

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082517\
 Data File : BF098033.D
 Acq On : 25 Aug 2017 16:32
 Operator : SJ/JU
 Sample : I4913-02
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TEC-BE2-3-12-COMP

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-BF081517.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	3.128	175	177	190	rBV	34648	71022	2.07%	0.207%
2	4.945	480	486	494	rVB	213764	318818	9.30%	0.928%
3	5.351	549	555	558	rBV	3020978	3315633	96.73%	9.656%
4	6.381	721	730	733	rBV	3056879	3427887	100.00%	9.983%
5	6.510	747	752	755	rBV	3208438	3271699	95.44%	9.528%
6	6.739	787	791	794	rBV	885373	743356	21.69%	2.165%
7	6.892	813	817	821	rBV	2499777	2463685	71.87%	7.175%
8	7.304	881	887	890	rBV	2100468	2116654	61.75%	6.164%
9	8.022	1004	1009	1012	rBV	1062954	950707	27.73%	2.769%
10	9.098	1186	1192	1195	rBV	3370450	3411787	99.53%	9.936%
11	9.492	1253	1259	1262	rBV	390714	325970	9.51%	0.949%
12	9.774	1301	1307	1310	rBV	995908	973631	28.40%	2.835%
13	9.980	1337	1342	1348	rBV	38379	41191	1.20%	0.120%
14	10.563	1435	1441	1444	rBV	1935096	1969890	57.47%	5.737%
15	10.680	1458	1461	1465	rBV	35669	41797	1.22%	0.122%
16	11.251	1554	1558	1562	rBV	1113316	980026	28.59%	2.854%
17	11.786	1644	1649	1652	rBV	78842	99092	2.89%	0.289%
18	11.874	1652	1664	1676	rVV3	272418	1152025	33.61%	3.355%
19	11.963	1676	1679	1687	rVB5	32479	51204	1.49%	0.149%
20	12.380	1742	1750	1758	rBV5	60986	169198	4.94%	0.493%
21	12.510	1768	1772	1782	rVB6	26674	65645	1.92%	0.191%
22	12.668	1796	1799	1800	rBV2	62473	61248	1.79%	0.178%
23	12.721	1800	1808	1819	rVB	909786	2404456	70.14%	7.002%
24	12.839	1823	1828	1832	rBV	2780664	2866699	83.63%	8.349%
25	13.321	1905	1910	1915	rVB	124087	123930	3.62%	0.361%
26	13.368	1915	1918	1920	rBV	42329	51021	1.49%	0.149%
27	13.398	1920	1923	1929	rVB3	73520	117920	3.44%	0.343%
28	13.645	1961	1965	1972	rVB6	25503	48221	1.41%	0.140%
29	13.739	1977	1981	1992	rVB	203945	281904	8.22%	0.821%
30	13.880	2001	2005	2009	rBV2	912186	996047	29.06%	2.901%
31	14.033	2027	2031	2040	rVB2	61347	116576	3.40%	0.339%
32	14.515	2111	2113	2116	rBV	42332	36196	1.06%	0.105%
33	14.562	2117	2121	2126	rVV2	43395	62014	1.81%	0.181%
34	14.792	2157	2160	2168	rBV7	32492	50629	1.48%	0.147%

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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

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35	14.868	2168	2173	2190	rVB7	139305	343513	10.02%	1.000%
36	15.086	2207	2210	2216	rVB3	31198	54814	1.60%	0.160%
37	15.298	2242	2246	2251	rBV	469412	548696	16.01%	1.598%
38	15.751	2320	2323	2328	rVB3	27028	40429	1.18%	0.118%
39	16.051	2371	2374	2383	rVB9	32639	73416	2.14%	0.214%
40	19.021	2873	2879	2890	rVB10	32224	99214	2.89%	0.289%

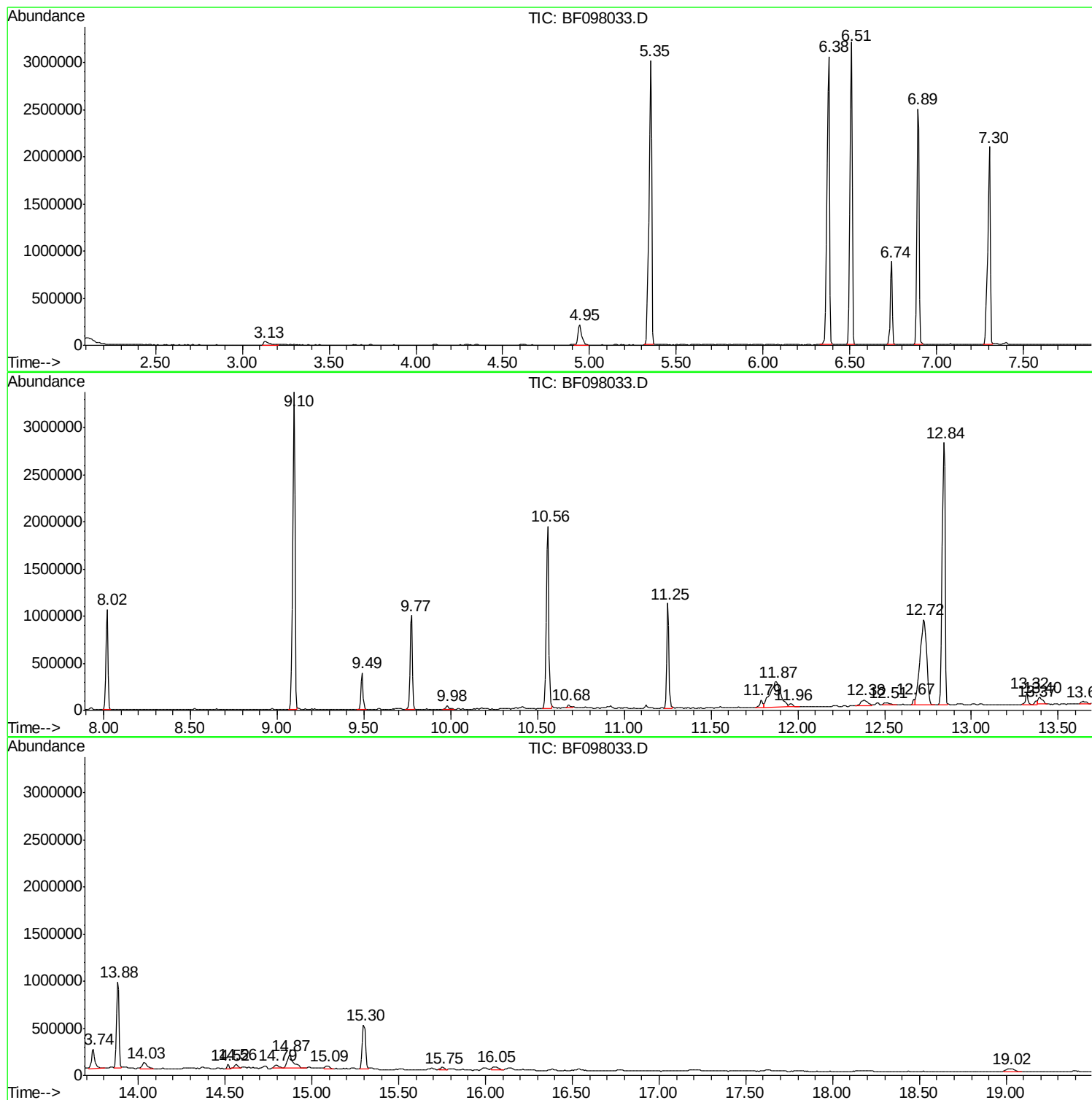
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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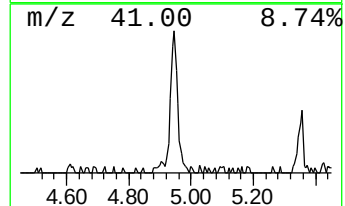
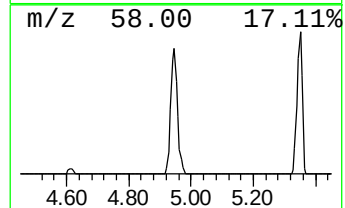
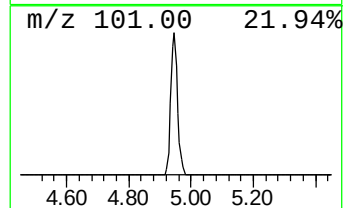
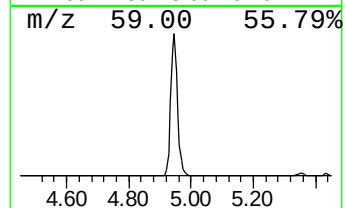
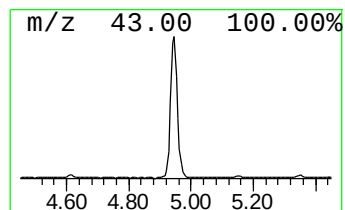
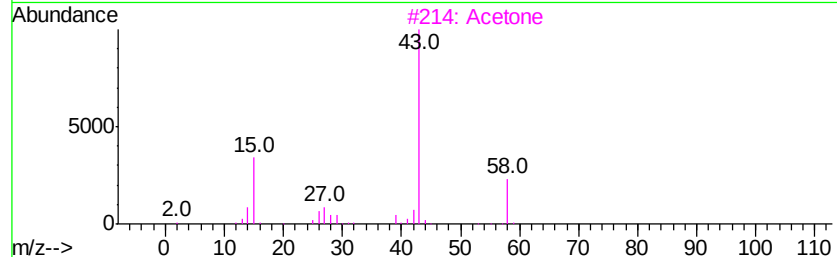
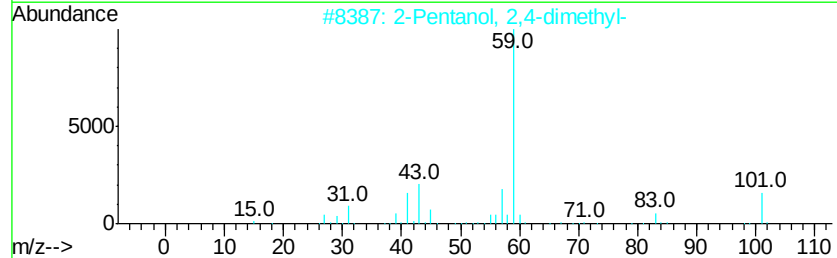
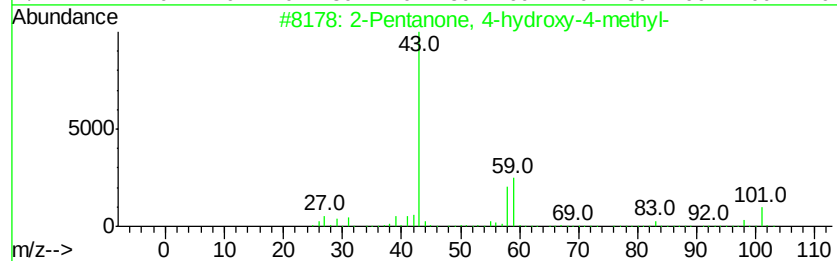
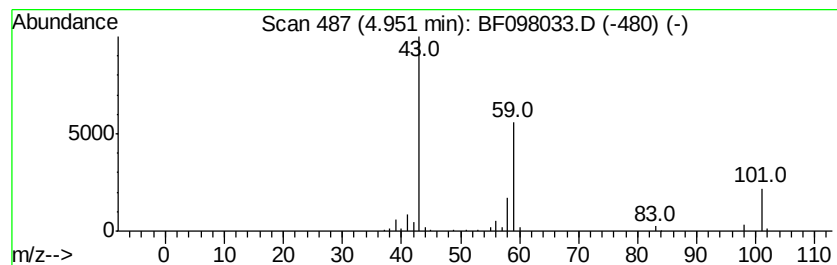
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.95	8.58 ng	318818	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	23
3		Acetone	58	C3H6O	000067-64-1	10
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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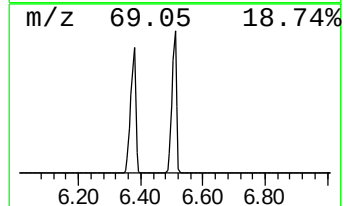
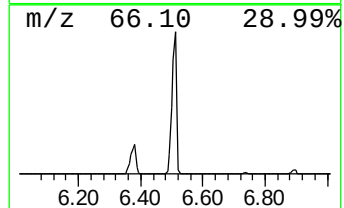
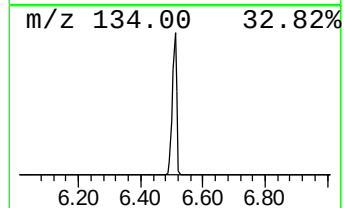
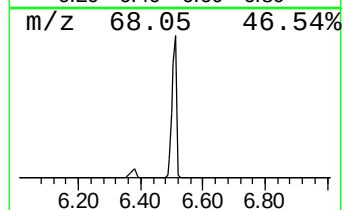
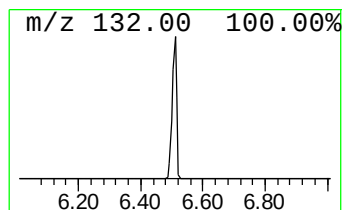
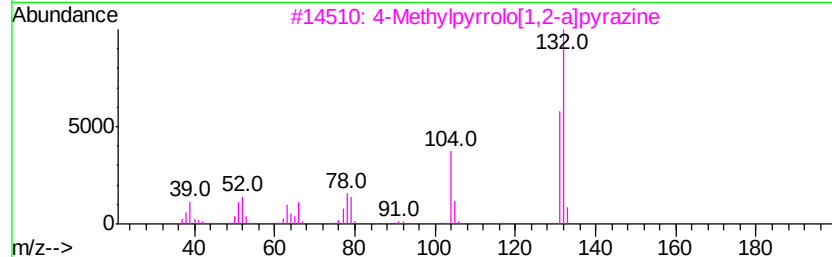
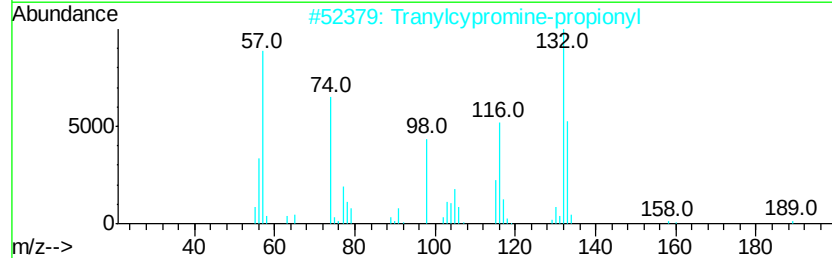
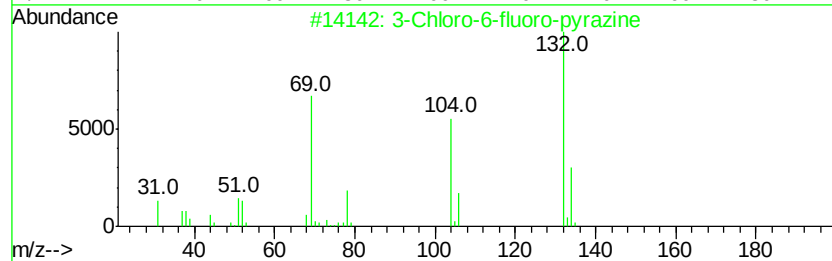
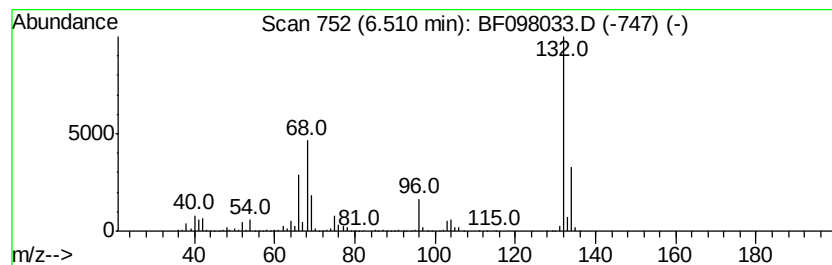
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	88.03 ng	3271700	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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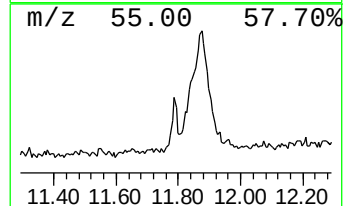
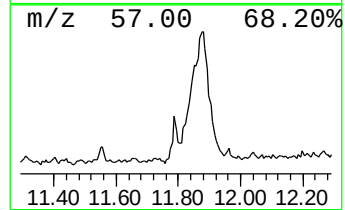
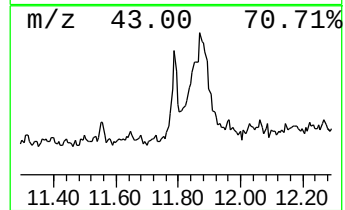
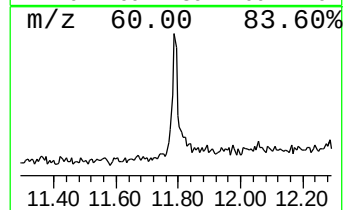
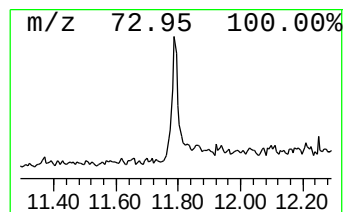
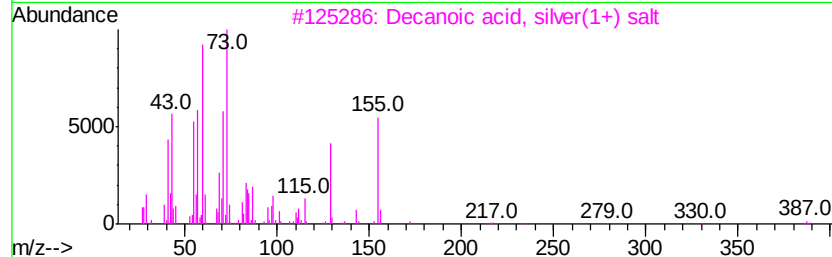
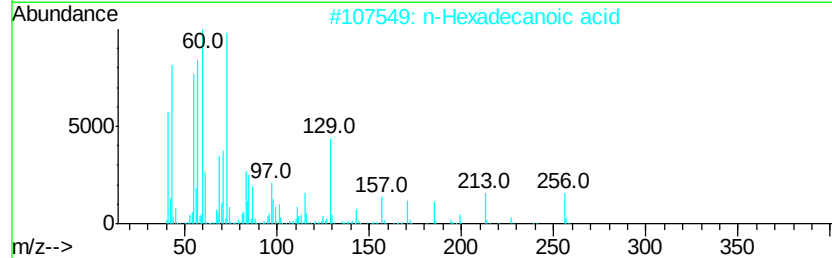
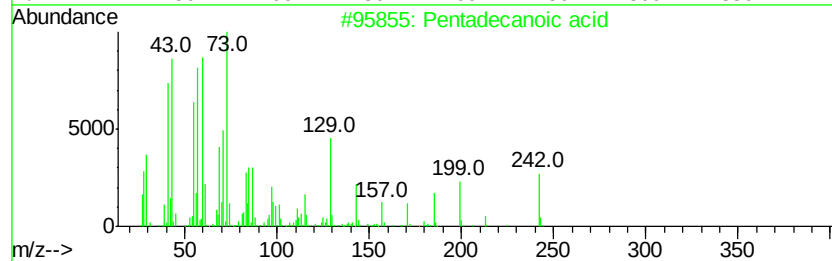
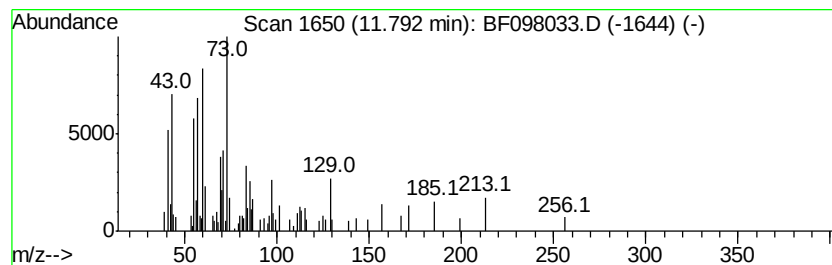
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Pentadecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	2.02 ng	99092	Phenanthrene-d10	11.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
3		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64
4		Dodecanoic acid	200	C12H24O2	000143-07-7	58
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	58



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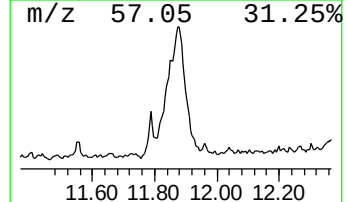
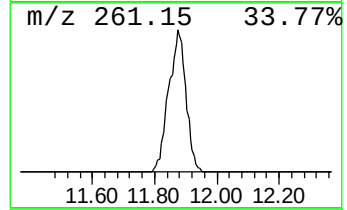
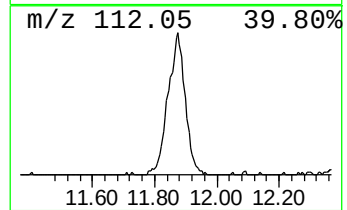
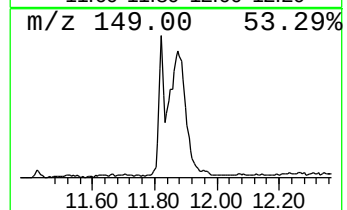
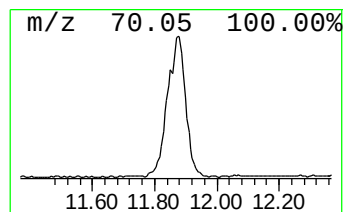
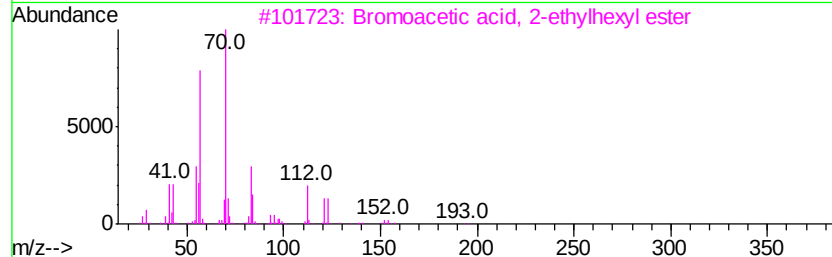
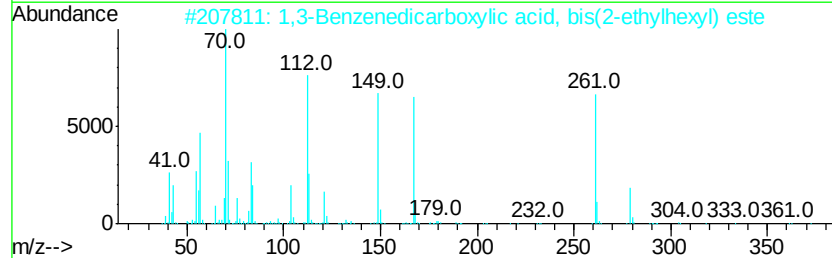
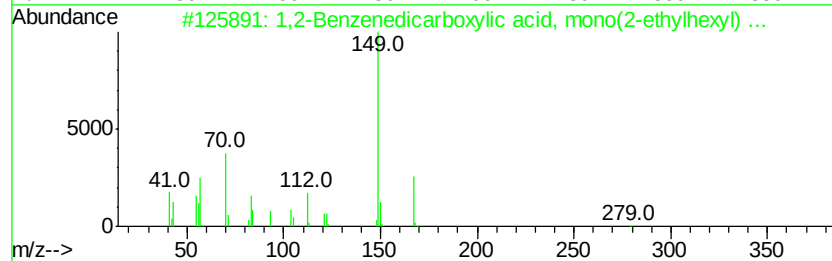
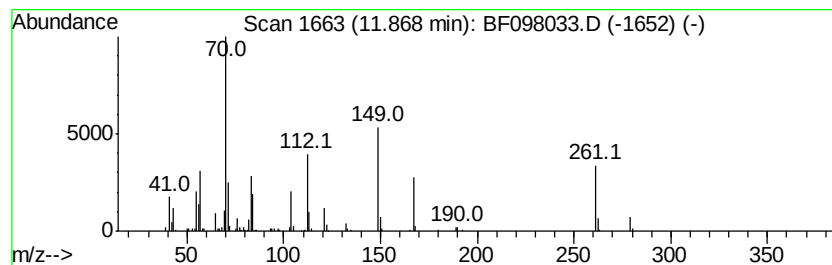
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1,2-Benzenedicarboxylic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	23.51 ng	1152030	Phenanthrene-d10	11.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,2-Benzenedicarboxylic acid, mo...	278	C16H22O4	004376-20-9	50
2		1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	46
3		Bromoacetic acid, 2-ethylhexyl e...	250	C10H19BrO2	068144-73-0	35
4		Carbonic acid, propargyl 2-ethyl...	212	C12H20O3	1000357-90-9	25
5		Phthalic acid, 3,5-difluoropheny...	418	C24H28F2O4	1000315-53-1	22



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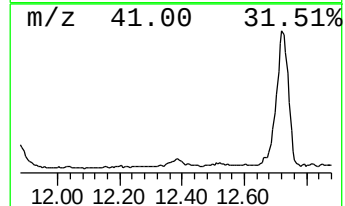
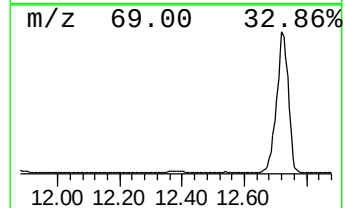
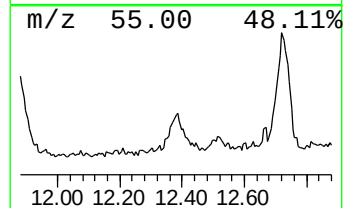
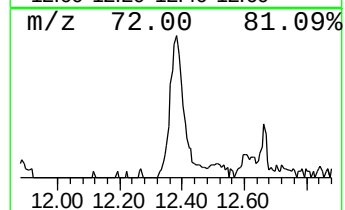
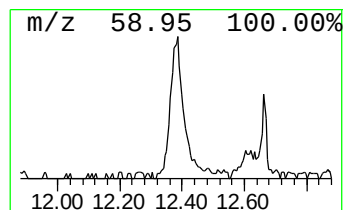
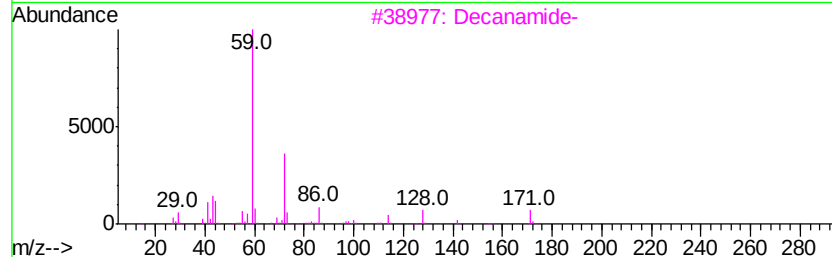
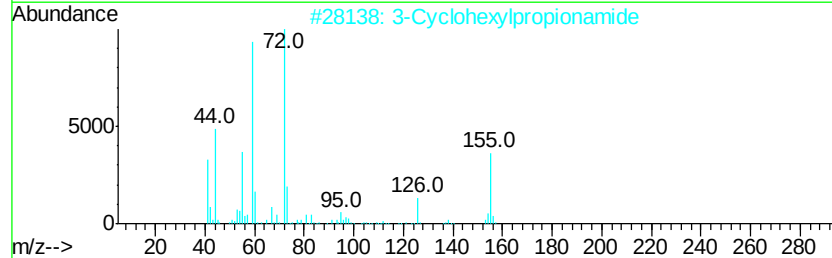
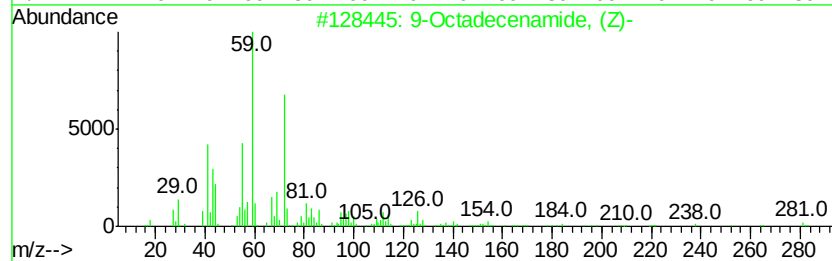
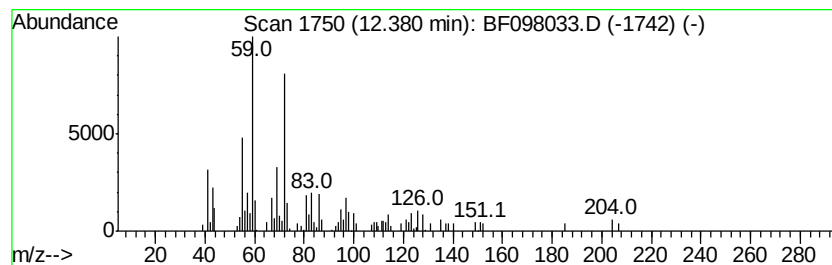
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Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.38	3.45 ng	169198	Phenanthrene-d10	11.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	78
2		3-Cyclohexylpropionamide	155	C9H17NO	004361-29-9	45
3		Decanamide-	171	C10H21NO	002319-29-1	38
4		Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	000498-81-7	35
5		Dodecanamide	199	C12H25NO	001120-16-7	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082517\
Data File : BF098033.D
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Operator : SJ/JU
Sample : I4913-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

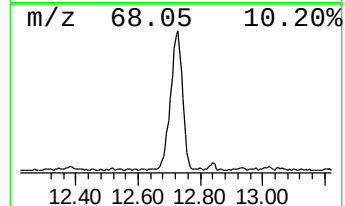
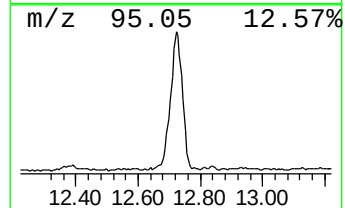
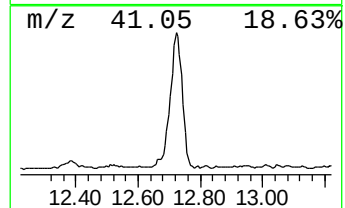
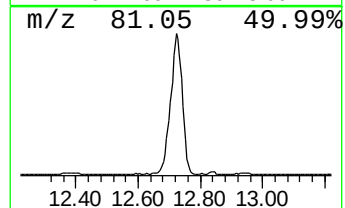
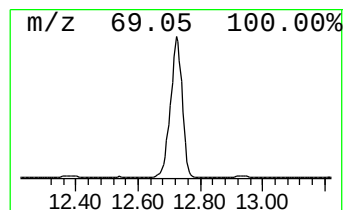
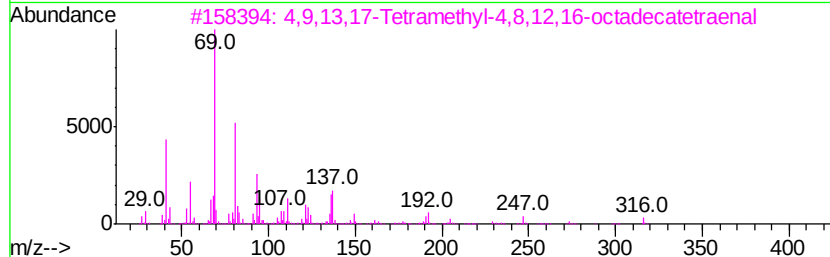
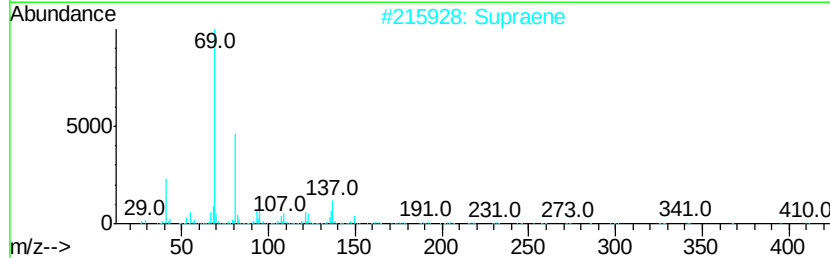
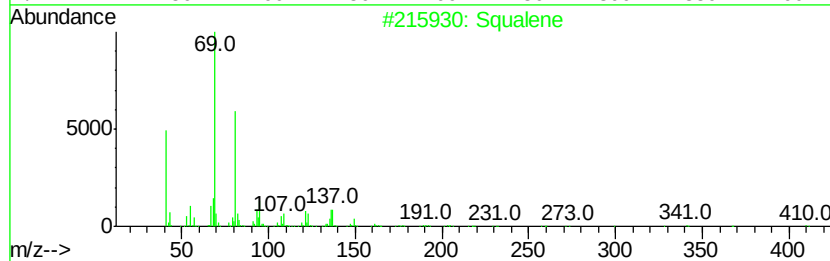
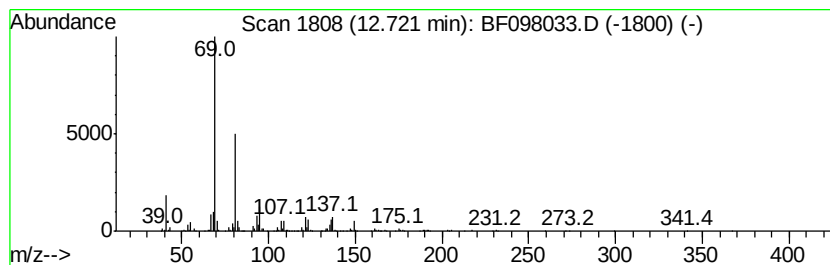
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ClientSampleId :
TEC-BE2-3-12-COMP

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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 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	48.28 ng	2404460	Chrysene-d12	13.89
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene	410 C30H50	000111-02-4	91
2	Supraene	410 C30H50	007683-64-9	86
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316 C22H36O	056882-09-8	83
4	1,5,9-Undecatriene, 2,6,10-trime...	192 C14H24	062951-96-6	78
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264 C17H28O2	004128-17-0	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF082517\
Data File : BF098033.D
Acq On : 25 Aug 2017 16:32
Operator : SJ/JU
Sample : I4913-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

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ClientSampleId :
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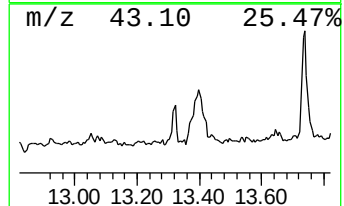
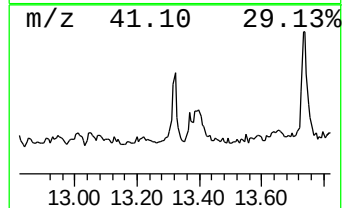
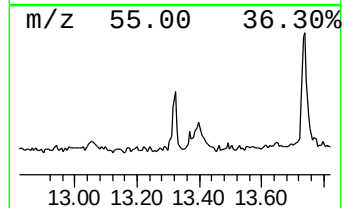
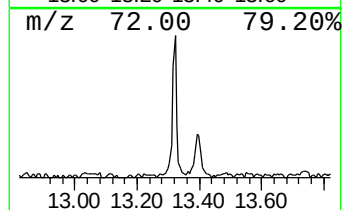
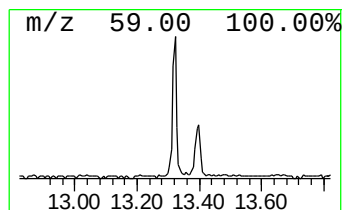
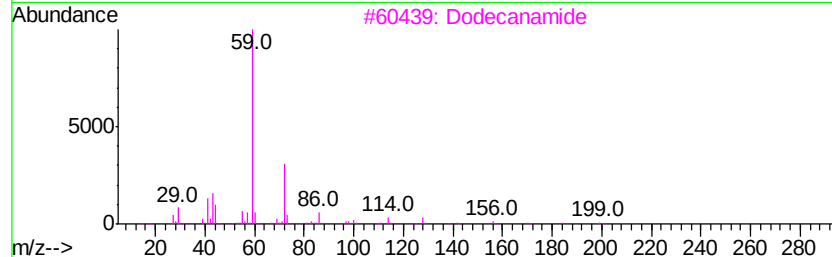
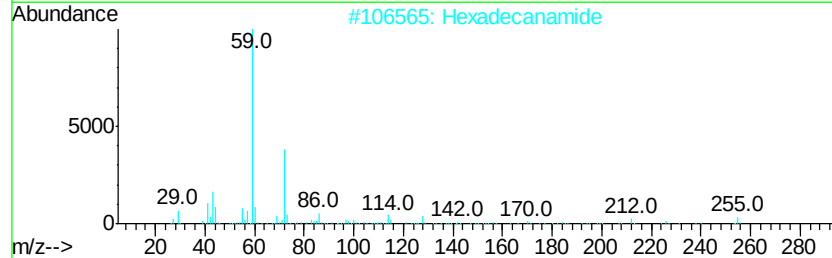
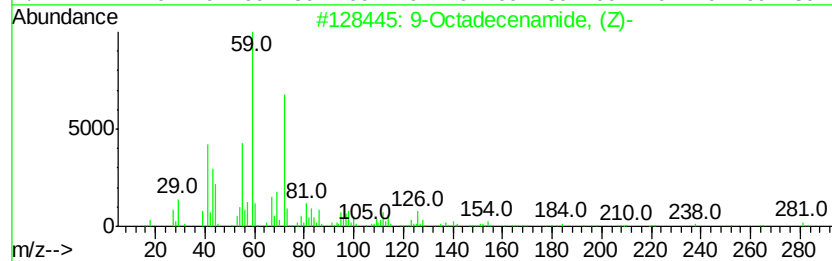
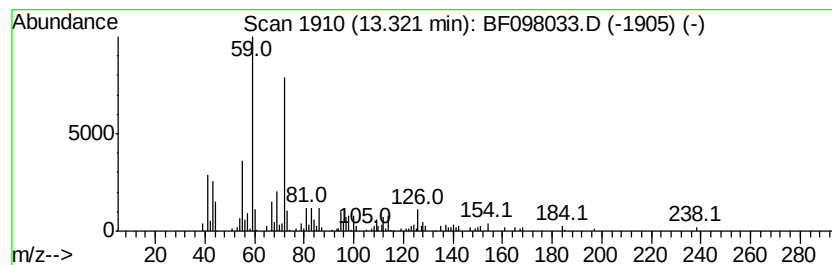
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecanamide Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.32	2.49 ng	123930	Chrysene-d12	13.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2		Hexadecanamide	255	C16H33NO	000629-54-9	53
3		Dodecanamide	199	C12H25NO	001120-16-7	47
4		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	47
5		Nonanamide	157	C9H19NO	001120-07-6	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082517\
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Acq On : 25 Aug 2017 16:32
Operator : SJ/JU
Sample : I4913-02
Misc :
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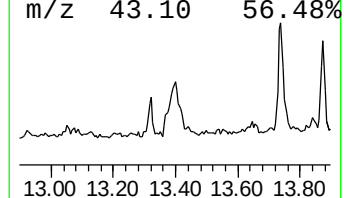
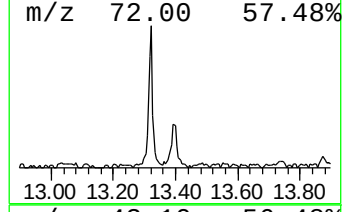
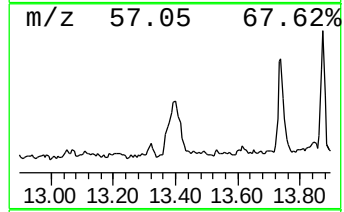
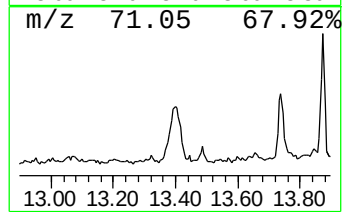
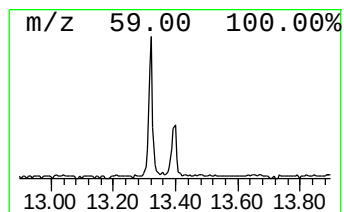
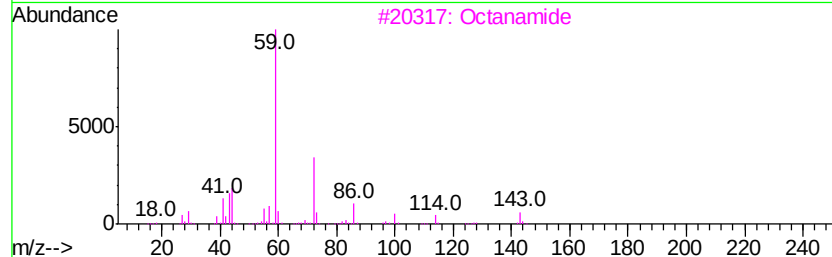
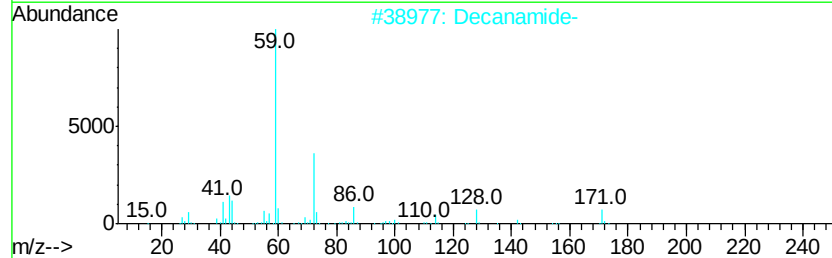
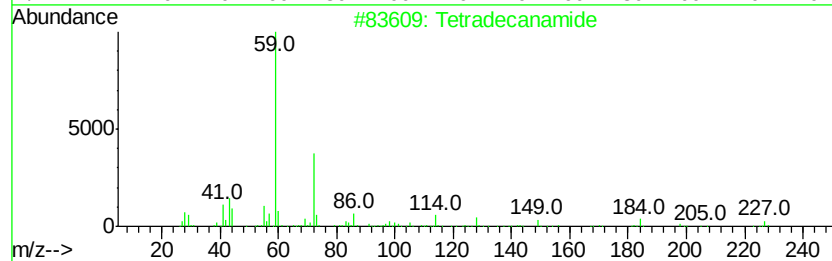
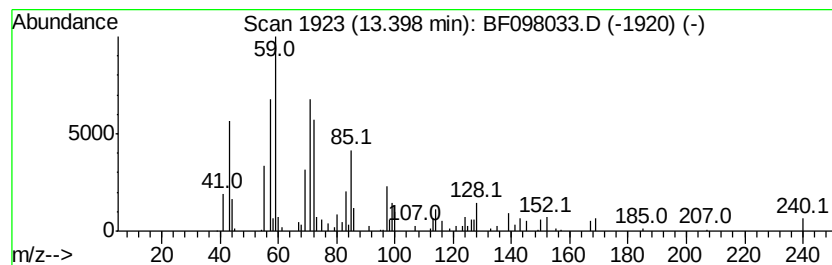
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown13.40 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.40	2.37 ng	117920	Chrysene-d12	13.89	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanamide	227	C14H29NO	000638-58-4	43
2	Decanamide-	171	C10H21NO	002319-29-1	43
3	Octanamide	143	C8H17NO	000629-01-6	38
4	Nonanamide	157	C9H19NO	001120-07-6	27
5	4-Heptanone, 2-methyl-	128	C8H16O	000626-33-5	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082517\
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Acq On : 25 Aug 2017 16:32
Operator : SJ/JU
Sample : I4913-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

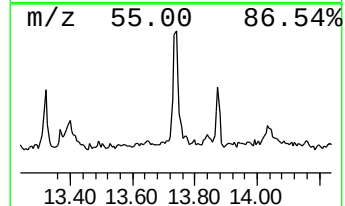
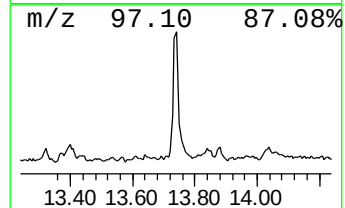
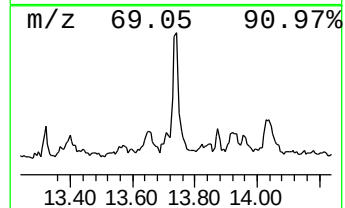
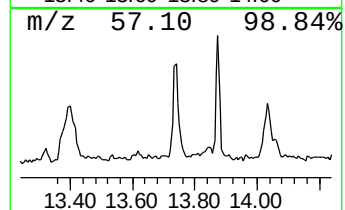
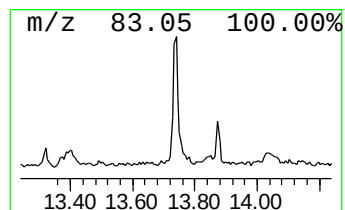
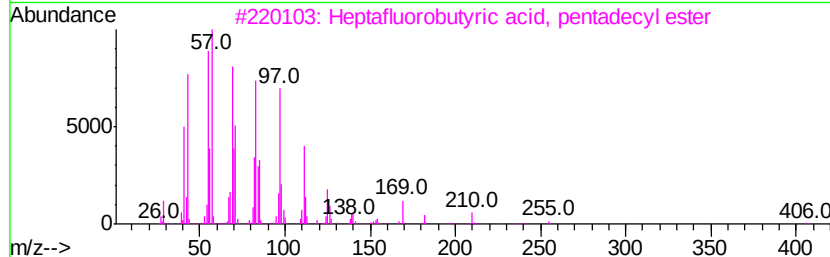
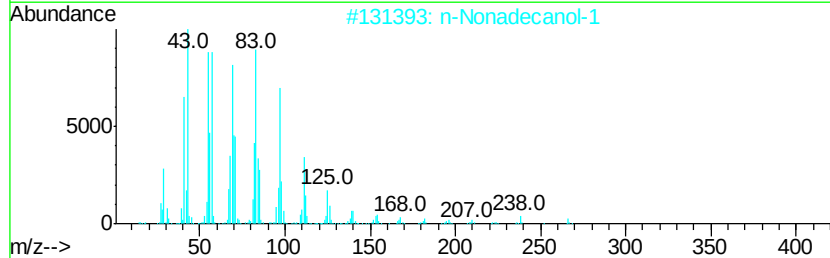
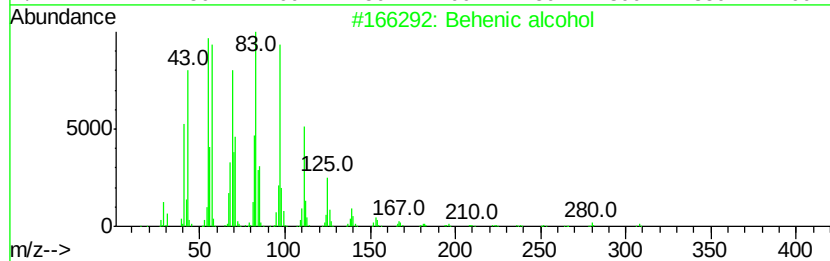
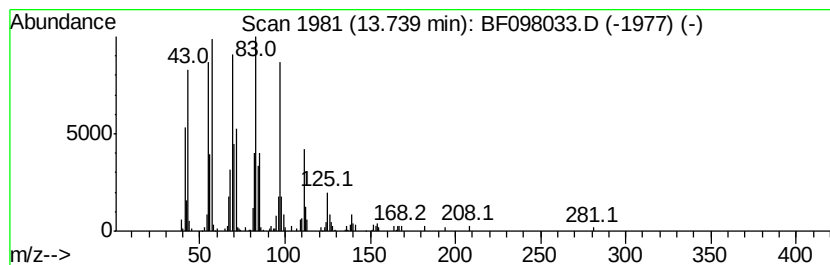
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Behenic alcohol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.74	5.66 ng	281904	Chrysene-d12	13.89	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	Heptafluorobutvric acid, pentade...	424	C19H31F7O2	959261-23-5	93
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082517\
Data File : BF098033.D
Acq On : 25 Aug 2017 16:32
Operator : SJ/JU
Sample : I4913-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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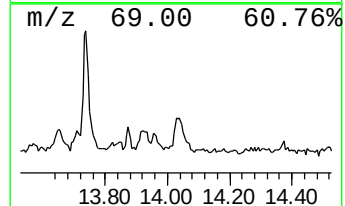
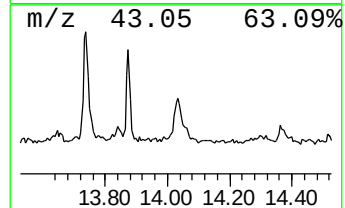
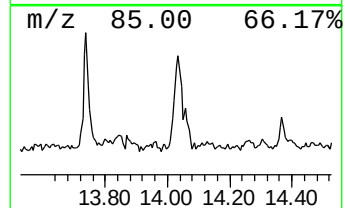
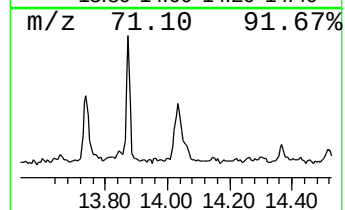
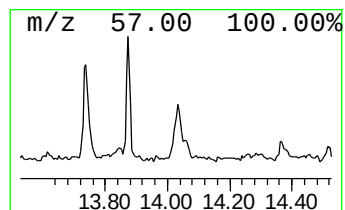
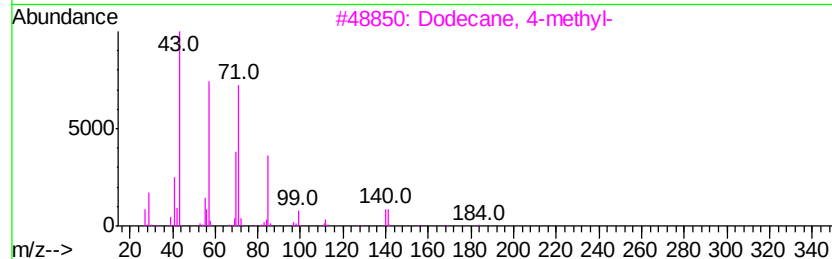
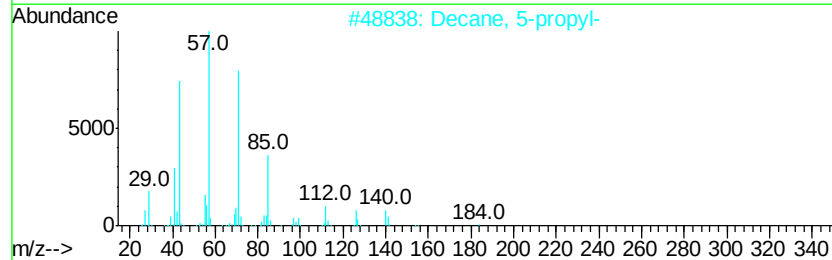
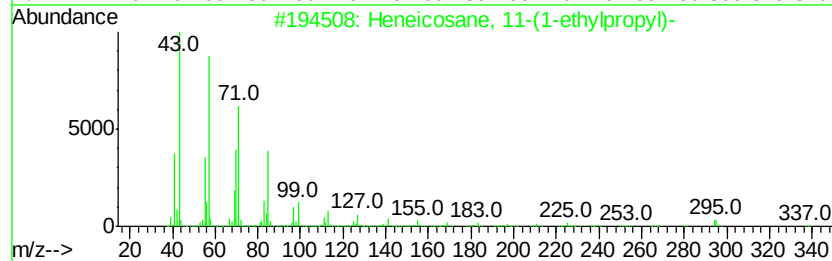
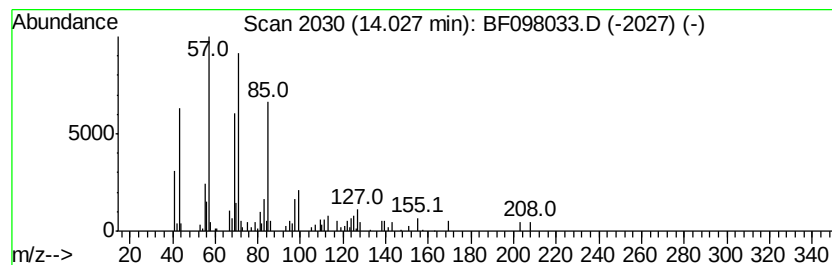
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heneicosane, 11-(1-ethylpro... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.03	2.34 ng	116576	Chrysene-d12	13.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	64
2		Decane, 5-propyl-	184	C13H28	017312-62-8	59
3		Dodecane, 4-methyl-	184	C13H28	006117-97-1	59
4		Undecane, 4,8-dimethyl-	184	C13H28	017301-33-6	59
5		Decane, 2,3,7-trimethyl-	184	C13H28	062238-13-5	59



Data Path : Z:\HPCHEM1\BNA F\DATA\BF082517\
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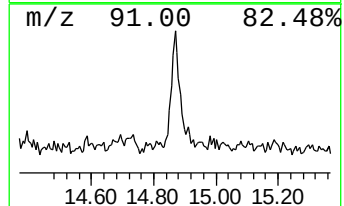
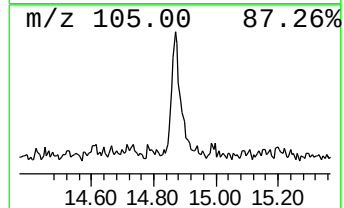
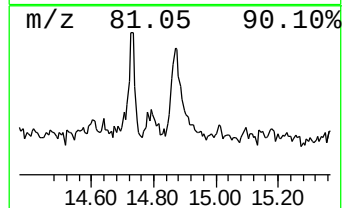
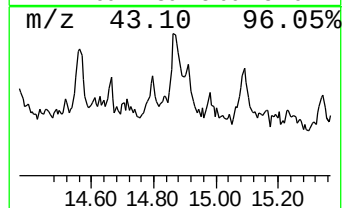
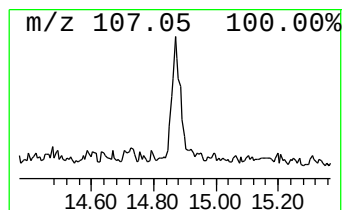
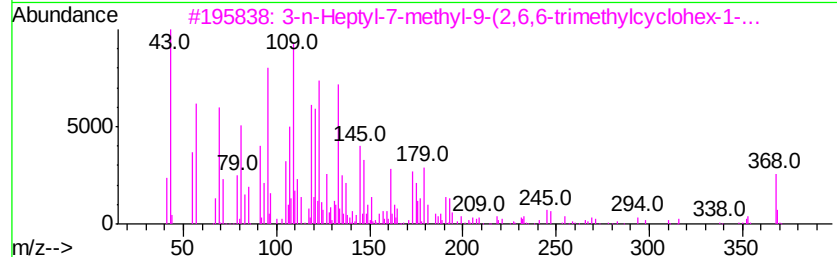
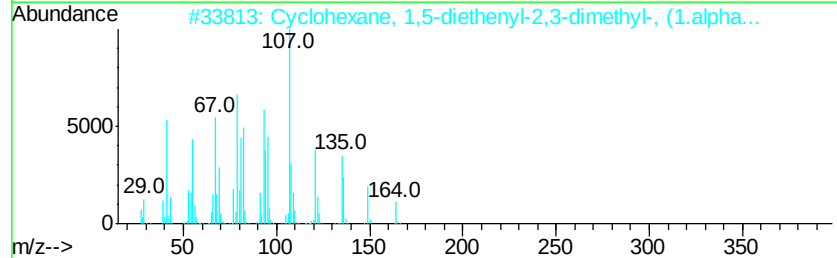
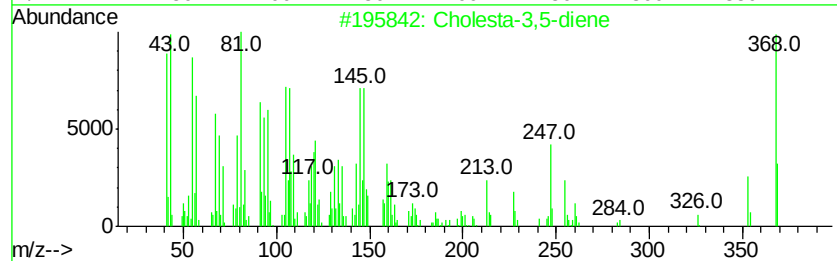
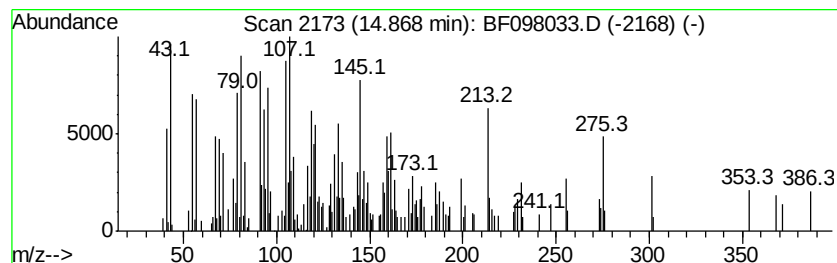
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Cholesta-3,5-diene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.87	12.52 ng	343513	Perylene-d12	15.30	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholesta-3,5-diene	368	C27H44	000747-90-0	86
2	Cyclohexane, 1,5-diethenyl-2,3-d...	164	C12H20	068779-14-6	44
3	3-n-Heptvl-7-methyl-9-(2,6,6-tri...	368	C26H400	1000216-09-3	18
4	4-Hydroxy-4-(4,6-dimethylcyclohe...	196	C12H2002	002316-79-2	14
5	Cyclohexane, 1,2-dimethyl-3,5-bi...	192	C14H24	074806-55-6	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082517\
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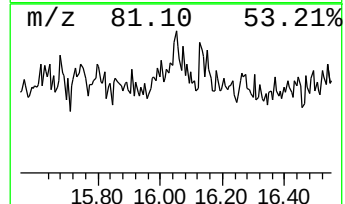
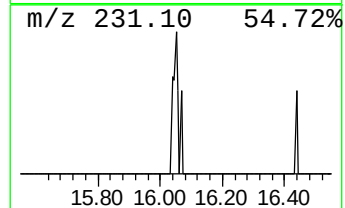
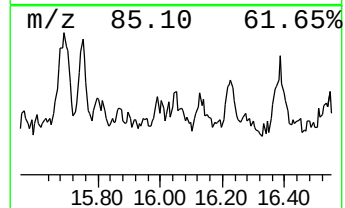
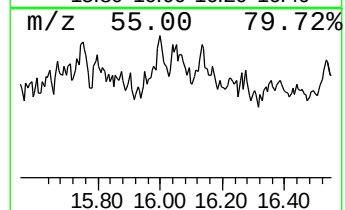
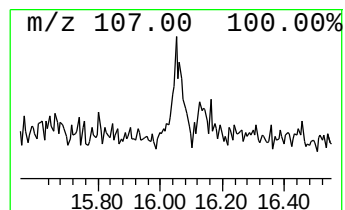
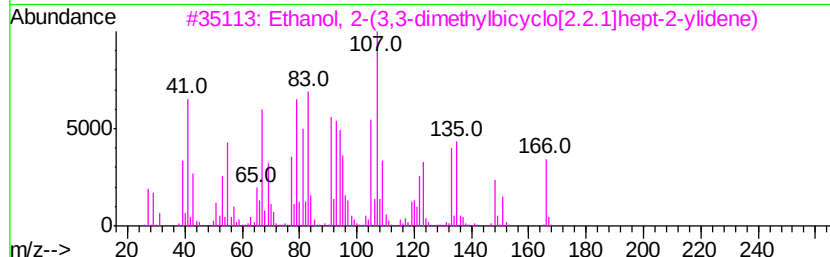
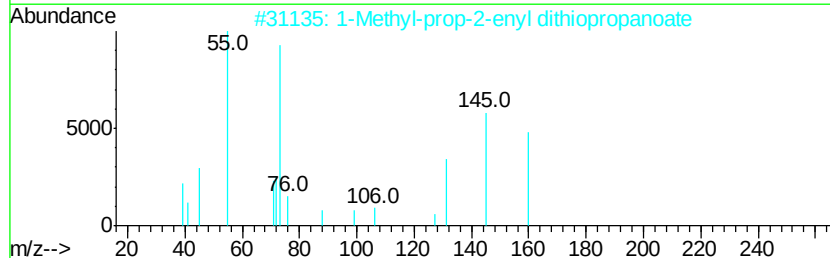
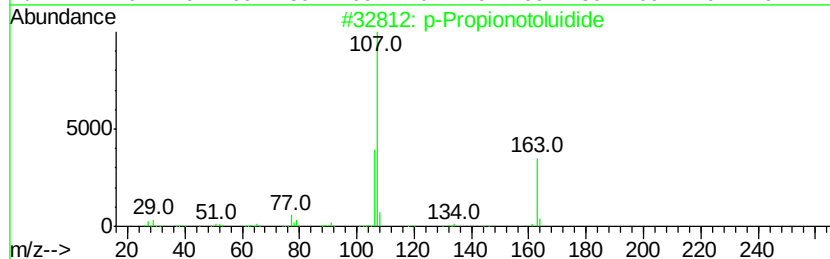
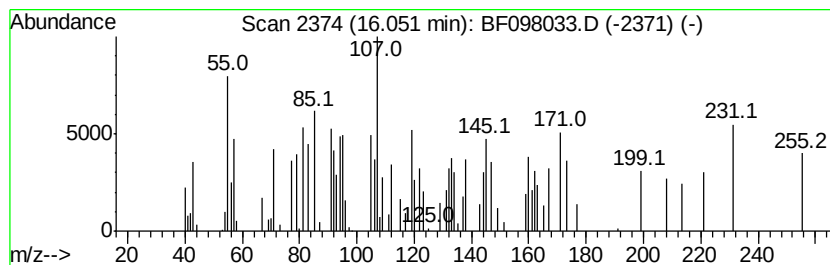
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown16.05 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.05	2.68 ng	73416	Perylene-d12	15.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	p-Propionotoluidide	163	C10H13NO	002759-55-9	11
2		1-Methyl-prop-2-enyl dithiopropa...	160	C7H12S2	065901-87-3	10
3		Ethanol, 2-(3,3-dimethylbicyclof...	166	C11H18O	002226-05-3	10
4		2-Oxazolidinone, 4-methyl-5-phen...	177	C10H11NO2	028044-22-6	10
5		Phosphorodiamidic acid, N,N'-dim...	200	C8H13N2O2P	001754-58-1	10



Data Path : Z:\HPCHEM1\BNA F\DATA\BF082517\
Data File : BF098033.D
Acq On : 25 Aug 2017 16:32
Operator : SJ/JU
Sample : I4913-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-BE2-3-12-COMP

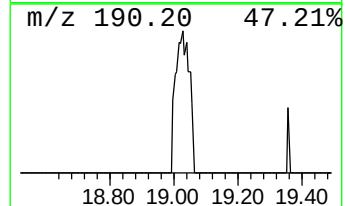
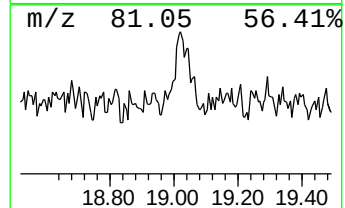
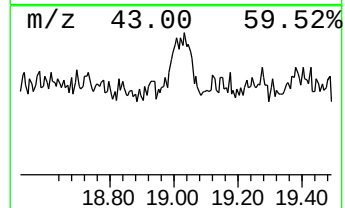
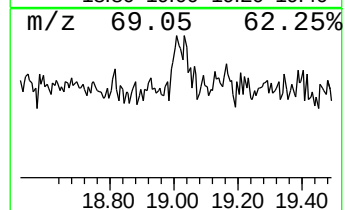
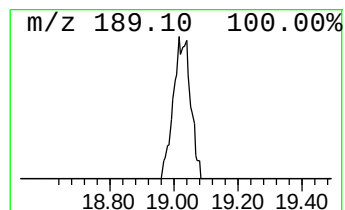
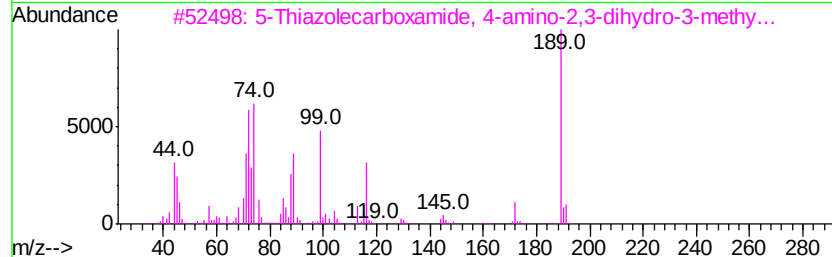
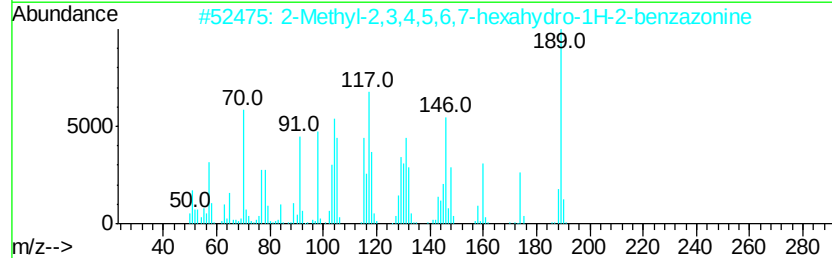
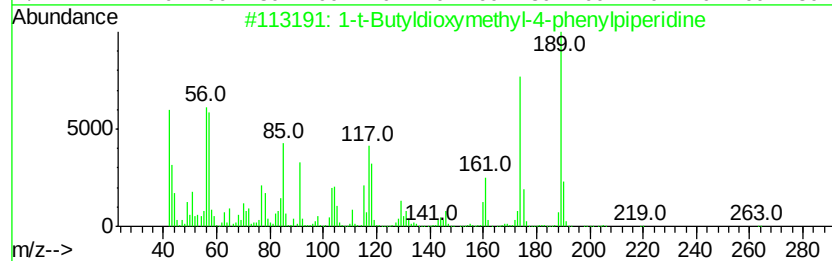
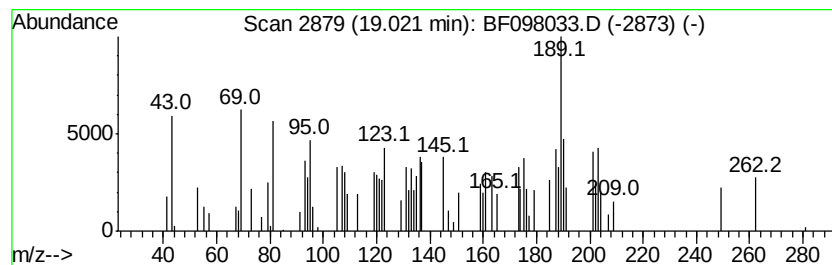
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown19.02 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.02	3.62 ng	99214	Perylene-d12	15.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-t-Butyldioxymethyl-4-phenylpip...	263	C16H25NO2	116437-26-4	22
2		2-Methyl-2,3,4,5,6,7-hexahydro-1...	189	C13H19N	078838-08-1	11
3		5-Thiazolecarboxamide, 4-amino-2...	189	C5H7N3OS2	1000338-08-9	11
4		Lilial	204	C14H20O	000080-54-6	10
5		(-)-1,2,2.alpha.,3,3,4,6,7,8,8.a...	204	C15H24	1000365-86-7	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082517\
 Data File : BF098033.D
 Acq On : 25 Aug 2017 16:32
 Operator : SJ/JU
 Sample : I4913-02
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TEC-BE2-3-12-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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...	4.95	8.6 ng		318818	1	6.74	743356	20.0
unknown6.51	6.51	88.0 ng		3271700	1	6.74	743356	20.0
Pentadecanoic acid	11.79	2.0 ng		99092	4	11.25	980026	20.0
1,2-Benzenedicarb...	11.87	23.5 ng		1152030	4	11.25	980026	20.0
9-Octadecenamide,...	12.38	3.5 ng		169198	4	11.25	980026	20.0
Squalene	12.72	48.3 ng		2404460	5	13.89	996047	20.0
Hexadecanamide	13.32	2.5 ng		123930	5	13.89	996047	20.0
unknown13.40	13.40	2.4 ng		117920	5	13.89	996047	20.0
Behenic alcohol	13.74	5.7 ng		281904	5	13.89	996047	20.0
Heneicosane, 11-(...	14.03	2.3 ng		116576	5	13.89	996047	20.0
Cholesta-3,5-diene	14.87	12.5 ng		343513	6	15.30	548696	20.0
unknown16.05	16.05	2.7 ng		73416	6	15.30	548696	20.0
unknown19.02	19.02	3.6 ng		99214	6	15.30	548696	20.0