

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091318\
 Data File : BF108982.D
 Acq On : 13 Sep 2018 23:19
 Operator : JU/SJ
 Sample : J4875-10
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 091118-DBRI-F-U-S

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	4.907	431	437	450	rBV2	144952	198336	4.28%	0.655%
2	5.331	505	509	513	rBV	1575618	1374457	29.65%	4.542%
3	6.354	679	683	690	rBV	1317837	1054227	22.74%	3.484%
4	6.496	700	707	710	rBV	2791851	2434794	52.52%	8.046%
5	6.725	743	746	750	rBV	982062	843007	18.18%	2.786%
6	6.890	769	774	777	rBV	3236153	3157827	68.12%	10.435%
7	7.290	836	842	845	rBV	2837888	2726105	58.81%	9.009%
8	8.007	960	964	968	rBV	1333141	1049325	22.64%	3.468%
9	9.089	1143	1148	1151	rBV	4964895	4635781	100.00%	15.320%
10	9.478	1210	1214	1217	rBV	498089	391643	8.45%	1.294%
11	9.760	1258	1262	1265	rBV	1333013	1190694	25.68%	3.935%
12	10.436	1374	1377	1381	rVB	82482	66817	1.44%	0.221%
13	10.542	1390	1395	1398	rBV	2253839	1983819	42.79%	6.556%
14	11.236	1509	1513	1516	rVB	1398634	1140939	24.61%	3.770%
15	11.772	1601	1604	1608	rBV	84314	85748	1.85%	0.283%
16	12.825	1778	1783	1786	rBV	4371076	4356634	93.98%	14.397%
17	13.066	1820	1824	1830	rBV	52830	47456	1.02%	0.157%
18	13.407	1879	1882	1885	rBV	77180	63983	1.38%	0.211%
19	13.736	1934	1938	1955	rBV	110315	166381	3.59%	0.550%
20	13.860	1955	1959	1963	rBV	1131739	1000479	21.58%	3.306%
21	14.048	1986	1991	1995	rBV	127655	112840	2.43%	0.373%
22	14.354	2039	2043	2046	rVB	127367	113835	2.46%	0.376%
23	14.648	2090	2093	2097	rBV	165149	161117	3.48%	0.532%
24	14.719	2101	2105	2109	rVB	290404	271539	5.86%	0.897%
25	14.966	2143	2147	2152	rBV	141585	156979	3.39%	0.519%
26	15.266	2193	2198	2203	rBV	826106	995911	21.48%	3.291%
27	15.324	2203	2208	2216	rVB	128975	161539	3.48%	0.534%
28	15.730	2271	2277	2285	rBV	90002	135759	2.93%	0.449%
29	16.195	2350	2356	2362	rVB	67666	121963	2.63%	0.403%
30	16.748	2445	2450	2457	rVB2	34488	60701	1.31%	0.201%

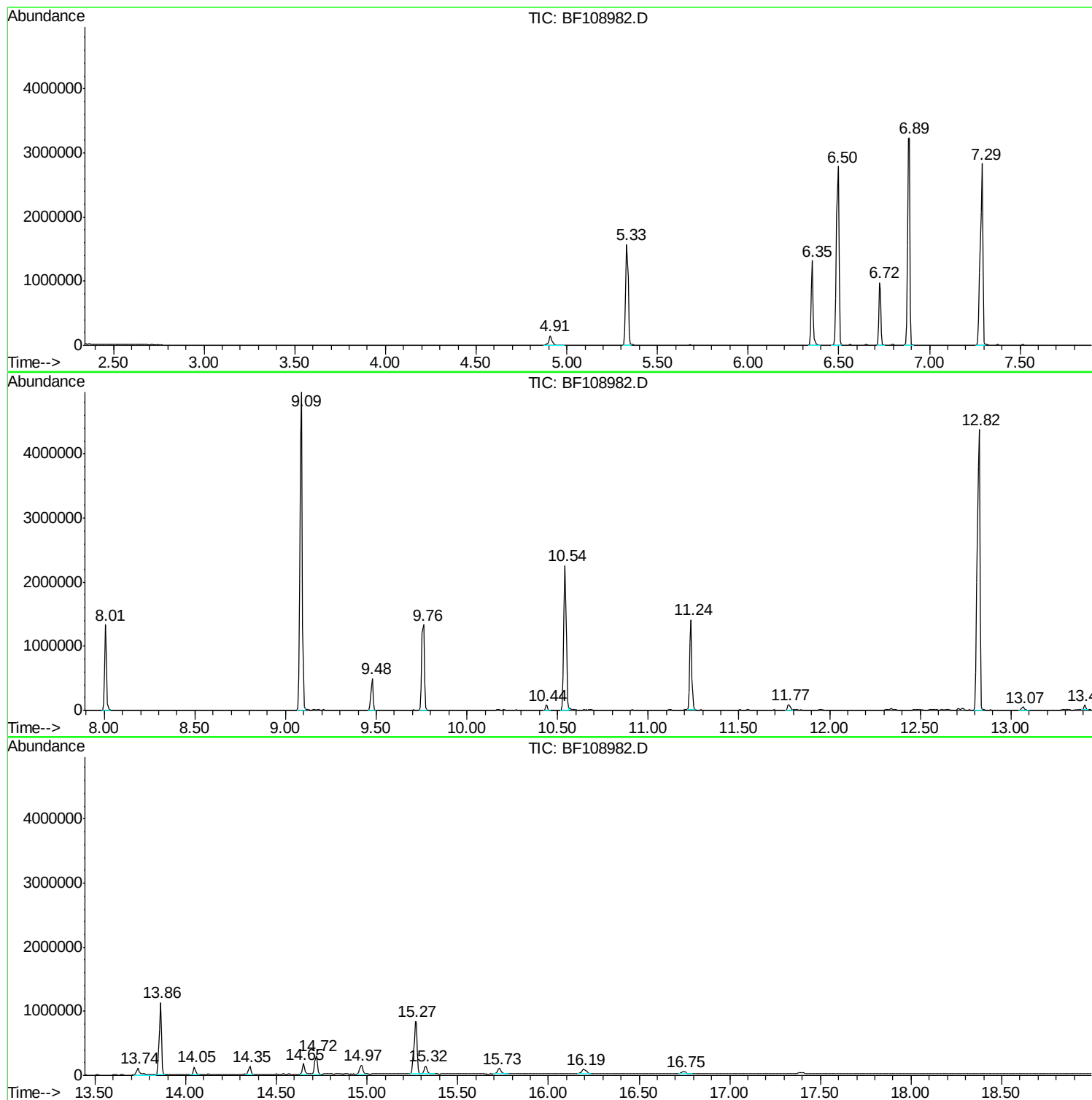
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Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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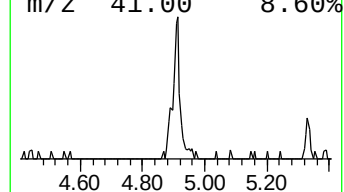
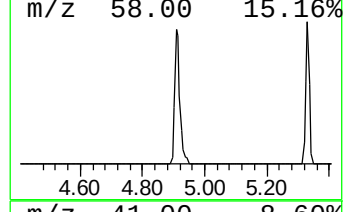
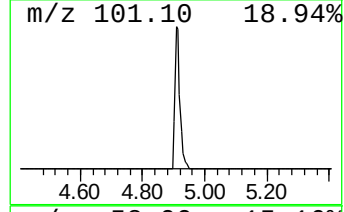
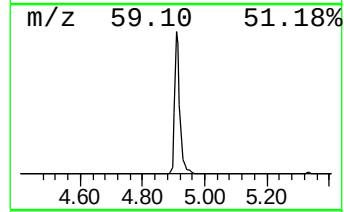
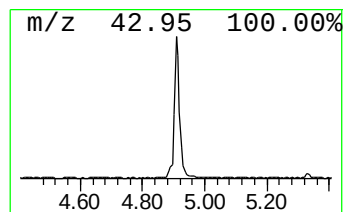
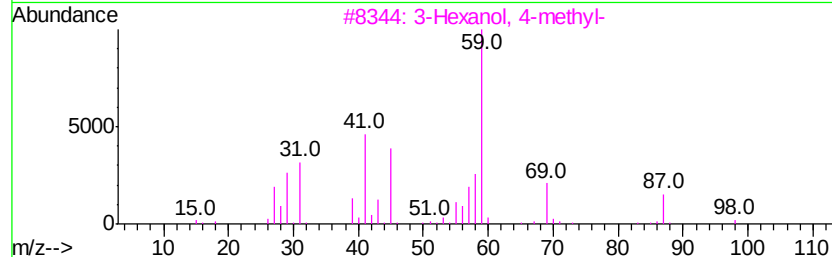
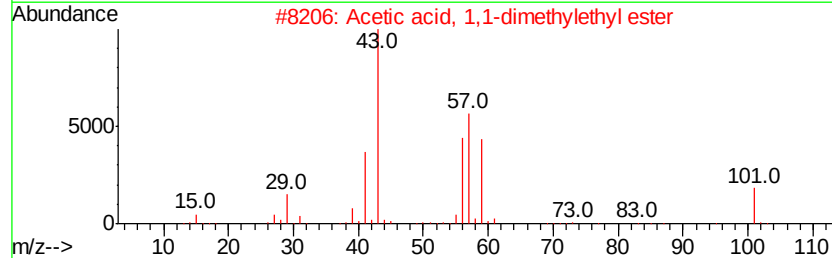
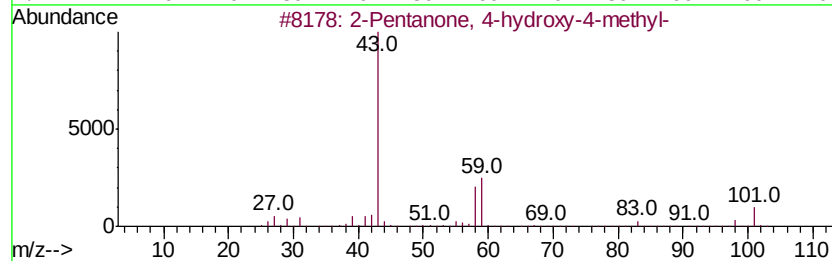
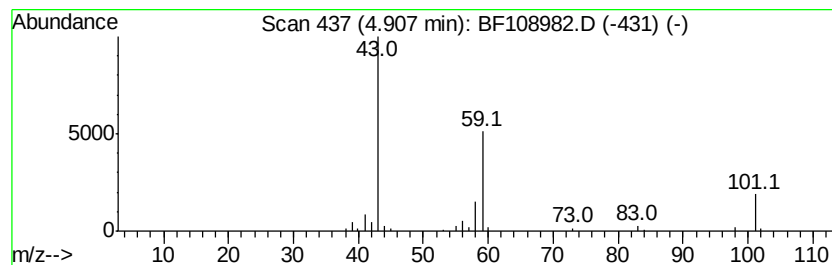
Instrument :
BNA_F
ClientSampleId :
091118-DBRI-F-U-S

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.91	4.71 ng	198336	1,4-Dichlorobenzene-d4	6.72	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25



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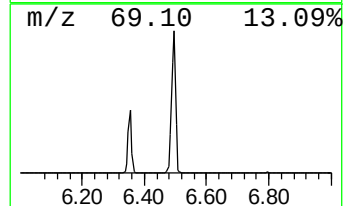
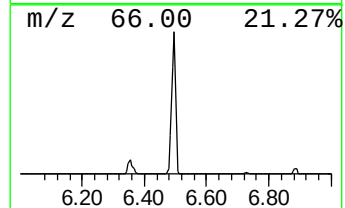
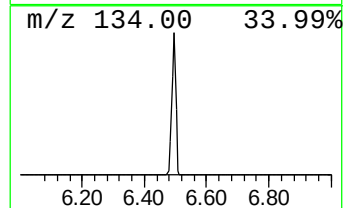
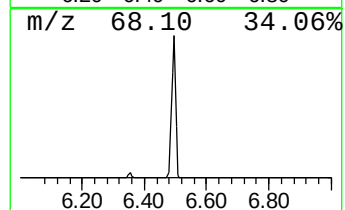
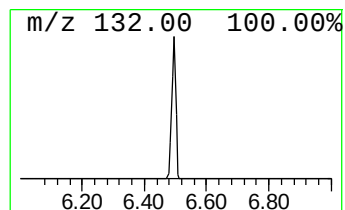
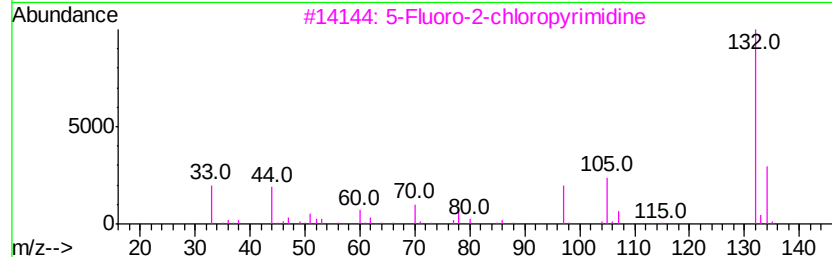
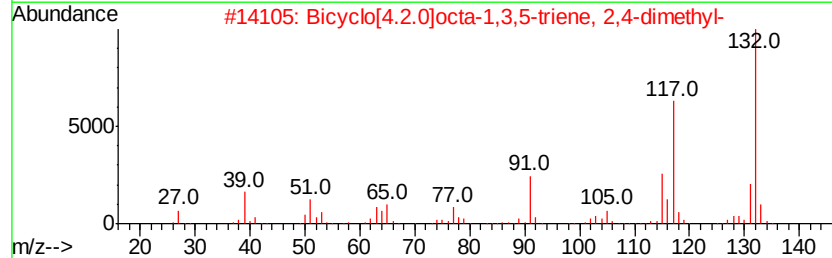
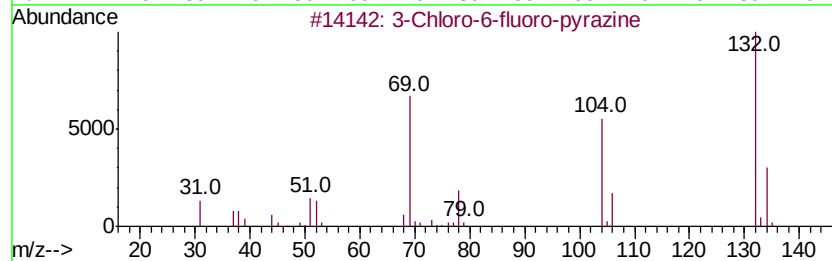
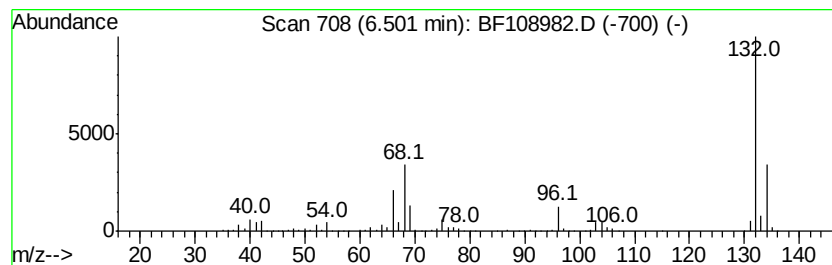
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.50 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	57.76 ng	2434790	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	Bicyclo[4.2.0]octa-1,3,5-triene,...			132	C10H12	028749-81-7	9
3	5-Fluoro-2-chloropyrimidine			132	C4H2ClFN2	062802-42-0	9
4	4-Chloro-2-fluoro-pyrimidine			132	C4H2ClFN2	051422-00-5	9
5	(E)-3-Chloro-2-methyl-2-pentenal			132	C6H9ClO	031357-76-3	9



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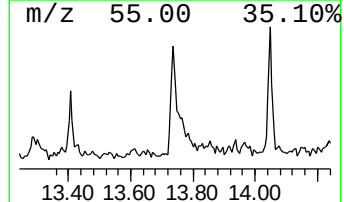
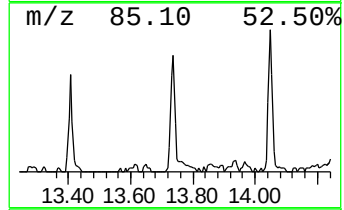
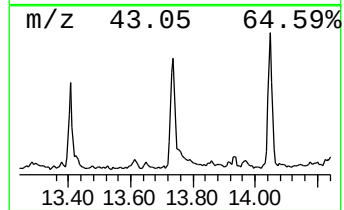
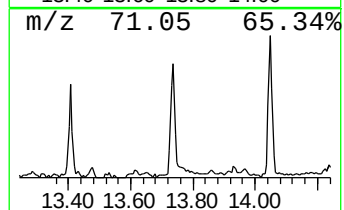
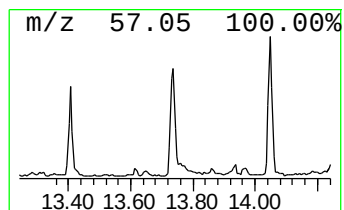
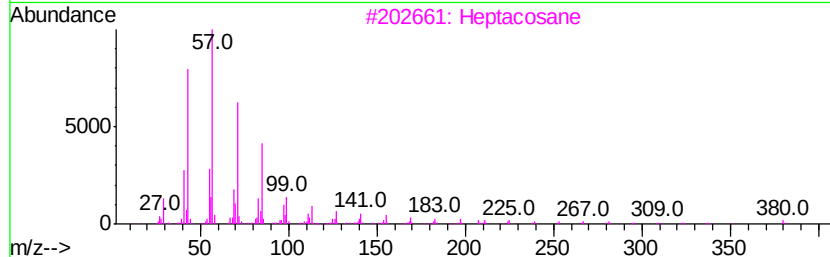
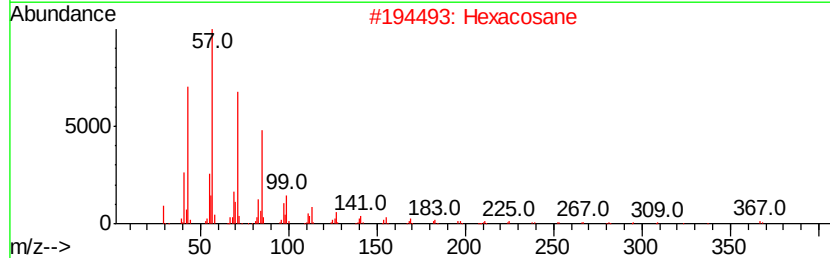
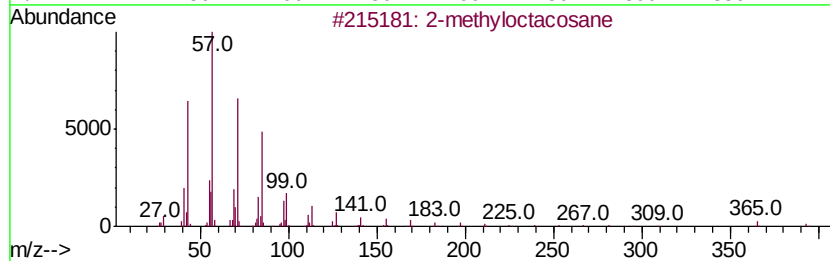
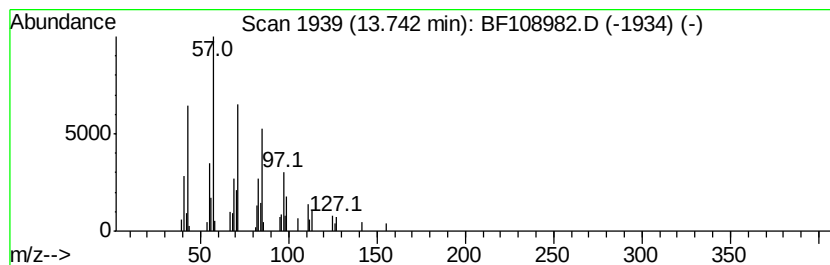
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	3.33 ng	166381	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heptacosane	380	C27H56	000593-49-7	91
4		Heneicosane	296	C21H44	000629-94-7	91
5		Tetratetracontane	619	C44H90	007098-22-8	91



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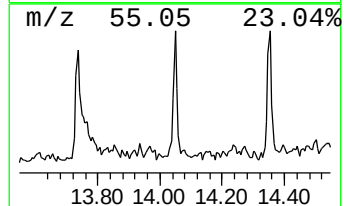
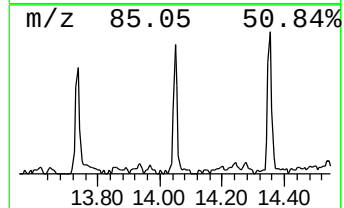
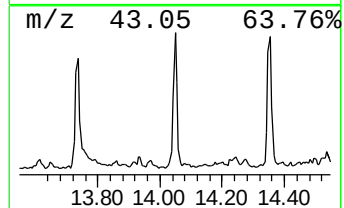
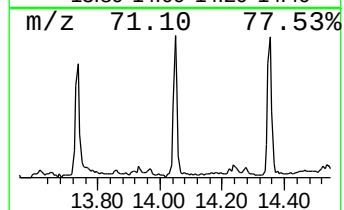
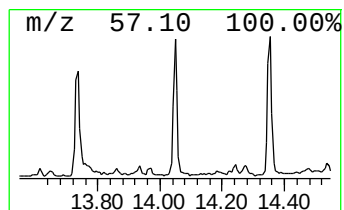
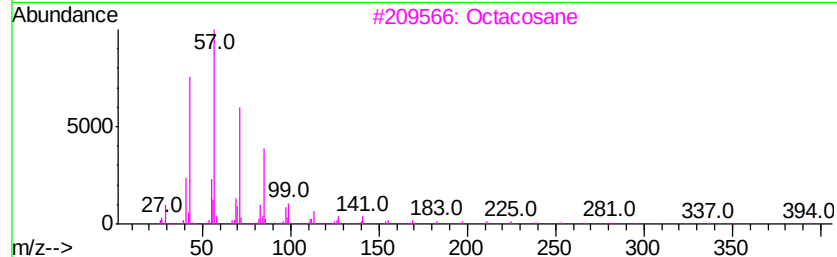
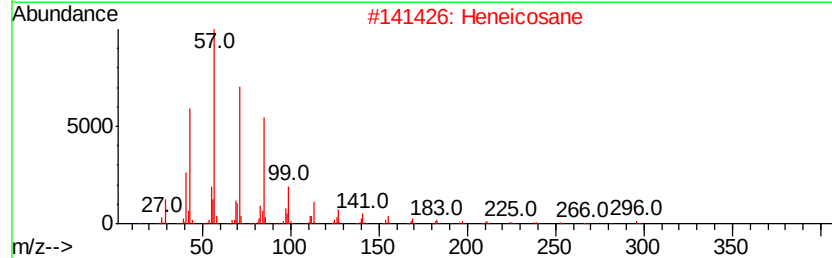
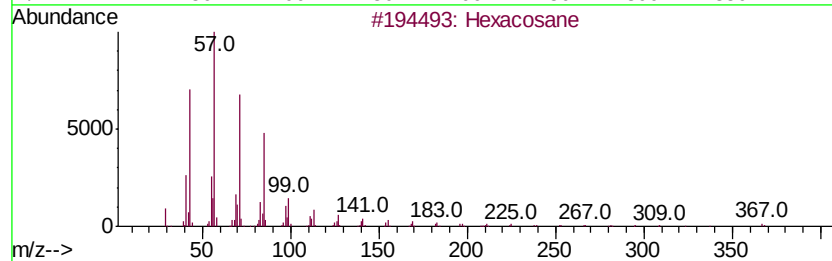
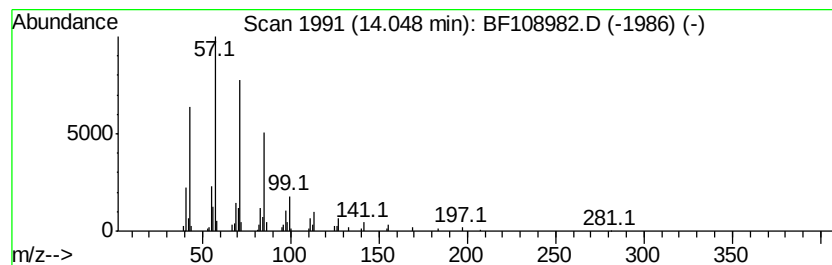
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.05	2.26 ng	112840	Chrysene-d12	13.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	91
2	Heneicosane		296	C21H44	000629-94-7	91
3	Octacosane		394	C28H58	000630-02-4	91
4	Tetracosane		338	C24H50	000646-31-1	90
5	Eicosane		282	C20H42	000112-95-8	90



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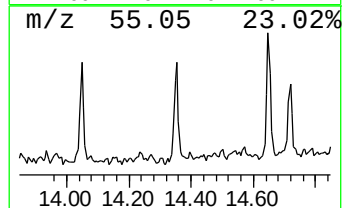
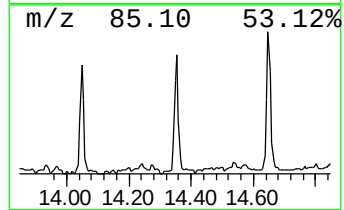
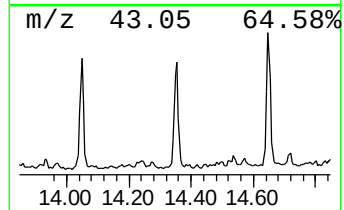
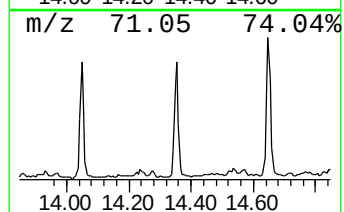
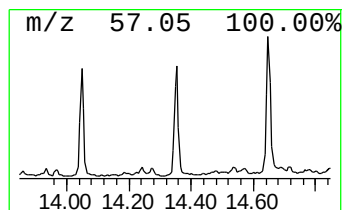
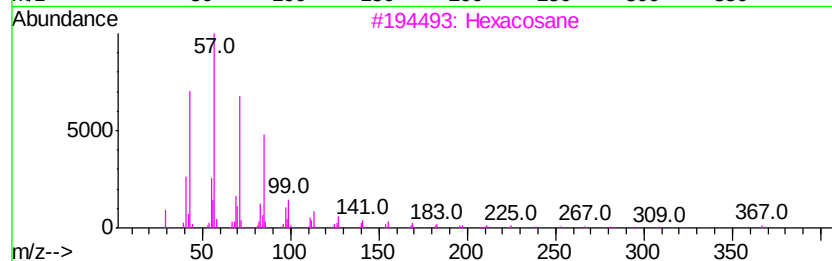
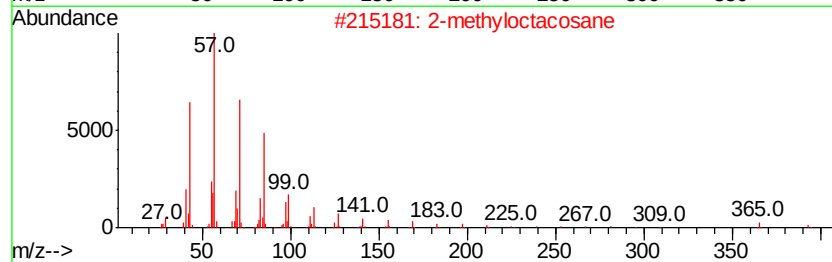
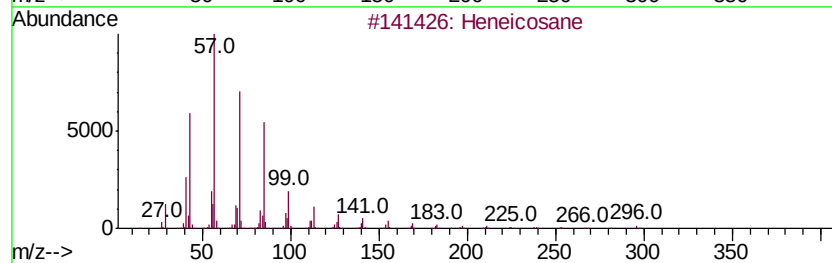
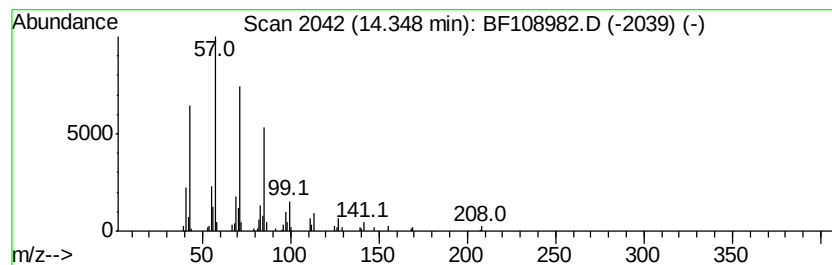
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 6 Heneicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	2.28 ng	113835	Chrysene-d12	13.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	2-methyloctacosane		408	C29H60	1000376-72-8	91
3	Hexacosane		366	C26H54	000630-01-3	90
4	Octacosane		394	C28H58	000630-02-4	87
5	Octadecane		254	C18H38	000593-45-3	87



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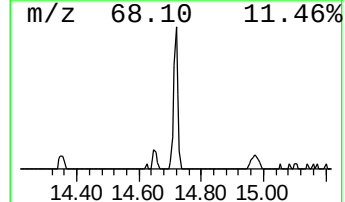
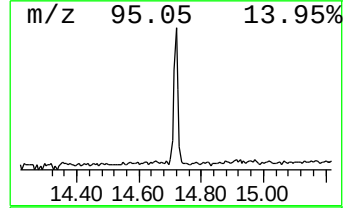
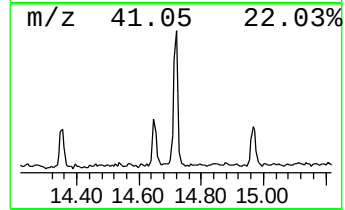
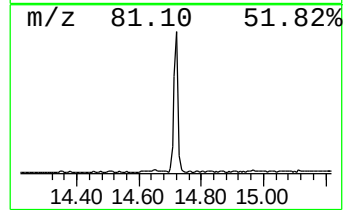
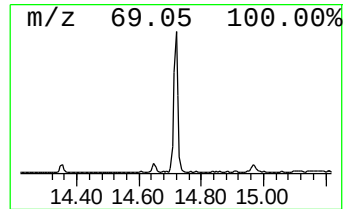
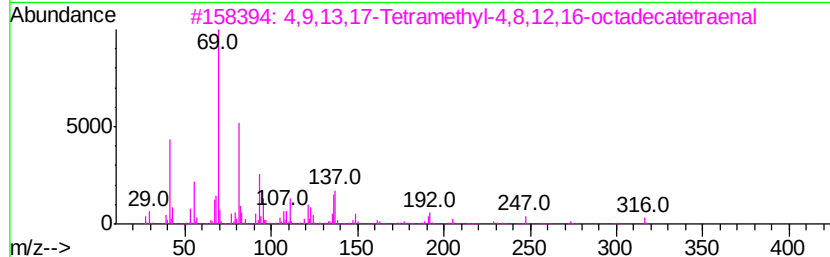
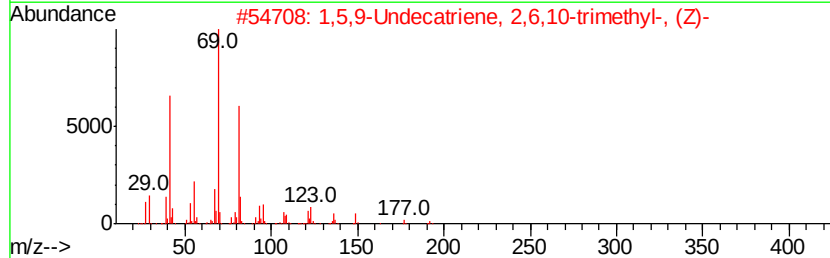
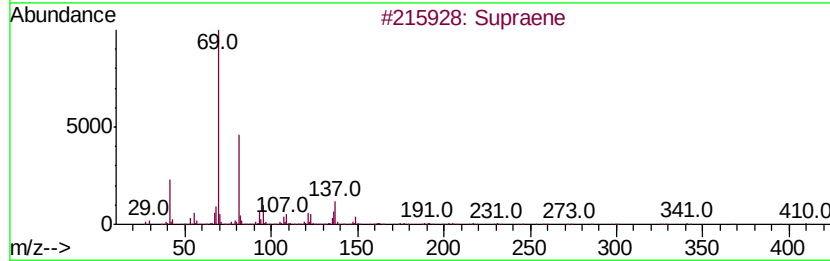
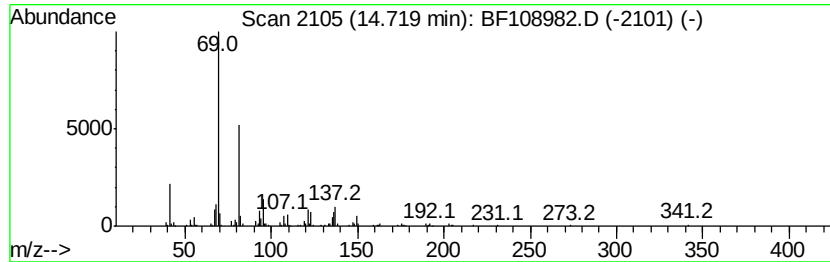
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	5.45 ng	271539	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	91
2		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	87
3		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H360	056882-09-8	83
4		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H280	066408-55-7	72
5		2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H2802	004128-17-0	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091318\
Data File : BF108982.D
Acq On : 13 Sep 2018 23:19
Operator : JU/SJ
Sample : J4875-10
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
091118-DBRI-F-U-S

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
2-Pentanone, 4-hy...	4.91	4.7	ng	198336	1	6.72	843007	20.0
unknown6.50	6.50	57.8	ng	2434790	1	6.72	843007	20.0
2-methyloctacosane	13.74	3.3	ng	166381	5	13.86	1000480	20.0
Hexacosane	14.05	2.3	ng	112840	5	13.86	1000480	20.0
Heneicosane	14.35	2.3	ng	113835	5	13.86	1000480	20.0
Supraene	14.72	5.5	ng	271539	6	15.27	995911	20.0