

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
 Data File : BF088627.D
 Acq On : 2 Jul 2016 20:04
 Operator : UM/SJ
 Sample : H3847-09
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S4-B3(0-12)C

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-BF063016.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	1.724	10	12	22	rVB	42554	98097	4.02%	0.431%
2	1.861	22	24	35	rVB	342222	609575	24.95%	2.678%
3	2.993	121	123	139	rBV	38770	106633	4.36%	0.469%
4	4.284	233	236	238	rVB	21404	30813	1.26%	0.135%
5	4.959	292	295	299	rBV	123715	165230	6.76%	0.726%
6	5.382	329	332	335	rBV	1734624	2151682	88.07%	9.454%
7	6.433	421	424	426	rBV	1743228	2443193	100.00%	10.735%
8	6.559	432	435	438	rBV	2362870	2162054	88.49%	9.499%
9	6.787	453	455	458	rBV	520279	691937	28.32%	3.040%
10	6.947	467	469	472	rVB	1801136	1704600	69.77%	7.489%
11	7.359	502	505	507	rBV	1707296	1620331	66.32%	7.119%
12	7.450	511	513	517	rBV	24163	25551	1.05%	0.112%
13	8.079	566	568	570	rBV	1195838	962474	39.39%	4.229%
14	9.153	660	662	665	rBV	2366300	2239003	91.64%	9.837%
15	9.553	695	697	699	rBV	475443	470945	19.28%	2.069%
16	9.828	719	721	723	rBV	1062904	916135	37.50%	4.025%
17	10.616	787	790	792	rBV	1005525	1208637	49.47%	5.310%
18	10.742	800	801	806	rVB	38174	39726	1.63%	0.175%
19	11.188	838	840	842	rBV	81393	80886	3.31%	0.355%
20	11.302	848	850	853	rBV	703301	738350	30.22%	3.244%
21	11.371	853	856	860	rVB2	23359	49603	2.03%	0.218%
22	11.542	869	871	876	rVV3	15643	30449	1.25%	0.134%
23	11.611	876	877	884	rVB	54422	77871	3.19%	0.342%
24	11.839	895	897	899	rBV	40759	41411	1.69%	0.182%
25	12.514	953	956	958	rBV	90063	90615	3.71%	0.398%
26	12.731	973	975	978	rBV	65036	100185	4.10%	0.440%
27	12.891	987	989	991	rBV	1751207	1561292	63.90%	6.860%
28	13.131	1006	1010	1012	rBV2	21634	30697	1.26%	0.135%
29	13.679	1056	1058	1059	rBV2	16696	27098	1.11%	0.119%
30	13.714	1059	1061	1065	rVV5	23188	63777	2.61%	0.280%
31	13.794	1066	1068	1072	rVB2	110495	140077	5.73%	0.615%
32	13.931	1077	1080	1085	rVB	803368	834825	34.17%	3.668%
33	14.114	1095	1096	1102	rBV4	14521	34247	1.40%	0.150%
34	14.434	1121	1124	1128	rBV4	27004	83703	3.43%	0.368%

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Integrator: RTE
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Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
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35	14.720	1147	1149	1152	rBV3	22861	48980	2.00%	0.215%
36	14.788	1153	1155	1159	rVB	48138	66044	2.70%	0.290%
37	14.857	1159	1161	1163	rBV2	20038	31673	1.30%	0.139%
38	14.937	1165	1168	1174	rBV	61248	135527	5.55%	0.595%
39	15.028	1174	1176	1182	rBV2	26989	67809	2.78%	0.298%
40	15.211	1190	1192	1195	rVB	35179	46635	1.91%	0.205%
41	15.268	1195	1197	1199	rBV	38610	40990	1.68%	0.180%
42	15.325	1199	1202	1205	rBV	433905	606644	24.83%	2.665%
43	15.794	1240	1243	1245	rBV	28777	47660	1.95%	0.209%
44	16.663	1317	1319	1322	rVB2	20192	36265	1.48%	0.159%

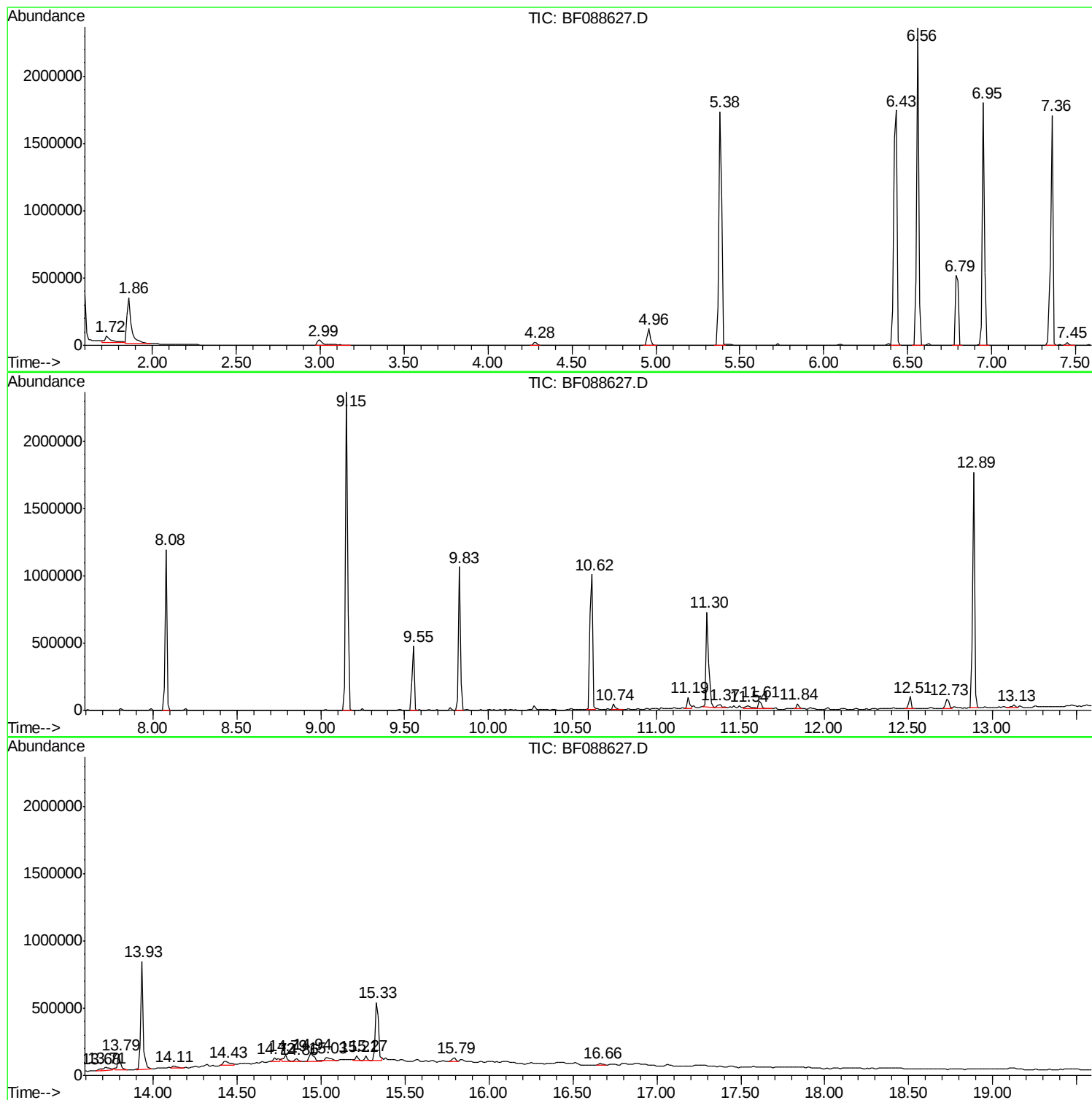
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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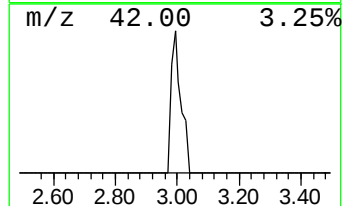
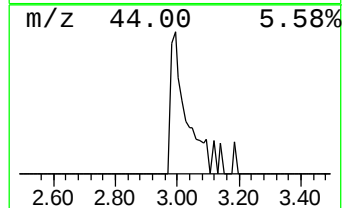
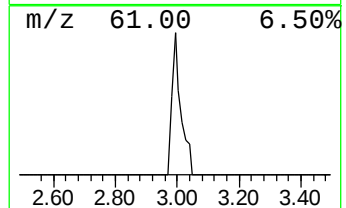
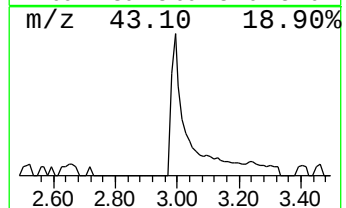
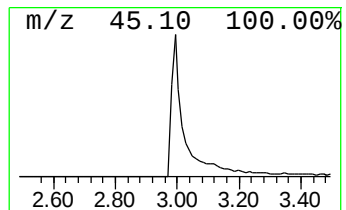
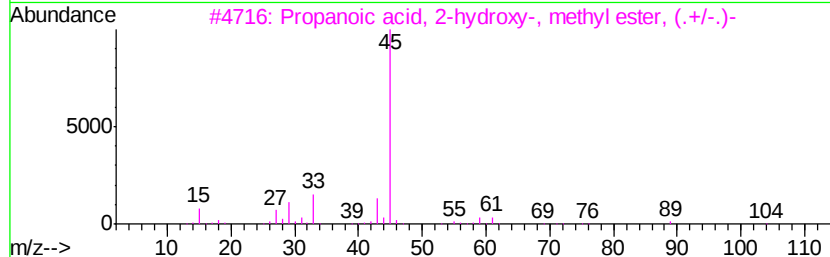
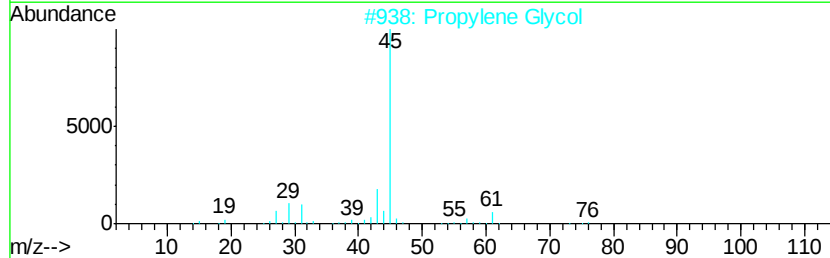
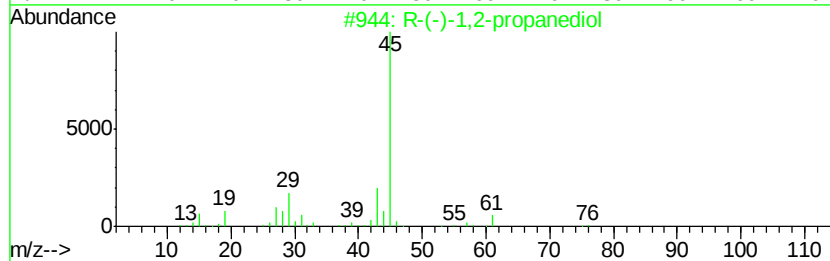
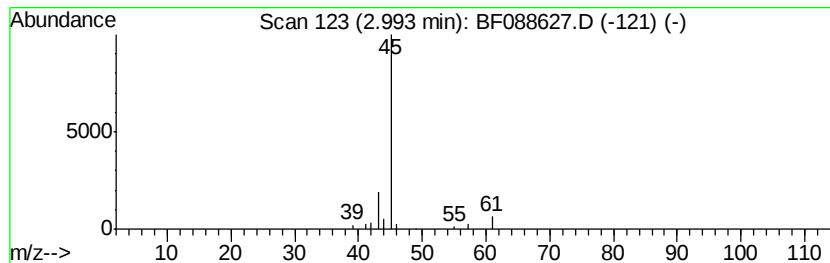
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TIC Library : C:\Database\NIST11.L
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Peak Number 3 R-(-)-1,2-propanediol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	3.08 ng	106633	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
2		Propylene Glycol	76	C3H8O2	000057-55-6	9
3		Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9
4		Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9



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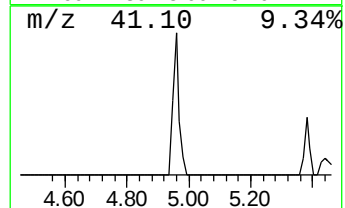
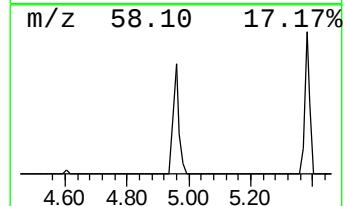
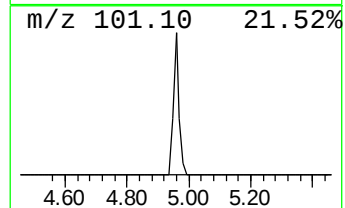
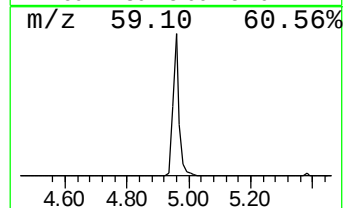
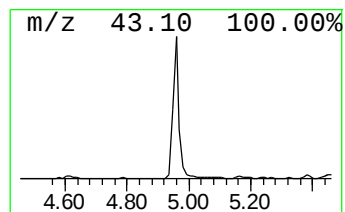
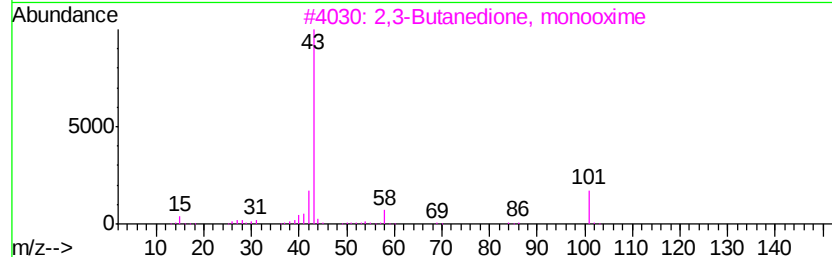
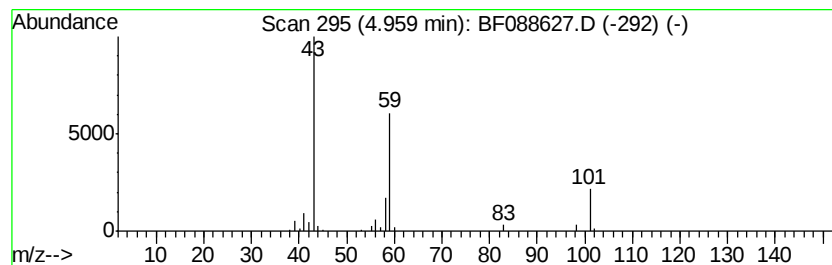
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	4.78 ng	165230	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
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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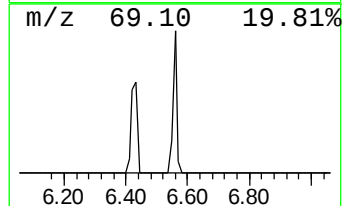
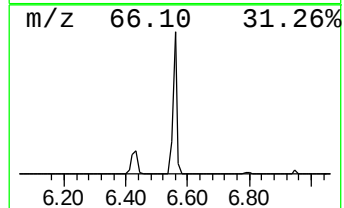
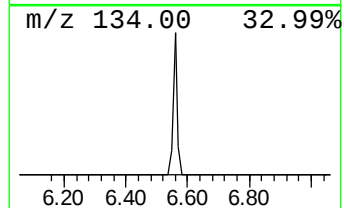
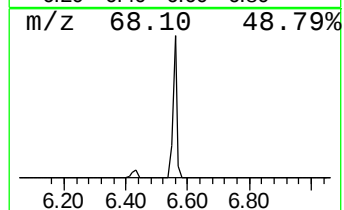
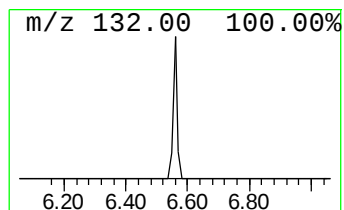
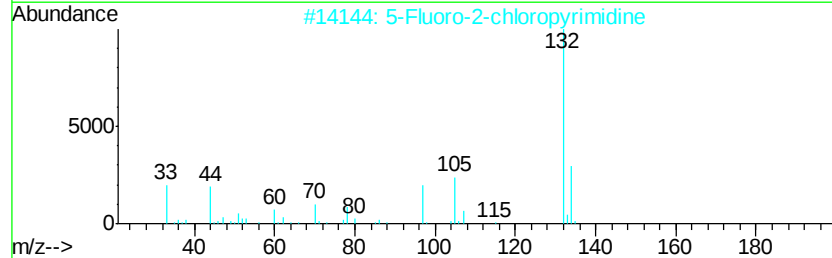
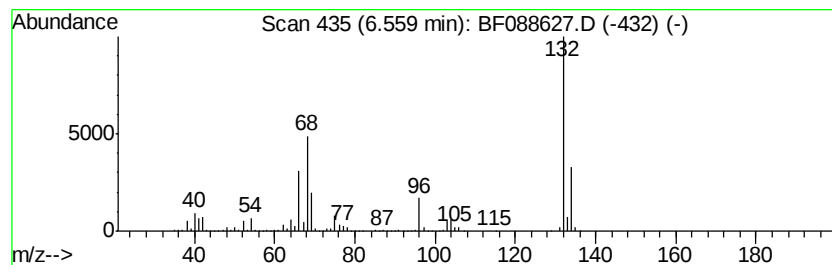
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	62.49 ng	2162050	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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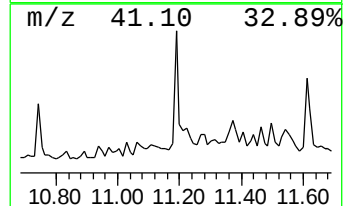
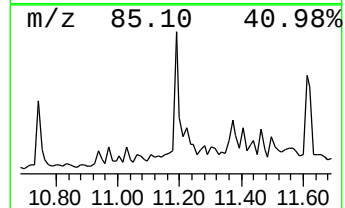
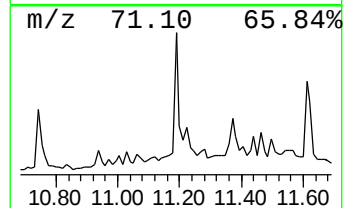
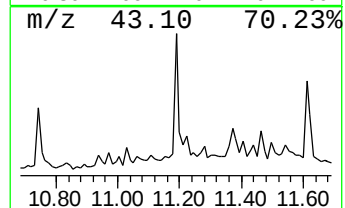
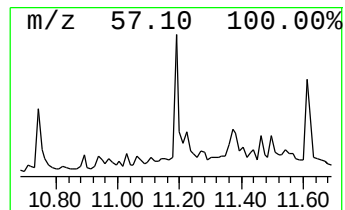
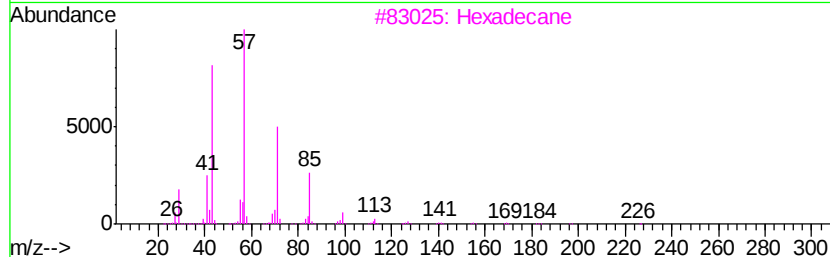
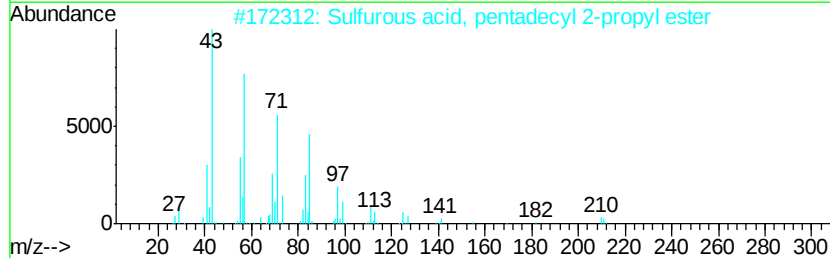
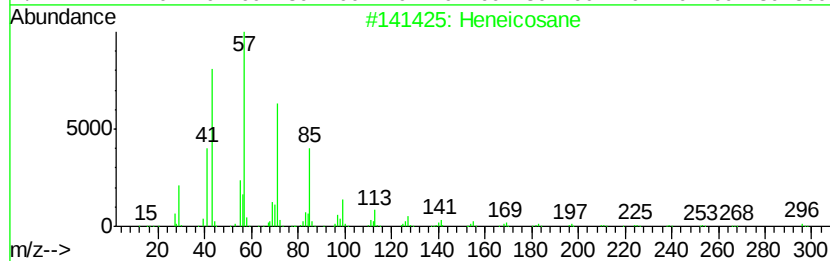
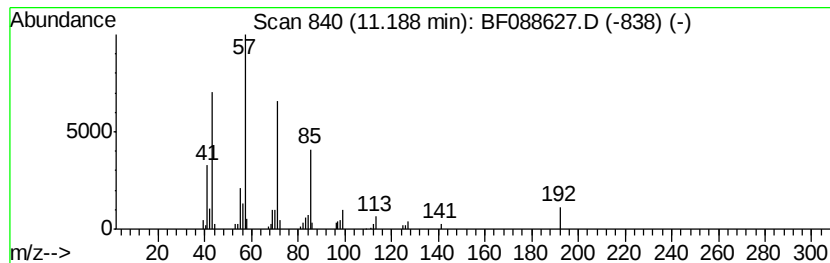
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TIC Library : C:\Database\NIST11.L
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Peak Number 7 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.19	2.19 ng	80886	Phenanthrene-d10	11.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	87
2		Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	86
3		Hexadecane	226	C16H34	000544-76-3	86
4		Octadecane	254	C18H38	000593-45-3	86
5		Tetratetracontane	619	C44H90	007098-22-8	80



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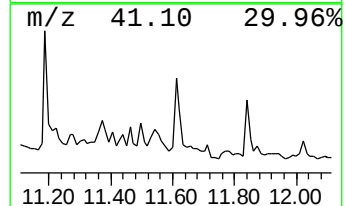
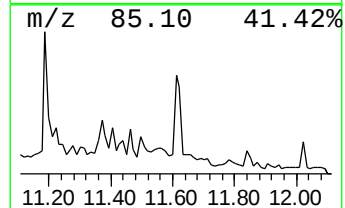
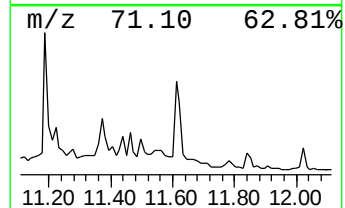
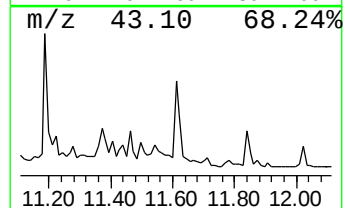
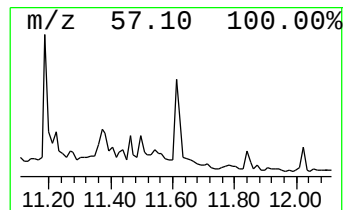
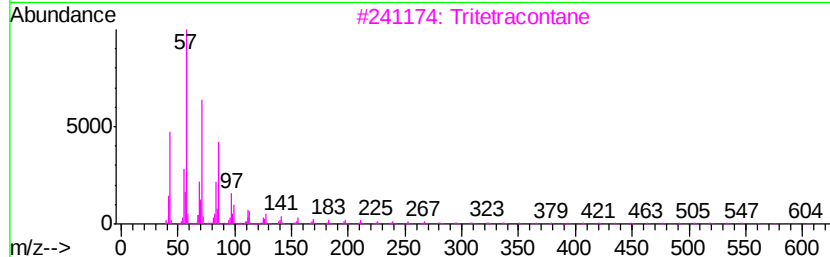
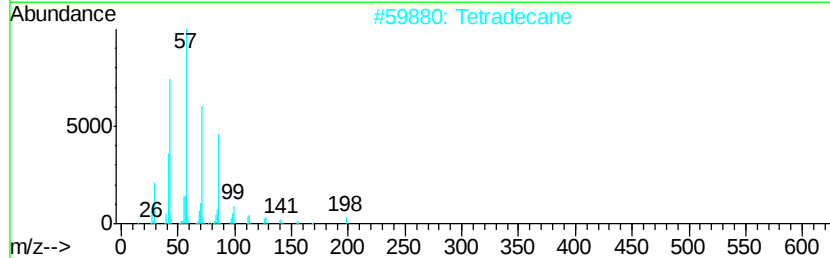
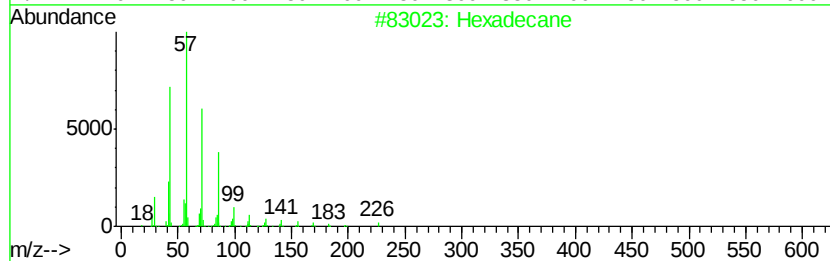
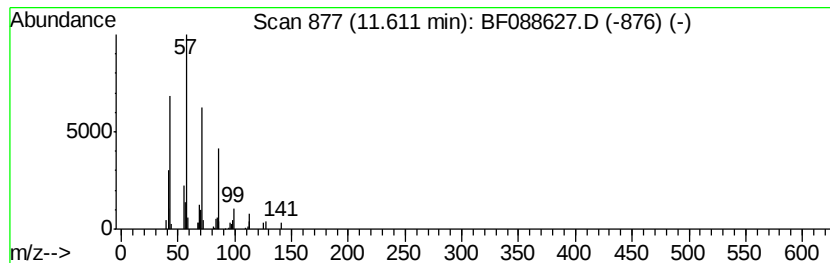
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Peak Number 8 Hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.61	2.11 ng	77871	Phenanthrene-d10	11.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	90
2		Tetradecane	198	C14H30	000629-59-4	90
3		Tritetracontane	605	C43H88	007098-21-7	90
4		Octacosane	394	C28H58	000630-02-4	87
5		Heneicosane	296	C21H44	000629-94-7	87



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ALS Vial : 18 Sample Multiplier: 1

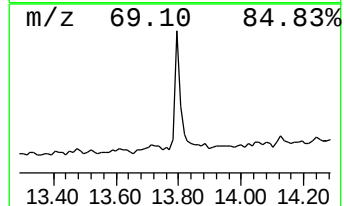
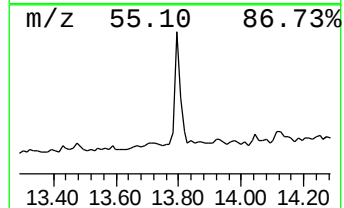
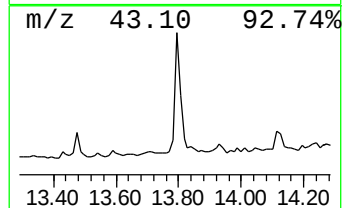
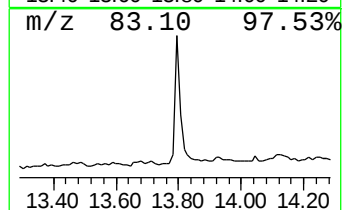
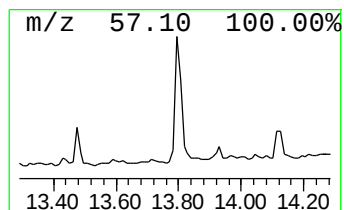
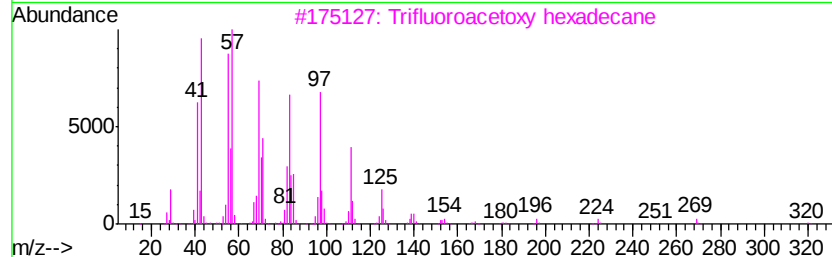
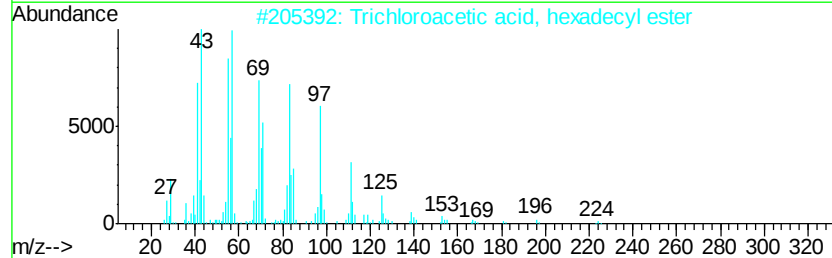
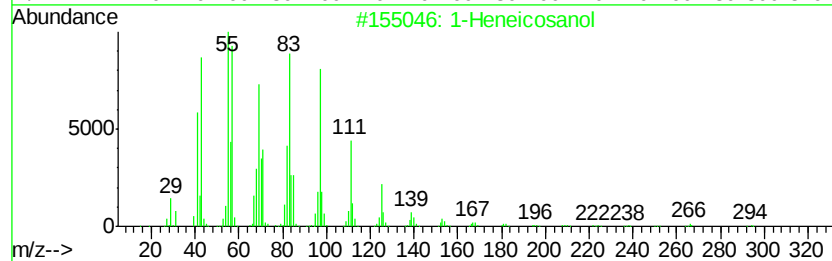
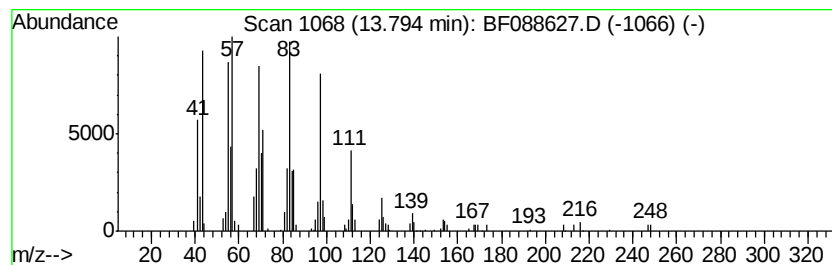
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ClientSampleId :
S4-B3(0-12)C

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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 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.79	3.36 ng	140077	Chrysene-d12	13.93	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
Data File : BF088627.D
Acq On : 2 Jul 2016 20:04
Operator : UM/SJ
Sample : H3847-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S4-B3(0-12)C

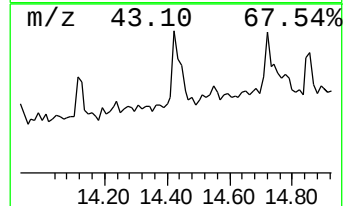
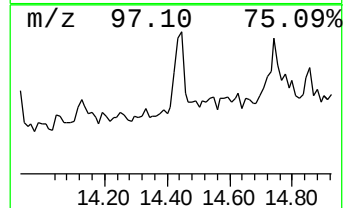
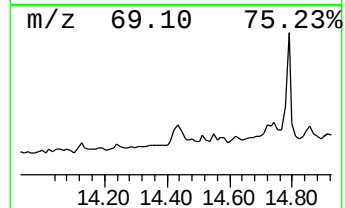
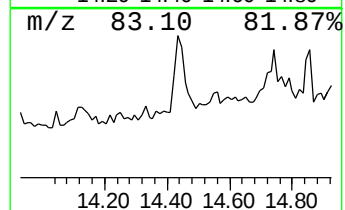
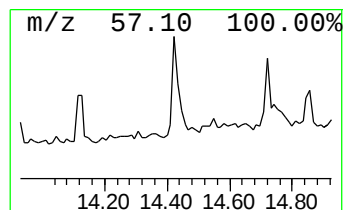
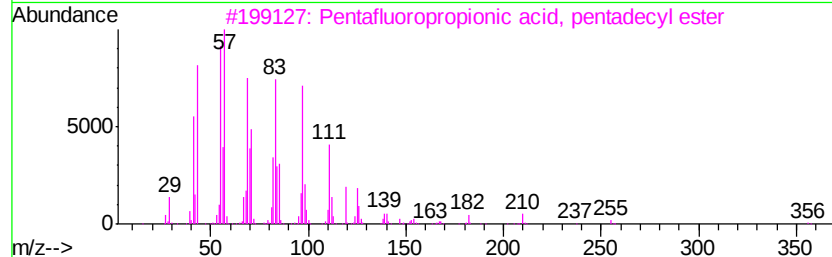
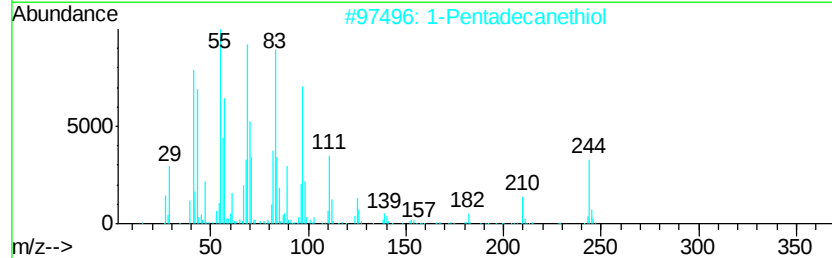
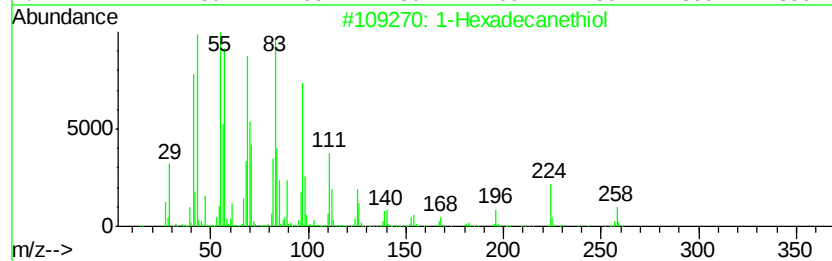
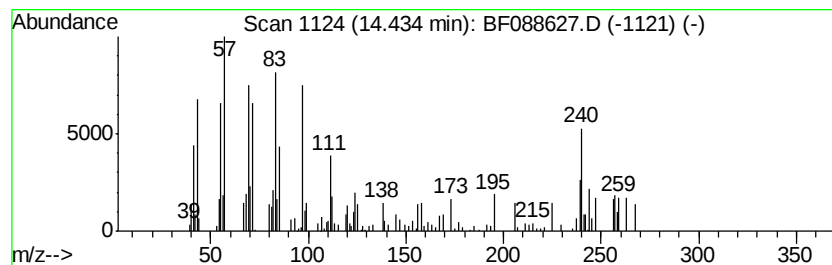
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Hexadecanethiol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.43	2.01 ng	83703	Chrysene-d12	13.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexadecanethiol	258	C16H34S	002917-26-2	64
2		1-Pentadecanethiol	244	C15H32S	025276-70-4	59
3		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	59
4		Dodecane, 6-cyclohexyl-	252	C18H36	013151-86-5	43
5		Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
Data File : BF088627.D
Acq On : 2 Jul 2016 20:04
Operator : UM/SJ
Sample : H3847-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S4-B3(0-12)C

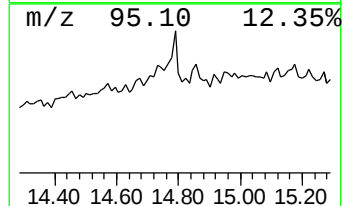
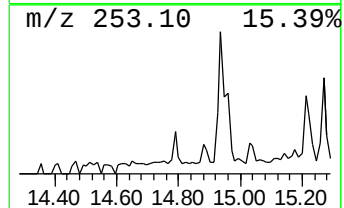
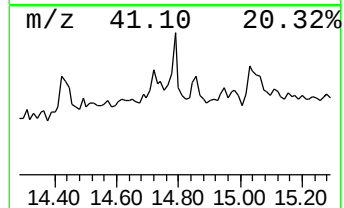
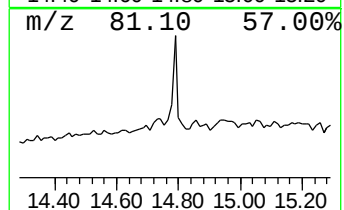
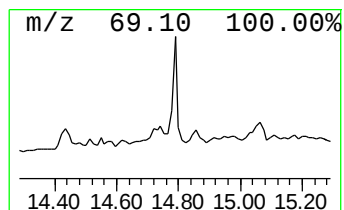
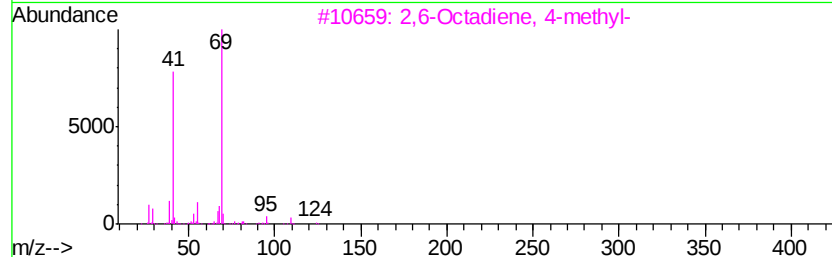
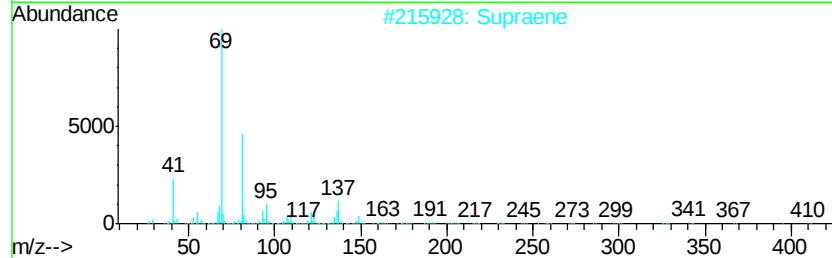
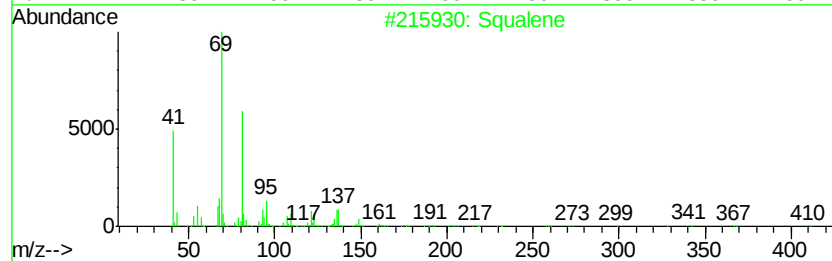
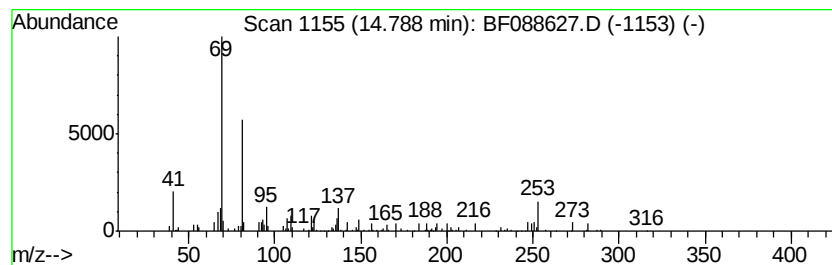
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Squalene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	2.18 ng	66044	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	60
2		Supraene	410	C30H50	007683-64-9	53
3		2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	47
4		2,6-Octadiene, 4,5-dimethyl-	138	C10H18	018476-57-8	47
5		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
Data File : BF088627.D
Acq On : 2 Jul 2016 20:04
Operator : UM/SJ
Sample : H3847-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

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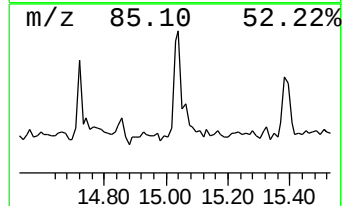
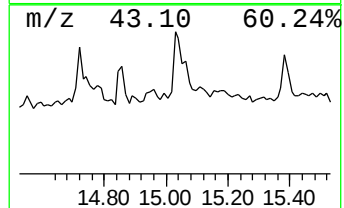
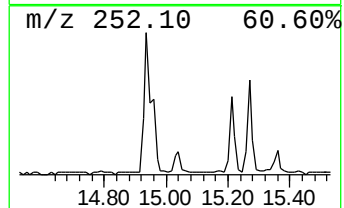
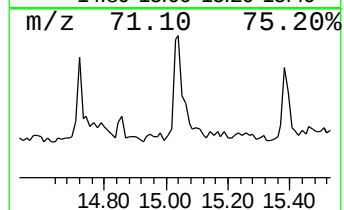
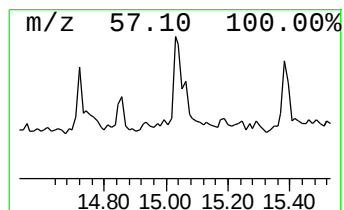
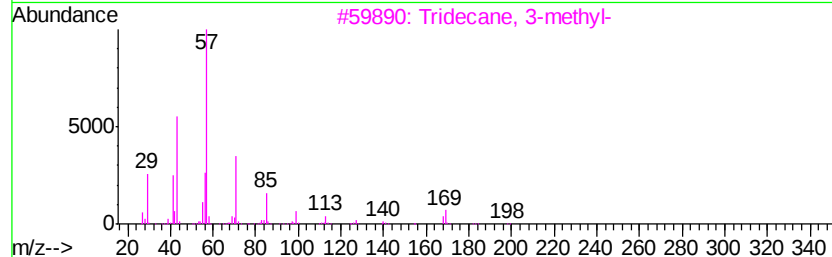
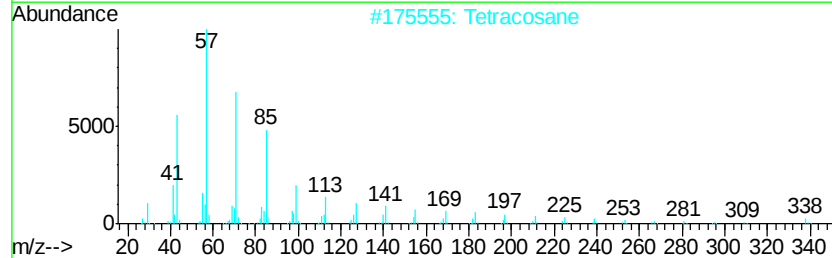
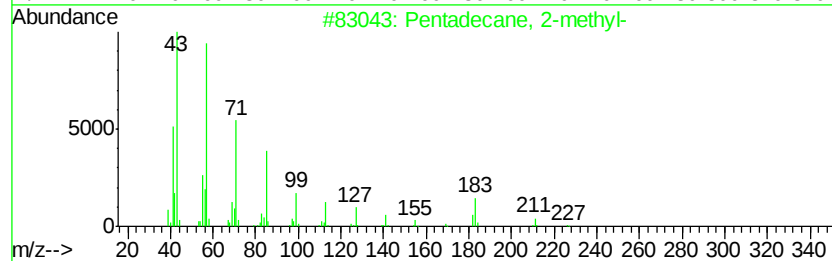
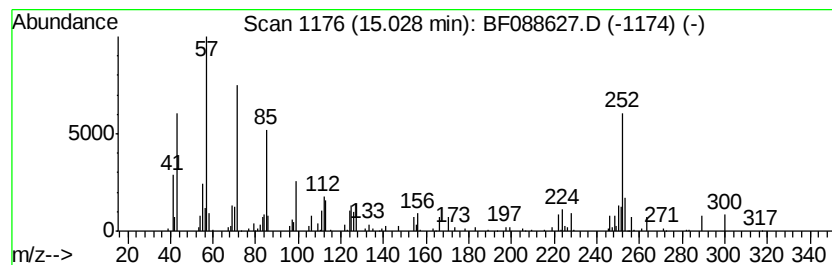
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Pentadecane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.03	2.24 ng	67809	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 2-methyl-	226	C16H34	001560-93-6	60
2		Tetracosane	338	C24H50	000646-31-1	47
3		Tridecane, 3-methyl-	198	C14H30	006418-41-3	47
4		Docosane	310	C22H46	000629-97-0	43
5		Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
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Acq On : 2 Jul 2016 20:04
Operator : UM/SJ
Sample : H3847-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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
R-(-)-1,2-propane...	2.99	3.1 ng		106633	1	6.80	691937	20.0
2-Pentanone, 4-hy...	4.96	4.8 ng		165230	1	6.80	691937	20.0
unknown6.56	6.56	62.5 ng		2162050	1	6.80	691937	20.0
Heneicosane	11.19	2.2 ng		80886	4	11.30	738350	20.0
Hexadecane	11.61	2.1 ng		77871	4	11.30	738350	20.0
1-Heneicosanol	13.79	3.4 ng		140077	5	13.93	834825	20.0
1-Hexadecanethiol	14.43	2.0 ng		83703	5	13.93	834825	20.0
Squalene	14.79	2.2 ng		66044	6	15.33	606644	20.0
Pentadecane, 2-me...	15.03	2.2 ng		67809	6	15.33	606644	20.0