

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
 Data File : BF112852.D
 Acq On : 5 Mar 2019 13:41
 Operator : JU/SJ
 Sample : K1704-12
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PST-028-SW003-022719

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-BF022719.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	5.357	551	556	559	rBV	3772799	3848220	84.80%	10.039%
2	6.034	667	671	674	rBV	71040	68791	1.52%	0.179%
3	6.381	724	730	739	rBV	3796813	4275686	94.23%	11.155%
4	6.451	739	742	746	rVB	156390	129691	2.86%	0.338%
5	6.516	748	753	756	rBV	4371108	4121985	90.84%	10.754%
6	6.745	788	792	795	rBV	1174543	951360	20.97%	2.482%
7	6.904	814	819	822	rBV	3150498	2953371	65.08%	7.705%
8	7.304	882	887	890	rBV	2609322	2539053	55.95%	6.624%
9	8.027	1005	1010	1033	rBV	1120538	1227966	27.06%	3.204%
10	9.104	1188	1193	1204	rBV	4578952	4537728	100.00%	11.838%
11	9.492	1255	1259	1265	rBV	243513	238300	5.25%	0.622%
12	9.774	1303	1307	1312	rBV	1398628	1306078	28.78%	3.407%
13	10.557	1436	1440	1456	rBV	2678826	2894399	63.79%	7.551%
14	11.010	1512	1517	1523	rVB	68899	98036	2.16%	0.256%
15	11.251	1554	1558	1566	rBV	1305969	1235882	27.24%	3.224%
16	11.792	1646	1650	1657	rBV2	268683	365491	8.05%	0.954%
17	11.851	1657	1660	1668	rVB2	44626	70443	1.55%	0.184%
18	12.333	1740	1742	1749	rVB	52138	51515	1.14%	0.134%
19	12.574	1780	1783	1797	rBV2	101699	206007	4.54%	0.537%
20	12.833	1823	1827	1831	rBV	3681673	3745398	82.54%	9.771%
21	13.321	1905	1910	1914	rBV3	38909	49245	1.09%	0.128%
22	13.745	1978	1982	1992	rBV2	186071	253771	5.59%	0.662%
23	13.880	2001	2005	2013	rBV	1141995	1086929	23.95%	2.836%
24	14.368	2085	2088	2095	rBV2	86268	120060	2.65%	0.313%
25	14.662	2135	2138	2142	rVB	87322	80934	1.78%	0.211%
26	14.733	2147	2150	2154	rVB	70290	67182	1.48%	0.175%
27	14.986	2189	2193	2196	rBV	92188	115619	2.55%	0.302%
28	15.292	2240	2245	2250	rBV	868481	1116106	24.60%	2.912%
29	15.339	2250	2253	2260	rVB	108003	148053	3.26%	0.386%
30	15.751	2319	2323	2328	rVB	80690	117693	2.59%	0.307%
31	15.809	2328	2333	2342	rBV10	23868	63579	1.40%	0.166%
32	16.221	2399	2403	2409	rVB2	56957	96444	2.13%	0.252%
33	16.780	2493	2498	2505	rVB3	80989	150164	3.31%	0.392%

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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PST-028-SW003-022719

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-BF022719.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

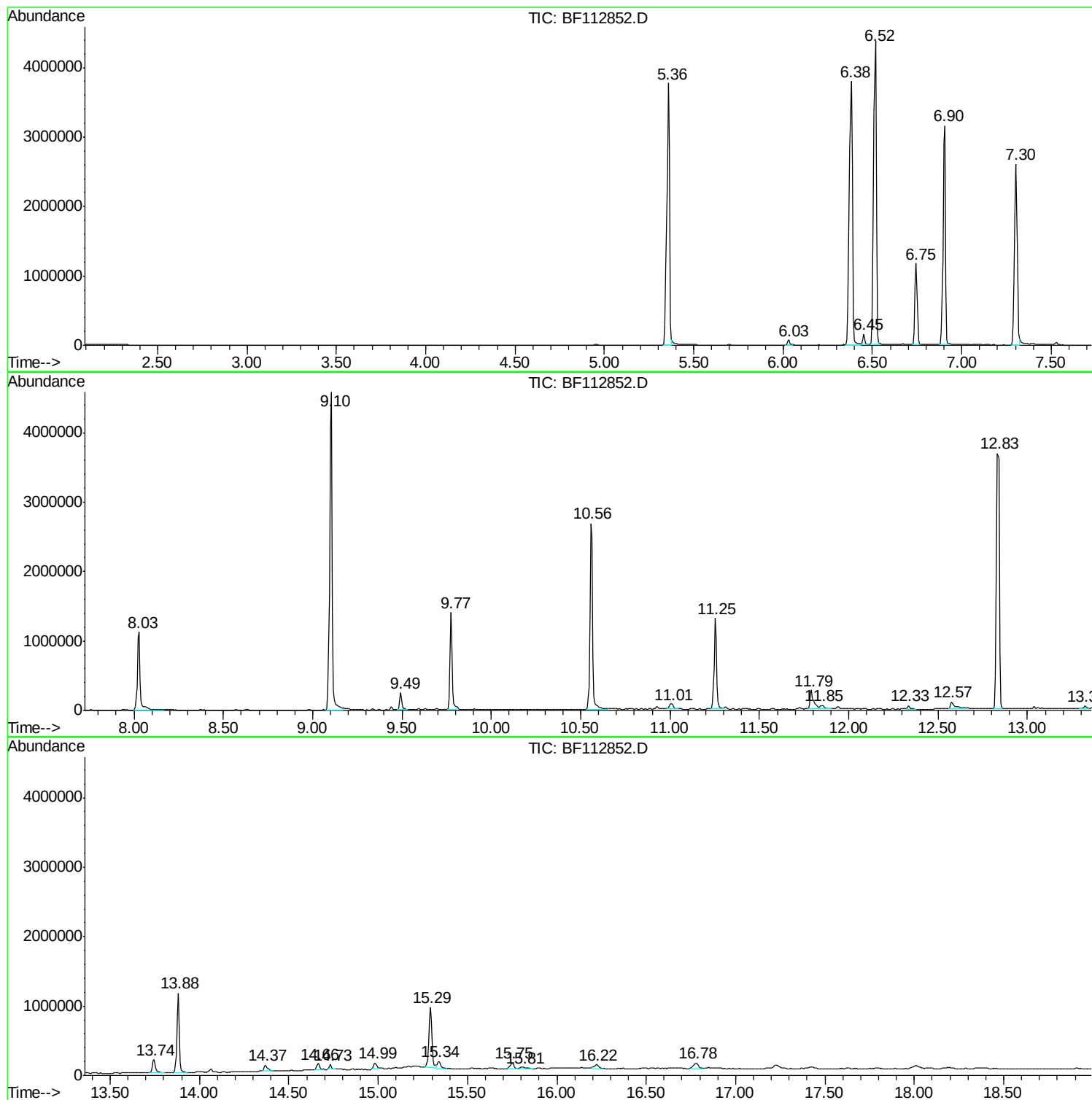
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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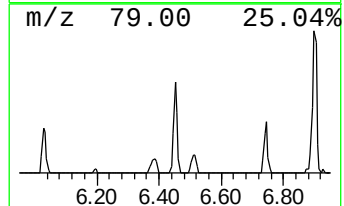
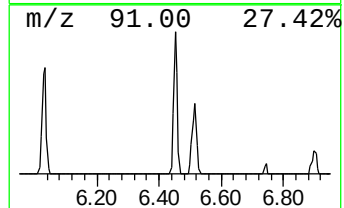
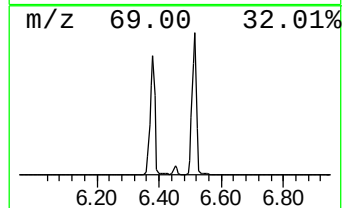
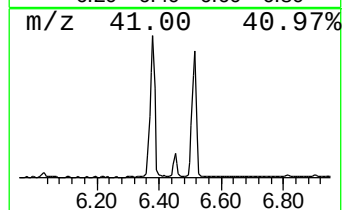
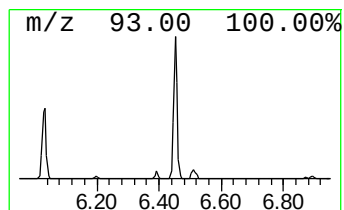
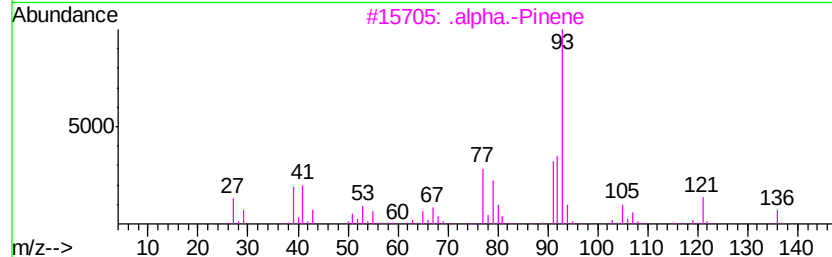
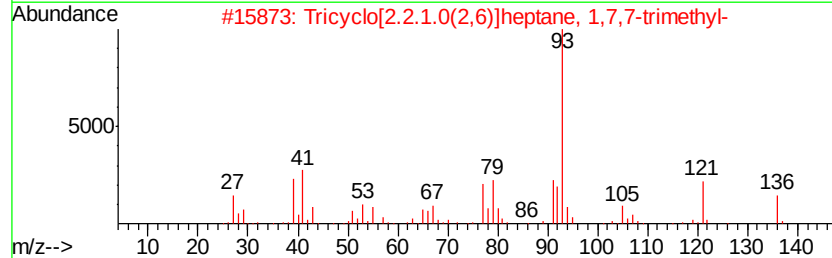
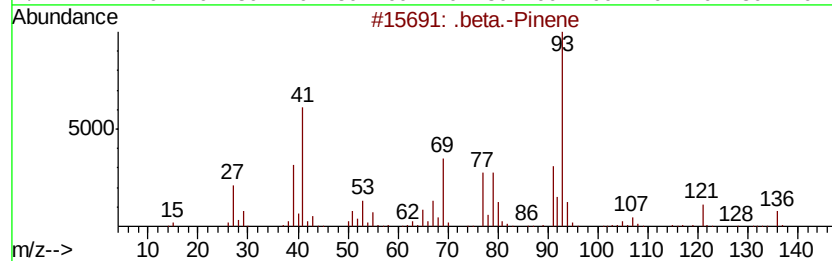
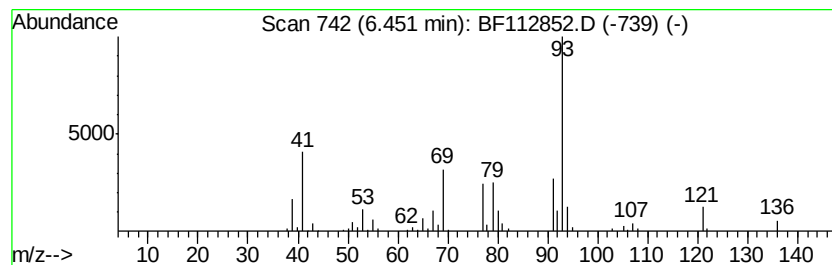
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 .beta.-Pinene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.45	2.73 ng	129691	1,4-Dichlorobenzene-d4	6.75	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Pinene	136	C10H16	000127-91-3	96
2	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	91
3	.alpha.-Pinene	136	C10H16	000080-56-8	87
4	Bicyclo[3.1.0]hexane, 4-methylen...	136	C10H16	003387-41-5	86
5	Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	83



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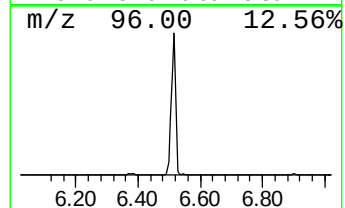
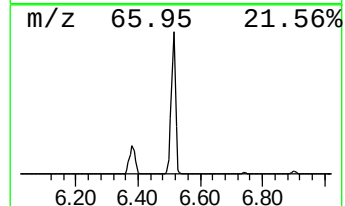
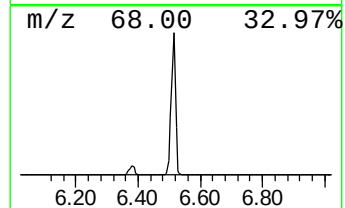
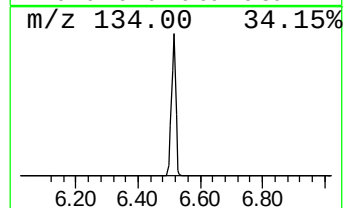
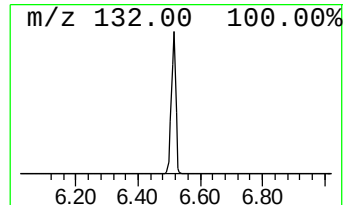
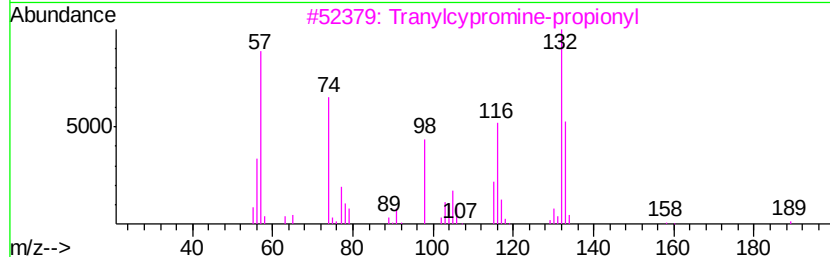
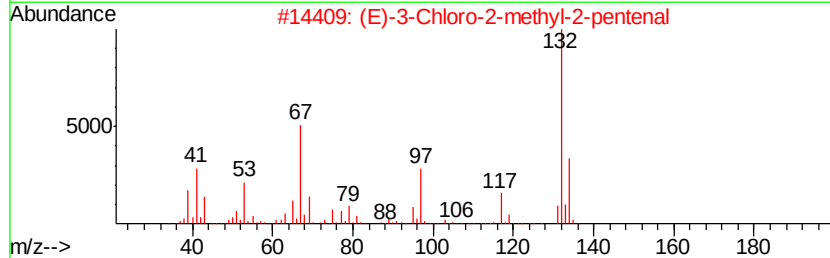
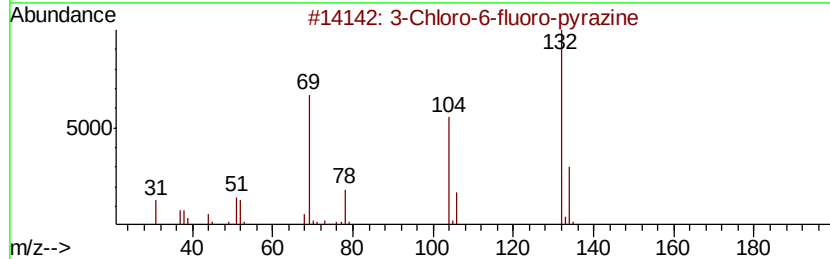
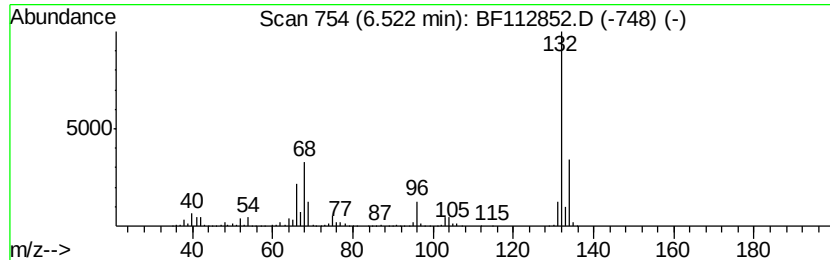
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	86.65 ng	4121990	1,4-Dichlorobenzene-d4	6.75

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		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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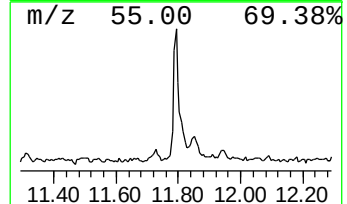
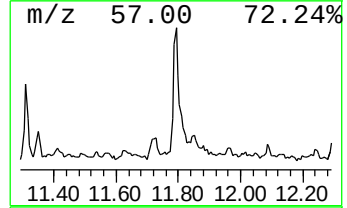
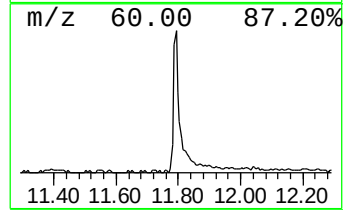
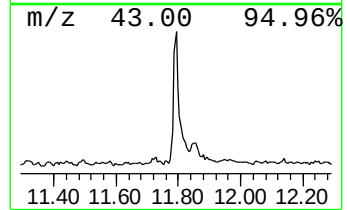
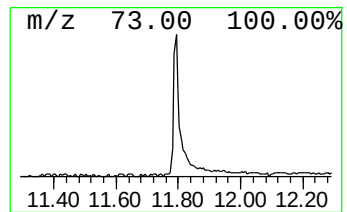
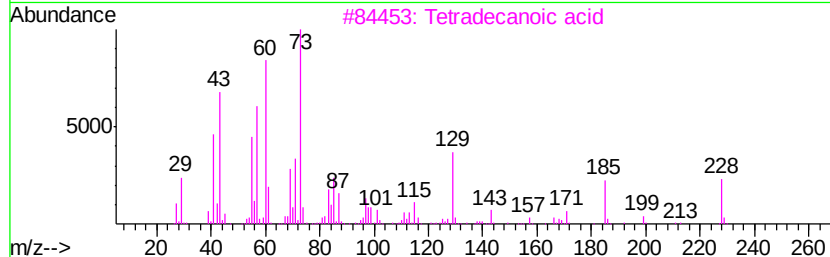
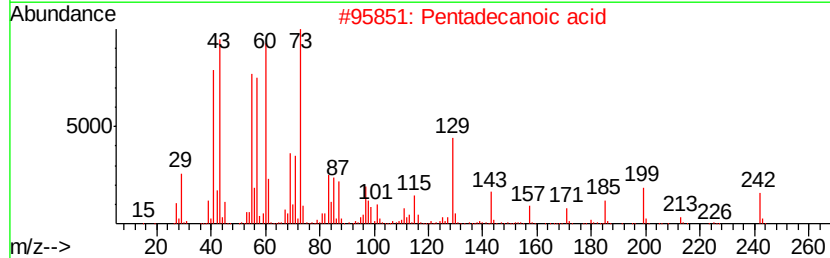
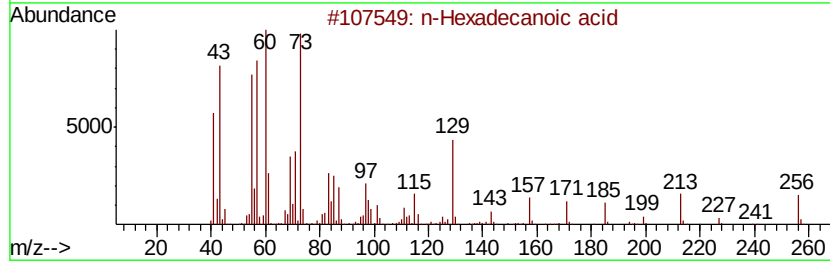
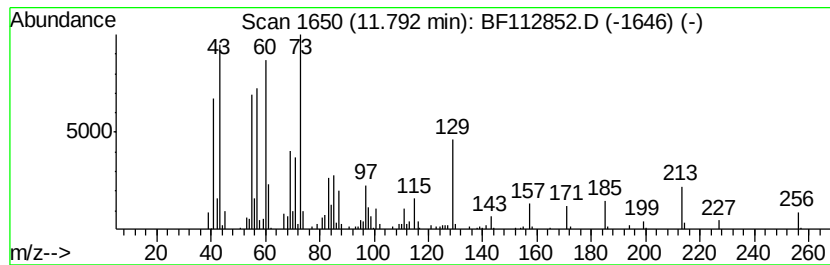
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.79	5.91 ng	365491	Phenanthrene-d10	11.25	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59



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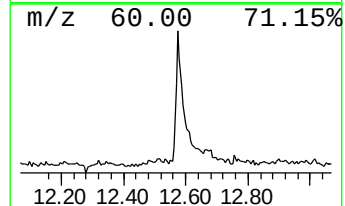
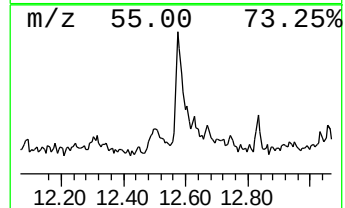
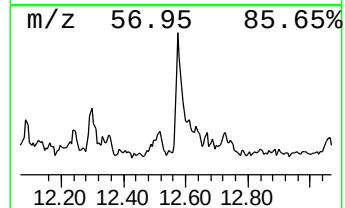
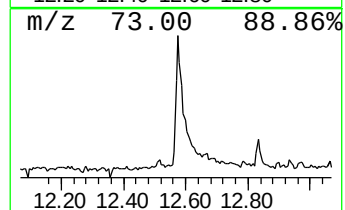
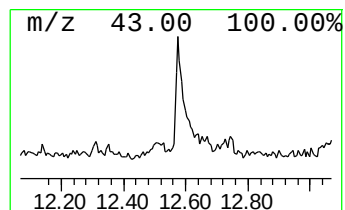
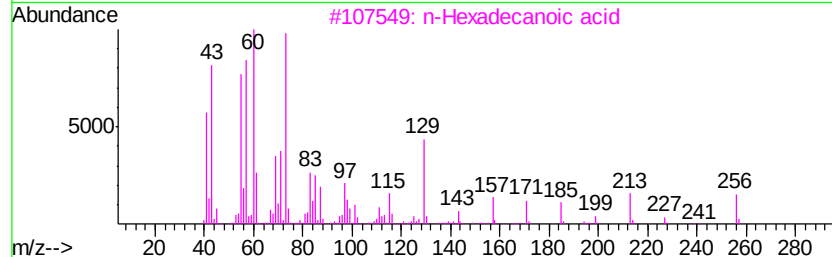
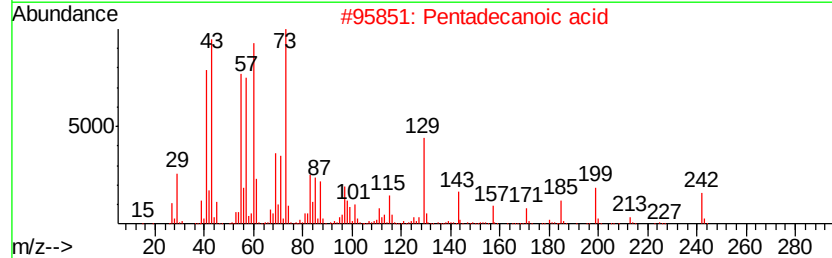
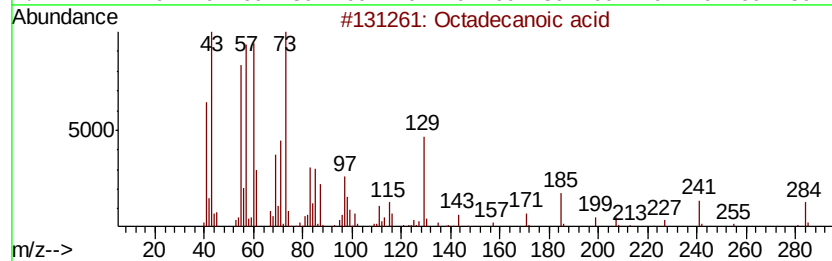
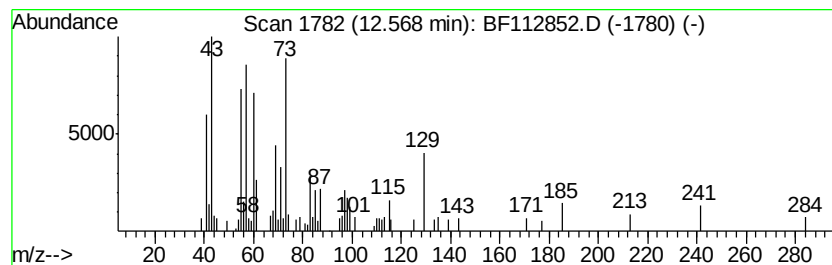
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.57	3.79 ng	206007	Chrysene-d12		13.88	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	97
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		n-Decanoic acid	172	C10H20O2	000334-48-5	52



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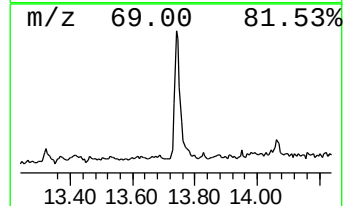
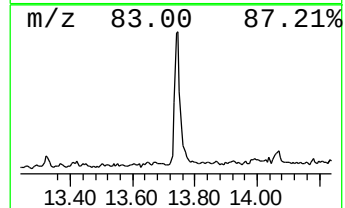
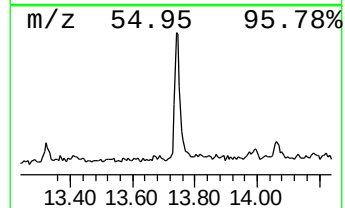
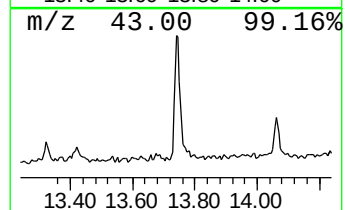
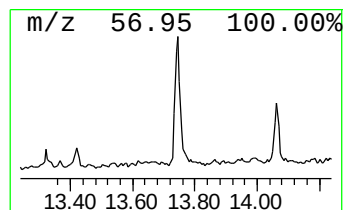
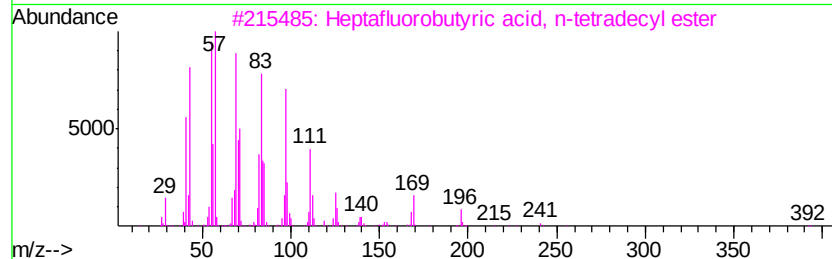
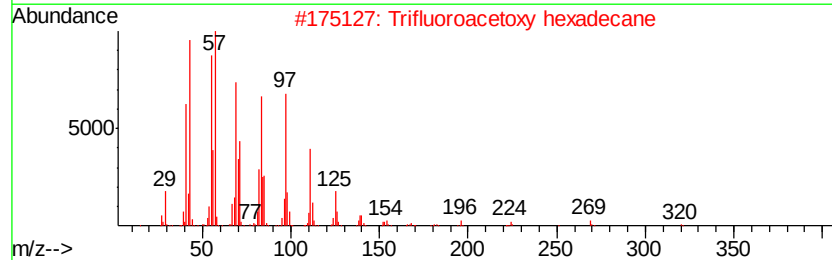
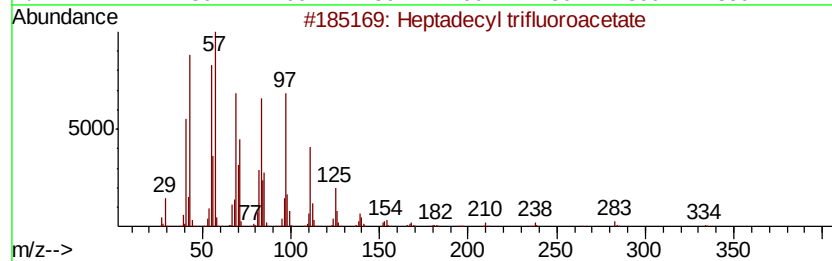
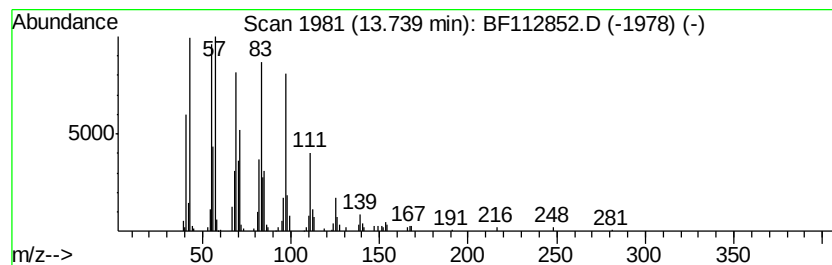
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Heptadecyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.74	4.67 ng	253771	Chrysene-d12		13.88	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	95
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
3		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
4		1-Heneicosanol	312	C21H44O	015594-90-8	93
5		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91



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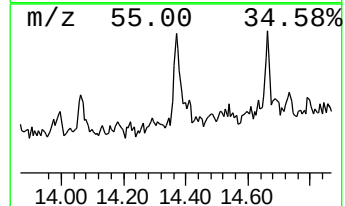
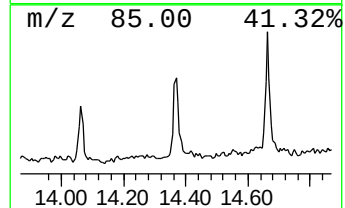
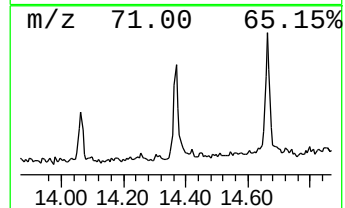
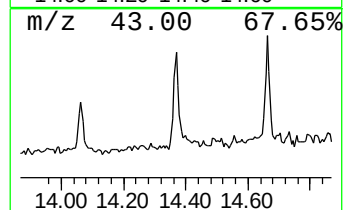
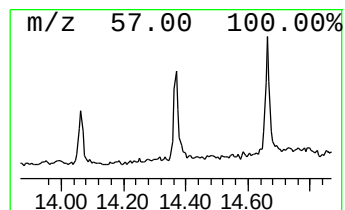
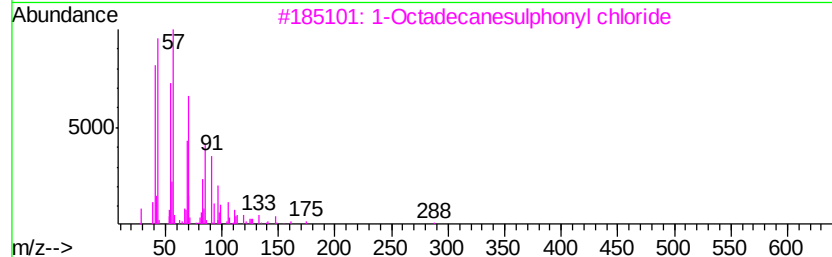
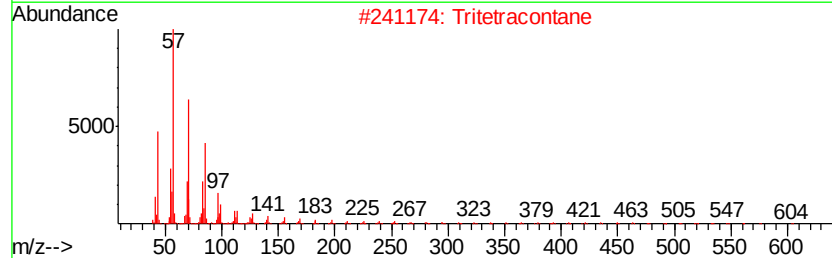
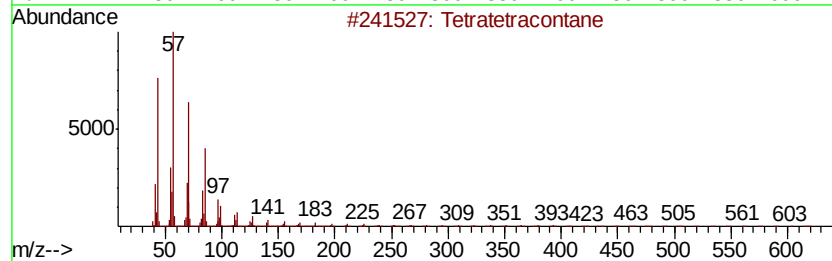
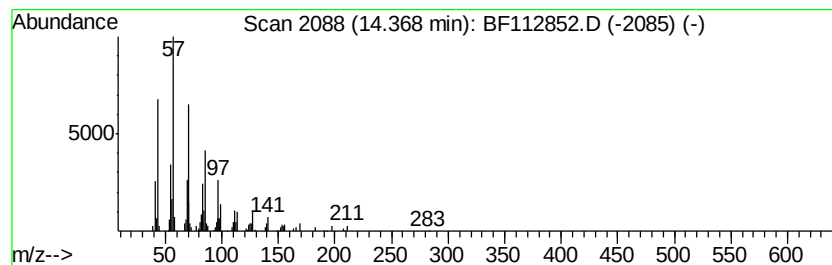
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetratetracontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.37	2.21 ng	120060	Chrysene-d12	13.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratetracontane	619	C44H90	007098-22-8	91
2		Tritetracontane	605	C43H88	007098-21-7	91
3		1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	91
4		Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	90
5		Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
Data File : BF112852.D
Acq On : 5 Mar 2019 13:41
Operator : JU/SJ
Sample : K1704-12
Misc :
ALS Vial : 6 Sample Multiplier: 1

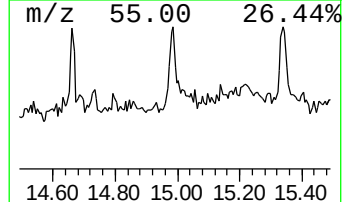
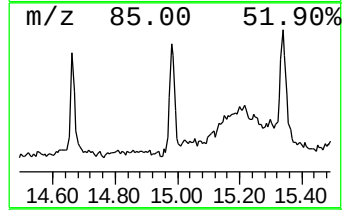
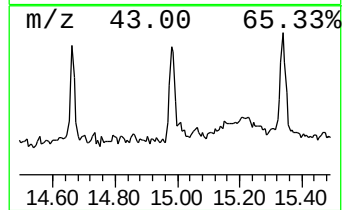
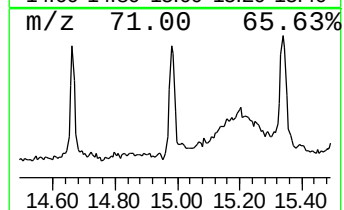
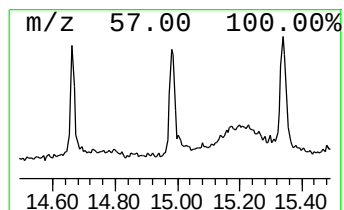
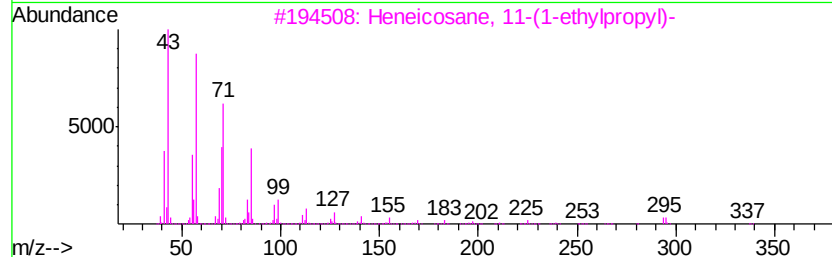
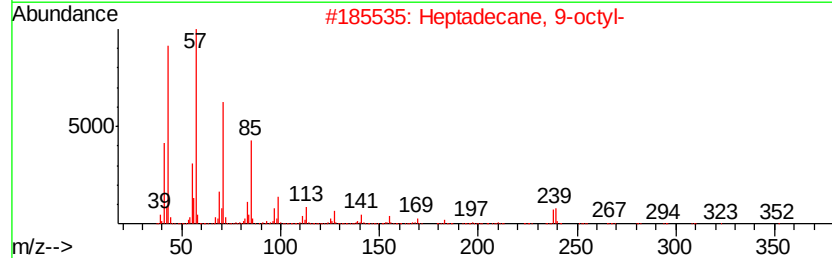
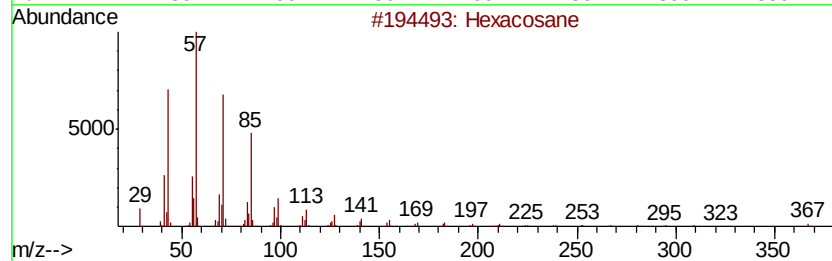
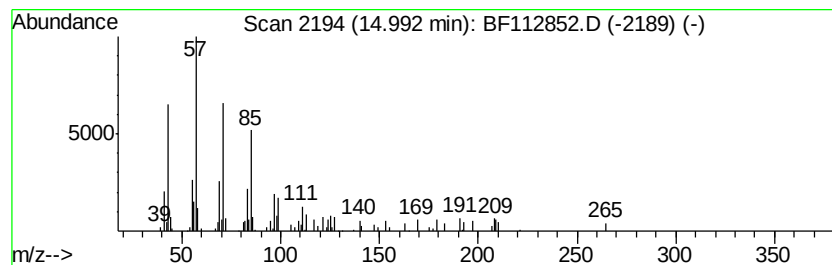
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PST-028-SW003-022719

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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 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	2.07 ng	115619	Perylene-d12	15.29
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexacosane	366 C26H54	000630-01-3	90
2	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	90
3	Heneicosane, 11-(1-ethylpropyl)-	366 C26H54	055282-11-6	87
4	Heptacosane	380 C27H56	000593-49-7	87
5	Heneicosane	296 C21H44	000629-94-7	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
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Sample : K1704-12
Misc :
ALS Vial : 6 Sample Multiplier: 1

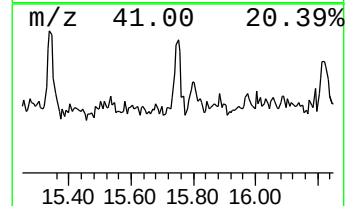
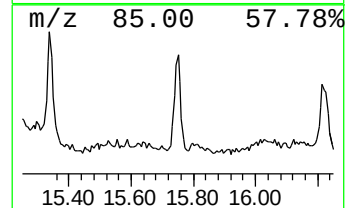
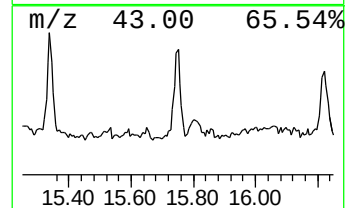
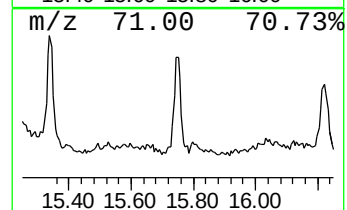
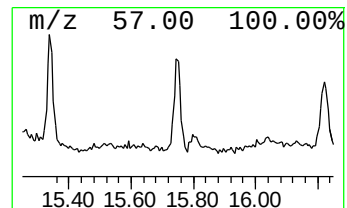
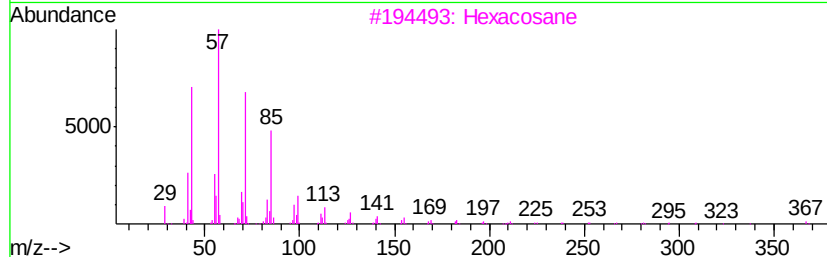
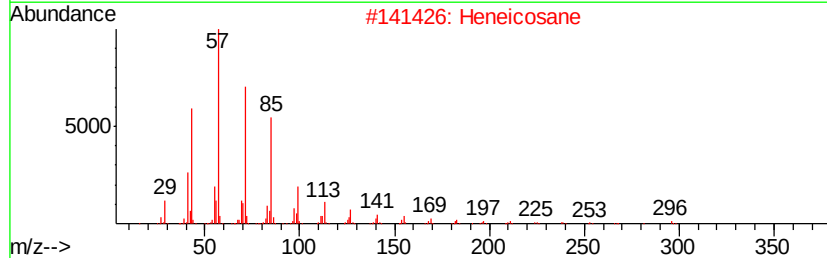
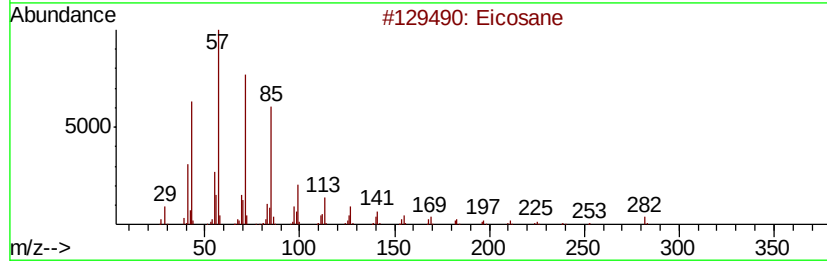
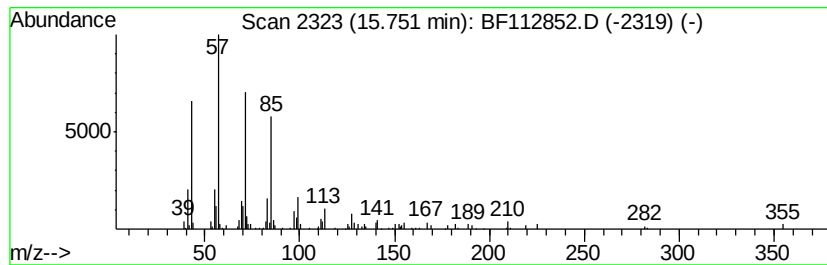
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.75	2.11 ng	117693	Perylene-d12	15.29
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	95
2	Heneicosane	296 C21H44	000629-94-7	90
3	Hexacosane	366 C26H54	000630-01-3	87
4	Hexadecane, 1-iodo-	352 C16H33I	000544-77-4	86
5	Heptadecane	240 C17H36	000629-78-7	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
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Acq On : 5 Mar 2019 13:41
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Sample : K1704-12
Misc :
ALS Vial : 6 Sample Multiplier: 1

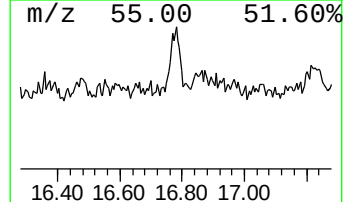
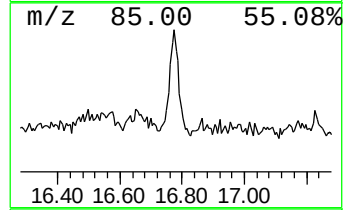
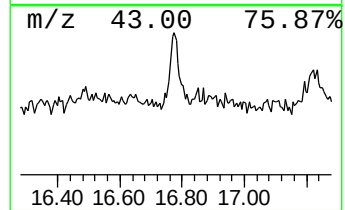
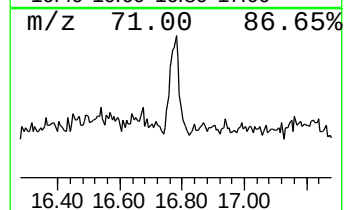
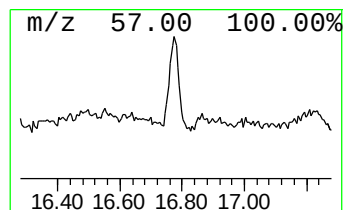
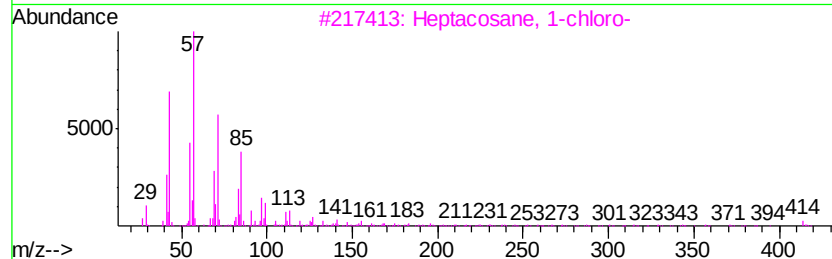
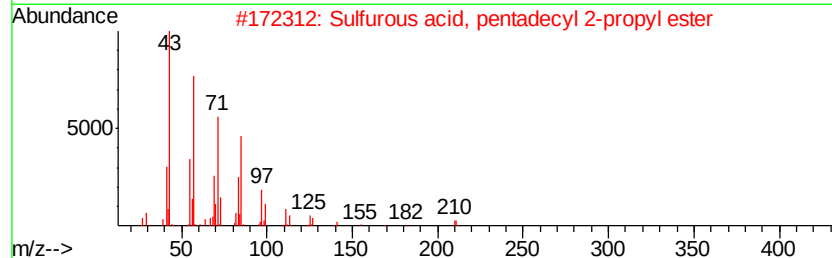
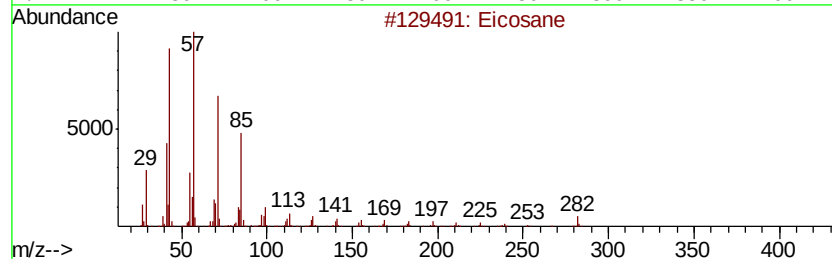
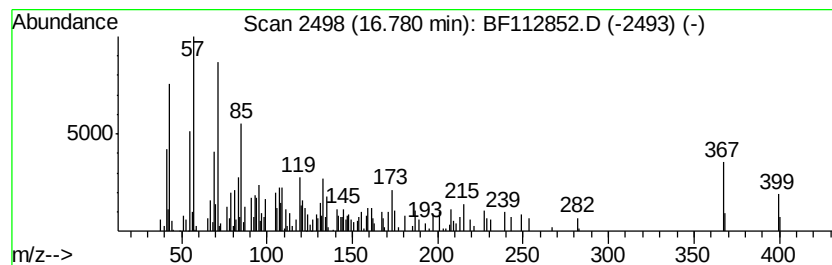
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.78	2.69 ng	150164	Perylene-d12	15.29
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	44
2	Sulfurous acid, pentadecyl 2-pro...	334 C18H38O3S	1000309-12-6	38
3	Heptacosane, 1-chloro-	414 C27H55Cl	062016-79-9	38
4	Heneicosane	296 C21H44	000629-94-7	35
5	Undecane, 2,3-dimethyl-	184 C13H28	017312-77-5	35



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030519\
Data File : BF112852.D
Acq On : 5 Mar 2019 13:41
Operator : JU/SJ
Sample : K1704-12
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown6.52	6.52	86.7	ng	4121990	1	6.75	951360	20.0
n-Hexadecanoic acid	11.79	5.9	ng	365491	4	11.25	1235880	20.0
Octadecanoic acid	12.57	3.8	ng	206007	5	13.88	1086930	20.0
Heptadecyl triflu...	13.74	4.7	ng	253771	5	13.88	1086930	20.0
Tetratetracontane	14.37	2.2	ng	120060	5	13.88	1086930	20.0
Hexacosane	14.99	2.1	ng	115619	6	15.29	1116110	20.0
Eicosane	15.75	2.1	ng	117693	6	15.29	1116110	20.0
Heneicosane	16.78	2.7	ng	150164	6	15.29	1116110	20.0