LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040422\
Data File : BF127632.D
Acq On : 04 Apr 2022 15:15
Operator : CG\JU
Sample : N2249-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-7D

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-BF032122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127632.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.457	537	539	571	rVB	1093124	1374482	42.74%	6.309%
2	6.475	709	712	735	rBV	730438	907248	28.21%	4.164%
3	6.834	769	773	780	rBV	513847	484410	15.06%	2.223%
4	7.404	866	870	881	rBV	2054147	1886310	58.66%	8.658%
5	8.116	987	991	1000	rBV	724501	645702	20.08%	2.964%
6	9.187	1169	1173	1177	rBV	2962484	2850668	88.64%	13.085%
7	9.292	1189	1191	1200	rVB	157316	168696	5.25%	0.774%
8	9.869	1286	1289	1298	rBV	899315	747079	23.23%	3.429%
9	10.669	1421	1425	1438	rBV	1923972	1988692	61.84%	9.128%
10	11.363	1540	1543	1553	rBV	943621	835243	25.97%	3.834%
11	11.875	1625	1630	1654	rVB	421997	788747	24.53%	3.620%
12	12.522	1736	1740	1744	rBV	56002	68140	2.12%	0.313%
13	12.663	1758	1764	1777	rBV	787196	1268441	39.44%	5.822%
14	12.880	1791	1801	1809	rBV3	146466	486833	15.14%	2.235%
15	12.951	1809	1813	1816	rVB	3493189	3215880	100.00%	14.761%
16	13.769	1945	1952	1960	rBV	302119	606970	18.87%	2.786%
17	14.016	1991	1994	2004	rBV	780056	770734	23.97%	3.538%
18	14.422	2056	2063	2067	rBV	368192	607322	18.89%	2.788%
19	14.827	2124	2132	2137	rVB	179015	263337	8.19%	1.209%
20	14.986	2154	2159	2172	rVB	237693	421757	13.11%	1.936%
21	15.504	2243	2247	2260	rBV2	346159	569029	17.69%	2.612%
22	15.627	2262	2268	2277	rVB2	121110	268879	8.36%	1.234%
23	16.374	2388	2395	2404	rBV	86279	199934	6.22%	0.918%
24	16.798	2461	2467	2478	rVB3	62010	166112	5.17%	0.762%
25	17.239	2536	2542	2543	rBV3	43975	71913	2.24%	0.330%
26	18.268	2711	2717	2728	rVB4	41114	123804	3.85%	0.568%

Sum of corrected areas: 21786362

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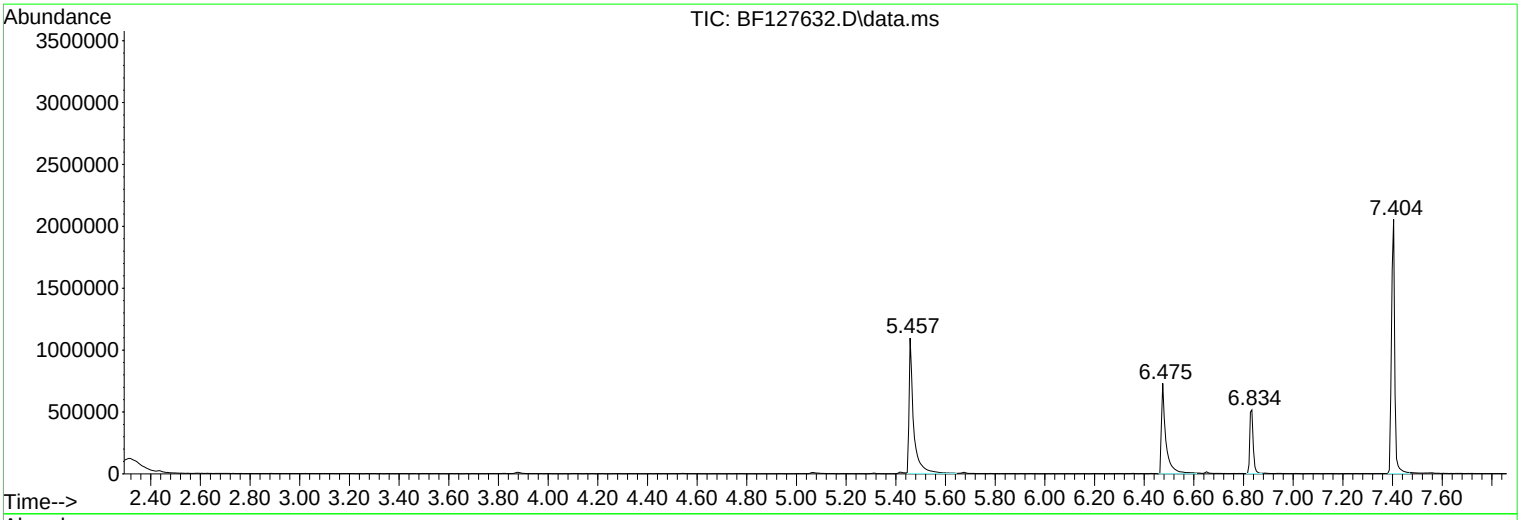
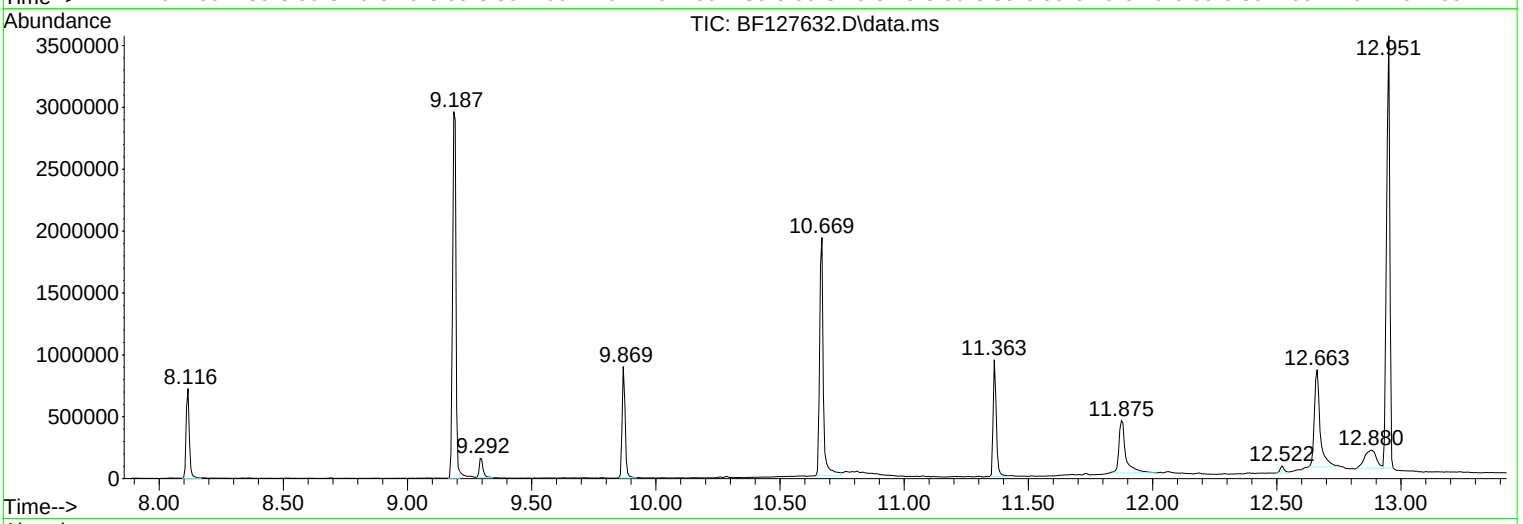
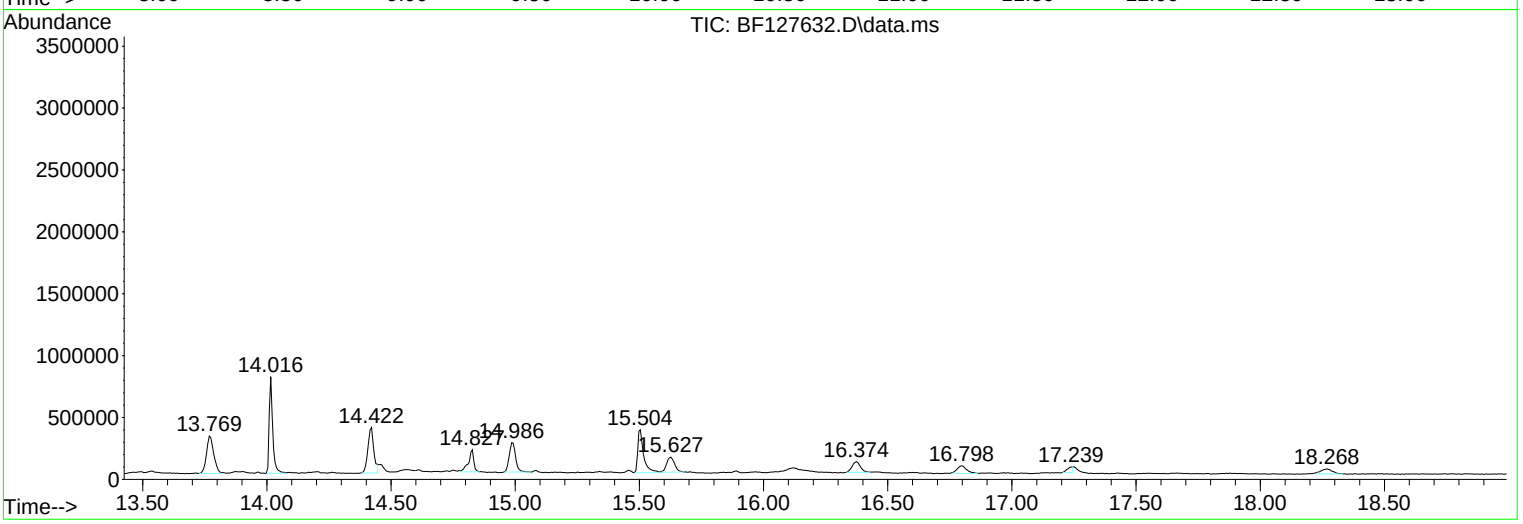
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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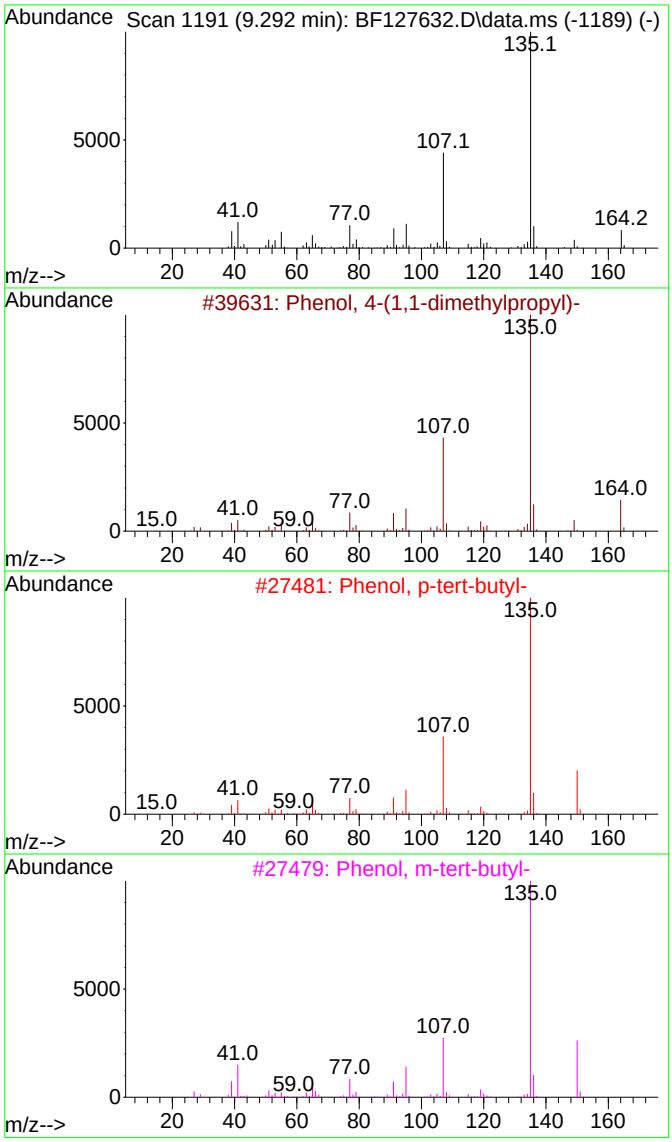
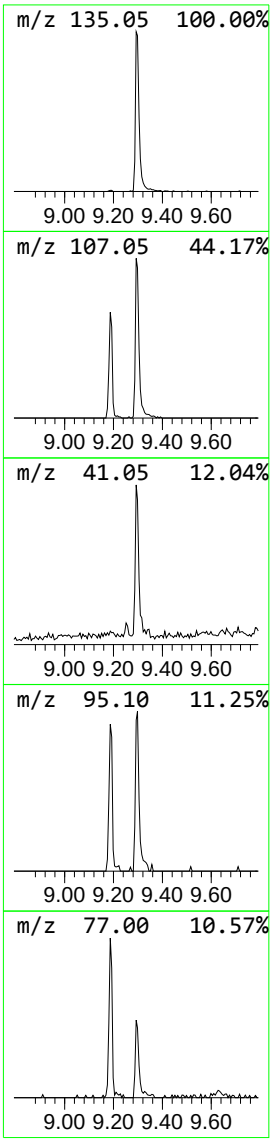
****
Peak Number 1 Phenol, 4-(1,1-dimethylprop... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.292	4.52 ng	168696	Acenaphthene-d10	9.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	95
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	86
3	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	64
4	4,4'-(1,2-diethylethylene)diphenol	270	C18H22O2	005635-50-7	64
5	Propane, 1,3-bis(ethylthio)-	164	C7H16S2	033672-52-5	58





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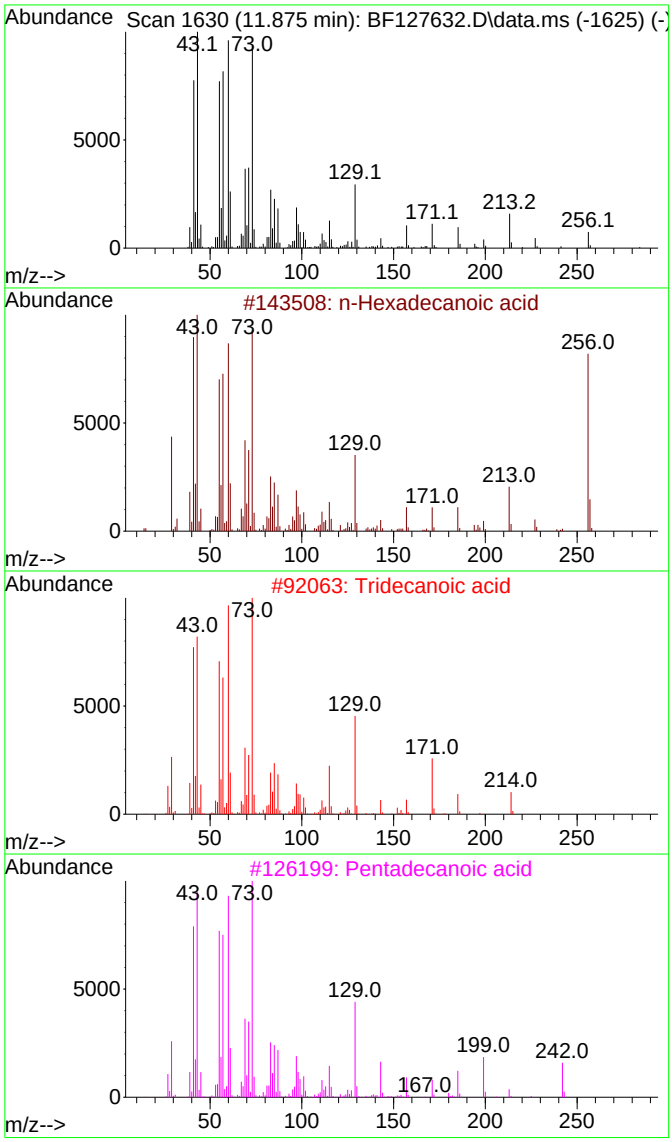
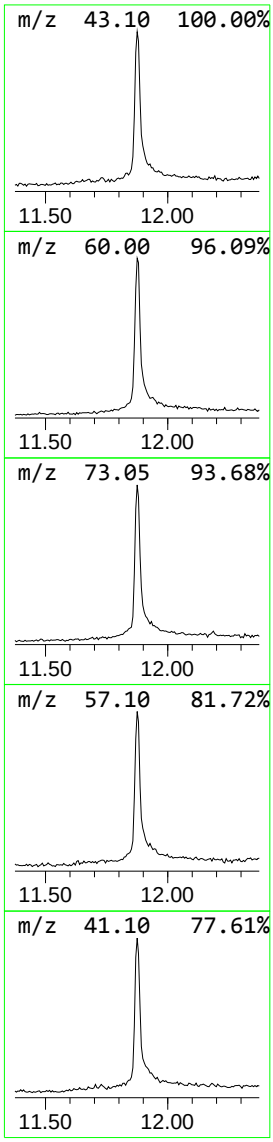
Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.875	18.89 ng	788747	Phenanthrene-d10	11.363

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Octadecanoic acid	284	C18H36O2	000057-11-4	64





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Sample : N2249-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-7D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.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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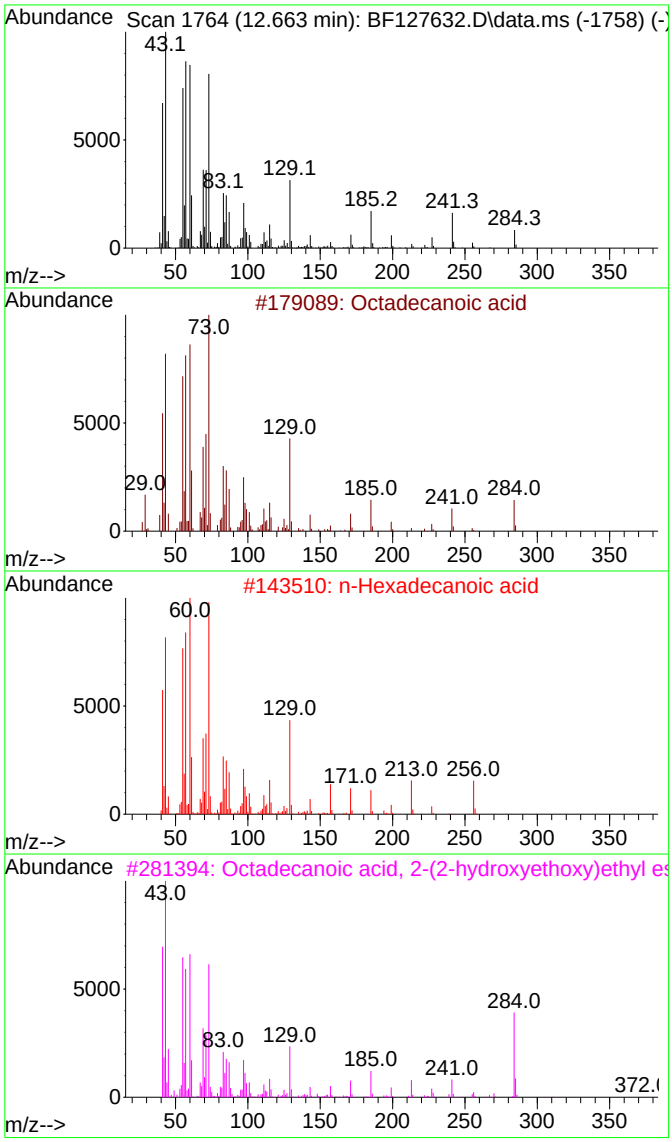
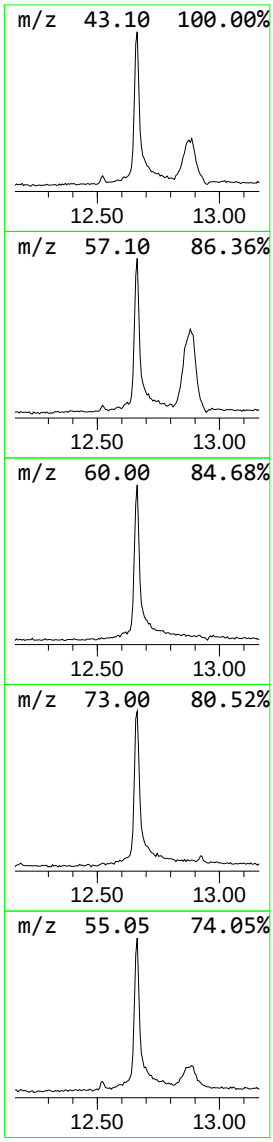
Peak Number 3 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.663	30.37 ng	1268440	Phenanthrene-d10	11.363

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Dodecanoic acid	200	C12H24O2	000143-07-7	68





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
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TIC Library : C:\Database\NIST20.L
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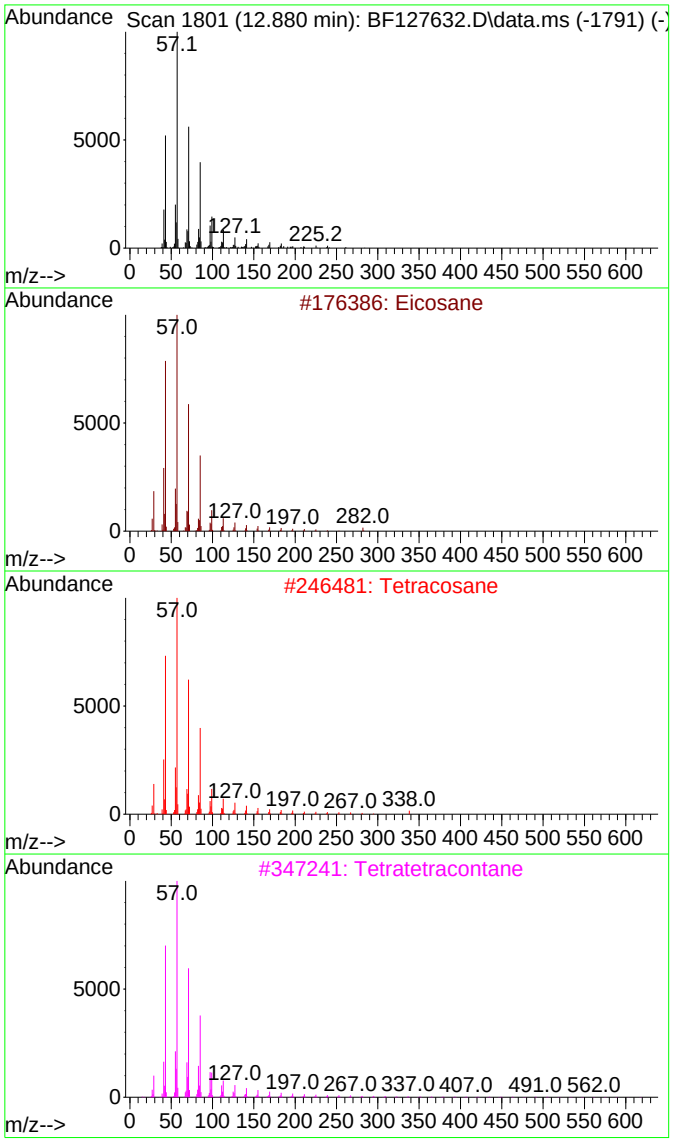
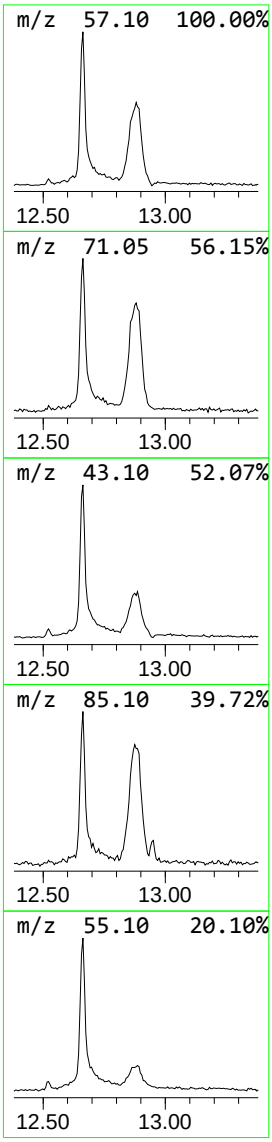
Peak Number 4 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.880	12.63 ng	486833	Chrysene-d12	14.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Tetracosane	338	C24H50	000646-31-1	90
3	Tetratetracontane	619	C44H90	007098-22-8	90
4	Pentacosane	352	C25H52	000629-99-2	90
5	Octacosane	394	C28H58	000630-02-4	90





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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-7D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
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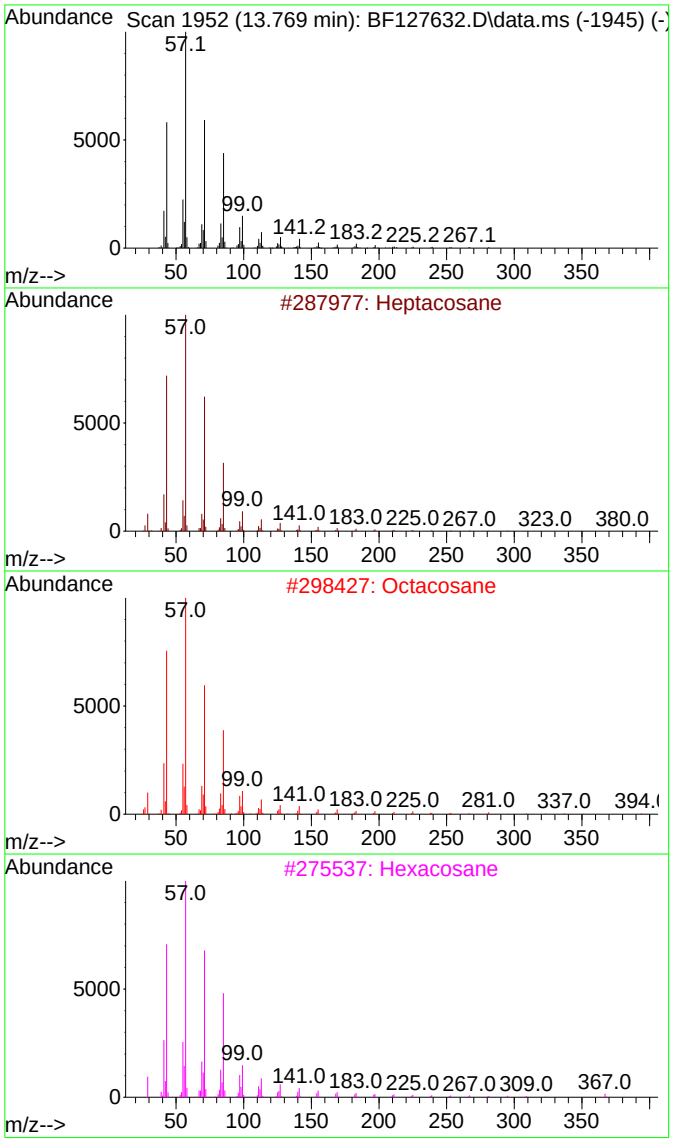
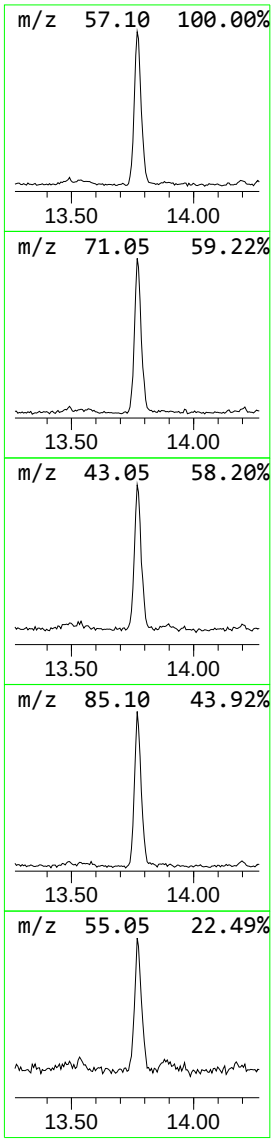
Peak Number 5 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.769	15.75 ng	606970	Chrysene-d12	14.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Heneicosane	296	C21H44	000629-94-7	90
5	Nonadecane	268	C19H40	000629-92-5	86





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Instrument :
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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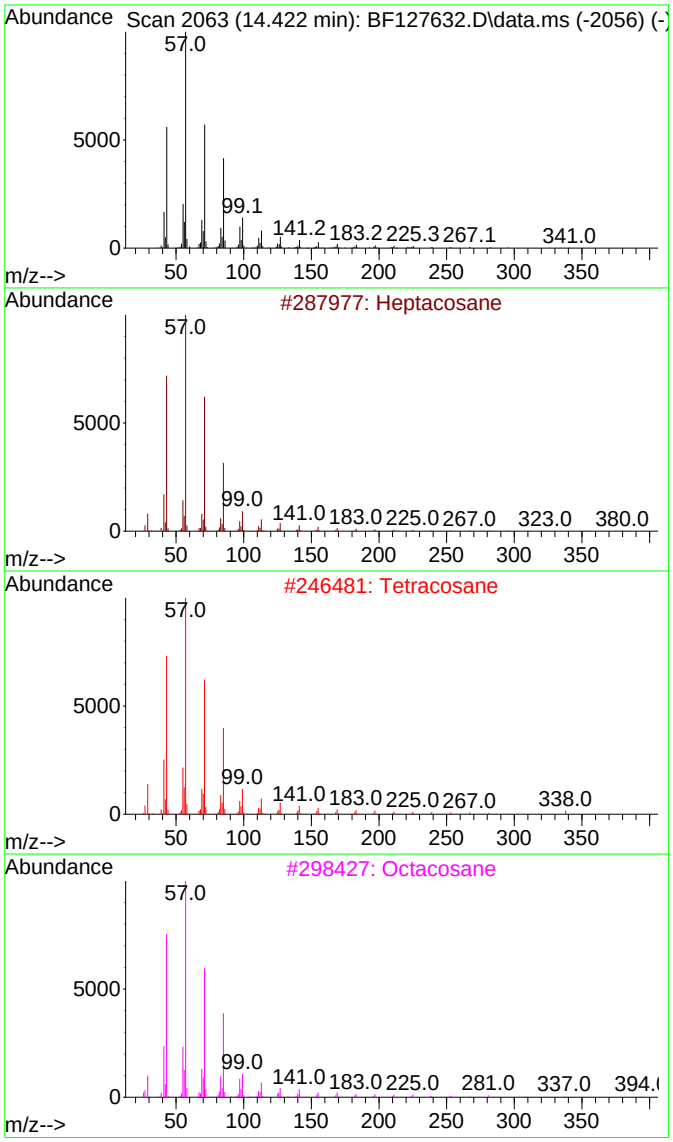
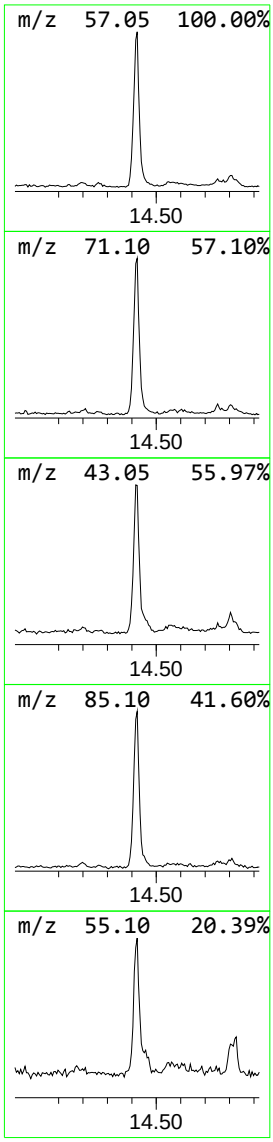
Peak Number 6 Tetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.422	15.76 ng	607322	Chrysene-d12	14.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Pentacosane	352	C25H52	000629-99-2	91
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90





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Sample : N2249-07
Misc :
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Instrument :
BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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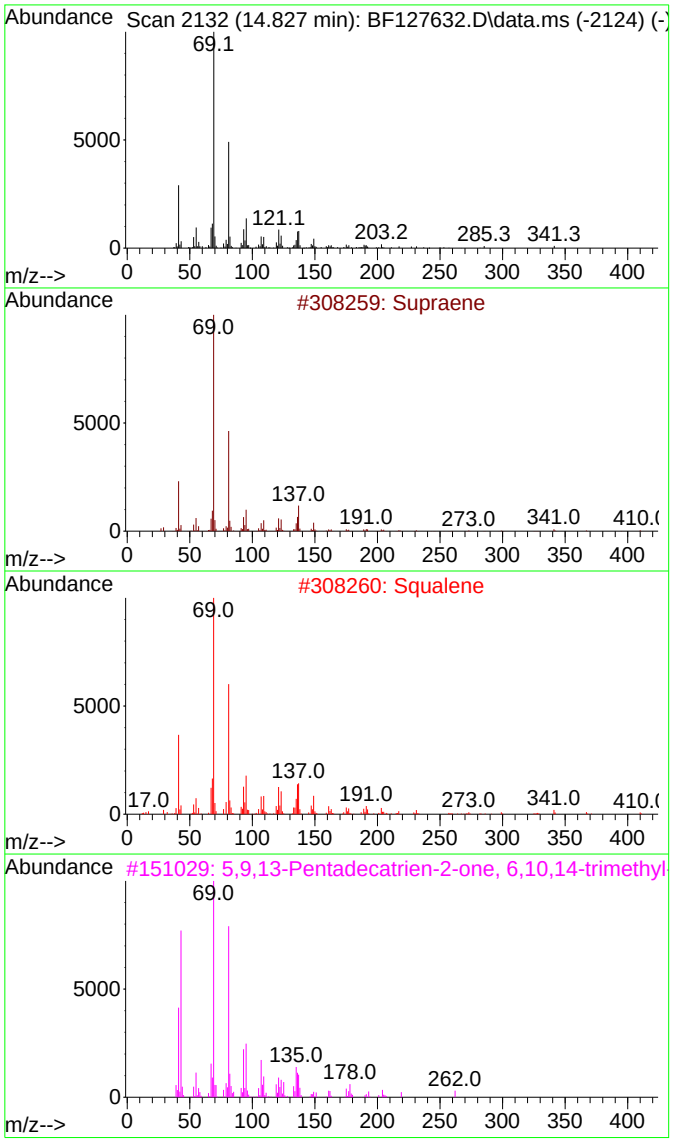
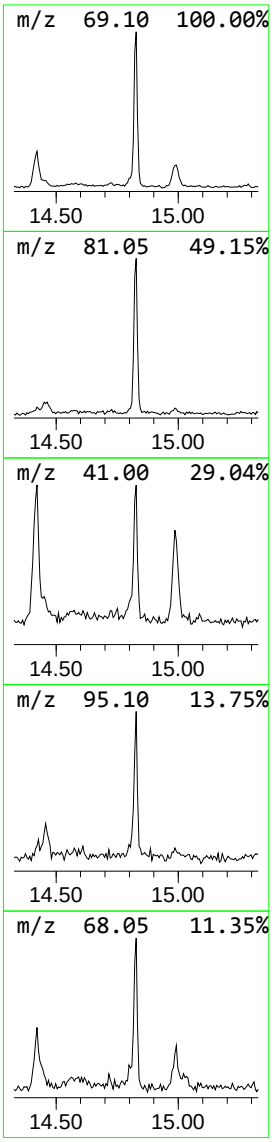
Peak Number 7 Supraene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.827	9.26 ng	263337	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	90
3	5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	72
4	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	58
5	5-Bromo-1-pentanol	166	C5H11BrO	034626-51-2	53





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ClientSampleId :
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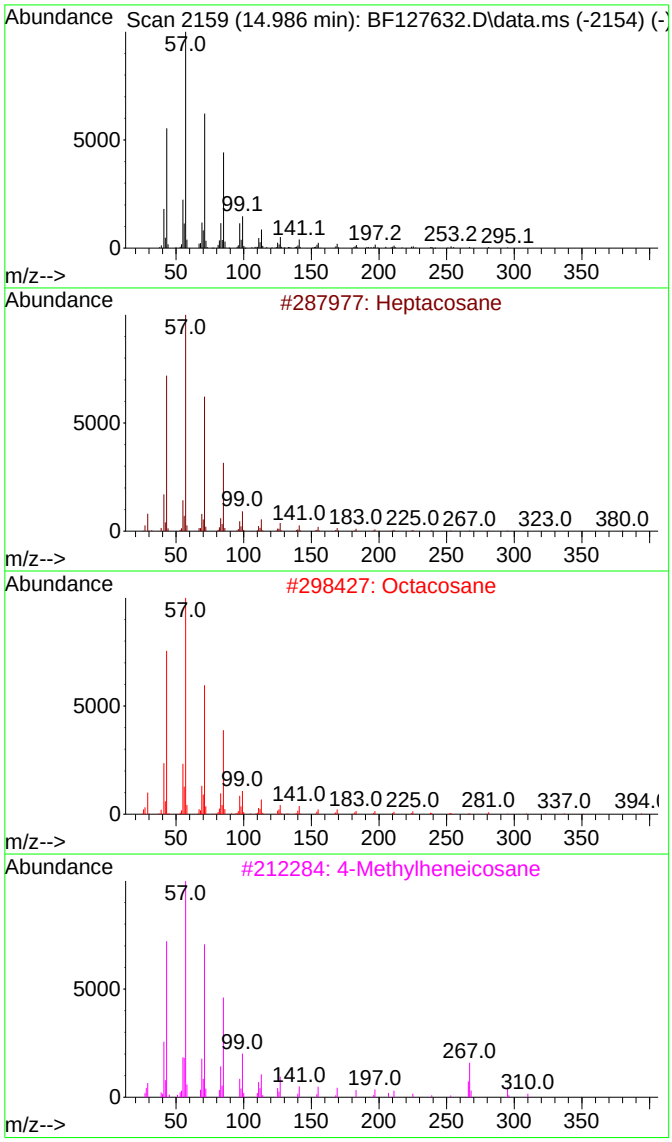
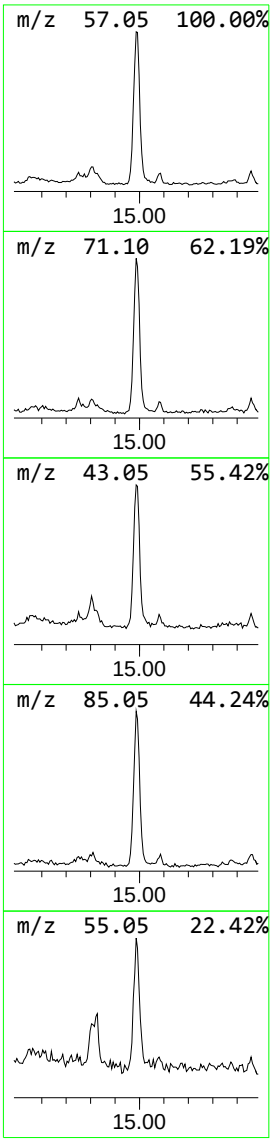
Peak Number 8 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.986	14.82 ng	421757	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	4-Methylheneicosane	310	C22H46	025117-29-7	91
4	Tetratetracontane	619	C44H90	007098-22-8	87
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	87





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.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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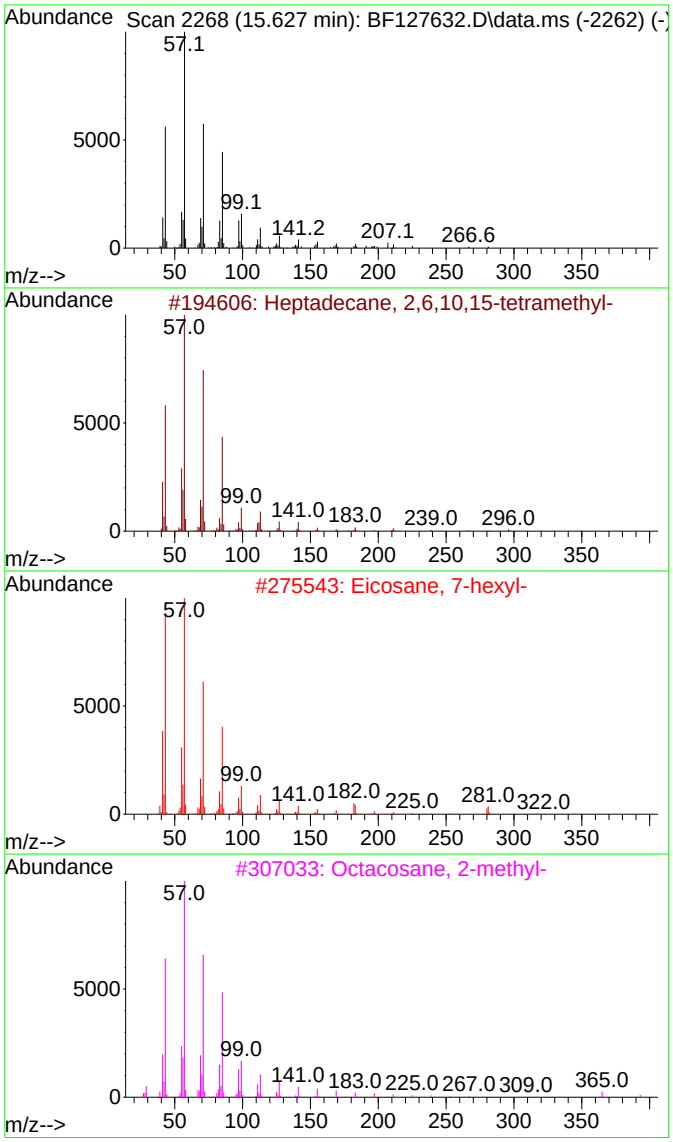
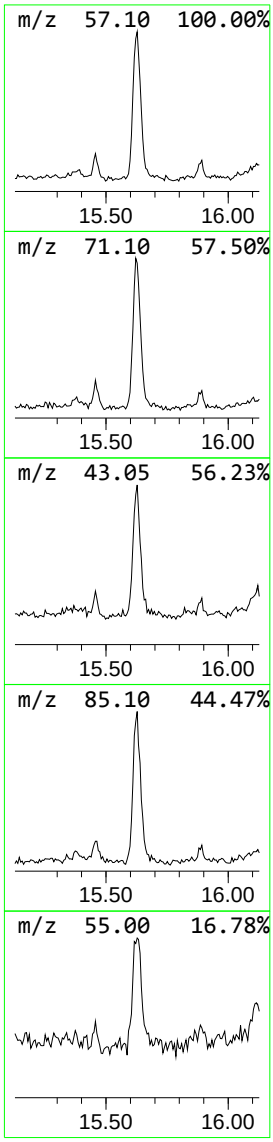
Peak Number 9 Heptadecane, 2,6,10,15-tetr... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.627	9.45 ng	268879	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
2	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
4	Docosane	310	C22H46	000629-97-0	86
5	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	86





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Operator : CG\JU
Sample : N2249-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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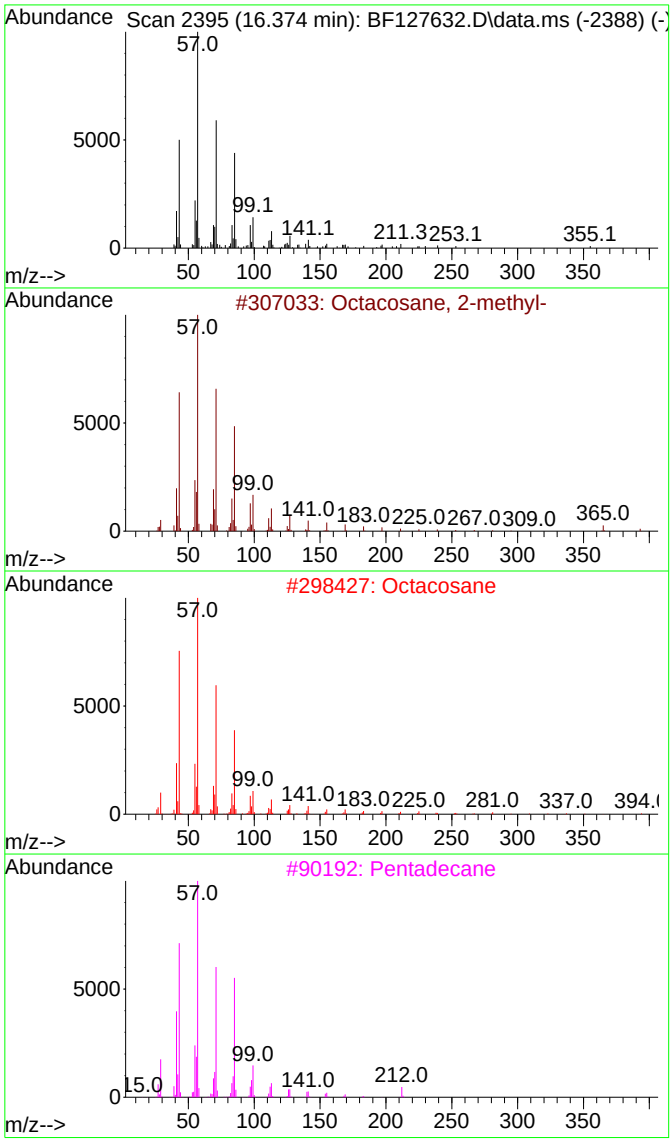
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

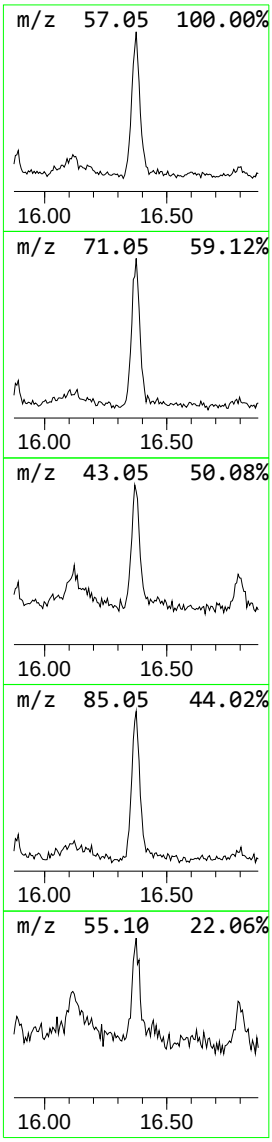
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Octacosane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.374	7.03 ng	199934	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
2	Octacosane	394	C28H58	000630-02-4	90
3	Pentadecane	212	C15H32	000629-62-9	72
4	Heptacosane	380	C27H56	000593-49-7	68
5	Hexadecane	226	C16H34	000544-76-3	64





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Data File : BF127632.D
Acq On : 04 Apr 2022 15:15
Operator : CG\JU
Sample : N2249-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-7D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

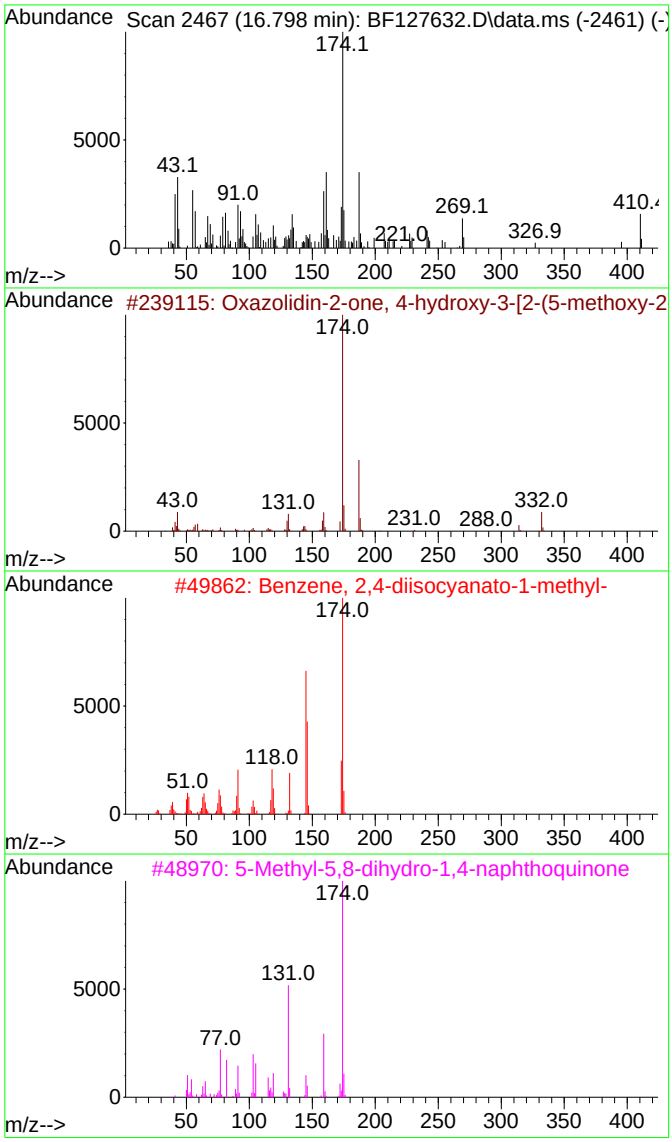
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

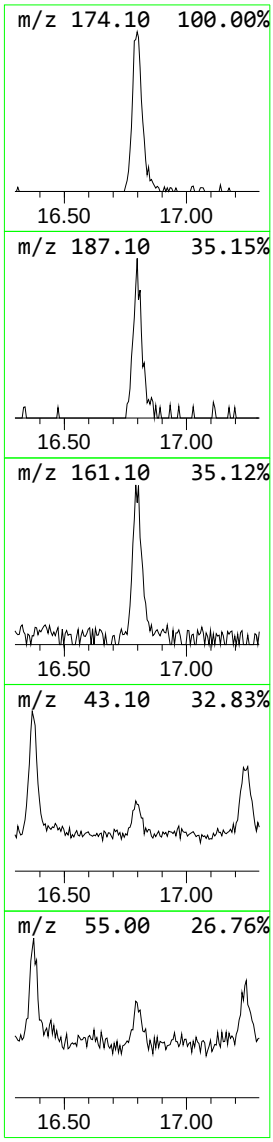
****

Peak Number 11 unknown16.798 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.798	5.84 ng	166112	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxazolidin-2-one, 4-hydroxy-3-[2...	332	C18H24N2O4	1000310-03-3	47
2	Benzene, 2,4-diisocyanato-1-methyl-	174	C9H6N2O2	000584-84-9	46
3	5-Methyl-5,8-dihydro-1,4-naphtho...	174	C11H10O2	086759-40-2	46
4	Pyrazole, 5-(4-methoxyphenyl)-	174	C10H10N2O	1000157-86-0	46
5	5,6-Dimethyl-1H-1,3-benzodiazole...	174	C10H10N2O	920484-85-1	43





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Data File : BF127632.D
Acq On : 04 Apr 2022 15:15
Operator : CG\JU
Sample : N2249-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-7D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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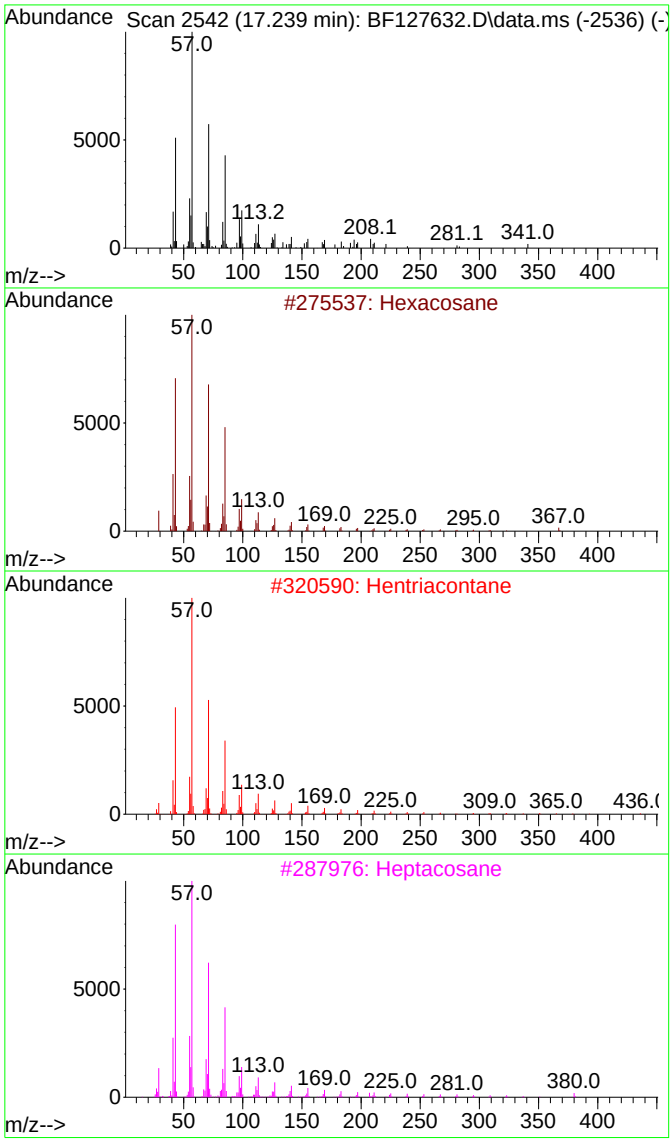
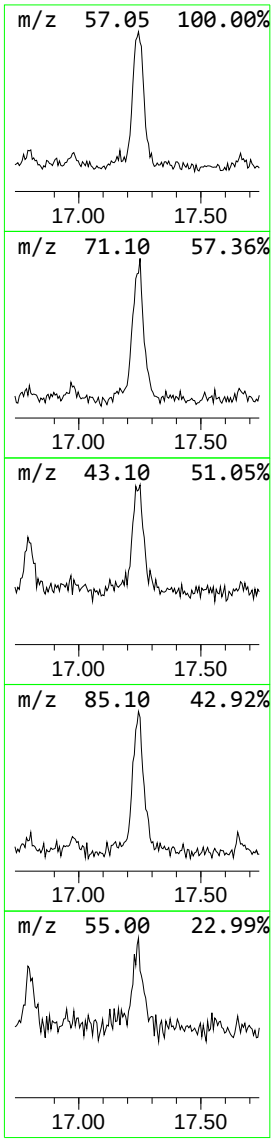
Peak Number 12 Hentriacontane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.239	2.53 ng	71913	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Hentriacontane	437	C31H64	000630-04-6	90
3	Heptacosane	380	C27H56	000593-49-7	87
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5	Pentacosane	352	C25H52	000629-99-2	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040422\
Data File : BF127632.D
Acq On : 04 Apr 2022 15:15
Operator : CG\JU
Sample : N2249-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-7D

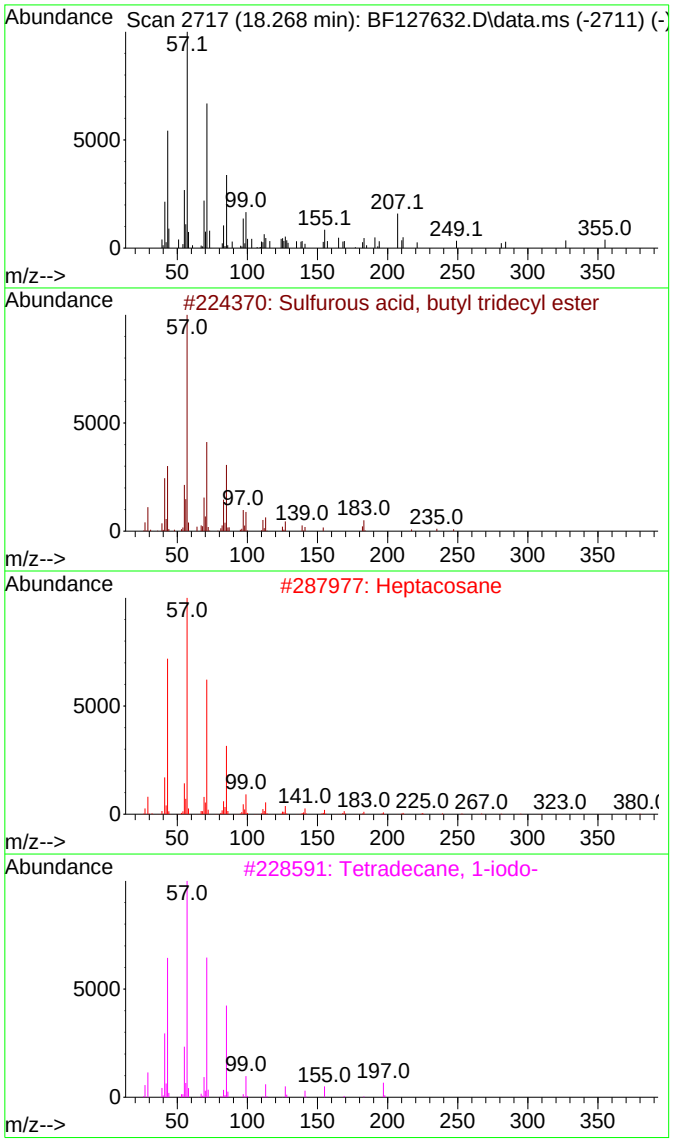
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

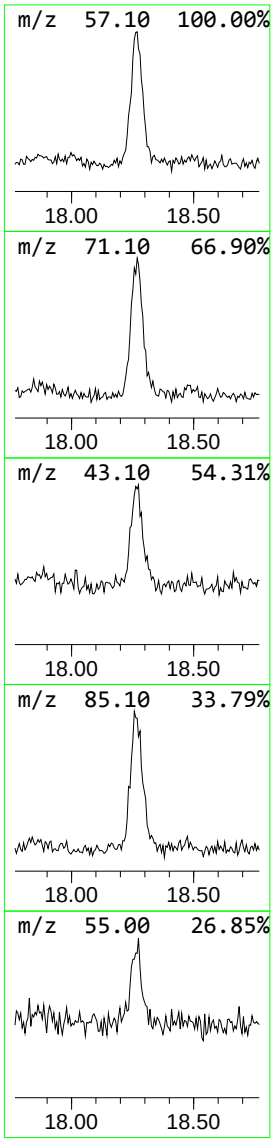
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 Sulfurous acid, butyl tride... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.268	4.35 ng	123804	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	59
2	Heptacosane	380	C27H56	000593-49-7	53
3	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	53
4	Nonane, 2-methyl-5-propyl-	184	C13H28	031081-17-1	50
5	Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040422\
Data File : BF127632.D
Acq On : 04 Apr 2022 15:15
Operator : CG\JU
Sample : N2249-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-7D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.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
Phenol, 4-(1,1-...	9.292	4.5	ng	168696	3	9.869	747079	20.0
n-Hexadecanoic ...	11.875	18.9	ng	788747	4	11.363	835243	20.0
Octadecanoic acid	12.663	30.4	ng	1268440	4	11.363	835243	20.0
Eicosane	12.880	12.6	ng	486833	5	14.016	770734	20.0
Heptacosane	13.769	15.8	ng	606970	5	14.016	770734	20.0
Tetracosane	14.422	15.8	ng	607322	5	14.016	770734	20.0
Supraene	14.827	9.3	ng	263337	6	15.504	569029	20.0
Octacosane	14.986	14.8	ng	421757	6	15.504	569029	20.0
Heptadecane, 2,...	15.627	9.4	ng	268879	6	15.504	569029	20.0
Octacosane, 2-m...	16.374	7.0	ng	199934	6	15.504	569029	20.0
unknown16.798	16.798	5.8	ng	166112	6	15.504	569029	20.0
Hentriacontane	17.239	2.5	ng	71913	6	15.504	569029	20.0
Sulfurous acid,...	18.268	4.3	ng	123804	6	15.504	569029	20.0