

Data Path : Z:\HPCHEM1\BNA_F\Data\BF091916\
 Data File : BF090122.D
 Acq On : 19 Sep 2016 16:03
 Operator : UM/SJ
 Sample : H4824-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 01

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-BF091516.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	1.690	6	9	39	rVB	765604	1950629	11.37%	1.506%
2	4.627	263	266	279	rBV	162528	304249	1.77%	0.235%
3	5.096	304	307	321	rBV	1257216	1855110	10.81%	1.433%
4	6.182	400	402	405	rBV	1248035	1153612	6.72%	0.891%
5	6.296	410	412	415	rBV	2559648	2815764	16.41%	2.175%
6	6.536	430	433	435	rBV	706267	823033	4.80%	0.636%
7	6.684	444	446	449	rBV	2314020	2801953	16.33%	2.164%
8	7.107	480	483	485	rBV	2173454	2598872	15.15%	2.007%
9	7.816	543	545	548	rBV	1034661	1088274	6.34%	0.840%
10	8.296	582	587	599	rVB2	68808	410914	2.40%	0.317%
11	8.639	607	617	626	rBV3	72360	401117	2.34%	0.310%
12	8.902	637	640	643	rBV	3765853	4002594	23.33%	3.091%
13	9.302	673	675	677	rVB	587203	503914	2.94%	0.389%
14	9.565	695	698	700	rBV	1544658	1376992	8.03%	1.063%
15	9.873	721	725	728	rBV	106564	230413	1.34%	0.178%
16	10.353	755	767	768	rBV2	2820952	5707801	33.27%	4.408%
17	10.433	768	774	775	rVV	2517744	9503324	55.40%	7.339%
18	10.468	775	777	779	rVB	3072151	4053991	23.63%	3.131%
19	10.582	785	787	792	rVB3	86673	178915	1.04%	0.138%
20	10.913	813	816	820	rBV2	73901	181254	1.06%	0.140%
21	11.039	824	827	829	rVV	955268	1254076	7.31%	0.969%
22	11.211	837	842	847	rBV3	331104	645144	3.76%	0.498%
23	11.394	854	858	863	rBV4	154302	336504	1.96%	0.260%
24	11.531	868	870	872	rVB	147019	188419	1.10%	0.146%
25	11.599	872	876	879	rBV2	601529	807327	4.71%	0.623%
26	11.702	882	885	886	rVV	387558	905516	5.28%	0.699%
27	11.736	886	888	896	rVB	586828	1271984	7.41%	0.982%
28	11.942	896	906	909	rBV	3941440	17155335	100.00%	13.249%
29	12.011	911	912	917	rVV2	480642	703036	4.10%	0.543%
30	12.091	917	919	921	rVV	386686	451590	2.63%	0.349%
31	12.125	921	922	924	rVB	194386	200865	1.17%	0.155%
32	12.376	941	944	950	rVB	613509	792010	4.62%	0.612%
33	12.582	960	962	964	rVV	1187925	1954988	11.40%	1.510%
34	12.628	964	966	968	rVV	3195427	4040737	23.55%	3.121%

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35	12.685	968	971	975	rVB4	149688	300826	1.75%	0.232%
36	12.845	981	985	986	rBV3	156944	376096	2.19%	0.290%
37	12.868	986	987	993	rVV	231050	279376	1.63%	0.216%
38	12.971	993	996	998	rVV2	523055	876264	5.11%	0.677%
39	13.028	998	1001	1003	rVV	2285786	3414111	19.90%	2.637%
40	13.291	1021	1024	1027	rBV	1296334	2706433	15.78%	2.090%
41	13.394	1027	1033	1036	rVV3	5336272	16013155	93.34%	12.367%
42	13.439	1036	1037	1041	rVV	649513	928127	5.41%	0.717%
43	13.508	1041	1043	1044	rVV	152273	253077	1.48%	0.195%
44	13.542	1044	1046	1048	rVV	1217594	1557017	9.08%	1.202%
45	13.645	1052	1055	1060	rBV2	1212289	1619930	9.44%	1.251%
46	13.771	1063	1066	1068	rBV	3569200	4127221	24.06%	3.187%
47	13.977	1081	1084	1085	rBV2	203621	247950	1.45%	0.191%
48	14.102	1092	1095	1097	rBV	3496749	3991495	23.27%	3.083%
49	14.251	1105	1108	1110	rBV	3177374	3165930	18.45%	2.445%
50	14.297	1110	1112	1113	rVV	197687	234197	1.37%	0.181%
51	14.365	1116	1118	1120	rBV	679648	928545	5.41%	0.717%
52	14.411	1120	1122	1124	rVV	2936768	3277714	19.11%	2.531%
53	14.468	1126	1127	1129	rVB	254028	241326	1.41%	0.186%
54	14.514	1129	1131	1135	rVB4	91582	209778	1.22%	0.162%
55	14.594	1135	1138	1140	rBV	242840	278099	1.62%	0.215%
56	14.708	1145	1148	1150	rBV	2499203	2769794	16.15%	2.139%
57	14.902	1162	1165	1167	rVV	151180	297166	1.73%	0.230%
58	14.971	1169	1171	1173	rBV	805306	961178	5.60%	0.742%
59	15.017	1173	1175	1180	rVB	1434955	2006928	11.70%	1.550%
60	15.382	1203	1207	1212	rBV	895953	1782937	10.39%	1.377%
61	15.451	1212	1213	1218	rVB3	156337	293743	1.71%	0.227%
62	15.542	1218	1221	1226	rBV5	73395	197813	1.15%	0.153%
63	15.783	1238	1242	1250	rVB	552468	1065156	6.21%	0.823%
64	16.251	1279	1283	1286	rBV	313953	669440	3.90%	0.517%
65	16.594	1309	1313	1323	rVB2	260388	686410	4.00%	0.530%
66	16.788	1325	1330	1333	rBV	157772	399547	2.33%	0.309%
67	17.154	1359	1362	1367	rVV3	64784	172801	1.01%	0.133%
68	17.440	1383	1387	1394	rVB	87515	280627	1.64%	0.217%
69	18.983	1517	1522	1528	rBV3	61143	223189	1.30%	0.172%

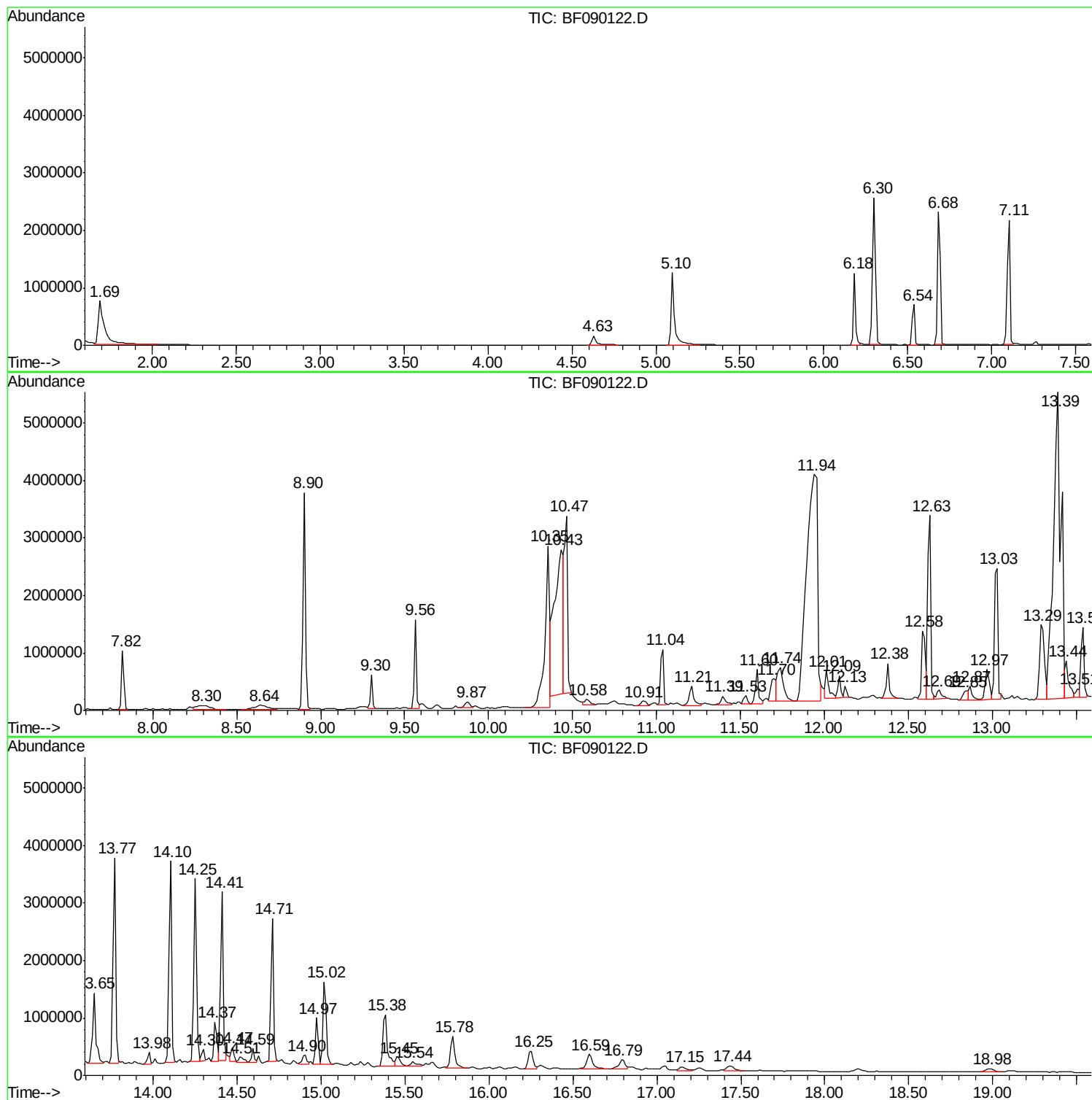
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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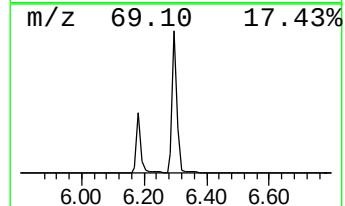
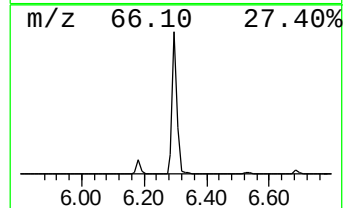
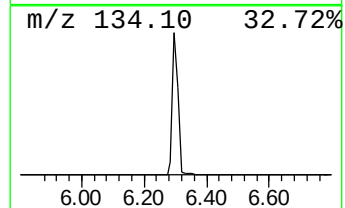
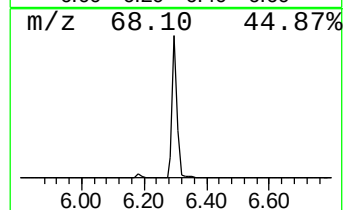
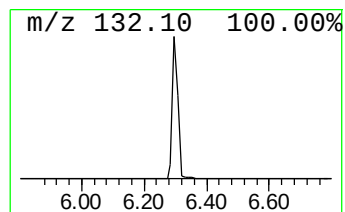
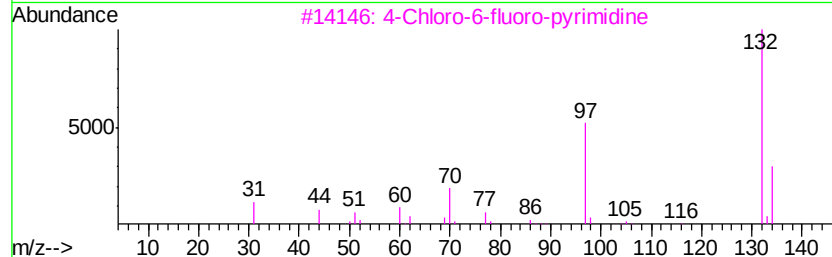
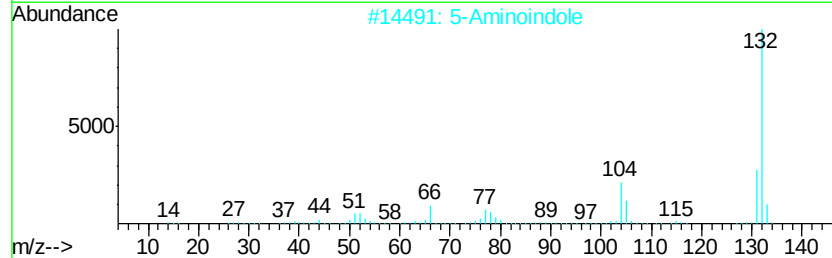
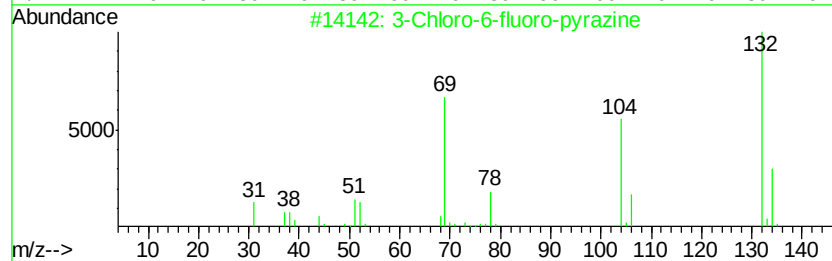
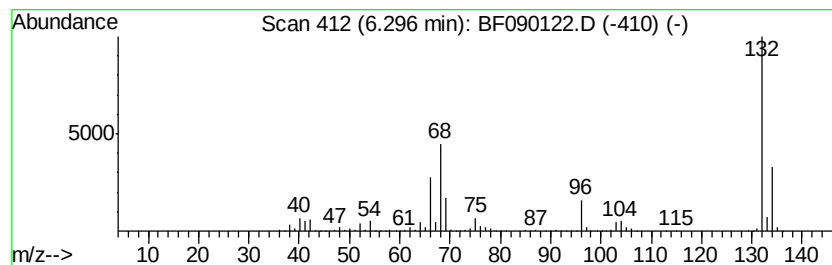
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.30 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.30	68.42 ng	2815760	1,4-Dichlorobenzene-d4	6.54

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4			1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5			4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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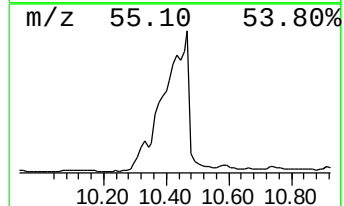
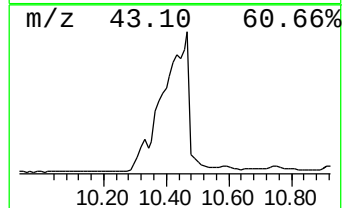
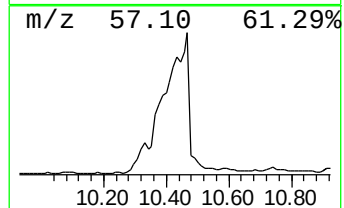
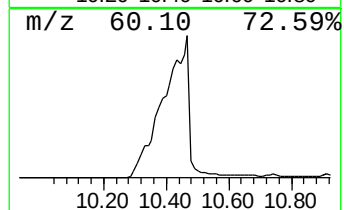
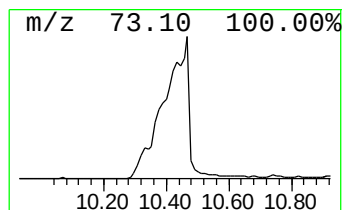
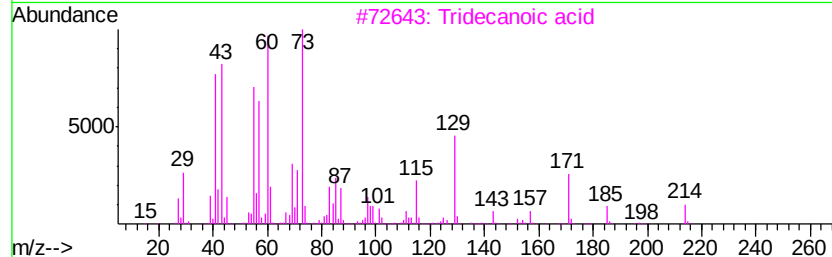
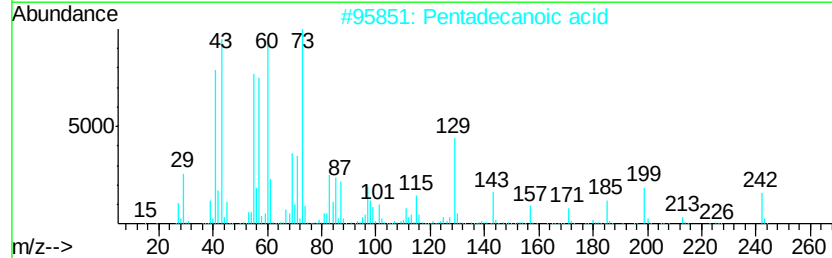
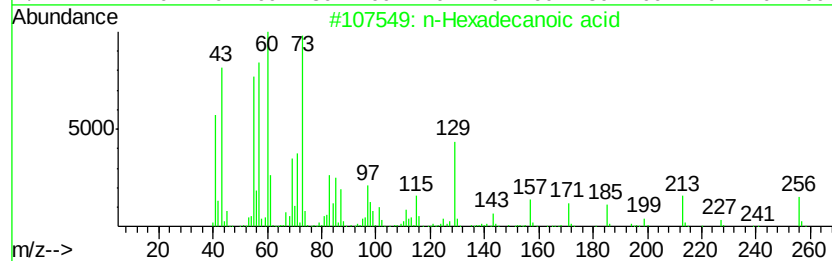
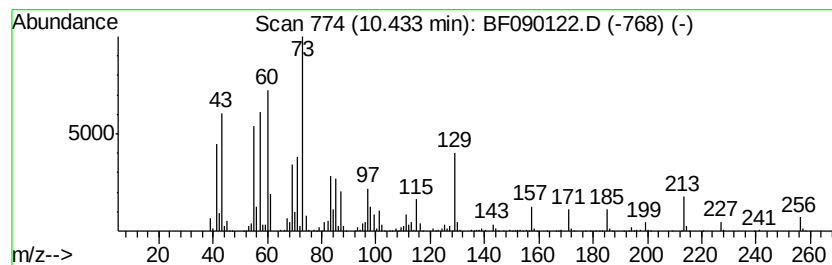
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.43	151.56 ng	9503320	Phenanthrene-d10		11.04
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	58
4	Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1000309-12-5	25
5	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	18



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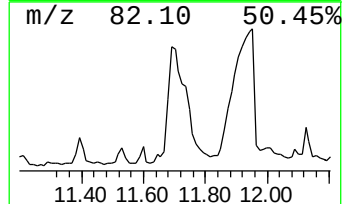
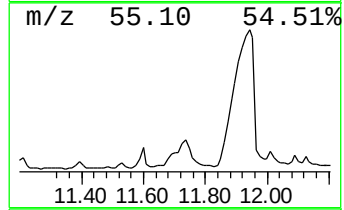
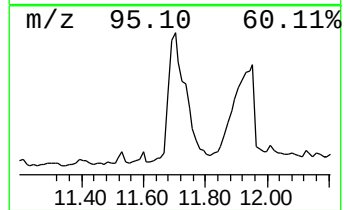
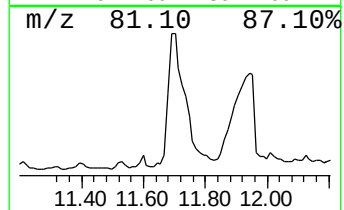
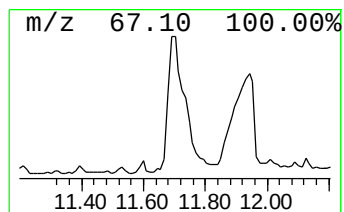
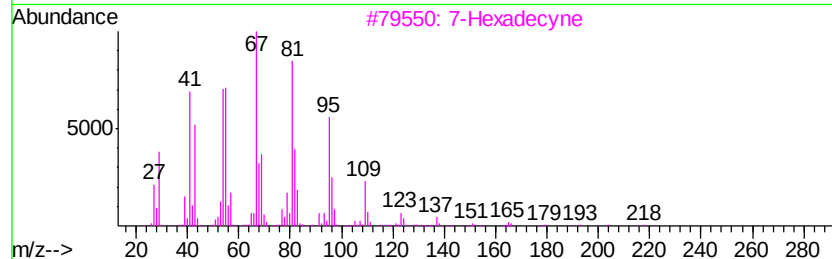
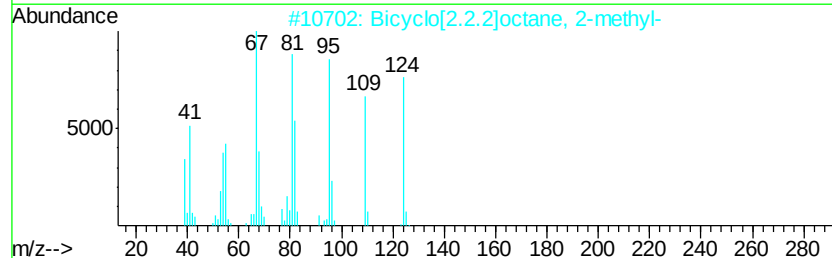
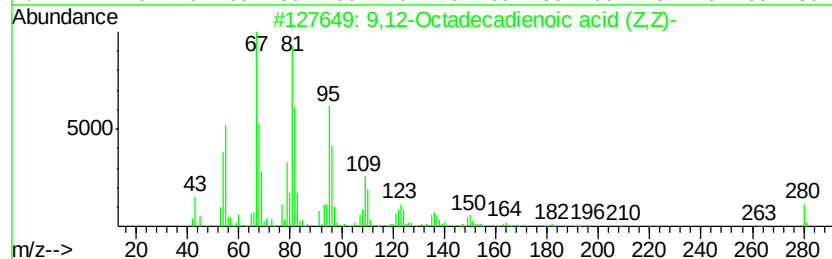
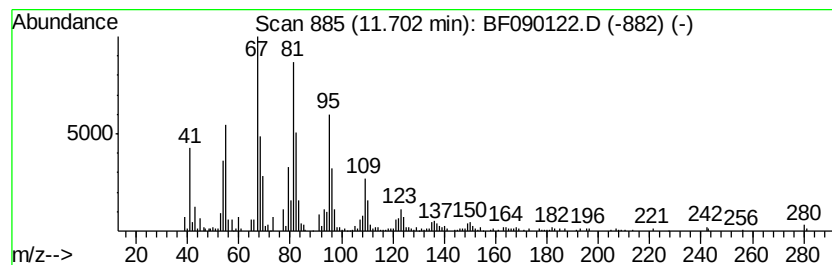
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 9,12-Octadecadienoic acid (... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	14.44 ng	905516	Phenanthrene-d10	11.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	99
2		Bicyclo[2.2.2]octane, 2-methyl-	124	C9H16	000766-53-0	87
3		7-Hexadecyne	222	C16H30	074685-28-2	86
4		6-Dodecyne	166	C12H22	006975-99-1	80
5		1-Pentadecyne	208	C15H28	000765-13-9	70



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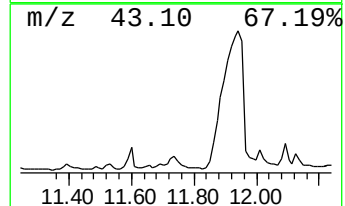
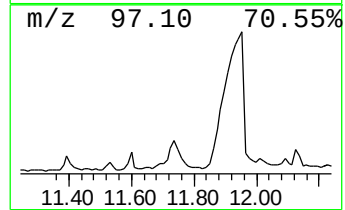
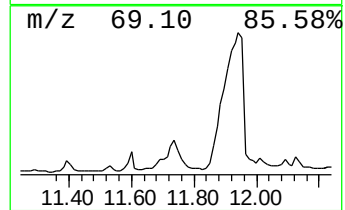
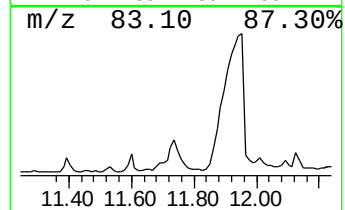
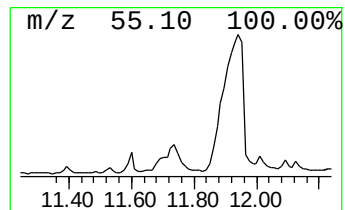
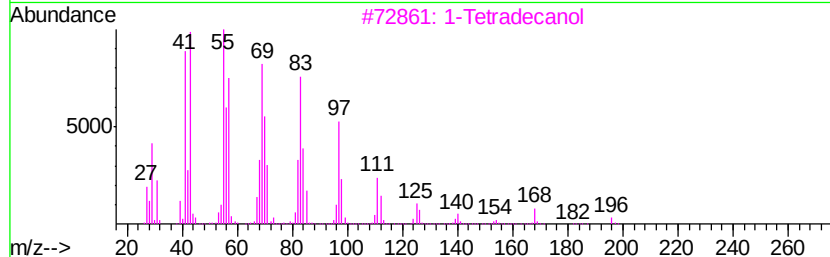
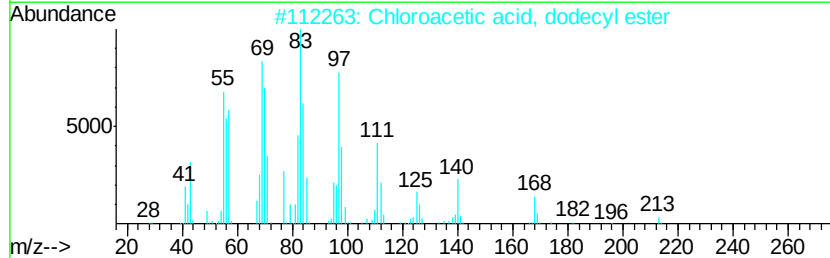
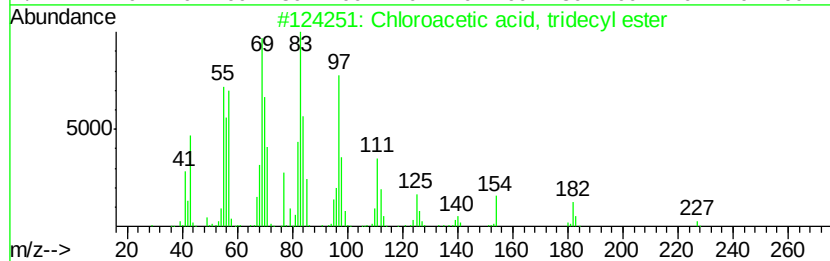
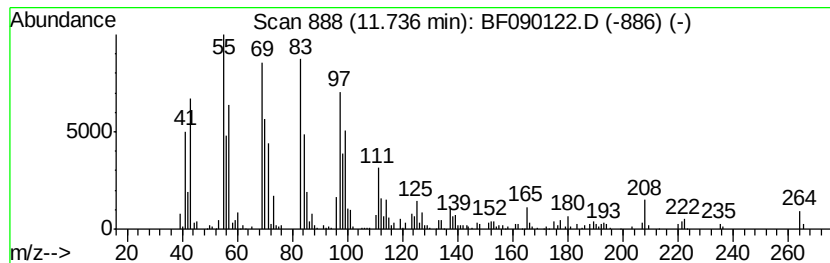
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Peak Number 7 Chloroacetic acid, tridecyl... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.74	20.29 ng	1271980	Phenanthrene-d10	11.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Chloroacetic acid, tridecyl ester	276	C15H29ClO2	018277-85-5	81
2		Chloroacetic acid, dodecyl ester	262	C14H27ClO2	006316-04-7	81
3		1-Tetradecanol	214	C14H30O	000112-72-1	68
4		Chloroacetic acid, tetradecyl ester	290	C16H31ClO2	018277-86-6	68
5		Acetic acid, trifluoro-, dodecyl...	282	C14H25F3O2	006222-00-0	68



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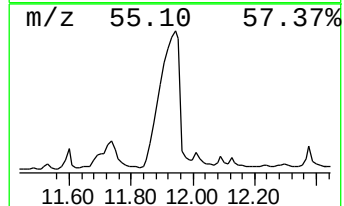
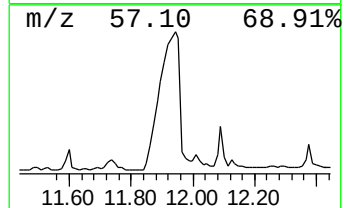
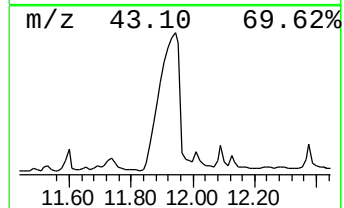
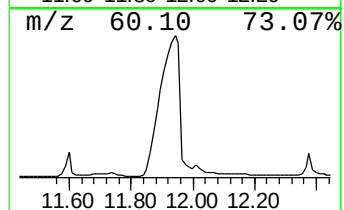
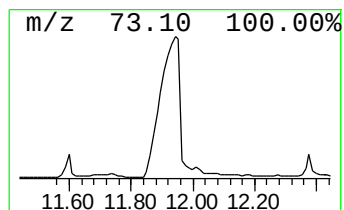
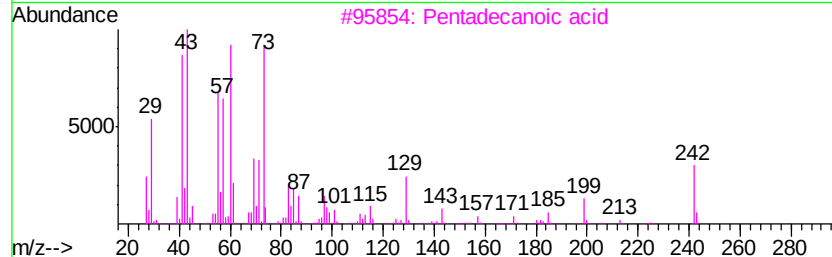
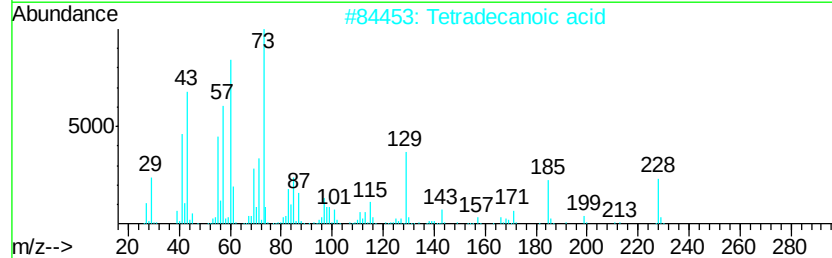
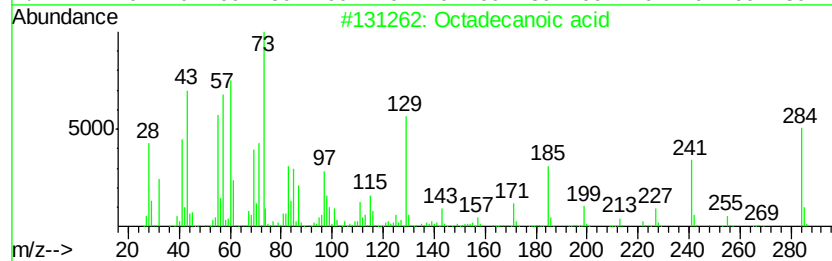
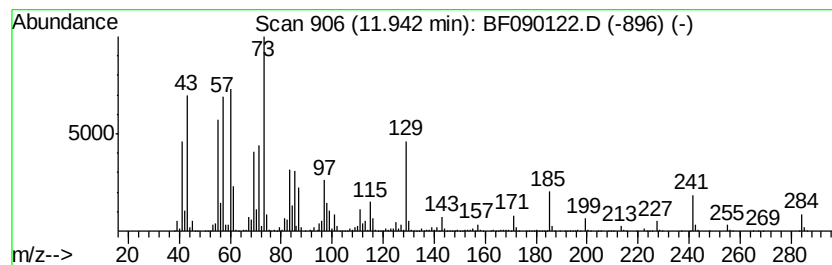
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	273.59 ng	17155300	Phenanthrene-d10	11.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		n-Decanoic acid	172	C10H20O2	000334-48-5	62
5		Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	25



Data Path : Z:\HPCHEM1\BNA_F\Data\BF091916\
Data File : BF090122.D
Acq On : 19 Sep 2016 16:03
Operator : UM/SJ
Sample : H4824-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

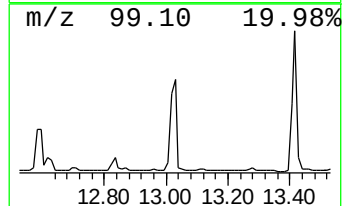
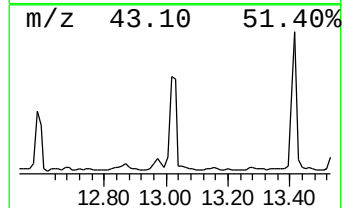
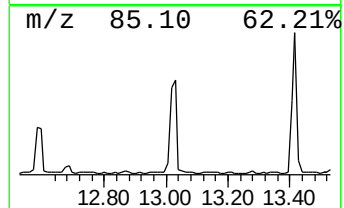
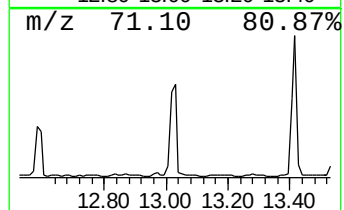
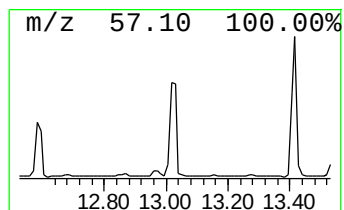
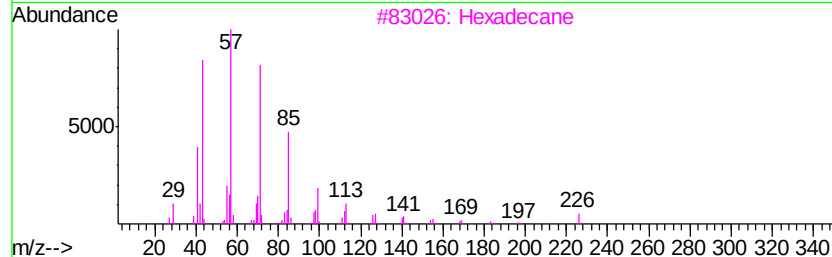
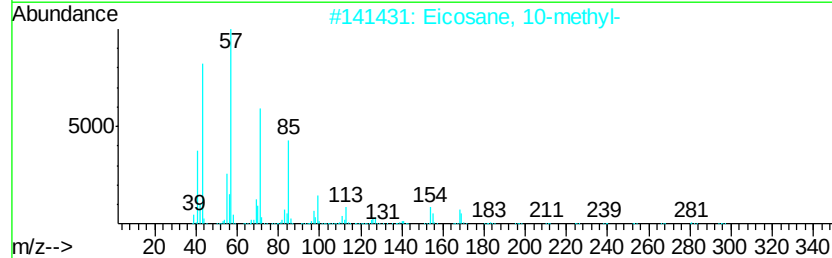
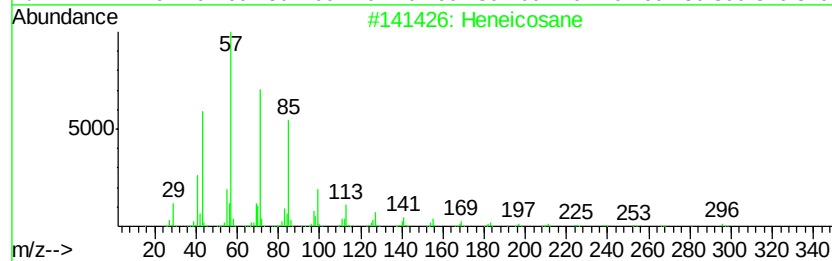
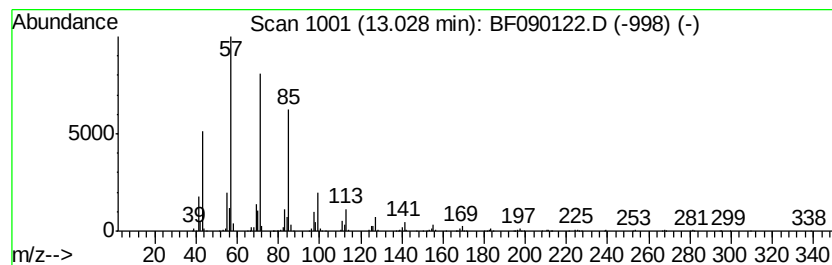
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.03	42.15 ng	3414110	Chrysene-d12	13.65	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	91
3	Hexadecane	226	C16H34	000544-76-3	90
4	Docosane	310	C22H46	000629-97-0	86
5	Heptacosane	380	C27H56	000593-49-7	83



Data Path : Z:\HPCHEM1\BNA_F\Data\BF091916\
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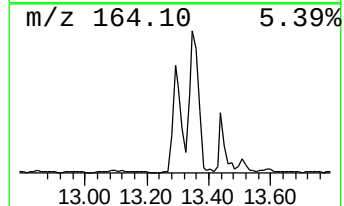
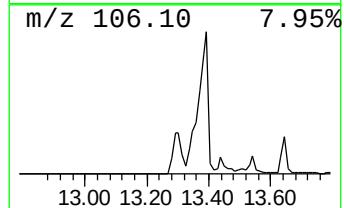
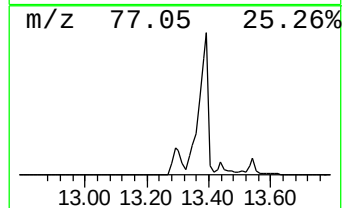
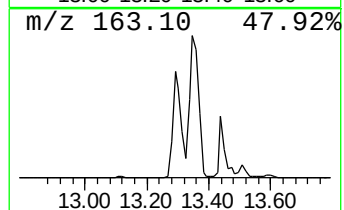
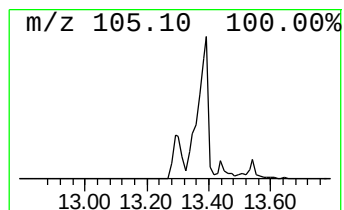
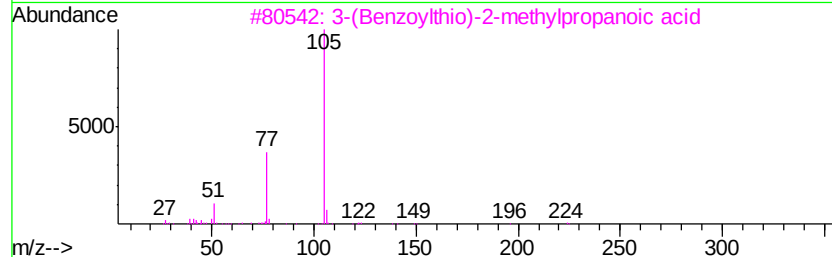
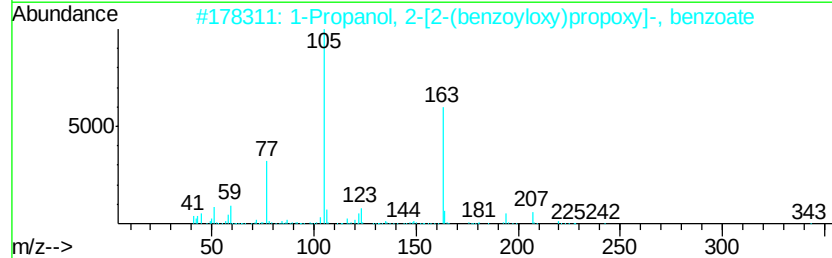
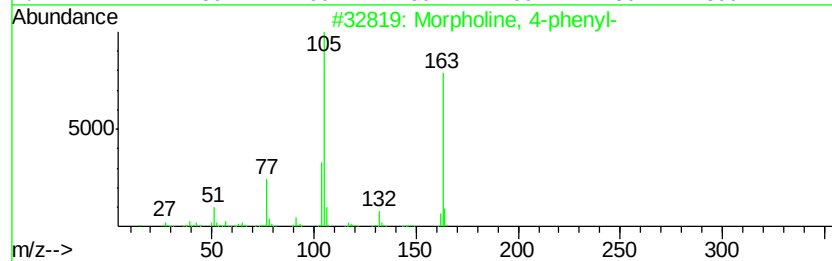
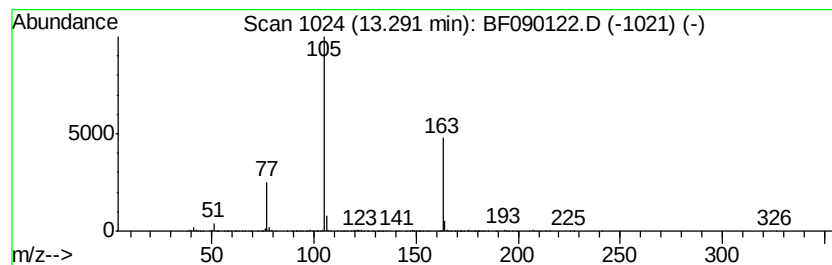
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Morpholine, 4-phenyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.29	33.41 ng	2706430	Chrysene-d12	13.65
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Morpholine, 4-phenyl-	163 C10H13NO	000092-53-5 72
2		1-Propanol, 2-[2-(benzoyloxy)pro...	342 C20H22O5	020109-39-1 40
3		3-(Benzoylthio)-2-methylpropanoi...	224 C11H12O3S	067714-34-5 38
4		Glyoxylic acid, phenyl-, (2'-ace...	268 C16H12O4	166538-12-1 38
5		(3-Phenylloxiran-2-yl)methyl benz...	254 C16H14O3	1000366-96-1 36



Data Path : Z:\HPCHEM1\BNA_F\Data\BF091916\
Data File : BF090122.D
Acq On : 19 Sep 2016 16:03
Operator : UM/SJ
Sample : H4824-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

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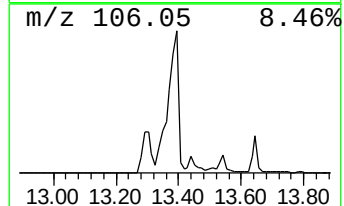
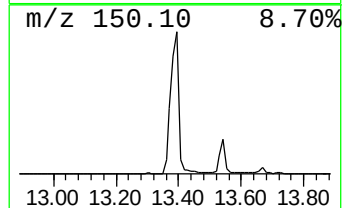
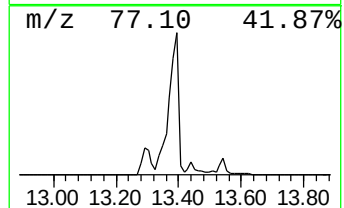
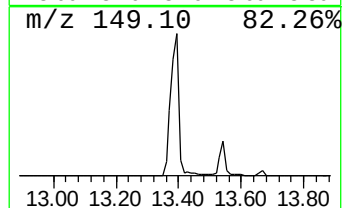
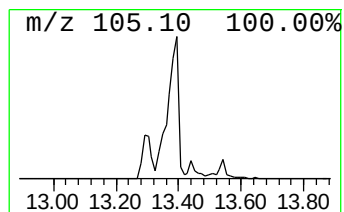
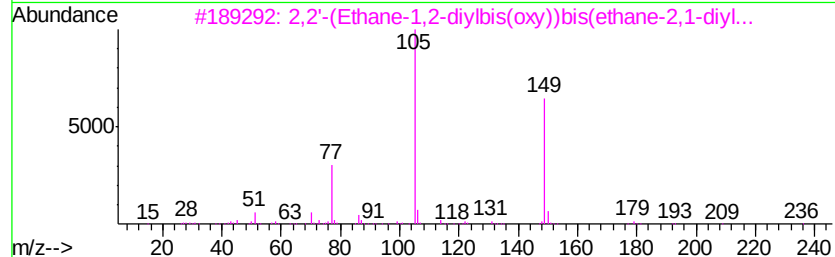
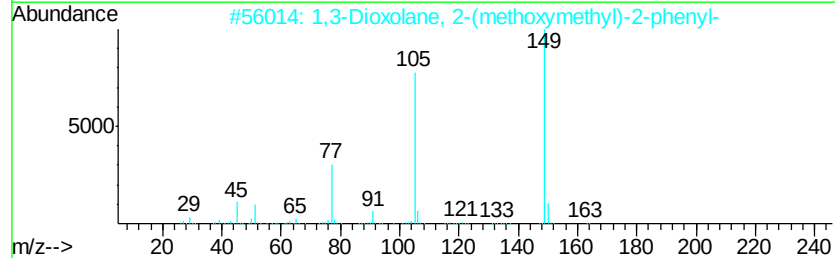
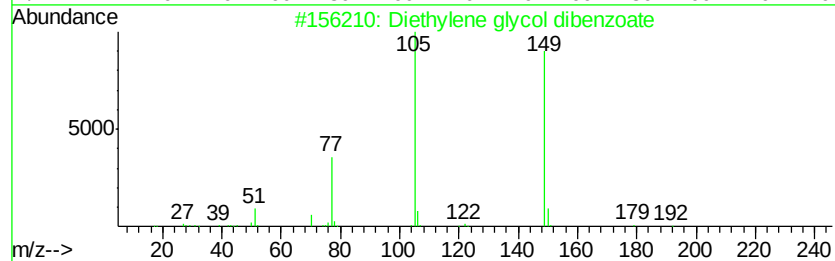
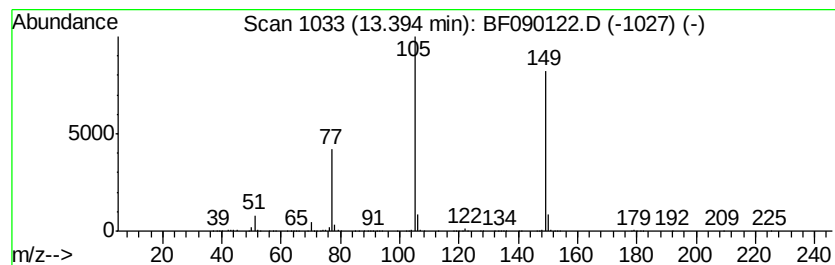
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Diethylene glycol dibenzoate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.39	197.70 ng	16013200	Chrysene-d12	13.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	80
2		1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	74
3		2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	74
4		2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	74
5		2,5,8,11-Tetraoxatridecan-13-yl ...	312	C16H24O6	1000366-96-7	50



Data Path : Z:\HPCHEM1\BNA_F\Data\BF091916\
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Acq On : 19 Sep 2016 16:03
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ALS Vial : 4 Sample Multiplier: 1

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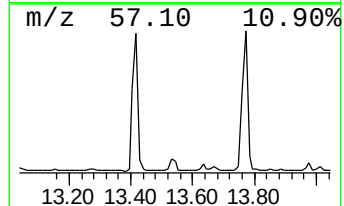
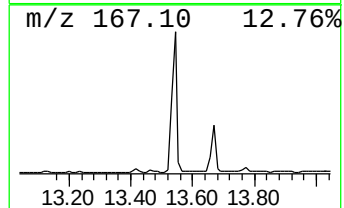
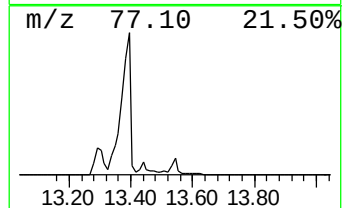
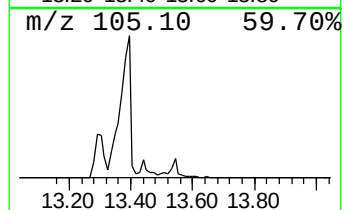
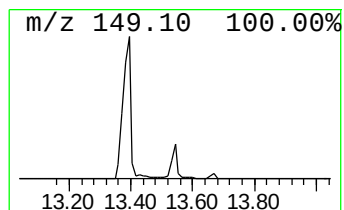
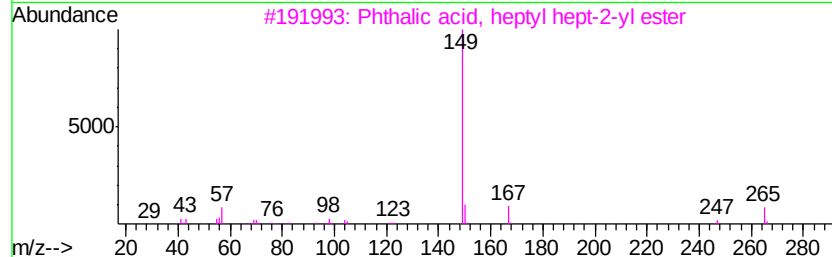
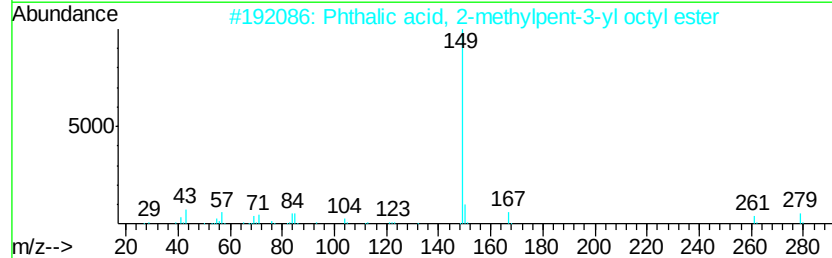
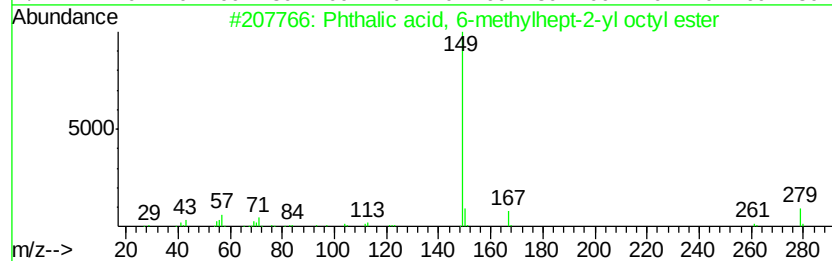
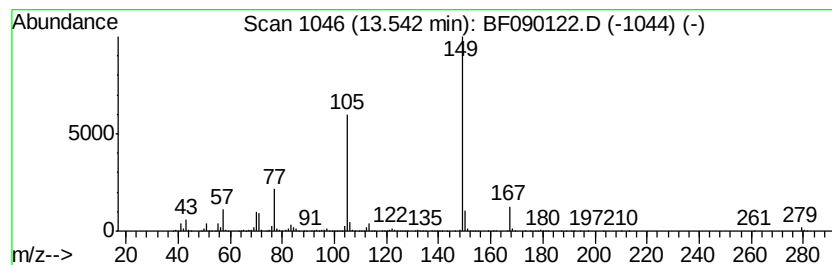
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Phthalic acid, 6-methylhept... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.54	19.22 ng	1557020	Chrysene-d12	13.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, 6-methylhept-2-yl...	390	C24H38O4	1000377-96-2	58
2		Phthalic acid, 2-methylpent-3-yl...	362	C22H34O4	1000356-91-3	53
3		Phthalic acid, heptyl hept-2-yl ...	362	C22H34O4	1000356-97-4	50
4		Phthalic acid, 2,3-dimethylpheny...	382	C24H30O4	1000357-09-0	50
5		Phthalic acid, heptyl 6-methylhe...	376	C23H36O4	1000377-96-1	50



Data Path : Z:\HPCHEM1\BNA_F\Data\BF091916\
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Misc :
ALS Vial : 4 Sample Multiplier: 1

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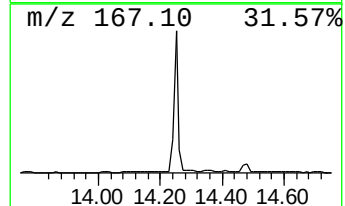
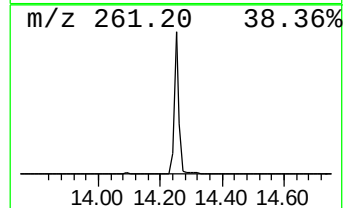
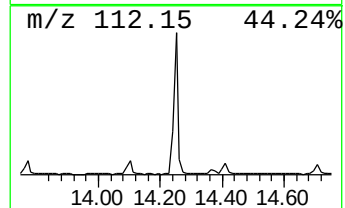
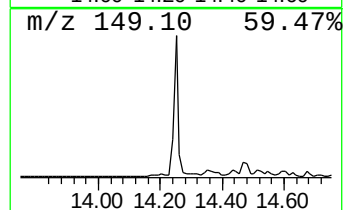
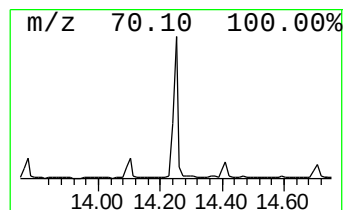
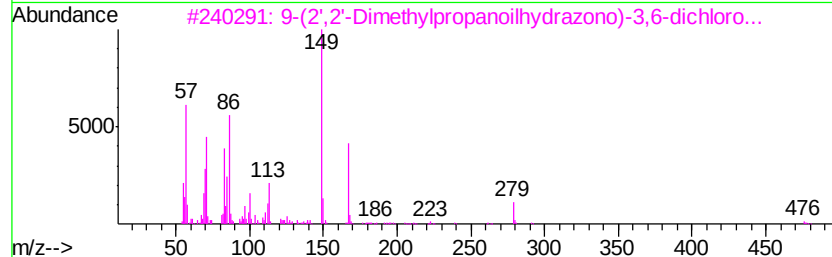
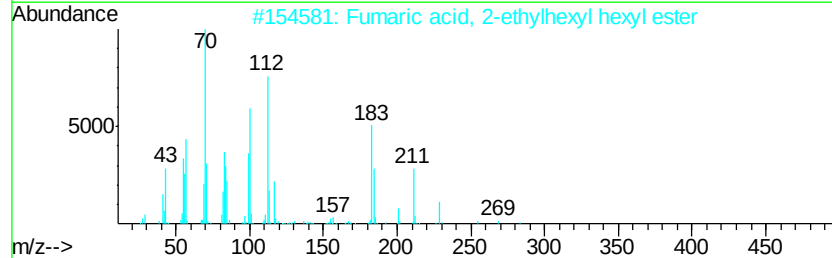
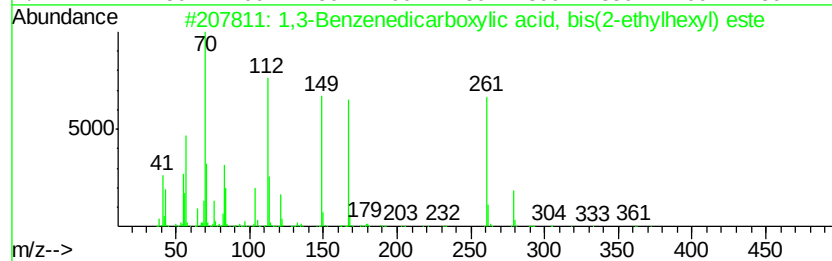
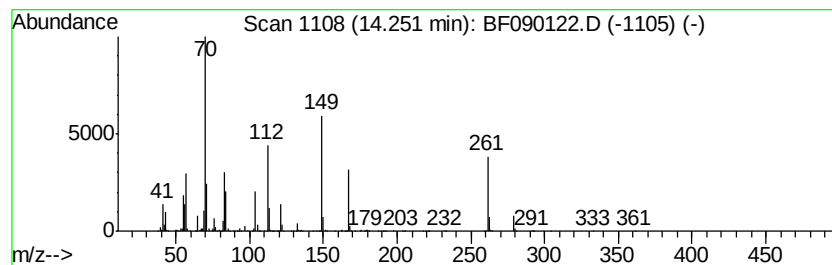
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 1,3-Benzenedicarboxylic aci... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.25	39.09 ng	3165930	Chrysene-d12	13.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	52
2		Fumaric acid, 2-ethylhexyl hexyl...	312	C18H32O4	1000339-14-1	22
3		9-(2',2'-Dimethylpropanoilhydraz...	576	C30H42Cl2N4O3	1000111-04-6	18
4		Cyclohexanamine, N-methyl-	113	C7H15N	000100-60-7	14
5		Diisooctyl phthalate	390	C24H38O4	000131-20-4	14



Data Path : Z:\HPCHEM1\BNA_F\Data\BF091916\
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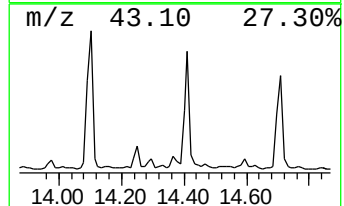
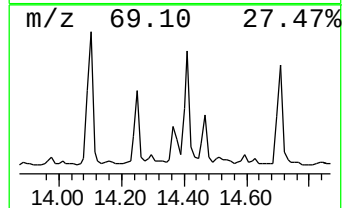
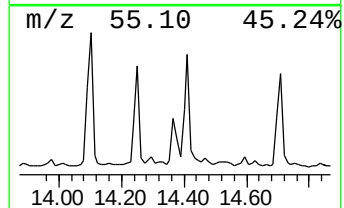
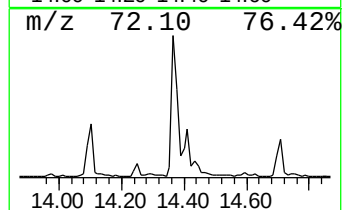
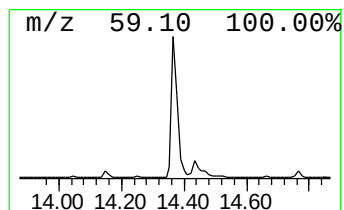
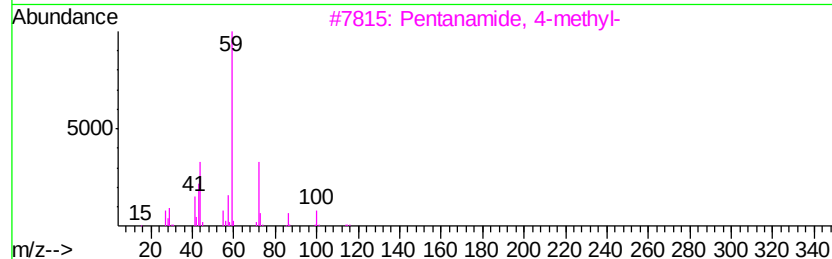
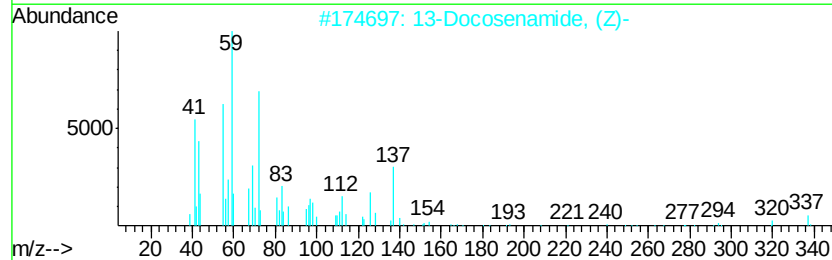
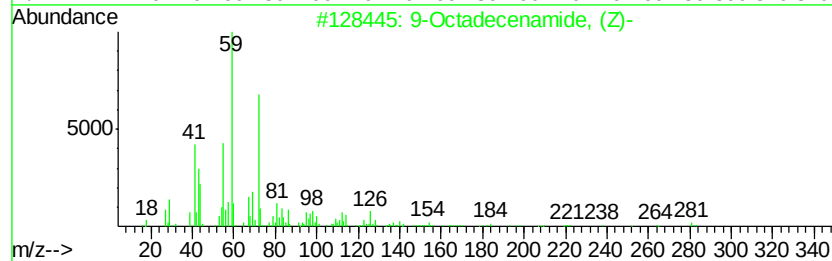
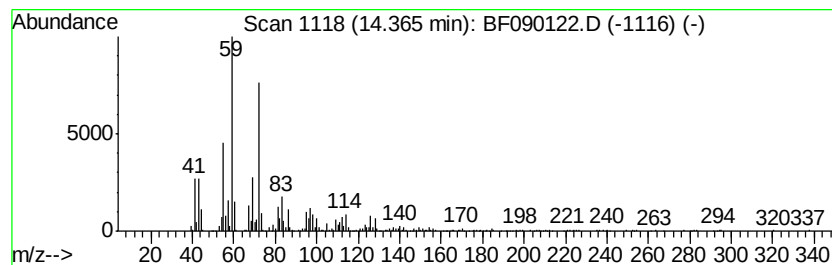
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 9-Octadecenamide, (Z)- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.37	19.32 ng	928545	Perylene-d12	14.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	72
3		Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	50
4		Hexadecanamide	255	C16H33NO	000629-54-9	47
5		Octadecanamide	283	C18H37NO	000124-26-5	47



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Acq On : 19 Sep 2016 16:03
Operator : UM/SJ
Sample : H4824-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
01

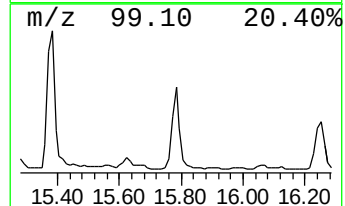
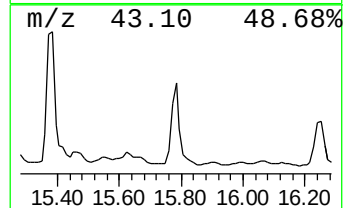
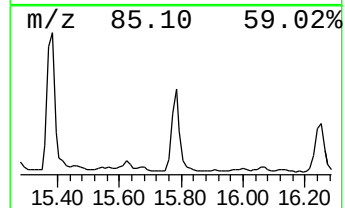
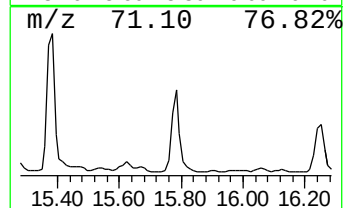
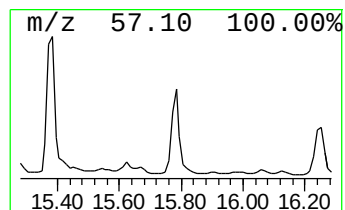
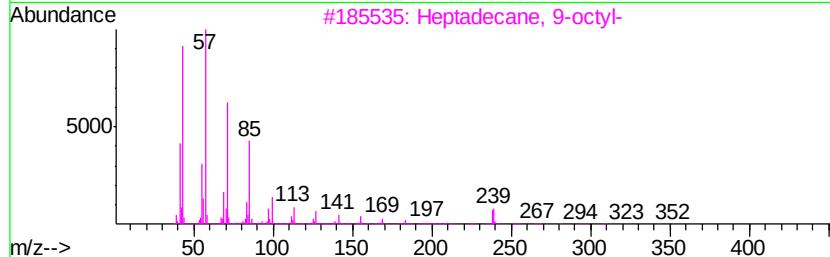
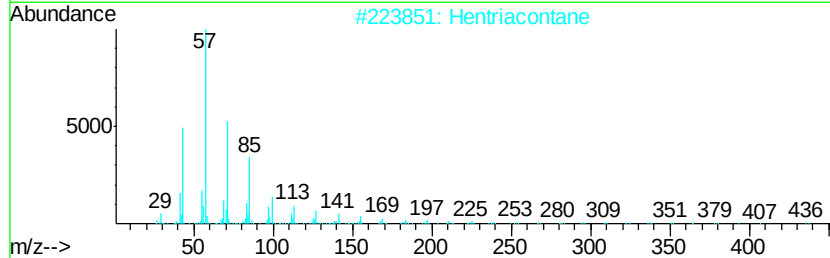
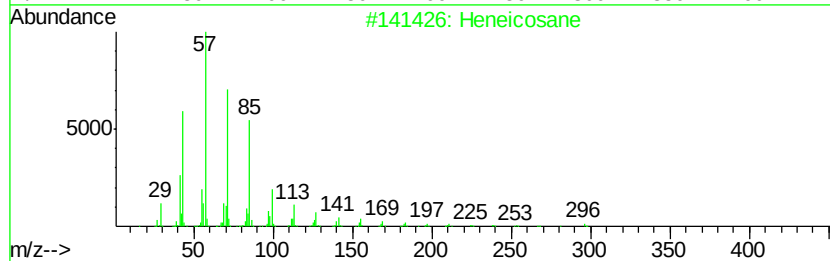
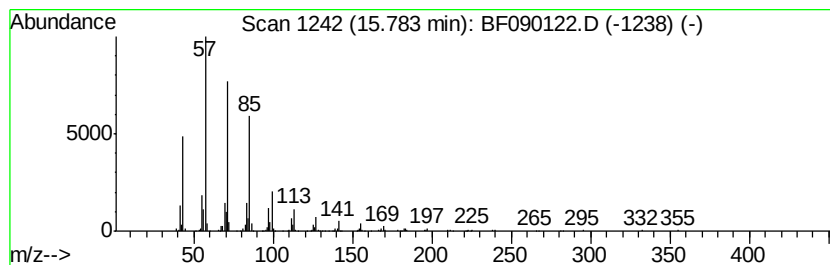
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Hentriacontane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.78	22.16 ng	1065160	Perylene-d12	14.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	90
2		Hentriacontane	437	C31H64	000630-04-6	80
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	80
4		Eicosane, 2-methyl-	296	C21H44	001560-84-5	80
5		Nonadecane	268	C19H40	000629-92-5	80



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 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091516.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
unknown6.30	6.30	68.4	ng	2815760	1	6.54	823033	20.0
n-Hexadecanoic acid	10.43	151.6	ng	9503320	4	11.04	1254080	20.0
9,12-Octadecadien...	11.70	14.4	ng	905516	4	11.04	1254080	20.0
Chloroacetic acid...	11.74	20.3	ng	1271980	4	11.04	1254080	20.0
Octadecanoic acid	11.94	273.6	ng	17155300	4	11.04	1254080	20.0
Heneicosane	13.03	42.1	ng	3414110	5	13.65	1619930	20.0
Morpholine, 4-phe...	13.29	33.4	ng	2706430	5	13.65	1619930	20.0
Diethylene glycol...	13.39	197.7	ng	16013200	5	13.65	1619930	20.0
Phthalic acid, 6-...	13.54	19.2	ng	1557020	5	13.65	1619930	20.0
1,3-Benzenedicarb...	14.25	39.1	ng	3165930	5	13.65	1619930	20.0
9-Octadecenamide, ...	14.37	19.3	ng	928545	6	14.97	961178	20.0
Hentriacontane	15.78	22.2	ng	1065160	6	14.97	961178	20.0