

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071619\
 Data File : BF115607.D
 Acq On : 16 Jul 2019 19:44
 Operator : HP/JU
 Sample : K3826-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RBR-200034

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

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-BF071219.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	2.193	11	18	32	rVB	1237380	1750543	36.56%	3.678%
2	5.510	576	582	585	rBV	4143543	4251024	88.79%	8.932%
3	6.510	746	752	755	rBV	3713576	4423914	92.40%	9.295%
4	6.657	772	777	780	rBV	4349091	4478441	93.54%	9.410%
5	6.881	812	815	819	rBV	1251280	1013242	21.16%	2.129%
6	7.039	838	842	845	rBV	3918425	3579071	74.76%	7.520%
7	7.439	905	910	913	rBV	2815269	2940030	61.41%	6.177%
8	8.163	1029	1033	1036	rBV	1562839	1265928	26.44%	2.660%
9	9.239	1211	1216	1219	rBV	5030404	4787717	100.00%	10.060%
10	9.628	1278	1282	1292	rVB	918501	748764	15.64%	1.573%
11	9.916	1327	1331	1335	rBV	1625919	1506939	31.48%	3.166%
12	10.704	1460	1465	1483	rBV	2985944	3153664	65.87%	6.626%
13	11.404	1580	1584	1586	rBV	1617864	1498275	31.29%	3.148%
14	11.422	1586	1587	1592	rVV	349642	307382	6.42%	0.646%
15	11.474	1592	1596	1599	rVB	58082	68499	1.43%	0.144%
16	11.927	1670	1673	1680	rVB2	397923	335175	7.00%	0.704%
17	12.610	1786	1789	1793	rBV	416155	377270	7.88%	0.793%
18	12.710	1803	1806	1810	rBV2	127807	130157	2.72%	0.273%
19	12.839	1822	1828	1831	rBV	339491	340807	7.12%	0.716%
20	12.986	1845	1853	1856	rBV	4453030	4357445	91.01%	9.156%
21	13.557	1948	1950	1959	rVB4	29883	50456	1.05%	0.106%
22	13.674	1965	1970	1975	rVB	71515	79184	1.65%	0.166%
23	13.786	1984	1989	1991	rBV2	35380	54140	1.13%	0.114%
24	13.904	2002	2009	2024	rVB5	163710	473848	9.90%	0.996%
25	14.039	2024	2032	2034	rBV	1278493	1370272	28.62%	2.879%
26	14.063	2034	2036	2044	rVB	187881	192904	4.03%	0.405%
27	14.204	2057	2060	2062	rBV	61984	56520	1.18%	0.119%
28	14.510	2106	2112	2115	rBV2	135803	165535	3.46%	0.348%
29	14.551	2115	2119	2121	rBV4	55897	80043	1.67%	0.168%
30	14.663	2135	2138	2144	rBV4	43119	73172	1.53%	0.154%
31	14.815	2161	2164	2168	rBV	131825	122563	2.56%	0.258%
32	14.892	2174	2177	2181	rBV2	81125	84337	1.76%	0.177%
33	14.962	2185	2189	2192	rBV2	128233	143654	3.00%	0.302%
34	15.074	2204	2208	2212	rBV2	132102	227602	4.75%	0.478%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.157	2218	2222	2226	rBV	208413	221676	4.63%	0.466%
36	15.227	2228	2234	2240	rVV4	73325	191176	3.99%	0.402%
37	15.380	2257	2260	2266	rVB	71119	80390	1.68%	0.169%
38	15.439	2267	2270	2276	rVV	92078	113632	2.37%	0.239%
39	15.509	2276	2282	2285	rVV	951784	1231542	25.72%	2.588%
40	15.539	2285	2287	2295	rVB	190741	235784	4.92%	0.495%
41	15.745	2318	2322	2325	rBV4	42793	55231	1.15%	0.116%
42	15.980	2357	2362	2369	rVB	207217	316692	6.61%	0.665%
43	16.098	2375	2382	2387	rBV8	48189	128535	2.68%	0.270%
44	16.492	2445	2449	2455	rVB	61680	100800	2.11%	0.212%
45	16.786	2494	2499	2508	rVB8	36990	76449	1.60%	0.161%
46	16.980	2526	2532	2539	rBV2	37562	84195	1.76%	0.177%
47	17.092	2545	2551	2558	rVB3	73674	158487	3.31%	0.333%
48	18.621	2806	2811	2821	rVB10	37650	110038	2.30%	0.231%

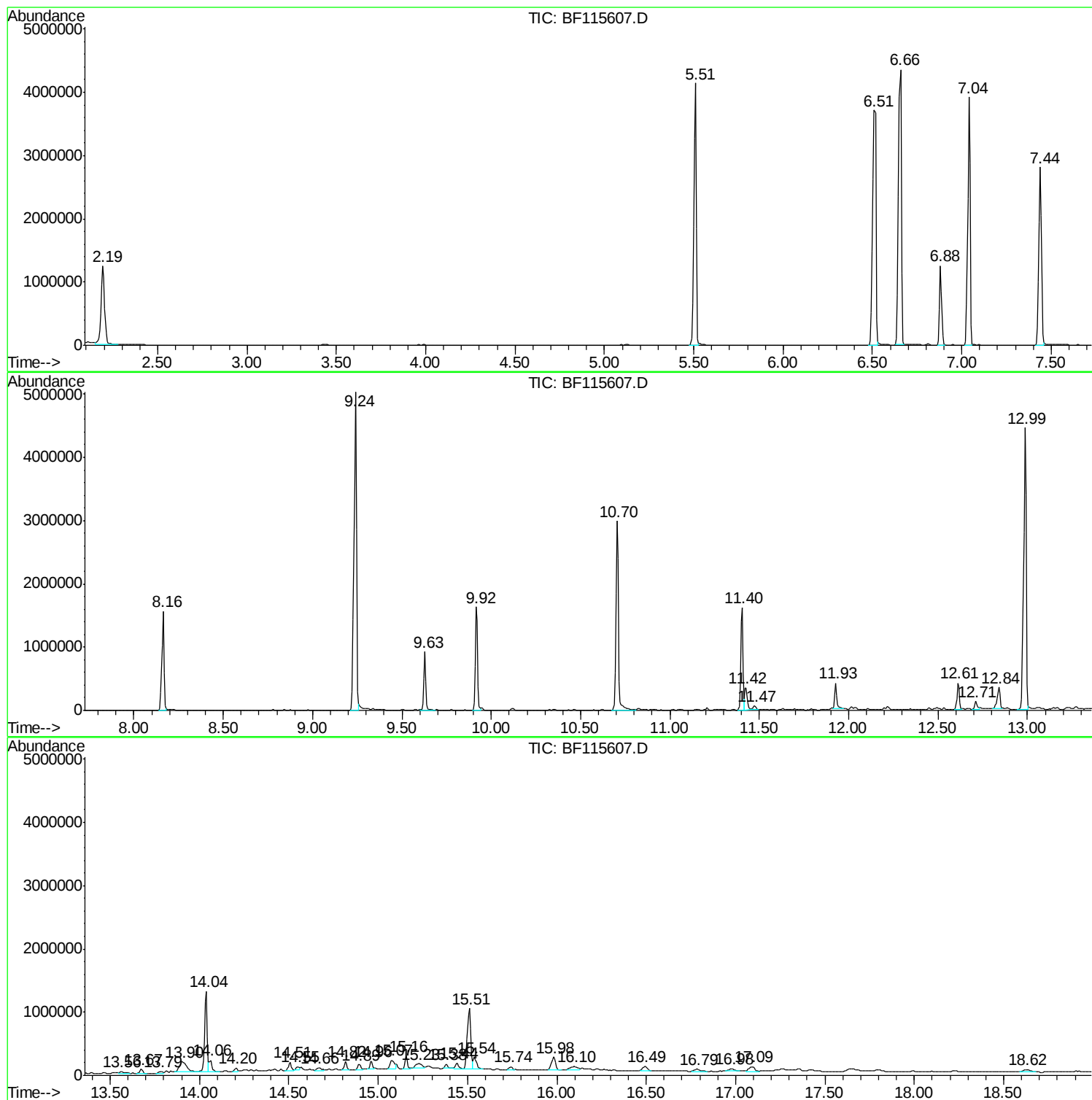
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Instrument :
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ClientSampled :
RBR-200034

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071219.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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Instrument :
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ClientSampleId :
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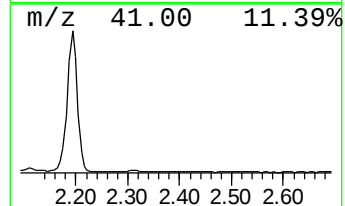
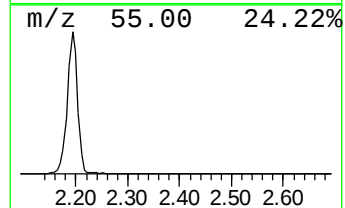
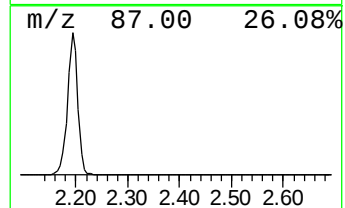
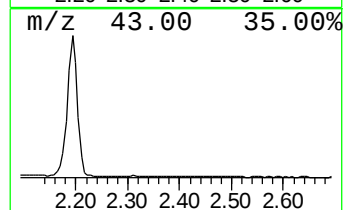
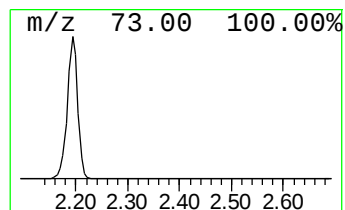
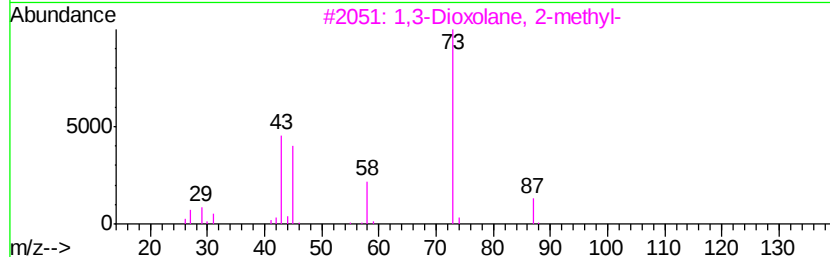
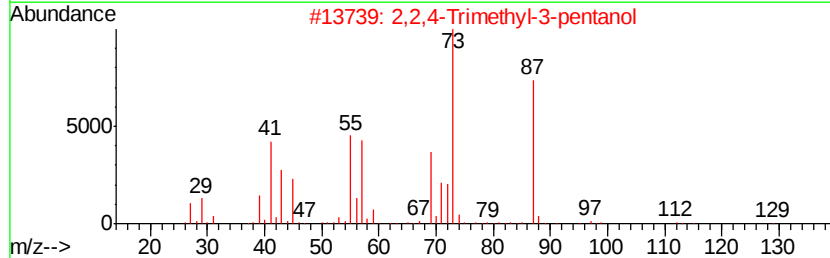
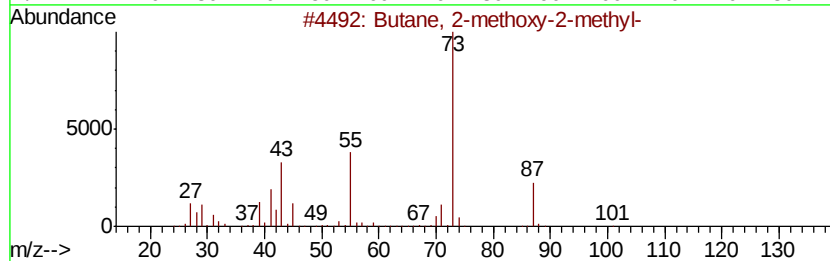
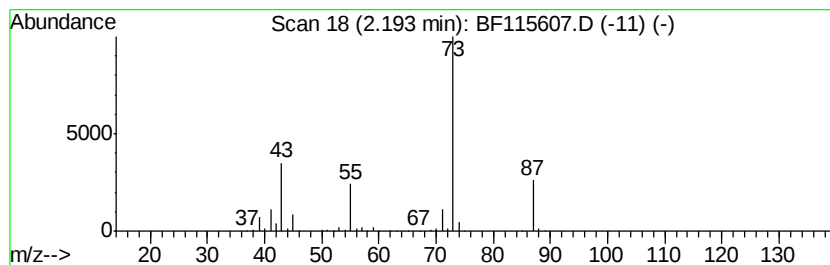
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.19	34.55 ng	1750540	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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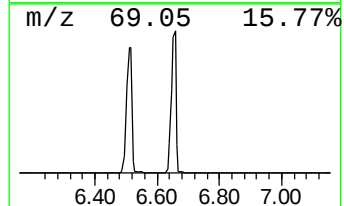
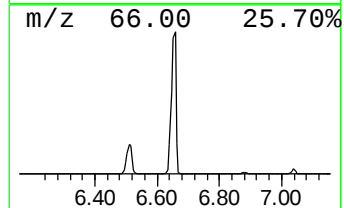
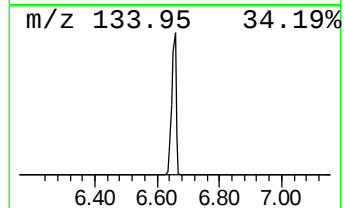
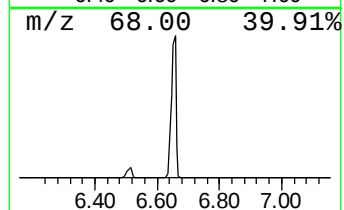
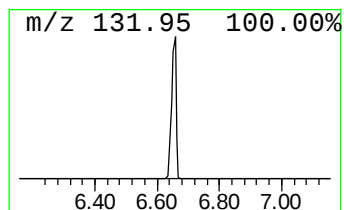
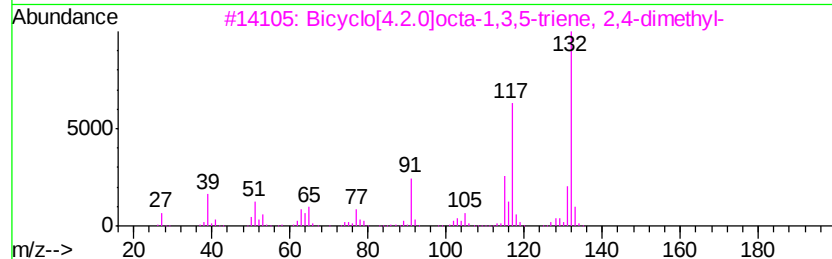
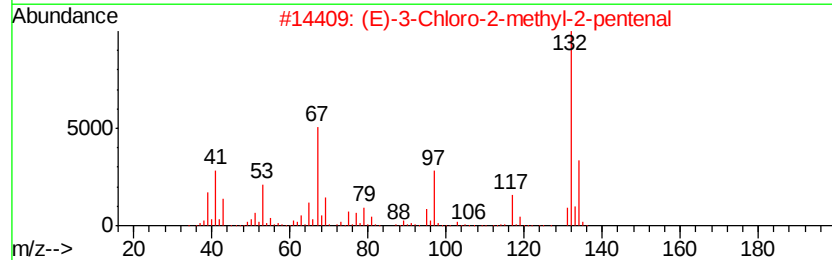
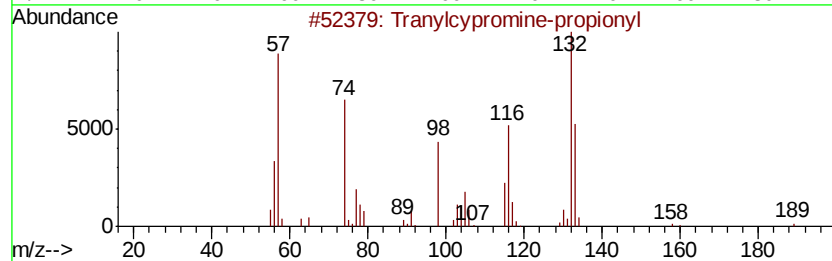
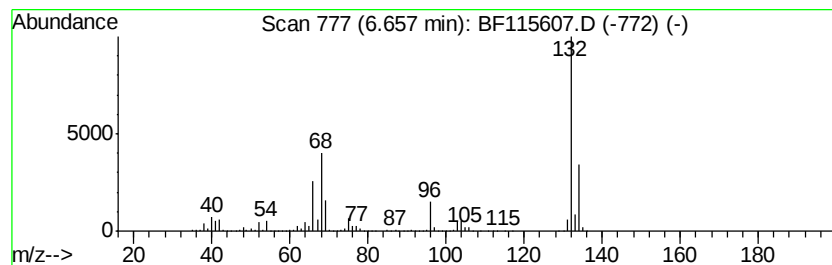
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	88.40 ng	4478440	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranlylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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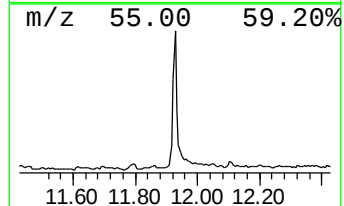
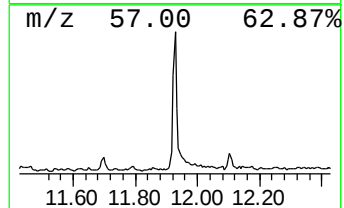
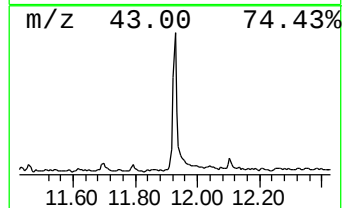
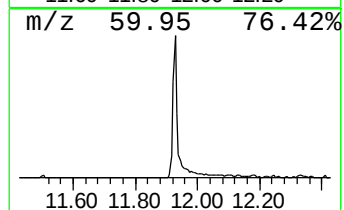
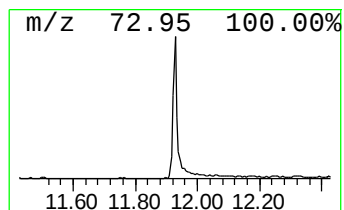
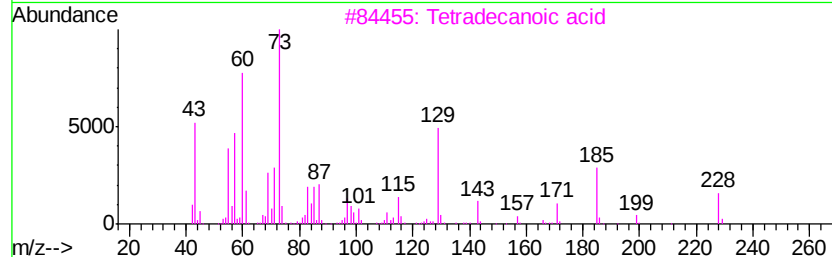
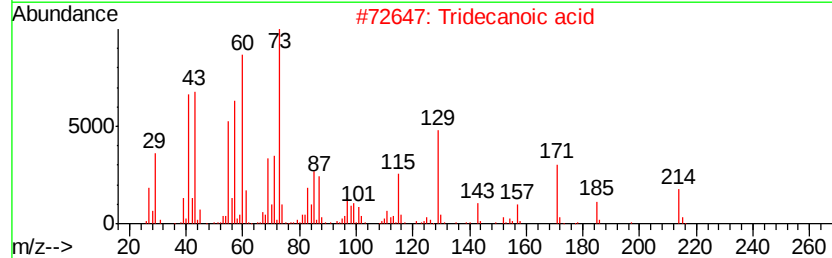
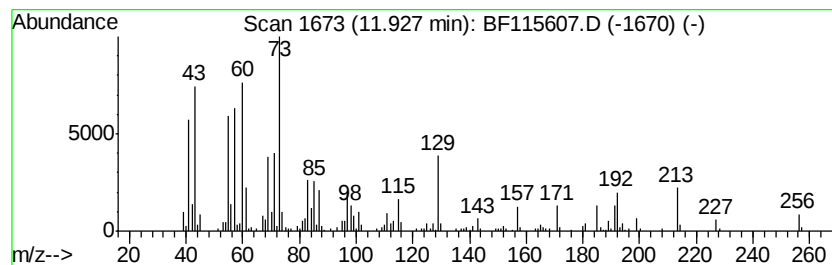
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	4.47 ng	335175	Phenanthrene-d10	11.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	89
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5		n-Decanoic acid	172	C10H20O2	000334-48-5	70



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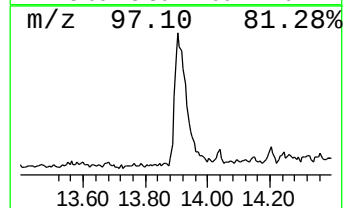
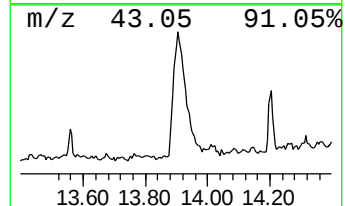
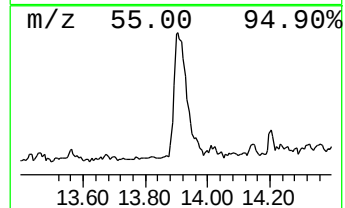
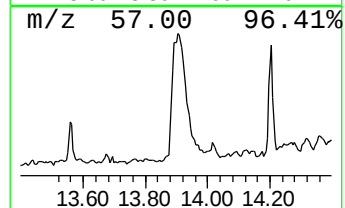
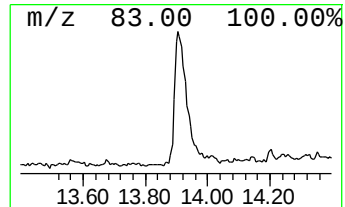
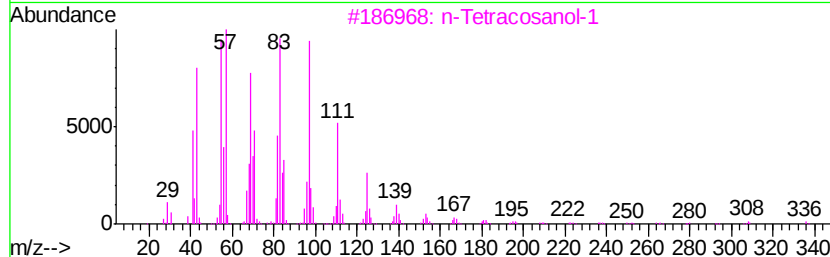
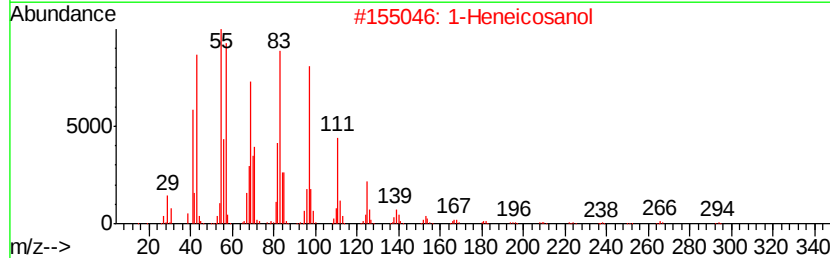
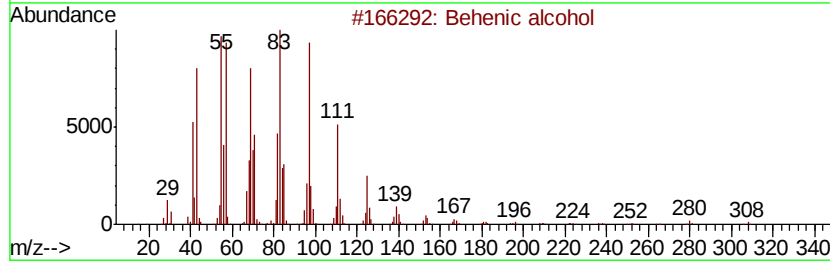
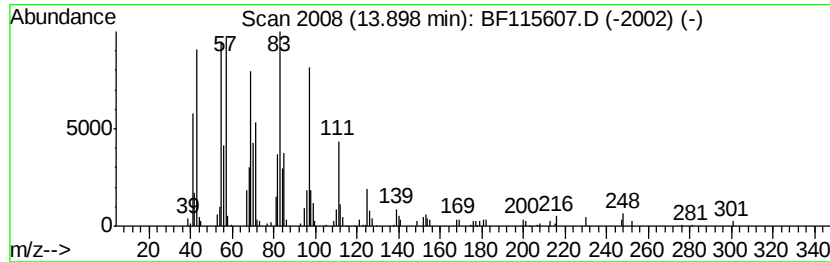
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Behenic alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.90	6.92 ng	473848	Chrysene-d12	14.04	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4	1-Heptacosanol	396	C27H56O	002004-39-9	95
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	95



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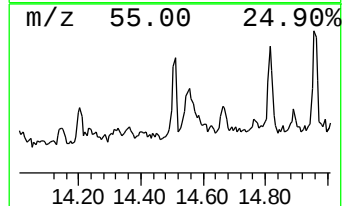
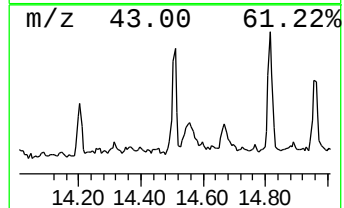
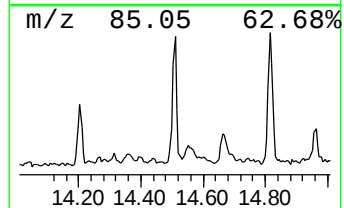
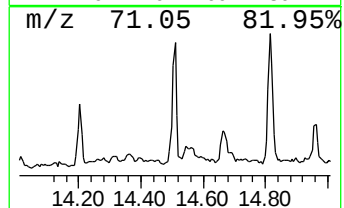
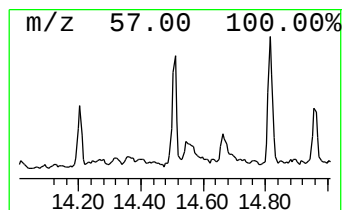
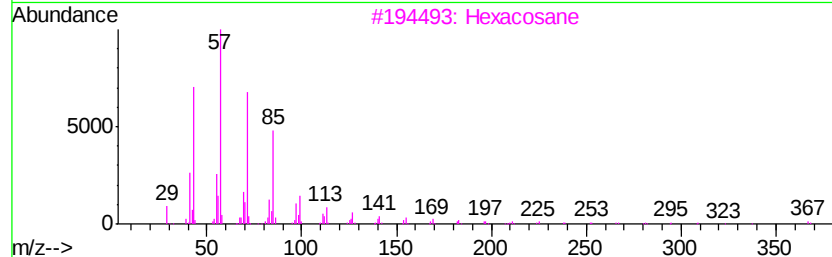
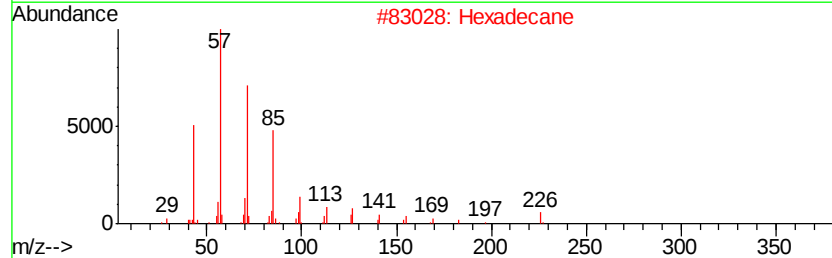
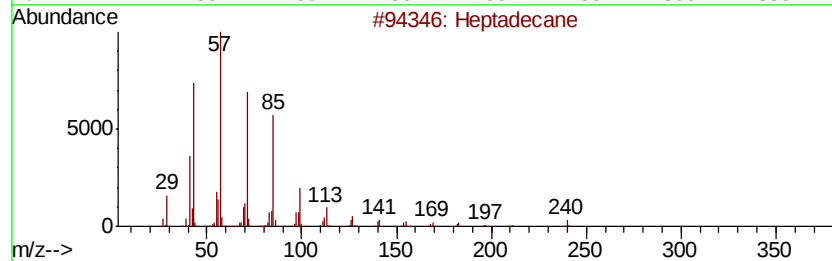
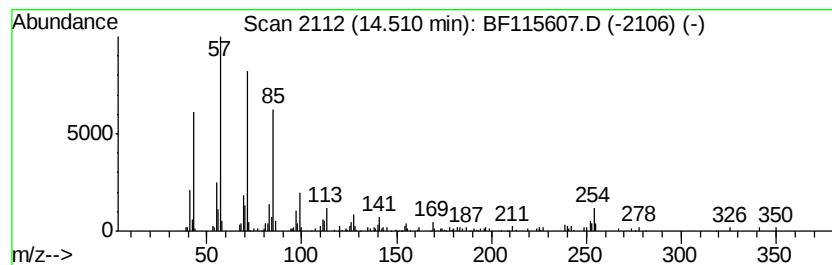
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.51	2.42 ng	165535	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	93
2	Hexadecane	226	C16H34	000544-76-3	91
3	Hexacosane	366	C26H54	000630-01-3	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071619\
Data File : BF115607.D
Acq On : 16 Jul 2019 19:44
Operator : HP/JU
Sample : K3826-01
Misc :
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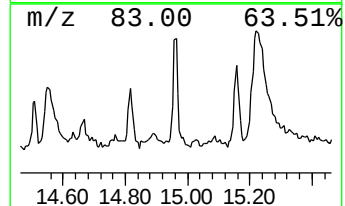
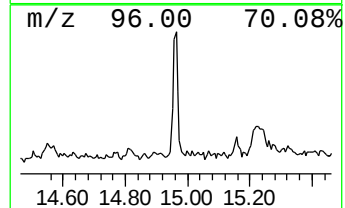
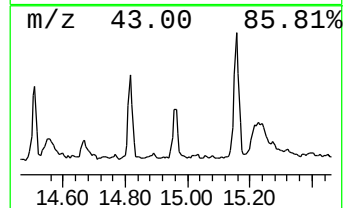
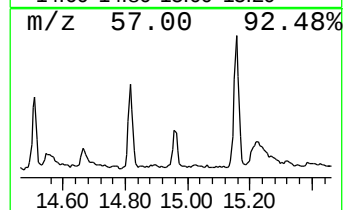
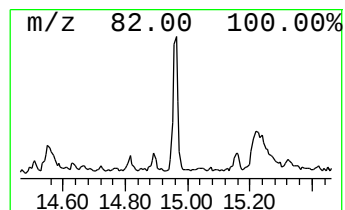
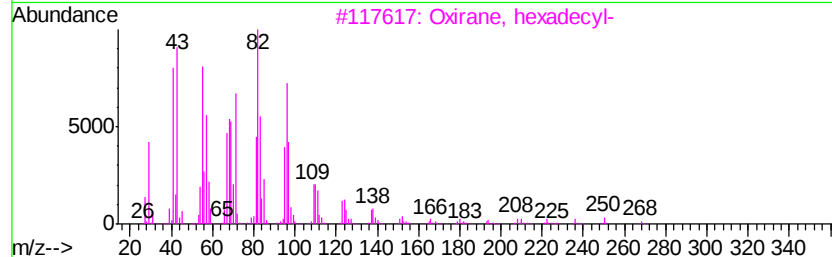
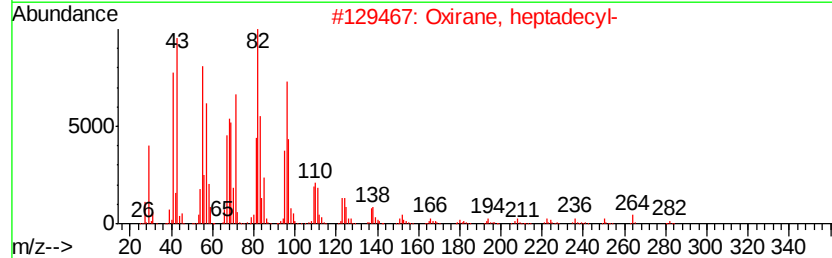
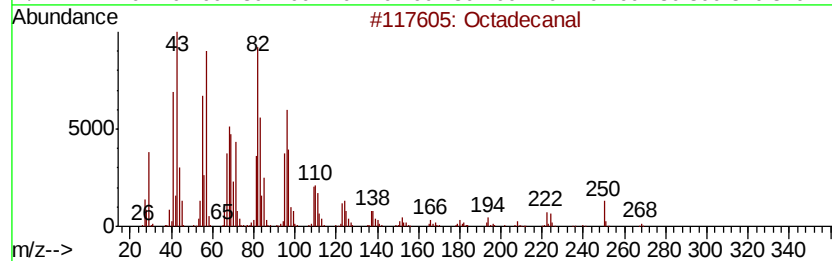
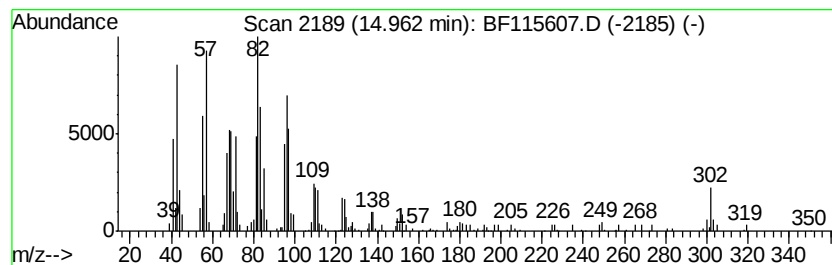
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanal Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	2.33 ng	143654	Perylene-d12	15.51
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octadecanal	268 C18H36O	000638-66-4	94
2	Oxirane, heptadecyl-	282 C19H38O	067860-04-2	91
3	Oxirane, hexadecyl-	268 C18H36O	007390-81-0	91
4	Heptadecanal	254 C17H34O	1000376-70-0	91
5	17-Octadecenal	266 C18H34O	056554-86-0	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071619\
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Sample : K3826-01
Misc :
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Instrument :
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ClientSampleId :
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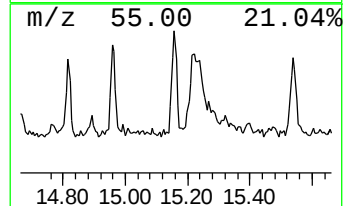
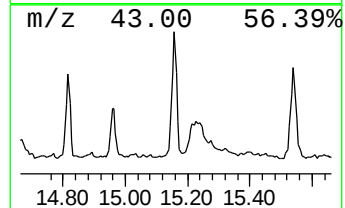
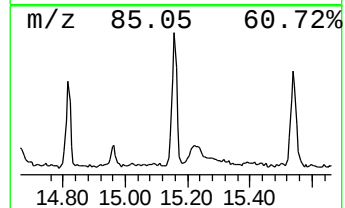
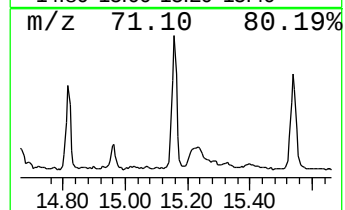
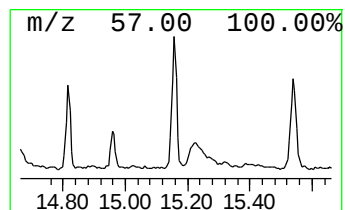
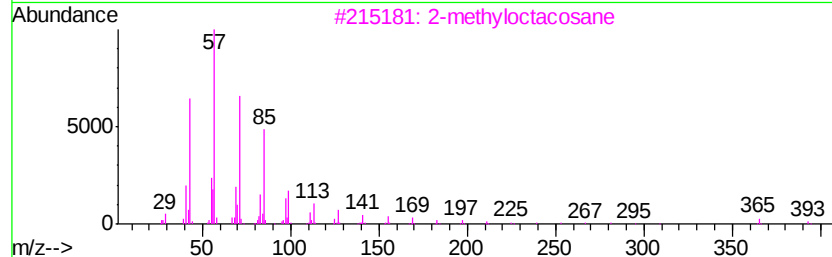
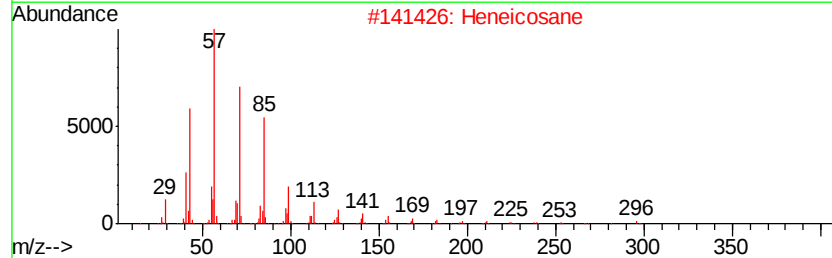
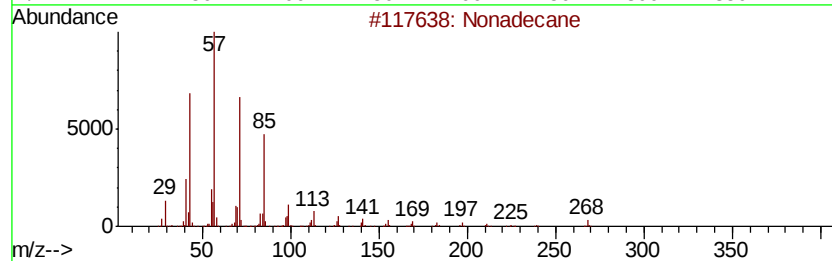
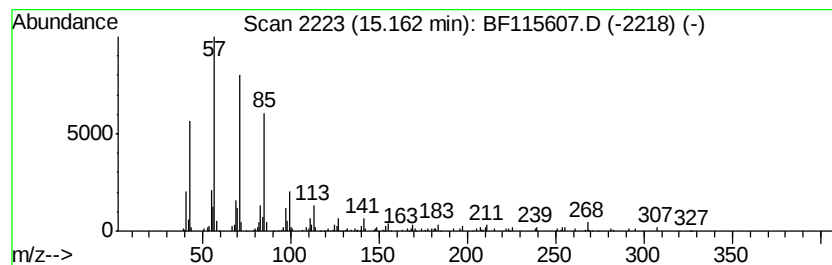
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.16	3.60 ng	221676	Perylene-d12	15.51

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	91
2	Heneicosane		296	C21H44	000629-94-7	90
3	2-methyloctacosane		408	C29H60	1000376-72-8	87
4	Octadecane, 1-iodo-		380	C18H37I	000629-93-6	87
5	Tetracosane		338	C24H50	000646-31-1	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071619\
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Sample : K3826-01
Misc :
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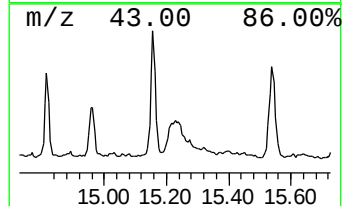
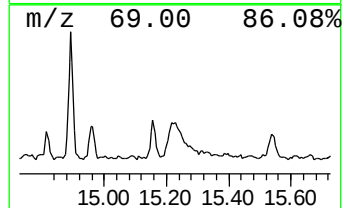
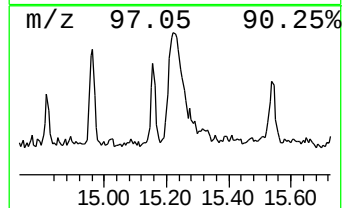
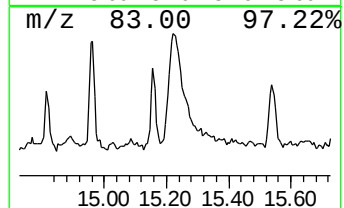
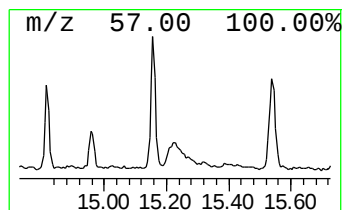
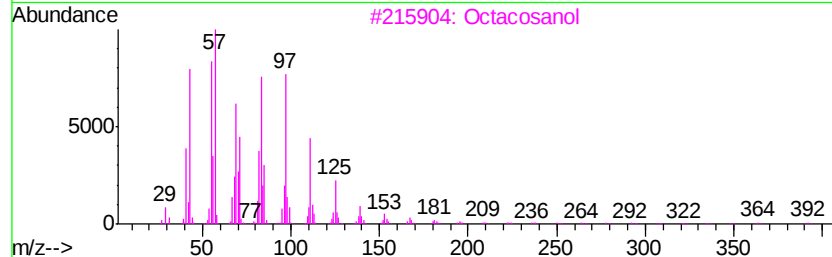
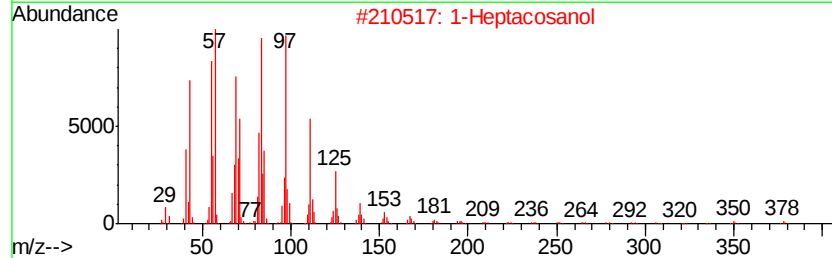
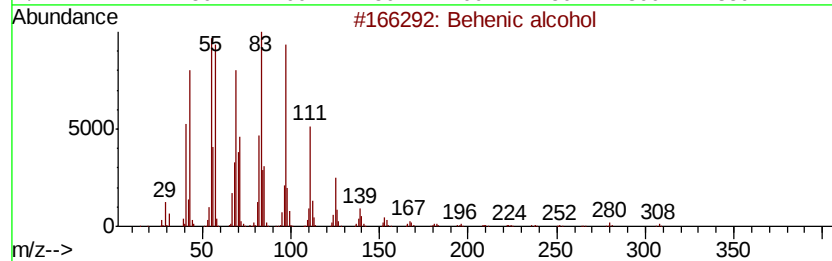
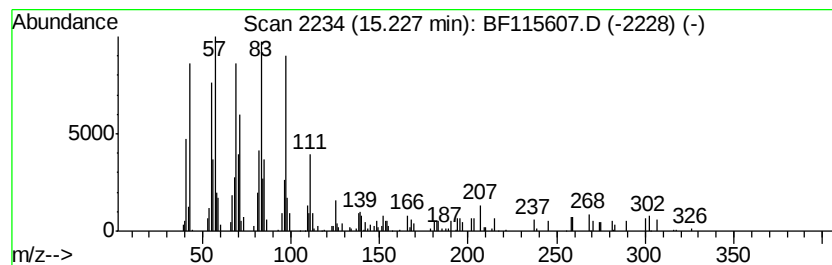
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Heptacosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.23	3.10 ng	191176	Perylene-d12	15.51
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Behenic alcohol	326 C22H46O	000661-19-8 87
2		1-Heptacosanol	396 C27H56O	002004-39-9 76
3		Octacosanol	410 C28H58O	000557-61-9 76
4		Pentafluoropropionic acid, penta...	374 C18H31F5O2	959092-08-1 74
5		1-Heneicosyl formate	340 C22H44O2	077899-03-7 74



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071619\
Data File : BF115607.D
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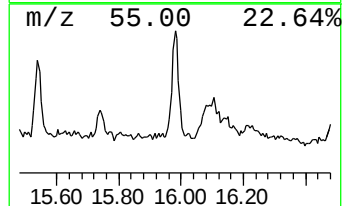
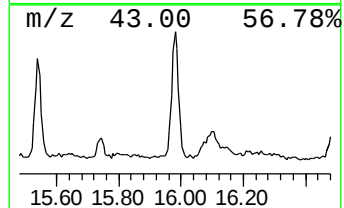
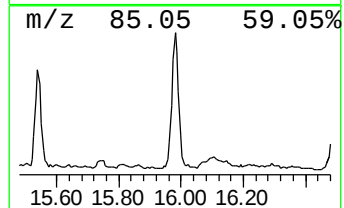
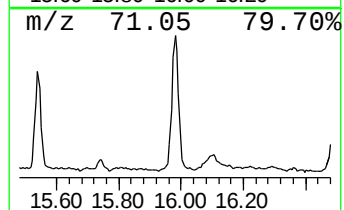
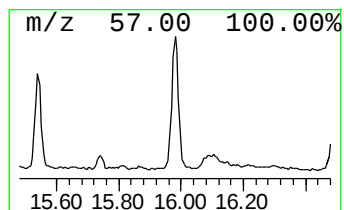
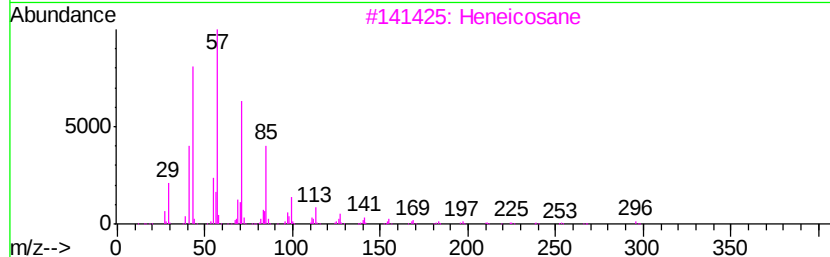
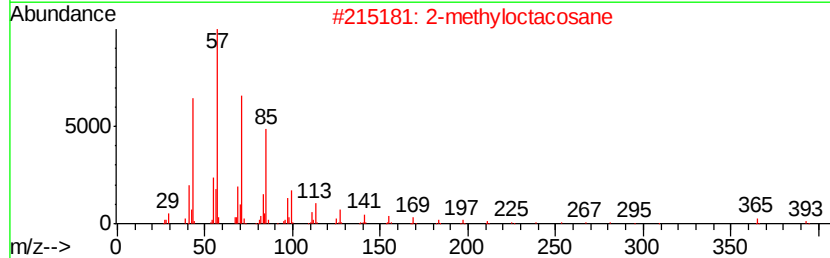
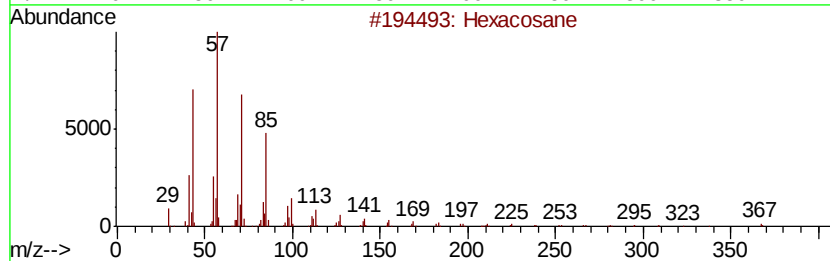
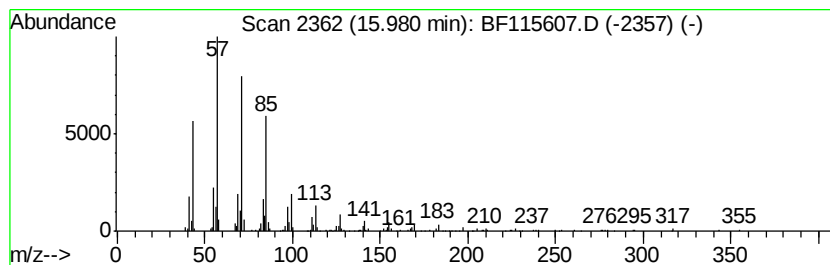
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.98	5.14 ng	316692	Perylene-d12	15.51

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			2-methyloctacosane	408	C29H60	1000376-72-8	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Docosane	310	C22H46	000629-97-0	91
5			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071619\
 Data File : BF115607.D
 Acq On : 16 Jul 2019 19:44
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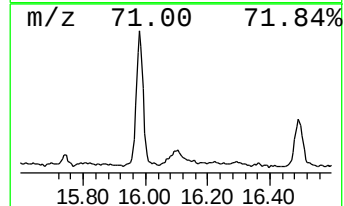
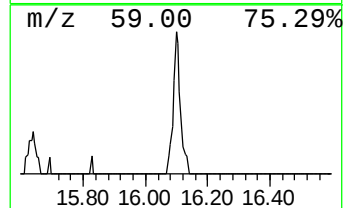
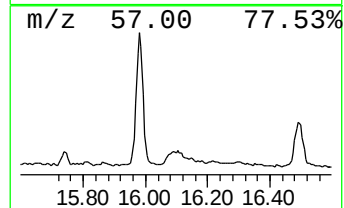
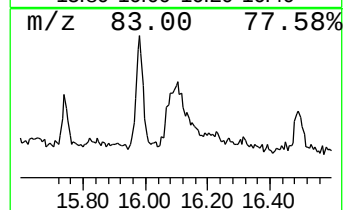
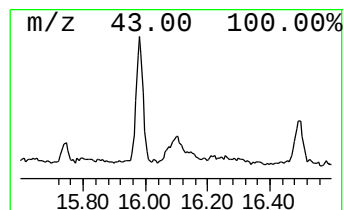
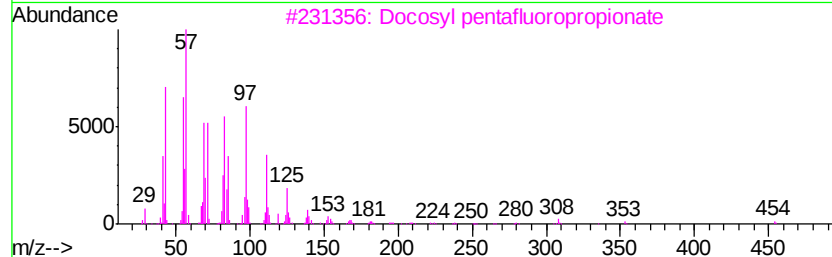
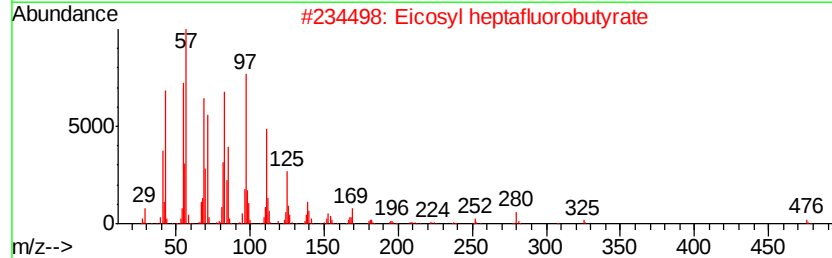
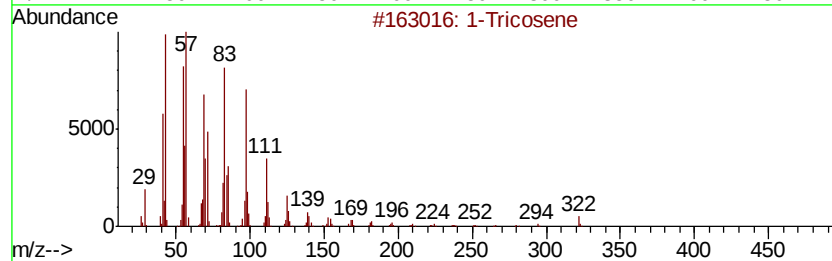
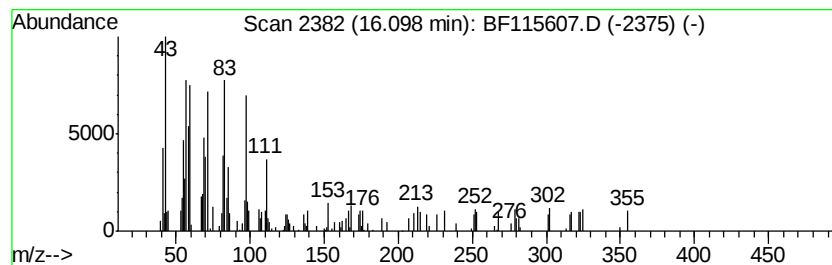
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 11 unknown16.10 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	2.09 ng	128535	Perylene-d12	15.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Tricosene	322	C23H46	018835-32-0	43
2		Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	41
3		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	41
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	41
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071619\
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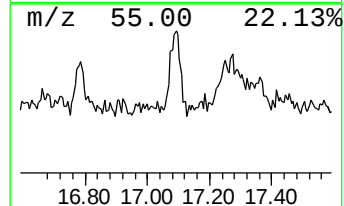
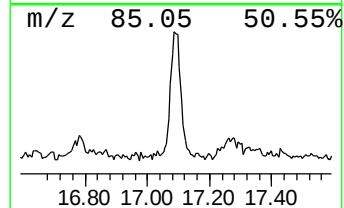
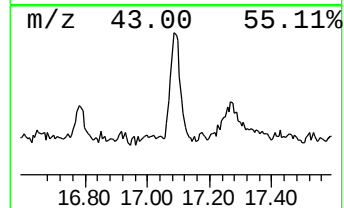
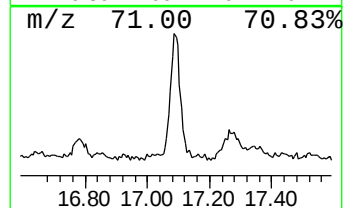
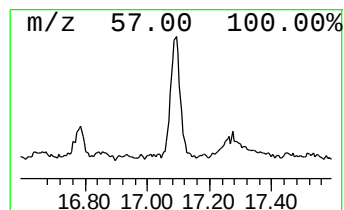
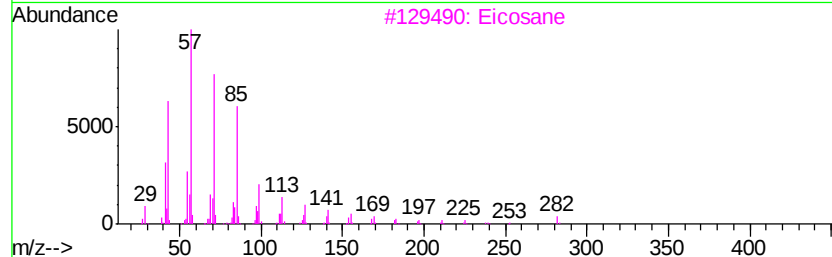
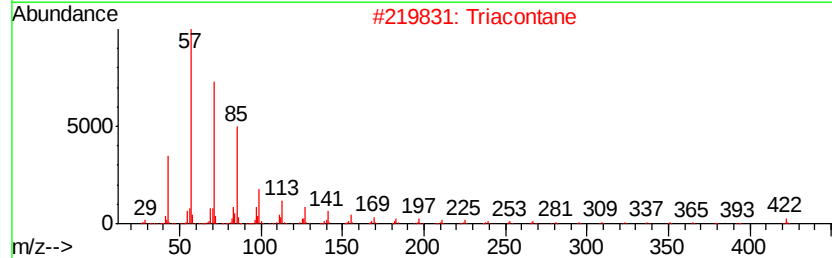
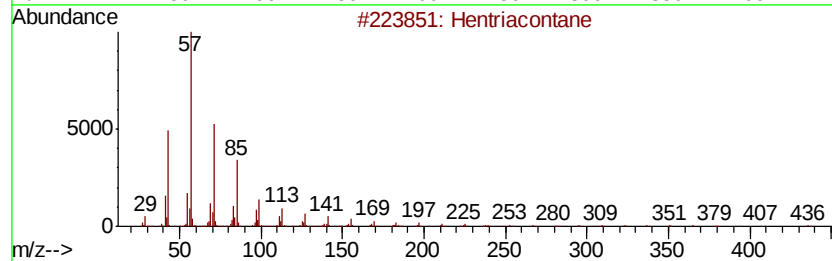
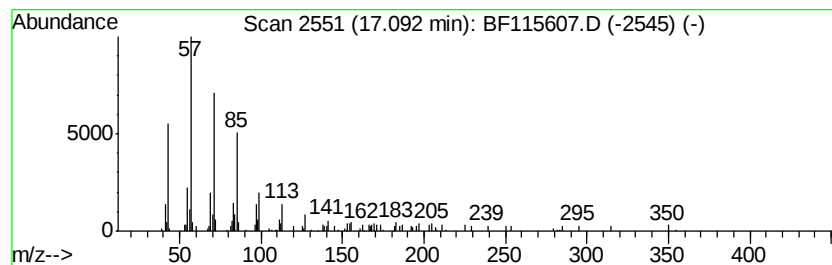
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hentriacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.09	2.57 ng	158487	Perylene-d12	15.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hentriacontane	437	C31H64	000630-04-6	90
2		Triacontane	422	C30H62	000638-68-6	90
3		Eicosane	282	C20H42	000112-95-8	90
4		Heneicosane	296	C21H44	000629-94-7	90
5		Docosane	310	C22H46	000629-97-0	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF071619\
Data File : BF115607.D
Acq On : 16 Jul 2019 19:44
Operator : HP/JU
Sample : K3826-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown6.66	6.66	88.4	ng	4478440	1	6.88	1013240	20.0
n-Hexadecanoic acid	11.93	4.5	ng	335175	4	11.40	1498280	20.0
Behenic alcohol	13.90	6.9	ng	473848	5	14.04	1370270	20.0
Heptadecane	14.51	2.4	ng	165535	5	14.04	1370270	20.0
Octadecanal	14.96	2.3	ng	143654	6	15.51	1231540	20.0
Nonadecane	15.16	3.6	ng	221676	6	15.51	1231540	20.0
1-Heptacosanol	15.23	3.1	ng	191176	6	15.51	1231540	20.0
Hexacosane	15.98	5.1	ng	316692	6	15.51	1231540	20.0
unknown16.10	16.10	2.1	ng	128535	6	15.51	1231540	20.0
Hentriacontane	17.09	2.6	ng	158487	6	15.51	1231540	20.0