

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
 Data File : BF102275.D
 Acq On : 20 Jan 2018 19:29
 Operator : SJ/JU
 Sample : J1210-10
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RT-2898

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:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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	4.928	478	483	493	rBV	182030	265403	7.02%	0.793%
2	5.334	547	552	555	rBV	3343350	3583843	94.77%	10.705%
3	6.363	721	727	732	rBV	2999892	3781711	100.00%	11.296%
4	6.492	744	749	752	rBV	3783172	3618095	95.67%	10.807%
5	6.722	784	788	791	rBV	1047442	914468	24.18%	2.731%
6	6.875	810	814	817	rBV	2995815	2758072	72.93%	8.238%
7	7.286	879	884	887	rBV	2164285	2271457	60.06%	6.785%
8	8.004	1001	1006	1009	rBV	1330416	1199742	31.72%	3.584%
9	8.557	1097	1100	1104	rBV	187013	161272	4.26%	0.482%
10	9.080	1183	1189	1192	rBV	4186953	3772450	99.76%	11.268%
11	9.474	1252	1256	1259	rBV	482502	413914	10.95%	1.236%
12	9.757	1299	1304	1307	rBV	1278086	1167660	30.88%	3.488%
13	10.469	1420	1425	1428	rBV	632850	491686	13.00%	1.469%
14	10.545	1433	1438	1441	rBV	1998834	1809800	47.86%	5.406%
15	11.239	1552	1556	1558	rBV	1082875	969552	25.64%	2.896%
16	11.257	1558	1559	1563	rVB	169695	133680	3.53%	0.399%
17	12.445	1758	1761	1765	rBV	229478	189790	5.02%	0.567%
18	12.674	1793	1800	1803	rBV	207509	202540	5.36%	0.605%
19	12.827	1821	1826	1829	rVB	2563386	2576591	68.13%	7.696%
20	13.298	1902	1906	1909	rBV	159904	140437	3.71%	0.419%
21	13.715	1974	1977	1985	rVB	440212	415037	10.97%	1.240%
22	13.874	1997	2004	2006	rBV	940637	1027318	27.17%	3.069%
23	13.898	2006	2008	2010	rVB	112321	86557	2.29%	0.259%
24	14.039	2030	2032	2036	rBV2	47076	48604	1.29%	0.145%
25	14.351	2081	2085	2088	rBV4	53446	71932	1.90%	0.215%
26	14.886	2173	2176	2179	rBV	113479	147317	3.90%	0.440%
27	14.962	2186	2189	2191	rBV	58099	59549	1.57%	0.178%
28	15.174	2223	2225	2232	rVB	67436	77009	2.04%	0.230%
29	15.233	2232	2235	2240	rVB	67290	80571	2.13%	0.241%
30	15.298	2241	2246	2249	rBV	509601	664688	17.58%	1.985%
31	15.733	2316	2320	2324	rVB	79633	103387	2.73%	0.309%
32	16.203	2396	2400	2404	rBV2	67459	96538	2.55%	0.288%
33	16.674	2476	2480	2486	rBV3	29265	70814	1.87%	0.212%
34	16.756	2491	2494	2501	rVB2	58685	107329	2.84%	0.321%

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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
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Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

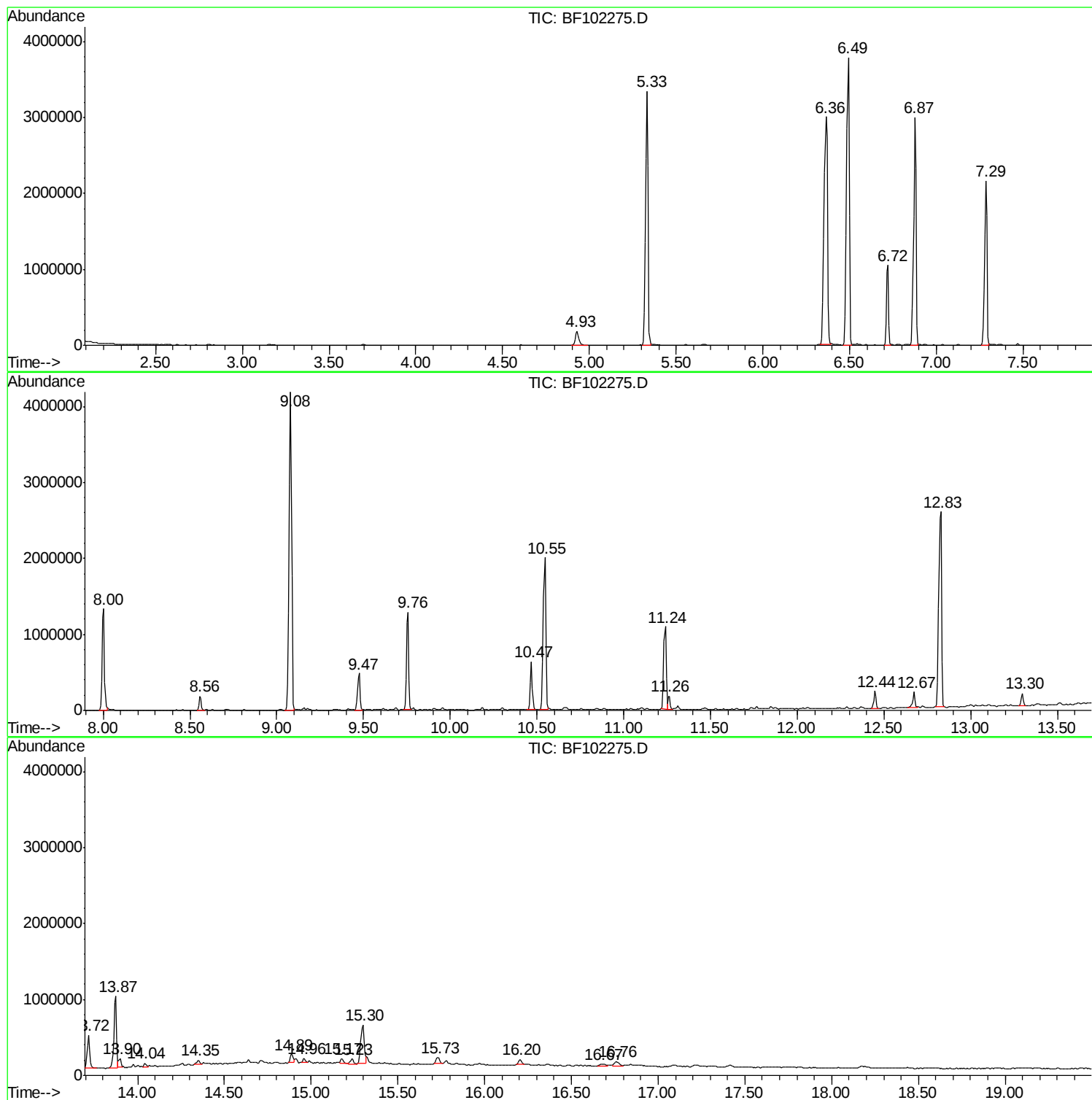
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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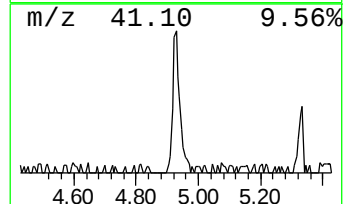
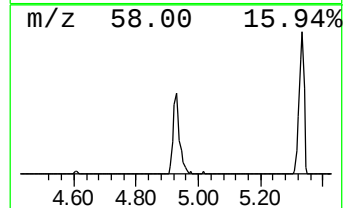
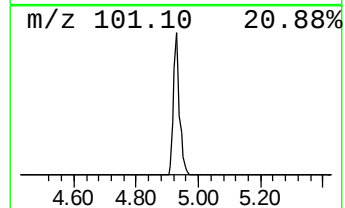
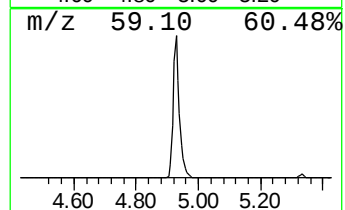
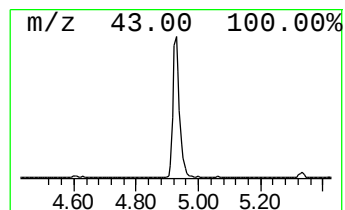
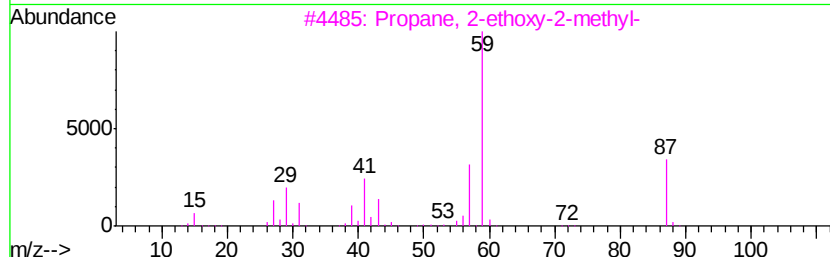
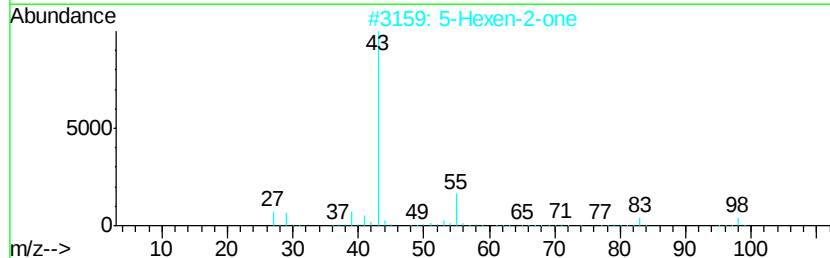
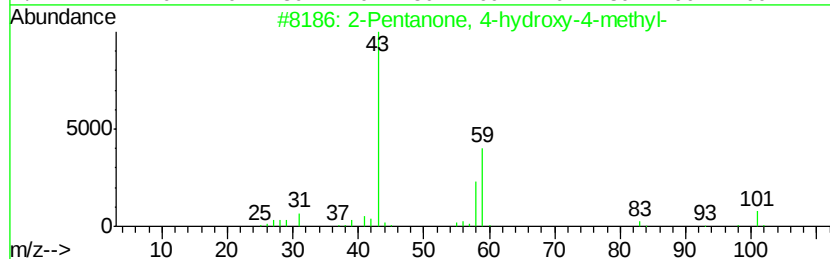
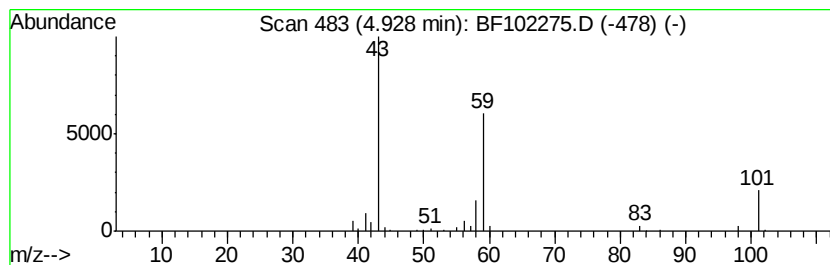
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	5.80 ng	265403	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	40		
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9		
3	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	9		
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9		
5	Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	9		



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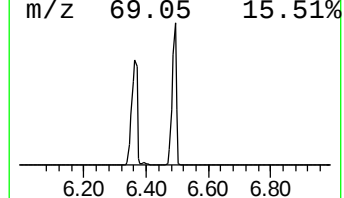
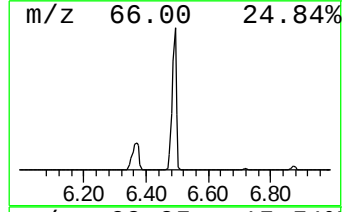
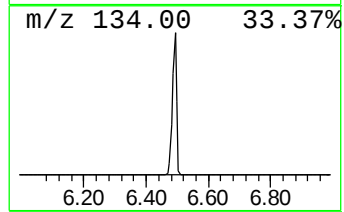
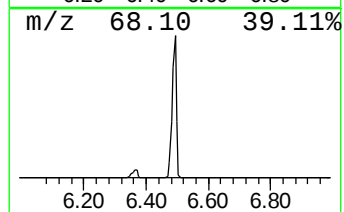
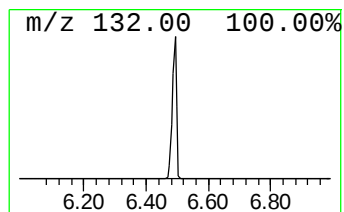
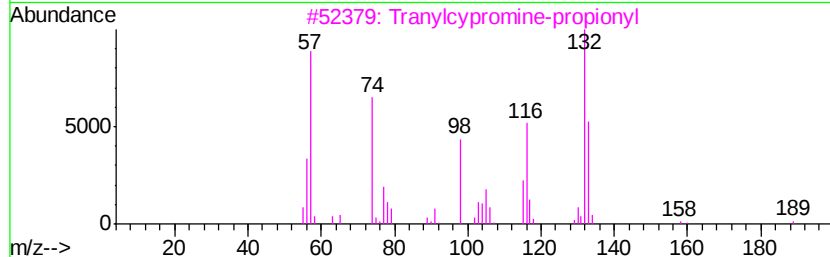
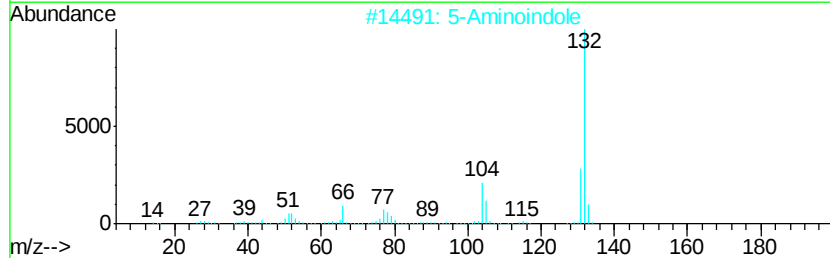
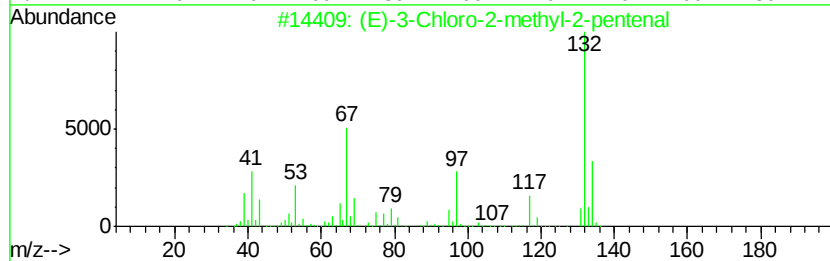
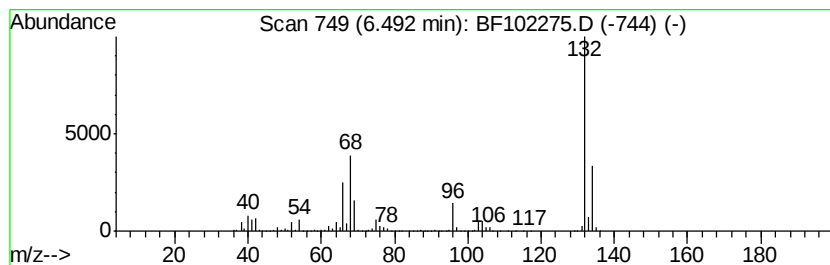
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	79.13 ng	3618100	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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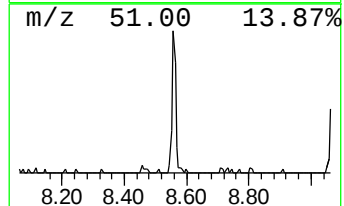
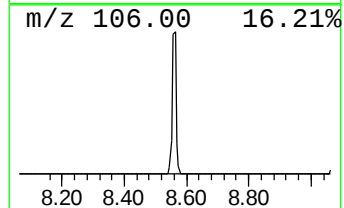
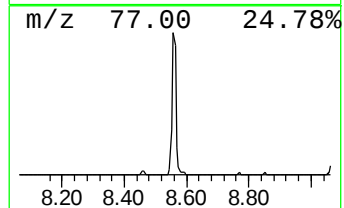
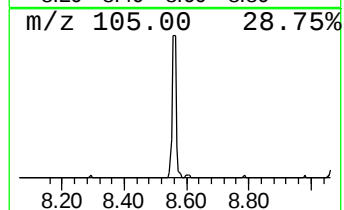
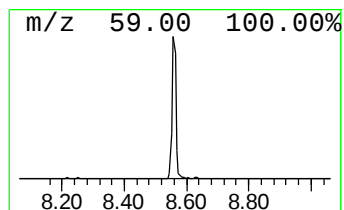
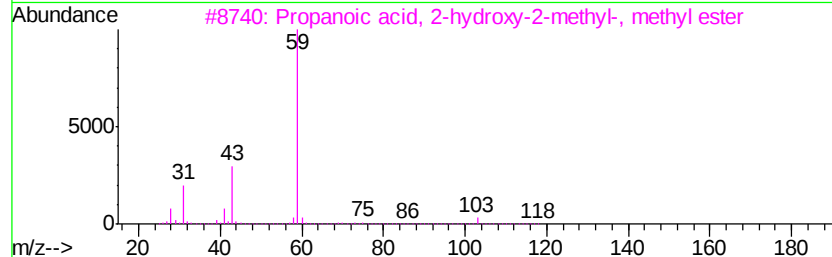
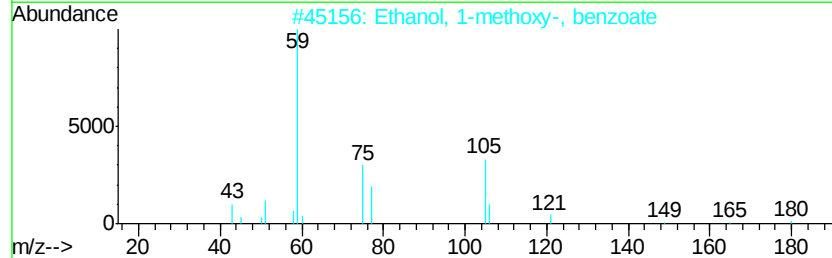
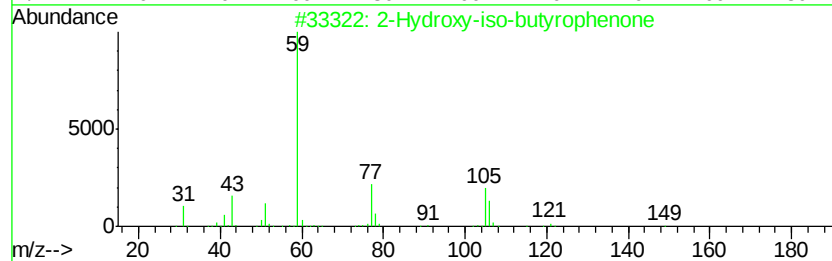
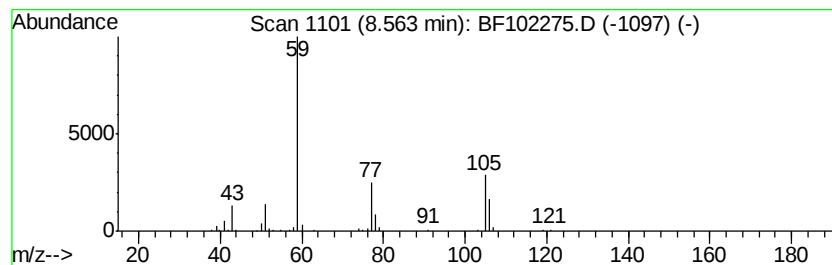
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.56	2.69 ng	161272	Napthalene-d8	8.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2		Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	72
3		Propanoic acid, 2-hydroxy-2-methyl-, methyl ester	118	C5H10O3	002110-78-3	9
4		Ethanone, 2-amino-1-phenyl-	135	C8H9NO	000613-89-8	9
5		Guanidine	59	CH5N3	000113-00-8	7



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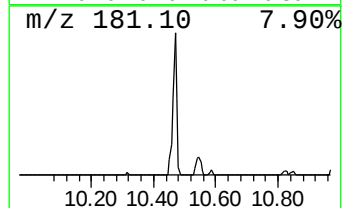
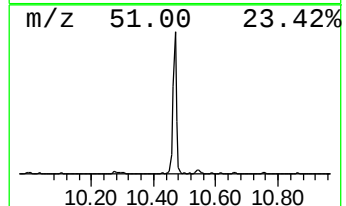
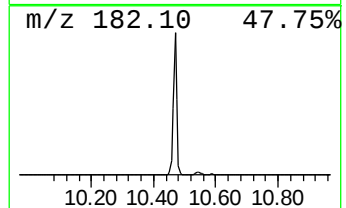
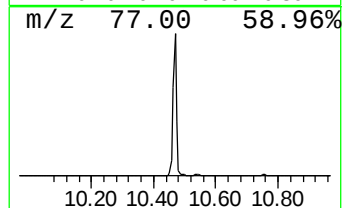
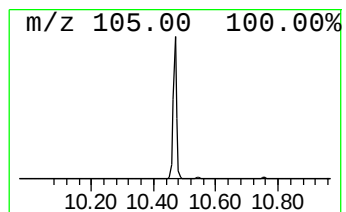
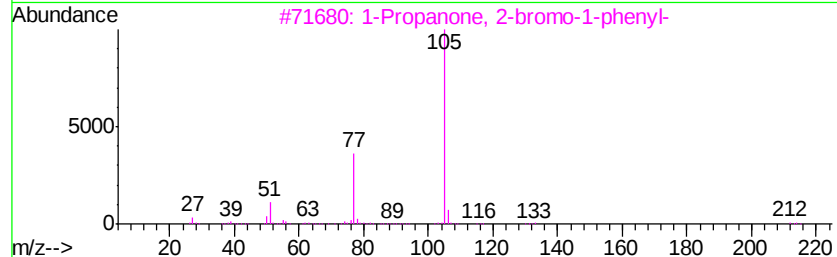
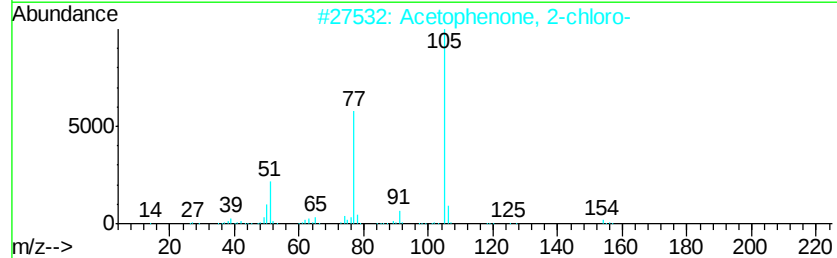
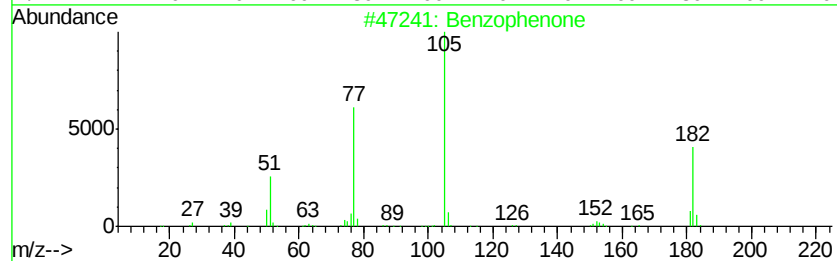
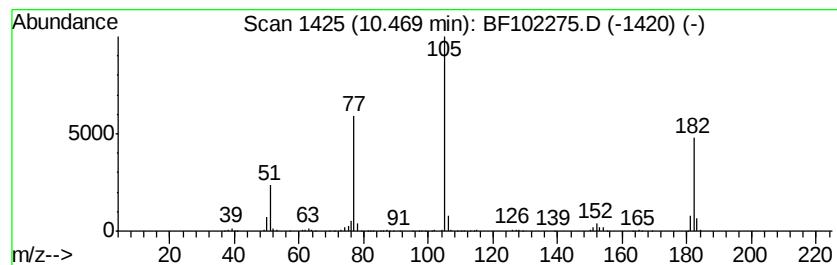
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.47	8.42 ng	491686	Acenaphthene-d10	9.76

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzophenone	182	C13H10O	000119-61-9	97
2		Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3		1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4		Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47
5		1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47



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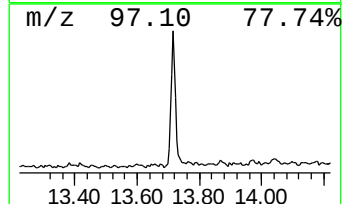
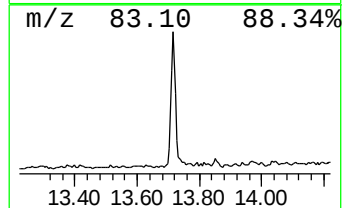
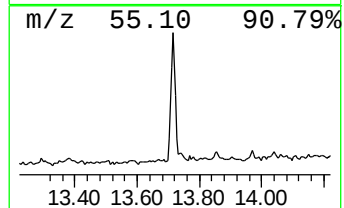
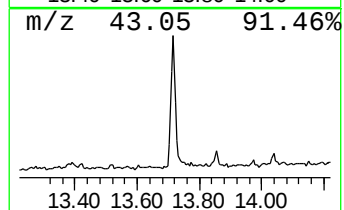
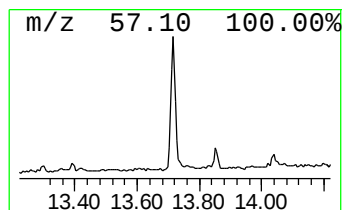
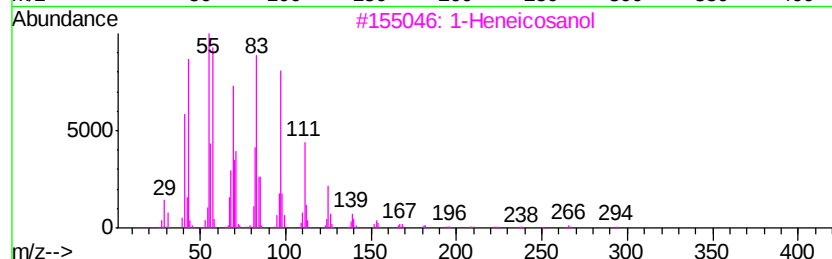
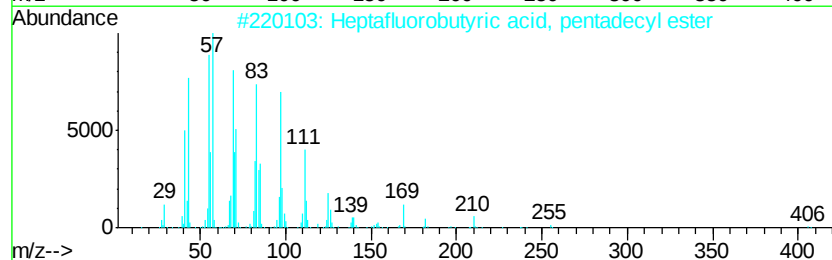
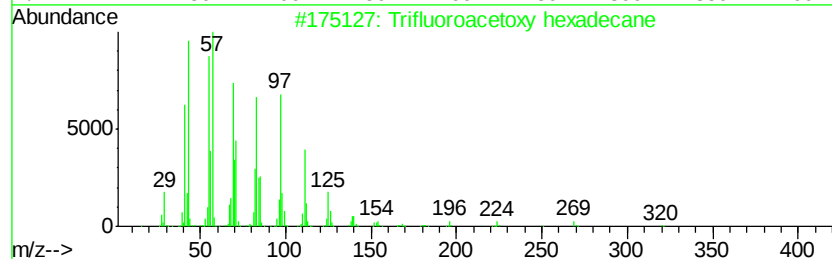
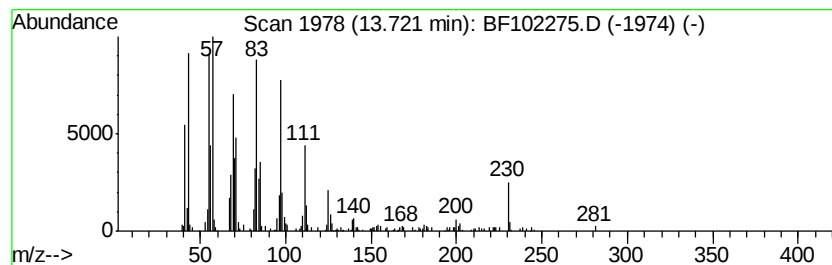
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	8.08 ng	415037	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3		1-Heneicosanol	312	C21H44O	015594-90-8	93
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5		n-Nonadecanol-1	284	C19H40O	001454-84-8	90



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ClientSampleId :
RT-2898

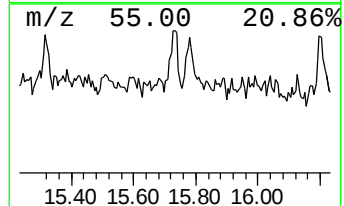
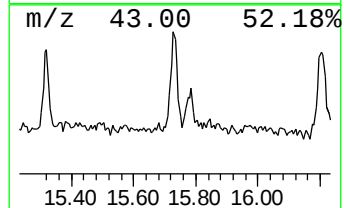
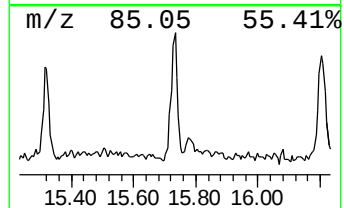
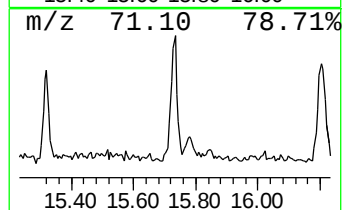
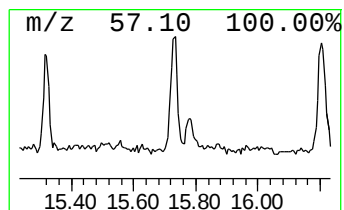
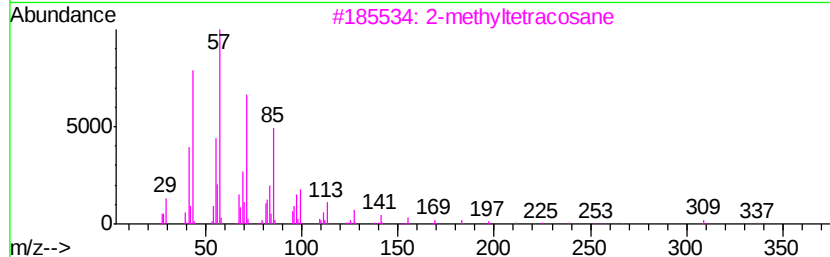
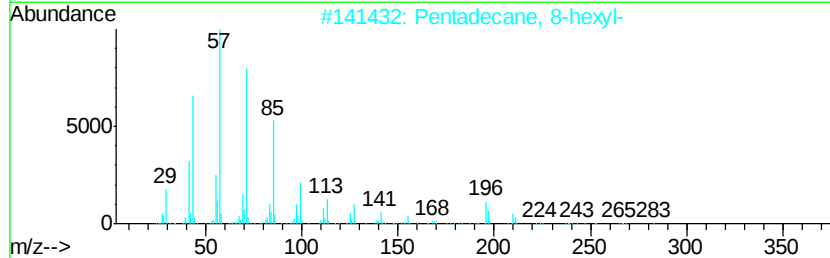
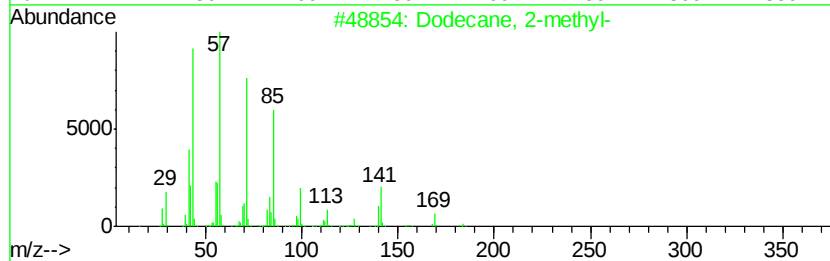
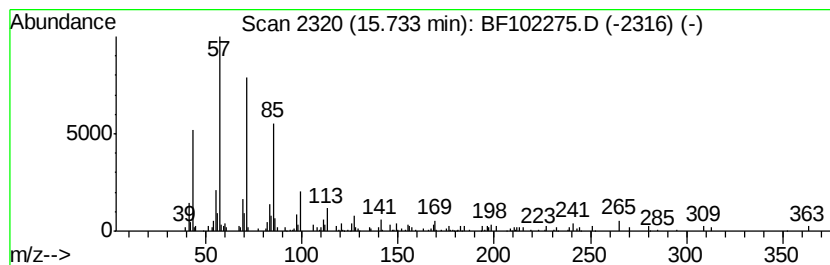
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Dodecane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.73	3.11 ng	103387	Perylene-d12	15.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	90
2		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	86
3		2-methyltetracosane	352	C25H52	1000376-72-6	86
4		triacontane	422	C30H62	000638-68-6	86
5		Tetracosane	338	C24H50	000646-31-1	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012018\
Data File : BF102275.D
Acq On : 20 Jan 2018 19:29
Operator : SJ/JU
Sample : J1210-10
Misc :
ALS Vial : 25 Sample Multiplier: 1

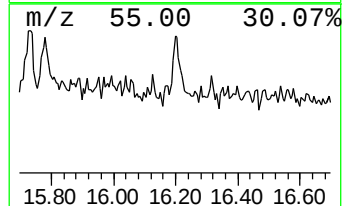
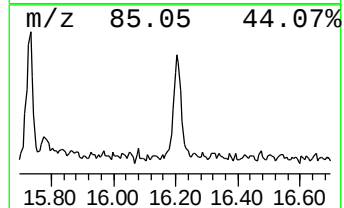
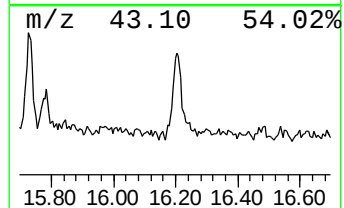
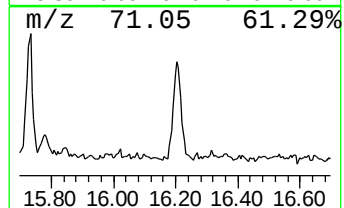
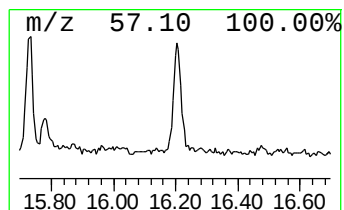
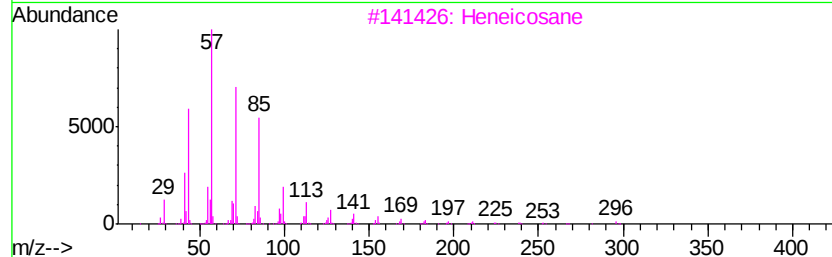
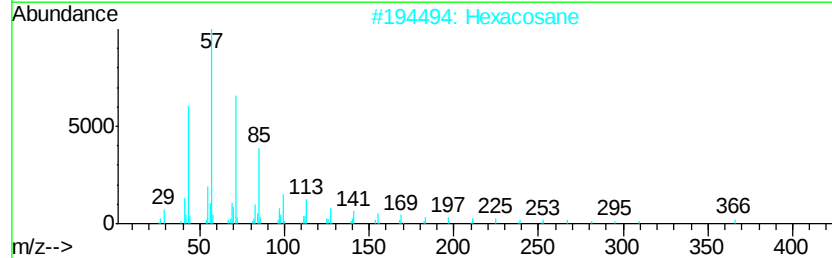
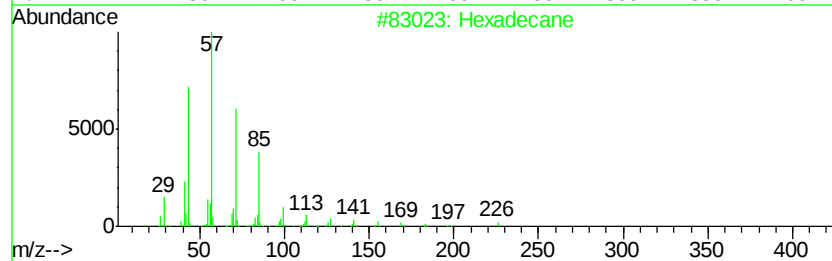
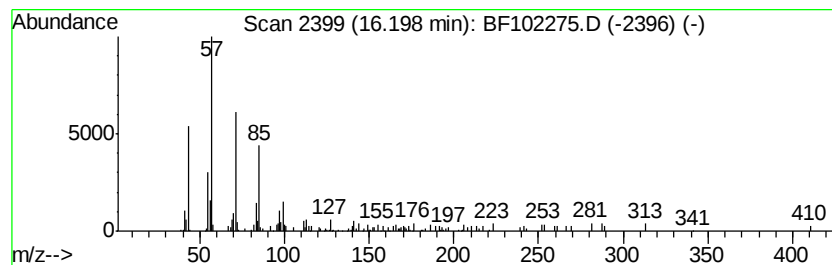
Instrument :
BNA_F
ClientSampleId :
RT-2898

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
16.20	2.90 ng	96538	Perylene-d12		15.30
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	93
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	87
4	Heptadecane	240	C17H36	000629-78-7	87
5	Octacosane	394	C28H58	000630-02-4	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012018\
Data File : BF102275.D
Acq On : 20 Jan 2018 19:29
Operator : SJ/JU
Sample : J1210-10
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-2898

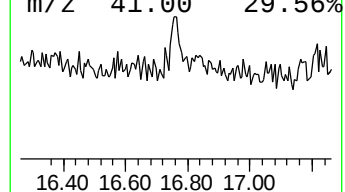
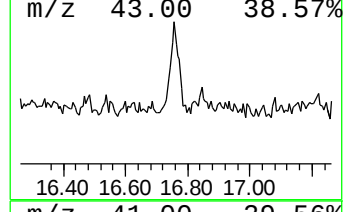
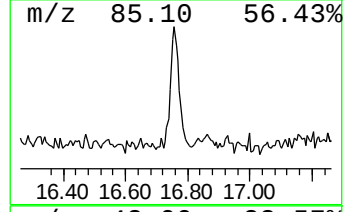
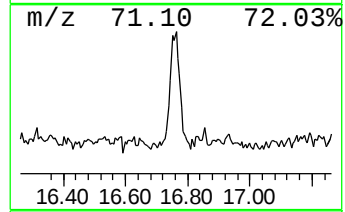
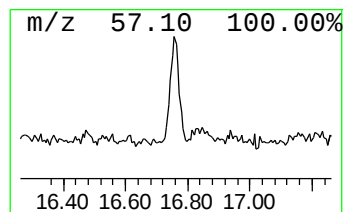
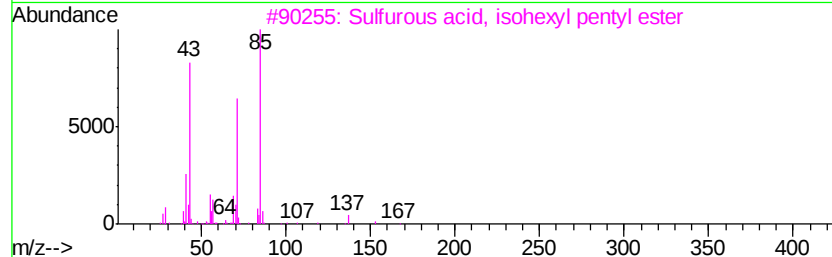
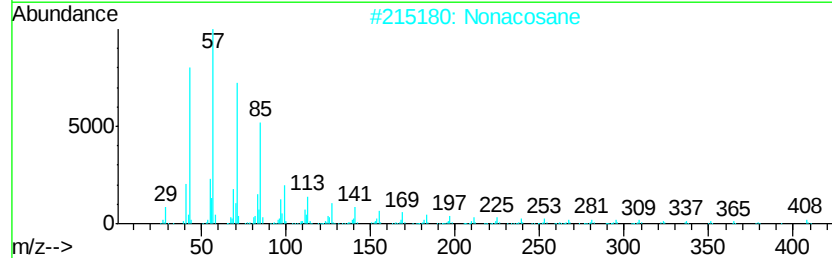
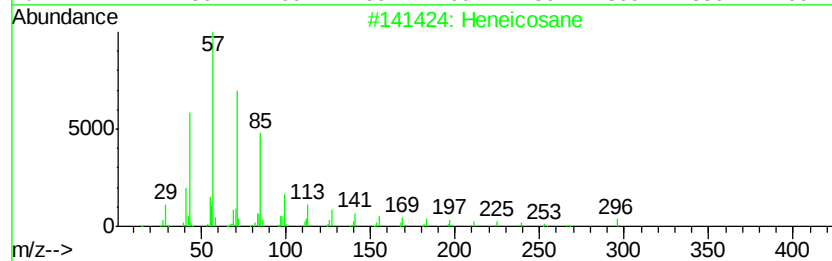
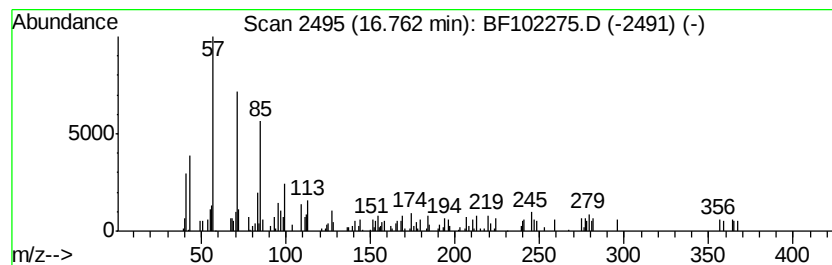
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.76	3.23 ng	107329	Perylene-d12	15.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	76
2		Nonacosane	408	C29H60	000630-03-5	59
3		Sulfurous acid, isohexyl pentyl ...	236	C11H24O3S	1000309-14-0	47
4		Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	47
5		6-Ethoxy-9-thia-bicyclo[3.3.1]no...	184	C10H16OS	1000187-29-2	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012018\
Data File : BF102275.D
Acq On : 20 Jan 2018 19:29
Operator : SJ/JU
Sample : J1210-10
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-2898

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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...	4.93	5.8	ng	265403	1	6.72	914468	20.0
unknown6.49	6.49	79.1	ng	3618100	1	6.72	914468	20.0
2-Hydroxy-iso-but...	8.56	2.7	ng	161272	2	8.00	1199740	20.0
Benzophenone	10.47	8.4	ng	491686	3	9.76	1167660	20.0
Trifluoroacetoxy ...	13.72	8.1	ng	415037	5	13.87	1027320	20.0
Dodecane, 2-methyl-	15.73	3.1	ng	103387	6	15.30	664688	20.0
Hexadecane	16.20	2.9	ng	96538	6	15.30	664688	20.0
Heneicosane	16.76	3.2	ng	107329	6	15.30	664688	20.0