

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
 Data File : BF083760.D
 Acq On : 14 Dec 2015 6:01
 Operator : UM/IZ
 Sample : G4648-03
 Misc :
 ALS Vial : 50 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-01(0-0.16)

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-BF121315.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	5.116	262	265	270	rVB	465671	582290	20.27%	2.074%
2	5.527	298	301	304	rBV	2407983	2507621	87.31%	8.932%
3	6.544	387	390	393	rBV	2335549	2515718	87.59%	8.961%
4	6.681	400	402	405	rBV	2158061	2853266	99.35%	10.163%
5	6.922	421	423	425	rBV	848739	847344	29.50%	3.018%
6	7.082	434	437	439	rVB	1759571	2292140	79.81%	8.165%
7	7.482	469	472	474	rBV	1730771	1941801	67.61%	6.917%
8	7.573	477	480	482	rBV	32329	51655	1.80%	0.184%
9	8.202	532	535	537	rBV	1334681	1114003	38.79%	3.968%
10	8.533	562	564	567	rBV	29137	33165	1.15%	0.118%
11	9.150	617	618	620	rVB	31752	32426	1.13%	0.116%
12	9.276	626	629	632	rBV	2817896	2872016	100.00%	10.230%
13	9.402	638	640	645	rVB	25170	35580	1.24%	0.127%
14	9.665	661	663	666	rBV	495063	504993	17.58%	1.799%
15	9.893	682	683	686	rVB	54262	39380	1.37%	0.140%
16	9.950	686	688	691	rBV	905194	1099309	38.28%	3.916%
17	10.396	723	727	728	rBV	91443	118069	4.11%	0.421%
18	10.613	743	746	749	rBV	39293	58850	2.05%	0.210%
19	10.739	754	757	759	rBV	1679595	1559633	54.30%	5.555%
20	10.865	766	768	772	rBV2	128149	145781	5.08%	0.519%
21	10.956	774	776	778	rVB2	46358	50673	1.76%	0.180%
22	11.059	783	785	787	rBV2	25190	40082	1.40%	0.143%
23	11.105	787	789	791	rBV2	31587	38322	1.33%	0.137%
24	11.139	791	792	794	rBV	49939	44790	1.56%	0.160%
25	11.310	804	807	809	rBV	79378	74224	2.58%	0.264%
26	11.436	816	818	820	rBV	1065818	949908	33.07%	3.384%
27	11.493	821	823	827	rVB	21634	36453	1.27%	0.130%
28	11.733	842	844	848	rBV	26790	35350	1.23%	0.126%
29	12.145	876	880	882	rBV2	20853	36584	1.27%	0.130%
30	12.419	901	904	908	rBV2	21061	45544	1.59%	0.162%
31	12.476	908	909	911	rVV	55770	56996	1.98%	0.203%
32	12.522	911	913	916	rVB3	16955	31041	1.08%	0.111%
33	12.636	922	923	925	rBV	39819	45141	1.57%	0.161%
34	12.671	925	926	929	rVB	44239	48995	1.71%	0.175%

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35	12.819	938	939	940	rBV	34842	37098	1.29%	0.132%
36	12.842	940	941	944	rVV2	170874	200855	6.99%	0.715%
37	12.922	947	948	949	rVB	73068	50719	1.77%	0.181%
38	13.014	954	956	958	rBV	1975561	1832585	63.81%	6.528%
39	13.174	968	970	971	rBV	65307	64916	2.26%	0.231%
40	13.254	975	977	980	rVV4	23515	38303	1.33%	0.136%
41	13.425	990	992	995	rBV3	15333	33449	1.16%	0.119%
42	13.505	996	999	1001	rVV	90460	125093	4.36%	0.446%
43	13.551	1001	1003	1005	rVV	218804	226210	7.88%	0.806%
44	13.596	1005	1007	1008	rVV	50611	57434	2.00%	0.205%
45	13.642	1010	1011	1012	rVV	87969	83612	2.91%	0.298%
46	13.676	1012	1014	1015	rVV	156626	151291	5.27%	0.539%
47	13.722	1015	1018	1020	rVB2	59377	105874	3.69%	0.377%
48	13.871	1029	1031	1033	rVB	50170	65991	2.30%	0.235%
49	13.916	1033	1035	1038	rBV3	71281	115181	4.01%	0.410%
50	13.985	1038	1041	1043	rBV	141433	163797	5.70%	0.583%
51	14.031	1043	1045	1046	rBV	67435	69717	2.43%	0.248%
52	14.065	1046	1048	1050	rVV	618125	685659	23.87%	2.442%
53	14.236	1061	1063	1065	rVB	59623	66880	2.33%	0.238%
54	14.294	1065	1068	1069	rBV	79487	85503	2.98%	0.305%
55	14.339	1069	1072	1074	rVB2	29774	52927	1.84%	0.189%
56	14.419	1077	1079	1081	rBV	29866	35822	1.25%	0.128%
57	14.545	1088	1090	1091	rBV	52655	53756	1.87%	0.191%
58	14.591	1091	1094	1096	rVV	60024	72152	2.51%	0.257%
59	14.739	1104	1107	1109	rBV2	53989	78269	2.73%	0.279%
60	14.785	1109	1111	1113	rVB2	26992	35433	1.23%	0.126%
61	14.842	1114	1116	1120	rBV	45628	61138	2.13%	0.218%
62	14.922	1121	1123	1125	rVB	25120	29677	1.03%	0.106%
63	15.174	1143	1145	1148	rBV2	35916	58041	2.02%	0.207%
64	15.505	1171	1174	1177	rBV	404295	597780	20.81%	2.129%

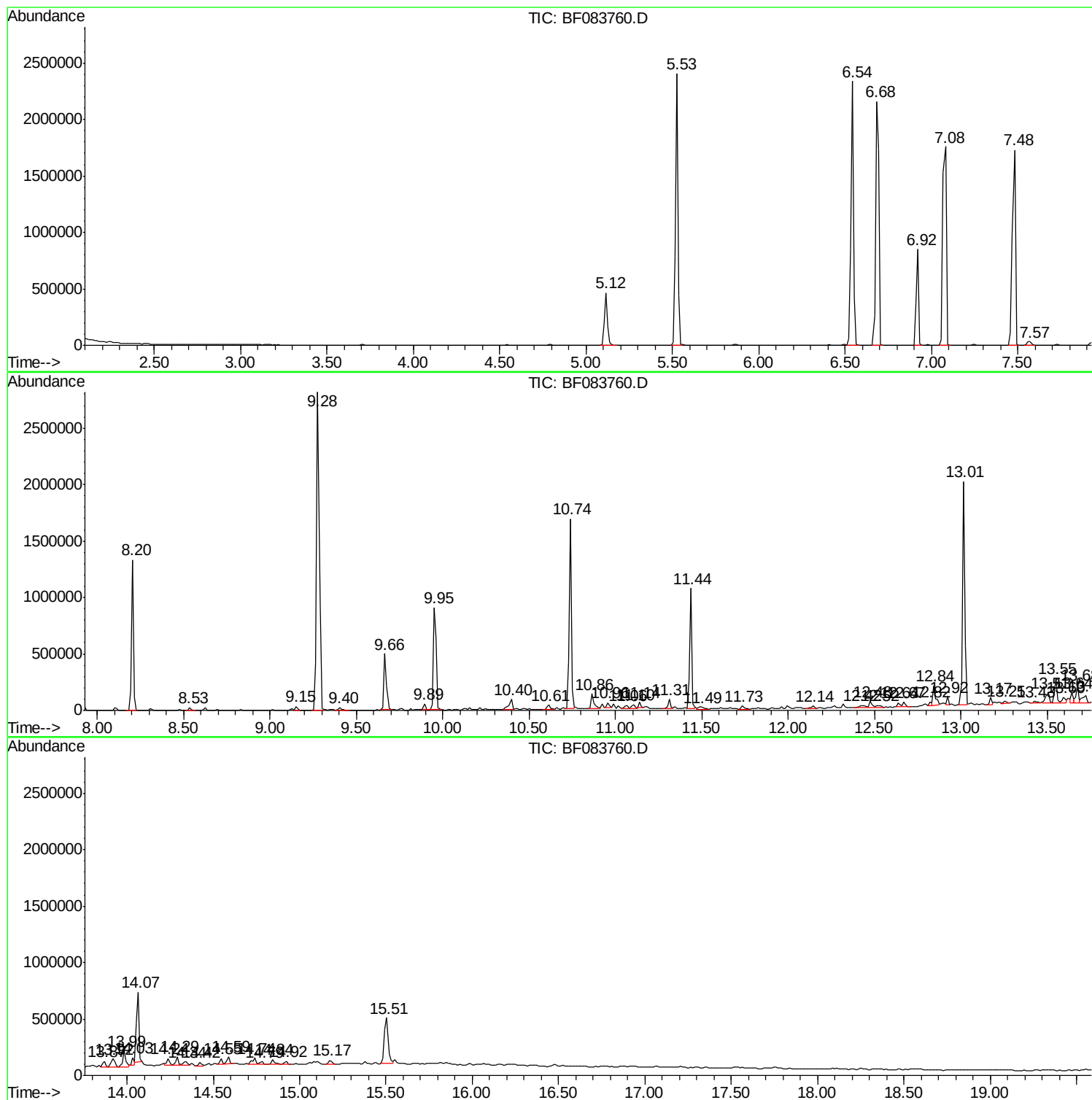
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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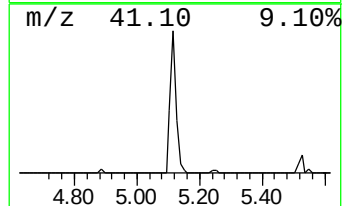
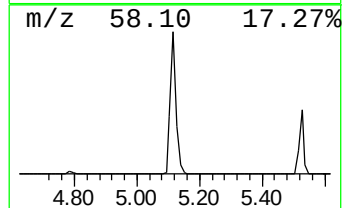
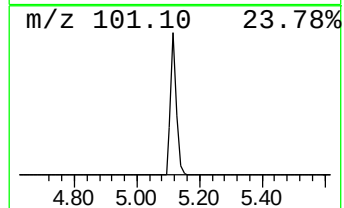
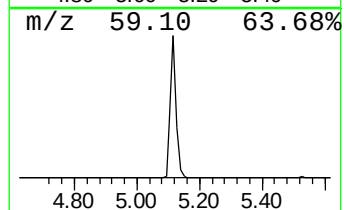
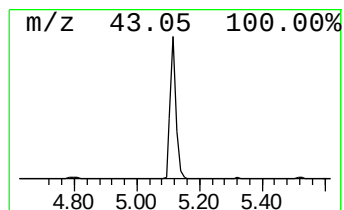
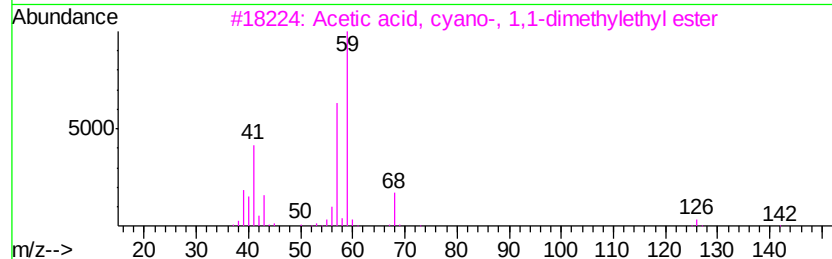
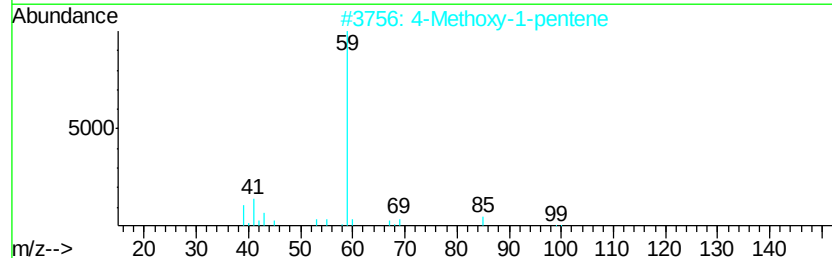
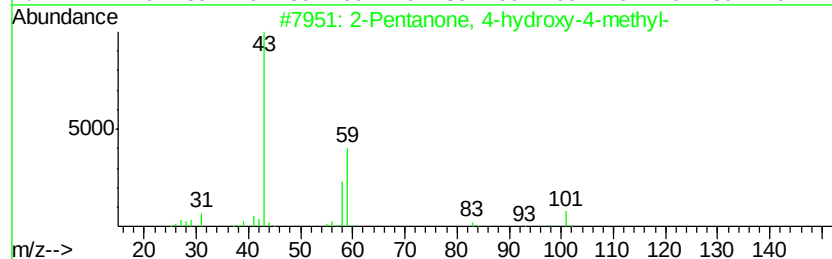
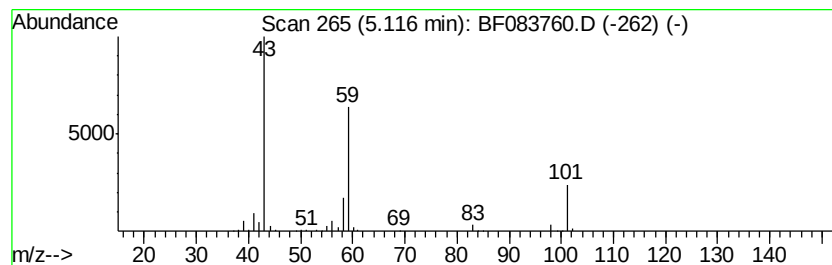
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	13.74 ng	582290	1,4-Dichlorobenzene-d4	6.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			4-Methoxy-1-pentene	100	C6H12O	098386-09-5	35
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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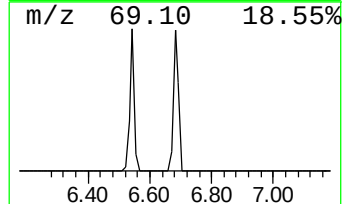
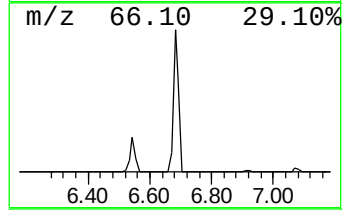
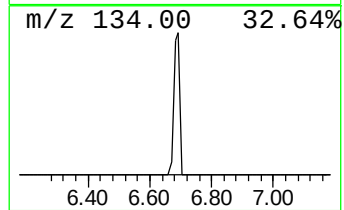
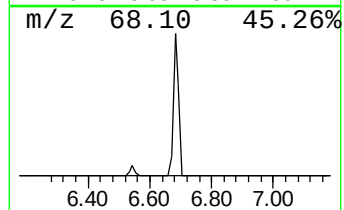
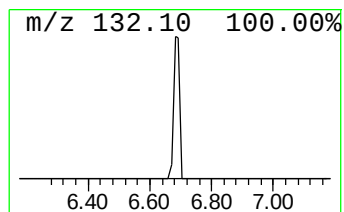
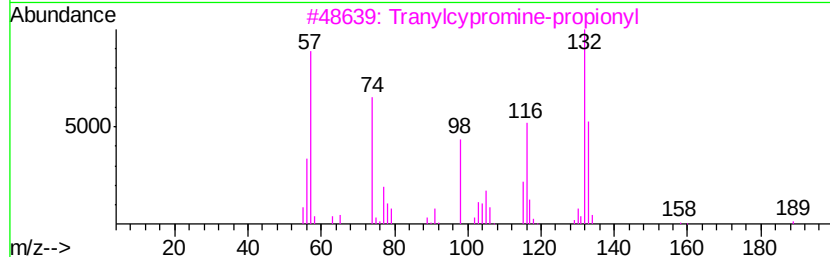
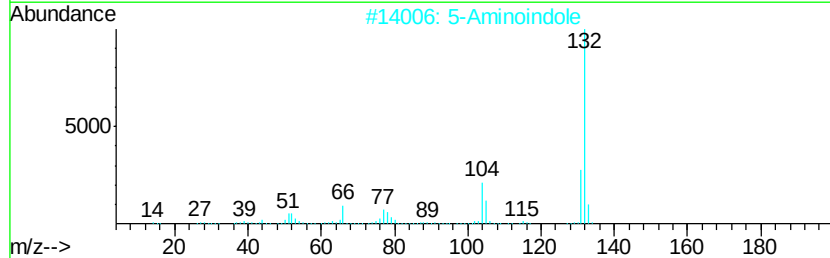
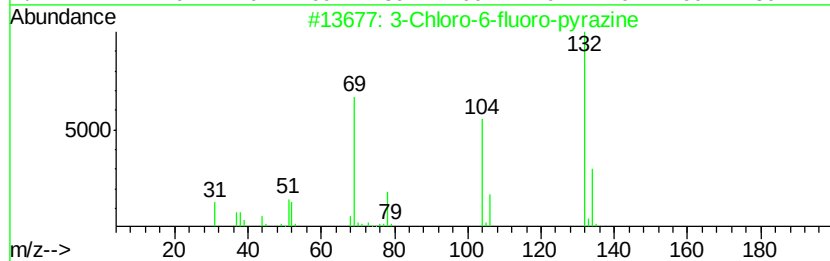
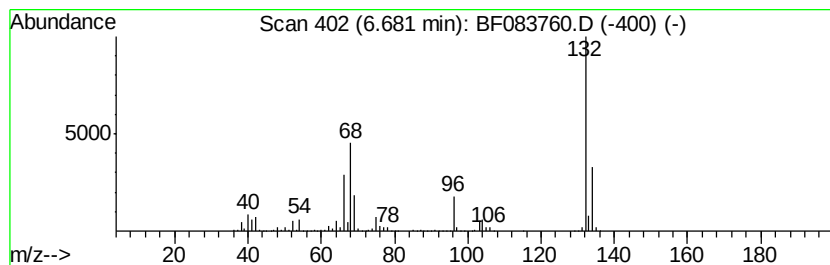
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	67.35 ng	2853270	1,4-Dichlorobenzene-d4	6.92

Hit#	of	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	Tranvlcy	promine-propionyl	189	C12H15NO	1000123-86-3	10
4	5-Fluoro-2-chloro	pyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Chloro-2-fluoro	pyrimidine	132	C4H2ClFN2	051422-00-5	9



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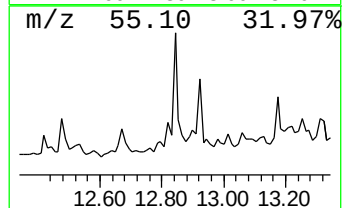
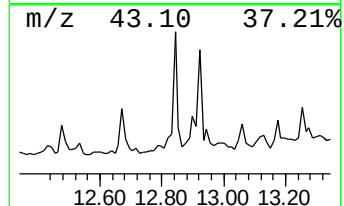
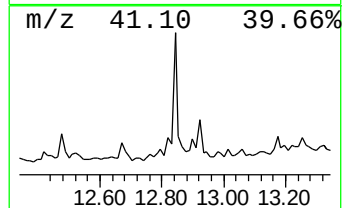
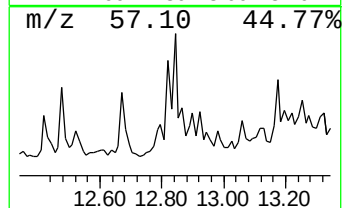
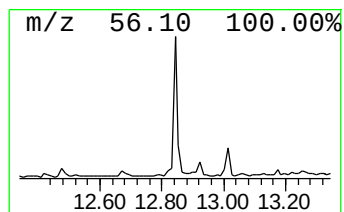
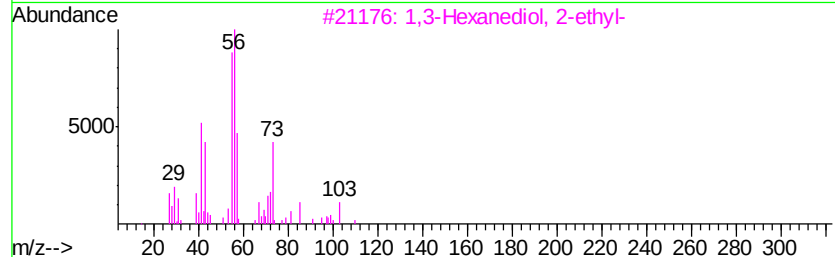
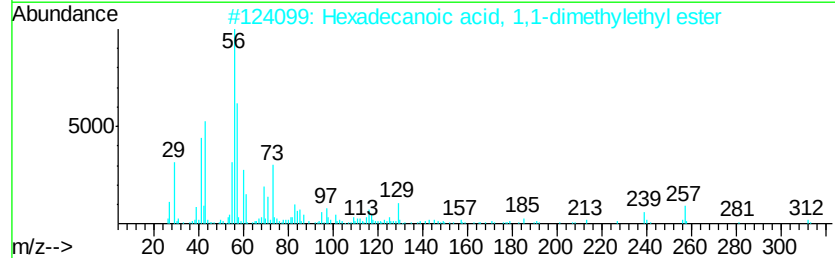
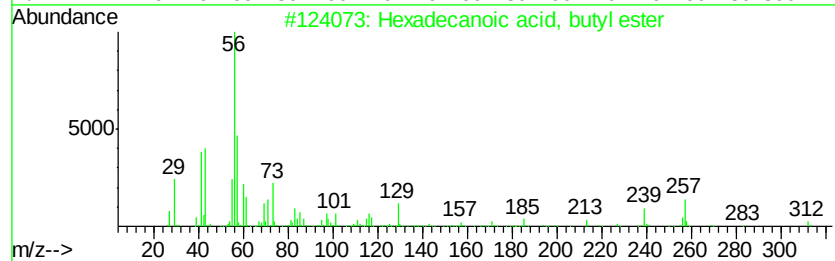
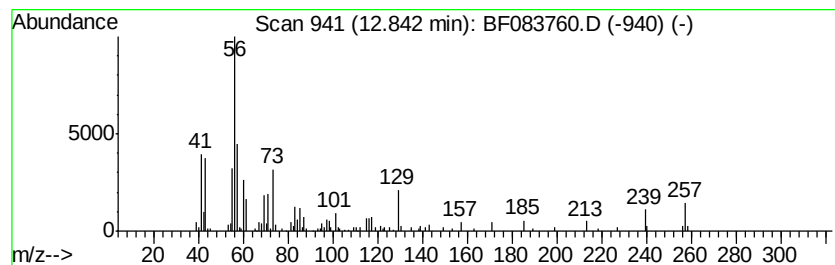
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.84	5.86 ng	200855	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	83
3		1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	32
4		Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	27
5		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27



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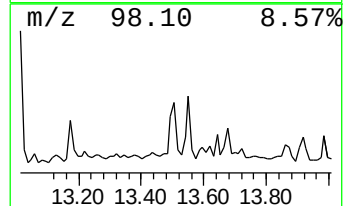
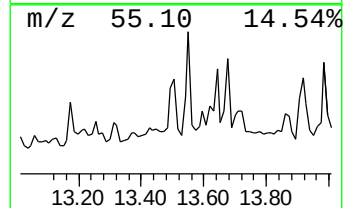
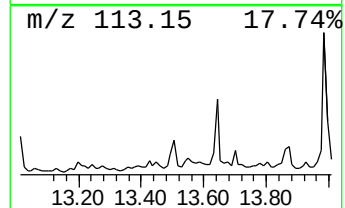
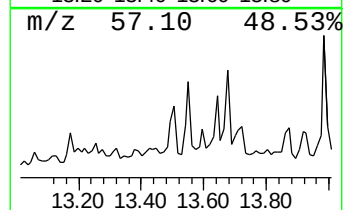
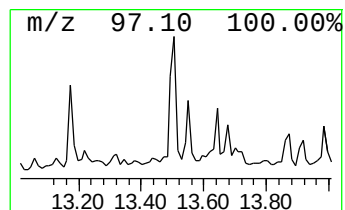
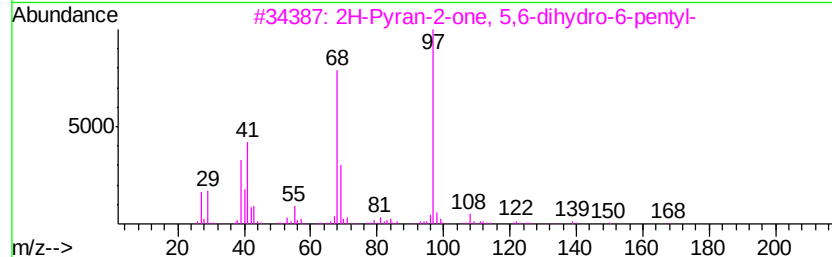
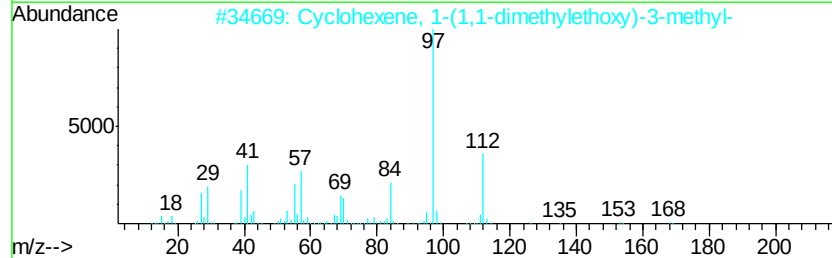
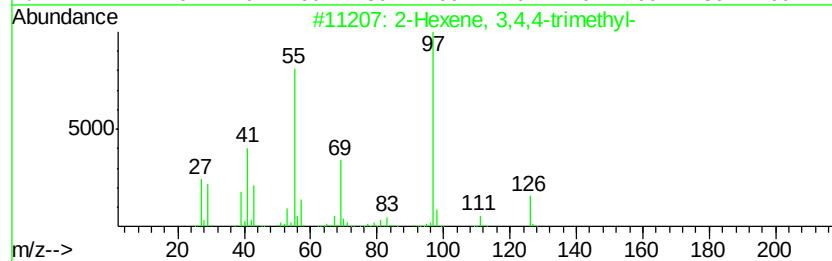
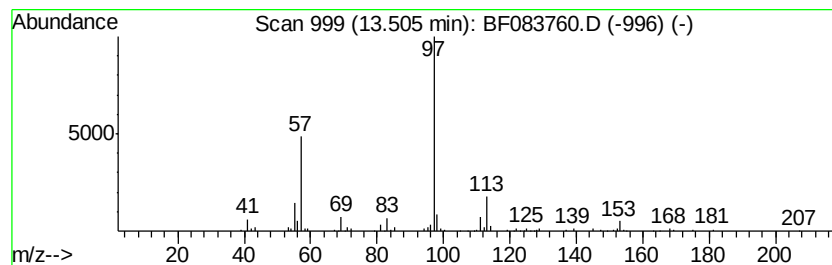
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Hexene, 3,4,4-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.51	3.65 ng	125093	Chrysene-d12	14.07
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-Hexene, 3,4,4-trimethyl-	126 C9H18	053941-19-8	59
2	Cyclohexene, 1-(1,1-dimethylethoxy)-	168 C11H20O	040648-24-6	59
3	2H-Pyran-2-one, 5,6-dihydro-6-pentyl-	168 C10H16O2	054814-64-1	53
4	Thiophene, 2-ethyl-	112 C6H8S	000872-55-9	45
5	Cyclohexane, 1,3-dimethyl-, cis-	112 C8H16	000638-04-0	42



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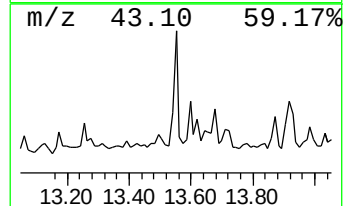
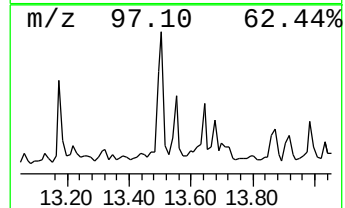
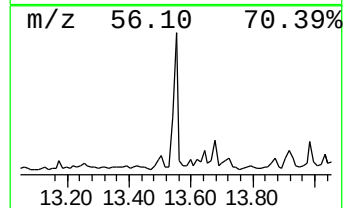
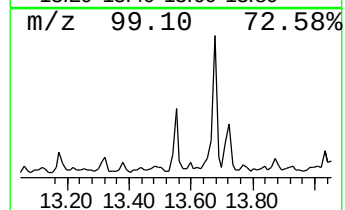
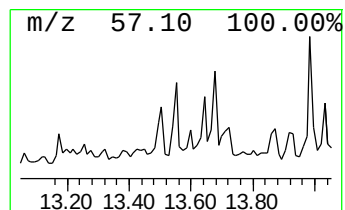
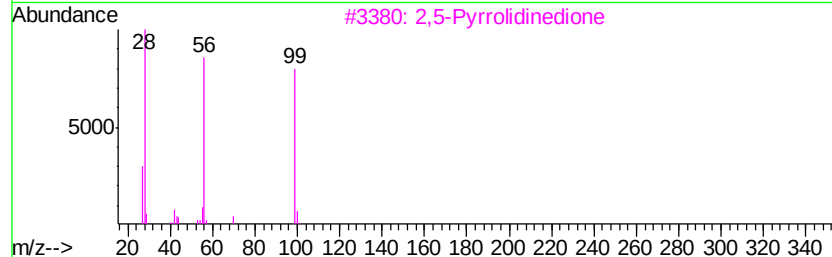
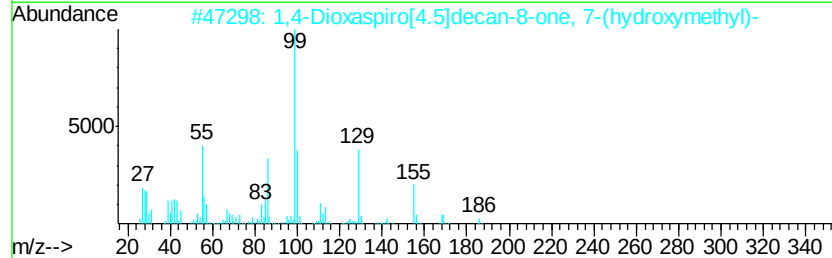
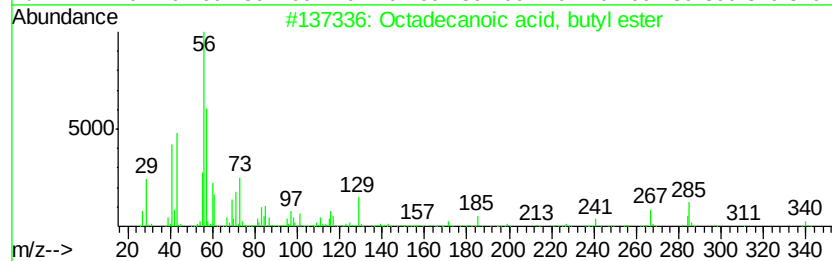
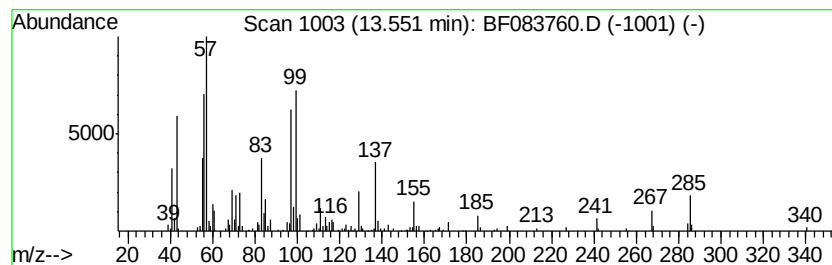
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	6.60 ng	226210	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	83
2		1,4-Dioxaspiro[4.5]decan-8-one, ...	186	C9H14O4	108177-20-4	35
3		2,5-Pyrrolidinedione	99	C4H5NO2	000123-56-8	25
4		2-Propylthiazole	127	C6H9NS	017626-75-4	15
5		2-Piperidinone	99	C5H9NO	000675-20-7	11



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083760.D
Acq On : 14 Dec 2015 6:01
Operator : UM/IZ
Sample : G4648-03
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-01(0-0.16)

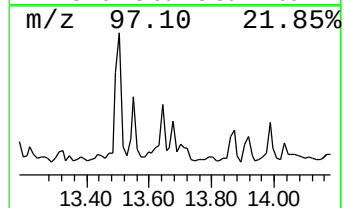
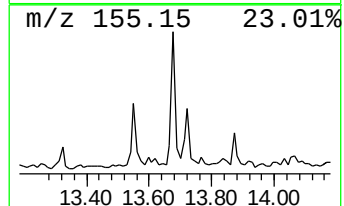
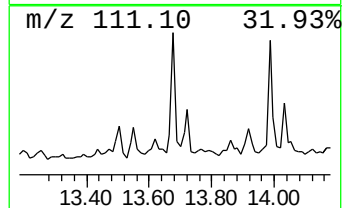
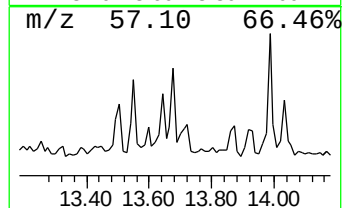
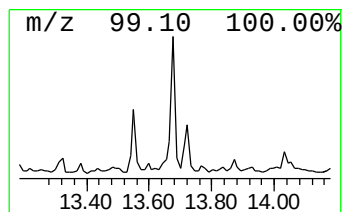
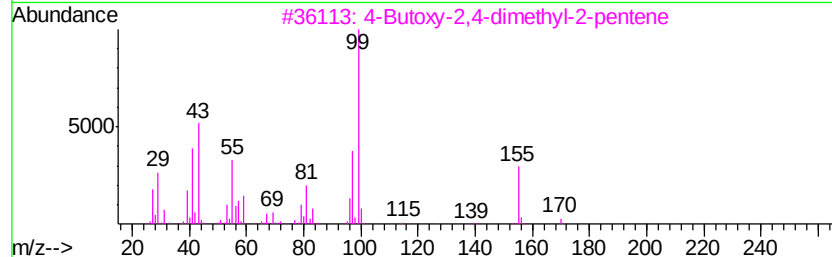
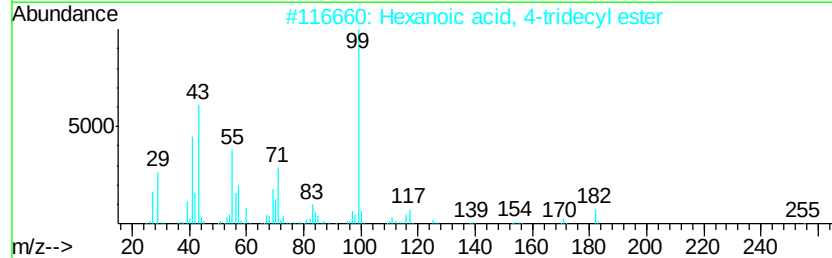
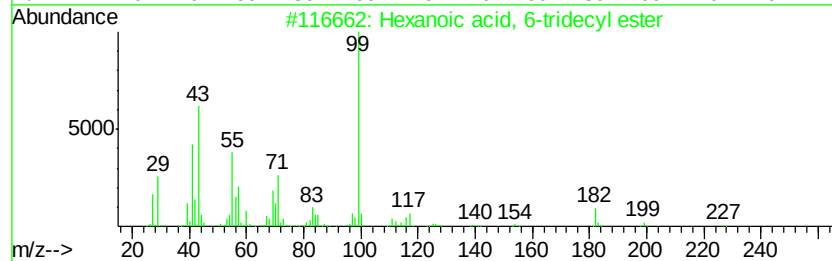
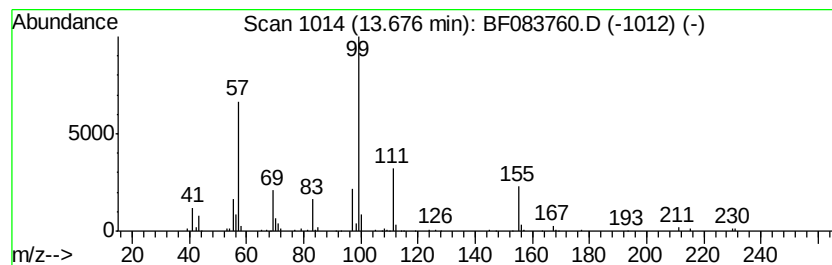
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown13.68 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	4.41 ng	151291	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 6-tridecyl ester	298	C19H38O2	1000279-29-5	37
2		Hexanoic acid, 4-tridecyl ester	298	C19H38O2	1000279-29-3	37
3		4-Butoxy-2,4-dimethyl-2-pentene	170	C11H22O	1000159-08-7	36
4		2-Propylthiazole	127	C6H9NS	017626-75-4	35
5		1-Pyrrolidinocarbonylmethyl pipe...	197	C10H19N3O	039890-45-4	33



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083760.D
Acq On : 14 Dec 2015 6:01
Operator : UM/IZ
Sample : G4648-03
Misc :
ALS Vial : 50 Sample Multiplier: 1

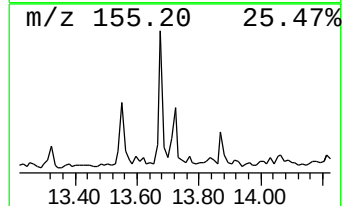
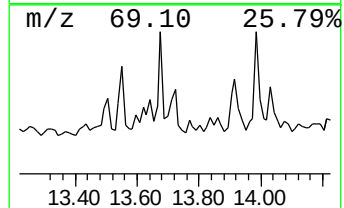
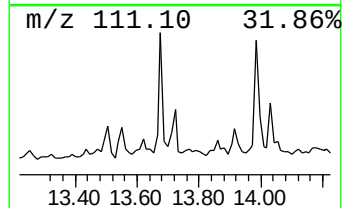
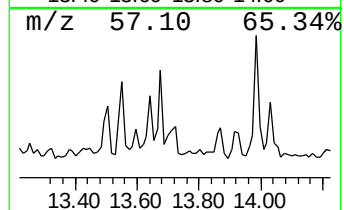
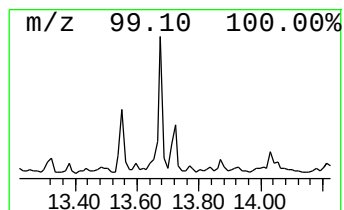
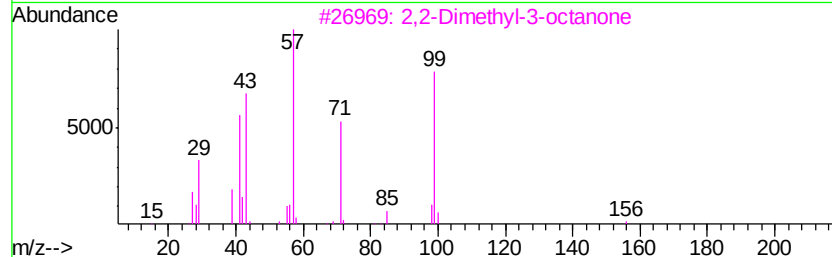
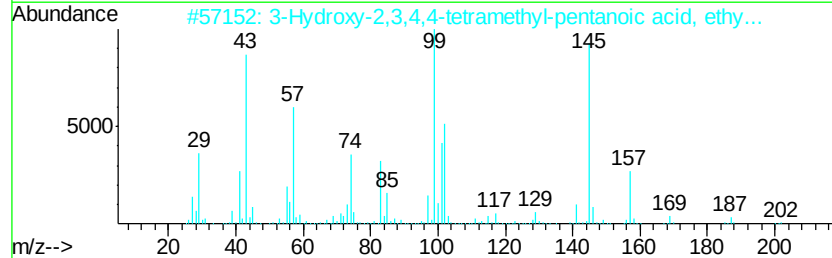
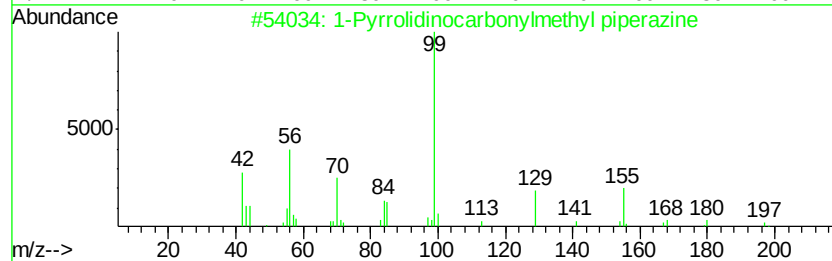
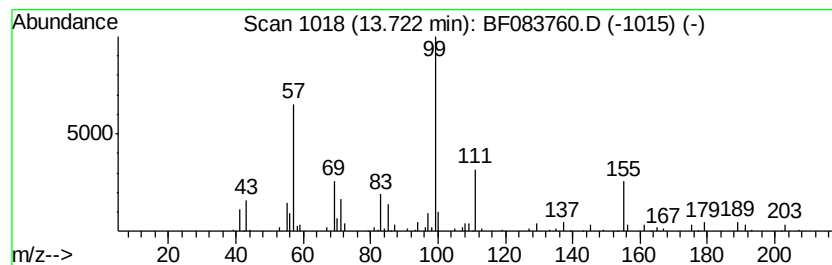
Instrument :
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ClientSampleId :
SB-01(0-0.16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Pyrrolidinocarbonylmethyl... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	3.09 ng	105874	Chrysene-d12	14.07
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1-Pyrrolidinocarbonylmethyl pipe...	197 C10H19N3O	039890-45-4 50
2		3-Hydroxy-2,3,4,4-tetramethyl-pe...	202 C11H22O3	1000194-64-5 50
3		2,2-Dimethyl-3-octanone	156 C10H20O	005340-64-7 38
4		3,3-Dimethyl-1-(6-methyl-tetrahy...	198 C12H22O2	343947-11-5 38
5		Silane, dimethyldi-2-propenyl-	140 C8H16Si	001113-12-8 38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083760.D
Acq On : 14 Dec 2015 6:01
Operator : UM/IZ
Sample : G4648-03
Misc :
ALS Vial : 50 Sample Multiplier: 1

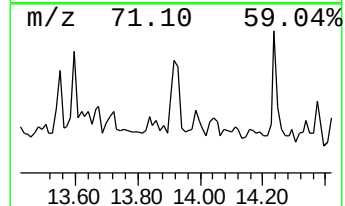
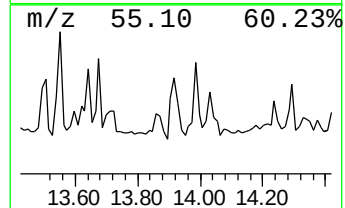
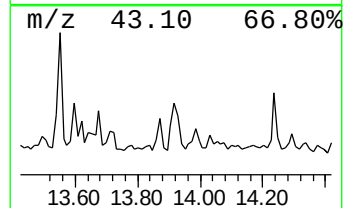
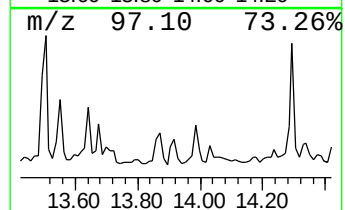
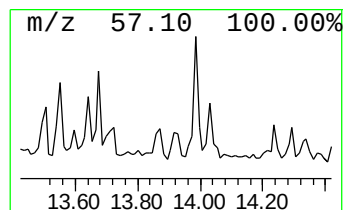
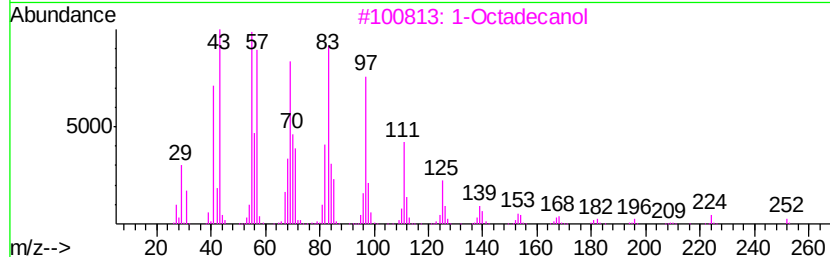
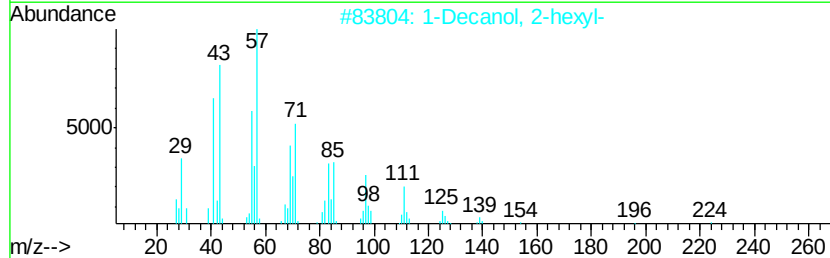
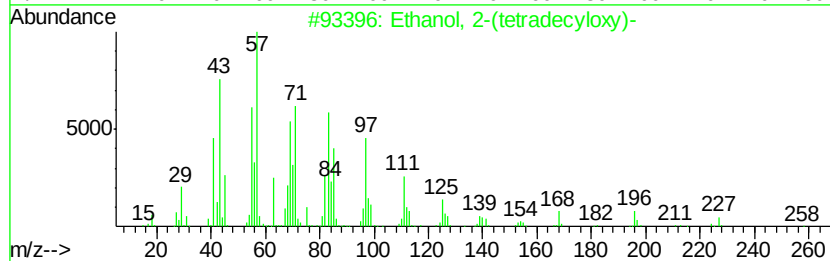
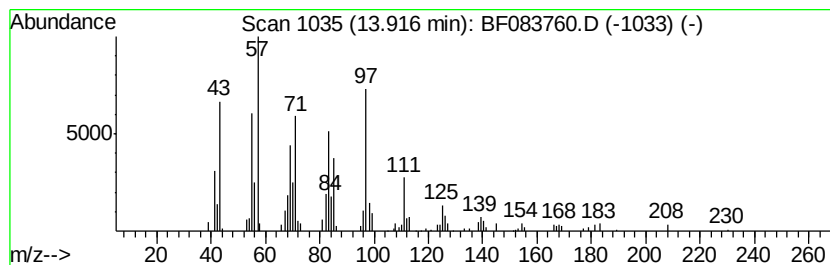
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Ethanol, 2-(tetradecyloxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.92	3.36 ng	115181	Chrysene-d12		14.07	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	62
2		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	52
3		1-Octadecanol	270	C18H38O	000112-92-5	50
4		1-Docosene	308	C22H44	001599-67-3	46
5		Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	45



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083760.D
Acq On : 14 Dec 2015 6:01
Operator : UM/IZ
Sample : G4648-03
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-01(0-0.16)

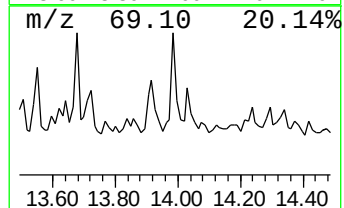
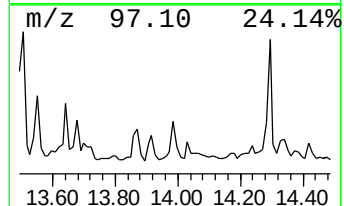
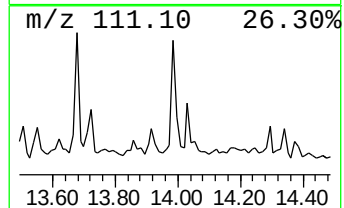
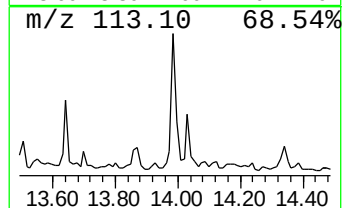
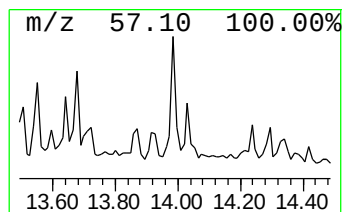
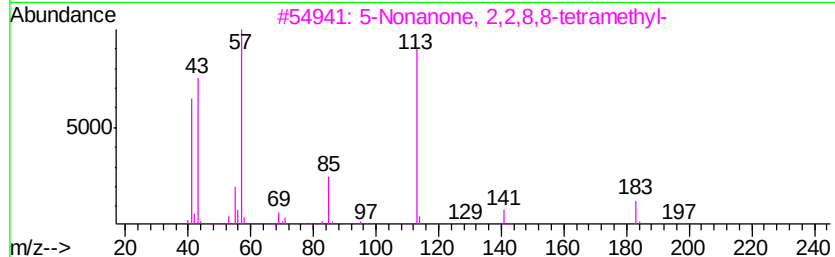
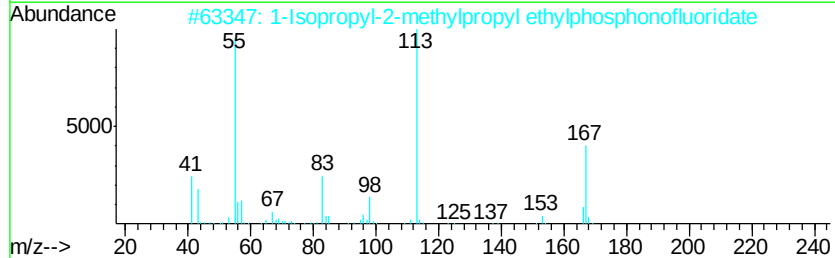
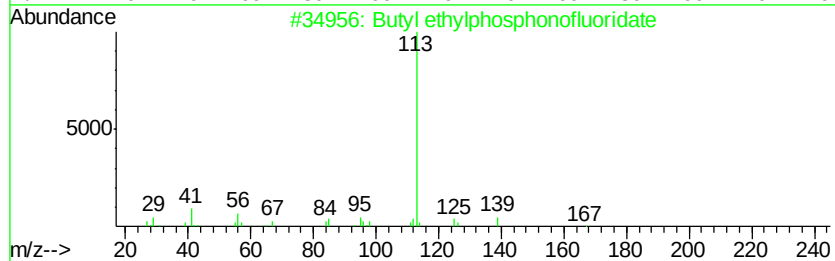
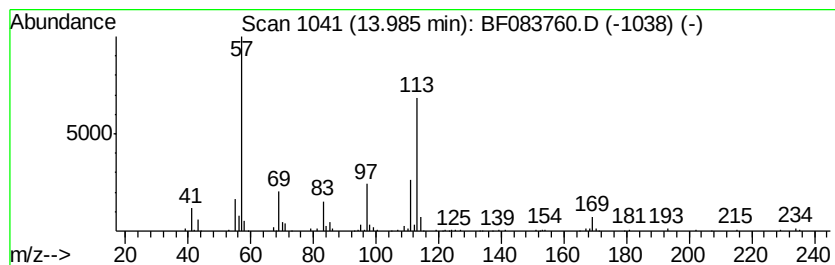
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown13.99 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.99	4.78 ng	163797	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butyl ethylphosphonofluoridate	168	C6H14F02P	018358-34-4	35
2		1-Isopropyl-2-methylpropyl ethyl...	210	C9H20F02P	1000298-33-2	35
3		5-Nonanone, 2,2,8,8-tetramethyl-	198	C13H26O	005709-95-5	32
4		Cyclohexaneethanol, 3-hydroxy-.b...	172	C10H20O2	057685-12-8	28
5		4-Fluoro-6-aminopyrimidine	113	C4H4FN3	051421-96-6	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083760.D
Acq On : 14 Dec 2015 6:01
Operator : UM/IZ
Sample : G4648-03
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-01(0-0.16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.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...	5.12	13.7	ng	582290	1	6.92	847344	20.0
unknown6.68	6.68	67.3	ng	2853270	1	6.92	847344	20.0
Hexadecanoic acid...	12.84	5.9	ng	200855	5	14.07	685659	20.0
2-Hexene, 3,4,4-t...	13.51	3.6	ng	125093	5	14.07	685659	20.0
Octadecanoic acid...	13.55	6.6	ng	226210	5	14.07	685659	20.0
unknown13.68	13.68	4.4	ng	151291	5	14.07	685659	20.0
1-Pyrrolidinocarb...	13.72	3.1	ng	105874	5	14.07	685659	20.0
Ethanol, 2-(tetra...	13.92	3.4	ng	115181	5	14.07	685659	20.0
unknown13.99	13.99	4.8	ng	163797	5	14.07	685659	20.0