LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082418\
Data File : BF108466.D
Acq On : 24 Aug 2018 16:31
Operator : JU/SJ
Sample : J4581-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q3-A1

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-BF080818.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	2.366	3	5	15	rVB	827758	911209	34.76%	3.089%
2	5.242	490	494	502	rVB	99663	124444	4.75%	0.422%
3	5.631	555	560	563	rBV	2495097	2370975	90.45%	8.038%
4	6.625	723	729	740	rVB	2427809	2620236	99.96%	8.884%
5	6.772	749	754	757	rBV	2692718	2548229	97.22%	8.639%
6	7.001	789	793	796	rBV	880556	819098	31.25%	2.777%
7	7.154	815	819	823	rBV	2066679	1761015	67.18%	5.970%
8	7.560	883	888	891	rBV	1721766	1661906	63.40%	5.634%
9	8.283	1006	1011	1014	rBV	1166494	1032358	39.38%	3.500%
10	9.354	1188	1193	1197	rBV	2880917	2621200	100.00%	8.887%
11	9.748	1256	1260	1263	rBV	527773	470090	17.93%	1.594%
12	10.042	1306	1310	1314	rBV2	1306380	1218518	46.49%	4.131%
13	10.672	1410	1417	1422	rBV6	15209	39400	1.50%	0.134%
14	10.836	1441	1445	1458	rBV	2105559	2042425	77.92%	6.925%
15	10.924	1458	1460	1465	rVB	28565	32518	1.24%	0.110%
16	11.377	1534	1537	1539	rBV	33168	27417	1.05%	0.093%
17	11.542	1561	1565	1567	rBV	1326648	1250491	47.71%	4.240%
18	11.560	1567	1568	1572	rVB	251642	197783	7.55%	0.671%
19	11.613	1572	1577	1581	rBV	52180	53463	2.04%	0.181%
20	11.766	1599	1603	1607	rBV	24063	29418	1.12%	0.100%
21	12.042	1644	1650	1653	rBV	428412	489584	18.68%	1.660%
22	12.160	1666	1670	1672	rBV3	42192	52352	2.00%	0.177%
23	12.366	1702	1705	1710	rVB	30155	30320	1.16%	0.103%
24	12.601	1740	1745	1747	rBV2	26421	40573	1.55%	0.138%
25	12.760	1768	1772	1776	rVB	366651	311547	11.89%	1.056%
26	12.830	1780	1784	1791	rBV3	89218	117209	4.47%	0.397%
27	12.989	1805	1811	1816	rBV	274871	349198	13.32%	1.184%
28	13.124	1830	1834	1837	rBV	2770615	2466840	94.11%	8.363%
29	13.201	1844	1847	1851	rBV2	19590	33674	1.28%	0.114%
30	13.330	1865	1869	1873	rVB2	54000	75933	2.90%	0.257%
31	13.383	1875	1878	1880	rBV	34910	28877	1.10%	0.098%
32	13.677	1924	1928	1931	rVB2	58726	58754	2.24%	0.199%
33	14.007	1980	1984	1986	rBV2	89737	89609	3.42%	0.304%
34	14.071	1991	1995	2004	rVB5	49672	115757	4.42%	0.392%

LSC Area Percent Report

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Acq On : 24 Aug 2018 16:31
Operator : JU/SJ
Sample : J4581-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q3-A1

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-BF080818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.195	2011	2016	2018	rBV	863507	903424	34.47%	3.063%
36	14.218	2018	2020	2027	rVB	107863	105121	4.01%	0.356%
37	14.318	2032	2037	2040	rBV2	98798	114713	4.38%	0.389%
38	14.630	2086	2090	2093	rBV	119626	112544	4.29%	0.382%
39	14.954	2140	2145	2149	rVB2	159391	194440	7.42%	0.659%
40	15.036	2155	2159	2163	rVB	138601	156872	5.98%	0.532%
41	15.277	2197	2200	2203	rBV	77022	116216	4.43%	0.394%
42	15.312	2203	2206	2215	rVB2	185151	251953	9.61%	0.854%
43	15.607	2252	2256	2262	rVB	49091	84853	3.24%	0.288%
44	15.677	2264	2268	2271	rBV	67941	79781	3.04%	0.270%
45	15.748	2272	2280	2285	rVV2	535916	931895	35.55%	3.159%
46	16.201	2352	2357	2365	rVB	145017	226884	8.66%	0.769%
47	16.754	2446	2451	2457	rVB2	71631	124242	4.74%	0.421%

Sum of corrected areas: 29495358

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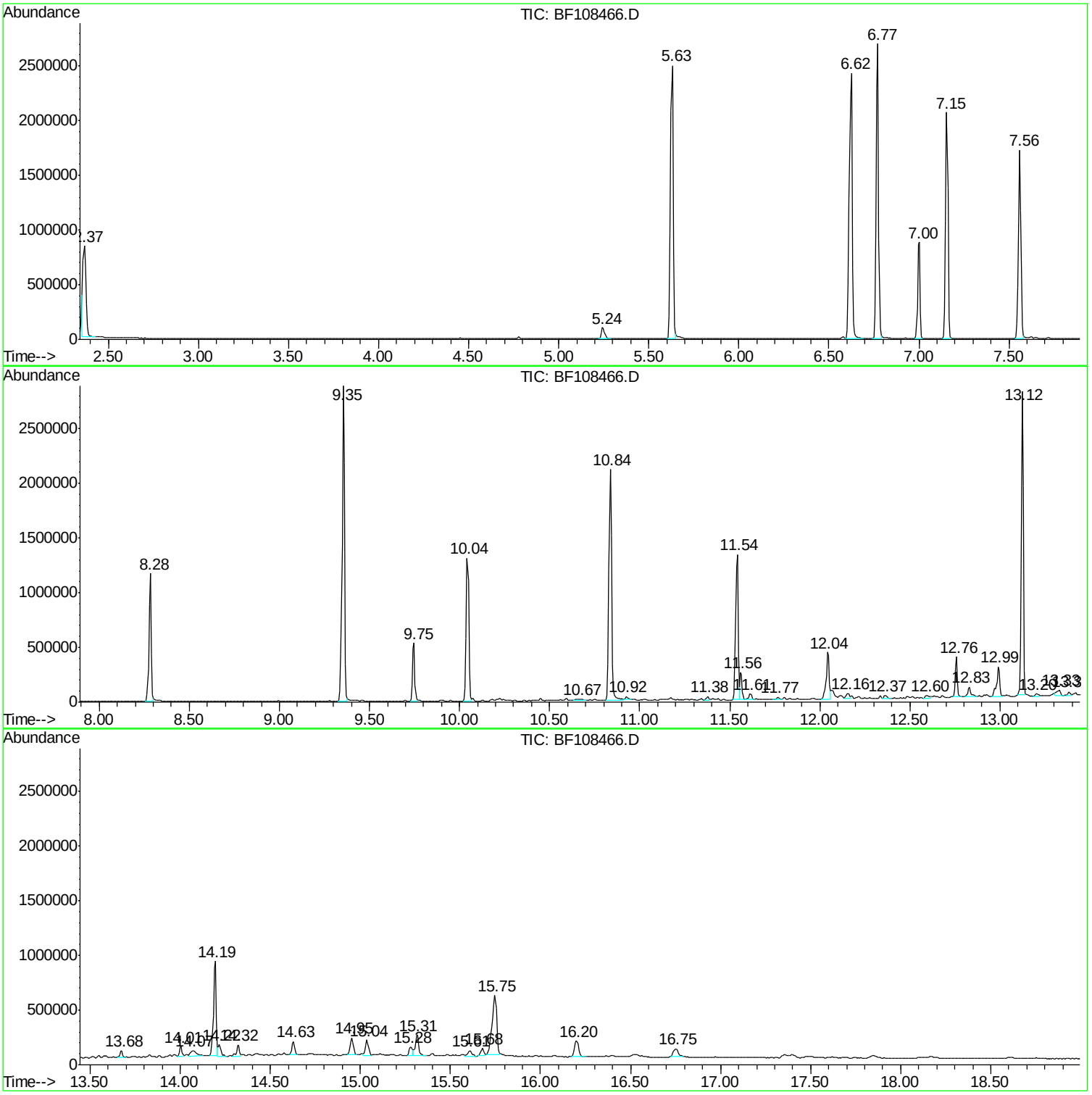
Instrument :
BNA_F
ClientSampleId :
EP1-Q3-A1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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\BF082418\
Data File : BF108466.D
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Misc :
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Instrument : BNA_F
ClientSampleId : EP1-Q3-A1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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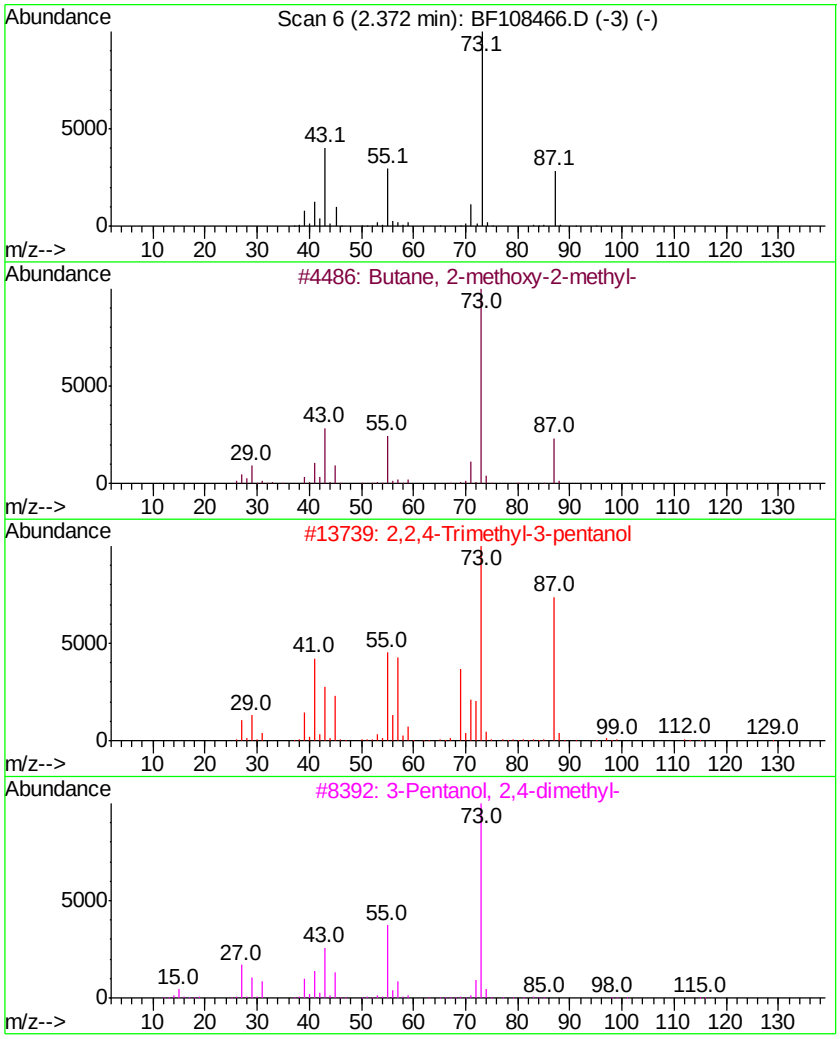
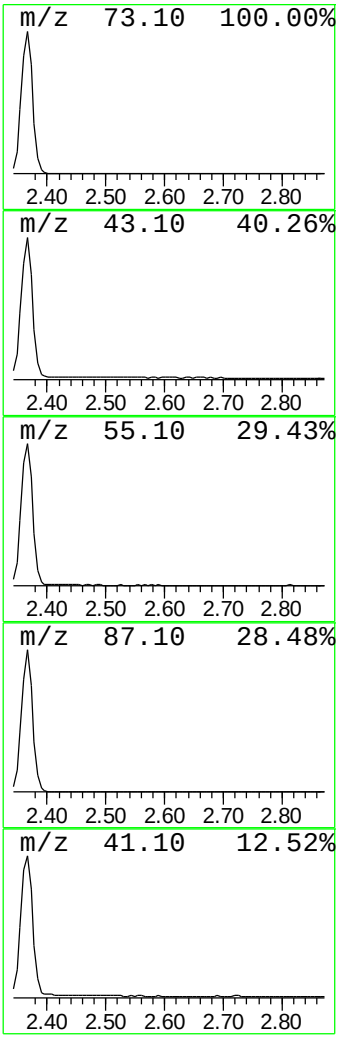
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.37	22.25 ng	911209	1,4-Dichlorobenzene-d4	7.00

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	39
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35





Library Search Compound Report

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Operator : JU/SJ
Sample : J4581-01
Misc :
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Instrument : BNA_F
ClientSampleId : EP1-Q3-A1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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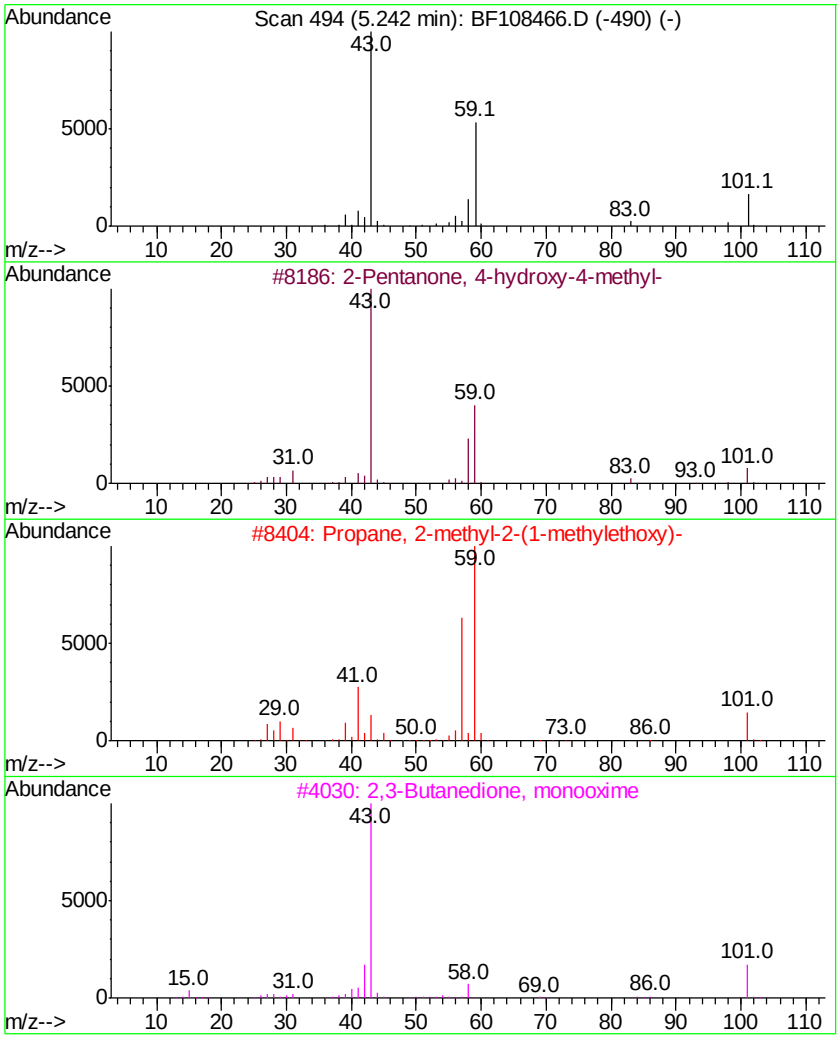
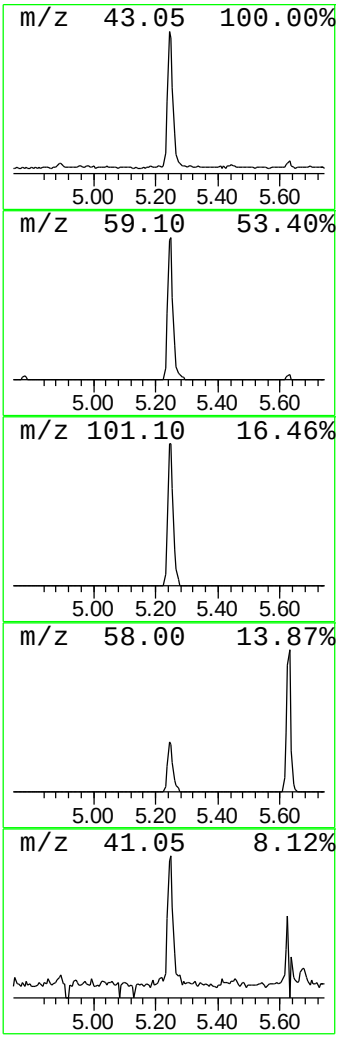
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	3.04 ng	124444	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9





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Data File : BF108466.D
Acq On : 24 Aug 2018 16:31
Operator : JU/SJ
Sample : J4581-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q3-A1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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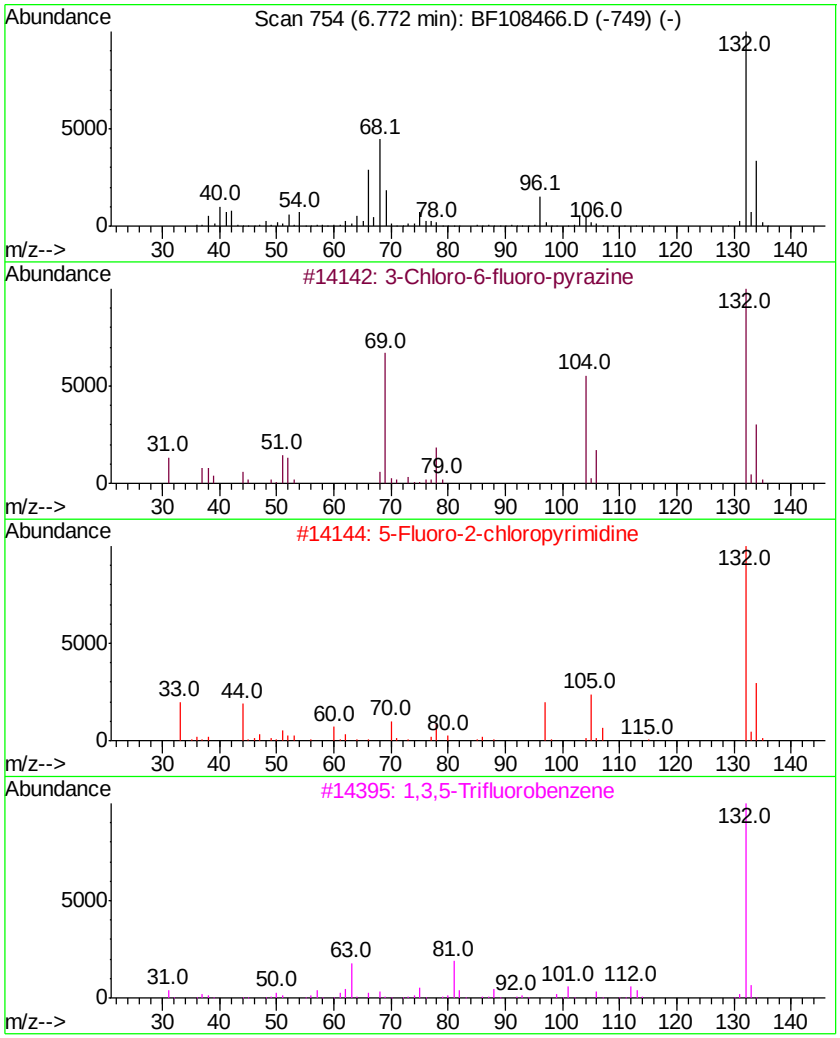
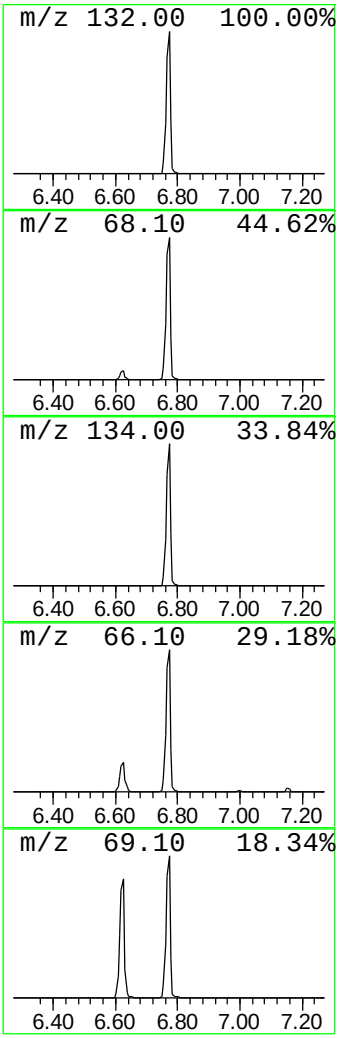
Peak Number 3 unknown6.77 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	62.22 ng	2548230	1,4-Dichlorobenzene-d4	7.00

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	16
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	Xenon	132	Xe	007440-63-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Instrument : BNA_F
ClientSampleId : EP1-Q3-A1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

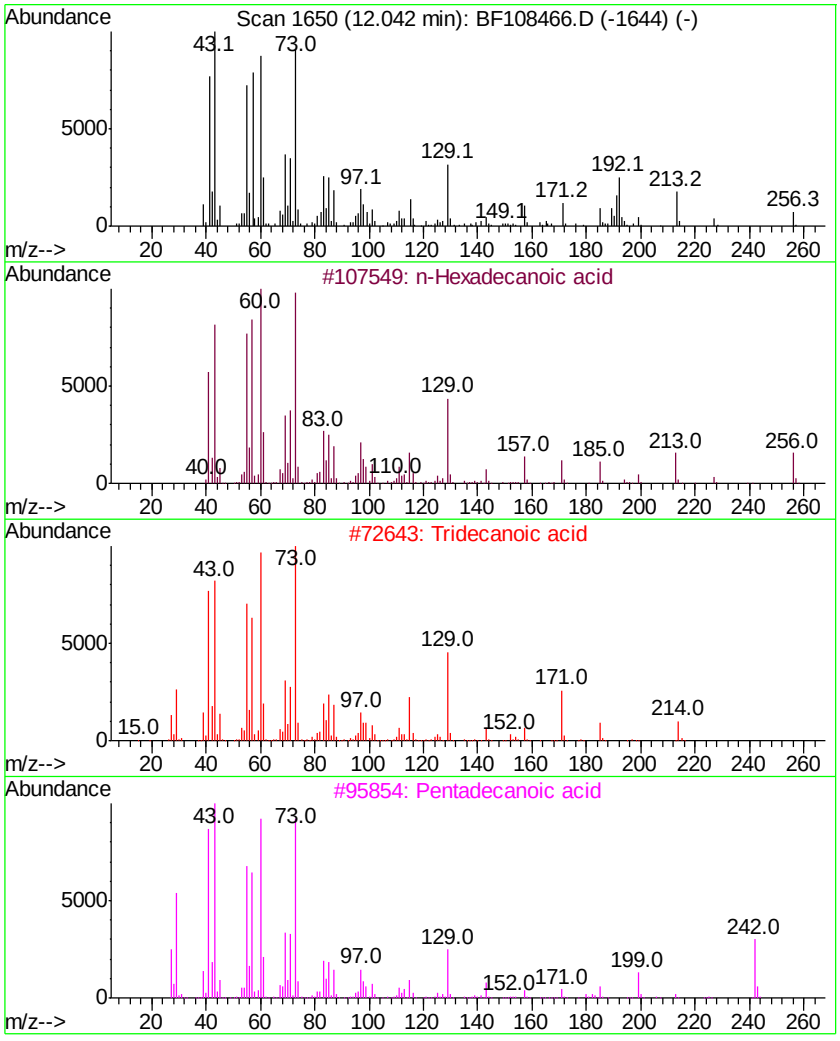
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

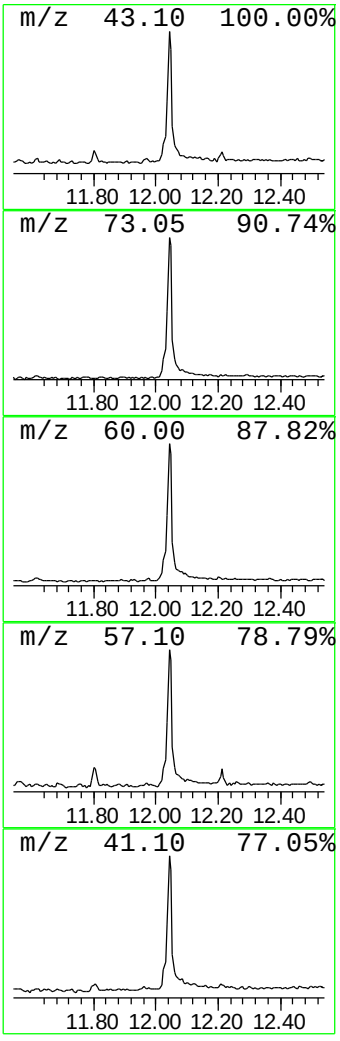
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.04	7.83 ng	489584	Phenanthrene-d10	11.54

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	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	n-Decanoic acid	172	C10H20O2	000334-48-5	53
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	53





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Sample : J4581-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q3-A1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
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TIC Library : C:\DATABASE\NIST11.L
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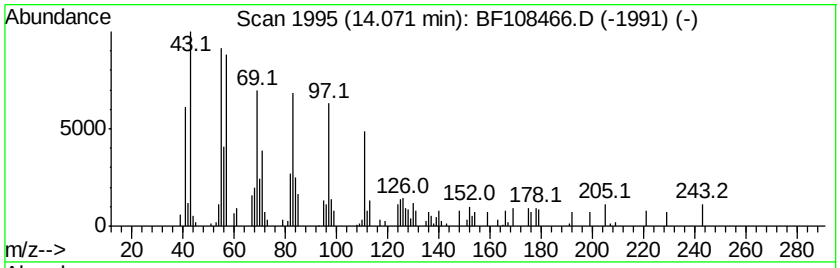
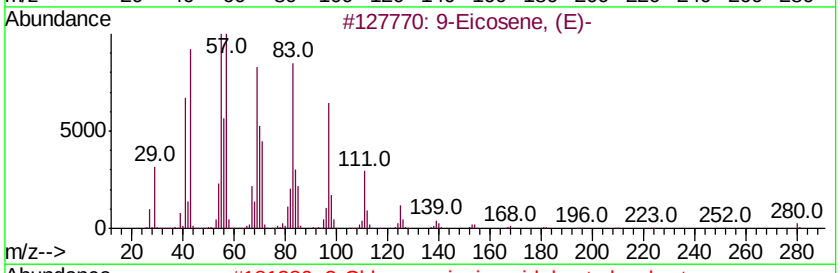
****

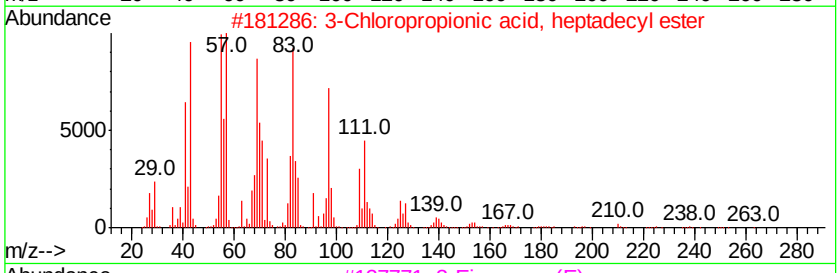
Peak Number 6 9-Eicosene, (E)- Concentration Rank 10

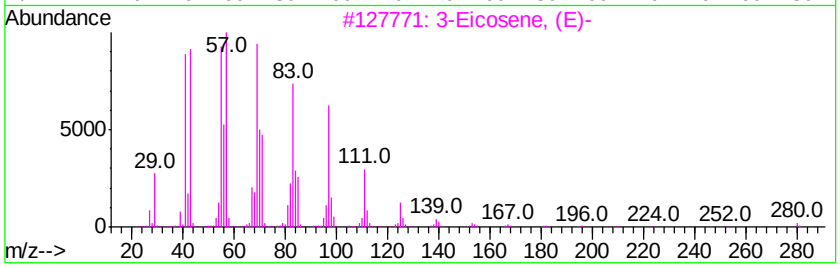
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.07	2.56 ng	115757	Chrysene-d12	14.19

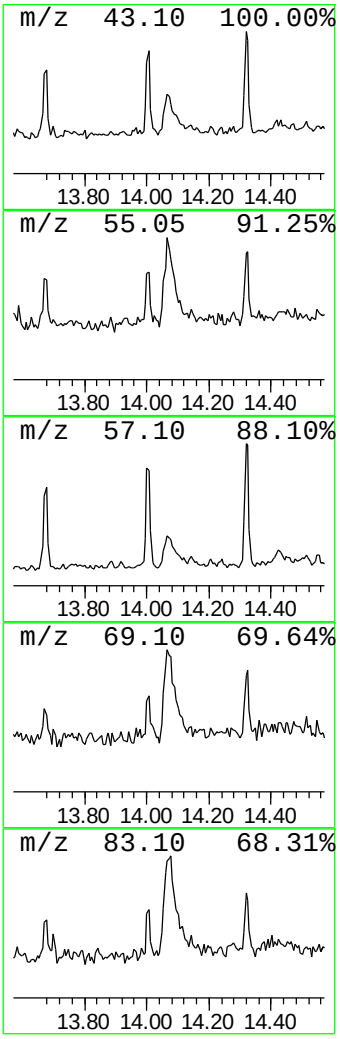
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Eicosene, (E)-	280	C20H40	074685-29-3	68
2	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	68
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	64
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	62
5	1-Hexadecanol	242	C16H34O	036653-82-4	58











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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q3-A1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

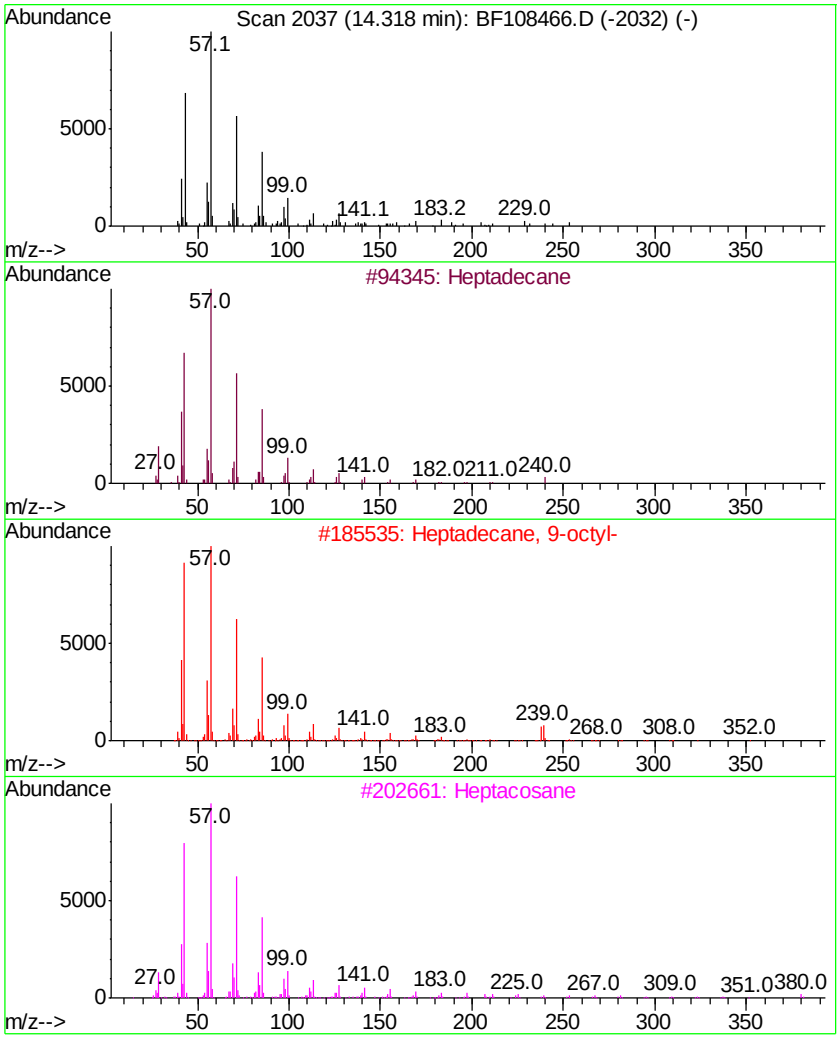
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

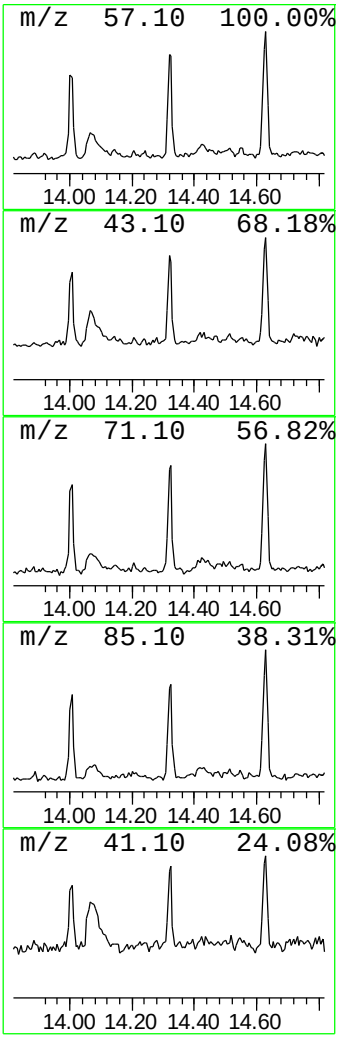
****

Peak Number 7 Heptadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.32	2.54 ng	114713	Chrysene-d12	14.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	93
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Heptacosane	380	C27H56	000593-49-7	87
4	Tetracosane	338	C24H50	000646-31-1	87
5	Hexatriacontane	507	C36H74	000630-06-8	87





Library Search Compound Report

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Operator : JU/SJ
Sample : J4581-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q3-A1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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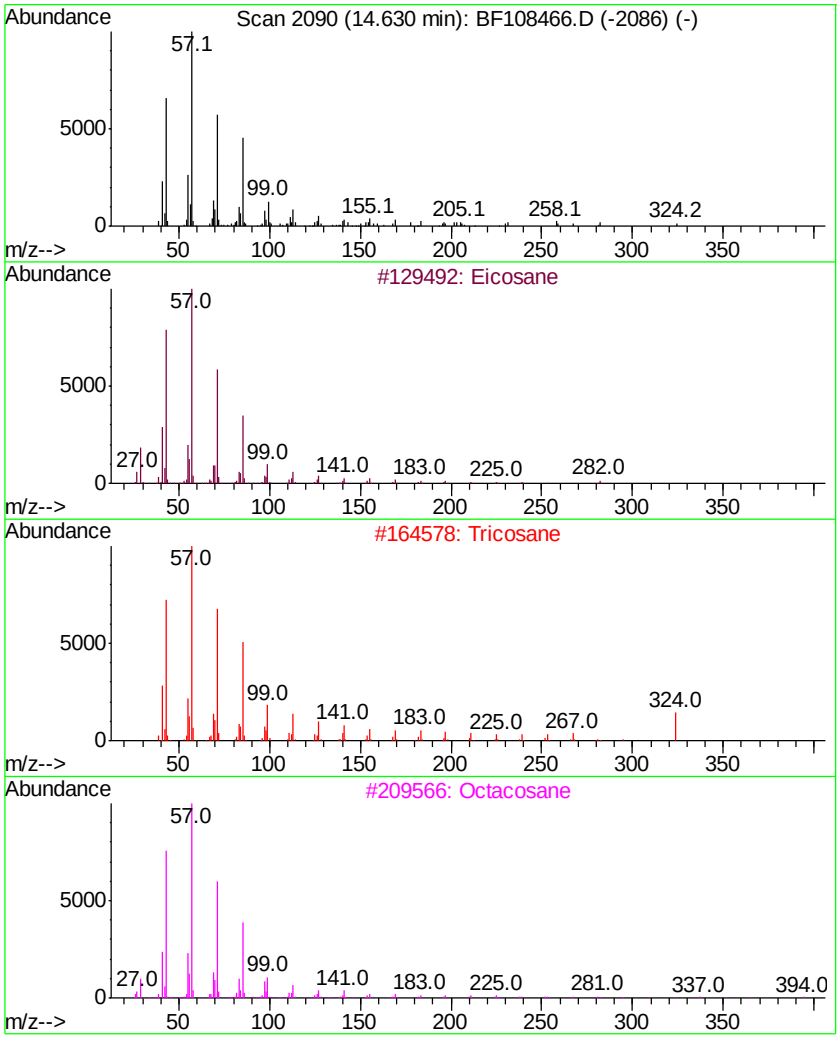
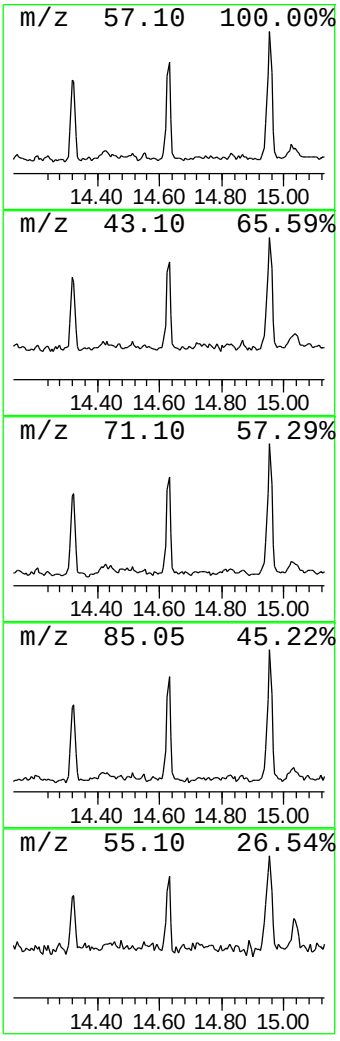
Peak Number 8 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	2.49 ng	112544	Chrysene-d12	14.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Tricosane	324	C23H48	000638-67-5	93
3	Octacosane	394	C28H58	000630-02-4	87
4	Tetracosane	338	C24H50	000646-31-1	87
5	Octadecane	254	C18H38	000593-45-3	83





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082418\
Data File : BF108466.D
Acq On : 24 Aug 2018 16:31
Operator : JU/SJ
Sample : J4581-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q3-A1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
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TIC Integration Parameters: LSCINT.P

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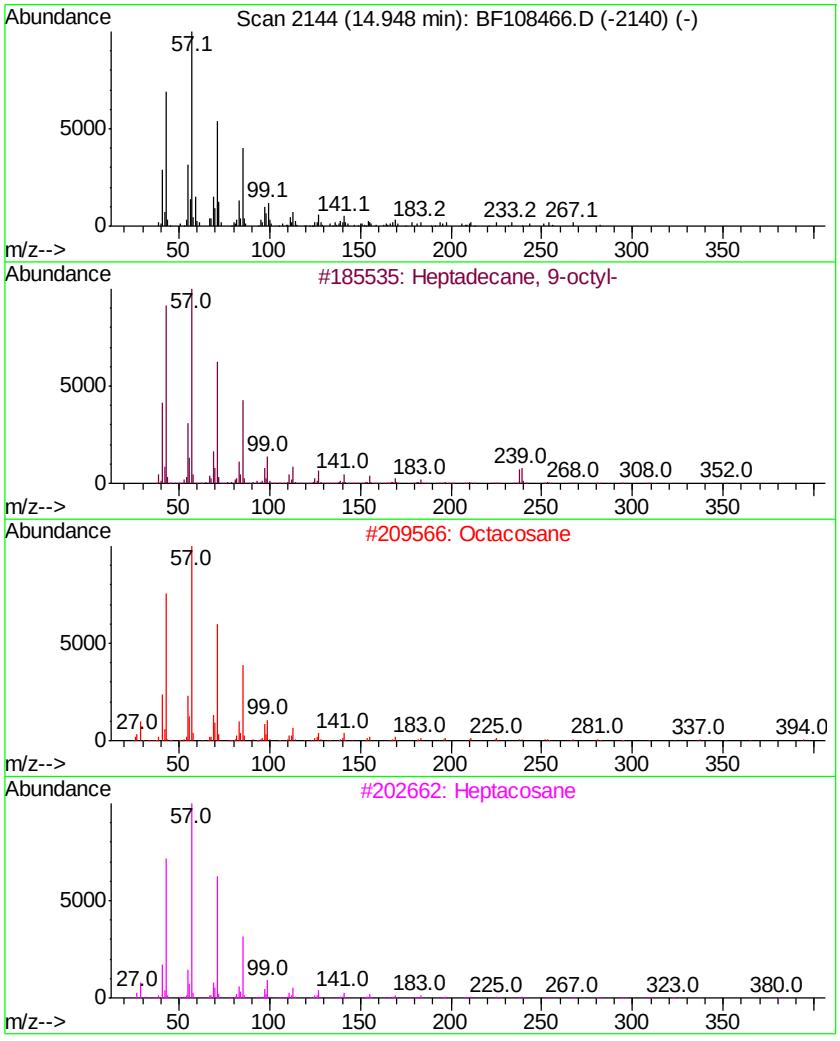
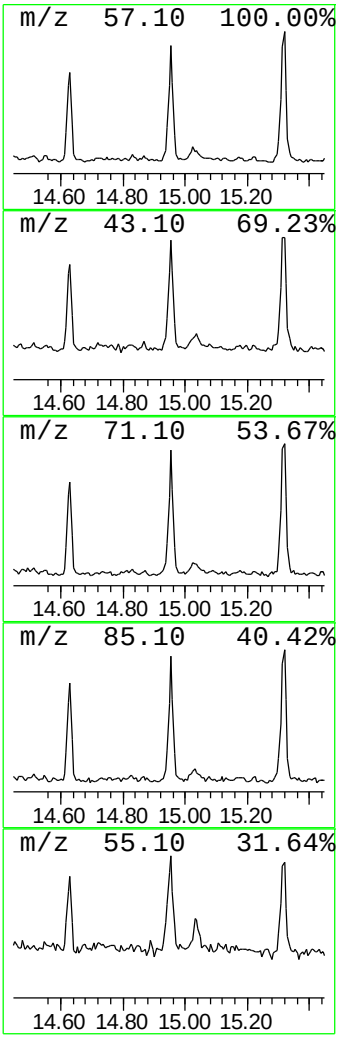
Peak Number 9 Heptadecane, 9-octyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	4.30 ng	194440	Chrysene-d12	14.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Docosane	310	C22H46	000629-97-0	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082418\
Data File : BF108466.D
Acq On : 24 Aug 2018 16:31
Operator : JU/SJ
Sample : J4581-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q3-A1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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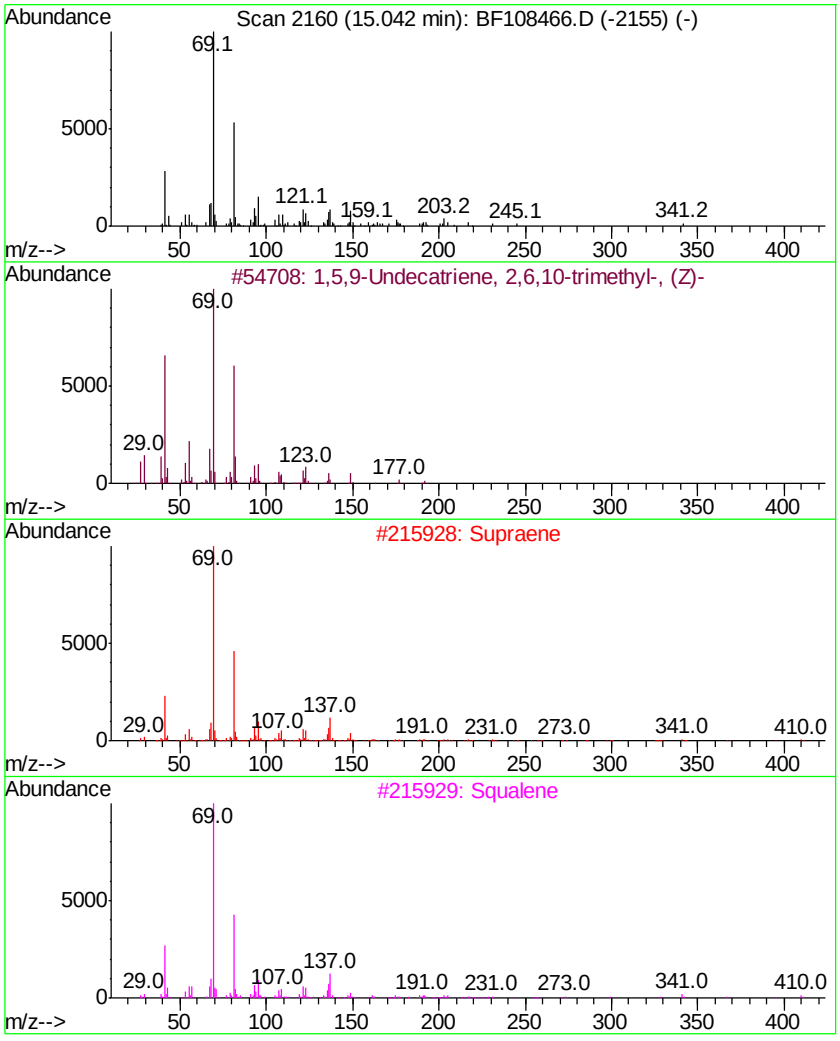
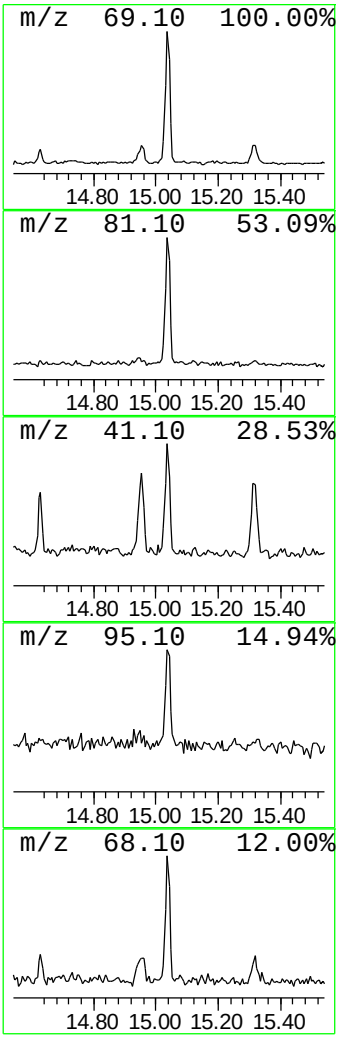
Peak Number 10 1,5,9-Undecatriene, 2,6,10-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.04	3.37 ng	156872	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	91
2	Supraene	410	C30H50	007683-64-9	91
3	Squalene	410	C30H50	000111-02-4	91
4	4,8,12-Tetradecatrienenitrile, 5...	245	C17H27N	005981-31-7	64
5	trans-Farnesol	222	C15H26O	000106-28-5	59





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Data File : BF108466.D
Acq On : 24 Aug 2018 16:31
Operator : JU/SJ
Sample : J4581-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q3-A1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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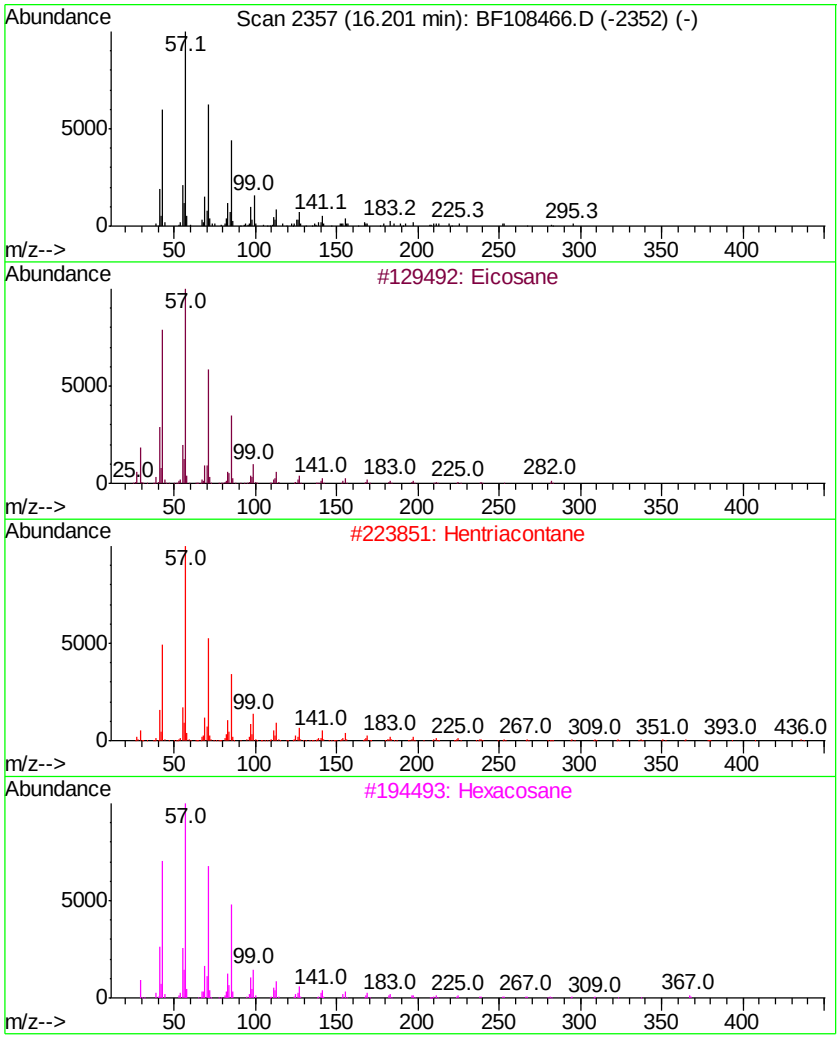
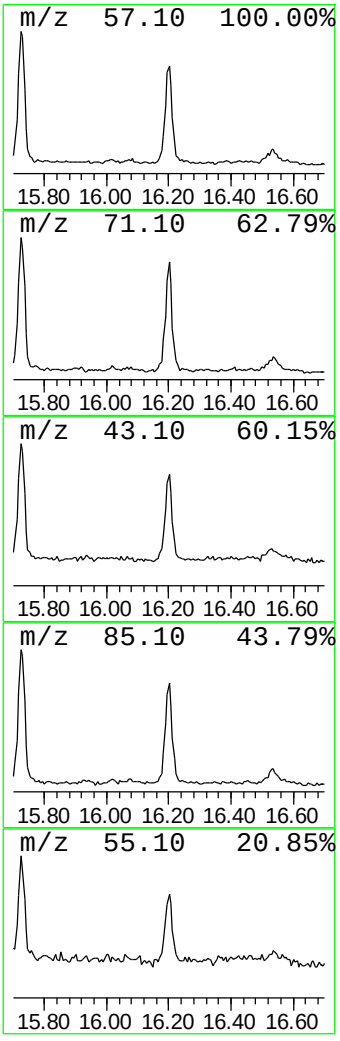
Peak Number 11 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.20	4.87 ng	226884	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Hentriacontane	437	C31H64	000630-04-6	90
3	Hexacosane	366	C26H54	000630-01-3	90
4	Heptacosane	380	C27H56	000593-49-7	90
5	Heneicosane	296	C21H44	000629-94-7	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082418\
Data File : BF108466.D
Acq On : 24 Aug 2018 16:31
Operator : JU/SJ
Sample : J4581-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q3-A1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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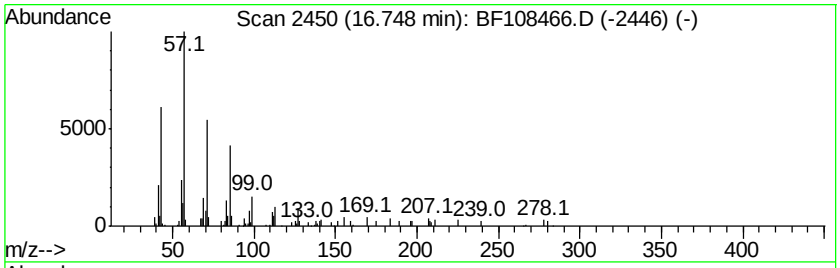
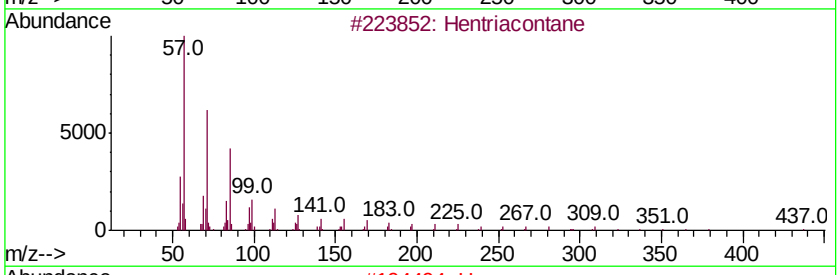
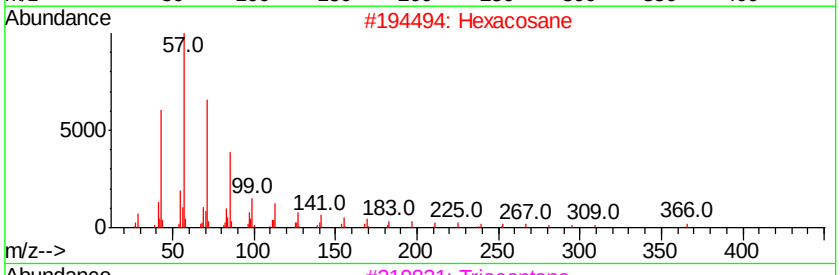
Peak Number 12 Hentriacontane Concentration Rank 9

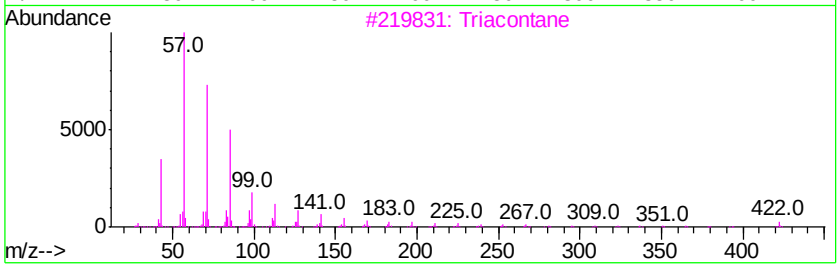
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.75	2.67 ng	124242	Perylene-d12	15.75

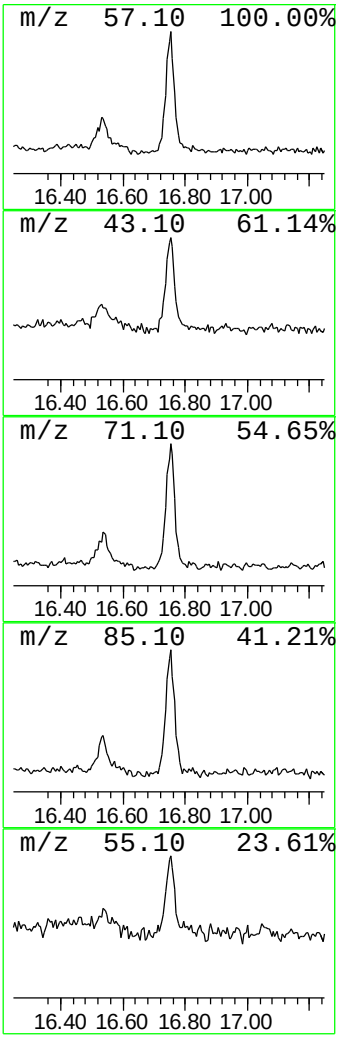
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	90
2	Hexacosane	366	C26H54	000630-01-3	90
3	Triacontane	422	C30H62	000638-68-6	87
4	Tetratetracontane	619	C44H90	007098-22-8	87
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86











Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082418\
Data File : BF108466.D
Acq On : 24 Aug 2018 16:31
Operator : JU/SJ
Sample : J4581-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q3-A1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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-methoxy...	2.37	22.3	ng	911209	1	7.00	819098	20.0
2-Pentanone, 4-hy...	5.24	3.0	ng	124444	1	7.00	819098	20.0
unknown6.77	6.77	62.2	ng	2548230	1	7.00	819098	20.0
n-Hexadecanoic acid	12.04	7.8	ng	489584	4	11.54	1250490	20.0
9-Eicosene, (E)-	14.07	2.6	ng	115757	5	14.19	903424	20.0
Heptadecane	14.32	2.5	ng	114713	5	14.19	903424	20.0
Eicosane	14.63	2.5	ng	112544	5	14.19	903424	20.0
Heptadecane, 9-oc...	14.95	4.3	ng	194440	5	14.19	903424	20.0
1,5,9-Undecatrien...	15.04	3.4	ng	156872	6	15.75	931895	20.0
Hexacosane	16.20	4.9	ng	226884	6	15.75	931895	20.0
Hentriacontane	16.75	2.7	ng	124242	6	15.75	931895	20.0