LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
Data File : BF113052.D
Acq On : 14 Mar 2019 16:23
Operator : JU/SJ
Sample : K1866-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-01-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-BF022719.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	5.345	549	554	557	rBV	3964015	3843080	79.06%	8.201%
2	6.375	723	729	745	rVB	3560695	4357215	89.64%	9.298%
3	6.498	745	750	753	rBV	4221318	4139974	85.17%	8.835%
4	6.728	785	789	792	rBV	1292149	1163975	23.94%	2.484%
5	6.881	811	815	819	rBV	3345982	3190479	65.63%	6.809%
6	7.286	878	884	887	rBV	2667063	2590113	53.28%	5.527%
7	8.010	1002	1007	1012	rBV	1411857	1440161	29.63%	3.073%
8	9.086	1184	1190	1200	rBV	4438059	4515736	92.90%	9.637%
9	9.475	1252	1256	1266	rVB	397697	353967	7.28%	0.755%
10	9.757	1299	1304	1318	rVB2	1819105	1613892	33.20%	3.444%
11	10.545	1432	1438	1441	rBV	3350768	3217151	66.18%	6.865%
12	11.233	1551	1555	1563	rBV	1800641	1780160	36.62%	3.799%
13	11.774	1643	1647	1657	rBV	1126762	1302071	26.79%	2.779%
14	12.439	1757	1760	1764	rBV	132763	142348	2.93%	0.304%
15	12.474	1764	1766	1775	rVB5	42338	67347	1.39%	0.144%
16	12.557	1776	1780	1791	rVV	471204	569311	11.71%	1.215%
17	12.668	1796	1799	1803	rVB	126232	120878	2.49%	0.258%
18	12.821	1819	1825	1828	rBV	4669675	4861050	100.00%	10.374%
19	13.057	1858	1865	1869	rBV3	79122	97552	2.01%	0.208%
20	13.398	1920	1923	1926	rVB	110680	86930	1.79%	0.186%
21	13.721	1974	1978	1990	rBV	580213	781347	16.07%	1.667%
22	13.863	1997	2002	2005	rBV	2031728	1981224	40.76%	4.228%
23	14.039	2028	2032	2038	rBV	252532	232869	4.79%	0.497%
24	14.339	2080	2083	2091	rVB	287704	295337	6.08%	0.630%
25	14.610	2126	2129	2131	rBV	360249	328144	6.75%	0.700%
26	14.633	2131	2133	2142	rVV	332818	404396	8.32%	0.863%
27	14.704	2142	2145	2150	rVB	179573	182567	3.76%	0.390%
28	14.868	2170	2173	2181	rVB2	64443	100780	2.07%	0.215%
29	14.951	2183	2187	2195	rVV	282811	332739	6.85%	0.710%
30	15.204	2227	2230	2235	rVB	54411	62744	1.29%	0.134%
31	15.268	2236	2241	2244	rVV	1564106	1794680	36.92%	3.830%
32	15.304	2244	2247	2254	rVB	252446	350195	7.20%	0.747%
33	15.709	2312	2316	2321	rVB	203038	264381	5.44%	0.564%
34	15.768	2322	2326	2333	rBV6	68404	154848	3.19%	0.330%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
Data File : BF113052.D
Acq On : 14 Mar 2019 16:23
Operator : JU/SJ
Sample : K1866-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-01-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-BF022719.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.174	2391	2395	2400	rVB	100836	140452	2.89%	0.300%

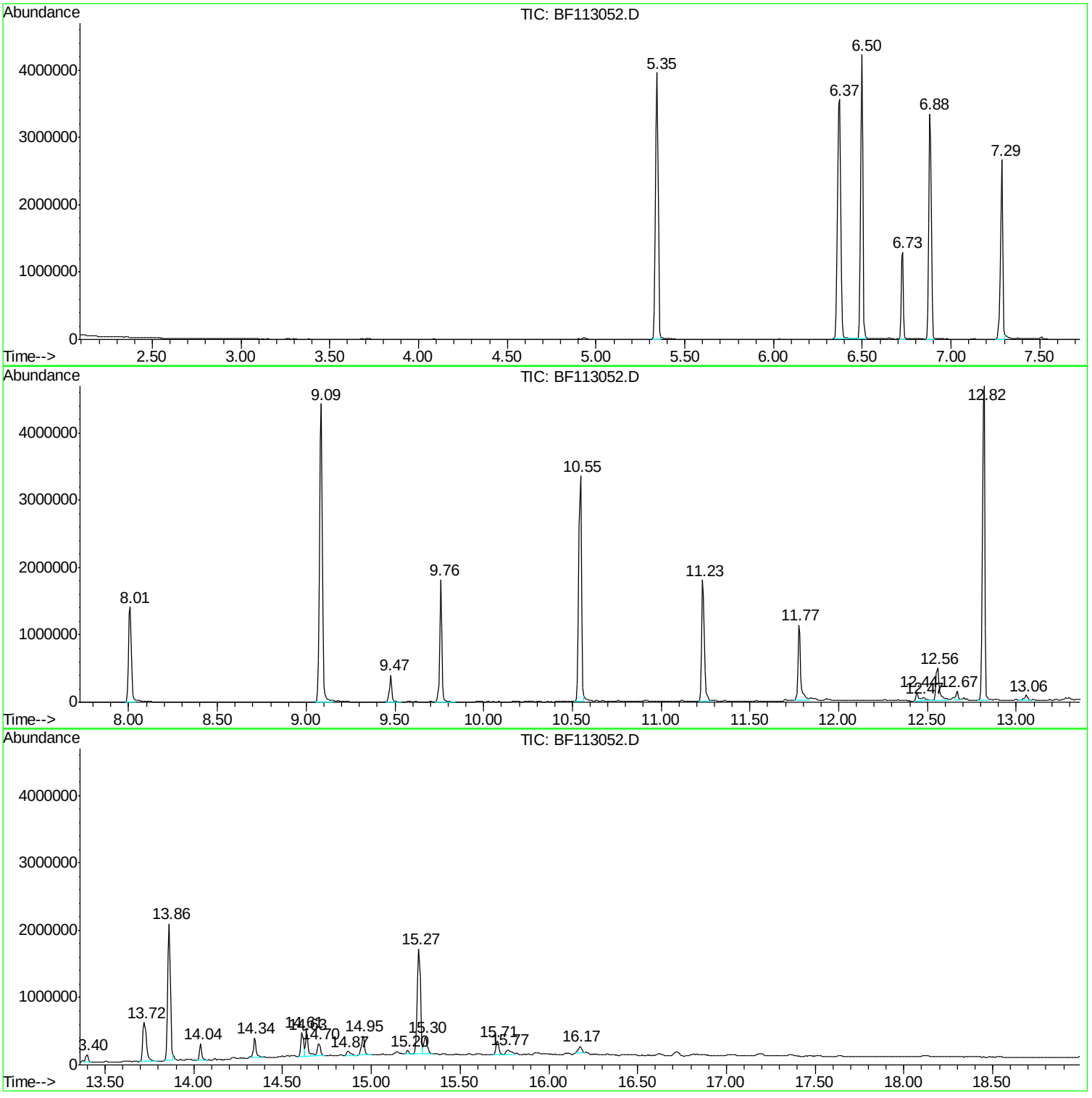
Sum of corrected areas: 46860093

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
Data File : BF113052.D
Acq On : 14 Mar 2019 16:23
Operator : JU/SJ
Sample : K1866-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-01-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
Data File : BF113052.D
Acq On : 14 Mar 2019 16:23
Operator : JU/SJ
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Misc :
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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

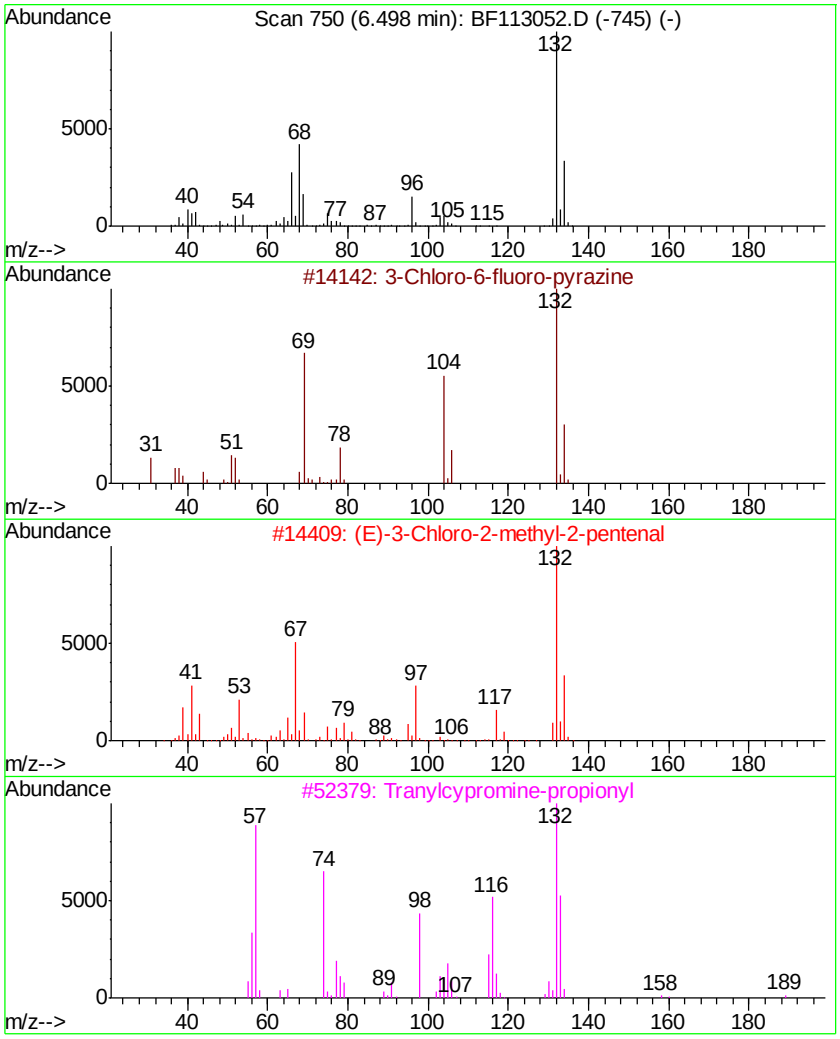
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

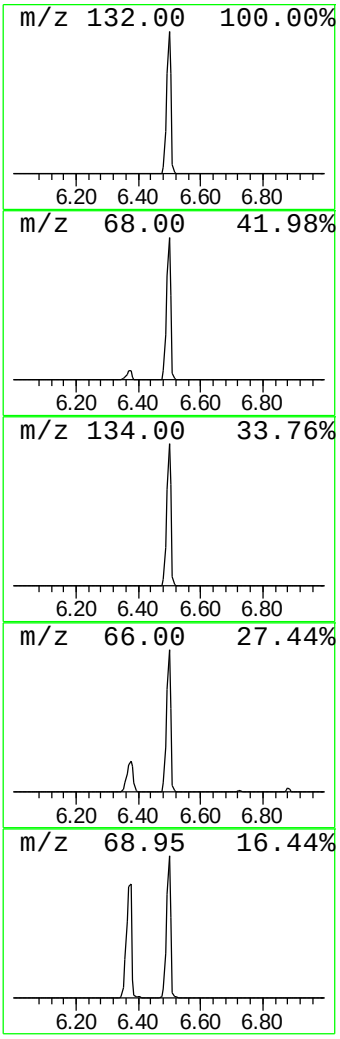
****

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	71.14 ng	4139970	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
Data File : BF113052.D
Acq On : 14 Mar 2019 16:23
Operator : JU/SJ
Sample : K1866-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-01-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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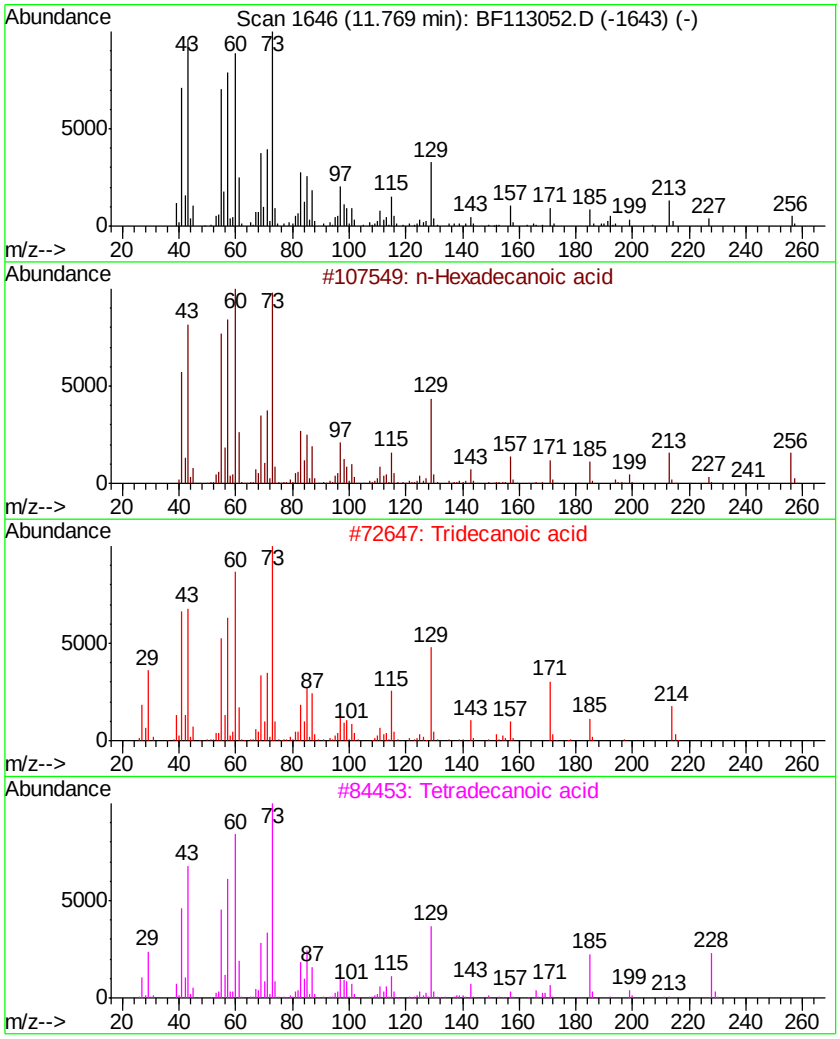
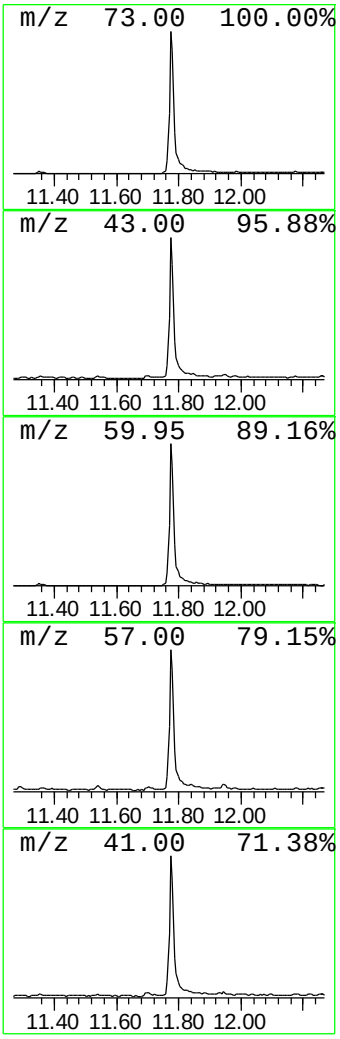
Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	14.63 ng	1302070	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5	Oxalic acid, dodecyl isobutyl ester	314	C18H34O4	1000309-37-7	25





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
Data File : BF113052.D
Acq On : 14 Mar 2019 16:23
Operator : JU/SJ
Sample : K1866-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-01-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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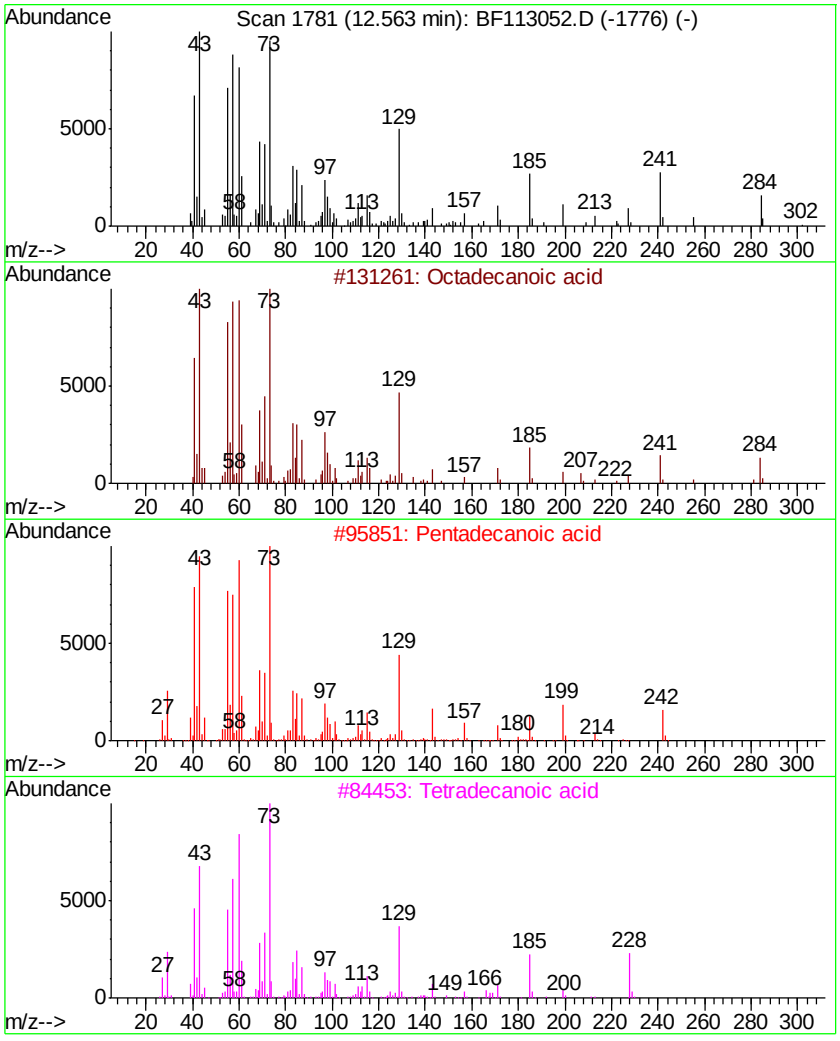
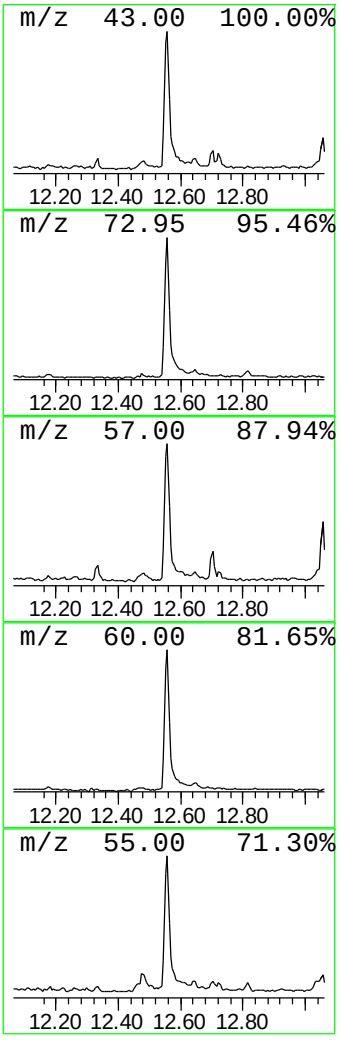
Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	5.75 ng	569311	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
5	Undecanoic acid	186	C11H22O2	000112-37-8	74





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
Data File : BF113052.D
Acq On : 14 Mar 2019 16:23
Operator : JU/SJ
Sample : K1866-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-01-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

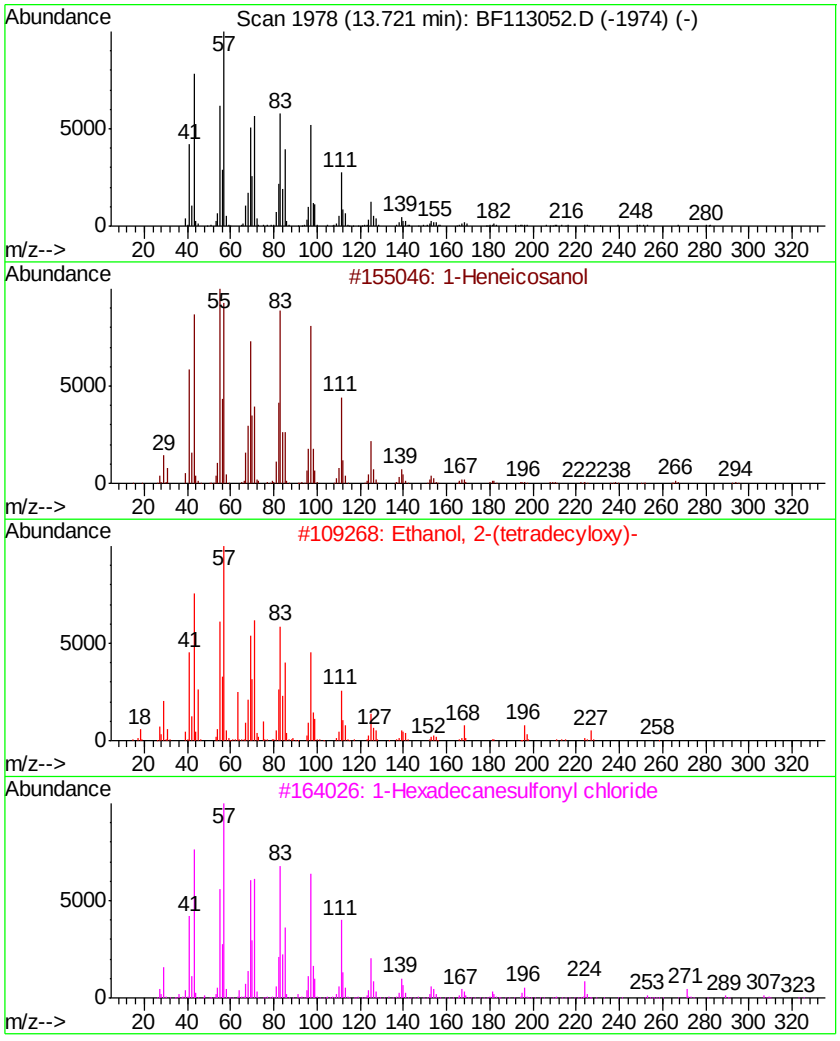
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

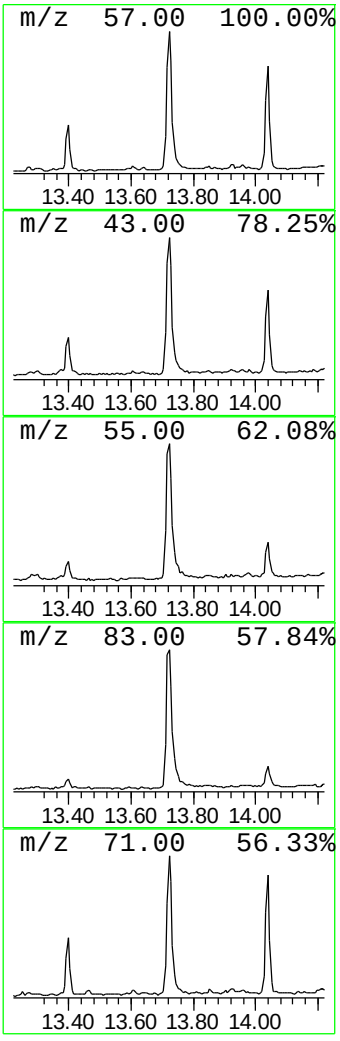
****

Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	7.89 ng	781347	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	92
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
4	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	90
5	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
Data File : BF113052.D
Acq On : 14 Mar 2019 16:23
Operator : JU/SJ
Sample : K1866-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-01-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

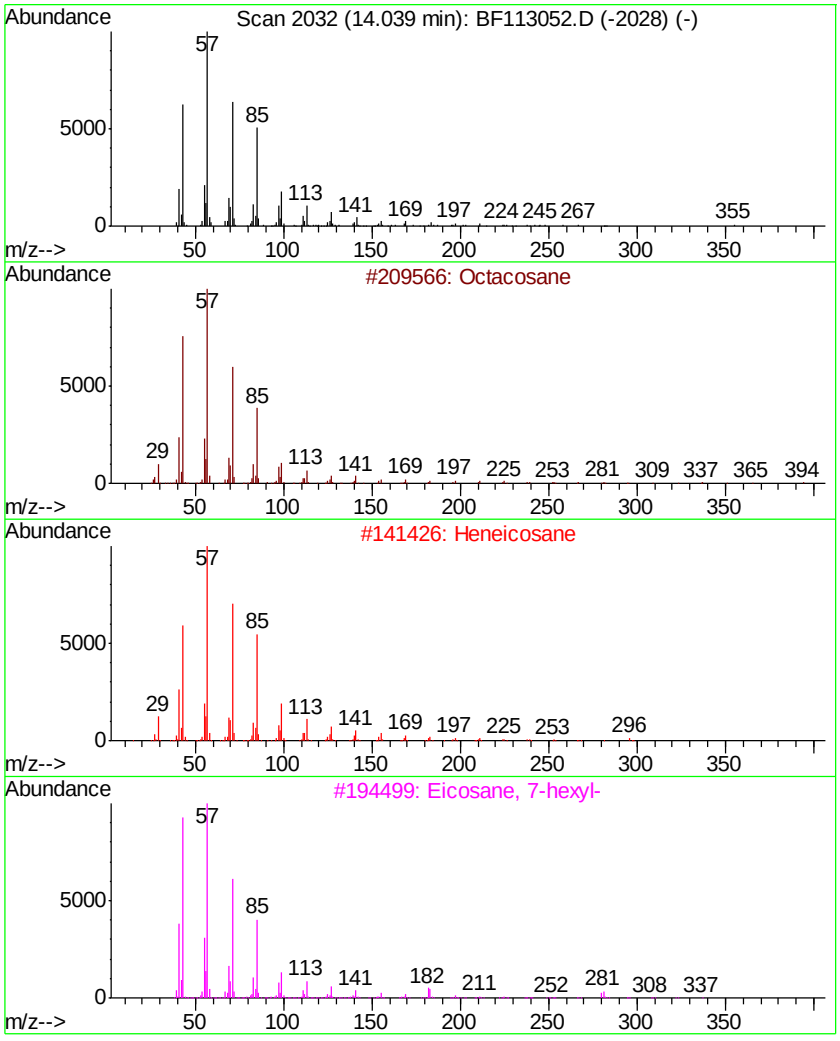
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

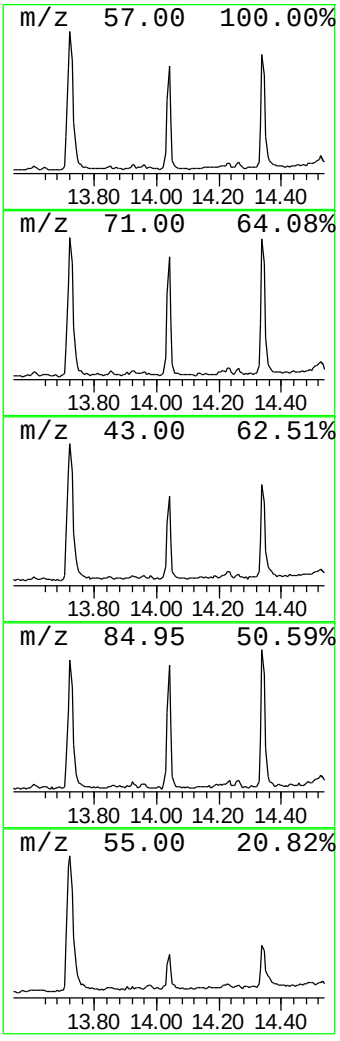
****

Peak Number 6 Octacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.04	2.35 ng	232869	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heneicosane	296	C21H44	000629-94-7	90
3	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
4	Hexadecane	226	C16H34	000544-76-3	87
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	83





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Data File : BF113052.D
Acq On : 14 Mar 2019 16:23
Operator : JU/SJ
Sample : K1866-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-01-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

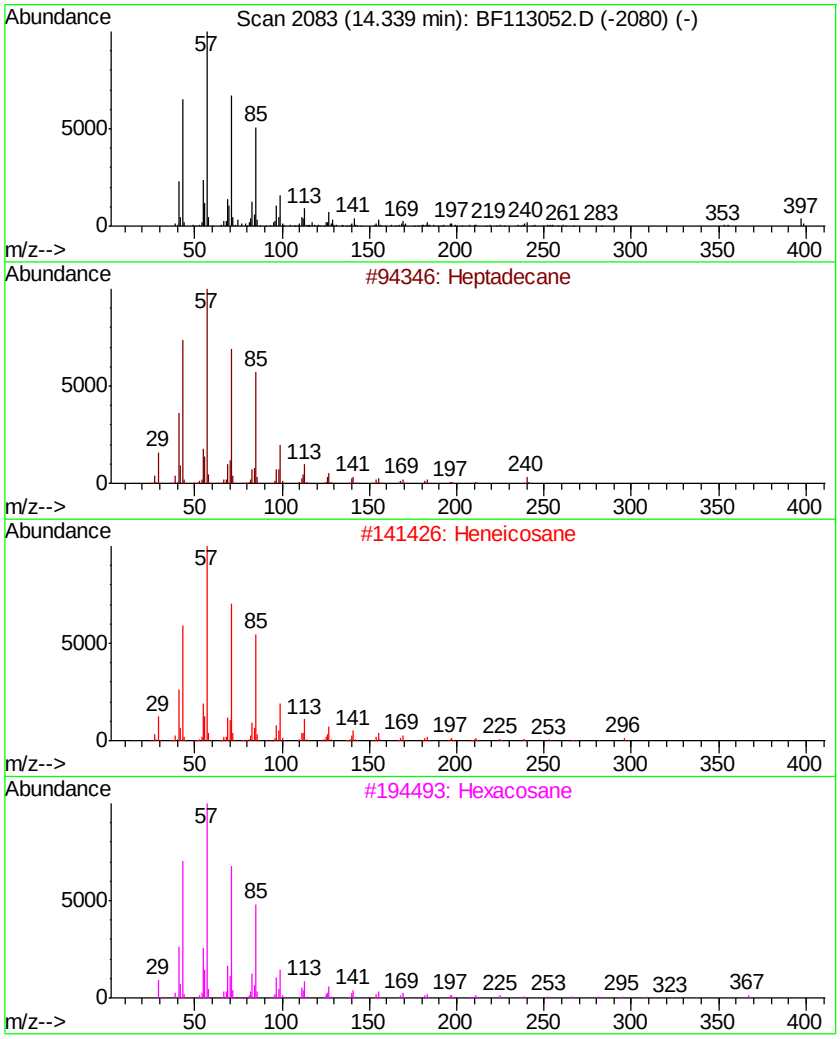
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

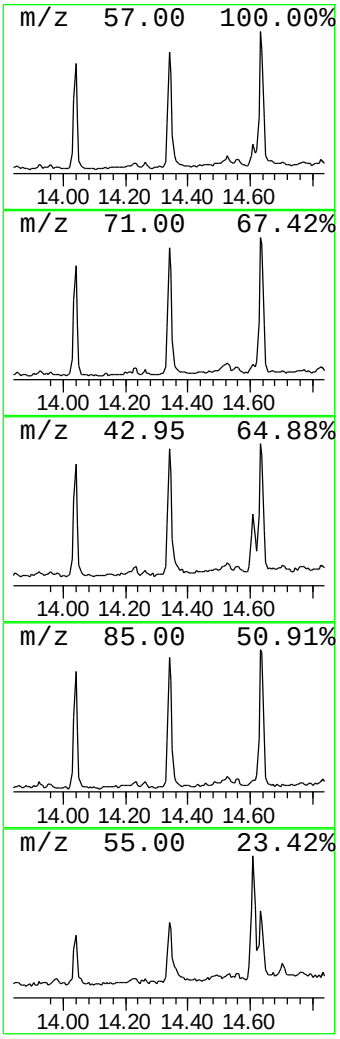
****

Peak Number 7 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	2.98 ng	295337	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	94
2	Heneicosane	296	C21H44	000629-94-7	90
3	Hexacosane	366	C26H54	000630-01-3	90
4	Triacontane	422	C30H62	000638-68-6	87
5	Eicosane	282	C20H42	000112-95-8	81





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
Data File : BF113052.D
Acq On : 14 Mar 2019 16:23
Operator : JU/SJ
Sample : K1866-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-01-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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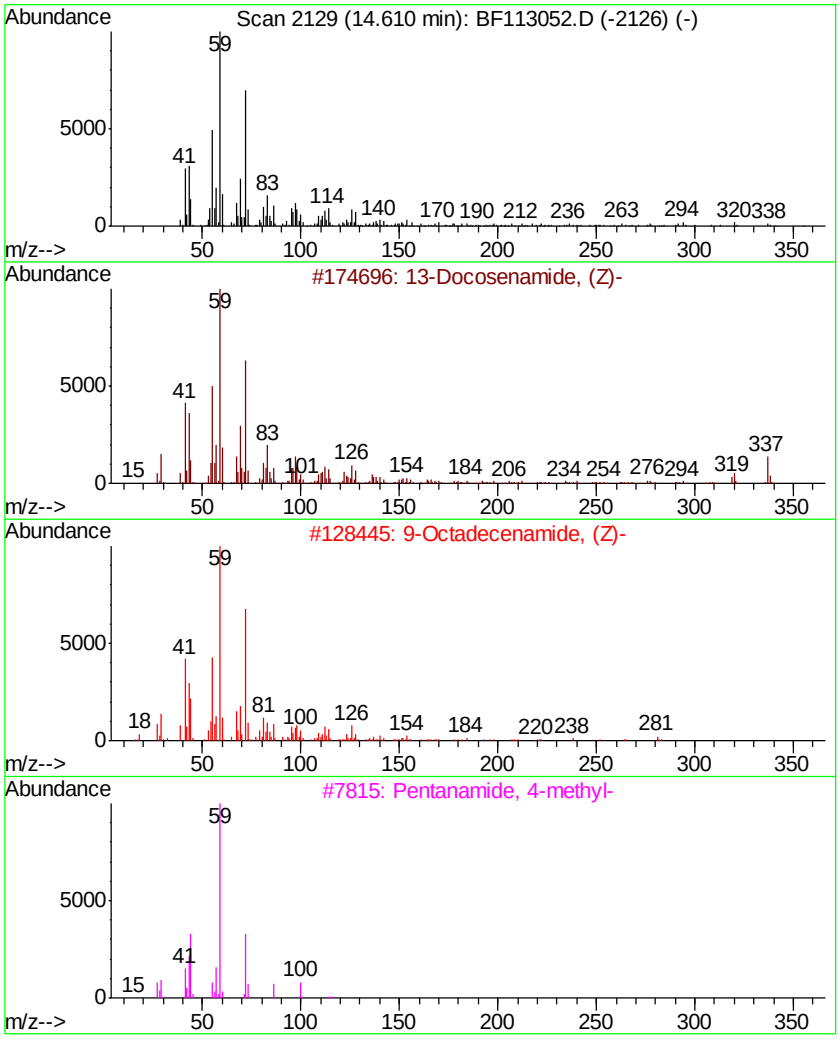
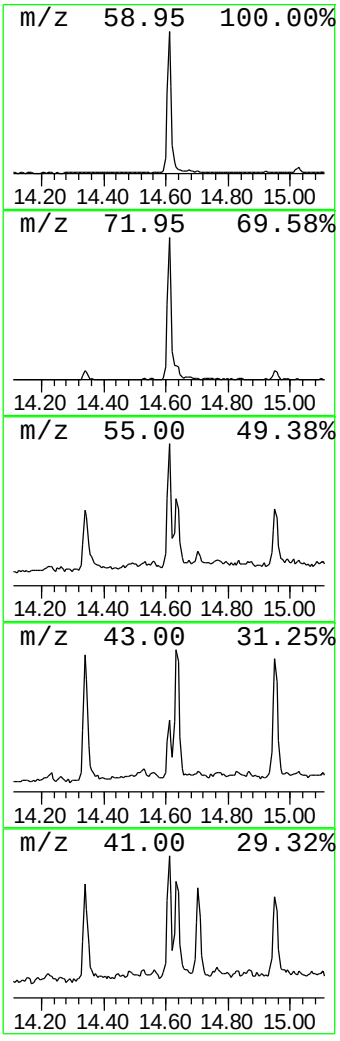
Peak Number 8 13-Docosenamide, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.61	3.66 ng	328144	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	94
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
3	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	59
4	Methyl 17-methoxy-10-methoxycarb...	386	C22H42O5	1000110-20-7	43
5	2-Hydroxy-2-methylundec-5-en-3-one	198	C12H22O2	1000191-46-2	38





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Sample : K1866-07
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ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-01-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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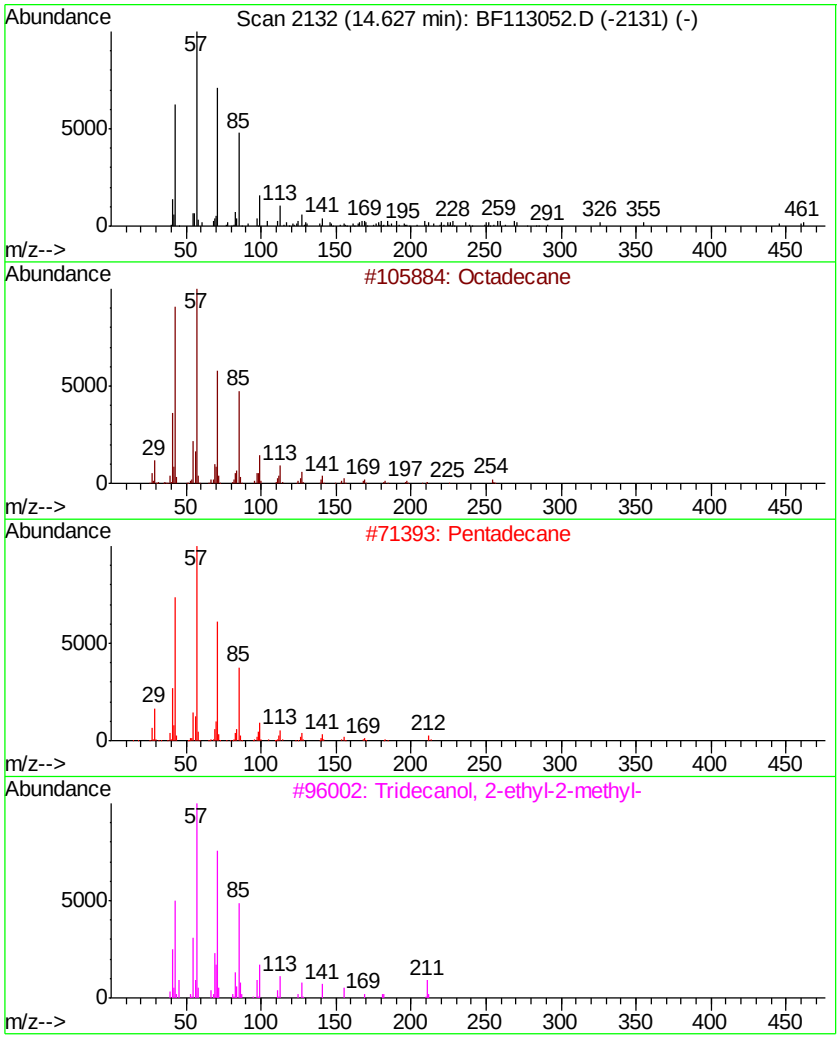
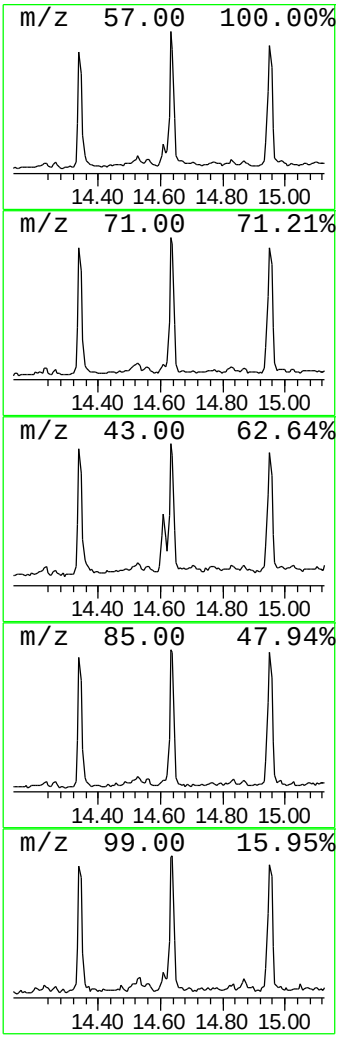
Peak Number 9 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	4.51 ng	404396	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	90
2	Pentadecane	212	C15H32	000629-62-9	90
3	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	83
4	Heptacosane	380	C27H56	000593-49-7	74
5	Undecane, 3-methyl-	170	C12H26	001002-43-3	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
Data File : BF113052.D
Acq On : 14 Mar 2019 16:23
Operator : JU/SJ
Sample : K1866-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-01-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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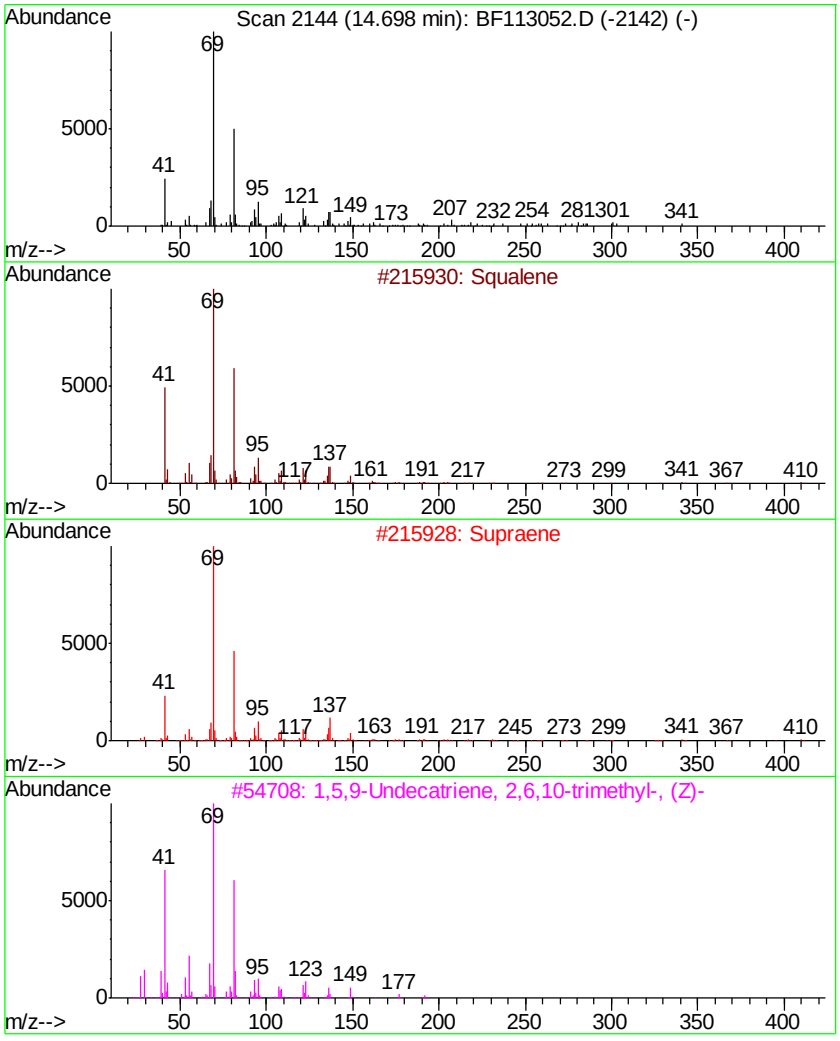
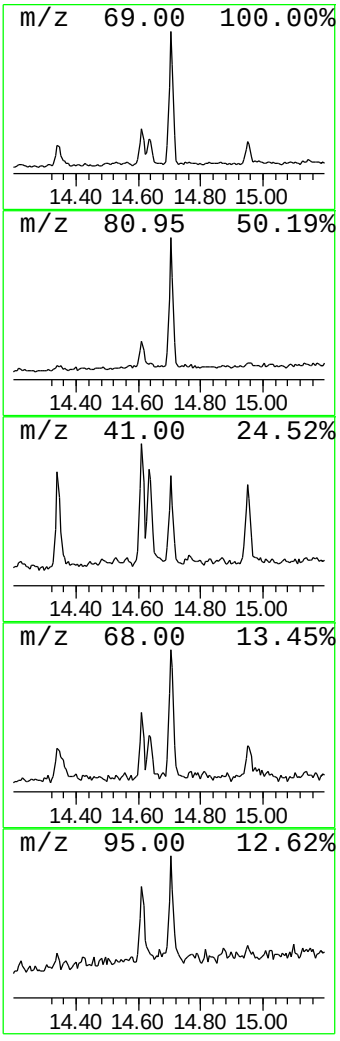
Peak Number 10 Squalene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.70	2.03 ng	182567	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	90
2	Supraene	410	C30H50	007683-64-9	90
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	74
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5	6,11-Dimethyl-2,6,10-dodecatrien...	208	C14H24O	1000196-53-3	53





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Acq On : 14 Mar 2019 16:23
Operator : JU/SJ
Sample : K1866-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-01-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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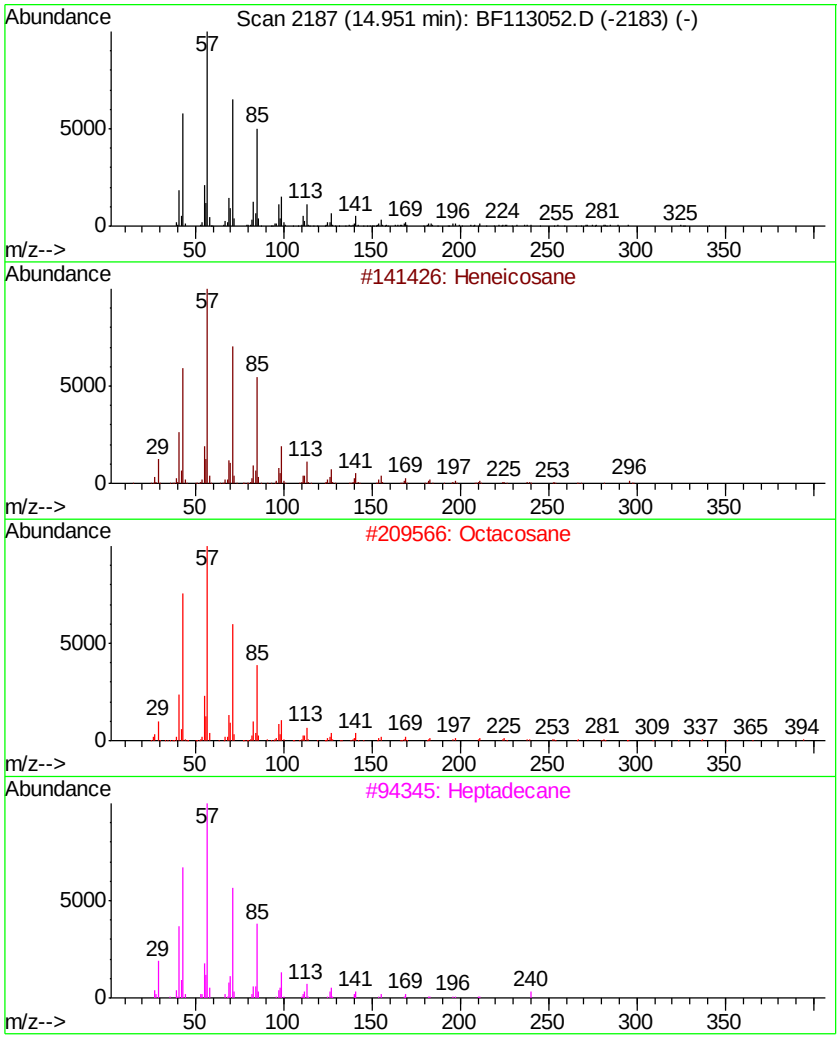
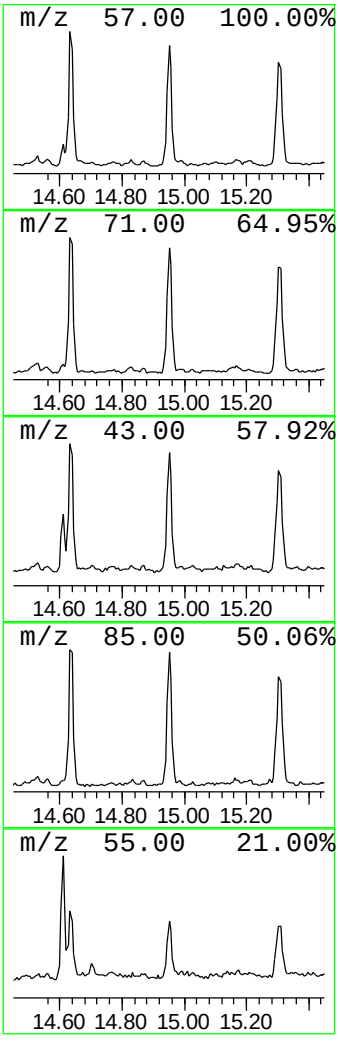
Peak Number 11 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	3.71 ng	332739	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heptadecane	240	C17H36	000629-78-7	90
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
5	Tridecane, 7-hexyl-	268	C19H40	007225-66-3	86





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Acq On : 14 Mar 2019 16:23
Operator : JU/SJ
Sample : K1866-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-01-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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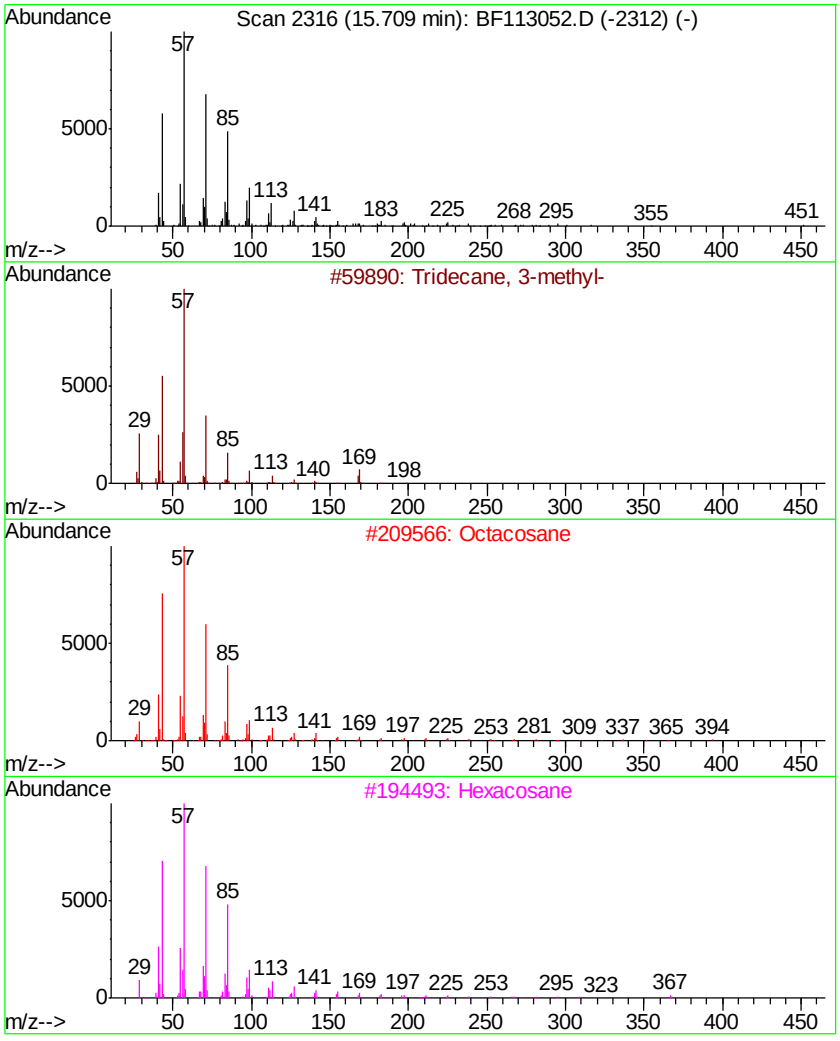
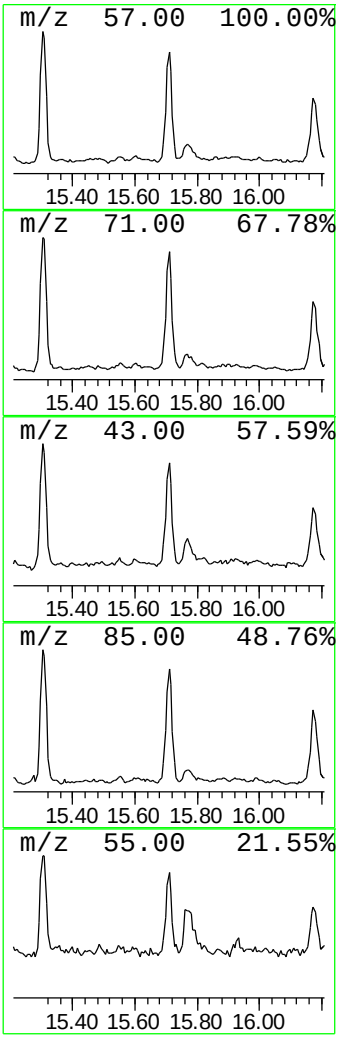
Peak Number 12 Tridecane, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	2.95 ng	264381	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 3-methyl-	198	C14H30	006418-41-3	87
2	Octacosane	394	C28H58	000630-02-4	87
3	Hexacosane	366	C26H54	000630-01-3	87
4	2-methyloctacosane	408	C29H60	1000376-72-8	87
5	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031419\
Data File : BF113052.D
Acq On : 14 Mar 2019 16:23
Operator : JU/SJ
Sample : K1866-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-01-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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
unknown6.50	6.50	71.1	ng	4139970	1	6.73	1163980	20.0
n-Hexadecanoic acid	11.77	14.6	ng	1302070	4	11.23	1780160	20.0
Octadecanoic acid	12.56	5.8	ng	569311	5	13.86	1981220	20.0
1-Heneicosanol	13.72	7.9	ng	781347	5	13.86	1981220	20.0
Octacosane	14.04	2.4	ng	232869	5	13.86	1981220	20.0
Heptadecane	14.34	3.0	ng	295337	5	13.86	1981220	20.0
13-Docosenamide, ...	14.61	3.7	ng	328144	6	15.27	1794680	20.0
Octadecane	14.63	4.5	ng	404396	6	15.27	1794680	20.0
Squalene	14.70	2.0	ng	182567	6	15.27	1794680	20.0
Heneicosane	14.95	3.7	ng	332739	6	15.27	1794680	20.0
Tridecane, 3-methyl-	15.71	3.0	ng	264381	6	15.27	1794680	20.0