

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010816\
 Data File : BF084348.D
 Acq On : 9 Jan 2016 2:21
 Operator : SJ/UM
 Sample : H1036-03
 Misc :
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-DRUM3

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

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

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.059	258	260	266	rVB	1466951	2145581	27.47%	3.019%
2	5.219	266	274	279	rVB	55695	158012	2.02%	0.222%
3	5.481	294	297	300	rBV	5869600	6015435	77.01%	8.463%
4	5.813	324	326	329	rBV	214427	337855	4.33%	0.475%
5	6.510	384	387	389	rBV	5913564	6439254	82.44%	9.059%
6	6.636	395	398	400	rBV	6249222	7437342	95.22%	10.463%
7	6.693	400	403	408	rVB	173412	269098	3.45%	0.379%
8	6.853	415	417	419	rBV	1934684	1540044	19.72%	2.167%
9	6.922	421	423	427	rBV	212633	398072	5.10%	0.560%
10	7.013	429	431	433	rVB	6442352	5724089	73.28%	8.053%
11	7.253	451	452	457	rVB3	59340	102710	1.31%	0.144%
12	7.424	463	467	469	rBV	4952238	5384801	68.94%	7.576%
13	7.893	504	508	511	rBV2	218932	444470	5.69%	0.625%
14	8.145	527	530	533	rVB	1553810	2464618	31.55%	3.467%
15	8.419	550	554	556	rVB2	112816	147938	1.89%	0.208%
16	8.659	571	575	580	rBV	124569	348060	4.46%	0.490%
17	8.785	582	586	590	rVB2	45128	100405	1.29%	0.141%
18	8.853	590	592	595	rBV	116888	112620	1.44%	0.158%
19	9.105	612	614	621	rVB	283755	334619	4.28%	0.471%
20	9.219	621	624	626	rBV	7909459	7810833	100.00%	10.989%
21	9.356	634	636	639	rBV	1213756	1146231	14.67%	1.613%
22	9.813	674	676	680	rVB	135263	154346	1.98%	0.217%
23	9.893	680	683	685	rBV	2515925	2310226	29.58%	3.250%
24	10.110	698	702	704	rBV2	140328	225272	2.88%	0.317%
25	10.316	715	720	723	rBV2	85668	187136	2.40%	0.263%
26	10.408	724	728	729	rBV	102204	114824	1.47%	0.162%
27	10.648	747	749	750	rBV	107342	111193	1.42%	0.156%
28	10.682	750	752	755	rVV2	4211648	5298518	67.84%	7.454%
29	10.796	759	762	767	rVB3	77775	156014	2.00%	0.219%
30	10.979	776	778	780	rBV	103301	125041	1.60%	0.176%
31	11.379	810	813	814	rBV	2650908	2334325	29.89%	3.284%
32	11.448	816	819	820	rBV2	73599	106775	1.37%	0.150%
33	12.796	934	937	938	rBV	83529	117459	1.50%	0.165%
34	12.968	949	952	955	rBV	7107626	7680571	98.33%	10.806%

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Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.871	1028	1031	1034	rBV	106210	144339	1.85%	0.203%
36	14.008	1041	1043	1046	rBV	1580673	1852992	23.72%	2.607%
37	15.437	1165	1168	1171	rBV	1016747	1298811	16.63%	1.827%

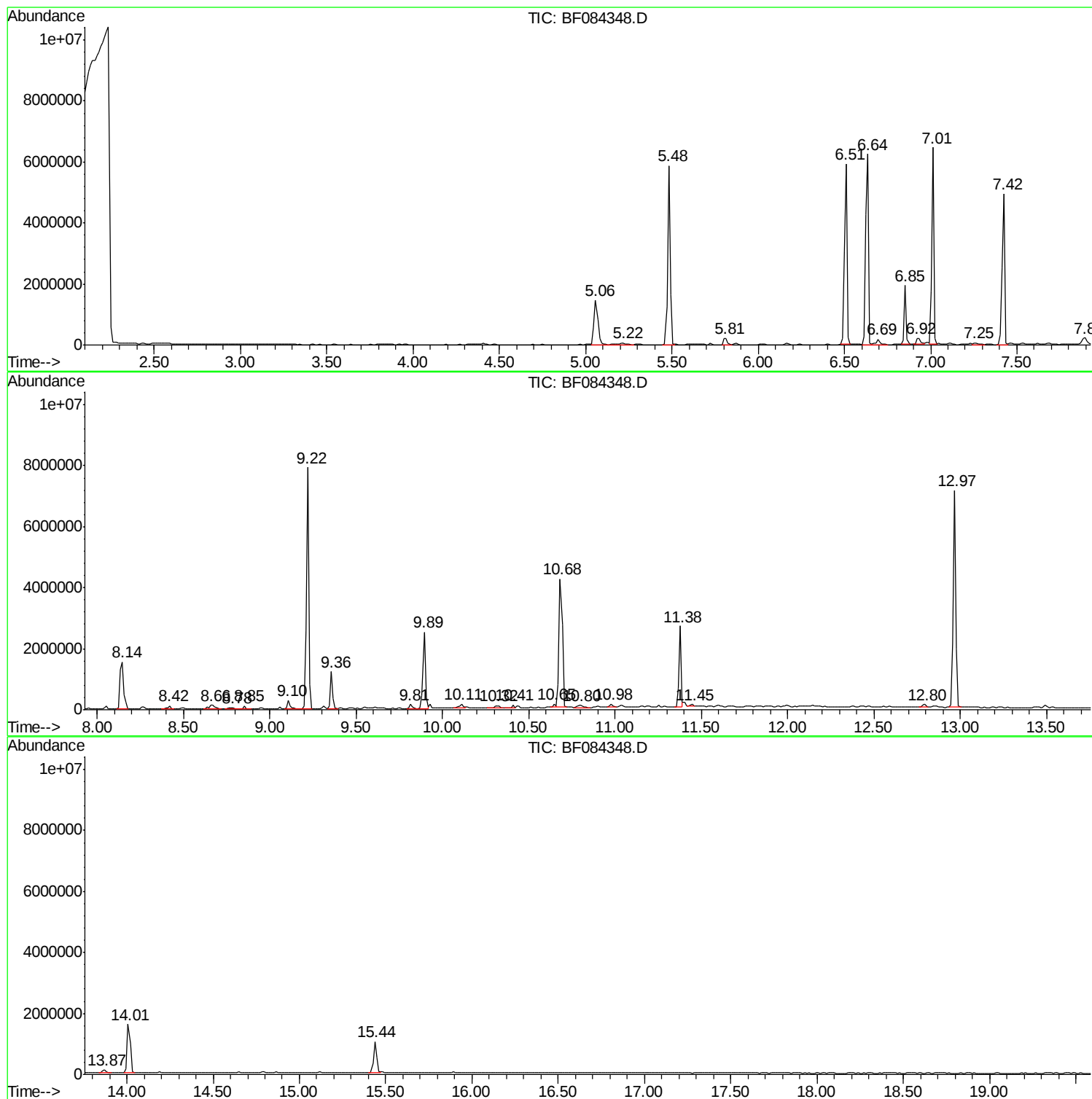
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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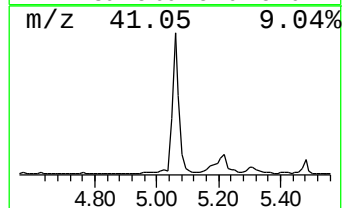
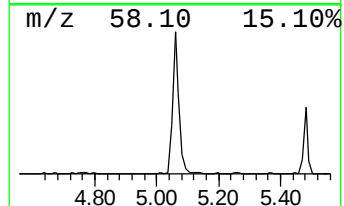
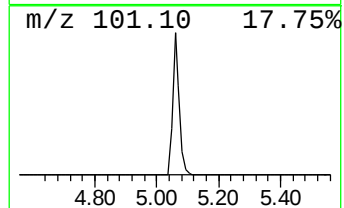
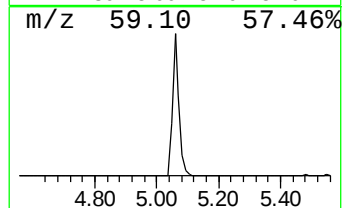
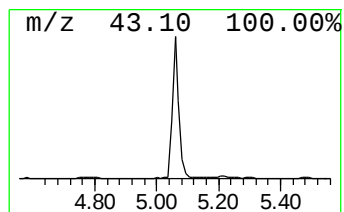
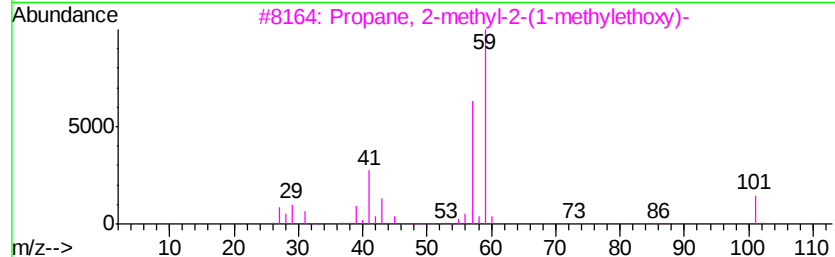
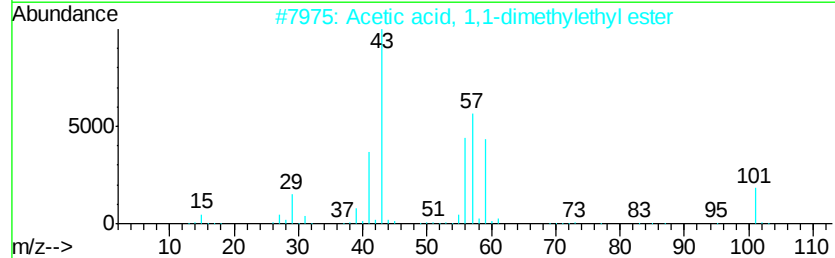
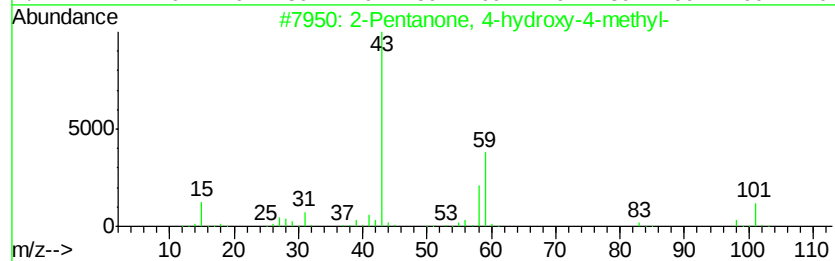
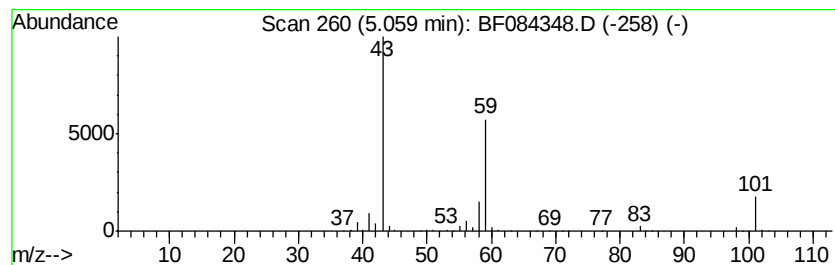
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	27.86 ng	2145580	1,4-Dichlorobenzene-d4	6.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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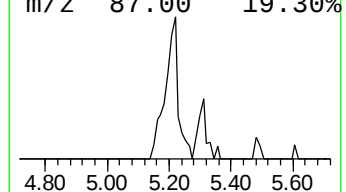
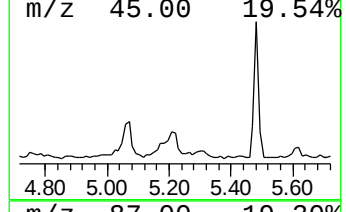
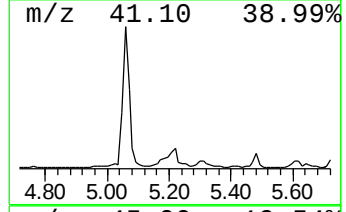
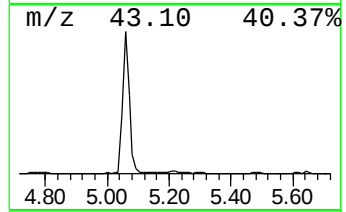
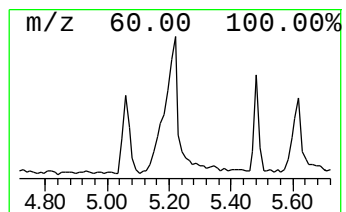
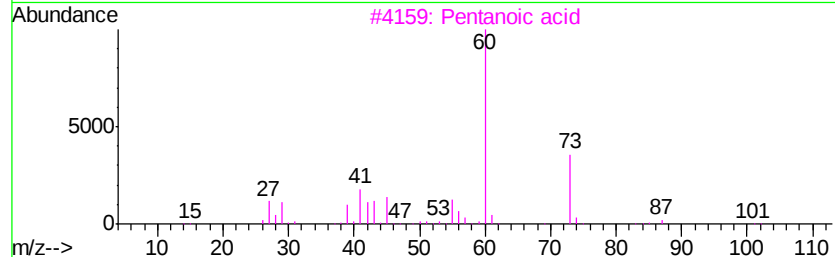
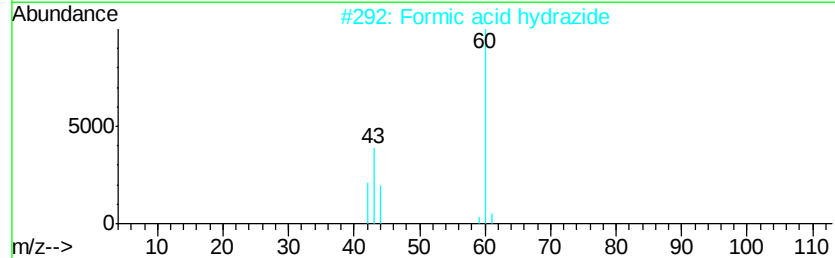
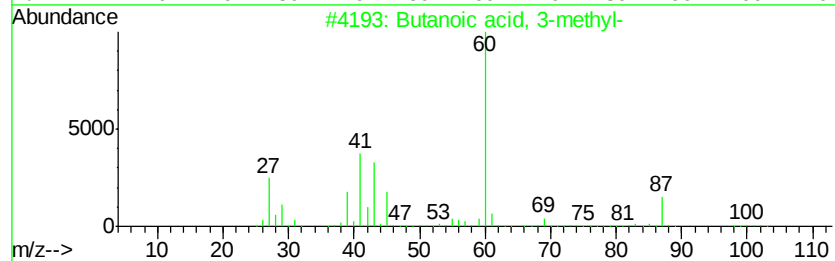
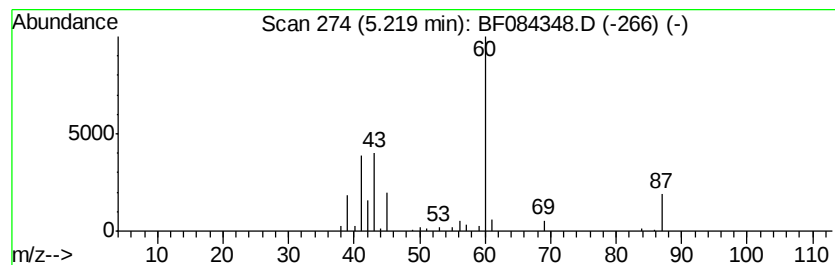
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butanoic acid, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	2.05 ng	158012	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	64
2		Formic acid hydrazide	60	CH4N2O	000624-84-0	47
3		Pentanoic acid	102	C5H10O2	000109-52-4	45
4		1-Pentanamine	87	C5H13N	000110-58-7	9
5		1,5-Pentanediol	104	C5H12O2	000111-29-5	9



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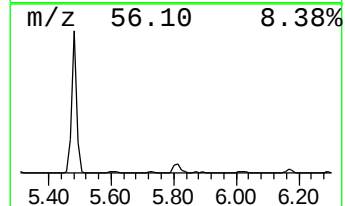
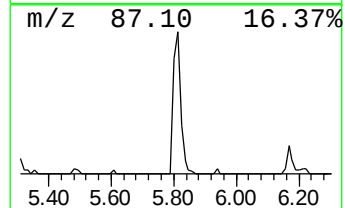
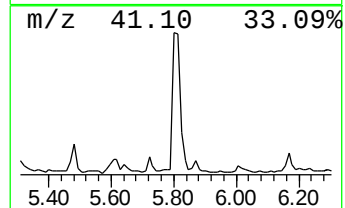
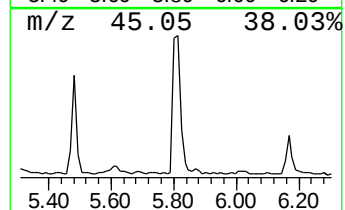
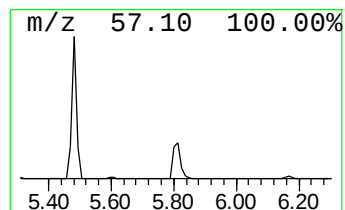
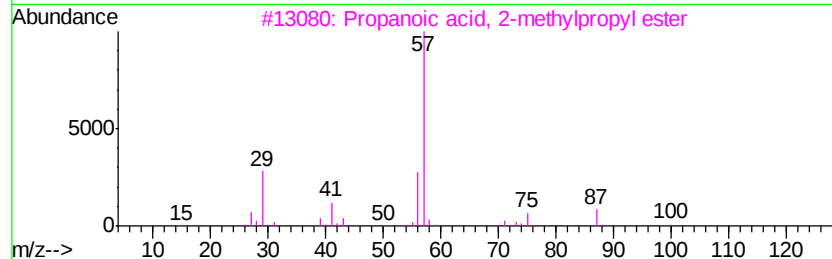
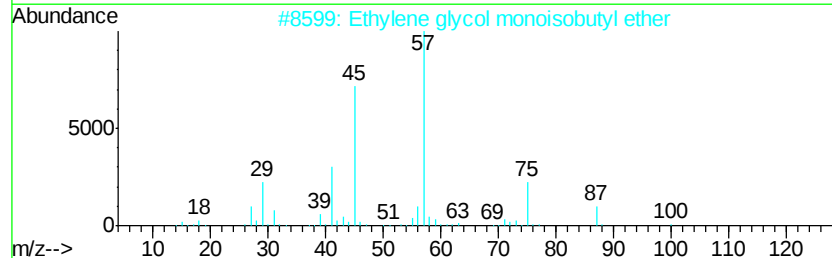
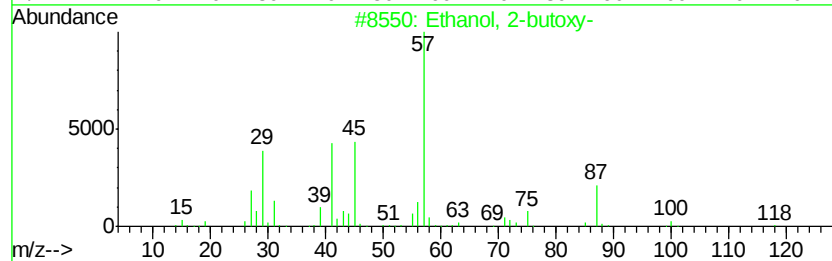
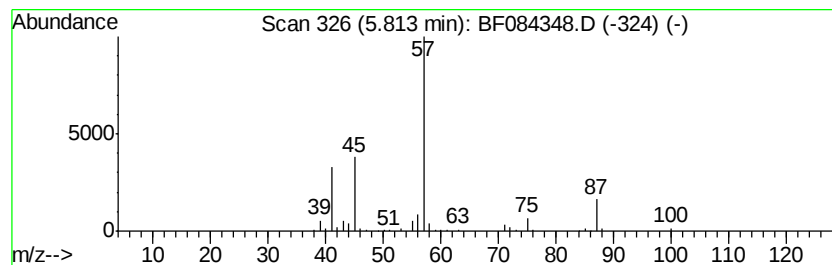
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-butoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.81	4.39 ng	337855	1,4-Dichlorobenzene-d4	6.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	78
2		Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	45
3		Propanoic acid, 2-methylpropyl e...	130	C7H14O2	000540-42-1	38
4		3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	37
5		Isobutyl ether	130	C8H18O	000628-55-7	25



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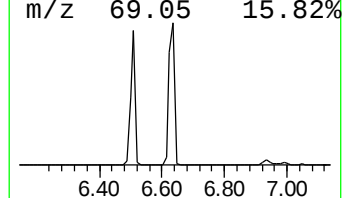
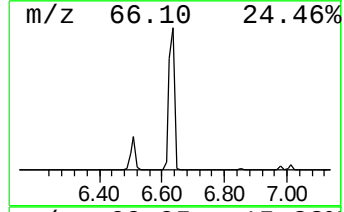
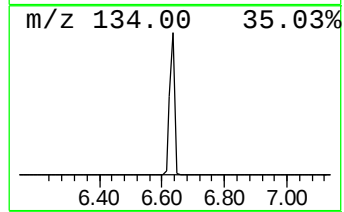
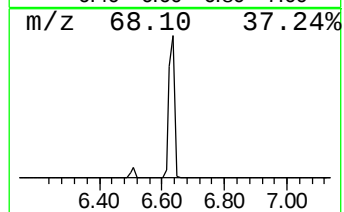
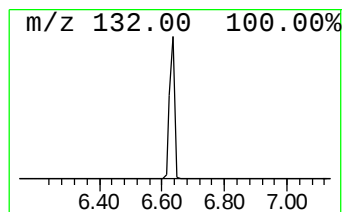
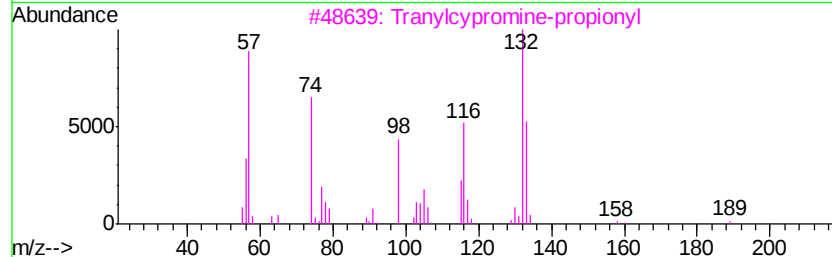
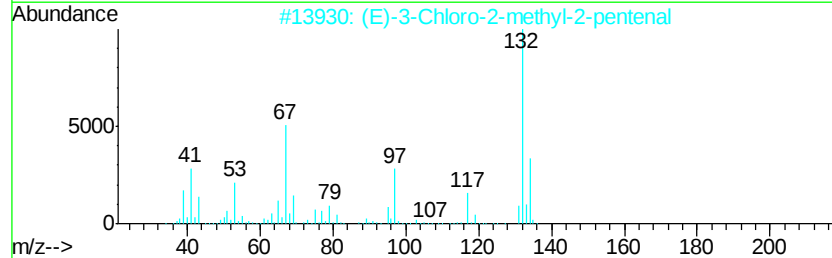
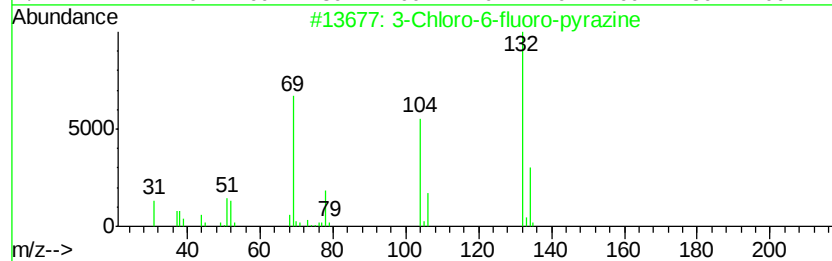
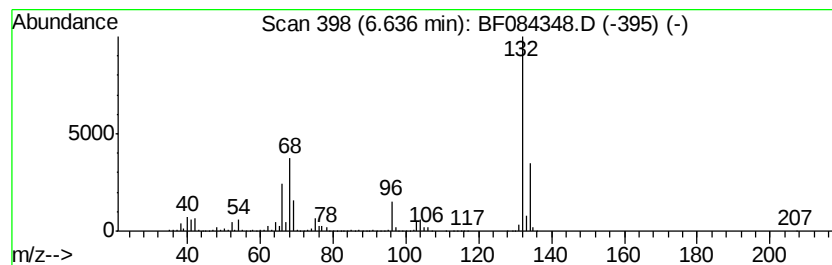
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	96.59 ng	7437340	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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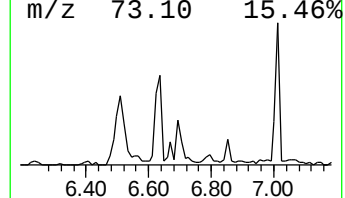
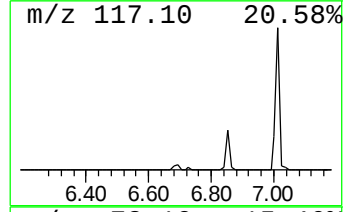
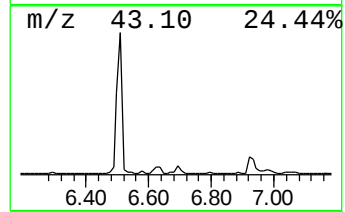
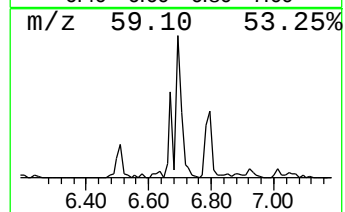
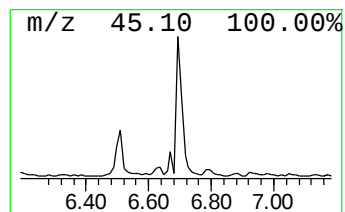
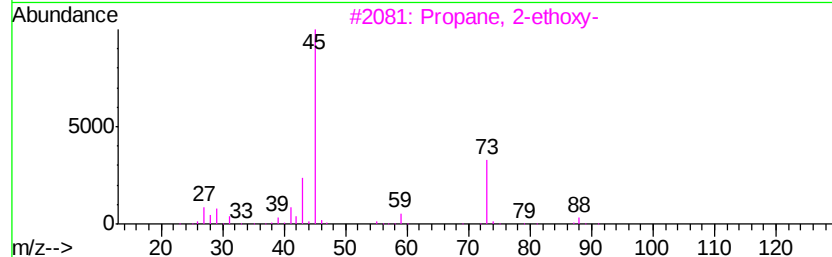
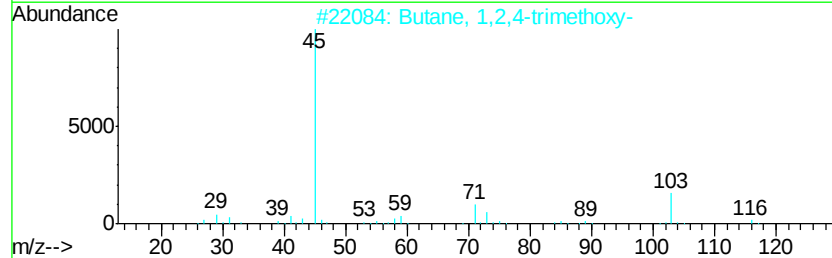
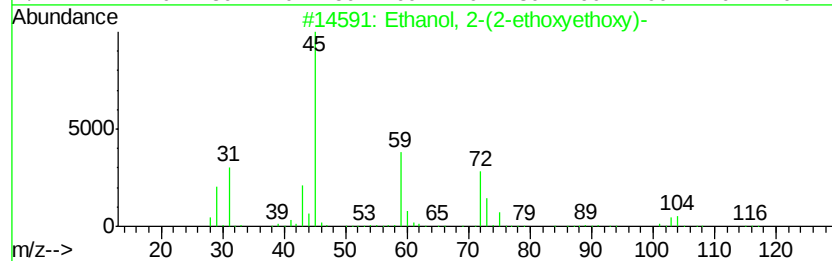
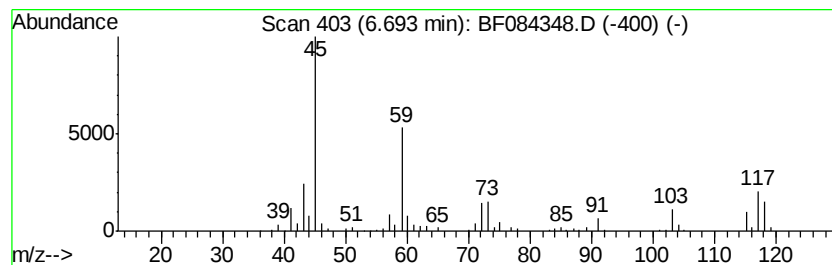
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	3.49 ng	269098	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	50
2		Butane, 1,2,4-trimethoxy-	148	C7H16O3	020637-48-3	43
3		Propane, 2-ethoxy-	88	C5H12O	000625-54-7	38
4		Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	37
5		Propane, 1-(1-ethoxyethoxy)-	132	C7H16O2	020680-10-8	37



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010816\
Data File : BF084348.D
Acq On : 9 Jan 2016 2:21
Operator : SJ/UM
Sample : H1036-03
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-DRUM3

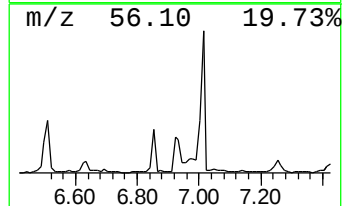
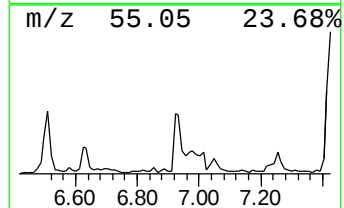
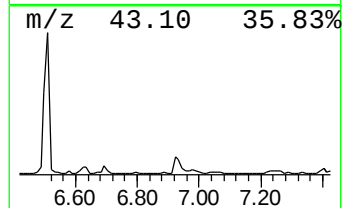
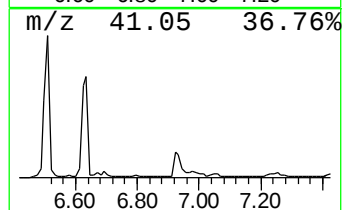
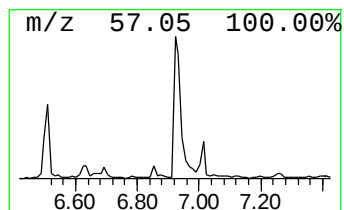
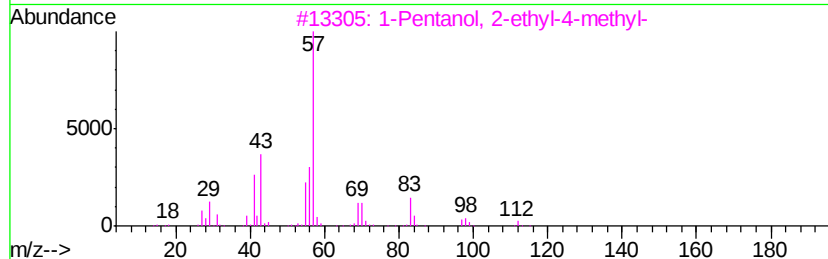
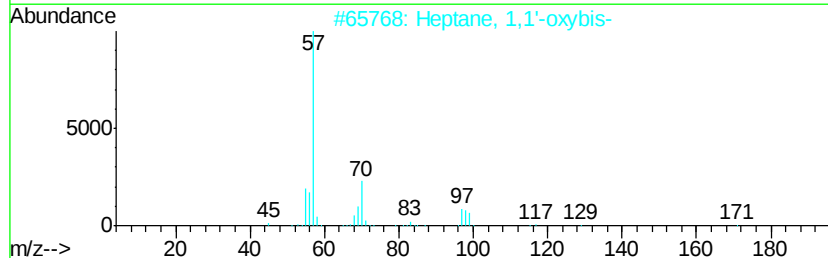
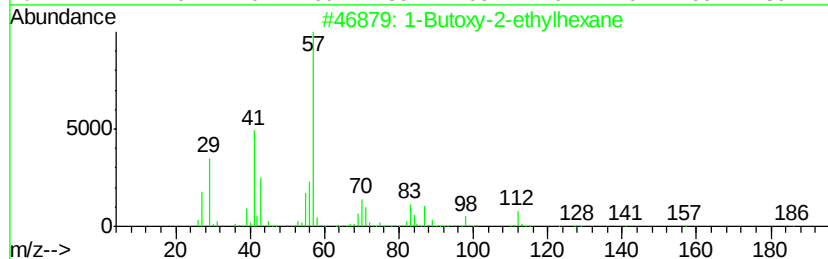
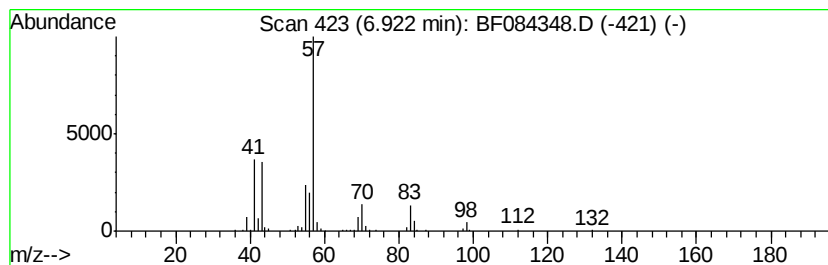
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Butoxy-2-ethylhexane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.92	5.17 ng	398072	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Butoxy-2-ethylhexane	186	C12H26O	062625-25-6	78
2		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	59
3		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
4		1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
5		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	53



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Data File : BF084348.D
Acq On : 9 Jan 2016 2:21
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Sample : H1036-03
Misc :
ALS Vial : 38 Sample Multiplier: 1

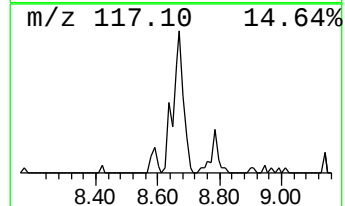
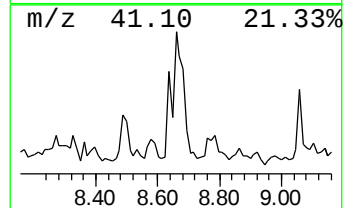
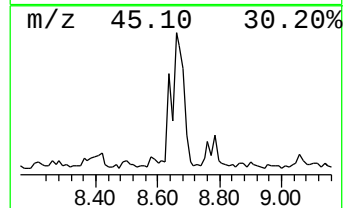
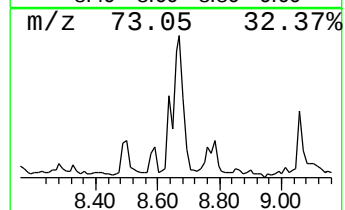
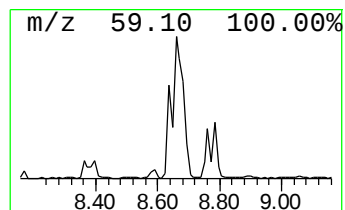
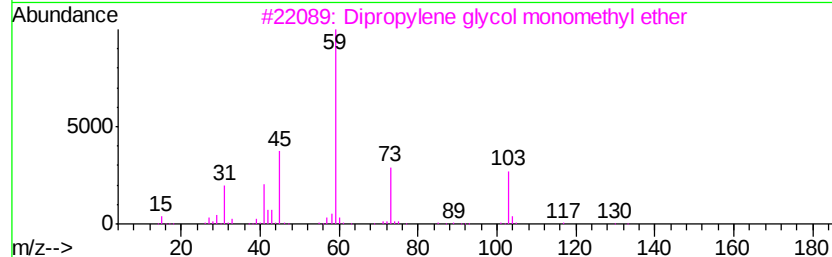
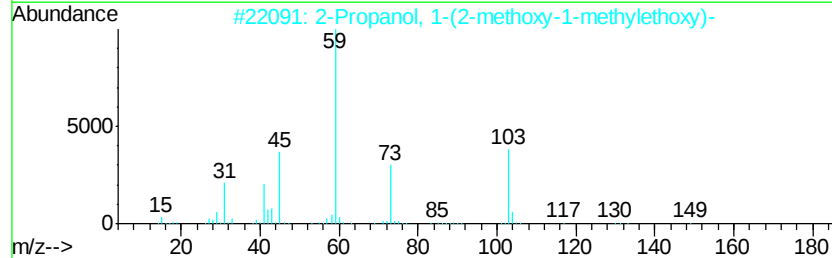
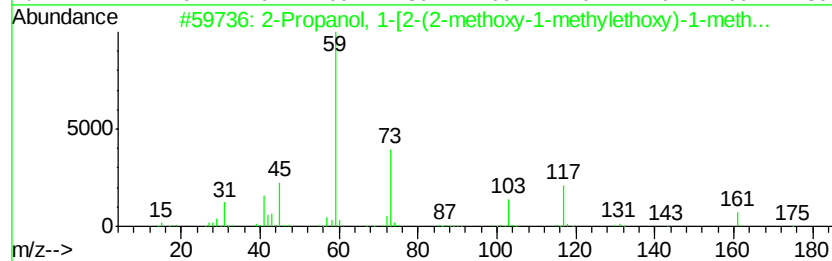
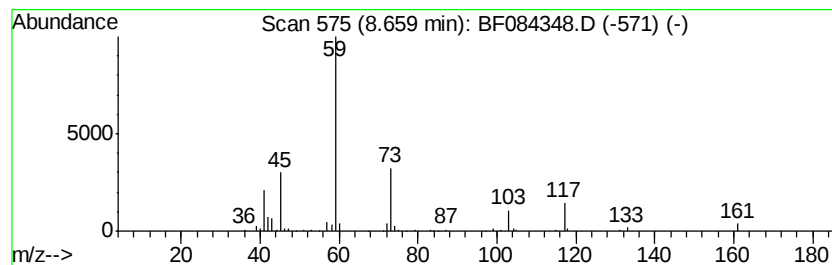
Instrument :
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ClientSampleId :
WC-DRUM3

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

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

Peak Number 8 2-Propanol, 1-[2-(2-methoxy... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.66	2.82 ng	348060	Naphthalene-d8	8.14
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-Propanol, 1-[2-(2-methoxy-1-me...	206 C10H22O4	020324-33-8	78
2	2-Propanol, 1-(2-methoxy-1-methy...	148 C7H16O3	020324-32-7	64
3	Dipropylene glycol monomethyl ether	148 C7H16O3	034590-94-8	56
4	Tri(1,2-propyleneglycol), monome...	206 C10H22O4	1000262-26-6	56
5	Propane, 1,2-dimethoxy-	104 C5H12O2	007778-85-0	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010816\
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Acq On : 9 Jan 2016 2:21
Operator : SJ/UM
Sample : H1036-03
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-DRUM3

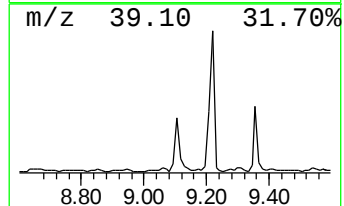
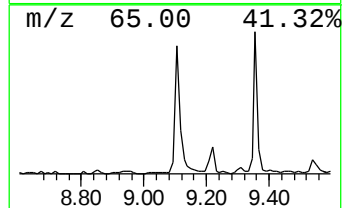
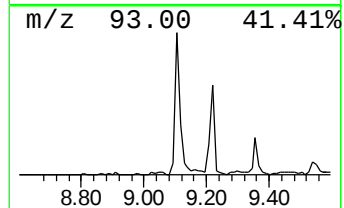
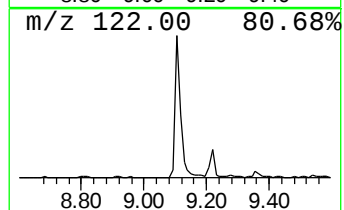
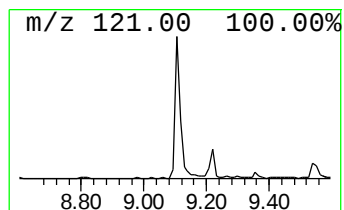
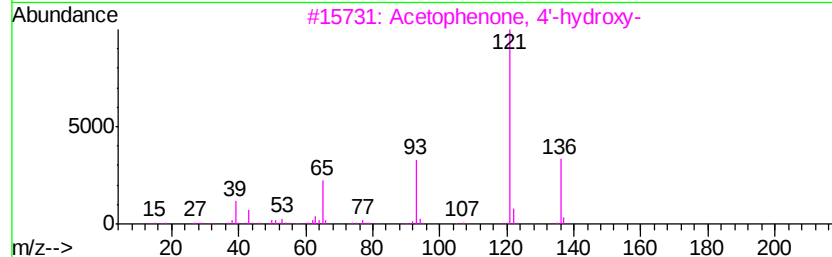
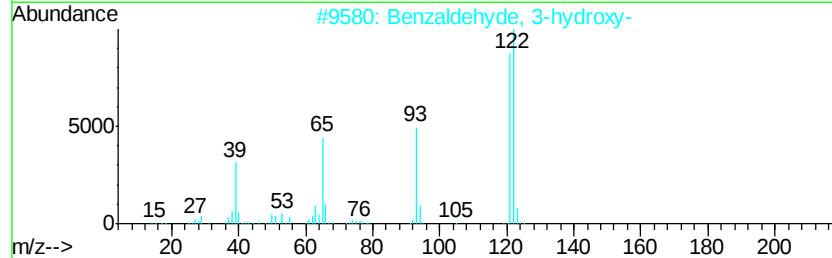
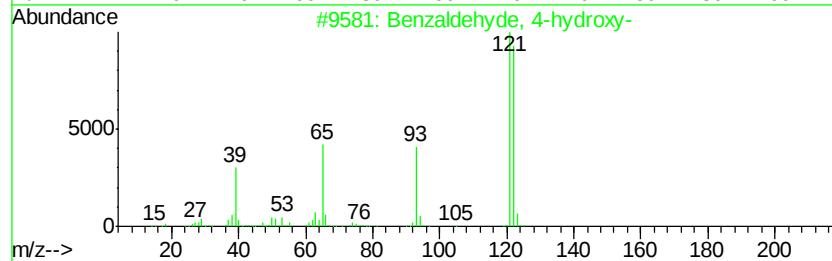
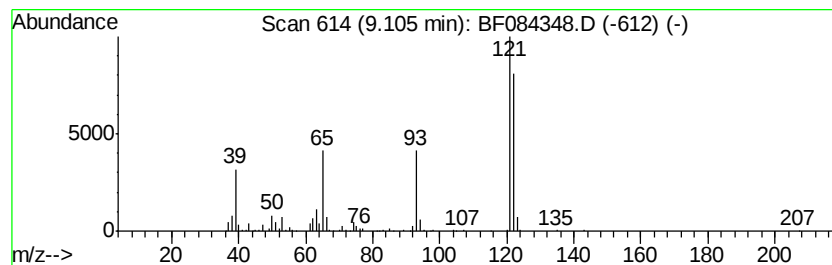
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzaldehyde, 4-hydroxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.10	2.90 ng	334619	Acenaphthene-d10	9.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzaldehyde, 4-hydroxy-	122	C7H6O2	000123-08-0	96
2		Benzaldehyde, 3-hydroxy-	122	C7H6O2	000100-83-4	81
3		Acetophenone, 4'-hydroxy-	136	C8H8O2	000099-93-4	59
4		3(2H)-Benzofuranone, 2-[(4-hydro...	268	C16H12O4	077764-93-3	52
5		3-Hydroxybenzoyl 2-nitrobenzylid...	285	C14H11N3O4	299929-40-1	45



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Misc :
ALS Vial : 38 Sample Multiplier: 1

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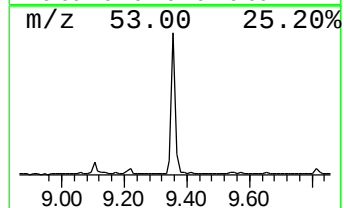
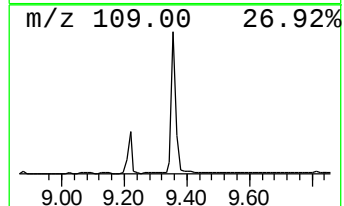
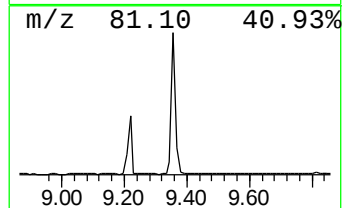
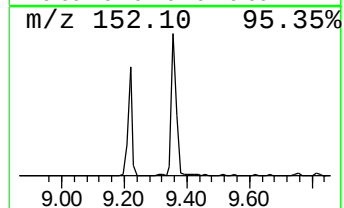
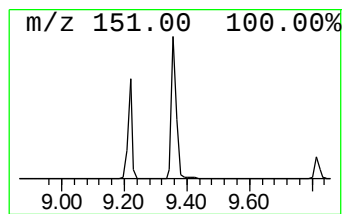
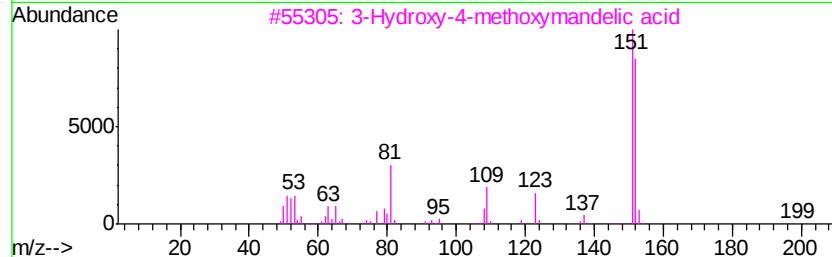
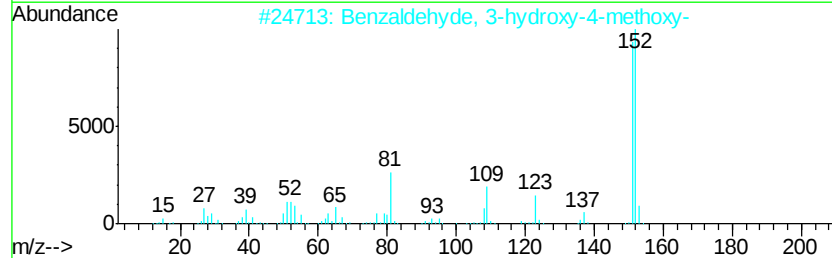
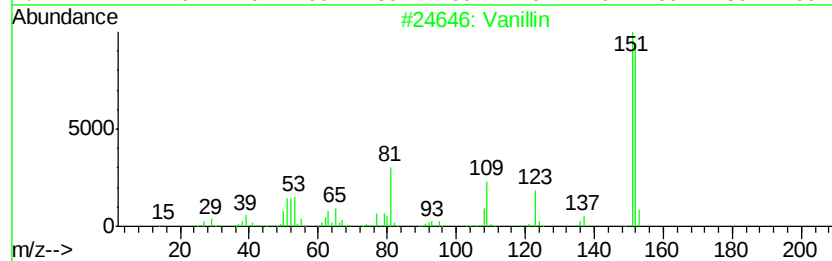
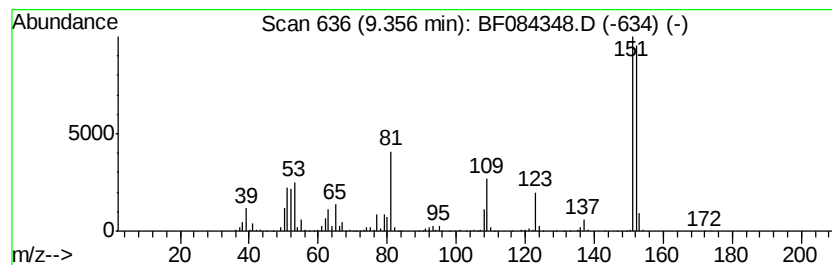
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Vanillin Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.36	9.92 ng	1146230	Acenaphthene-d10	9.89

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-methoxybenzaldehyde	152	C8H8O3	018278-34-7	64
5		Benzaldehyde, 3-(chloroacetoxy)-...	228	C10H9ClO4	066267-38-7	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010816\
 Data File : BF084348.D
 Acq On : 9 Jan 2016 2:21
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 Sample : H1036-03
 Misc :
 ALS Vial : 38 Sample Multiplier: 1

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

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.06	27.9	ng	2145580	1	6.85	1540040	20.0
Butanoic acid, 3-...	5.22	2.0	ng	158012	1	6.85	1540040	20.0
Ethanol, 2-butoxy-	5.81	4.4	ng	337855	1	6.85	1540040	20.0
unknown6.64	6.64	96.6	ng	7437340	1	6.85	1540040	20.0
Ethanol, 2-(2-eth...	6.69	3.5	ng	269098	1	6.85	1540040	20.0
1-Butoxy-2-ethylh...	6.92	5.2	ng	398072	1	6.85	1540040	20.0
2-Propanol, 1-[2-...	8.66	2.8	ng	348060	2	8.14	2464620	20.0
Benzaldehyde, 4-h...	9.10	2.9	ng	334619	3	9.89	2310230	20.0
Vanillin	9.36	9.9	ng	1146230	3	9.89	2310230	20.0