LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081717\
Data File : BF097807.D
Acq On : 18 Aug 2017 1:09
Operator : SJ/JU
Sample : I4761-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RUSB-06

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:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.969	486	490	501	rVB	236331	309569	10.33%	1.139%
2	5.381	555	560	564	rBV	2638135	2792152	93.21%	10.274%
3	6.404	729	734	740	rBV	2686552	2995667	100.00%	11.022%
4	6.545	753	758	761	rBV	2890162	2745809	91.66%	10.103%
5	6.775	793	797	800	rBV	1153844	901125	30.08%	3.316%
6	6.934	820	824	827	rBV	2346017	2072839	69.19%	7.627%
7	7.340	888	893	896	rBV	1803637	1671798	55.81%	6.151%
8	8.057	1011	1015	1019	rBV	1320044	1086737	36.28%	3.999%
9	9.134	1194	1198	1202	rBV	2770941	2609671	87.11%	9.602%
10	9.528	1262	1265	1270	rVB	332647	253569	8.46%	0.933%
11	9.810	1309	1313	1317	rVB2	1089142	957879	31.98%	3.524%
12	10.251	1386	1388	1391	rVB	47545	35426	1.18%	0.130%
13	10.598	1442	1447	1450	rBV	1371896	1250695	41.75%	4.602%
14	10.722	1465	1468	1477	rVB	58332	60131	2.01%	0.221%
15	11.292	1561	1565	1568	rBV	1000278	862307	28.79%	3.173%
16	11.316	1568	1569	1572	rVB	58320	33840	1.13%	0.125%
17	12.504	1767	1771	1775	rBV	143292	116639	3.89%	0.429%
18	12.710	1803	1806	1807	rBV	54865	46337	1.55%	0.170%
19	12.727	1807	1809	1813	rVB	121053	115281	3.85%	0.424%
20	12.822	1822	1825	1828	rVB	55030	40440	1.35%	0.149%
21	12.880	1831	1835	1839	rVB	2338749	2115965	70.63%	7.786%
22	13.780	1983	1988	1996	rBV4	255505	304884	10.18%	1.122%
23	13.927	2008	2013	2016	rBV	1079142	1042260	34.79%	3.835%
24	13.951	2016	2017	2025	rVB	91653	69621	2.32%	0.256%
25	14.039	2025	2032	2035	rBV5	24801	37354	1.25%	0.137%
26	14.110	2040	2044	2048	rBV2	49219	58551	1.95%	0.215%
27	14.416	2092	2096	2102	rBV	215393	276862	9.24%	1.019%
28	14.716	2144	2147	2155	rVB2	37194	64703	2.16%	0.238%
29	14.851	2166	2170	2174	rBV	205414	211323	7.05%	0.778%
30	14.945	2182	2186	2189	rBV	69395	102205	3.41%	0.376%
31	15.045	2198	2203	2204	rBV	107512	139501	4.66%	0.513%
32	15.063	2204	2206	2213	rVB	215362	261409	8.73%	0.962%
33	15.233	2233	2235	2240	rVB	40258	43730	1.46%	0.161%
34	15.292	2242	2245	2249	rVV	52698	56572	1.89%	0.208%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081717\
Data File : BF097807.D
Acq On : 18 Aug 2017 1:09
Operator : SJ/JU
Sample : I4761-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RUSB-06

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:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.357	2251	2256	2262	rVV	565485	690249	23.04%	2.540%
36	15.410	2262	2265	2268	rVB	41614	50065	1.67%	0.184%
37	15.604	2294	2298	2304	rVB	89112	129452	4.32%	0.476%
38	15.833	2332	2337	2341	rBV	98346	155012	5.17%	0.570%
39	15.880	2341	2345	2351	rVV3	66474	121094	4.04%	0.446%
40	15.945	2353	2356	2365	rVB6	31985	60516	2.02%	0.223%
41	16.592	2461	2466	2473	rBV2	108660	193615	6.46%	0.712%
42	17.327	2589	2591	2596	rVB5	23252	35298	1.18%	0.130%

Sum of corrected areas: 27178152

LSC Report - Integrated Chromatogram

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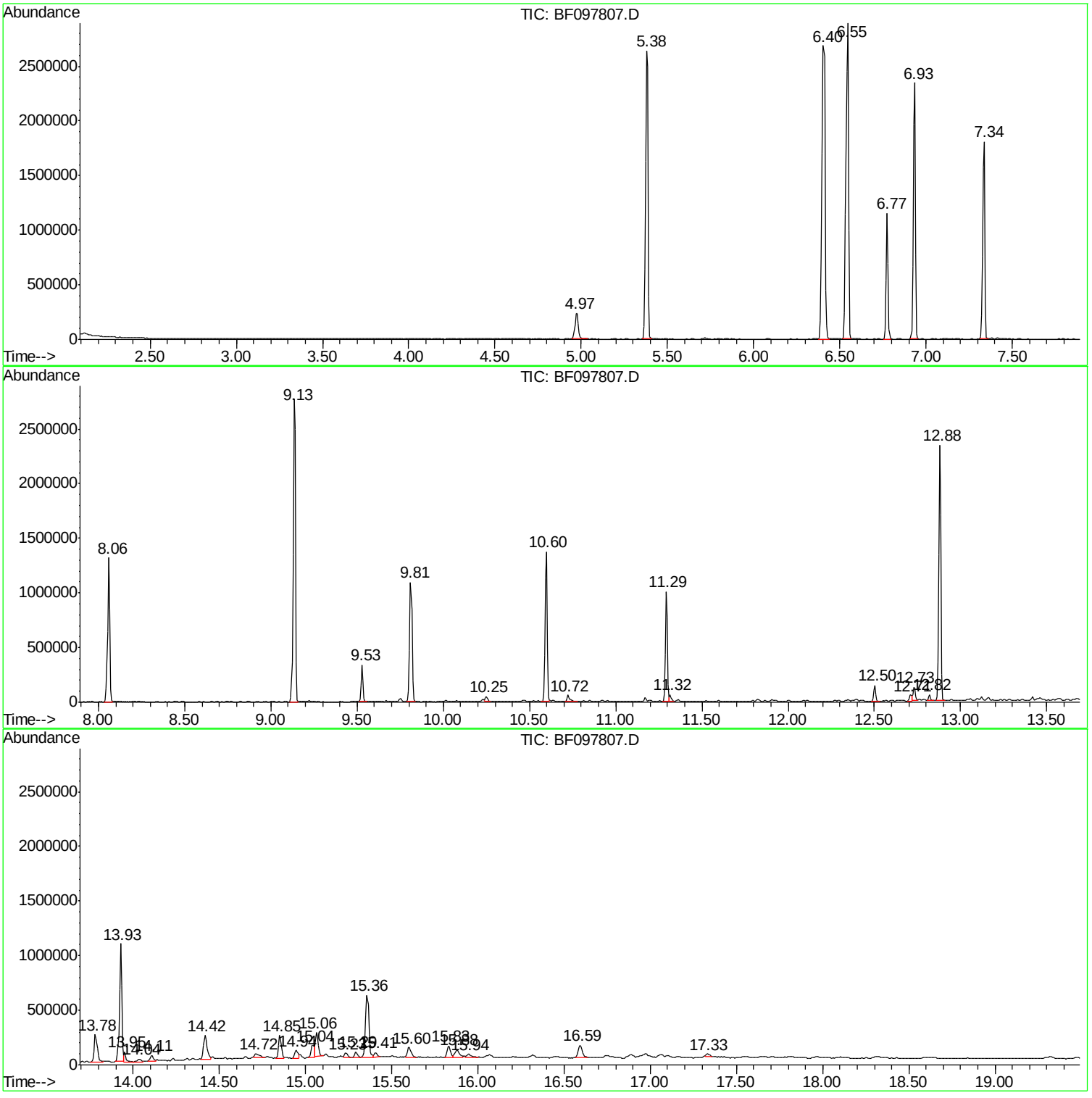
Operator : SJ/JU
Sample : I4761-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RUSB-06

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081717\
Data File : BF097807.D
Acq On : 18 Aug 2017 1:09
Operator : SJ/JU
Sample : I4761-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RUSB-06

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

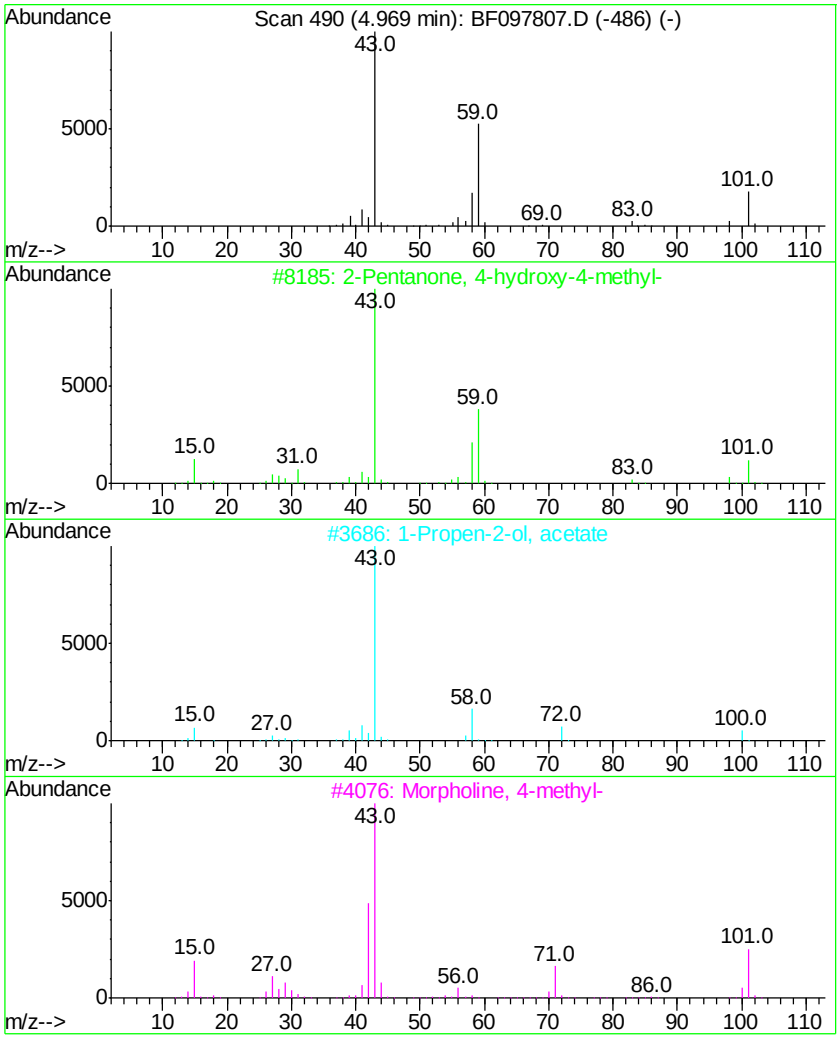
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

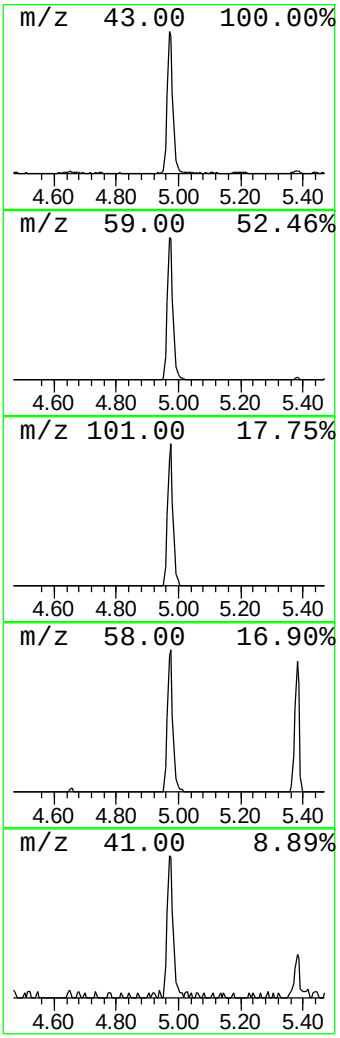
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	6.87 ng	309569	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Acetone	58	C3H6O	000067-64-1	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

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Acq On : 18 Aug 2017 1:09
Operator : SJ/JU
Sample : I4761-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RUSB-06

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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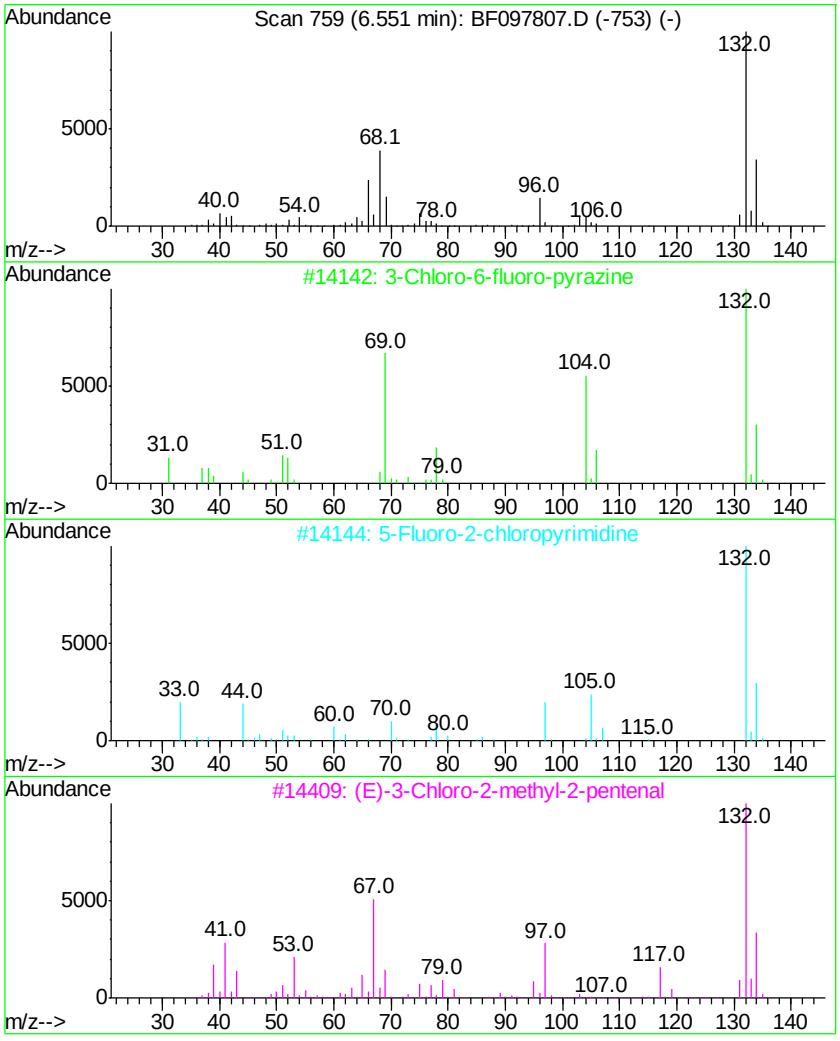
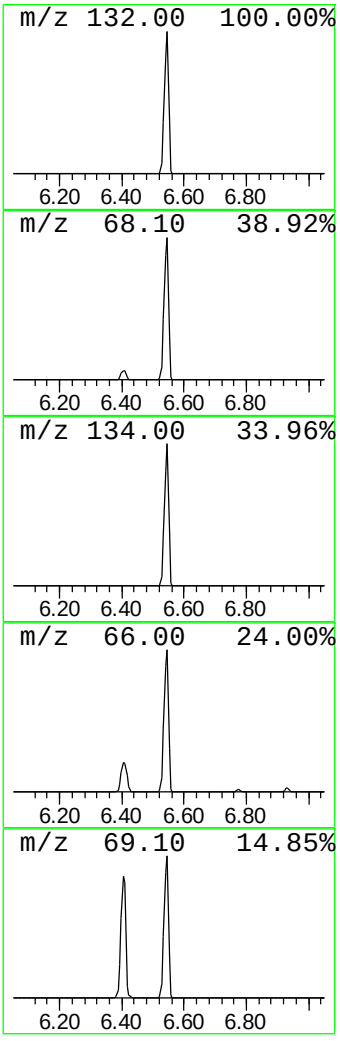
Peak Number 2 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	60.94 ng	2745810	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081717\
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Acq On : 18 Aug 2017 1:09
Operator : SJ/JU
Sample : I4761-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RUSB-06

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

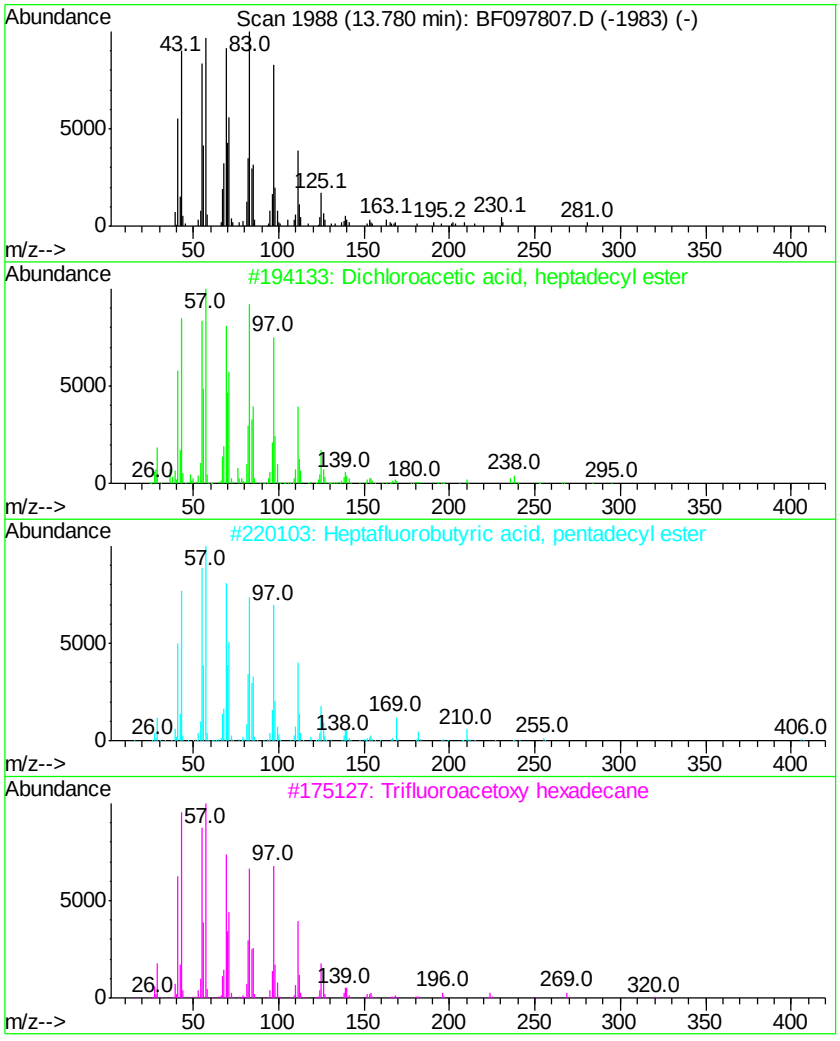
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

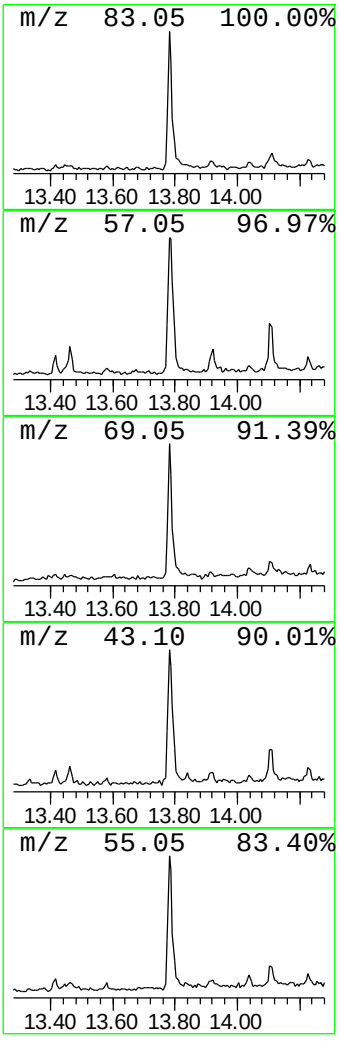
****

Peak Number 5 Dichloroacetic acid, heptad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.78	5.85 ng	304884	Chrysene-d12	13.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF081717\
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Operator : SJ/JU
Sample : I4761-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RUSB-06

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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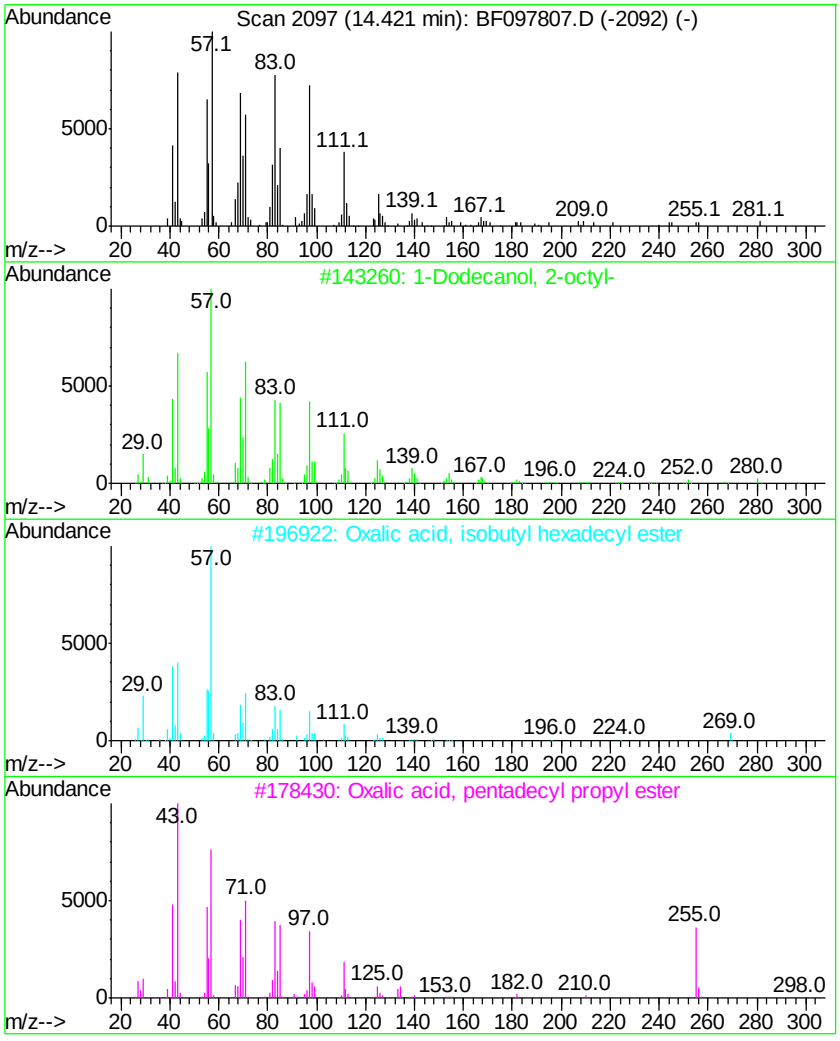
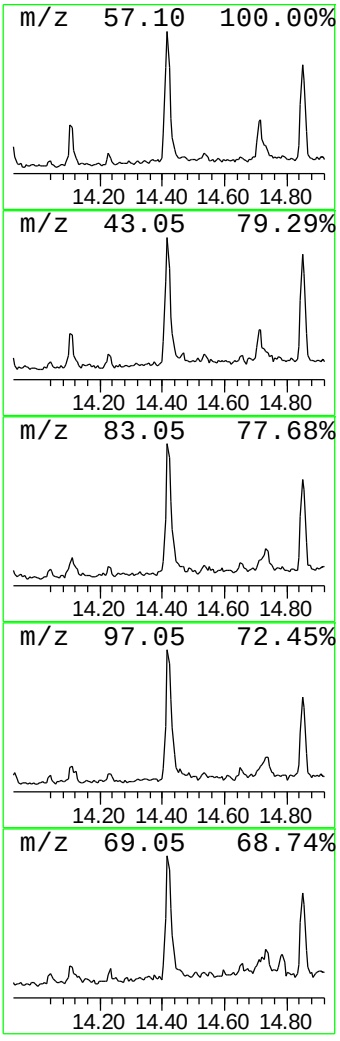
Peak Number 6 1-Dodecanol, 2-octyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.42	5.31 ng	276862	Chrysene-d12	13.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
2	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
3	Oxalic acid, pentadecyl propyl e...	342	C20H38O4	1000309-26-8	91
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	90
5	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF081717\
Data File : BF097807.D
Acq On : 18 Aug 2017 1:09
Operator : SJ/JU
Sample : I4761-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RUSB-06

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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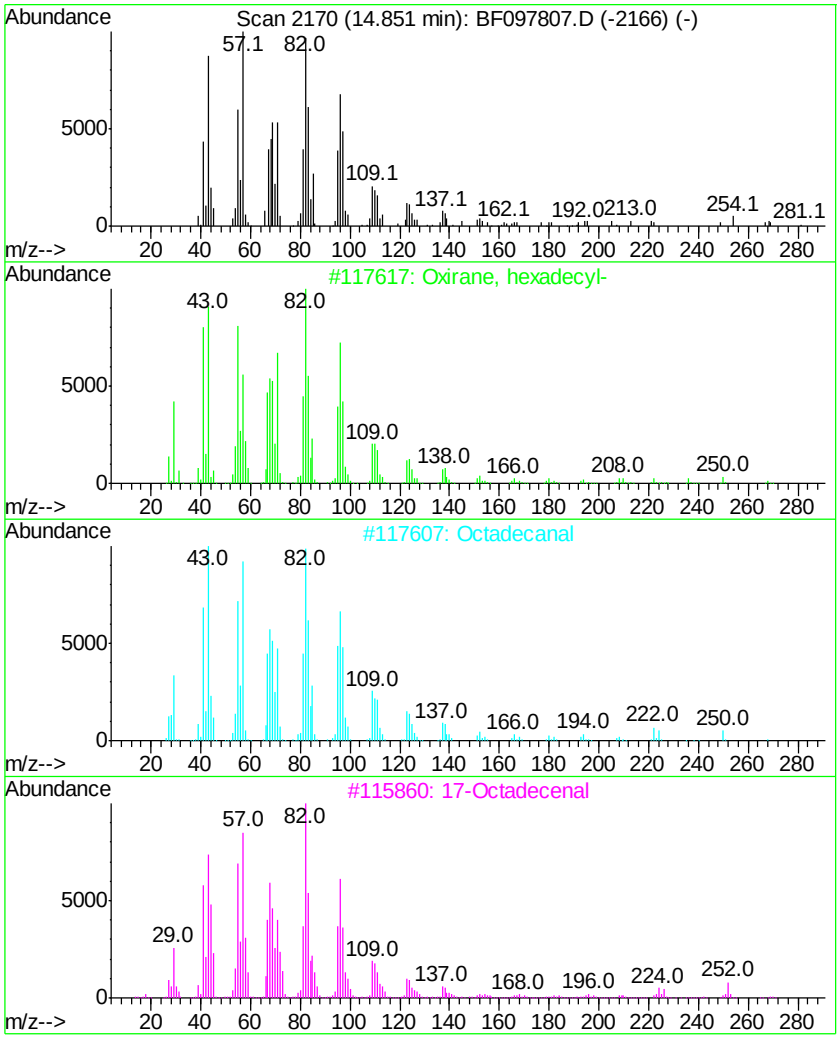
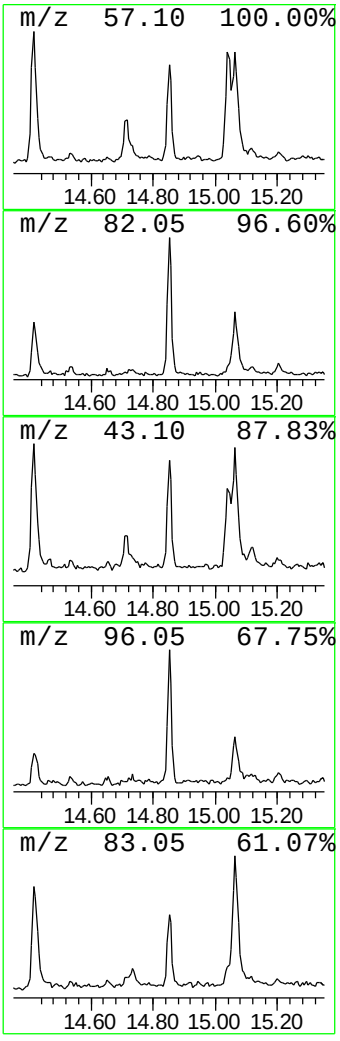
Peak Number 7 Oxirane, hexadecyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.85	6.12 ng	211323	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	94
2	Octadecanal	268	C18H36O	000638-66-4	94
3	17-Octadecenal	266	C18H34O	056554-86-0	90
4	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	90
5	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	87





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Sample : I4761-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RUSB-06

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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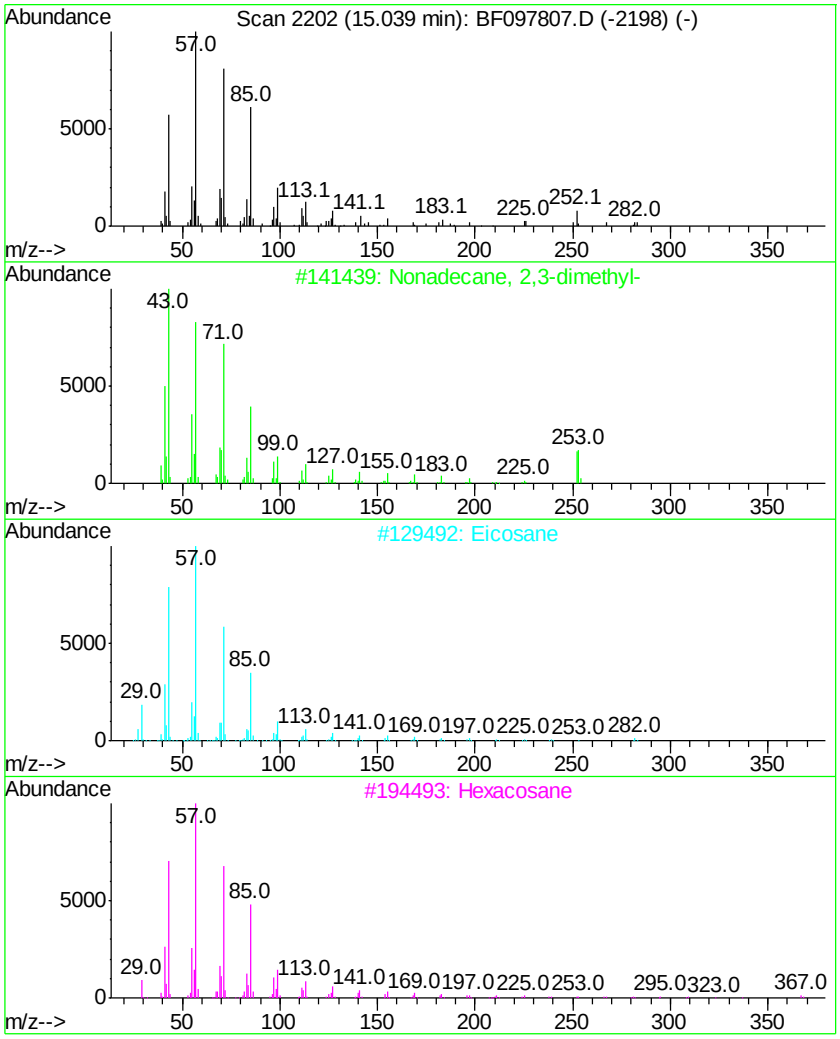
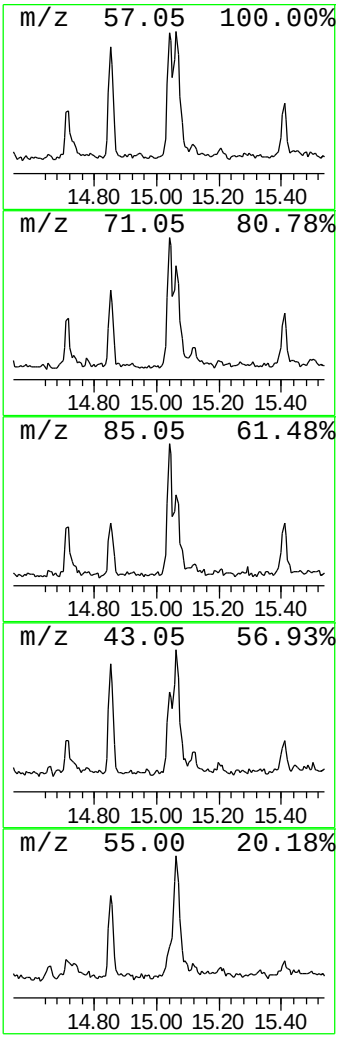
Peak Number 8 Nonadecane, 2,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.04	4.04 ng	139501	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 2,3-dimethyl-	296	C21H44	075163-99-4	90
2	Eicosane	282	C20H42	000112-95-8	87
3	Hexacosane	366	C26H54	000630-01-3	87
4	Octacosane	394	C28H58	000630-02-4	87
5	Heneicosane	296	C21H44	000629-94-7	83





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : RUSB-06

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

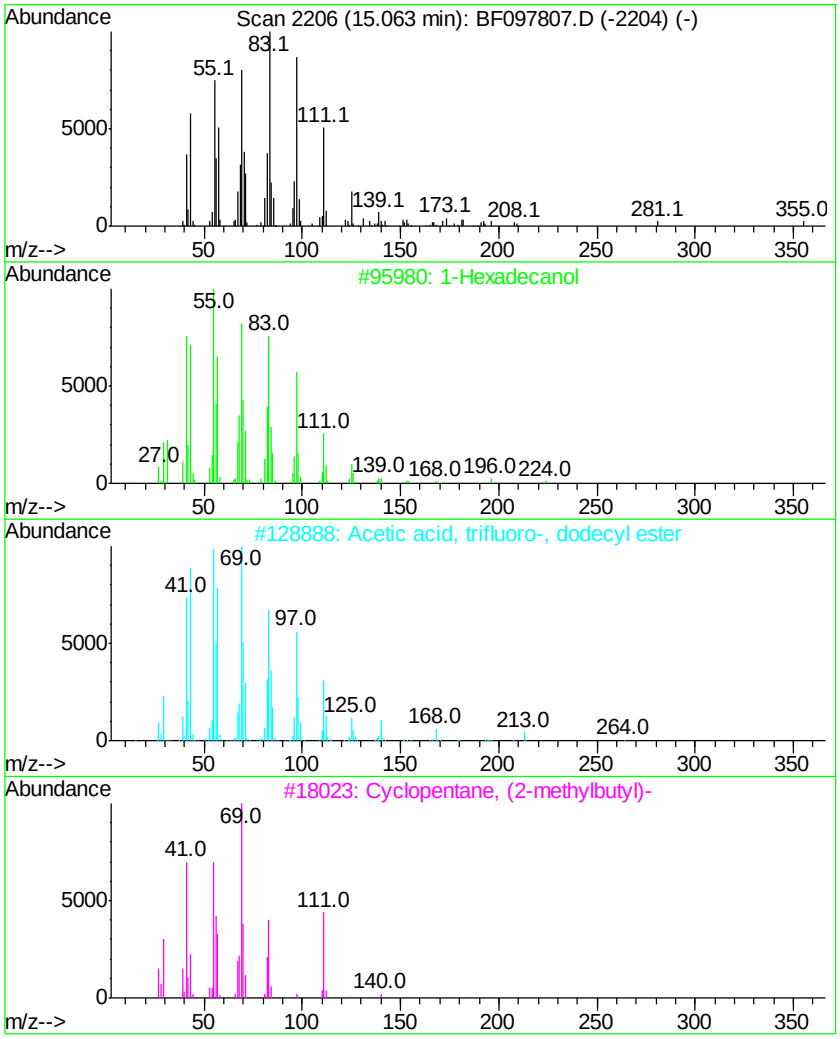
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

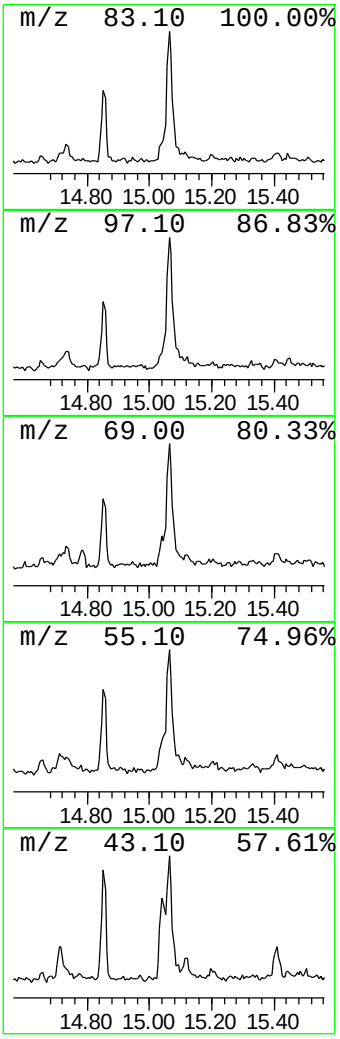
****

Peak Number 9 1-Hexadecanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	7.57 ng	261409	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	58
2	Acetic acid, trifluoro-, dodecyl...	282	C14H25F3O2	006222-00-0	49
3	Cyclopentane, (2-methylbutyl)-	140	C10H20	053366-38-4	46
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	43
5	1-Octadecanol	270	C18H38O	000112-92-5	43





Data Path : Z:\HPCHEM1\BNA F\DATA\BF081717\
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Sample : I4761-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RUSB-06

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

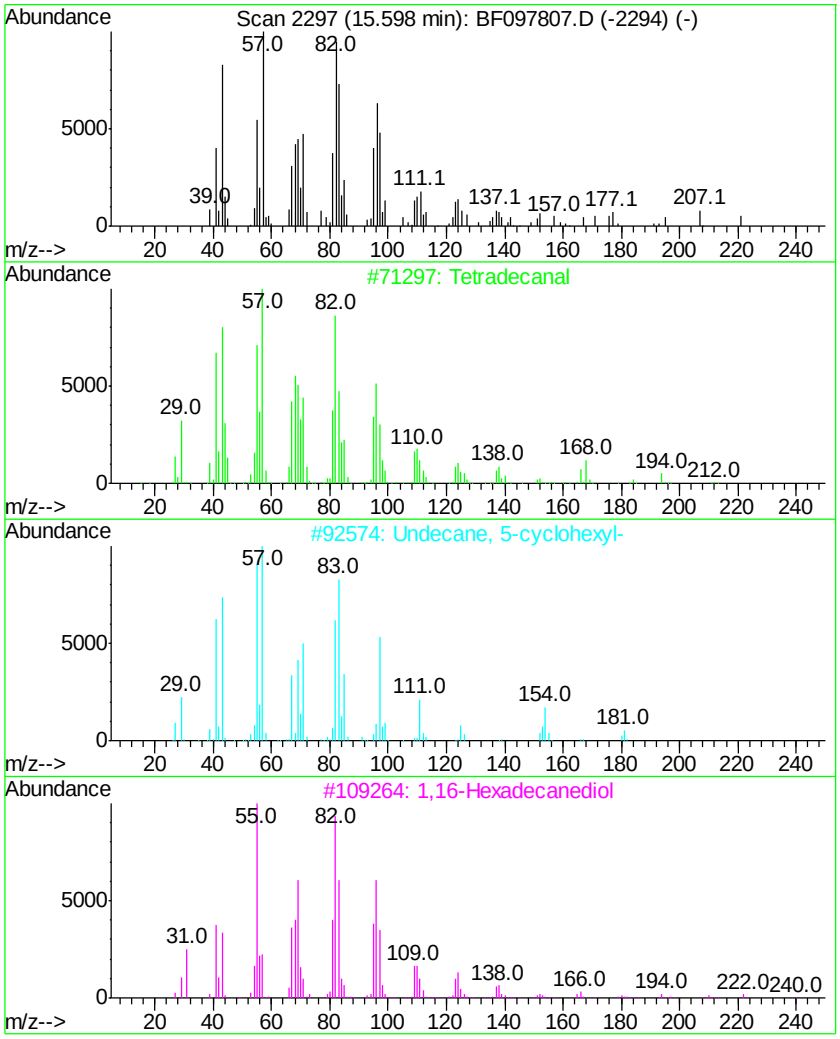
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

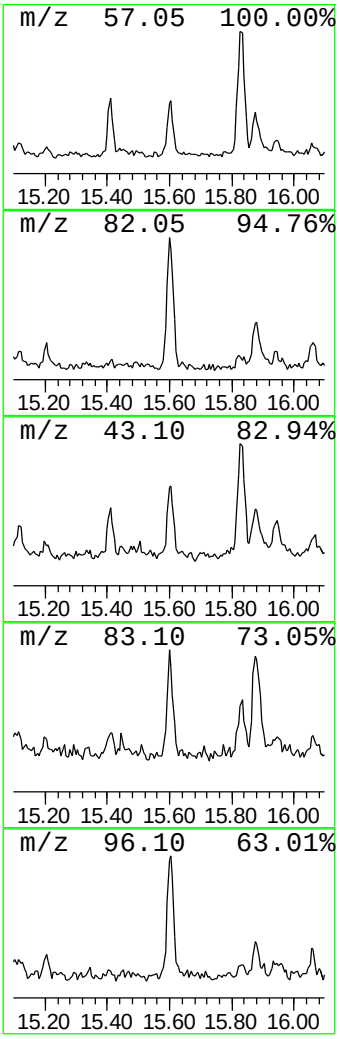
****

Peak Number 10 Tetradecanal Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.60	3.75 ng	129452	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanal	212	C14H28O	000124-25-4	58
2	Undecane, 5-cyclohexyl-	238	C17H34	013151-80-9	49
3	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	43
4	Dodecane, 5-cyclohexyl-	252	C18H36	013151-85-4	43
5	8-Azabicyclo[3.2.1]octan-3-ol, 8...	141	C8H15NO	000120-29-6	38





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Data File : BF097807.D
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Sample : I4761-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RUSB-06

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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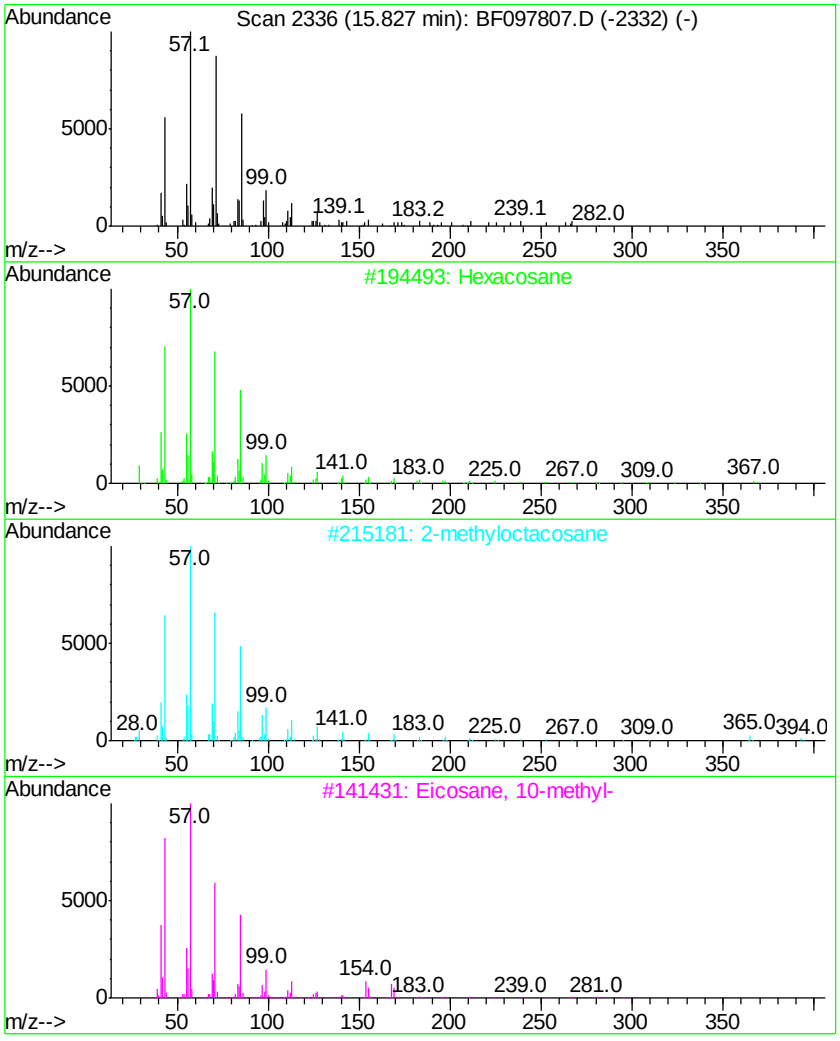
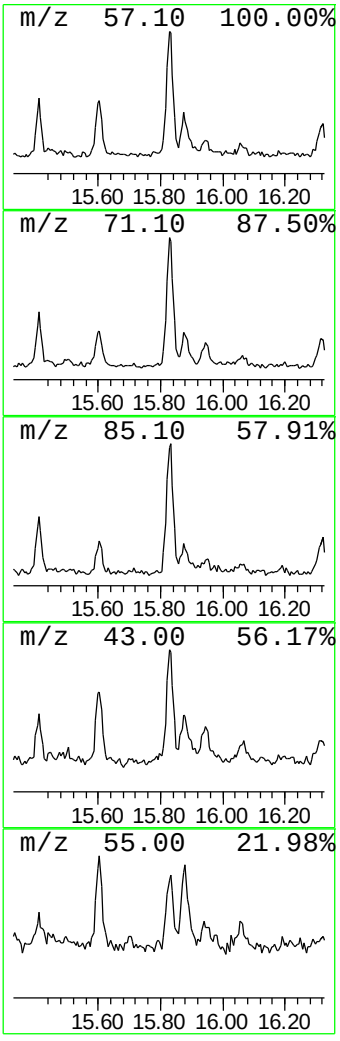
Peak Number 11 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.83	4.49 ng	155012	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	2-methyloctacosane	408	C29H60	1000376-72-8	90
3	Eicosane, 10-methyl-	296	C21H44	054833-23-7	87
4	Tetracosane	338	C24H50	000646-31-1	86
5	Heptadecane	240	C17H36	000629-78-7	86





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081717\
Data File : BF097807.D
Acq On : 18 Aug 2017 1:09
Operator : SJ/JU
Sample : I4761-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RUSB-06

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

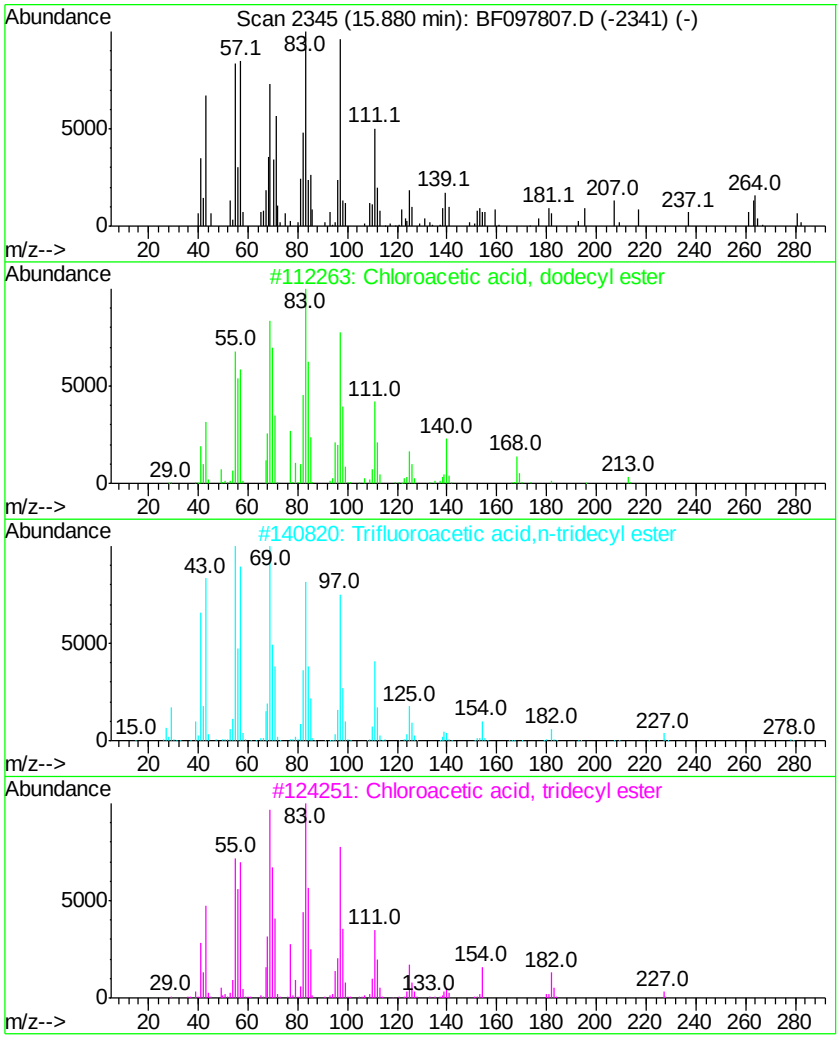
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

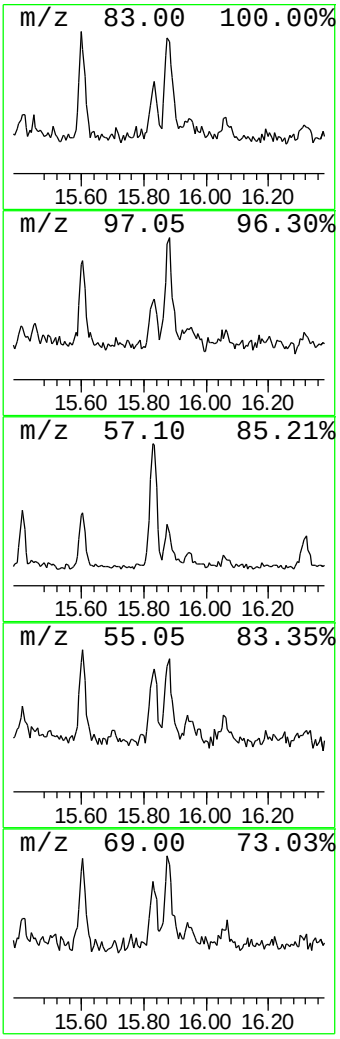
****

Peak Number 12 Chloroacetic acid, dodecyl ... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.88	3.51 ng	121094	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Chloroacetic acid, dodecyl ester	262	C14H27ClO2	006316-04-7	80
2	Trifluoroacetic acid,n-tridecyl ...	296	C15H27F3O2	053800-02-5	80
3	Chloroacetic acid, tridecyl ester	276	C15H29ClO2	018277-85-5	80
4	Octacosanol	410	C28H58O	000557-61-9	80
5	1-Heptacosanol	396	C27H56O	002004-39-9	70





Data Path : Z:\HPCHEM1\BNA F\DATA\BF081717\
Data File : BF097807.D
Acq On : 18 Aug 2017 1:09
Operator : SJ/JU
Sample : I4761-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RUSB-06

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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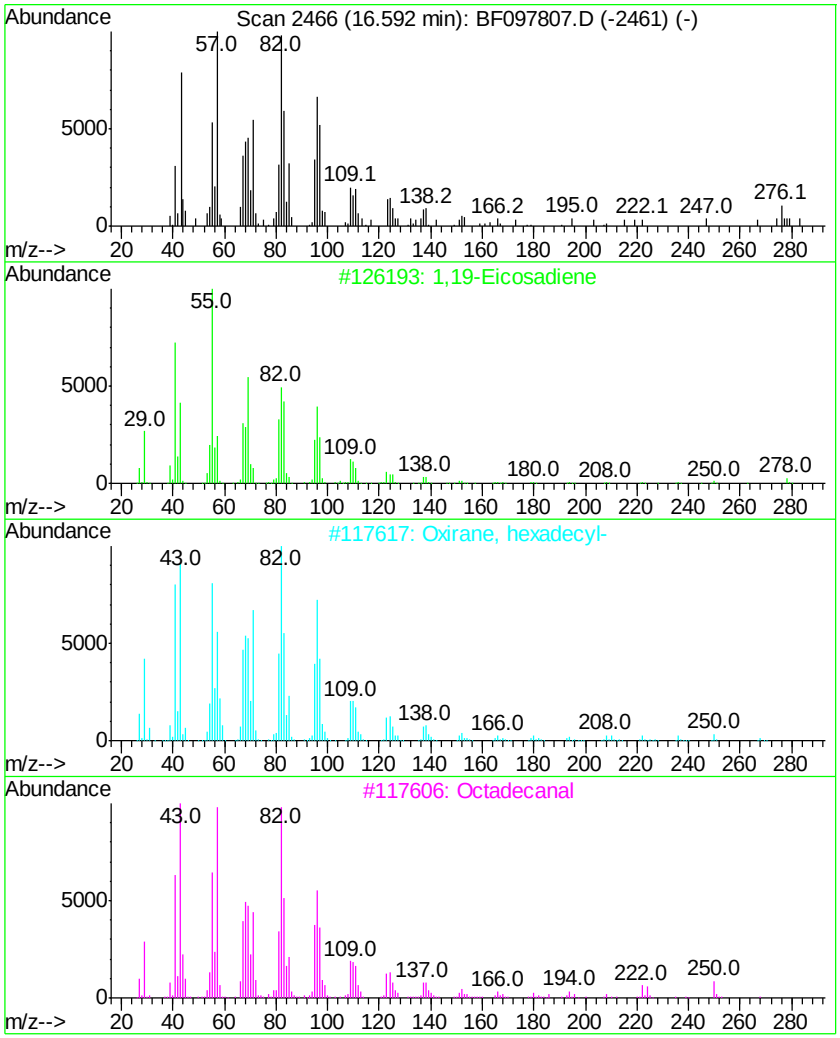
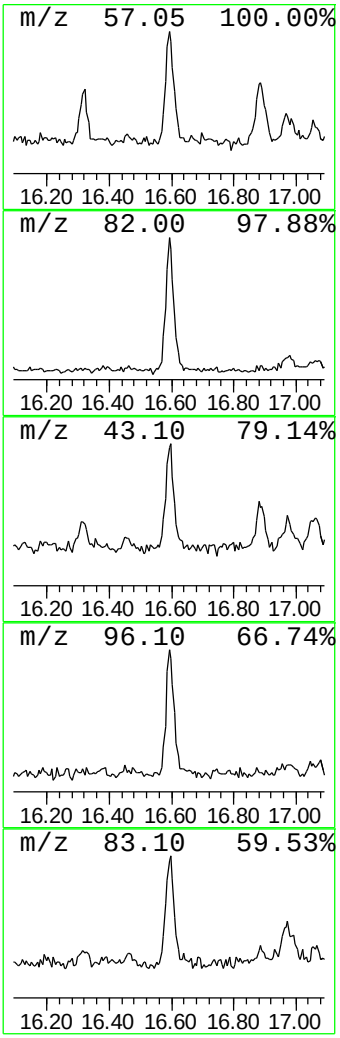
Peak Number 13 1,19-Eicosadiene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.59	5.61 ng	193615	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	92
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
3	Octadecanal	268	C18H36O	000638-66-4	83
4	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	68
5	Hexadecanal	240	C16H32O	000629-80-1	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081717\
Data File : BF097807.D
Acq On : 18 Aug 2017 1:09
Operator : SJ/JU
Sample : I4761-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RUSB-06

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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
2-Pentanone, 4-hy...	4.97	6.9	ng	309569	1	6.77	901125	20.0
unknown6.55	6.55	60.9	ng	2745810	1	6.77	901125	20.0
Dichloroacetic ac...	13.78	5.8	ng	304884	5	13.93	1042260	20.0
1-Dodecanol, 2-oc...	14.42	5.3	ng	276862	5	13.93	1042260	20.0
Oxirane, hexadecyl-	14.85	6.1	ng	211323	6	15.36	690249	20.0
Nonadecane, 2,3-d...	15.04	4.0	ng	139501	6	15.36	690249	20.0
1-Hexadecanol	15.06	7.6	ng	261409	6	15.36	690249	20.0
Tetradecanal	15.60	3.8	ng	129452	6	15.36	690249	20.0
Hexacosane	15.83	4.5	ng	155012	6	15.36	690249	20.0
Chloroacetic acid...	15.88	3.5	ng	121094	6	15.36	690249	20.0
1,19-Eicosadiene	16.59	5.6	ng	193615	6	15.36	690249	20.0