

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120518\
 Data File : BF111125.D
 Acq On : 5 Dec 2018 23:33
 Operator : JU/SJ
 Sample : J6198-01 2X
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SA-06-120318

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	4.999	488	495	501	rVB2	290332	371942	5.37%	0.505%
2	5.410	560	565	568	rBV	6806635	6091700	87.88%	8.263%
3	6.428	733	738	746	rBV	7522335	6931950	100.00%	9.403%
4	6.569	758	762	766	rBV	7089318	6406885	92.43%	8.690%
5	6.804	798	802	806	rBV	4173465	3280057	47.32%	4.449%
6	6.963	825	829	832	rVB	5541872	4411279	63.64%	5.983%
7	7.363	891	897	900	rBV	4353116	3984612	57.48%	5.405%
8	7.587	927	935	939	rBV2	54101	77569	1.12%	0.105%
9	8.087	1016	1020	1023	rBV	5601632	4367077	63.00%	5.924%
10	8.522	1091	1094	1099	rBV3	74123	88841	1.28%	0.121%
11	8.692	1119	1123	1125	rBV	140160	127833	1.84%	0.173%
12	9.122	1193	1196	1199	rVB3	106600	88022	1.27%	0.119%
13	9.163	1199	1203	1206	rBV	7213139	5564514	80.27%	7.548%
14	9.257	1215	1219	1222	rBV2	198416	188016	2.71%	0.255%
15	9.551	1267	1269	1272	rBV	677372	560989	8.09%	0.761%
16	9.781	1306	1308	1311	rVB	202476	165615	2.39%	0.225%
17	9.839	1314	1318	1322	rVV2	5106427	4250248	61.31%	5.765%
18	10.022	1345	1349	1351	rBV3	43783	75183	1.08%	0.102%
19	10.110	1360	1364	1368	rBV3	65591	83259	1.20%	0.113%
20	10.281	1390	1393	1396	rVB	234393	185034	2.67%	0.251%
21	10.504	1424	1431	1434	rBV	129668	161823	2.33%	0.219%
22	10.622	1447	1451	1454	rBV	3810886	3067761	44.26%	4.161%
23	10.757	1471	1474	1475	rBV	242640	214469	3.09%	0.291%
24	11.204	1547	1550	1553	rBV2	207868	183251	2.64%	0.249%
25	11.233	1553	1555	1559	rVB	113786	110965	1.60%	0.151%
26	11.322	1566	1570	1572	rBV	4179672	3432110	49.51%	4.655%
27	11.345	1572	1574	1577	rVV	265838	211048	3.04%	0.286%
28	11.392	1579	1582	1585	rVB2	93648	97506	1.41%	0.132%
29	11.628	1619	1622	1624	rBV	176274	143804	2.07%	0.195%
30	11.728	1635	1639	1645	rVB	1042734	814093	11.74%	1.104%
31	11.851	1657	1660	1665	rBV	411795	385927	5.57%	0.523%
32	11.933	1671	1674	1676	rBV3	87636	83302	1.20%	0.113%
33	12.033	1689	1691	1693	rBV	124394	103031	1.49%	0.140%
34	12.410	1752	1755	1757	rBV	2697324	2285050	32.96%	3.099%

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Instrument :
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ClientSampleId :
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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

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

35	12.433	1757	1759	1762	rVB	1924364	1494935	21.57%	2.028%
36	12.527	1771	1775	1779	rBV2	503682	644559	9.30%	0.874%
37	12.580	1779	1784	1789	rBV6	91579	137892	1.99%	0.187%
38	12.639	1791	1794	1797	rBV	222486	233892	3.37%	0.317%
39	12.757	1808	1814	1817	rBV	441746	489938	7.07%	0.665%
40	12.798	1818	1821	1823	rVB	157410	135096	1.95%	0.183%
41	12.904	1835	1839	1843	rBV	4220211	3582736	51.68%	4.860%
42	13.151	1878	1881	1885	rBV	268996	247519	3.57%	0.336%
43	13.492	1937	1939	1942	rBV	240048	223574	3.23%	0.303%
44	13.816	1990	1994	2002	rVB3	464532	694851	10.02%	0.942%
45	13.951	2013	2017	2020	rBV	2874278	2950578	42.56%	4.002%
46	13.980	2020	2022	2025	rVB	154889	113222	1.63%	0.154%
47	14.139	2046	2049	2052	rVB	340132	271481	3.92%	0.368%
48	14.445	2098	2101	2104	rBV	390887	341179	4.92%	0.463%
49	14.745	2149	2152	2159	rBV	424396	457849	6.60%	0.621%
50	15.074	2206	2208	2212	rVB	403712	427294	6.16%	0.580%
51	15.392	2258	2262	2266	rVB	1594586	1769671	25.53%	2.400%
52	15.451	2269	2272	2276	rVB	398475	492681	7.11%	0.668%
53	15.874	2341	2344	2349	rVB2	301284	420682	6.07%	0.571%

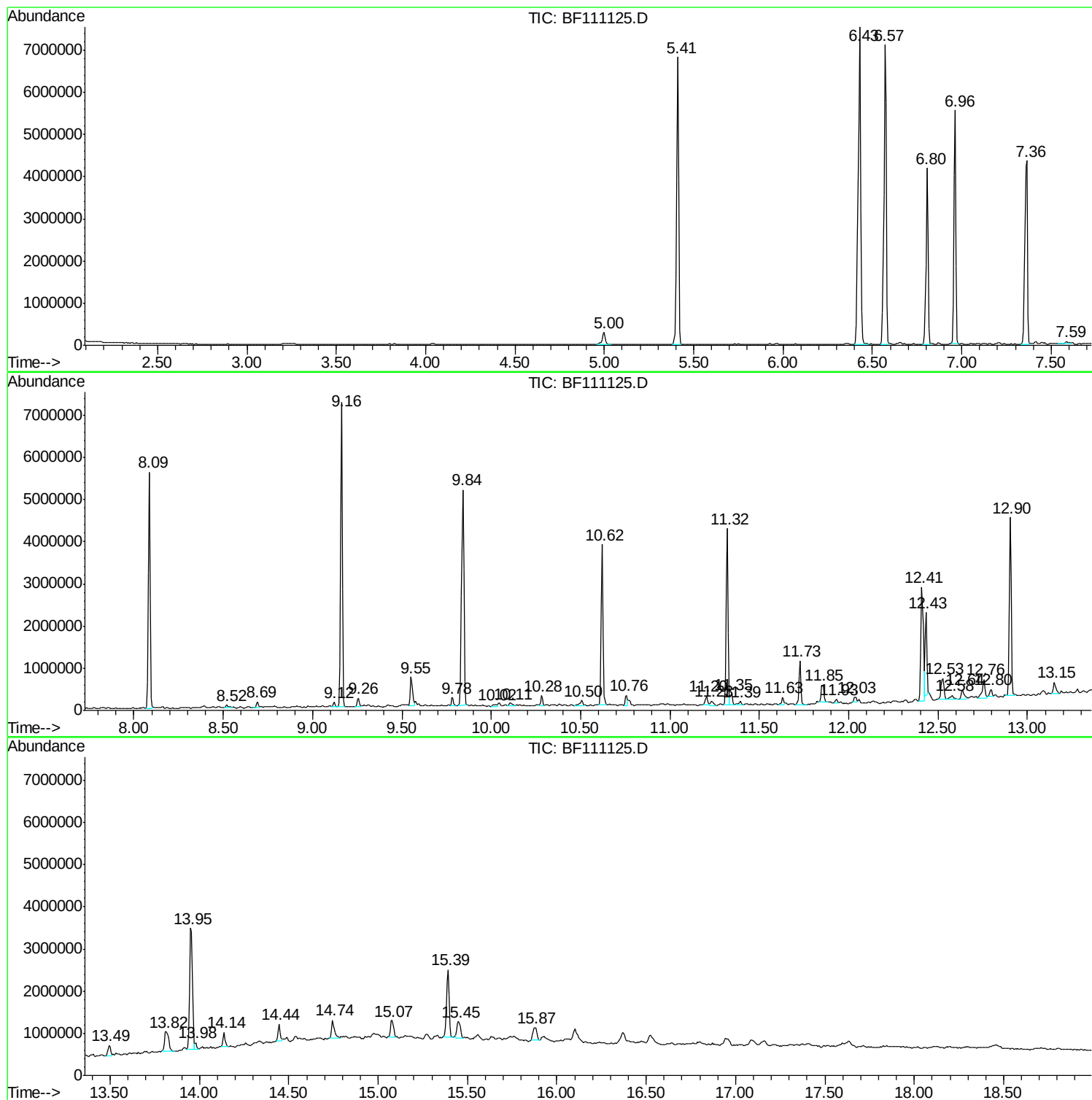
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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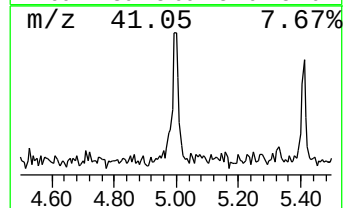
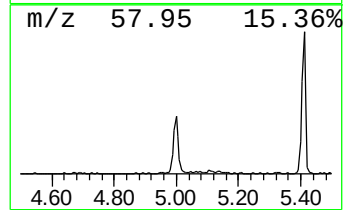
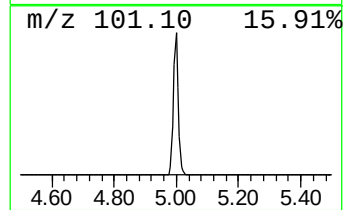
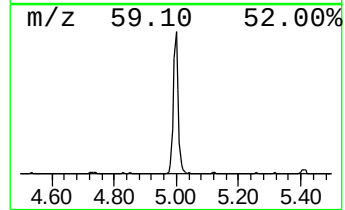
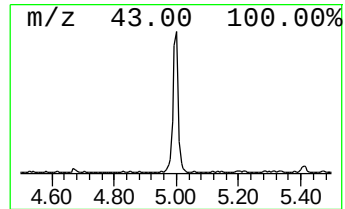
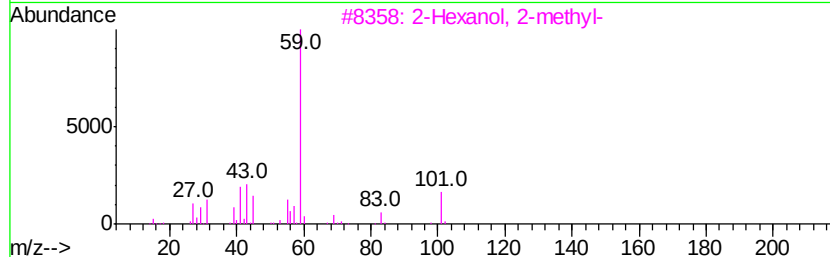
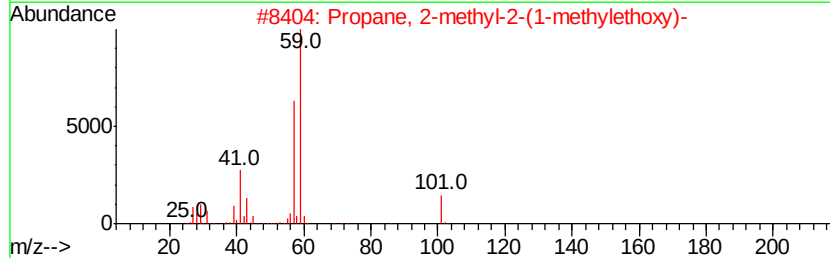
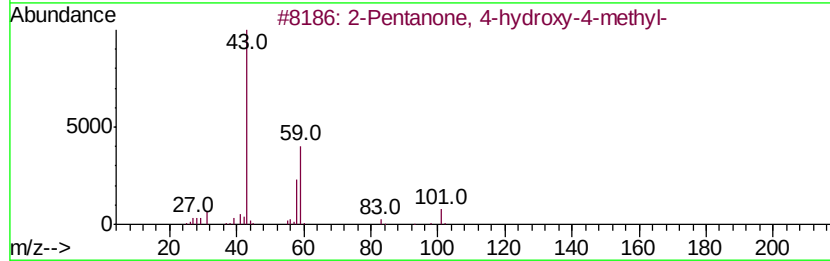
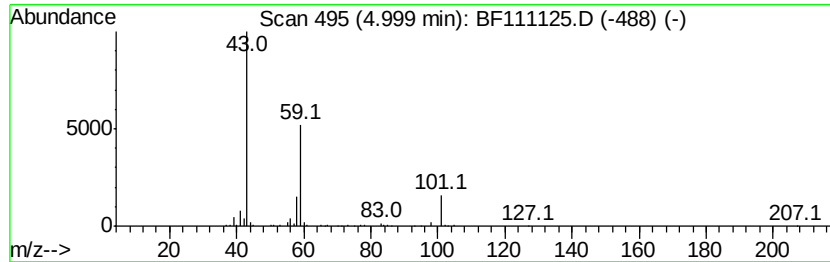
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.00	2.27 ng	371942	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	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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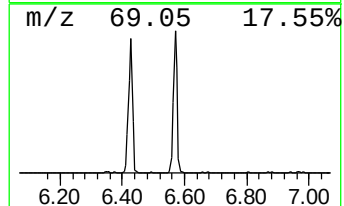
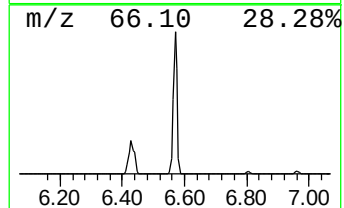
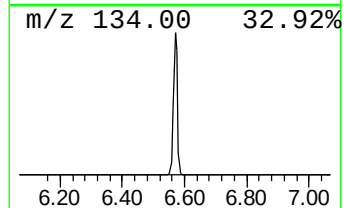
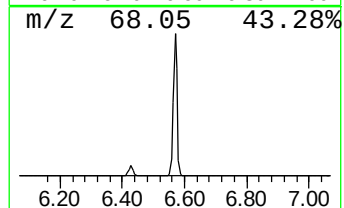
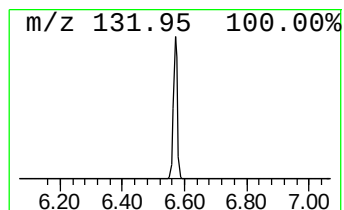
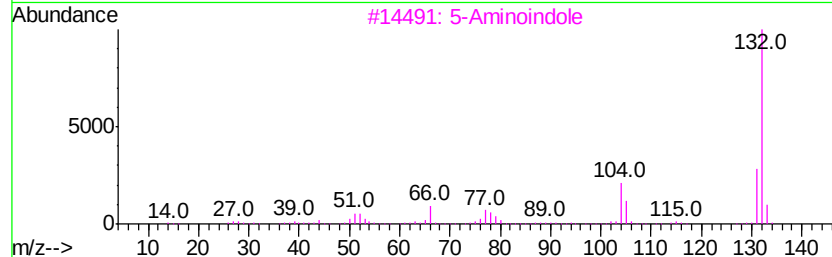
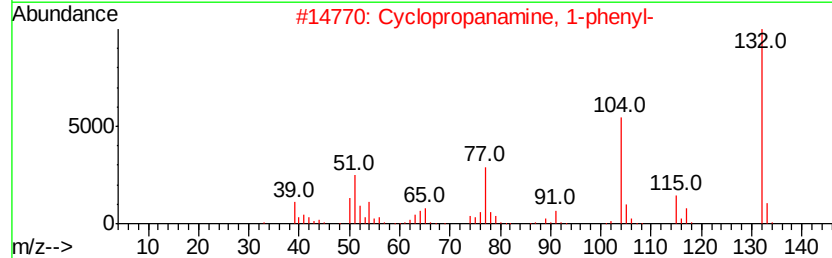
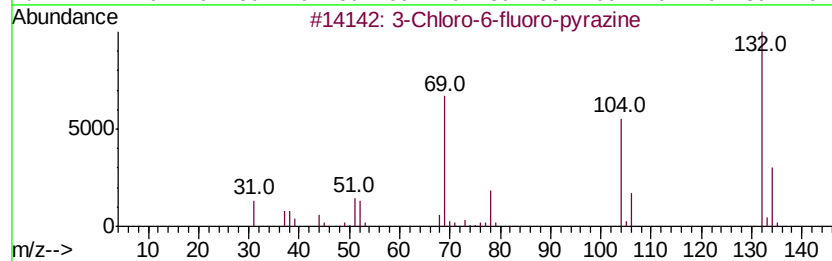
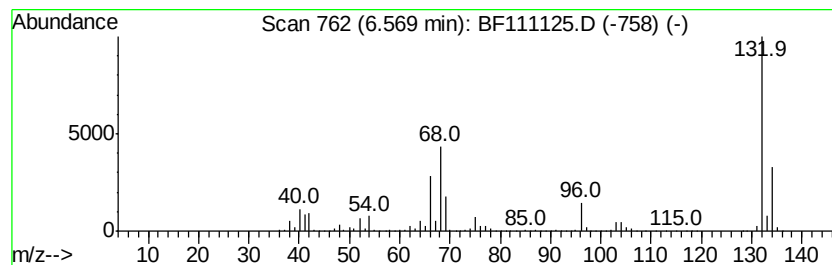
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	39.07 ng	6406890	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		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	14
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9



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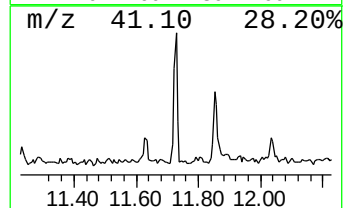
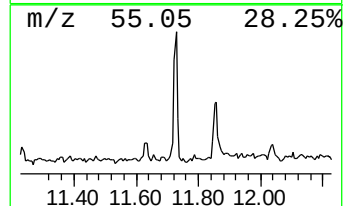
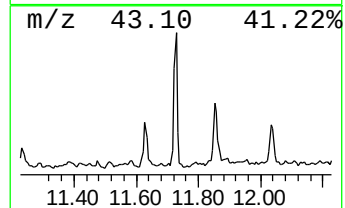
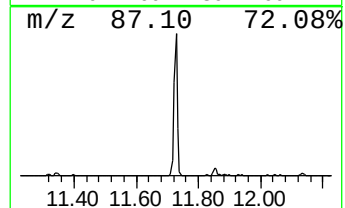
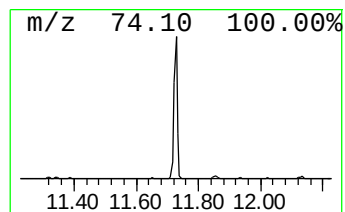
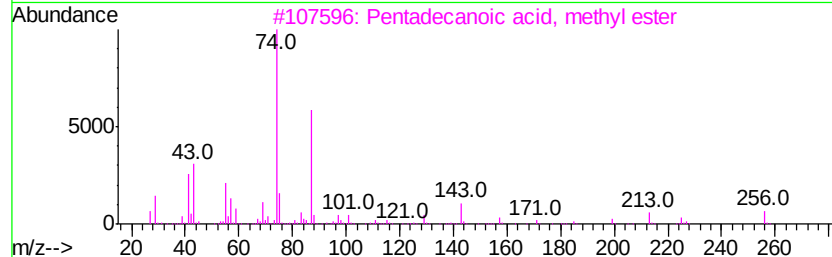
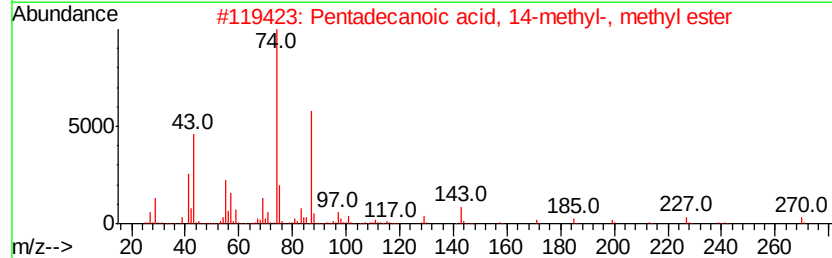
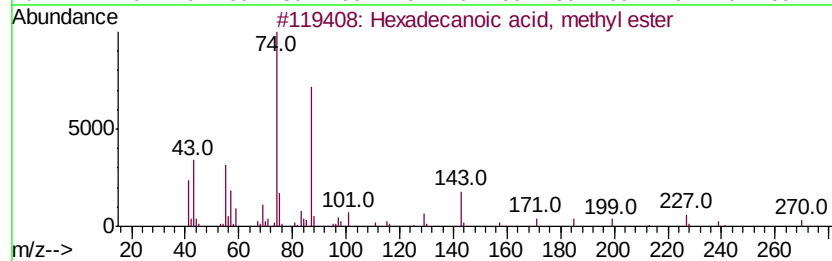
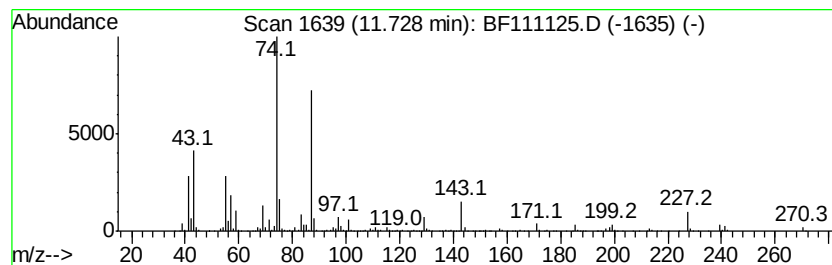
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.73	4.74 ng	814093	Phenanthrene-d10	11.32		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	92
2		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
3		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
4		Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	86
5		Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	86



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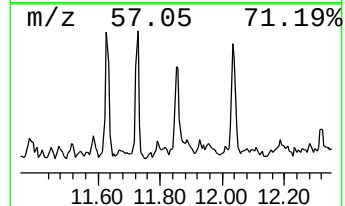
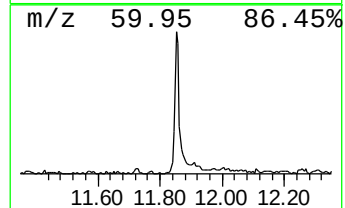
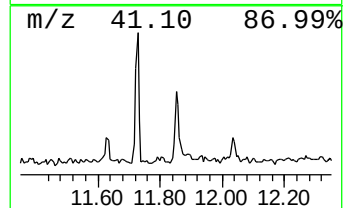
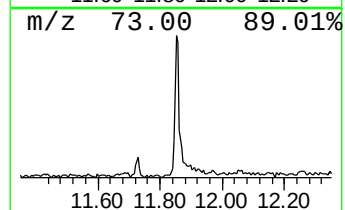
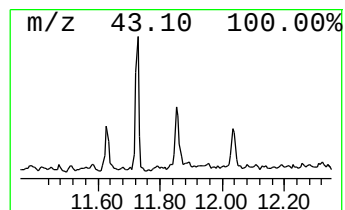
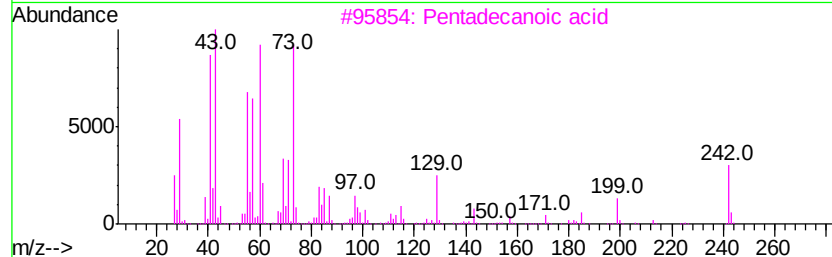
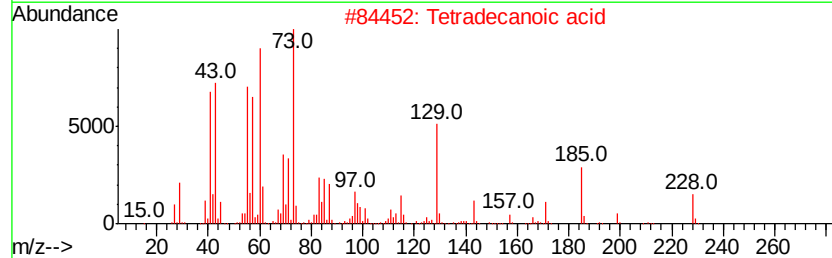
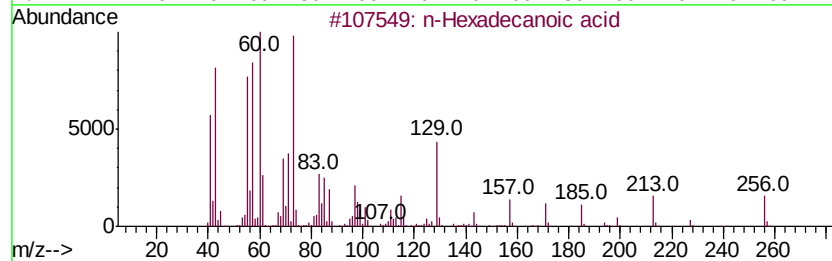
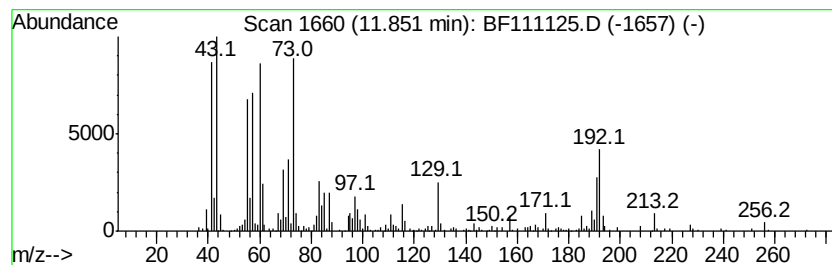
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.85	2.25 ng	385927	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	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	62
4	Tridecanoic acid	214	C13H26O2	000638-53-9	60
5	Undecanoic acid	186	C11H22O2	000112-37-8	52



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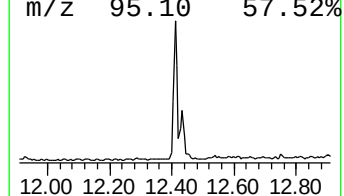
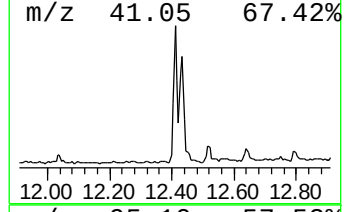
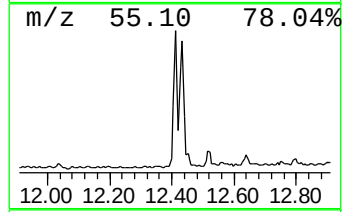
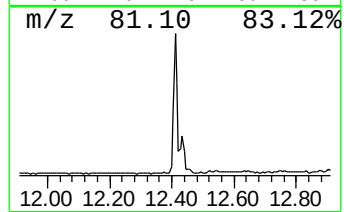
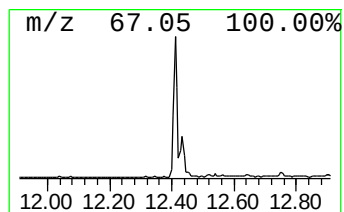
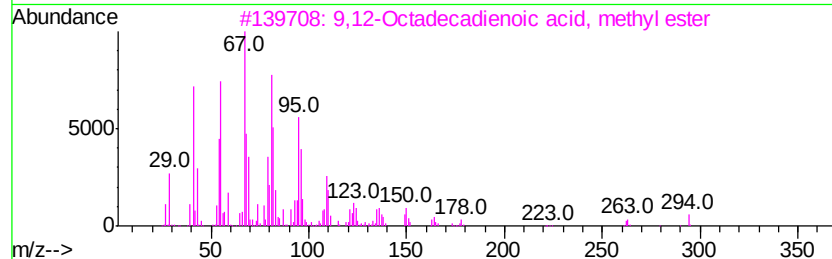
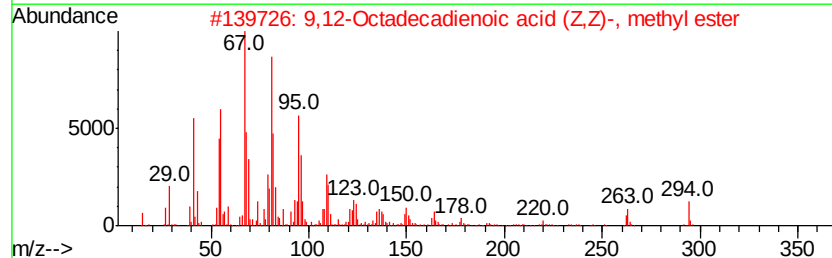
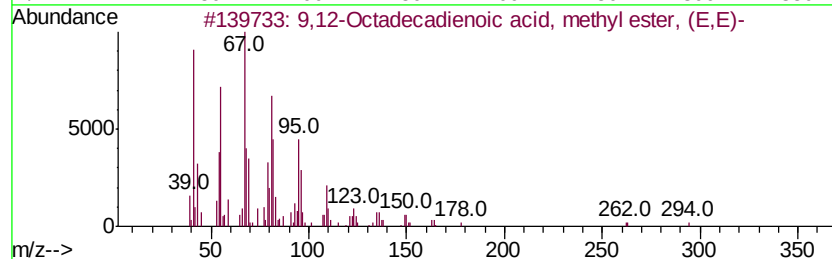
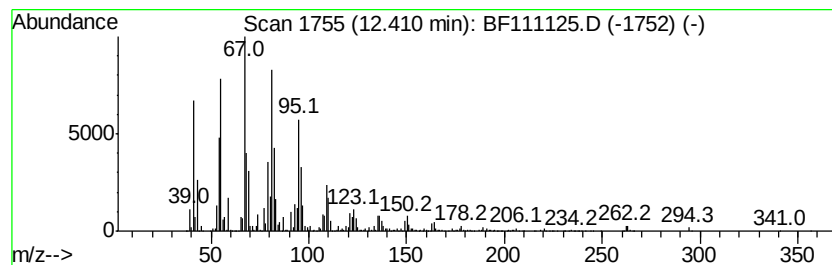
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.41	13.32 ng	2285050	Phenanthrene-d10	11.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2		9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
3		9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
4		Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	99
5		10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120518\
Data File : BF111125.D
Acq On : 5 Dec 2018 23:33
Operator : JU/SJ
Sample : J6198-01 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

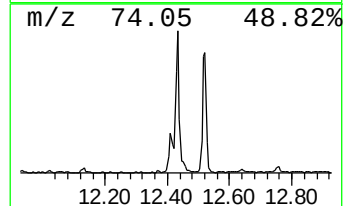
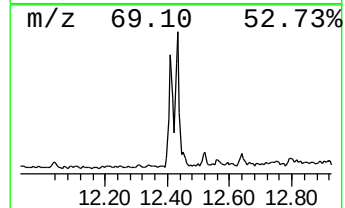
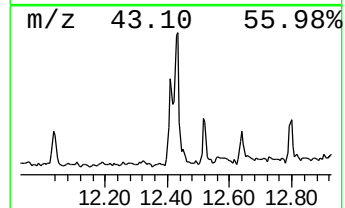
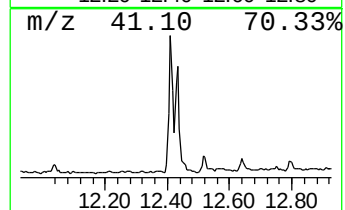
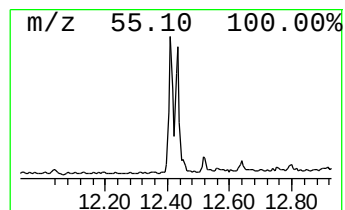
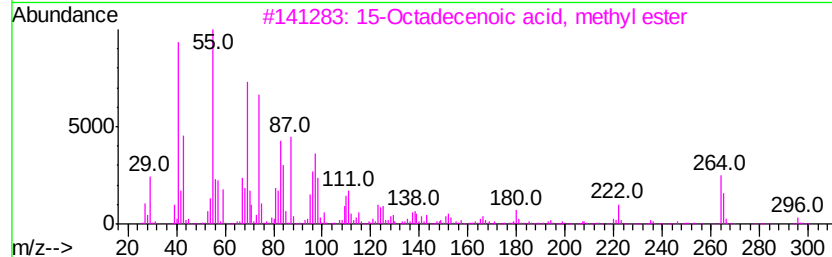
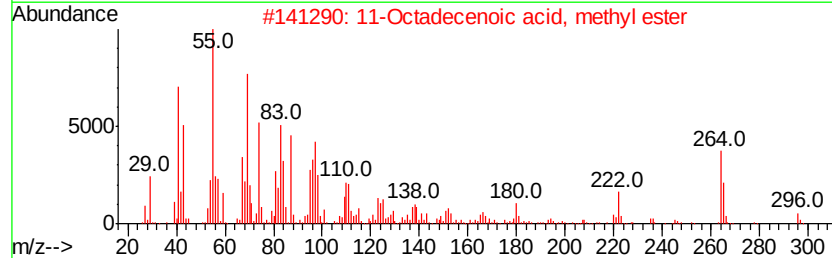
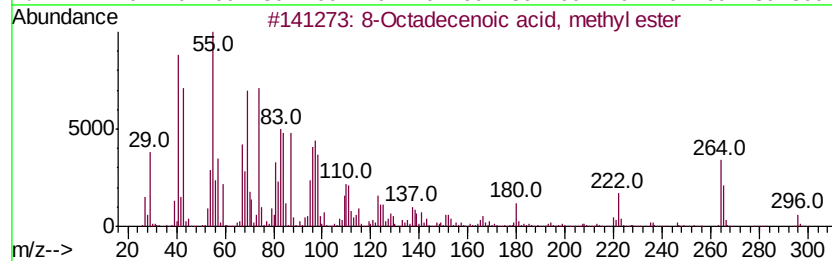
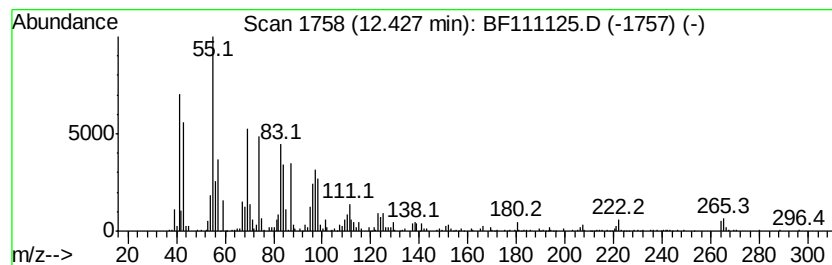
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 8-Octadecenoic acid, methyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.43	8.71 ng	1494940	Phenanthrene-d10	11.32	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	99
2	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	98
3	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	98
4	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	98
5	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	97



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120518\
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Sample : J6198-01 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

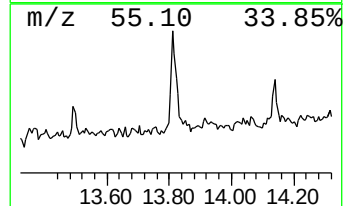
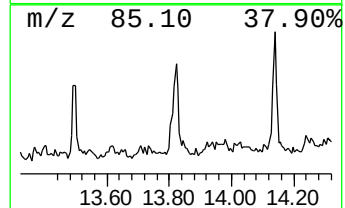
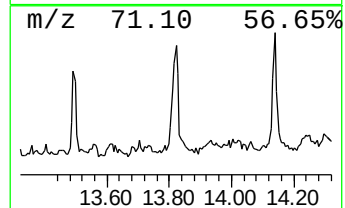
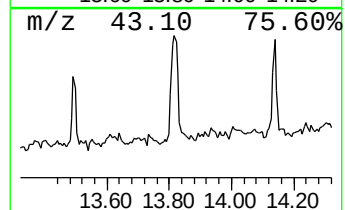
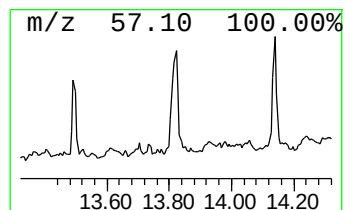
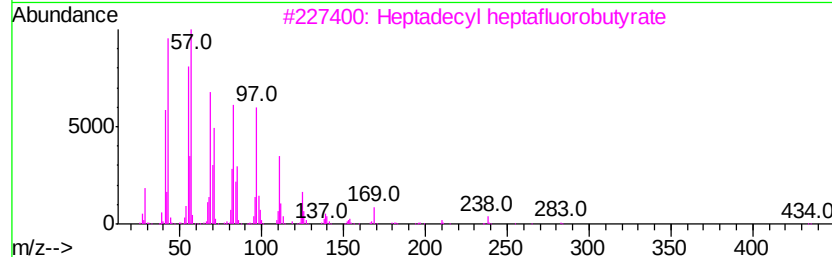
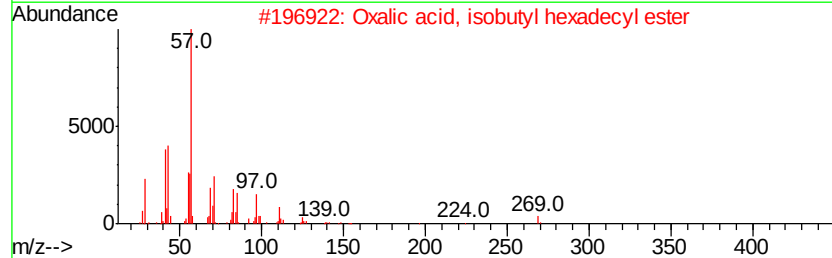
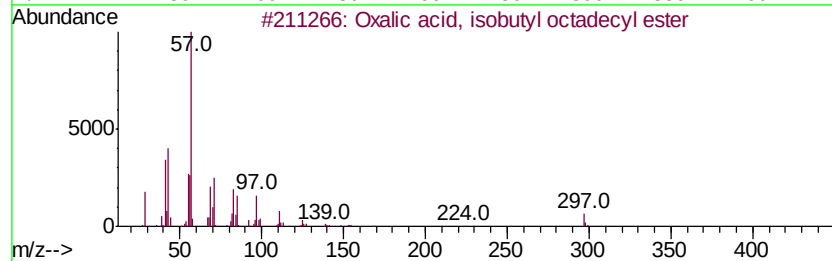
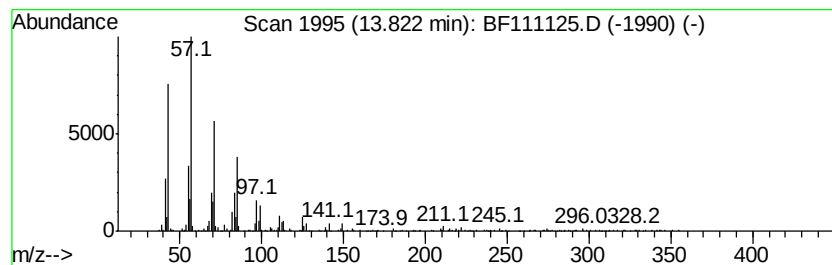
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Oxalic acid, isobutyl octadecyl... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.82	4.71 ng	694851	Chrysene-d12	13.96		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	91
2		Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
3		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	81
4		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	81
5		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120518\
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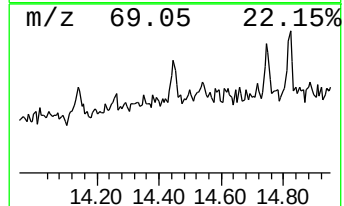
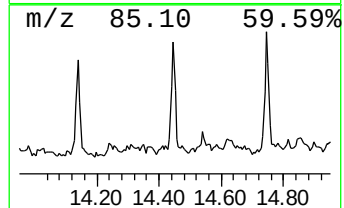
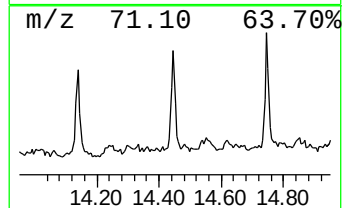
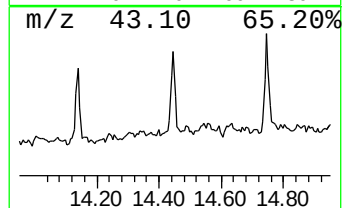
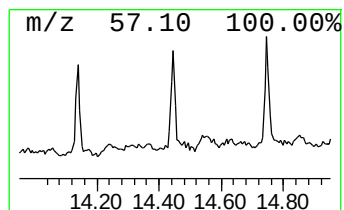
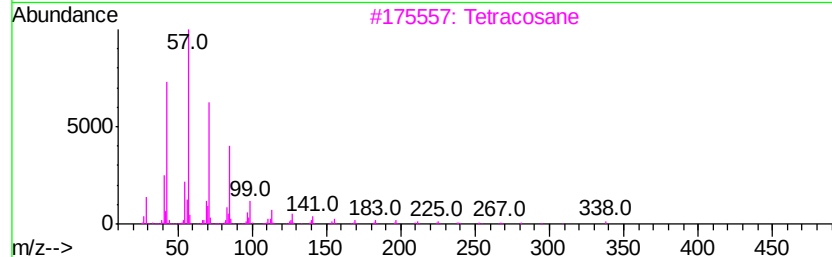
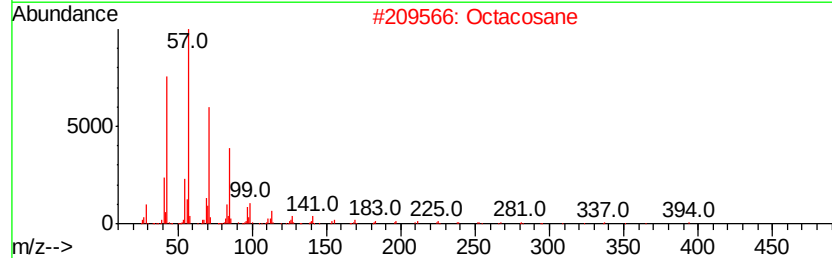
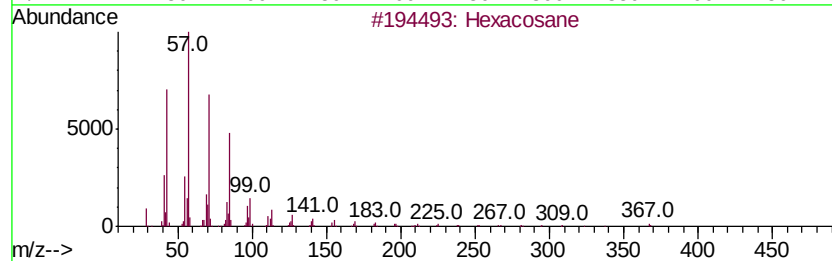
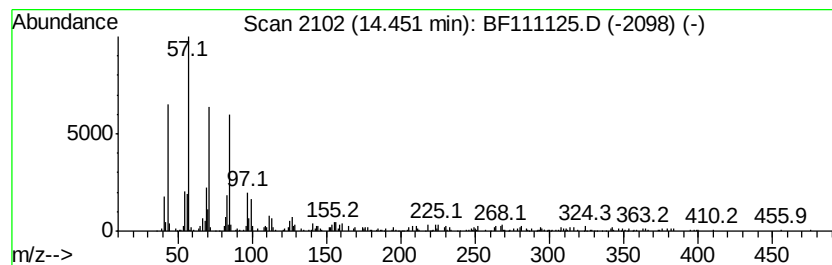
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	2.31 ng	341179	Chrysene-d12	13.96
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexacosane	366 C26H54	000630-01-3	90
2	Octacosane	394 C28H58	000630-02-4	90
3	Tetracosane	338 C24H50	000646-31-1	90
4	Nonadecane	268 C19H40	000629-92-5	90
5	Tridecane, 6-propyl-	226 C16H34	055045-10-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120518\
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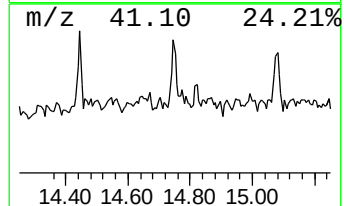
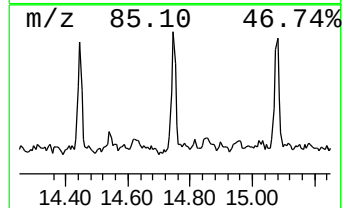
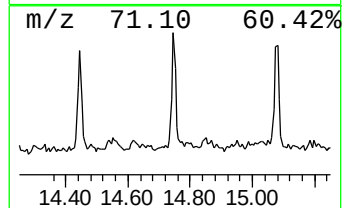
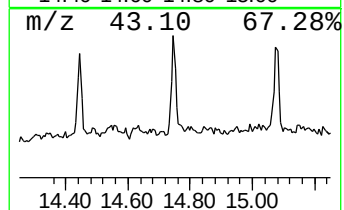
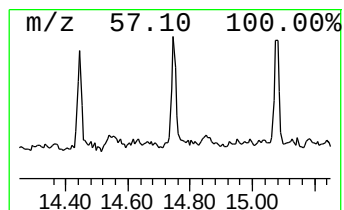
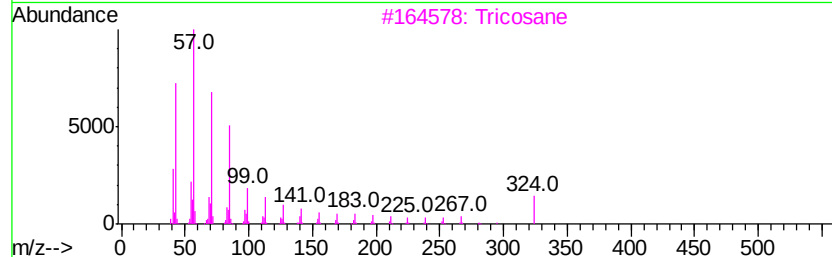
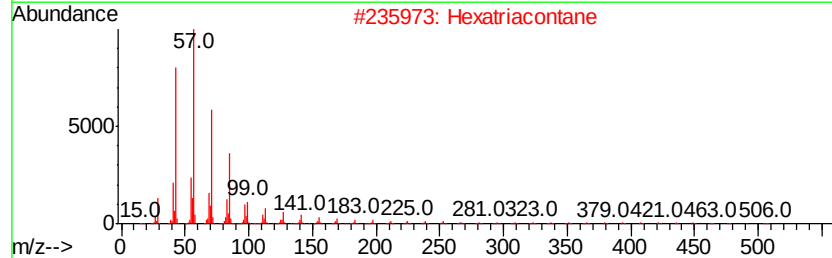
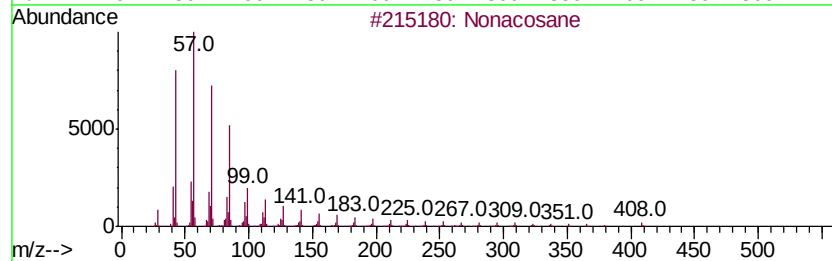
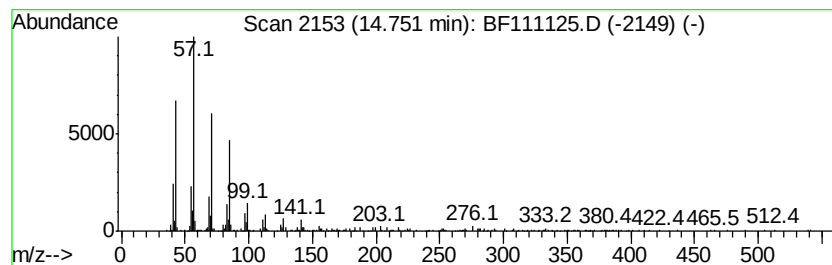
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Nonacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	5.17 ng	457849	Perylene-d12	15.39
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Nonacosane	408 C29H60	000630-03-5	87
2	Hexatriacontane	507 C36H74	000630-06-8	86
3	Tricosane	324 C23H48	000638-67-5	83
4	Tridecane, 1-iodo-	310 C13H27I	035599-77-0	80
5	Octacosane	394 C28H58	000630-02-4	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120518\
Data File : BF111125.D
Acq On : 5 Dec 2018 23:33
Operator : JU/SJ
Sample : J6198-01 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

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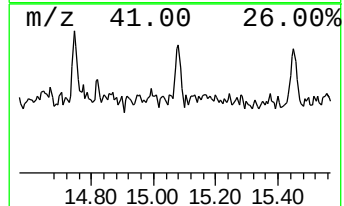
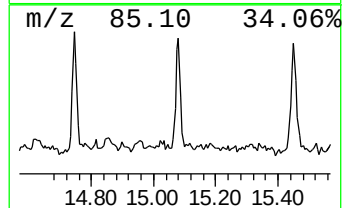
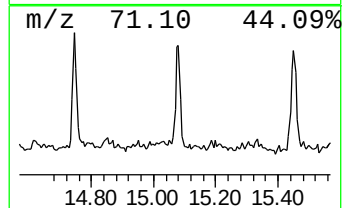
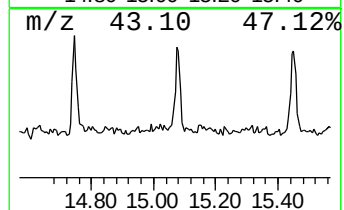
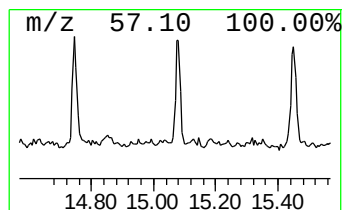
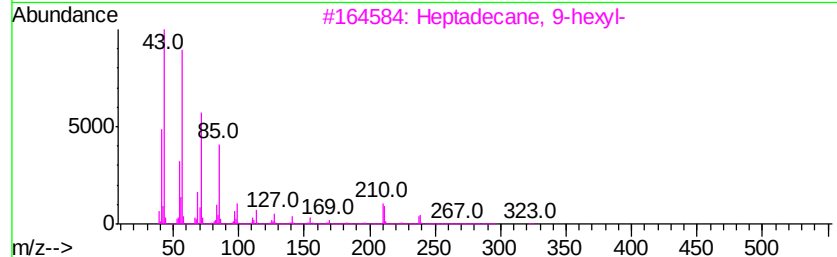
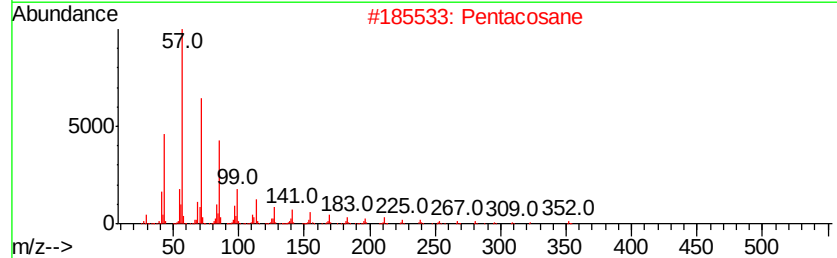
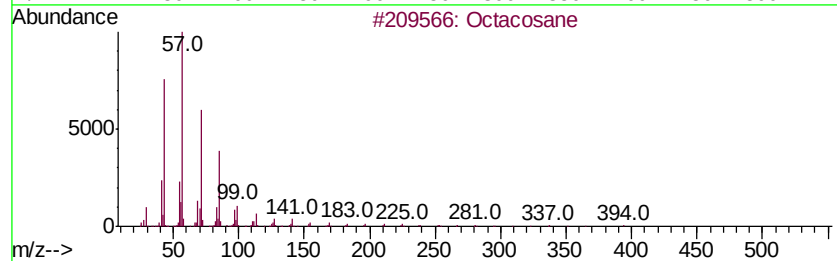
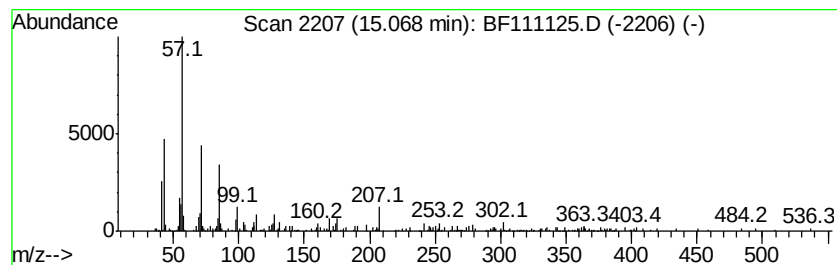
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	4.83 ng	427294	Perylene-d12	15.39

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	95
2			Pentacosane	352	C25H52	000629-99-2	91
3			Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	91
4			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	91
5			Hexadecane	226	C16H34	000544-76-3	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120518\
Data File : BF111125.D
Acq On : 5 Dec 2018 23:33
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Misc :
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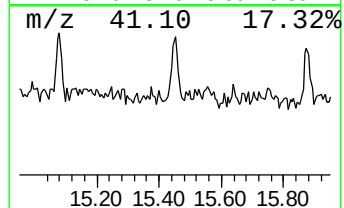
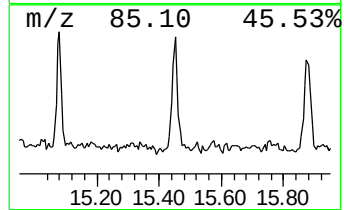
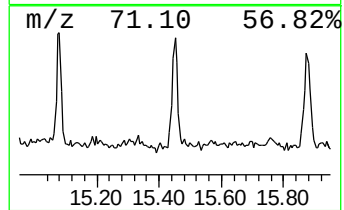
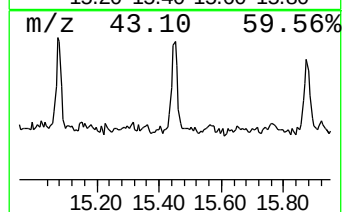
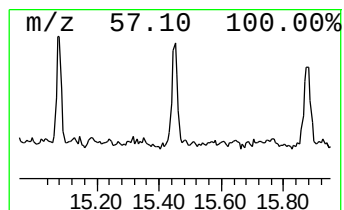
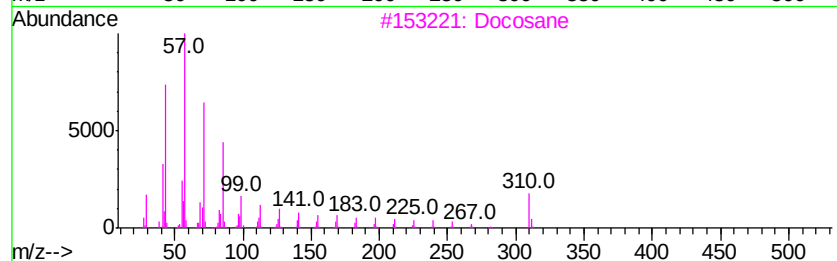
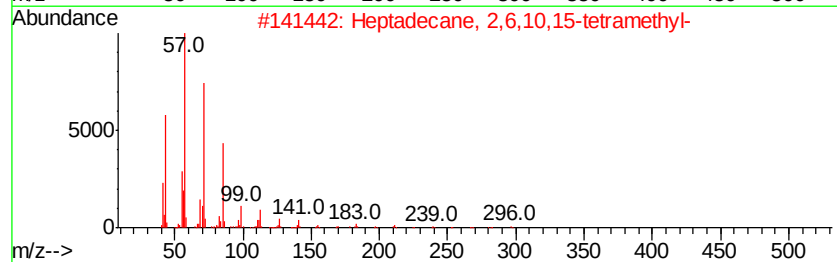
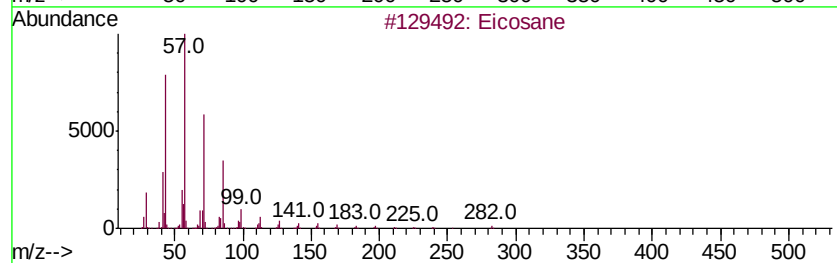
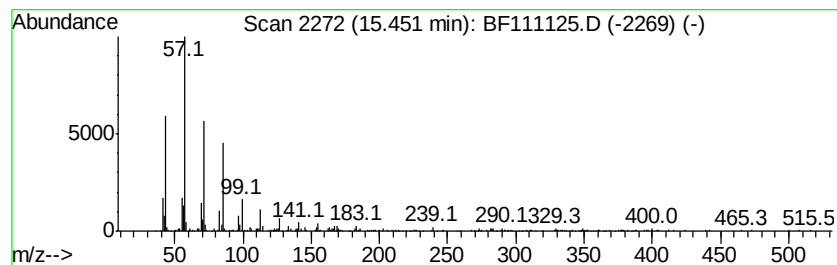
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.45	5.57 ng	492681	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	93
2		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
3		Docosane	310	C22H46	000629-97-0	90
4		Pentacosane	352	C25H52	000629-99-2	90
5		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF120518\
Data File : BF111125.D
Acq On : 5 Dec 2018 23:33
Operator : JU/SJ
Sample : J6198-01 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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
2-Pentanone, 4-hy...	5.00	2.3	ng	371942	1	6.80	3280060	20.0
unknown6.57	6.57	39.1	ng	6406890	1	6.80	3280060	20.0
Hexadecanoic acid...	11.73	4.7	ng	814093	4	11.32	3432110	20.0
n-Hexadecanoic acid	11.85	2.3	ng	385927	4	11.32	3432110	20.0
9,12-Octadecadien...	12.41	13.3	ng	2285050	4	11.32	3432110	20.0
8-Octadecenoic ac...	12.43	8.7	ng	1494940	4	11.32	3432110	20.0
Oxalic acid, isob...	13.82	4.7	ng	694851	5	13.96	2950580	20.0
Hexacosane	14.45	2.3	ng	341179	5	13.96	2950580	20.0
Nonacosane	14.75	5.2	ng	457849	6	15.39	1769670	20.0
Octacosane	15.07	4.8	ng	427294	6	15.39	1769670	20.0
Eicosane	15.45	5.6	ng	492681	6	15.39	1769670	20.0