

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010615\
 Data File : BF076762.D
 Acq On : 6 Jan 2015 16:54
 Operator : IZ / TP
 Sample : G1011-03
 Misc : W
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW3

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-BF121714.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	1.133	3	4	9	rVB2	11732	19898	1.21%	0.167%
2	1.498	35	36	44	rBV	38819	79753	4.86%	0.669%
3	2.001	77	80	84	rVB2	8938	16755	1.02%	0.141%
4	2.116	84	90	93	rBV	16440	29557	1.80%	0.248%
5	2.630	130	135	139	rBV2	8346	16987	1.03%	0.142%
6	4.219	272	274	281	rBV	160366	283490	17.26%	2.377%
7	4.893	331	333	338	rBV	370777	559446	34.06%	4.692%
8	6.139	441	442	446	rVB	22770	30657	1.87%	0.257%
9	6.207	446	448	451	rBV	63602	63332	3.86%	0.531%
10	6.322	455	458	464	rBV2	350220	376265	22.91%	3.155%
11	6.413	464	466	469	rBV	875064	1028409	62.61%	8.625%
12	6.710	489	492	494	rBV	247526	241919	14.73%	2.029%
13	6.779	494	498	500	rVV2	61387	73418	4.47%	0.616%
14	6.893	506	508	510	rBV	1011497	942845	57.40%	7.907%
15	7.042	519	521	523	rBV2	26853	33446	2.04%	0.280%
16	7.076	523	524	527	rVV	41865	54123	3.29%	0.454%
17	7.145	527	530	532	rVV2	110241	145121	8.83%	1.217%
18	7.225	535	537	539	rVB	33874	33827	2.06%	0.284%
19	7.419	549	554	557	rBV2	857154	908529	55.31%	7.619%
20	7.476	557	559	564	rVV2	14037	24051	1.46%	0.202%
21	7.545	564	565	567	rVV2	11958	17614	1.07%	0.148%
22	7.579	567	568	570	rVB	36147	30626	1.86%	0.257%
23	7.693	575	578	579	rVV	85503	77153	4.70%	0.647%
24	7.728	579	581	583	rVB	103938	103535	6.30%	0.868%
25	7.853	589	592	593	rBV	19564	18077	1.10%	0.152%
26	7.888	593	595	596	rVV	33768	35976	2.19%	0.302%
27	7.910	596	597	602	rVV2	35219	52989	3.23%	0.444%
28	7.990	602	604	608	rVB2	63500	111965	6.82%	0.939%
29	8.059	608	610	611	rBV	30270	31284	1.90%	0.262%
30	8.116	611	615	617	rVB3	17804	35293	2.15%	0.296%
31	8.173	617	620	622	rVB	15350	19974	1.22%	0.168%
32	8.253	625	627	628	rBV	12745	17432	1.06%	0.146%
33	8.299	628	631	633	rVV	354455	404853	24.65%	3.395%
34	8.356	633	636	640	rVB2	46286	99099	6.03%	0.831%

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Integration Parameters: rteint.p
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

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35	8.562	652	654	658 rBV	11367	17171	1.05%	0.144%
36	8.665	660	663	665 rVB2	22192	27699	1.69%	0.232%
37	8.722	665	668	673 rVB3	7626	17092	1.04%	0.143%
38	8.802	673	675	676 rBV	16436	23338	1.42%	0.196%
39	8.893	679	683	685 rBV	17456	21162	1.29%	0.177%
40	8.939	685	687	690 rBV2	12099	20108	1.22%	0.169%
41	9.019	690	694	697 rBV3	11403	29269	1.78%	0.245%
42	9.648	747	749	752 rVB	1410705	1500890	91.37%	12.587%
43	10.448	817	819	822 rBV	435591	392978	23.92%	3.296%
44	11.419	901	904	907 rBV	1031424	1025213	62.41%	8.598%
45	12.265	975	978	980 rBV	385465	404194	24.61%	3.390%
46	14.254	1149	1152	1155 rBV	1668544	1642632	100.00%	13.776%
47	15.466	1255	1258	1259 rBV	23370	35477	2.16%	0.298%
48	15.500	1259	1261	1264 rVB	354951	396525	24.14%	3.325%
49	17.180	1405	1408	1411 rBV	302647	352812	21.48%	2.959%

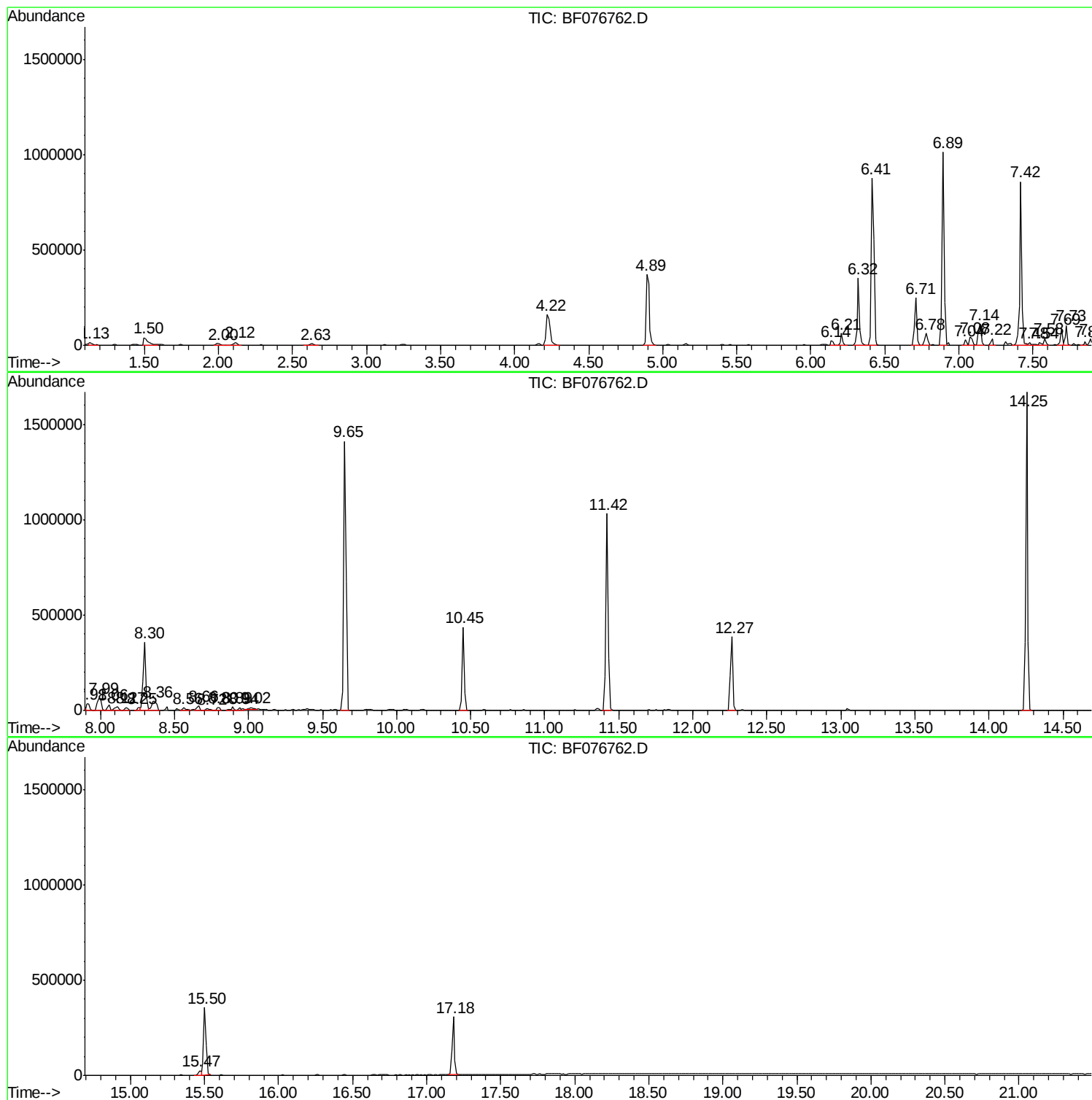
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121714.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
BNA_F
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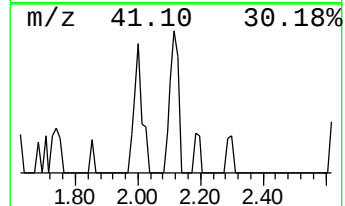
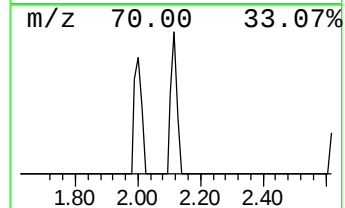
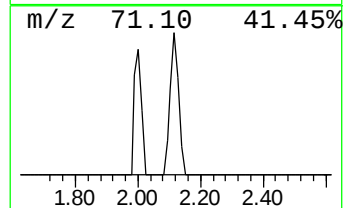
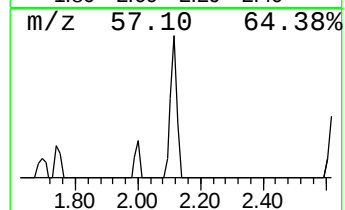
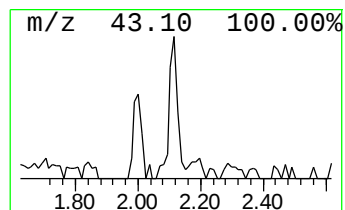
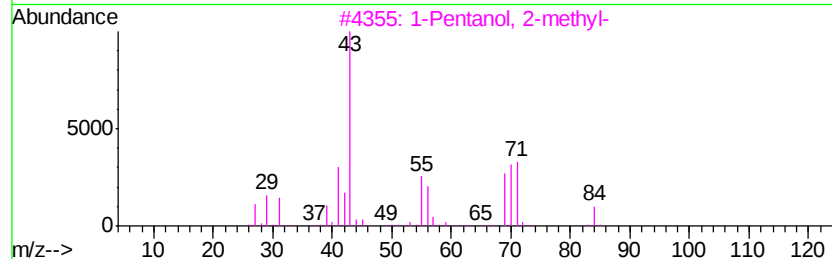
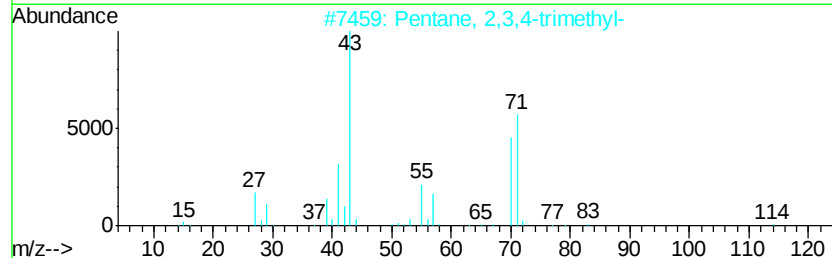
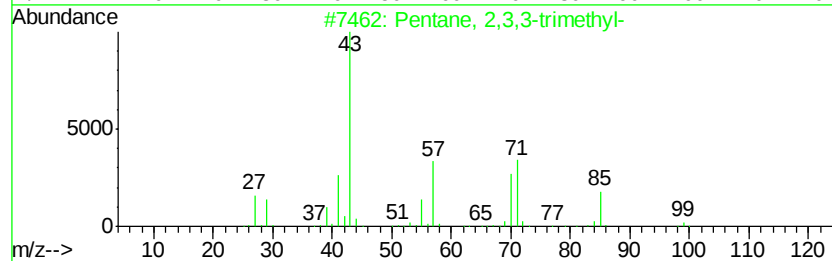
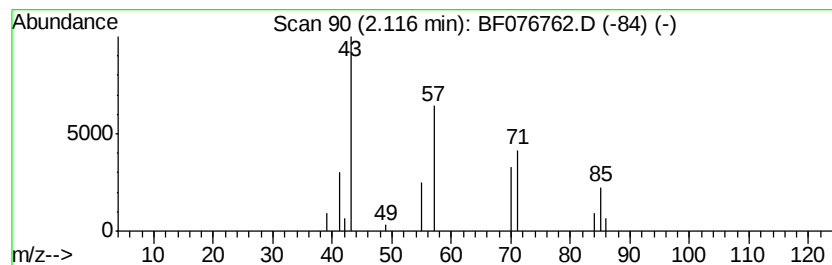
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121714.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown2.12 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	2.44 ng	29557	1,4-Dichlorobenzene-d4	6.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	40
2			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	36
3			1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	36
4			Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	9
5			2-Butanone, 1-chloro-3,3-dimethyl-	134	C6H11ClO	013547-70-1	9



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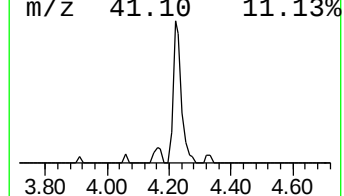
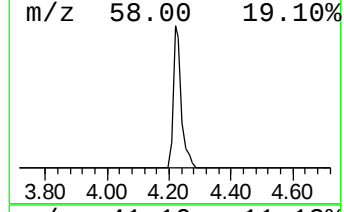
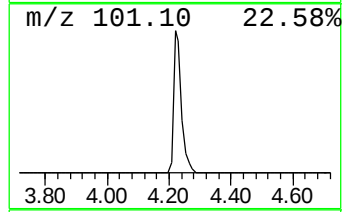
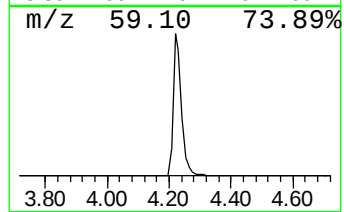
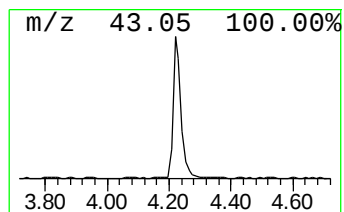
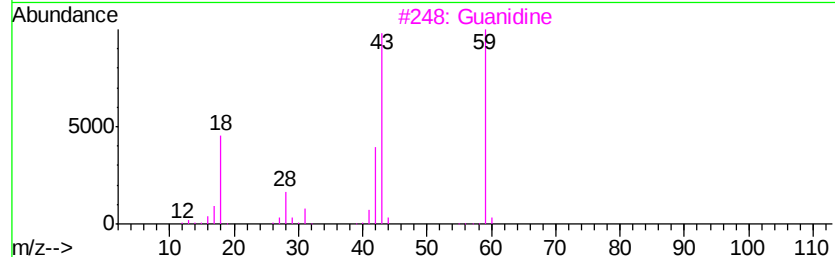
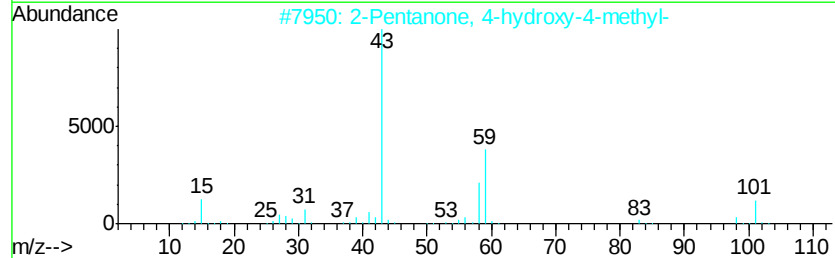
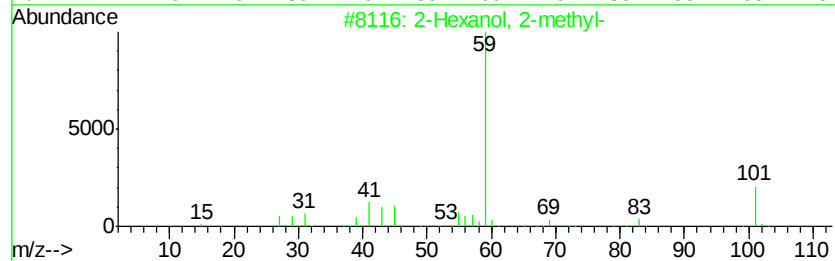
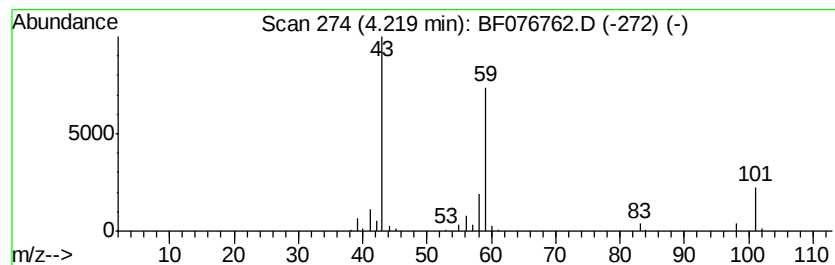
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Hexanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.22	23.44 ng	283490	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	53
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
3		Guanidine	59	CH5N3	000113-00-8	38
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	37
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	32



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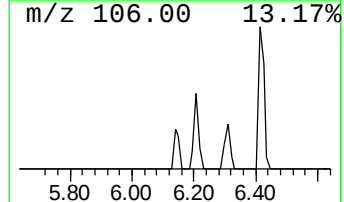
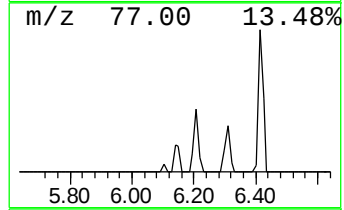
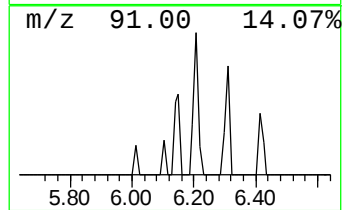
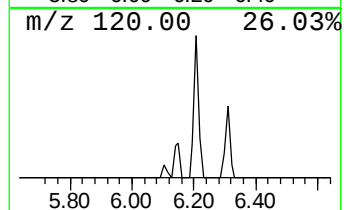
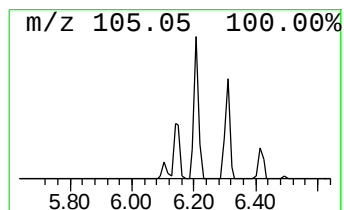
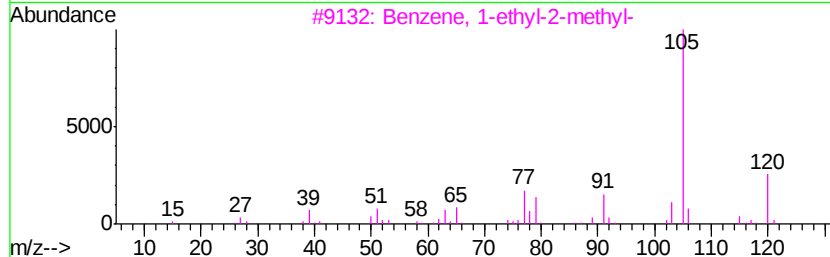
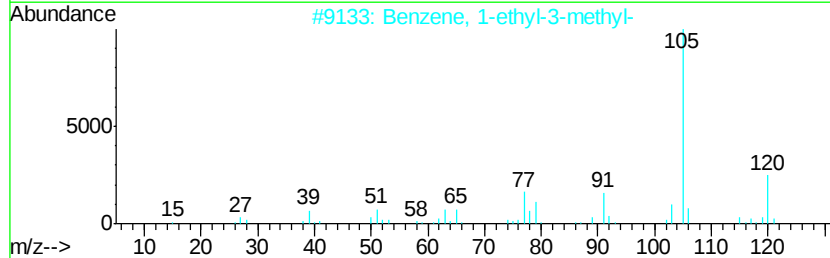
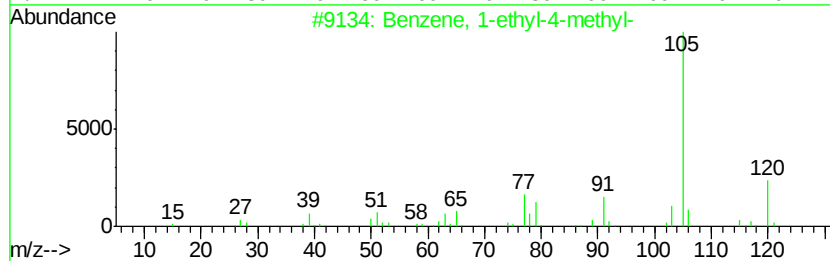
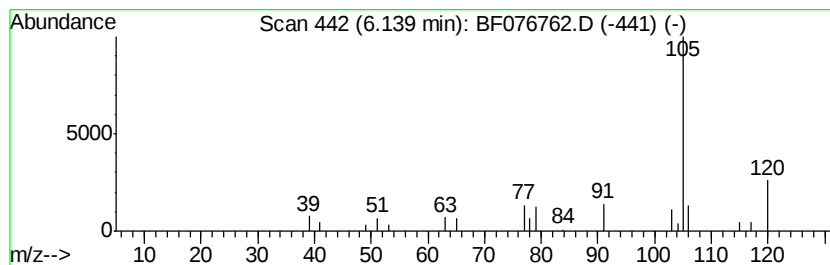
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121714.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Benzene, 1-ethyl-4-methyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.14	2.53 ng	30657	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90
2		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	87
3		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	83
4		Benzene, (1-methylethyl)-	120	C9H12	000098-82-8	80
5		1-Hexene, 6-phenyl-4-(1-phenylet...	280	C20H24O	1000190-48-6	53



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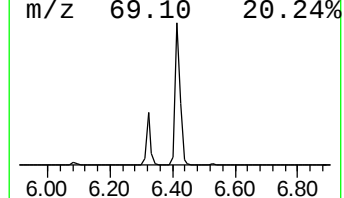
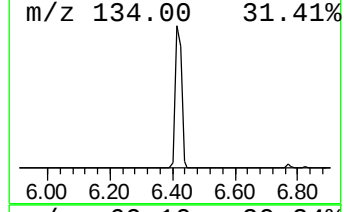
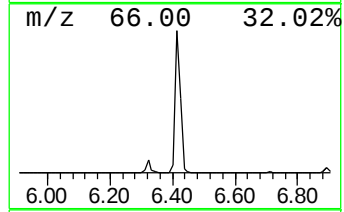
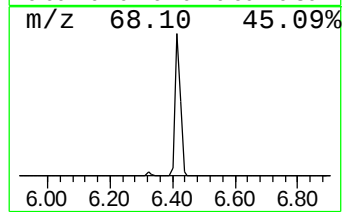
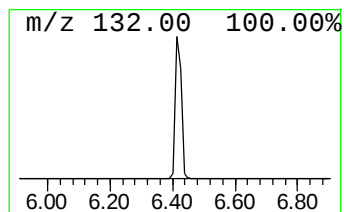
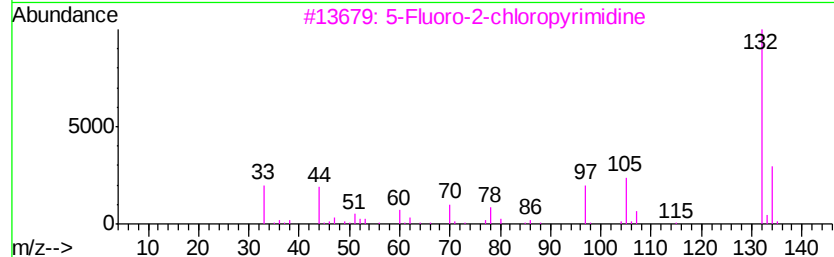
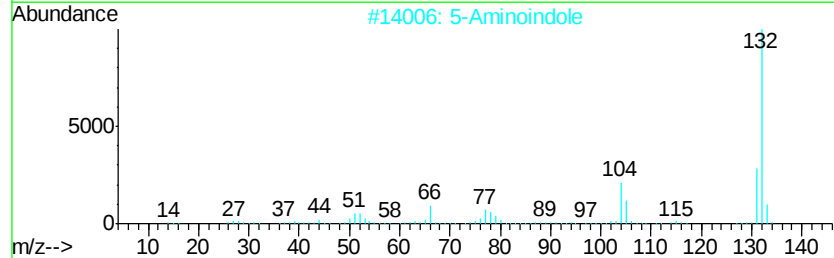
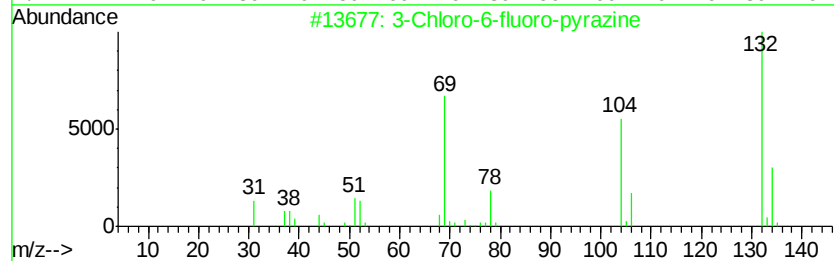
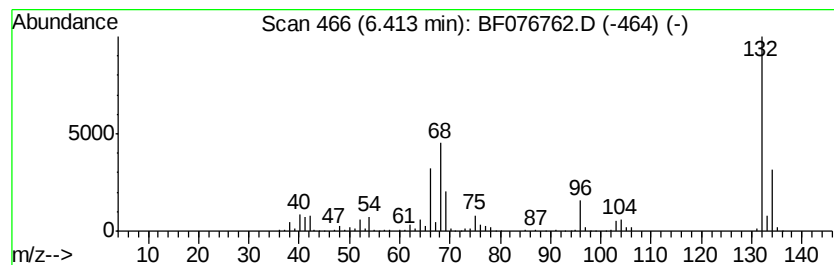
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown6.41 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.41	85.02 ng	1028410	1,4-Dichlorobenzene-d4	6.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	27
3			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4			(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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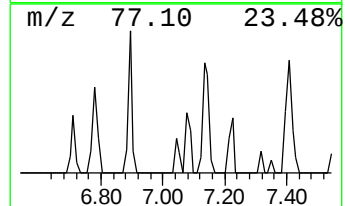
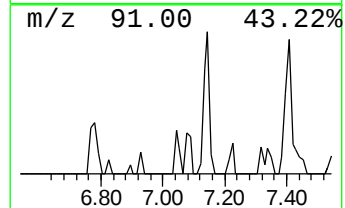
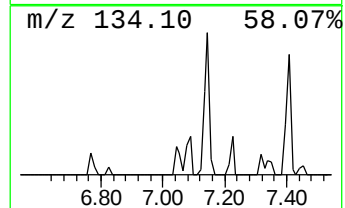
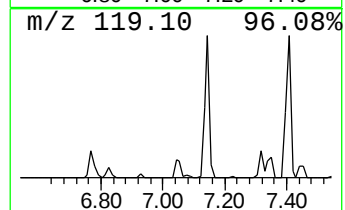
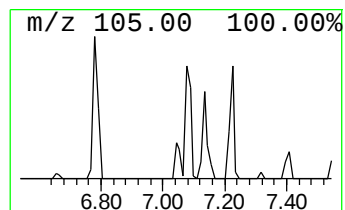
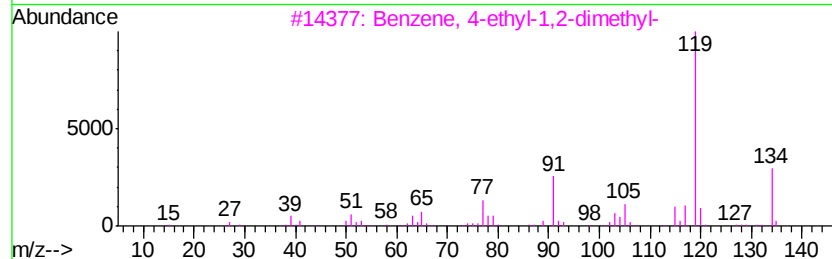
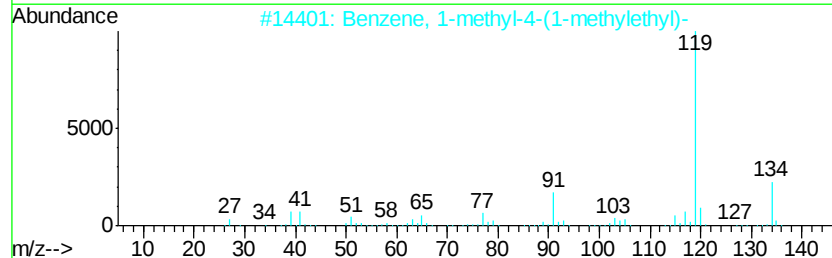
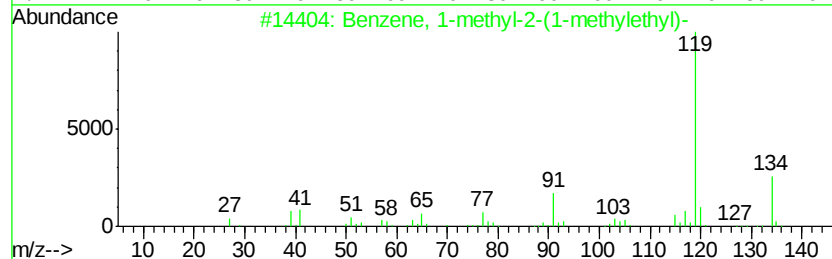
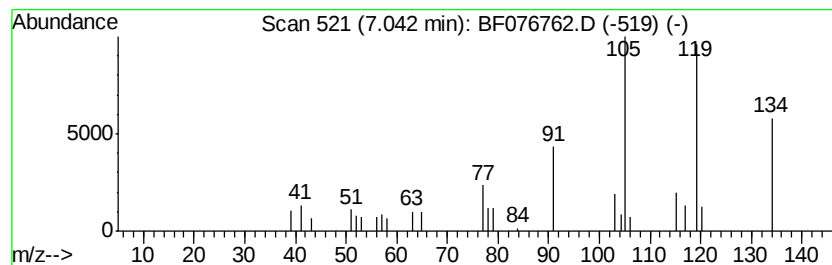
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzene, 1-methyl-2-(1-meth... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.04	2.77 ng	33446	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-methyl-2-(1-methyleth...	134	C10H14	000527-84-4	59
2		Benzene, 1-methyl-4-(1-methyleth...	134	C10H14	000099-87-6	53
3		Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	37
4		Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	37
5		Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	37



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010615\
Data File : BF076762.D
Acq On : 6 Jan 2015 16:54
Operator : IZ / TP
Sample : G1011-03
Misc : W
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW3

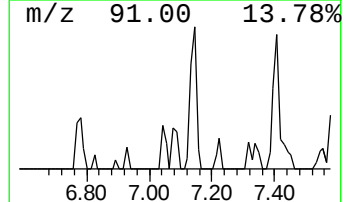
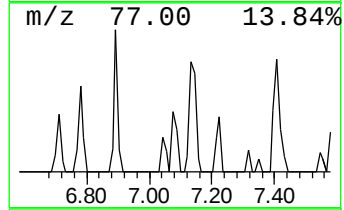
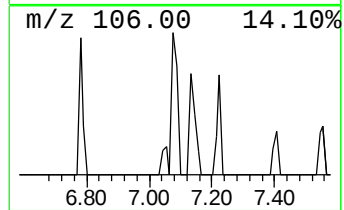
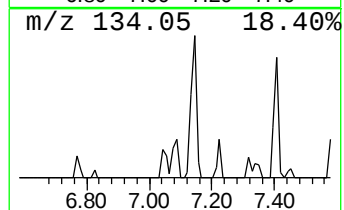
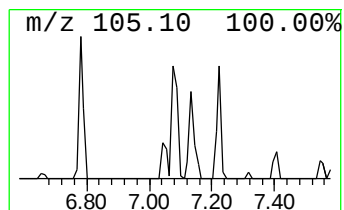
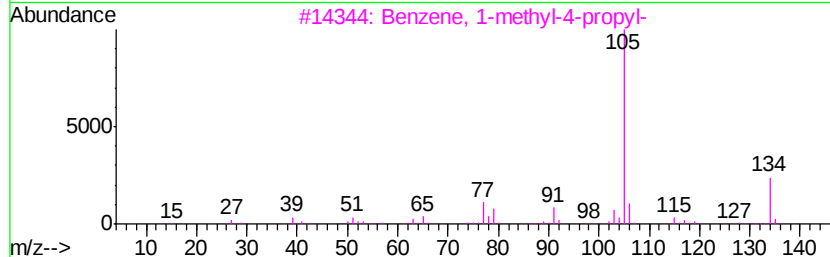
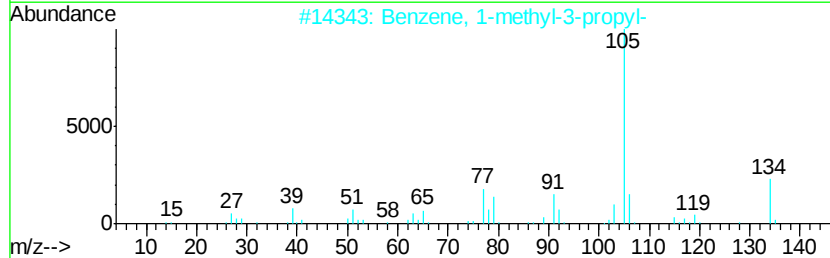
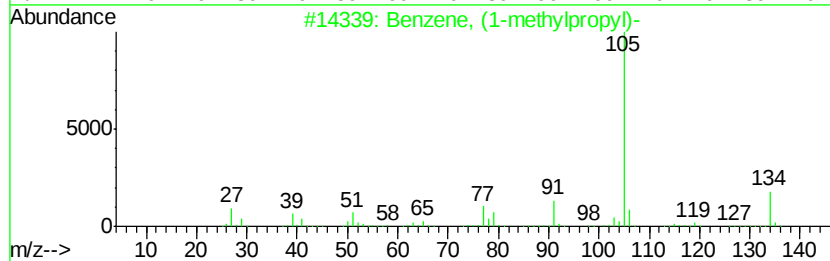
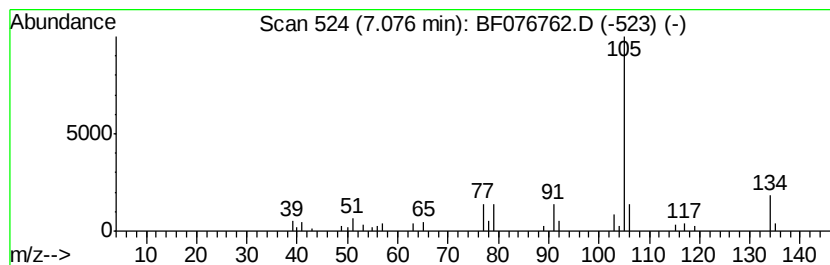
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzene, (1-methylpropyl)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.08	4.47 ng	54123	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	87
2		Benzene, 1-methyl-3-propyl-	134	C10H14	001074-43-7	81
3		Benzene, 1-methyl-4-propyl-	134	C10H14	001074-55-1	80
4		Oxirane, 2-methyl-2-phenyl-	134	C9H10O	002085-88-3	80
5		Benzeneacetaldehyde, .alpha.-met...	134	C9H10O	000093-53-8	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010615\
Data File : BF076762.D
Acq On : 6 Jan 2015 16:54
Operator : IZ / TP
Sample : G1011-03
Misc : W
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW3

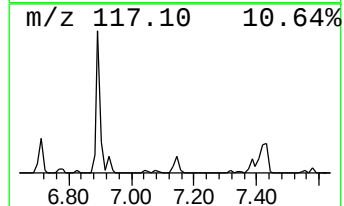
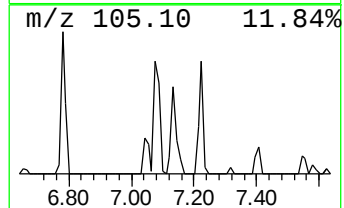
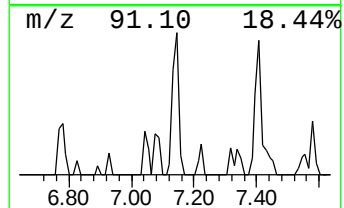
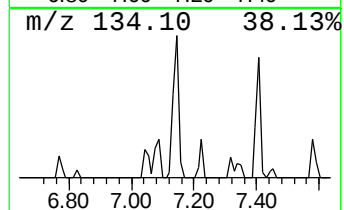
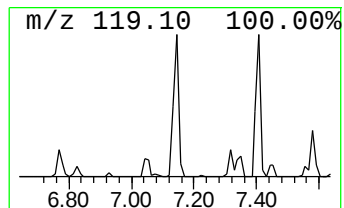
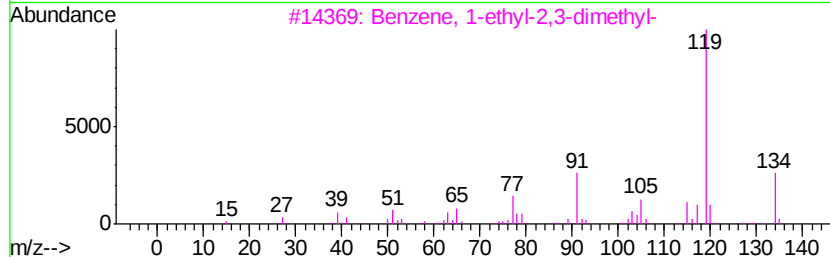
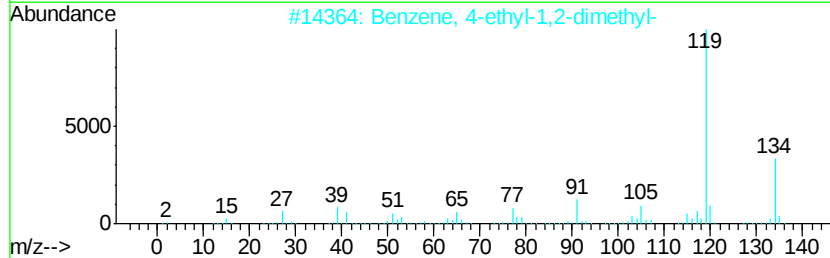
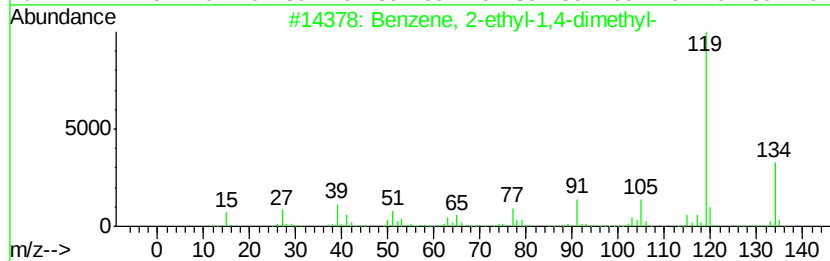
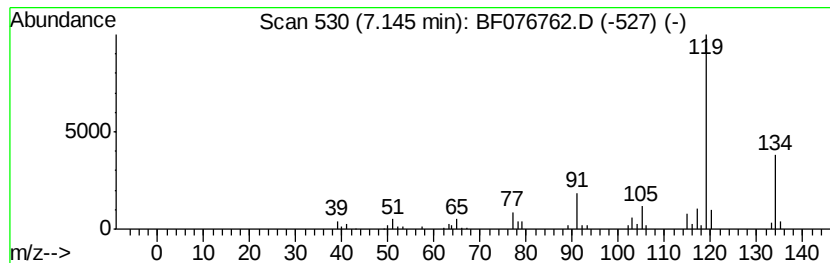
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.14	12.00 ng	145121	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
2		Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
3		Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
4		Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94
5		Benzene, 1-methyl-2-(1-methyleth...	134	C10H14	000527-84-4	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010615\
Data File : BF076762.D
Acq On : 6 Jan 2015 16:54
Operator : IZ / TP
Sample : G1011-03
Misc : W
ALS Vial : 12 Sample Multiplier: 1

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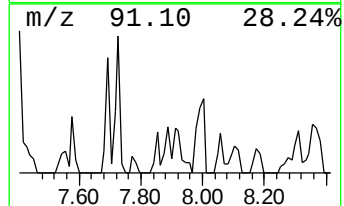
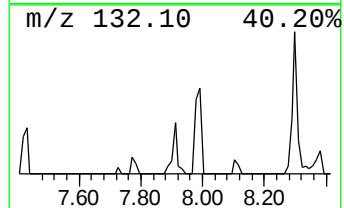
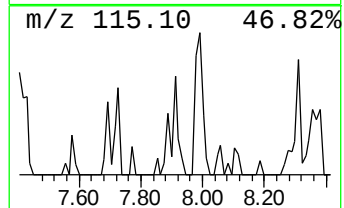
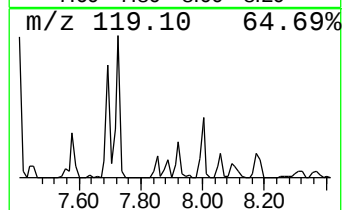
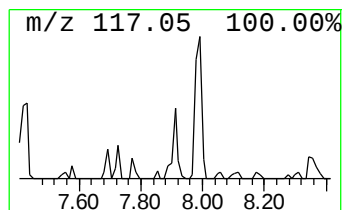
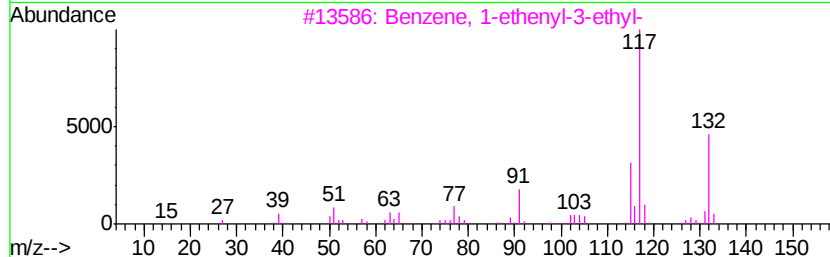
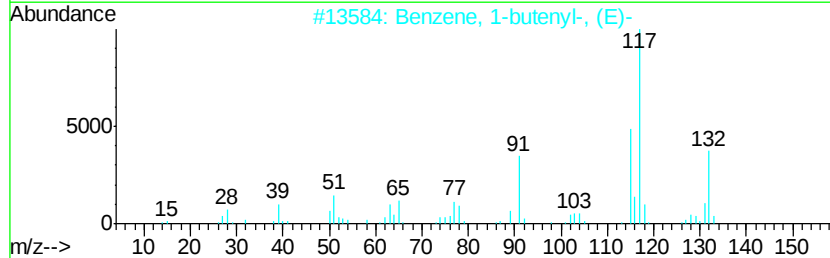
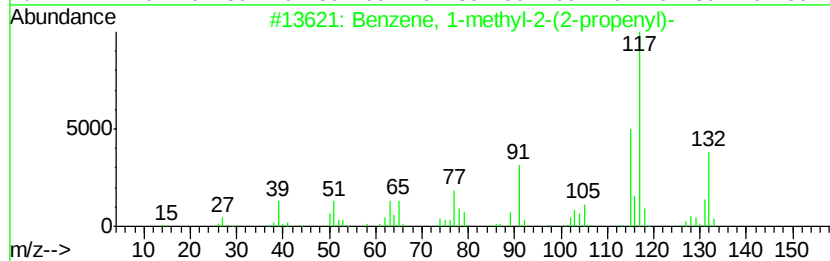
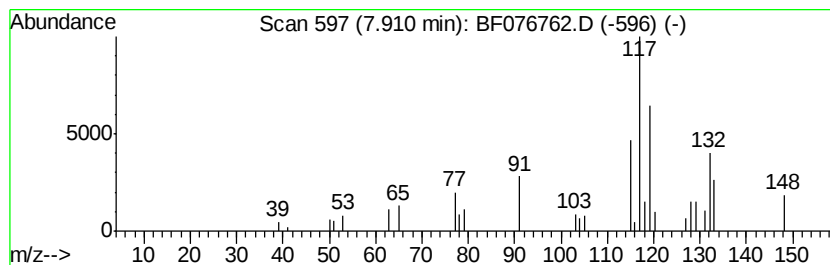
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Benzene, 1-methyl-2-(2-prop... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.91	2.62 ng	52989	Napthalene-d8	8.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	58
2		Benzene, 1-butenyl-, (E)-	132	C10H12	001005-64-7	58
3		Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	58
4		Benzene, 2-butenyl-	132	C10H12	001560-06-1	52
5		Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010615\
Data File : BF076762.D
Acq On : 6 Jan 2015 16:54
Operator : IZ / TP
Sample : G1011-03
Misc : W
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW3

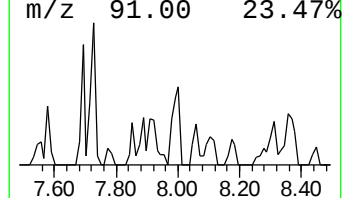
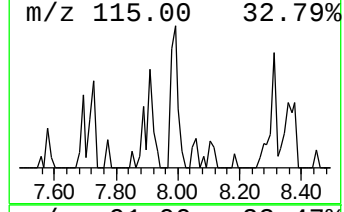
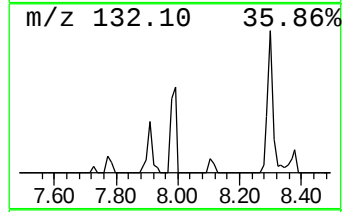
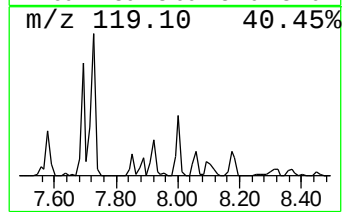
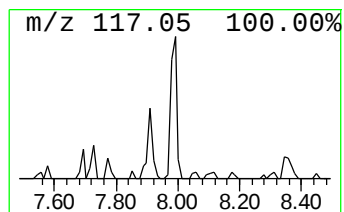
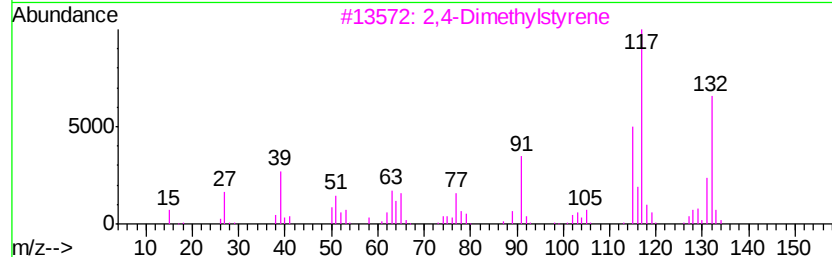
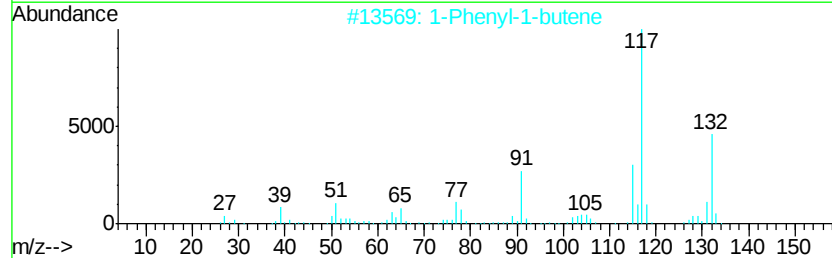
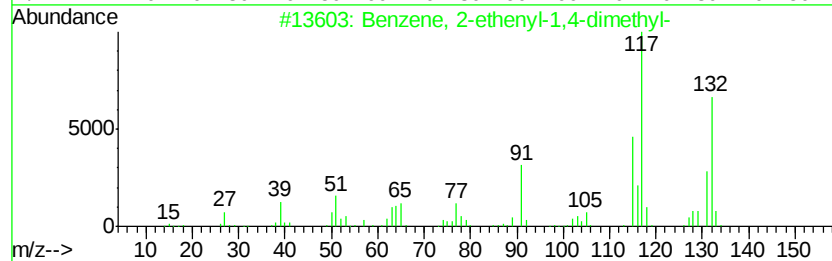
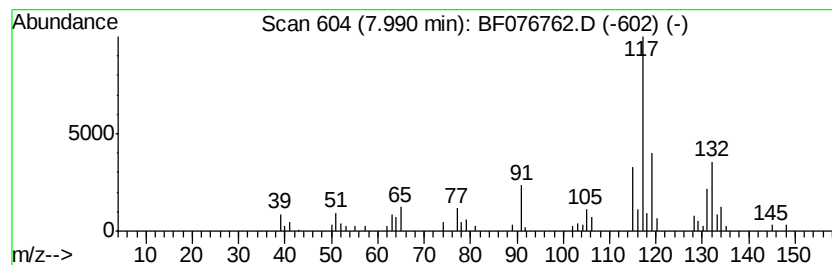
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.99	5.53 ng	111965	Naphthalene-d8	8.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
2			1-Phenyl-1-butene	132	C10H12	000824-90-8	92
3			2,4-Dimethylstyrene	132	C10H12	002234-20-0	89
4			3-Phenylbut-1-ene	132	C10H12	000934-10-1	70
5			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	70



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010615\
Data File : BF076762.D
Acq On : 6 Jan 2015 16:54
Operator : IZ / TP
Sample : G1011-03
Misc : W
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW3

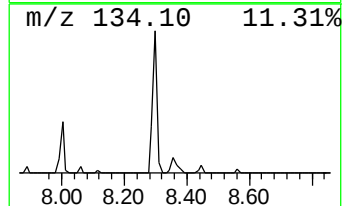
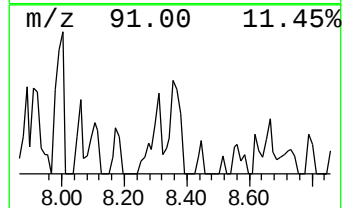
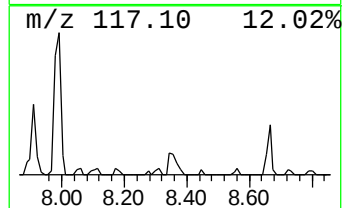
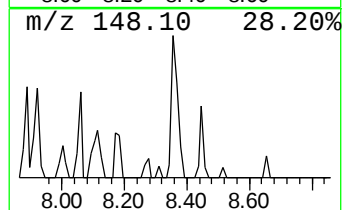
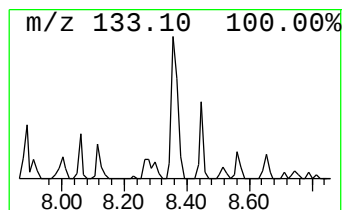
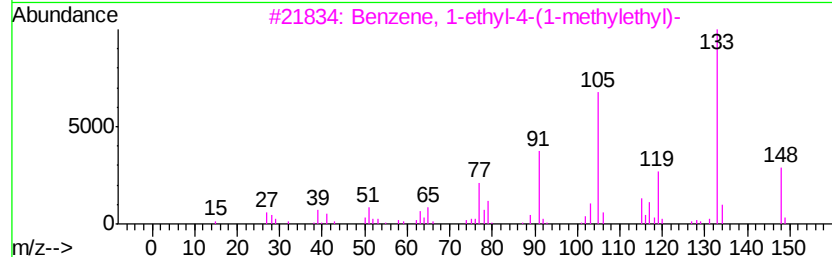
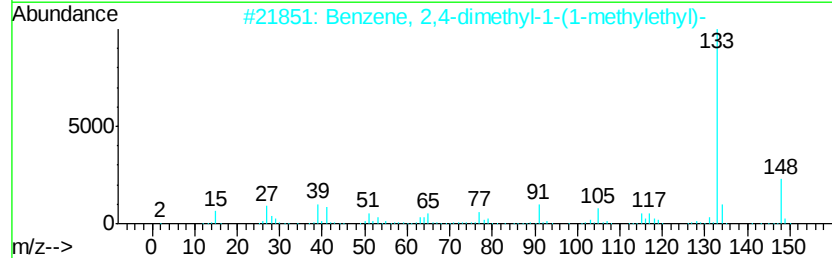
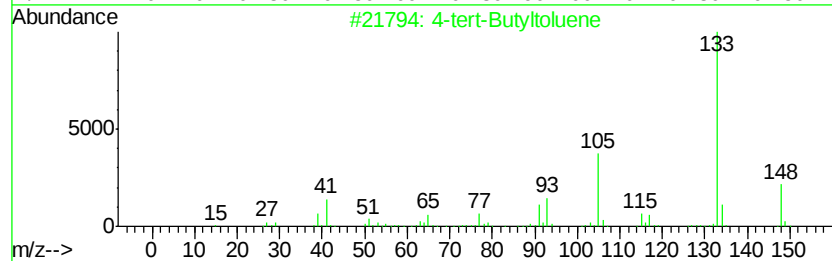
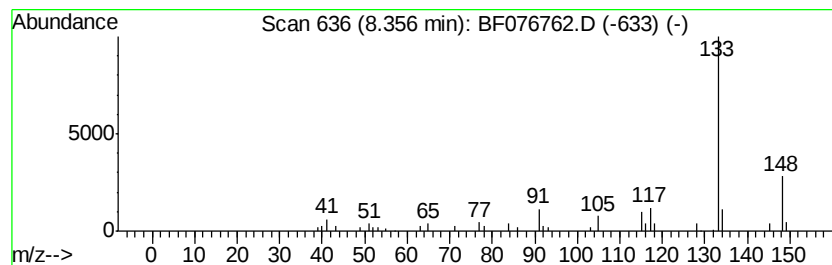
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 4-tert-Butyltoluene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.36	4.90 ng	99099	Naphthalene-d8	8.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-tert-Butyltoluene	148	C11H16	000098-51-1	90
2		Benzene, 2,4-dimethyl-1-(1-methy...	148	C11H16	004706-89-2	87
3		Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	004218-48-8	86
4		Benzene, pentamethyl-	148	C11H16	000700-12-9	86
5		Benzene, 1,4-dimethyl-2-(1-methy...	148	C11H16	004132-72-3	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010615\
Data File : BF076762.D
Acq On : 6 Jan 2015 16:54
Operator : IZ / TP
Sample : G1011-03
Misc : W
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121714.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
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Benzene, 1-ethyl-...	6.14	2.5	ng	30657	1	6.71	241919	20.0
unknown6.41	6.41	85.0	ng	1028410	1	6.71	241919	20.0
Benzene, 1-methyl...	7.04	2.8	ng	33446	1	6.71	241919	20.0
Benzene, (1-methy...	7.08	4.5	ng	54123	1	6.71	241919	20.0
Benzene, 2-ethyl-...	7.14	12.0	ng	145121	1	6.71	241919	20.0
Benzene, 1-methyl...	7.91	2.6	ng	52989	2	8.30	404853	20.0
Benzene, 2-etheny...	7.99	5.5	ng	111965	2	8.30	404853	20.0
4-tert-Butyltoluene	8.36	4.9	ng	99099	2	8.30	404853	20.0