

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082019\
 Data File : BG042371.D
 Acq On : 20 Aug 2019 23:47
 Operator : HP/JU
 Sample : K4385-13
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 T8-C-(0-2)

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG081919.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.128	3	7	31	rVB	662398	1577286	63.57%	6.940%
2	5.572	415	423	439	rBV	680146	1271494	51.24%	5.595%
3	7.176	687	696	714	rBV	763258	1435109	57.84%	6.315%
4	7.546	747	759	772	rBV	820867	1517941	61.17%	6.679%
5	8.010	830	838	846	rBV	240910	426574	17.19%	1.877%
6	8.334	886	893	902	rBV	753037	1323333	53.33%	5.823%
7	9.174	1029	1036	1047	rBV	472170	870022	35.06%	3.828%
8	10.831	1309	1318	1331	rBV	306927	617314	24.88%	2.716%
9	13.110	1702	1706	1712	rVB2	122798	194569	7.84%	0.856%
10	13.287	1728	1736	1742	rBV	1538546	2481353	100.00%	10.918%
11	13.457	1760	1765	1772	rBV	211125	371633	14.98%	1.635%
12	14.092	1868	1873	1880	rBV2	724050	1227400	49.46%	5.401%
13	14.209	1889	1893	1902	rVB2	204277	367976	14.83%	1.619%
14	14.415	1922	1928	1933	rBV3	373836	812106	32.73%	3.573%
15	14.503	1939	1943	1950	rVB	969812	1472570	59.35%	6.480%
16	14.579	1950	1956	1960	rBV3	221538	480291	19.36%	2.113%
17	14.638	1961	1966	1968	rBV	501805	800488	32.26%	3.522%
18	14.667	1968	1971	1980	rVB	577728	939984	37.88%	4.136%
19	14.761	1984	1987	1992	rVB2	164425	288681	11.63%	1.270%
20	15.190	2057	2060	2064	rBV3	232945	354556	14.29%	1.560%
21	15.390	2090	2094	2099	rBV4	319827	580571	23.40%	2.555%
22	15.461	2102	2106	2113	rVB2	943805	1589004	64.04%	6.992%
23	16.166	2221	2226	2230	rBV2	1050091	1726112	69.56%	7.595%

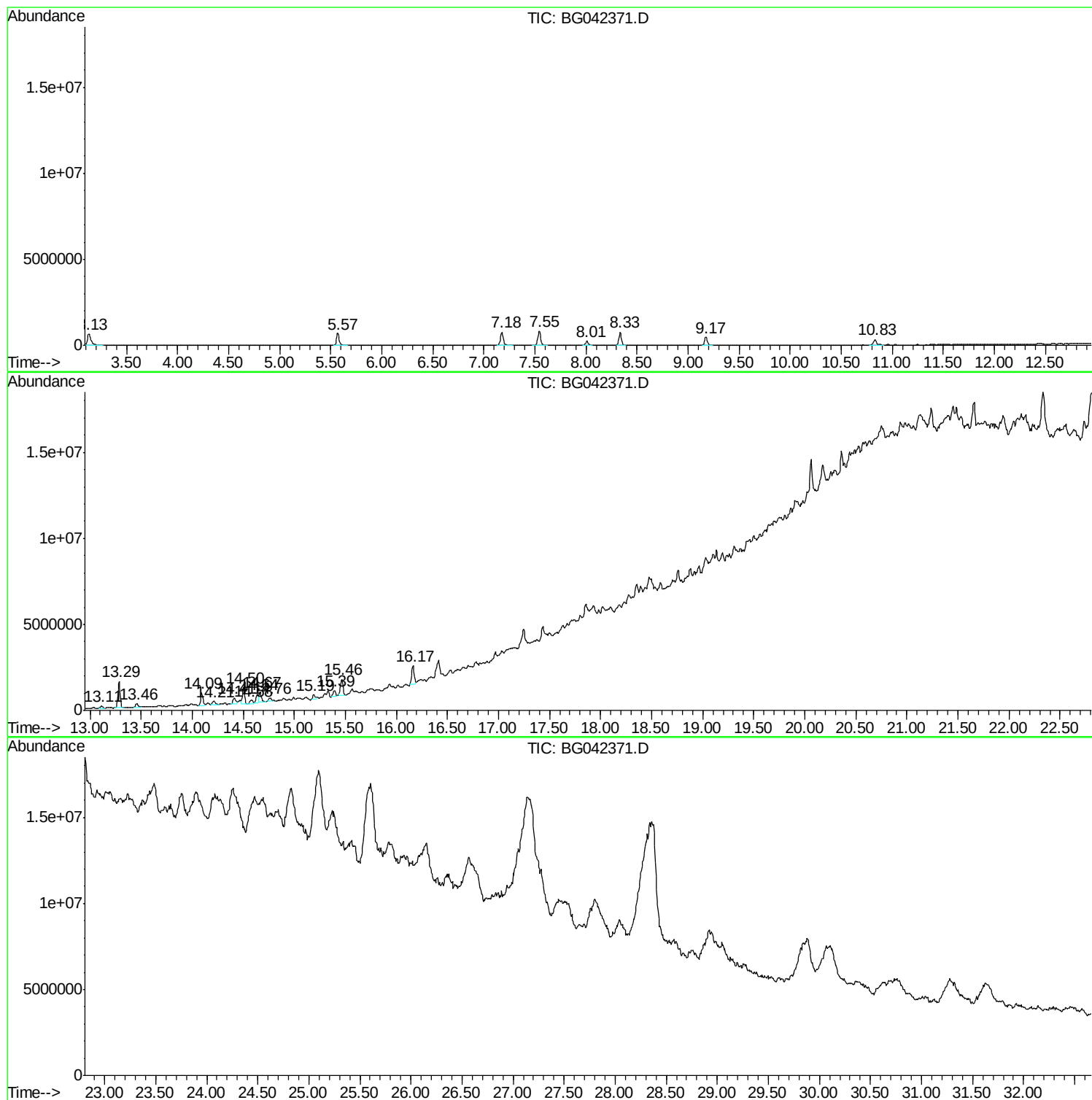
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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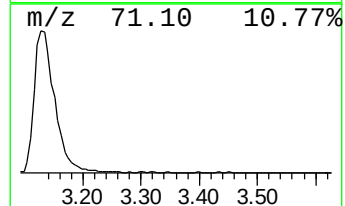
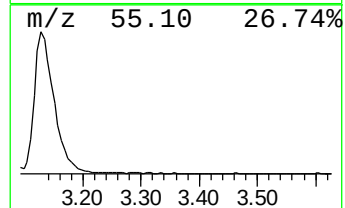
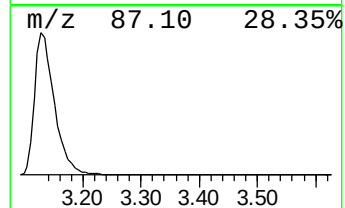
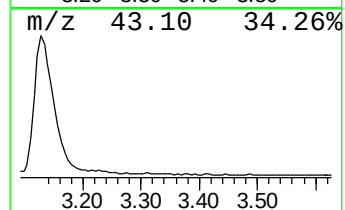
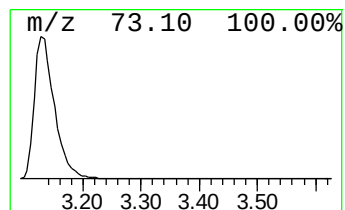
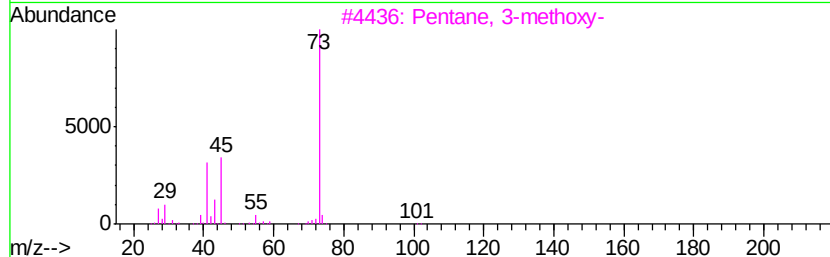
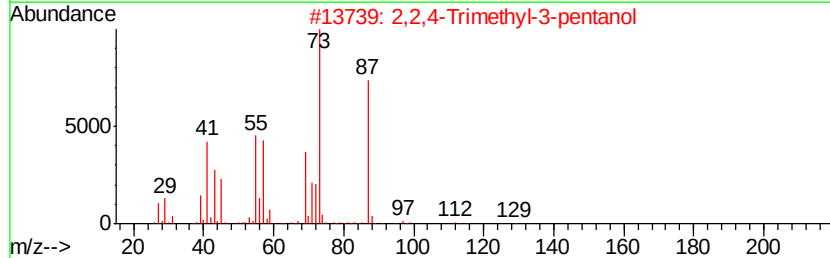
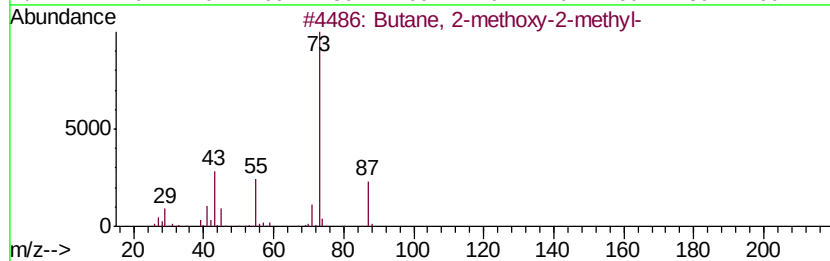
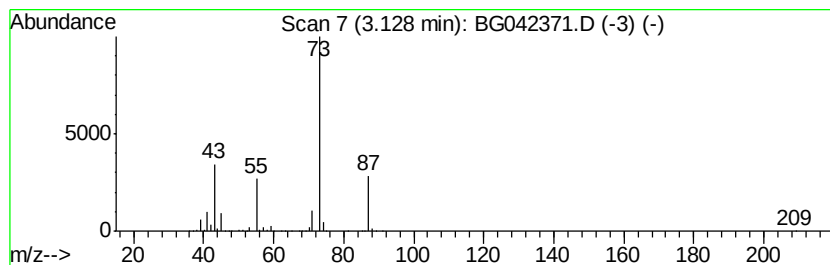
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	73.95 ng	1577290	1,4-Dichlorobenzene-d4	8.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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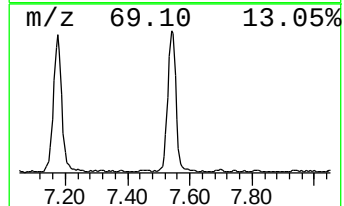
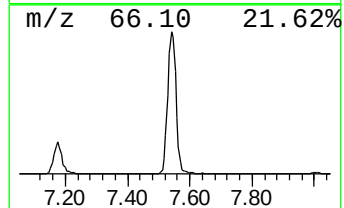
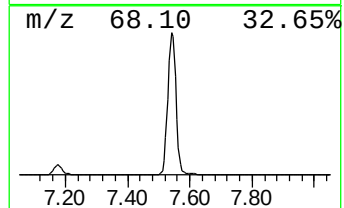
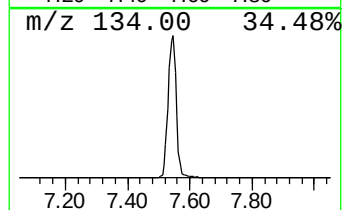
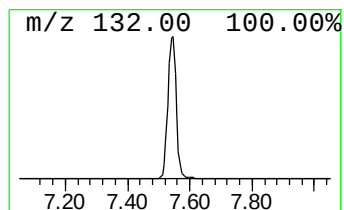
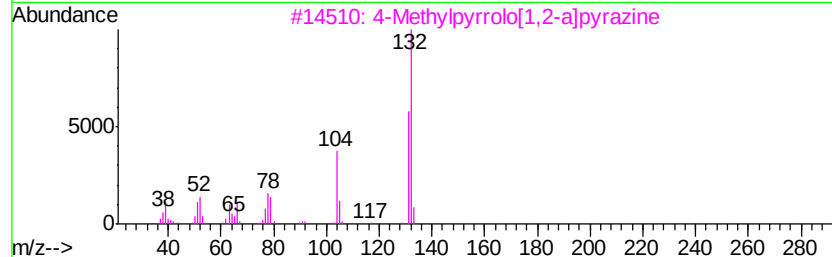
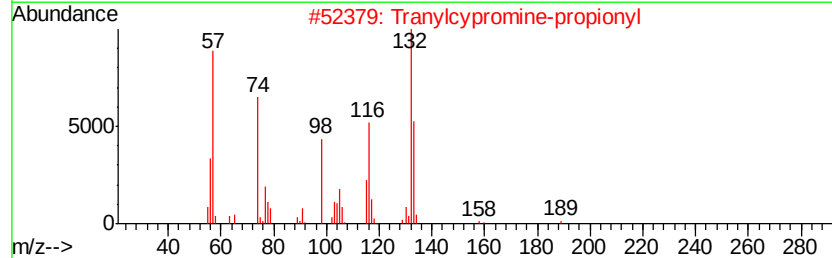
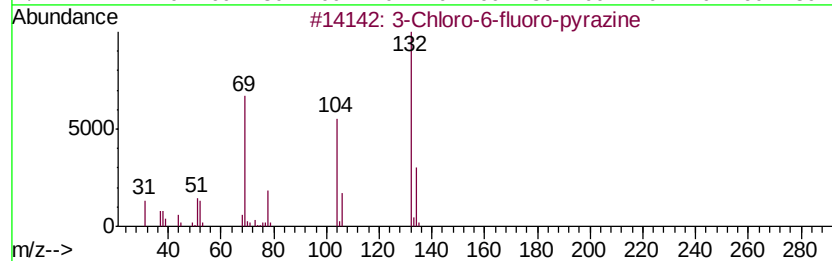
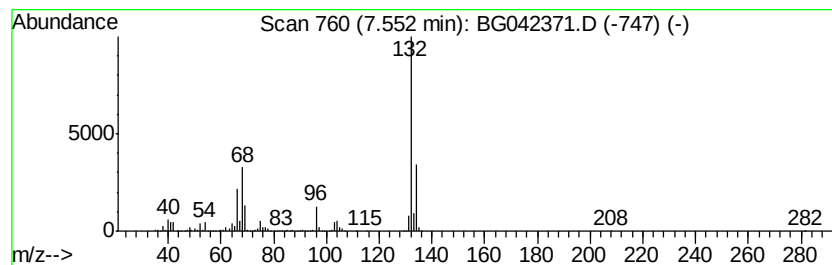
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.55 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.55	71.17 ng	1517940	1,4-Dichlorobenzene-d4	8.01

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3			4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5			1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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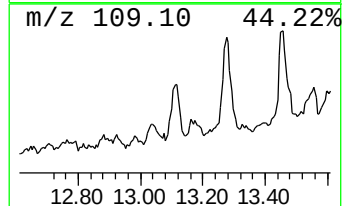
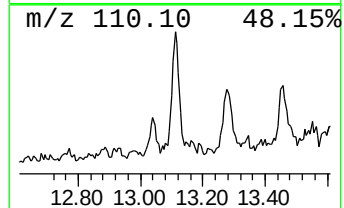
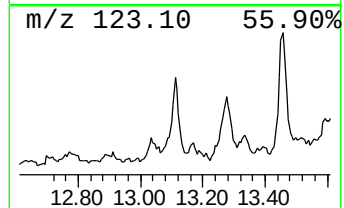
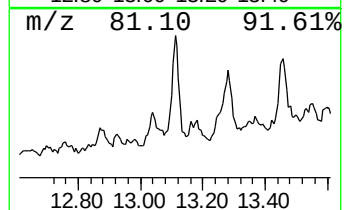
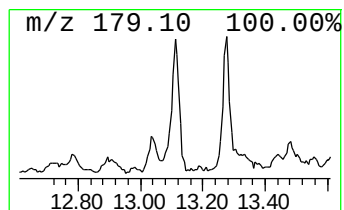
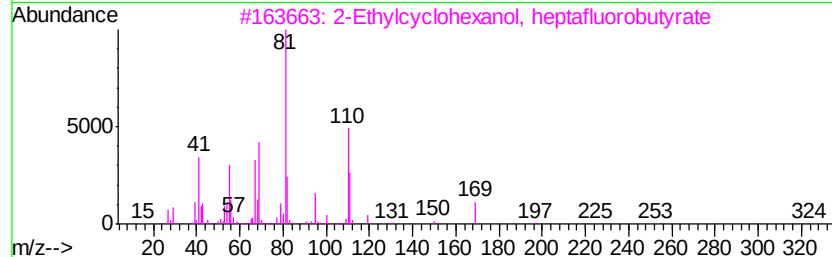
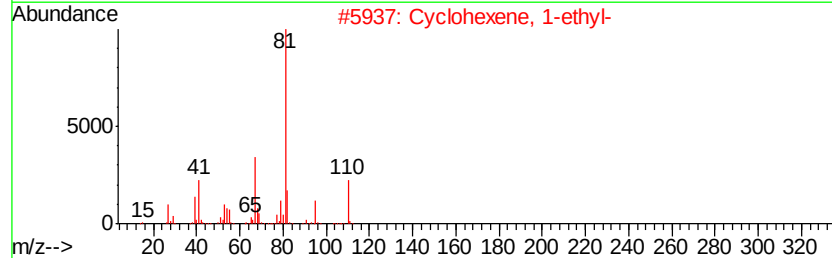
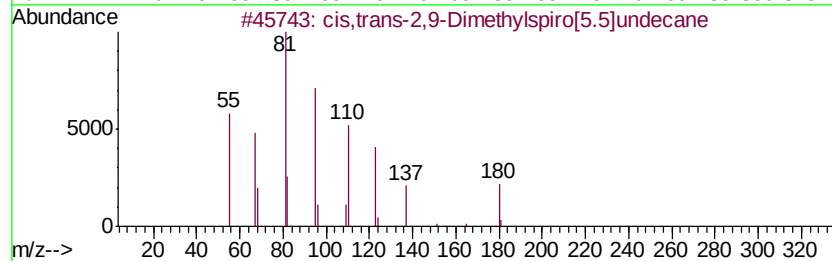
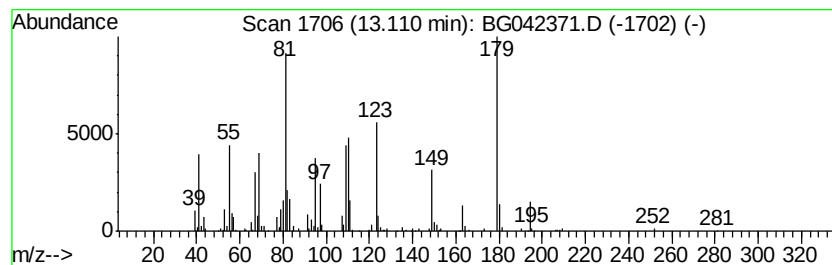
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Peak Number 4 unknown13.11 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.11	4.14 ng	194569	Acenaphthene-d10	14.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	cis,trans-2,9-Dimethylspiro[5.5]undecane	180	C13H24	095530-74-8	27
2		Cyclohexene, 1-ethyl-	110	C8H14	001453-24-3	25
3		2-Ethylcyclohexanol, heptafluoro...	324	C12H15F7O2	959079-92-6	22
4		4-Ethylcyclohexene	110	C8H14	003742-42-5	22
5		1H-Purin-2-amine, 6-methoxy-N-me...	179	C7H9N5O	050704-44-4	22



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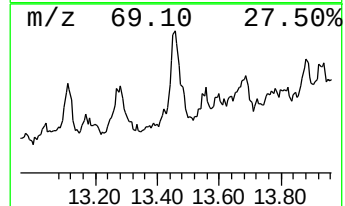
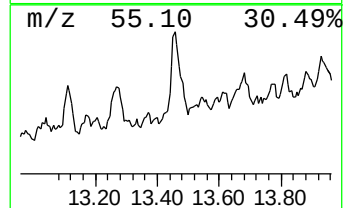
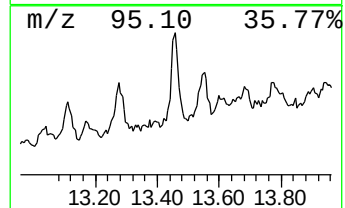
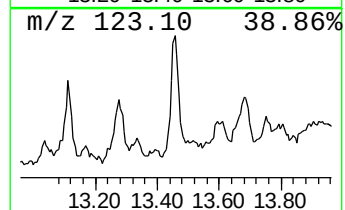
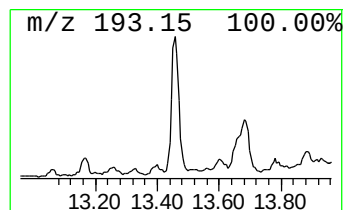
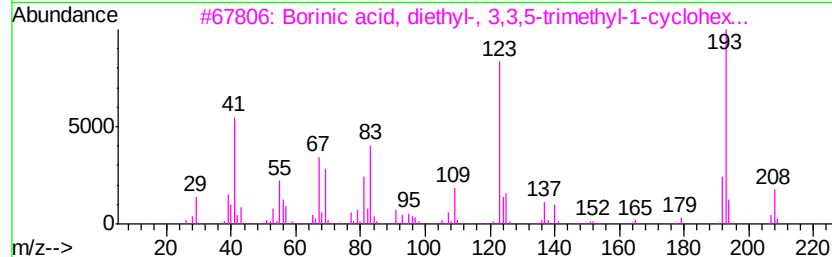
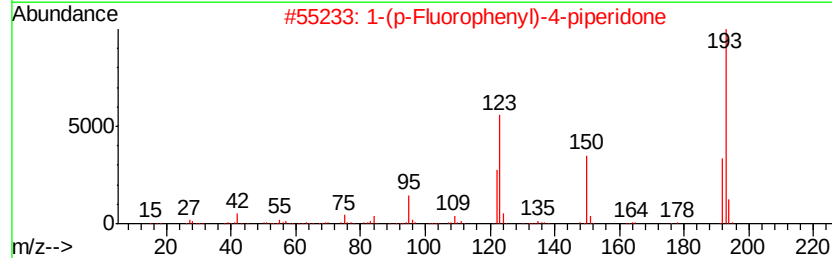
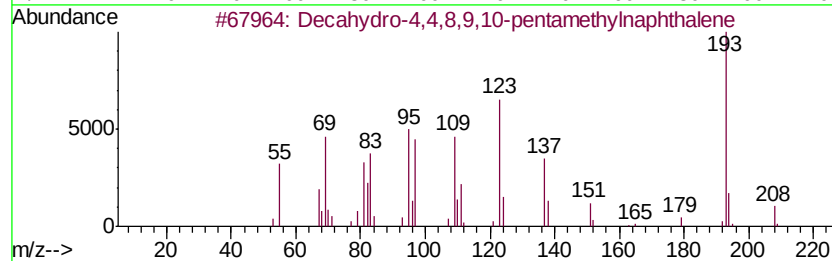
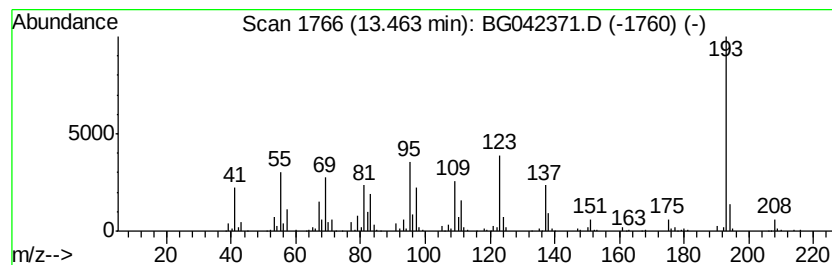
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Peak Number 5 Decahydro-4,4,8,9,10-pentam... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.46	7.91 ng	371633	Acenaphthene-d10	14.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	92
2		1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	43
3		Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	37
4		[1,1'-Biphenyl]-4-acetonitrile	193	C14H11N	031603-77-7	27
5		2-Amino-4-(trifluoromethyl)benze...	193	C7H6F3NS	004274-38-8	25



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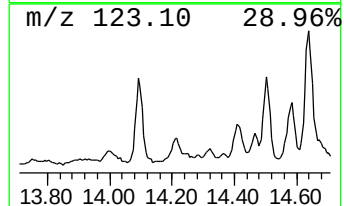
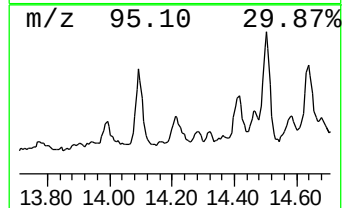
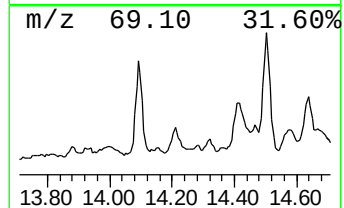
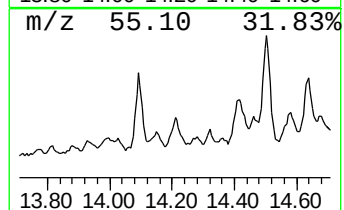
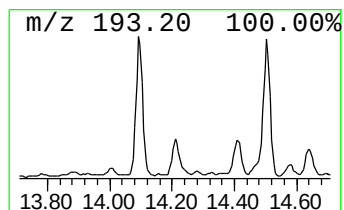
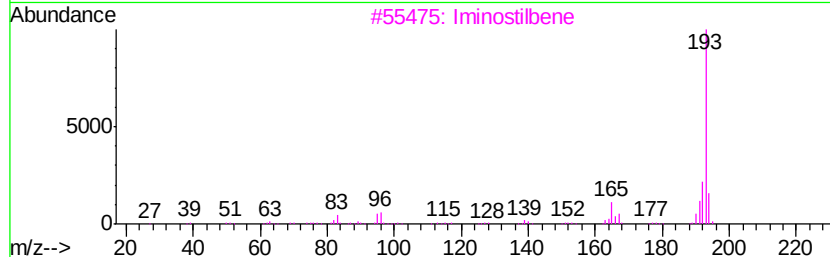
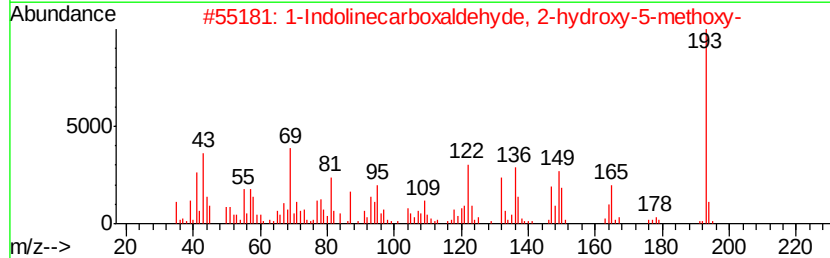
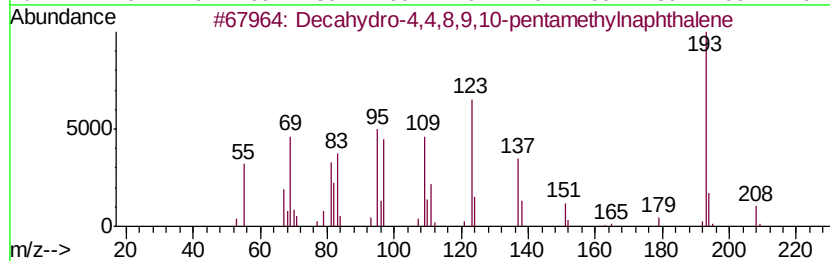
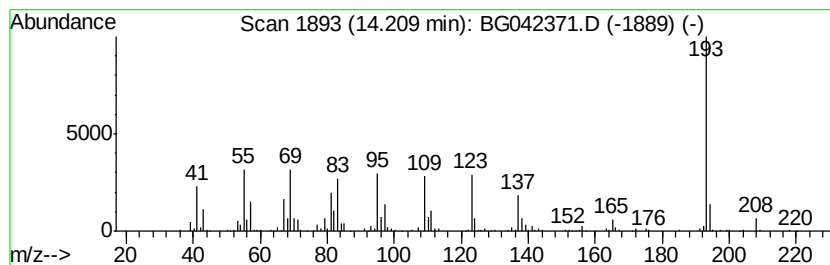
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Peak Number 6 1-Indolinecarboxaldehyde, 2... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.21	7.83 ng	367976	Acenaphthene-d10	14.67	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	86
2	1-Indolinecarboxaldehyde, 2-hydr...	193	C10H11N03	013303-70-3	50
3	Iminostilbene	193	C14H11N	000256-96-2	46
4	S-Phenyl 5-(phenylthio)pentaneth...	302	C17H18S2	1000234-40-7	40
5	Acridine, 9-methyl-	193	C14H11N	000611-64-3	35



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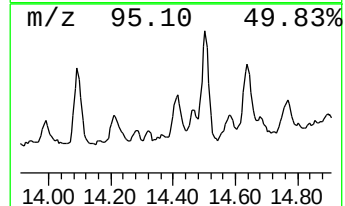
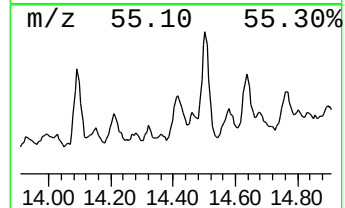
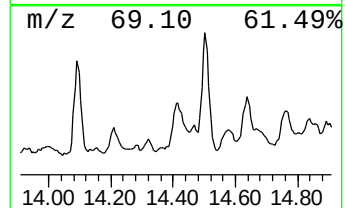
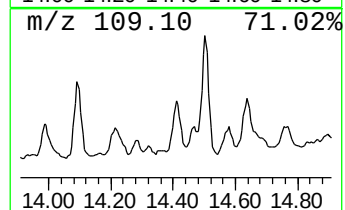
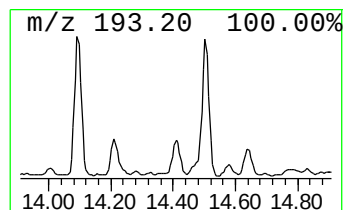
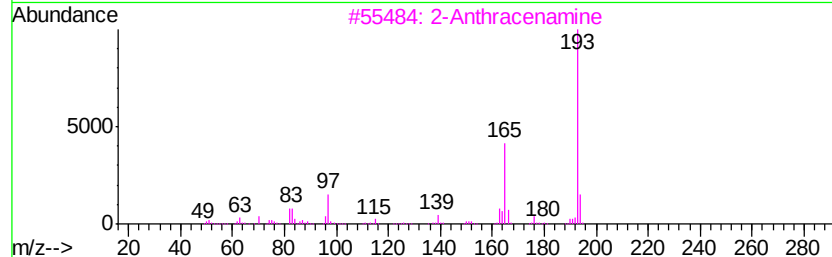
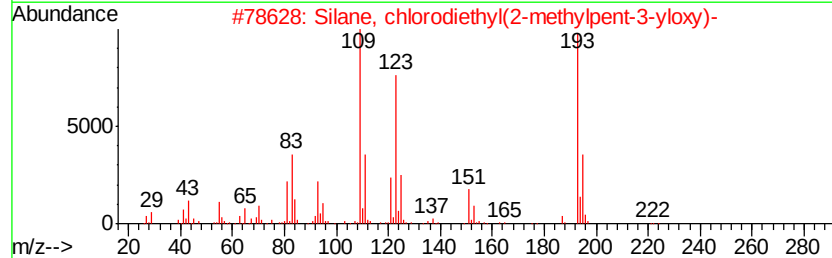
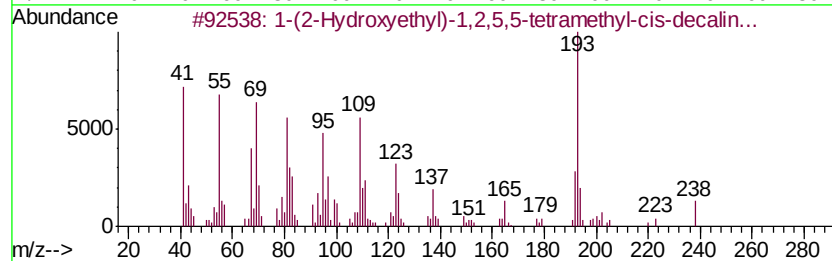
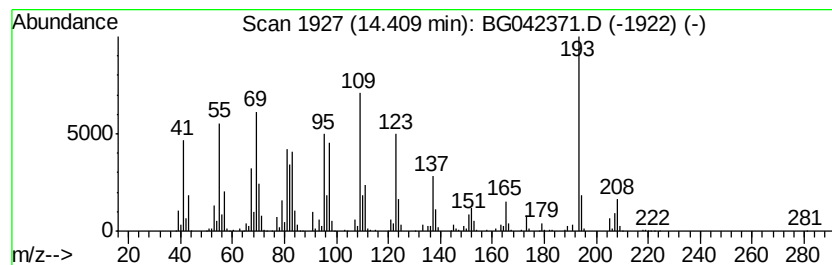
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ClientSampleId :
T8-C-(0-2)

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1-(2-Hydroxyethyl)-1,2,5,5-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.41	17.28 ng	812106	Acenaphthene-d10	14.67
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1-(2-Hydroxyethyl)-1,2,5,5-tetra...	238 C16H30O	1000298-97-4 64
2		Silane, chlorodiethyl(2-methylpe...	222 C10H23ClOSi	1000363-79-1 53
3		2-Anthracenamine	193 C14H11N	000613-13-8 42
4		2(1H)-Naphthalenone, octahydro-4...	194 C13H22O	054699-31-9 38
5		2,6-Heptadienal, 2,4-dimethyl-	138 C9H14O	085136-08-9 35



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082019\
Data File : BG042371.D
Acq On : 20 Aug 2019 23:47
Operator : HP/JU
Sample : K4385-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
T8-C-(0-2)

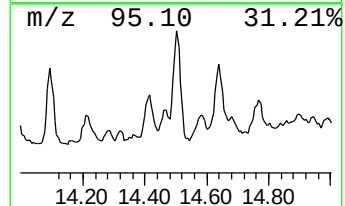
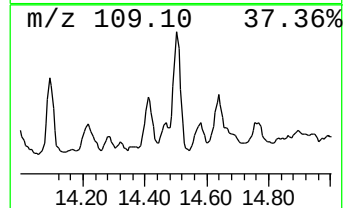
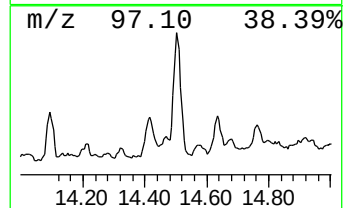
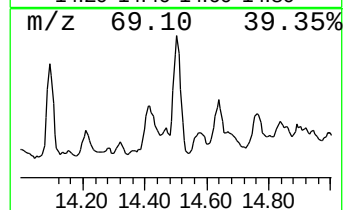
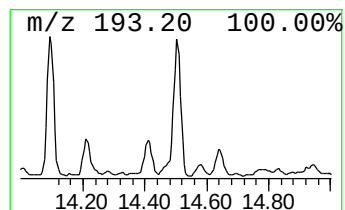
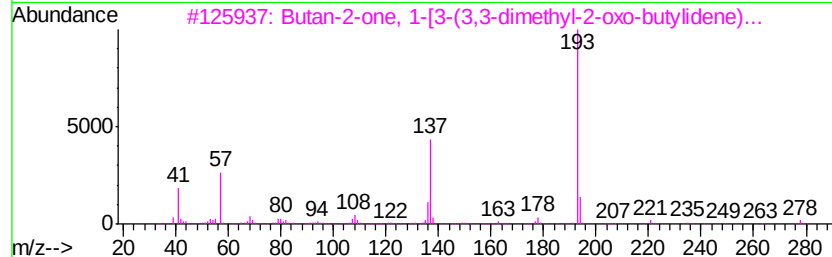
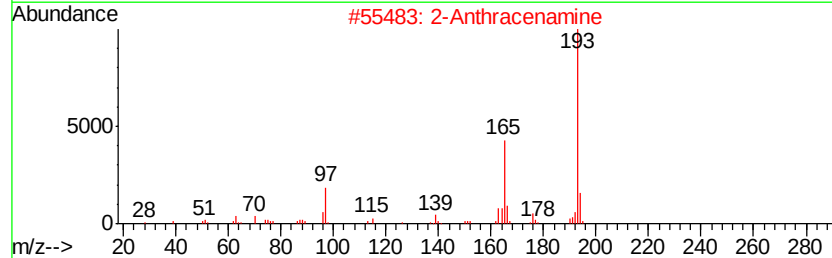
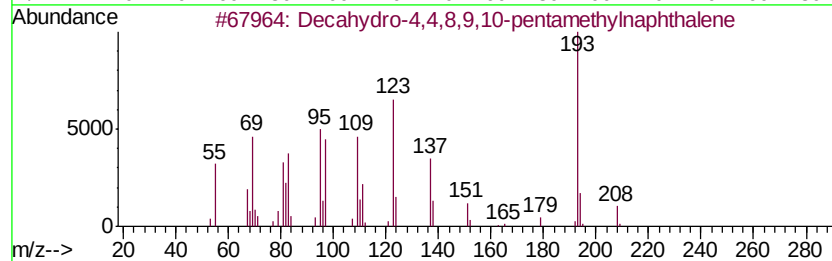
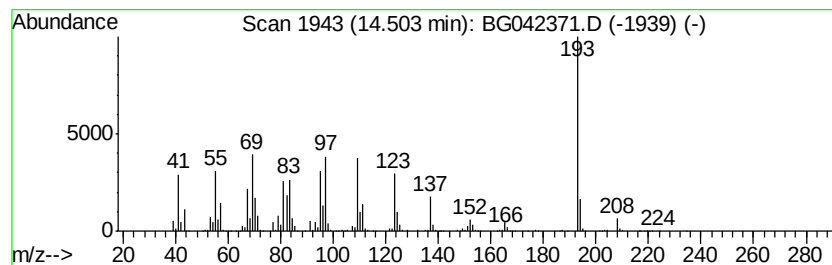
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown14.50 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	31.33 ng	1472570	Acenaphthene-d10	14.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	62
2		2-Anthracenamine	193	C14H11N	000613-13-8	46
3		Butan-2-one, 1-[3-(3,3-dimethyl-...	278	C16H26N2O2	1000303-34-2	35
4		2-Phenylindolizine	193	C14H11N	025379-20-8	35
5		2-Aminophenanthrene	193	C14H11N	003366-65-2	27



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082019\
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Sample : K4385-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

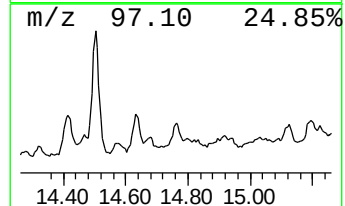
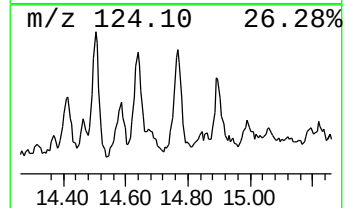
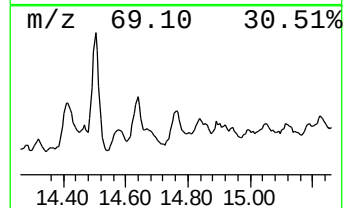
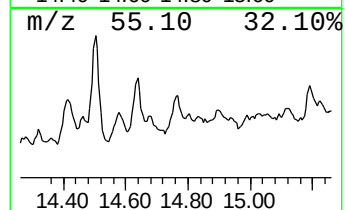
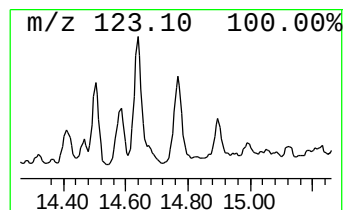
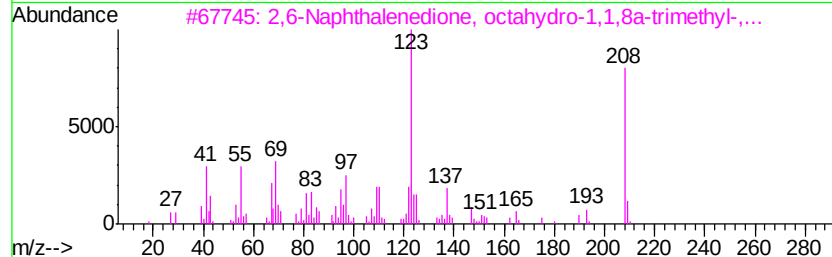
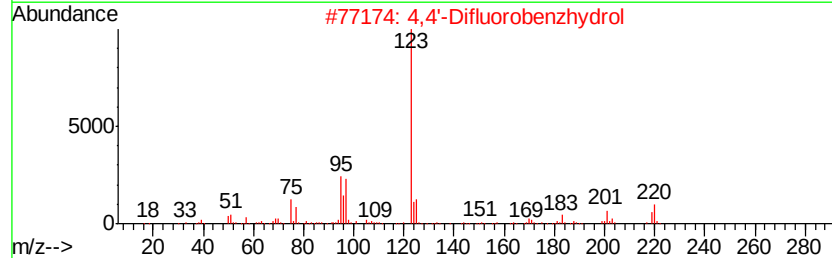
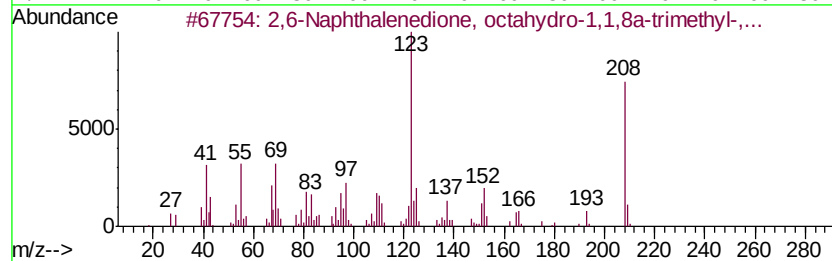
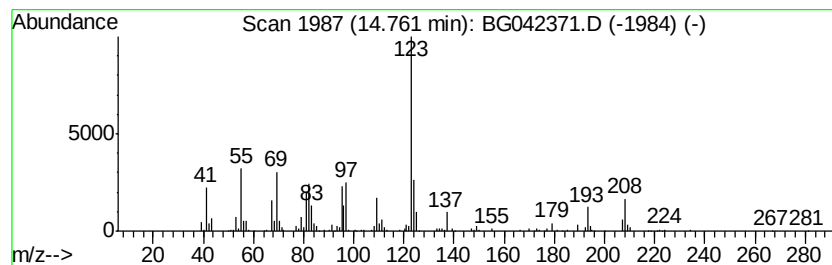
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 2,6-Naphthalenedione, octah... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.76	6.14 ng	288681	Acenaphthene-d10		14.67
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Naphthalenedione, octahydro-...	208	C13H20O2	057289-17-5	64
2	4,4'-Difluorobenzhydrol	220	C13H10F2O	000365-24-2	45
3	2,6-Naphthalenedione, octahydro-...	208	C13H20O2	057289-16-4	45
4	Benzamide, 4-fluoro-N-methallyl-	193	C11H12FN0	1000340-31-9	43
5	Cyclohexene, 1,5,5-trimethyl-6-a...	180	C12H20O	211563-96-1	42



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082019\
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Operator : HP/JU
Sample : K4385-13
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ALS Vial : 11 Sample Multiplier: 1

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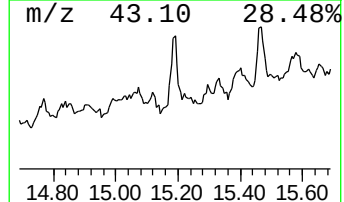
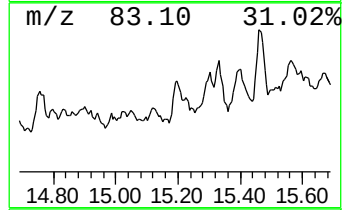
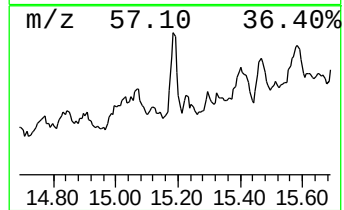
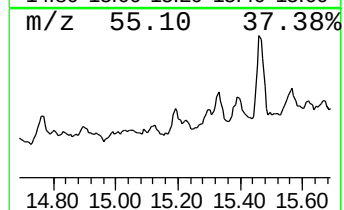
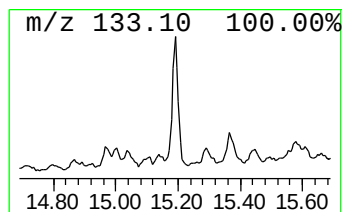
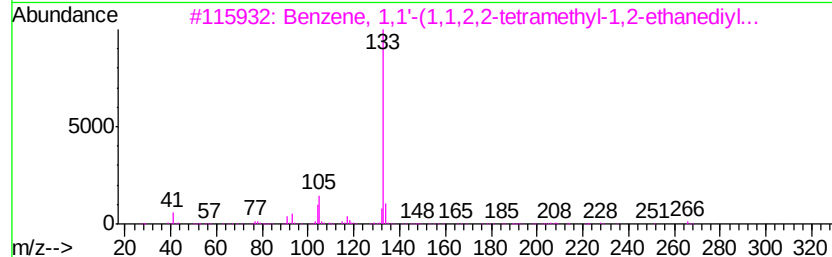
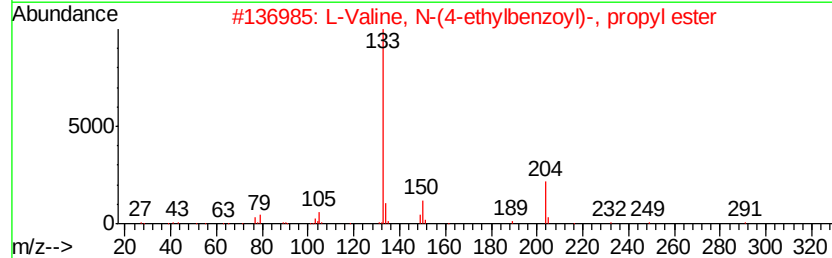
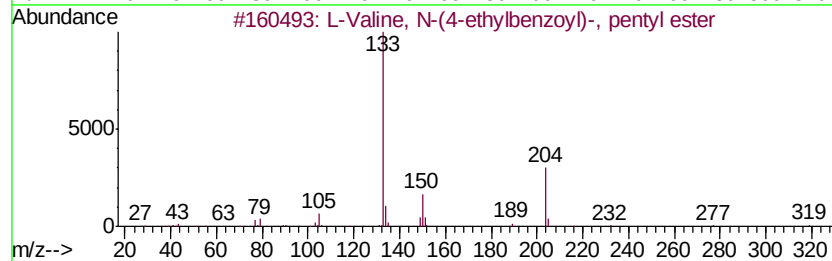
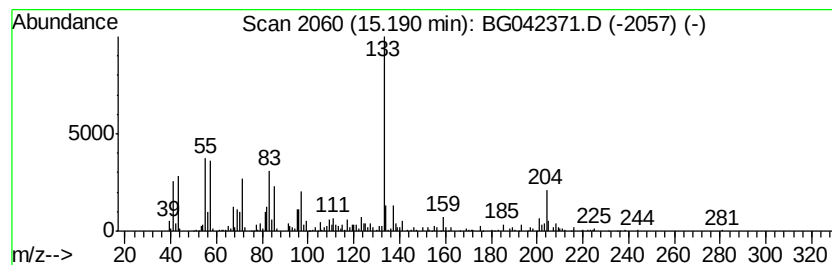
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown15.19 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.19	7.54 ng	354556	Acenaphthene-d10	14.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	L-Valine, N-(4-ethylbenzoyl)-, p...	319	C19H29N03	1000346-63-0	38
2		L-Valine, N-(4-ethylbenzoyl)-, p...	291	C17H25N03	1000346-62-9	38
3		Benzene, 1,1'-(1,1,2,2-tetrameth...	266	C20H26	000734-17-8	35
4		Glycine, N-(4-ethylbenzoyl)-, is...	263	C15H21N03	1000314-51-4	35
5		1H-Benzimidazol-5-amine	133	C7H7N3	000934-22-5	30



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082019\
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Acq On : 20 Aug 2019 23:47
Operator : HP/JU
Sample : K4385-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

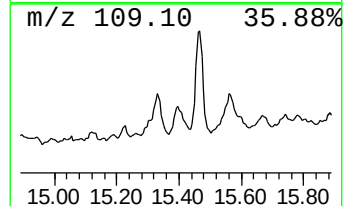
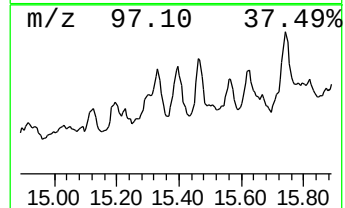
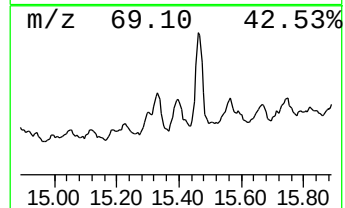
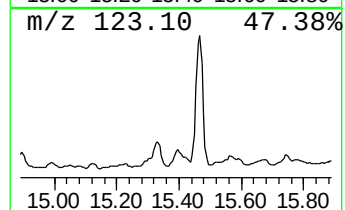
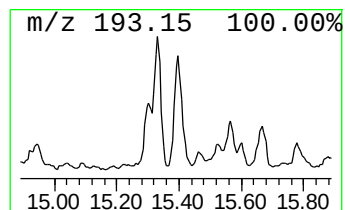
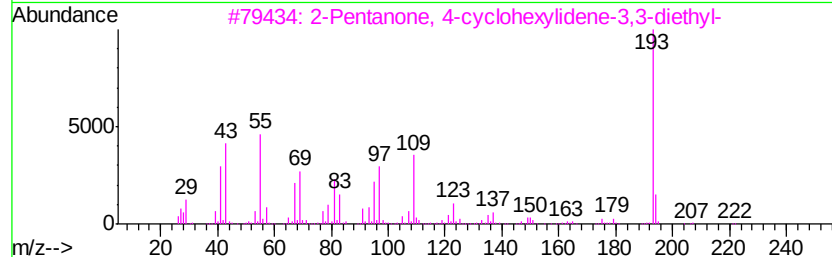
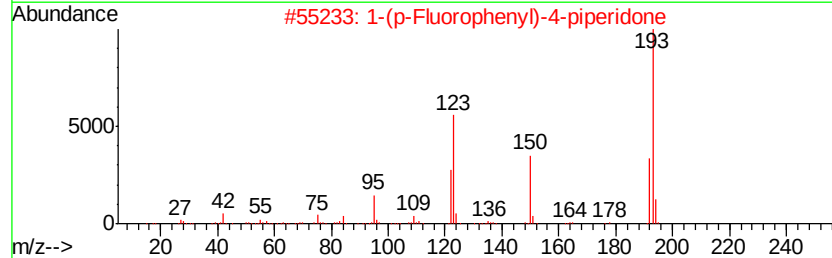
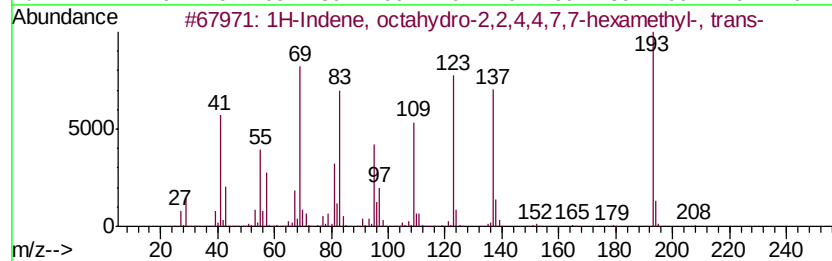
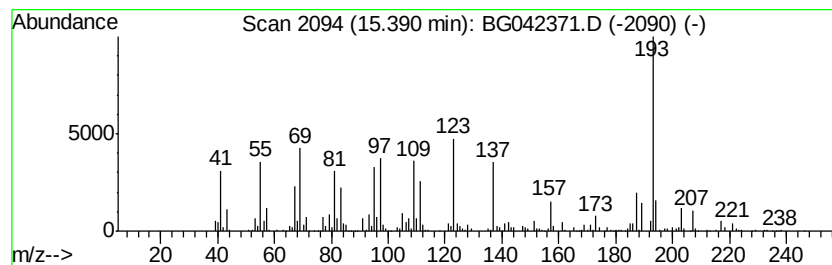
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 1H-Indene, octahydro-2,2,4,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.39	12.35 ng	580571	Acenaphthene-d10	14.67		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	58
2		1-(p-Fluorophenyl)-4-piperidone	193	C11H12FN0	1000238-56-7	46
3		2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	43
4		S-Phenyl 5-(phenylthio)pentaneth...	302	C17H18OS2	1000234-40-7	43
5		Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	37



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082019\
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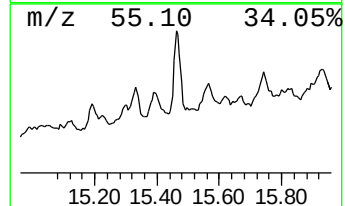
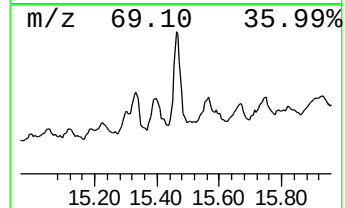
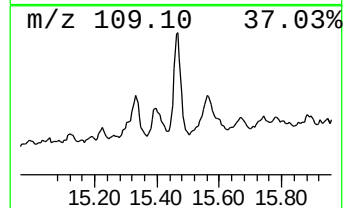
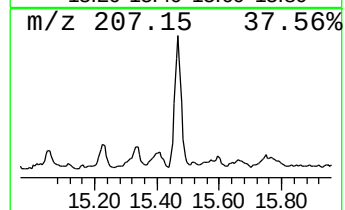
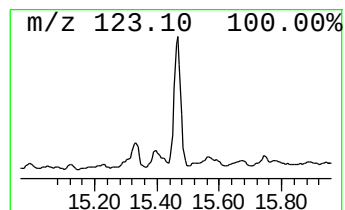
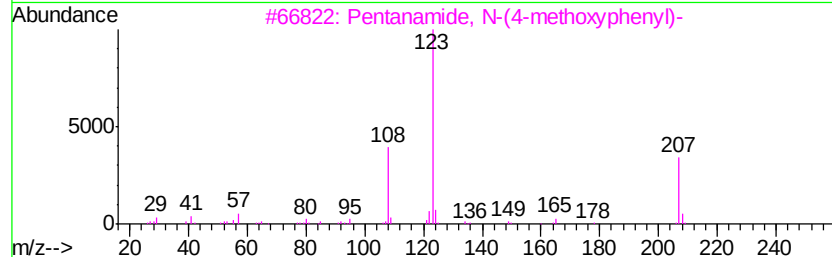
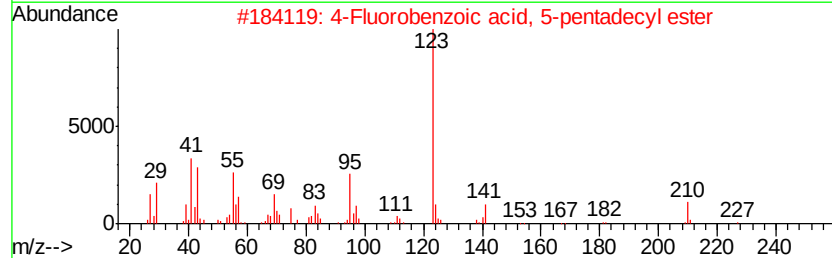
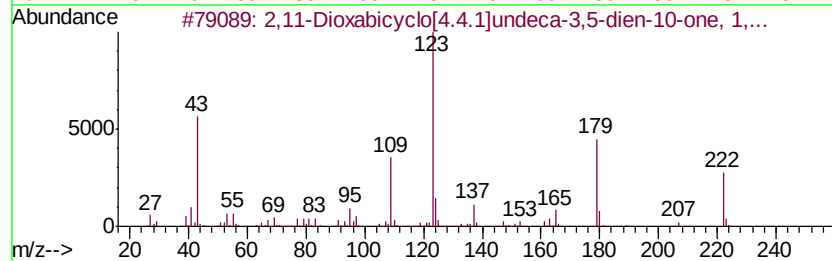
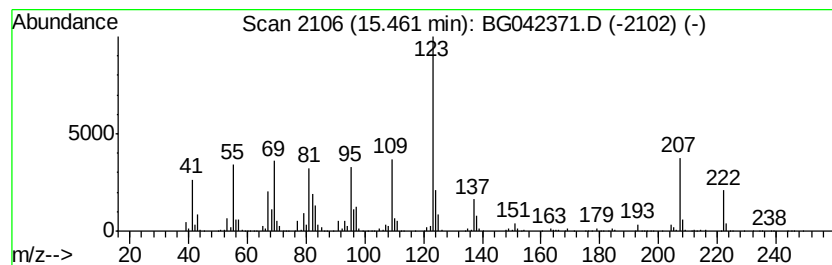
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 2,11-Dioxabicyclo[4.4.1]und... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.46	33.81 ng	1589000	Acenaphthene-d10	14.67
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2,11-Dioxabicyclo[4.4.1]undeca-3...	222	C13H18O3	070412-52-1 53
2	4-Fluorobenzoic acid, 5-pentadec...	350	C22H35FO2	1000280-68-6 47
3	Pentanamide, N-(4-methoxyphenyl)-	207	C12H17NO2	1000306-89-3 45
4	1-Trimethylsilylpent-1-en-4-yne	138	C8H14Si	079516-25-9 43
5	1-(1-Ethyl-2,3-dimethyl-cyclopen...	166	C11H18O	1000185-18-6 38



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG082019\
Data File : BG042371.D
Acq On : 20 Aug 2019 23:47
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Sample : K4385-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
T8-C-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG081919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.13	74.0	ng	1577290	1	8.01	426574	20.0
unknown7.55	7.55	71.2	ng	1517940	1	8.01	426574	20.0
unknown13.11	13.11	4.1	ng	194569	3	14.67	939984	20.0
Decahydro-4,4,8,9...	13.46	7.9	ng	371633	3	14.67	939984	20.0
1-Indolinecarboxa...	14.21	7.8	ng	367976	3	14.67	939984	20.0
1-(2-Hydroxyethyl...	14.41	17.3	ng	812106	3	14.67	939984	20.0
unknown14.50	14.50	31.3	ng	1472570	3	14.67	939984	20.0
2,6-Naphthalenedi...	14.76	6.1	ng	288681	3	14.67	939984	20.0
unknown15.19	15.19	7.5	ng	354556	3	14.67	939984	20.0
1H-Indene, octahy...	15.39	12.4	ng	580571	3	14.67	939984	20.0
2,11-Dioxabicyclo...	15.46	33.8	ng	1589000	3	14.67	939984	20.0