

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082015\
 Data File : BF081132.D
 Acq On : 20 Aug 2015 19:08
 Operator : UM/IZ
 Sample : G3345-02
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TEC-2

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-BF081715.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	4.447	222	224	230	rVB	12276	20215	1.01%	0.110%
2	4.676	242	244	247	rBV	294969	392006	19.57%	2.135%
3	5.133	282	284	287	rBV	392941	490573	24.49%	2.672%
4	5.499	315	316	320	rVB	22406	27645	1.38%	0.151%
5	6.219	374	379	381	rBV2	261796	417864	20.86%	2.276%
6	6.333	387	389	392	rBV	801044	763481	38.11%	4.158%
7	6.425	396	397	403	rVB2	15350	25866	1.29%	0.141%
8	6.516	403	405	408	rBV	11996	20993	1.05%	0.114%
9	6.573	408	410	412	rVV	550256	463356	23.13%	2.524%
10	6.607	412	413	415	rVV	131734	127350	6.36%	0.694%
11	6.653	415	417	421	rVV	95005	150796	7.53%	0.821%
12	6.733	421	424	426	rVV	1347206	1419845	70.88%	7.733%
13	6.767	426	427	433	rVB2	38524	63553	3.17%	0.346%
14	6.905	437	439	441	rBV2	25856	24086	1.20%	0.131%
15	6.985	444	446	452	rVB	67686	83116	4.15%	0.453%
16	7.145	457	460	462	rVV2	1240520	1427060	71.24%	7.773%
17	7.179	462	463	467	rVV2	22106	45250	2.26%	0.246%
18	7.236	467	468	470	rVV	25019	46581	2.33%	0.254%
19	7.293	470	473	474	rVV	61097	99404	4.96%	0.541%
20	7.327	474	476	480	rVB2	23449	41321	2.06%	0.225%
21	7.407	480	483	486	rBV	17449	24915	1.24%	0.136%
22	7.682	496	507	509	rBV	189070	678842	33.89%	3.697%
23	7.785	513	516	520	rVV3	37639	81145	4.05%	0.442%
24	7.865	520	523	524	rVV	522119	625740	31.24%	3.408%
25	7.899	524	526	527	rVV	63074	63999	3.19%	0.349%
26	8.002	531	535	537	rVV3	25646	48601	2.43%	0.265%
27	8.105	540	544	545	rVV2	17032	33146	1.65%	0.181%
28	8.139	545	547	550	rVV3	126056	169509	8.46%	0.923%
29	8.185	550	551	554	rVV	81019	120141	6.00%	0.654%
30	8.242	554	556	558	rVV3	27378	43095	2.15%	0.235%
31	8.299	558	561	564	rVB5	24643	50470	2.52%	0.275%
32	8.448	571	574	576	rBV2	22228	44205	2.21%	0.241%
33	8.619	584	589	591	rBV	248529	478001	23.86%	2.603%
34	8.665	591	593	596	rVB	34770	52045	2.60%	0.283%

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35	8.882	610	612	615 rBV	64851	68118	3.40%	0.371%
36	8.939	615	617	620 rVB	1637355	2003126	100.00%	10.910%
37	9.042	623	626	627 rVV	15264	21788	1.09%	0.119%
38	9.088	627	630	632 rVV2	343085	370506	18.50%	2.018%
39	9.122	632	633	636 rVB2	19932	21685	1.08%	0.118%
40	9.271	644	646	649 rVB	24855	22273	1.11%	0.121%
41	9.339	651	652	654 rVB	104043	78651	3.93%	0.428%
42	9.453	659	662	664 rBV2	15704	31473	1.57%	0.171%
43	9.488	664	665	667 rBV	36151	38245	1.91%	0.208%
44	9.545	667	670	672 rVB2	87097	122481	6.11%	0.667%
45	9.602	673	675	677 rVB2	519572	620074	30.96%	3.377%
46	9.831	694	695	698 rBV3	73416	75450	3.77%	0.411%
47	9.888	698	700	704 rVB3	31525	56295	2.81%	0.307%
48	10.036	711	713	714 rBV	23769	32276	1.61%	0.176%
49	10.059	714	715	717 rVB	29578	24820	1.24%	0.135%
50	10.151	721	723	725 rVB2	18676	21232	1.06%	0.116%
51	10.208	726	728	731 rVB	18743	29568	1.48%	0.161%
52	10.265	731	733	735 rBV	100641	101217	5.05%	0.551%
53	10.391	740	744	746 rVB	654946	710769	35.48%	3.871%
54	10.448	746	749	751 rBV	20763	25380	1.27%	0.138%
55	10.505	751	754	755 rBV	114579	106491	5.32%	0.580%
56	10.528	755	756	759 rVB2	44230	48851	2.44%	0.266%
57	10.585	759	761	763 rBV2	29616	33087	1.65%	0.180%
58	10.699	770	771	774 rBV2	47507	47148	2.35%	0.257%
59	10.756	774	776	779 rVB3	36877	60271	3.01%	0.328%
60	10.848	781	784	786 rBV	105788	126382	6.31%	0.688%
61	10.974	792	795	797 rBV2	381840	398090	19.87%	2.168%
62	11.031	797	800	802 rVV	95081	84513	4.22%	0.460%
63	11.076	802	804	810 rVV	725823	681487	34.02%	3.712%
64	11.202	813	815	817 rBV	57572	65333	3.26%	0.356%
65	11.294	818	823	826 rBV4	20374	75579	3.77%	0.412%
66	11.636	851	853	856 rBV2	98574	122566	6.12%	0.668%
67	11.682	856	857	860 rVV	40664	40748	2.03%	0.222%
68	11.796	863	867	871 rVV	61529	94042	4.69%	0.512%
69	11.854	871	872	880 rVB7	22749	34281	1.71%	0.187%
70	12.322	911	913	915 rBV	12035	20326	1.01%	0.111%
71	12.368	915	917	919 rVB	79893	91279	4.56%	0.497%

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72	12.414	919	921	927	rVB	28994	43860	2.19%	0.239%
73	12.551	931	933	940	rBV4	10840	25654	1.28%	0.140%
74	12.665	940	943	945	rBV	1910141	1827224	91.22%	9.952%
75	13.031	973	975	978	rBV	121867	117201	5.85%	0.638%
76	13.248	992	994	998	rBV4	10280	21918	1.09%	0.119%
77	13.580	1021	1023	1027	rBV	45767	58296	2.91%	0.318%
78	13.694	1030	1033	1035	rBV	528907	493437	24.63%	2.688%
79	14.551	1106	1108	1110	rVB	190713	172139	8.59%	0.938%
80	15.031	1147	1150	1153	rBV	289824	305973	15.27%	1.667%
81	16.734	1295	1299	1304	rBV6	7483	24205	1.21%	0.132%

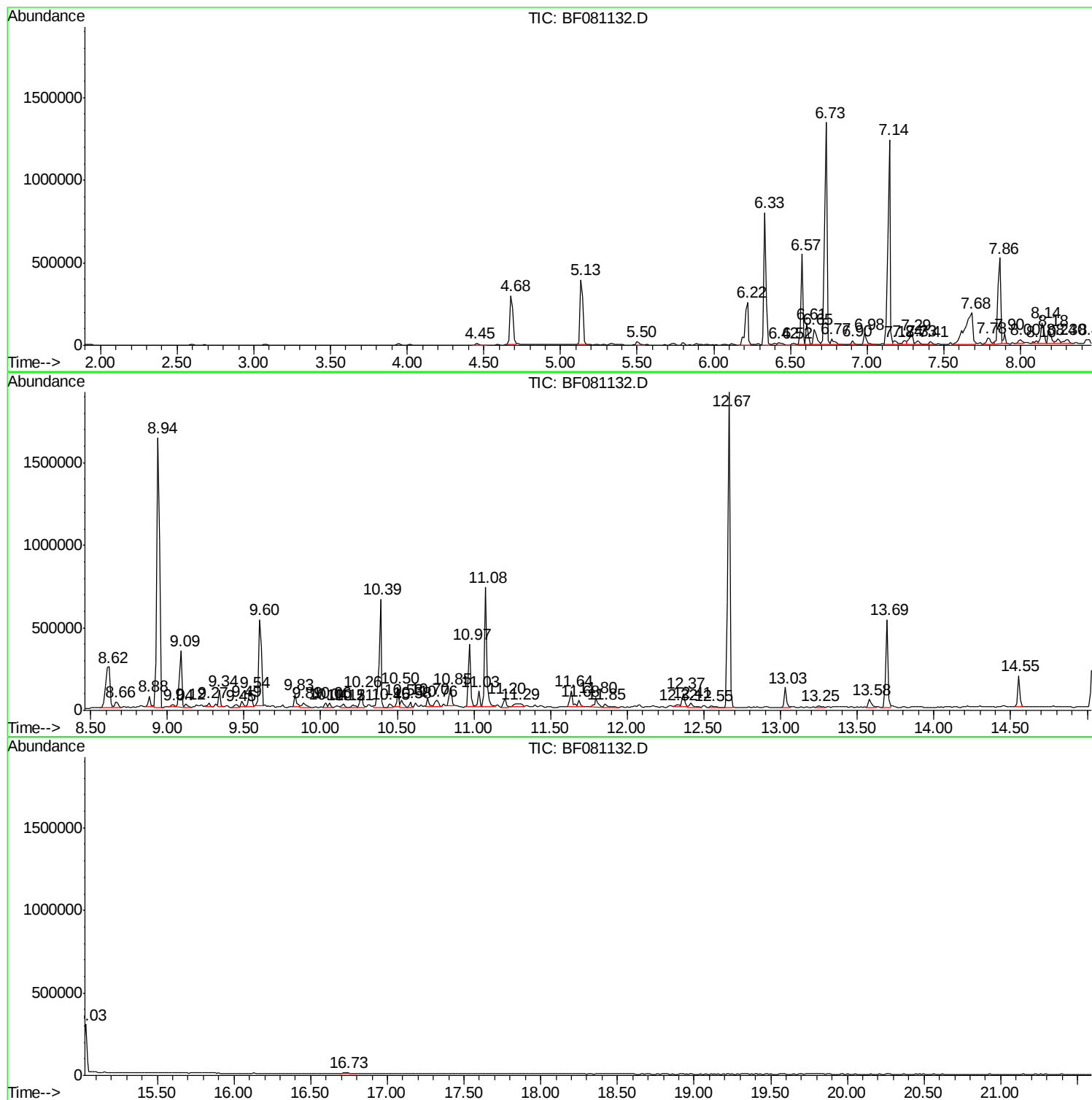
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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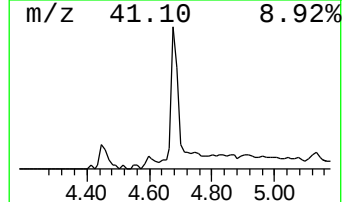
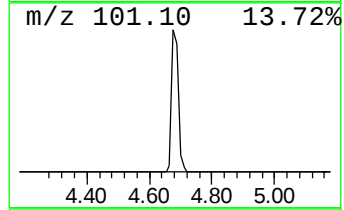
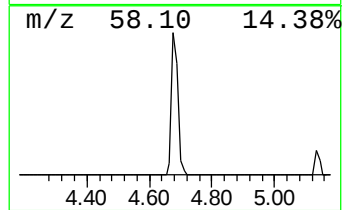
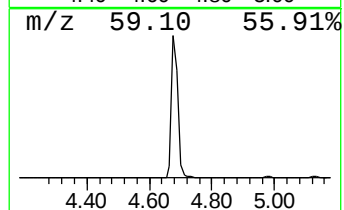
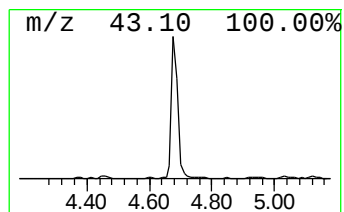
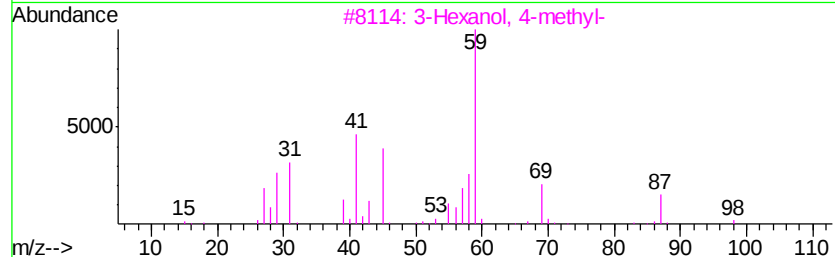
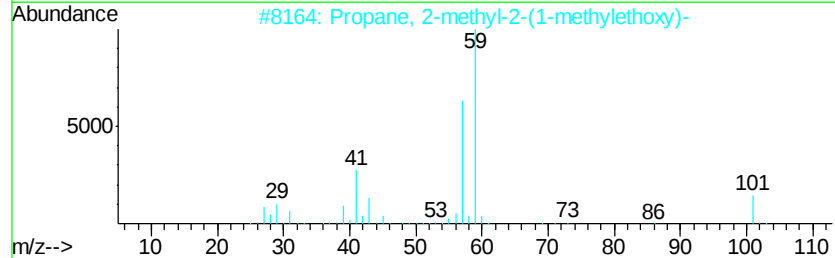
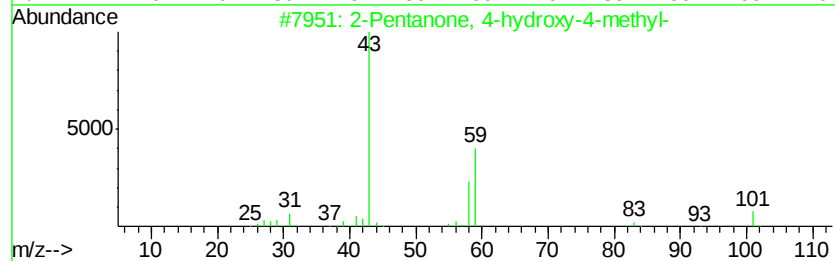
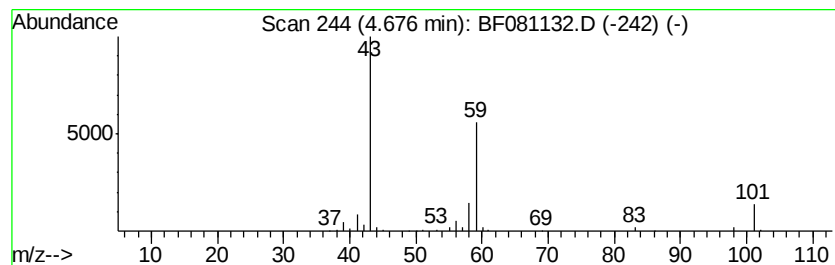
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.68	16.92 ng	392006	1,4-Dichlorobenzene-d4	6.57

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32



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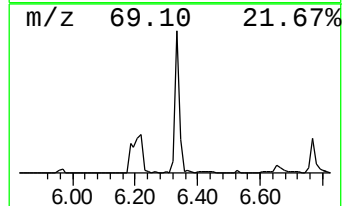
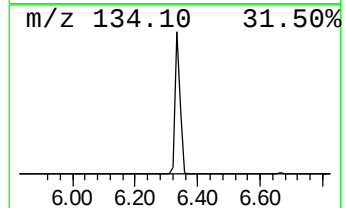
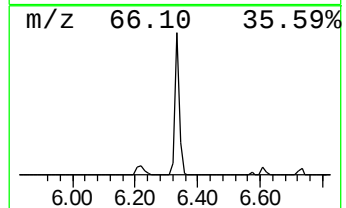
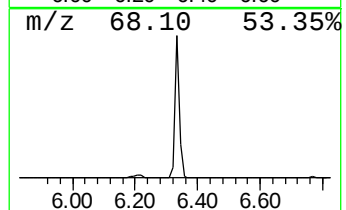
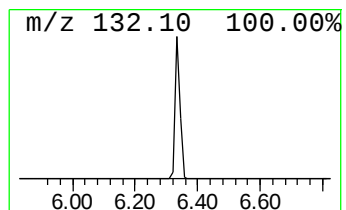
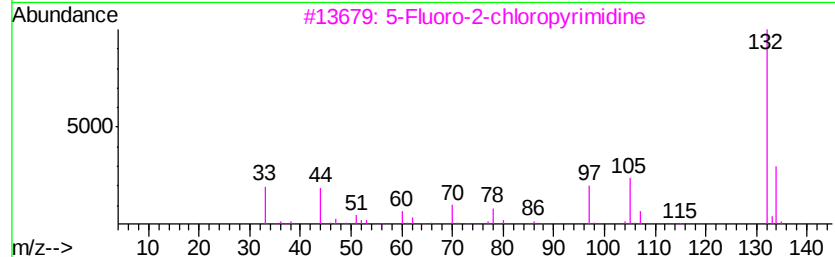
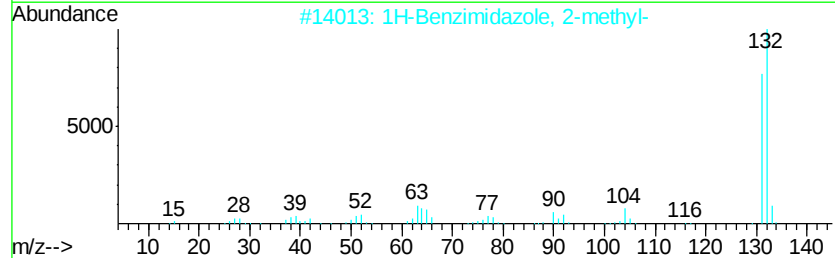
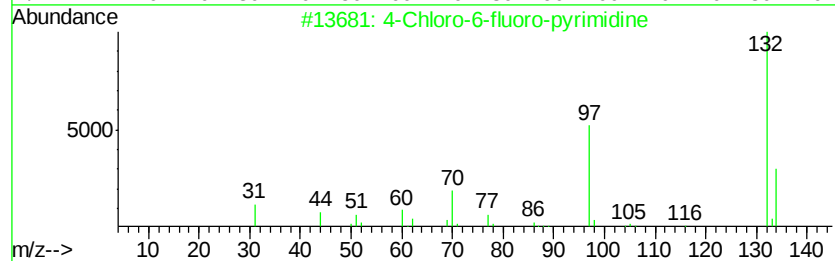
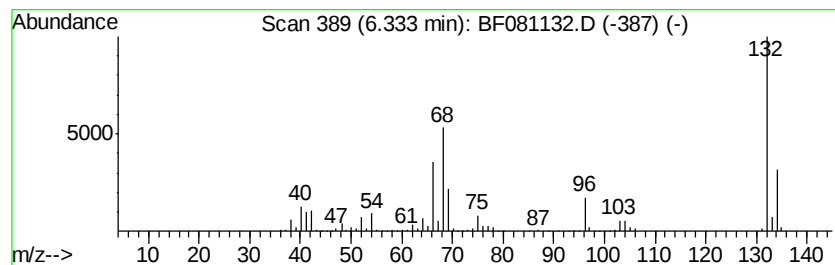
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.33 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.33	32.95 ng	763481	1,4-Dichlorobenzene-d4	6.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	25
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5		5-Aminoindole	132	C8H8N2	005192-03-0	10



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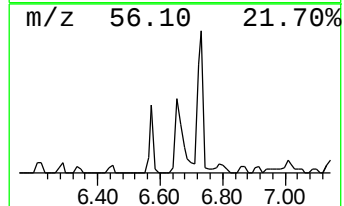
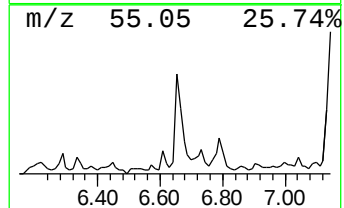
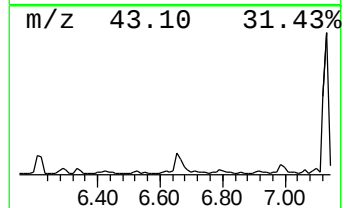
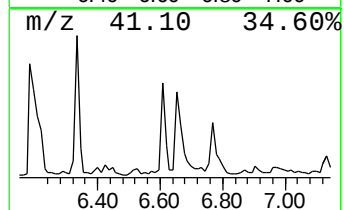
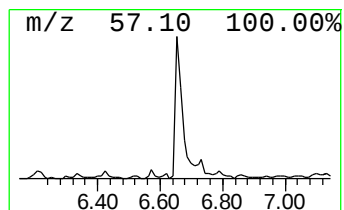
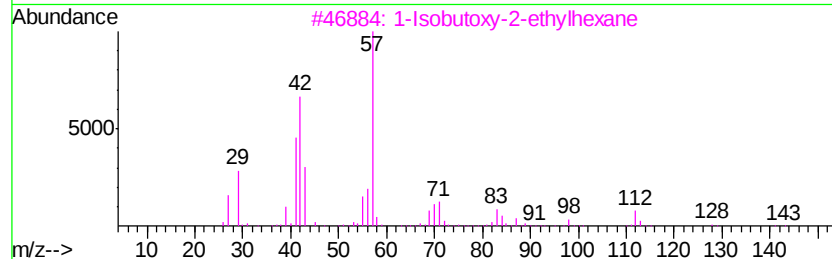
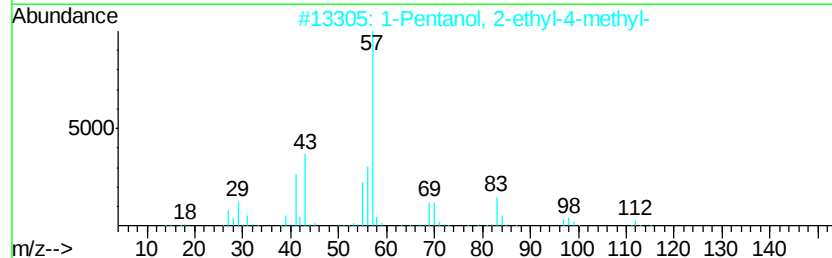
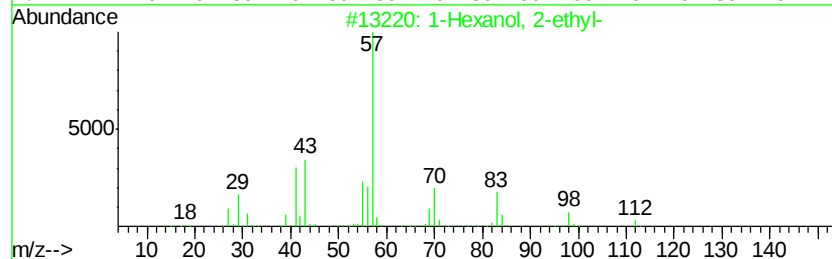
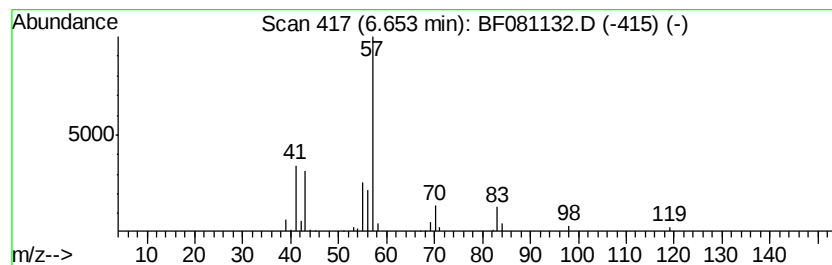
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	6.51 ng	150796	1,4-Dichlorobenzene-d4	6.57

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	53
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50
3			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	39
4			3-Undecene, 6-methyl-, (E)-	168	C12H24	074630-52-7	38
5			1-Pentene, 4,4-dimethyl-	98	C7H14	000762-62-9	37



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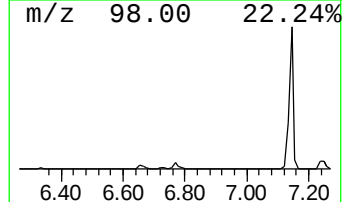
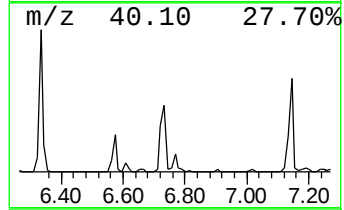
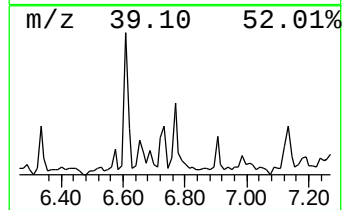
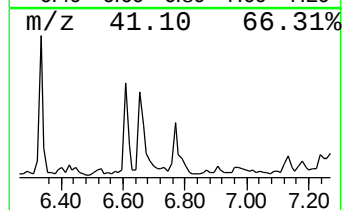
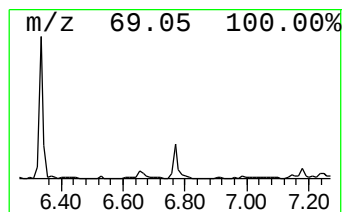
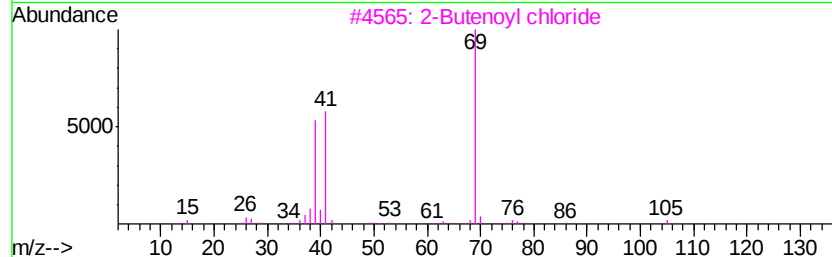
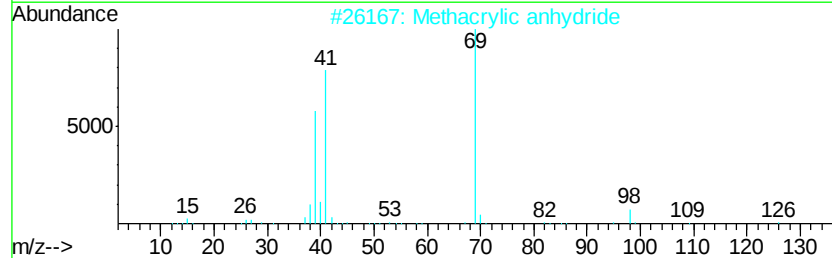
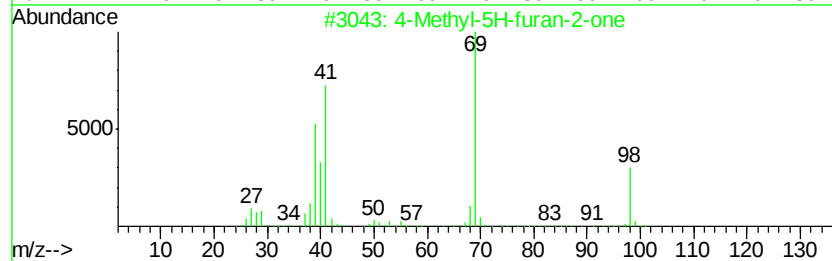
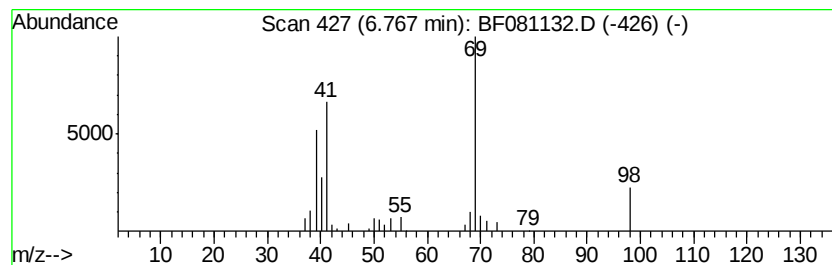
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 4-Methyl-5H-furan-2-one Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	2.74 ng	63553	1,4-Dichlorobenzene-d4	6.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Methyl-5H-furan-2-one	98	C5H6O2	006124-79-4	91
2		Methacrylic anhydride	154	C8H10O3	000760-93-0	72
3		2-Butenoyl chloride	104	C4H5ClO	010487-71-5	64
4		Crotonyl isothiocyanate	127	C5H5NOS	060034-28-8	59
5		Methacryloyl chloride	104	C4H5ClO	000920-46-7	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082015\
Data File : BF081132.D
Acq On : 20 Aug 2015 19:08
Operator : UM/IZ
Sample : G3345-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TEC-2

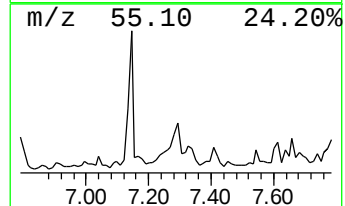
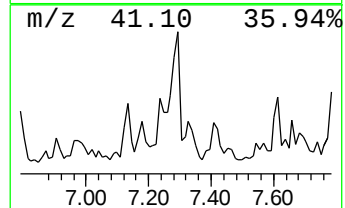
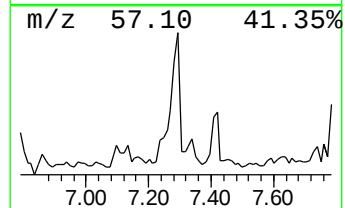
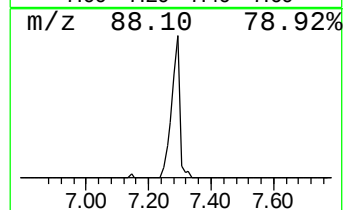
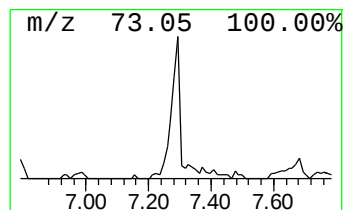
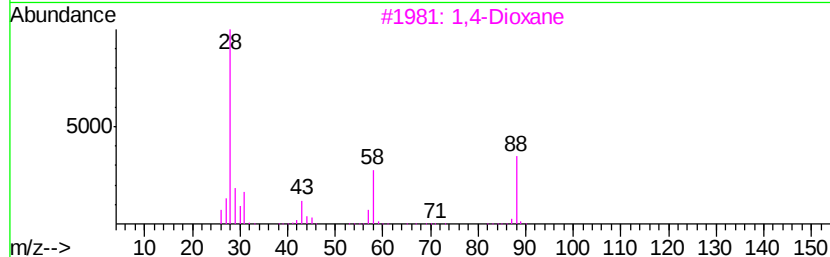
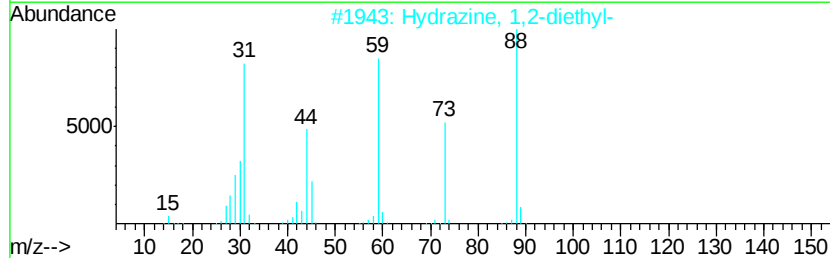
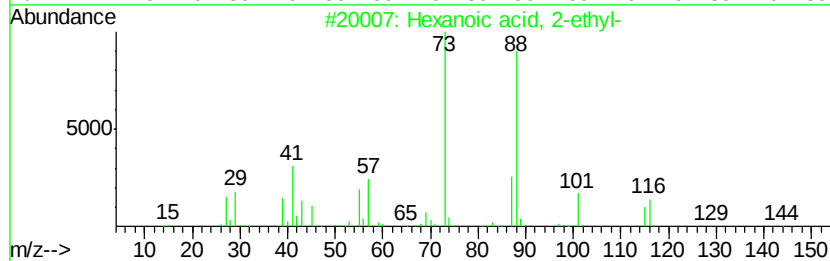
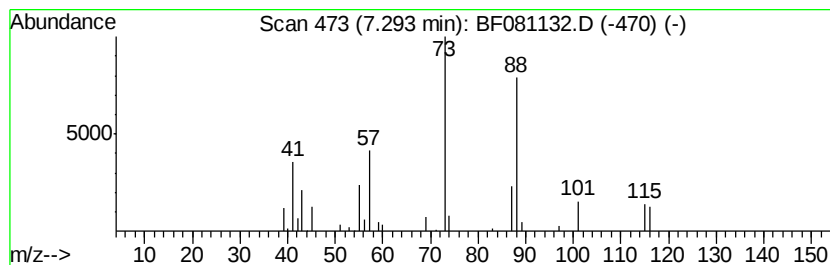
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexanoic acid, 2-ethyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.29	3.18 ng	99404	Naphthalene-d8	7.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	78
2			Hydrazine, 1,2-diethyl-	88	C4H12N2	001615-80-1	50
3			1,4-Dioxane	88	C4H8O2	000123-91-1	47
4			Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	45
5			Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	33



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082015\
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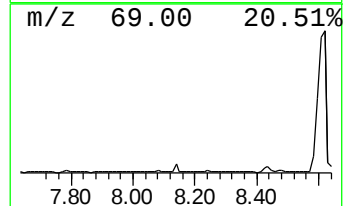
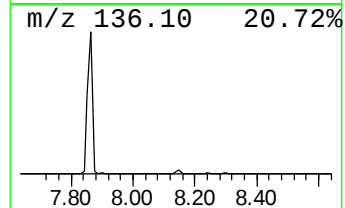
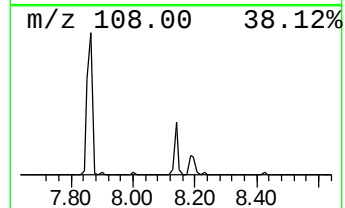
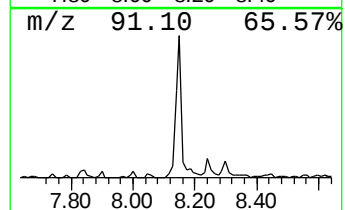
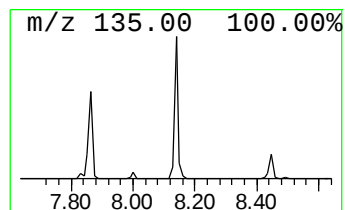
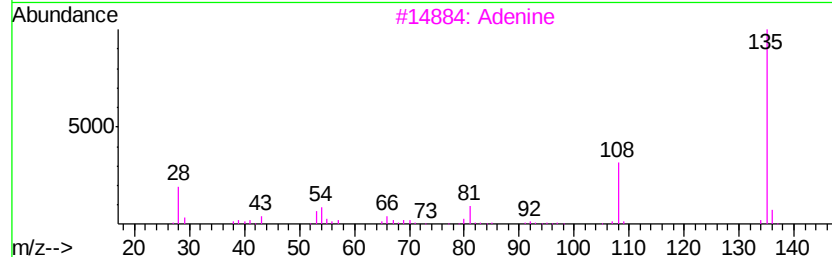
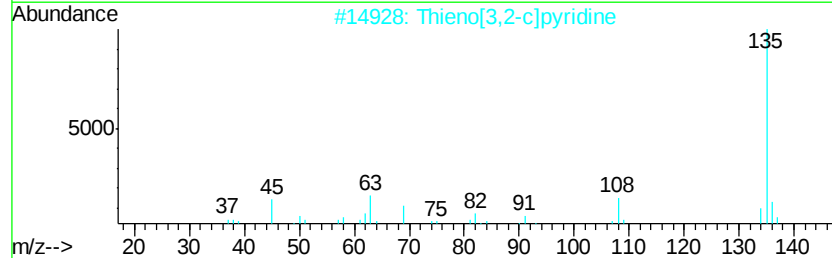
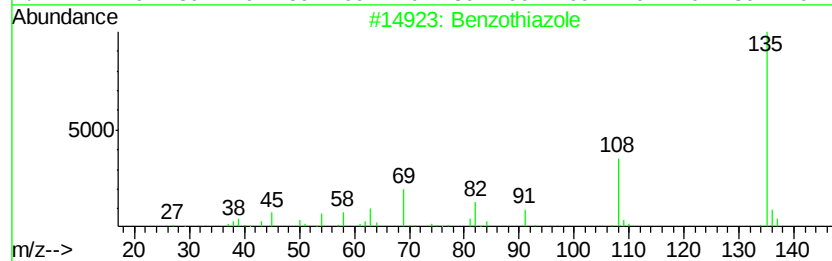
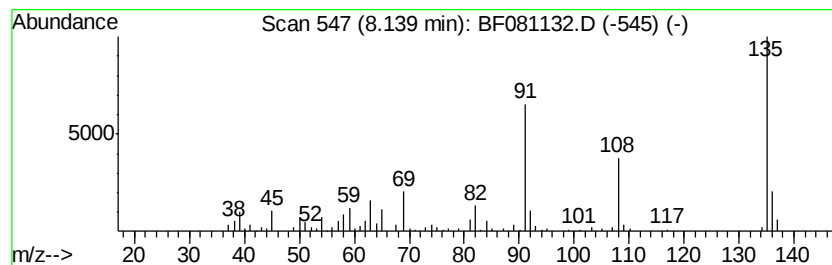
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzothiazole Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.14	5.42 ng	169509	Napthalene-d8	7.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzothiazole	135	C7H5NS	000095-16-9	81
2		Thieno[3,2-c]pyridine	135	C7H5NS	000272-14-0	60
3		Adenine	135	C5H5N5	000073-24-5	58
4		1,2-Benzisothiazole	135	C7H5NS	000272-16-2	52
5		Thieno[2,3-c]pyridine	135	C7H5NS	000272-12-8	52



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082015\
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ClientSampleId :
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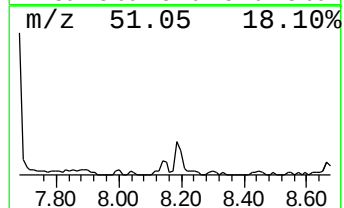
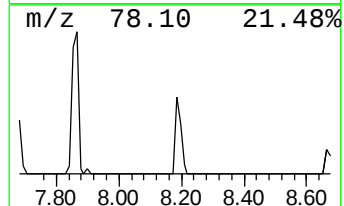
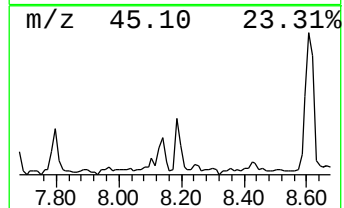
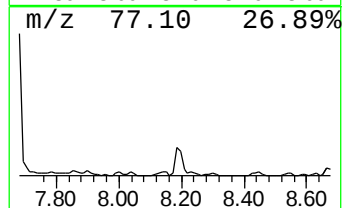
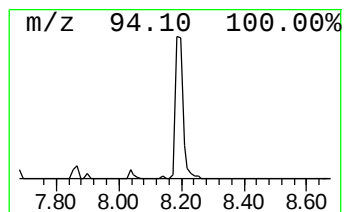
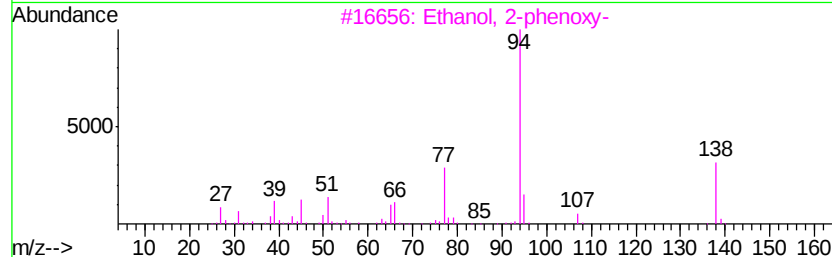
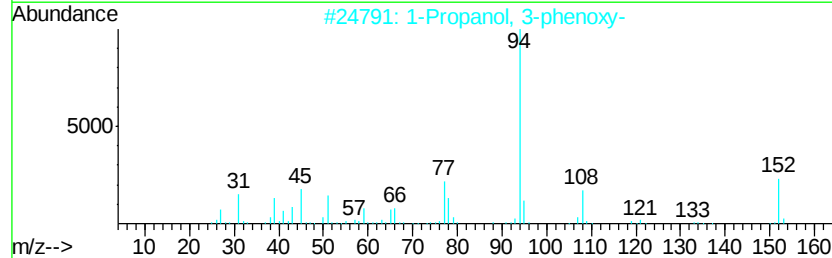
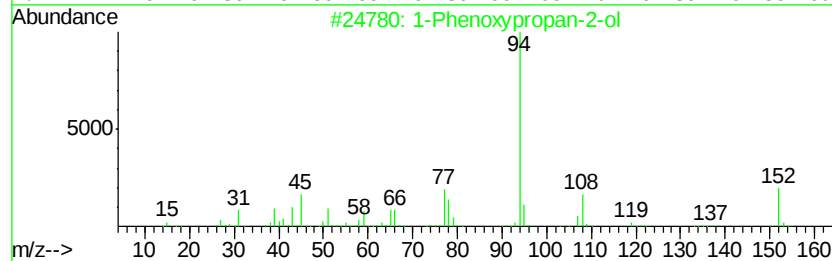
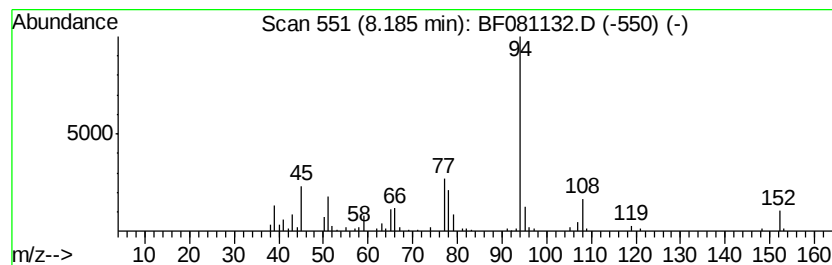
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Phenoxypropan-2-ol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.18	3.84 ng	120141	Napthalene-d8	7.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
2		1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	72
3		Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	59
4		1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	53
5		Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082015\
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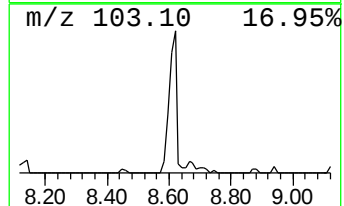
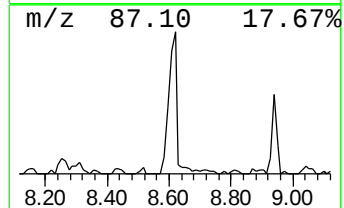
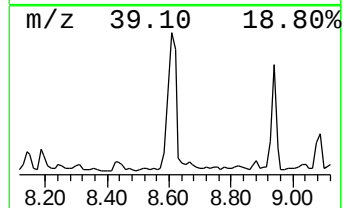
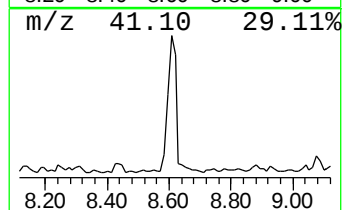
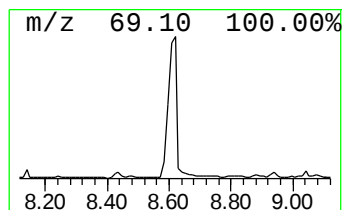
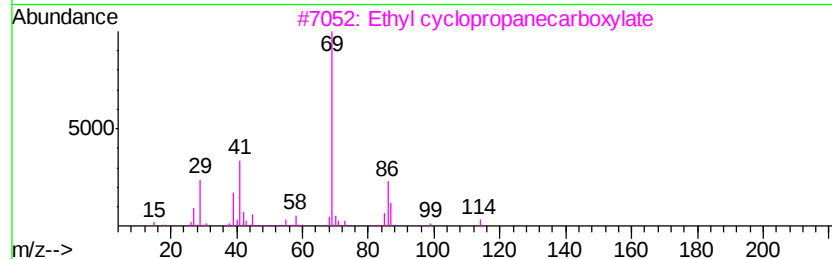
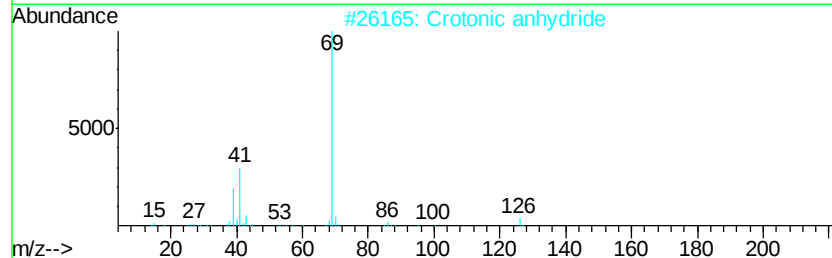
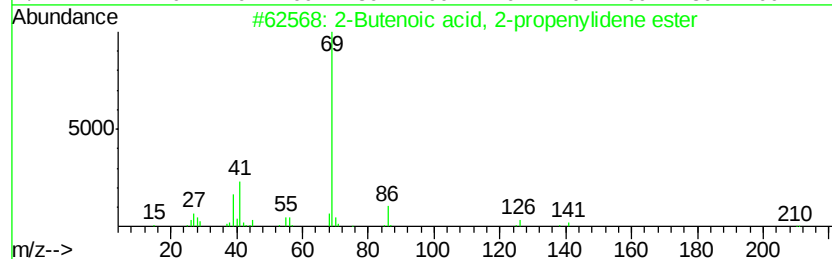
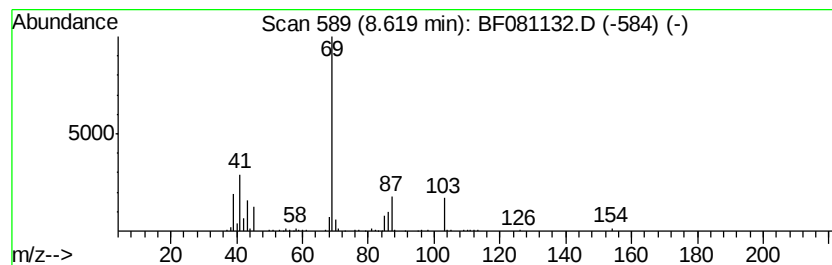
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown8.62 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.62	15.28 ng	478001	Naphthalene-d8	7.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	36	
2	Crotonic anhydride	154	C8H10O3	000623-68-7	9	
3	Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	9	
4	Cyclopropanecarboxylic acid,isop...	128	C7H12O2	006887-83-8	9	
5	(E)-2-Butenoic acid propyl ester	128	C7H12O2	010352-87-1	9	



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Acq On : 20 Aug 2015 19:08
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Instrument :
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ClientSampleId :
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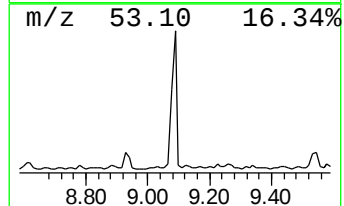
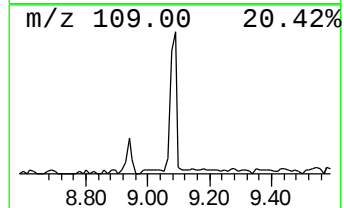
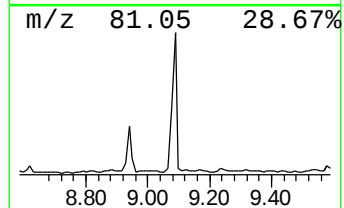
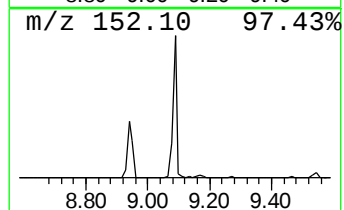
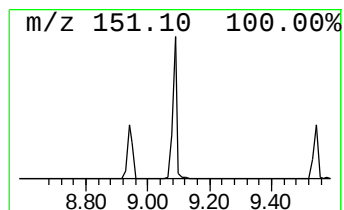
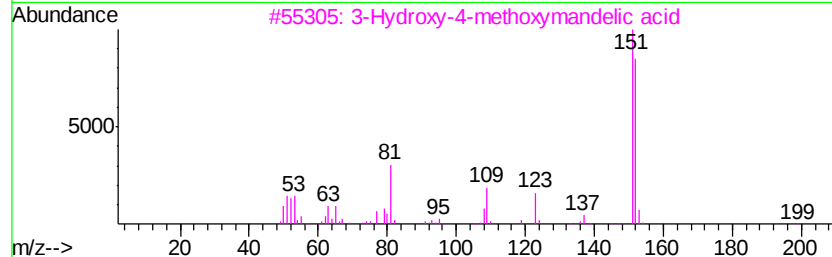
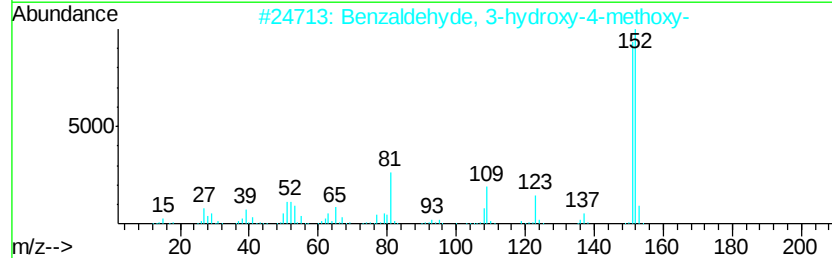
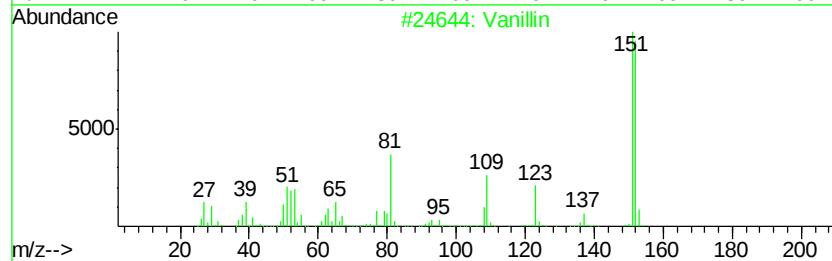
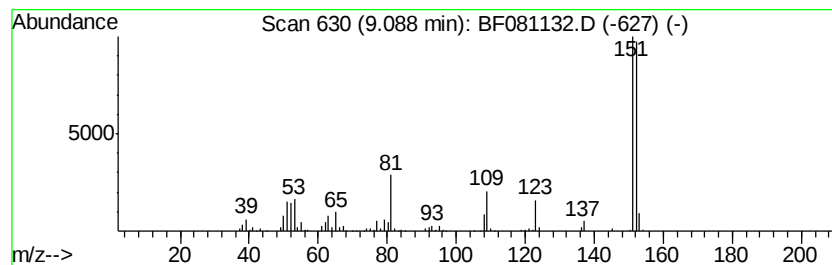
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Vanillin Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.09	11.95 ng	370506	Acenaphthene-d10	9.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Vanillin	152	C8H8O3	000121-33-5	98
2		Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	96
3		3-Hydroxy-4-methoxymandelic acid	198	C9H10O5	003695-24-7	91
4		Vanillin lactoside	476	C20H28O13	1000129-94-7	72
5		Benzaldehyde, 2,4-dihydroxy-6-me...	152	C8H8O3	000487-69-4	64



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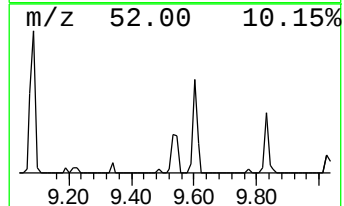
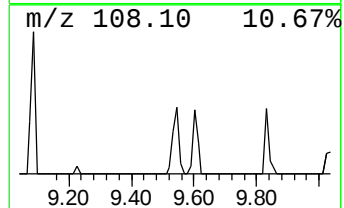
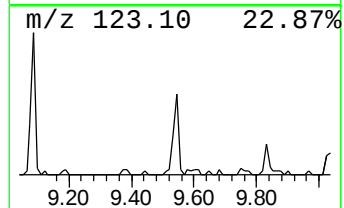
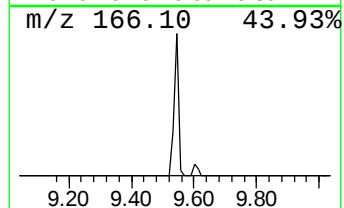
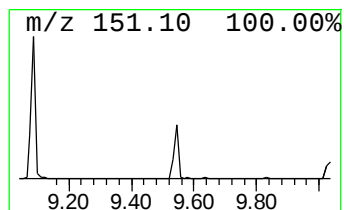
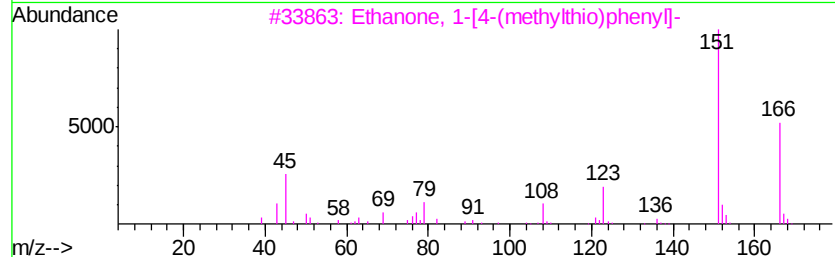
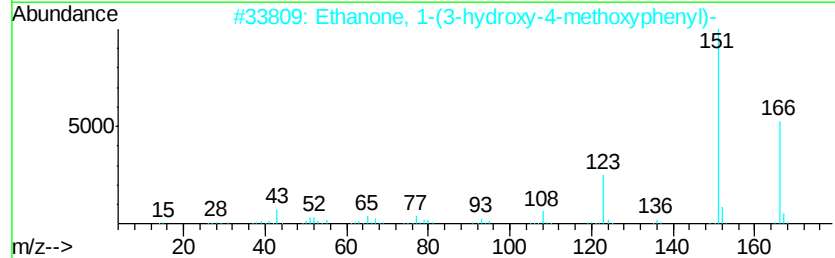
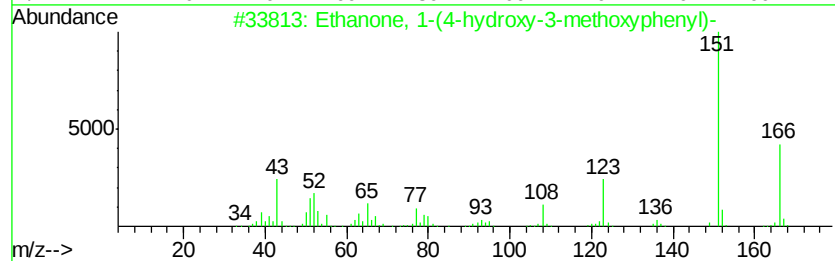
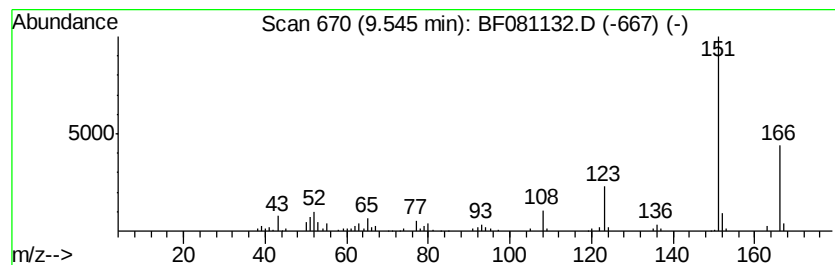
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Ethanone, 1-(4-hydroxy-3-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.54	3.95 ng	122481	Acenaphthene-d10	9.60

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-(4-hydroxy-3-methoxy...	166	C9H10O3	000498-02-2	94		
2	Ethanone, 1-(3-hydroxy-4-methoxy...	166	C9H10O3	006100-74-9	93		
3	Ethanone, 1-[4-(methylthio)phenyl]-	166	C9H10OS	001778-09-2	80		
4	1,4-Benzenediol, 2-(1,1-dimethyl...	166	C10H14O2	001948-33-0	72		
5	Ethanone, 1-(2-hydroxy-4-methoxy...	166	C9H10O3	000552-41-0	72		



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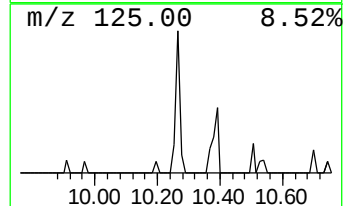
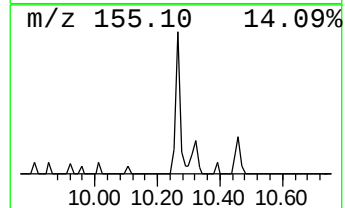
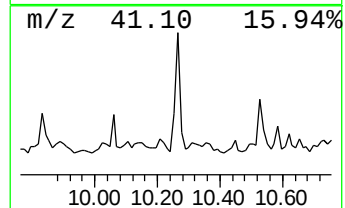
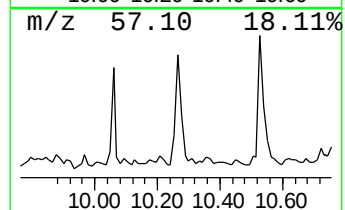
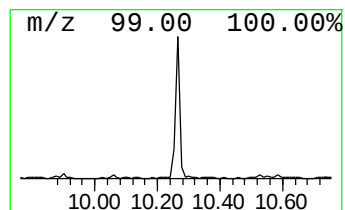
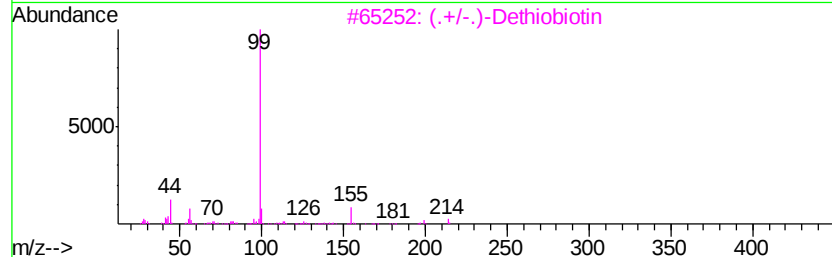
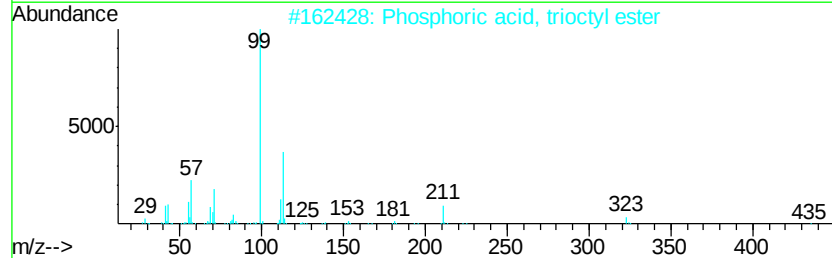
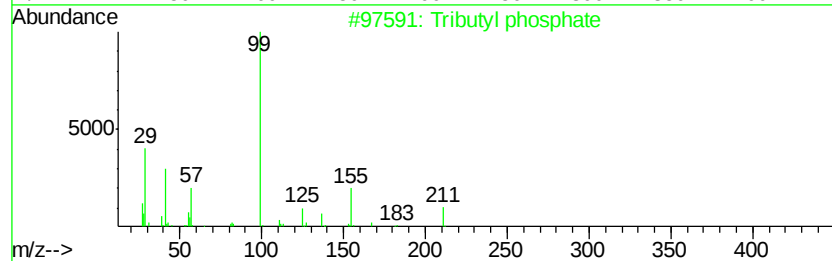
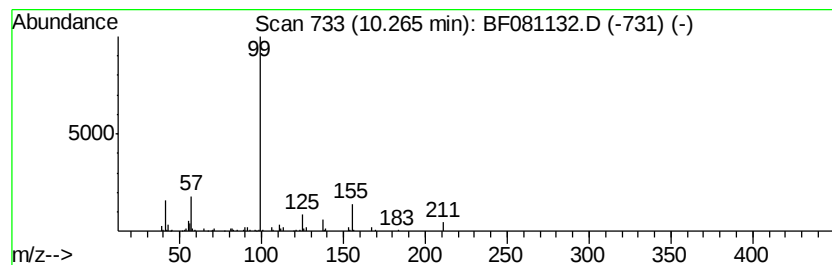
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ClientSampleId :
TEC-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Tributyl phosphate Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.26	3.26 ng	101217	Acenaphthene-d10	9.60
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Tributyl phosphate	266 C12H27O4P	000126-73-8 90
2		Phosphoric acid, trioctyl ester	434 C24H51O4P	001806-54-8 50
3		(.+/-)-Dethiobiotin	214 C10H18N2O3	000636-20-4 36
4		3-Hydroxy-2,3,4,4-tetramethyl-pe...	202 C11H22O3	1000194-64-5 28
5		3,5-Diamino-1,2,4-triazole	99 C2H5N5	001455-77-2 9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082015\
Data File : BF081132.D
Acq On : 20 Aug 2015 19:08
Operator : UM/IZ
Sample : G3345-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-2

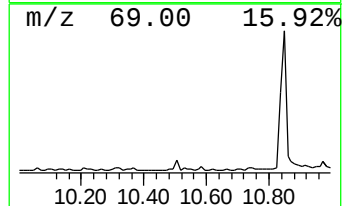
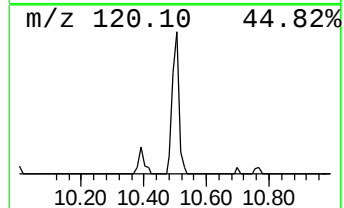
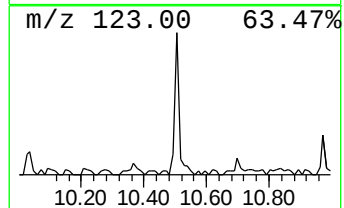
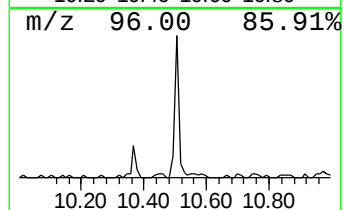
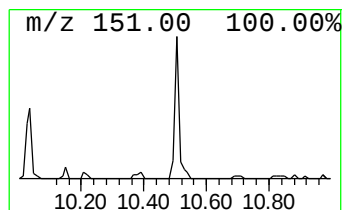
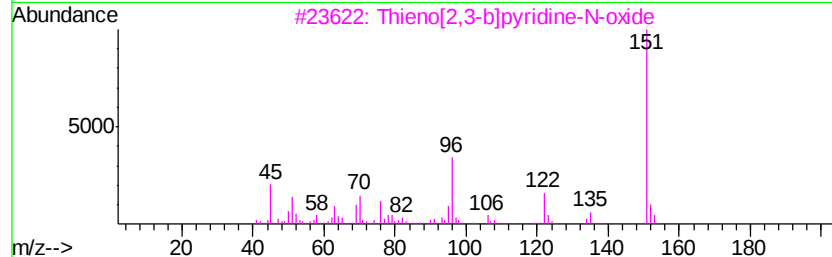
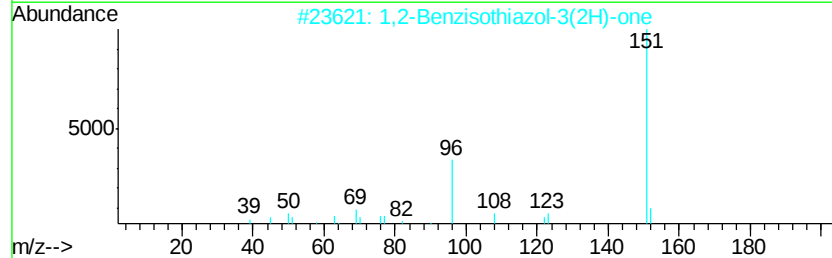
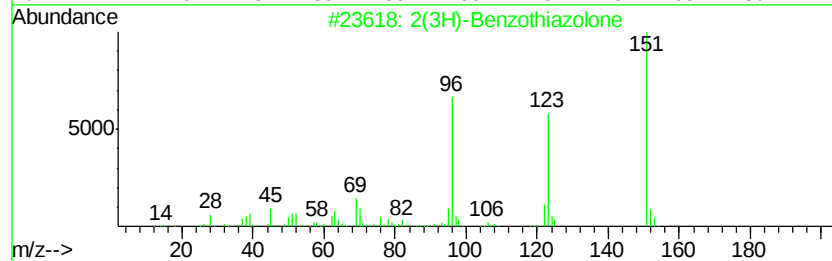
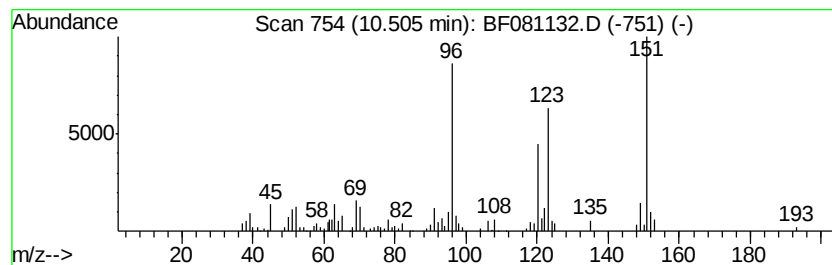
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 2(3H)-Benzothiazolone Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.50	3.13 ng	106491	Phenanthrene-d10	11.08

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	93
2			1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	64
3			Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	46
4			6-Methyl-7-oxo-4,7-dihydro-triaz...	151	C5H5N5O	057250-39-2	35
5			2(3H)-Benzoxazolethione	151	C7H5NOS	002382-96-9	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082015\
Data File : BF081132.D
Acq On : 20 Aug 2015 19:08
Operator : UM/IZ
Sample : G3345-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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TEC-2

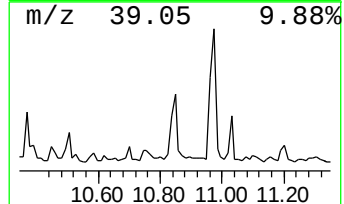
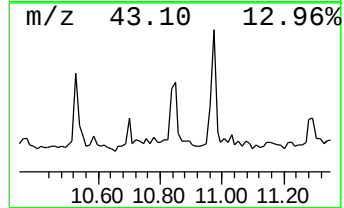
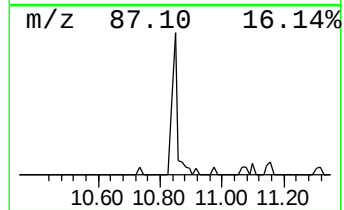
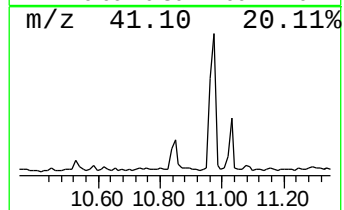
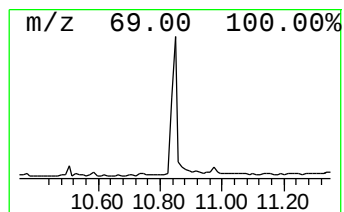
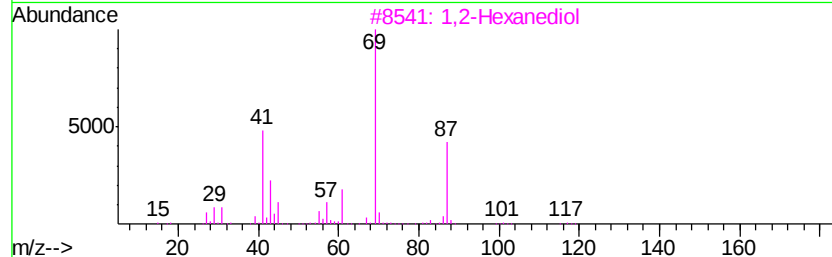
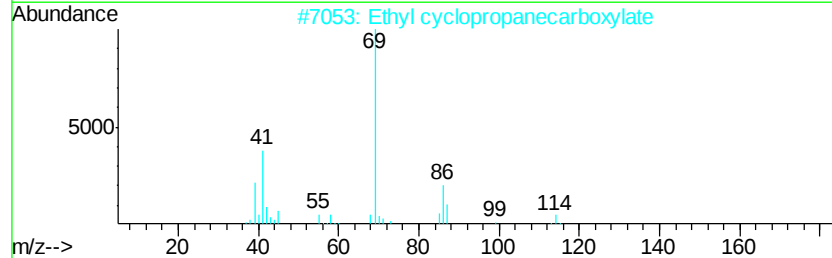
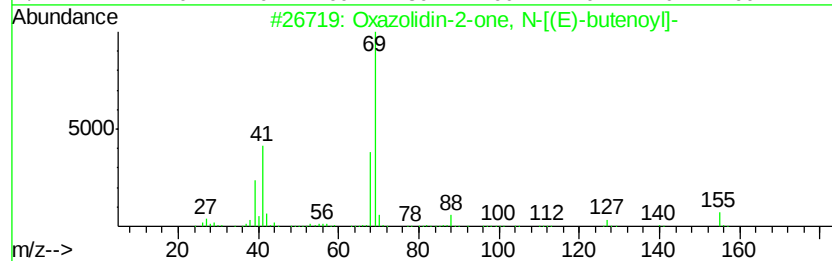
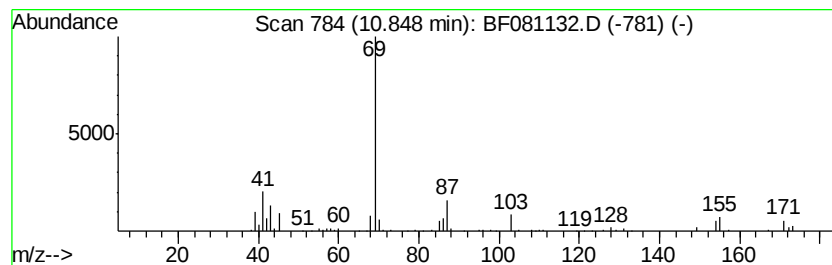
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Oxazolidin-2-one, N-[(E)-bu... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.85	3.71 ng	126382	Phenanthrene-d10	11.08

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxazolidin-2-one, N-[(E)-butenoyl]-	155	C7H9NO3	1000156-45-5	52
2			Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	45
3			1,2-Hexanediol	118	C6H14O2	006920-22-5	42
4			Cyclopropanecarboxylic acid, isop...	128	C7H12O2	006887-83-8	36
5			2-Decene, 2-methyl-	154	C11H22	023381-92-2	33



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082015\
Data File : BF081132.D
Acq On : 20 Aug 2015 19:08
Operator : UM/IZ
Sample : G3345-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-2

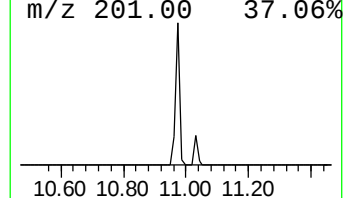
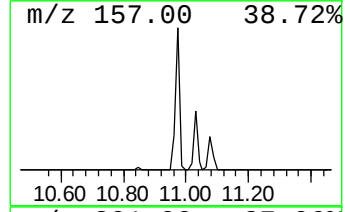
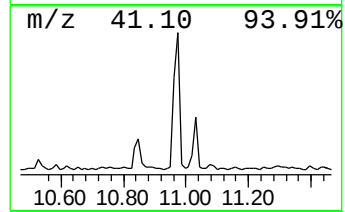
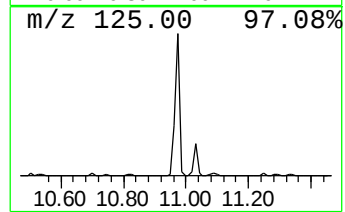
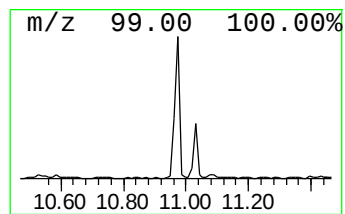
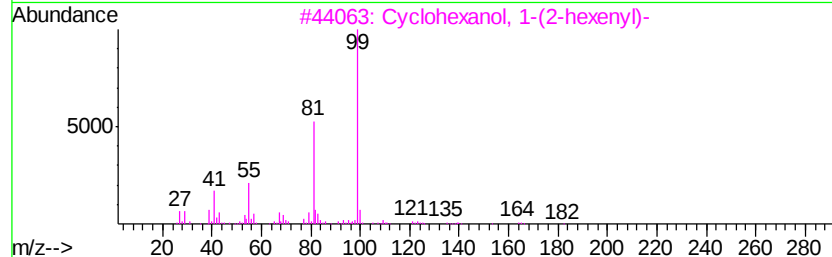
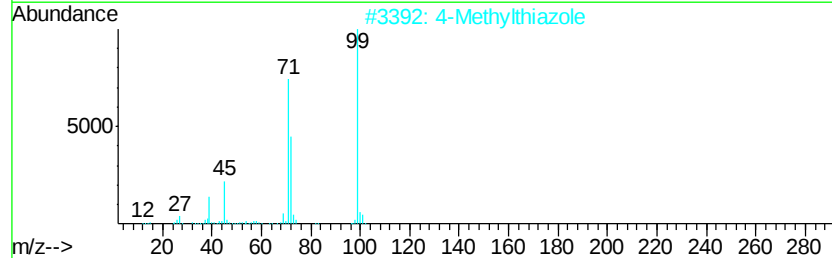
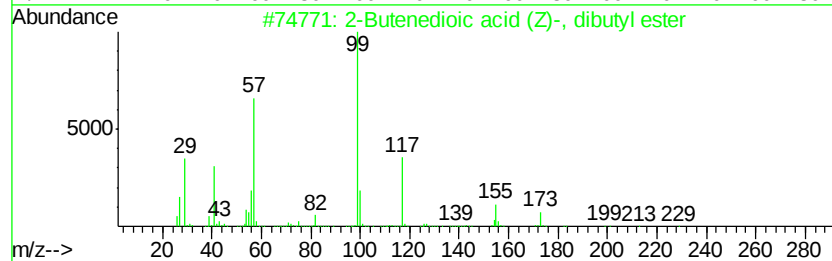
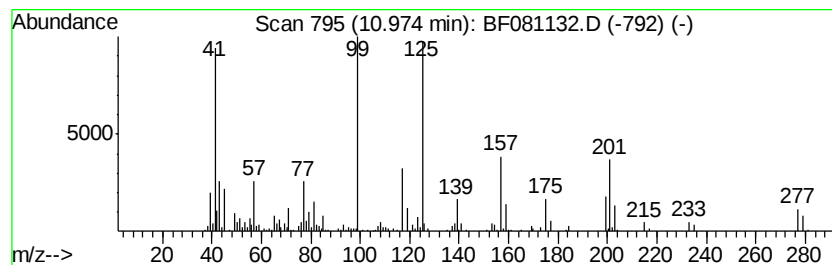
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown10.97 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.97	11.68 ng	398090	Phenanthrene-d10	11.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Butenedioic acid (Z)-, dibutyl...	228	C12H20O4	000105-76-0	22
2		4-Methylthiazole	99	C4H5NS	000693-95-8	18
3		Cyclohexanol, 1-(2-hexenyl)-	182	C12H22O	054655-47-9	14
4		Isopropylphosphonic acid, dihept...	320	C17H37O3P	1000273-18-5	14
5		2,4,6-Pyrimidinetriamine	125	C4H7N5	001004-38-2	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082015\
Data File : BF081132.D
Acq On : 20 Aug 2015 19:08
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Misc :
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Instrument :
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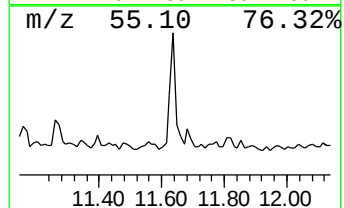
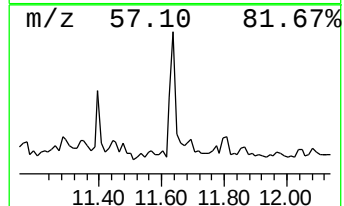
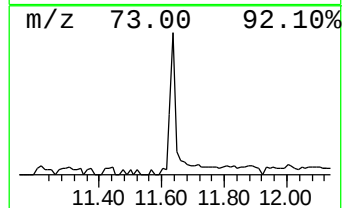
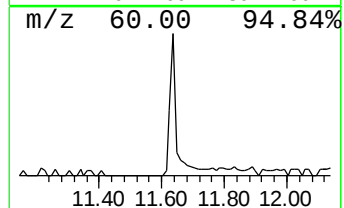
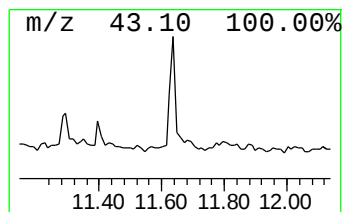
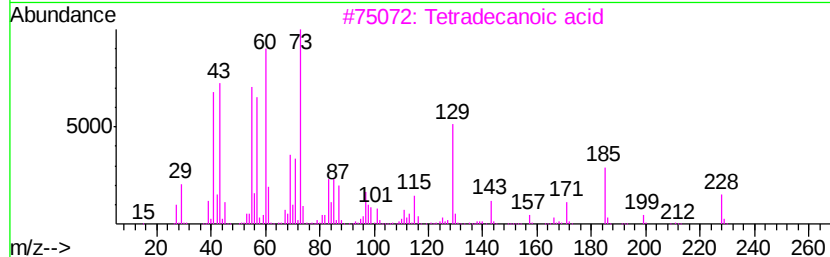
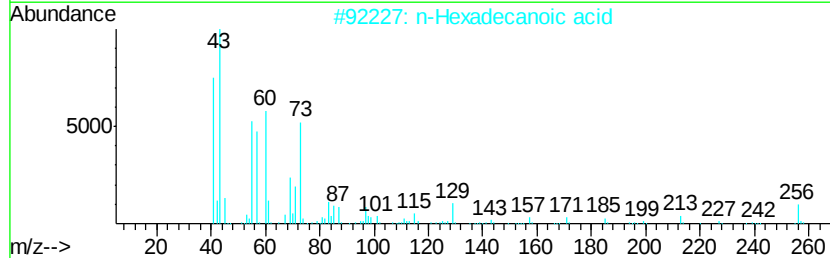
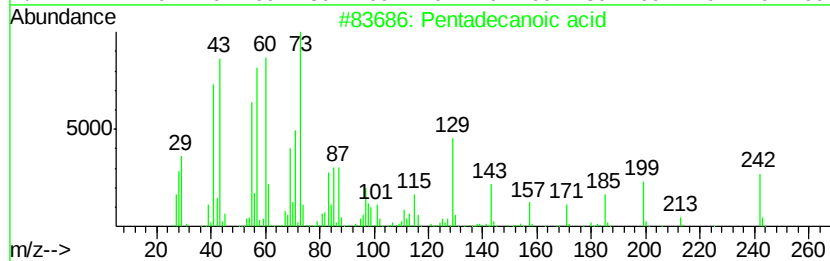
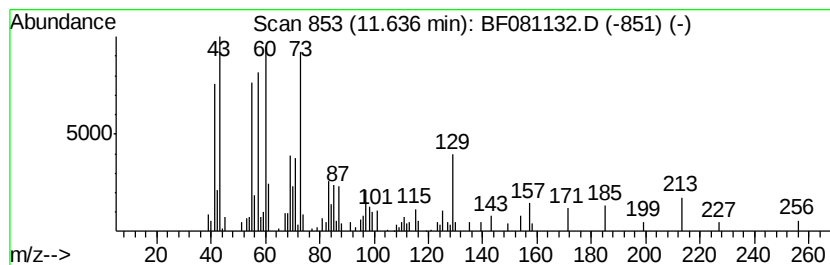
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Pentadecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.64	3.60 ng	122566	Phenanthrene-d10	11.08

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	72
5			Undecanoic acid	186	C11H22O2	000112-37-8	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082015\
Data File : BF081132.D
Acq On : 20 Aug 2015 19:08
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Sample : G3345-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TEC-2

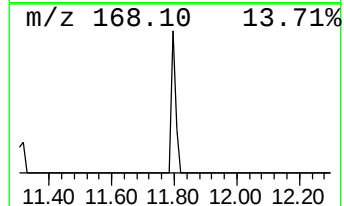
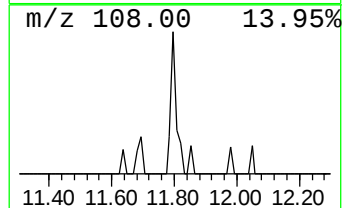
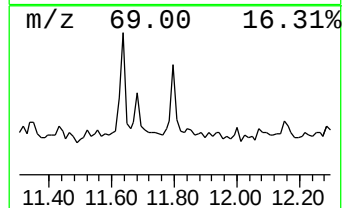
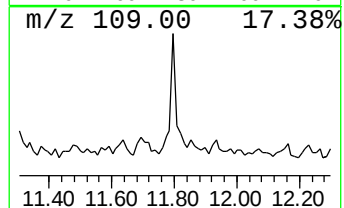
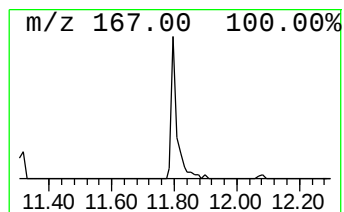
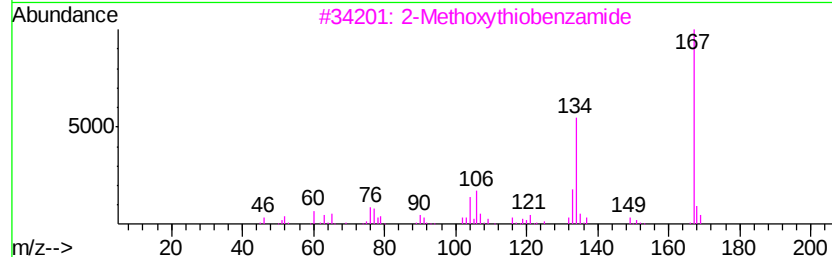
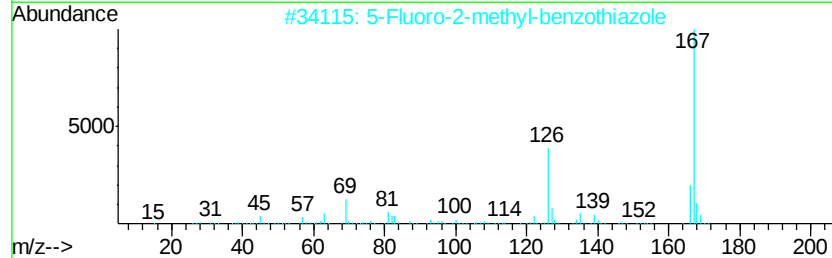
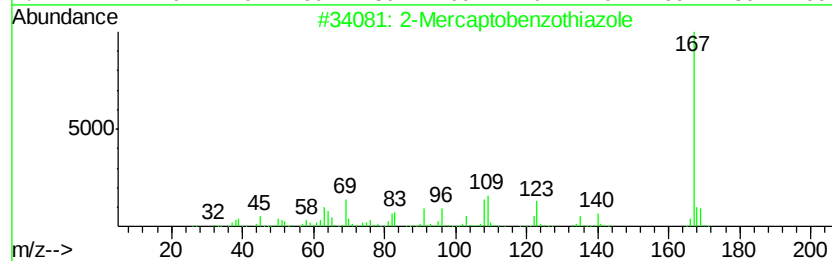
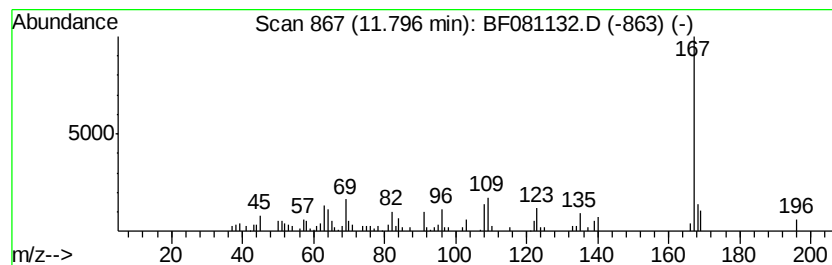
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 2-Mercaptobenzothiazole Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.80	2.76 ng	94042	Phenanthrene-d10	11.08

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	97
2			5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	52
3			2-Methoxythiobenzamide	167	C8H9NOS	042590-97-6	50
4			Thiazolo[3,2-a]pyridinium, 2,3-d...	167	C8H9NOS	023003-43-2	47
5			3-Amino-4-methoxybenzoic acid	167	C8H9NO3	002840-76-8	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082015\
Data File : BF081132.D
Acq On : 20 Aug 2015 19:08
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ClientSampleId :
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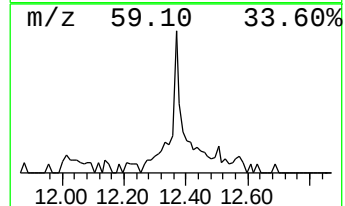
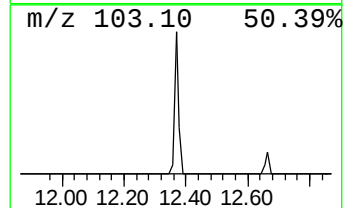
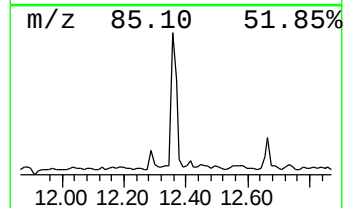
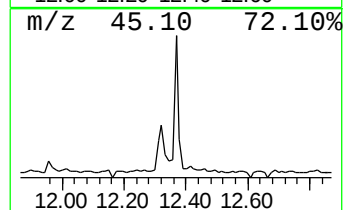
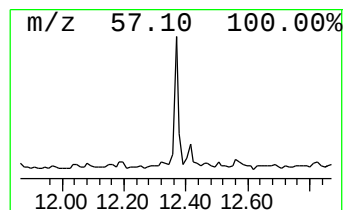
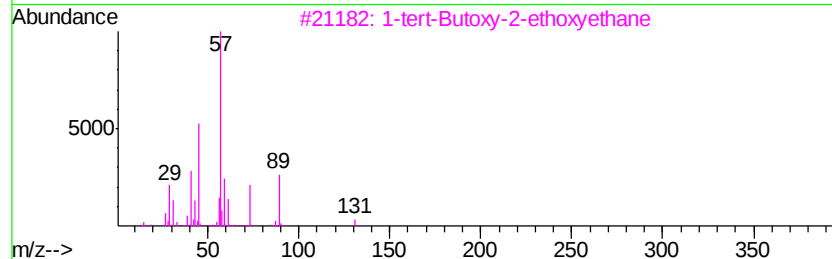
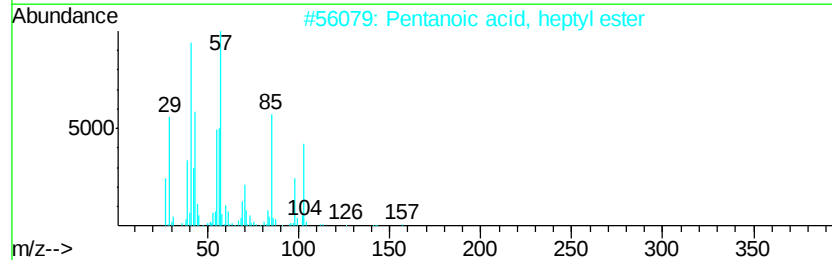
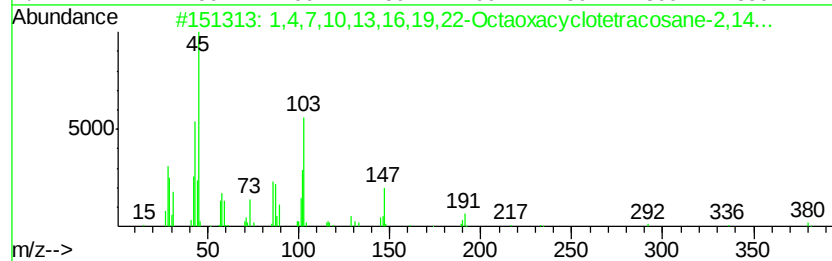
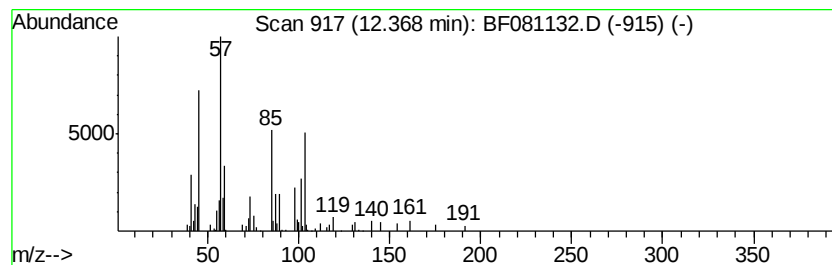
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 unknown12.37 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.37	2.68 ng	91279	Phenanthrene-d10	11.08

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4,7,10,13,16,19,22-Octaoxacycl...	380	C16H28O10	1000221-60-1	37		
2	Pentanoic acid, heptyl ester	200	C12H24O2	005451-80-9	37		
3	1-tert-Butoxy-2-ethoxyethane	146	C8H18O2	051422-54-9	35		
4	1-Butene-3-ethoxy	100	C6H12O	001476-08-0	35		
5	Dimethyl diglycolcarbonate	222	C8H14O7	087292-23-7	35		



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082015\
Data File : BF081132.D
Acq On : 20 Aug 2015 19:08
Operator : UM/IZ
Sample : G3345-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-2

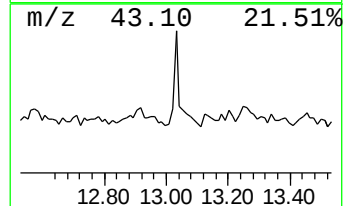
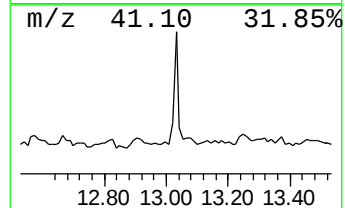
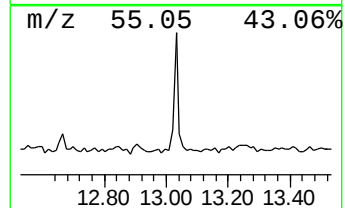
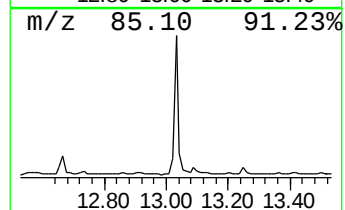
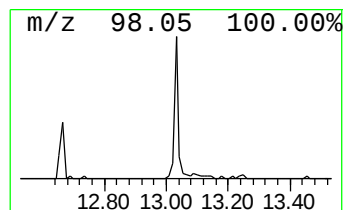
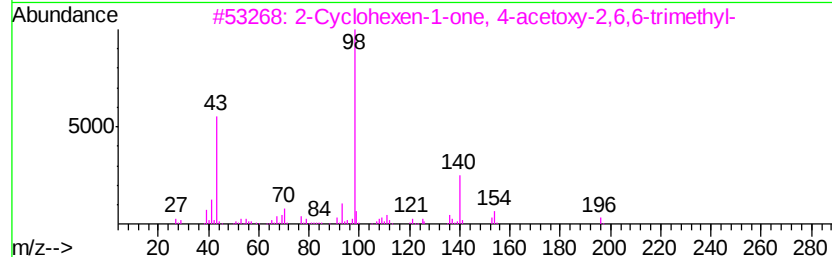
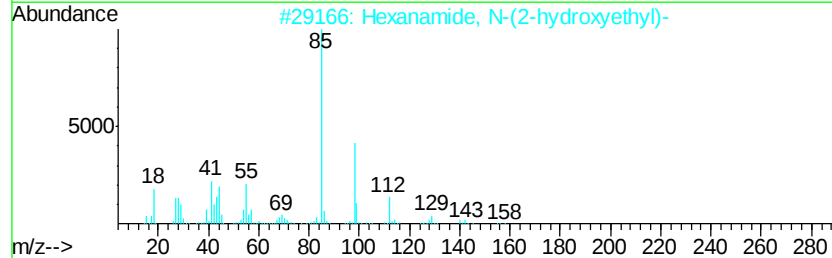
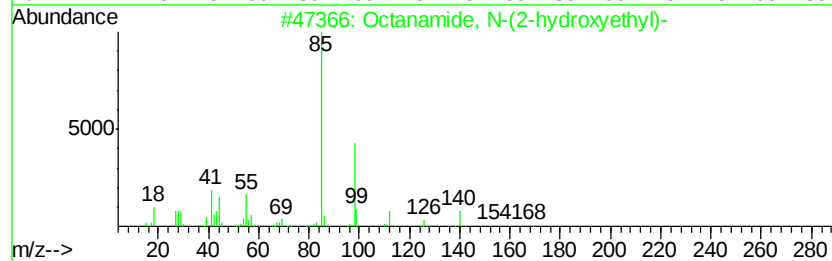
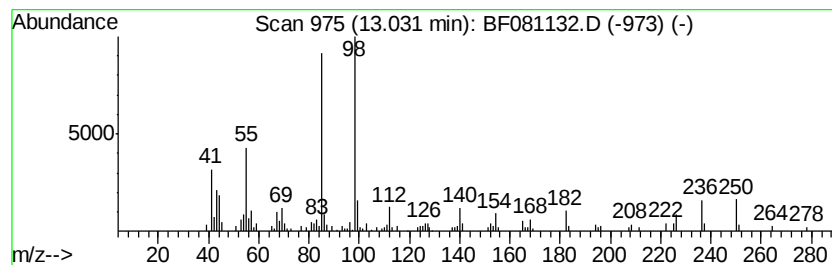
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown13.03 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.03	4.75 ng	117201	Chrysene-d12	13.69

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octanamide, N-(2-hydroxyethyl)-	187	C10H21NO2	007112-02-9	43
2			Hexanamide, N-(2-hydroxyethyl)-	159	C8H17NO2	007726-06-9	35
3			2-Cyclohexen-1-one, 4-acetoxy-2,...	196	C11H16O3	1000197-29-5	27
4			3-Acetyl-dihydro-tomatidine	459	C29H49NO3	1000256-70-2	27
5			5,6,22,16(0)-Tetrahydrosolasodine	417	C27H47NO2	1000256-07-0	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082015\
Data File : BF081132.D
Acq On : 20 Aug 2015 19:08
Operator : UM/IZ
Sample : G3345-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-2

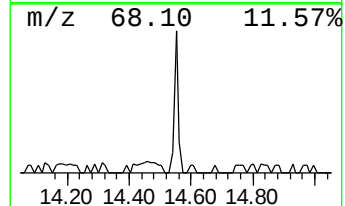
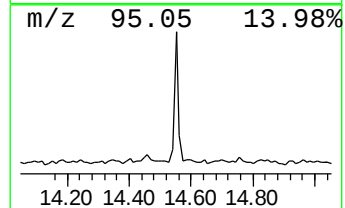
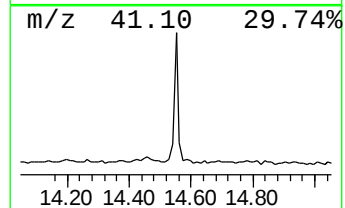
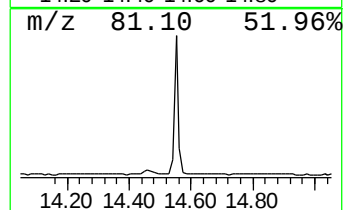
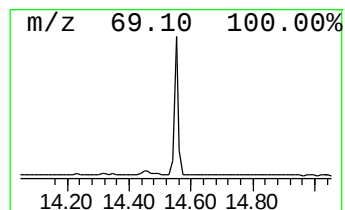
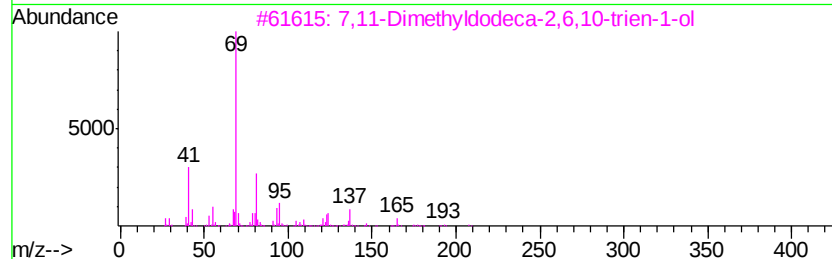
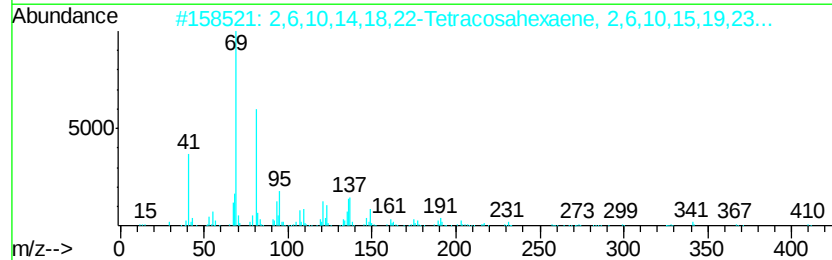
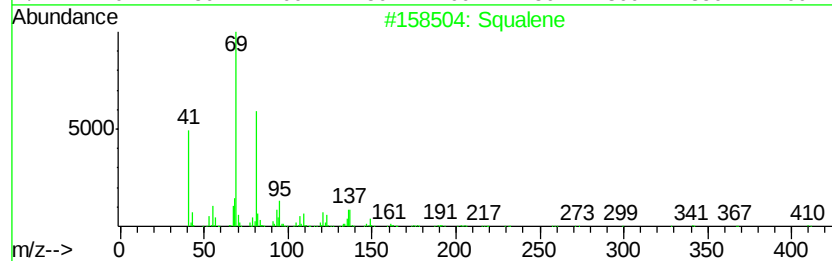
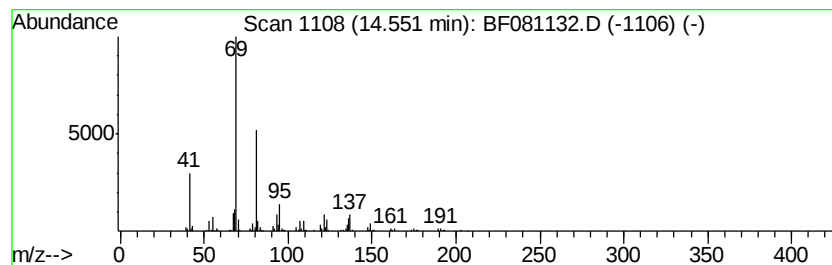
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.55	11.25 ng	172139	Perylene-d12	15.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	91
2		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	91
3		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	53
5		1,5-Heptadiene, 3,4-dimethyl-	124	C9H16	1000061-77-9	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082015\
 Data File : BF081132.D
 Acq On : 20 Aug 2015 19:08
 Operator : UM/IZ
 Sample : G3345-02
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TEC-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.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...	4.68	16.9	ng	392006	1	6.57	463356	20.0
unknown6.33	6.33	33.0	ng	763481	1	6.57	463356	20.0
1-Hexanol, 2-ethyl-	6.65	6.5	ng	150796	1	6.57	463356	20.0
4-Methyl-5H-furan...	6.77	2.7	ng	63553	1	6.57	463356	20.0
Hexanoic acid, 2-...	7.29	3.2	ng	99404	2	7.86	625740	20.0
Benzothiazole	8.14	5.4	ng	169509	2	7.86	625740	20.0
1-Phenoxypropan-2-ol	8.18	3.8	ng	120141	2	7.86	625740	20.0
unknown8.62	8.62	15.3	ng	478001	2	7.86	625740	20.0
Vanillin	9.09	11.9	ng	370506	3	9.60	620074	20.0
Ethanone, 1-(4-hy...	9.54	4.0	ng	122481	3	9.60	620074	20.0
Tributyl phosphate	10.26	3.3	ng	101217	3	9.60	620074	20.0
2(3H)-Benzothiazo...	10.50	3.1	ng	106491	4	11.08	681487	20.0
Oxazolidin-2-one,...	10.85	3.7	ng	126382	4	11.08	681487	20.0
unknown10.97	10.97	11.7	ng	398090	4	11.08	681487	20.0
Pentadecanoic acid	11.64	3.6	ng	122566	4	11.08	681487	20.0
2-Mercaptobenzoth...	11.80	2.8	ng	94042	4	11.08	681487	20.0
unknown12.37	12.37	2.7	ng	91279	4	11.08	681487	20.0
unknown13.03	13.03	4.8	ng	117201	5	13.69	493437	20.0
Squalene	14.55	11.3	ng	172139	6	15.03	305973	20.0