LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022719\
Data File : BF112723.D
Acq On : 27 Feb 2019 17:07
Operator : JU/SJ
Sample : K1594-29
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-4(4-5)

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	548	554	557	rBV	3695493	3558041	96.47%	9.657%
2	6.369	722	728	731	rBV	3765670	3688398	100.00%	10.010%
3	6.504	747	751	755	rBV	3914225	3675848	99.66%	9.976%
4	6.739	787	791	794	rBV	1329639	1076789	29.19%	2.922%
5	6.810	799	803	807	rVB	60115	49996	1.36%	0.136%
6	6.892	814	817	821	rVB	3066999	2791030	75.67%	7.575%
7	7.292	881	885	888	rBV	2424888	2250088	61.00%	6.107%
8	8.016	1005	1008	1012	rBV	1575708	1321846	35.84%	3.588%
9	9.092	1187	1191	1195	rBV	4113177	3608331	97.83%	9.793%
10	9.374	1236	1239	1242	rBV	53791	43936	1.19%	0.119%
11	9.486	1254	1258	1261	rBV	308856	260511	7.06%	0.707%
12	9.769	1302	1306	1309	rVB	1414870	1295942	35.14%	3.517%
13	10.545	1434	1438	1442	rBV	2208896	1904805	51.64%	5.170%
14	11.239	1552	1556	1560	rVB	1406634	1158953	31.42%	3.145%
15	11.457	1590	1593	1596	rBV	56823	45235	1.23%	0.123%
16	11.780	1643	1648	1658	rBV	402446	518267	14.05%	1.407%
17	12.486	1762	1768	1775	rBV8	45366	101416	2.75%	0.275%
18	12.568	1776	1782	1794	rBV	885724	1184674	32.12%	3.215%
19	12.698	1801	1804	1821	rVB	267978	348700	9.45%	0.946%
20	12.821	1821	1825	1829	rBV	3066411	2732881	74.09%	7.417%
21	13.727	1976	1979	1989	rBV	274988	331417	8.99%	0.899%
22	13.862	1998	2002	2009	rVB	1563215	1366369	37.05%	3.708%
23	14.056	2031	2035	2038	rBV	117737	114167	3.10%	0.310%
24	14.362	2083	2087	2092	rBV	170882	171835	4.66%	0.466%
25	14.656	2134	2137	2145	rVV	194732	201115	5.45%	0.546%
26	14.727	2145	2149	2153	rVB	236918	235795	6.39%	0.640%
27	14.974	2187	2191	2199	rVB	235083	263584	7.15%	0.715%
28	15.268	2236	2241	2246	rVB	1184085	1363839	36.98%	3.701%
29	15.333	2247	2252	2257	rVB	251010	318376	8.63%	0.864%
30	15.739	2316	2321	2325	rBV	241273	346562	9.40%	0.941%
31	15.780	2325	2328	2332	rVV6	34878	52398	1.42%	0.142%
32	15.945	2354	2356	2366	rVB4	64586	107994	2.93%	0.293%
33	16.209	2396	2401	2407	rVB	143085	253188	6.86%	0.687%
34	16.756	2490	2494	2500	rVB2	58617	103480	2.81%	0.281%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022719\
Data File : BF112723.D
Acq On : 27 Feb 2019 17:07
Operator : JU/SJ
Sample : K1594-29
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-4(4-5)

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

Sum of corrected areas: 36845806

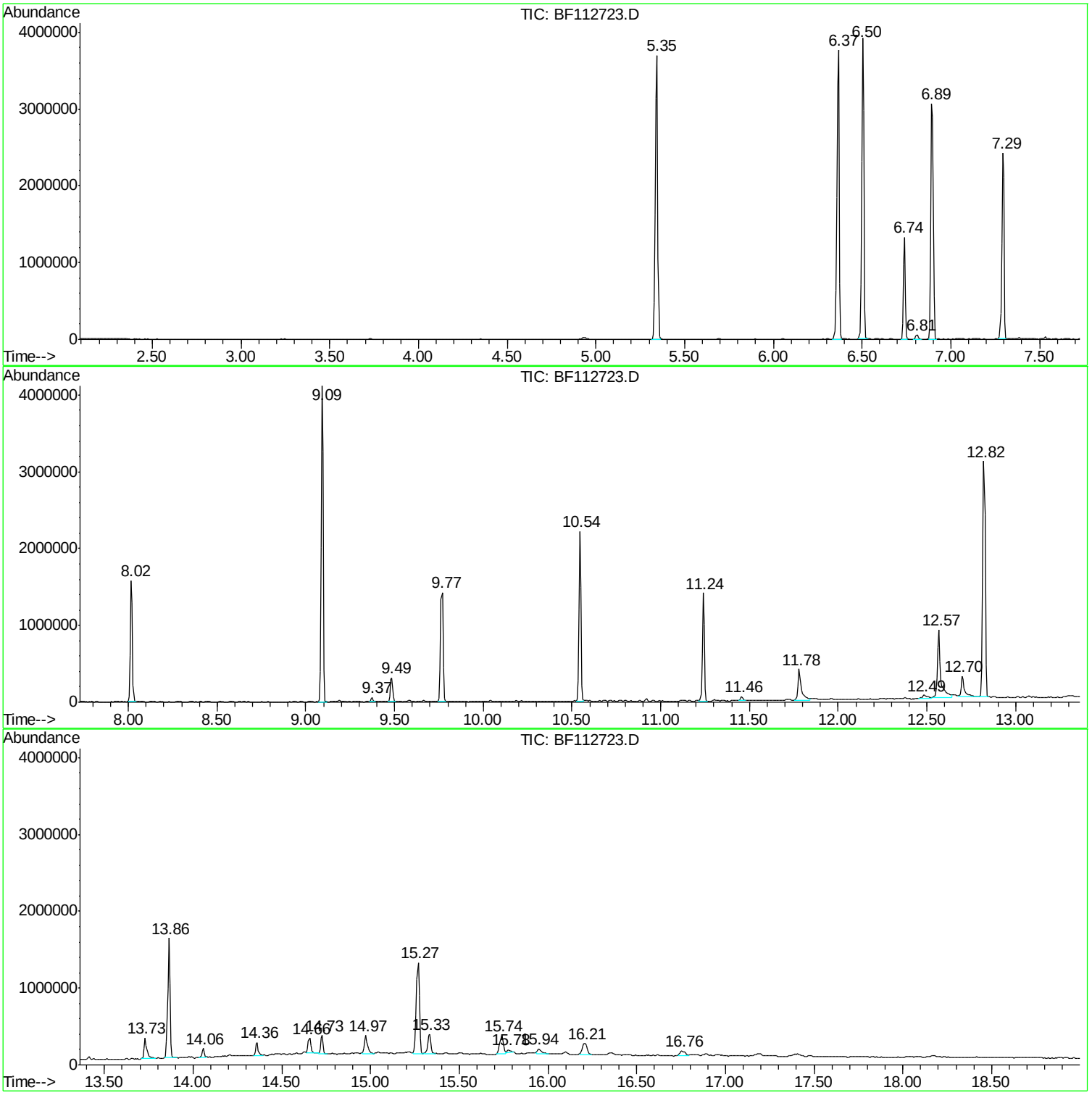
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022719\
Data File : BF112723.D
Acq On : 27 Feb 2019 17:07
Operator : JU/SJ
Sample : K1594-29
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-4(4-5)

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\BF022719\
Data File : BF112723.D
Acq On : 27 Feb 2019 17:07
Operator : JU/SJ
Sample : K1594-29
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-4(4-5)

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

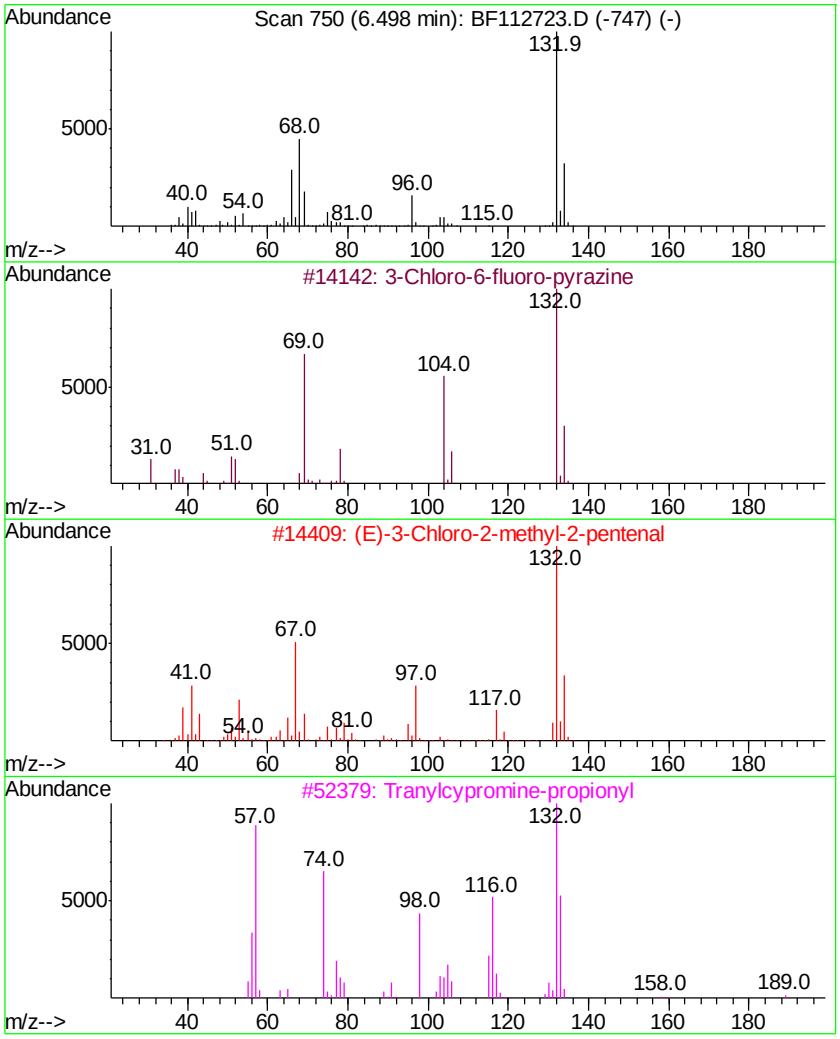
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

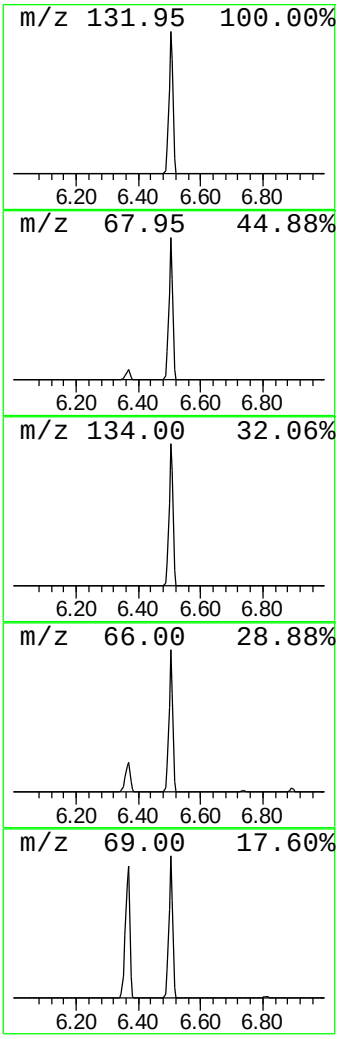
****

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	68.27 ng	3675850	1,4-Dichlorobenzene-d4	6.74

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	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022719\
Data File : BF112723.D
Acq On : 27 Feb 2019 17:07
Operator : JU/SJ
Sample : K1594-29
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-4(4-5)

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

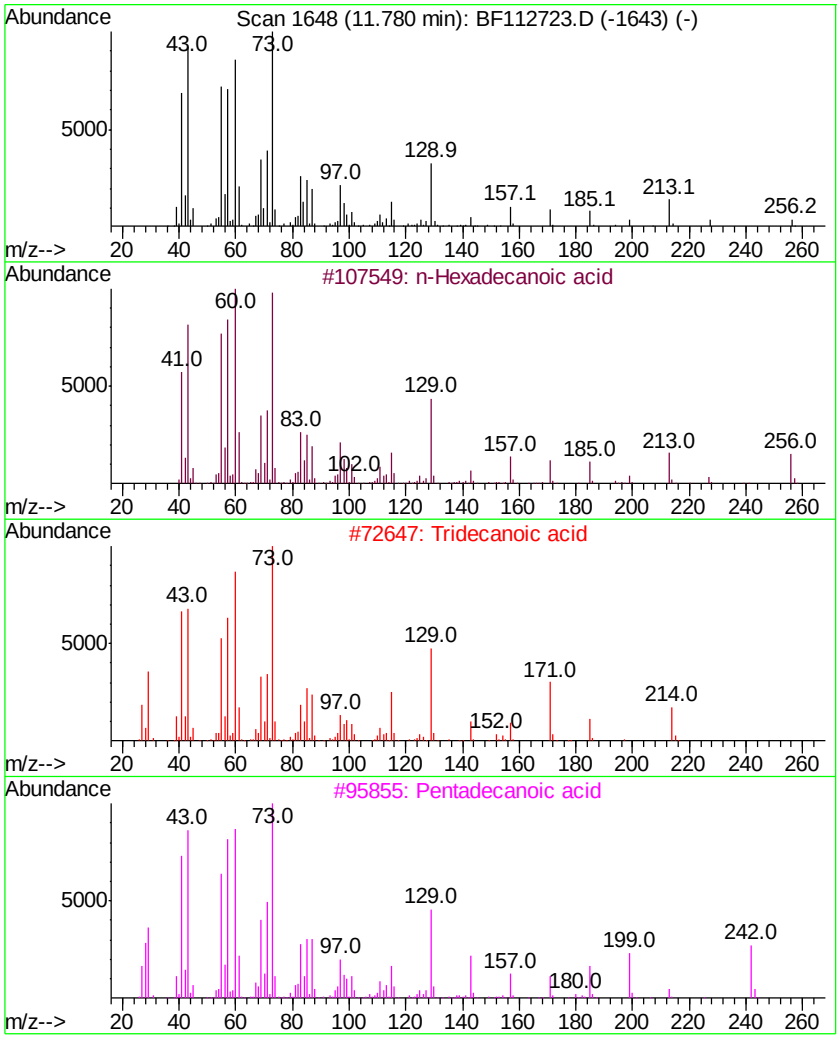
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

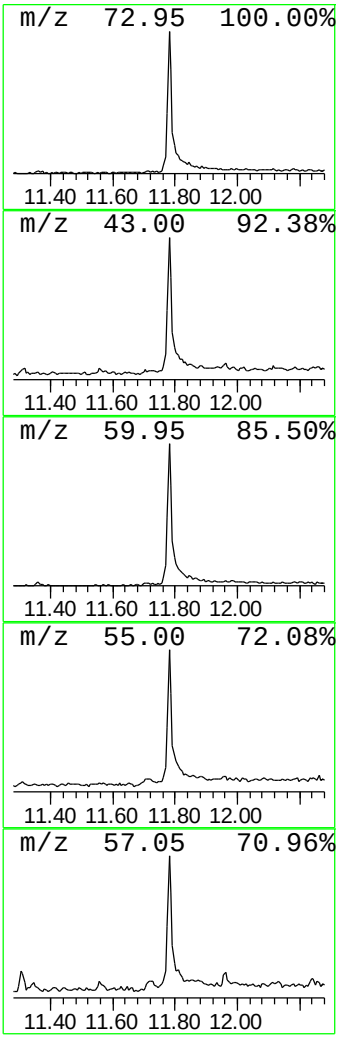
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	8.94 ng	518267	Phenanthrene-d10	11.24

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	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	Nonanoic acid	158	C9H18O2	000112-05-0	43





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022719\
Data File : BF112723.D
Acq On : 27 Feb 2019 17:07
Operator : JU/SJ
Sample : K1594-29
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-4(4-5)

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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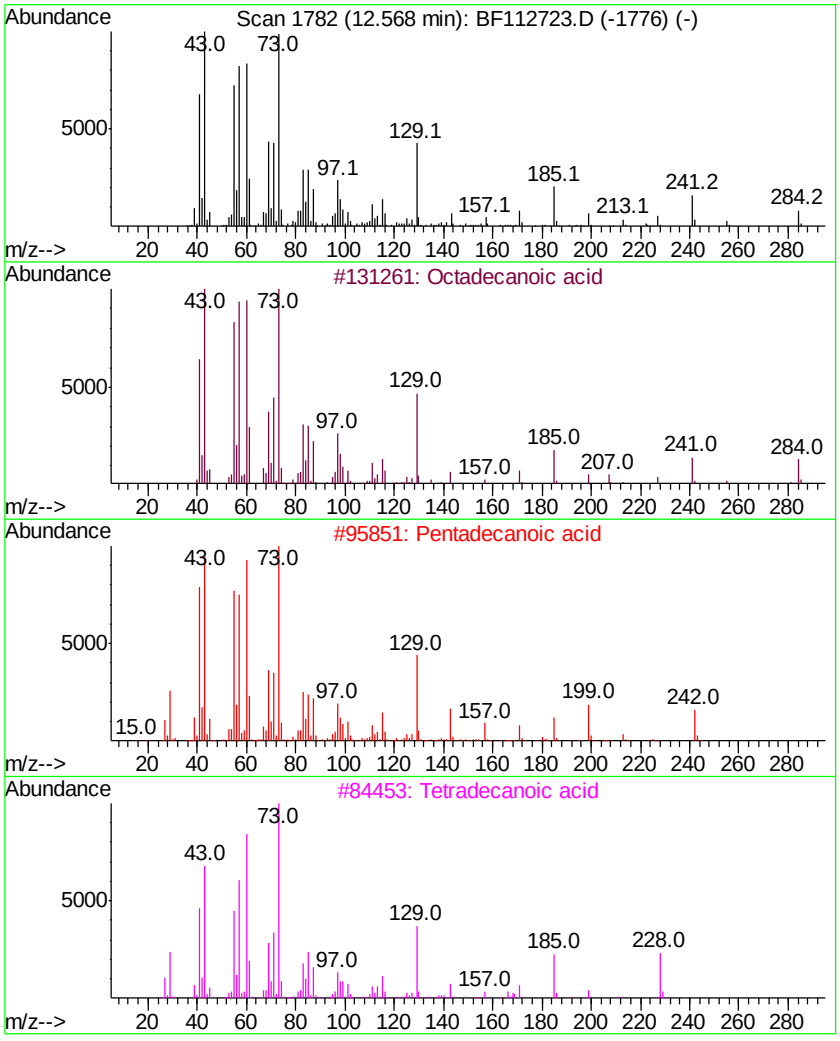
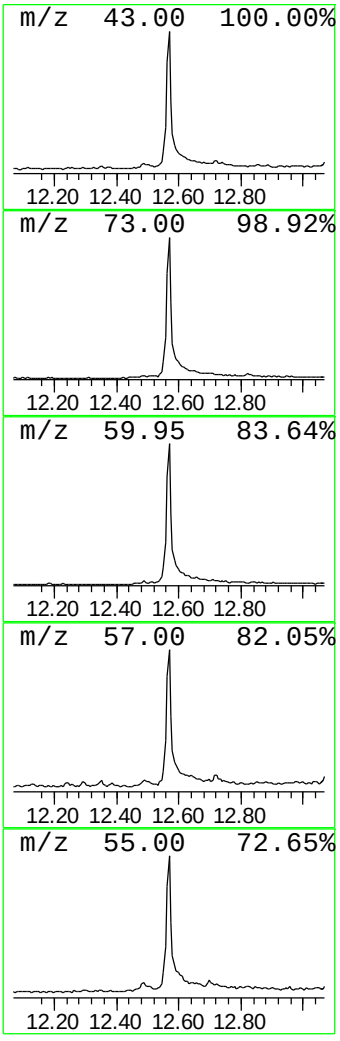
Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	17.34 ng	1184670	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	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022719\
Data File : BF112723.D
Acq On : 27 Feb 2019 17:07
Operator : JU/SJ
Sample : K1594-29
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-4(4-5)

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

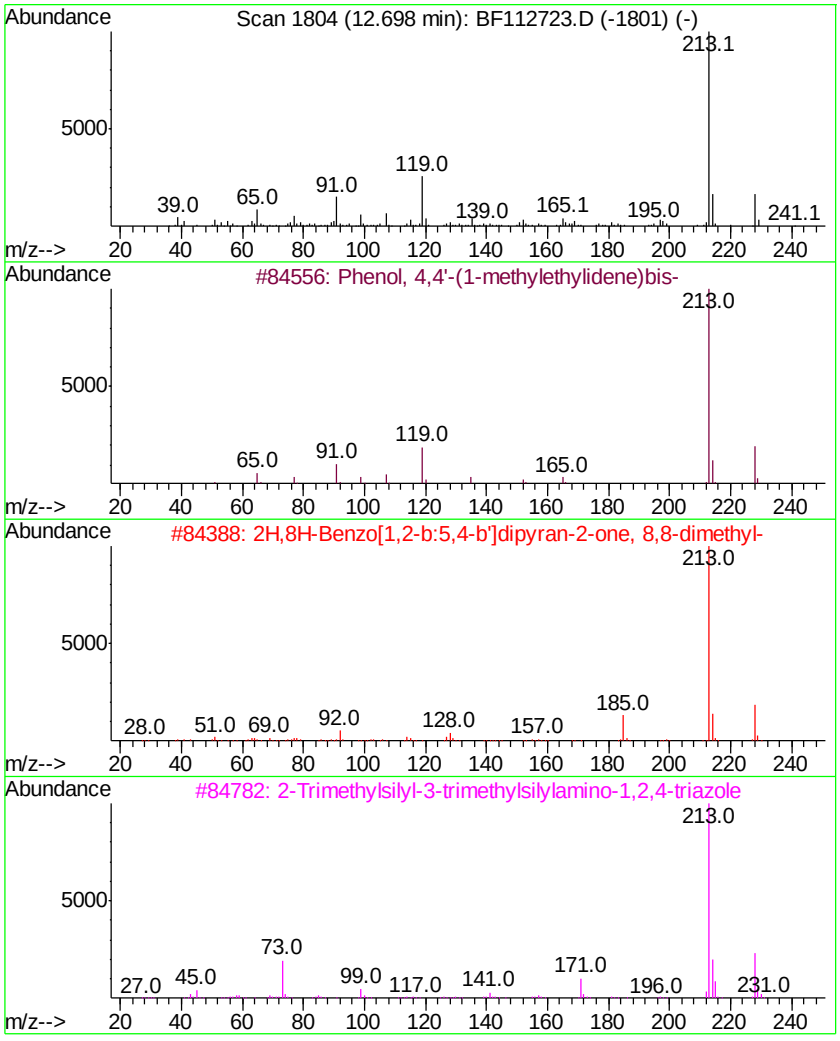
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

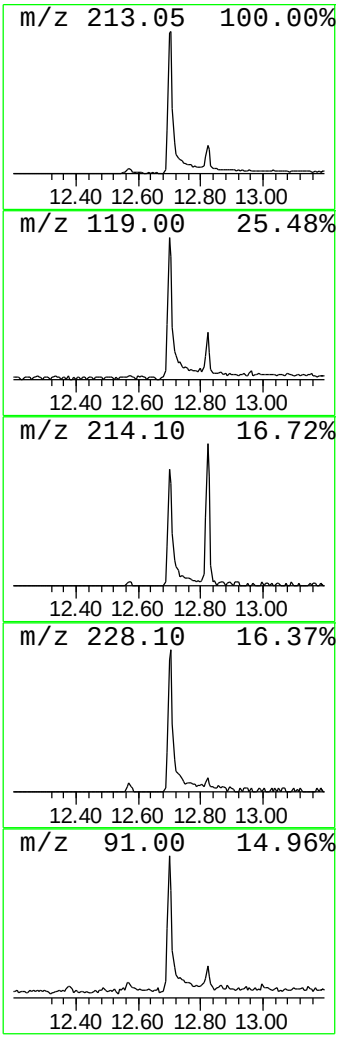
****

Peak Number 5 Phenol, 4,4'-(1-methylethyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	5.10 ng	348700	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	95
2	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	58
3	2-Trimethylsilyl-3-trimethylsily...	228	C8H20N4Si2	1000373-05-5	58
4	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	58
5	6-Bromo-2-(methylamino)tropone	213	C8H8BrNO	1000241-43-1	50





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022719\
Data File : BF112723.D
Acq On : 27 Feb 2019 17:07
Operator : JU/SJ
Sample : K1594-29
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-4(4-5)

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

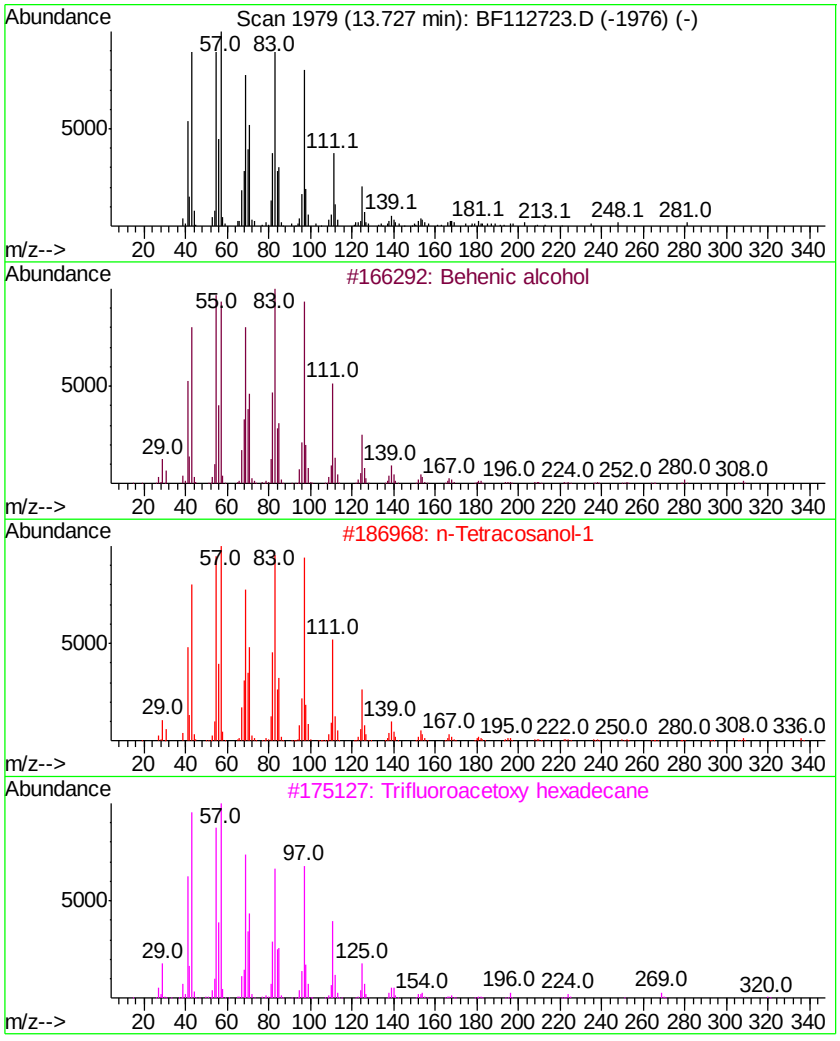
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

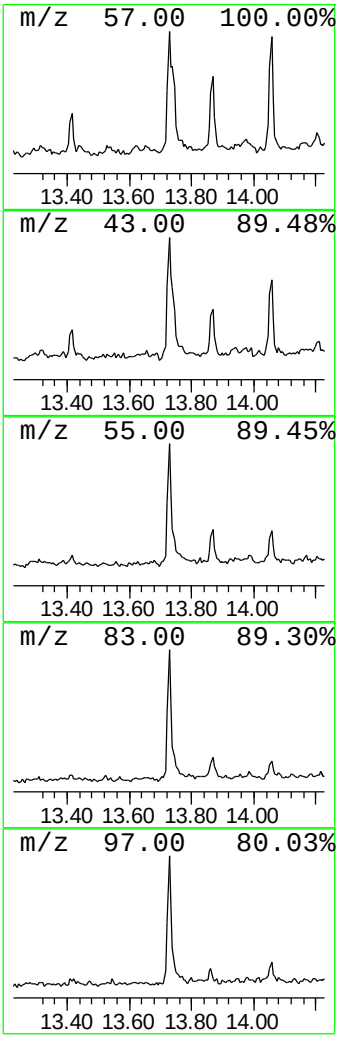
****

Peak Number 6 Behenic alcohol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	4.85 ng	331417	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91





Library Search Compound Report

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Data File : BF112723.D
Acq On : 27 Feb 2019 17:07
Operator : JU/SJ
Sample : K1594-29
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-4(4-5)

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

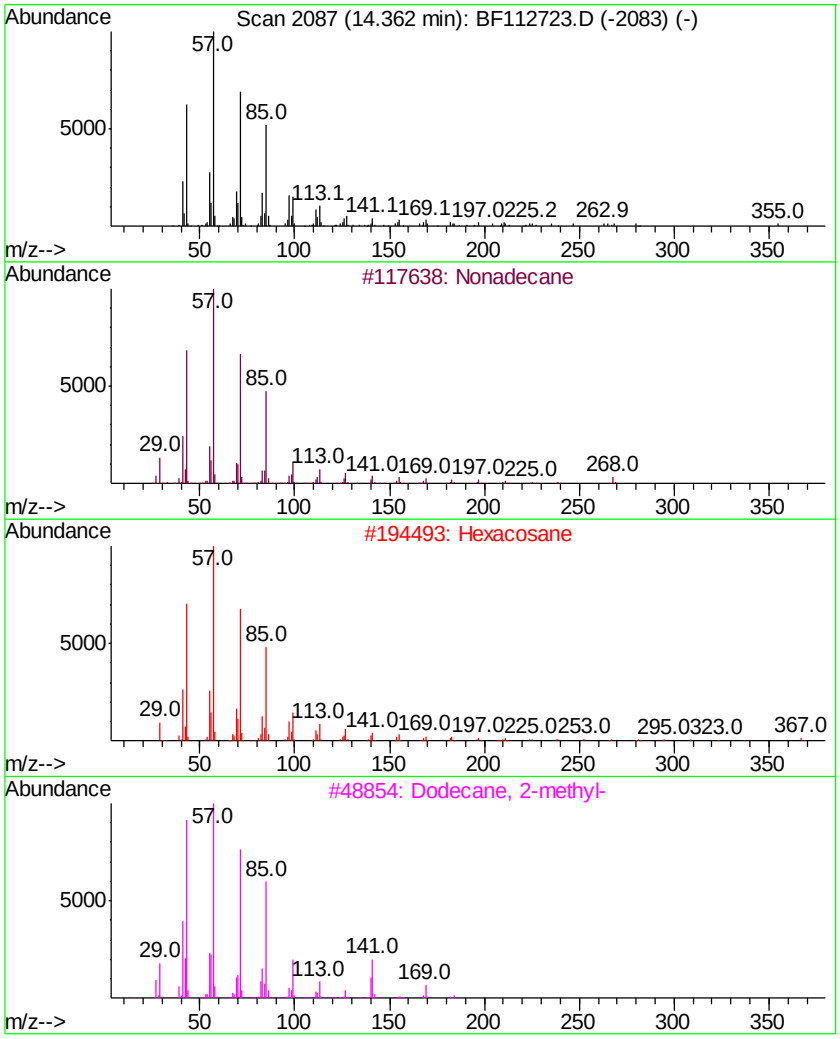
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

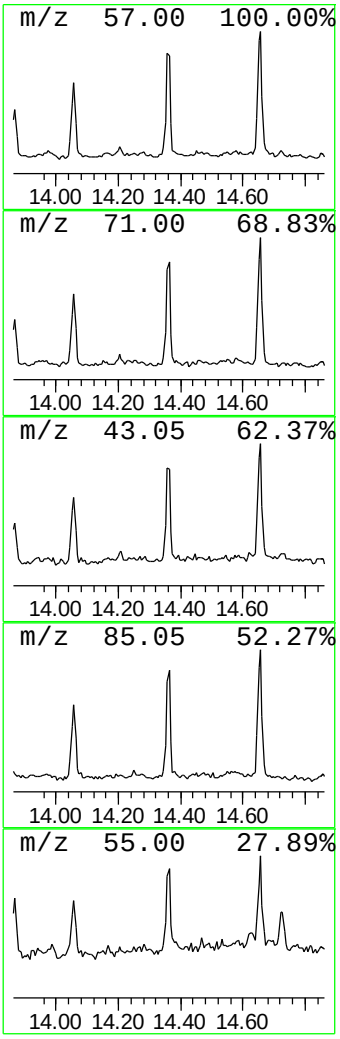
****

Peak Number 7 Nonadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	2.52 ng	171835	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	95
2	Hexacosane	366	C26H54	000630-01-3	90
3	Dodecane, 2-methyl-	184	C13H28	001560-97-0	90
4	Heptadecane	240	C17H36	000629-78-7	87
5	Tetracosane	338	C24H50	000646-31-1	87





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Data File : BF112723.D
Acq On : 27 Feb 2019 17:07
Operator : JU/SJ
Sample : K1594-29
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-4(4-5)

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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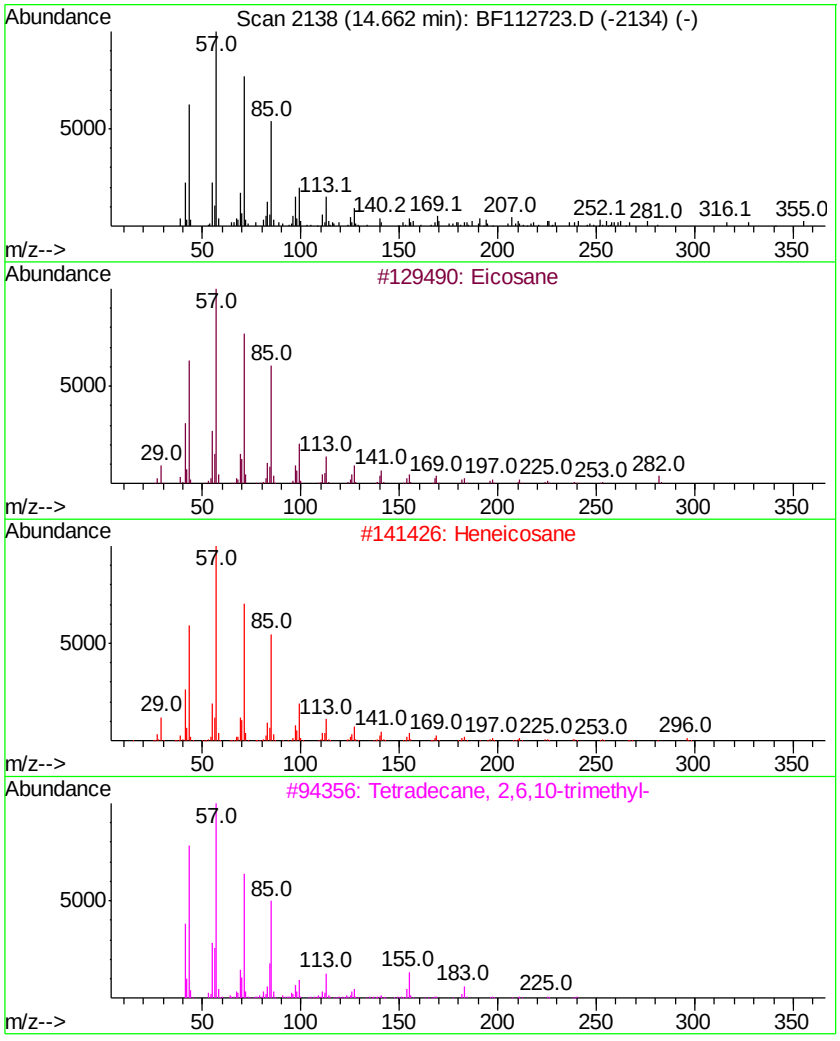
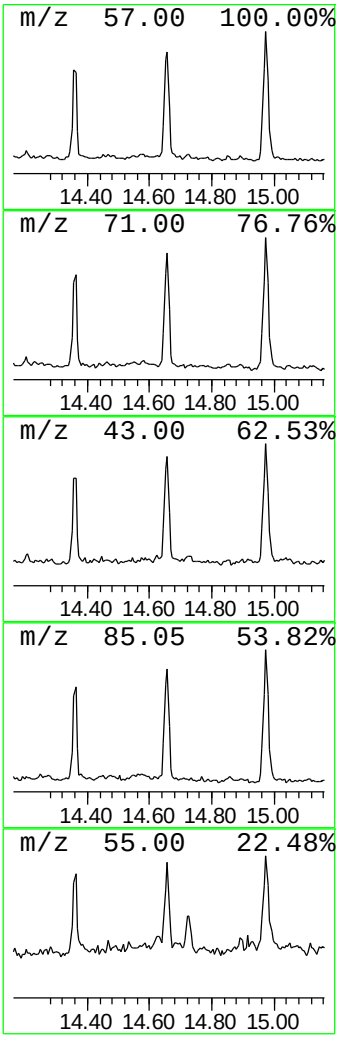
Peak Number 8 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	2.95 ng	201115	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Heneicosane	296	C21H44	000629-94-7	87
3	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	83
4	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	72
5	Octacosane	394	C28H58	000630-02-4	68





Library Search Compound Report

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Data File : BF112723.D
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Sample : K1594-29
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-4(4-5)

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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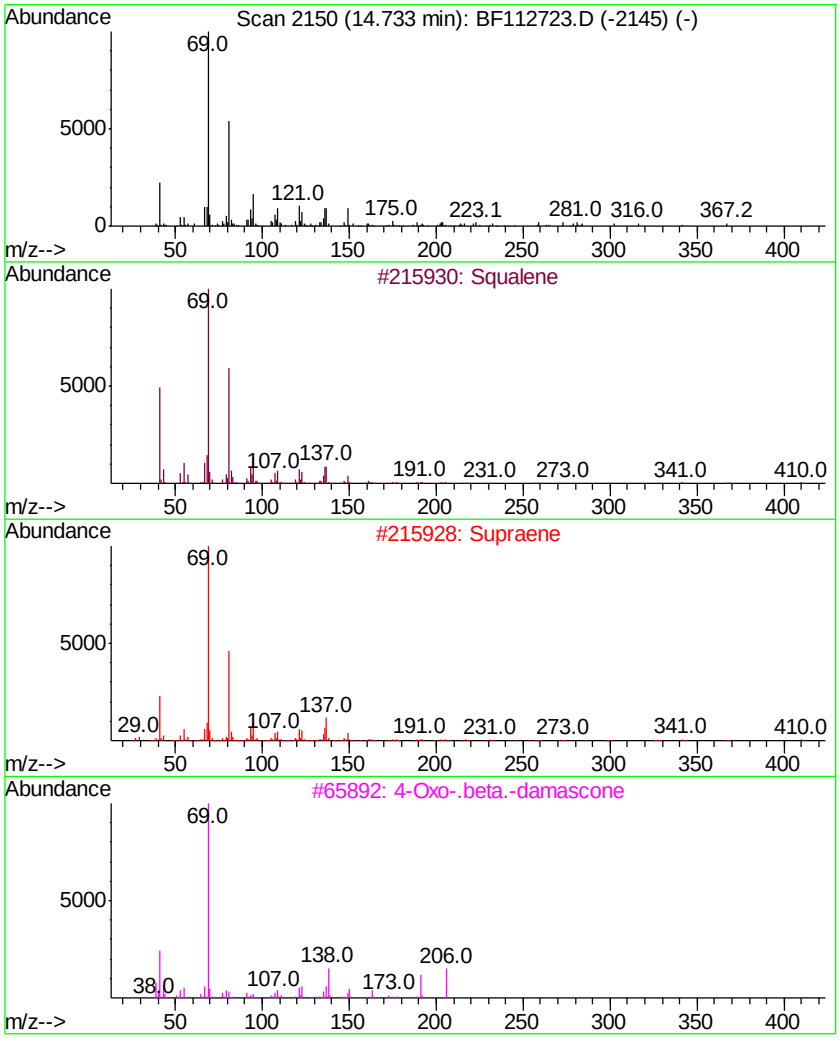
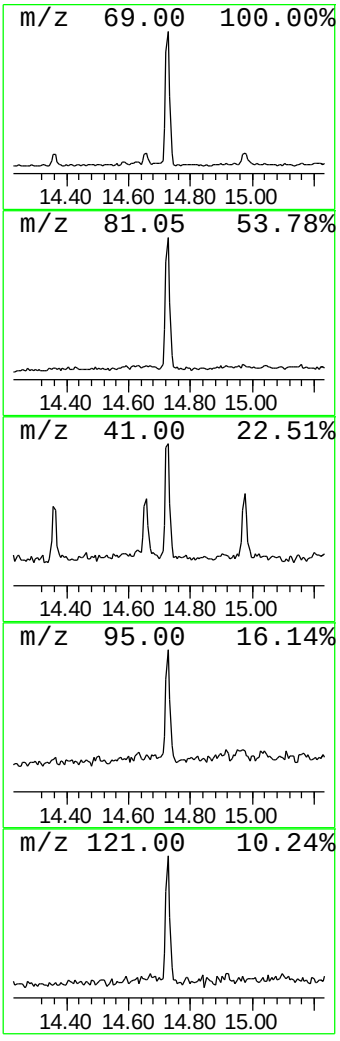
Peak Number 9 Squalene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	3.46 ng	235795	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	4-Oxo-.beta.-damascone	206	C13H18O2	053398-08-6	72
4	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	72
5	Trideca-1,3,7,11-tetraene-1,1-di...	268	C18H24N2	1000159-88-9	50





Library Search Compound Report

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Data File : BF112723.D
Acq On : 27 Feb 2019 17:07
Operator : JU/SJ
Sample : K1594-29
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-4(4-5)

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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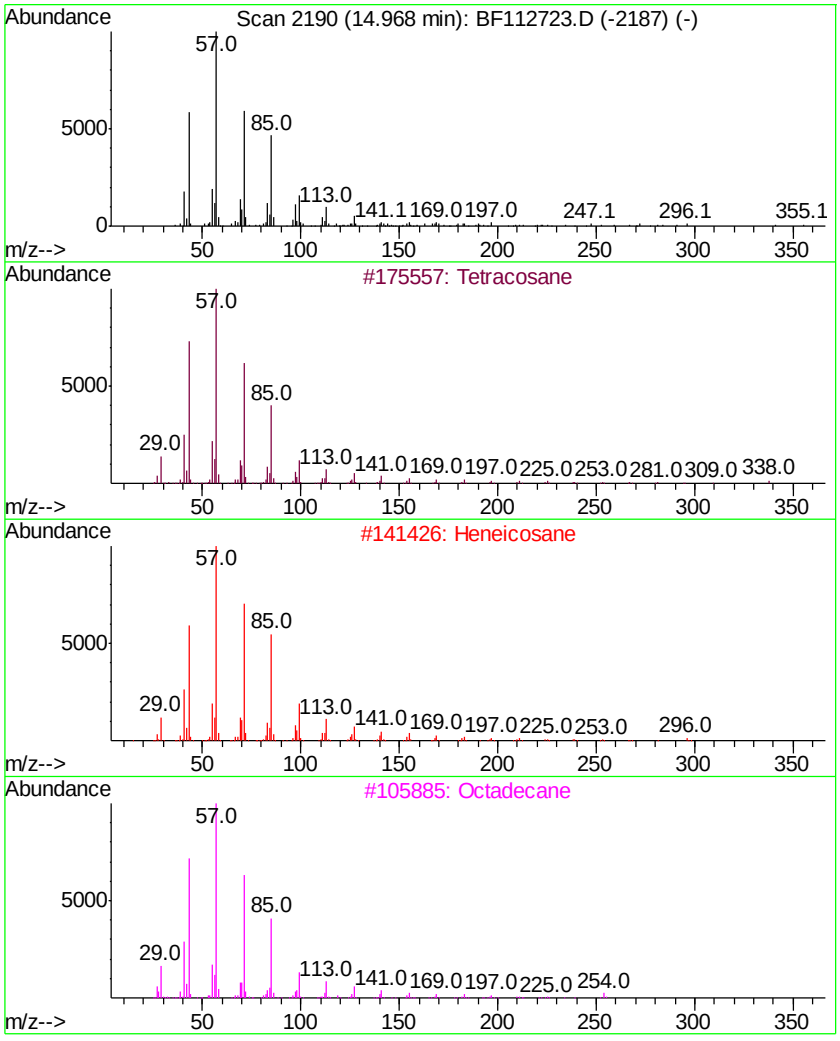
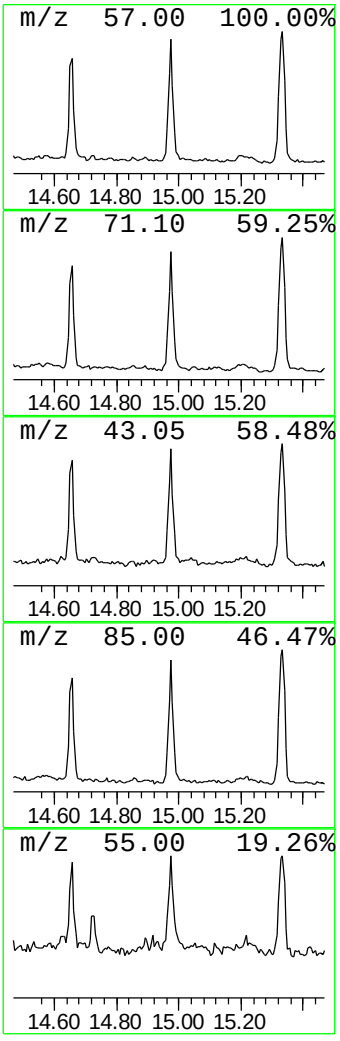
Peak Number 10 Tetracosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	3.87 ng	263584	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Heneicosane	296	C21H44	000629-94-7	90
3	Octadecane	254	C18H38	000593-45-3	87
4	Nonadecane	268	C19H40	000629-92-5	87
5	Eicosane	282	C20H42	000112-95-8	86





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Acq On : 27 Feb 2019 17:07
Operator : JU/SJ
Sample : K1594-29
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-4(4-5)

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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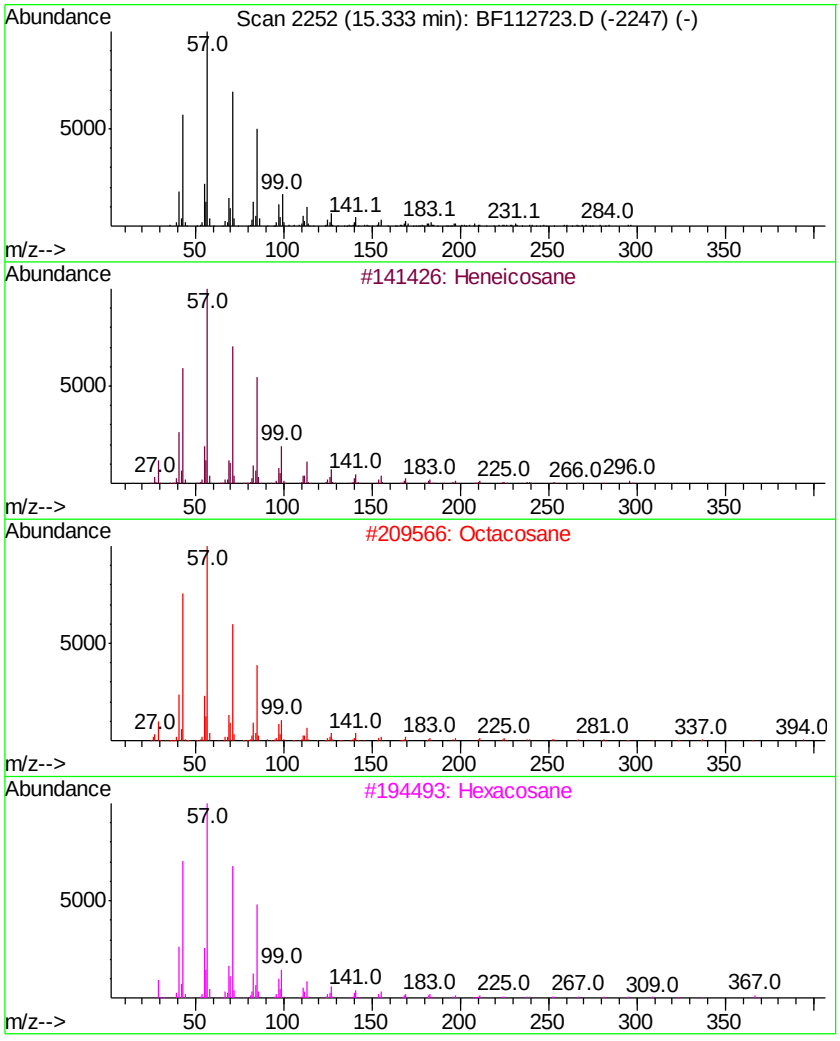
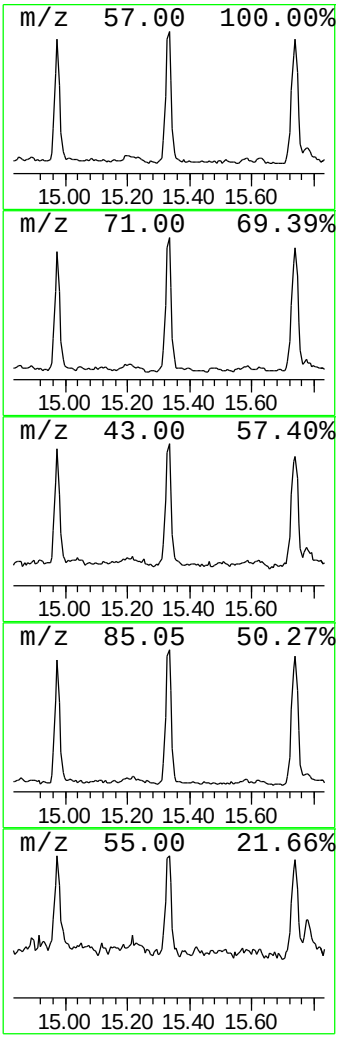
Peak Number 11 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.33	4.67 ng	318376	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	97
2	Octacosane	394	C28H58	000630-02-4	91
3	Hexacosane	366	C26H54	000630-01-3	90
4	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87
5	Octadecane	254	C18H38	000593-45-3	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022719\
Data File : BF112723.D
Acq On : 27 Feb 2019 17:07
Operator : JU/SJ
Sample : K1594-29
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-4(4-5)

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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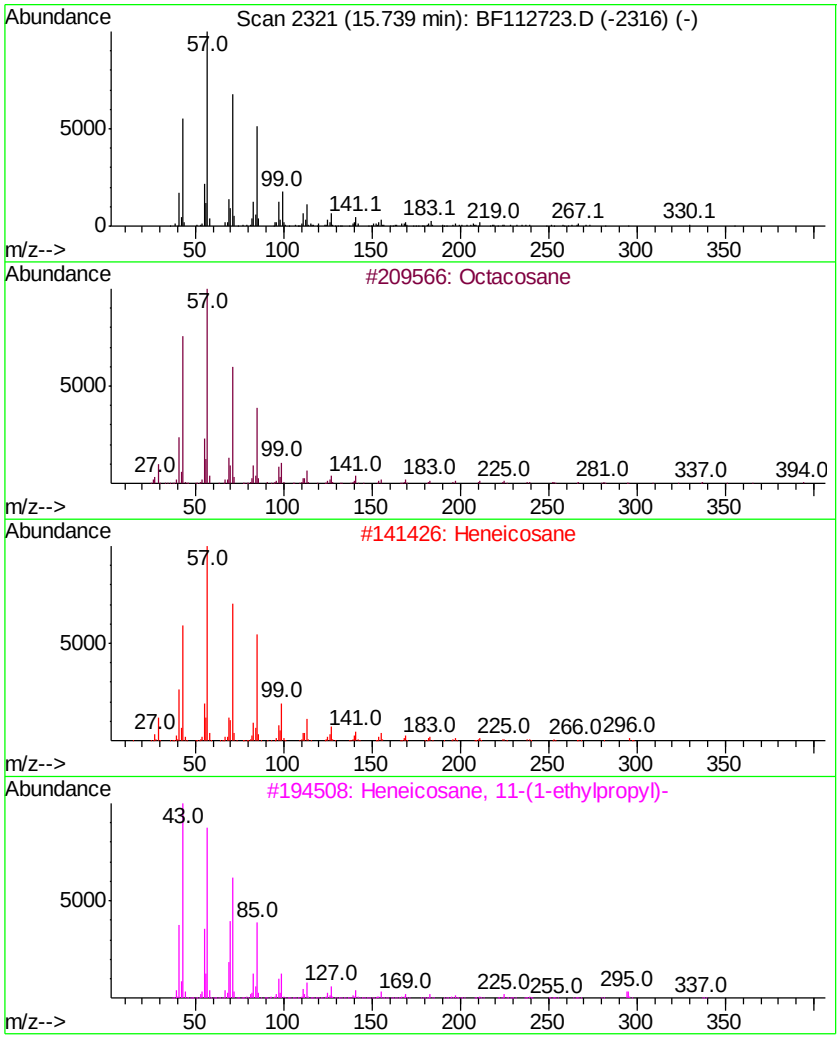
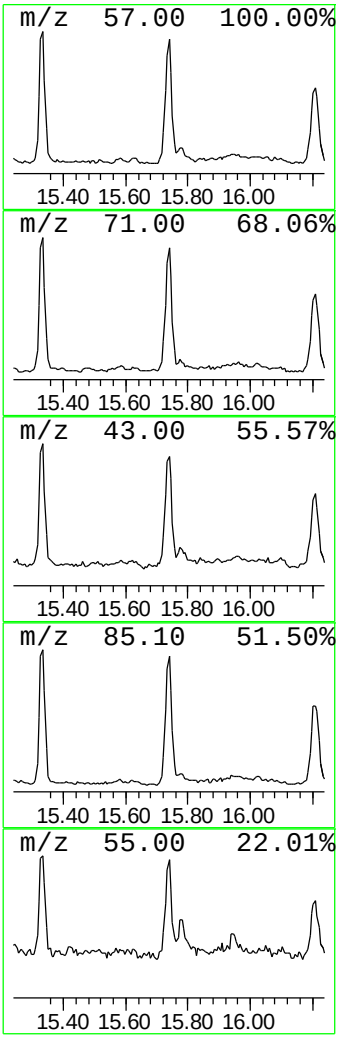
Peak Number 12 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	5.08 ng	346562	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	90
5	Tetratetracontane	619	C44H90	007098-22-8	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF022719\
Data File : BF112723.D
Acq On : 27 Feb 2019 17:07
Operator : JU/SJ
Sample : K1594-29
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-4(4-5)

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	68.3	ng	3675850	1	6.74	1076790	20.0
n-Hexadecanoic acid	11.78	8.9	ng	518267	4	11.24	1158950	20.0
Octadecanoic acid	12.57	17.3	ng	1184670	5	13.86	1366370	20.0
Phenol, 4,4'-(1-m...	12.70	5.1	ng	348700	5	13.86	1366370	20.0
Behenic alcohol	13.73	4.8	ng	331417	5	13.86	1366370	20.0
Nonadecane	14.36	2.5	ng	171835	5	13.86	1366370	20.0
Eicosane	14.66	3.0	ng	201115	6	15.27	1363840	20.0
Squalene	14.73	3.5	ng	235795	6	15.27	1363840	20.0
Tetracosane	14.97	3.9	ng	263584	6	15.27	1363840	20.0
Heneicosane	15.33	4.7	ng	318376	6	15.27	1363840	20.0
Octacosane	15.74	5.1	ng	346562	6	15.27	1363840	20.0