

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120718\
 Data File : BF111196.D
 Acq On : 7 Dec 2018 19:32
 Operator : JU/SJ
 Sample : J6214-11
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-4(3-5)

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-BF120518.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	5.004	489	496	502	rVB	544758	691754	7.70%	0.795%
2	5.416	561	566	569	rBV	7894958	7539348	83.93%	8.662%
3	6.428	733	738	743	rBV	7426422	8191943	91.19%	9.411%
4	6.575	758	763	766	rBV	7635946	7598045	84.58%	8.729%
5	6.804	798	802	805	rBV	3760498	2843042	31.65%	3.266%
6	6.963	825	829	832	rVB	7418410	6651415	74.04%	7.642%
7	7.363	892	897	900	rBV	6232308	5750265	64.01%	6.606%
8	8.087	1016	1020	1023	rBV	4536414	3836197	42.70%	4.407%
9	9.163	1198	1203	1206	rBV	10720736	8983243	100.00%	10.321%
10	9.551	1266	1269	1272	rBV	979940	765868	8.53%	0.880%
11	9.839	1314	1318	1322	rBV	4918583	4154995	46.25%	4.774%
12	10.622	1447	1451	1455	rBV	5111769	4467566	49.73%	5.133%
13	11.322	1566	1570	1572	rBV	3884766	3221907	35.87%	3.702%
14	11.345	1572	1574	1577	rVV	502490	386554	4.30%	0.444%
15	11.392	1577	1582	1586	rVB	145567	137137	1.53%	0.158%
16	11.857	1657	1661	1665	rBV2	1343227	1310436	14.59%	1.506%
17	11.933	1670	1674	1676	rBV2	177258	183061	2.04%	0.210%
18	12.369	1745	1748	1751	rBV	101667	107137	1.19%	0.123%
19	12.527	1772	1775	1779	rBV	917223	805600	8.97%	0.926%
20	12.639	1790	1794	1800	rBV	914941	890026	9.91%	1.023%
21	12.757	1808	1814	1817	rBV	932853	902322	10.04%	1.037%
22	12.910	1836	1840	1843	rBV	7039076	6466528	71.98%	7.429%
23	12.980	1846	1852	1855	rBV4	80829	111809	1.24%	0.128%
24	13.086	1868	1870	1873	rVB	121766	102456	1.14%	0.118%
25	13.151	1878	1881	1884	rVB	206185	164697	1.83%	0.189%
26	13.192	1884	1888	1890	rBV	101116	111001	1.24%	0.128%
27	13.492	1936	1939	1942	rBV	257313	210410	2.34%	0.242%
28	13.704	1970	1975	1978	rBV2	65351	107411	1.20%	0.123%
29	13.821	1991	1995	2000	rVB	556672	581779	6.48%	0.668%
30	13.951	2009	2017	2020	rBV	2787746	3183293	35.44%	3.657%
31	13.974	2020	2021	2024	rVB	283988	229152	2.55%	0.263%
32	14.139	2045	2049	2052	rVB	470220	413765	4.61%	0.475%
33	14.445	2097	2101	2104	rBV	454672	430795	4.80%	0.495%
34	14.745	2149	2152	2160	rVB	453937	420568	4.68%	0.483%

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Instrument :
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ClientSampleId :
SB-4(3-5)

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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.821	2161	2165	2169	rVV	182368	200667	2.23%	0.231%
36	14.980	2188	2192	2199	rVB	229239	435406	4.85%	0.500%
37	15.074	2204	2208	2212	rBV2	355584	408718	4.55%	0.470%
38	15.268	2238	2241	2247	rVB	152098	180069	2.00%	0.207%
39	15.327	2247	2251	2257	rVB	228081	281715	3.14%	0.324%
40	15.392	2257	2262	2266	rBV	2074373	2417466	26.91%	2.777%
41	15.451	2268	2272	2278	rVB	267985	361017	4.02%	0.415%
42	15.874	2339	2344	2349	rBV	201911	294742	3.28%	0.339%
43	16.368	2424	2428	2433	rVB2	115815	195834	2.18%	0.225%
44	16.792	2497	2500	2508	rVB3	104364	184722	2.06%	0.212%
45	17.215	2568	2572	2577	rBV2	82900	130446	1.45%	0.150%

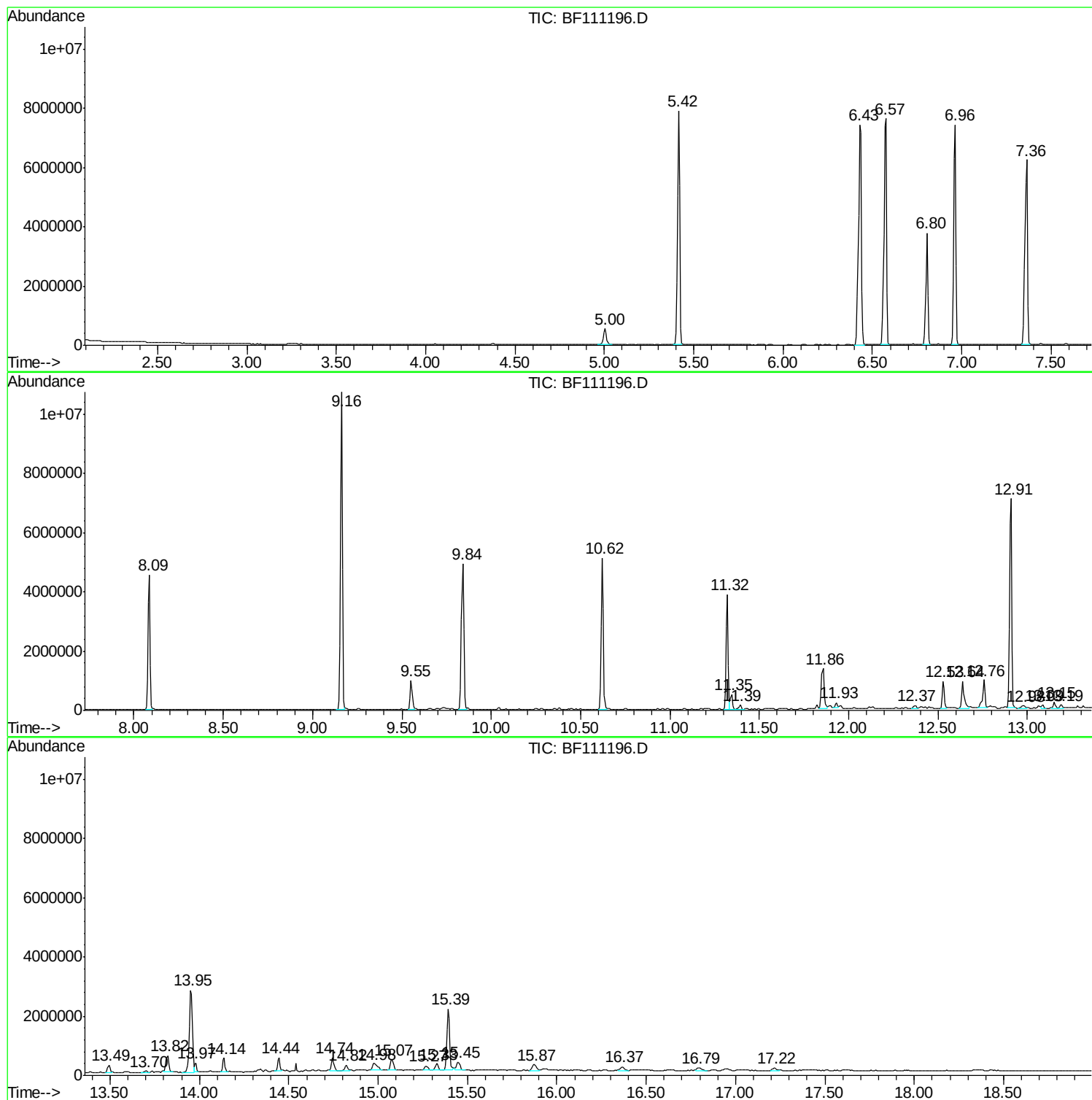
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Instrument :
BNA_F
ClientSampled :
SB-4(3-5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120518.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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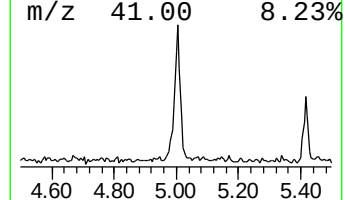
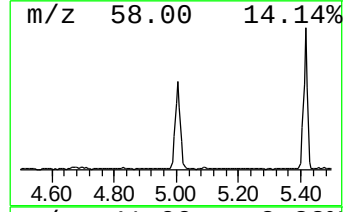
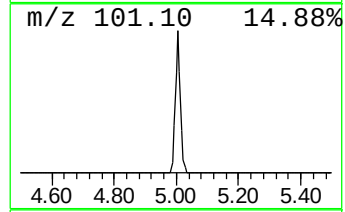
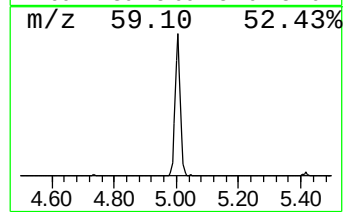
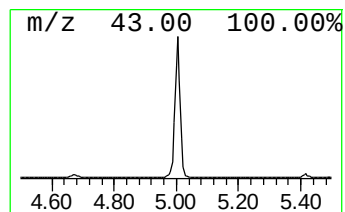
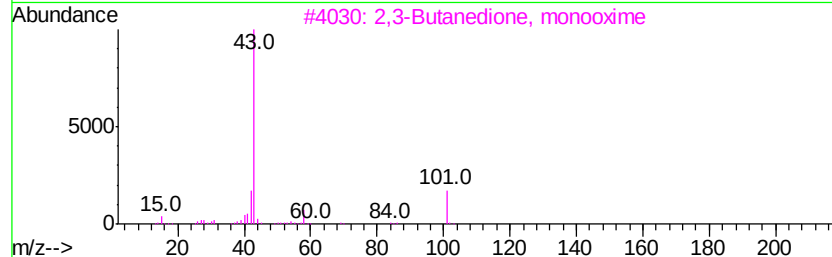
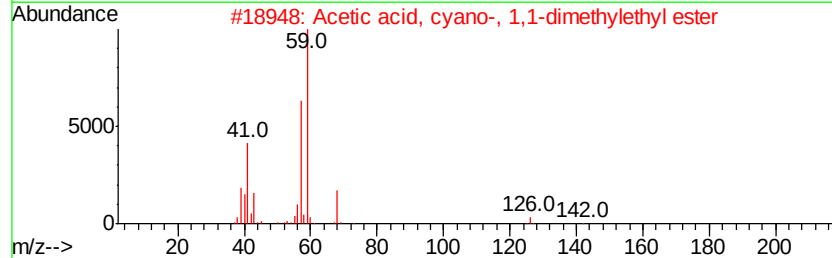
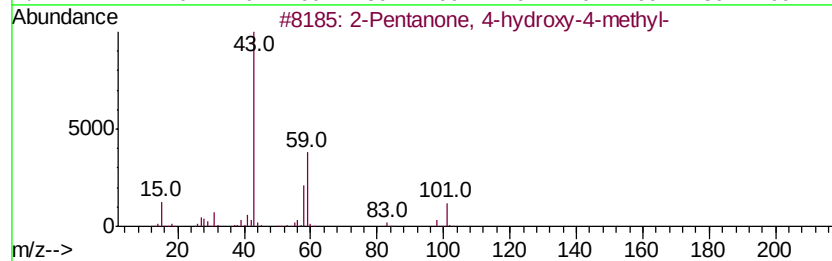
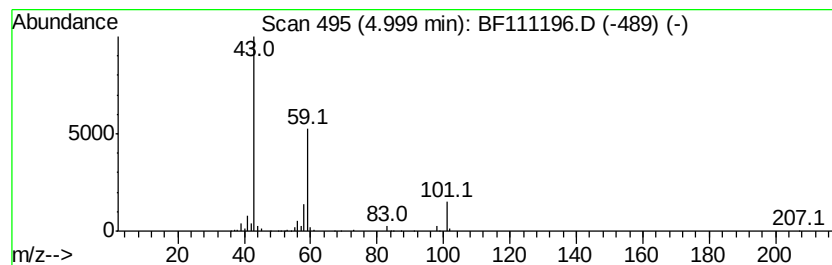
Instrument :
BNA_F
ClientSampleId :
SB-4(3-5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.00	4.87 ng	691754	1,4-Dichlorobenzene-d4	6.80	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	9
5	Ethanol, pentamethyl-	116	C7H16O	000594-83-2	9



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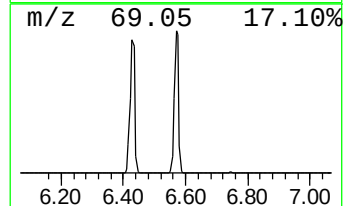
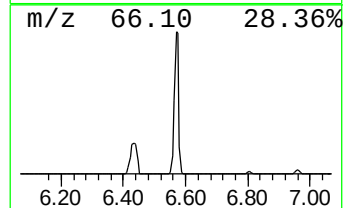
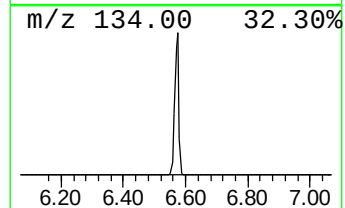
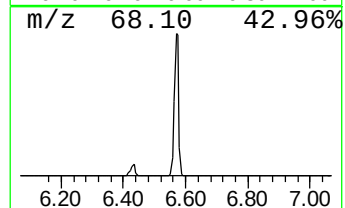
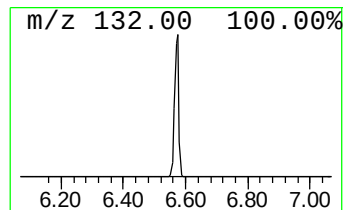
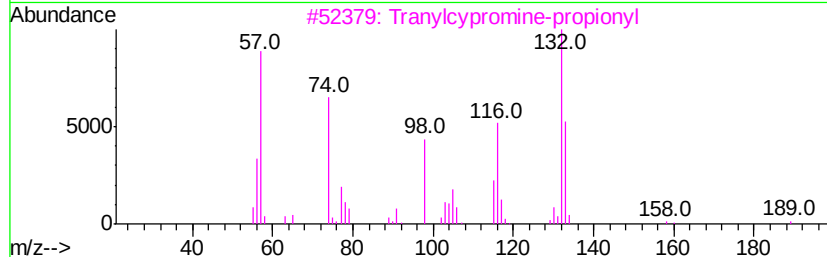
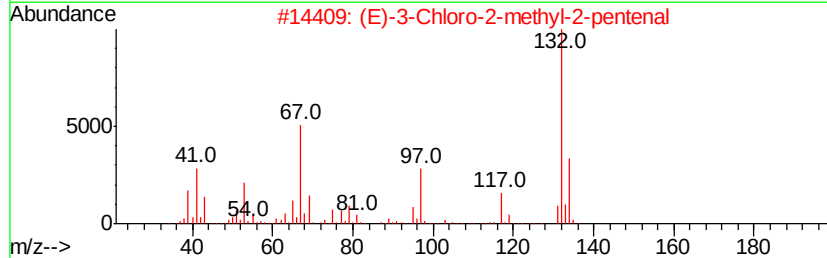
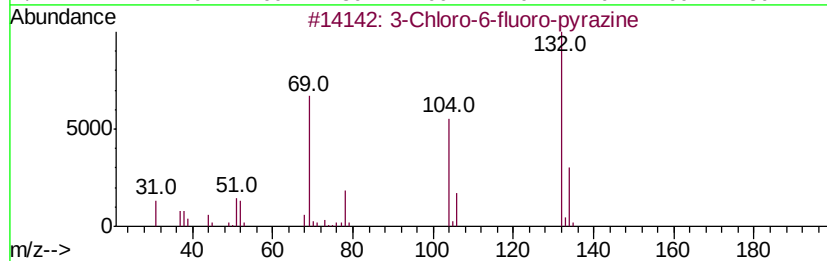
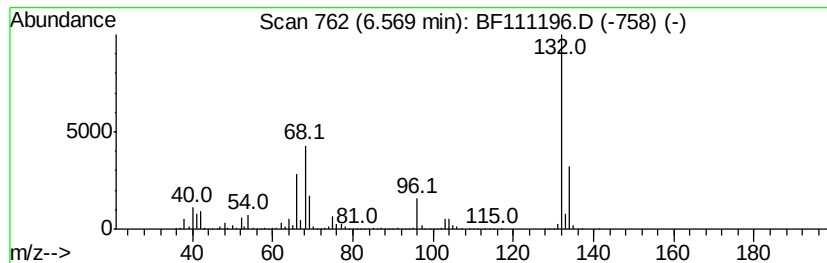
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	53.45 ng	7598050	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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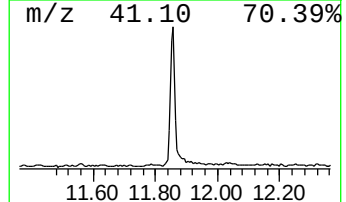
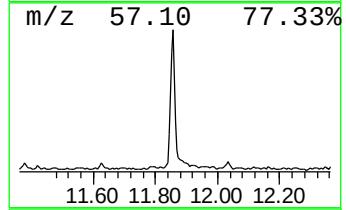
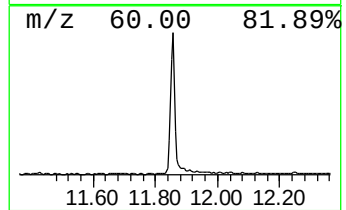
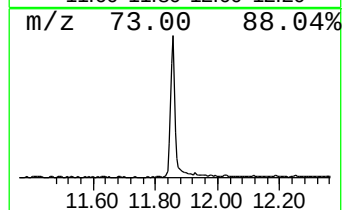
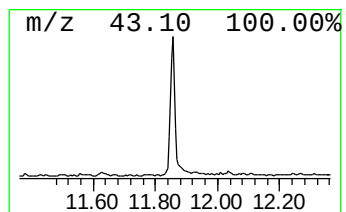
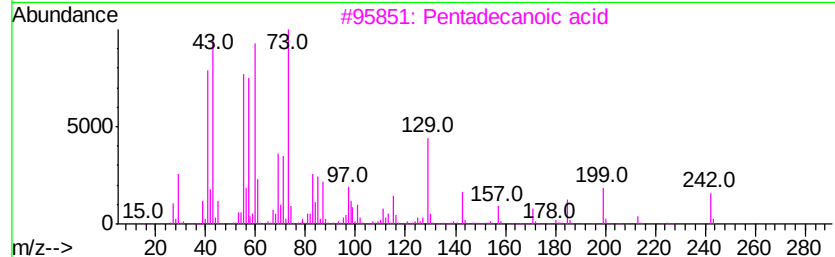
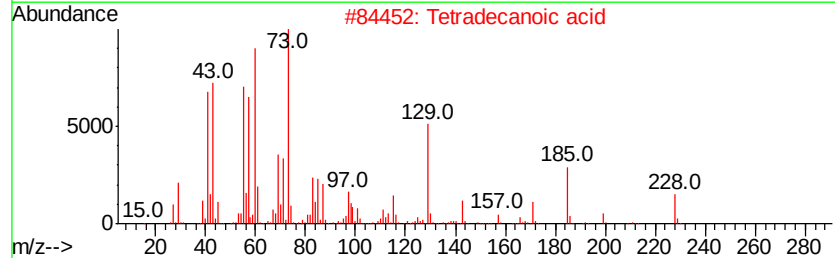
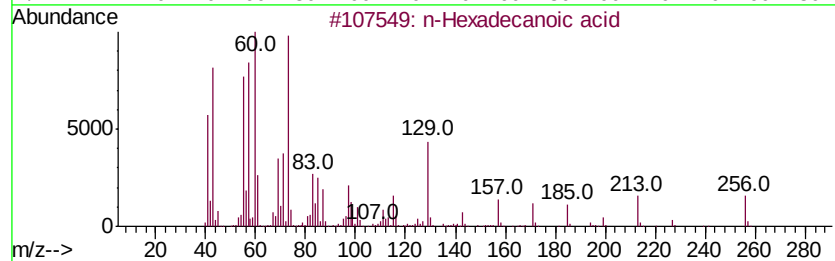
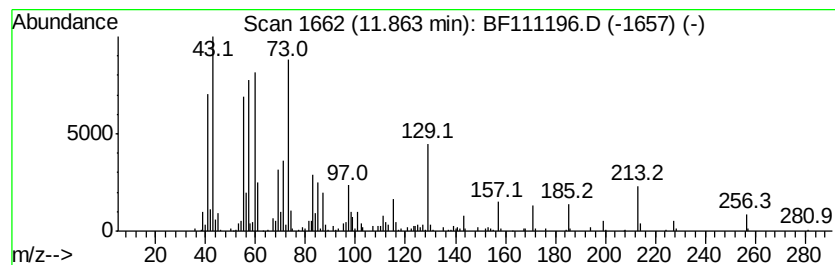
Instrument :
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.86	8.13 ng	1310440	Phenanthrene-d10		11.32	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	97
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Tridecanoic acid	214	C13H26O2	000638-53-9	72
5		Undecanoic acid	186	C11H22O2	000112-37-8	68



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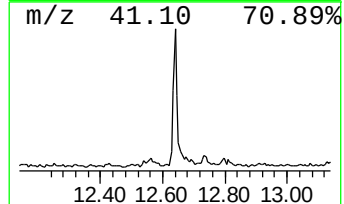
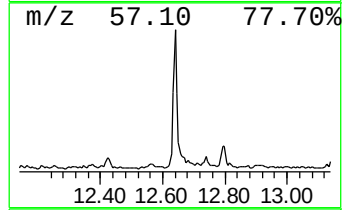
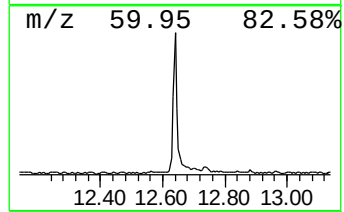
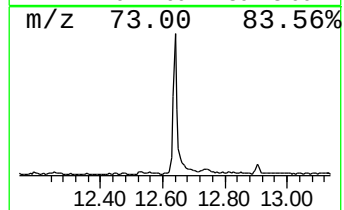
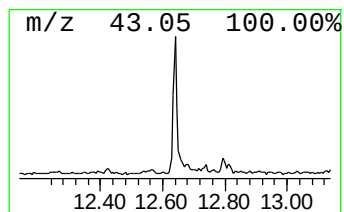
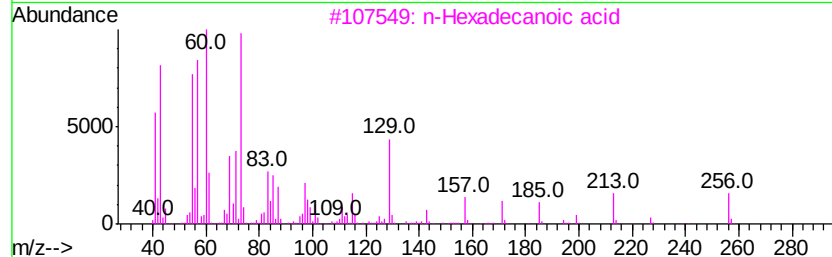
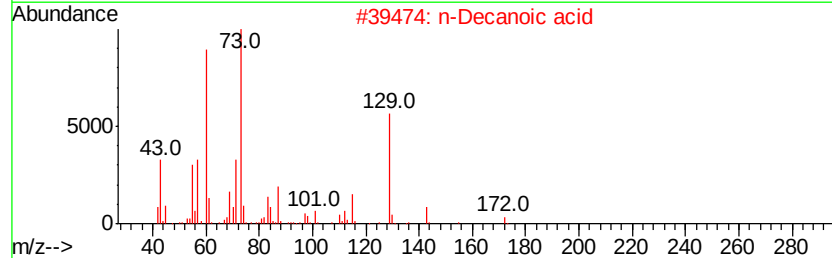
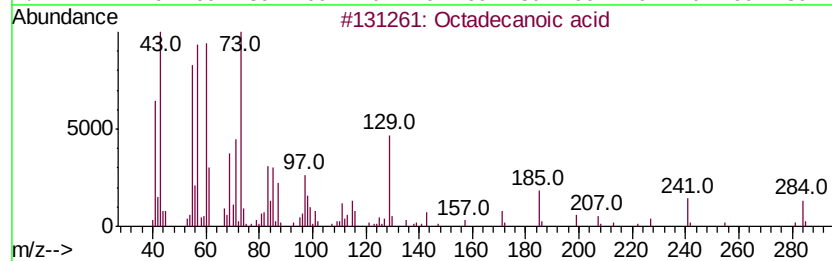
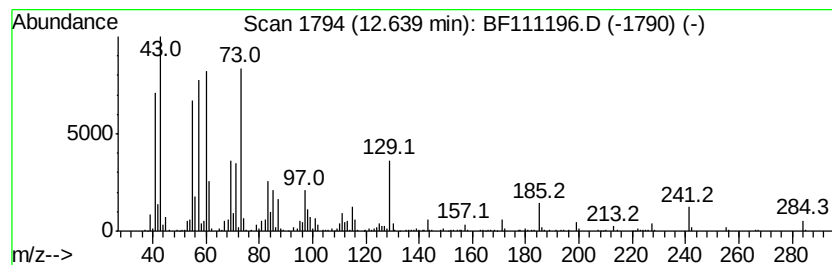
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	5.59 ng	890026	Chrysene-d12	13.96

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		n-Decanoic acid	172	C10H20O2	000334-48-5	91
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	64



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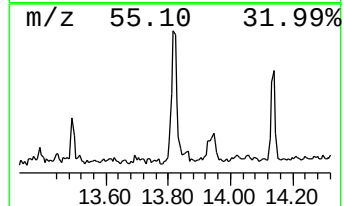
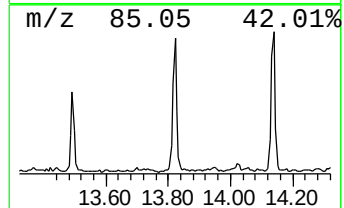
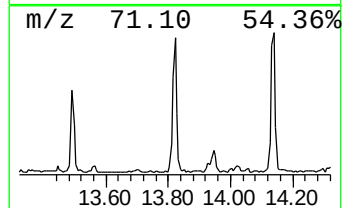
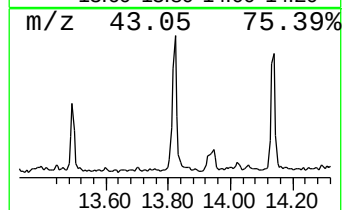
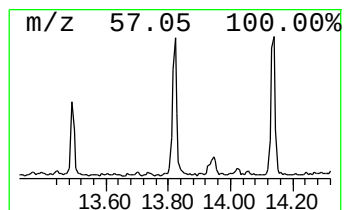
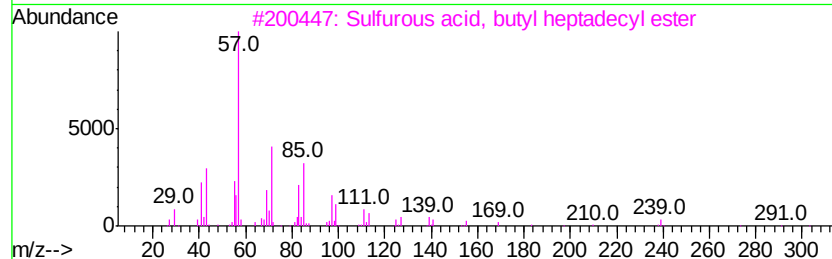
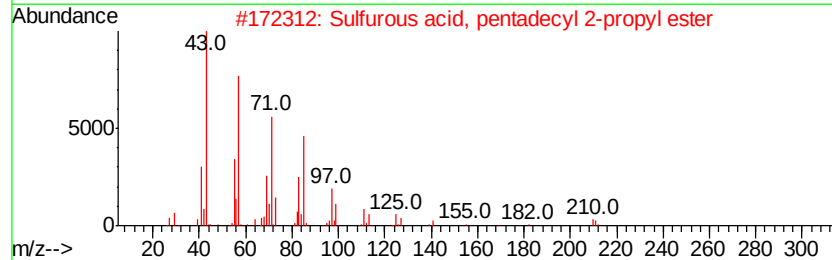
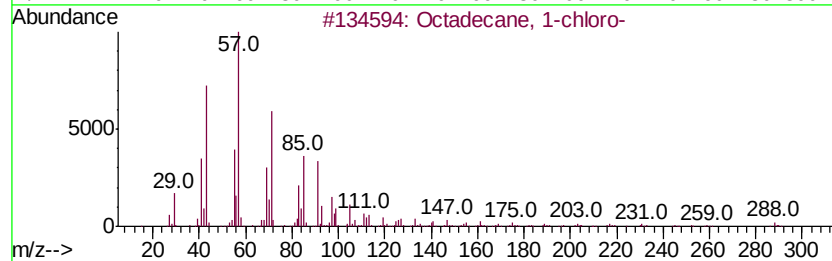
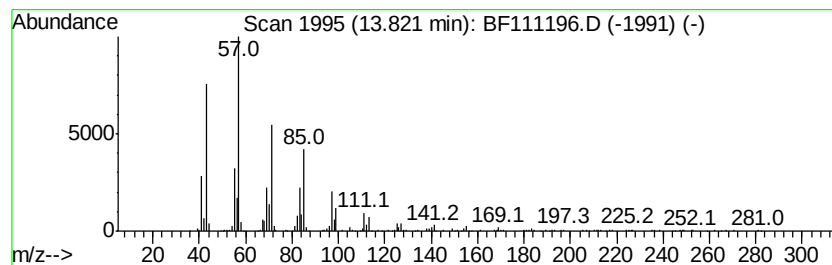
Instrument :
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ClientSampleId :
SB-4(3-5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecane, 1-chloro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.82	3.66 ng	581779	Chrysene-d12	13.96	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	90
2	Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	90
3	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	74
4	Tridecane	184	C13H28	000629-50-5	64
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	62



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120718\
 Data File : BF111196.D
 Acq On : 7 Dec 2018 19:32
 Operator : JU/SJ
 Sample : J6214-11
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

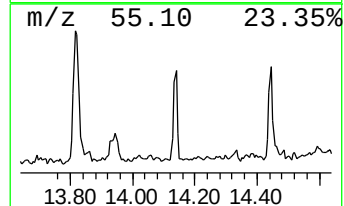
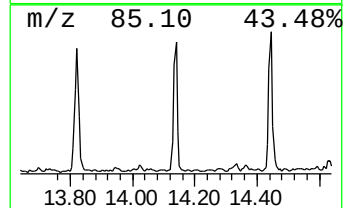
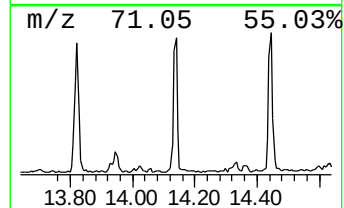
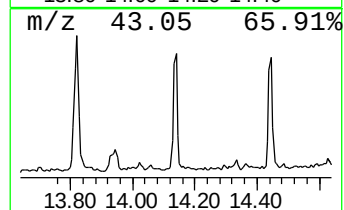
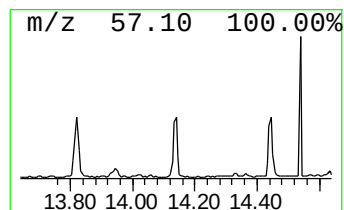
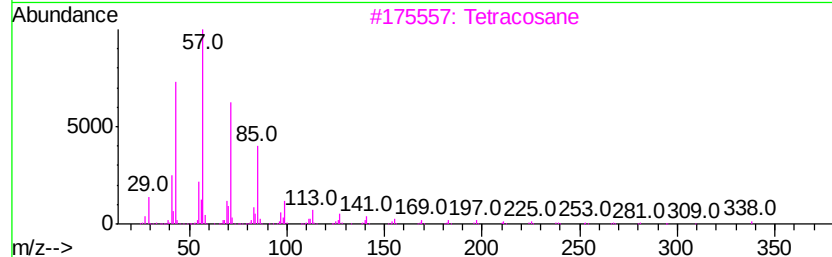
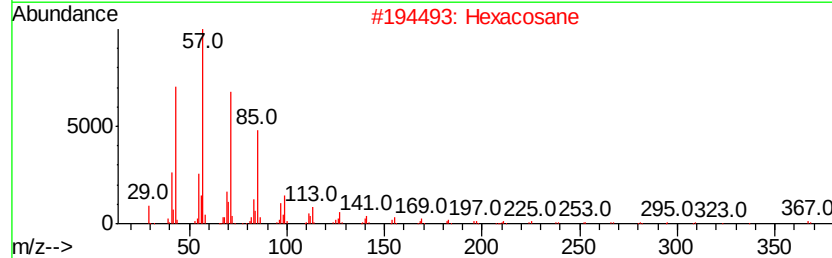
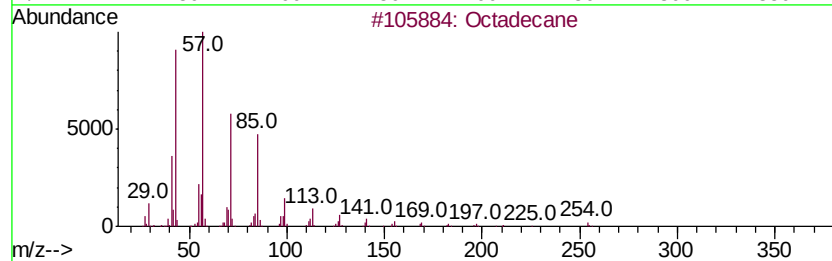
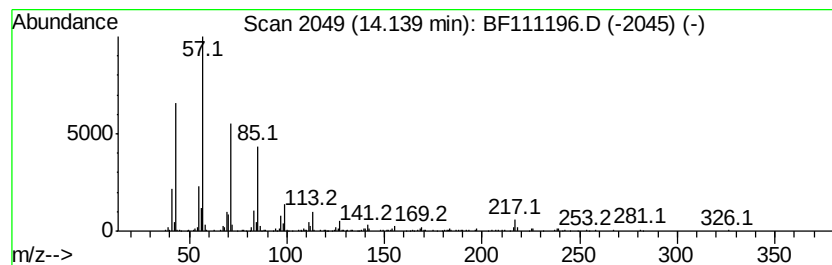
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 ClientSampleId :
 SB-4(3-5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120518.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 7 Octadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.14	2.60 ng	413765	Chrysene-d12	13.96
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octadecane	254 C18H38	000593-45-3	90
2	Hexacosane	366 C26H54	000630-01-3	90
3	Tetracosane	338 C24H50	000646-31-1	90
4	Octacosane	394 C28H58	000630-02-4	90
5	Eicosane	282 C20H42	000112-95-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120718\
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Operator : JU/SJ
Sample : J6214-11
Misc :
ALS Vial : 20 Sample Multiplier: 1

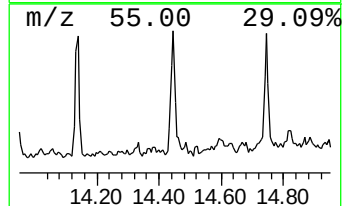
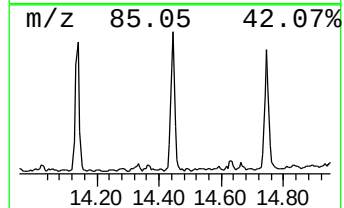
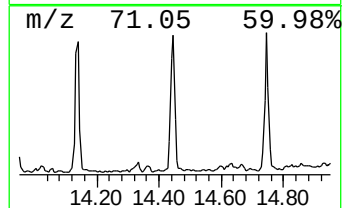
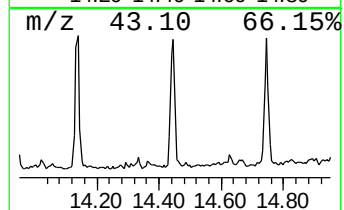
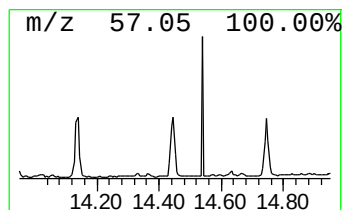
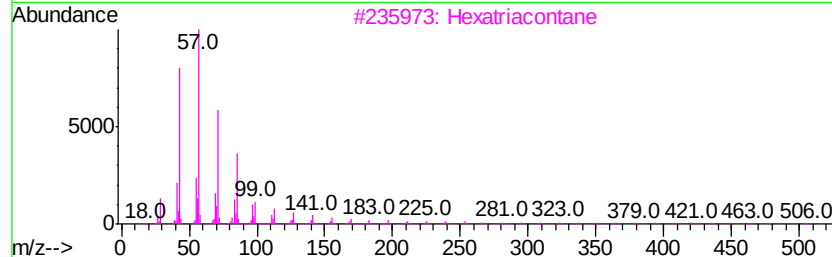
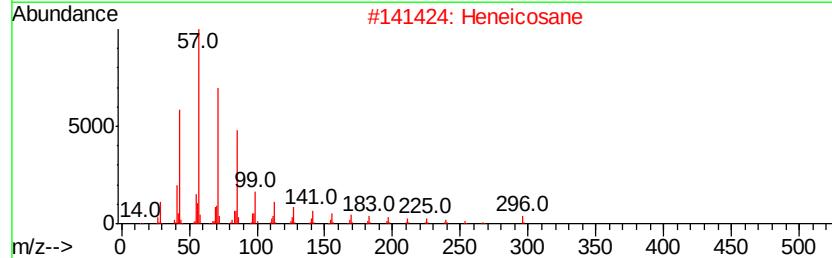
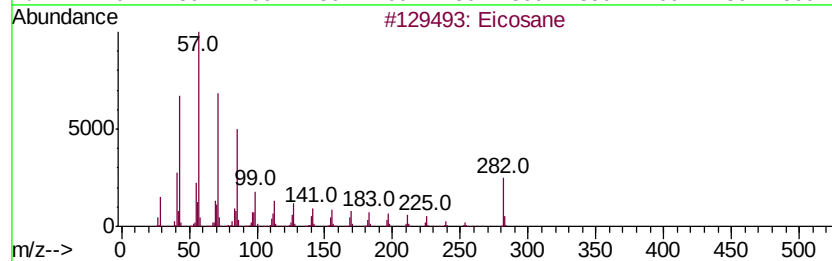
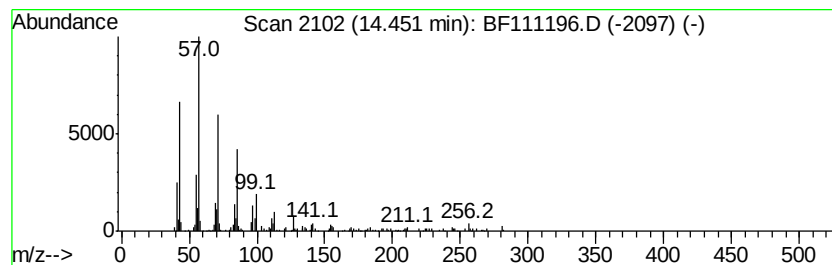
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SB-4(3-5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	2.71 ng	430795	Chrysene-d12	13.96
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane		282 C20H42	000112-95-8 86
2	Heneicosane		296 C21H44	000629-94-7 86
3	Hexatriacontane		507 C36H74	000630-06-8 83
4	1-Iodoundecane		282 C11H23I	004282-44-4 81
5	Tridecane, 1-iodo-		310 C13H27I	035599-77-0 80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120718\
Data File : BF111196.D
Acq On : 7 Dec 2018 19:32
Operator : JU/SJ
Sample : J6214-11
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-4(3-5)

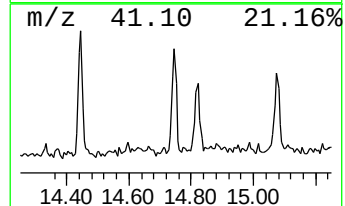
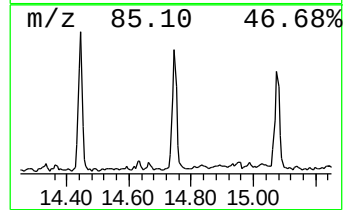
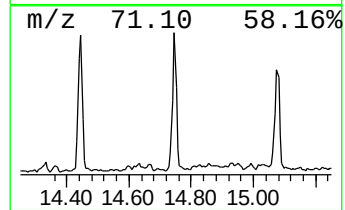
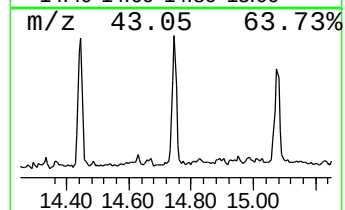
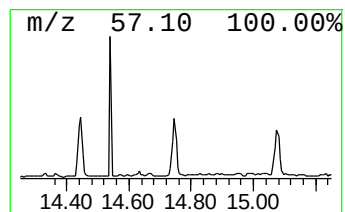
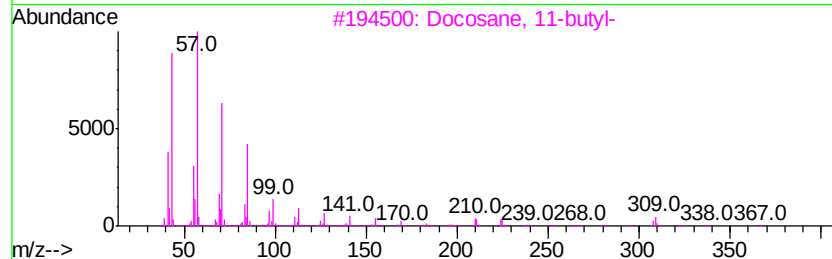
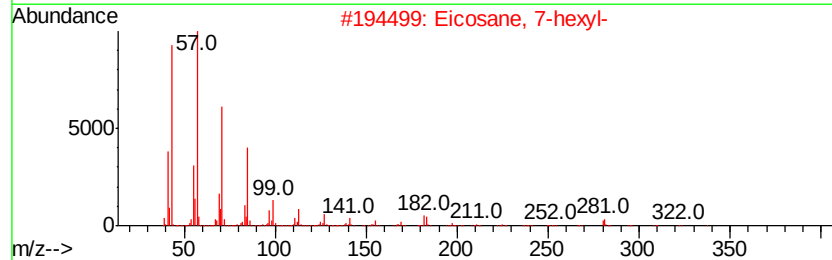
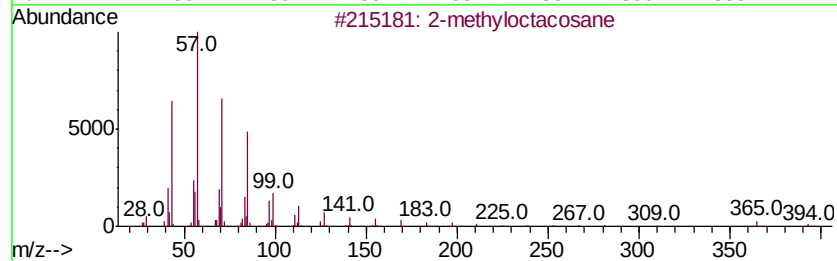
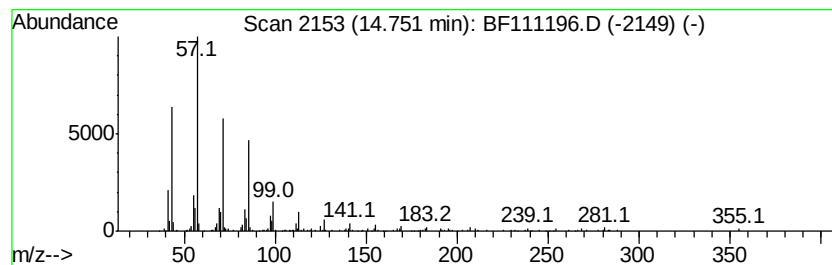
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-methyloctacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	3.48 ng	420568	Perylene-d12	15.39

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane		408	C29H60	1000376-72-8	90
2	Eicosane, 7-hexyl-		366	C26H54	055333-99-8	90
3	Docosane, 11-butyl-		366	C26H54	013475-76-8	90
4	Pentacosane		352	C25H52	000629-99-2	90
5	Heptacosane		380	C27H56	000593-49-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120718\
Data File : BF111196.D
Acq On : 7 Dec 2018 19:32
Operator : JU/SJ
Sample : J6214-11
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-4(3-5)

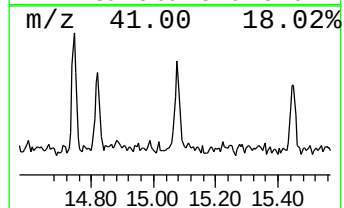
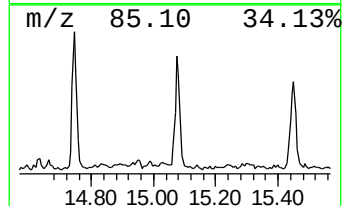
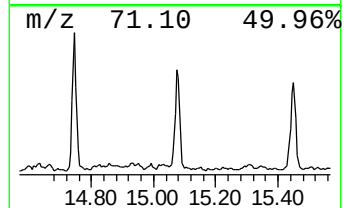
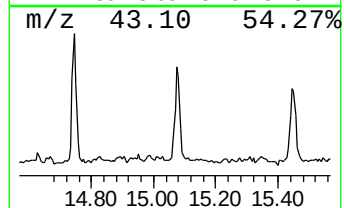
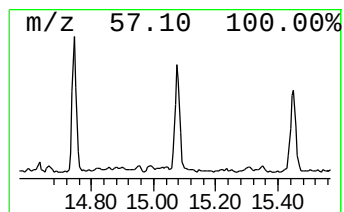
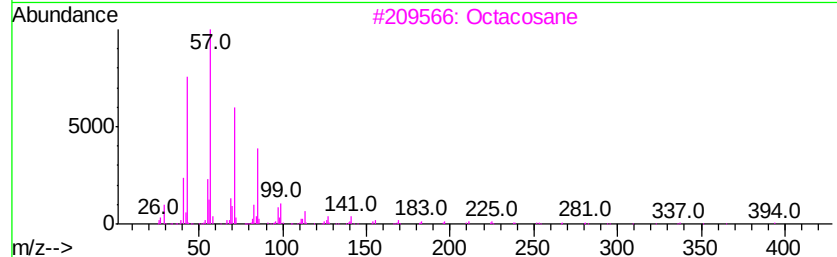
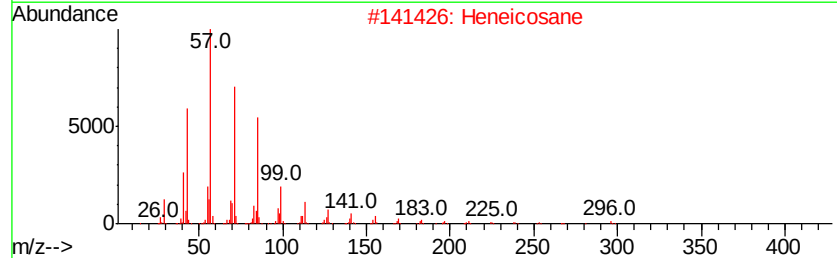
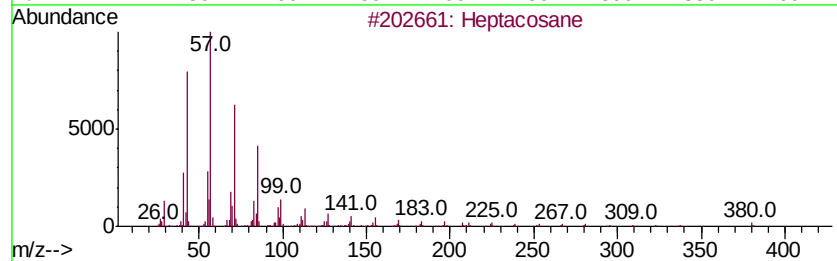
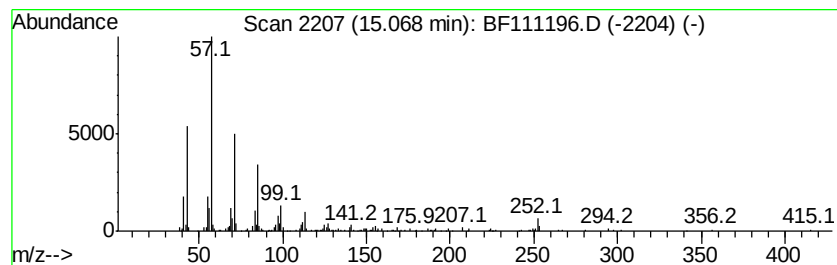
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	3.38 ng	408718	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	87
2		Heneicosane	296	C21H44	000629-94-7	87
3		Octacosane	394	C28H58	000630-02-4	87
4		Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87
5		Docosane, 11-butyl-	366	C26H54	013475-76-8	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120718\
 Data File : BF111196.D
 Acq On : 7 Dec 2018 19:32
 Operator : JU/SJ
 Sample : J6214-11
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
 SB-4(3-5)

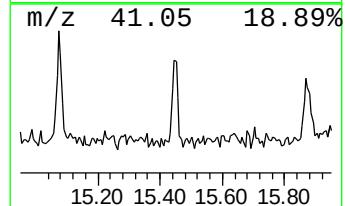
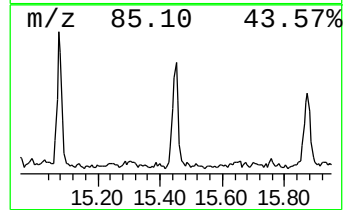
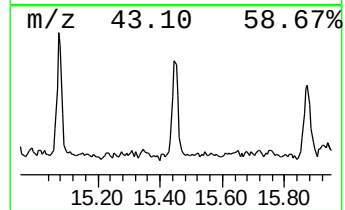
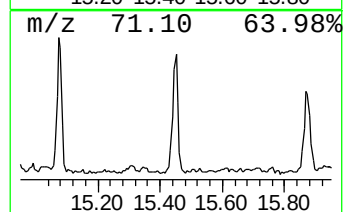
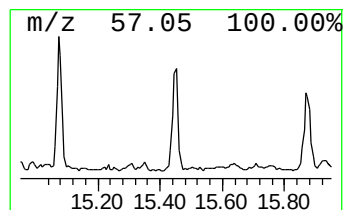
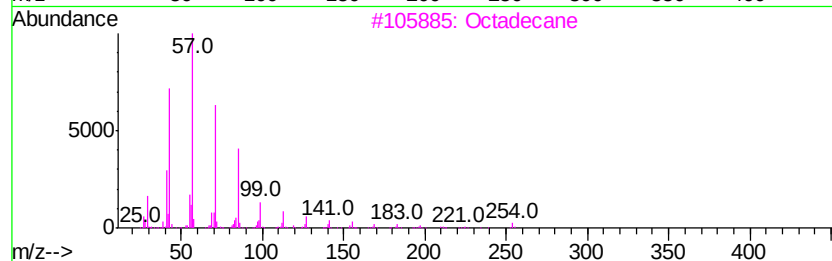
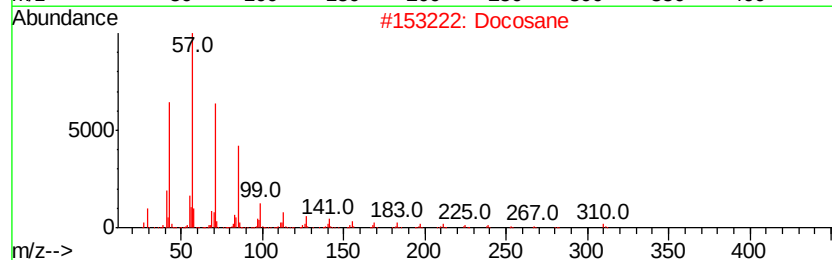
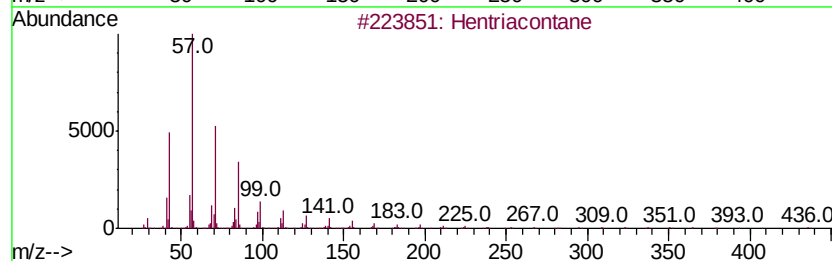
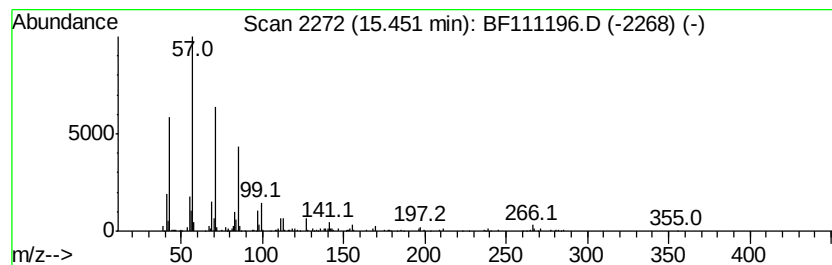
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 11 Hentriacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.45	2.99 ng	361017	Perylene-d12	15.39

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	91
2	Docosane		310	C22H46	000629-97-0	87
3	Octadecane		254	C18H38	000593-45-3	87
4	Hexadecane		226	C16H34	000544-76-3	86
5	Heptacosane		380	C27H56	000593-49-7	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120718\
Data File : BF111196.D
Acq On : 7 Dec 2018 19:32
Operator : JU/SJ
Sample : J6214-11
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-4(3-5)

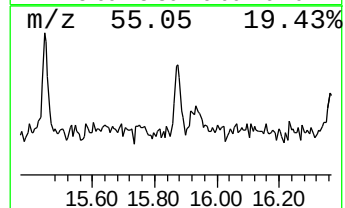
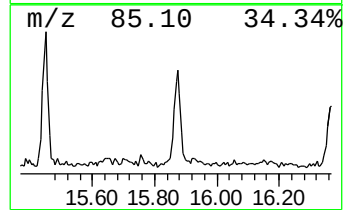
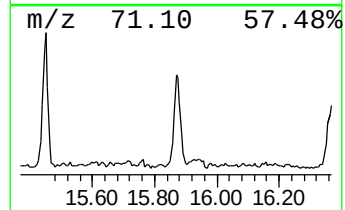
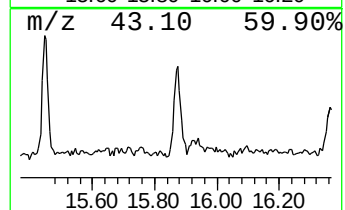
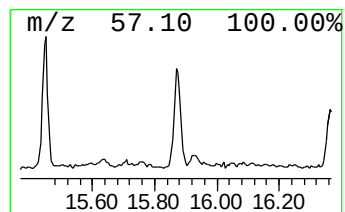
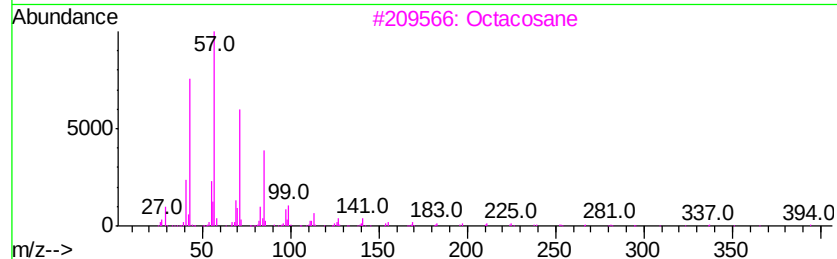
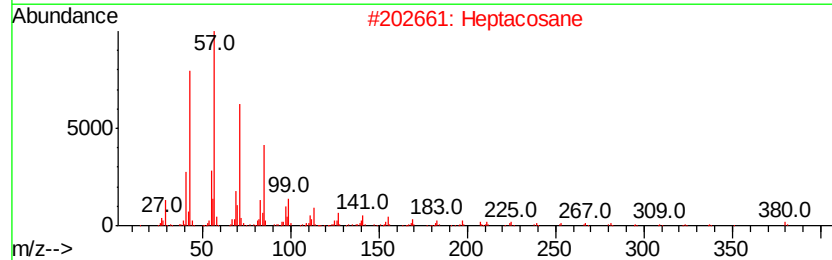
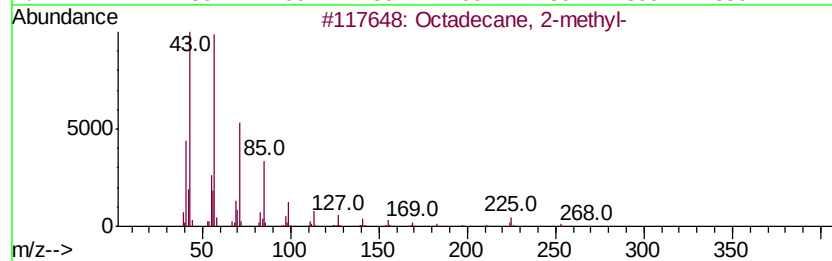
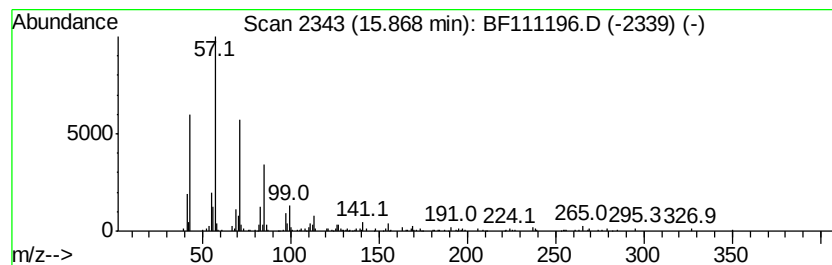
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octadecane, 2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.87	2.44 ng	294742	Perylene-d12	15.39

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
2			Heptacosane	380	C27H56	000593-49-7	90
3			Octacosane	394	C28H58	000630-02-4	90
4			Hexacosane	366	C26H54	000630-01-3	90
5			Hexatriacontane	507	C36H74	000630-06-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF120718\
Data File : BF111196.D
Acq On : 7 Dec 2018 19:32
Operator : JU/SJ
Sample : J6214-11
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-4(3-5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120518.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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unknown6.57	6.57	53.5 ng		7598050	1	6.80	2843040	20.0
n-Hexadecanoic acid	11.86	8.1 ng		1310440	4	11.32	3221910	20.0
Octadecanoic acid	12.64	5.6 ng		890026	5	13.96	3183290	20.0
Octadecane, 1-chl...	13.82	3.7 ng		581779	5	13.96	3183290	20.0
Octadecane	14.14	2.6 ng		413765	5	13.96	3183290	20.0
Eicosane	14.45	2.7 ng		430795	5	13.96	3183290	20.0
2-methyloctacosane	14.75	3.5 ng		420568	6	15.39	2417470	20.0
Heptacosane	15.07	3.4 ng		408718	6	15.39	2417470	20.0
Hentriacontane	15.45	3.0 ng		361017	6	15.39	2417470	20.0
Octadecane, 2-met...	15.87	2.4 ng		294742	6	15.39	2417470	20.0