LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051521\
Data File : BF123938.D
Acq On : 15 May 2021 11:33
Operator : JU/CG
Sample : M2383-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KTW-03

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-BF051421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123938.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	9	16	22	rVB	1537199	1987467	95.69%	15.013%
2	5.104	507	513	517	rVB2	14994	23037	1.11%	0.174%
3	5.504	577	581	585	rVB	638809	587633	28.29%	4.439%
4	6.504	747	751	756	rBV	391698	363977	17.52%	2.749%
5	6.898	815	818	822	rBV	357273	285945	13.77%	2.160%
6	6.957	825	828	831	rBV	52963	42200	2.03%	0.319%
7	7.463	908	914	917	rBV	1111549	1030922	49.63%	7.787%
8	8.180	1033	1036	1040	rBV	418672	369983	17.81%	2.795%
9	9.263	1215	1220	1223	rBV	2362990	1918277	92.36%	14.491%
10	9.651	1283	1286	1290	rBV	26452	24153	1.16%	0.182%
11	9.939	1331	1335	1338	rVB	558163	443307	21.34%	3.349%
12	10.039	1348	1352	1355	rBV	41054	38690	1.86%	0.292%
13	10.727	1464	1469	1472	rBV	1690806	1472336	70.89%	11.122%
14	10.945	1498	1506	1508	rBV7	21350	52709	2.54%	0.398%
15	11.427	1584	1588	1591	rBV	569088	497548	23.95%	3.758%
16	11.527	1600	1605	1609	rBV4	22297	28194	1.36%	0.213%
17	11.951	1672	1677	1681	rBV	208405	200355	9.65%	1.513%
18	12.092	1697	1701	1703	rBV4	23815	24814	1.19%	0.187%
19	12.115	1703	1705	1711	rVB5	29762	39796	1.92%	0.301%
20	12.733	1806	1810	1813	rBV4	77819	80676	3.88%	0.609%
21	13.015	1854	1858	1861	rBV	2184121	2077037	100.00%	15.690%
22	13.286	1896	1904	1913	rVB3	44658	107989	5.20%	0.816%
23	13.909	2007	2010	2016	rBV2	152421	158424	7.63%	1.197%
24	14.027	2024	2030	2032	rBV3	44270	75903	3.65%	0.573%
25	14.062	2032	2036	2040	rVB	459888	450747	21.70%	3.405%
26	14.545	2114	2118	2121	rBV4	20835	24608	1.18%	0.186%
27	14.615	2123	2130	2133	rBV2	51661	95212	4.58%	0.719%
28	14.645	2133	2135	2141	rVB5	30237	43636	2.10%	0.330%
29	14.939	2180	2185	2188	rBV	83055	92808	4.47%	0.701%
30	15.203	2223	2230	2237	rBV2	49031	88051	4.24%	0.665%
31	15.556	2284	2290	2294	rBV	272691	341999	16.47%	2.583%
32	15.874	2338	2344	2350	rBV2	32177	55558	2.67%	0.420%
33	16.098	2378	2382	2387	rVB5	21304	30588	1.47%	0.231%
34	16.250	2404	2408	2419	rVB7	22696	58842	2.83%	0.444%
35	16.668	2477	2479	2487	rVB6	17287	24745	1.19%	0.187%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051521\
Data File : BF123938.D
Acq On : 15 May 2021 11:33
Operator : JU/CG
Sample : M2383-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KTW-03

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-BF051421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

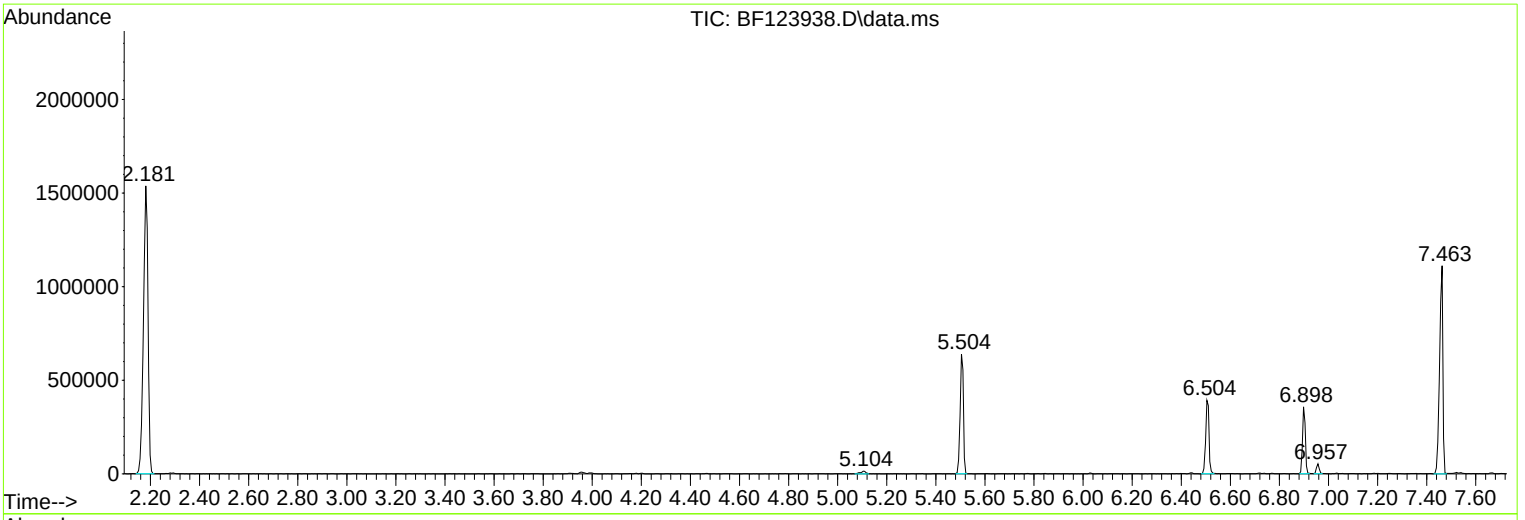
Sum of corrected areas: 13238166

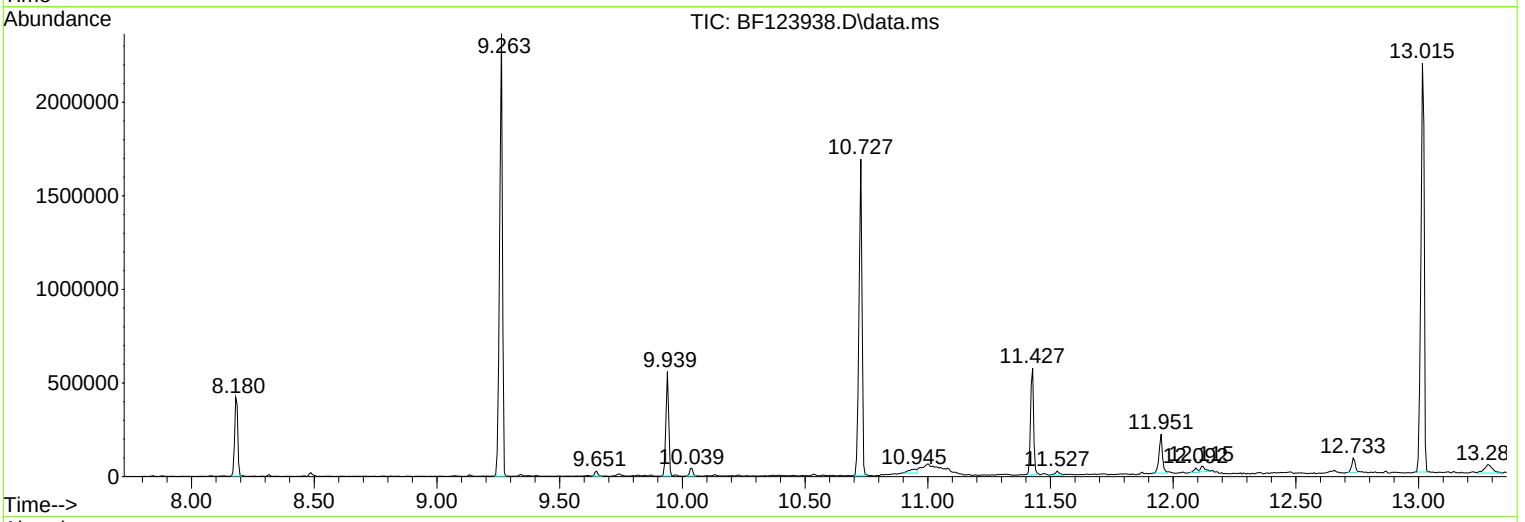
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051521\
Data File : BF123938.D
Acq On : 15 May 2021 11:33
Operator : JU/CG
Sample : M2383-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

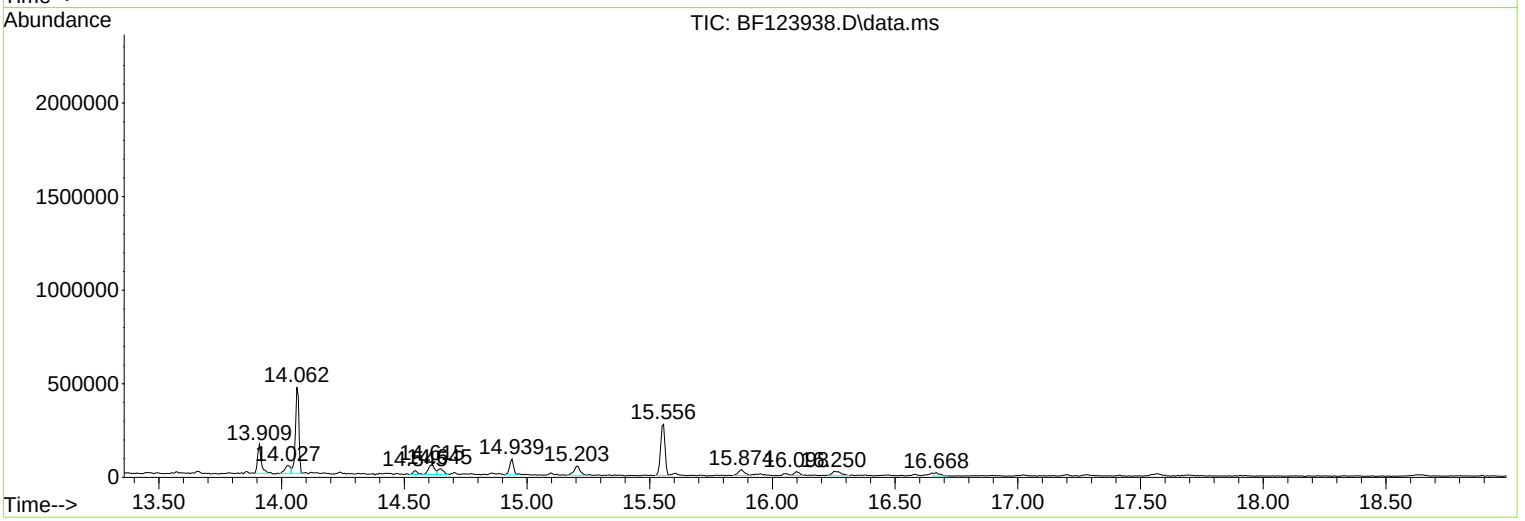
Instrument :
BNA_F
ClientSampleId :
KTW-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051521\
Data File : BF123938.D
Acq On : 15 May 2021 11:33
Operator : JU/CG
Sample : M2383-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KTW-03

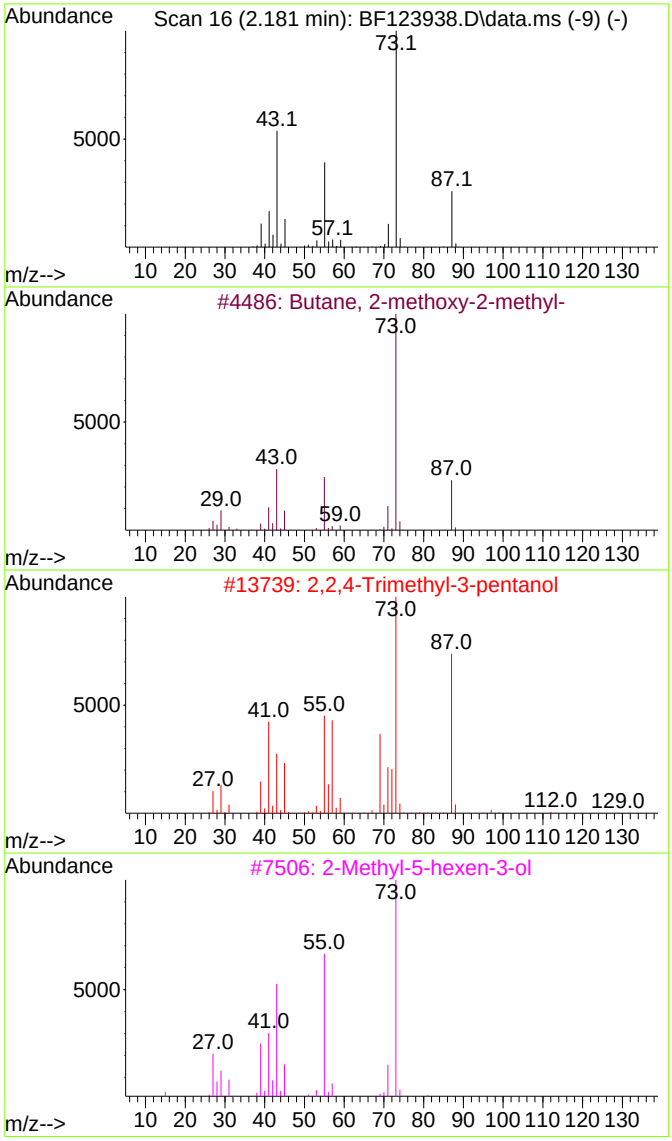
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

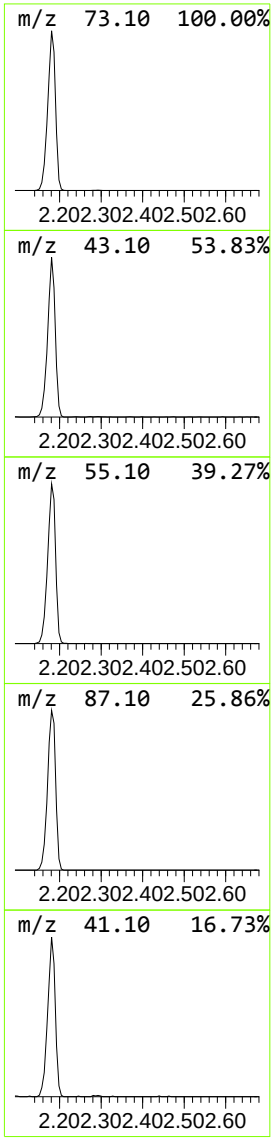
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	139.01 ng	1987470	1,4-Dichlorobenzene-d4	6.898

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	38
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	t-Butyl nitrite	103	C4H9NO2	000540-80-7	9





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Data File : BF123938.D
Acq On : 15 May 2021 11:33
Operator : JU/CG
Sample : M2383-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KTW-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

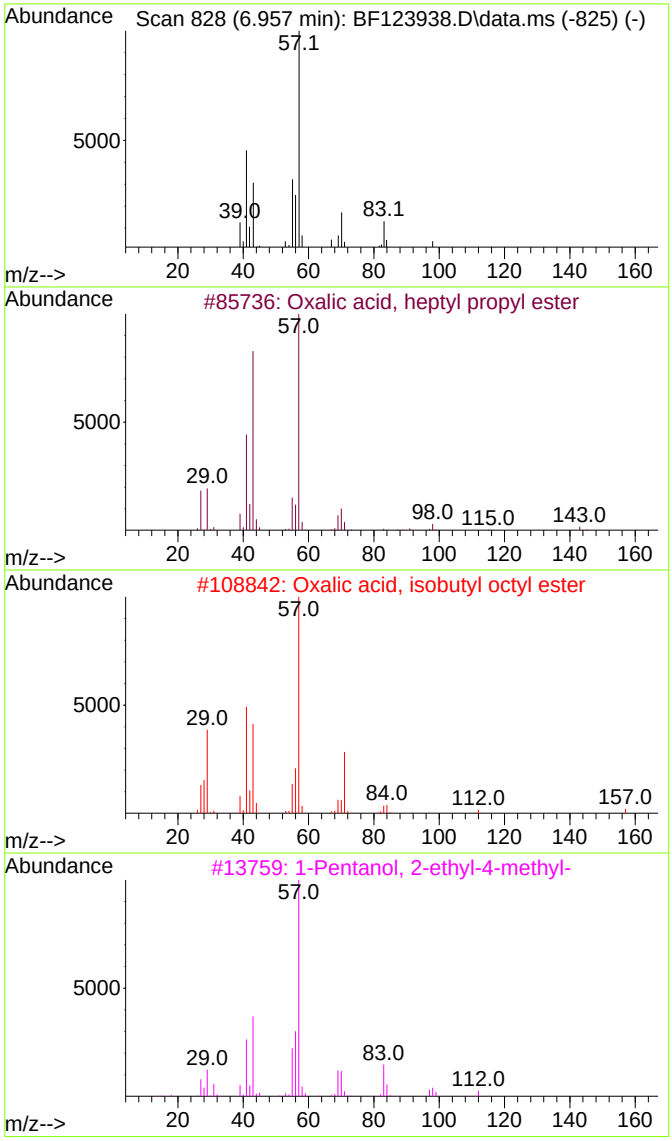
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

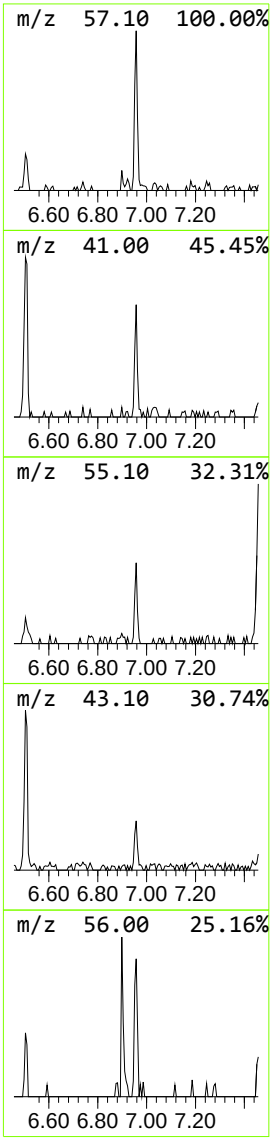
****

Peak Number 2 unknown6.957 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.957	2.95 ng	42200	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, heptyl propyl ester	230	C12H22O4	1000309-26-0	40
2	Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	40
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	37
4	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	37
5	Acetic acid, dichloro-, heptyl e...	226	C9H16Cl2O2	083004-97-1	36





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051521\
Data File : BF123938.D
Acq On : 15 May 2021 11:33
Operator : JU/CG
Sample : M2383-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KTW-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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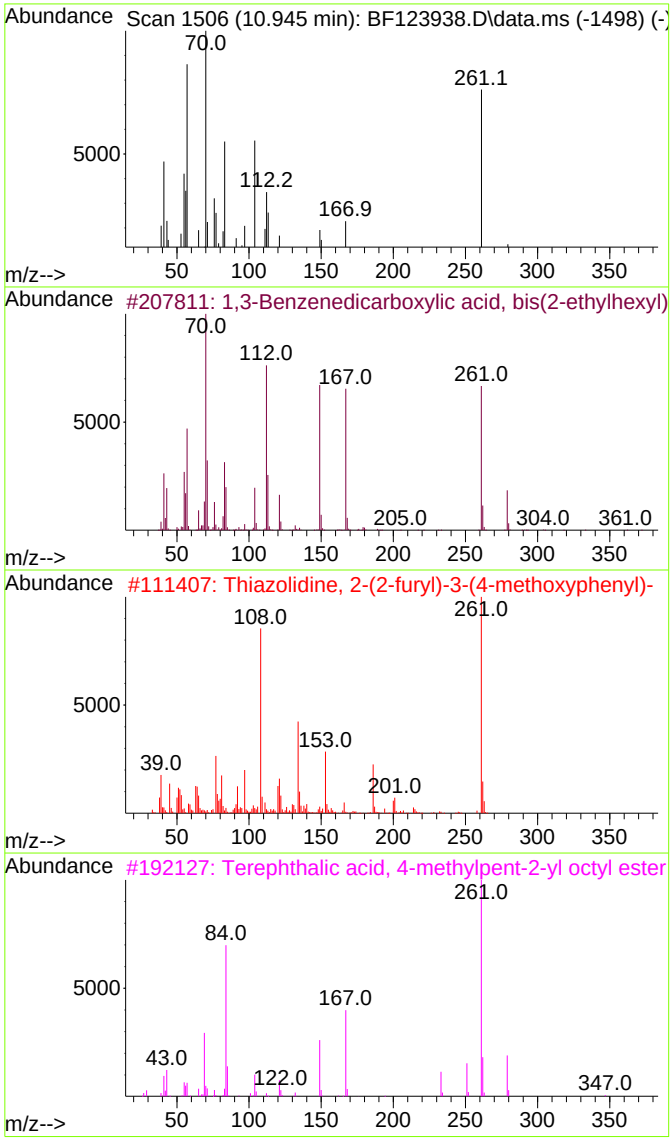
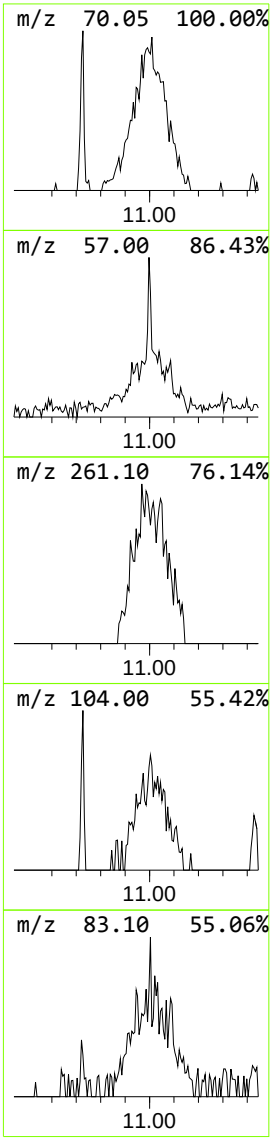
Peak Number 3 unknown10.945 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.945	2.12 ng	52709	Phenanthrene-d10	11.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	17
2	Thiazolidine, 2-(2-furyl)-3-(4-m...	261	C14H15NO2S	100710-99-4	14
3	Terephthalic acid, 4-methylpent-...	362	C22H34O4	1000356-26-2	12
4	2-Undecenal	168	C11H20O	002463-77-6	12
5	Dichloroacetic acid, 2-octyl ester	240	C10H18Cl2O2	096980-53-9	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051521\
Data File : BF123938.D
Acq On : 15 May 2021 11:33
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Sample : M2383-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KTW-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

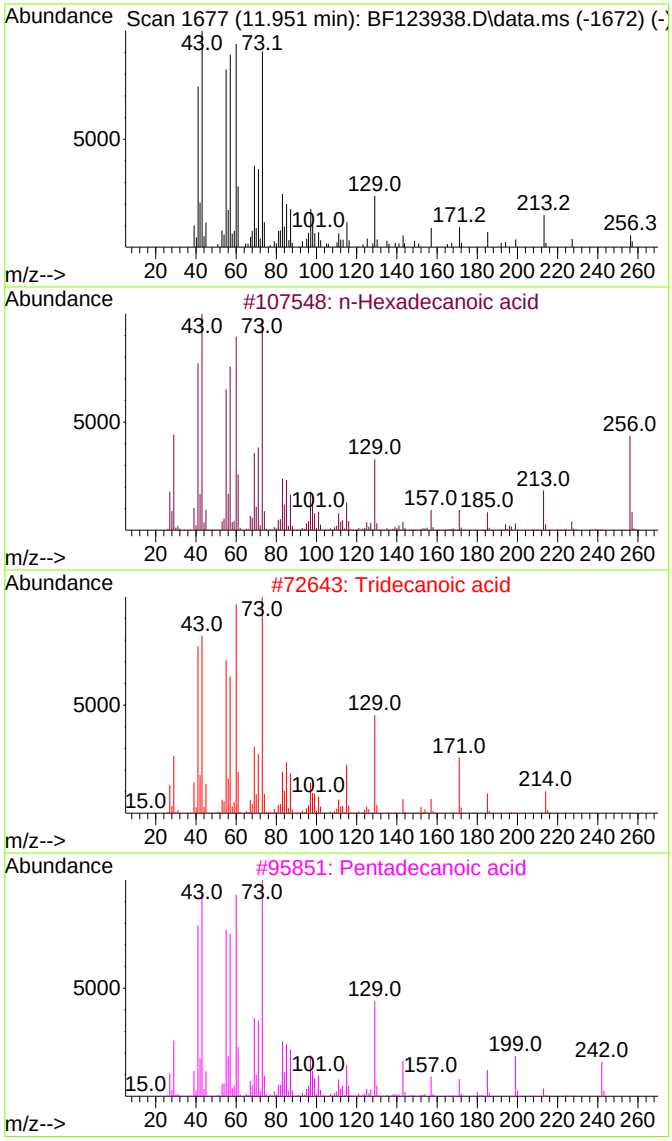
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

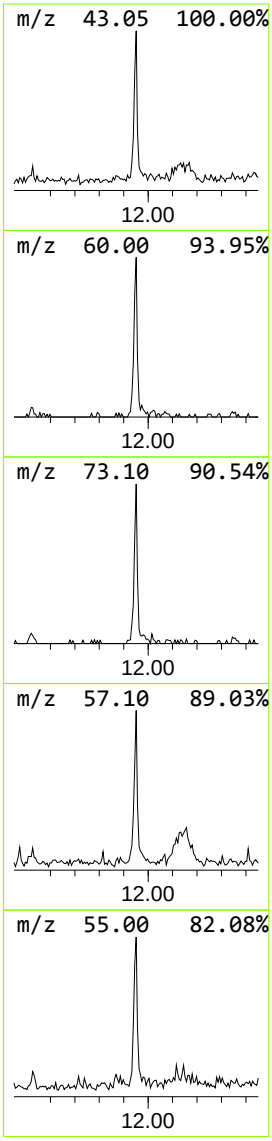
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	8.05 ng	200355	Phenanthrene-d10	11.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Undecanoic acid	186	C11H22O2	000112-37-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051521\
Data File : BF123938.D
Acq On : 15 May 2021 11:33
Operator : JU/CG
Sample : M2383-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KTW-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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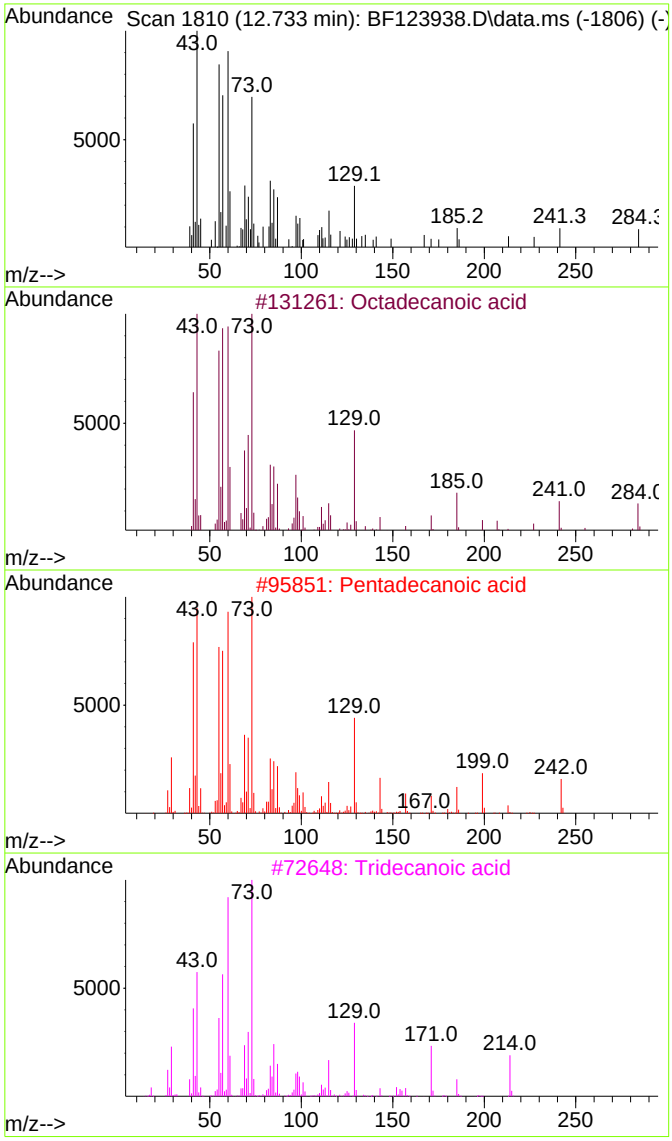
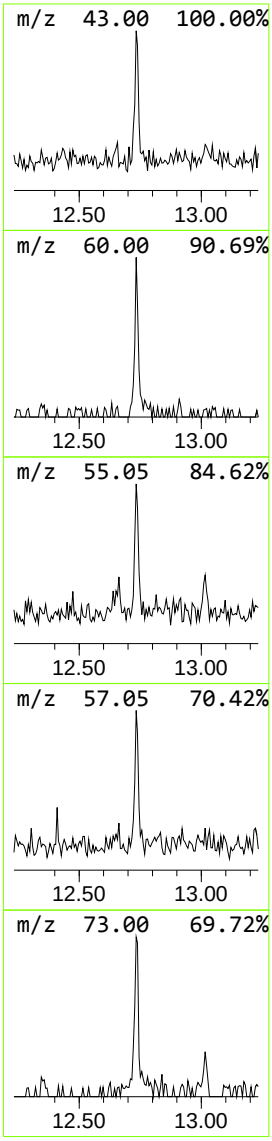
Peak Number 5 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.733	3.24 ng	80676	Phenanthrene-d10	11.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	91
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
3	Tridecanoic acid	214	C13H26O2	000638-53-9	53
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	53
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051521\
Data File : BF123938.D
Acq On : 15 May 2021 11:33
Operator : JU/CG
Sample : M2383-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KTW-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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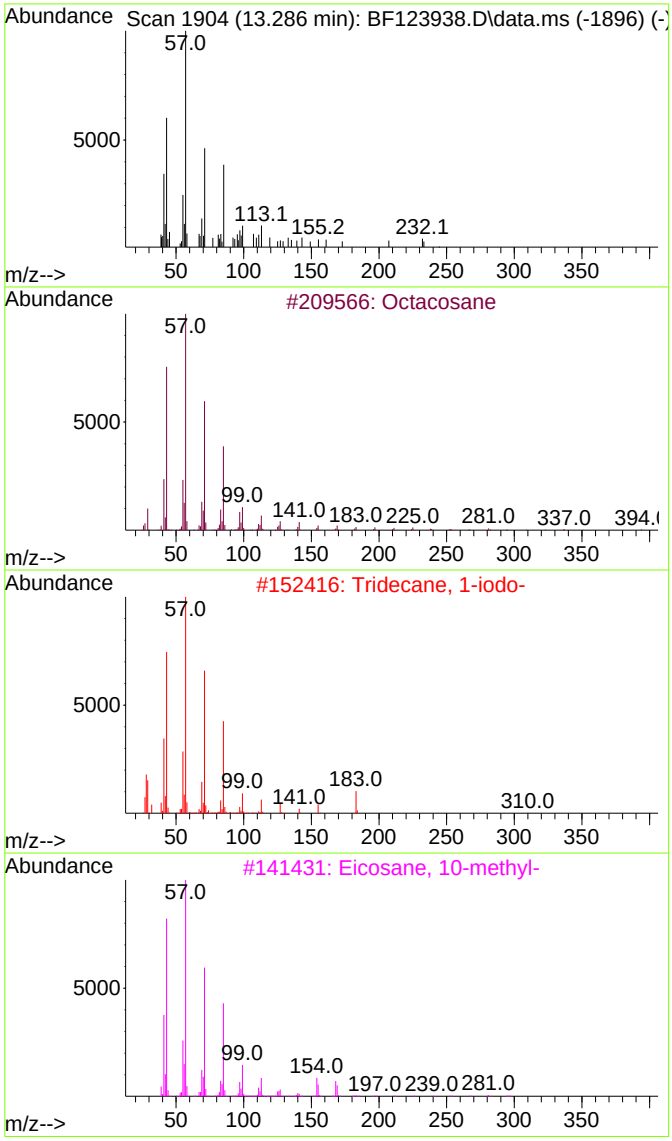
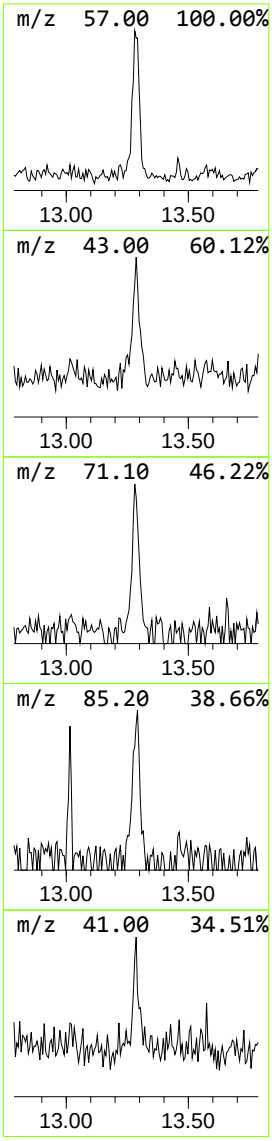
Peak Number 6 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.286	4.79 ng	107989	Chrysene-d12	14.062

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	72
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	72
3	Eicosane, 10-methyl-	296	C21H44	054833-23-7	64
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	64
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	64





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Data File : BF123938.D
Acq On : 15 May 2021 11:33
Operator : JU/CG
Sample : M2383-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KTW-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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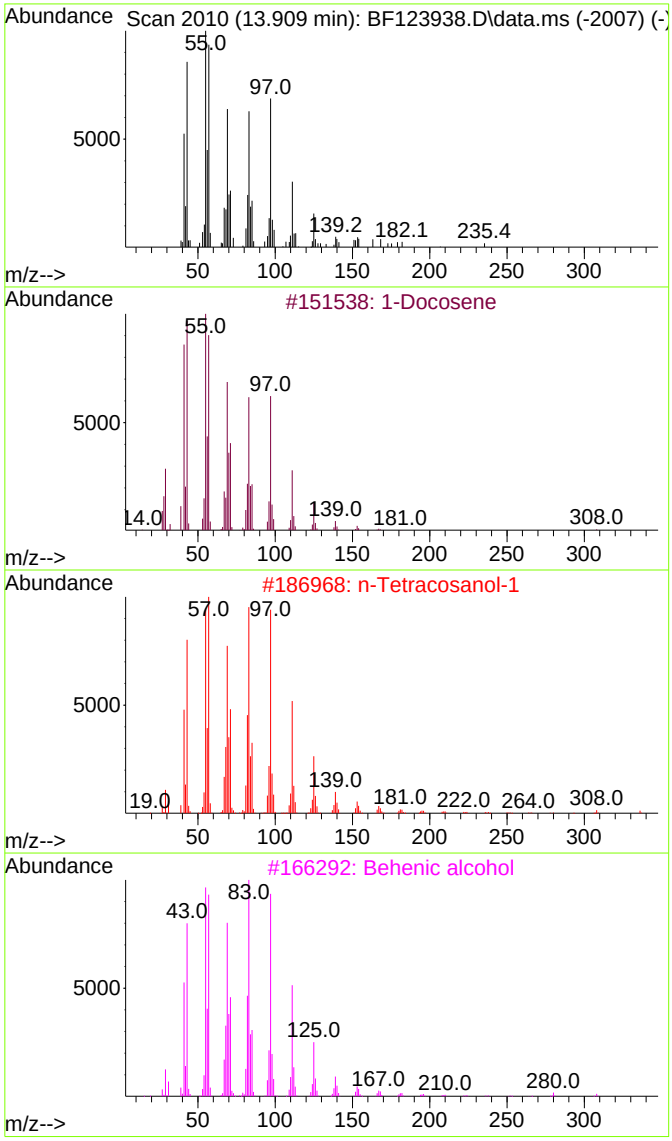
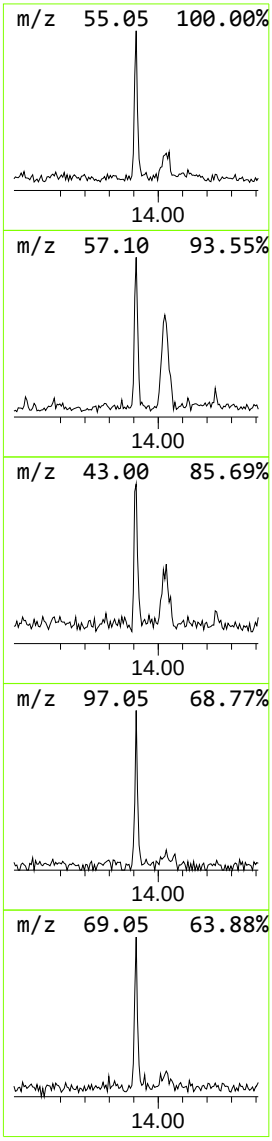
Peak Number 7 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	7.03 ng	158424	Chrysene-d12	14.062

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	91
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
3	Behenic alcohol	326	C22H46O	000661-19-8	87
4	Octacosanol	410	C28H58O	000557-61-9	87
5	1-Heptacosanol	396	C27H56O	002004-39-9	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051521\
Data File : BF123938.D
Acq On : 15 May 2021 11:33
Operator : JU/CG
Sample : M2383-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KTW-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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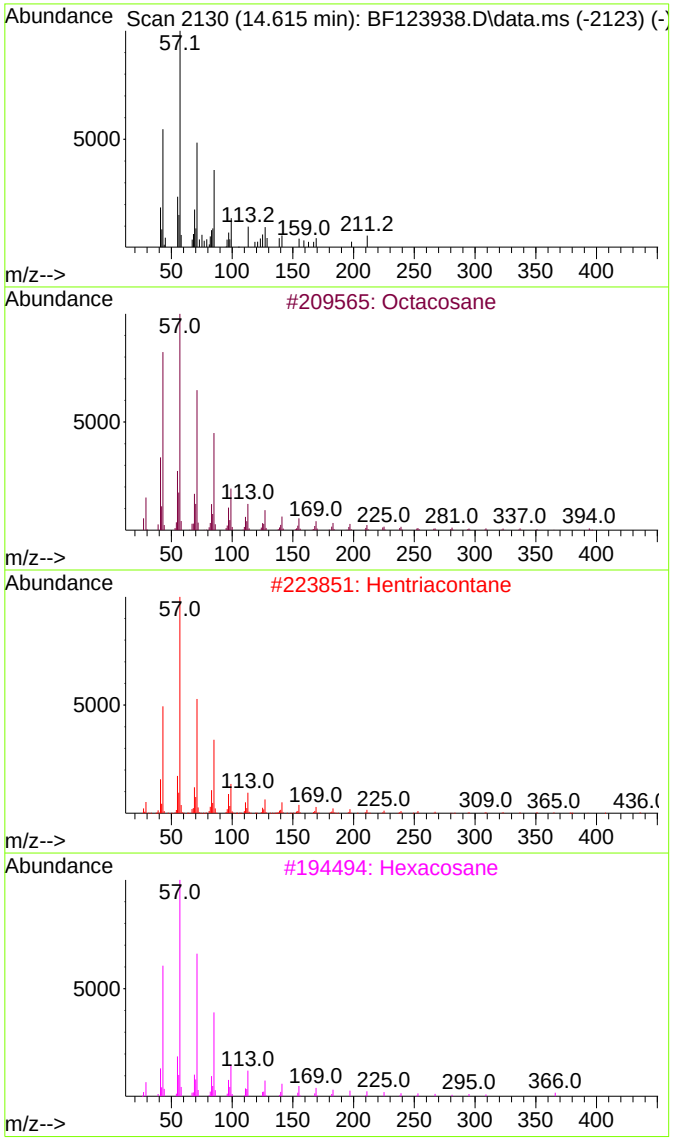
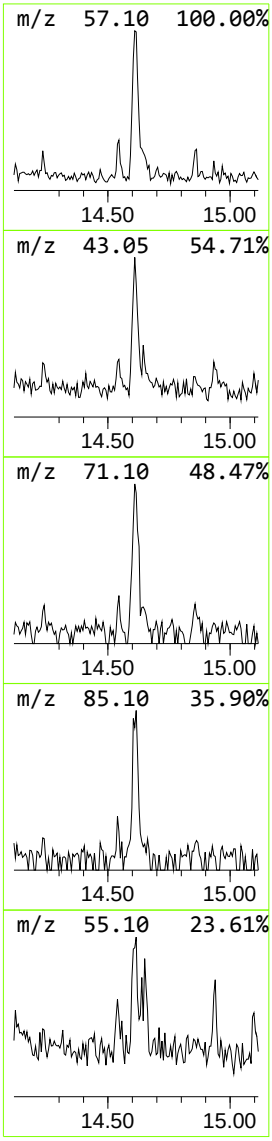
Peak Number 8 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.615	4.22 ng	95212	Chrysene-d12	14.062

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	87
2	Hentriacontane	437	C31H64	000630-04-6	86
3	Hexacosane	366	C26H54	000630-01-3	86
4	Sulfurous acid, butyl pentadecyl...	348	C19H40O3S	1000309-18-2	86
5	Tetratetracontane	619	C44H90	007098-22-8	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051521\
Data File : BF123938.D
Acq On : 15 May 2021 11:33
Operator : JU/CG
Sample : M2383-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KTW-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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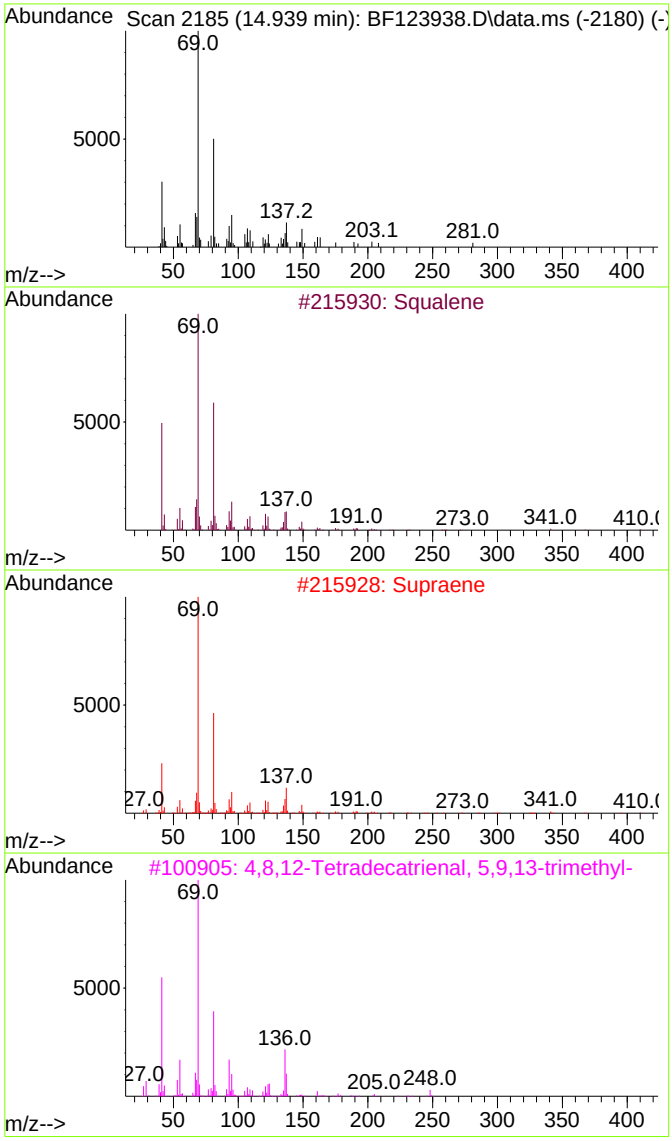
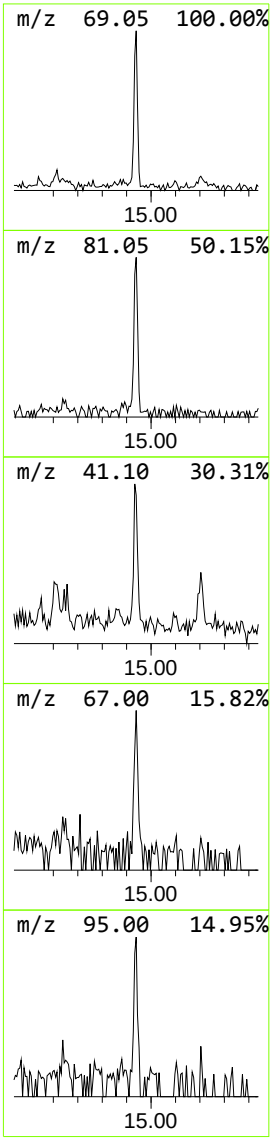
Peak Number 9 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.939	5.43 ng	92808	Perylene-d12	15.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	80
2	Supraene	410	C30H50	007683-64-9	72
3	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5	1,3-Dioxolan-2-one, 3-methyl-3-(...	264	C16H24O3	336879-76-6	59





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Data File : BF123938.D
Acq On : 15 May 2021 11:33
Operator : JU/CG
Sample : M2383-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KTW-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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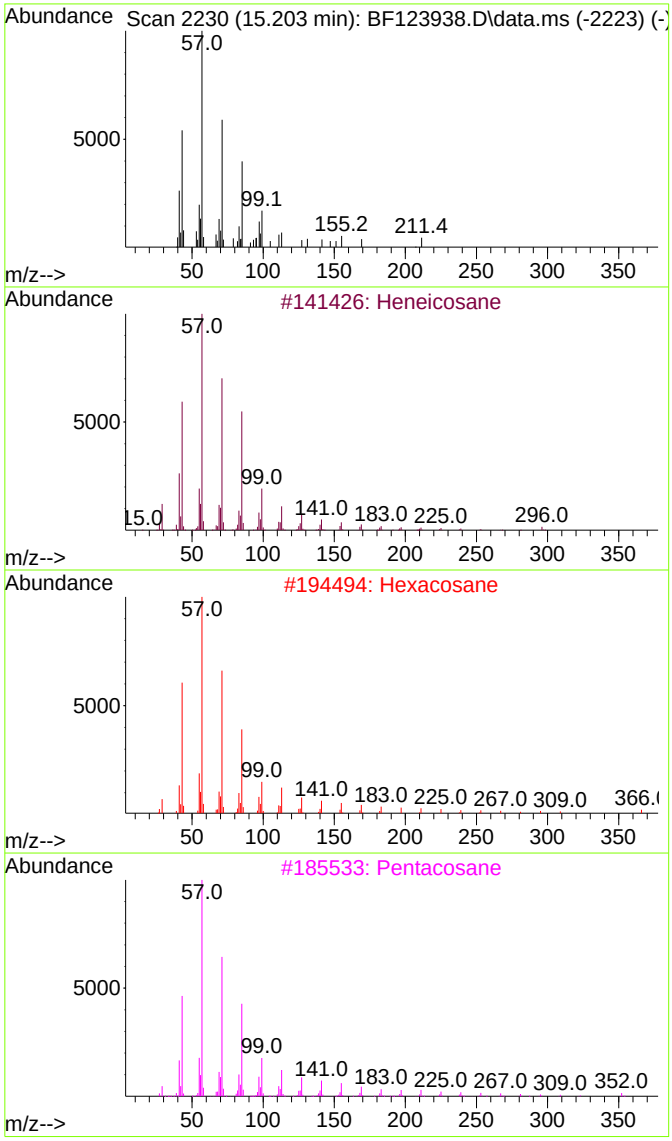
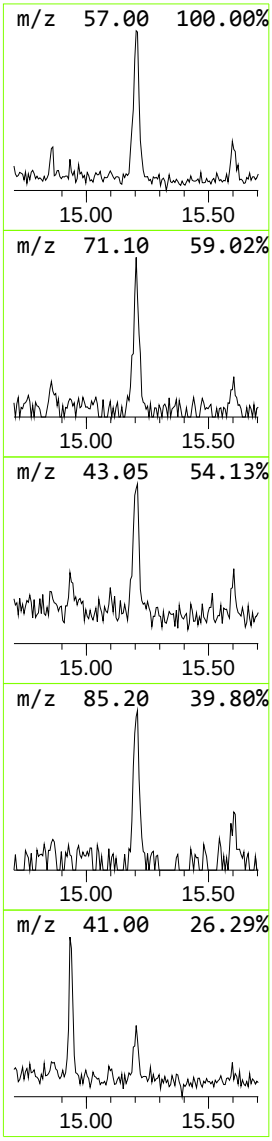
Peak Number 10 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.204	5.15 ng	88051	Perylene-d12	15.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	83
2	Hexacosane	366	C26H54	000630-01-3	72
3	Pentacosane	352	C25H52	000629-99-2	72
4	Octacosane	394	C28H58	000630-02-4	72
5	10-Methylnonadecane	282	C20H42	056862-62-5	64





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Acq On : 15 May 2021 11:33
Operator : JU/CG
Sample : M2383-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KTW-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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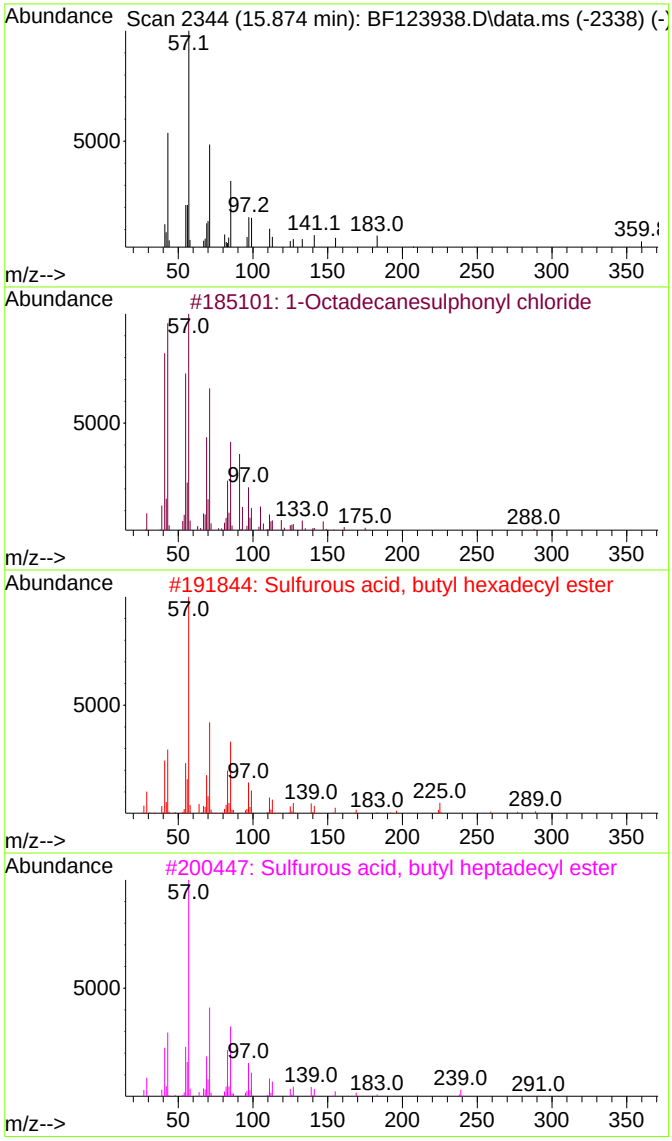
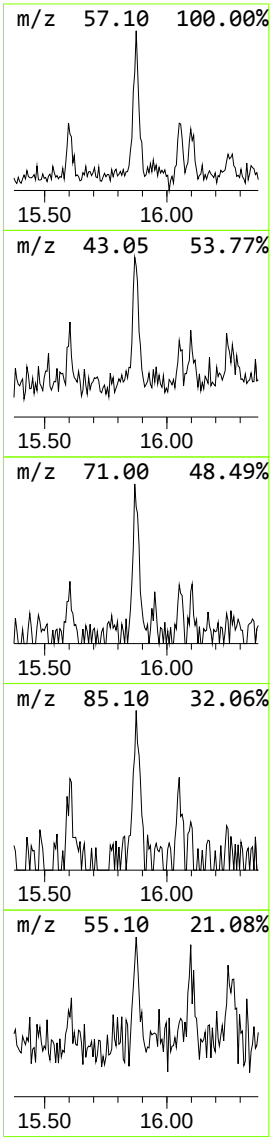
Peak Number 11 1-Octadecanesulphonyl chloride Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.874	3.25 ng	55558	Perylene-d12	15.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	86
2	Sulfurous acid, butyl hexadecyl ...	362	C20H42O3S	1000309-18-3	78
3	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	78
4	Undecane, 3,9-dimethyl-	184	C13H28	017301-31-4	64
5	Heptacosane	380	C27H56	000593-49-7	64





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Data File : BF123938.D
Acq On : 15 May 2021 11:33
Operator : JU/CG
Sample : M2383-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KTW-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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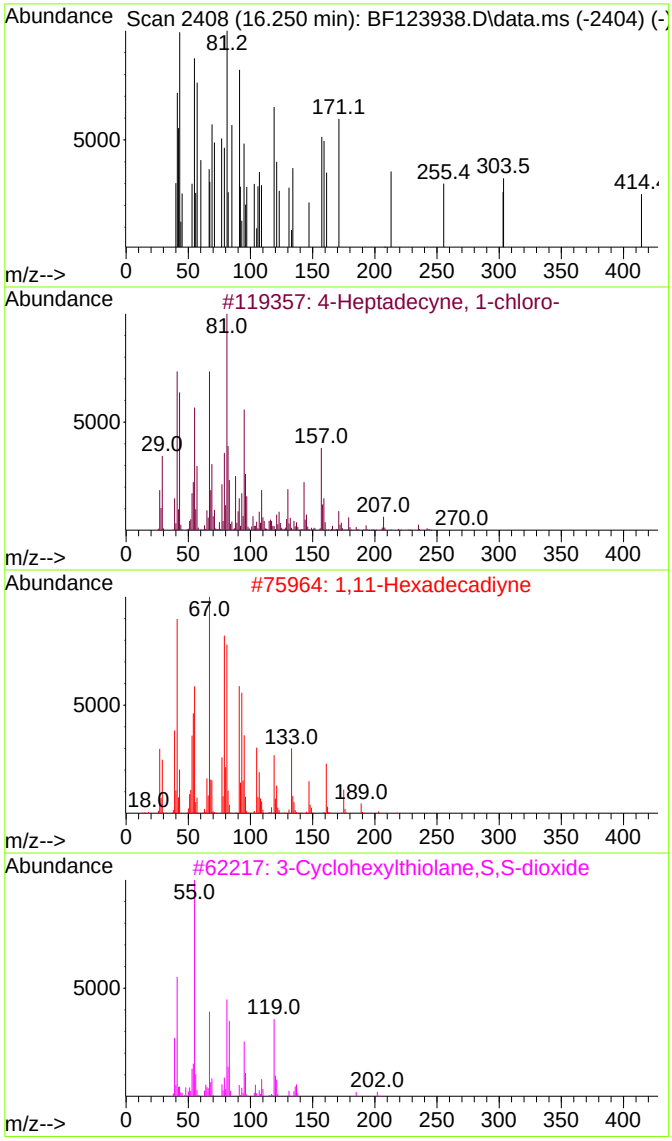
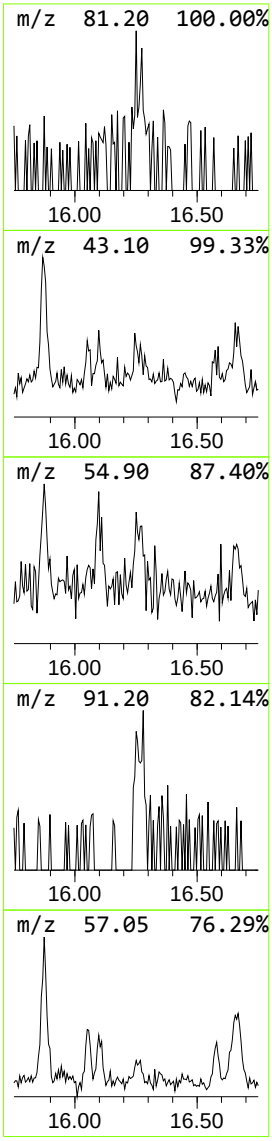
Peak Number 12 unknown16.250 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.250	3.44 ng	58842	Perylene-d12	15.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptadecyne, 1-chloro-	270	C17H31Cl	056554-73-5	22
2	1,11-Hexadecadiyne	218	C16H26	071673-32-0	12
3	3-Cyclohexylthiolane,S,S-dioxide	202	C10H18O2S	071053-08-2	12
4	Undec-10-ynoic acid	182	C11H18O2	002777-65-3	12
5	1-Nonyne	124	C9H16	003452-09-3	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051521\
Data File : BF123938.D
Acq On : 15 May 2021 11:33
Operator : JU/CG
Sample : M2383-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KTW-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.181	139.0	ng	1987470	1	6.898	285945	20.0
unknown6.957	6.957	3.0	ng	42200	1	6.898	285945	20.0
unknown10.945	10.945	2.1	ng	52709	4	11.427	497548	20.0
n-Hexadecanoic ...	11.951	8.1	ng	200355	4	11.427	497548	20.0
Octadecanoic acid	12.733	3.2	ng	80676	4	11.427	497548	20.0
Octacosane	13.286	4.8	ng	107989	5	14.062	450747	20.0
1-Docosene	13.910	7.0	ng	158424	5	14.062	450747	20.0
Hentriacontane	14.615	4.2	ng	95212	5	14.062	450747	20.0
Squalene	14.939	5.4	ng	92808	6	15.556	341999	20.0
Heneicosane	15.204	5.2	ng	88051	6	15.556	341999	20.0
1-Octadecanesul...	15.874	3.3	ng	55558	6	15.556	341999	20.0
unknown16.250	16.250	3.4	ng	58842	6	15.556	341999	20.0