

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011816\
 Data File : BF084540.D
 Acq On : 18 Jan 2016 17:24
 Operator : SJ/UM
 Sample : H1140-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SYS-DIS-011416

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	4.258	188	190	191	rBV	267135	327864	2.88%	0.335%
2	4.956	249	251	254	rBV	1235755	1279814	11.22%	1.308%
3	5.047	256	259	261	rVB	677868	785580	6.89%	0.803%
4	5.401	287	290	292	rBV	881877	1190795	10.44%	1.217%
5	5.790	322	324	326	rBV	163960	161664	1.42%	0.165%
6	6.156	354	356	359	rBV	444095	497077	4.36%	0.508%
7	6.464	378	383	386	rBV	7365615	11402412	100.00%	11.652%
8	6.567	389	392	394	rVV	1748270	2135381	18.73%	2.182%
9	6.613	394	396	399	rVB	426115	532664	4.67%	0.544%
10	6.796	409	412	414	rBV	1600619	1827807	16.03%	1.868%
11	6.944	423	425	428	rVB	2766197	2783224	24.41%	2.844%
12	7.219	445	449	453	rBV	218078	365710	3.21%	0.374%
13	7.356	458	461	464	rBV	2464058	2432294	21.33%	2.485%
14	7.482	469	472	474	rBV	7126937	7340822	64.38%	7.501%
15	7.573	478	480	482	rVB2	112854	138080	1.21%	0.141%
16	7.607	482	483	485	rBV	256565	322058	2.82%	0.329%
17	7.744	492	495	497	rVB	775393	880557	7.72%	0.900%
18	7.802	497	500	501	rBV2	144236	167787	1.47%	0.171%
19	8.076	520	524	527	rBV	2221485	2563153	22.48%	2.619%
20	8.133	527	529	530	rVV	299218	291673	2.56%	0.298%
21	8.179	530	533	534	rVV2	122671	206795	1.81%	0.211%
22	8.224	534	537	538	rVV3	95230	160808	1.41%	0.164%
23	8.270	538	541	544	rVB3	138712	216856	1.90%	0.222%
24	8.362	544	549	551	rBV2	66550	160277	1.41%	0.164%
25	8.533	559	564	566	rBV	84349	150011	1.32%	0.153%
26	8.579	566	568	569	rVV	111960	176972	1.55%	0.181%
27	8.613	569	571	573	rVV	1529088	1595659	13.99%	1.631%
28	8.647	573	574	578	rVB2	145550	143570	1.26%	0.147%
29	8.716	578	580	582	rBV2	76602	131392	1.15%	0.134%
30	8.762	582	584	587	rVB3	169152	214992	1.89%	0.220%
31	8.842	587	591	593	rBV2	361317	443214	3.89%	0.453%
32	8.956	596	601	603	rBV	95316	207206	1.82%	0.212%
33	9.013	603	606	607	rVV3	118100	247981	2.17%	0.253%
34	9.047	607	609	610	rVV	298160	294439	2.58%	0.301%

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35	9.105	612	614	615 rBV	133498	116340	1.02%	0.119%
36	9.162	615	619	621 rVB	3934242	4907969	43.04%	5.015%
37	9.265	624	628	632 rVB3	260424	506446	4.44%	0.518%
38	9.379	632	638	640 rBV	730199	807046	7.08%	0.825%
39	9.459	641	645	646 rBV3	126480	242995	2.13%	0.248%
40	9.482	646	647	650 rVV3	123775	186794	1.64%	0.191%
41	9.562	650	654	655 rVV	622695	962456	8.44%	0.984%
42	9.585	655	656	661 rVB5	65745	144447	1.27%	0.148%
43	9.710	665	667	669 rVB	331117	319421	2.80%	0.326%
44	9.768	669	672	674 rBV	441675	665702	5.84%	0.680%
45	9.836	674	678	680 rVV	2730735	3265383	28.64%	3.337%
46	9.882	680	682	684 rVV3	98076	184921	1.62%	0.189%
47	10.065	696	698	699 rBV2	141021	171824	1.51%	0.176%
48	10.099	699	701	702 rVV	227174	345830	3.03%	0.353%
49	10.133	702	704	706 rVV	1546612	1514251	13.28%	1.547%
50	10.168	706	707	709 rVB	696097	636603	5.58%	0.651%
51	10.270	713	716	718 rVV2	648983	743612	6.52%	0.760%
52	10.430	726	730	732 rBV	3885667	5982499	52.47%	6.113%
53	10.488	732	735	738 rVB2	1248761	1684782	14.78%	1.722%
54	10.579	741	743	744 rVV	462524	513420	4.50%	0.525%
55	10.625	744	747	748 rVV2	1632292	1967766	17.26%	2.011%
56	10.659	748	750	752 rVB2	682135	879614	7.71%	0.899%
57	10.716	752	755	756 rBV	711045	1046371	9.18%	1.069%
58	10.750	756	758	760 rVV	1602480	2088648	18.32%	2.134%
59	10.785	760	761	762 rVB	344048	237648	2.08%	0.243%
60	10.910	770	772	776 rVB	657805	651059	5.71%	0.665%
61	11.013	779	781	783 rBV	782143	727609	6.38%	0.744%
62	11.070	785	786	790 rVB4	80760	157397	1.38%	0.161%
63	11.196	792	797	798 rBV2	224797	508210	4.46%	0.519%
64	11.322	805	808	809 rVB	1922261	2472629	21.69%	2.527%
65	11.585	825	831	832 rBV4	203989	422045	3.70%	0.431%
66	11.642	832	836	839 rVV2	498539	837515	7.35%	0.856%
67	11.722	840	843	844 rVV	3446376	3639523	31.92%	3.719%
68	11.756	844	846	848 rVV	1392953	1240733	10.88%	1.268%
69	11.802	848	850	853 rVV2	351786	545210	4.78%	0.557%
70	11.871	853	856	857 rVV	697586	779105	6.83%	0.796%
71	11.951	861	863	865 rVB2	258204	283859	2.49%	0.290%

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72	12.065	872	873	875	rVB2	156986	118796	1.04%	0.121%
73	12.111	875	877	880	rBV3	310406	395365	3.47%	0.404%
74	12.225	885	887	891	rVB3	218738	261294	2.29%	0.267%
75	12.305	891	894	895	rBV2	255967	363786	3.19%	0.372%
76	12.373	899	900	905	rBV5	119087	286335	2.51%	0.293%
77	12.476	907	909	911	rVB	235377	210922	1.85%	0.216%
78	12.591	916	919	920	rBV2	127145	193588	1.70%	0.198%
79	12.648	923	924	930	rVB5	159560	272652	2.39%	0.279%
80	12.854	940	942	944	rBV	163203	222551	1.95%	0.227%
81	12.899	944	946	949	rVV	2739578	3265015	28.63%	3.336%
82	12.956	949	951	953	rVB	132856	139761	1.23%	0.143%
83	13.071	957	961	963	rVB5	136189	328454	2.88%	0.336%
84	13.128	964	966	970	rVV5	104391	157557	1.38%	0.161%
85	13.219	973	974	977	rVV2	171541	181768	1.59%	0.186%
86	13.276	977	979	981	rVB	146274	162613	1.43%	0.166%
87	13.574	1002	1005	1008	rBV2	191396	273527	2.40%	0.280%
88	13.699	1013	1016	1018	rVB2	462368	589347	5.17%	0.602%
89	13.814	1023	1026	1031	rVV	1224418	1464917	12.85%	1.497%
90	13.894	1031	1033	1036	rVV2	190082	241210	2.12%	0.246%
91	13.951	1036	1038	1041	rVB	2218900	2275441	19.96%	2.325%
92	14.797	1110	1112	1114	rVB	138497	151043	1.32%	0.154%
93	15.368	1159	1162	1164	rBV	1127061	1704159	14.95%	1.741%
94	15.860	1203	1205	1211	rVB4	68959	153419	1.35%	0.157%
95	16.271	1239	1241	1247	rVB3	62983	158188	1.39%	0.162%
96	16.900	1293	1296	1303	rVB8	39963	123467	1.08%	0.126%

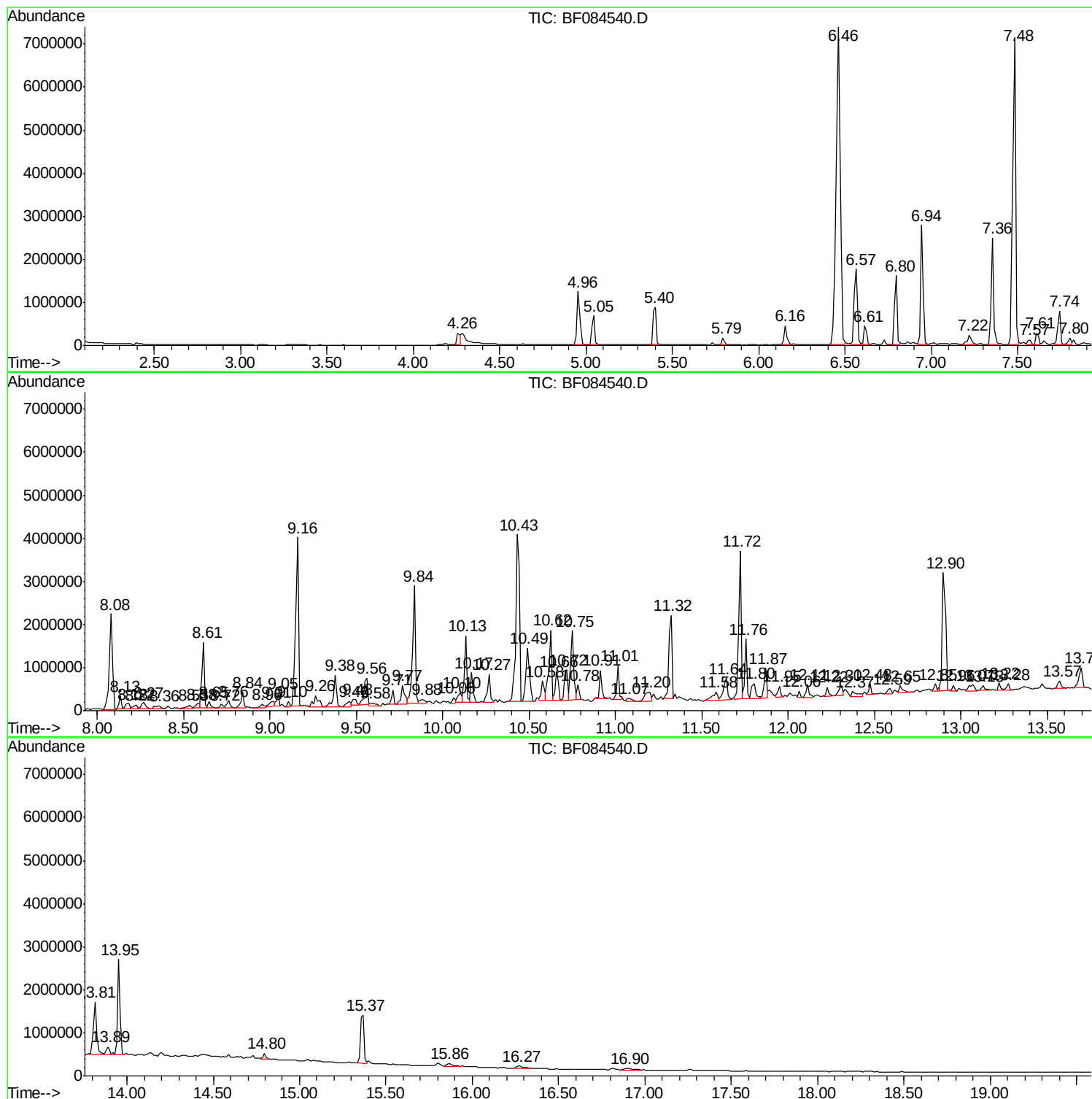
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF123115.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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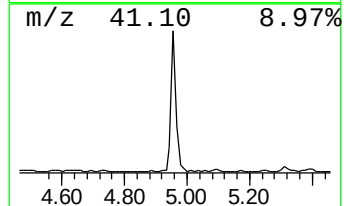
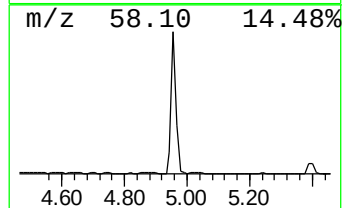
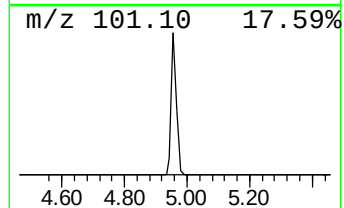
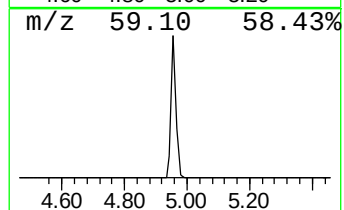
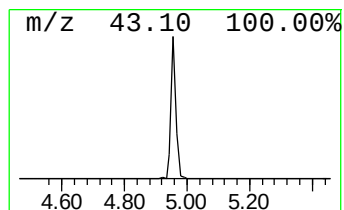
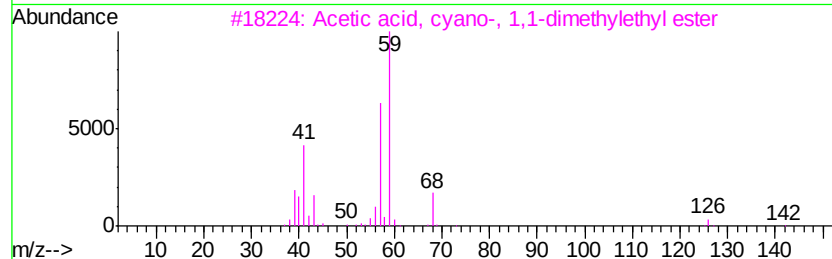
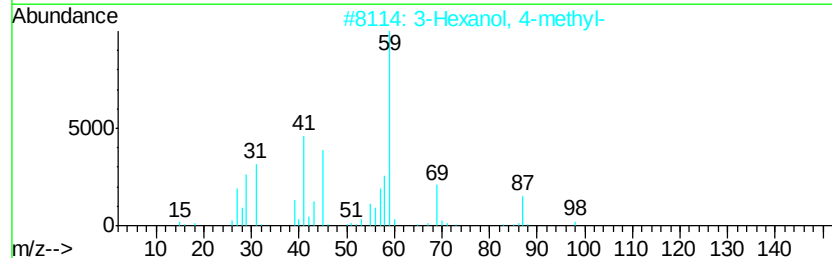
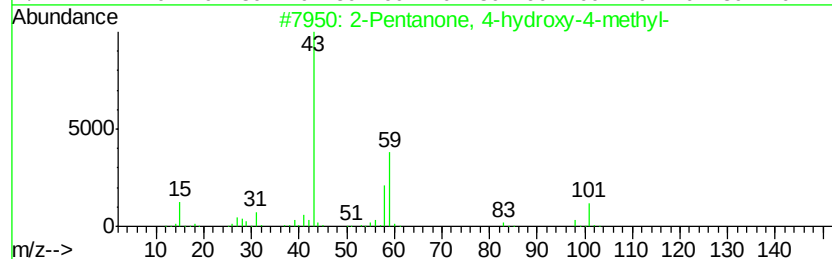
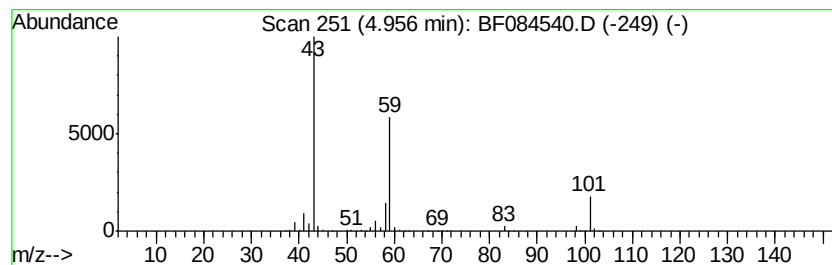
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	14.00 ng	1279810	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	59
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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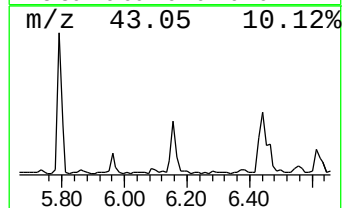
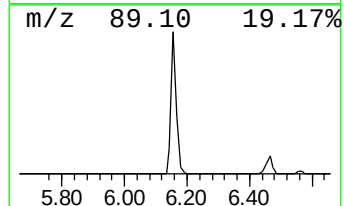
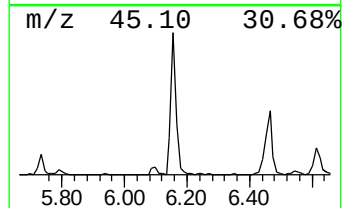
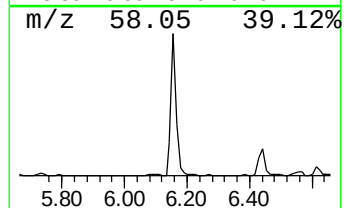
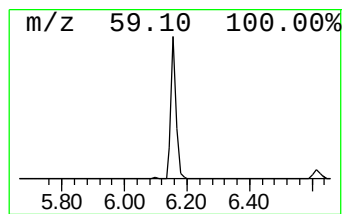
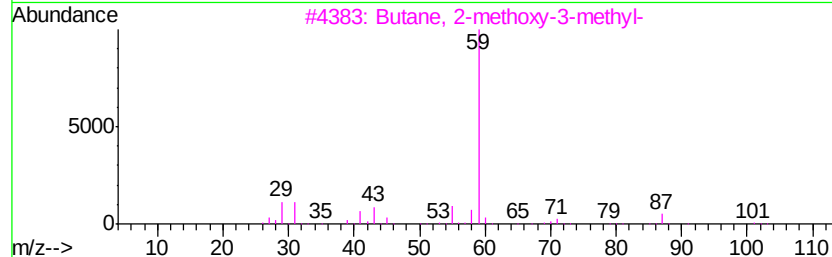
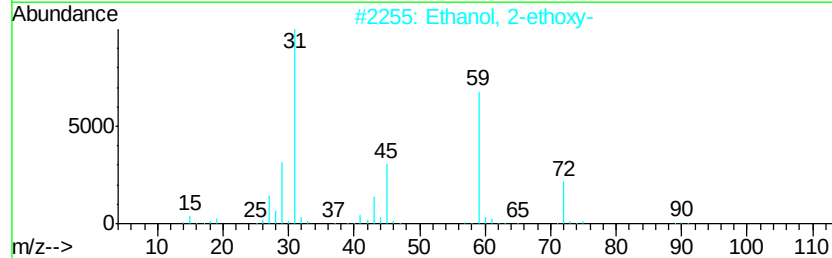
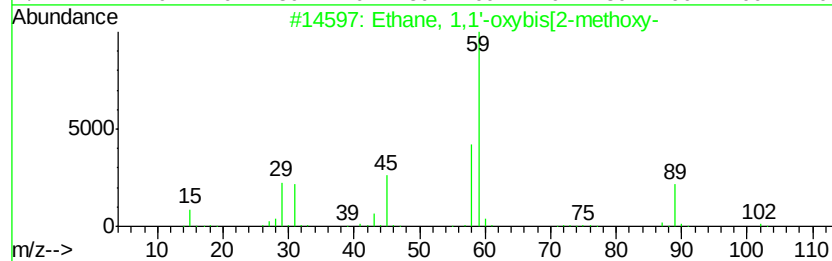
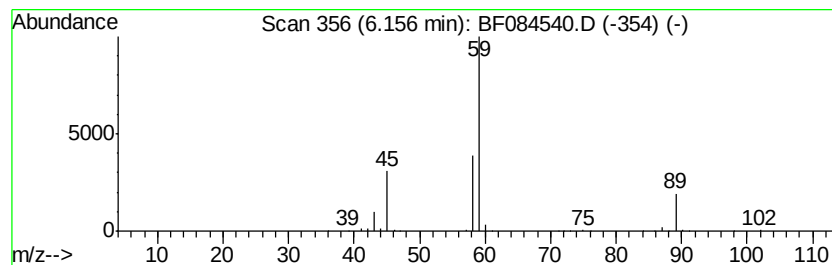
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Ethane, 1,1'-oxybis[2-methoxy- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.16	5.44 ng	497077	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethane, 1,1'-oxybis[2-methoxy-	134	C6H14O3	000111-96-6	83
2		Ethanol, 2-ethoxy-	90	C4H10O2	000110-80-5	9
3		Butane, 2-methoxy-3-methyl-	102	C6H14O	062016-49-3	9
4		Pentane, 2-methoxy-	102	C6H14O	006795-88-6	9
5		1,2-Butanediol	90	C4H10O2	000584-03-2	9



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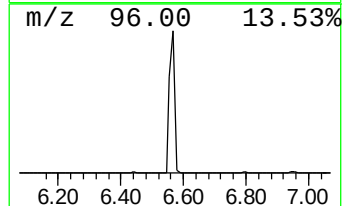
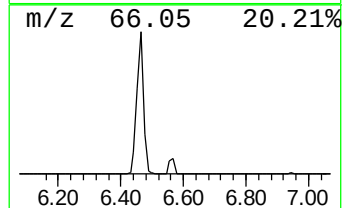
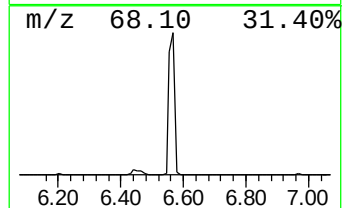
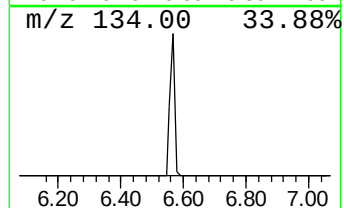
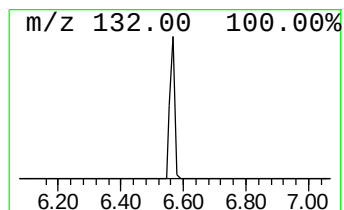
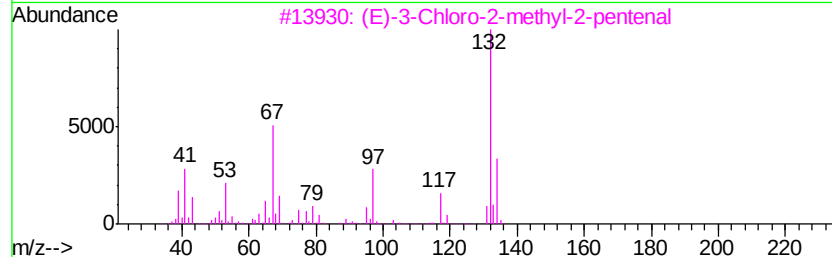
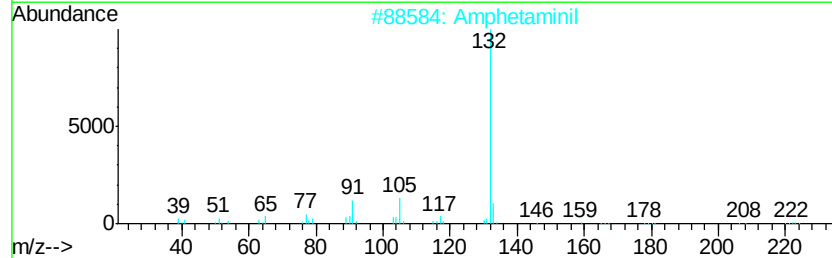
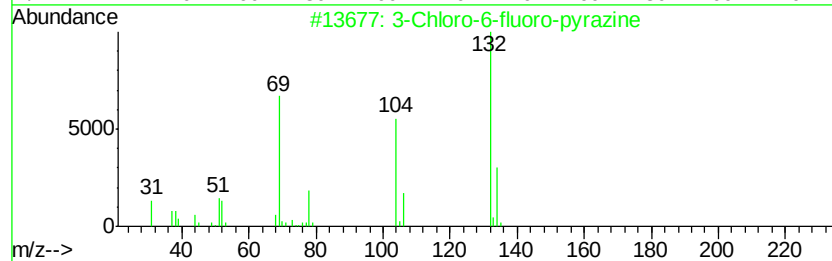
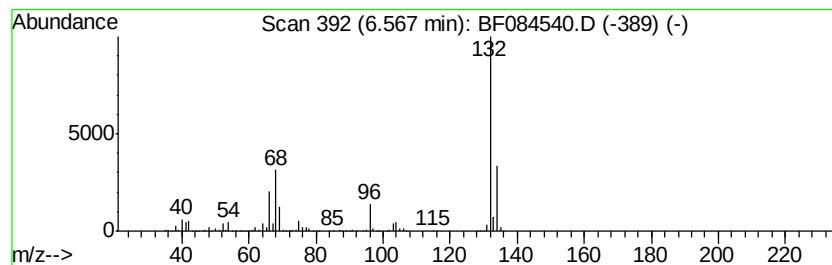
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.57 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	23.37 ng	2135380	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	38
2		Amphetaminil	250	C17H18N2	017590-01-1	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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ALS Vial : 4 Sample Multiplier: 1

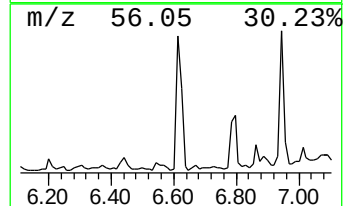
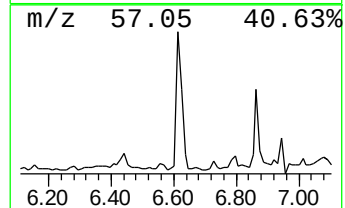
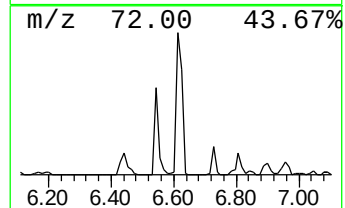
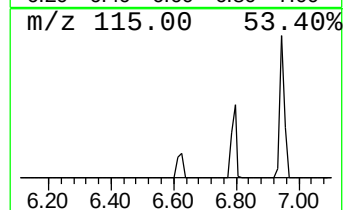
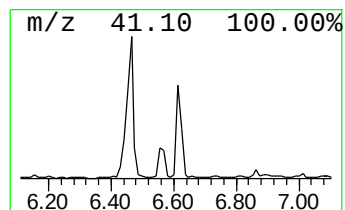
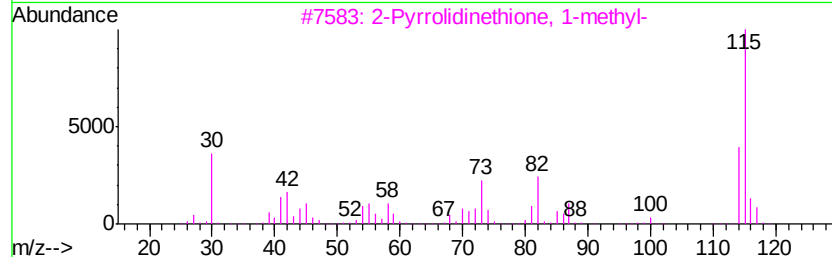
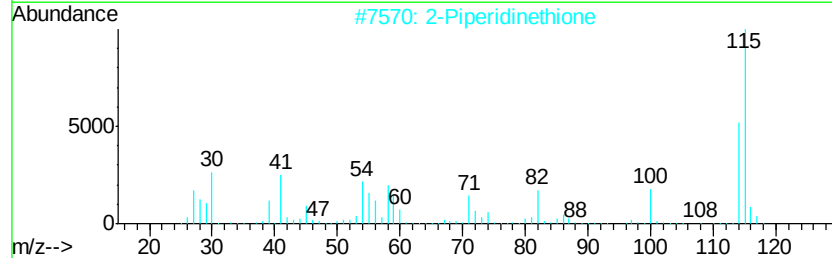
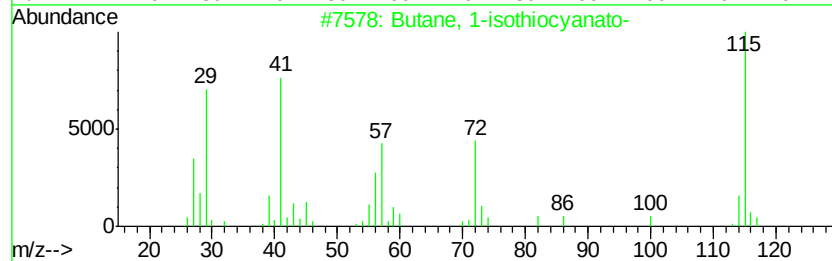
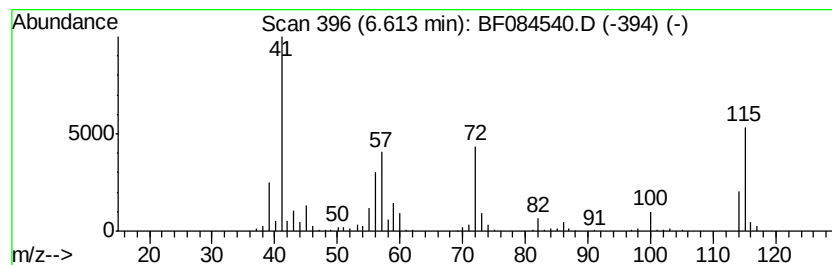
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Butane, 1-isothiocyanato- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.61	5.83 ng	532664	1,4-Dichlorobenzene-d4	6.80	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 1-isothiocyanato-	115	C5H9NS	000592-82-5	87
2	2-Piperidinethione	115	C5H9NS	013070-01-4	32
3	2-Pyrrolidinethione, 1-methyl-	115	C5H9NS	010441-57-3	25
4	Isobutyl isothiocyanate	115	C5H9NS	000591-82-2	25
5	Butanedioic acid, dimethyl ester	146	C6H10O4	000106-65-0	17



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011816\
Data File : BF084540.D
Acq On : 18 Jan 2016 17:24
Operator : SJ/UM
Sample : H1140-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SYS-DIS-011416

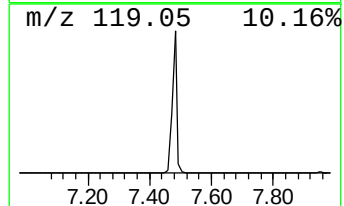
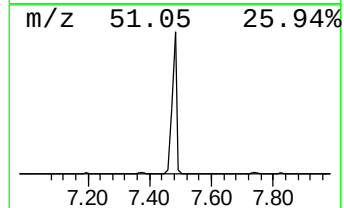
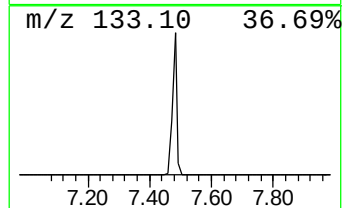
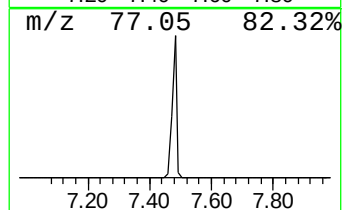
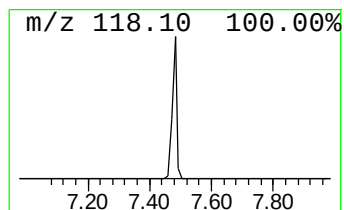
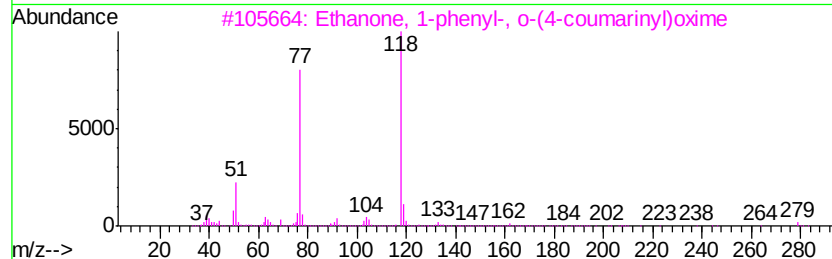
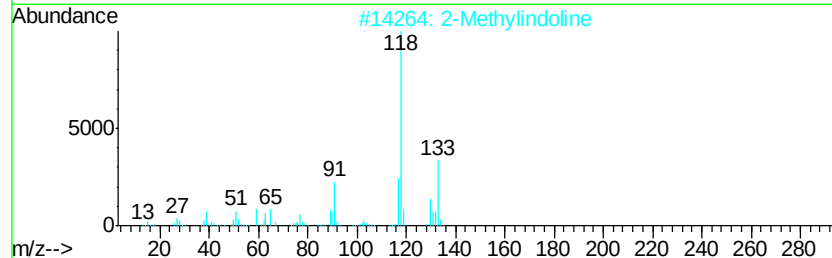
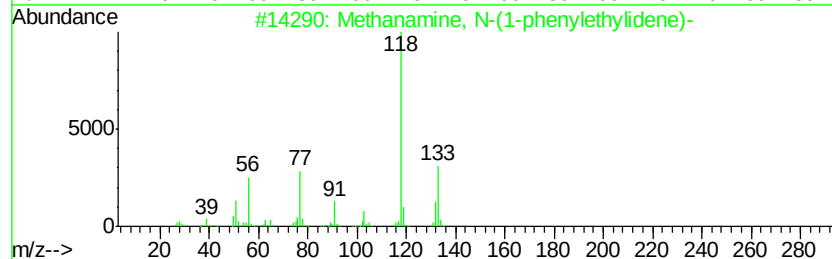
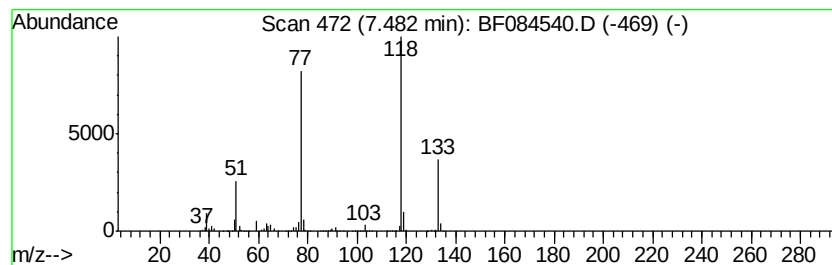
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown7.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.48	57.28 ng	7340820	Napthalene-d8	8.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methanamine, N-(1-phenylethylidene...	133	C9H11N	006907-71-7	40
2		2-Methylindoline	133	C9H11N	006872-06-6	38
3		Ethanone, 1-phenyl-, o-(4-coumar...	279	C17H13NO3	034605-11-3	35
4		1H-Indazole	118	C7H6N2	000271-44-3	30
5		Cyanic acid, phenyl ester	119	C7H5NO	001122-85-6	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011816\
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Sample : H1140-01
Misc :
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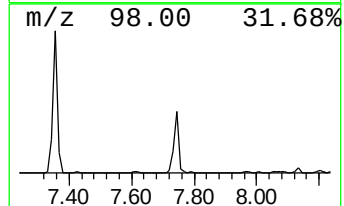
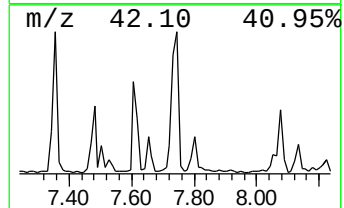
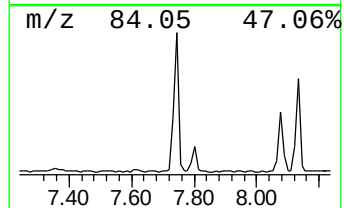
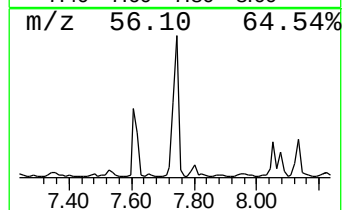
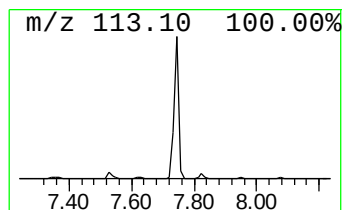
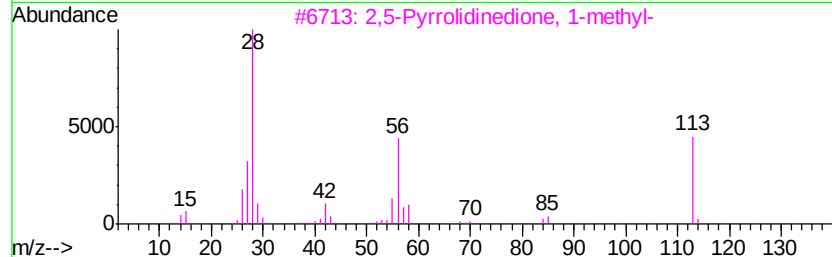
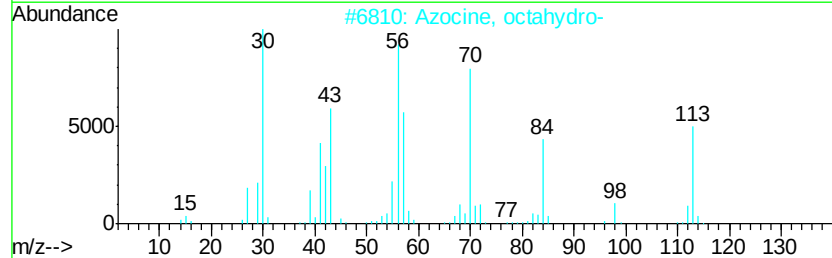
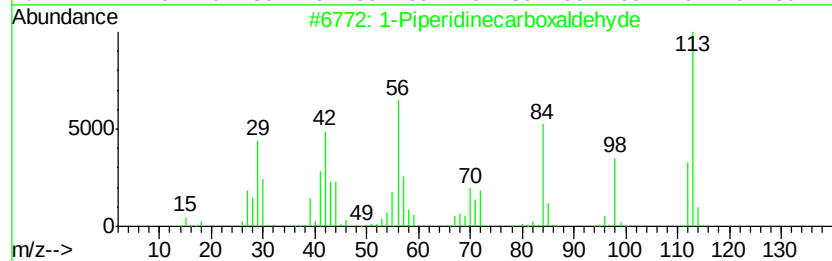
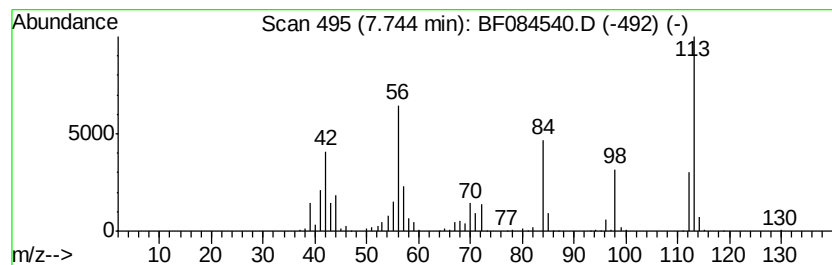
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Piperidinecarboxaldehyde Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.		
7.74	6.87 ng	880557	Napthalene-d8	8.08		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Piperidinecarboxaldehyde	113	C6H11NO	002591-86-8	98
2		Azocine, octahydro-	113	C7H15N	001121-92-2	40
3		2,5-Pyrrolidinedione, 1-methyl-	113	C5H7NO2	001121-07-9	38
4		Caprolactam	113	C6H11NO	000105-60-2	37
5		Isothiazole, 4,5-dimethyl-	113	C5H7NS	027330-47-8	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011816\
Data File : BF084540.D
Acq On : 18 Jan 2016 17:24
Operator : SJ/UM
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Misc :
ALS Vial : 4 Sample Multiplier: 1

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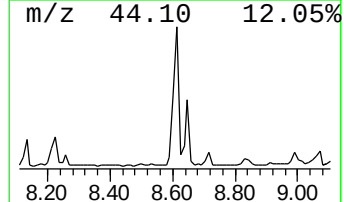
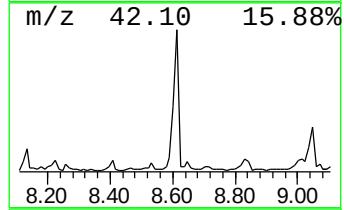
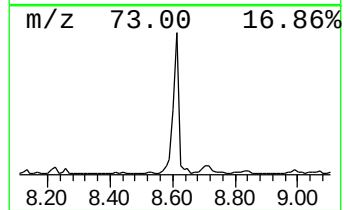
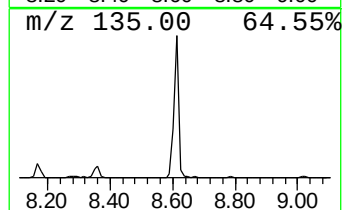
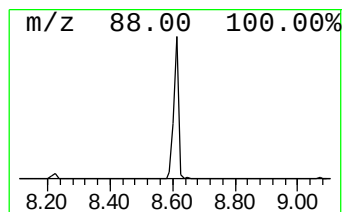
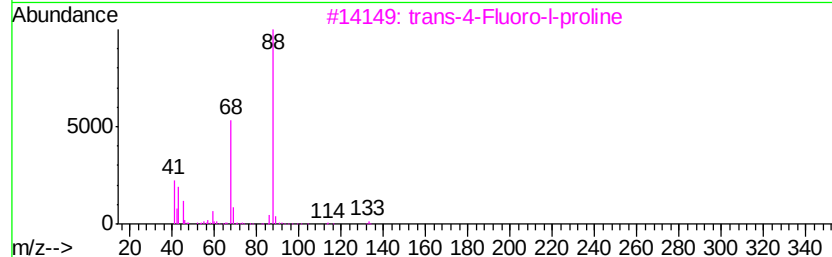
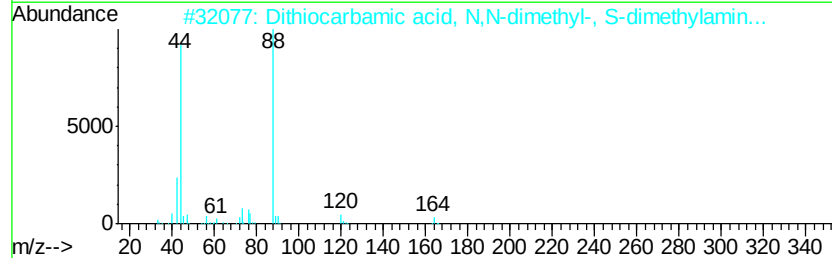
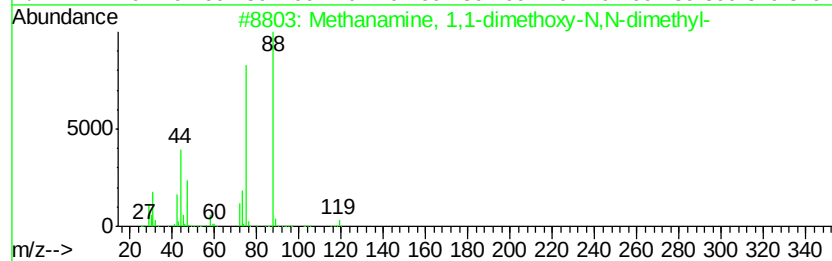
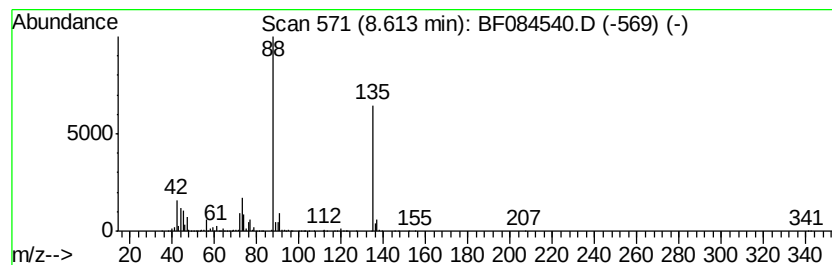
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown8.61 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.61	12.45 ng	1595660	Naphthalene-d8	8.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methanamine, 1,1-dimethoxy-N,N-d...	119	C5H13NO2	004637-24-5	38
2		Dithiocarbamic acid, N,N-dimethy...	164	C5H12N2S2	002801-22-1	37
3		trans-4-Fluoro-l-proline	133	C5H8FN02	1000132-55-8	35
4		Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	28
5		Dithiocarbamic acid, N,N-dimethy...	204	C8H16N2S2	066232-66-4	25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011816\
Data File : BF084540.D
Acq On : 18 Jan 2016 17:24
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Instrument :
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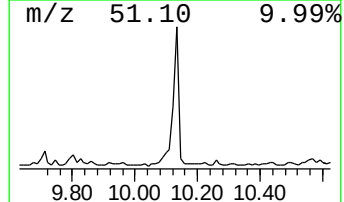
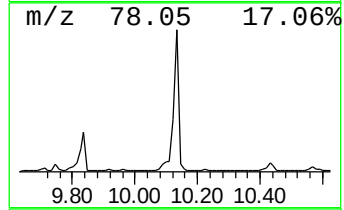
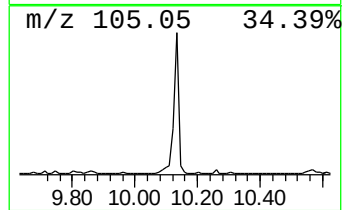
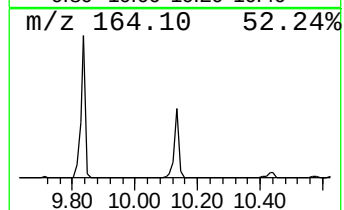
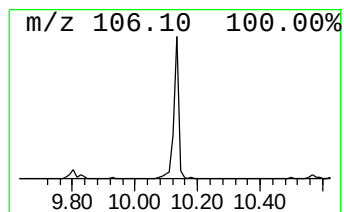
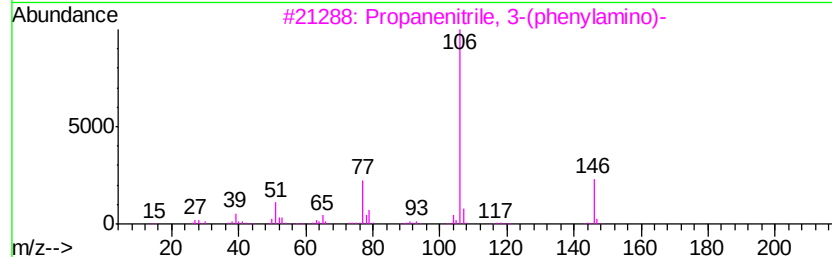
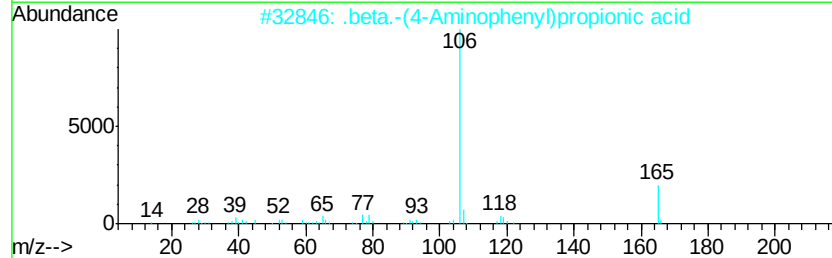
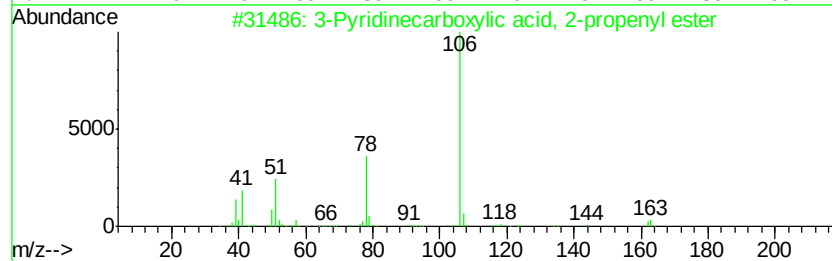
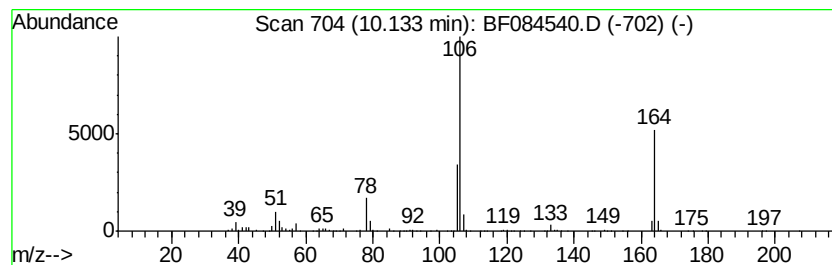
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown10.13 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.13	9.27 ng	1514250	Acenaphthene-d10	9.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Pyridinecarboxylic acid, 2-pro...	163	C9H9NO2	025635-12-5	47
2		.beta.-(4-Aminophenyl)propionic ...	165	C9H11NO2	002393-17-1	38
3		Propanenitrile, 3-(phenylamino)-	146	C9H10N2	001075-76-9	25
4		1-Propanone, 1-(3-pyridinyl)-	135	C8H9NO	001570-48-5	23
5		(5-tert-Butyl-5-hydroxy-3-triflu...	315	C14H16F3N3O2	1000297-18-2	23



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011816\
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Acq On : 18 Jan 2016 17:24
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Sample : H1140-01
Misc :
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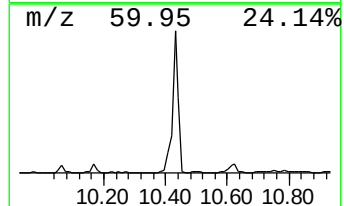
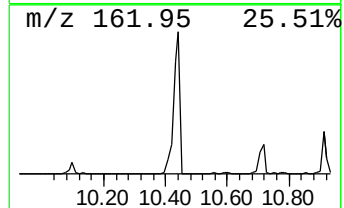
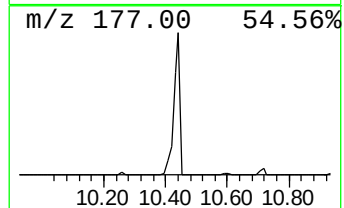
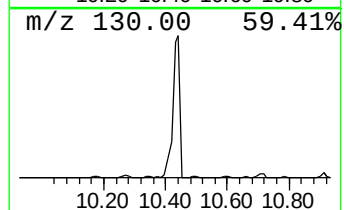
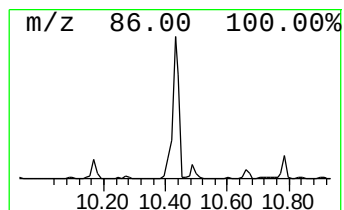
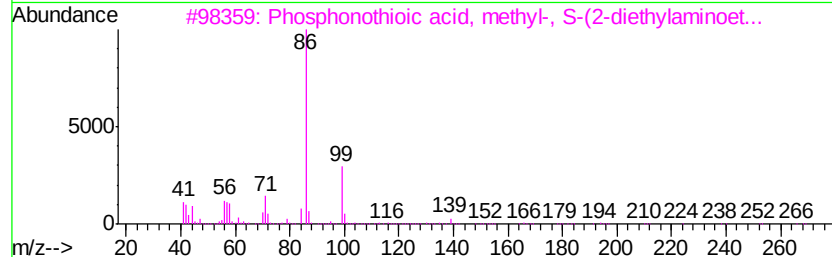
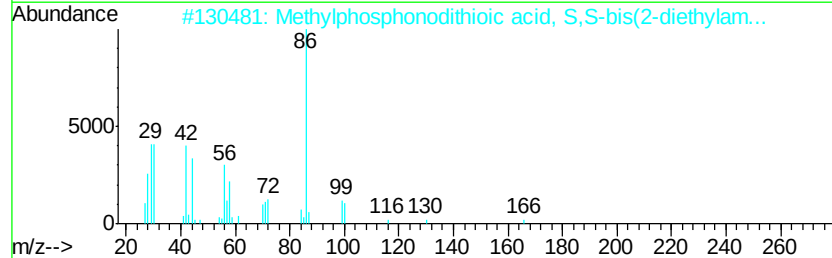
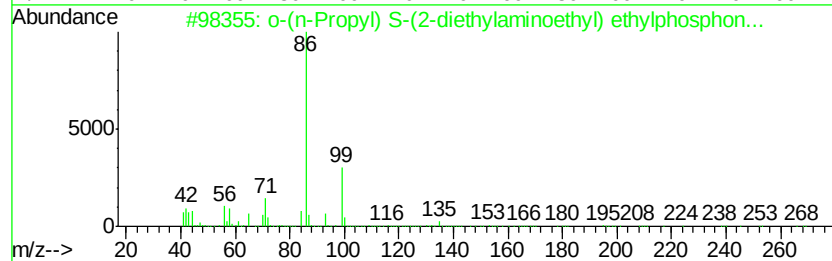
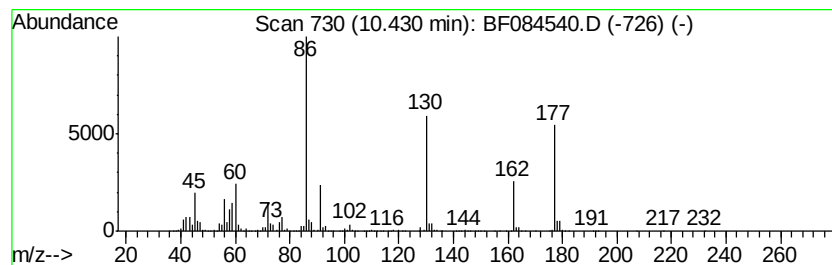
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown10.43 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.43	36.64 ng	5982500	Acenaphthene-d10	9.84	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-(n-Propyl) S-(2-diethylaminoet...	267	C11H26N02PS	1000273-61-8	22
2	Methylphosphonodithioic acid, S,...	326	C13H31N20PS2	092030-06-3	22
3	Phosphonothioic acid, methyl-, S...	267	C11H26N02PS	159939-87-4	22
4	Imidazole, 4-fluoro-	86	C3H3FN2	030086-17-0	22
5	3(2H)-Thiophenone, 2-ethyldihydro-	130	C6H10OS	052662-38-1	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011816\
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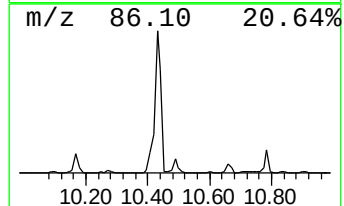
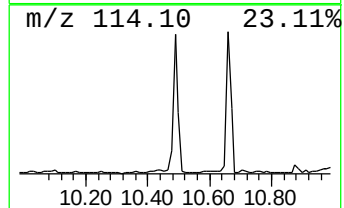
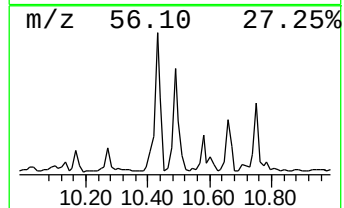
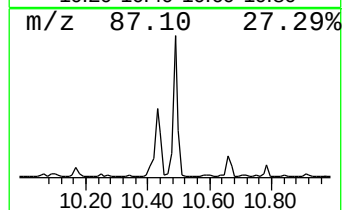
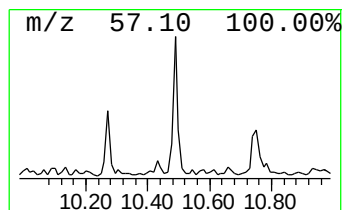
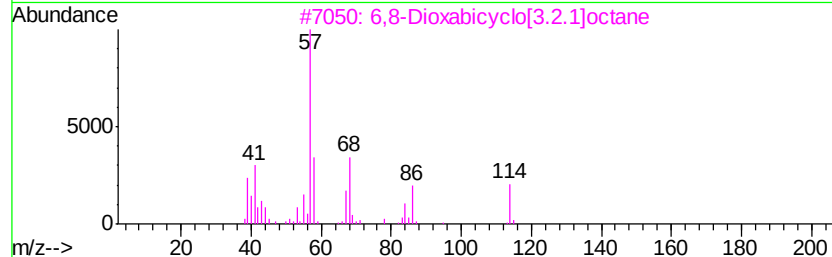
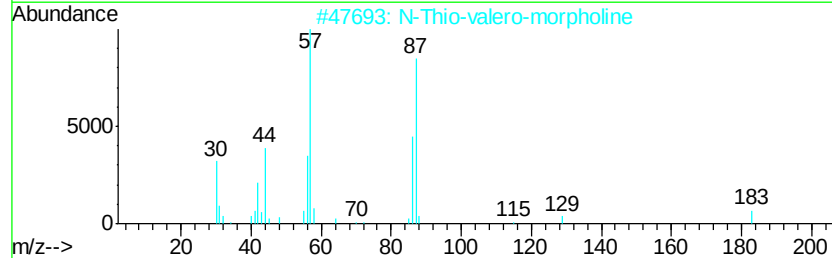
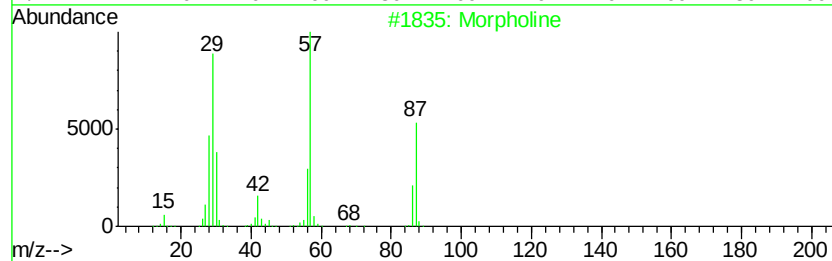
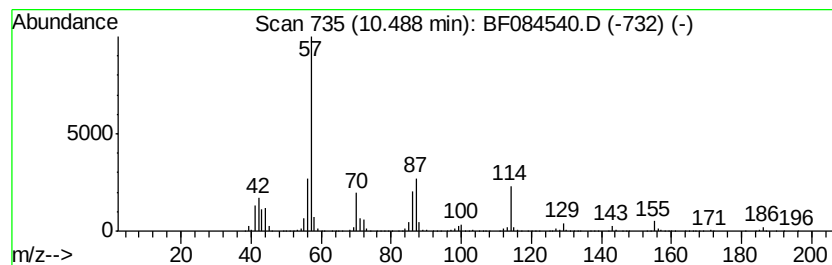
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown10.49 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.49	10.32 ng	1684780	Acenaphthene-d10		9.84
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine	87	C4H9NO	000110-91-8	38
2	N-Thio-valero-morpholine	187	C9H17NOS	002832-99-7	38
3	6,8-Dioxabicyclo[3.2.1]octane	114	C6H10O2	000280-16-0	38
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	25
5	n-Butyro-morpholine	157	C8H15NO2	005327-51-5	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011816\
Data File : BF084540.D
Acq On : 18 Jan 2016 17:24
Operator : SJ/UM
Sample : H1140-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SYS-DIS-011416

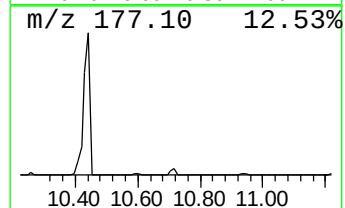
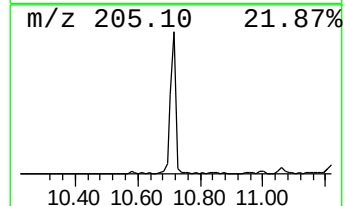
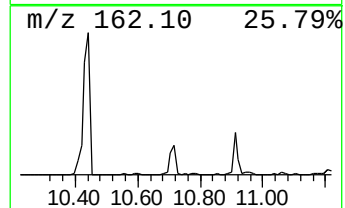
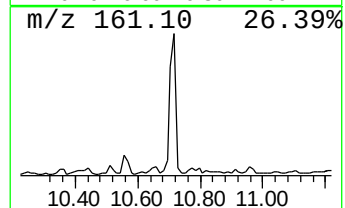
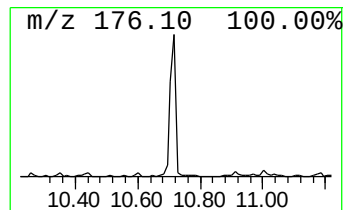
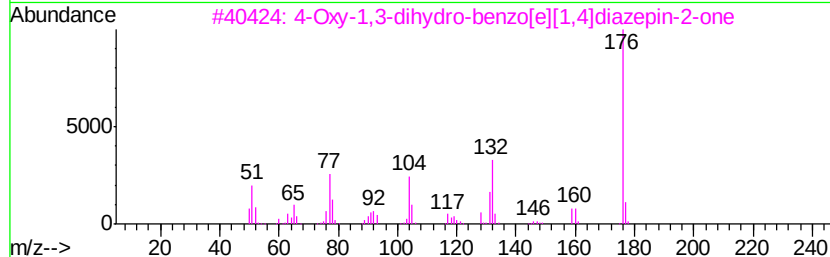
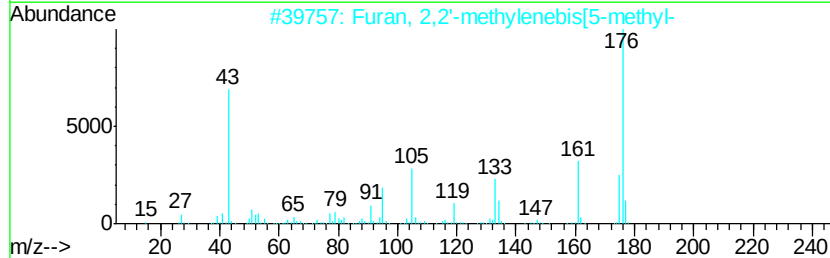
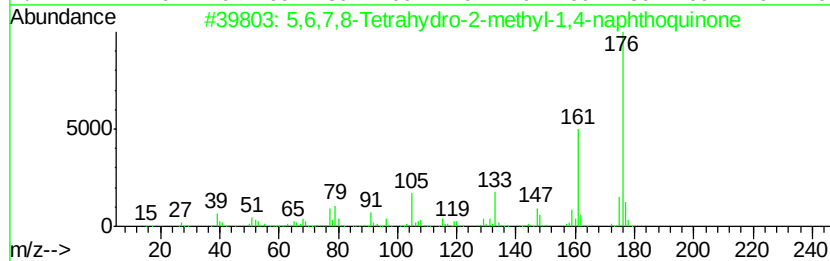
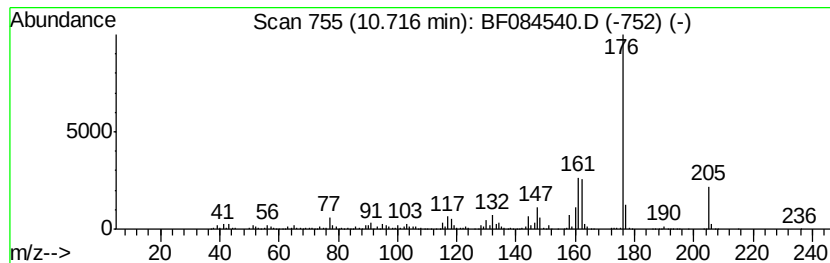
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 5,6,7,8-Tetrahydro-2-methyl... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.72	8.46 ng	1046370	Phenanthrene-d10	11.32

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5,6,7,8-Tetrahydro-2-methyl-1,4-...	176	C11H12O2	000058-26-4	52
2			Furan, 2,2'-methylenebis[5-methyl-	176	C11H12O2	013679-43-1	47
3			4-Oxy-1,3-dihydro-benzo[e][1,4]d...	176	C9H8N2O2	016780-57-7	43
4			4(5H)-Oxazolone, 2-amino-5-phenyl-	176	C9H8N2O2	002152-34-3	43
5			cis-2,4-Dimethoxy-.beta.-methyl-...	223	C11H13NO4	015804-78-1	42



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011816\
Data File : BF084540.D
Acq On : 18 Jan 2016 17:24
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Misc :
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Instrument :
BNA_F
ClientSampleId :
SYS-DIS-011416

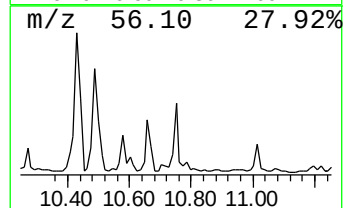
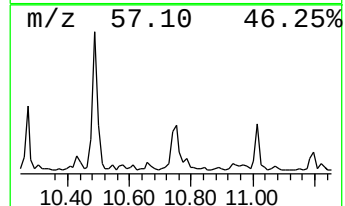
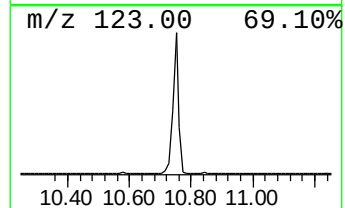
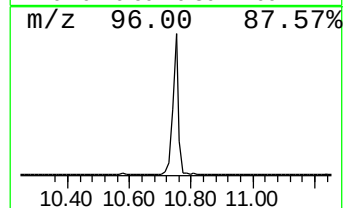
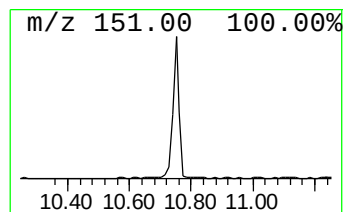
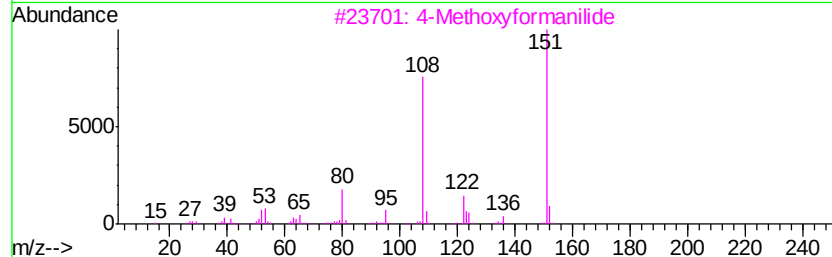
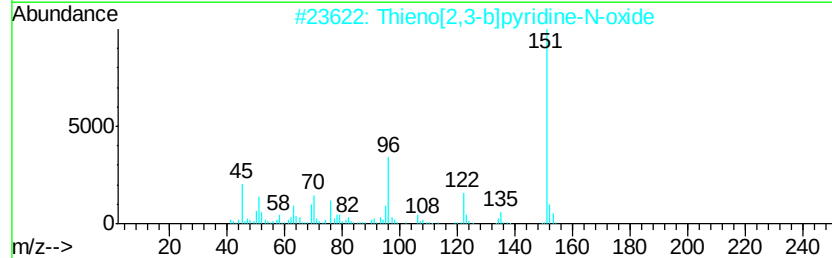
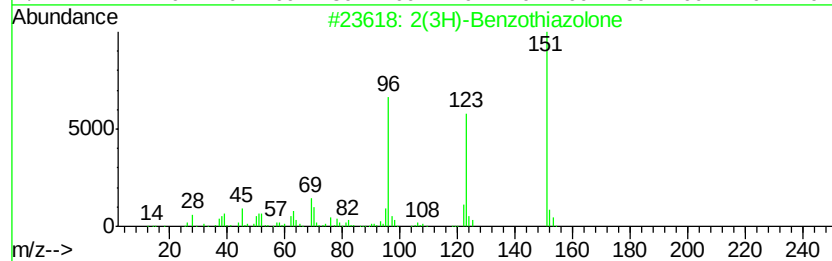
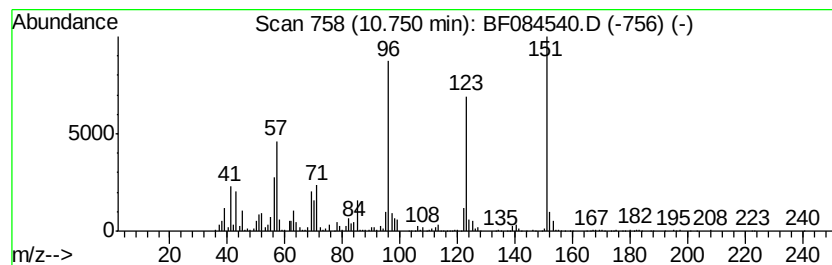
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 2(3H)-Benzothiazolone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	16.89 ng	2088650	Phenanthrene-d10	11.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	96
2		Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	35
3		4-Methoxyformanilide	151	C8H9NO2	023896-88-0	27
4		5-Cyclohexyl-1-pentene	152	C11H20	005729-54-4	25
5		1H-Imidazo[4,5-b]pyridine-2-thiol	151	C6H5N3S	029448-81-5	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011816\
Data File : BF084540.D
Acq On : 18 Jan 2016 17:24
Operator : SJ/UM
Sample : H1140-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

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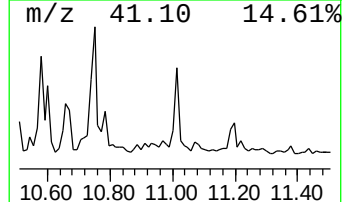
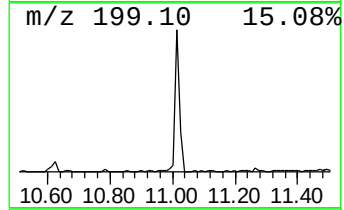
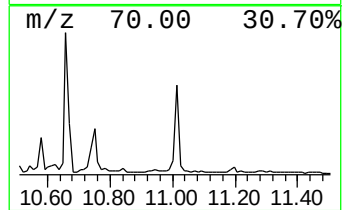
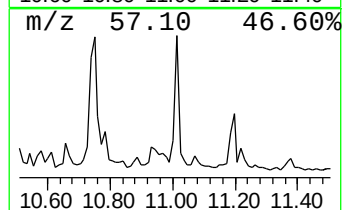
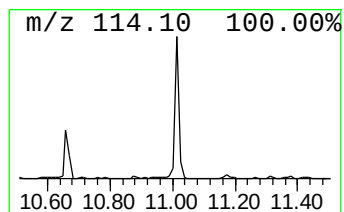
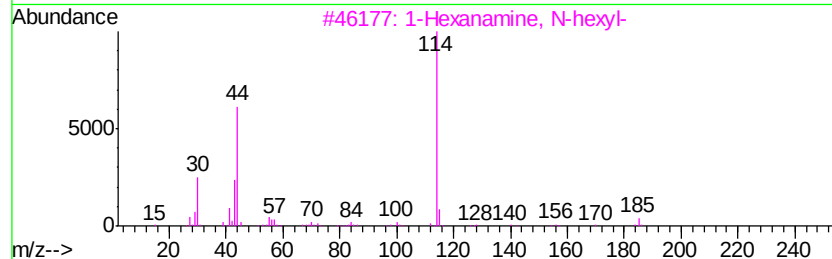
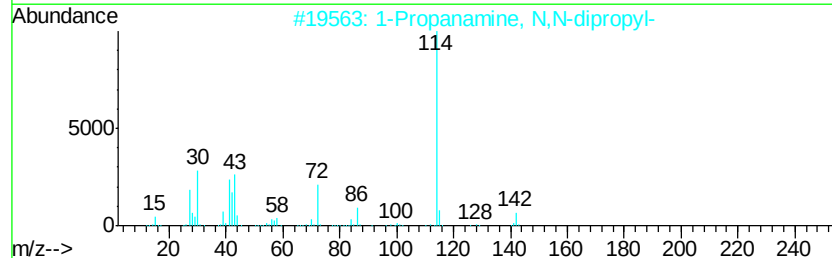
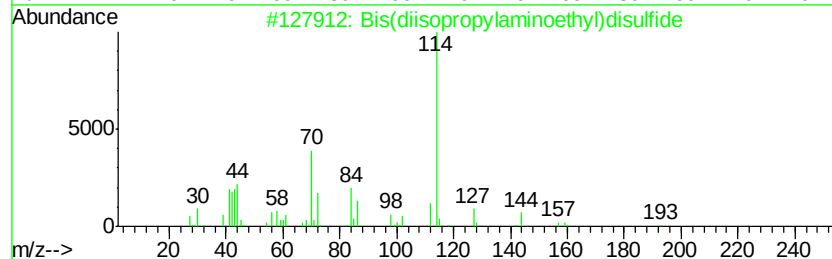
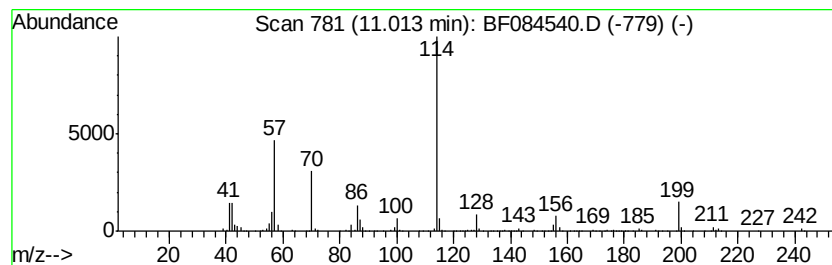
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown11.01 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.01	5.89 ng	727609	Phenanthrene-d10	11.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bis(diisopropylaminoethyl)disulfide	320	C16H36N2S2	065332-44-7	42
2		1-Propanamine, N,N-dipropyl-	143	C9H21N	000102-69-2	37
3		1-Hexanamine, N-hexyl-	185	C12H27N	000143-16-8	37
4		Methylthiophosphonic acid, o-ter...	353	C15H36N02PSSi	1000273-24-2	33
5		[2-(Diisopropylamino)ethyl]-(2-m...	221	C10H23NS2	168885-96-9	33



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011816\
Data File : BF084540.D
Acq On : 18 Jan 2016 17:24
Operator : SJ/UM
Sample : H1140-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SYS-DIS-011416

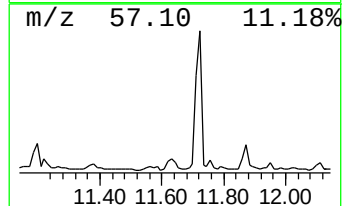
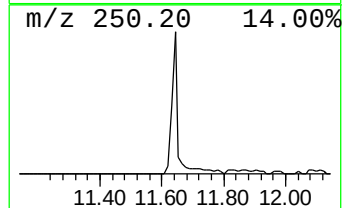
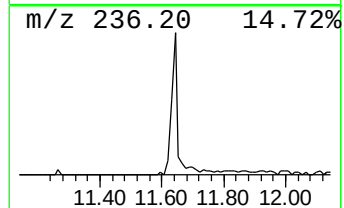
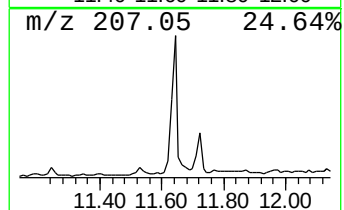
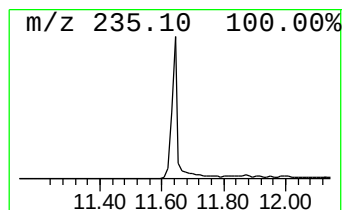
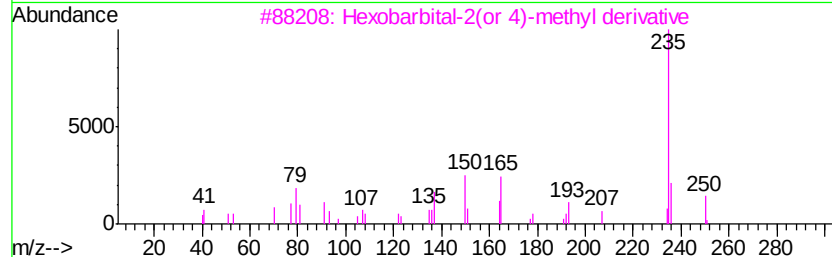
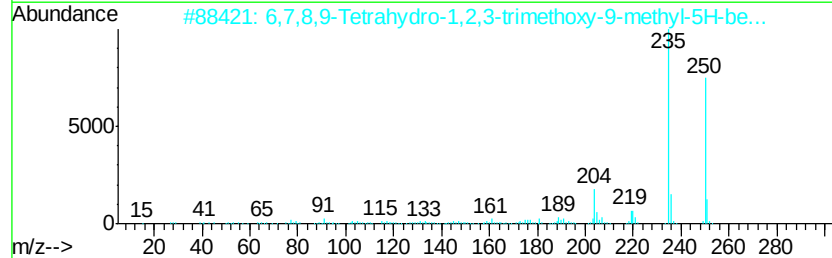
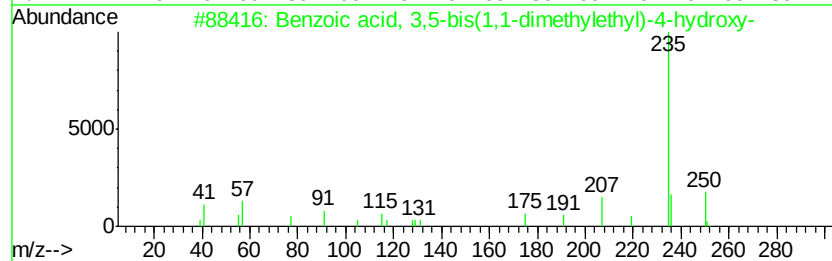
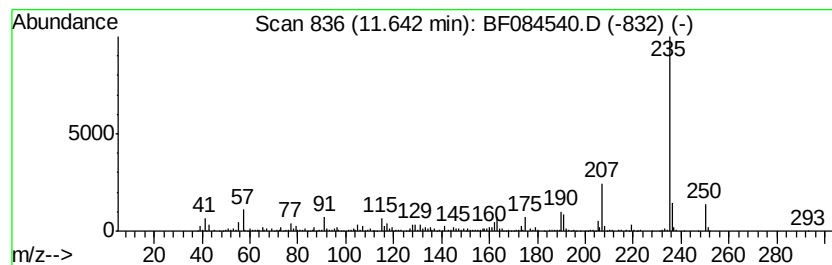
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Benzoic acid, 3,5-bis(1,1-d... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.64	6.77 ng	837515	Phenanthrene-d10	11.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzoic acid, 3,5-bis(1,1-dimeth...	250	C15H22O3	001421-49-4	90
2		6,7,8,9-Tetrahydro-1,2,3-trimeth...	250	C15H22O3	1000242-60-6	59
3		Hexobarbital-2(or 4)-methvl deri...	250	C13H18N2O3	1000123-51-5	59
4		Benzenesulfonamide, 4-amino-N-(3...	299	C15H13N3O2S	028970-84-5	50
5		1,3-Benzenedicarboxylic acid, 5-...	250	C14H18O4	016308-65-9	50



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011816\
Data File : BF084540.D
Acq On : 18 Jan 2016 17:24
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Instrument :
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ClientSampleId :
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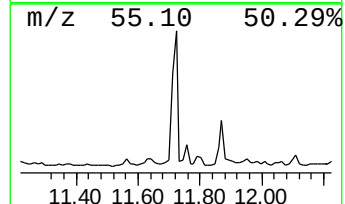
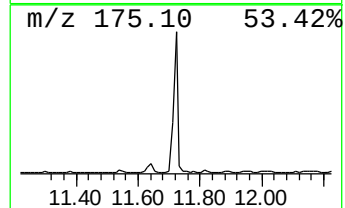
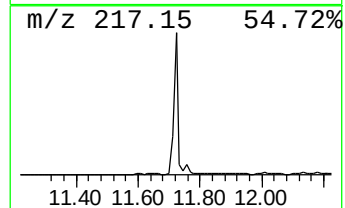
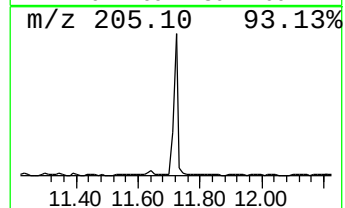
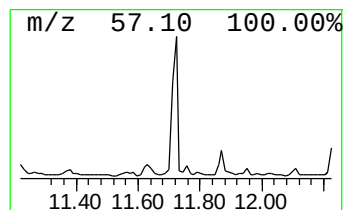
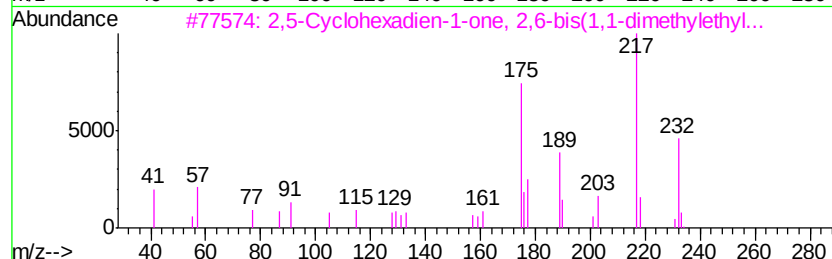
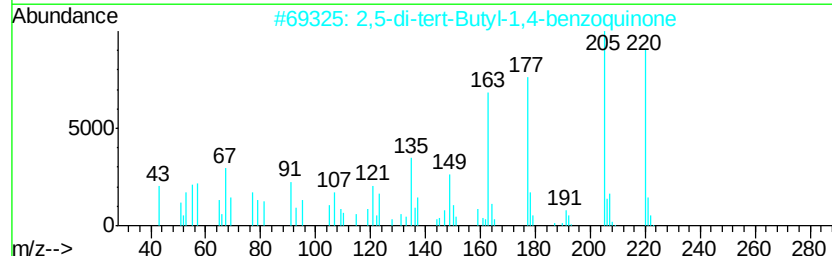
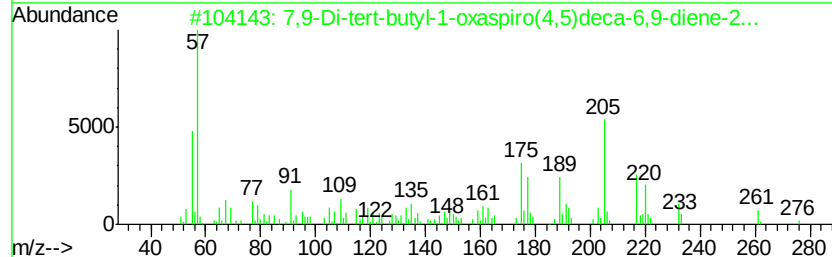
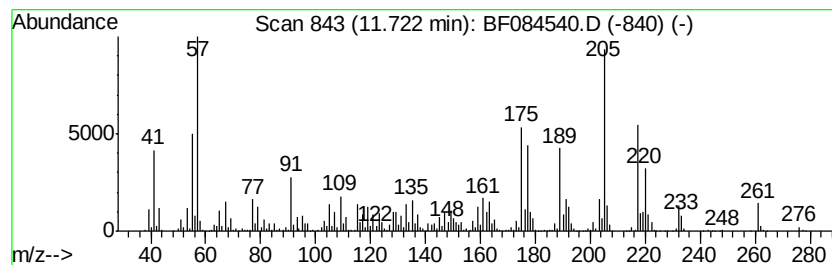
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.72	29.44 ng	3639520	Phenanthrene-d10	11.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	99
2		2,5-di-tert-Butyl-1,4-benzoquinone	220	C14H20O2	002460-77-7	45
3		2,5-Cyclohexadien-1-one, 2,6-bis...	232	C16H24O	006738-27-8	42
4		1,3-Pentadiene, 1,1-diphenyl-, (Z)-	220	C17H16	015295-31-5	38
5		Butylated Hydroxytoluene	220	C15H24O	000128-37-0	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011816\
Data File : BF084540.D
Acq On : 18 Jan 2016 17:24
Operator : SJ/UM
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ALS Vial : 4 Sample Multiplier: 1

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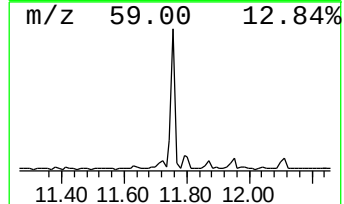
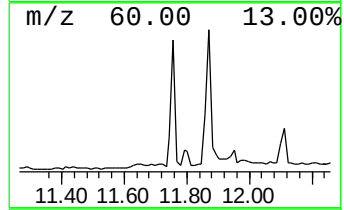
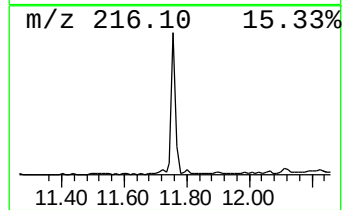
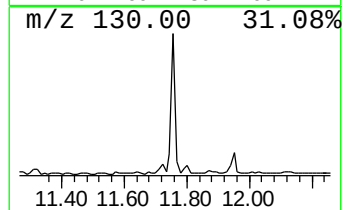
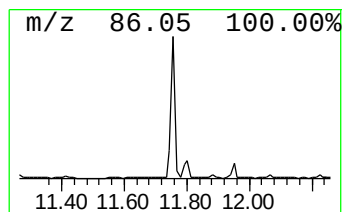
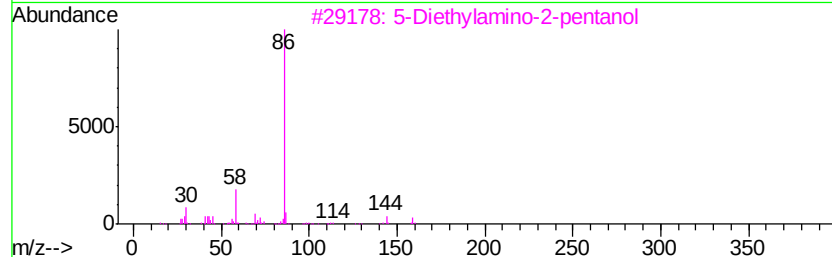
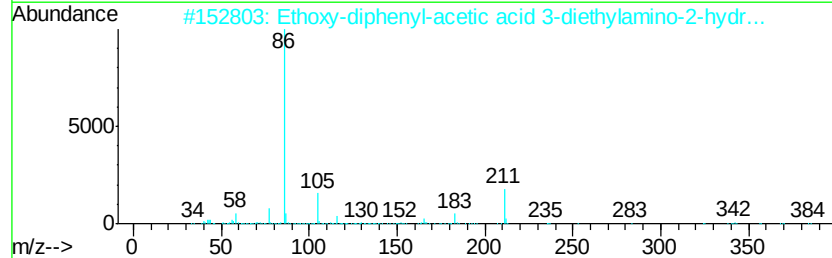
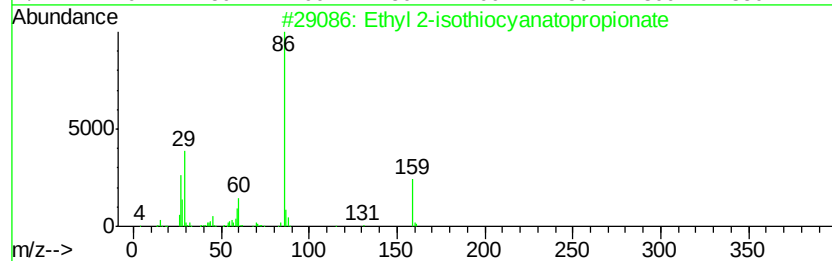
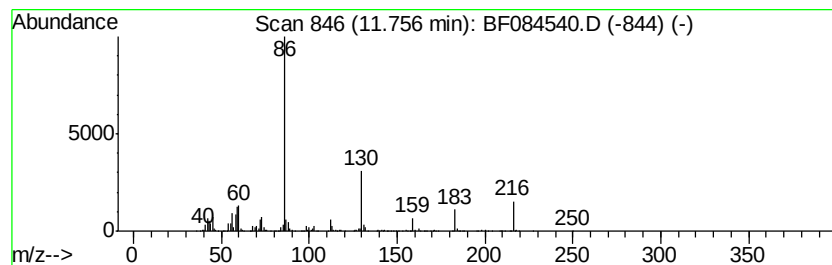
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Ethyl 2-isothiocyanatopropi... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.76	10.04 ng	1240730	Phenanthrene-d10	11.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethyl 2-isothiocyanatopropionate	159	C6H9N02S	039574-16-8	53
2		Ethoxy-diphenyl-acetic acid 3-di...	385	C23H31N04	087415-97-2	43
3		5-Diethylamino-2-pentanol	159	C9H21NO	005412-69-1	43
4		Imidazole, 4-fluoro-	86	C3H3FN2	030086-17-0	43
5		Dicyclomine	309	C19H35N02	000077-19-0	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011816\
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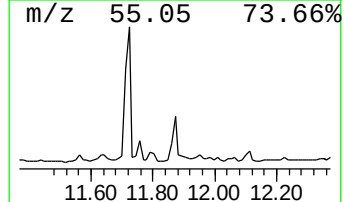
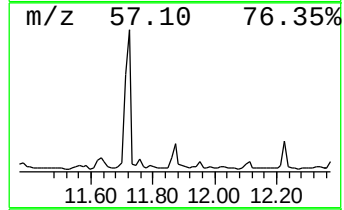
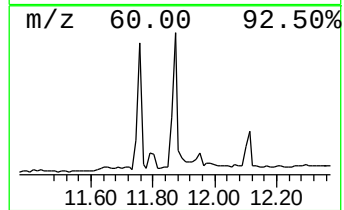
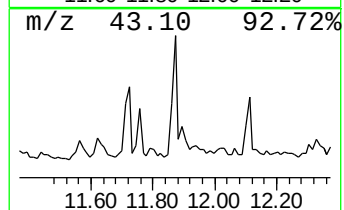
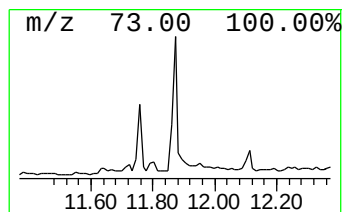
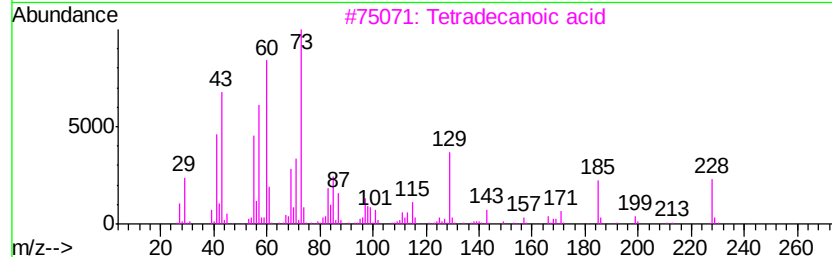
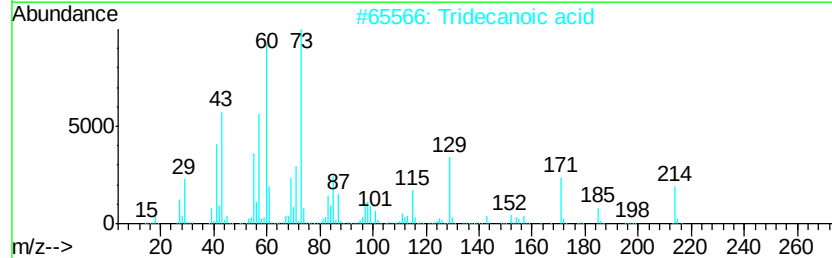
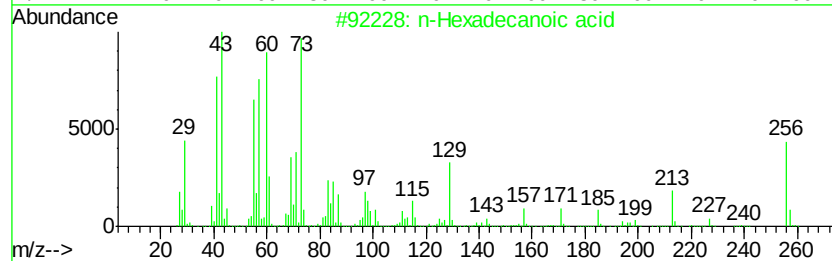
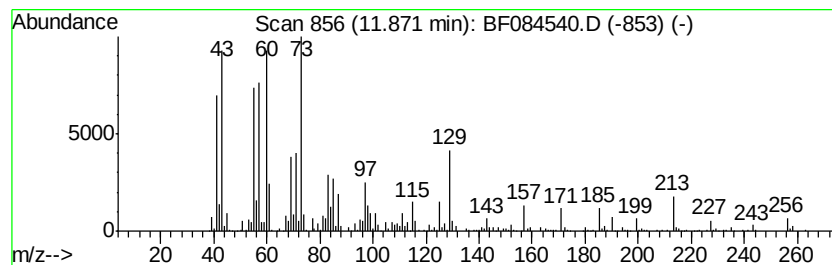
Instrument :
BNA_F
ClientSampleId :
SYS-DIS-011416

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 19 n-Hexadecanoic acid Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.87	6.30 ng	779105	Phenanthrene-d10	11.32	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011816\
Data File : BF084540.D
Acq On : 18 Jan 2016 17:24
Operator : SJ/UM
Sample : H1140-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SYS-DIS-011416

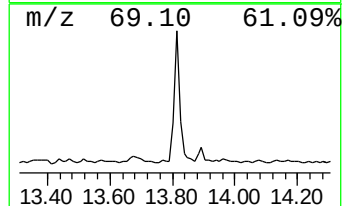
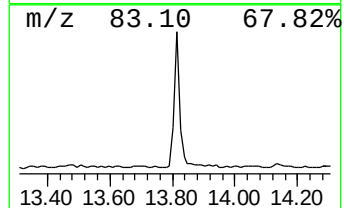
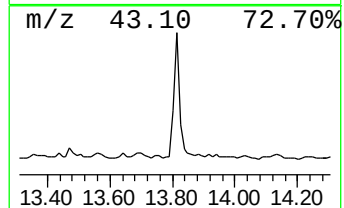
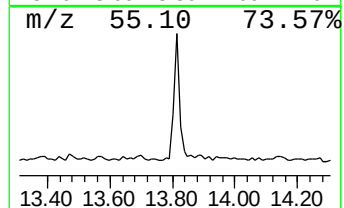
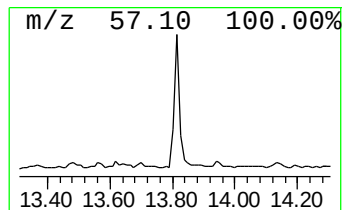
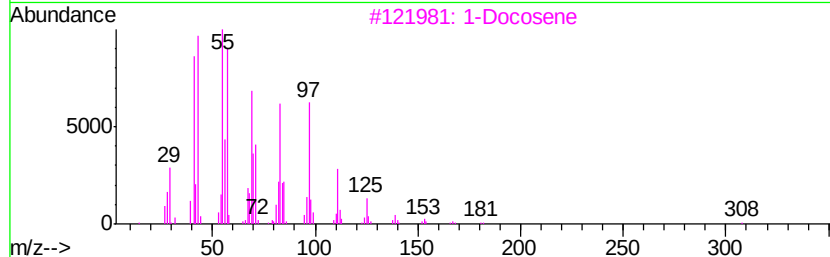
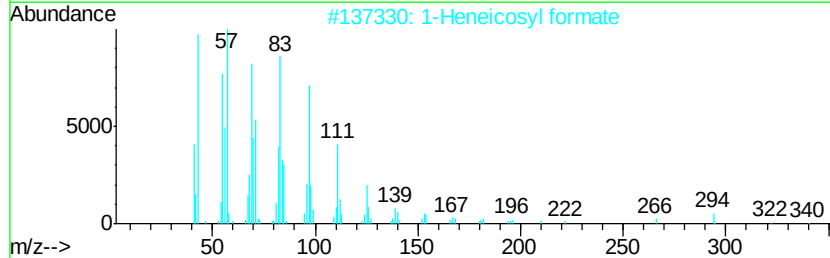
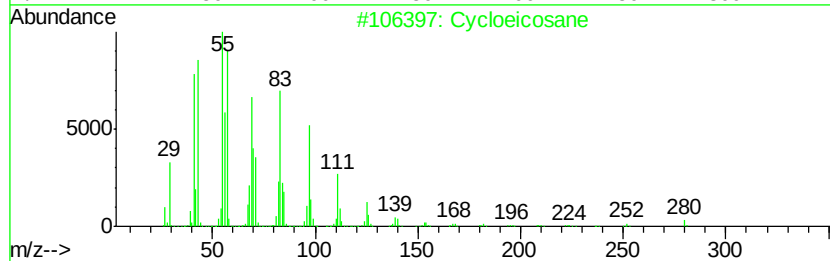
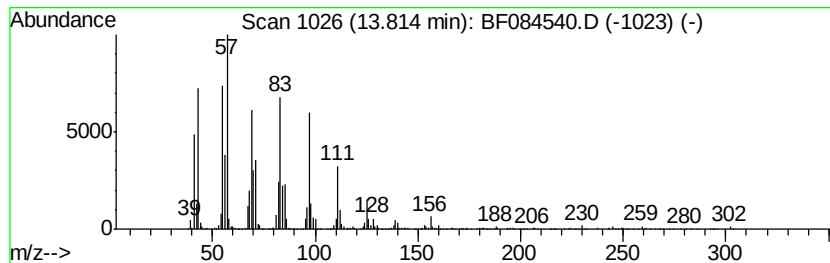
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Cycloeicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	12.88 ng	1464920	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cycloeicosane	280	C20H40	000296-56-0	99
2		1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
3		1-Docosene	308	C22H44	001599-67-3	91
4		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
5		5-Eicosene, (E)-	280	C20H40	074685-30-6	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011816\
 Data File : BF084540.D
 Acq On : 18 Jan 2016 17:24
 Operator : SJ/UM
 Sample : H1140-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SYS-DIS-011416

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...	4.96	14.0	ng	1279810	1	6.80	1827810	20.0
Ethane, 1,1'-oxyb...	6.16	5.4	ng	497077	1	6.80	1827810	20.0
unknown6.57	6.57	23.4	ng	2135380	1	6.80	1827810	20.0
Butane, 1-isothio...	6.61	5.8	ng	532664	1	6.80	1827810	20.0
unknown7.48	7.48	57.3	ng	7340820	2	8.08	2563150	20.0
1-Piperidinecarbo...	7.74	6.9	ng	880557	2	8.08	2563150	20.0
unknown8.61	8.61	12.4	ng	1595660	2	8.08	2563150	20.0
unknown10.13	10.13	9.3	ng	1514250	3	9.84	3265380	20.0
unknown10.43	10.43	36.6	ng	5982500	3	9.84	3265380	20.0
unknown10.49	10.49	10.3	ng	1684780	3	9.84	3265380	20.0
5,6,7,8-Tetrahydr...	10.72	8.5	ng	1046370	4	11.32	2472630	20.0
2(3H)-Benzothiazo...	10.75	16.9	ng	2088650	4	11.32	2472630	20.0
unknown11.01	11.01	5.9	ng	727609	4	11.32	2472630	20.0
Benzoic acid, 3,5...	11.64	6.8	ng	837515	4	11.32	2472630	20.0
7,9-Di-tert-butyl...	11.72	29.4	ng	3639520	4	11.32	2472630	20.0
Ethyl 2-isothiocy...	11.76	10.0	ng	1240730	4	11.32	2472630	20.0
n-Hexadecanoic acid	11.87	6.3	ng	779105	4	11.32	2472630	20.0
Cycloeicosane	13.81	12.9	ng	1464920	5	13.95	2275440	20.0