

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
 Data File : BF093604.D
 Acq On : 13 Mar 2017 13:52
 Operator : SJ/MA
 Sample : I2174-19
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 D-64

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-BF030717.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	2.355	38	41	44	rBV	81283	141644	3.01%	0.326%
2	2.412	44	46	55	rVB	63936	152969	3.25%	0.353%
3	3.098	103	106	122	rBV	403323	879074	18.68%	2.026%
4	4.161	195	199	214	rBV	983972	1751536	37.22%	4.037%
5	4.390	217	219	222	rBV	41891	73810	1.57%	0.170%
6	4.458	222	225	227	rVV	318892	477411	10.15%	1.100%
7	4.870	259	261	271	rBV	317185	558238	11.86%	1.287%
8	5.316	298	300	326	rBV	3084397	4574670	97.22%	10.544%
9	6.333	387	389	391	rBV	316352	366856	7.80%	0.846%
10	6.367	391	392	400	rVV	2945835	4084238	86.80%	9.413%
11	6.481	400	402	405	rVB	4361538	4277337	90.90%	9.858%
12	6.710	420	422	431	rVB	895514	945372	20.09%	2.179%
13	6.859	433	435	438	rBV	3182588	3268336	69.46%	7.533%
14	7.019	447	449	455	rVB	255322	286242	6.08%	0.660%
15	7.281	470	472	485	rBV	2769480	3080918	65.47%	7.101%
16	7.453	485	487	501	rVV2	357461	917597	19.50%	2.115%
17	8.002	532	535	546	rBV	1163542	1354550	28.79%	3.122%
18	8.162	546	549	555	rBV	71985	153356	3.26%	0.353%
19	8.390	567	569	579	rVB2	38874	98421	2.09%	0.227%
20	9.076	627	629	632	rBV	3423262	4705499	100.00%	10.845%
21	9.373	653	655	660	rBV	117119	271272	5.76%	0.625%
22	9.716	683	685	687	rBV	67151	119739	2.54%	0.276%
23	9.762	687	689	691	rVV	844706	1033623	21.97%	2.382%
24	10.047	711	714	721	rBV	271325	666494	14.16%	1.536%
25	10.150	721	723	733	rVB2	191869	488085	10.37%	1.125%
26	10.550	756	758	761	rBV2	1951738	2599994	55.25%	5.992%
27	11.248	817	819	824	rBV	1402647	1331024	28.29%	3.068%
28	12.836	955	958	961	rBV	3916887	3862613	82.09%	8.903%
29	13.899	1049	1051	1060	rVB	635537	761489	16.18%	1.755%
30	15.328	1174	1176	1182	rVB2	55650	105391	2.24%	0.243%

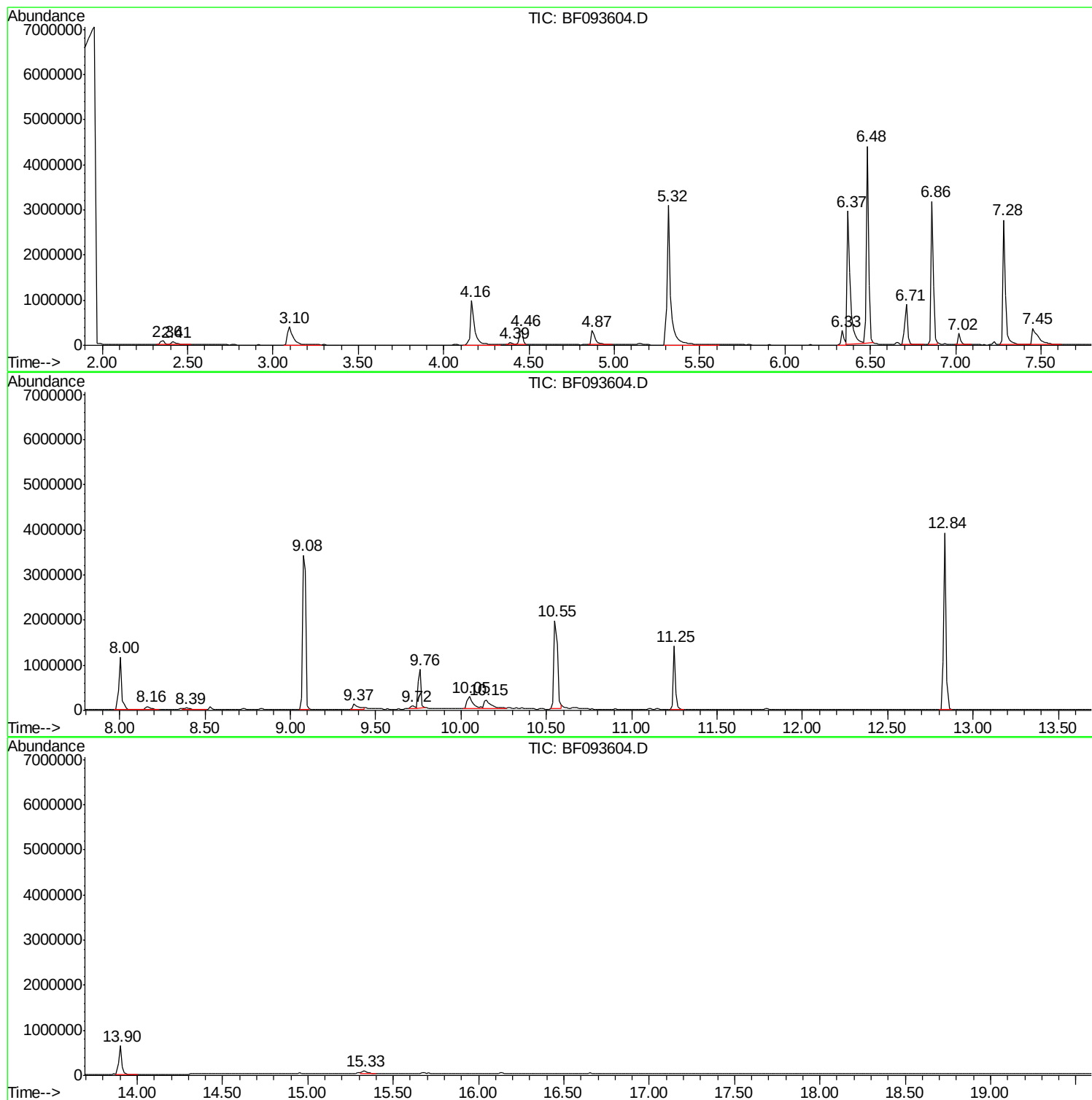
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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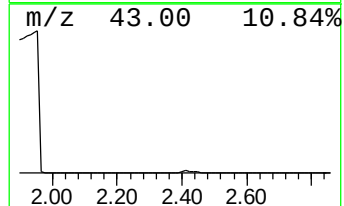
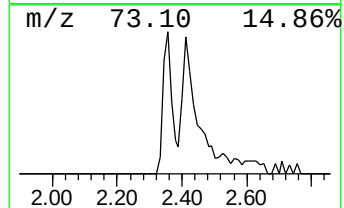
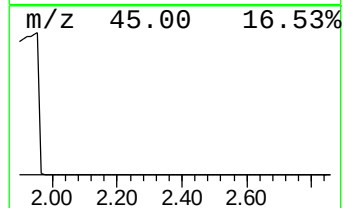
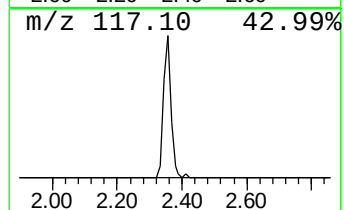
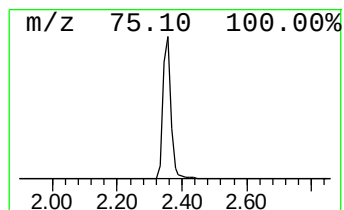
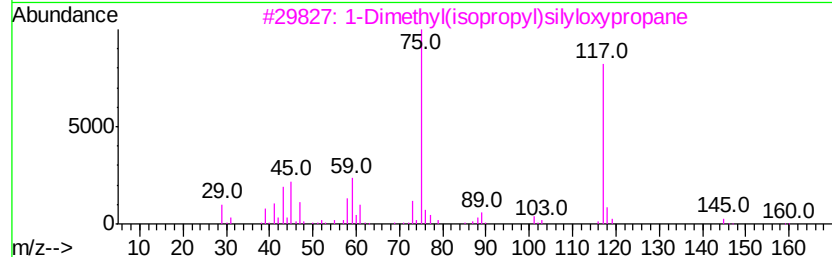
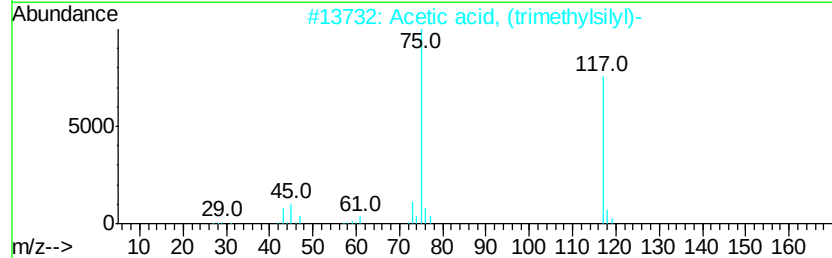
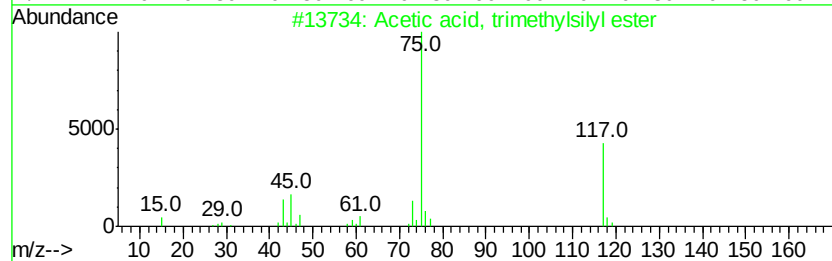
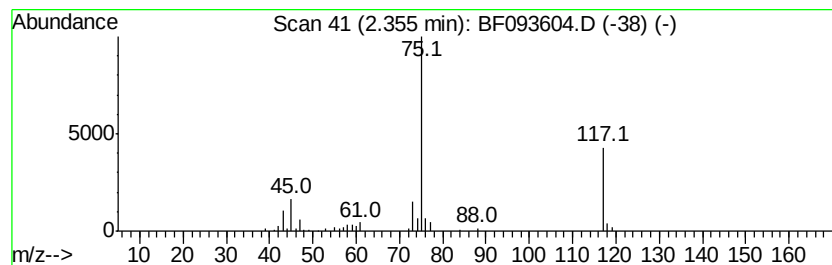
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Acetic acid, trimethylsilyl... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.36	3.00 ng	141644	1,4-Dichlorobenzene-d4	6.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, trimethylsilyl ester	132	C5H12O2Si	018147-36-9	90
2			Acetic acid, (trimethylsilyl)-	132	C5H12O2Si	002345-38-2	83
3			1-Dimethyl(isopropyl)silyloxypro...	160	C8H20O2Si	1000279-89-4	64
4			Silane, trimethyl(1-methylethoxy)-	132	C6H16O2Si	001825-64-5	56
5			2-Dichloromethyl(dimethyl)silylo...	200	C6H14Cl2OSi	018209-57-9	56



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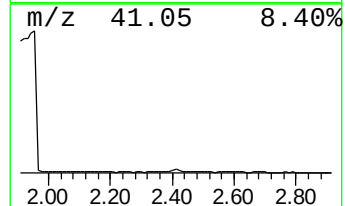
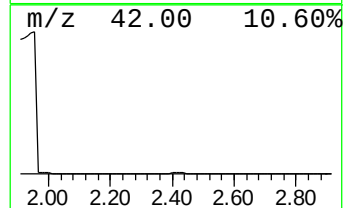
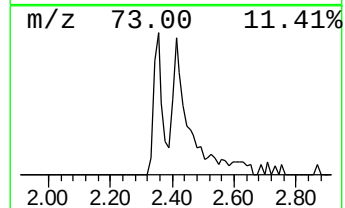
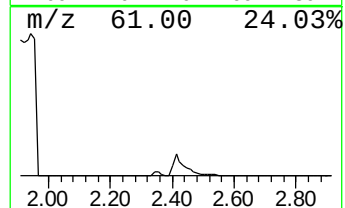
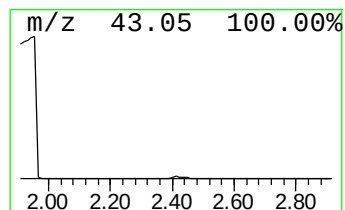
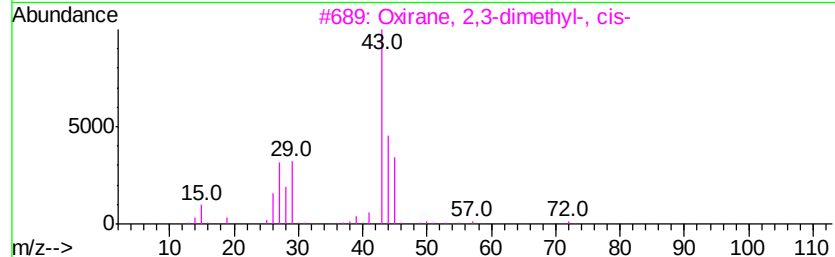
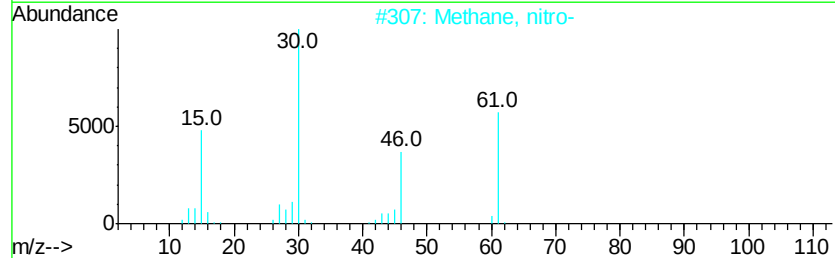
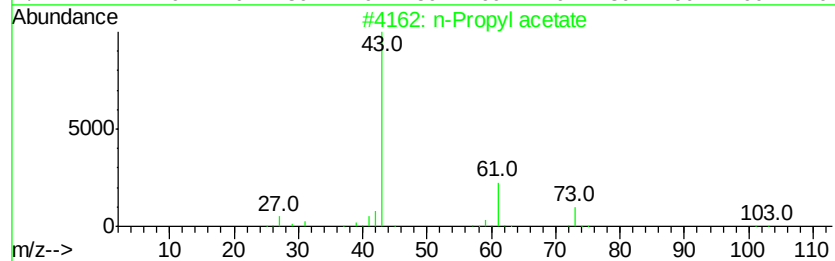
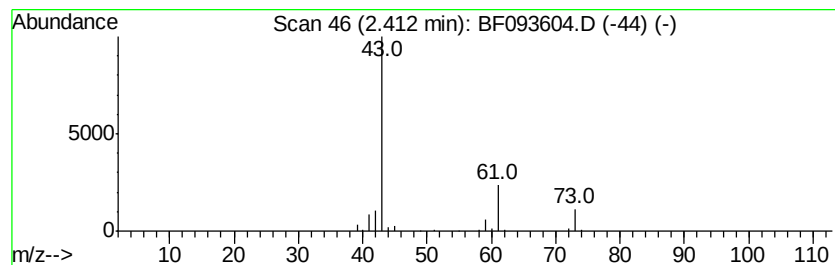
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 n-Propyl acetate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.41	3.24 ng	152969	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Propyl acetate	102	C5H10O2	000109-60-4	72
2		Methane, nitro-	61	CH3NO2	000075-52-5	5
3		Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	5
4		1-Butanamine	73	C4H11N	000109-73-9	5
5		Isobutylamine	73	C4H11N	000078-81-9	5



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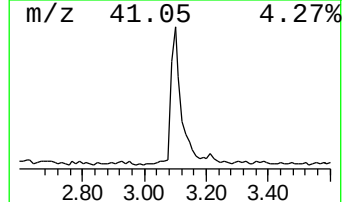
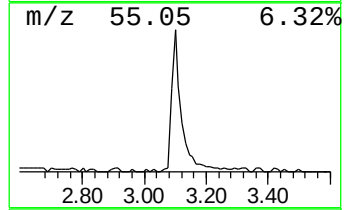
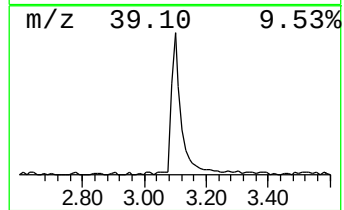
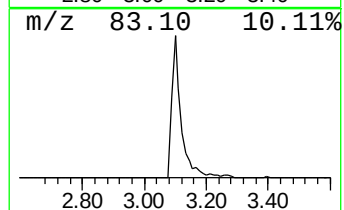
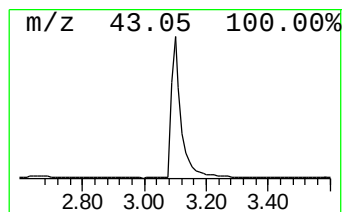
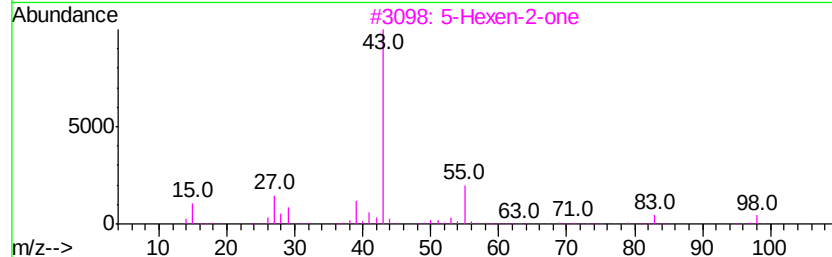
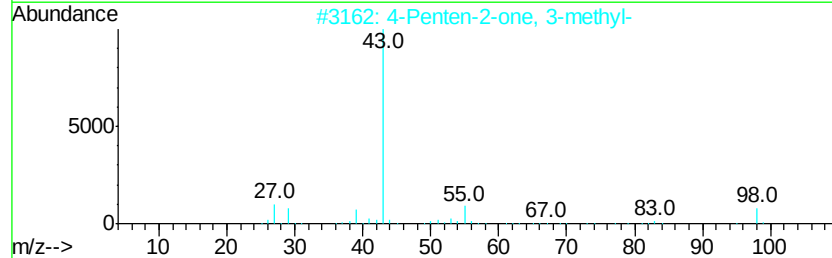
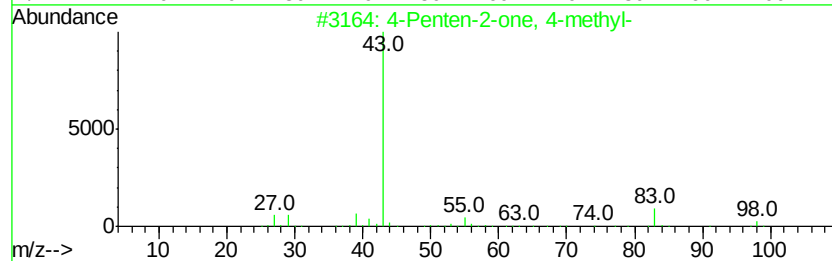
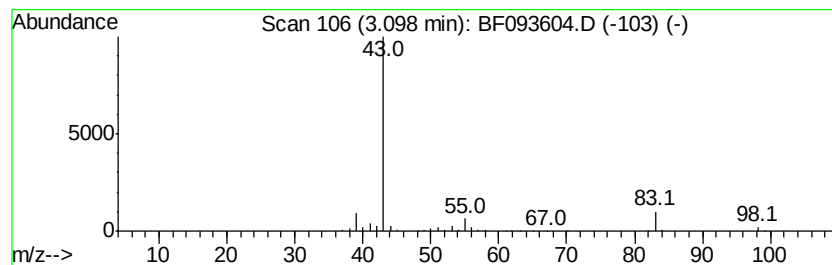
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 3 4-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.10	18.60 ng	879074	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	72
2		4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	50
3		5-Hexen-2-one	98	C6H10O	000109-49-9	40
4		3,5-Hexadien-2-ol	98	C6H10O	003280-51-1	37
5		Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	12



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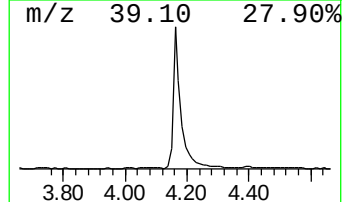
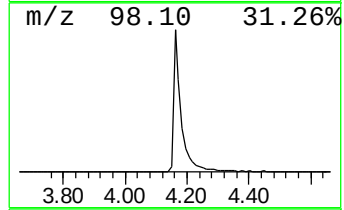
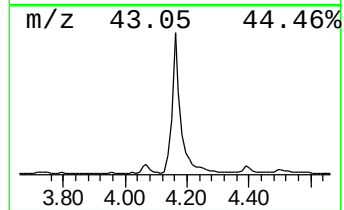
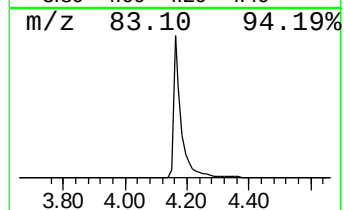
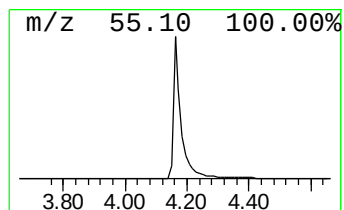
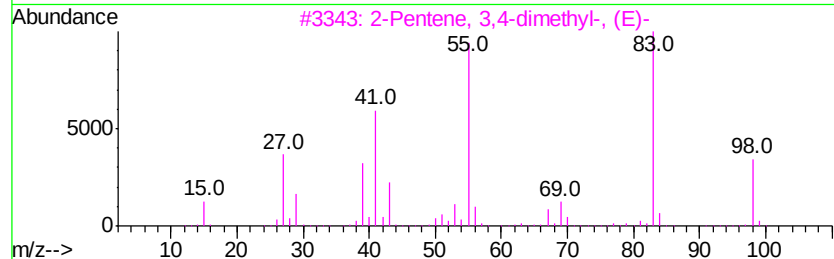
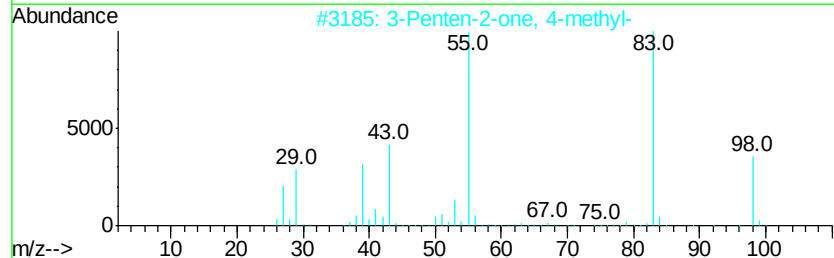
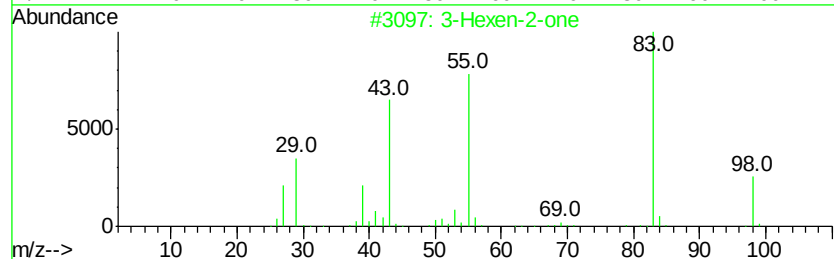
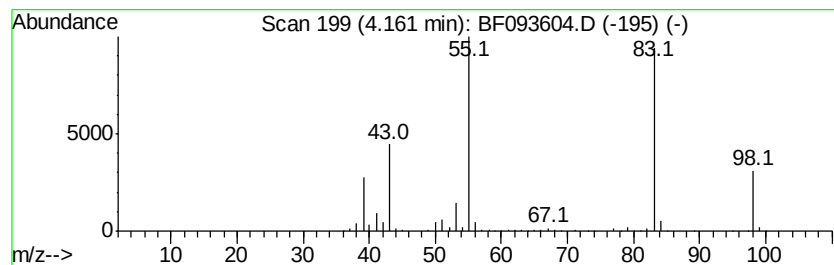
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 3-Hexen-2-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.16	37.06 ng	1751540	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



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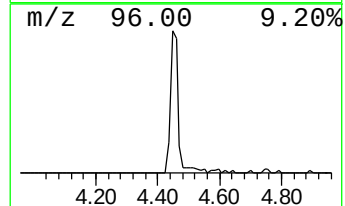
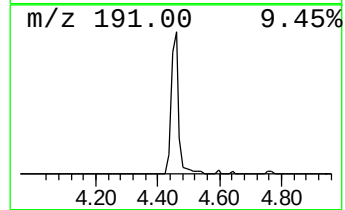
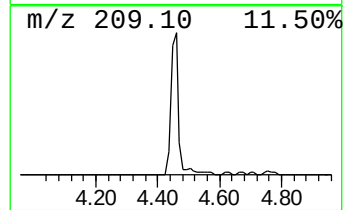
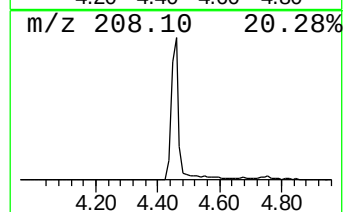
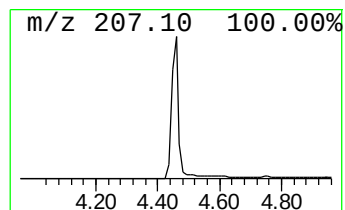
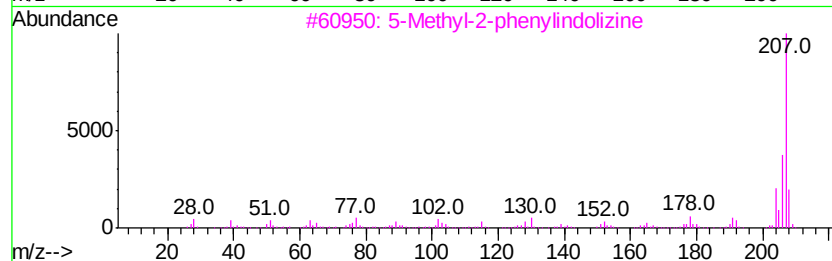
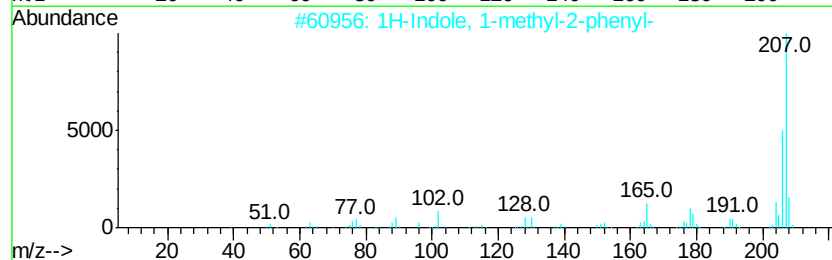
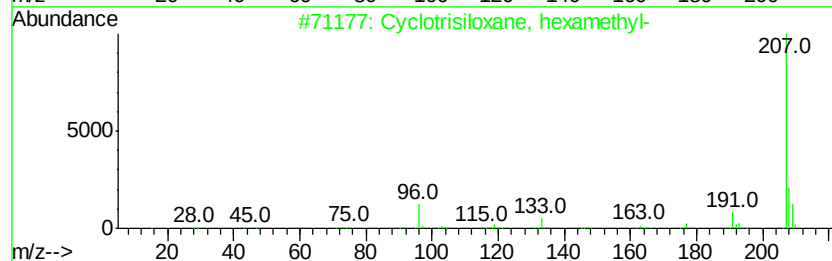
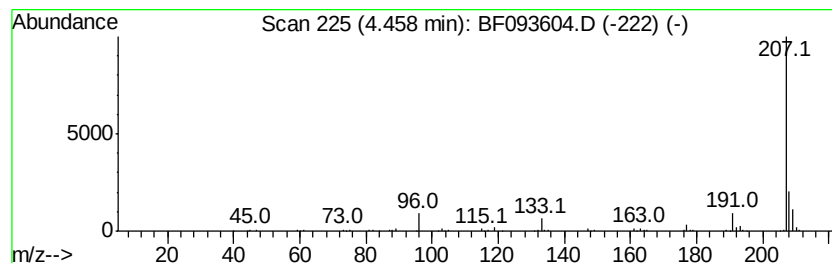
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclotrisiloxane, hexamethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.46	10.10 ng	477411	1,4-Dichlorobenzene-d4	6.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclotrisiloxane, hexamethyl-	222	C6H18O3Si3	000541-05-9	91
2		1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	39
3		5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	38
4		Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	38
5		1-Methyl-3-phenylindole	207	C15H13N	030020-98-5	9



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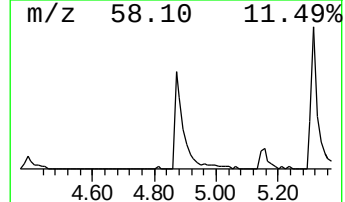
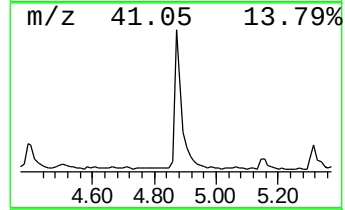
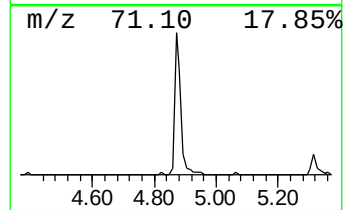
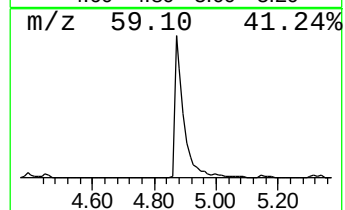
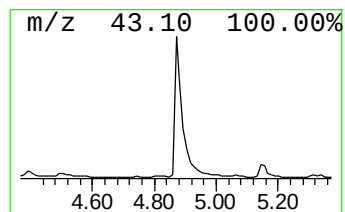
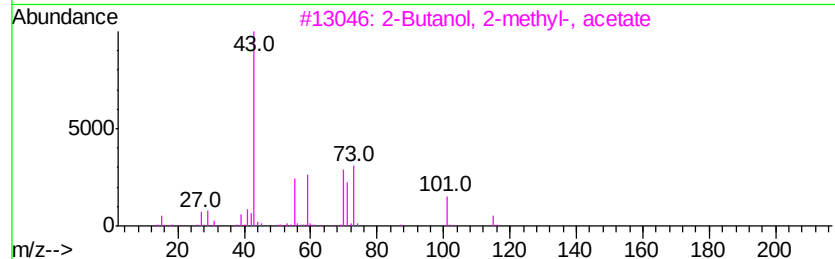
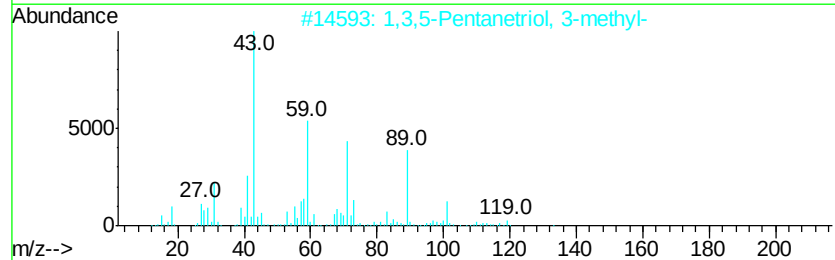
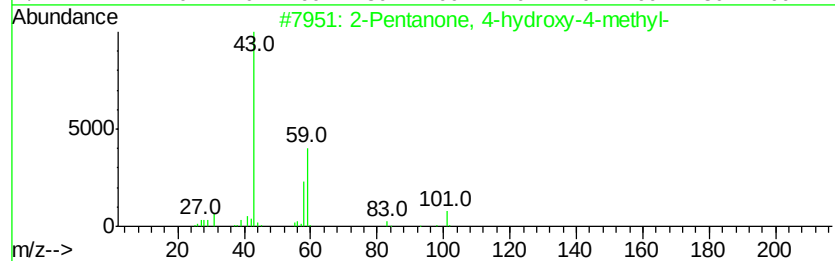
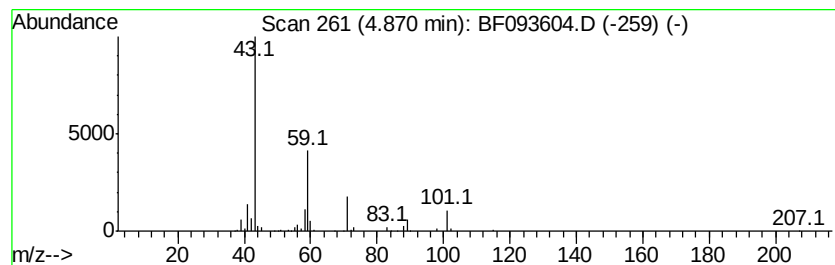
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	11.81 ng	558238	1,4-Dichlorobenzene-d4	6.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			1,3,5-Pentanetriol, 3-methyl-	134	C6H14O3	007564-64-9	38
3			2-Butanol, 2-methyl-, acetate	130	C7H14O2	000625-16-1	17
4			2-Pentanone, 5-(acetyloxy)-	144	C7H12O3	005185-97-7	12
5			2,3-Pentanedione, 4-methyl-	114	C6H10O2	007493-58-5	10



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093604.D
Acq On : 13 Mar 2017 13:52
Operator : SJ/MA
Sample : I2174-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D-64

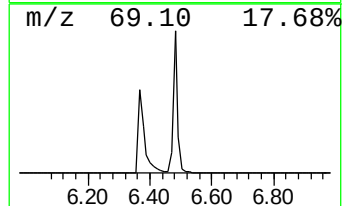
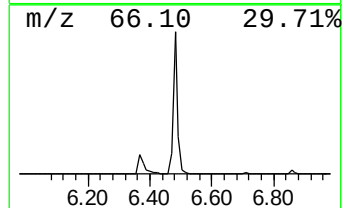
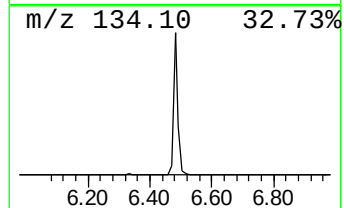
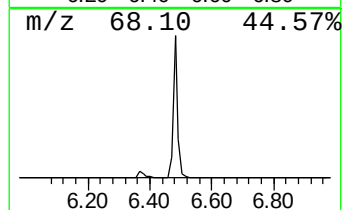
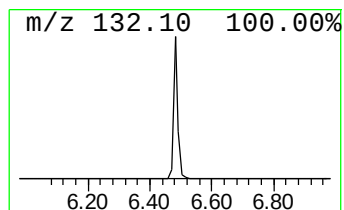
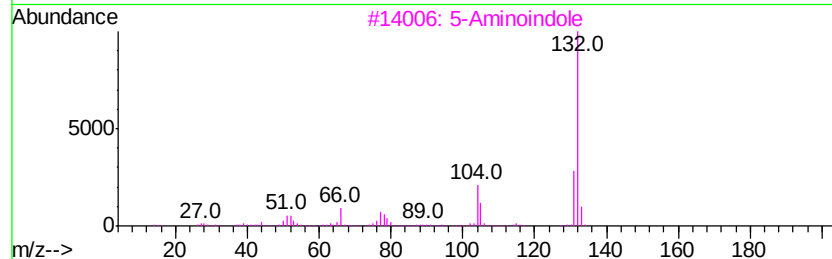
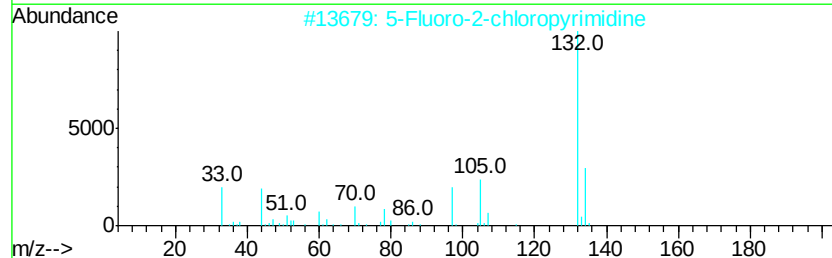
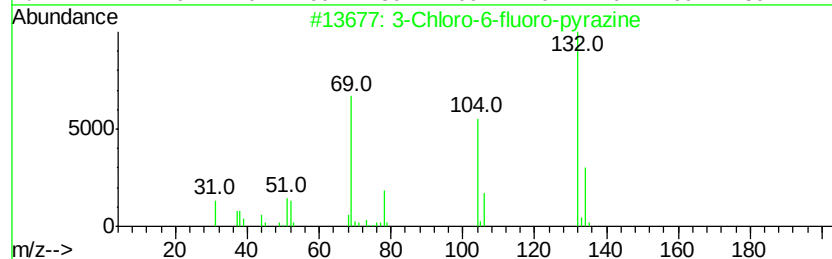
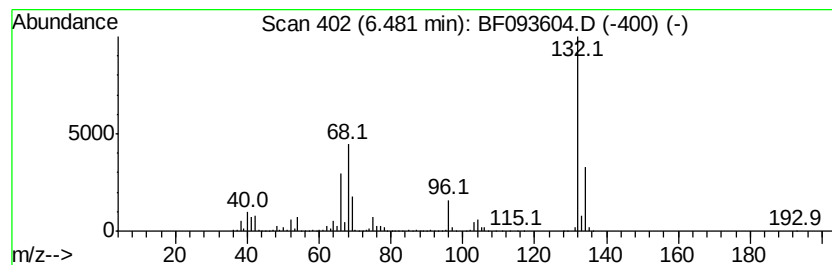
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	90.49 ng	4277340	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
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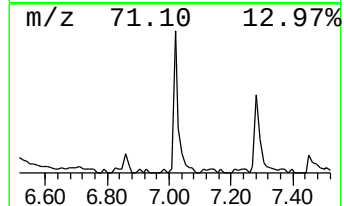
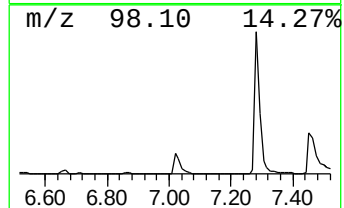
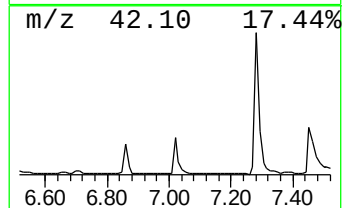
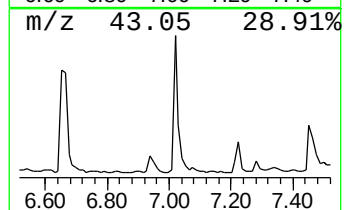
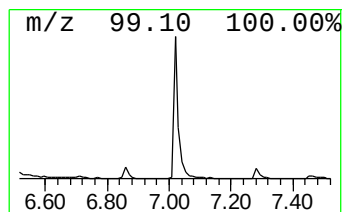
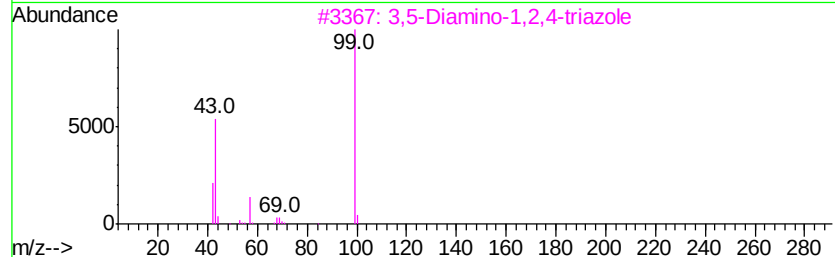
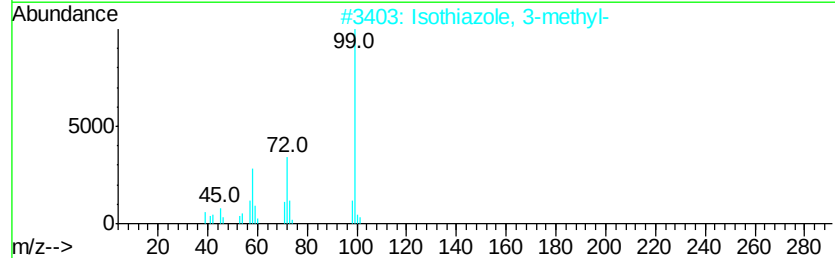
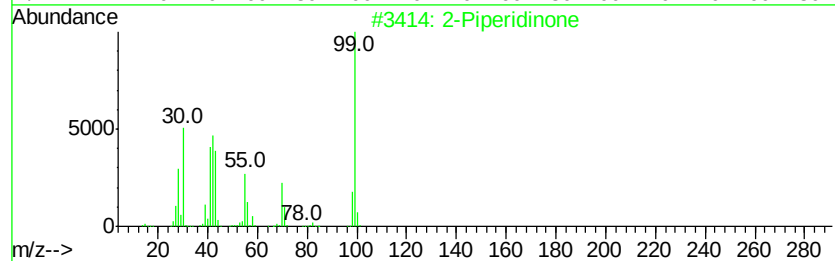
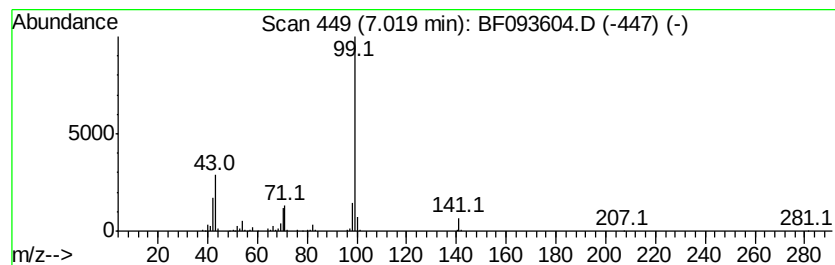
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-Piperidinone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.02	6.06 ng	286242	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Piperidinone	99	C5H9NO	000675-20-7	72
2		Isothiazole, 3-methyl-	99	C4H5NS	000693-92-5	53
3		3,5-Diamino-1,2,4-triazole	99	C2H5N5	001455-77-2	40
4		Cyclohexanol, 1-(2-nitropropyl)-	187	C9H17NO3	103077-77-6	38
5		2-Pyrrolidinone, 1-methyl-	99	C5H9NO	000872-50-4	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
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Sample : I2174-19
Misc :
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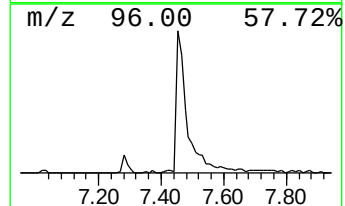
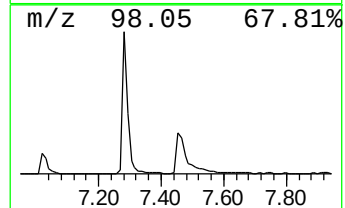
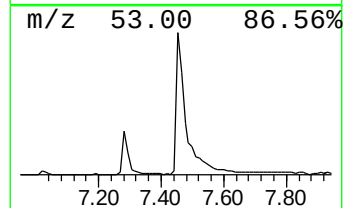
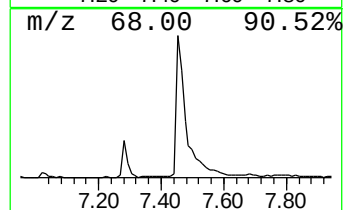
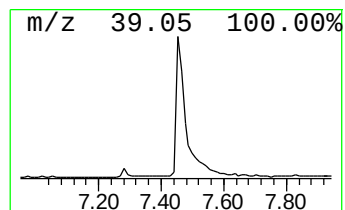
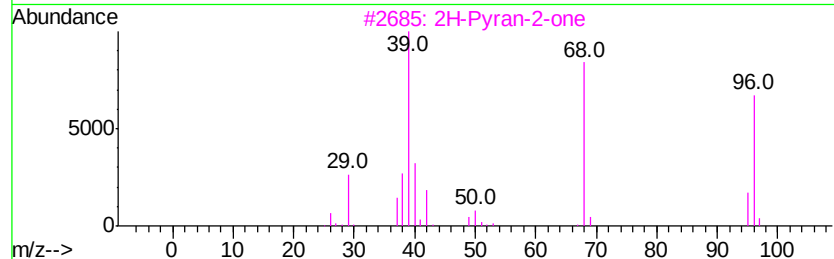
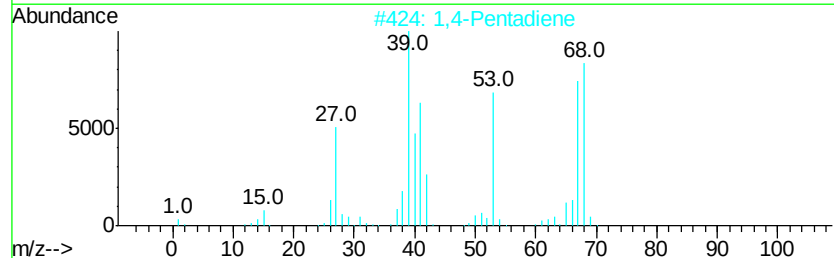
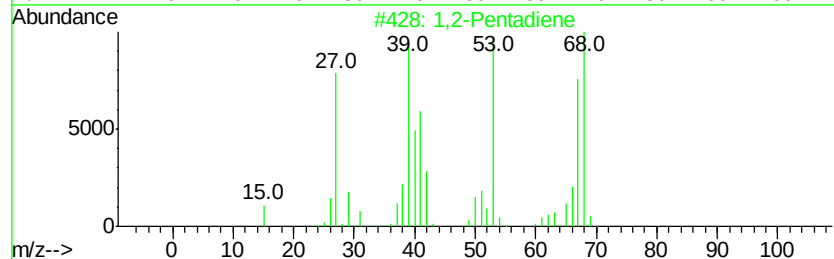
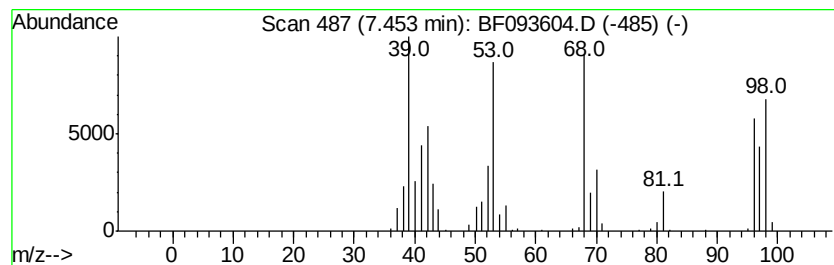
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1,2-Pentadiene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.45	13.55 ng	917597	Naphthalene-d8	8.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Pentadiene	68	C5H8	000591-95-7	81
2		1,4-Pentadiene	68	C5H8	000591-93-5	50
3		2H-Pyran-2-one	96	C5H4O2	000504-31-4	50
4		3,4-Pentadienal	82	C5H6O	004009-55-6	50
5		3(2H)-Pyridazinone	96	C4H4N2O	000504-30-3	49



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
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Sample : I2174-19
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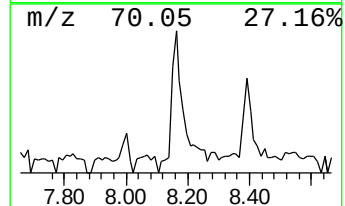
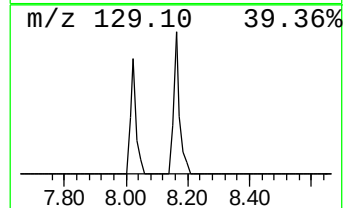
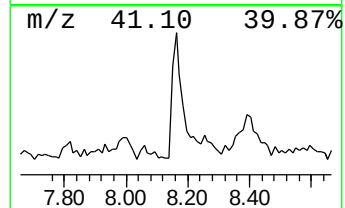
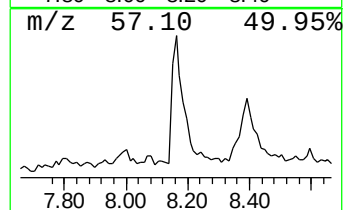
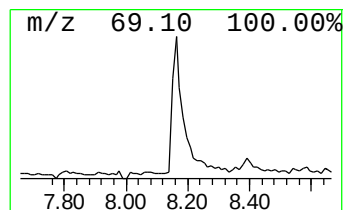
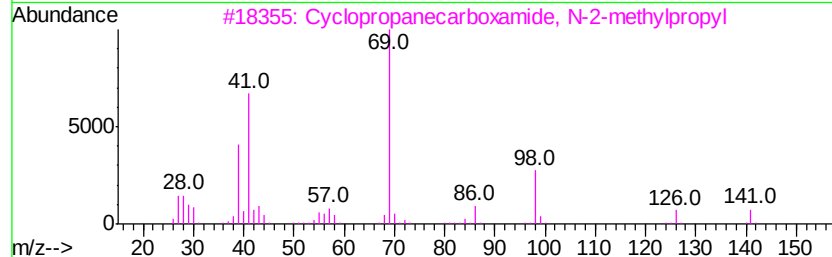
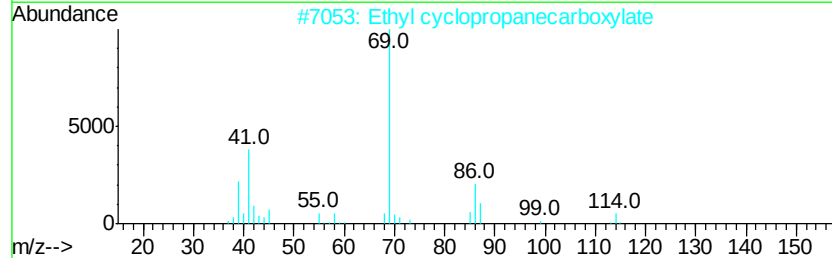
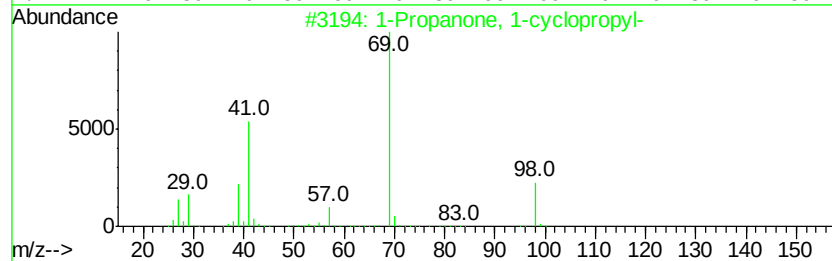
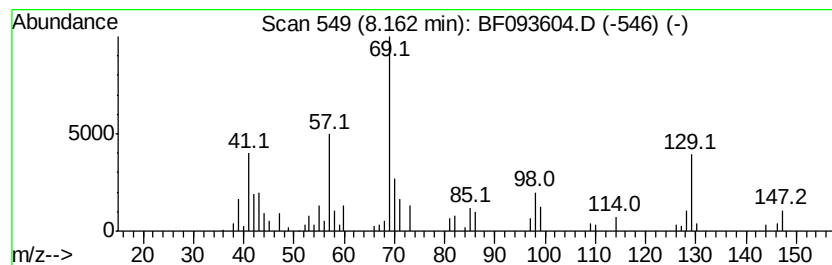
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown8.16 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.16	2.26 ng	153356	Napthalene-d8	8.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Propanone, 1-cvclopropyl-	98	C6H10O	006704-19-4	32
2		Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	25
3		Cyclopropanecarboxamide, N-2-met...	141	C8H15NO	122348-69-0	25
4		Hexane, 3-chloro-3-methyl-	134	C7H15Cl	043197-78-0	23
5		Cyclopropane, 1,1-dichloro-2-(1,...	194	C9H16Cl2	054824-03-2	23



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
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Misc :
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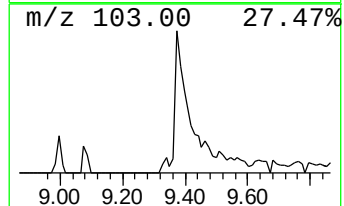
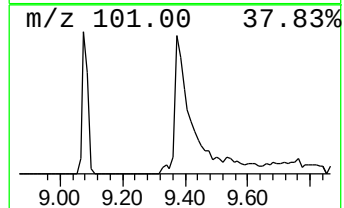
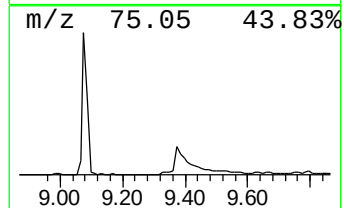
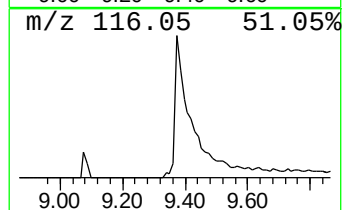
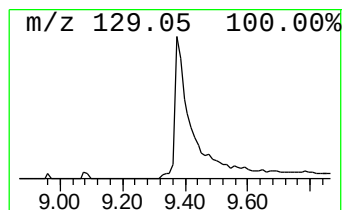
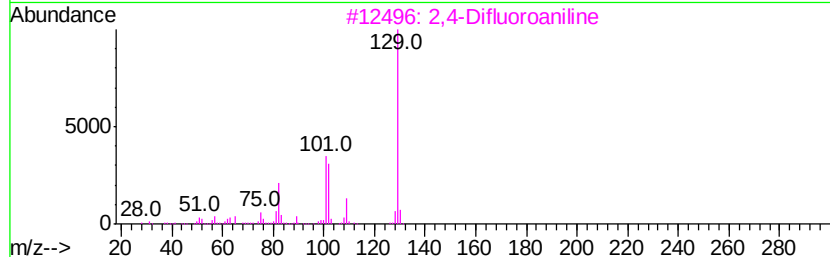
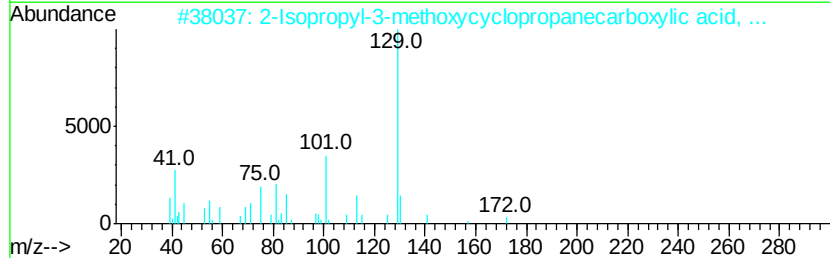
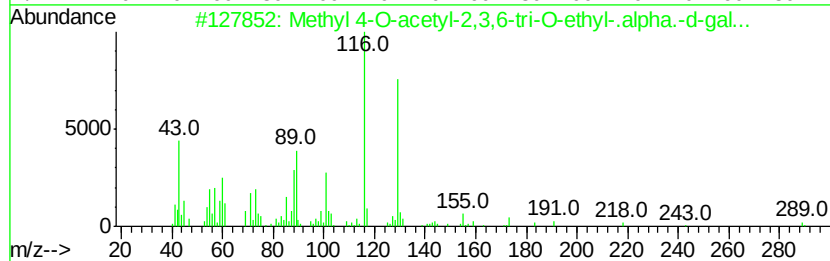
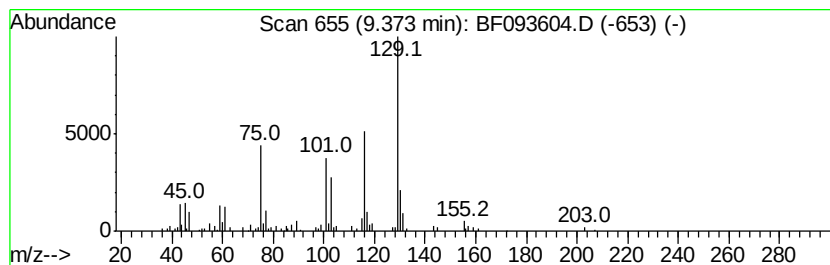
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown9.37 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.37	5.25 ng	271272	Acenaphthene-d10	9.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methyl 4-O-acetyl-2,3,6-tri-O-et...	320	C15H28O7	1000101-86-7	37
2		2-Isopropyl-3-methoxycyclopropan...	172	C9H16O3	122775-10-4	32
3		2,4-Difluoroaniline	129	C6H5F2N	000367-25-9	27
4		2,3-Difluoroaniline	129	C6H5F2N	004519-40-8	27
5		3,4-Difluoroaniline	129	C6H5F2N	003863-11-4	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
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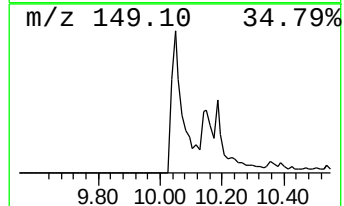
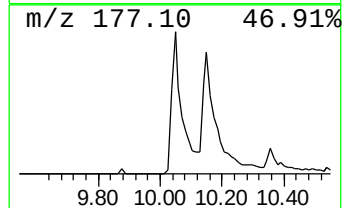
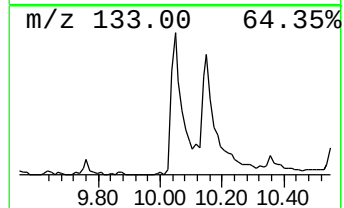
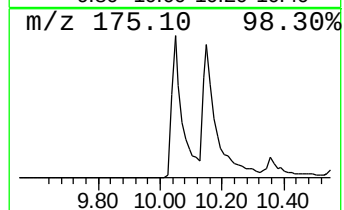
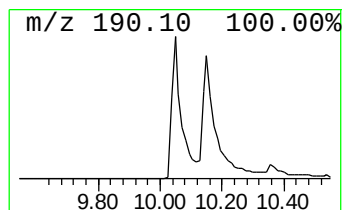
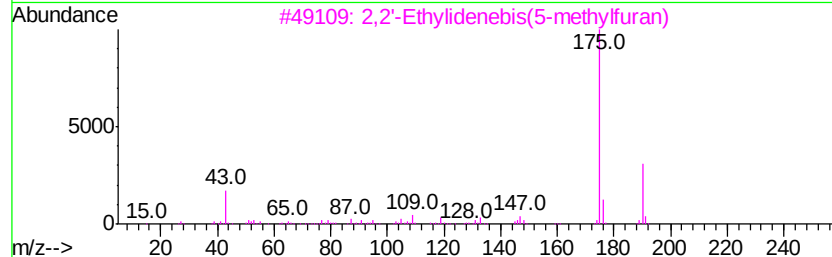
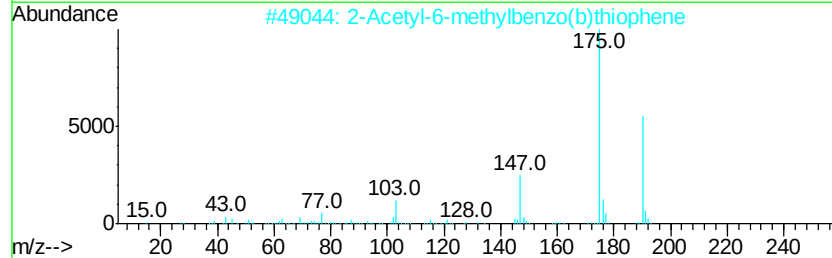
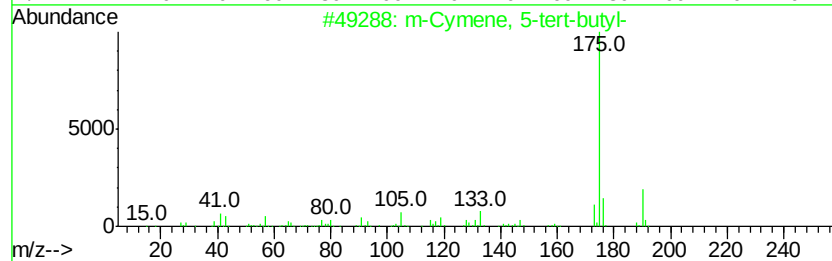
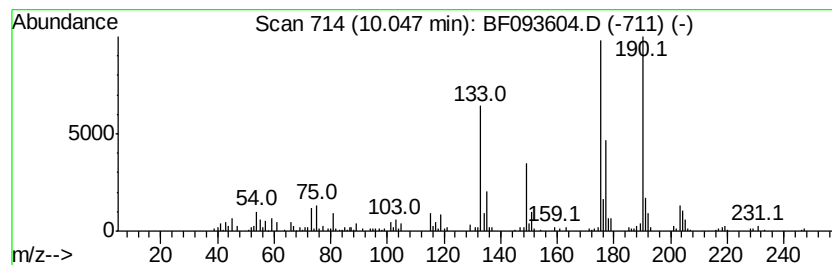
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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Peak Number 13 unknown10.05 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.05	12.90 ng	666494	Acenaphthene-d10	9.76	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	m-Cymene, 5-tert-butyl-	190	C14H22	029577-19-3	47
2	2-Acetyl-6-methylbenzo(b)thiophene	190	C11H10OS	001467-89-6	46
3	2,2'-Ethylidenebis(5-methylfuran)	190	C12H14O2	003209-79-8	43
4	2H-1-Benzopyran, 7-methoxy-2,2-d...	190	C12H14O2	017598-02-6	38
5	Pyrazol-5(4H)-one, 3-(4-methoxyp...	190	C10H10N2O2	001578-89-8	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
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ALS Vial : 9 Sample Multiplier: 1

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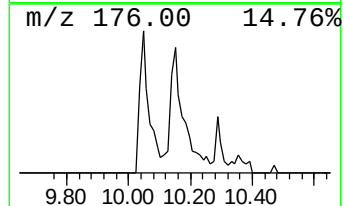
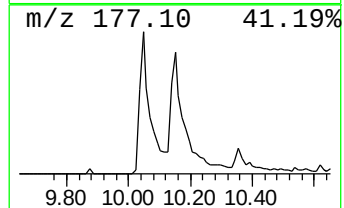
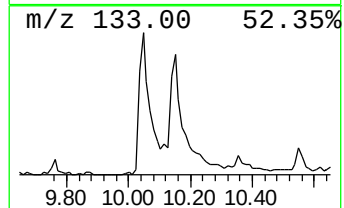
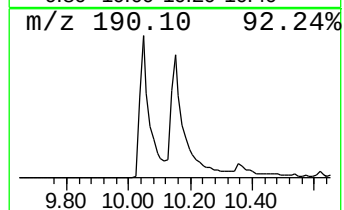
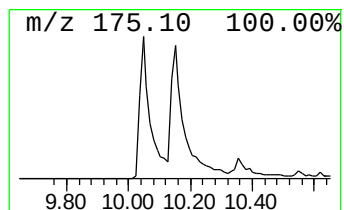
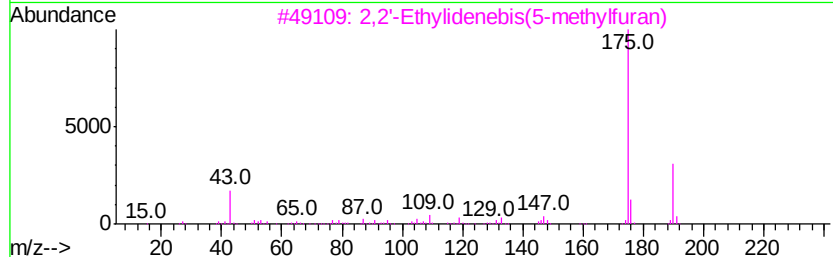
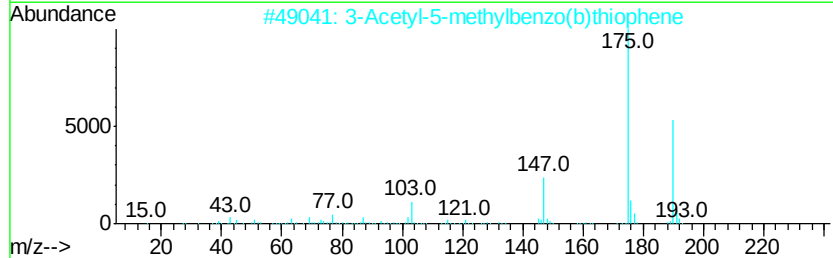
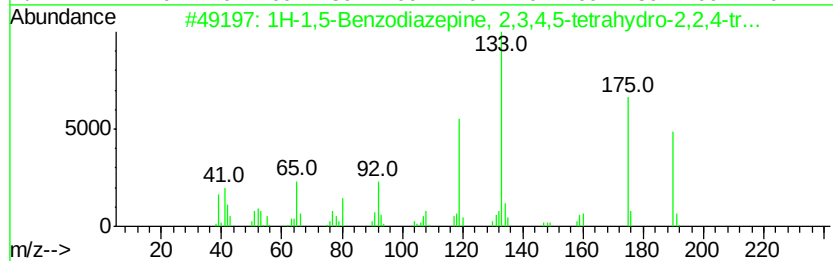
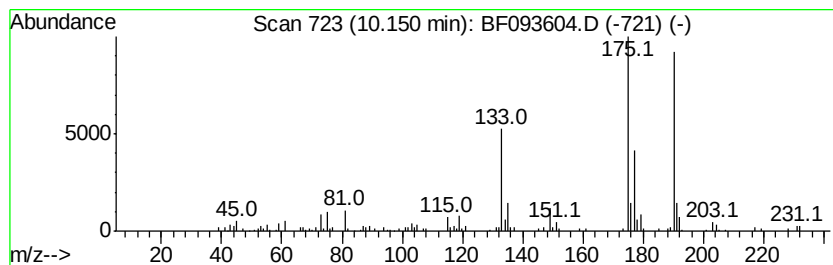
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 1H-1,5-Benzodiazepine, 2,3,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.15	9.44 ng	488085	Acenaphthene-d10	9.76

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-1,5-Benzodiazepine, 2,3,4,5-t...	190	C12H18N2	040358-38-1	59
2			3-Acetyl-5-methylbenzo(b)thiophene	190	C11H10OS	002046-76-6	52
3			2,2'-Ethylidenebis(5-methylfuran)	190	C12H14O2	003209-79-8	47
4			Disiloxane, 1,1,3,3-tetramethyl-...	362	C16H34O5Si2	000126-80-7	43
5			Ketone, 7-methoxy-2-benzofuranyl...	190	C11H10O3	043071-52-9	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
Data File : BF093604.D
Acq On : 13 Mar 2017 13:52
Operator : SJ/MA
Sample : I2174-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D-64

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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
Acetic acid, trim...	2.36	3.0	ng	141644	1	6.71	945372	20.0
n-Propyl acetate	2.41	3.2	ng	152969	1	6.71	945372	20.0
4-Penten-2-one, 4...	3.10	18.6	ng	879074	1	6.71	945372	20.0
3-Hexen-2-one	4.16	37.1	ng	1751540	1	6.71	945372	20.0
Cyclotrisiloxane,...	4.46	10.1	ng	477411	1	6.71	945372	20.0
2-Pentanone, 4-hy...	4.87	11.8	ng	558238	1	6.71	945372	20.0
unknown6.48	6.48	90.5	ng	4277340	1	6.71	945372	20.0
2-Piperidinone	7.02	6.1	ng	286242	1	6.71	945372	20.0
1,2-Pentadiene	7.45	13.6	ng	917597	2	8.00	1354550	20.0
unknown8.16	8.16	2.3	ng	153356	2	8.00	1354550	20.0
unknown9.37	9.37	5.3	ng	271272	3	9.76	1033620	20.0
unknown10.05	10.05	12.9	ng	666494	3	9.76	1033620	20.0
1H-1,5-Benzodiaze...	10.15	9.4	ng	488085	3	9.76	1033620	20.0