

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122118\
 Data File : BF111682.D
 Acq On : 21 Dec 2018 12:48
 Operator : JU/SJ
 Sample : J6353-06
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P001-SS003-0002-01

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-BF121918.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	2.216	17	22	31	rVB	59262	84122	2.28%	0.203%
2	3.428	225	228	241	rVB	15986	36891	1.00%	0.089%
3	5.116	510	515	521	rVB	168262	199910	5.42%	0.482%
4	5.516	578	583	587	rBV	3138046	3135348	85.06%	7.562%
5	6.522	748	754	764	rBV	3522193	3685865	100.00%	8.889%
6	6.663	774	778	782	rBV	3755095	3319840	90.07%	8.007%
7	6.892	814	817	821	rBV	1390562	1203541	32.65%	2.903%
8	7.051	840	844	847	rBV	3010916	2435392	66.07%	5.874%
9	7.451	907	912	915	rBV	2723952	2408202	65.34%	5.808%
10	8.175	1031	1035	1038	rBV	1867702	1583261	42.95%	3.818%
11	9.251	1213	1218	1221	rBV	3823106	3098400	84.06%	7.473%
12	9.639	1281	1284	1287	rBV	428510	316171	8.58%	0.763%
13	9.933	1329	1334	1337	rBV	2041781	1798958	48.81%	4.339%
14	10.128	1358	1367	1371	rBV2	67720	87382	2.37%	0.211%
15	10.333	1399	1402	1410	rVB2	116772	168632	4.58%	0.407%
16	10.716	1462	1467	1470	rBV	2635205	2255602	61.20%	5.440%
17	11.075	1522	1528	1531	rVB6	47036	67860	1.84%	0.164%
18	11.275	1559	1562	1567	rVB3	61777	67835	1.84%	0.164%
19	11.416	1582	1586	1589	rBV	2144816	1811298	49.14%	4.368%
20	11.810	1650	1653	1656	rBV	134597	116207	3.15%	0.280%
21	11.951	1670	1677	1693	rVB	2046745	2739827	74.33%	6.608%
22	12.633	1789	1793	1794	rBV3	128012	151535	4.11%	0.365%
23	12.651	1794	1796	1801	rVV	199751	240291	6.52%	0.580%
24	12.733	1803	1810	1821	rVV	2060315	2667576	72.37%	6.434%
25	12.821	1823	1825	1828	rVB2	91592	80270	2.18%	0.194%
26	12.874	1831	1834	1837	rBV	150076	149573	4.06%	0.361%
27	12.998	1851	1855	1858	rBV	3457986	2900526	78.69%	6.995%
28	13.045	1858	1863	1866	rBV2	84311	148070	4.02%	0.357%
29	13.774	1982	1987	1995	rBV2	174053	375303	10.18%	0.905%
30	13.892	2004	2007	2015	rVB	581519	535752	14.54%	1.292%
31	14.051	2029	2034	2037	rBV	1495485	1452888	39.42%	3.504%
32	14.351	2080	2085	2090	rBV	241922	382628	10.38%	0.923%
33	15.527	2280	2285	2289	rBV2	980191	1171409	31.78%	2.825%
34	16.015	2366	2368	2372	rVV2	58831	71679	1.94%	0.173%

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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	16.062	2373	2376	2389	rvB4	133387	363579	9.86%	0.877%
36	16.262	2408	2410	2419	rvB6	69809	152009	4.12%	0.367%

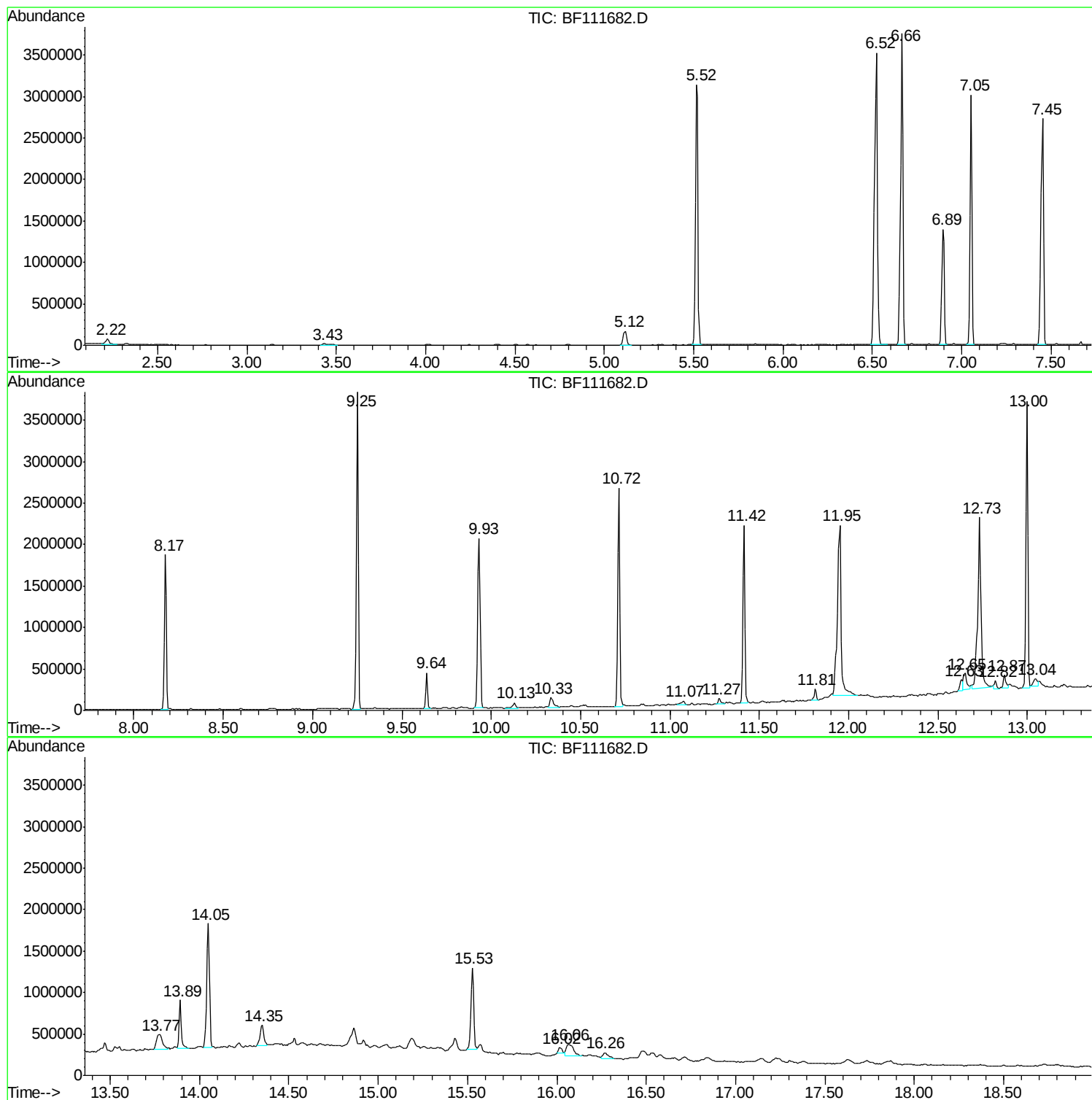
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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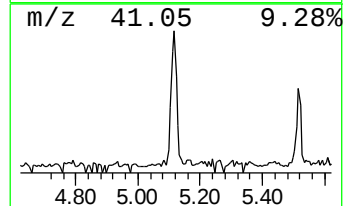
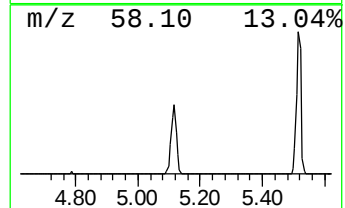
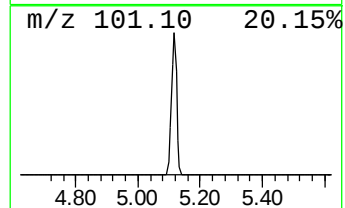
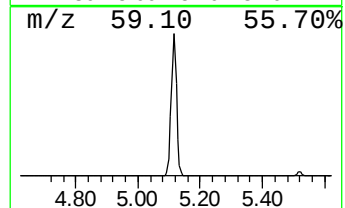
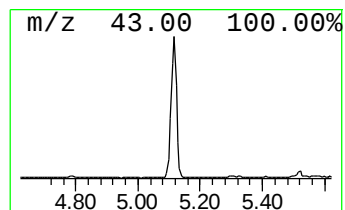
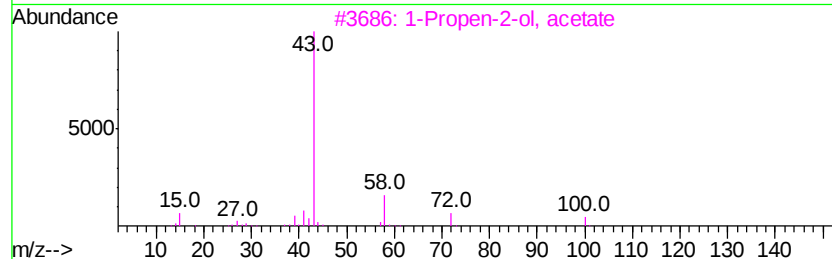
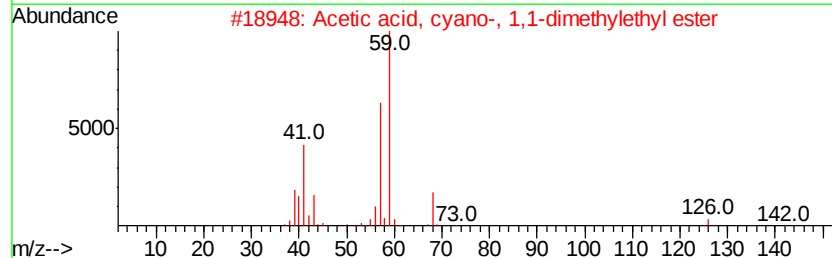
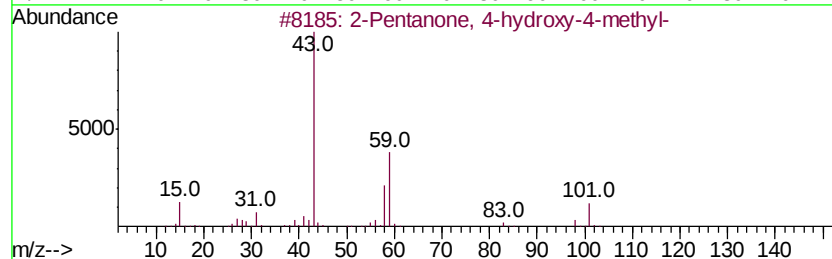
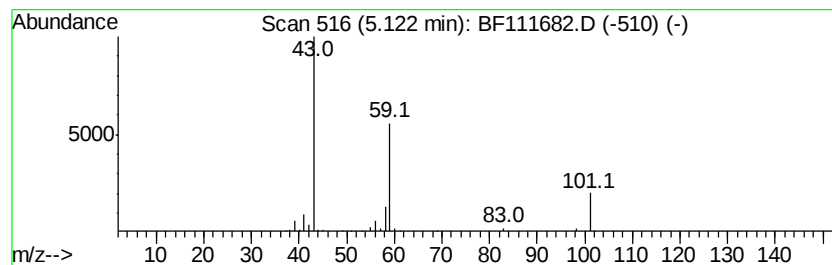
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	3.32 ng	199910	1,4-Dichlorobenzene-d4	6.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64	
2	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25	
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10	
4	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9	
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	



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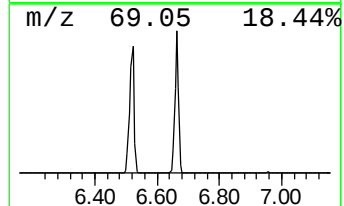
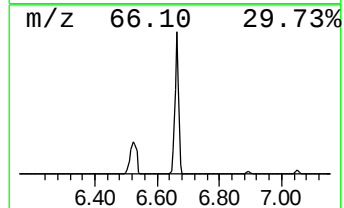
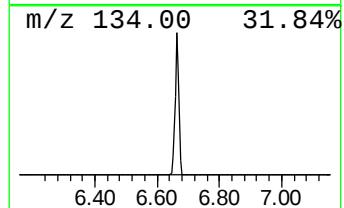
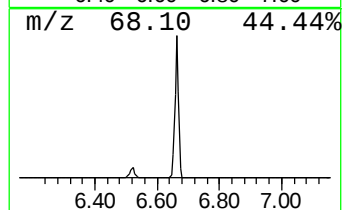
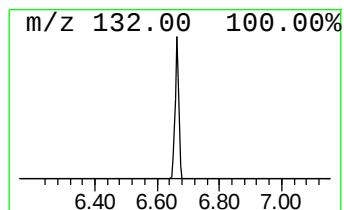
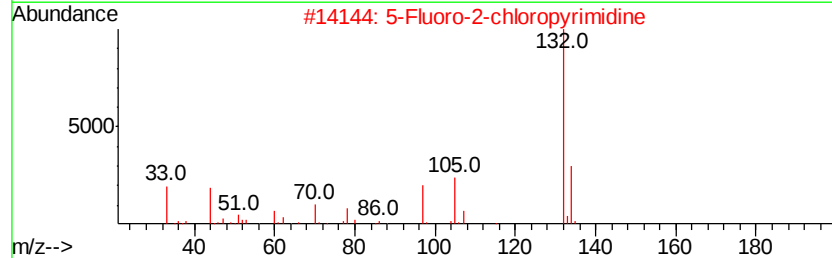
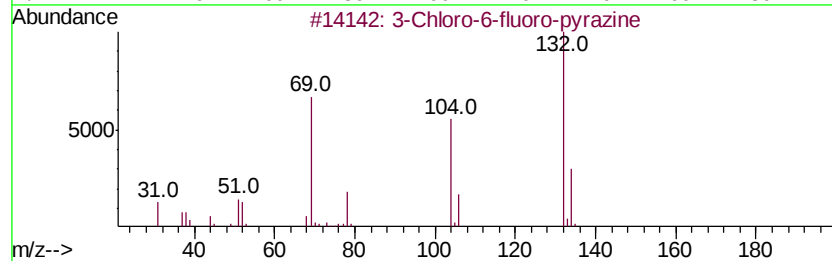
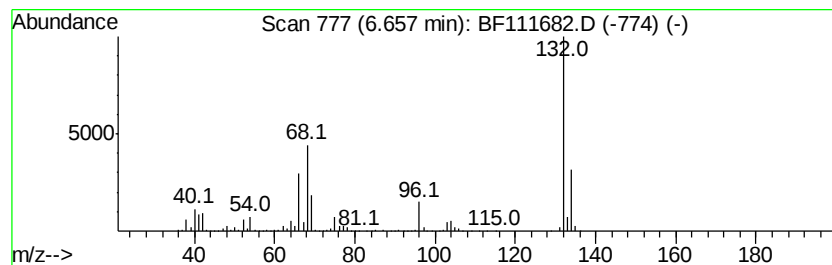
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	55.17 ng	3319840	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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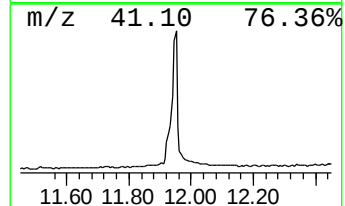
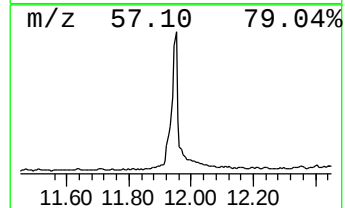
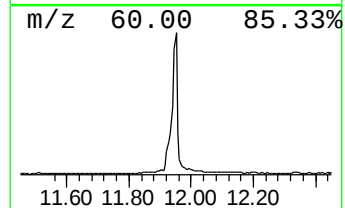
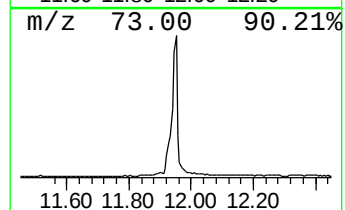
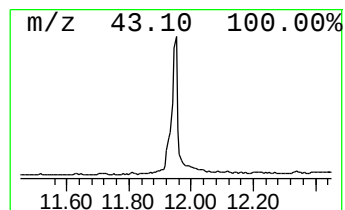
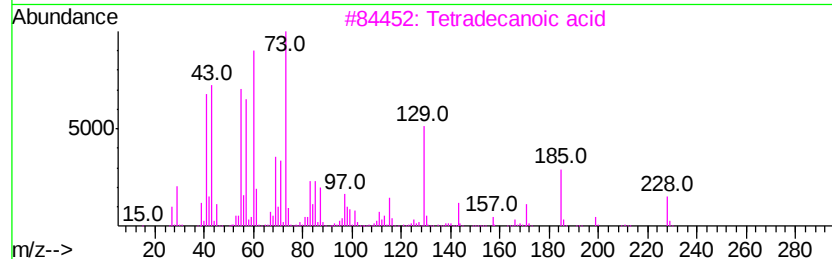
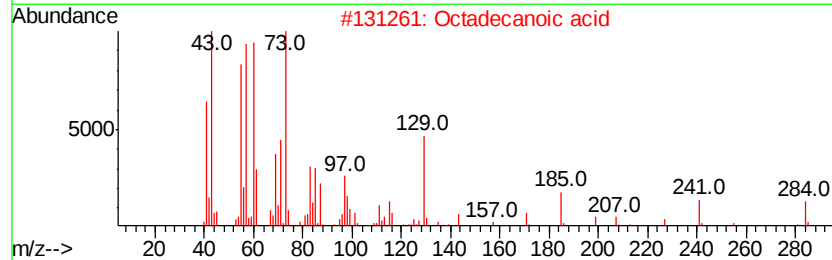
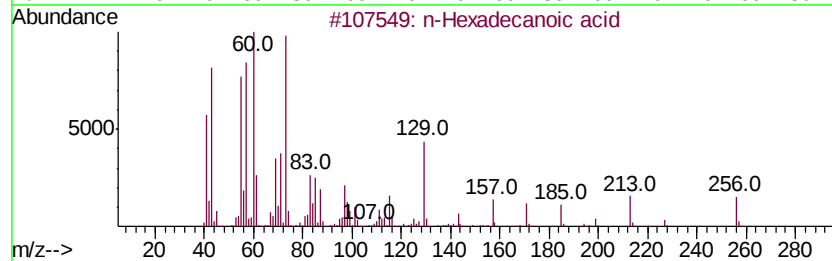
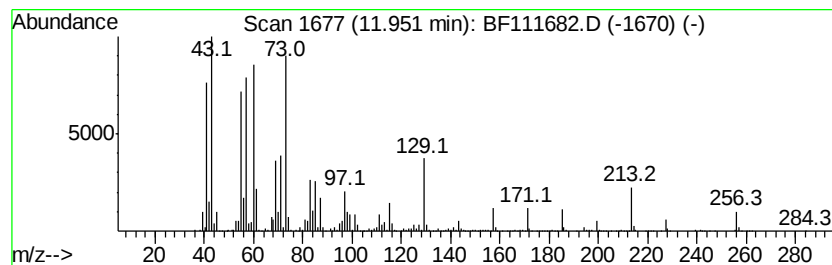
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.95	30.25 ng	2739830	Phenanthrene-d10		11.42
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Octadecanoic acid	284	C18H36O2	000057-11-4	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Tridecanoic acid	214	C13H26O2	000638-53-9	80



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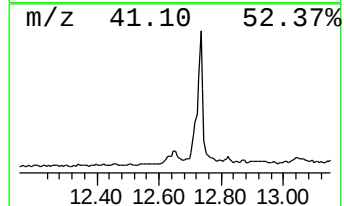
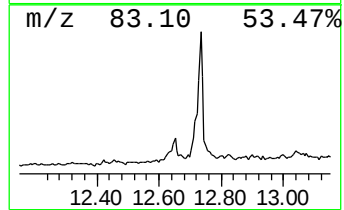
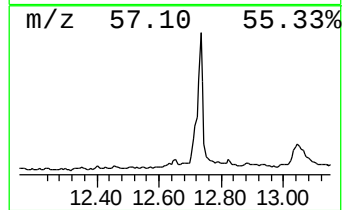
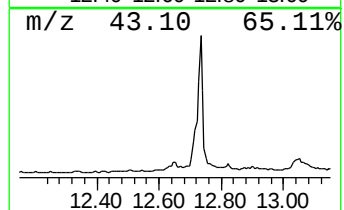
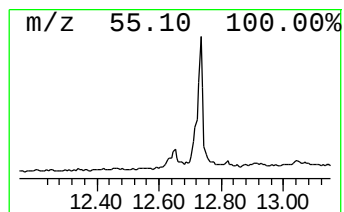
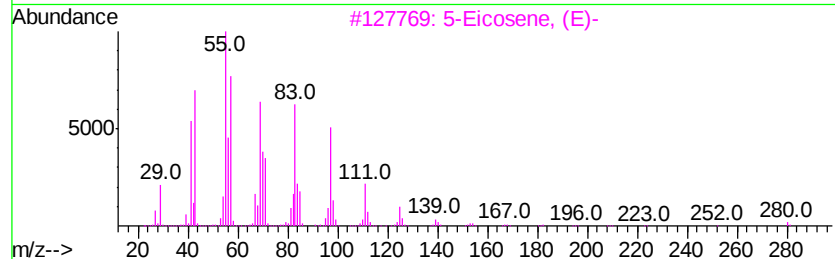
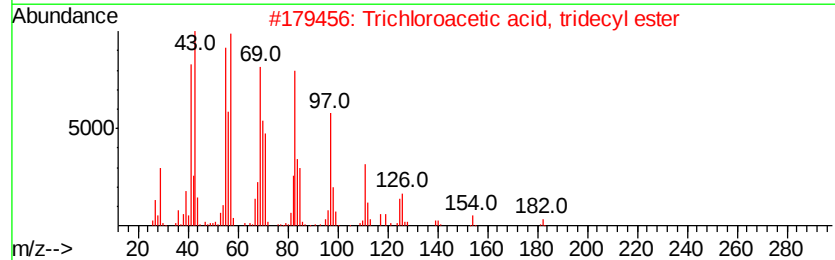
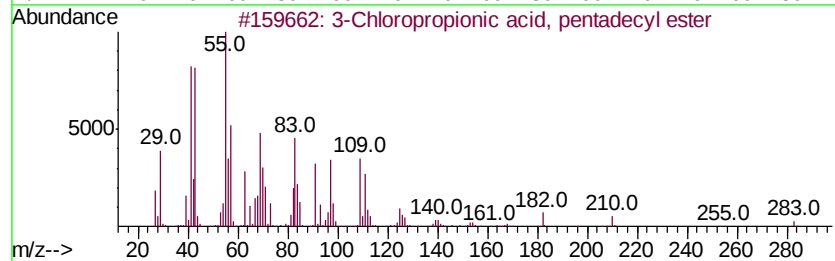
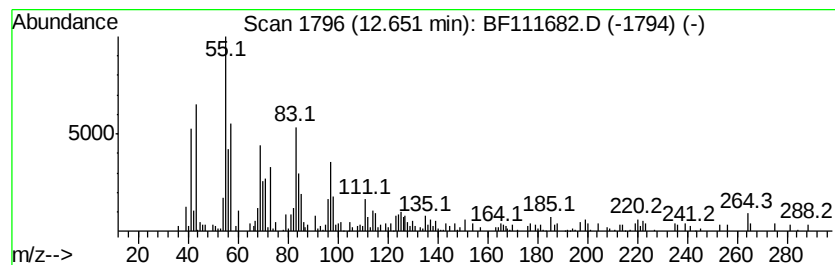
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 3-Chloropropionic acid, pen... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	2.65 ng	240291	Phenanthrene-d10	11.42

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Chloropropionic acid, pentadec...	318	C18H35ClO2	1000281-77-6	64
2		Trichloroacetic acid, tridecyl e...	344	C15H27Cl3O2	074339-51-8	64
3		5-Eicosene, (E)-	280	C20H40	074685-30-6	53
4		1-Octadecene	252	C18H36	000112-88-9	53
5		1-Tridecene	182	C13H26	002437-56-1	52



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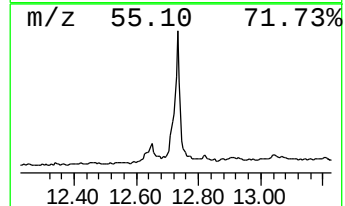
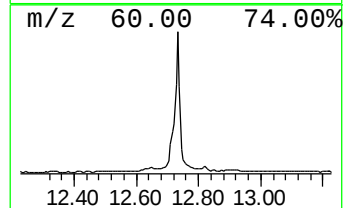
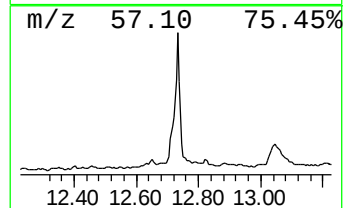
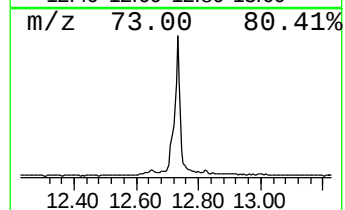
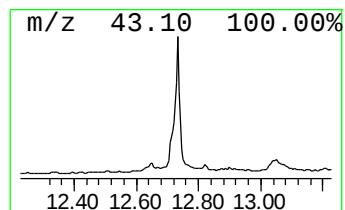
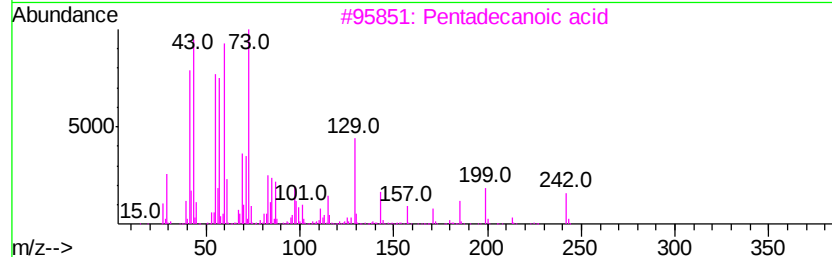
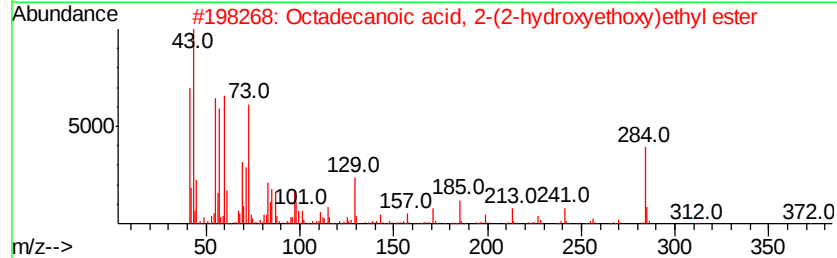
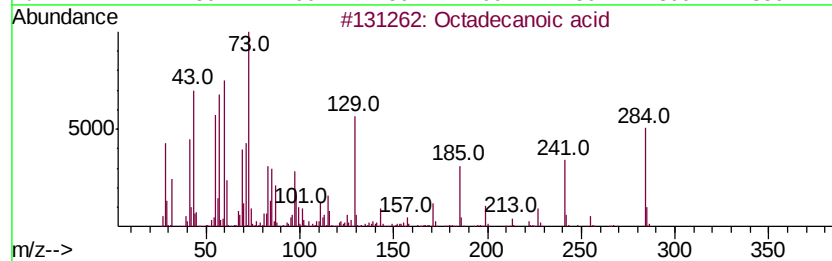
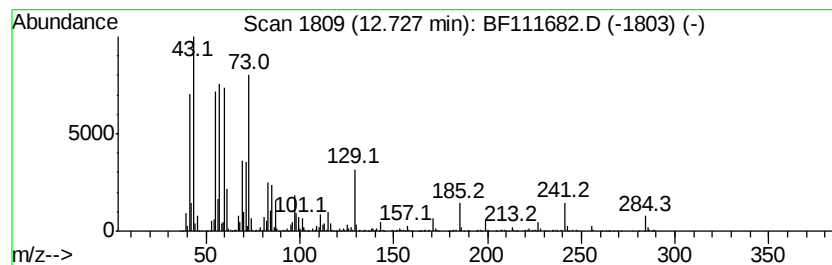
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	29.45 ng	2667580	Phenanthrene-d10	11.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
5		Undecanoic acid	186	C11H22O2	000112-37-8	70



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122118\
Data File : BF111682.D
Acq On : 21 Dec 2018 12:48
Operator : JU/SJ
Sample : J6353-06
Misc :
ALS Vial : 3 Sample Multiplier: 1

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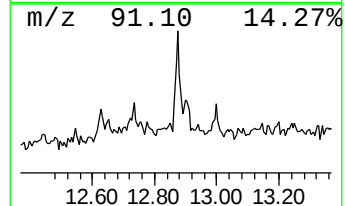
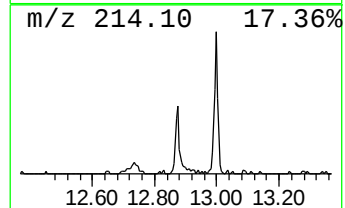
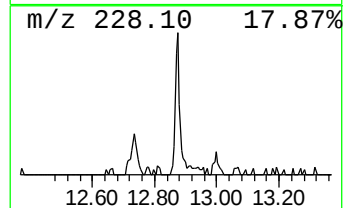
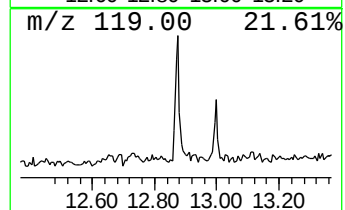
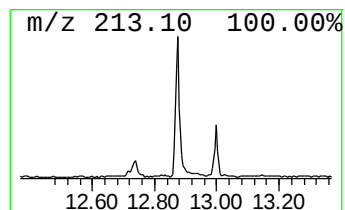
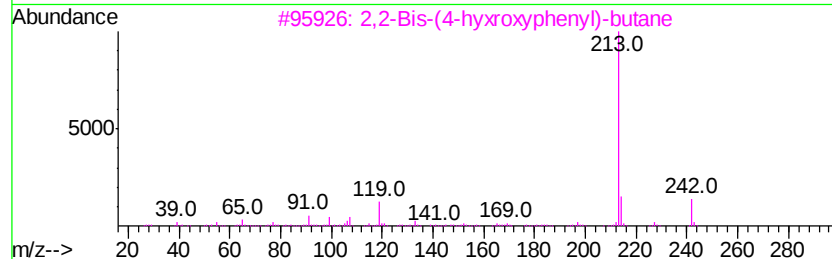
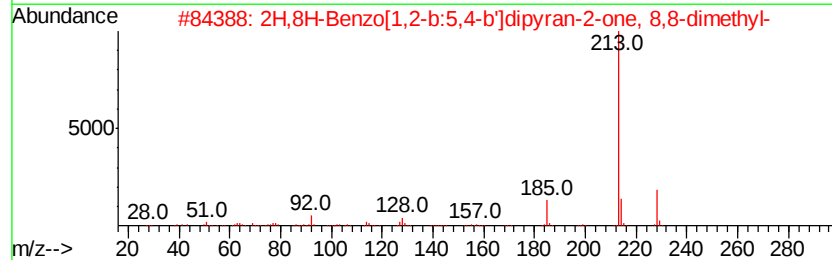
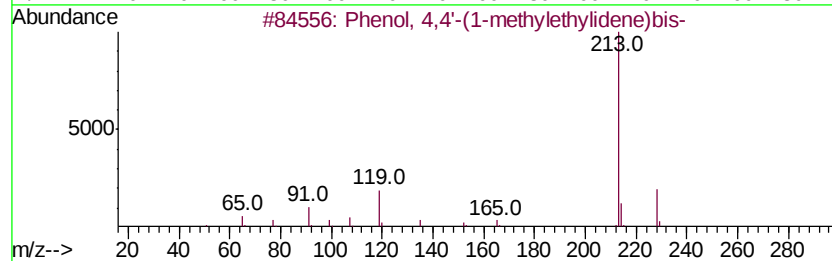
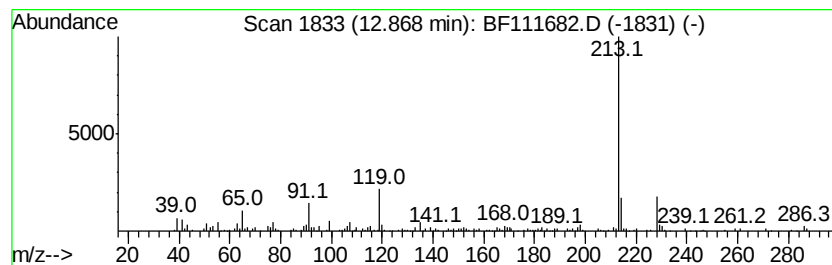
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Phenol, 4,4'-(1-methylethyl... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.87	2.06 ng	149573	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	93
2		2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	59
3		2,2-Bis-(4-hydroxyphenyl)-butane	242	C16H18O2	000077-40-7	50
4		2,5-bis(Trimethylsilyl)thiophene	228	C10H20SSi2	017906-71-7	45
5		2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	45



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122118\
 Data File : BF111682.D
 Acq On : 21 Dec 2018 12:48
 Operator : JU/SJ
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Instrument :
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 ClientSampleId :
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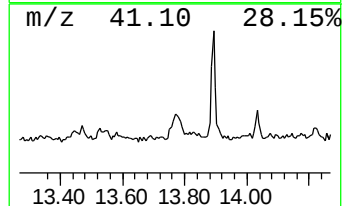
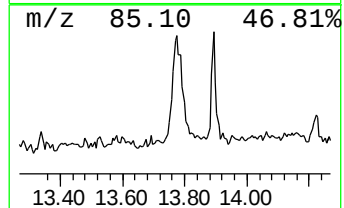
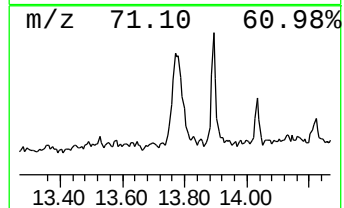
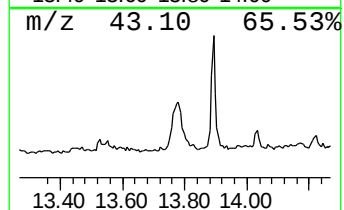
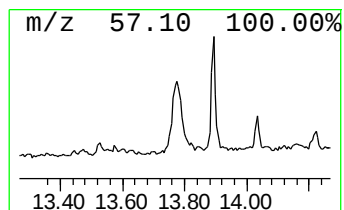
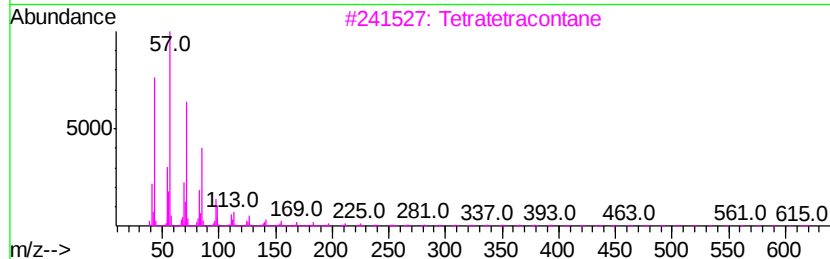
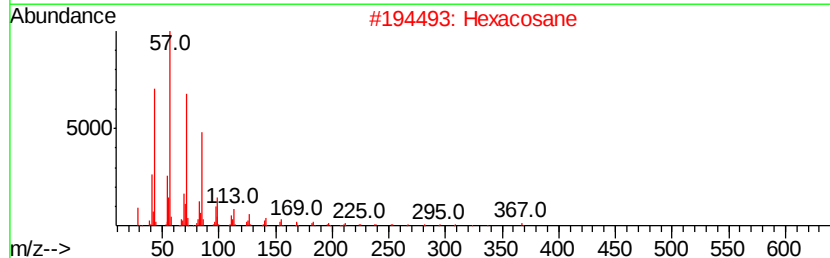
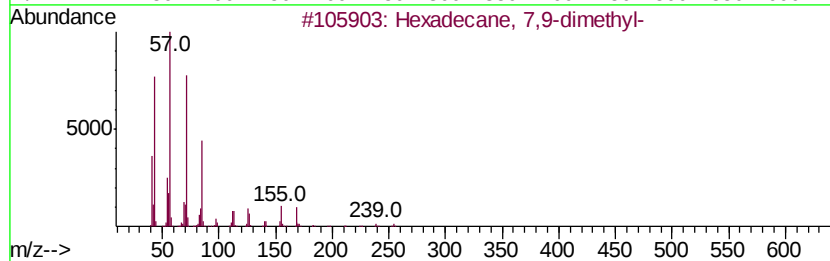
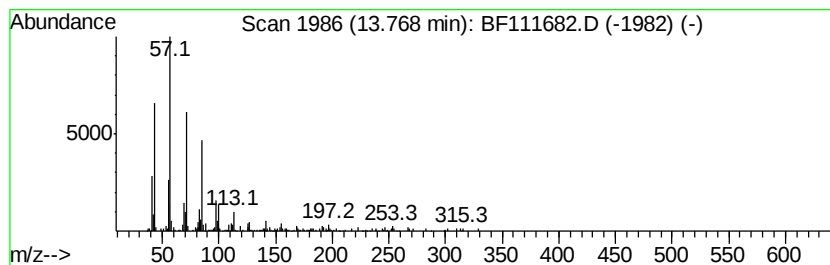
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 8 Hexadecane, 7,9-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	5.17 ng	375303	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	90
2		Hexacosane	366	C26H54	000630-01-3	90
3		Tetratetracontane	619	C44H90	007098-22-8	90
4		2-methyloctacosane	408	C29H60	1000376-72-8	90
5		Heneicosane	296	C21H44	000629-94-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122118\
Data File : BF111682.D
Acq On : 21 Dec 2018 12:48
Operator : JU/SJ
Sample : J6353-06
Misc :
ALS Vial : 3 Sample Multiplier: 1

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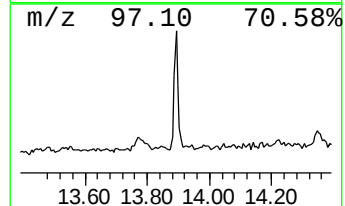
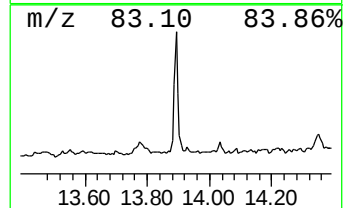
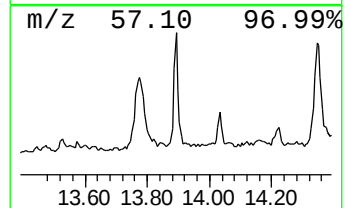
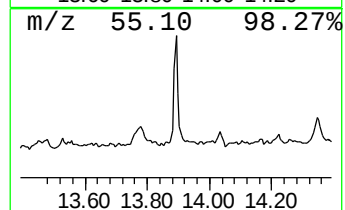
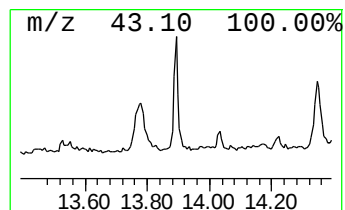
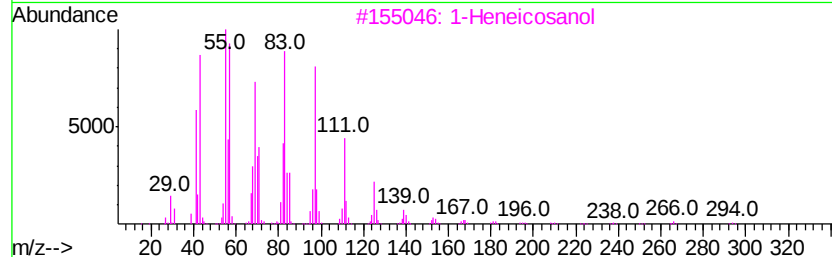
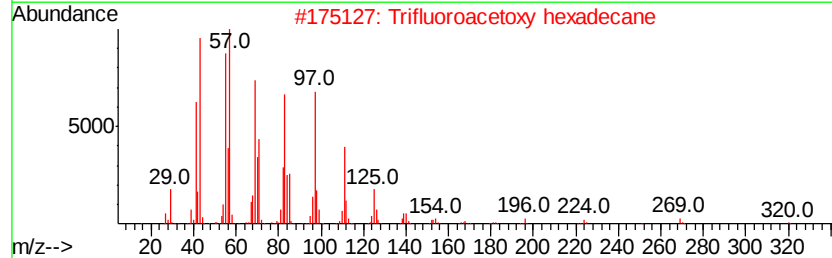
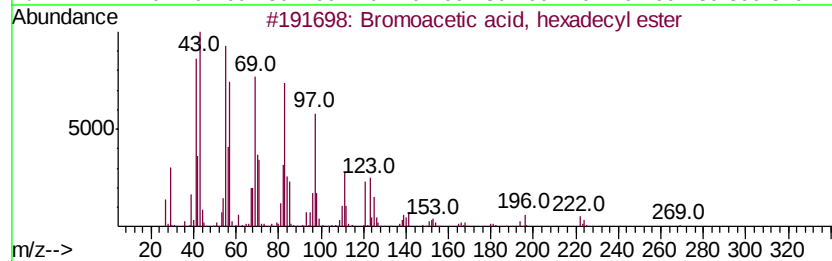
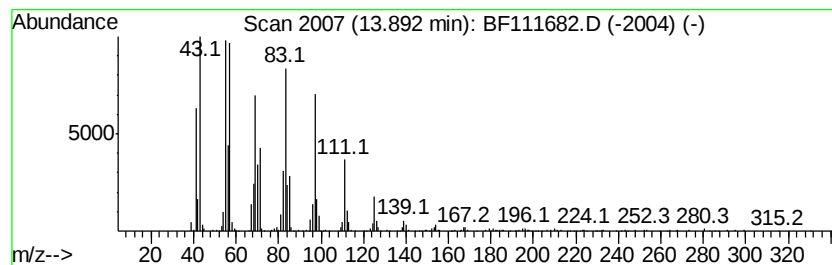
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Bromoacetic acid, hexadecyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	7.37 ng	535752	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3		1-Heneicosanol	312	C21H44O	015594-90-8	94
4		1-Docosene	308	C22H44	001599-67-3	94
5		Behenic alcohol	326	C22H46O	000661-19-8	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122118\
Data File : BF111682.D
Acq On : 21 Dec 2018 12:48
Operator : JU/SJ
Sample : J6353-06
Misc :
ALS Vial : 3 Sample Multiplier: 1

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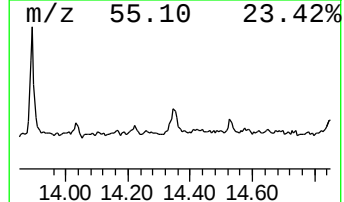
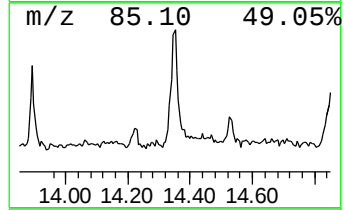
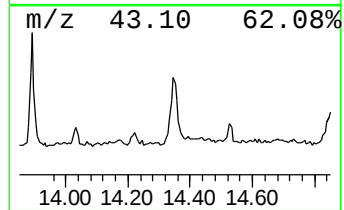
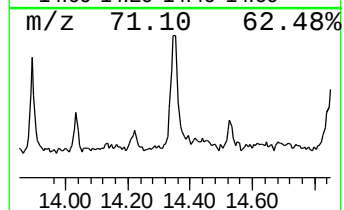
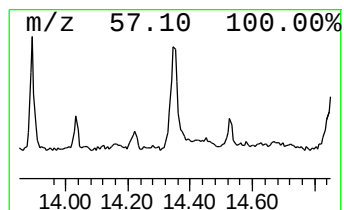
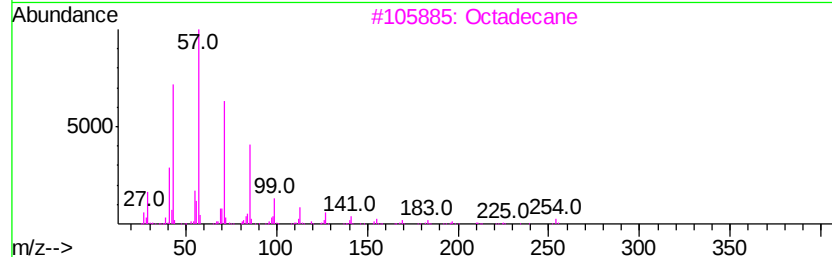
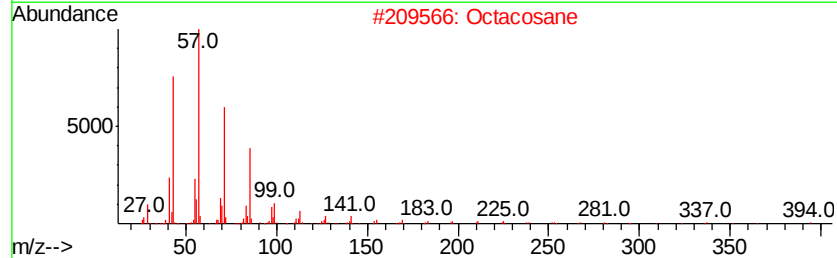
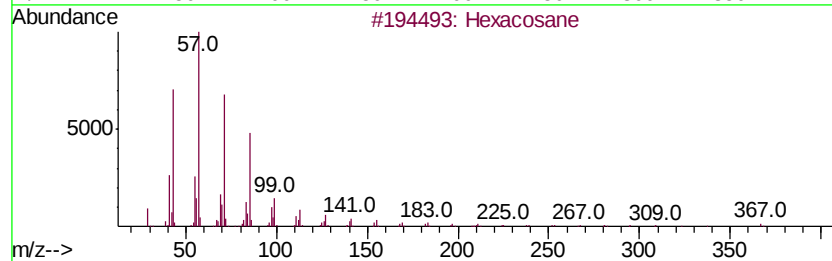
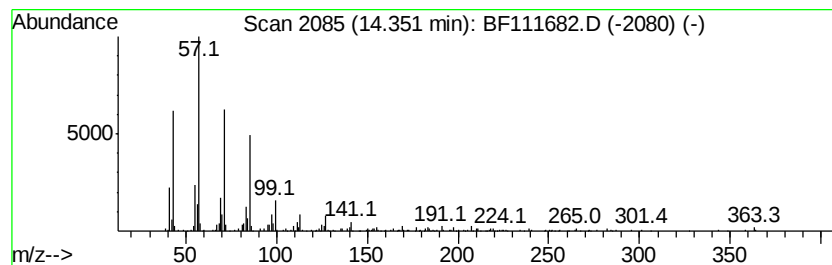
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	5.27 ng	382628	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	87
2		Octacosane	394	C28H58	000630-02-4	87
3		Octadecane	254	C18H38	000593-45-3	83
4		Heneicosane	296	C21H44	000629-94-7	83
5		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122118\
Data File : BF111682.D
Acq On : 21 Dec 2018 12:48
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Sample : J6353-06
Misc :
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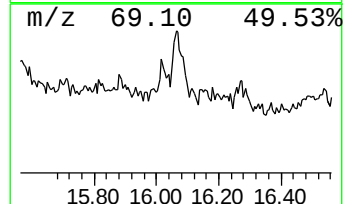
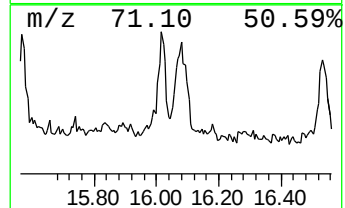
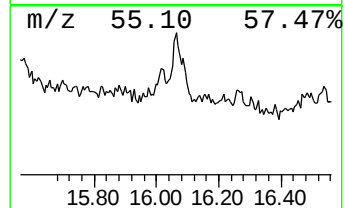
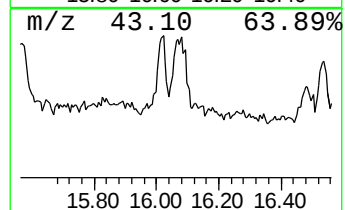
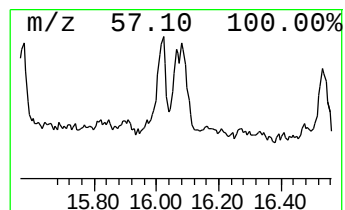
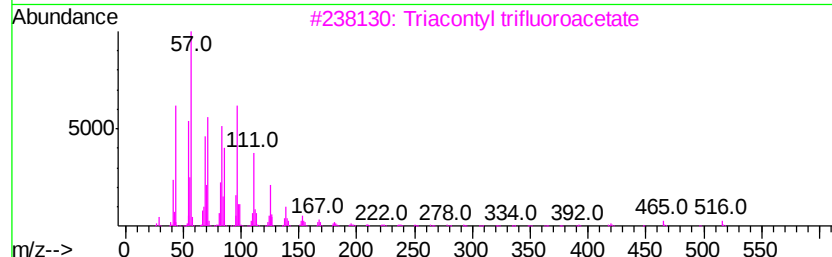
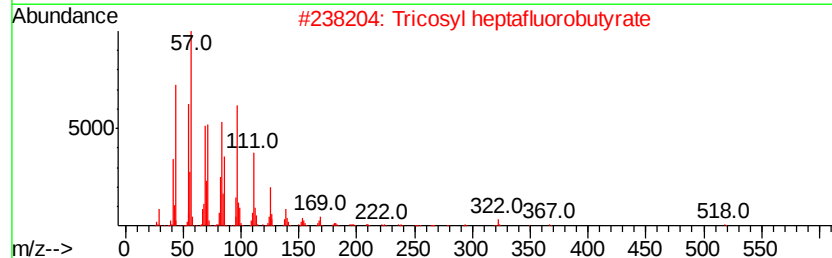
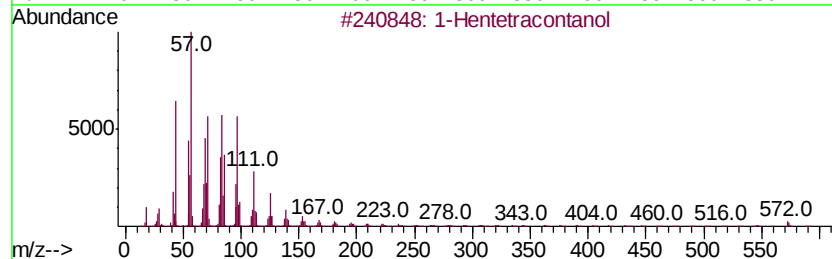
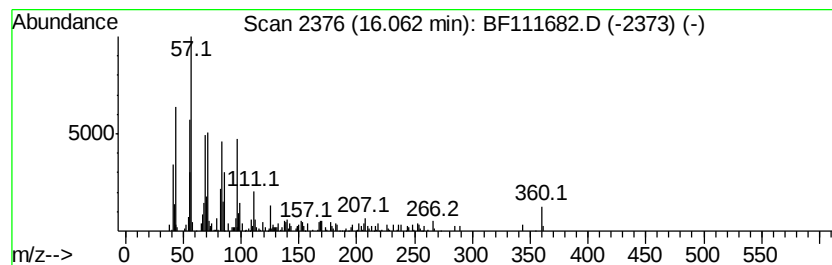
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Hentetracontanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD			R.T.	
16.06	6.21 ng	363579	Perylene-d12			15.53	
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hentetracontanol	593	C41H84O	040710-42-7	83
2			Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	80
3			Triacosyl trifluoroacetate	534	C32H61F3O2	1000351-75-7	80
4			Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	80
5			Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122118\
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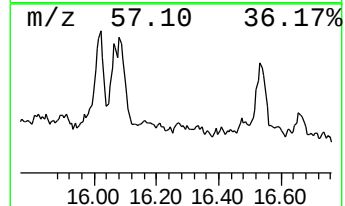
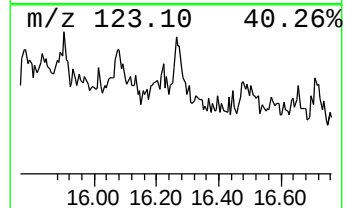
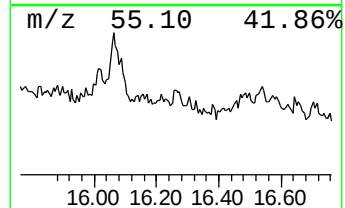
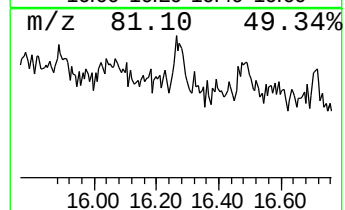
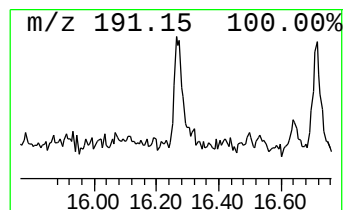
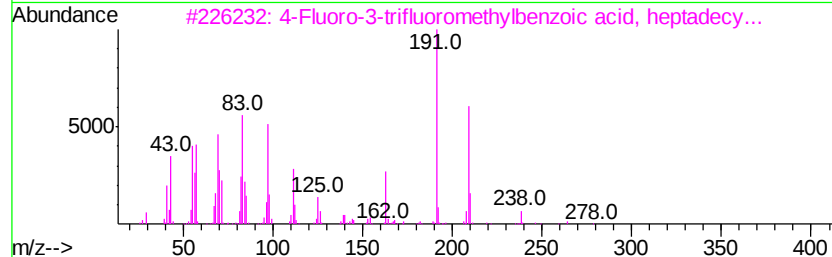
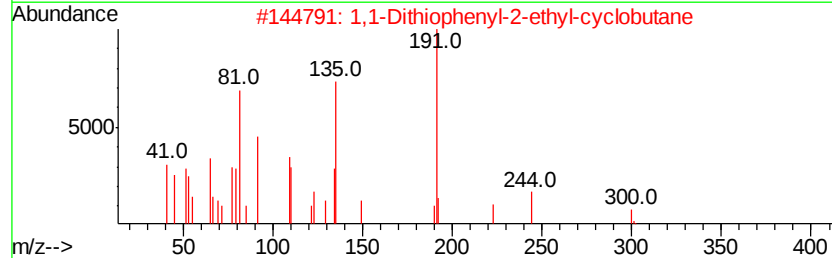
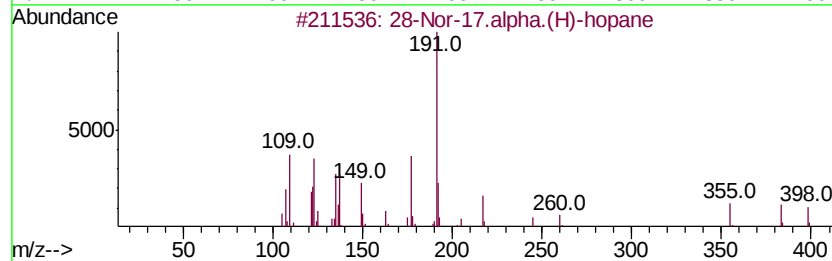
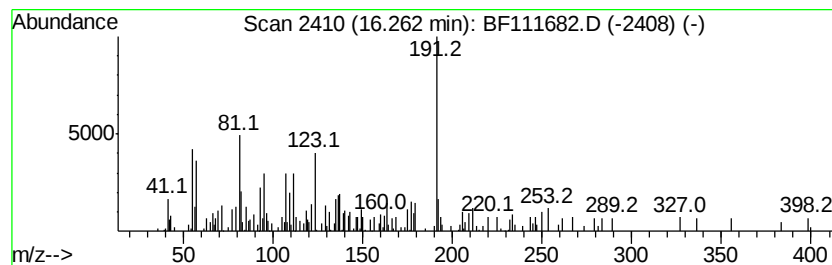
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown16.26 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.26	2.60 ng	152009	Perylene-d12	15.53		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	28-Nor-17.alpha.(H)-hopane		398	C29H50	053584-60-4	46
2	1,1-Dithiophenyl-2-ethyl-cyclobu...		300	C18H20S2	122732-87-0	35
3	4-Fluoro-3-trifluoromethylbenzoi...		446	C25H38F4O2	1000338-92-9	35
4	Terephthalic acid, isopropyl pro...		250	C14H18O4	1000323-75-8	30
5	N-[[2-Oxo-1,2'-bi(tricyclo[3.3.1...		355	C23H33N02	1000305-39-6	30



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF122118\
Data File : BF111682.D
Acq On : 21 Dec 2018 12:48
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Sample : J6353-06
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P001-SS003-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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
2-Pentanone, 4-hy...	5.12	3.3	ng	199910	1	6.89	1203540	20.0
unknown6.66	6.66	55.2	ng	3319840	1	6.89	1203540	20.0
n-Hexadecanoic acid	11.95	30.3	ng	2739830	4	11.42	1811300	20.0
3-Chloropropionic...	12.65	2.6	ng	240291	4	11.42	1811300	20.0
Octadecanoic acid	12.73	29.4	ng	2667580	4	11.42	1811300	20.0
Phenol, 4,4'-(1-m...	12.87	2.1	ng	149573	5	14.05	1452890	20.0
Hexadecane, 7,9-d...	13.77	5.2	ng	375303	5	14.05	1452890	20.0
Bromoacetic acid,...	13.89	7.4	ng	535752	5	14.05	1452890	20.0
Hexacosane	14.35	5.3	ng	382628	5	14.05	1452890	20.0
1-Hentetracontanol	16.06	6.2	ng	363579	6	15.53	1171410	20.0
unknown16.26	16.26	2.6	ng	152009	6	15.53	1171410	20.0