LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
Data File : BF113051.D
Acq On : 14 Mar 2019 15:55
Operator : JU/SJ
Sample : K1866-15
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-12-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	5.351	549	555	558	rBV	4385318	5199363	81.14%	8.364%
2	6.381	723	730	734	rBV2	4338167	6002179	93.67%	9.655%
3	6.504	745	751	754	rBV	5044072	5477037	85.48%	8.811%
4	6.728	785	789	792	rBV	1447441	1271510	19.84%	2.045%
5	6.887	811	816	819	rBV	4527102	4225686	65.95%	6.798%
6	7.292	878	885	888	rBV	3206397	3674685	57.35%	5.911%
7	8.010	1002	1007	1024	rBV	1479200	1624573	25.35%	2.613%
8	9.086	1184	1190	1193	rBV	5878259	5934626	92.62%	9.547%
9	9.475	1252	1256	1265	rVB	601737	518367	8.09%	0.834%
10	9.757	1298	1304	1317	rBV2	2120111	1957172	30.54%	3.148%
11	10.545	1432	1438	1442	rBV	4033090	4546311	70.95%	7.313%
12	11.233	1551	1555	1558	rBV	2072006	2042544	31.88%	3.286%
13	11.780	1643	1648	1656	rBV	1583554	1792407	27.97%	2.883%
14	11.869	1661	1663	1670	rVB2	58547	66042	1.03%	0.106%
15	12.439	1756	1760	1765	rBV	380825	381523	5.95%	0.614%
16	12.557	1774	1780	1793	rBV	828374	945753	14.76%	1.521%
17	12.669	1793	1799	1802	rVV	346722	350315	5.47%	0.564%
18	12.821	1816	1825	1828	rBV2	5795681	6407684	100.00%	10.308%
19	13.057	1862	1865	1869	rVB2	122631	125056	1.95%	0.201%
20	13.398	1920	1923	1926	rBV	155694	124903	1.95%	0.201%
21	13.721	1973	1978	1987	rBV2	673782	876035	13.67%	1.409%
22	13.863	1996	2002	2005	rBV	2346137	2358596	36.81%	3.794%
23	13.886	2005	2006	2011	rVB	183198	111797	1.74%	0.180%
24	14.039	2028	2032	2037	rBV	294914	282814	4.41%	0.455%
25	14.251	2063	2068	2071	rBV4	36663	68830	1.07%	0.111%
26	14.345	2080	2084	2091	rBV	320536	372052	5.81%	0.599%
27	14.610	2126	2129	2132	rBV	522286	559101	8.73%	0.899%
28	14.639	2132	2134	2141	rVV	383121	403139	6.29%	0.649%
29	14.704	2143	2145	2152	rVB2	84410	94017	1.47%	0.151%
30	14.868	2169	2173	2182	rBV	163604	328456	5.13%	0.528%
31	14.951	2183	2187	2196	rVB2	326884	427347	6.67%	0.687%
32	15.151	2218	2221	2227	rVB	82147	95963	1.50%	0.154%
33	15.210	2227	2231	2235	rVV	100721	129255	2.02%	0.208%
34	15.274	2236	2242	2245	rVV	1636371	2183255	34.07%	3.512%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
Data File : BF113051.D
Acq On : 14 Mar 2019 15:55
Operator : JU/SJ
Sample : K1866-15
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-12-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	15.304	2245	2247	2255	rVB2	273832	351139	5.48%	0.565%
36	15.710	2312	2316	2321	rVB	215999	297014	4.64%	0.478%
37	15.762	2321	2325	2337	rVB5	100360	253388	3.95%	0.408%
38	16.174	2391	2395	2399	rBV2	97111	158694	2.48%	0.255%
39	16.315	2415	2419	2423	rBV6	32814	75446	1.18%	0.121%
40	16.627	2468	2472	2475	rBV2	43117	69972	1.09%	0.113%

Sum of corrected areas: 62164046

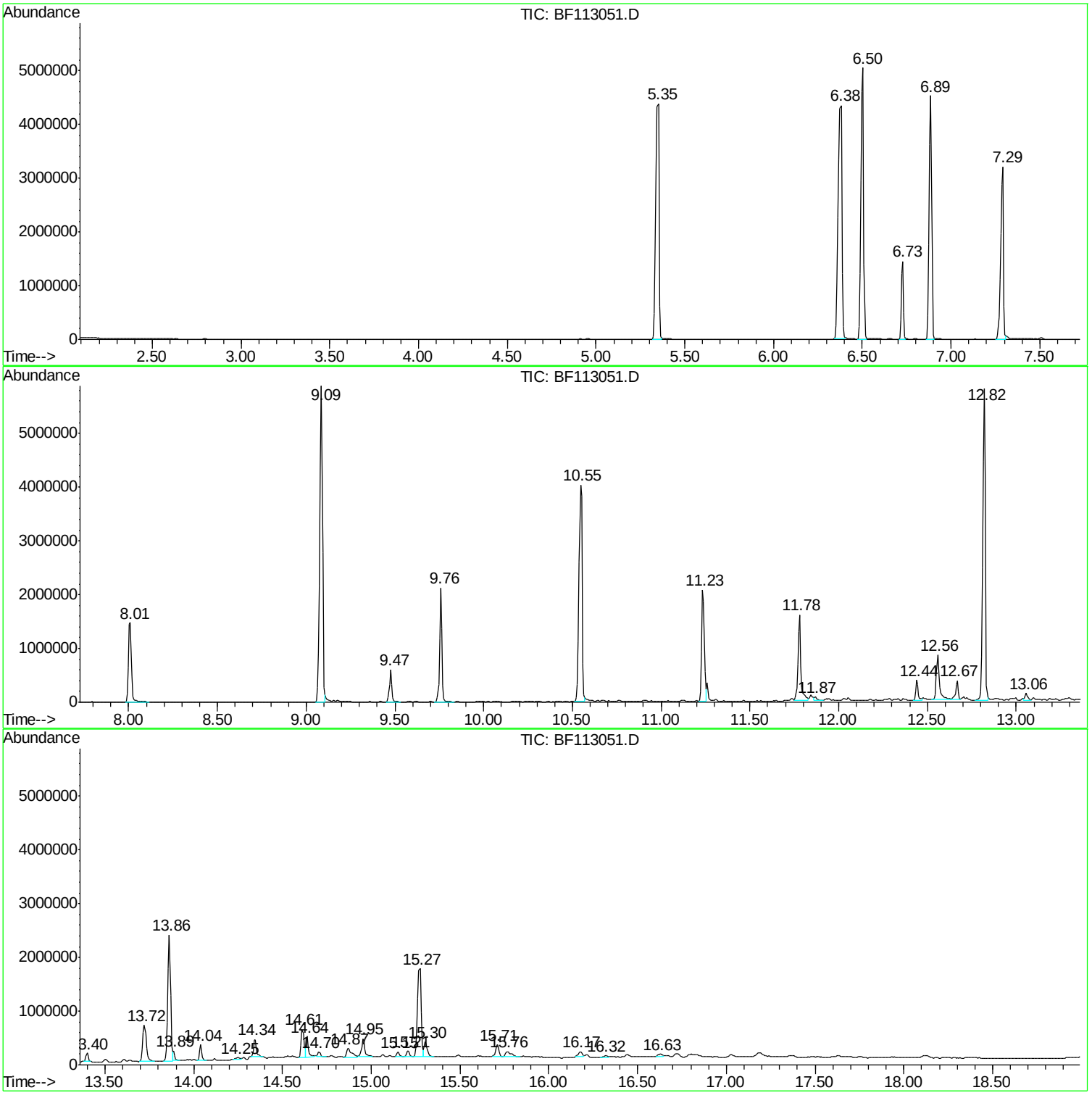
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
Data File : BF113051.D
Acq On : 14 Mar 2019 15:55
Operator : JU/SJ
Sample : K1866-15
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-12-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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
Data File : BF113051.D
Acq On : 14 Mar 2019 15:55
Operator : JU/SJ
Sample : K1866-15
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-12-COMP

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

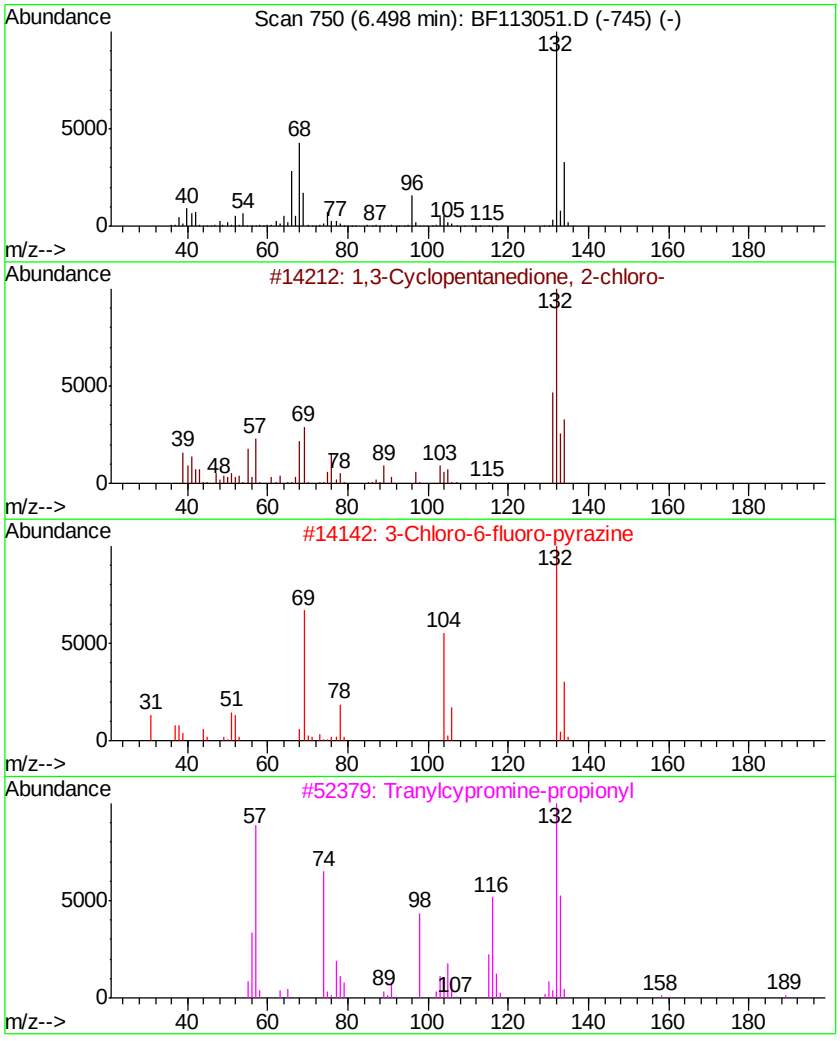
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

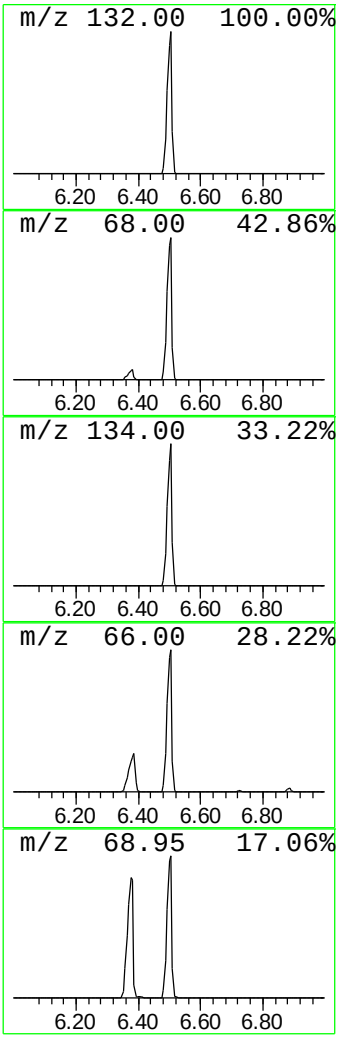
****

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	86.15 ng	5477040	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	47
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
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Operator : JU/SJ
Sample : K1866-15
Misc :
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Instrument : BNA_F
ClientSampleId : MR-MH-12-COMP

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

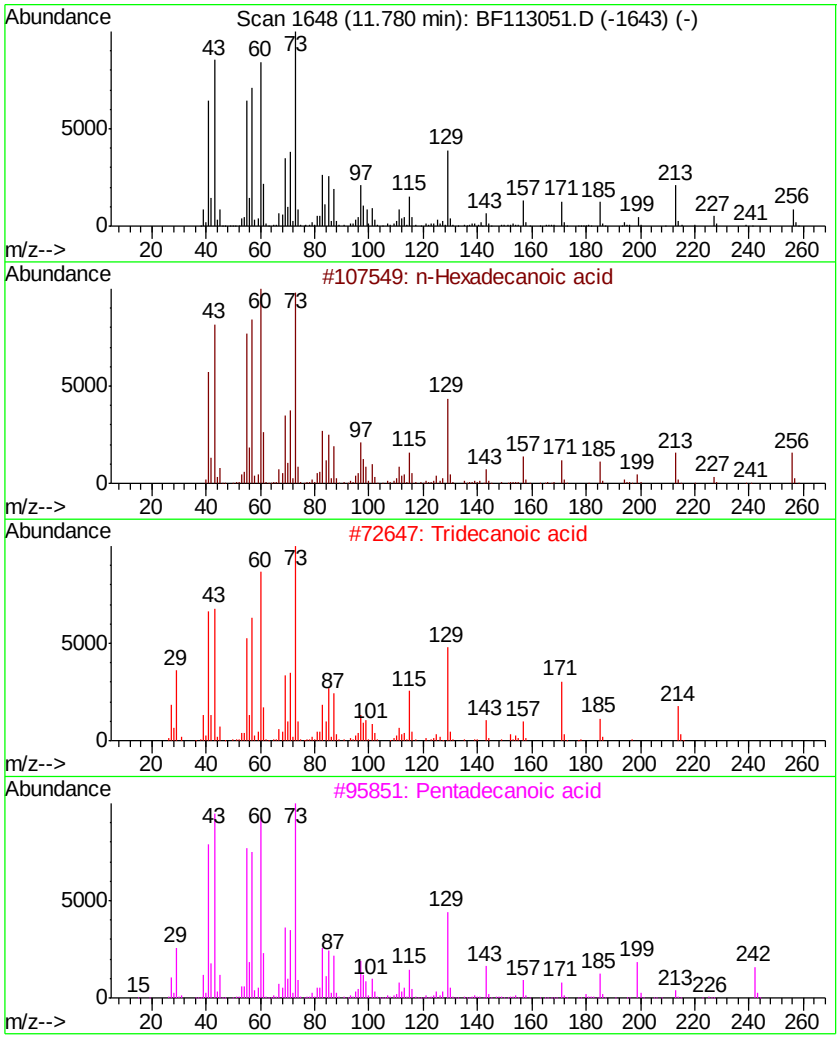
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

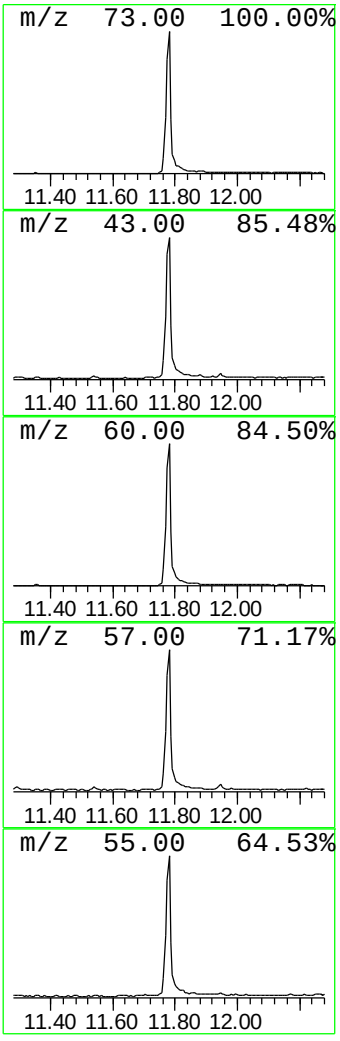
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	17.55 ng	1792410	Phenanthrene-d10	11.23

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	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
Data File : BF113051.D
Acq On : 14 Mar 2019 15:55
Operator : JU/SJ
Sample : K1866-15
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-12-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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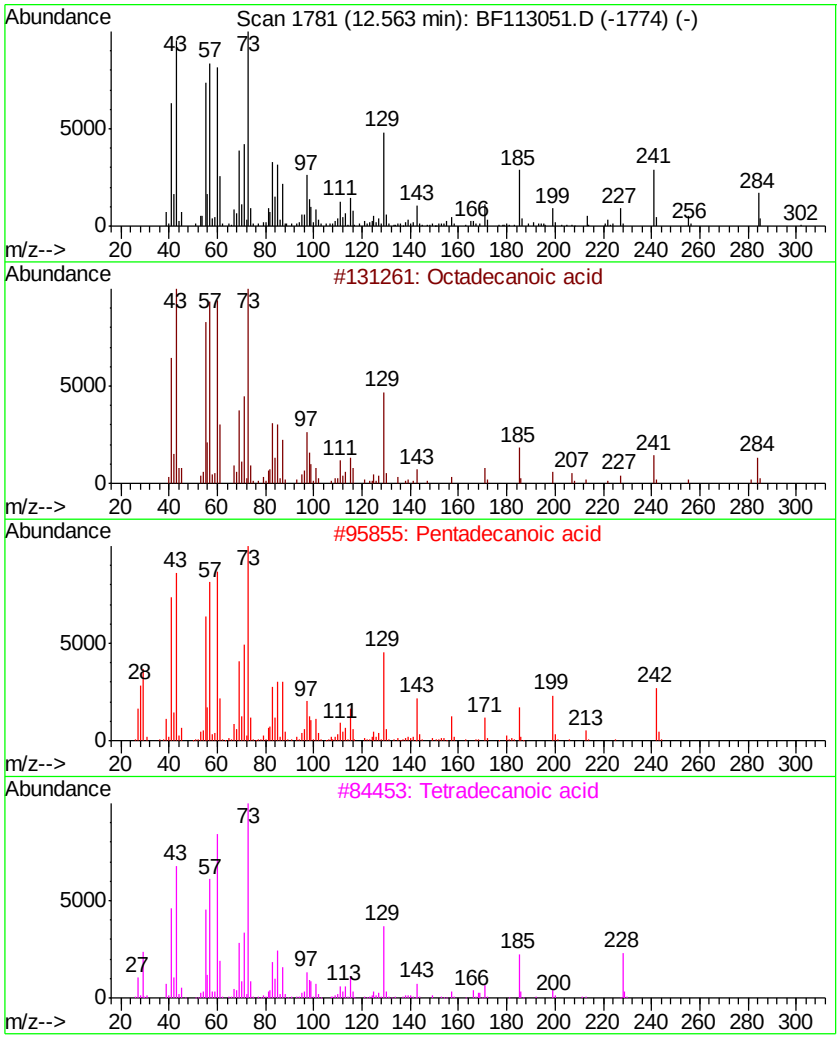
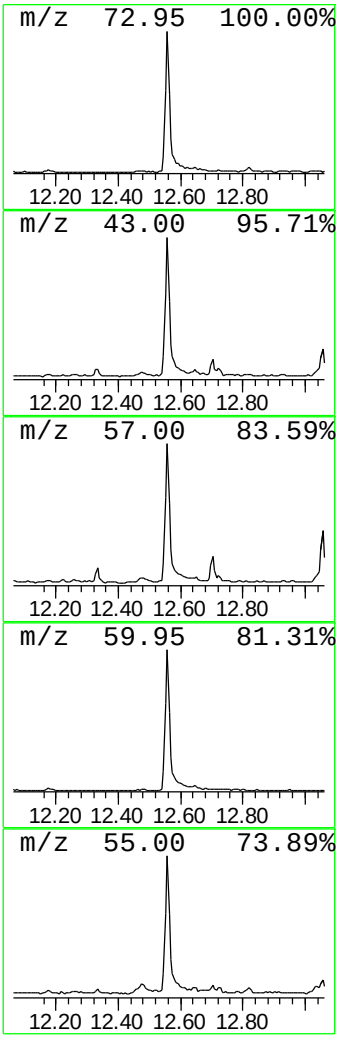
Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	8.02 ng	945753	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	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Tridecanoic acid	214	C13H26O2	000638-53-9	68





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
Data File : BF113051.D
Acq On : 14 Mar 2019 15:55
Operator : JU/SJ
Sample : K1866-15
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-12-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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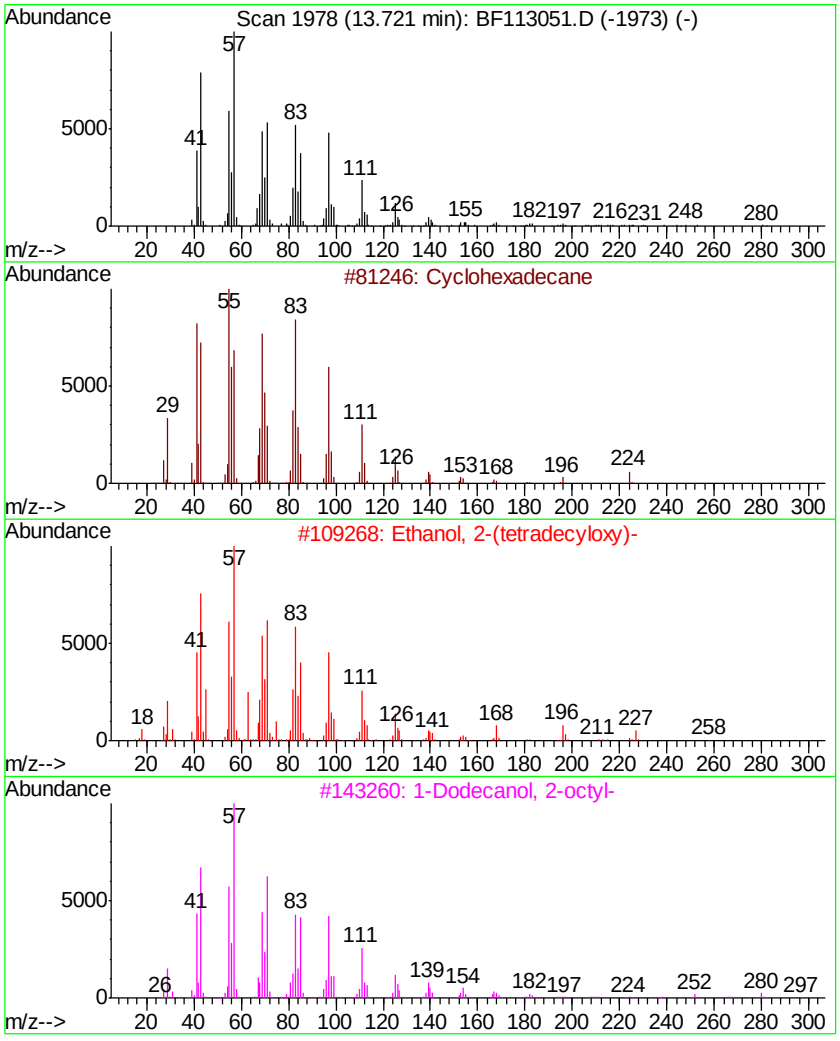
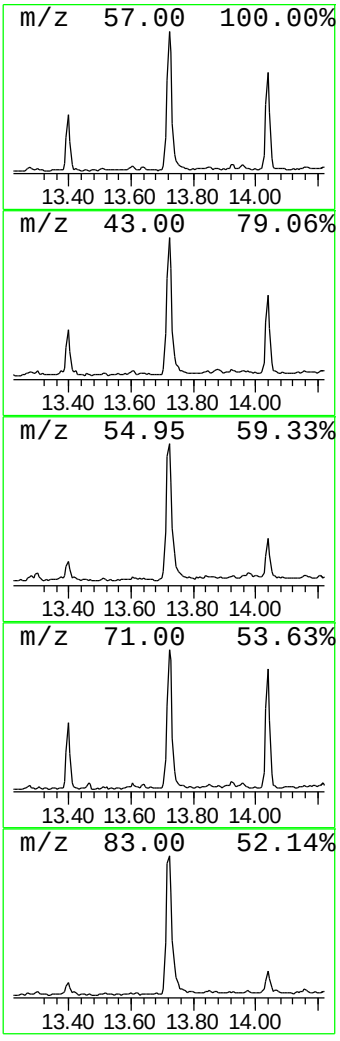
Peak Number 5 Cyclohexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	7.43 ng	876035	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	92
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
4	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
5	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
Data File : BF113051.D
Acq On : 14 Mar 2019 15:55
Operator : JU/SJ
Sample : K1866-15
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-12-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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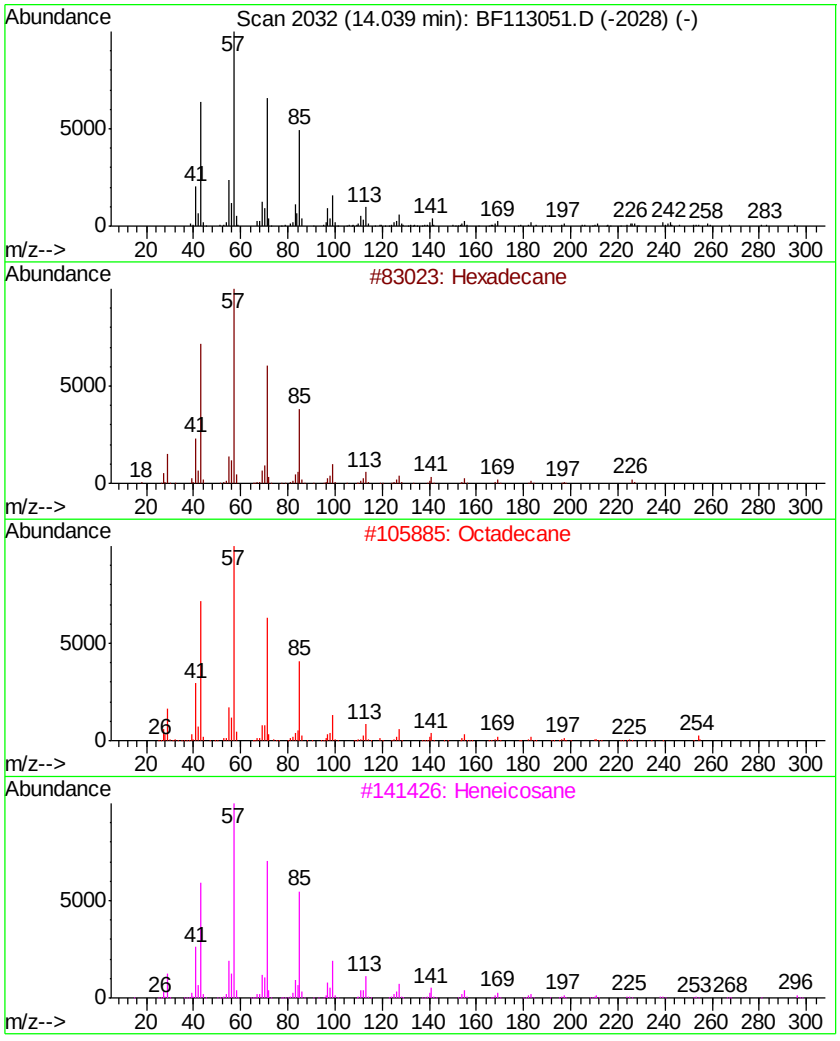
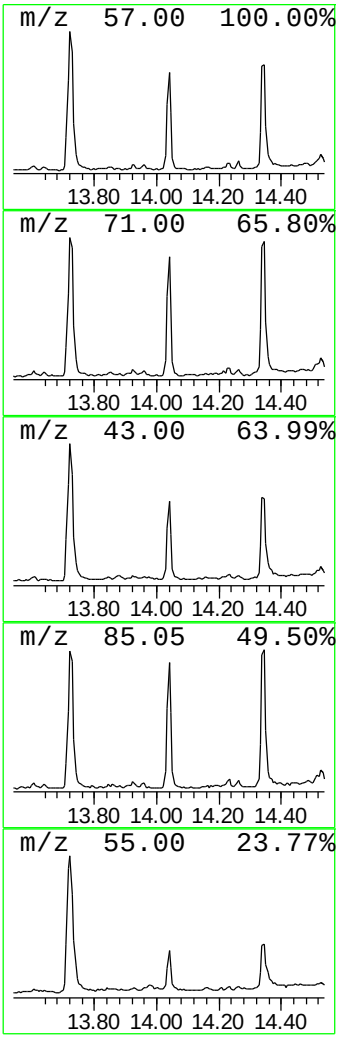
Peak Number 6 Hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.04	2.40 ng	282814	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	95
2	Octadecane	254	C18H38	000593-45-3	93
3	Heneicosane	296	C21H44	000629-94-7	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
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Operator : JU/SJ
Sample : K1866-15
Misc :
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Instrument : BNA_F
ClientSampleId : MR-MH-12-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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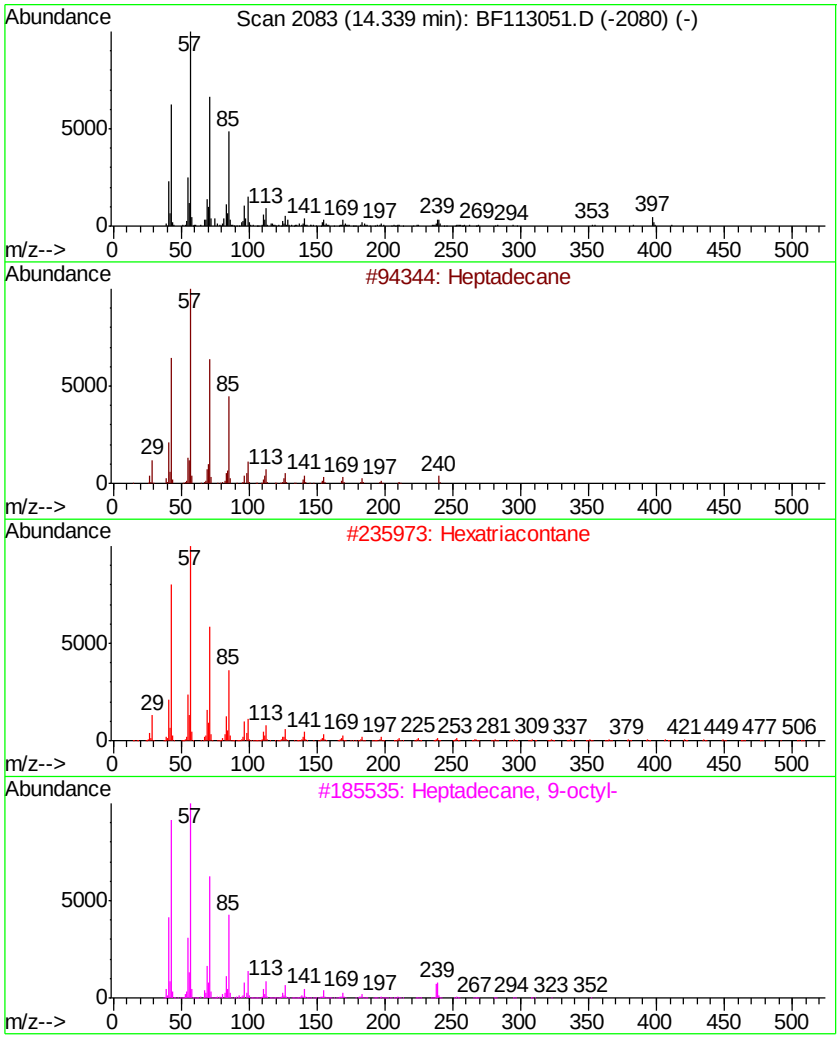
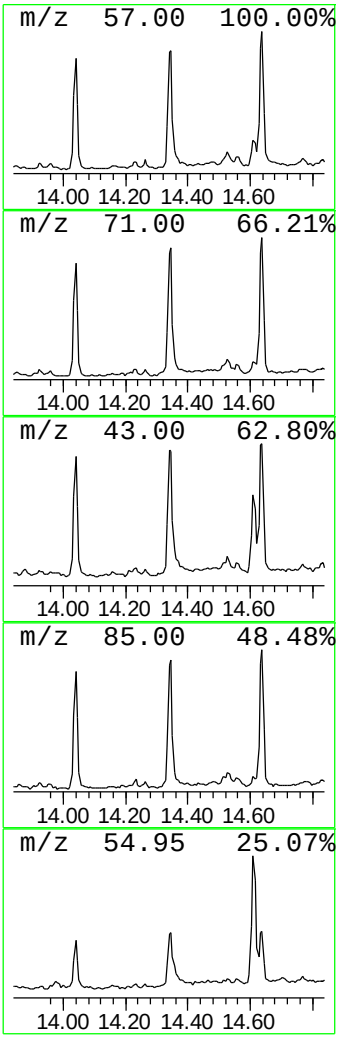
Peak Number 7 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	3.15 ng	372052	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	94
2	Hexatriacontane	507	C36H74	000630-06-8	90
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Tetratetracontane	619	C44H90	007098-22-8	90





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Sample : K1866-15
Misc :
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Instrument : BNA_F
ClientSampleId : MR-MH-12-COMP

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

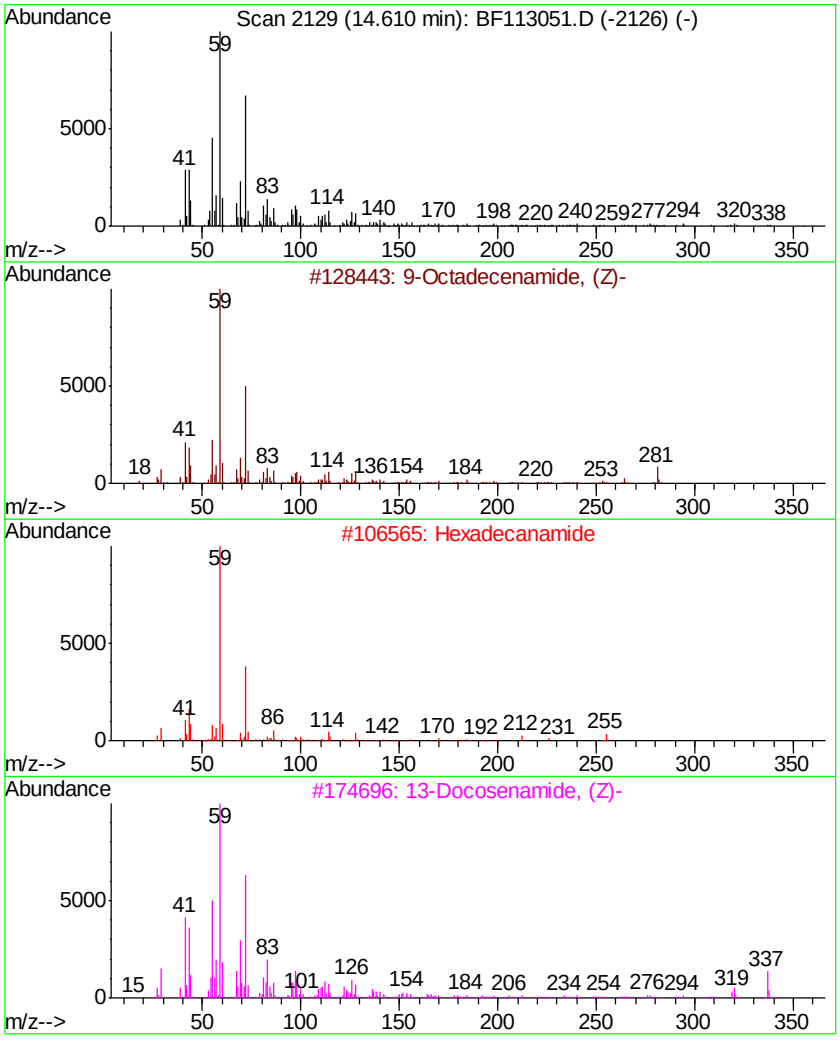
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

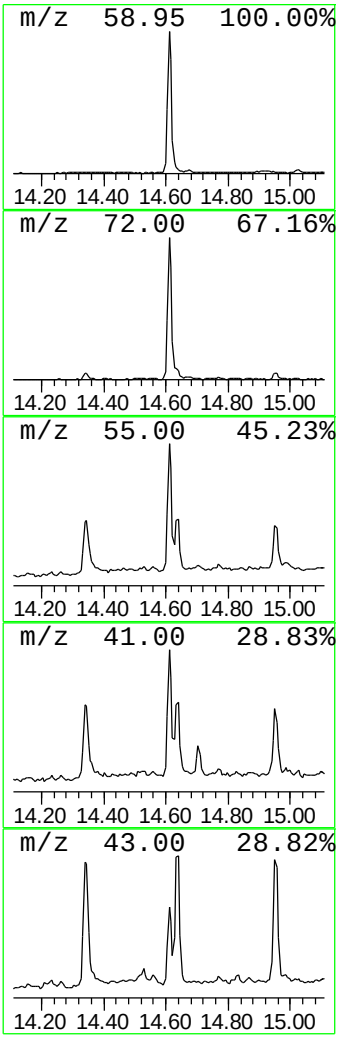
****

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.61	5.12 ng	559101	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2	Hexadecanamide	255	C16H33NO	000629-54-9	78
3	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	64
4	d-Glucosamine	179	C6H13NO5	000090-77-7	59
5	2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	43





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
Data File : BF113051.D
Acq On : 14 Mar 2019 15:55
Operator : JU/SJ
Sample : K1866-15
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-12-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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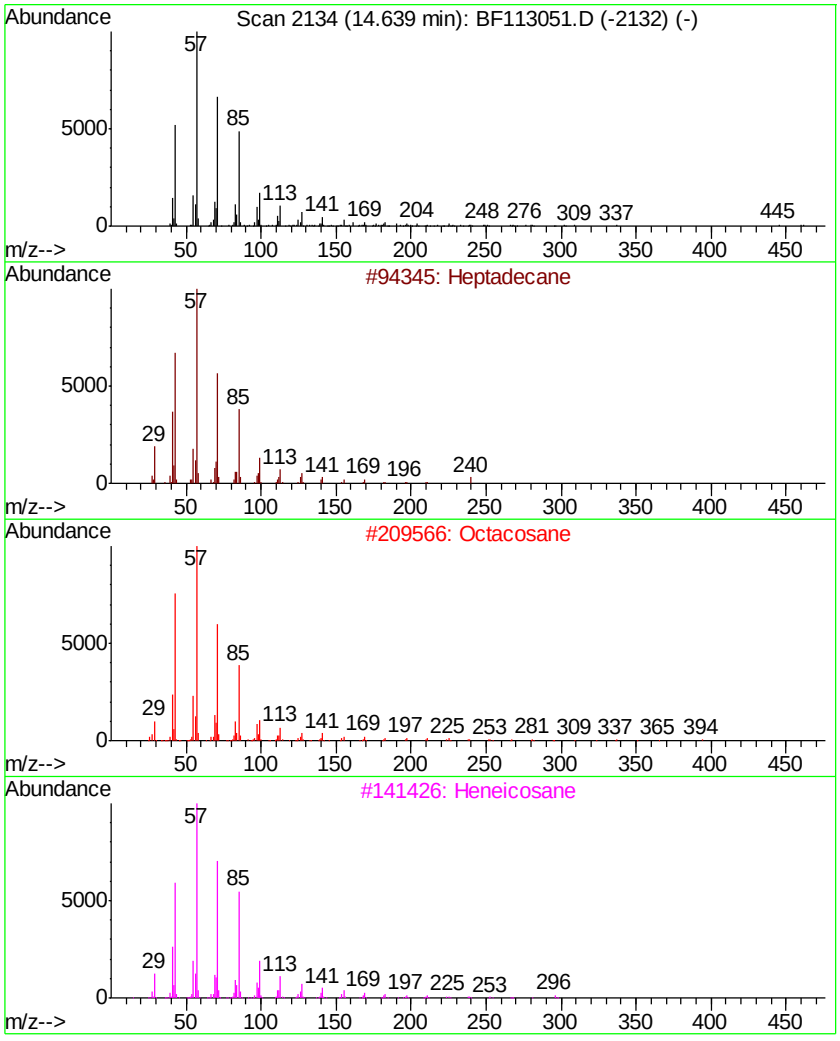
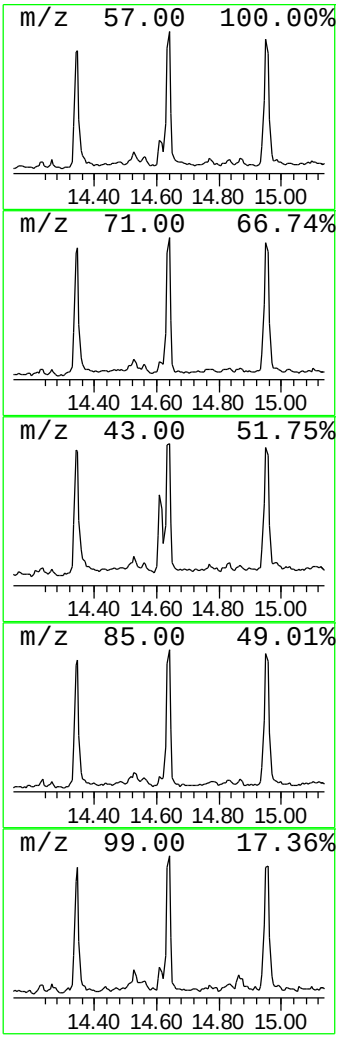
Peak Number 9 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	3.69 ng	403139	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heneicosane	296	C21H44	000629-94-7	83
4	Dodecane	170	C12H26	000112-40-3	83
5	Tridecane, 6-propyl-	226	C16H34	055045-10-8	83





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031419\
Data File : BF113051.D
Acq On : 14 Mar 2019 15:55
Operator : JU/SJ
Sample : K1866-15
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-12-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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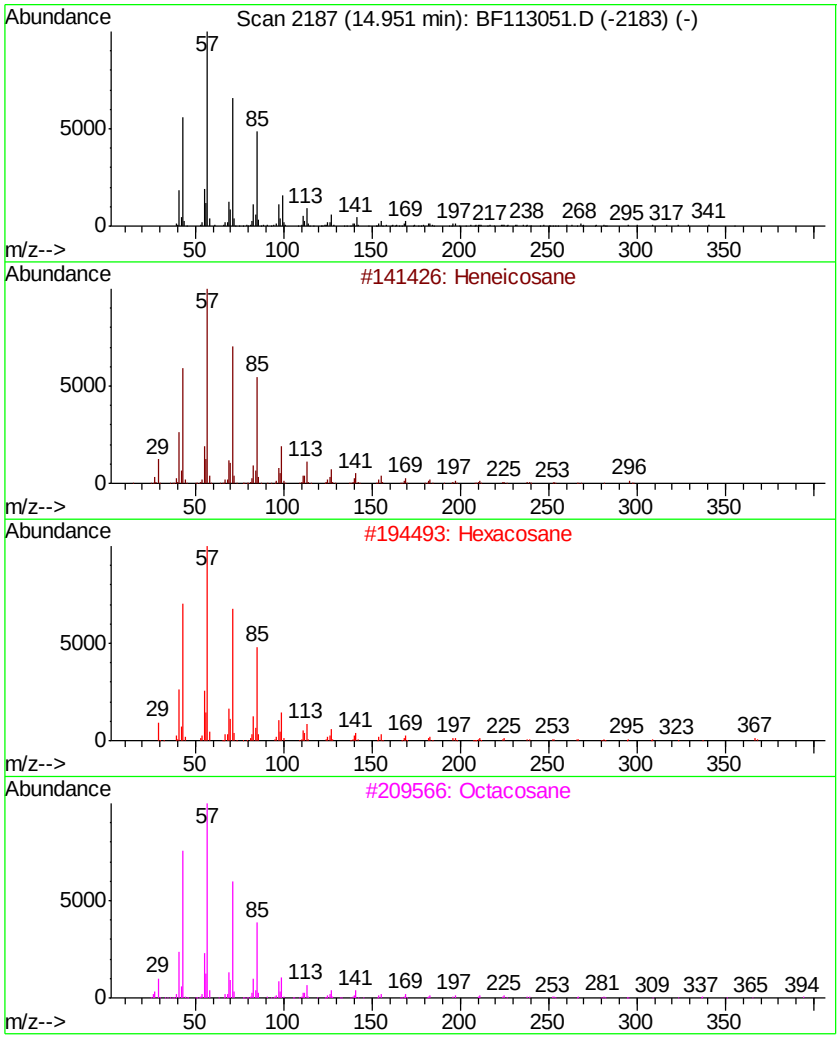
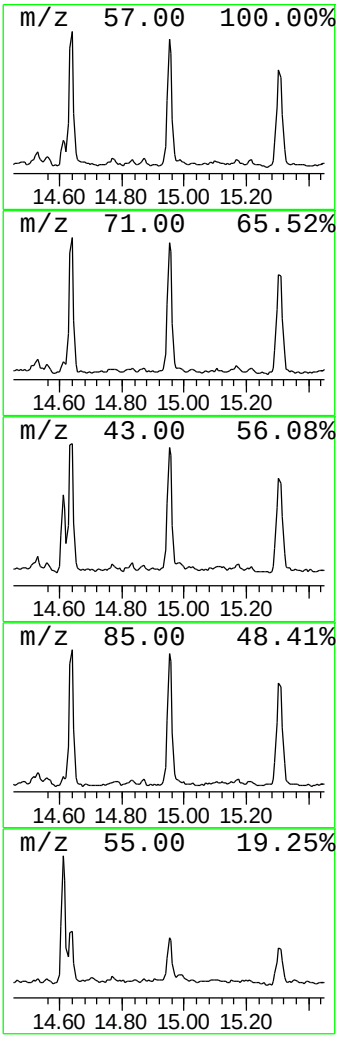
Peak Number 11 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	3.91 ng	427347	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Nonadecane	268	C19H40	000629-92-5	90





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Acq On : 14 Mar 2019 15:55
Operator : JU/SJ
Sample : K1866-15
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-12-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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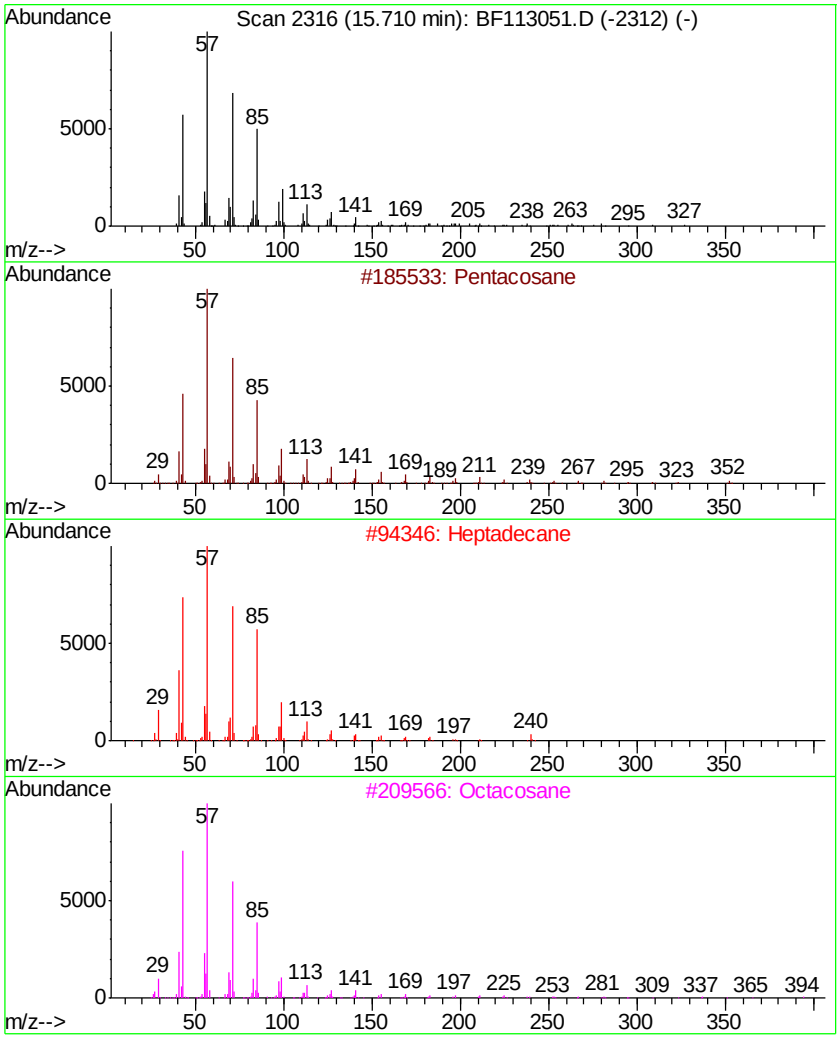
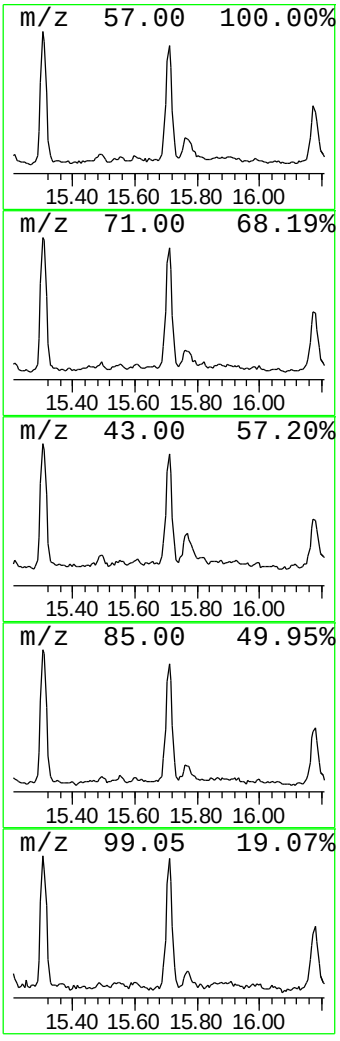
Peak Number 12 Pentacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	2.72 ng	297014	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	90
2	Heptadecane	240	C17H36	000629-78-7	86
3	Octacosane	394	C28H58	000630-02-4	83
4	Tridecane, 7-hexyl-	268	C19H40	007225-66-3	81
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80





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Data File : BF113051.D
Acq On : 14 Mar 2019 15:55
Operator : JU/SJ
Sample : K1866-15
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-12-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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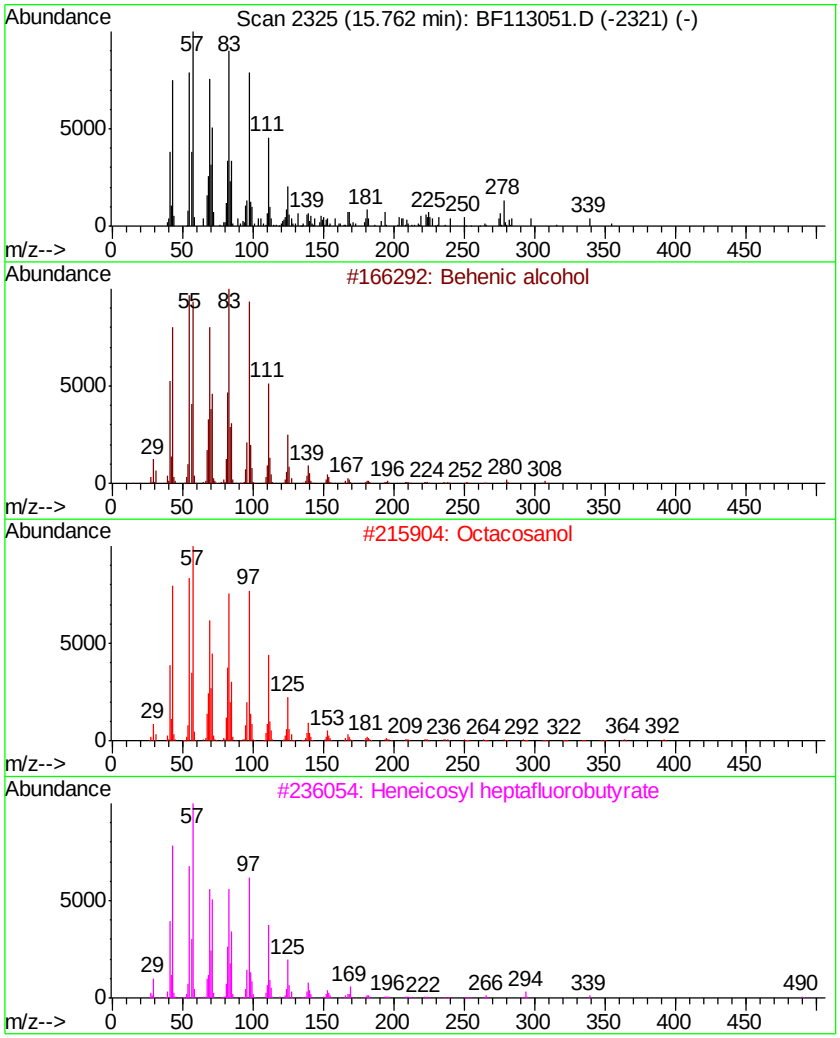
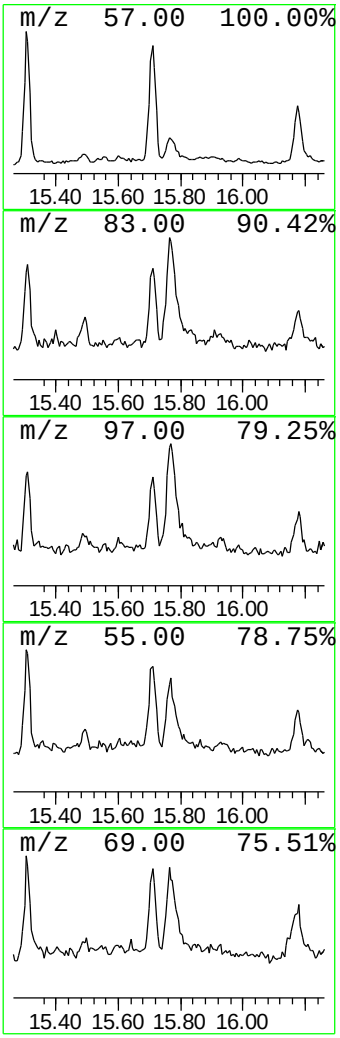
Peak Number 13 Behenic alcohol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.76	2.32 ng	253388	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	87
2	Octacosanol	410	C28H58O	000557-61-9	81
3	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	70
4	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	70
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	70





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031419\
Data File : BF113051.D
Acq On : 14 Mar 2019 15:55
Operator : JU/SJ
Sample : K1866-15
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-MH-12-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	86.2	ng	5477040	1	6.73	1271510	20.0
n-Hexadecanoic acid	11.78	17.6	ng	1792410	4	11.23	2042540	20.0
Octadecanoic acid	12.56	8.0	ng	945753	5	13.86	2358600	20.0
Cyclohexadecane	13.72	7.4	ng	876035	5	13.86	2358600	20.0
Hexadecane	14.04	2.4	ng	282814	5	13.86	2358600	20.0
Heptadecane	14.34	3.1	ng	372052	5	13.86	2358600	20.0
9-Octadecenamide,...	14.61	5.1	ng	559101	6	15.27	2183260	20.0
Octacosane	14.64	3.7	ng	403139	6	15.27	2183260	20.0
Heneicosane	14.95	3.9	ng	427347	6	15.27	2183260	20.0
Pentacosane	15.71	2.7	ng	297014	6	15.27	2183260	20.0
Behenic alcohol	15.76	2.3	ng	253388	6	15.27	2183260	20.0