

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090518\
 Data File : BF108818.D
 Acq On : 6 Sep 2018 11:38
 Operator : JU/SJ
 Sample : J4724-10
 Misc :
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EP1-SUT-UST-09

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-BF090518.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	4.925	435	440	452	rVB	110916	133286	3.92%	0.396%
2	5.342	506	511	514	rBV	3231094	2858864	84.05%	8.499%
3	6.025	623	627	630	rBV	415388	351716	10.34%	1.046%
4	6.366	680	685	688	rBV	3436619	3081924	90.61%	9.162%
5	6.501	704	708	711	rBV	3578876	3053217	89.76%	9.076%
6	6.566	717	719	726	rVB	75853	62150	1.83%	0.185%
7	6.737	744	748	751	rBV	1977605	1539609	45.26%	4.577%
8	6.889	771	774	778	rVB	2655494	2440341	71.74%	7.255%
9	7.289	838	842	845	rBV	2026600	1846188	54.28%	5.488%
10	7.719	912	915	920	rVB2	53974	63206	1.86%	0.188%
11	8.019	962	966	969	rBV	2334119	1878910	55.24%	5.586%
12	8.148	985	988	990	rBV	51567	39066	1.15%	0.116%
13	9.095	1144	1149	1152	rBV	3746040	3401412	100.00%	10.112%
14	9.483	1211	1215	1218	rBV	1298338	924499	27.18%	2.748%
15	9.766	1259	1263	1267	rBV2	2183745	1801154	52.95%	5.354%
16	10.548	1392	1396	1399	rBV	1717236	1413465	41.56%	4.202%
17	11.242	1510	1514	1517	rBV	1881161	1487001	43.72%	4.420%
18	11.783	1602	1606	1615	rBV2	122503	154713	4.55%	0.460%
19	12.666	1752	1756	1760	rBV2	84759	94361	2.77%	0.281%
20	12.824	1779	1783	1786	rBV	3159294	2555654	75.14%	7.597%
21	12.936	1799	1802	1804	rVB	76149	65630	1.93%	0.195%
22	13.189	1842	1845	1849	rBV	98641	94939	2.79%	0.282%
23	13.366	1872	1875	1878	rBV2	69123	56474	1.66%	0.168%
24	13.730	1934	1937	1947	rBV	437857	499405	14.68%	1.485%
25	13.865	1956	1960	1964	rBV	1838086	1642166	48.28%	4.882%
26	14.060	1990	1993	1996	rBV	48740	57426	1.69%	0.171%
27	14.124	2001	2004	2007	rVV3	58413	61567	1.81%	0.183%
28	14.360	2042	2044	2047	rBV	69178	73401	2.16%	0.218%
29	14.660	2092	2095	2099	rVB	94483	100259	2.95%	0.298%
30	14.724	2103	2106	2110	rVB	251348	257297	7.56%	0.765%
31	14.977	2146	2149	2153	rVB	97326	102508	3.01%	0.305%
32	15.271	2195	2199	2205	rVB	1101164	1309217	38.49%	3.892%
33	15.742	2275	2279	2284	rBV	91200	137845	4.05%	0.410%

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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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

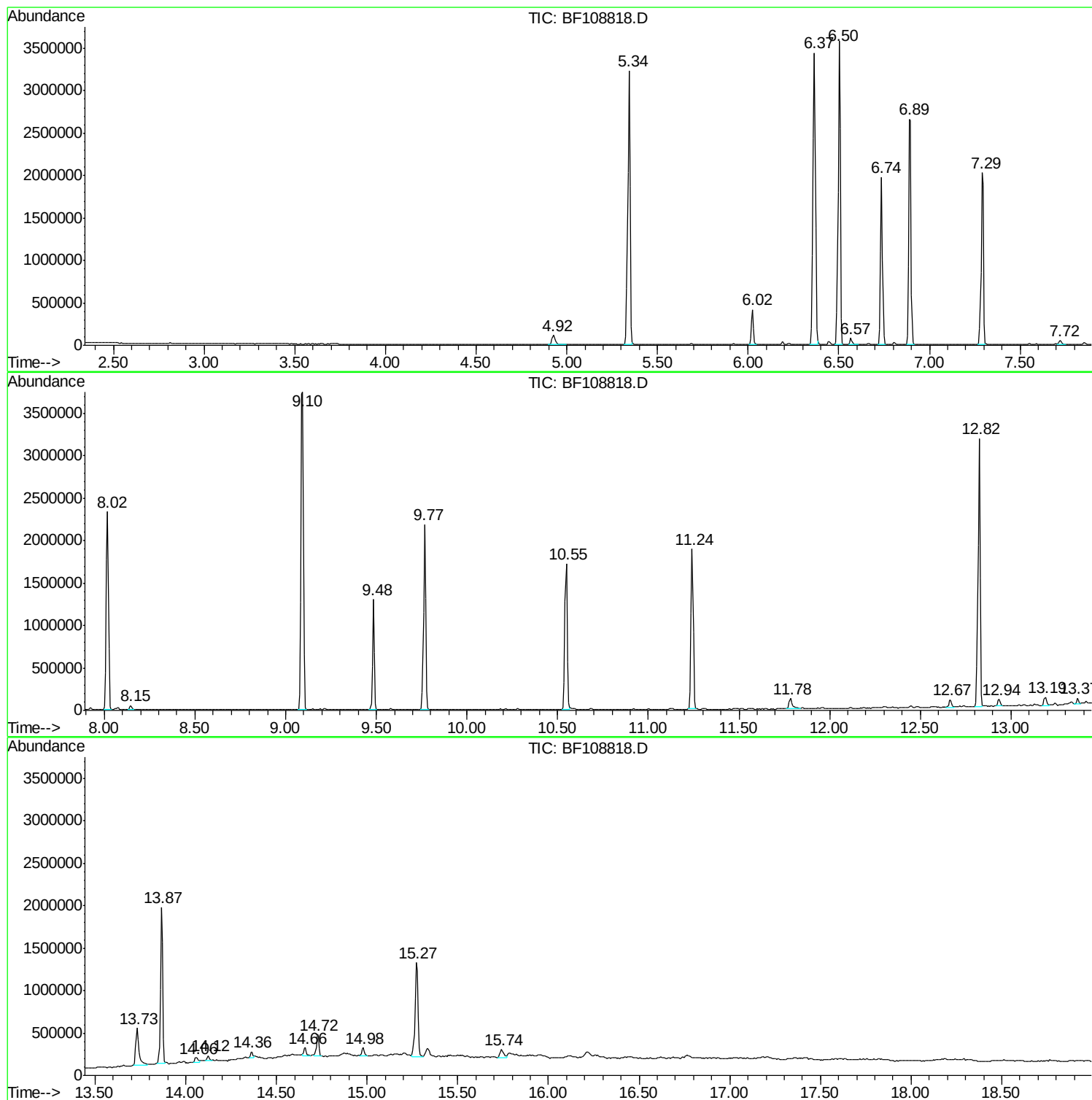
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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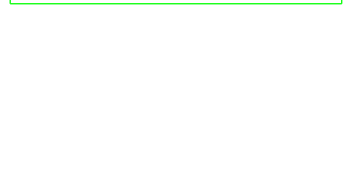
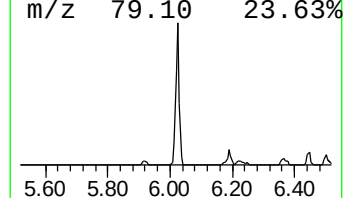
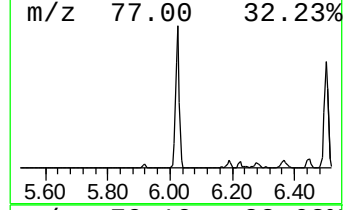
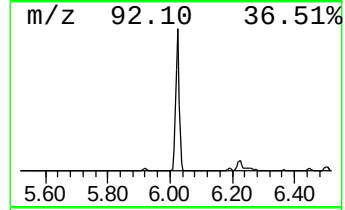
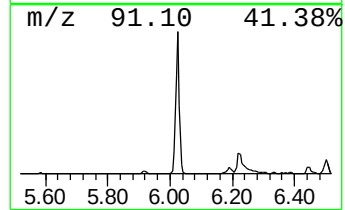
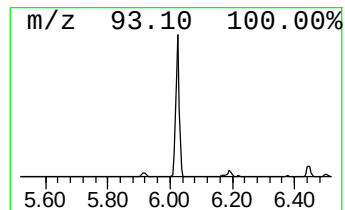
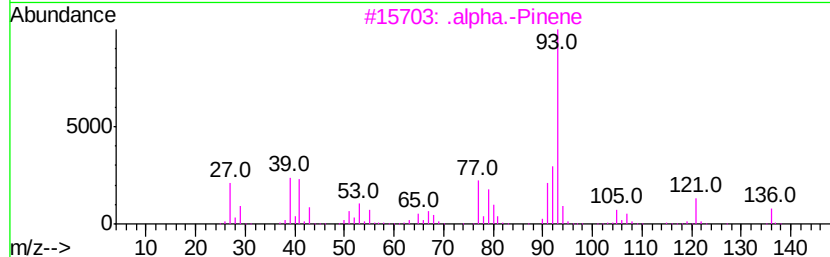
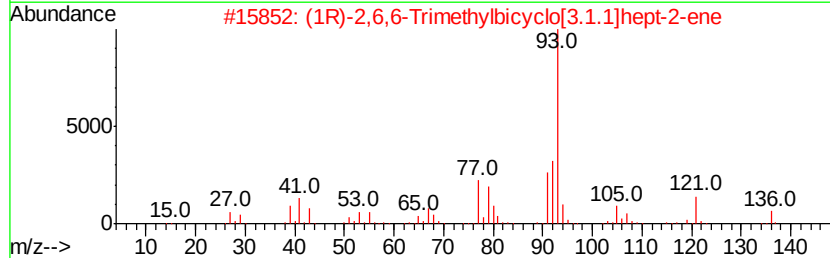
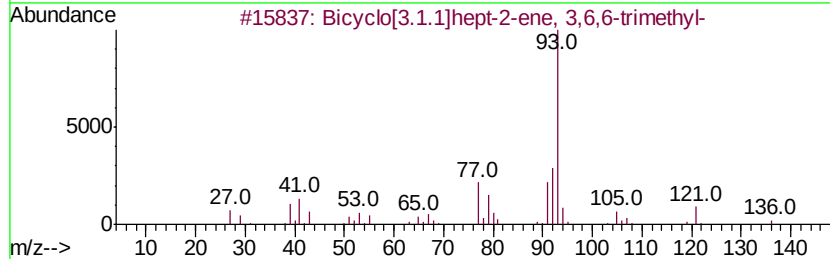
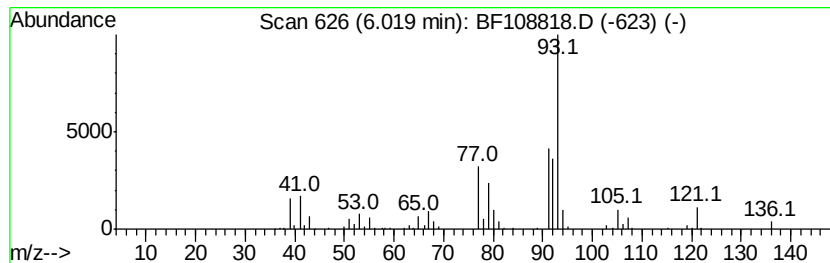
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Bicyclo[3.1.1]hept-2-ene, 3... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.02	4.57 ng	351716	1,4-Dichlorobenzene-d4	6.74	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	94
2	(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-70-8	94
3	.alpha.-Pinene	136	C10H16	000080-56-8	94
4	Tricyclo[2.2.1.0(2,6)]heptane, 1,4-dichloro-	136	C10H16	000508-32-7	91
5	.gamma.-Terpinene	136	C10H16	000099-85-4	91



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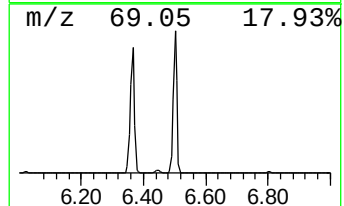
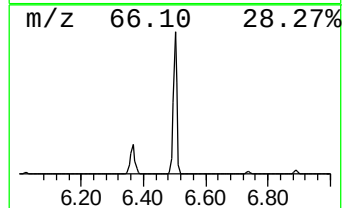
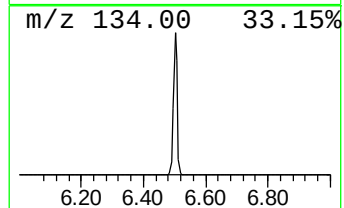
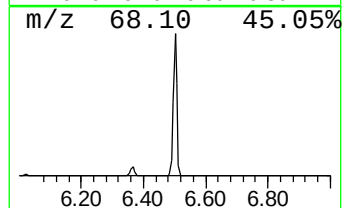
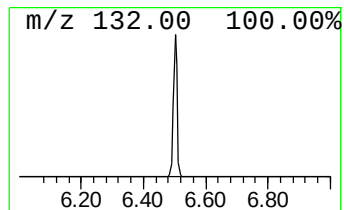
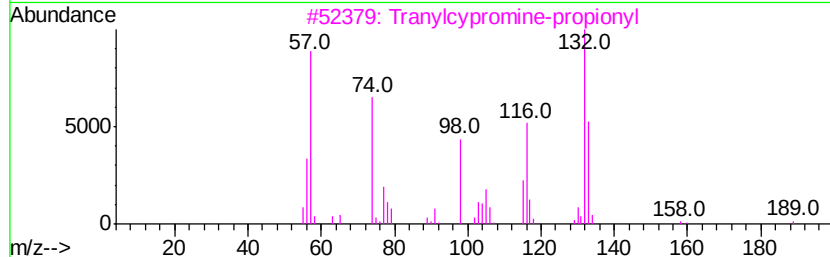
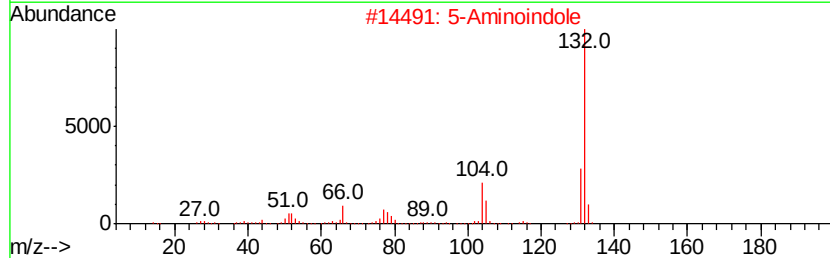
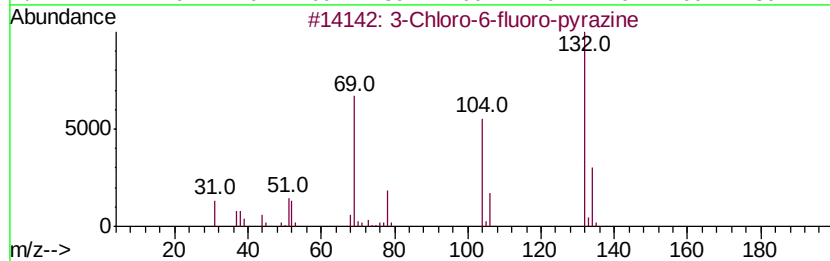
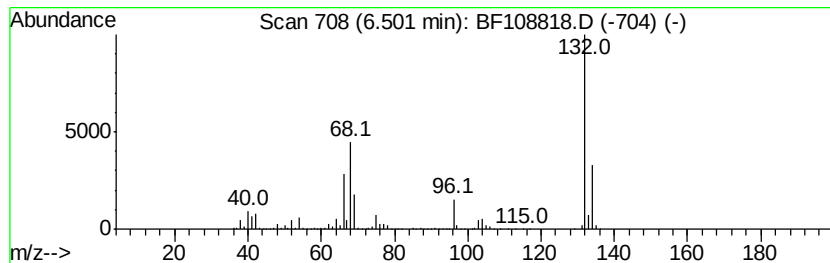
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	39.66 ng	3053220	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	5-Aminoindole	132	C8H8N2	005192-03-0	12	
3	Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10	
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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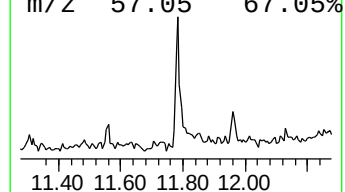
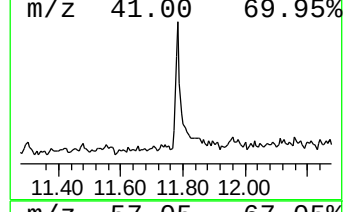
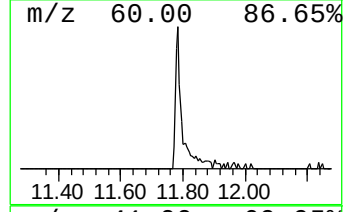
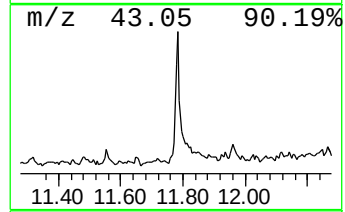
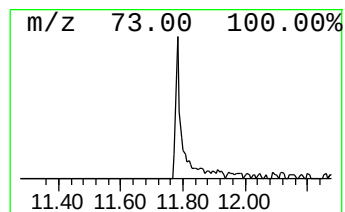
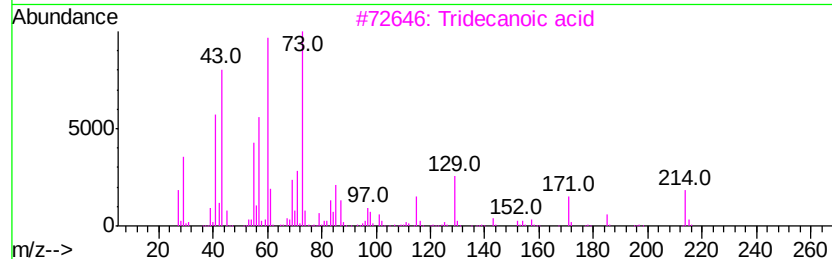
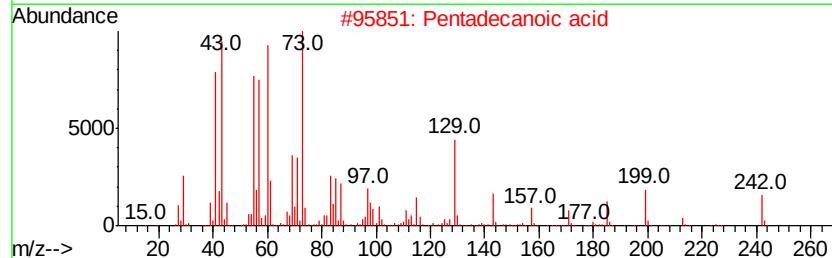
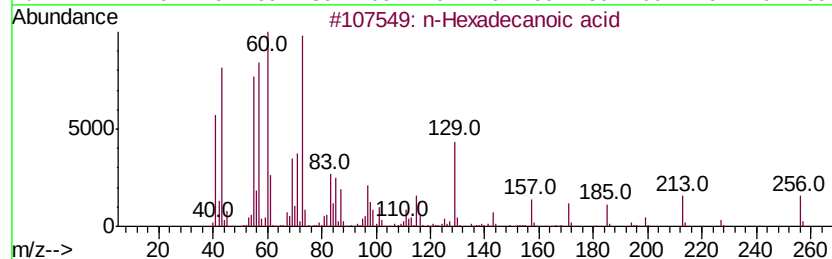
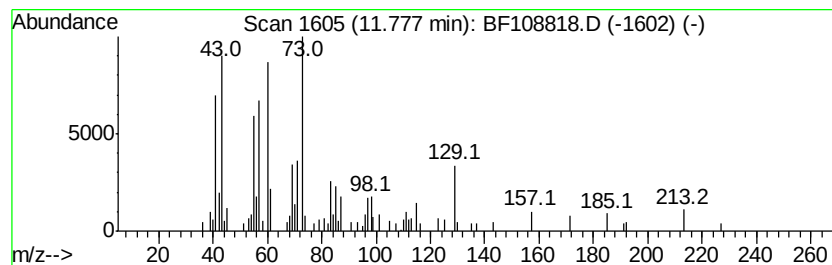
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.78	2.08 ng	154713	Phenanthrene-d10		11.24
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	72



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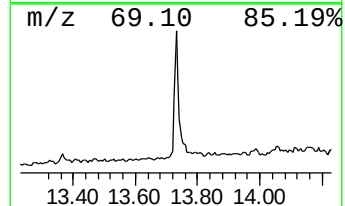
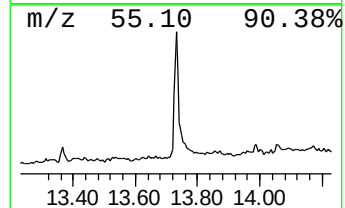
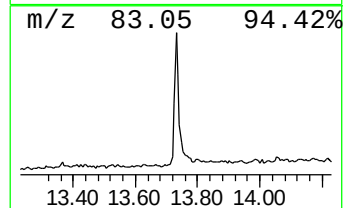
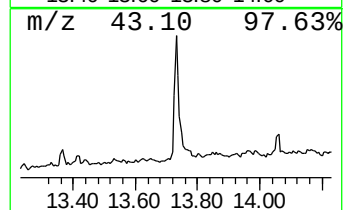
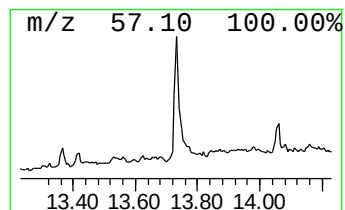
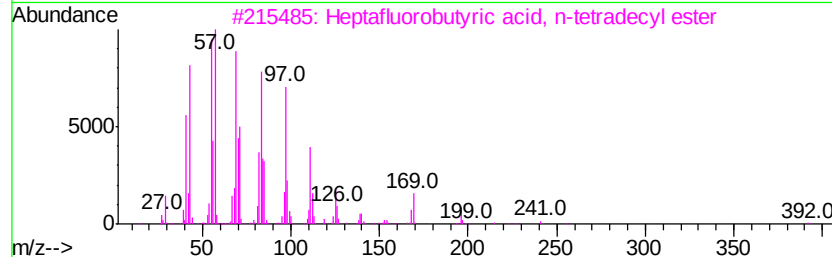
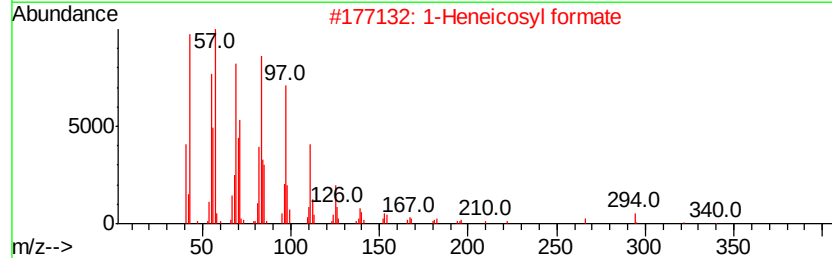
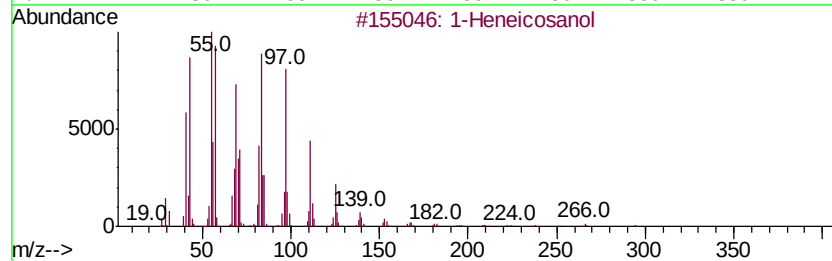
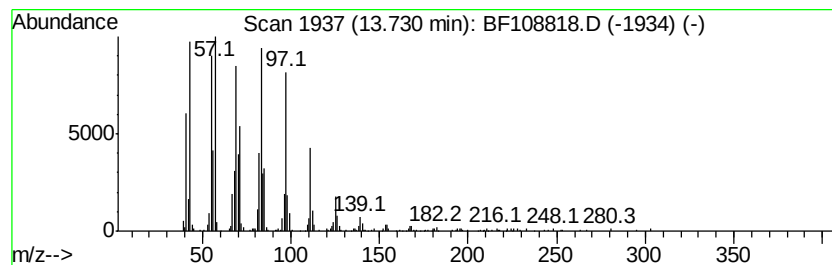
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	6.08 ng	499405	Chrysene-d12	13.87
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1-Heneicosanol	312 C21H44O	015594-90-8 95
2		1-Heneicosyl formate	340 C22H44O2	077899-03-7 95
3		Heptafluorobutyric acid, n-tetra...	410 C18H29F7O2	007365-36-8 94
4		Heptafluorobutyric acid, pentade...	424 C19H31F7O2	959261-23-5 94
5		Trifluoroacetic acid, pentadecyl...	324 C17H31F3O2	959010-23-2 94



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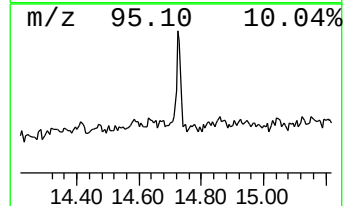
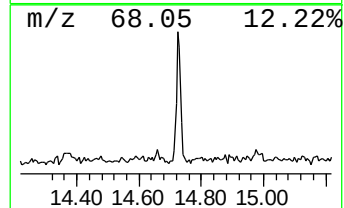
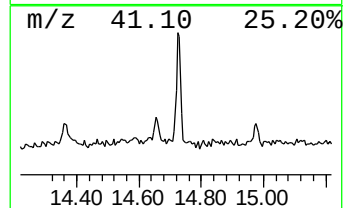
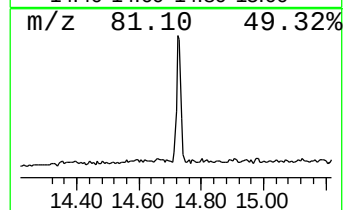
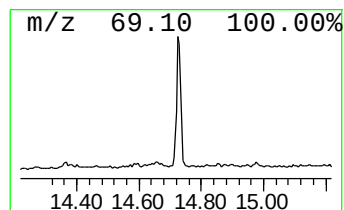
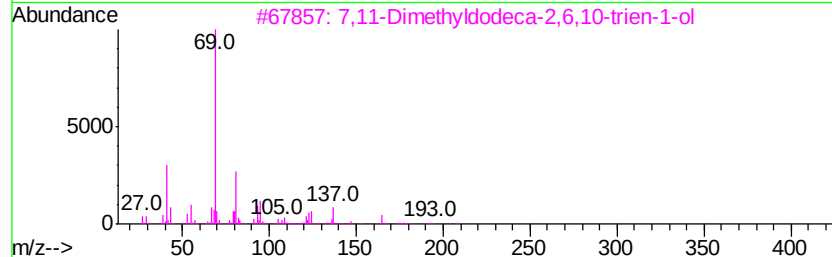
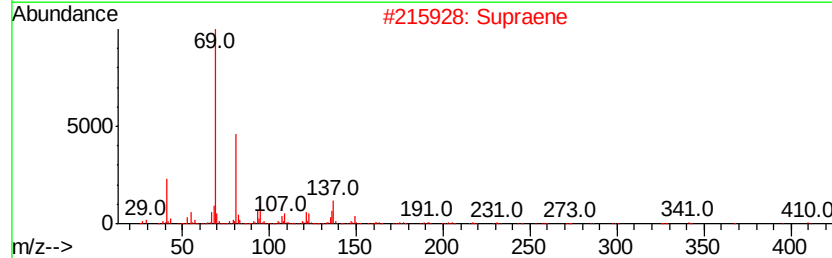
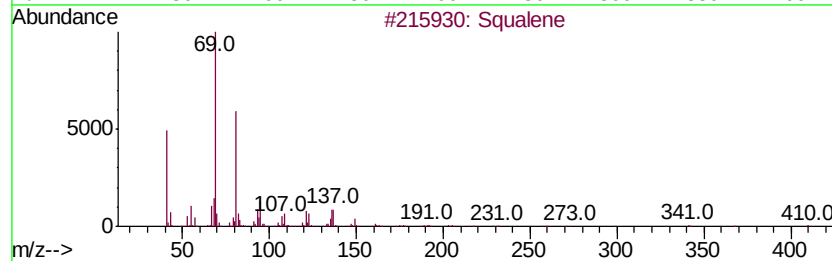
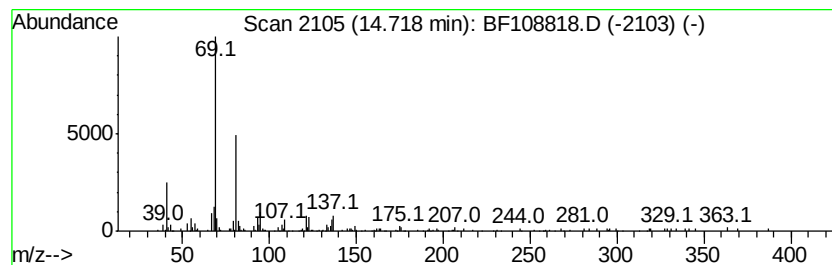
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	3.93 ng	257297	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
4		2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	58
5		1,5-Heptadiene, 3,3-dimethyl-, (E)-	124	C9H16	067682-47-7	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090518\
Data File : BF108818.D
Acq On : 6 Sep 2018 11:38
Operator : JU/SJ
Sample : J4724-10
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-SUT-UST-09

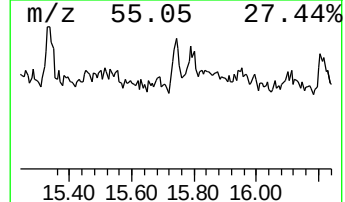
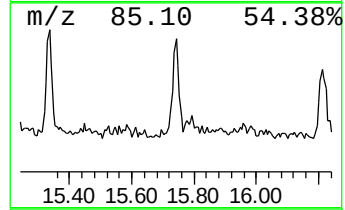
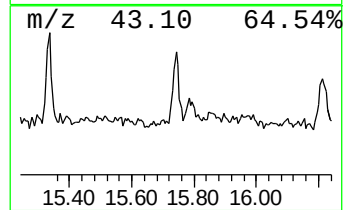
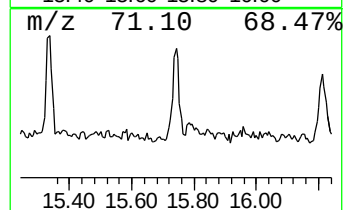
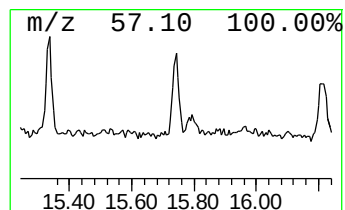
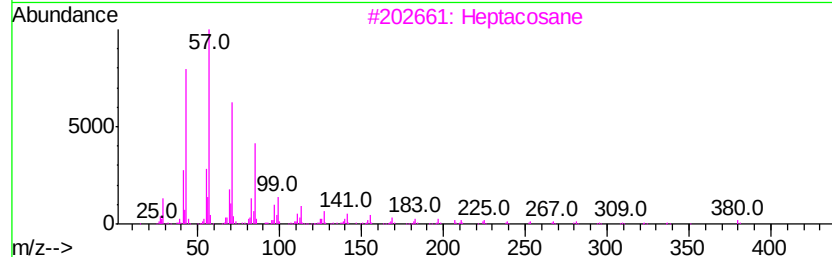
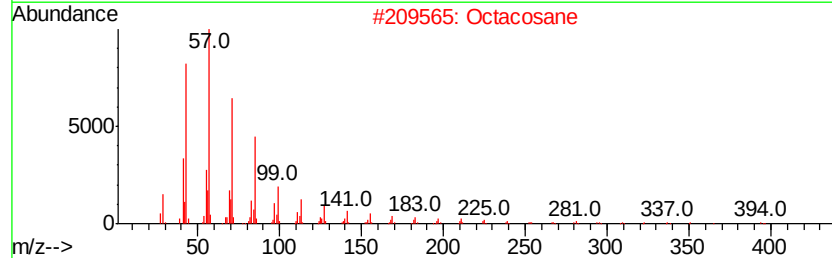
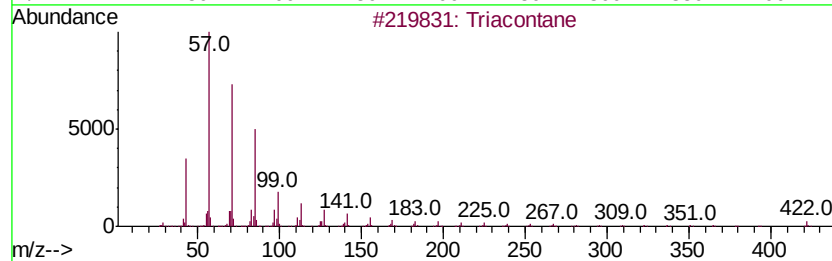
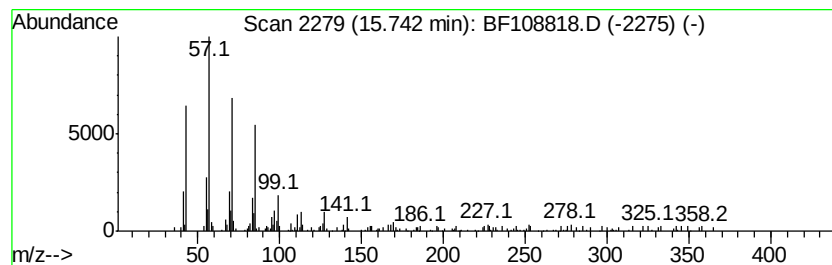
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Triacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	2.11 ng	137845	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Triacontane	422	C30H62	000638-68-6	87
2		Octacosane	394	C28H58	000630-02-4	87
3		Heptacosane	380	C27H56	000593-49-7	87
4		Tetracosane	338	C24H50	000646-31-1	87
5		Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090518\
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Acq On : 6 Sep 2018 11:38
Operator : JU/SJ
Sample : J4724-10
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-SUT-UST-09

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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
Bicyclo[3.1.1]hep...	6.02	4.6 ng		351716	1	6.74	1539610	20.0
unknown6.50	6.50	39.7 ng		3053220	1	6.74	1539610	20.0
n-Hexadecanoic acid	11.78	2.1 ng		154713	4	11.24	1487000	20.0
1-Heneicosanol	13.73	6.1 ng		499405	5	13.87	1642170	20.0
Squalene	14.72	3.9 ng		257297	6	15.27	1309220	20.0
Triacontane	15.74	2.1 ng		137845	6	15.27	1309220	20.0