

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
 Data File : BF102248.D
 Acq On : 20 Jan 2018 5:33
 Operator : SJ/JU
 Sample : J1113-13
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-17-3.5-4.0

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:\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	4.922	477	482	491	rVB	161248	236798	7.17%	0.824%
2	5.334	547	552	555	rBV	3220399	3220501	97.48%	11.206%
3	6.363	721	727	730	rBV	2984152	3186659	96.45%	11.089%
4	6.492	744	749	752	rBV	3373930	3229243	97.74%	11.237%
5	6.716	784	787	791	rBV	952992	797728	24.15%	2.776%
6	6.875	810	814	817	rBV	2990938	2517454	76.20%	8.760%
7	7.286	878	884	887	rBV	2149774	2037933	61.68%	7.091%
8	7.469	911	915	921	rVB	44513	36867	1.12%	0.128%
9	7.998	1001	1005	1009	rBV	1153541	1042197	31.55%	3.627%
10	9.080	1183	1189	1192	rBV	3633823	3303842	100.00%	11.496%
11	9.475	1251	1256	1258	rBV	267186	233805	7.08%	0.814%
12	9.686	1288	1292	1295	rBV	159094	115561	3.50%	0.402%
13	9.751	1299	1303	1307	rVB	1090974	1015404	30.73%	3.533%
14	10.186	1373	1377	1380	rVB	169376	140036	4.24%	0.487%
15	10.404	1408	1414	1416	rBV	42908	54162	1.64%	0.188%
16	10.539	1431	1437	1441	rBV	1690827	1660448	50.26%	5.778%
17	10.657	1454	1457	1465	rVB	144487	141928	4.30%	0.494%
18	11.104	1530	1533	1536	rBV	70663	57916	1.75%	0.202%
19	11.233	1552	1555	1559	rBV	924873	846084	25.61%	2.944%
20	12.645	1791	1795	1798	rBV	294282	223970	6.78%	0.779%
21	12.721	1805	1808	1811	rVB	94132	75086	2.27%	0.261%
22	12.821	1821	1825	1828	rBV	2291805	2129279	64.45%	7.409%
23	13.304	1902	1907	1911	rBV2	31788	37232	1.13%	0.130%
24	13.351	1911	1915	1918	rBV	158192	134481	4.07%	0.468%
25	13.715	1973	1977	1982	rBV	235158	232980	7.05%	0.811%
26	13.874	1999	2004	2007	rBV	730482	717086	21.70%	2.495%
27	14.039	2029	2032	2038	rBV	49304	44547	1.35%	0.155%
28	14.345	2080	2084	2090	rBV2	65298	82659	2.50%	0.288%
29	14.639	2129	2134	2139	rBV3	45516	62012	1.88%	0.216%
30	14.962	2185	2189	2192	rBV	40591	43336	1.31%	0.151%
31	15.292	2240	2245	2249	rBV	629907	762734	23.09%	2.654%
32	15.727	2316	2319	2324	rBV	43039	47043	1.42%	0.164%
33	15.774	2324	2327	2333	rVB8	25322	40474	1.23%	0.141%
34	16.204	2396	2400	2404	rBV	33138	46125	1.40%	0.160%

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Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-17-3.5-4.0

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

35	16.756	2490	2494	2500	rVB4	25053	42179	1.28%	0.147%
36	16.821	2503	2505	2515	rVB10	21102	44341	1.34%	0.154%
37	17.203	2566	2570	2580	rVB9	44750	98221	2.97%	0.342%

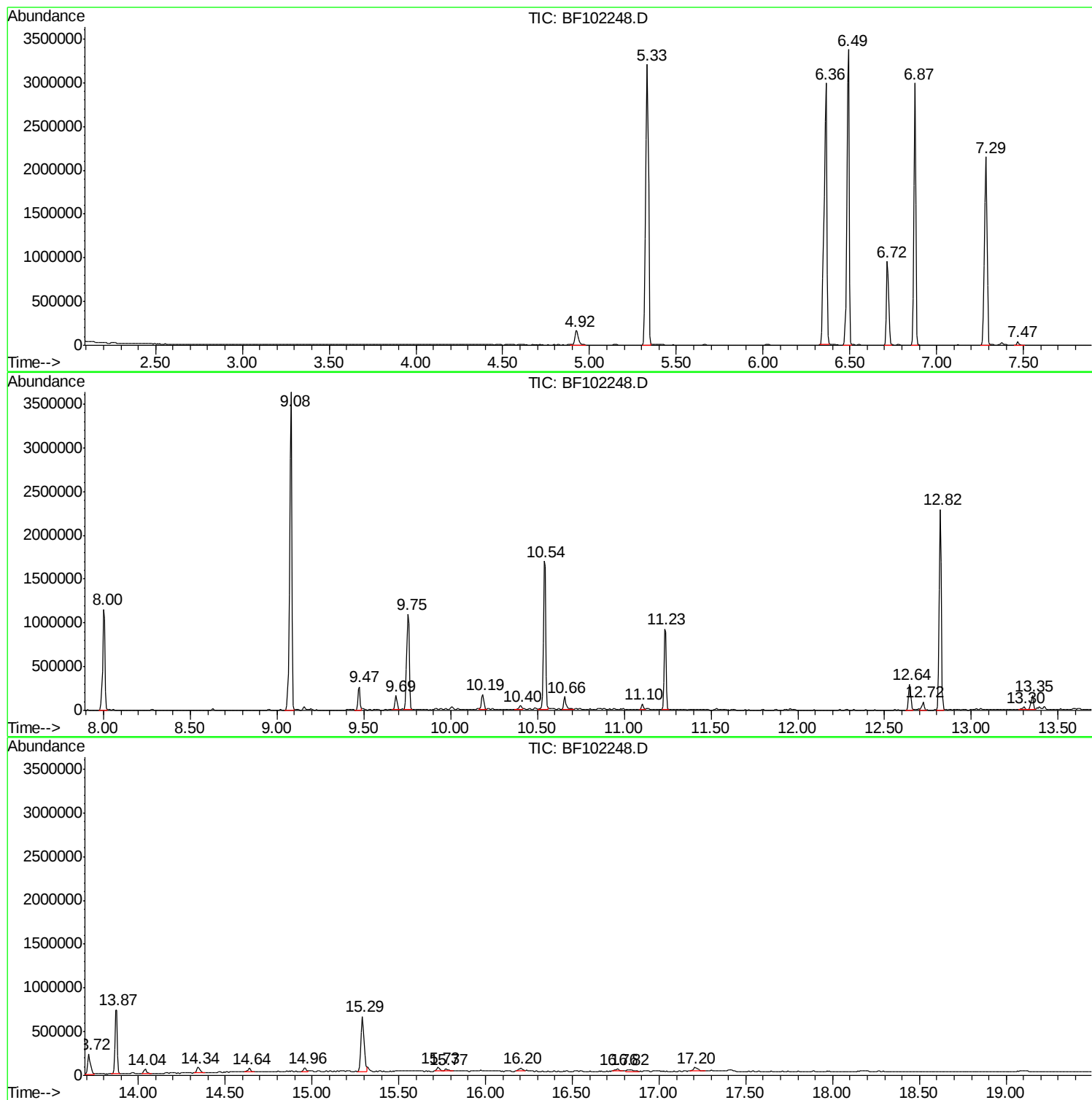
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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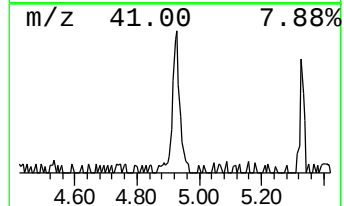
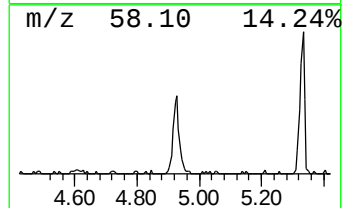
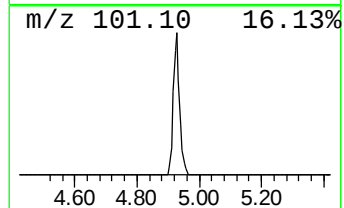
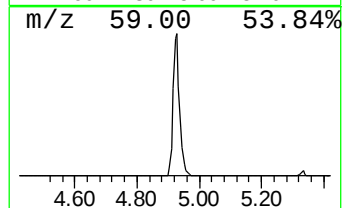
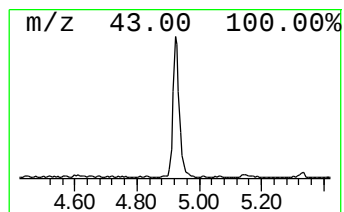
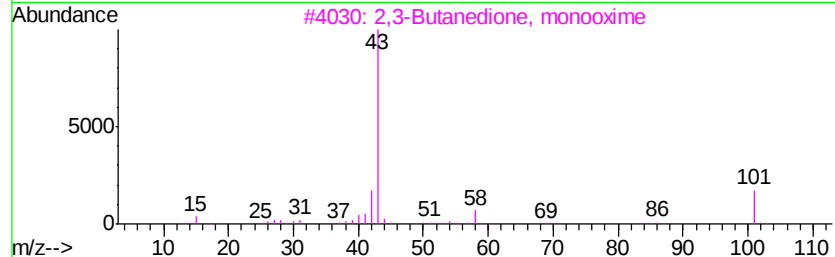
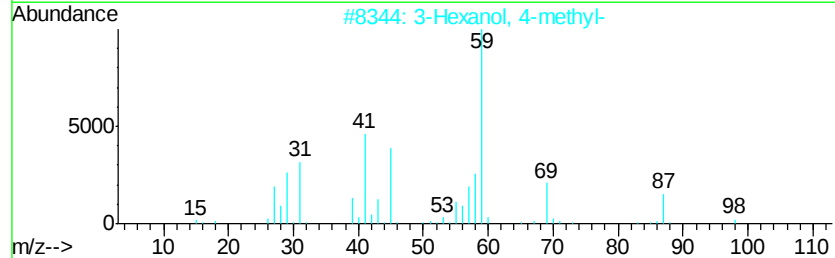
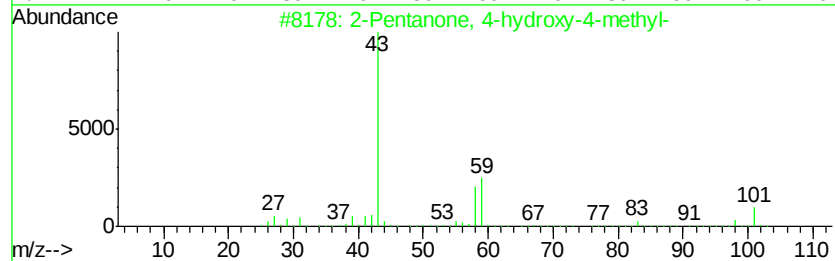
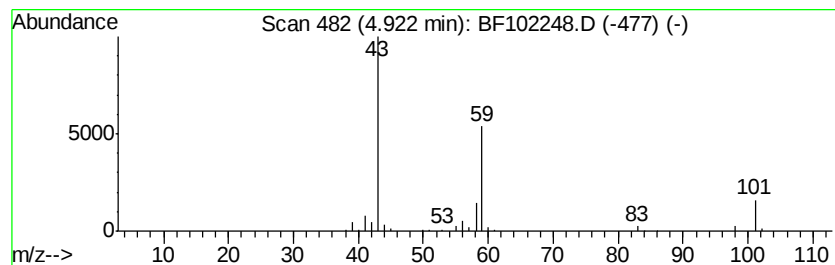
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	5.94 ng	236798	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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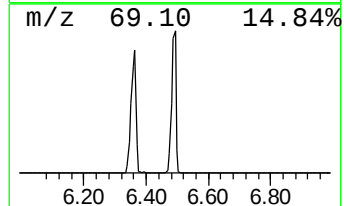
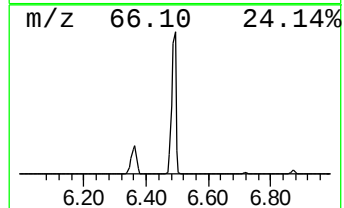
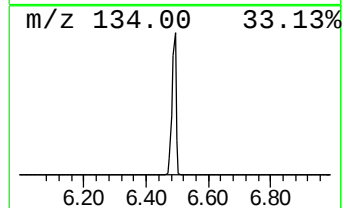
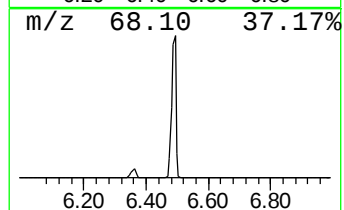
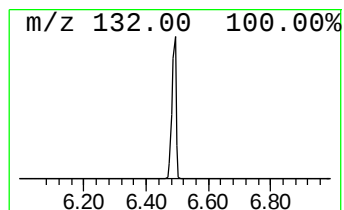
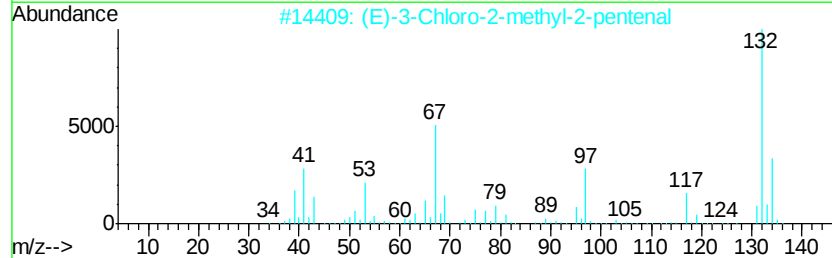
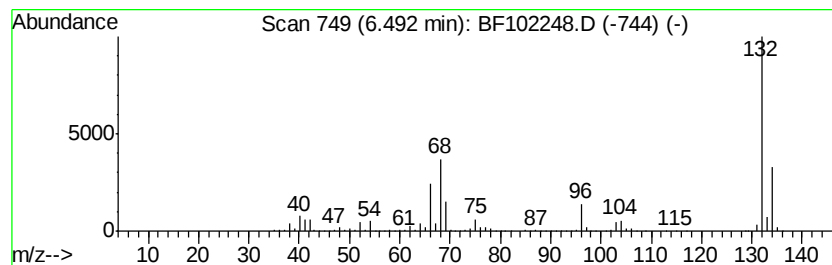
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	80.96 ng	3229240	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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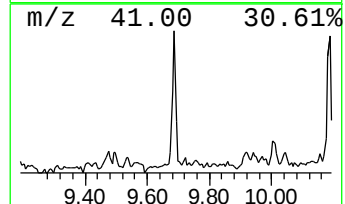
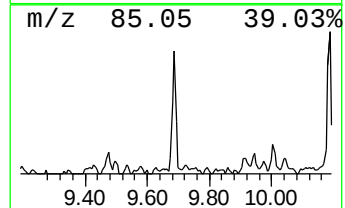
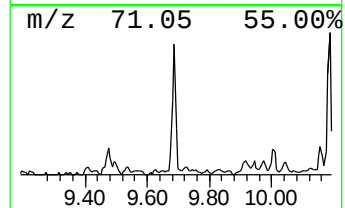
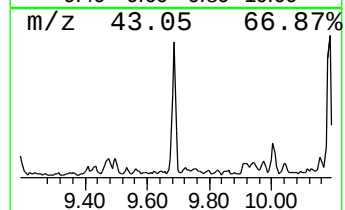
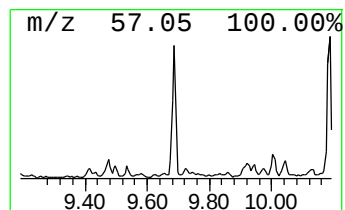
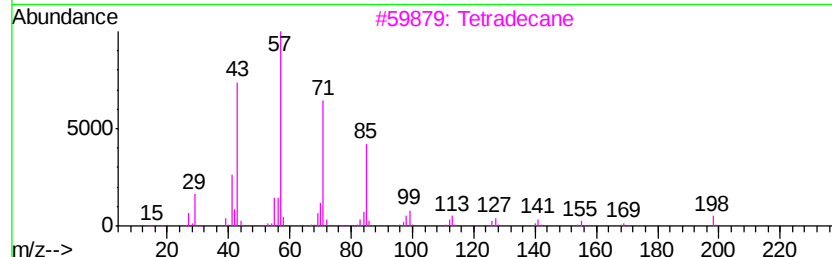
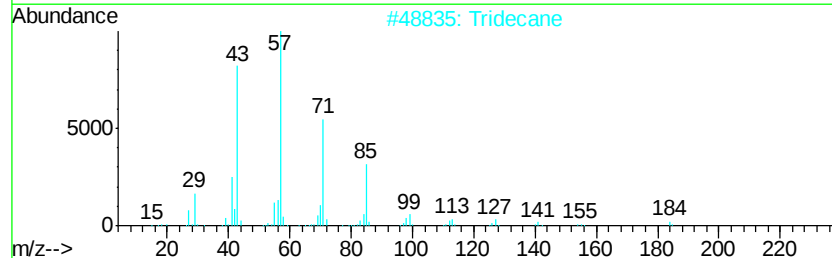
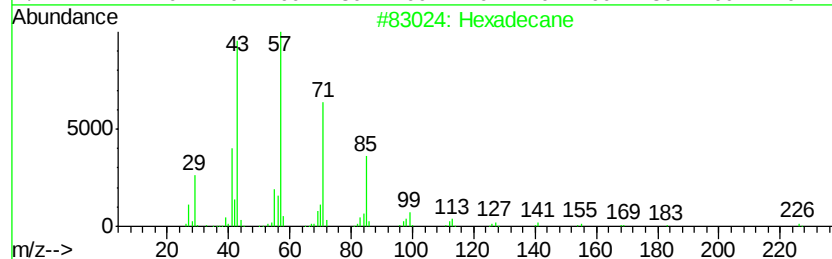
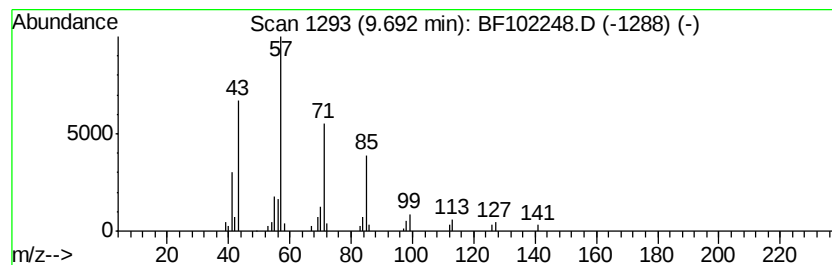
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.69	2.28 ng	115561	Acenaphthene-d10	9.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	91
2		Tridecane	184	C13H28	000629-50-5	86
3		Tetradecane	198	C14H30	000629-59-4	86
4		Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	72
5		Undecane	156	C11H24	001120-21-4	64



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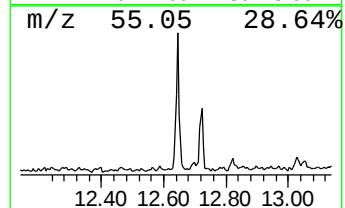
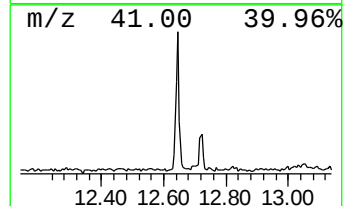
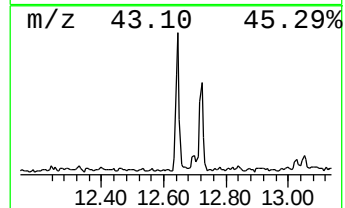
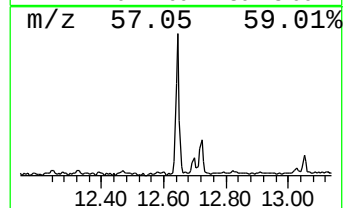
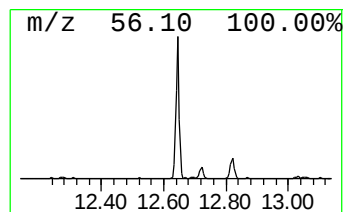
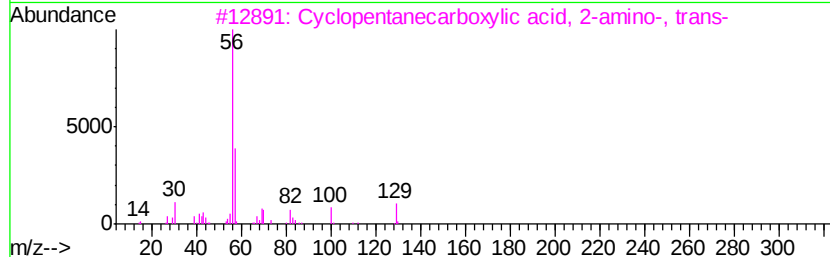
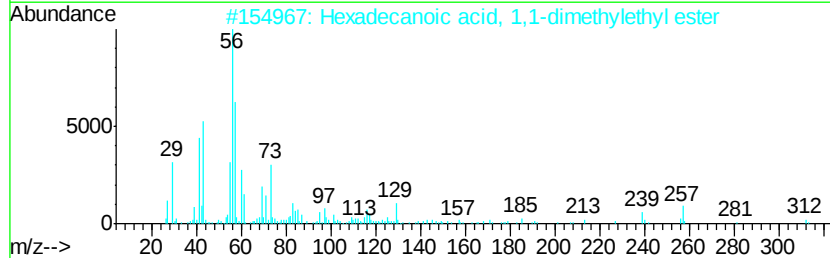
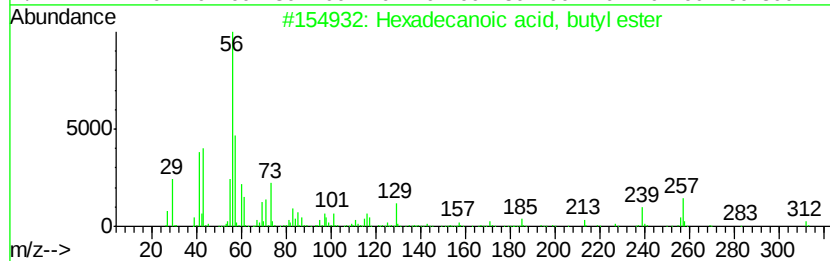
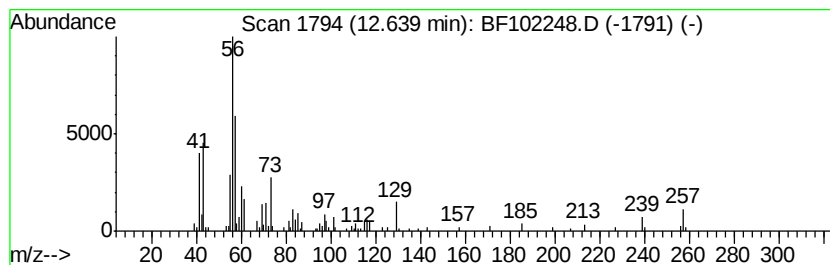
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	6.25 ng	223970	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	92
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	43
3		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	38
4		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5		Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	32



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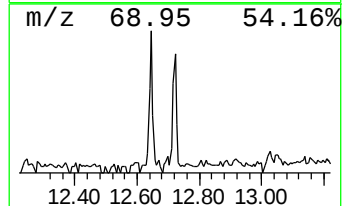
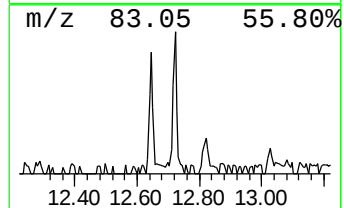
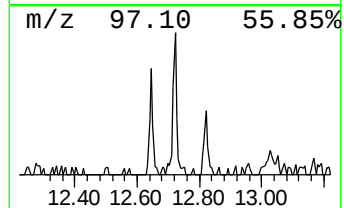
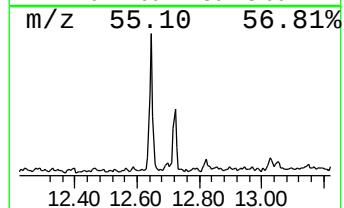
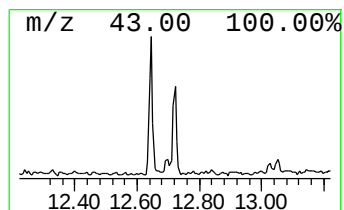
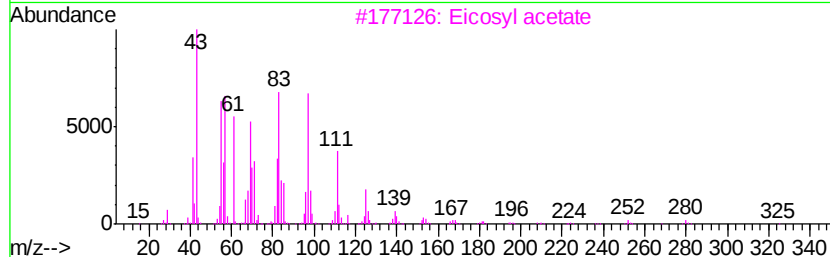
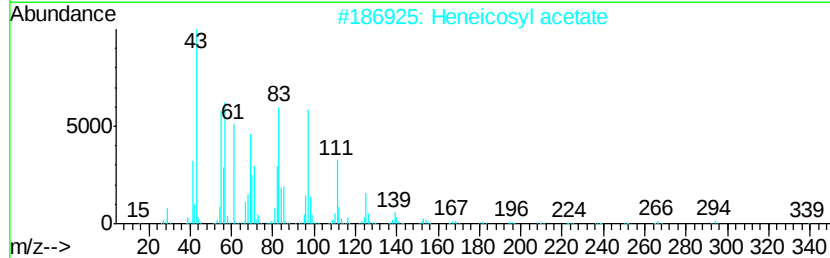
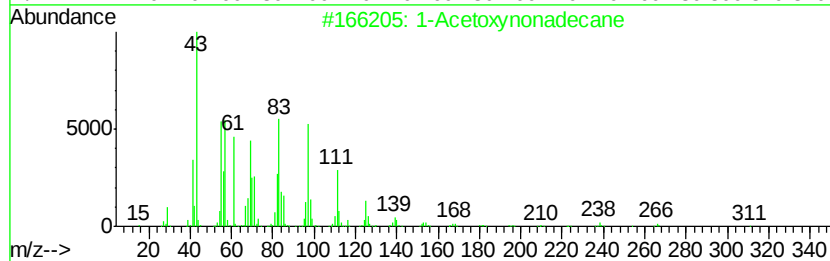
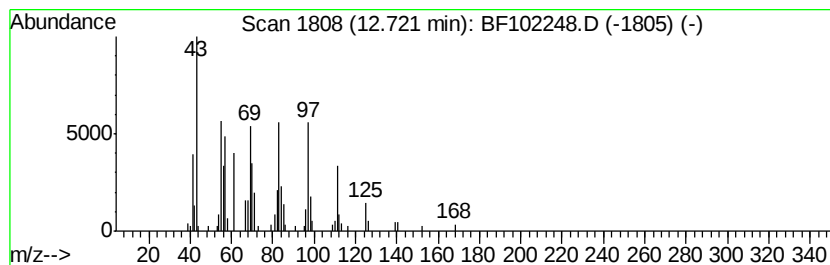
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 1-Acetoxy-nonadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	2.09 ng	75086	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Acetoxy-nonadecane	326	C21H42O2	001577-43-1	91
2		Heneicosyl acetate	354	C23H46O2	1000351-77-3	91
3		Eicosyl acetate	340	C22H44O2	1000351-77-9	91
4		Heptadecyl acetate	298	C19H38O2	000822-20-8	91
5		1-Docosanol, acetate	368	C24H48O2	000822-26-4	83



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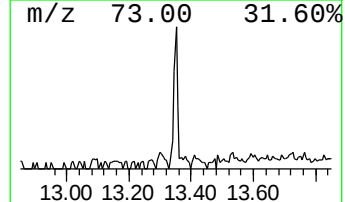
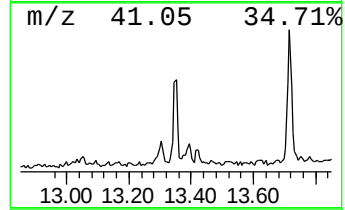
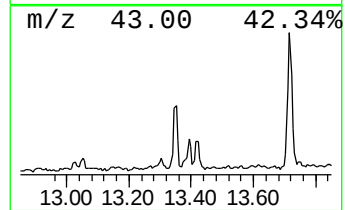
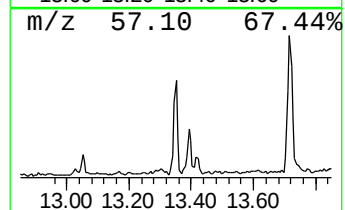
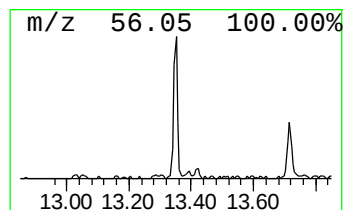
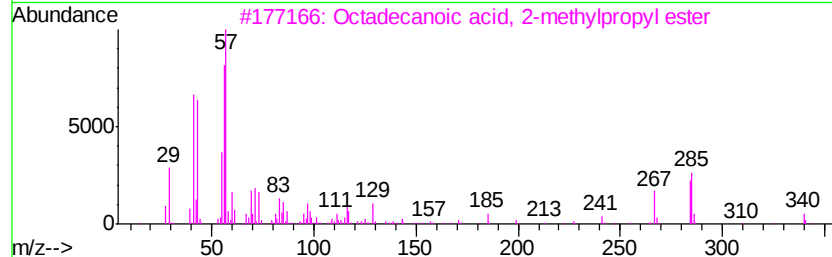
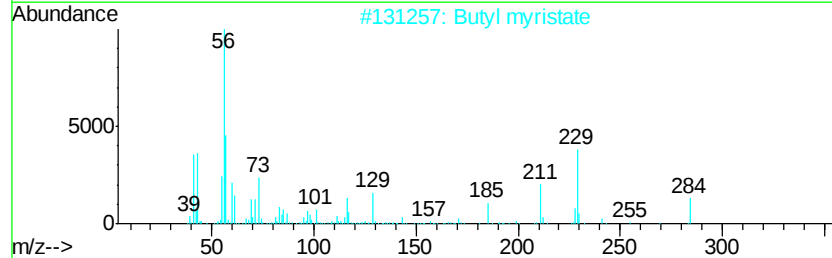
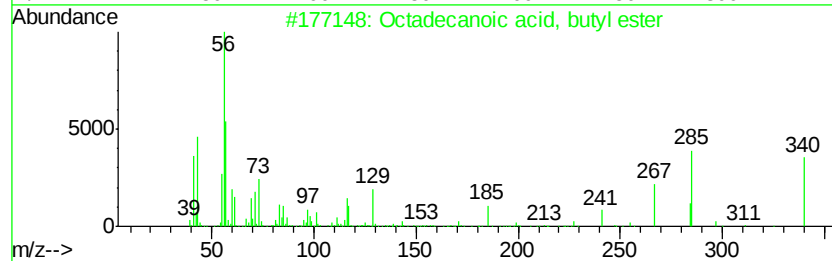
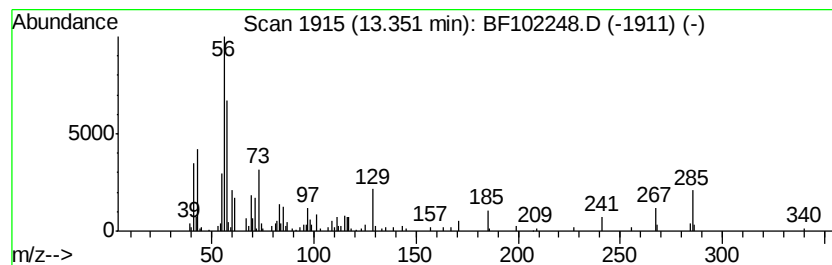
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	3.75 ng	134481	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2		Butyl myristate	284	C18H36O2	000110-36-1	64
3		Octadecanoic acid, 2-methylpropyl ester	340	C22H44O2	000646-13-9	43
4		1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	37
5		Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102248.D
Acq On : 20 Jan 2018 5:33
Operator : SJ/JU
Sample : J1113-13
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-17-3.5-4.0

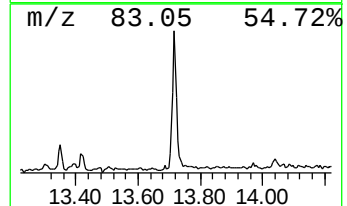
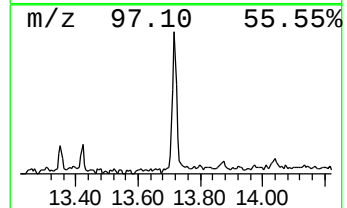
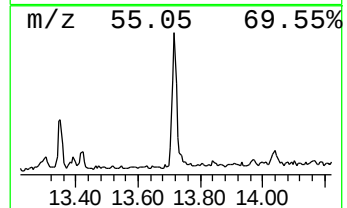
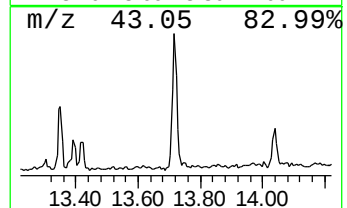
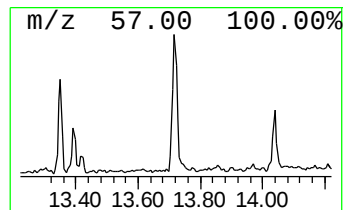
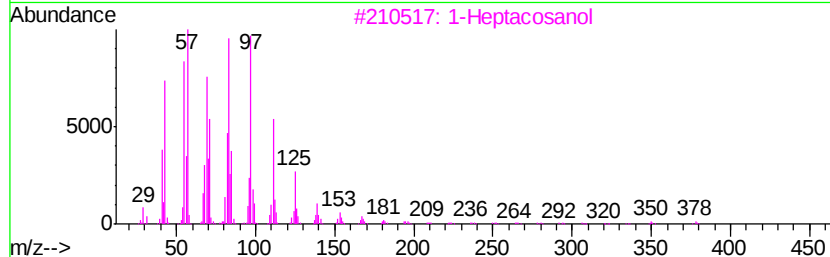
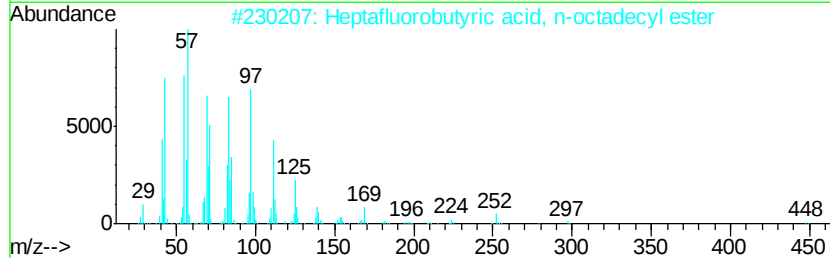
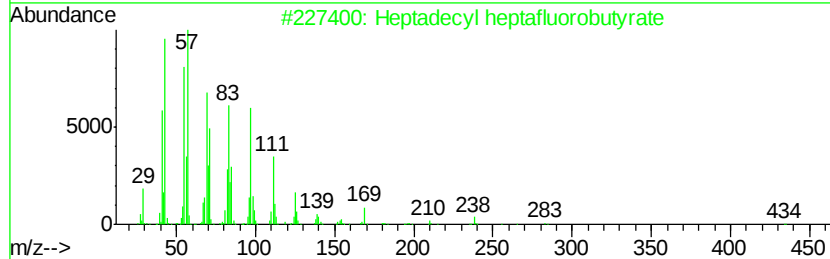
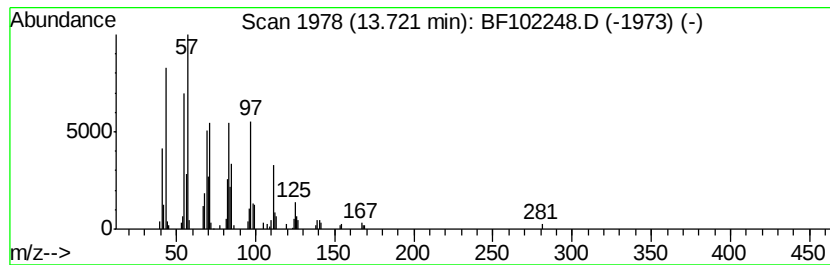
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	6.50 ng	232980	Chrysene-d12	13.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2			Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	91
3			1-Heptacosanol	396	C27H56O	002004-39-9	91
4			Pentafluoropropionic acid, octadecyl ester	416	C21H37F5O2	959261-25-7	91
5			Heptafluorobutyric acid, pentadecyl ester	424	C19H31F7O2	959261-23-5	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011918\
Data File : BF102248.D
Acq On : 20 Jan 2018 5:33
Operator : SJ/JU
Sample : J1113-13
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-17-3.5-4.0

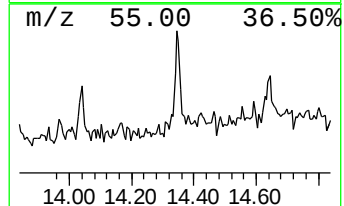
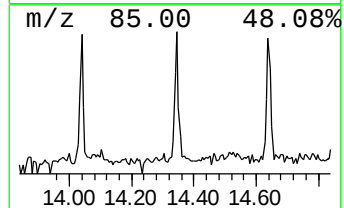
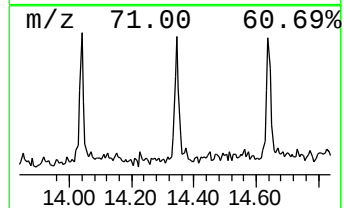
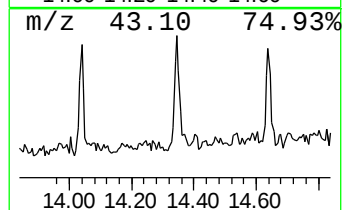
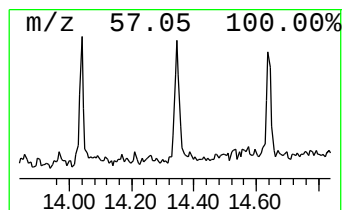
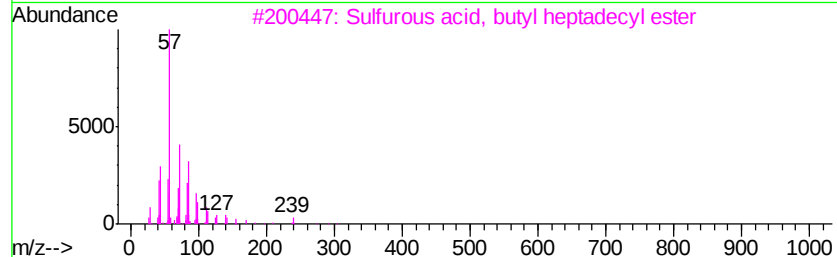
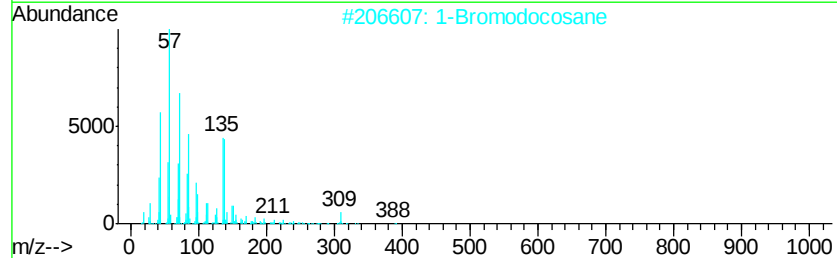
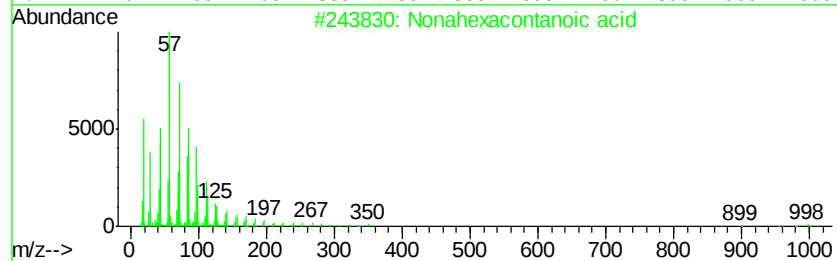
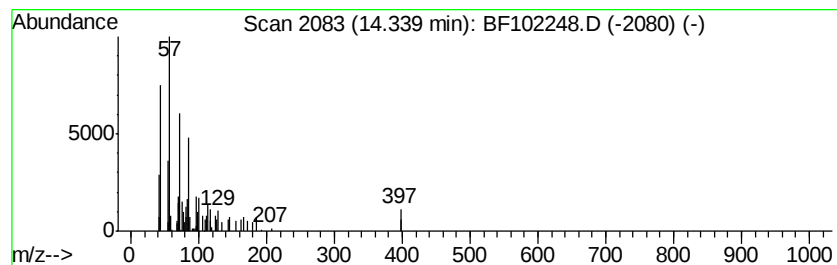
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Nonaheptacontanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	2.31 ng	82659	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonaheptacontanoic acid	999	C69H138O2	040710-32-5	90
2		1-Bromodocosane	388	C22H45Br	006938-66-5	87
3		Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	86
4		Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	86
5		Tetracosane	338	C24H50	000646-31-1	68



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011918\
Data File : BF102248.D
Acq On : 20 Jan 2018 5:33
Operator : SJ/JU
Sample : J1113-13
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-17-3.5-4.0

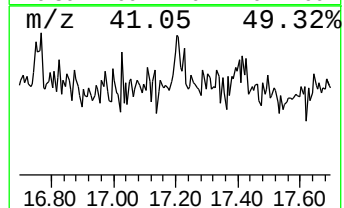
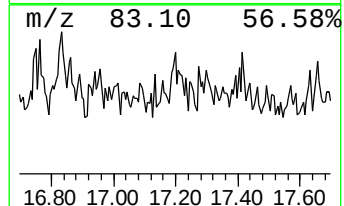
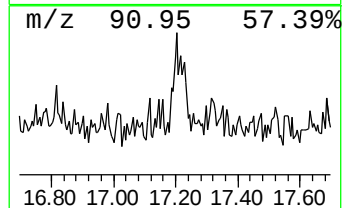
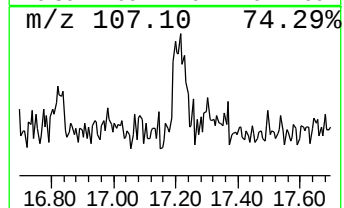
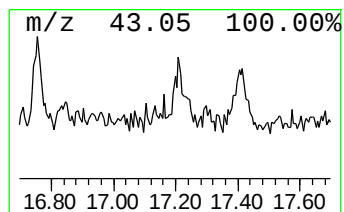
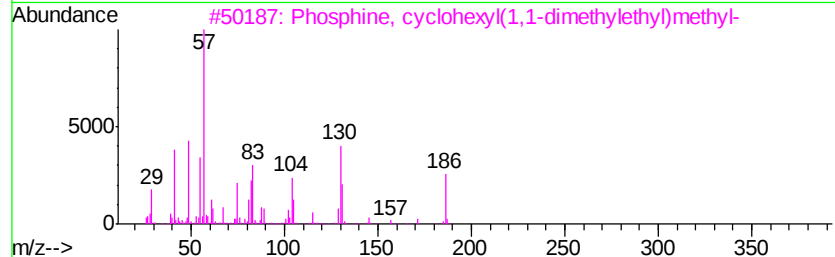
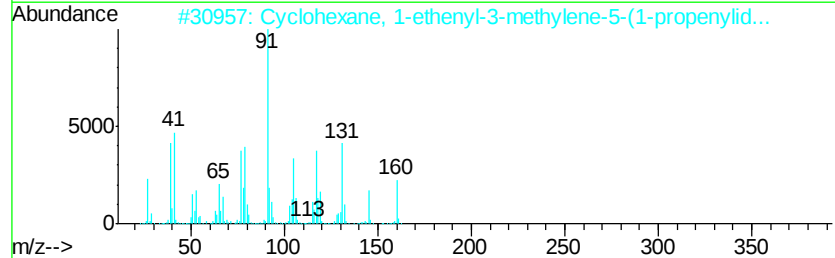
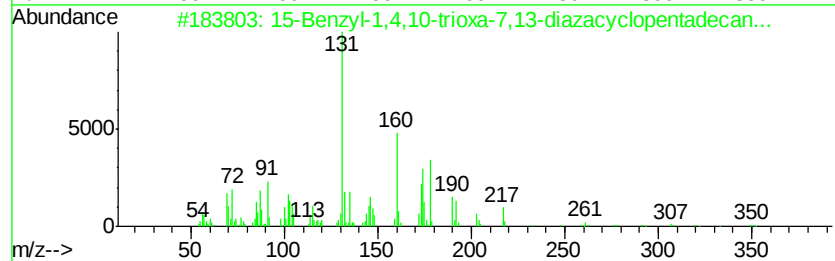
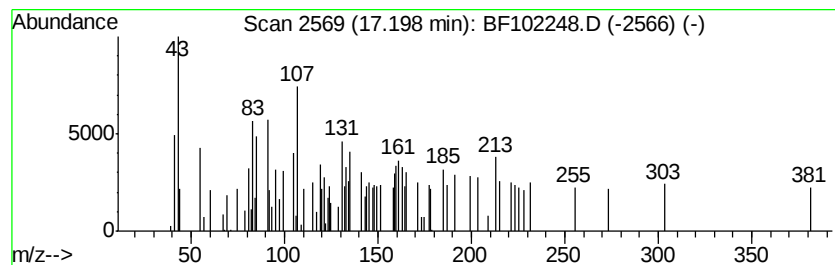
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown17.20 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.20	2.58 ng	98221	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	15-Benzyl-1,4,10-trioxa-7,13-dia...	350	C17H22N2O6	074229-37-1	14
2		Cyclohexane, 1-ethenyl-3-methyle...	160	C12H16	061142-28-7	11
3		Phosphine, cyclohexyl(1,1-dimeth...	186	C11H23P	074685-81-7	10
4		4-Methyl-2H-benzopyrane	146	C10H10O	021776-94-3	10
5		Propanedinitrile, (4-oxocyclohex...	160	C9H8N2O	083928-81-8	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011918\
Data File : BF102248.D
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Operator : SJ/JU
Sample : J1113-13
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-17-3.5-4.0

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...	4.92	5.9	ng	236798	1	6.72	797728	20.0
unknown6.49	6.49	81.0	ng	3229240	1	6.72	797728	20.0
Hexadecane	9.69	2.3	ng	115561	3	9.75	1015400	20.0
Hexadecanoic acid...	12.64	6.3	ng	223970	5	13.87	717086	20.0
1-Acetoxynonadecane	12.72	2.1	ng	75086	5	13.87	717086	20.0
Octadecanoic acid...	13.35	3.8	ng	134481	5	13.87	717086	20.0
Heptadecyl hepta...	13.72	6.5	ng	232980	5	13.87	717086	20.0
Nonahexacontanoic...	14.34	2.3	ng	82659	5	13.87	717086	20.0
unknown17.20	17.20	2.6	ng	98221	6	15.29	762734	20.0