

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020822\
 Data File : BG052328.D
 Acq On : 8 Feb 2022 20:44
 Operator : CG/JU
 Sample : N1387-07
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 24801

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

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

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG052328.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.758	377	386	402	rVB	477716	789135	46.68%	7.612%
2	7.374	653	661	673	rBV	521014	934464	55.28%	9.014%
3	8.226	795	806	817	rBV	121295	236049	13.96%	2.277%
4	9.400	999	1006	1013	rBV	347006	630200	37.28%	6.079%
5	11.069	1284	1290	1297	rVB	168166	307861	18.21%	2.970%
6	13.090	1631	1634	1641	rVB6	46678	91764	5.43%	0.885%
7	13.495	1697	1703	1709	rBV	885408	1431694	84.69%	13.810%
8	14.311	1837	1842	1845	rBV	401752	642204	37.99%	6.195%
9	14.405	1854	1858	1869	rVB4	353185	743321	43.97%	7.170%
10	14.523	1875	1878	1883	rBV2	319499	415430	24.57%	4.007%
11	14.629	1891	1896	1902	rBV5	418976	1069240	63.25%	10.314%
12	14.717	1907	1911	1916	rVB	1075641	1690549	100.00%	16.307%
13	15.680	2072	2075	2083	rVB	985406	1385342	81.95%	13.363%

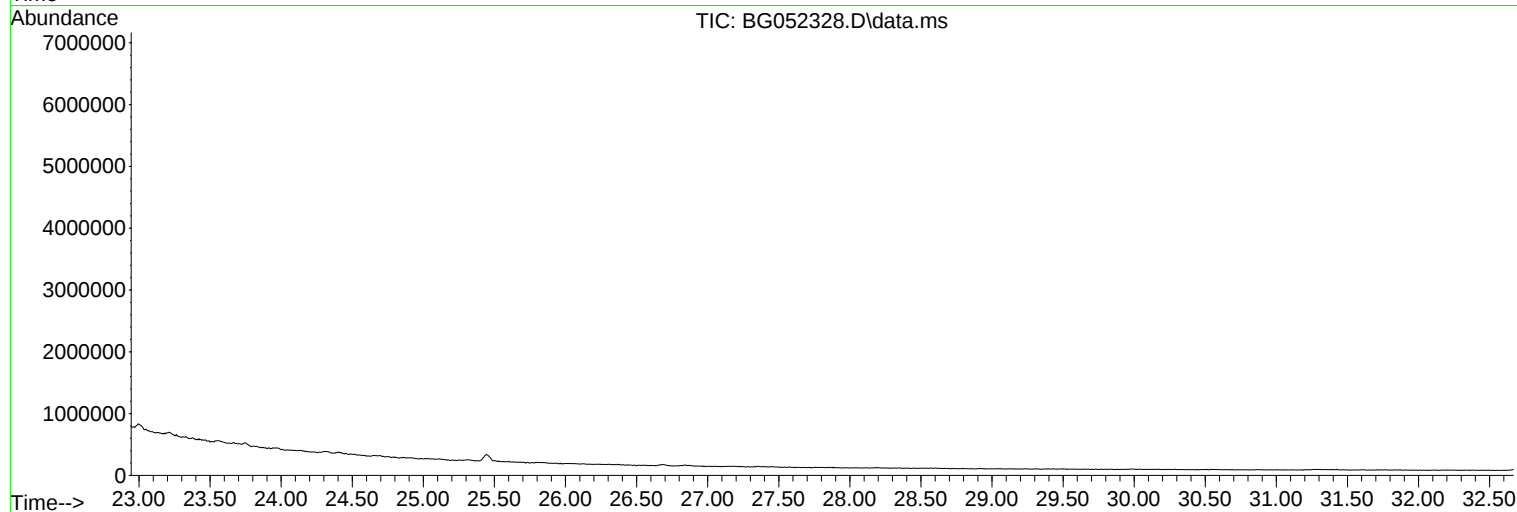
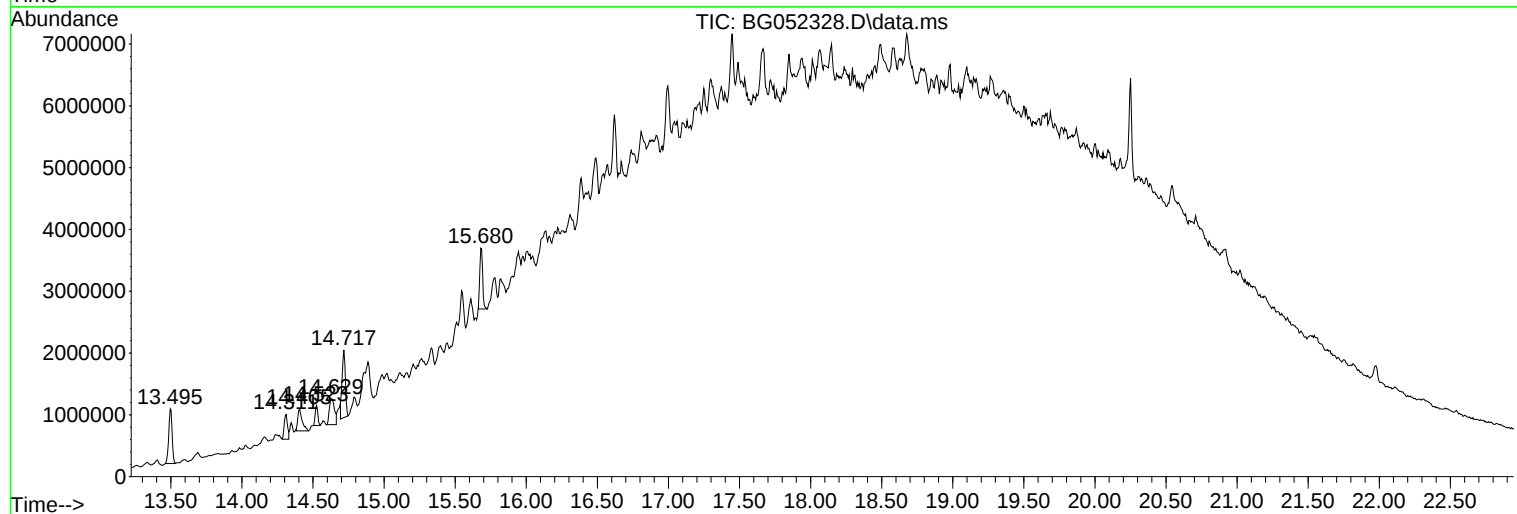
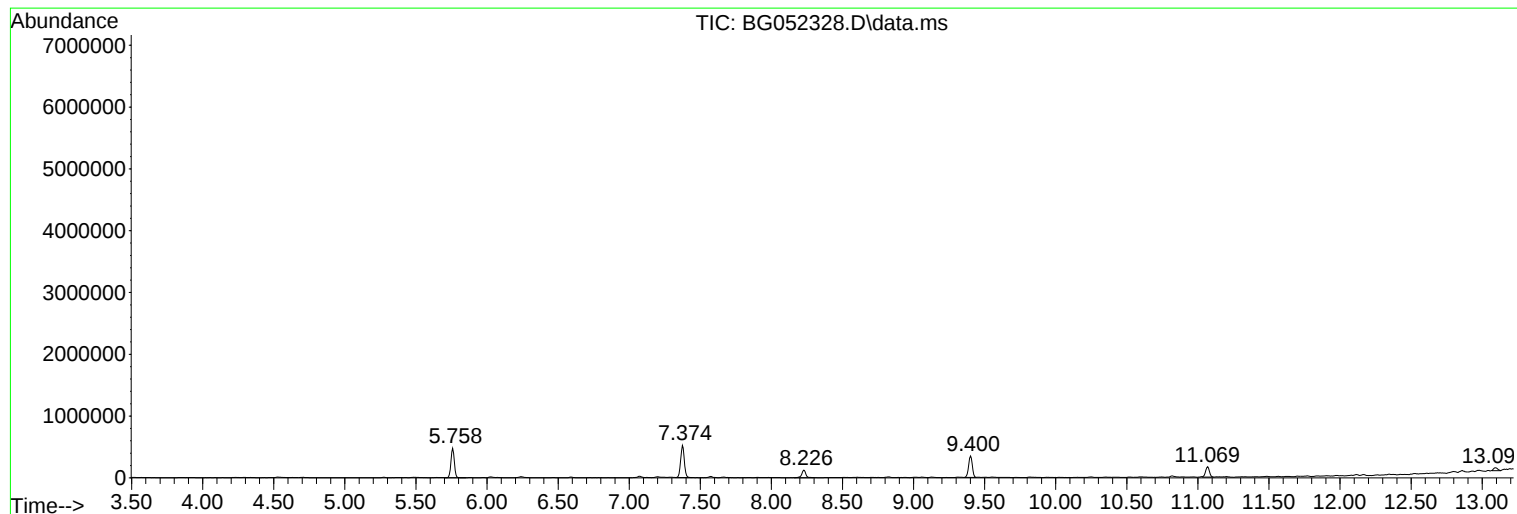
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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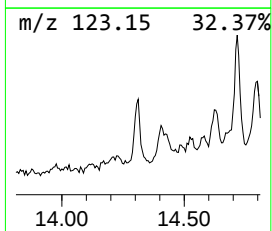
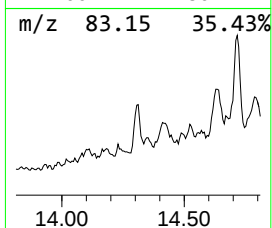
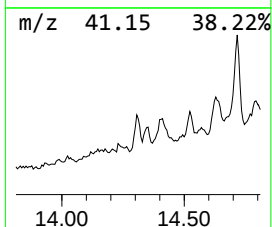
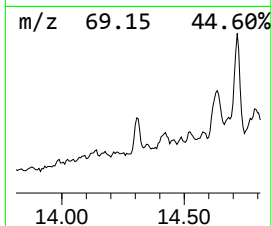
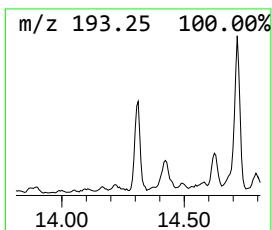
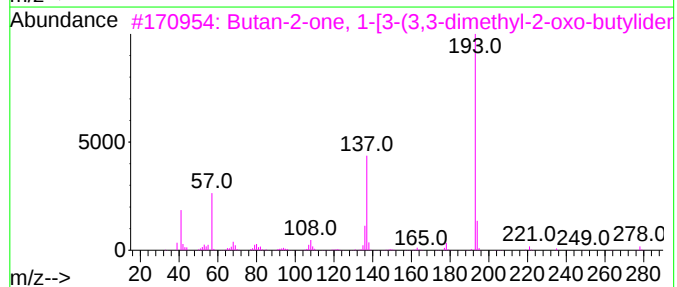
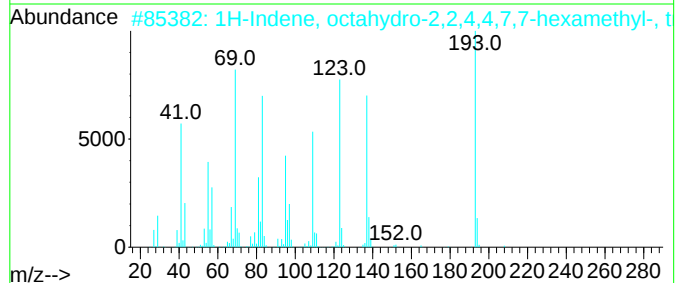
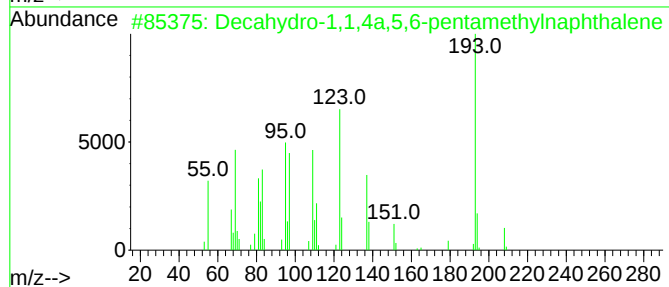
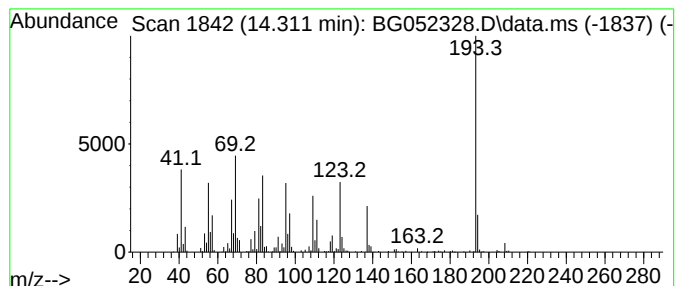
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.311	7.60 ng	642204	Acenaphthene-d10	14.881	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	70
2	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	45
3	Butan-2-one, 1-[3-(3,3-dimethyl-...	278	C16H26N2O2	1000303-34-2	38
4	S-Phenyl 5-(phenylthio)pentaneth...	302	C17H18OS2	1000234-40-7	38
5	Acridine, 9-methyl-	193	C14H11N	000611-64-3	38



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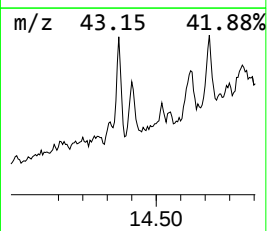
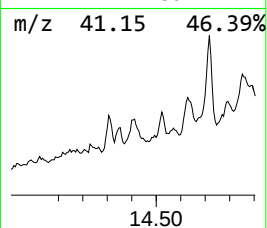
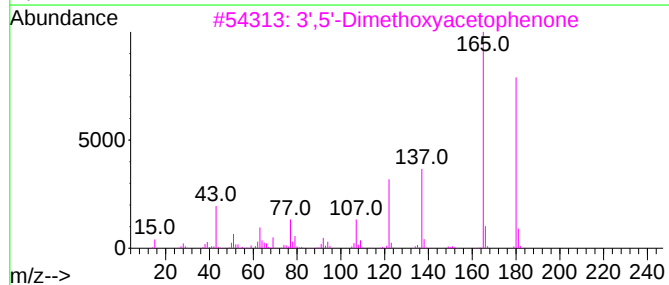
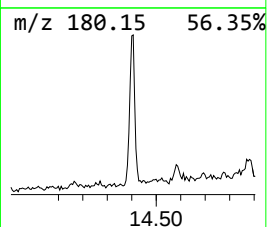
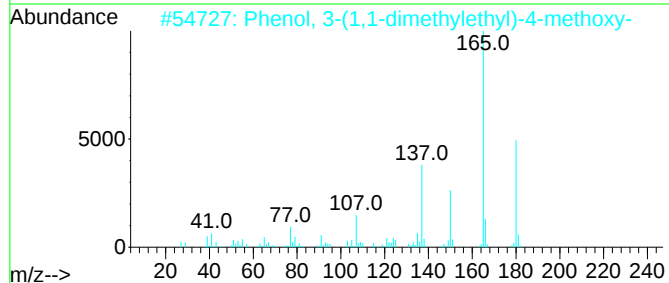
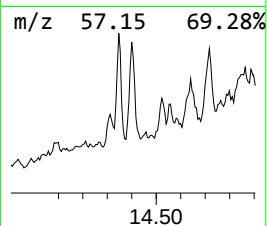
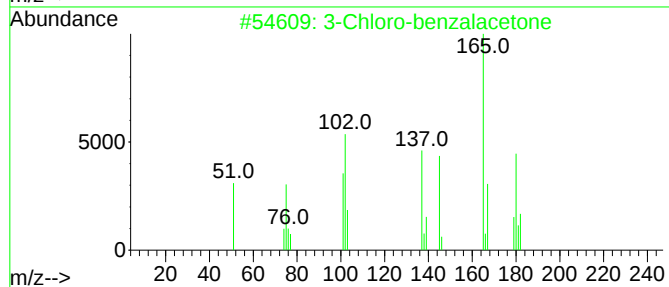
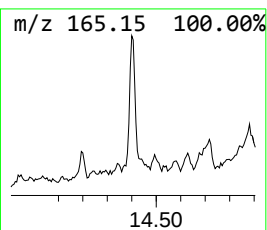
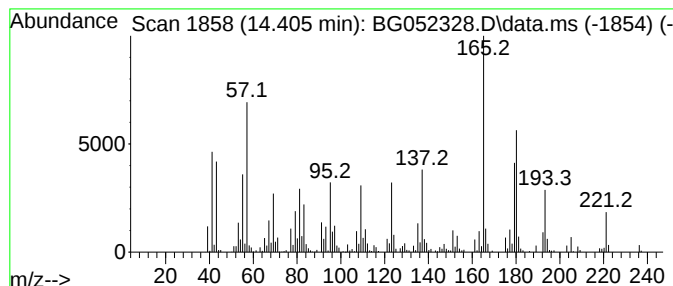
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Chloro-benzalacetone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.405	8.79 ng	743321	Acenaphthene-d10	14.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-benzalacetone	180	C10H9ClO	1000146-90-5	87
2			Phenol, 3-(1,1-dimethylethyl)-4-...	180	C11H16O2	000088-32-4	55
3			3',5'-Dimethoxyacetophenone	180	C10H12O3	039151-19-4	55
4			3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	46
5			4a,9a-Methano-9H-fluorene	180	C14H12	019540-84-2	45



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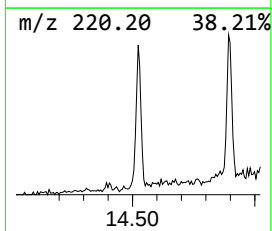
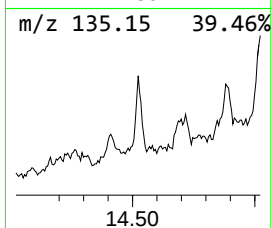
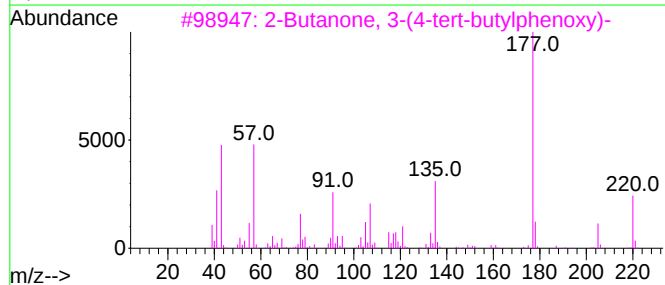
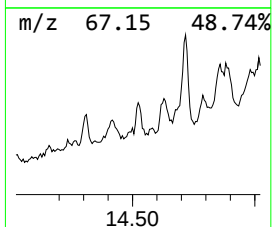
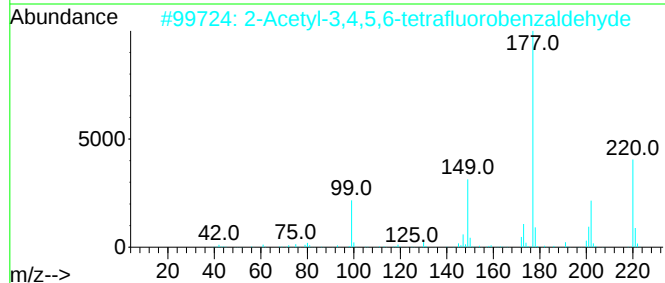
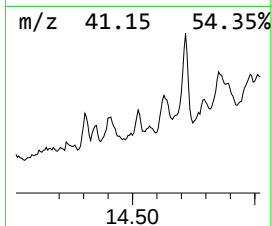
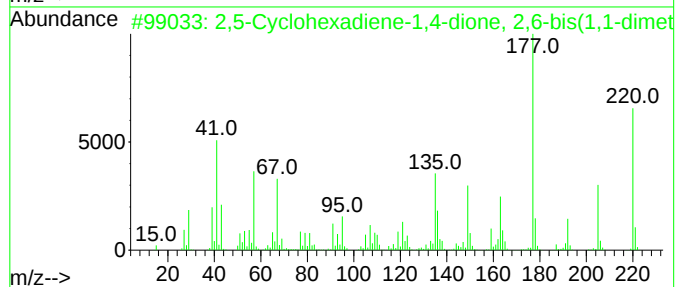
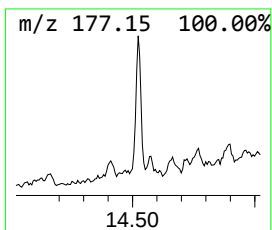
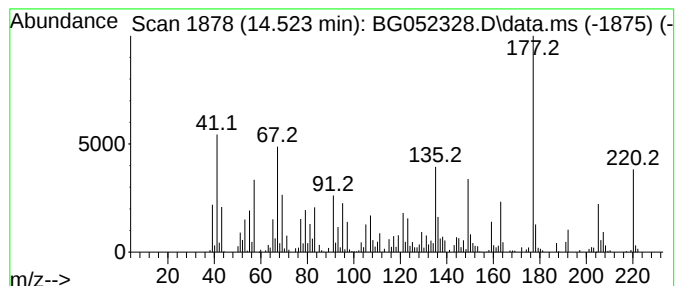
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Peak Number 3 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.523	4.91 ng	415430	Acenaphthene-d10	14.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	95
2			2-Acetyl-3,4,5,6-tetrafluorobenz...	220	C9H4F4O2	1000461-12-2	46
3			2-Butanone, 3-(4-tert-butylpheno...	220	C14H20O2	160875-28-5	45
4			4-Propylbenzaldehyde diethyl acetal	222	C14H22O2	089557-35-7	38
5			Propanamine, 2-(1-adamantyl)-2-m...	207	C14H25N	885284-11-7	35



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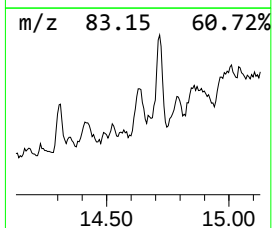
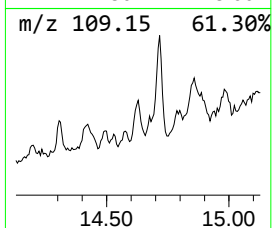
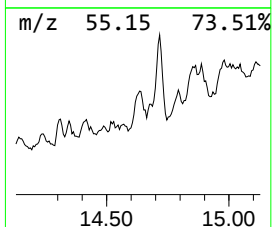
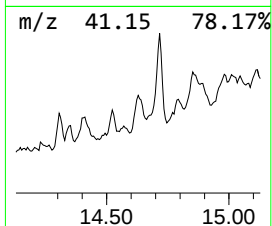
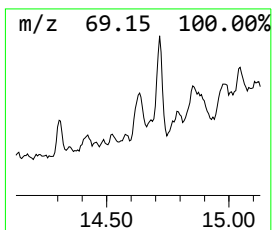
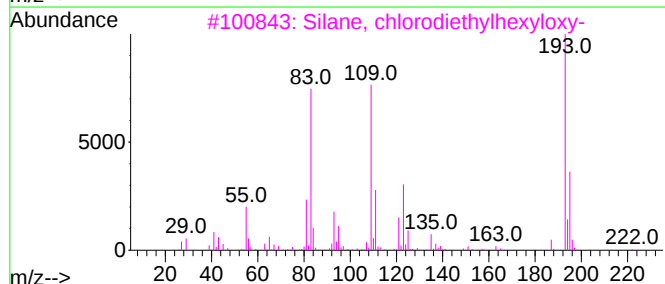
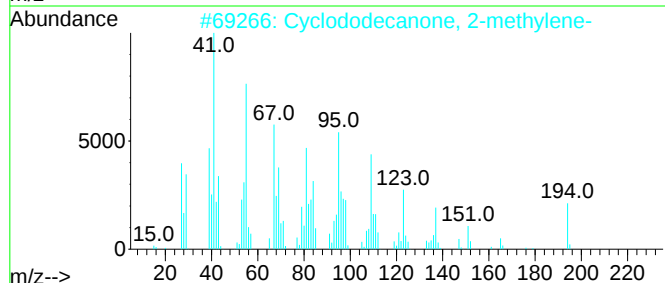
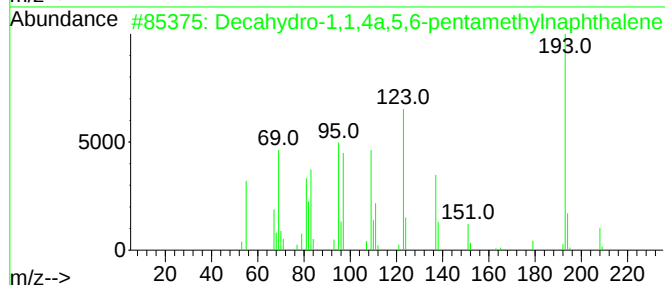
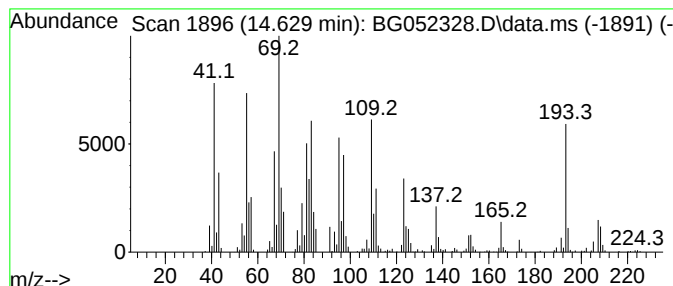
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown14.629 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.629	12.65 ng	1069240	Acenaphthene-d10	14.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	93
2			Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	38
3			Silane, chlorodiethylhexyloxy-	222	C10H23ClOSi	1000363-74-4	38
4			Cyclopropanemethanol, .alpha.,2-...	182	C12H22O	121959-70-4	38
5			Neopentylidenecyclohexane	152	C11H20	039546-80-0	38



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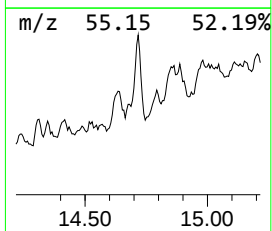
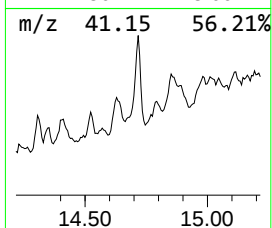
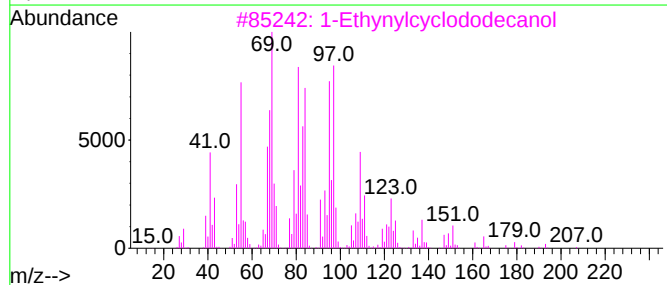
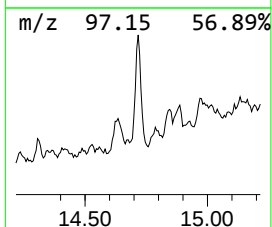
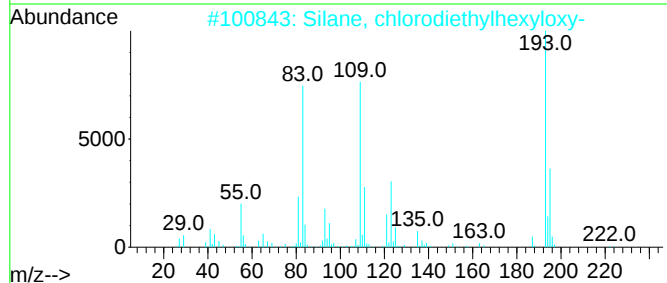
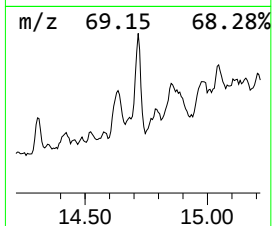
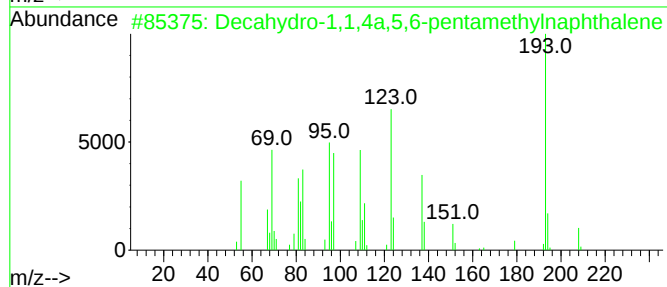
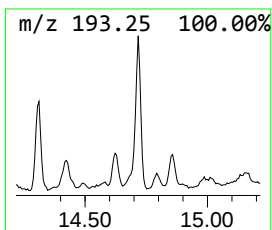
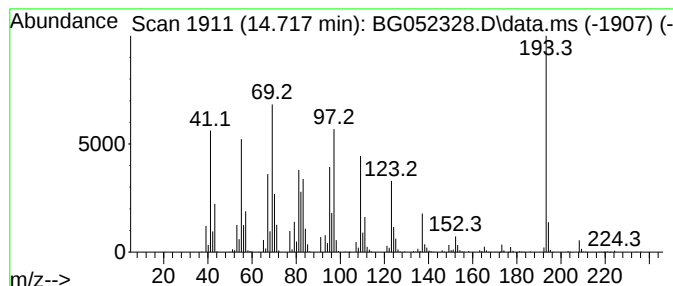
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Peak Number 5 unknown14.717 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.717	20.00 ng	1690550	Acenaphthene-d10	14.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	53
2			Silane, chlorodiethylhexyloxy-	222	C10H23ClOSi	1000363-74-4	37
3			1-Ethynylcyclododecanol	208	C14H24O	1000484-40-4	32
4			Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	30
5			2-propenamide, N-(2,6-dihydroxyp...	193	C10H11NO3	1000395-98-7	27



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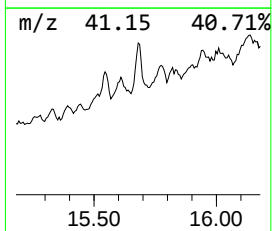
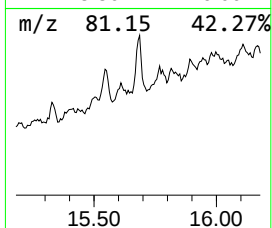
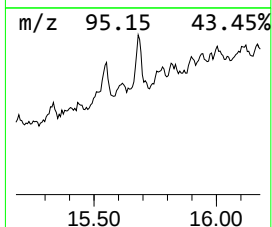
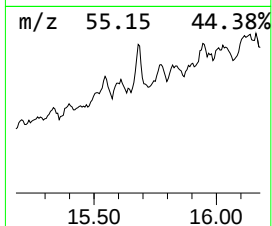
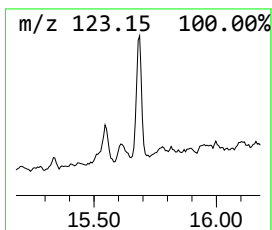
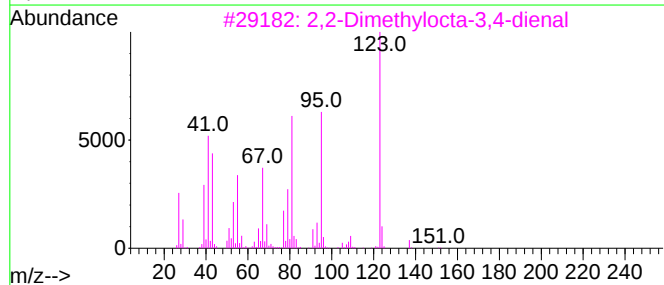
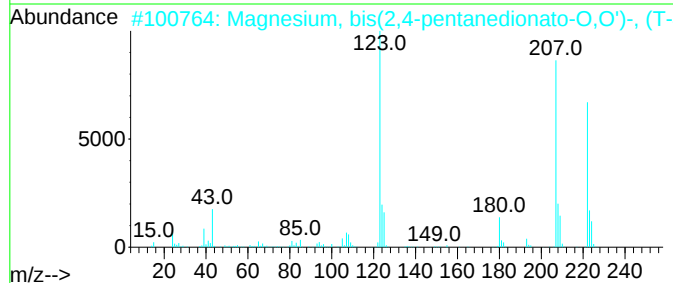
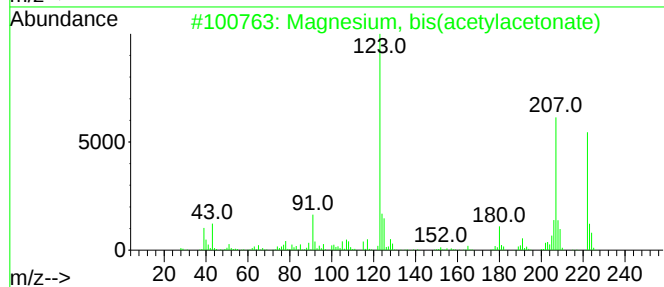
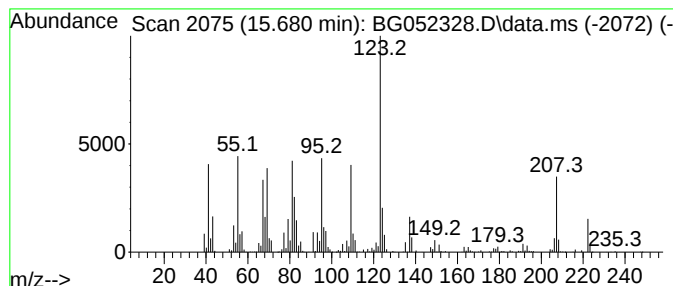
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown15.680 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.680	16.39 ng	1385340	Acenaphthene-d10	14.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Magnesium, bis(acetylacetonate)	222	C10H14MgO4	068488-07-3	46
2			Magnesium, bis(2,4-pentanedionat...	222	C10H14MgO4	014024-56-7	46
3			2,2-Dimethylocta-3,4-dienal	152	C10H16O	000590-71-6	43
4			Benzene-1,2,3-triamine	123	C6H9N3	1000316-45-3	43
5			1-Trimethylsilylpent-1-en-4-yne	138	C8H14Si	079516-25-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020822\
Data File : BG052328.D
Acq On : 8 Feb 2022 20:44
Operator : CG/JU
Sample : N1387-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
24801

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Decahydro-1,1,4...	14.311	7.6	ng	642204	3	14.881	1690550	20.0
3-Chloro-benzal...	14.405	8.8	ng	743321	3	14.881	1690550	20.0
2,5-Cyclohexadi...	14.523	4.9	ng	415430	3	14.881	1690550	20.0
unknown14.629	14.629	12.7	ng	1069240	3	14.881	1690550	20.0
unknown14.717	14.717	20.0	ng	1690550	3	14.881	1690550	20.0
unknown15.680	15.680	16.4	ng	1385340	3	14.881	1690550	20.0