

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010416\
 Data File : BF084251.D
 Acq On : 4 Jan 2016 20:52
 Operator : UM/SJ
 Sample : G4987-01
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DRUM(116-142)COMPOSITE

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-BF123115.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	2.167	5	7	13	rVB2	64063	124243	2.04%	0.205%
2	2.258	13	15	20	rVB2	42026	76402	1.25%	0.126%
3	2.396	20	27	28	rBV	115393	506751	8.31%	0.838%
4	5.082	260	262	265	rVB	1329428	1559392	25.58%	2.579%
5	5.516	297	300	302	rBV	4798130	5924812	97.17%	9.800%
6	6.465	381	383	385	rBV	532142	646450	10.60%	1.069%
7	6.545	387	390	395	rVB	4117324	6097151	100.00%	10.085%
8	6.670	398	401	403	rBV	4136568	5919976	97.09%	9.792%
9	6.887	418	420	422	rBV	1849630	1575760	25.84%	2.606%
10	7.047	431	434	436	rBV	4963919	4469267	73.30%	7.392%
11	7.082	436	437	440	rVB	58792	64984	1.07%	0.107%
12	7.459	467	470	472	rVB	3400246	4028538	66.07%	6.663%
13	7.550	475	478	482	rVB	90551	113657	1.86%	0.188%
14	7.916	505	510	513	rVB2	58979	70522	1.16%	0.117%
15	8.088	523	525	527	rBV	298123	270993	4.44%	0.448%
16	8.179	530	533	535	rBV	2242903	2213585	36.31%	3.661%
17	8.248	537	539	542	rBV	413901	386562	6.34%	0.639%
18	9.253	624	627	630	rBV	6506945	6030660	98.91%	9.975%
19	9.653	659	662	664	rBV	2122088	1887479	30.96%	3.122%
20	9.688	664	665	668	rVV	75788	86833	1.42%	0.144%
21	9.745	668	670	672	rVB	66338	82828	1.36%	0.137%
22	9.871	677	681	684	rBV3	48802	87809	1.44%	0.145%
23	9.928	684	686	689	rVB	1952164	2204814	36.16%	3.647%
24	10.076	697	699	701	rBV	215781	193197	3.17%	0.320%
25	10.293	716	718	721	rBV	127535	137770	2.26%	0.228%
26	10.362	721	724	726	rVV2	119344	139785	2.29%	0.231%
27	10.579	740	743	747	rBV	33818	67057	1.10%	0.111%
28	10.716	753	755	758	rBV2	3268799	3841747	63.01%	6.354%
29	10.842	764	766	772	rVB	103291	159999	2.62%	0.265%
30	11.265	801	803	804	rBV	70909	78122	1.28%	0.129%
31	11.288	804	805	806	rVB	93098	66578	1.09%	0.110%
32	11.414	814	816	819	rBV	2352392	2066327	33.89%	3.418%
33	11.642	833	836	840	rBV	88624	133162	2.18%	0.220%
34	13.002	952	955	957	rBV	5364326	4706428	77.19%	7.785%

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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

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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.905	1031	1034	1039	rBV	129087	162427	2.66%	0.269%
36	14.054	1044	1047	1049	rBV	1306897	1474578	24.18%	2.439%
37	14.522	1087	1088	1090	rBV	56112	83178	1.36%	0.138%
38	14.831	1113	1115	1117	rVB	77339	71875	1.18%	0.119%
39	14.900	1119	1121	1124	rBV	98908	147172	2.41%	0.243%
40	15.163	1141	1144	1146	rBV	98663	112415	1.84%	0.186%
41	15.494	1170	1173	1175	rBV	1004168	1374148	22.54%	2.273%
42	15.528	1175	1176	1180	rVB	106376	145490	2.39%	0.241%
43	15.963	1211	1214	1216	rBV	98152	175147	2.87%	0.290%
44	16.443	1253	1256	1261	rBV	100200	197987	3.25%	0.327%
45	17.026	1304	1307	1310	rBV	82241	166682	2.73%	0.276%
46	17.711	1363	1367	1372	rVB	70964	175990	2.89%	0.291%
47	18.511	1434	1437	1442	rVB2	52238	152173	2.50%	0.252%

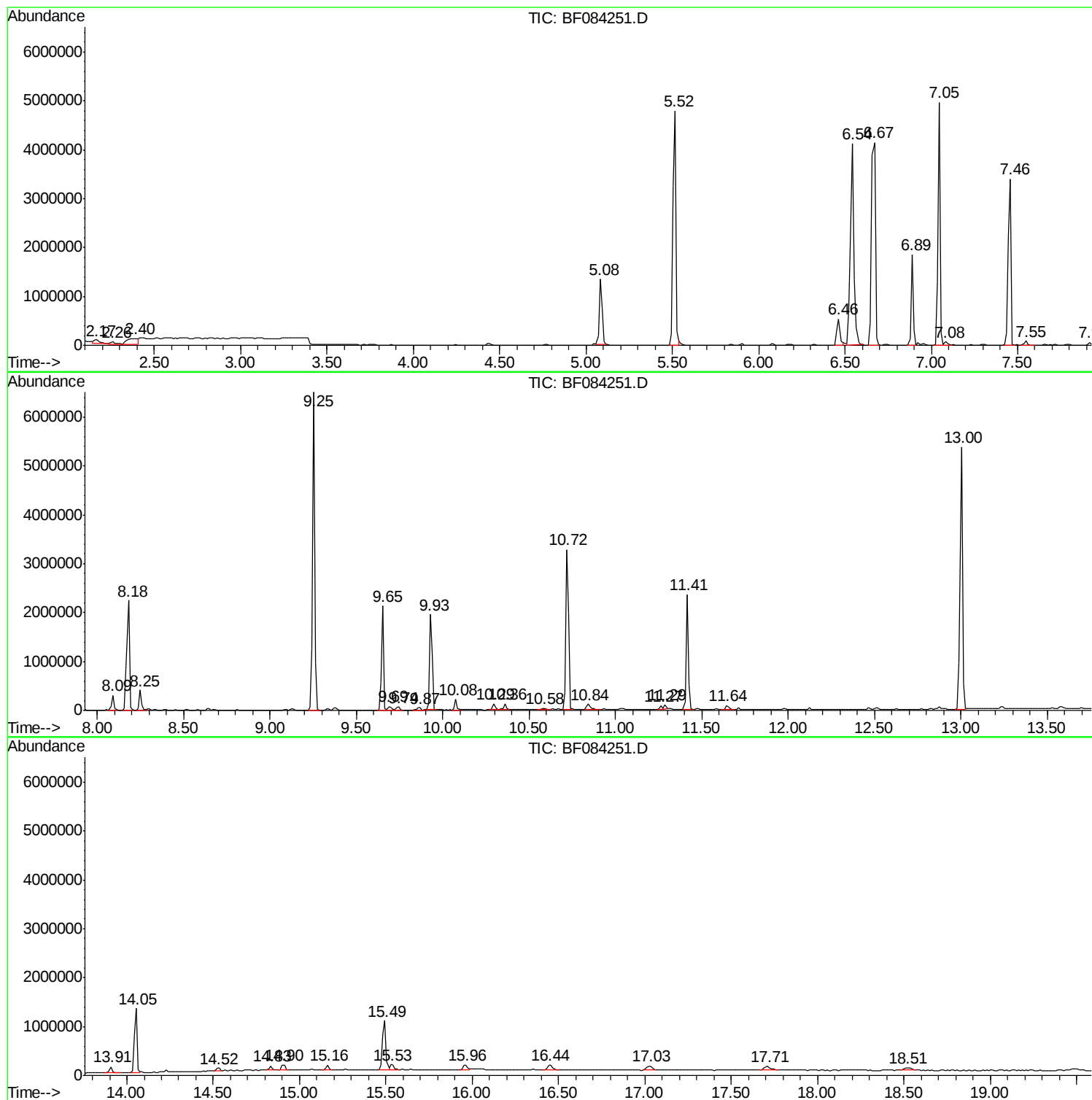
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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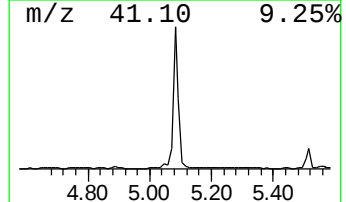
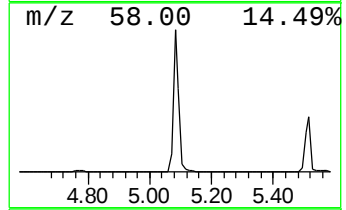
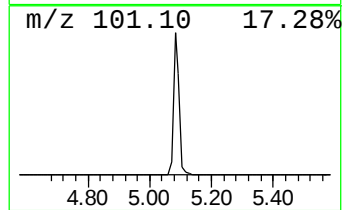
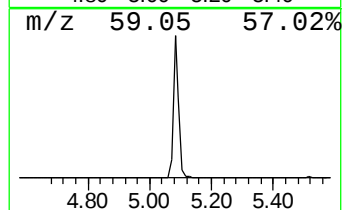
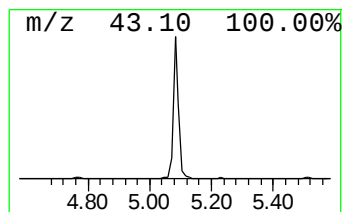
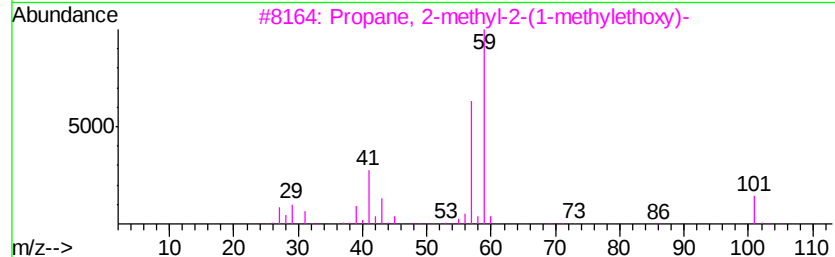
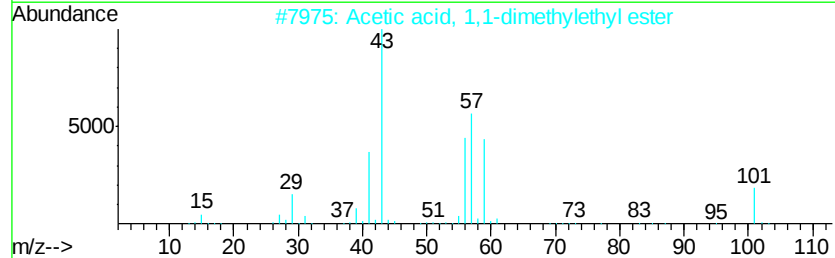
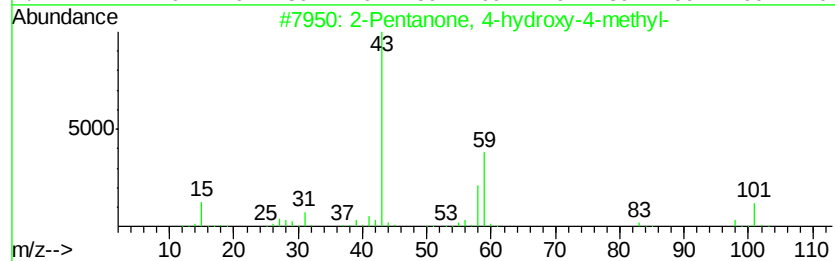
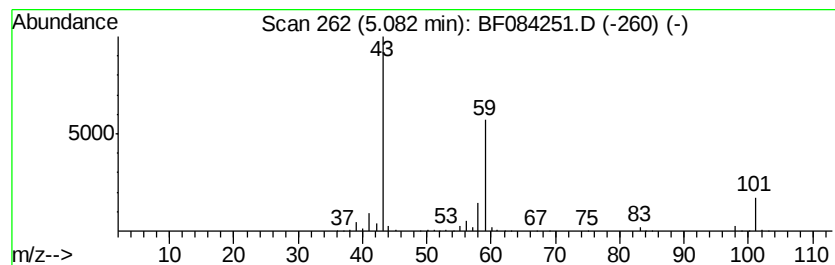
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	19.79 ng	1559390	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32



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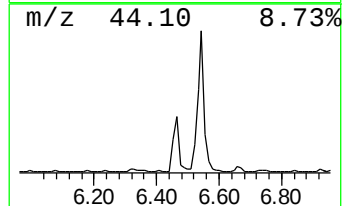
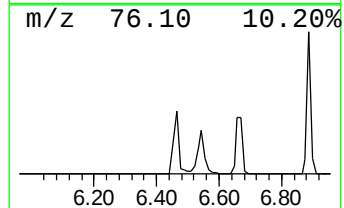
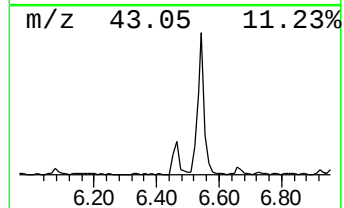
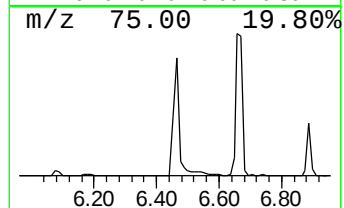
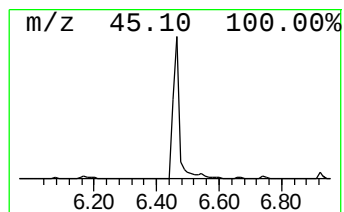
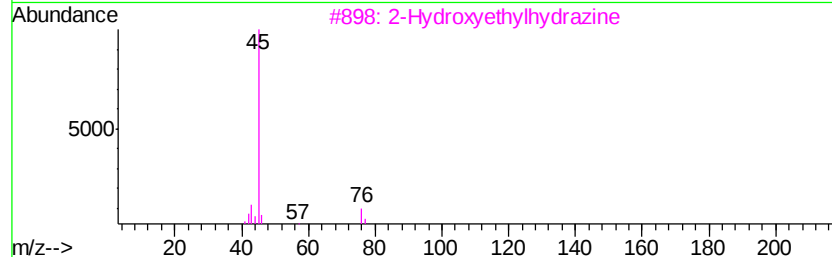
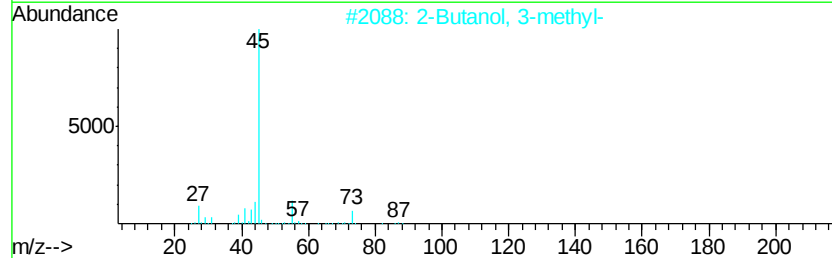
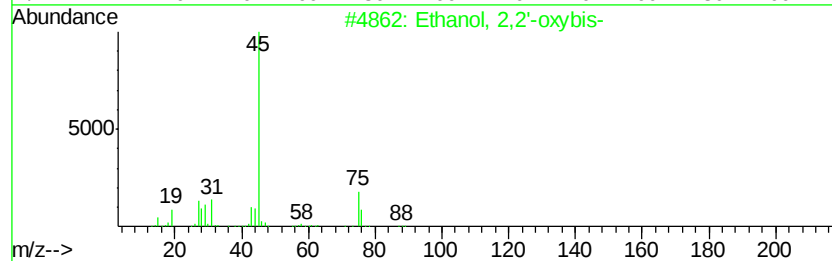
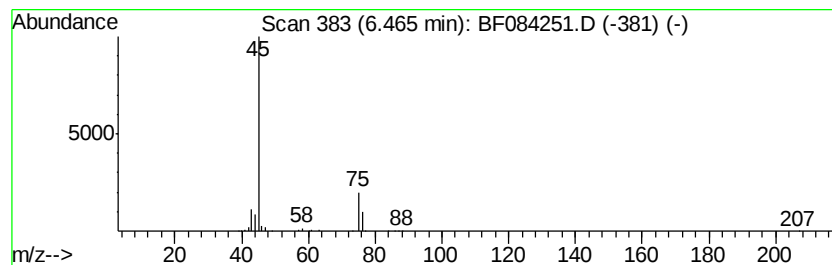
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2,2'-oxybis- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	8.20 ng	646450	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2,2'-oxybis-	106	C4H10O3	000111-46-6	83
2		2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	42
3		2-Hydroxyethylhydrazine	76	C2H8N2O	000109-84-2	9
4		Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5		Ethanol, 2-methoxy-	76	C3H8O2	000109-86-4	9



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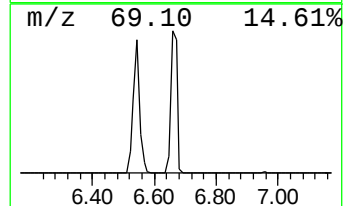
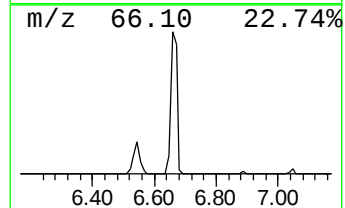
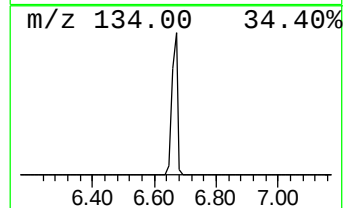
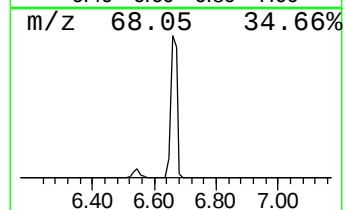
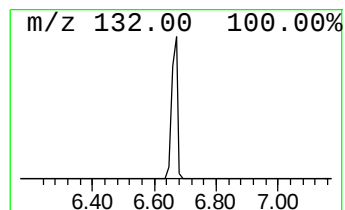
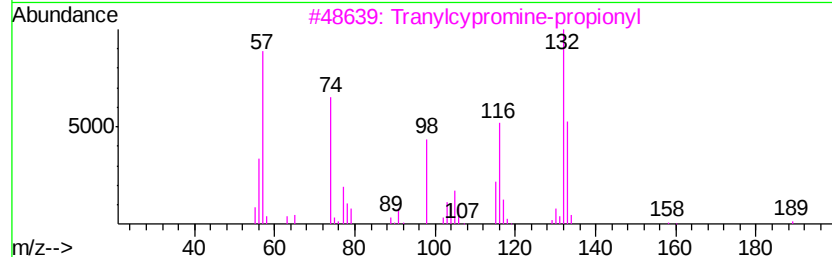
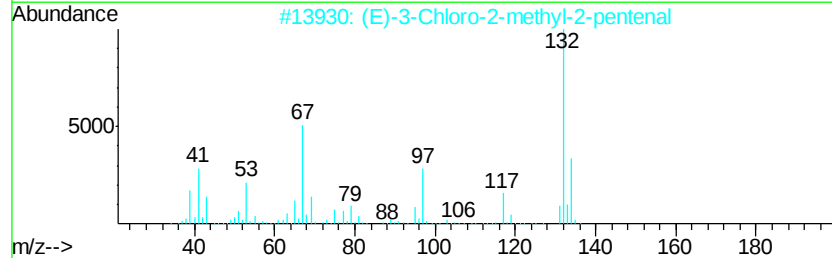
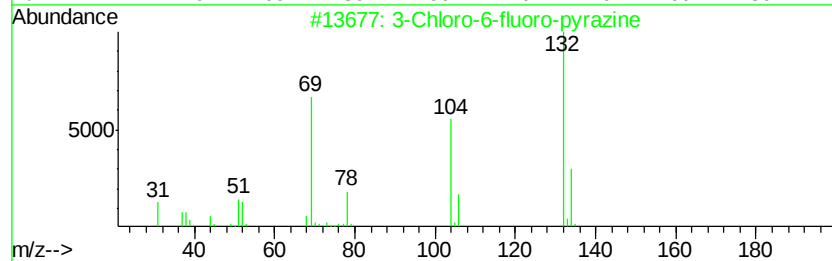
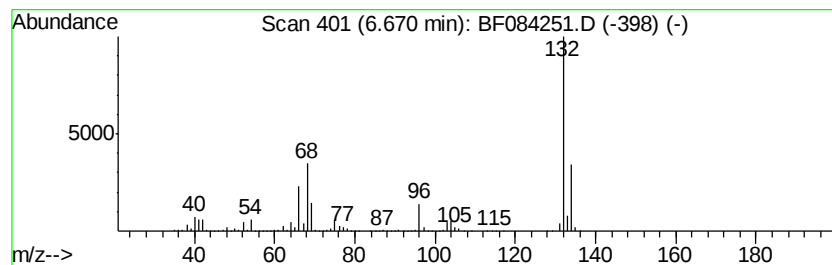
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	75.14 ng	5919980	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	16
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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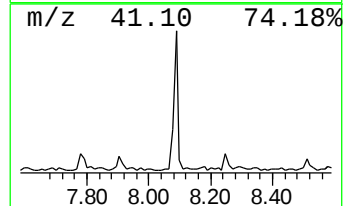
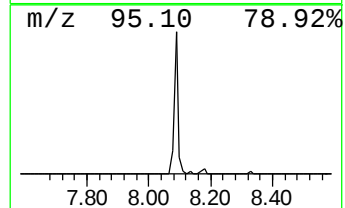
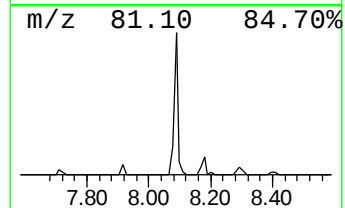
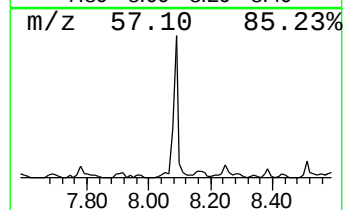
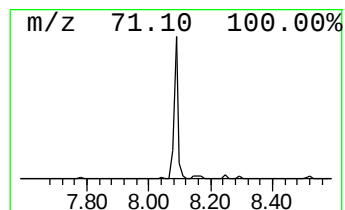
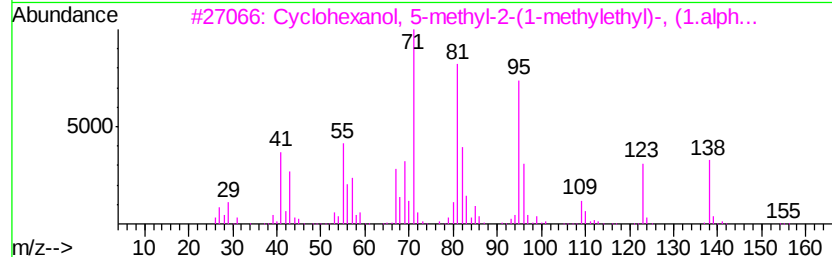
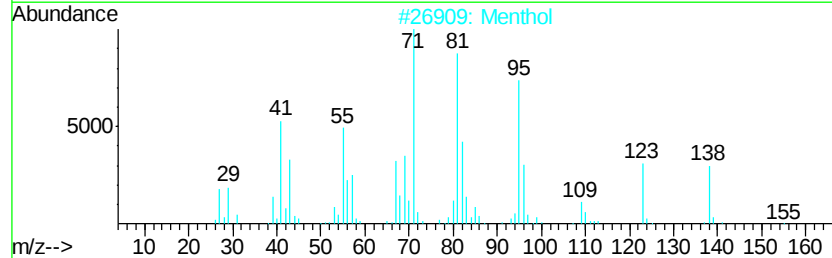
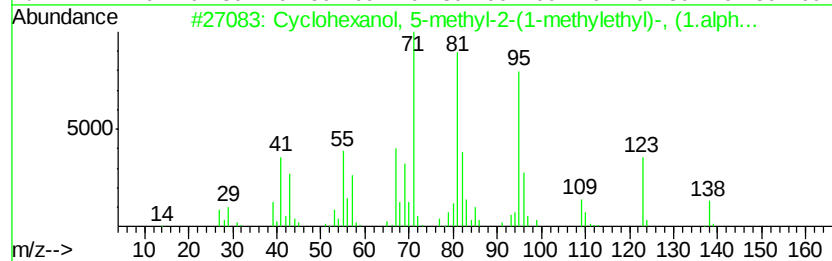
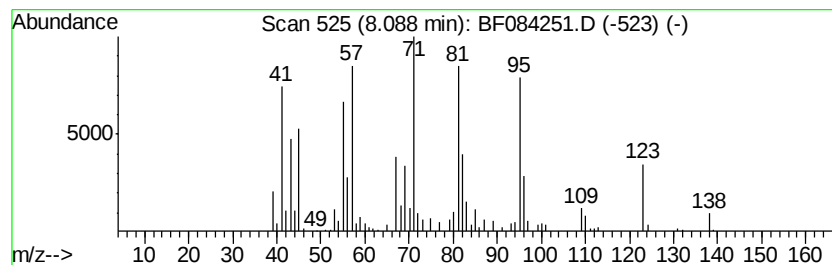
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Cyclohexanol, 5-methyl-2-(1... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.09	2.45 ng	270993	Naphthalene-d8	8.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	015356-70-4	90
2		Menthol	156	C10H20O	001490-04-6	83
3		Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	000089-78-1	83
4		Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	002216-51-5	83
5		Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	002216-52-6	80



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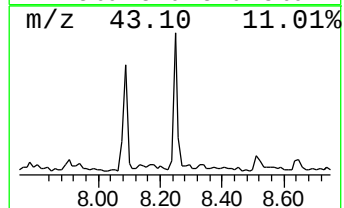
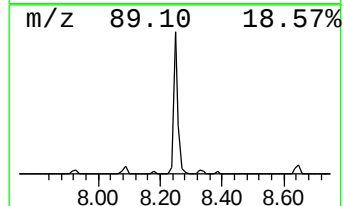
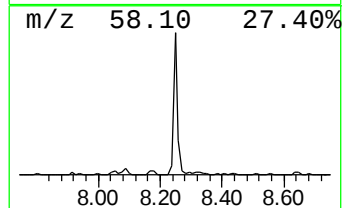
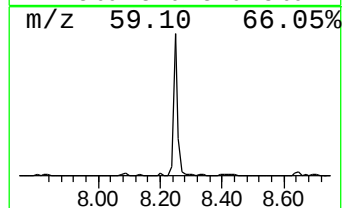
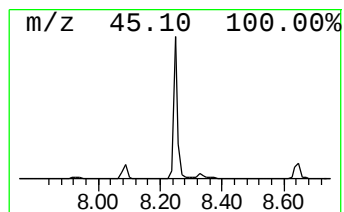
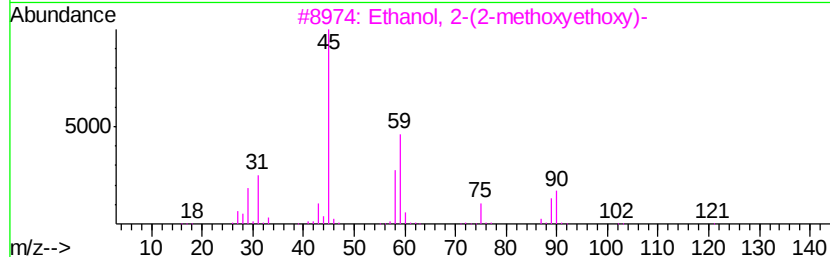
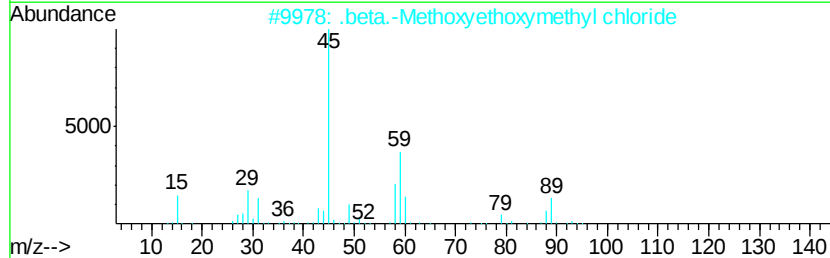
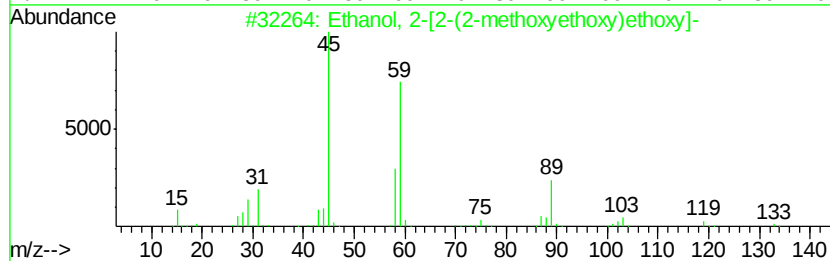
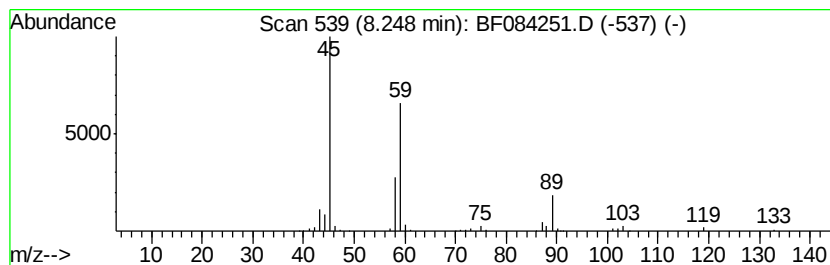
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Ethanol, 2-[2-(2-methoxyeth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.25	3.49 ng	386562	Naphthalene-d8	8.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-[2-(2-methoxvethoxy)e...	164	C7H16O4	000112-35-6	90
2		.beta.-Methoxvethoxymethyl chloride	124	C4H9ClO2	003970-21-6	78
3		Ethanol, 2-(2-methoxvethoxy)-	120	C5H12O3	000111-77-3	74
4		2,5,8,11,14-Pentaoxahexadecan-16-ol	252	C11H24O6	023778-52-1	64
5		Triethylene glycol	150	C6H14O4	000112-27-6	50



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010416\
Data File : BF084251.D
Acq On : 4 Jan 2016 20:52
Operator : UM/SJ
Sample : G4987-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DRUM(116-142)COMPOSITE

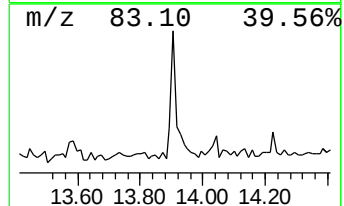
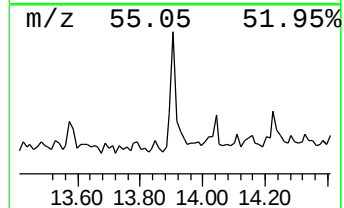
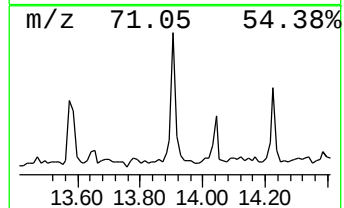
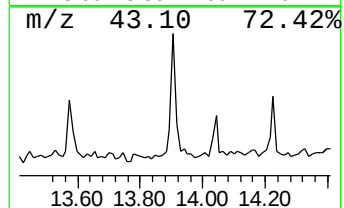
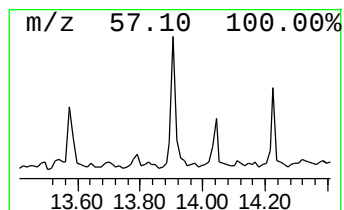
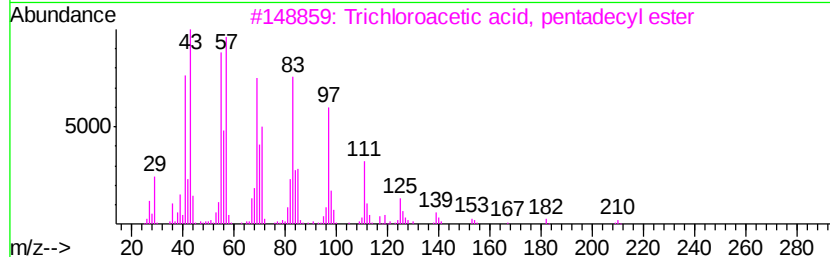
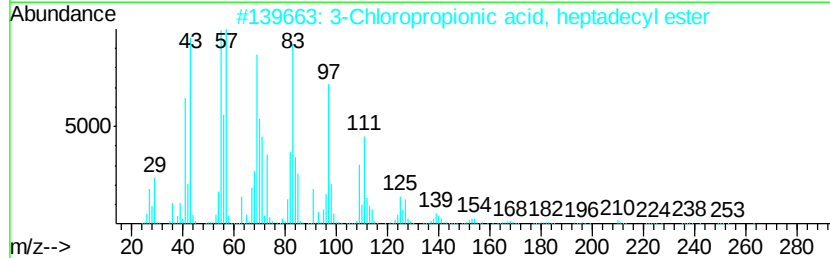
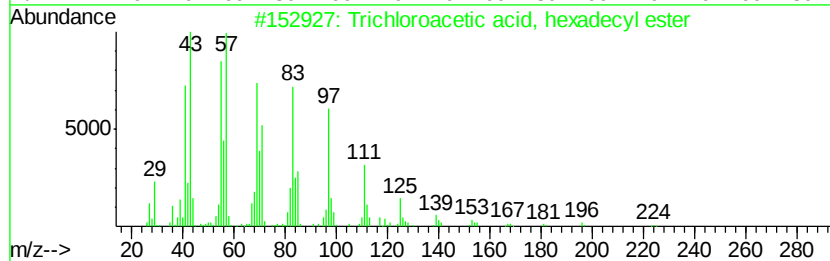
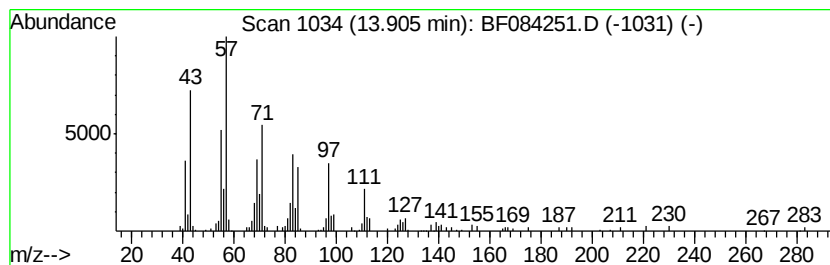
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Trichloroacetic acid, hexad... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.91	2.20 ng	162427	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	64
2		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	62
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	58
4		1-Nonadecanol	284	C19H40O	001454-84-8	58
5		Acetic acid, octadecyl ester	312	C20H40O2	000822-23-1	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010416\
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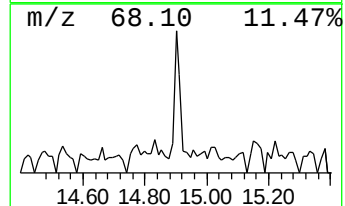
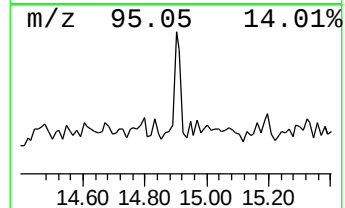
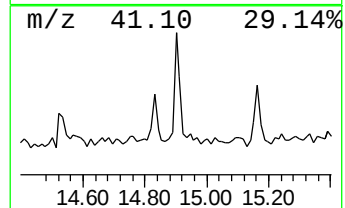
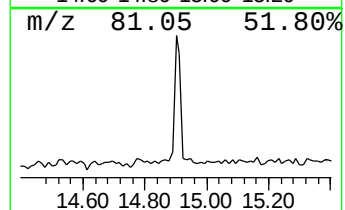
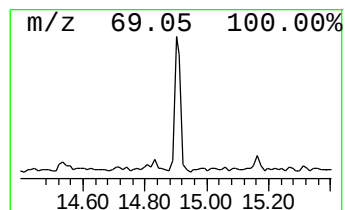
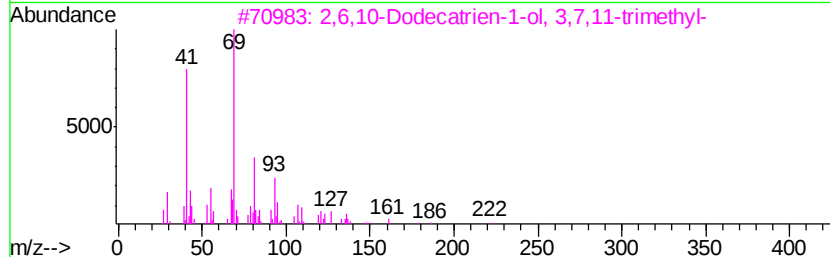
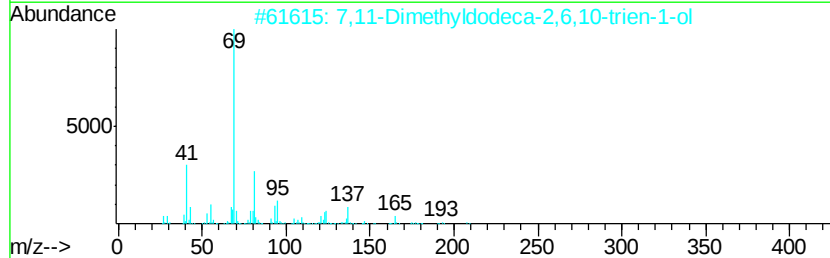
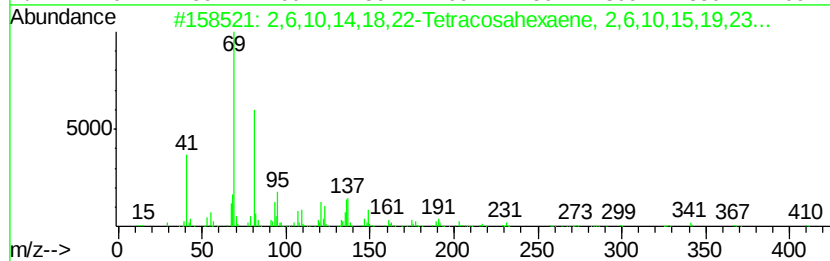
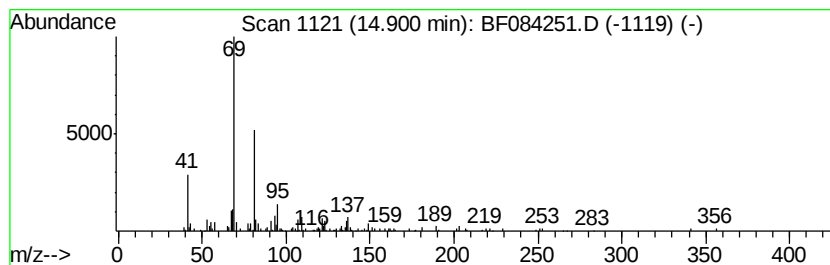
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DRUM(116-142)COMPOSITE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 2,6,10,14,18,22-Tetracosahexaene... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.90	2.14 ng	147172	Perylene-d12	15.49
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2,6,10,14,18,22-Tetracosahexaene...	410 C30H50	000111-02-4	86
2	7,11-Dimethyldodeca-2,6,10-trien...	208 C14H24O	125529-10-4	80
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222 C15H26O	004602-84-0	72
4	Hexadeca-2,6,10,14-tetraen-1-ol,...	290 C20H34O	007614-21-3	72
5	4,9,13,17-Tetramethyl-4,8,12,16-...	316 C22H36O	056882-09-8	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010416\
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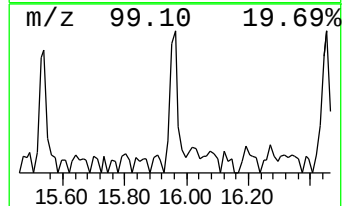
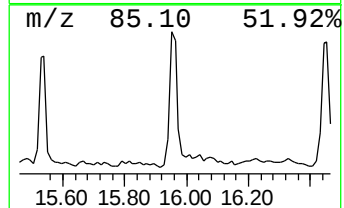
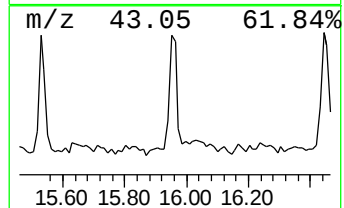
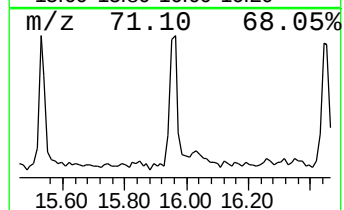
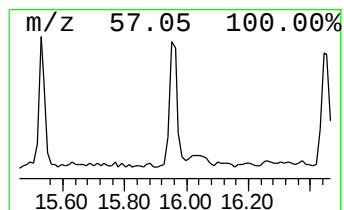
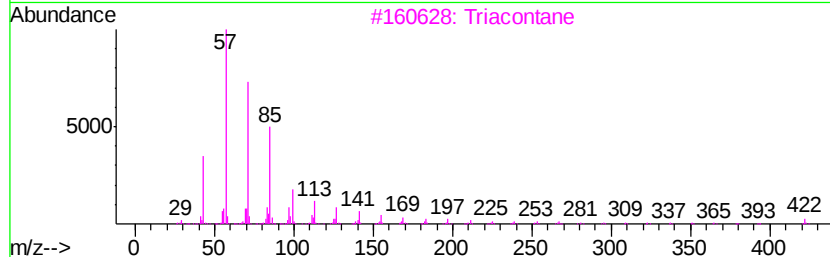
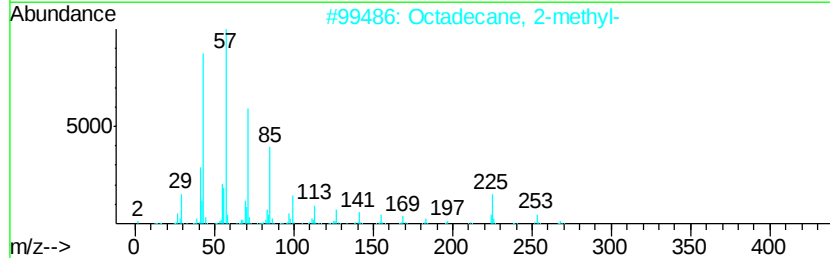
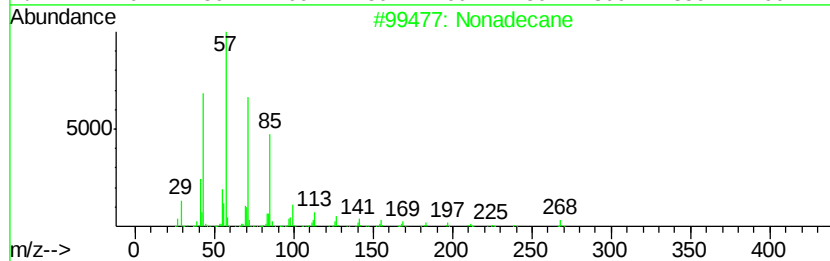
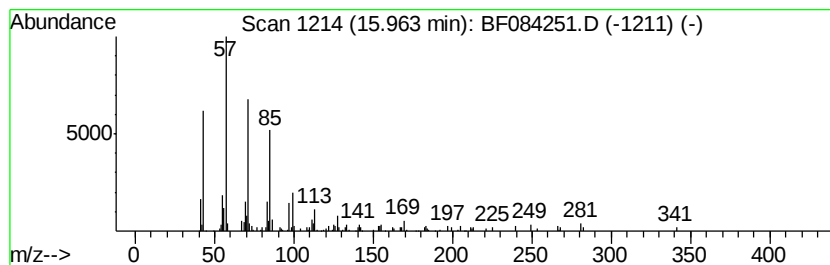
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.96	2.55 ng	175147	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	90
2		Octadecane, 2-methyl-	268	C19H40	001560-88-9	86
3		Triacontane	422	C30H62	000638-68-6	86
4		Hexacosane	366	C26H54	000630-01-3	86
5		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010416\
Data File : BF084251.D
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ClientSampleId :
DRUM(116-142)COMPOSITE

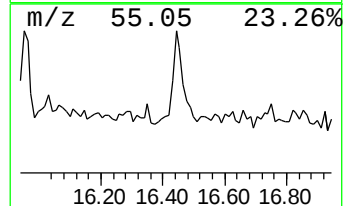
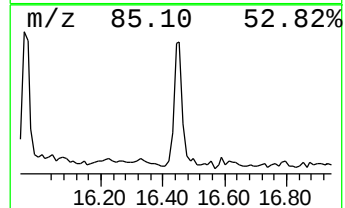
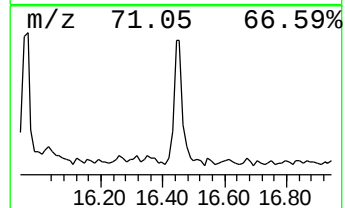
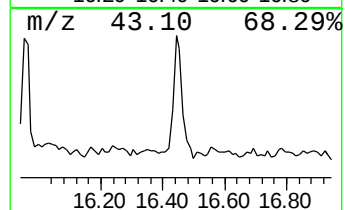
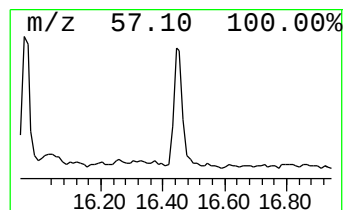
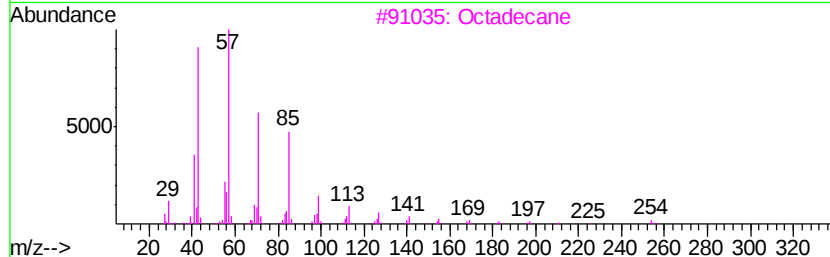
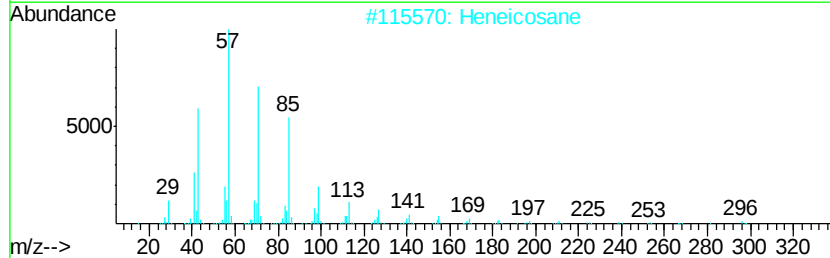
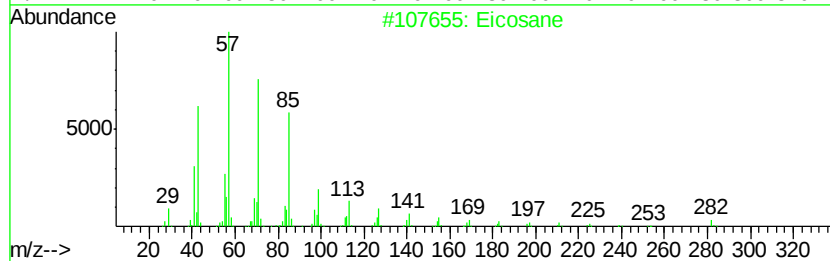
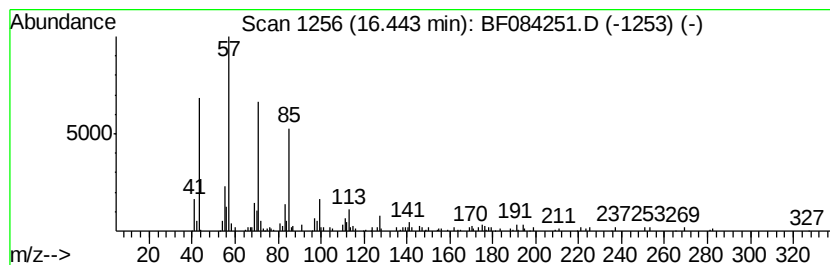
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.44	2.88 ng	197987	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	90
2		Heneicosane	296	C21H44	000629-94-7	87
3		Octadecane	254	C18H38	000593-45-3	83
4		Nonadecane	268	C19H40	000629-92-5	83
5		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010416\
Data File : BF084251.D
Acq On : 4 Jan 2016 20:52
Operator : UM/SJ
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ClientSampleId :
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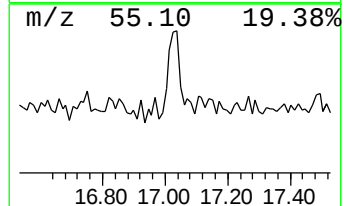
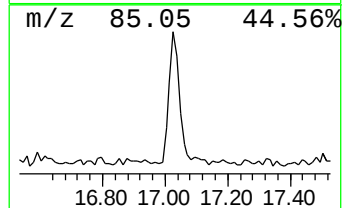
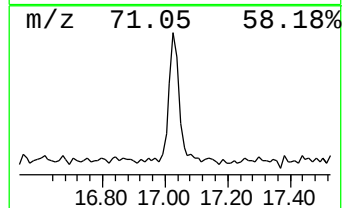
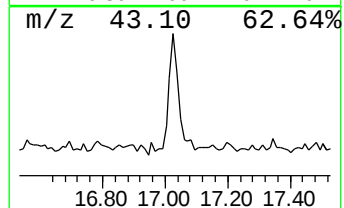
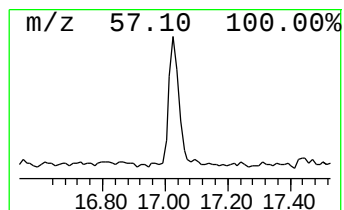
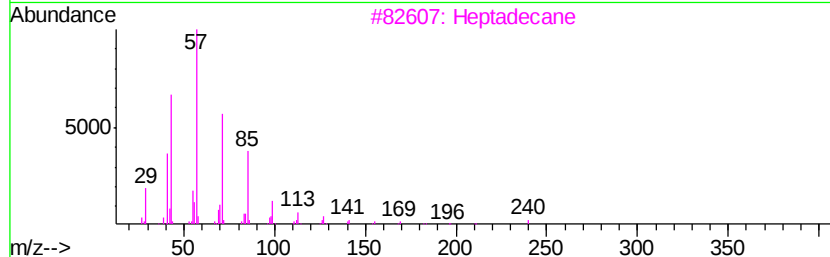
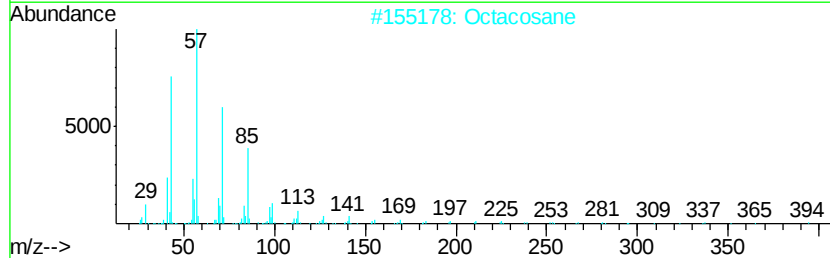
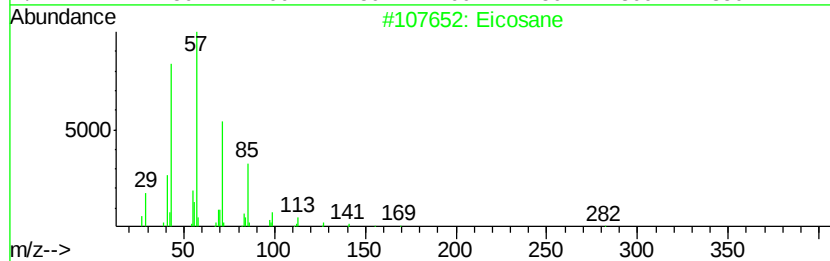
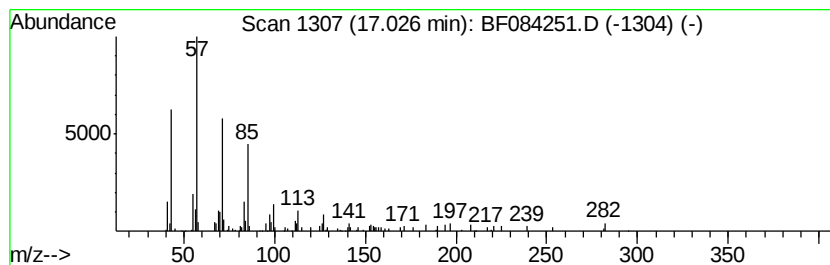
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Octacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.03	2.43 ng	166682	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	93
2		Octacosane	394	C28H58	000630-02-4	87
3		Heptadecane	240	C17H36	000629-78-7	83
4		Pentacosane	352	C25H52	000629-99-2	83
5		Tetracosane	338	C24H50	000646-31-1	83



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010416\
Data File : BF084251.D
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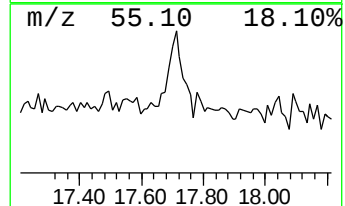
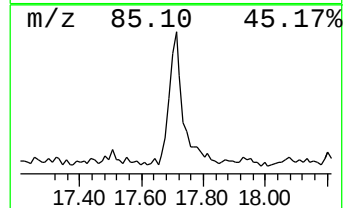
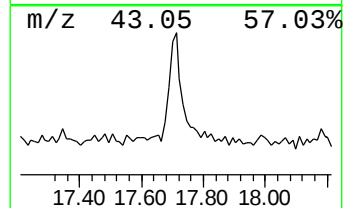
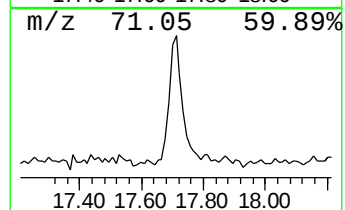
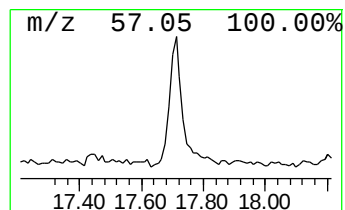
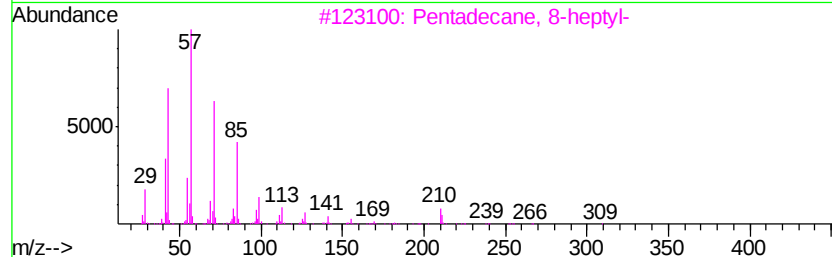
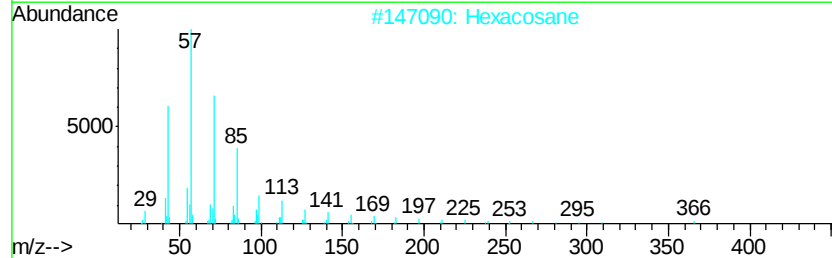
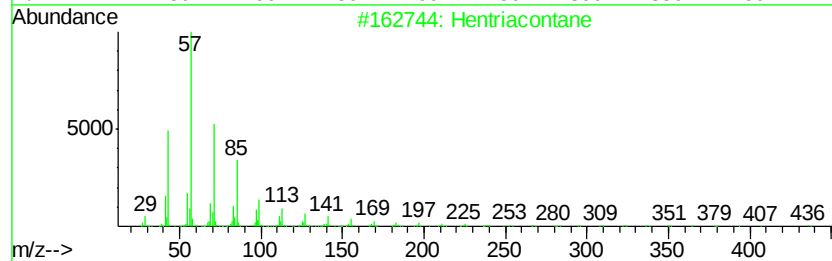
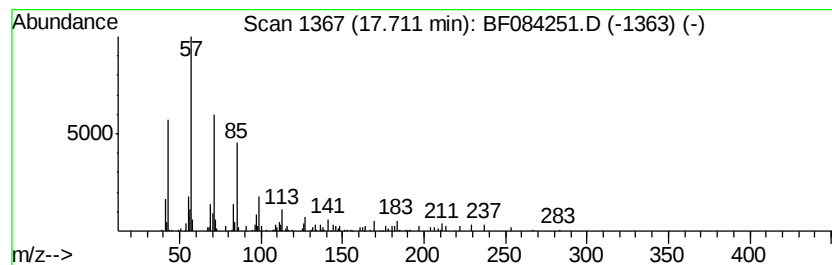
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Hentriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.71	2.56 ng	175990	Perylene-d12	15.49

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	87
2			Hexacosane	366	C26H54	000630-01-3	87
3			Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	87
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
5			Heptacosane	380	C27H56	000593-49-7	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010416\
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ALS Vial : 21 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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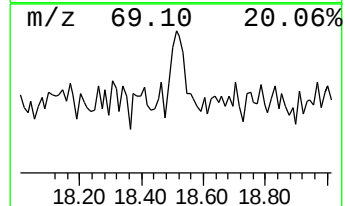
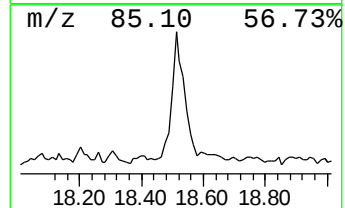
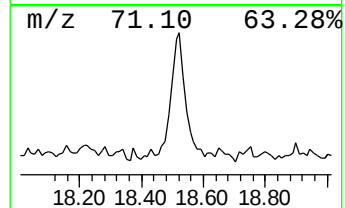
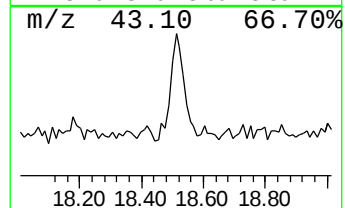
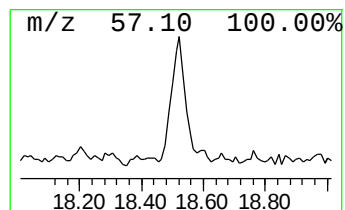
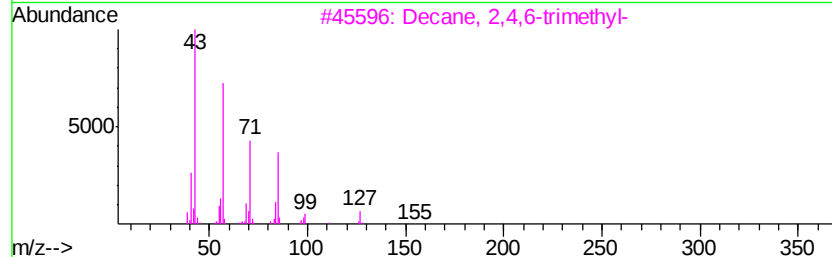
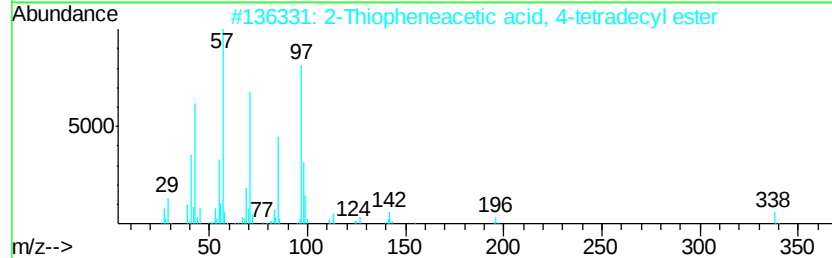
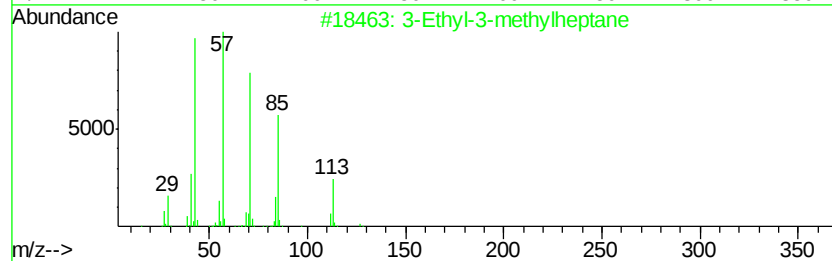
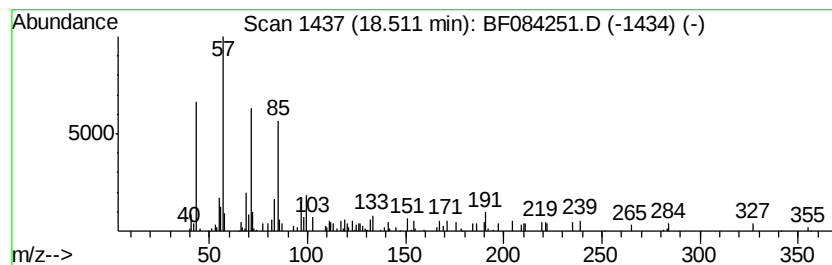
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 unknown18.51 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.51	2.21 ng	152173	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Ethyl-3-methylheptane	142	C10H22	017302-01-1	47
2		2-Thiopheneacetic acid, 4-tetrad...	338	C20H34O2S	1000280-67-0	47
3		Decane, 2,4,6-trimethyl-	184	C13H28	062108-27-4	47
4		Heptadecane	240	C17H36	000629-78-7	47
5		Undecane, 4-ethyl-	184	C13H28	017312-59-3	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010416\
 Data File : BF084251.D
 Acq On : 4 Jan 2016 20:52
 Operator : UM/SJ
 Sample : G4987-01
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DRUM(116-142)COMPOSITE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.08	19.8	ng	1559390	1	6.89	1575760	20.0
Ethanol, 2,2'-oxy...	6.46	8.2	ng	646450	1	6.89	1575760	20.0
unknown6.67	6.67	75.1	ng	5919980	1	6.89	1575760	20.0
Cyclohexanol, 5-m...	8.09	2.5	ng	270993	2	8.18	2213590	20.0
Ethanol, 2-[2-(2-...	8.25	3.5	ng	386562	2	8.18	2213590	20.0
Trichloroacetic a...	13.91	2.2	ng	162427	5	14.05	1474580	20.0
2,6,10,14,18,22-T...	14.90	2.1	ng	147172	6	15.49	1374150	20.0
Nonadecane	15.96	2.5	ng	175147	6	15.49	1374150	20.0
Eicosane	16.44	2.9	ng	197987	6	15.49	1374150	20.0
Octacosane	17.03	2.4	ng	166682	6	15.49	1374150	20.0
Hentriacontane	17.71	2.6	ng	175990	6	15.49	1374150	20.0
unknown18.51	18.51	2.2	ng	152173	6	15.49	1374150	20.0