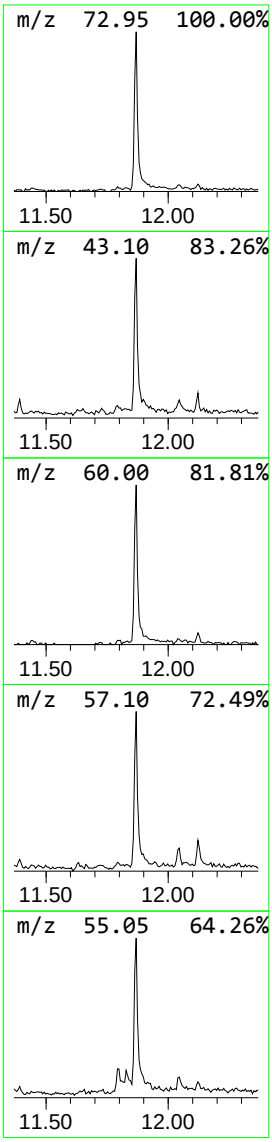
Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.869	7.75 ng	257180	Phenanthrene-d10	11.328

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120123\
Data File : BF136364.D
Acq On : 02 Dec 2023 06:48
Operator : CG\JU
Sample : 05521-04
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-2-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.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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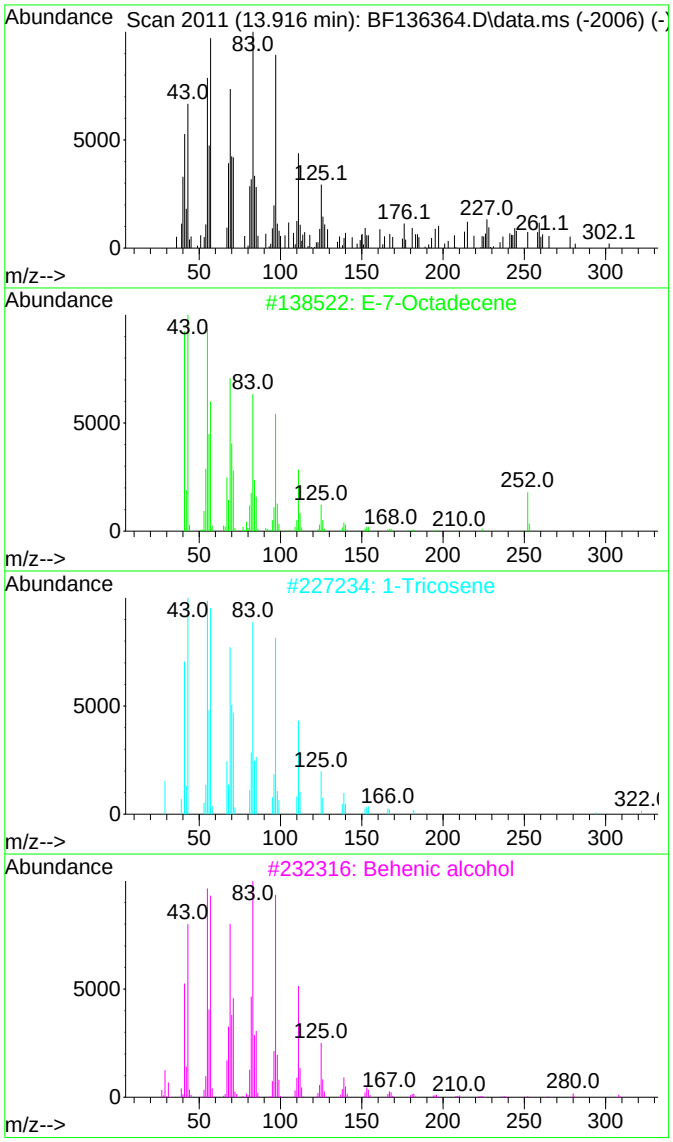
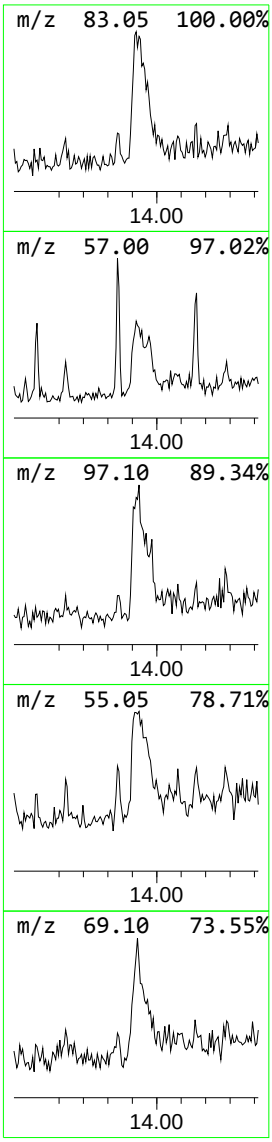
Peak Number 2 E-7-Octadecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.916	2.48 ng	108721	Chrysene-d12	13.980

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-7-Octadecene	252	C18H36	1000130-92-0	93
2	1-Tricosene	322	C23H46	018835-32-0	91
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	1-Tetracosene	336	C24H48	010192-32-2	91
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120123\
Data File : BF136364.D
Acq On : 02 Dec 2023 06:48
Operator : CG\JU
Sample : 05521-04
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-2-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.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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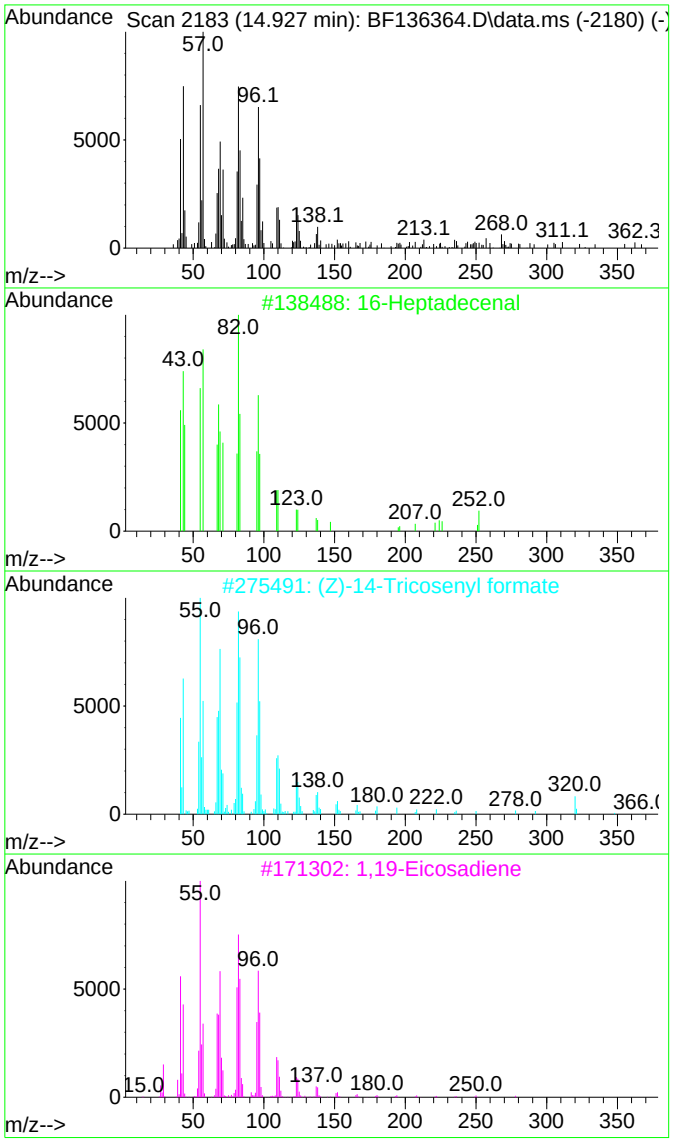
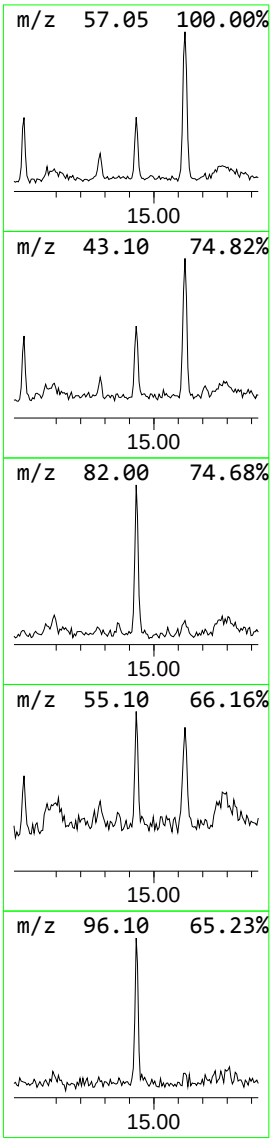
Peak Number 3 16-Heptadecenal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.927	4.23 ng	112109	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	16-Heptadecenal	252	C17H32O	1010144-57-9	93
2	(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	93
3	1,19-Eicosadiene	278	C20H38	014811-95-1	90
4	Octadecanal	268	C18H36O	000638-66-4	81
5	Oxirane, tetradecyl-	240	C16H32O	007320-37-8	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120123\
Data File : BF136364.D
Acq On : 02 Dec 2023 06:48
Operator : CG\JU
Sample : 05521-04
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-2-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.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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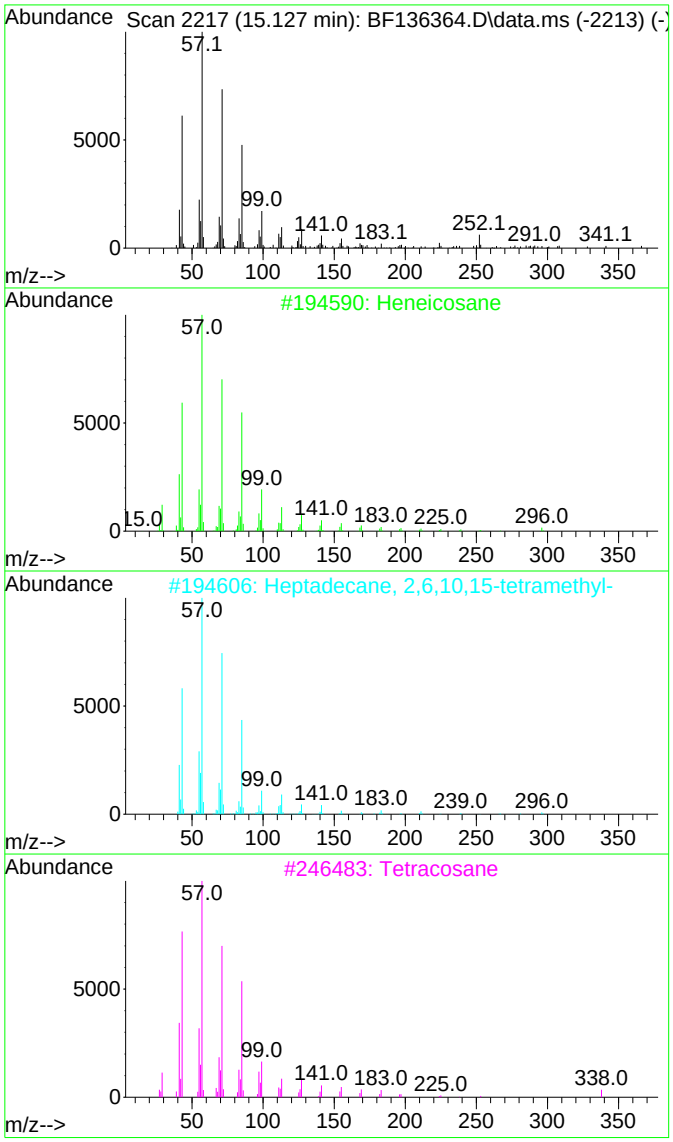
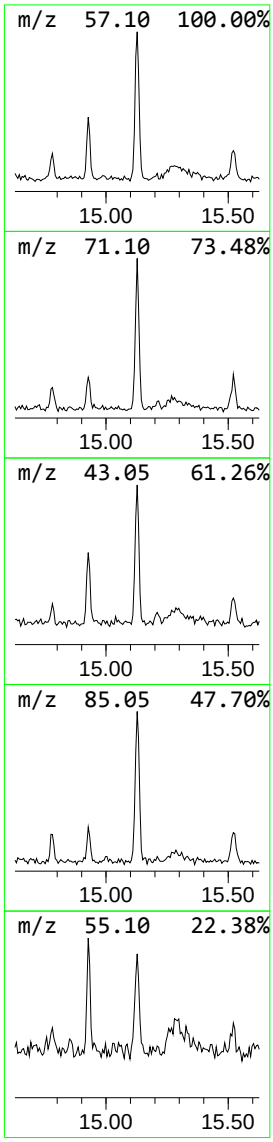
Peak Number 4 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.127	6.18 ng	163722	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	95
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
3	Tetracosane	338	C24H50	000646-31-1	90
4	Pentacosane	352	C25H52	000629-99-2	90
5	Docosane	310	C22H46	000629-97-0	87





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Sample : 05521-04
Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.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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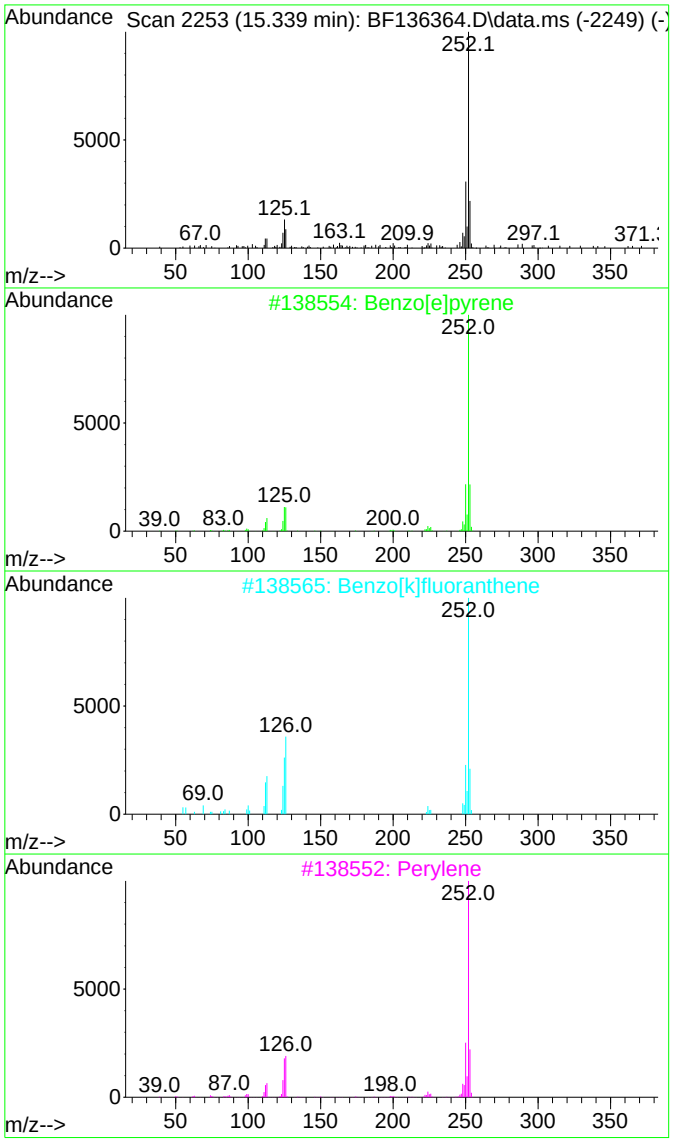
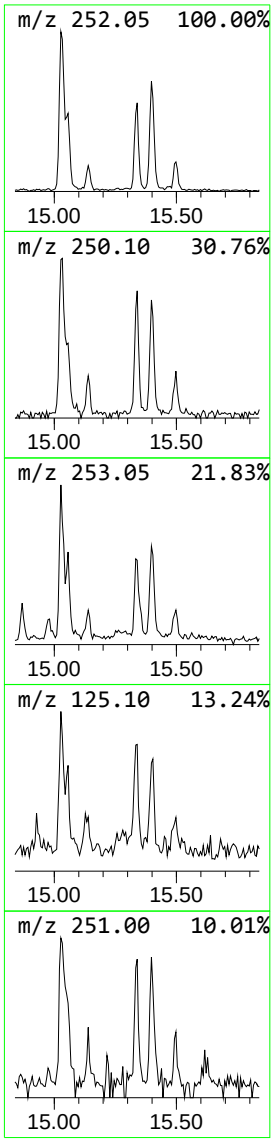
Peak Number 5 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.339	3.18 ng	84077	Perylene-d12	15.468

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	93
3	Perylene	252	C20H12	000198-55-0	90
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
5	Benzo[a]pyrene	252	C20H12	000050-32-8	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120123\
Data File : BF136364.D
Acq On : 02 Dec 2023 06:48
Operator : CG\JU
Sample : 05521-04
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.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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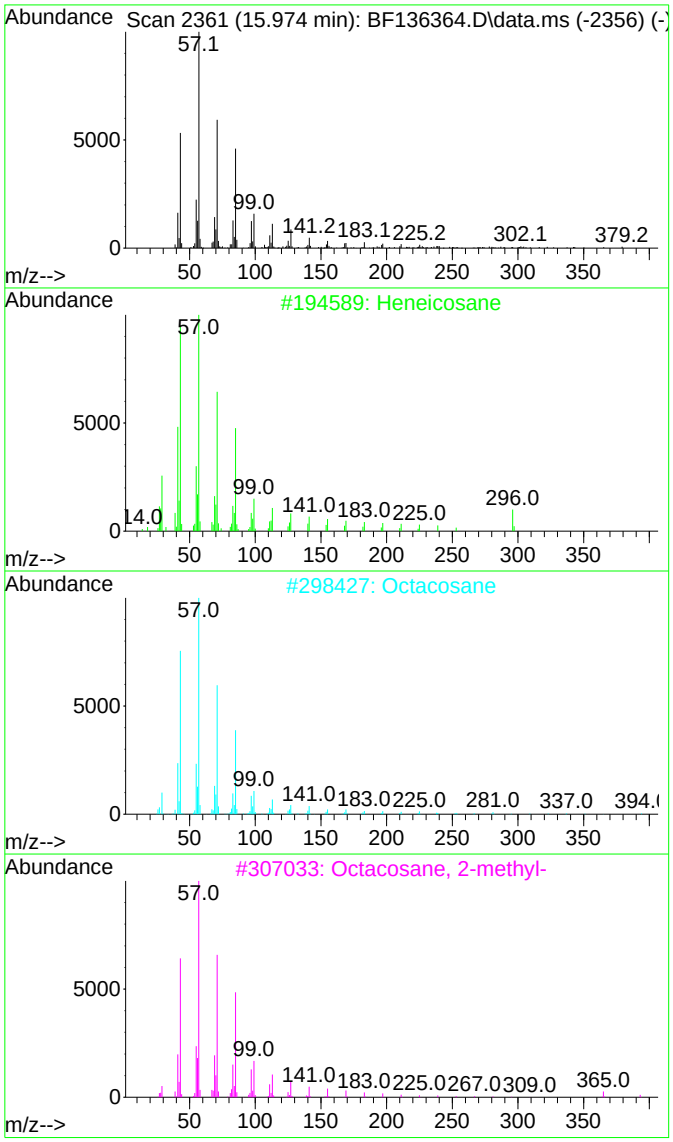
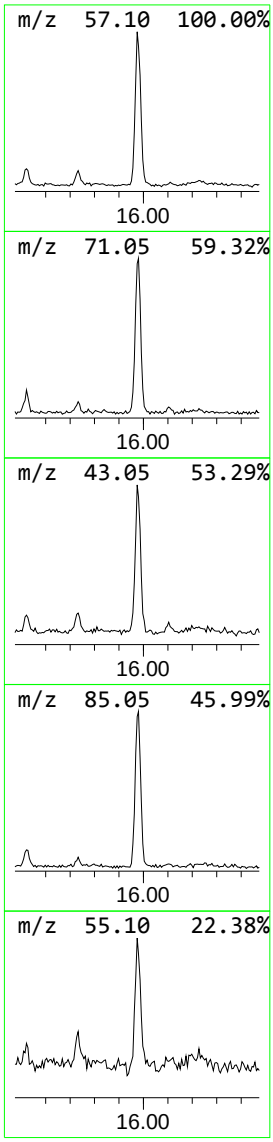
Peak Number 6 Octacosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.974	13.36 ng	353855	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	93
2	Octacosane	394	C28H58	000630-02-4	91
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4	Eicosane	282	C20H42	000112-95-8	91
5	Tetratetracontane	619	C44H90	007098-22-8	91





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Data File : BF136364.D
Acq On : 02 Dec 2023 06:48
Operator : CG\JU
Sample : 05521-04
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-2-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.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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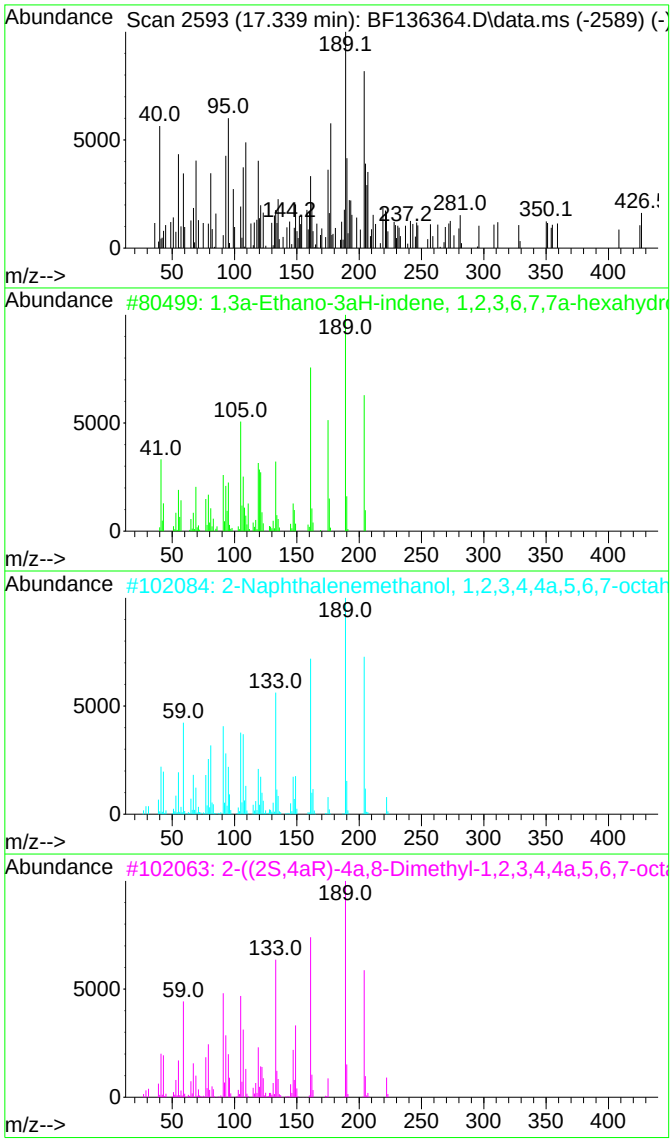
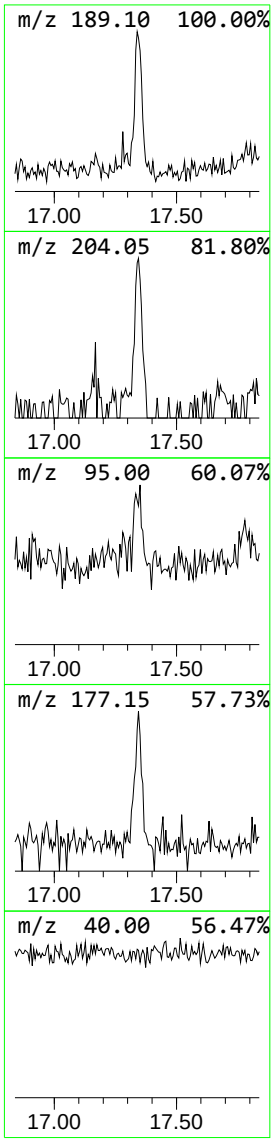
Peak Number 7 unknown17.339 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.339	2.50 ng	66200	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3a-Ethano-3aH-indene, 1,2,3,6,...	204	C15H24	004545-68-0	45
2	2-Naphthalenemethanol, 1,2,3,4,4...	222	C15H26O	001209-71-8	43
3	2-((2S,4aR)-4a,8-Dimethyl-1,2,3,...	222	C15H26O	117066-77-0	43
4	(-)-1,2,2.alpha.,3,3,4,6,7,8,8.a...	204	C15H24	1000365-86-7	41
5	2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	207297-57-2	41





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120123\
Data File : BF136364.D
Acq On : 02 Dec 2023 06:48
Operator : CG\JU
Sample : 05521-04
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-2-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.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
n-Hexadecanoic ...	11.869	7.8	ng	257180	4	11.328	663549	20.0
E-7-Octadecene	13.916	2.5	ng	108721	5	13.980	876332	20.0
16-Heptadecenal	14.927	4.2	ng	112109	6	15.468	529536	20.0
Heneicosane	15.127	6.2	ng	163722	6	15.468	529536	20.0
Benzo[e]pyrene	15.339	3.2	ng	84077	6	15.468	529536	20.0
Octacosane	15.974	13.4	ng	353855	6	15.468	529536	20.0
unknown17.339	17.339	2.5	ng	66200	6	15.468	529536	20.0