

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
 Data File : BF086735.D
 Acq On : 6 May 2016 20:33
 Operator : UM/SJ
 Sample : H2802-06
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-4

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-BF050416.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	3.516	121	125	129	rVB	78354	145413	2.51%	0.205%
2	4.041	169	171	174	rVV	160568	282237	4.86%	0.399%
3	4.247	187	189	196	rVB	56438	88864	1.53%	0.126%
4	4.750	231	233	242	rBV	637865	1126433	19.41%	1.592%
5	4.899	244	246	250	rVV	97959	191013	3.29%	0.270%
6	5.013	253	256	261	rVV2	77766	147867	2.55%	0.209%
7	5.093	261	263	265	rVV	53646	75195	1.30%	0.106%
8	5.241	274	276	279	rVV	100156	174112	3.00%	0.246%
9	5.310	281	282	288	rVV	1496826	2190617	37.74%	3.096%
10	5.493	295	298	303	rVV	515822	690414	11.89%	0.976%
11	5.573	303	305	308	rVV	96262	139413	2.40%	0.197%
12	5.630	308	310	312	rVV	72543	72900	1.26%	0.103%
13	5.676	312	314	316	rVV	194864	257229	4.43%	0.363%
14	5.722	316	318	326	rVB3	196140	512471	8.83%	0.724%
15	5.893	331	333	338	rBV	426117	530916	9.15%	0.750%
16	5.962	338	339	340	rBV	119728	113668	1.96%	0.161%
17	6.144	353	355	360	rVV	800744	1209146	20.83%	1.709%
18	6.236	360	363	366	rVV3	789392	1343017	23.14%	1.898%
19	6.293	366	368	372	rVV3	211928	538273	9.27%	0.761%
20	6.373	373	375	378	rVV	1120972	1608600	27.71%	2.273%
21	6.442	378	381	383	rVV	989505	1380439	23.78%	1.951%
22	6.487	383	385	388	rVV	3781526	4519768	77.87%	6.387%
23	6.533	388	389	390	rVV	110585	106100	1.83%	0.150%
24	6.556	390	391	393	rVV2	159284	218199	3.76%	0.308%
25	6.590	393	394	399	rVB3	137295	244689	4.22%	0.346%
26	6.670	399	401	402	rBV	143172	137918	2.38%	0.195%
27	6.704	402	404	407	rVB	1285900	1175860	20.26%	1.662%
28	6.762	407	409	413	rBV	420050	578085	9.96%	0.817%
29	6.830	413	415	416	rBV2	129096	184500	3.18%	0.261%
30	6.864	416	418	420	rVV	3967519	4322939	74.48%	6.109%
31	6.956	422	426	429	rBV	293645	663775	11.44%	0.938%
32	7.013	429	431	432	rVV	439475	408559	7.04%	0.577%
33	7.059	434	435	438	rVB	352204	279440	4.81%	0.395%
34	7.127	438	441	443	rBV2	506254	1177516	20.29%	1.664%

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 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	7.162	443	444	446	rVV2	471631	426188	7.34%	0.602%
36	7.207	446	448	451	rVB3	253227	374327	6.45%	0.529%
37	7.276	451	454	456	rBV	2542751	4170309	71.85%	5.893%
38	7.310	456	457	460	rVB2	228368	207634	3.58%	0.293%
39	7.367	460	462	463	rVB	160224	170473	2.94%	0.241%
40	7.413	463	466	469	rVB2	263775	381264	6.57%	0.539%
41	7.482	469	472	475	rVB5	92447	216467	3.73%	0.306%
42	7.562	475	479	481	rBV4	151994	331557	5.71%	0.469%
43	7.607	481	483	485	rBV2	94056	145631	2.51%	0.206%
44	7.665	486	488	491	rVB2	244117	311990	5.37%	0.441%
45	7.722	491	493	495	rBV	493152	533014	9.18%	0.753%
46	7.813	495	501	504	rBV4	664322	1522299	26.23%	2.151%
47	7.882	505	507	508	rVB	122619	120632	2.08%	0.170%
48	7.927	508	511	514	rBV3	164428	421700	7.27%	0.596%
49	7.996	514	517	519	rVB	1491602	1629149	28.07%	2.302%
50	8.042	519	521	523	rVB3	76765	75773	1.31%	0.107%
51	8.087	523	525	526	rVB	135398	122771	2.12%	0.173%
52	8.133	528	529	531	rBV	77883	142437	2.45%	0.201%
53	8.179	531	533	535	rVB2	230698	239476	4.13%	0.338%
54	8.225	535	537	538	rVB	164716	157790	2.72%	0.223%
55	8.282	540	542	544	rBV	228408	291296	5.02%	0.412%
56	8.316	544	545	547	rVB	219929	181514	3.13%	0.256%
57	8.396	547	552	556	rBV3	593624	1425179	24.55%	2.014%
58	8.465	556	558	559	rVV2	135646	139591	2.40%	0.197%
59	8.590	565	569	573	rVB5	192789	425016	7.32%	0.601%
60	8.659	573	575	576	rBV	78464	105241	1.81%	0.149%
61	8.693	576	578	581	rVB3	158913	278230	4.79%	0.393%
62	8.750	581	583	584	rBV	85847	104114	1.79%	0.147%
63	8.785	584	586	587	rBV	117775	109077	1.88%	0.154%
64	8.876	591	594	597	rBV4	130027	376293	6.48%	0.532%
65	8.956	597	601	602	rVV3	419525	610483	10.52%	0.863%
66	8.990	602	604	607	rVV2	409187	831564	14.33%	1.175%
67	9.070	607	611	614	rVB	4080486	5804515	100.00%	8.202%
68	9.116	614	615	618	rVB	101223	110140	1.90%	0.156%
69	9.173	618	620	623	rBV4	119994	263871	4.55%	0.373%
70	9.230	623	625	627	rBV	1354328	1253451	21.59%	1.771%
71	9.322	631	633	634	rBV2	129307	215008	3.70%	0.304%

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72	9.390	638	639	641 rBV2	75049	141535	2.44%	0.200%
73	9.482	645	647	648 rBV	239914	289667	4.99%	0.409%
74	9.573	654	655	658 rVB	112334	126083	2.17%	0.178%
75	9.619	658	659	662 rBV3	163267	205628	3.54%	0.291%
76	9.688	662	665	668 rBV3	193846	320589	5.52%	0.453%
77	9.745	668	670	672 rVB	1889716	1708565	29.44%	2.414%
78	9.825	676	677	681 rVB4	118335	139596	2.40%	0.197%
79	9.905	681	684	687 rBV3	199094	434269	7.48%	0.614%
80	9.985	689	691	693 rBV2	223405	242858	4.18%	0.343%
81	10.145	703	705	706 rBV	67908	114554	1.97%	0.162%
82	10.179	706	708	710 rVB	701821	637957	10.99%	0.902%
83	10.236	710	713	714 rBV3	69308	116034	2.00%	0.164%
84	10.533	736	739	742 rVB3	2746861	3754302	64.68%	5.305%
85	10.648	747	749	751 rBV2	117815	147115	2.53%	0.208%
86	10.762	757	759	761 rBV3	101344	161682	2.79%	0.228%
87	10.911	770	772	776 rBV3	169830	255963	4.41%	0.362%
88	11.219	797	799	802 rBV	1358952	1517173	26.14%	2.144%
89	11.265	802	803	808 rVB2	114062	205647	3.54%	0.291%
90	11.768	845	847	852 rVB2	800401	826585	14.24%	1.168%
91	12.099	874	876	879 rBV	49625	78495	1.35%	0.111%
92	12.305	892	894	899 rVB	56960	80269	1.38%	0.113%
93	12.476	905	909	913 rVV4	71704	218820	3.77%	0.309%
94	12.557	913	916	918 rVV	640825	965340	16.63%	1.364%
95	12.808	935	938	940 rBV	4276151	4374322	75.36%	6.181%
96	12.842	940	941	946 rVB	217752	212648	3.66%	0.300%
97	13.699	1014	1016	1021 rBV2	131798	162774	2.80%	0.230%
98	13.848	1027	1029	1032 rBV	1307619	1263785	21.77%	1.786%
99	14.922	1121	1123	1127 rBV	45721	71121	1.23%	0.101%
100	15.231	1147	1150	1158 rVB	703256	931484	16.05%	1.316%

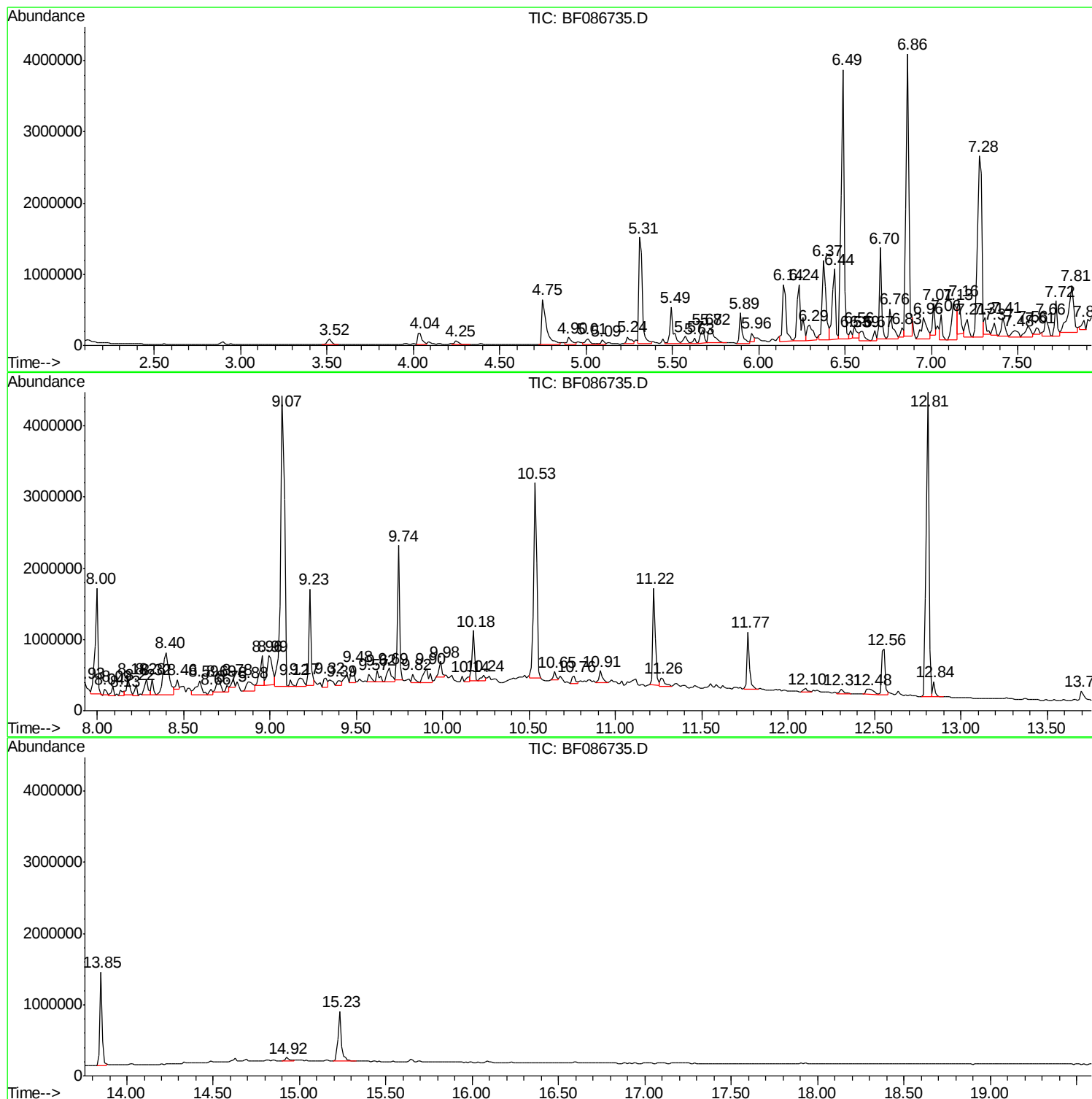
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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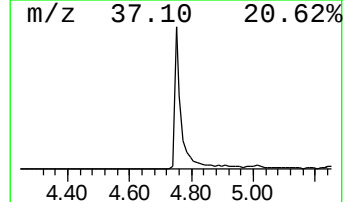
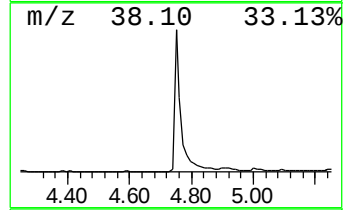
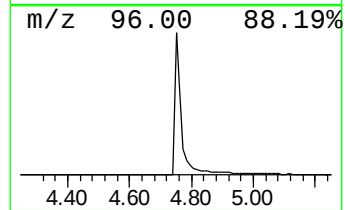
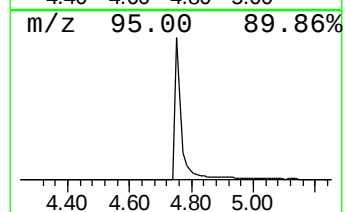
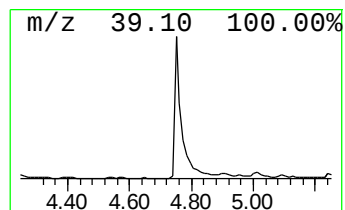
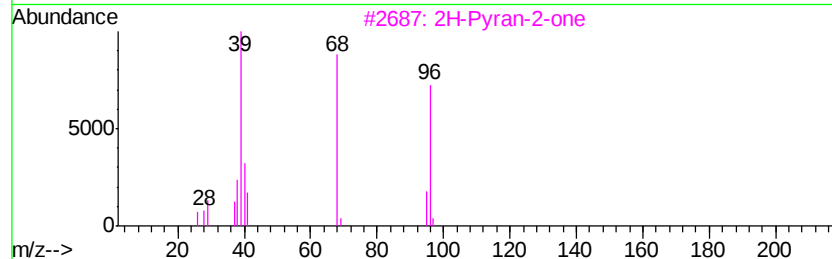
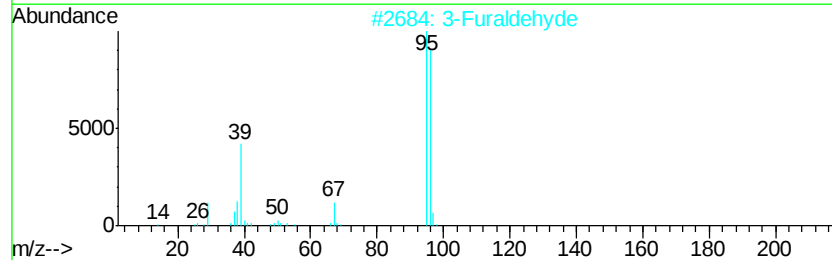
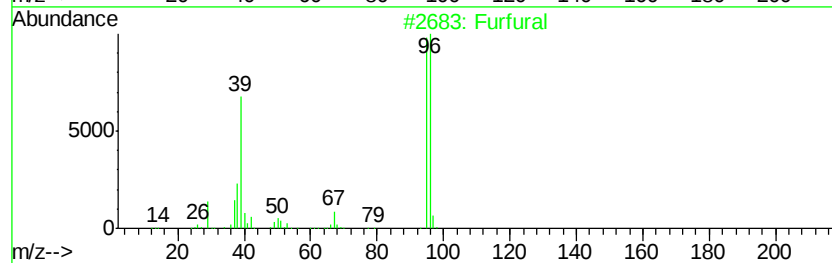
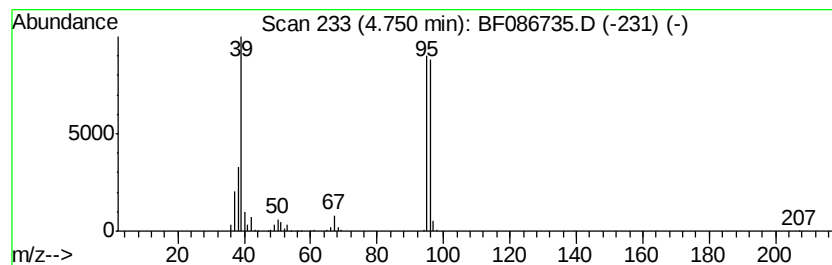
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Furfural Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.75	38.32 ng	1126430	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furfural	96	C5H4O2	000098-01-1	97
2	3-Furaldehyde	96	C5H4O2	000498-60-2	91
3	2H-Pyran-2-one	96	C5H4O2	000504-31-4	64
4	Furan, 2,4-dimethyl-	96	C6H8O	003710-43-8	50
5	1-Propyne, 3-chloro-	74	C3H3Cl	000624-65-7	36



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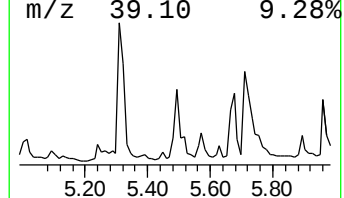
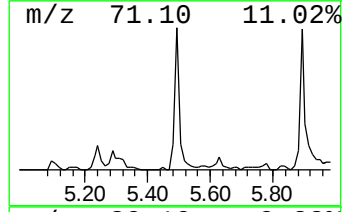
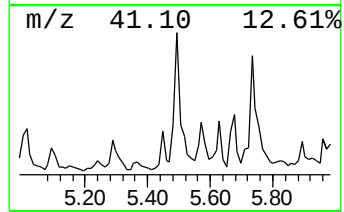
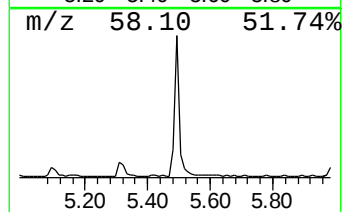
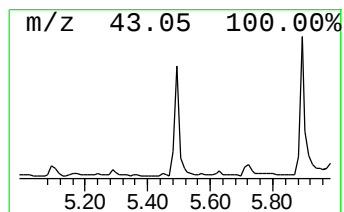
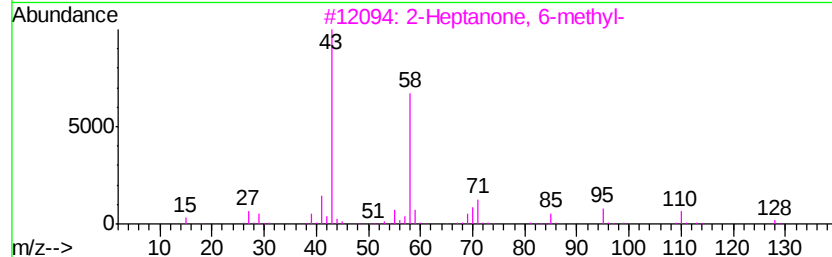
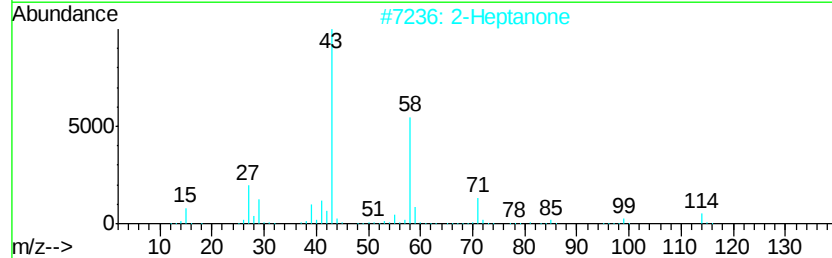
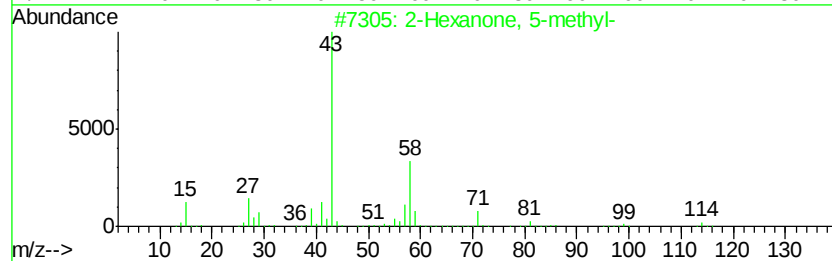
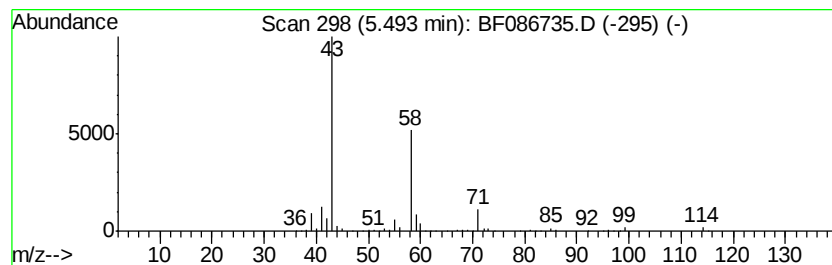
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Hexanone, 5-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.49	23.49 ng	690414	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	80
2		2-Heptanone	114	C7H14O	000110-43-0	72
3		2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	50
4		8-Hydroxy-2-octanone	144	C8H16O2	025368-54-1	50
5		2-Hexanone	100	C6H12O	000591-78-6	45



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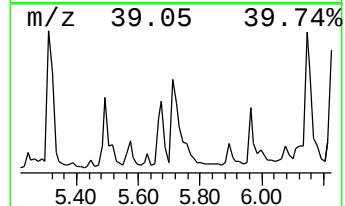
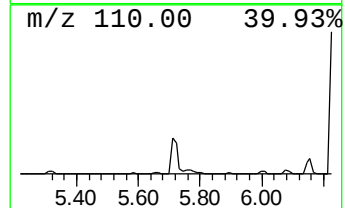
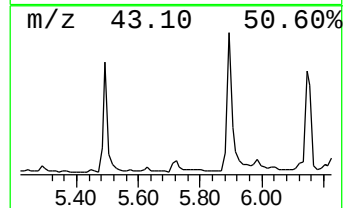
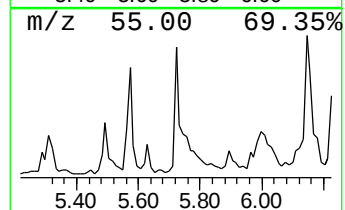
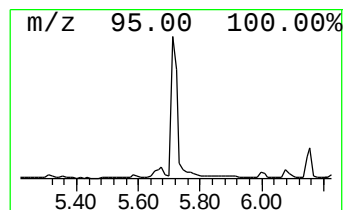
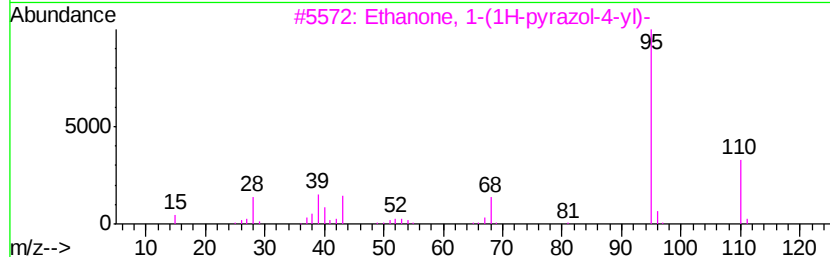
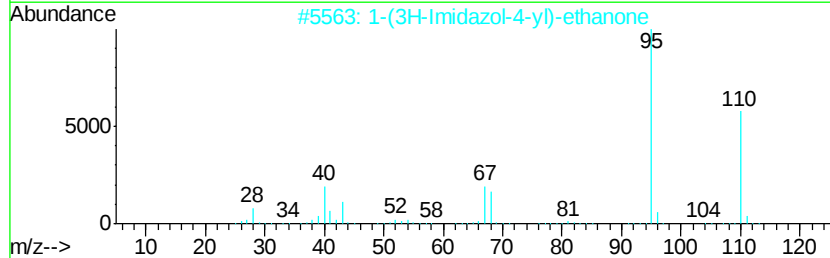
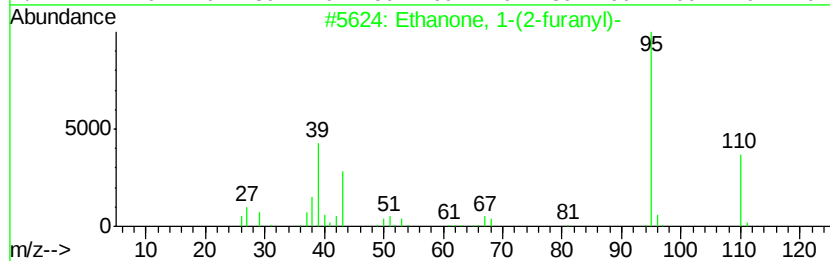
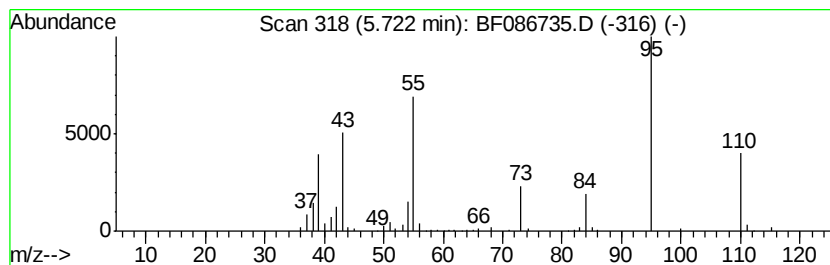
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanone, 1-(2-furanyl)- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	17.43 ng	512471	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanone, 1-(2-furanyl)-	110	C6H6O2	001192-62-7	62
2		1-(3H-Imidazol-4-yl)-ethanone	110	C5H6N2O	061985-25-9	38
3		Ethanone, 1-(1H-pyrazol-4-yl)-	110	C5H6N2O	025016-16-4	37
4		1H-Imidazole, 2-ethyl-4-methyl-	110	C6H10N2	000931-36-2	12
5		2(5H)-Furanone	84	C4H4O2	000497-23-4	11



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ClientSampleId :
MW-4

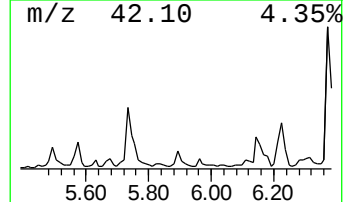
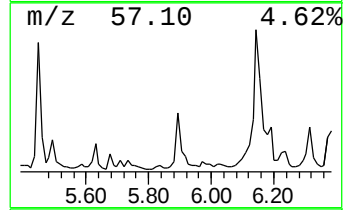
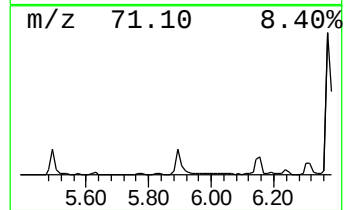
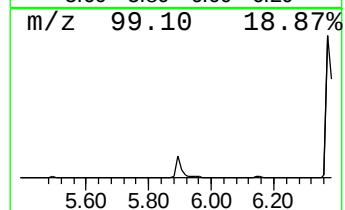
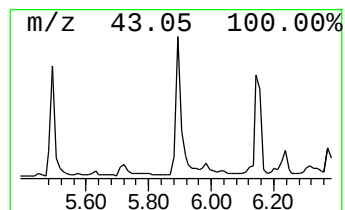
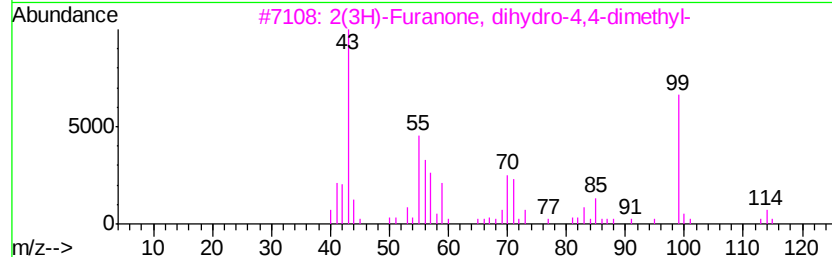
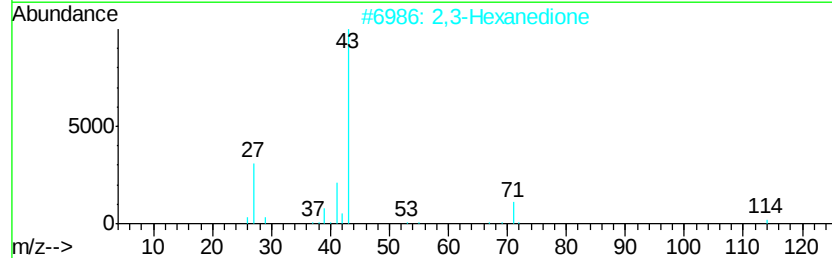
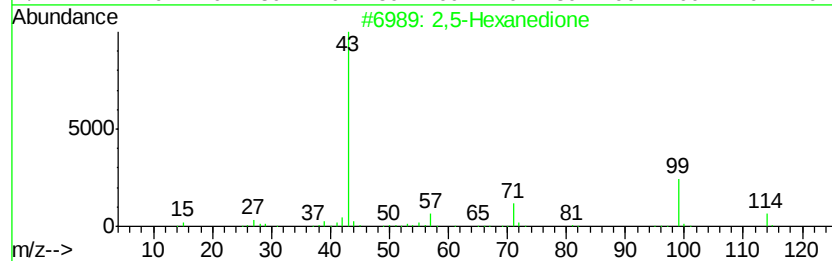
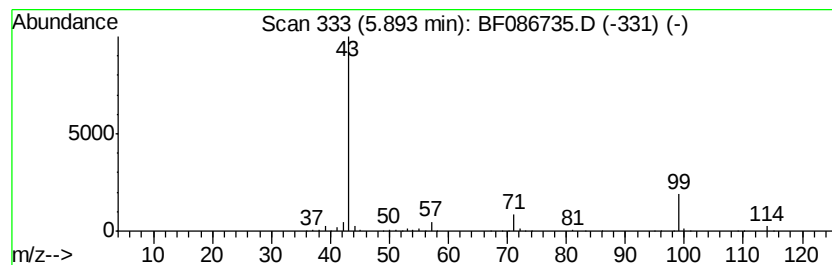
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 2,5-Hexanedione Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.89	18.06 ng	530916	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Hexanedione	114	C6H10O2	000110-13-4	59
2	2,3-Hexanedione	114	C6H10O2	003848-24-6	40
3	2(3H)-Furanone, dihydro-4,4-dime...	114	C6H10O2	013861-97-7	32
4	2-Hexanone, 3-methyl-	114	C7H14O	002550-21-2	25
5	2-Pentanone, 3-ethyl-	114	C7H14O	006137-03-7	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086735.D
Acq On : 6 May 2016 20:33
Operator : UM/SJ
Sample : H2802-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
MW-4

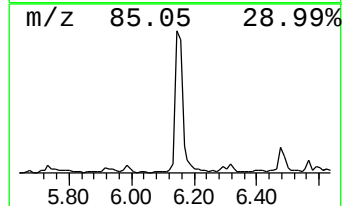
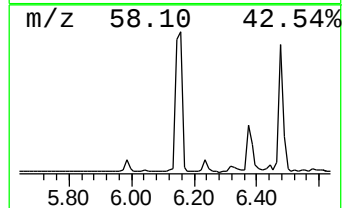
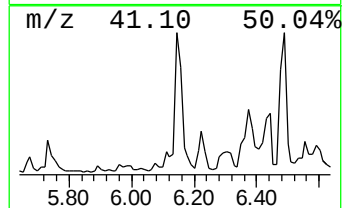
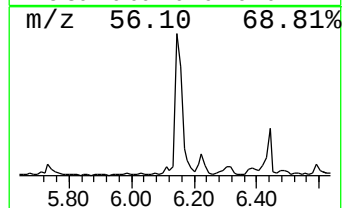
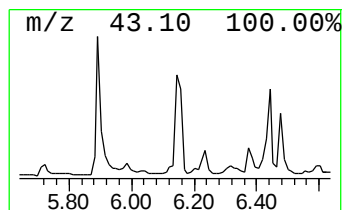
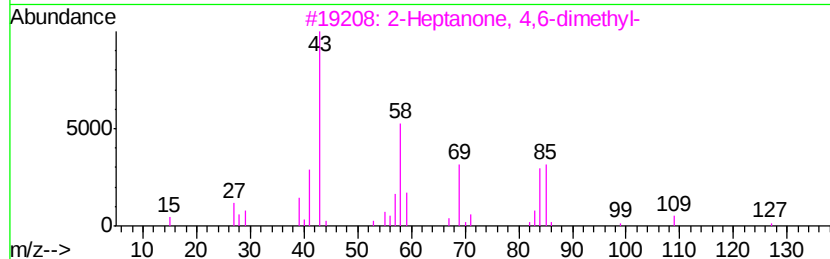
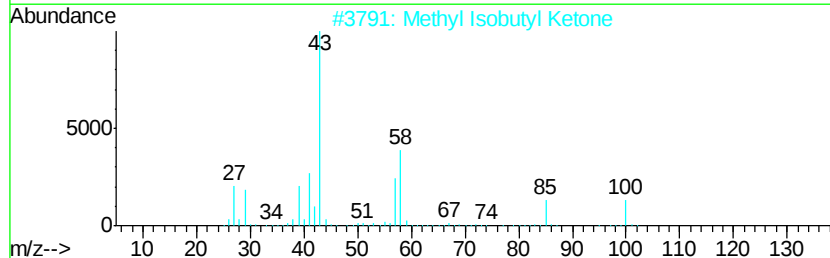
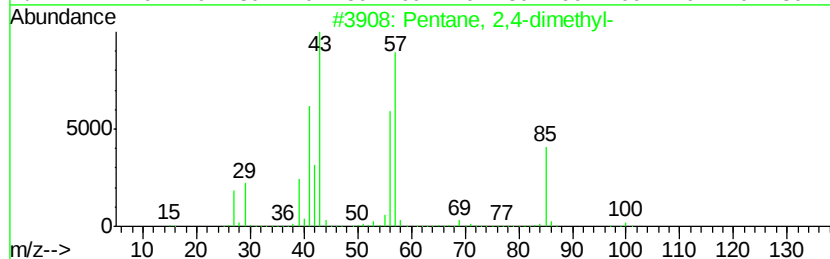
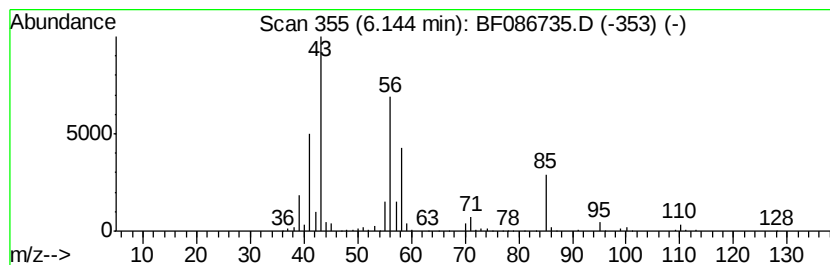
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown6.14 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.14	41.13 ng	1209150	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	38
2		Methyl Isobutyl Ketone	100	C6H12O	000108-10-1	37
3		2-Heptanone, 4,6-dimethyl-	142	C9H18O	019549-80-5	37
4		Pentanal, 2-methyl-	100	C6H12O	000123-15-9	35
5		3,5-Dimethyl-1,6-heptadien-4-ol	140	C9H16O	019549-66-7	32



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086735.D
Acq On : 6 May 2016 20:33
Operator : UM/SJ
Sample : H2802-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

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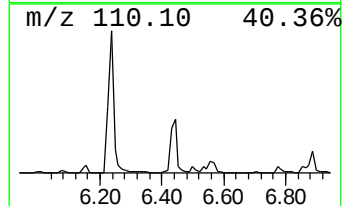
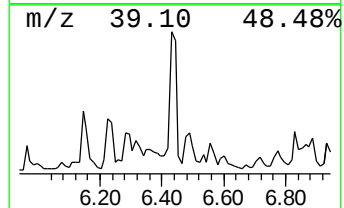
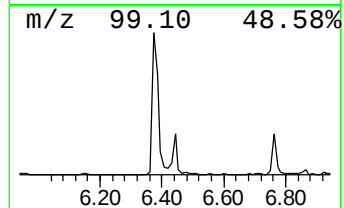
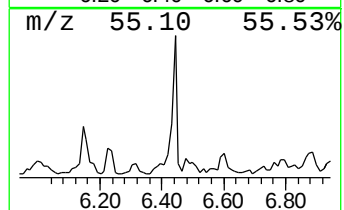
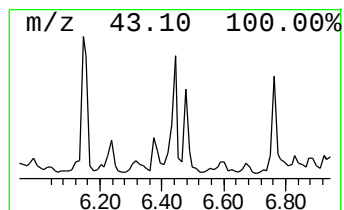
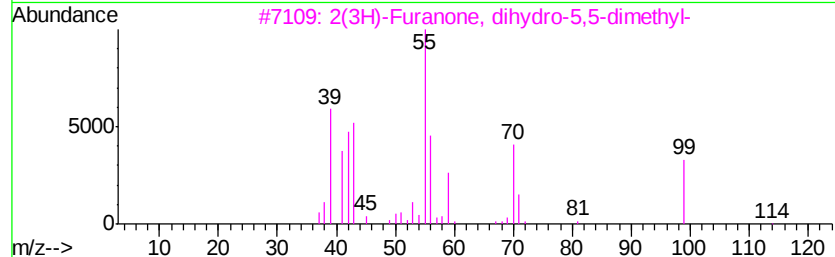
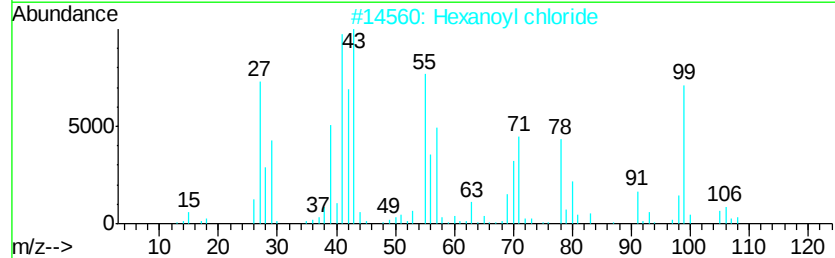
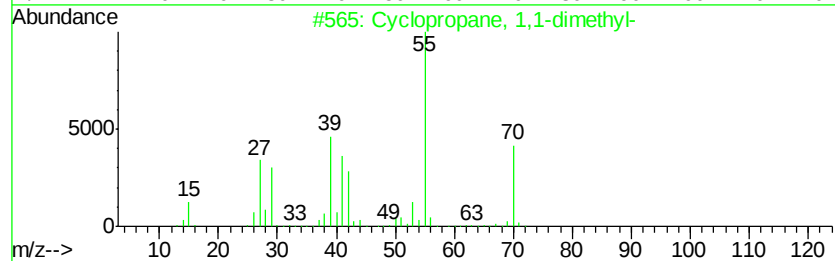
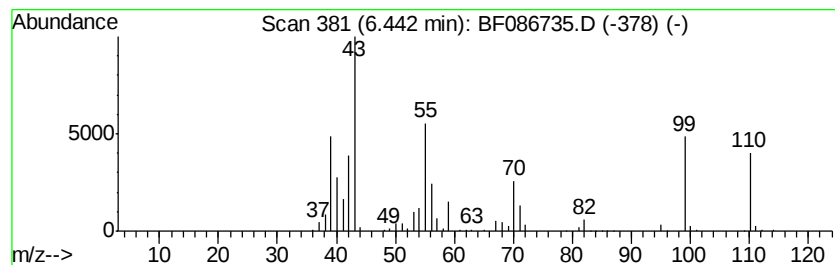
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown6.44 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.44	46.96 ng	1380440	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	38
2		Hexanoyl chloride	134	C6H11ClO	000142-61-0	37
3		2(3H)-Furanone, dihydro-5,5-dime...	114	C6H10O2	003123-97-5	30
4		3-Pentenoic acid, 4-methyl-	114	C6H10O2	000504-85-8	27
5		1-Pyrrolidinecarboxaldehyde	99	C5H9NO	003760-54-1	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086735.D
Acq On : 6 May 2016 20:33
Operator : UM/SJ
Sample : H2802-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

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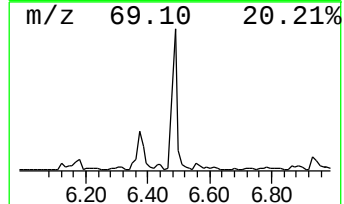
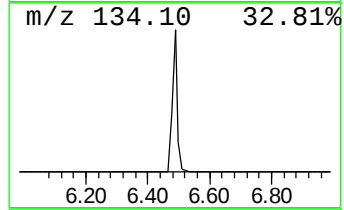
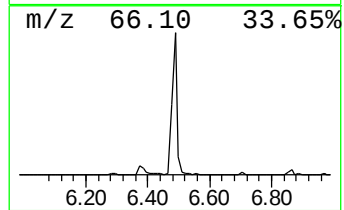
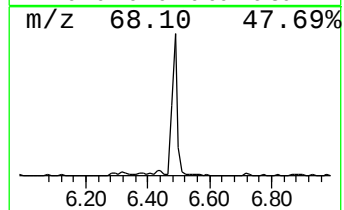
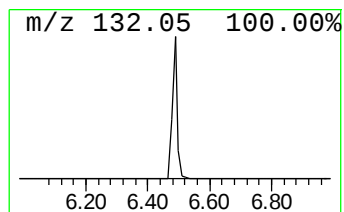
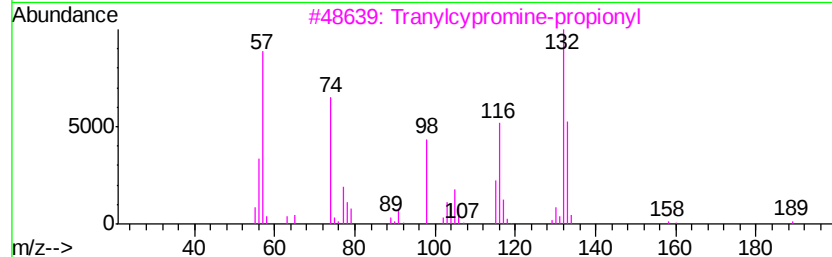
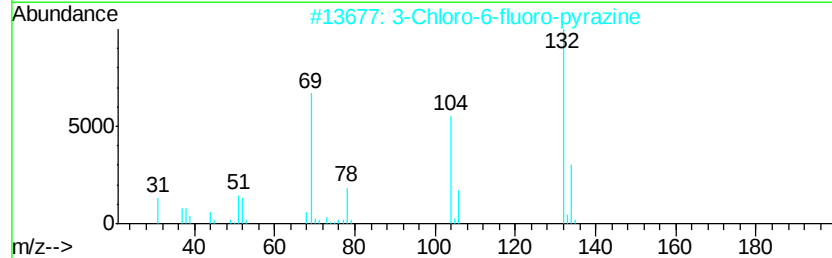
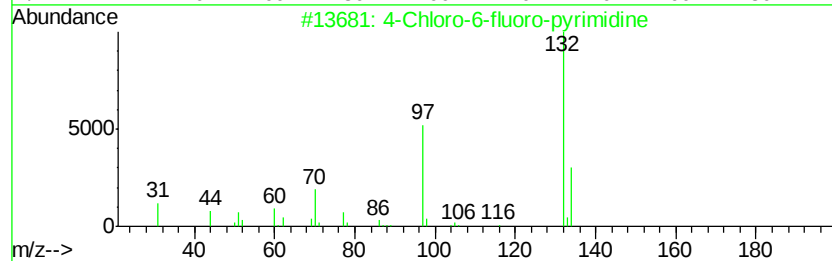
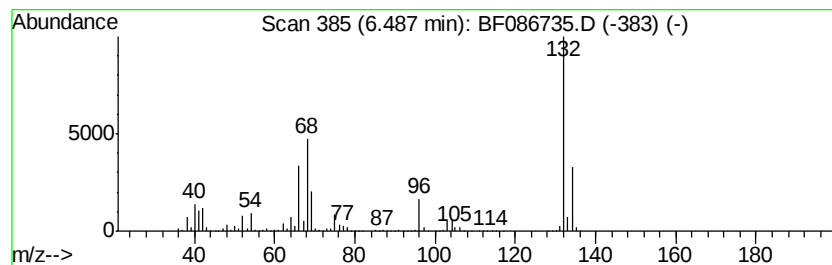
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	153.75 ng	4519770	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086735.D
Acq On : 6 May 2016 20:33
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Misc :
ALS Vial : 10 Sample Multiplier: 1

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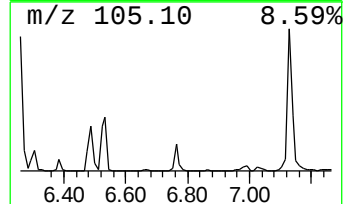
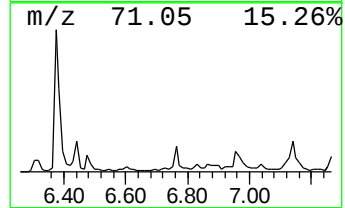
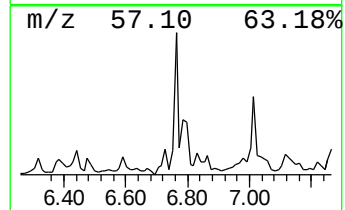
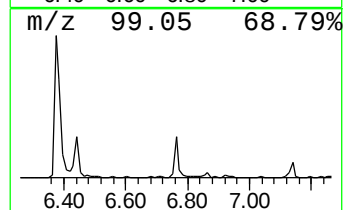
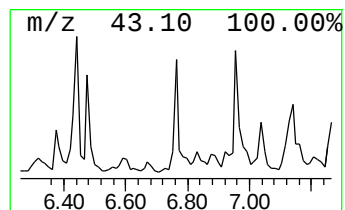
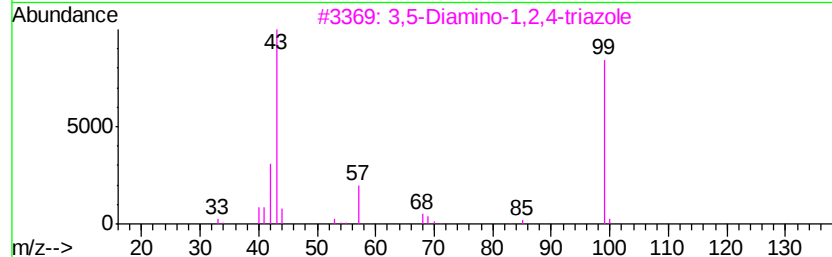
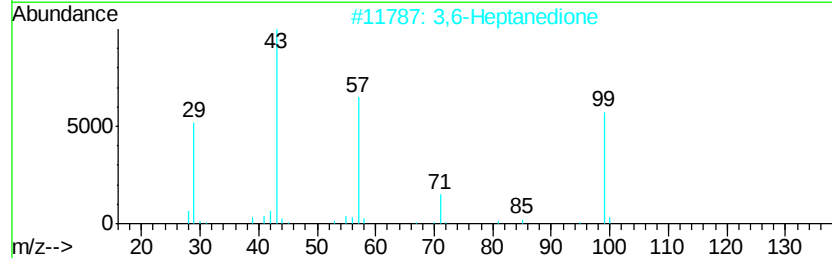
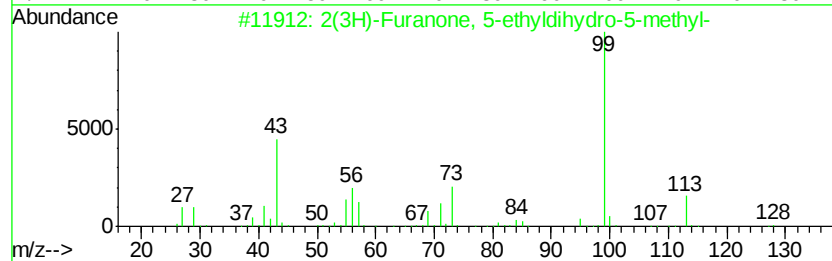
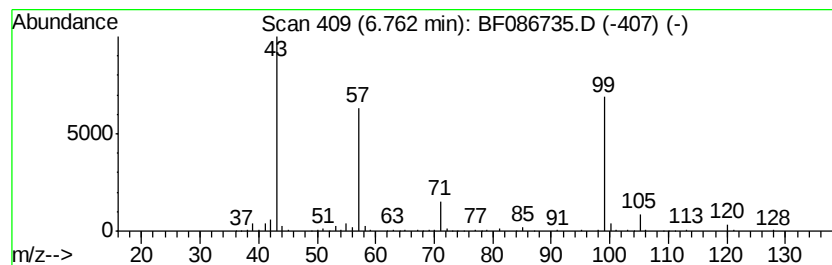
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2(3H)-Furanone, 5-ethylidihy... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.76	19.67 ng	578085	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2(3H)-Furanone, 5-ethylidihydro-5...	128	C7H12O2	002865-82-9	72
2		3,6-Heptanedione	128	C7H12O2	001703-51-1	47
3		3,5-Diamino-1,2,4-triazole	99	C2H5N5	001455-77-2	45
4		Hexanoic acid, anhydride	214	C12H22O3	002051-49-2	38
5		4-Piperidinone	99	C5H9NO	041661-47-6	37



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086735.D
Acq On : 6 May 2016 20:33
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Misc :
ALS Vial : 10 Sample Multiplier: 1

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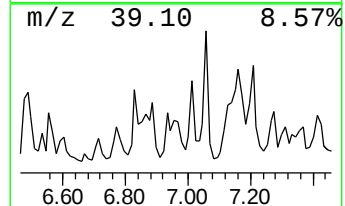
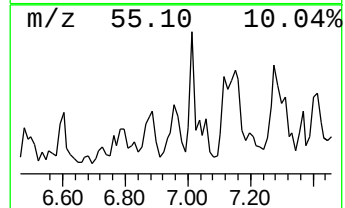
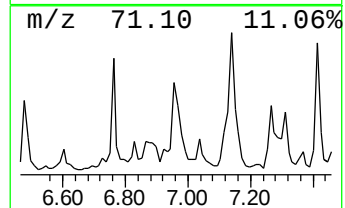
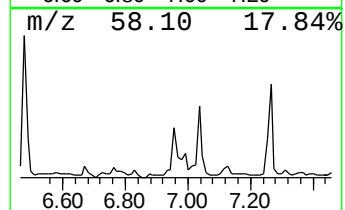
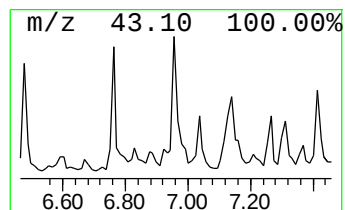
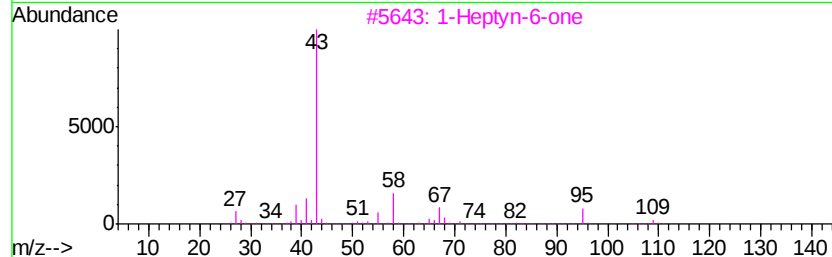
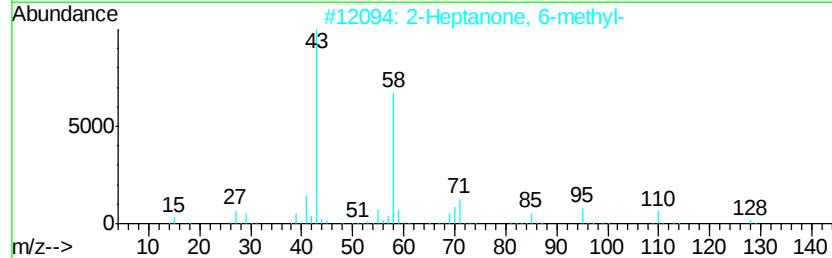
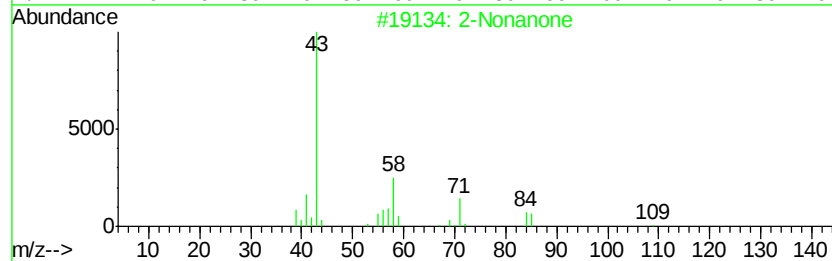
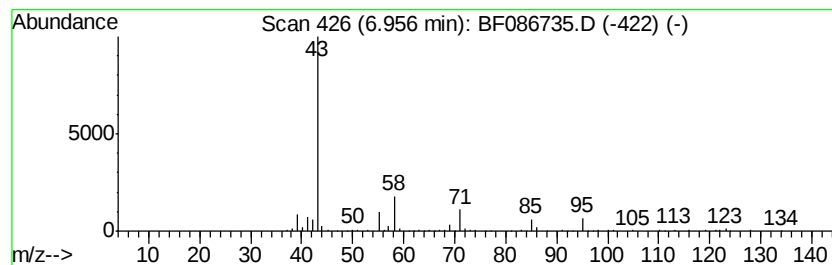
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2-Nonanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.96	22.58 ng	663775	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Nonanone	142	C9H18O	000821-55-6	50
2			2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	38
3			1-Heptyn-6-one	110	C7H10O	000928-39-2	37
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	32
5			2-Octanone	128	C8H16O	000111-13-7	28



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086735.D
Acq On : 6 May 2016 20:33
Operator : UM/SJ
Sample : H2802-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-4

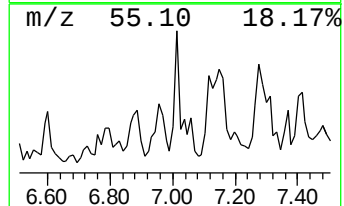
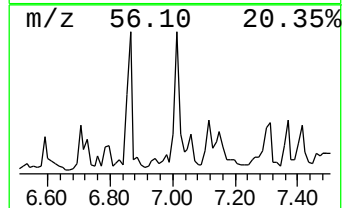
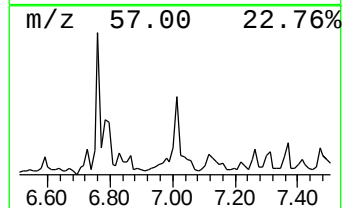
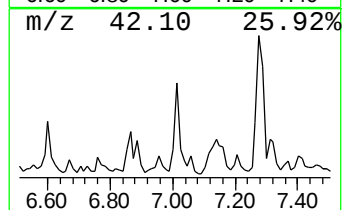
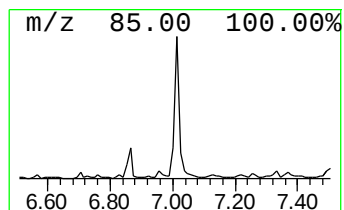
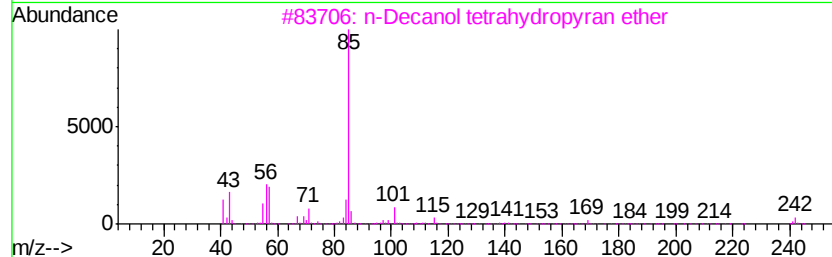
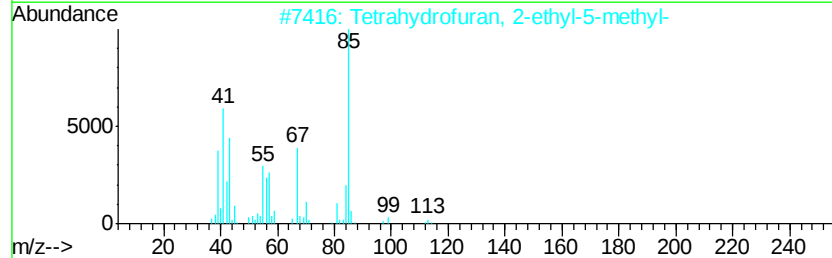
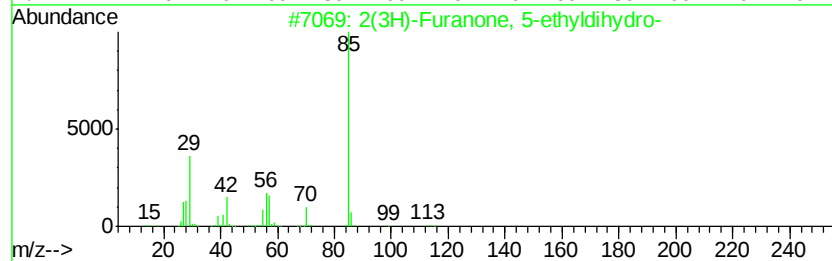
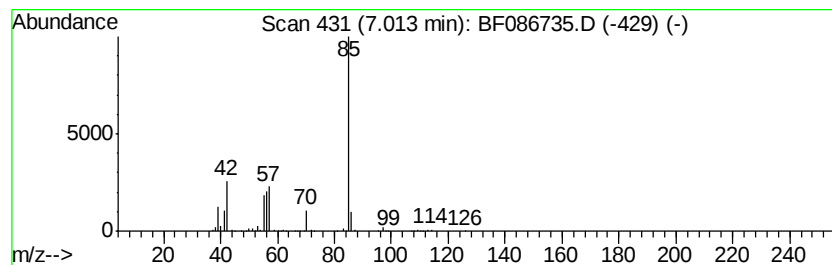
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2(3H)-Furanone, 5-ethylidihy... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.01	13.90 ng	408559	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2(3H)-Furanone, 5-ethylidihydro-	114	C6H10O2	000695-06-7	78
2			Tetrahydrofuran, 2-ethyl-5-methyl-	114	C7H14O	000931-39-5	64
3			n-Decanol tetrahydropyran ether	242	C15H30O2	110477-35-5	45
4			2-Pyrrolidinone	85	C4H7NO	000616-45-5	9
5			Carbonic acid, dihexyl ester	230	C13H26O3	007523-15-1	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086735.D
Acq On : 6 May 2016 20:33
Operator : UM/SJ
Sample : H2802-06
Misc :
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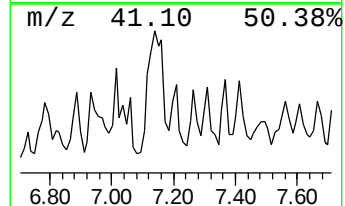
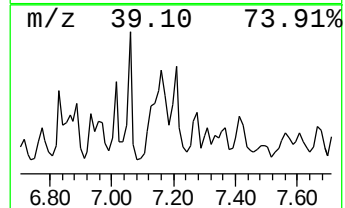
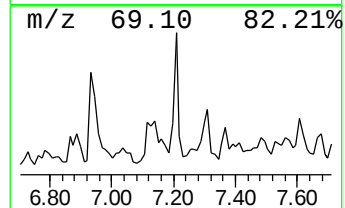
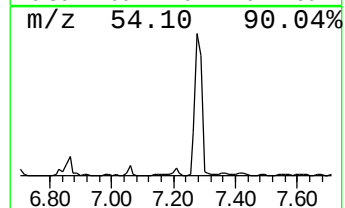
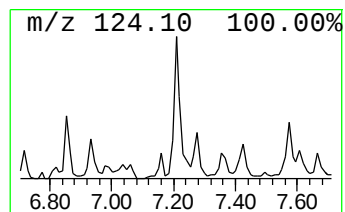
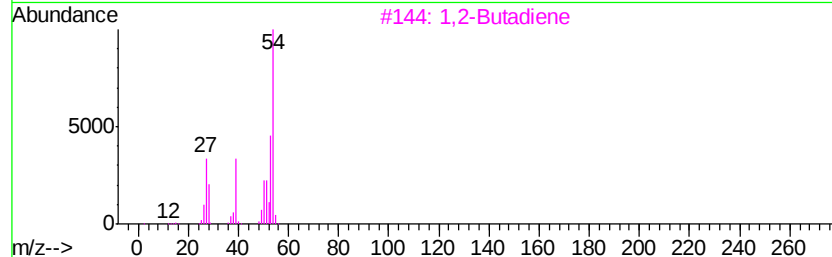
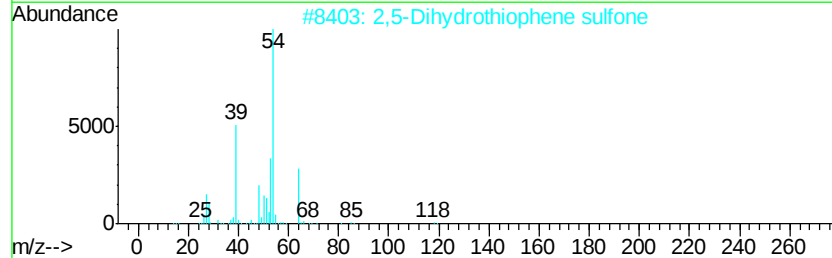
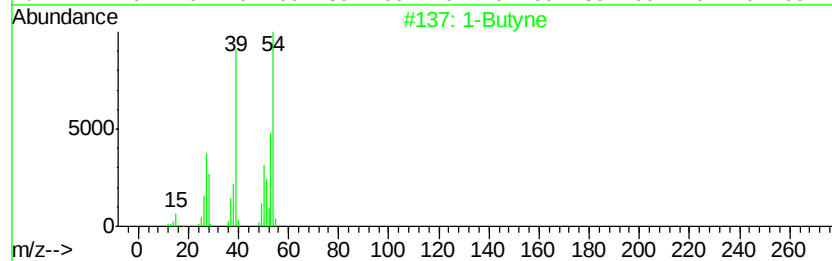
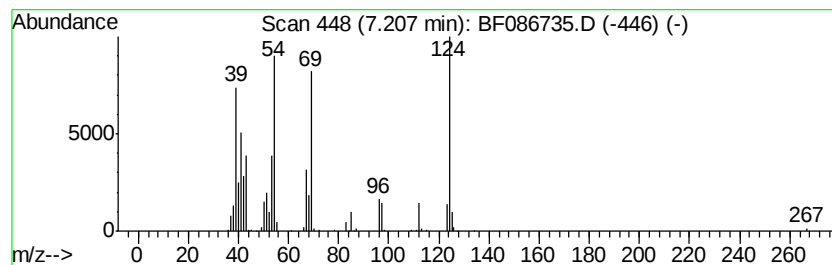
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Butyne Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.21	12.73 ng	374327	1,4-Dichlorobenzene-d4	6.70
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Butyne	54 C4H6	000107-00-6	64
2	2,5-Dihydrothiophene sulfone	118 C4H6O2S	000077-79-2	64
3	1,2-Butadiene	54 C4H6	000590-19-2	64
4	Cycloheptanone, oxime	127 C7H13NO	002158-31-8	40
5	Spiro[3.3]heptane-2,6-dione	124 C7H8O2	020061-23-8	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086735.D
Acq On : 6 May 2016 20:33
Operator : UM/SJ
Sample : H2802-06
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Instrument :
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ClientSampleId :
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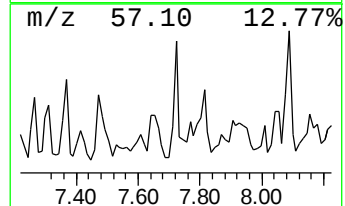
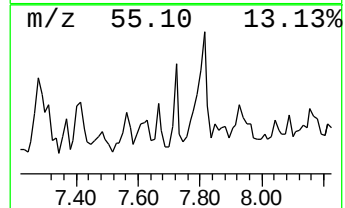
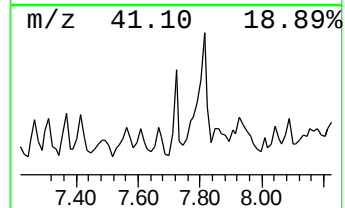
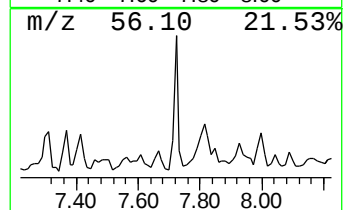
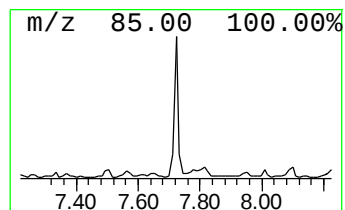
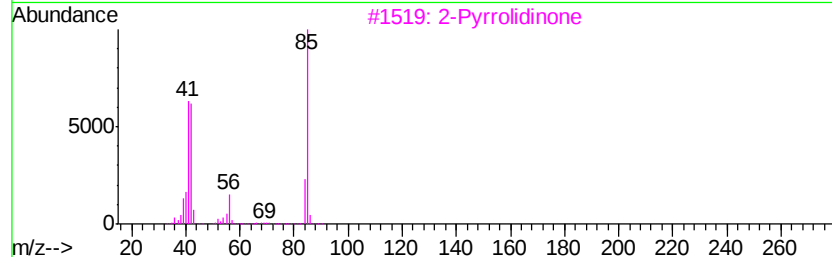
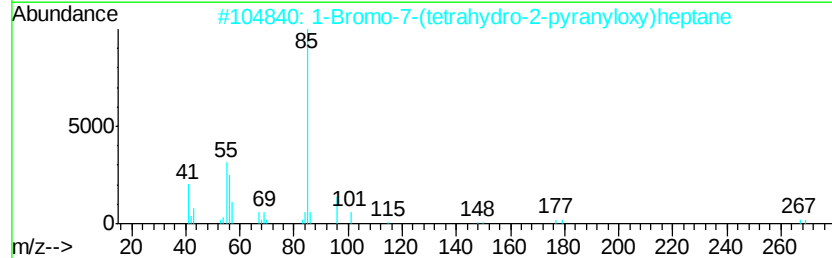
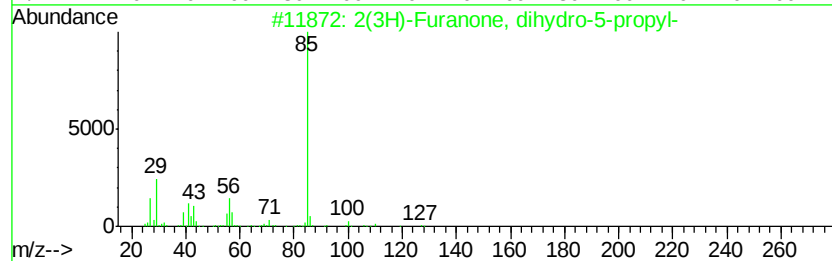
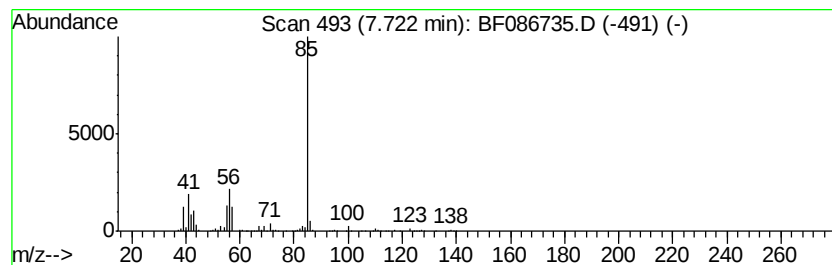
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 2(3H)-Furanone, dihydro-5-p... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.72	13.09 ng	533014	Napthalene-d8	8.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2(3H)-Furanone, dihydro-5-propyl-	128	C7H12O2	000105-21-5	72
2		1-Bromo-7-(tetrahydro-2-pyranylo...	278	C12H23BrO2	010160-25-5	72
3		2-Pyrrolidinone	85	C4H7NO	000616-45-5	64
4		Oxetane, 2-ethyl-3-methyl-	100	C6H12O	053778-62-4	64
5		Carbonic acid, dihexyl ester	230	C13H26O3	007523-15-1	56



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086735.D
Acq On : 6 May 2016 20:33
Operator : UM/SJ
Sample : H2802-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

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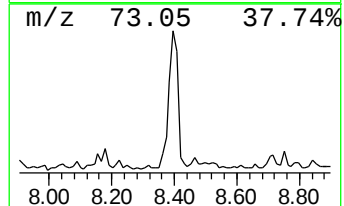
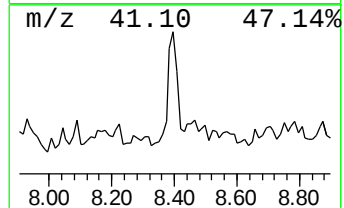
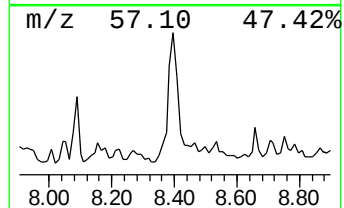
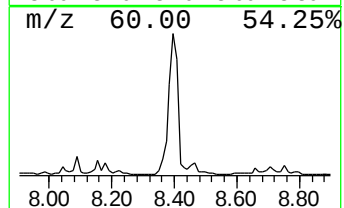
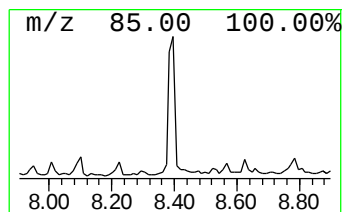
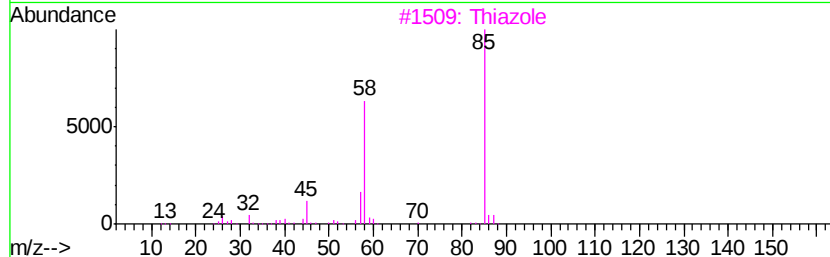
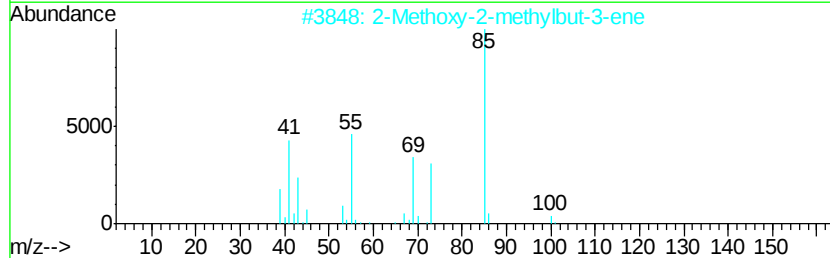
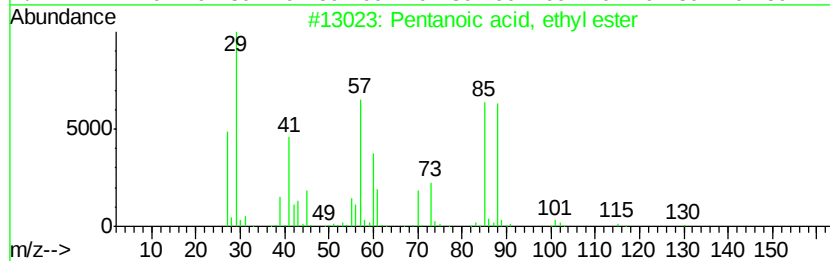
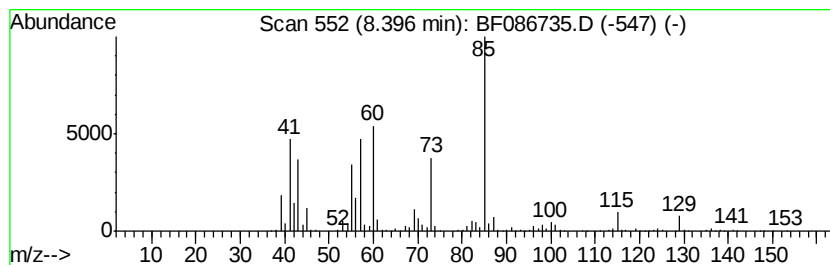
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Pentanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.40	34.99 ng	1425180	Napthalene-d8	8.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentanoic acid, ethyl ester	130	C7H14O2	000539-82-2	50
2		2-Methoxy-2-methylbut-3-ene	100	C6H12O	040426-44-6	49
3		Thiazole	85	C3H3NS	000288-47-1	43
4		2(3H)-Furanone, 5-hexyldihydro-	170	C10H18O2	000706-14-9	38
5		2(3H)-Furanone, 5-butyldihydro-	142	C8H14O2	000104-50-7	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086735.D
Acq On : 6 May 2016 20:33
Operator : UM/SJ
Sample : H2802-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

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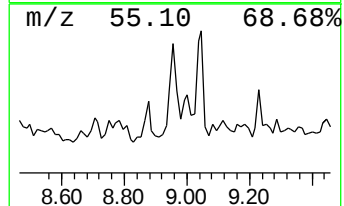
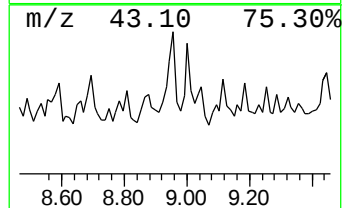
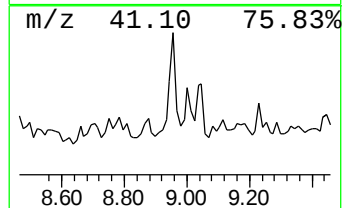
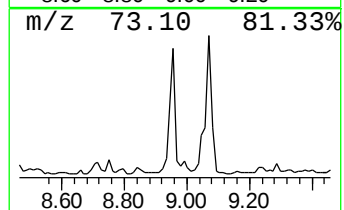
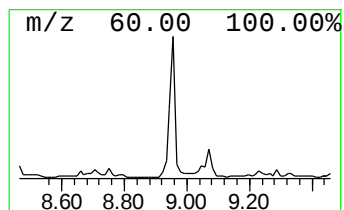
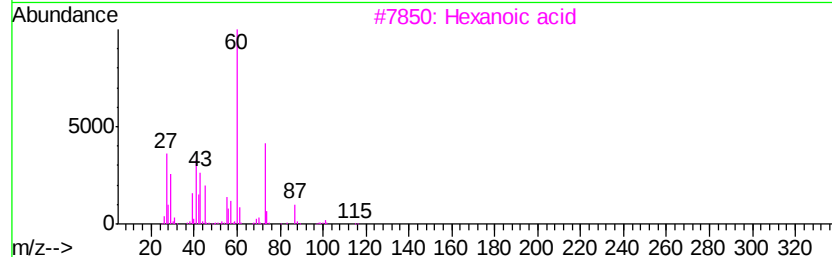
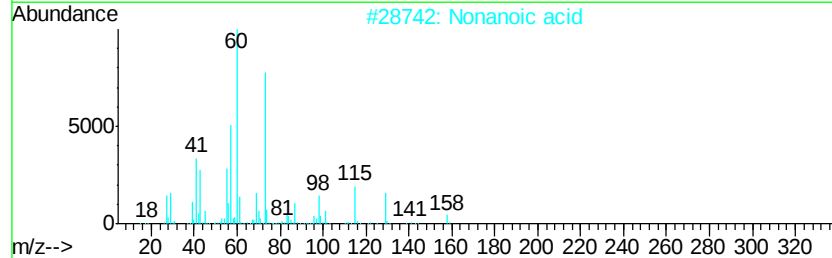
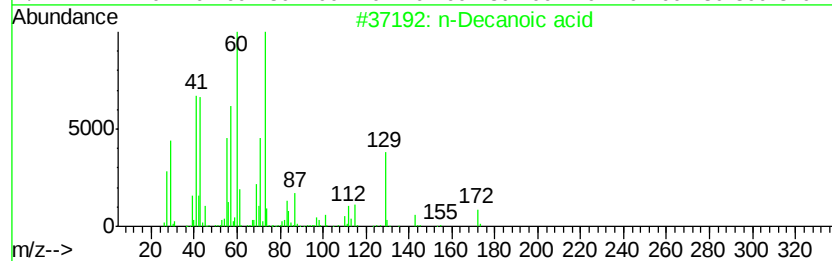
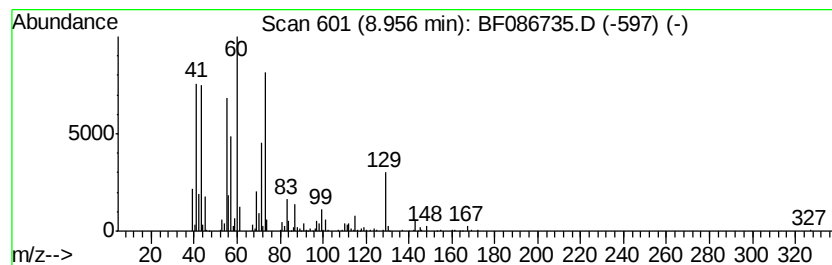
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 n-Decanoic acid Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.96	14.29 ng	610483	Acenaphthene-d10	9.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Decanoic acid	172	C10H20O2	000334-48-5	80
2		Nonanoic acid	158	C9H18O2	000112-05-0	47
3		Hexanoic acid	116	C6H12O2	000142-62-1	47
4		11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	43
5		Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086735.D
Acq On : 6 May 2016 20:33
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Sample : H2802-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

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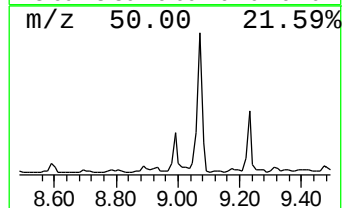
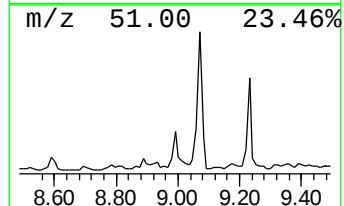
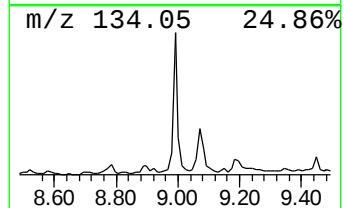
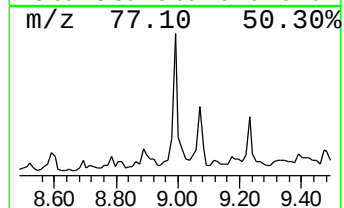
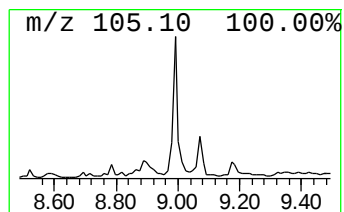
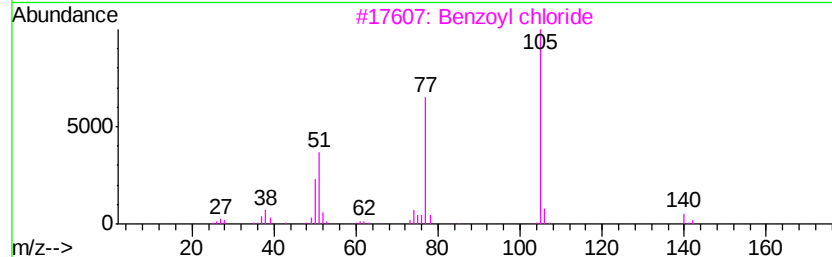
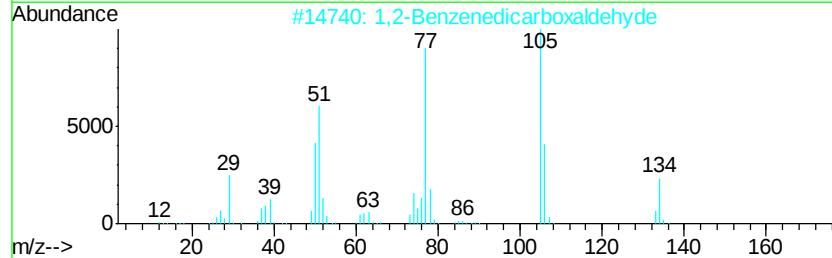
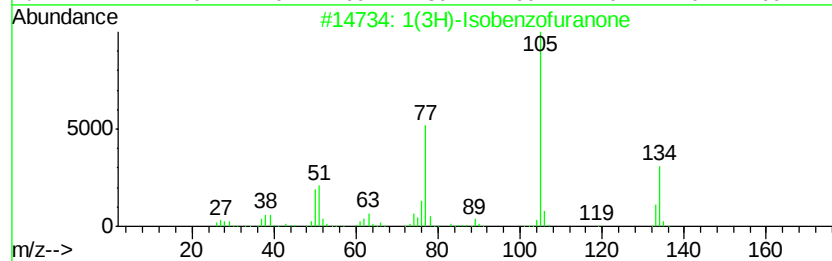
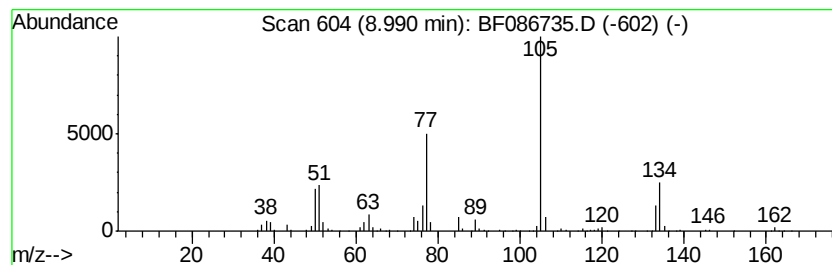
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 1(3H)-Isobenzofuranone Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.99	19.47 ng	831564	Acenaphthene-d10	9.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1(3H)-Isobenzofuranone	134	C8H6O2	000087-41-2	96
2		1,2-Benzenedicarboxaldehyde	134	C8H6O2	000643-79-8	72
3		Benzoyl chloride	140	C7H5ClO	000098-88-4	58
4		Benzoyl bromide	184	C7H5BrO	000618-32-6	53
5		1-Propanone, 1-phenyl-	134	C9H10O	000093-55-0	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
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Misc :
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Instrument :
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ClientSampleId :
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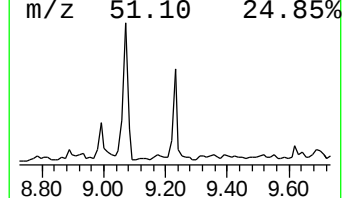
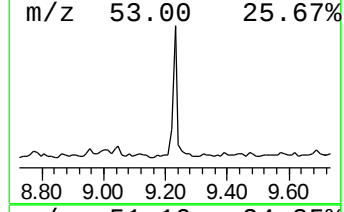
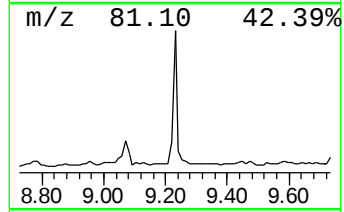
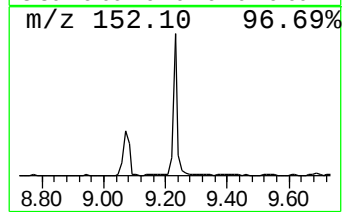
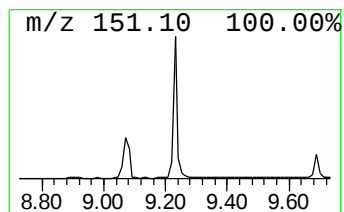
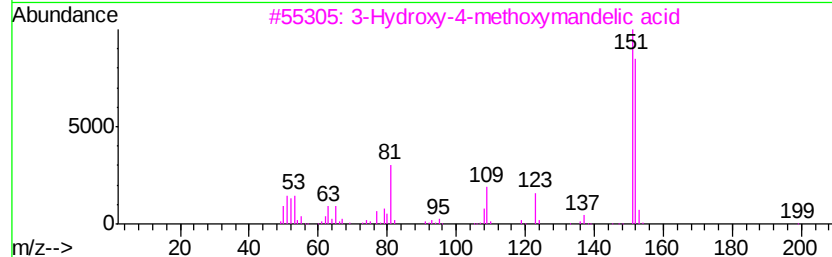
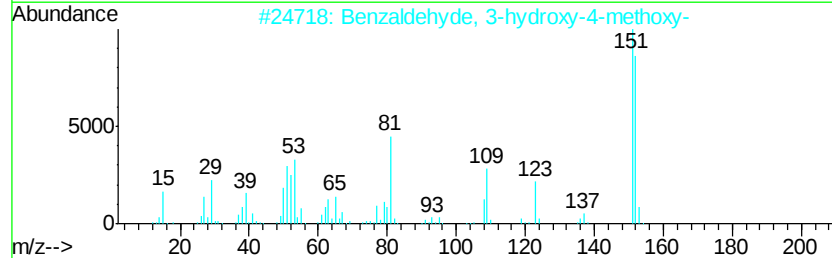
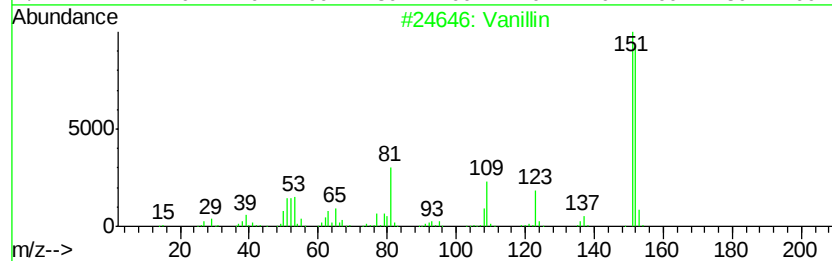
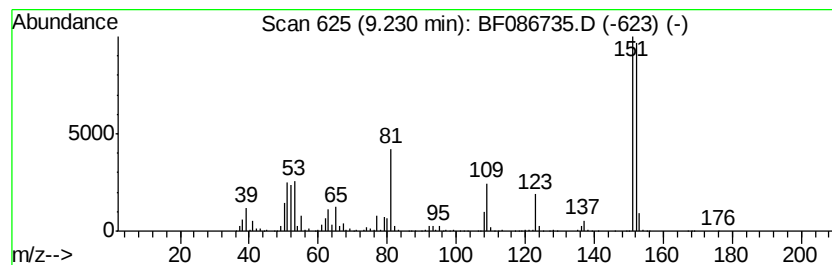
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Vanillin Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.23	29.35 ng	1253450	Acenaphthene-d10	9.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Vanillin	152	C8H8O3	000121-33-5	97
2		Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	97
3		3-Hydroxy-4-methoxymandelic acid	198	C9H10O5	003695-24-7	91
4		4-Hydroxy-2-methoxybenaldehyde	152	C8H8O3	018278-34-7	62
5		Benzaldehyde, 2-hydroxy-4-methoxy-	152	C8H8O3	000673-22-3	46



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Data File : BF086735.D
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ClientSampleId :
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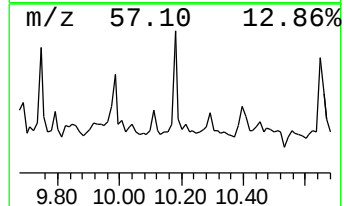
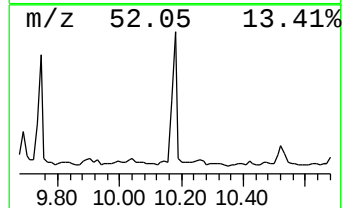
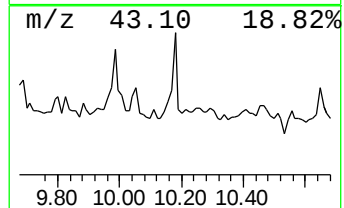
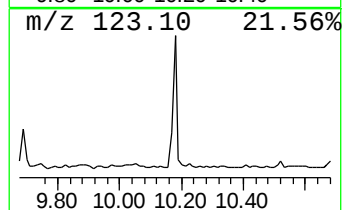
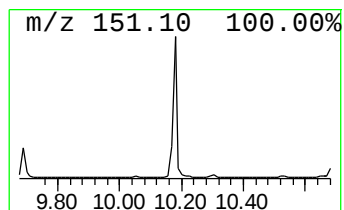
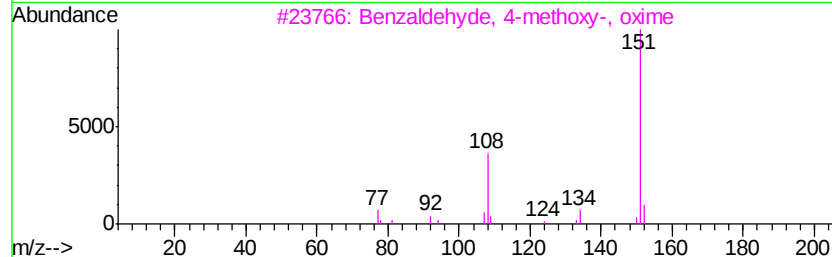
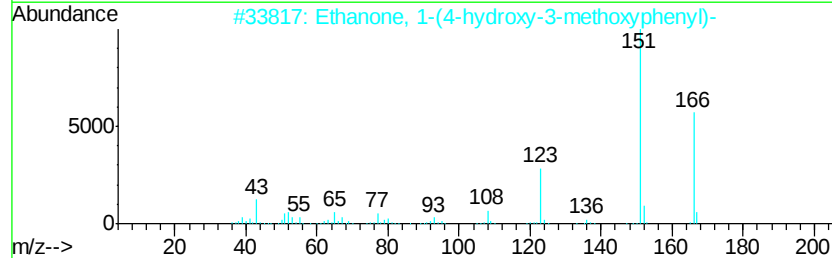
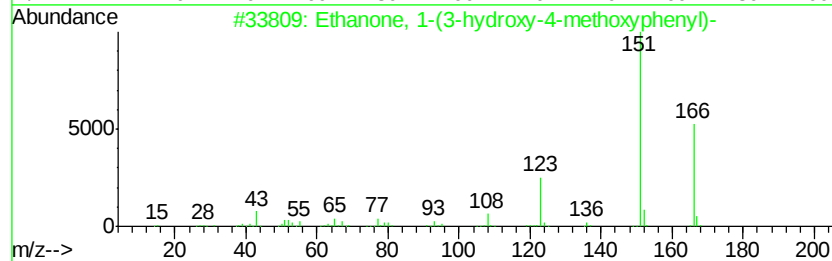
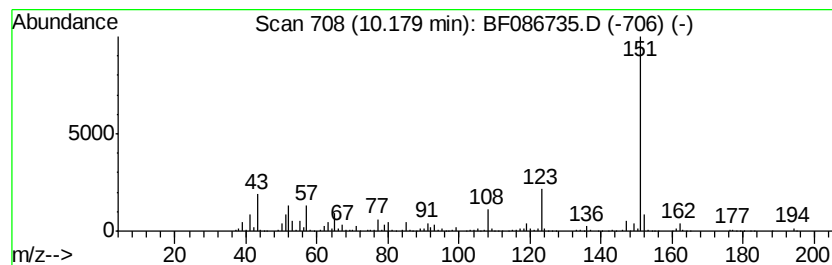
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Ethanone, 1-(3-hydroxy-4-me... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.18	14.94 ng	637957	Acenaphthene-d10	9.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanone, 1-(3-hydroxy-4-methoxy...	166	C9H10O3	006100-74-9	64
2		Ethanone, 1-(4-hydroxy-3-methoxy...	166	C9H10O3	000498-02-2	64
3		Benzaldehyde, 4-methoxy-, oxime	151	C8H9NO2	003235-04-9	50
4		3-Hydroxy-4-methoxymandelic acid	198	C9H10O5	003695-24-7	45
5		Ethanone, 1-(2-hydroxy-6-methoxy...	166	C9H10O3	000703-23-1	42



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086735.D
Acq On : 6 May 2016 20:33
Operator : UM/SJ
Sample : H2802-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4

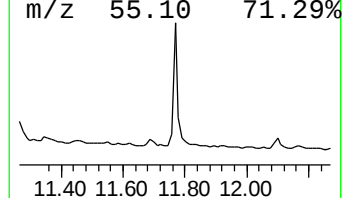
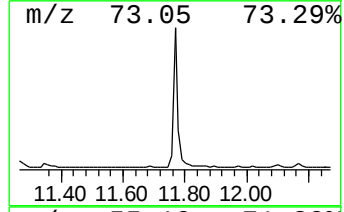
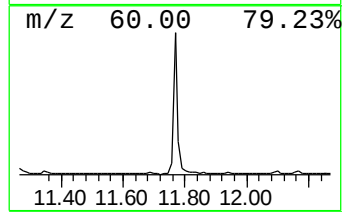
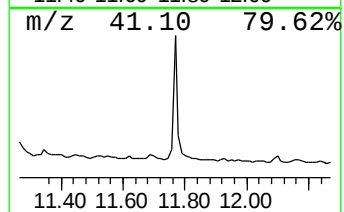
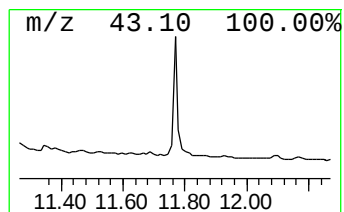
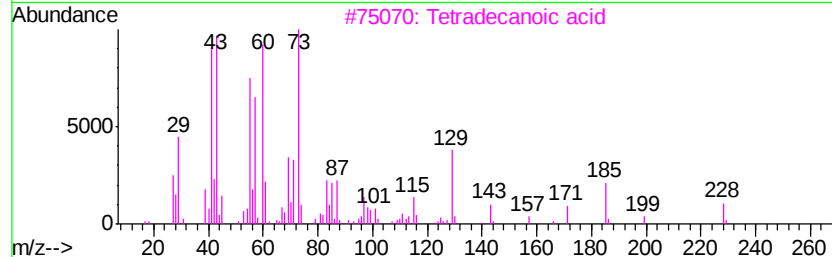
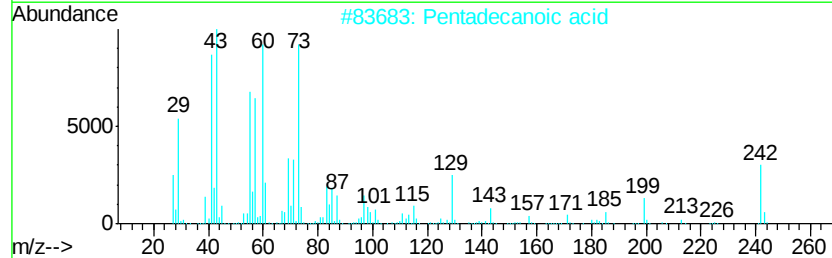
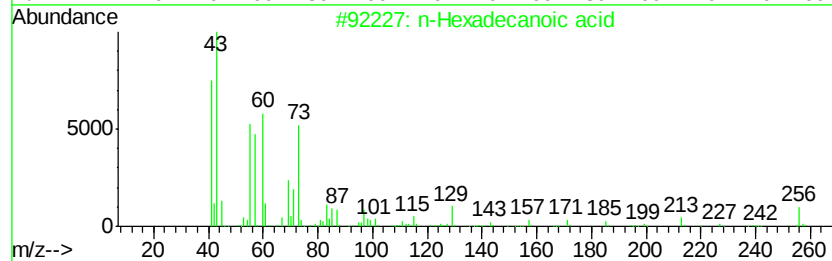
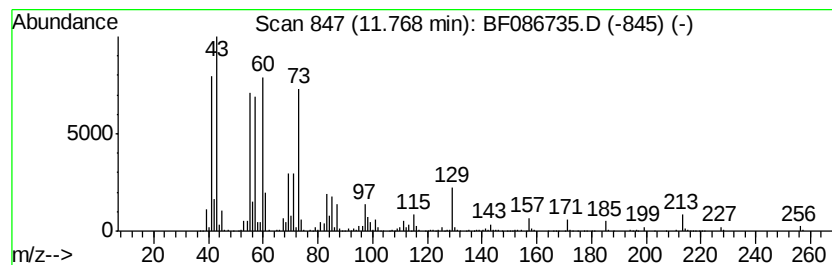
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	21.79 ng	826585	Phenanthrene-d10	11.22

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4			Undecanoic acid	186	C11H22O2	000112-37-8	83
5			Tridecanoic acid	214	C13H26O2	000638-53-9	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086735.D
Acq On : 6 May 2016 20:33
Operator : UM/SJ
Sample : H2802-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4

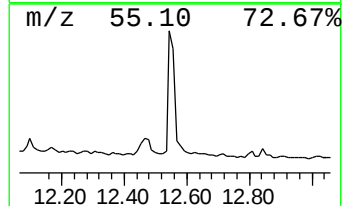
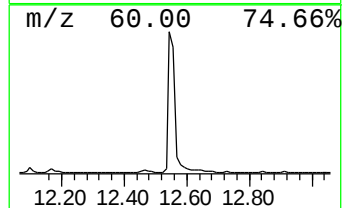
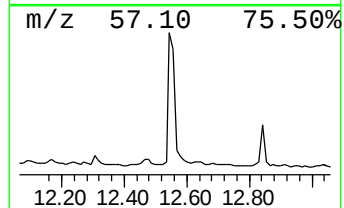
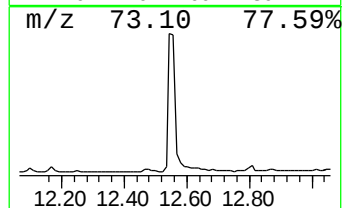
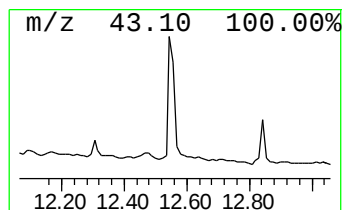
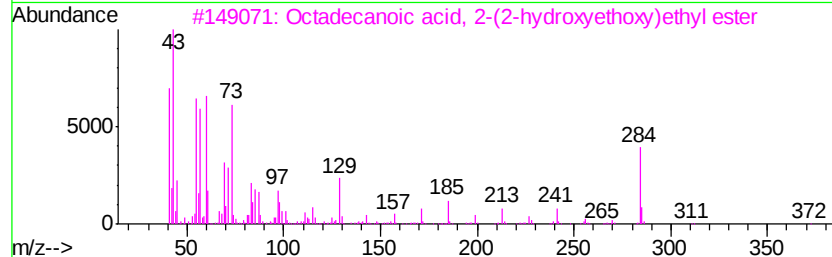
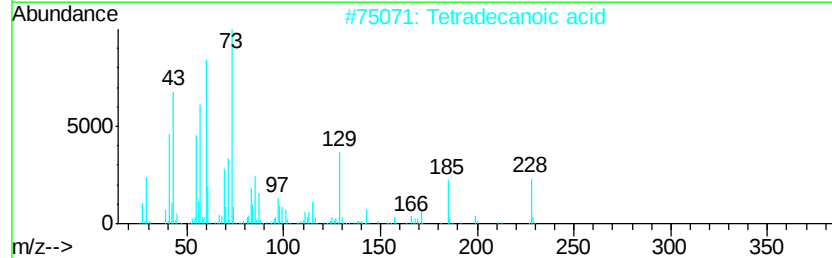
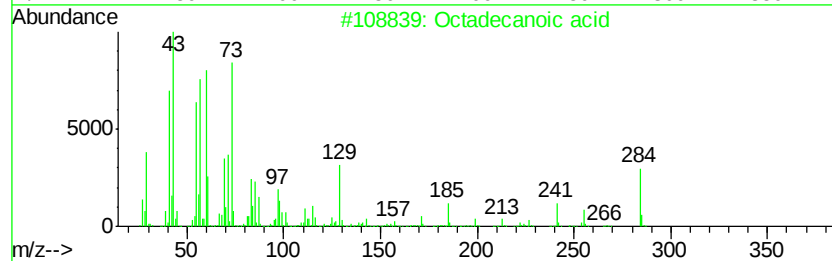
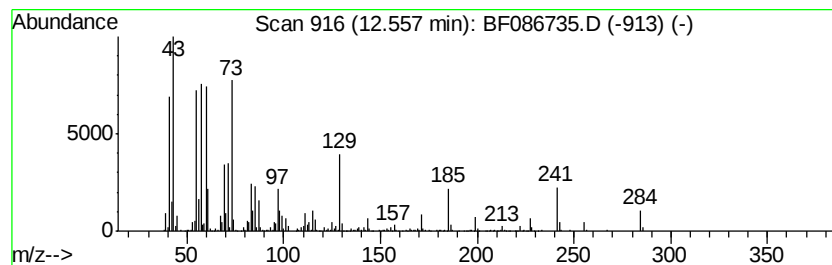
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	30.55 ng	965340	Chrysene-d12	13.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
3		Octadecanoic acid, 2-(2-hydroxyethoxy)ethyl ester	372	C22H44O4	000106-11-6	59
4		Tridecanoic acid	214	C13H26O2	000638-53-9	53
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
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 Acq On : 6 May 2016 20:33
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 Sample : H2802-06
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.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
Furfural	4.75	38.3	ng	1126430	1	6.70	1175860	40.0
2-Hexanone, 5-met...	5.49	23.5	ng	690414	1	6.70	1175860	40.0
Ethanone, 1-(2-fu...	5.72	17.4	ng	512471	1	6.70	1175860	40.0
2,5-Hexanedione	5.89	18.1	ng	530916	1	6.70	1175860	40.0
unknown6.14	6.14	41.1	ng	1209150	1	6.70	1175860	40.0
unknown6.44	6.44	47.0	ng	1380440	1	6.70	1175860	40.0
unknown6.49	6.49	153.8	ng	4519770	1	6.70	1175860	40.0
2(3H)-Furanone, 5...	6.76	19.7	ng	578085	1	6.70	1175860	40.0
2-Nonanone	6.96	22.6	ng	663775	1	6.70	1175860	40.0
2(3H)-Furanone, 5...	7.01	13.9	ng	408559	1	6.70	1175860	40.0
1-Butyne	7.21	12.7	ng	374327	1	6.70	1175860	40.0
2(3H)-Furanone, d...	7.72	13.1	ng	533014	2	8.00	1629150	40.0
Pentanoic acid, e...	8.40	35.0	ng	1425180	2	8.00	1629150	40.0
n-Decanoic acid	8.96	14.3	ng	610483	3	9.74	1708570	40.0
1(3H)-Isobenzofur...	8.99	19.5	ng	831564	3	9.74	1708570	40.0
Vanillin	9.23	29.4	ng	1253450	3	9.74	1708570	40.0
Ethanone, 1-(3-hy...	10.18	14.9	ng	637957	3	9.74	1708570	40.0
n-Hexadecanoic acid	11.77	21.8	ng	826585	4	11.22	1517170	40.0
Octadecanoic acid	12.56	30.6	ng	965340	5	13.85	1263790	40.0