

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091222\
 Data File : BG054919.D
 Acq On : 12 Sep 2022 23:49
 Operator : CG/JU
 Sample : N4562-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 CHRT-2046

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-BG082522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054919.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.207	319	326	337	rVB	59910	100885	3.23%	0.494%
2	5.688	400	408	423	rBV	605033	1035955	33.14%	5.074%
3	7.304	674	683	695	rBV	604953	1092266	34.94%	5.350%
4	8.144	818	826	831	rBV	150118	267369	8.55%	1.309%
5	9.319	1017	1026	1036	rBV	385482	708393	22.66%	3.469%
6	10.735	1258	1267	1276	rBV3	38612	95647	3.06%	0.468%
7	10.970	1300	1307	1312	rBV	207983	384890	12.31%	1.885%
8	13.403	1714	1721	1727	rVB	1100841	1736734	55.55%	8.506%
9	13.562	1740	1748	1753	rBV8	26652	77744	2.49%	0.381%
10	13.644	1754	1762	1768	rBV7	44894	126275	4.04%	0.618%
11	14.096	1834	1839	1845	rVB2	316688	483218	15.46%	2.367%
12	14.484	1899	1905	1909	rBV	498228	881540	28.20%	4.317%
13	14.602	1921	1925	1930	rVB2	198275	300900	9.62%	1.474%
14	14.778	1951	1955	1961	rVB	306793	502039	16.06%	2.459%
15	14.842	1961	1966	1977	rBV6	148192	460095	14.72%	2.253%
16	15.559	2085	2088	2092	rVB	306393	405724	12.98%	1.987%
17	16.276	2207	2210	2218	rBV	587797	1003325	32.09%	4.914%
18	21.687	3128	3131	3146	rVB2	711191	1366390	43.71%	6.692%
19	21.834	3151	3156	3163	rVV3	1103330	2851235	91.20%	13.964%
20	21.899	3164	3167	3179	rVB	1118221	1848291	59.12%	9.052%
21	24.161	3544	3552	3567	rBV2	659707	3126346	100.00%	15.312%
22	25.077	3701	3708	3720	rVB	540928	1562772	49.99%	7.654%

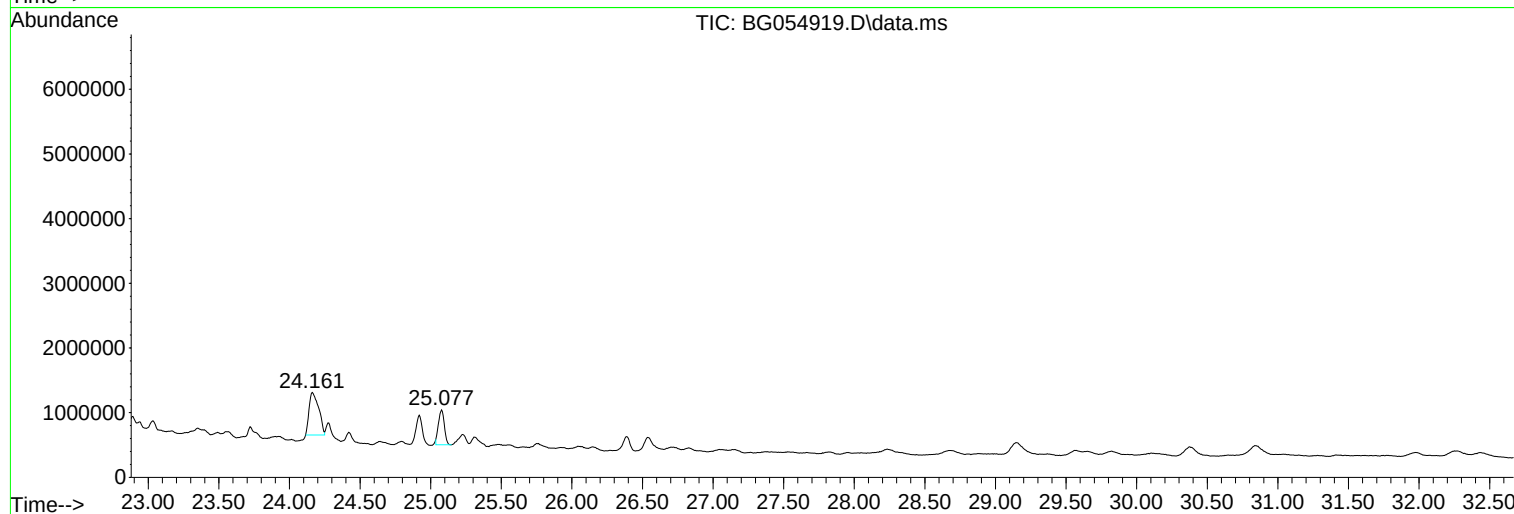
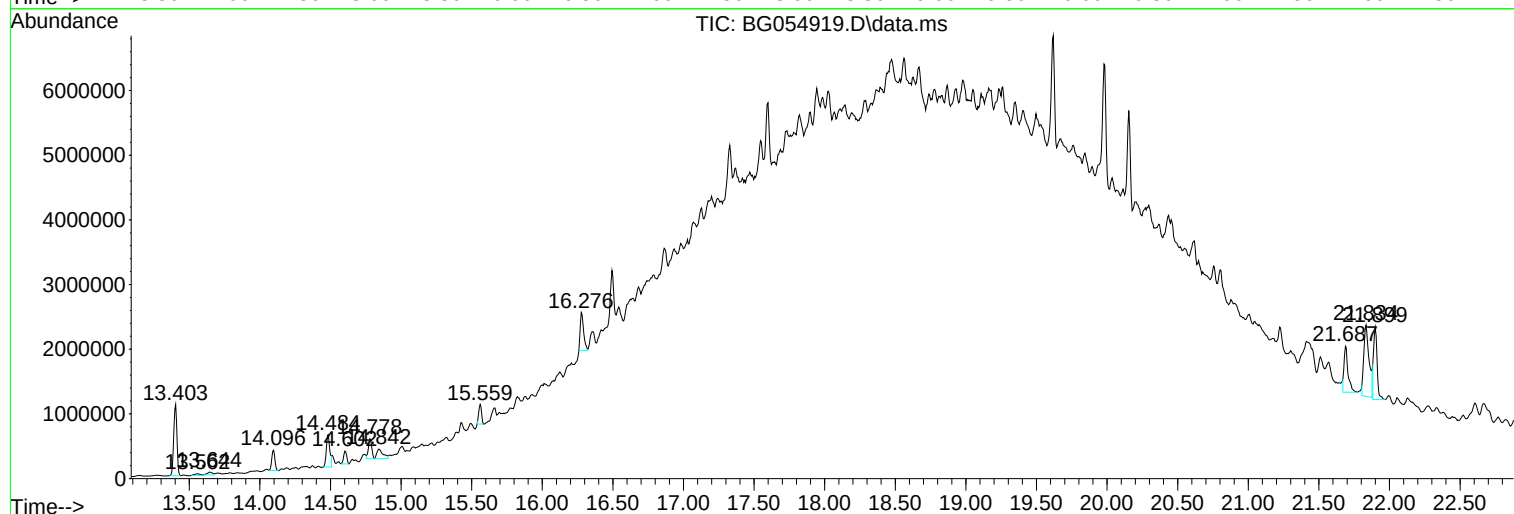
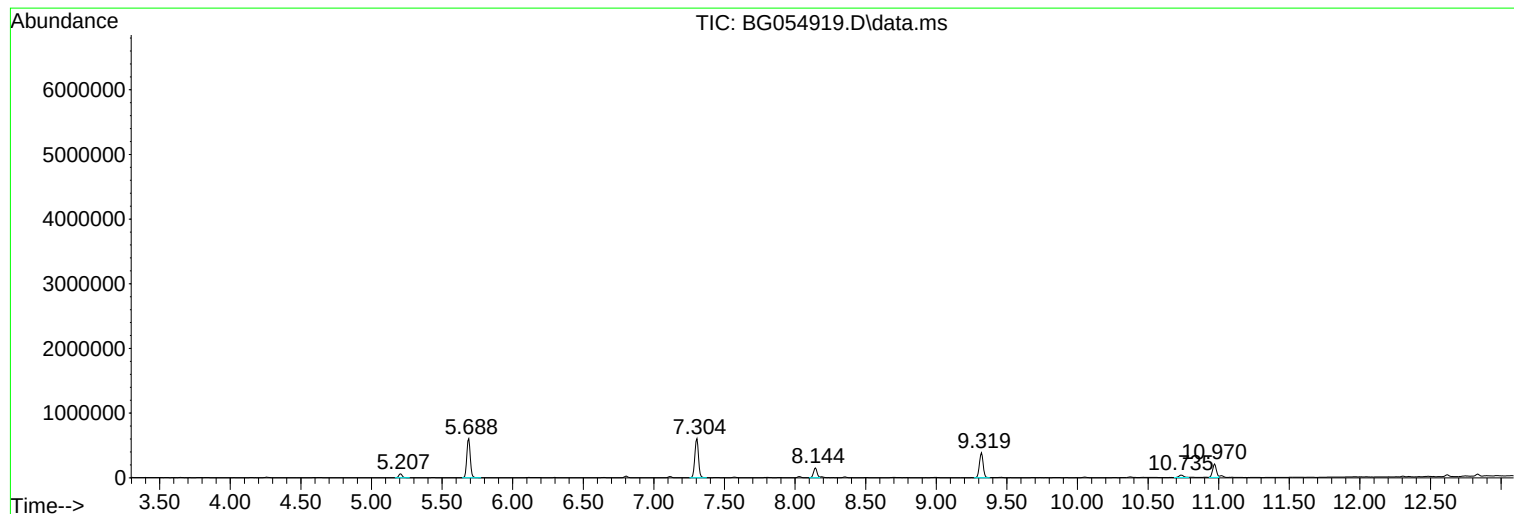
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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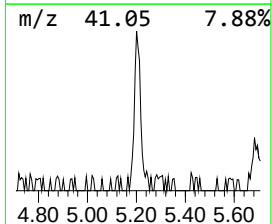
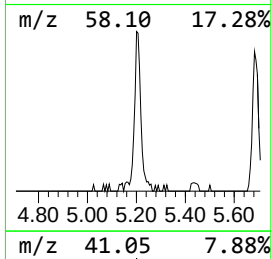
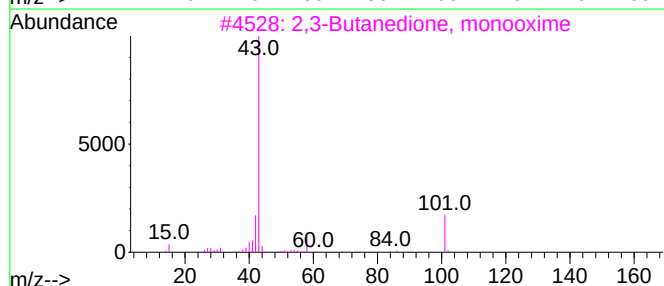
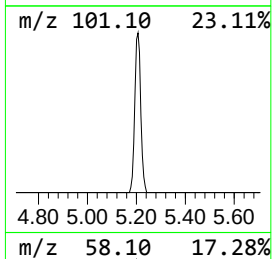
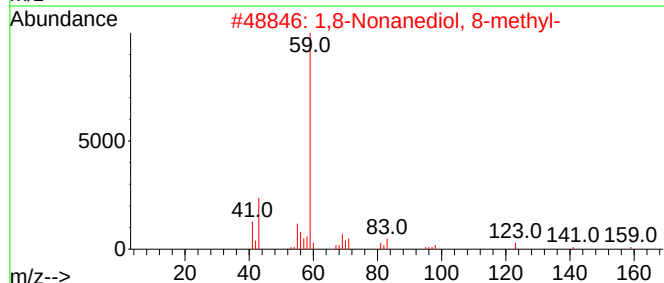
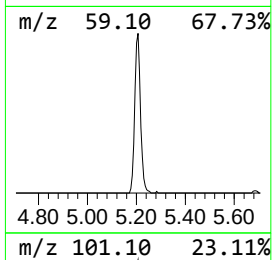
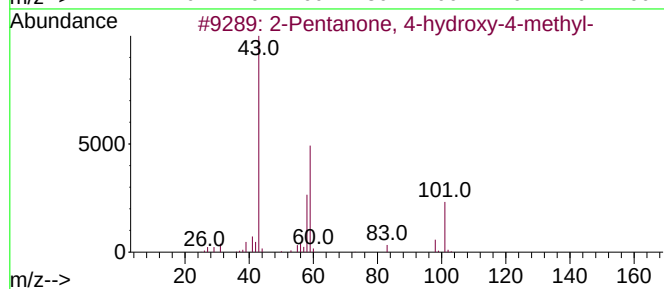
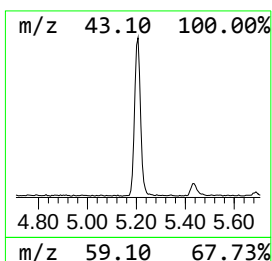
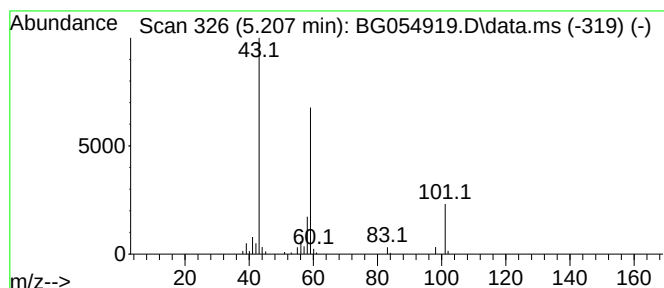
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.207	7.55 ng	100885	1,4-Dichlorobenzene-d4	8.144

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25		
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23		



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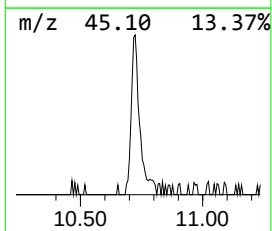
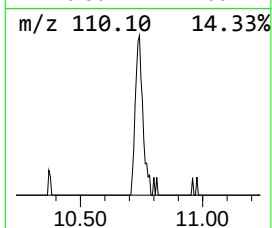
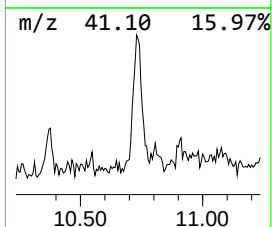
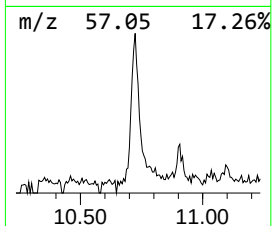
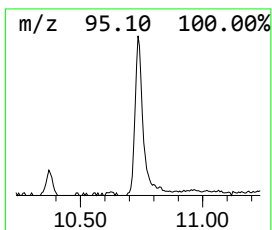
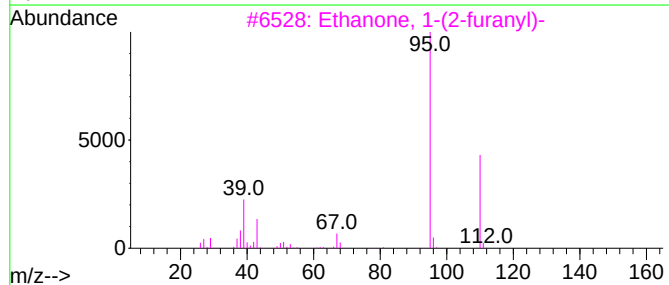
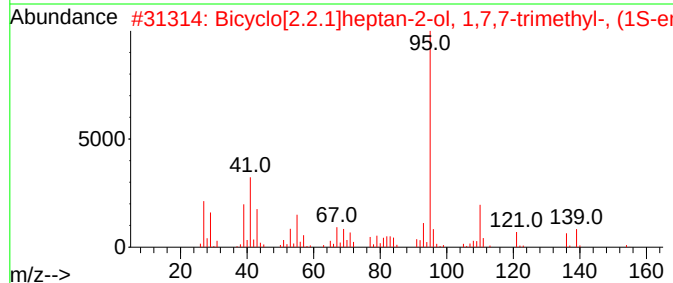
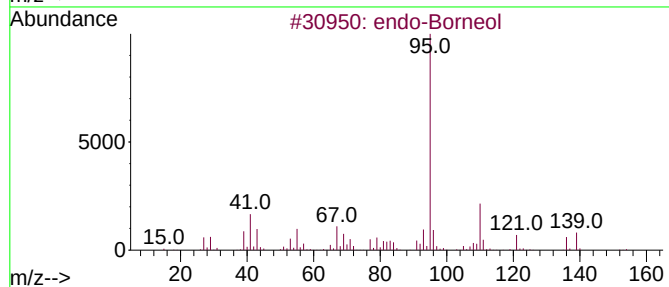
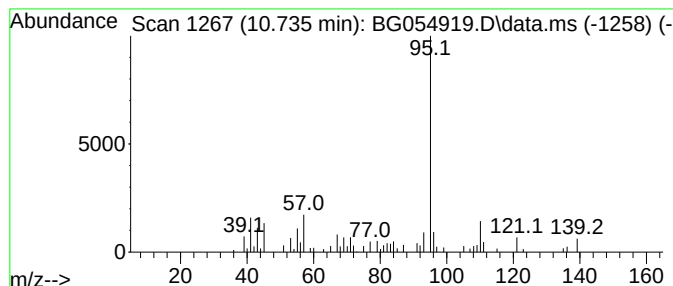
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 endo-Borneol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.736	4.97 ng	95647	Naphthalene-d8	10.970

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			endo-Borneol	154	C10H18O	000507-70-0	72
2			Bicyclo[2.2.1]heptan-2-ol, 1,7,7...	154	C10H18O	000464-45-9	72
3			Ethanone, 1-(2-furanyl)-	110	C6H6O2	001192-62-7	50
4			2-Amino-4-methylbut-2-enenitrile	110	C6H10N2	1000197-39-9	50
5			Furan, 2-ethyl-5-methyl-	110	C7H10O	001703-52-2	49



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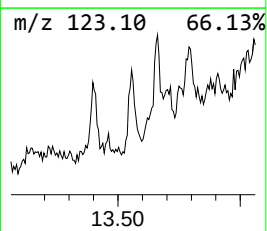
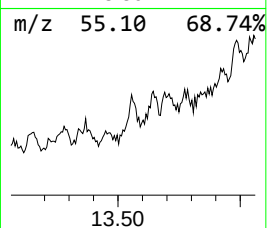
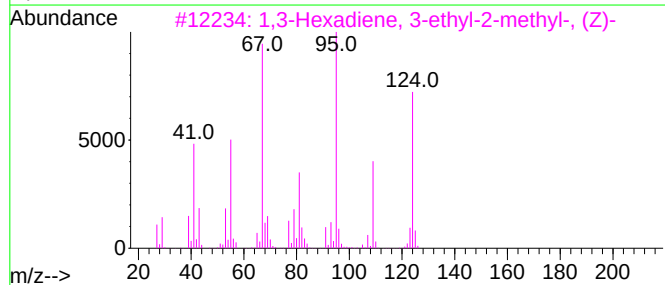
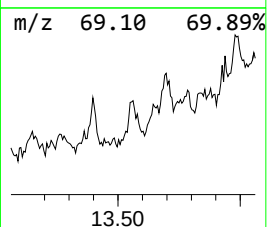
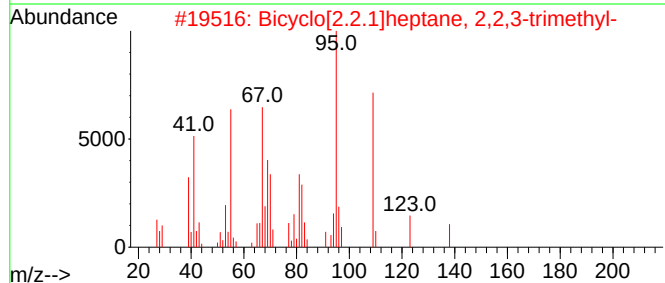
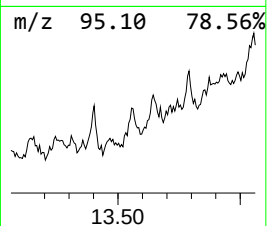
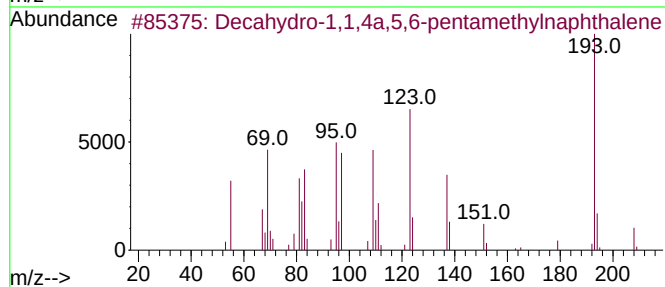
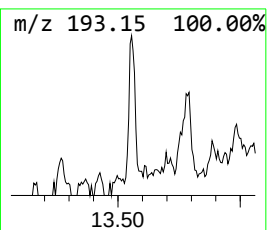
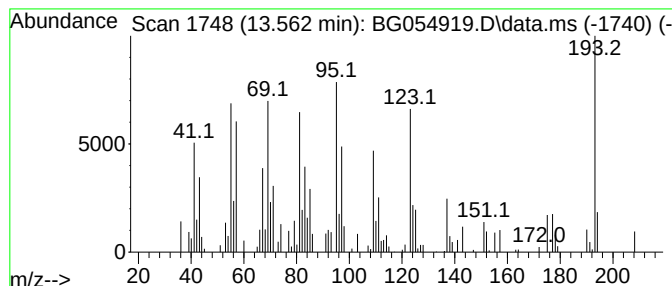
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Peak Number 3 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.562	3.10 ng	77744	Acenaphthene-d10	14.778

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	93
2			Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	000473-19-8	38
3			1,3-Hexadiene, 3-ethyl-2-methyl-...	124	C9H16	074752-97-9	30
4			Butanoic acid, 3-methyl-, 3,7-di...	240	C15H28O2	068922-10-1	30
5			Pyrimidine, 5-formamido-	123	C5H5N3O	056621-84-2	22



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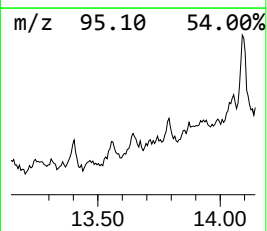
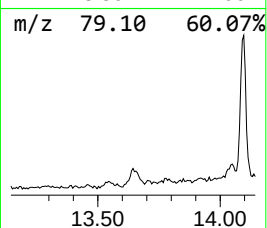
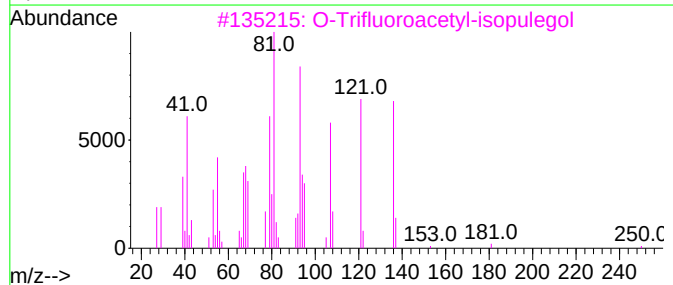
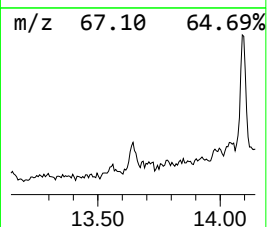
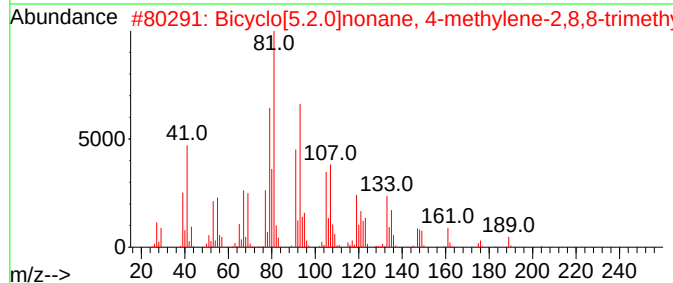
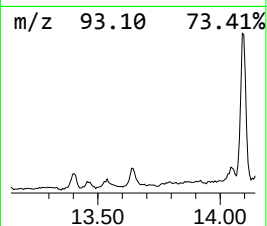
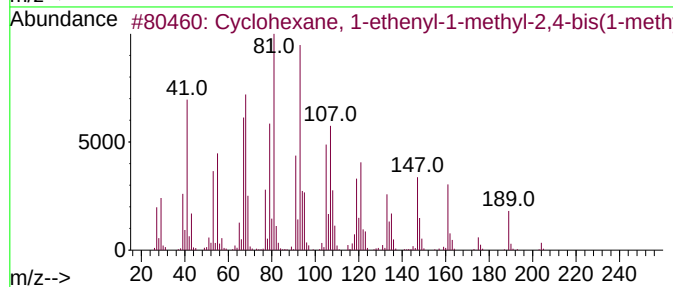
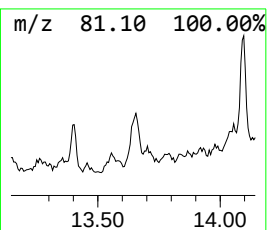
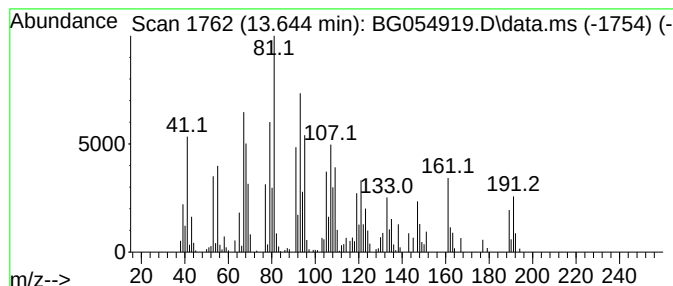
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Peak Number 4 Cyclohexane, 1-ethenyl-1-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.644	5.03 ng	126275	Acenaphthene-d10	14.778

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-ethenyl-1-methyl-...	204	C15H24	000515-13-9	62
2			Bicyclo[5.2.0]nonane, 4-methylen...	204	C15H24	1000159-38-2	45
3			O-Trifluoroacetyl-isopulegol	250	C12H17F3O2	028587-54-4	43
4			1,5-Cycloundecadiene, 9-(1-methy...	190	C14H22	062338-55-0	30
5			3-Tetradecen-5-yne, (E)-	192	C14H24	074744-44-8	30



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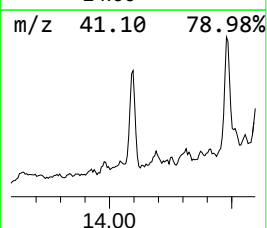
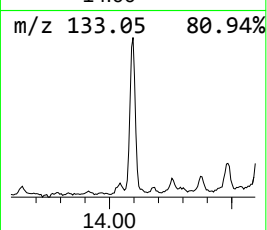
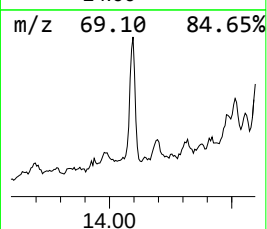
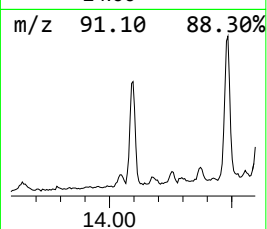
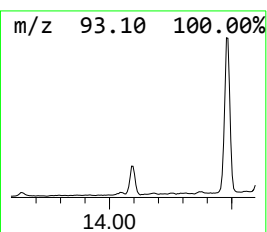
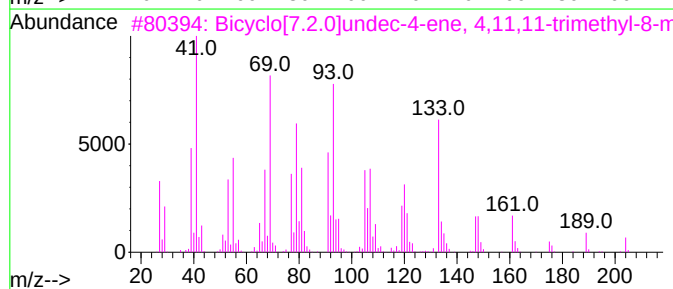
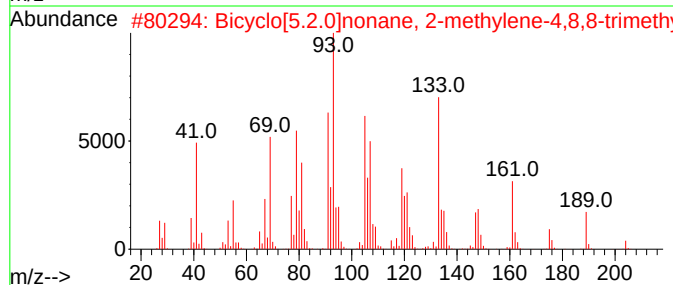
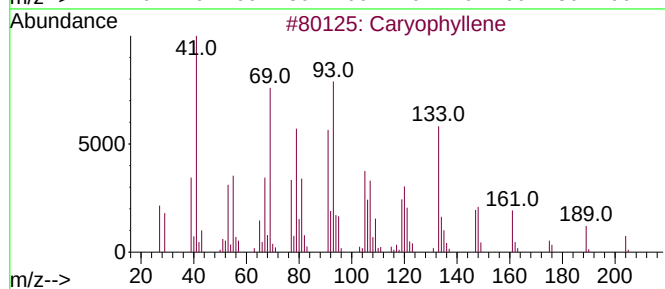
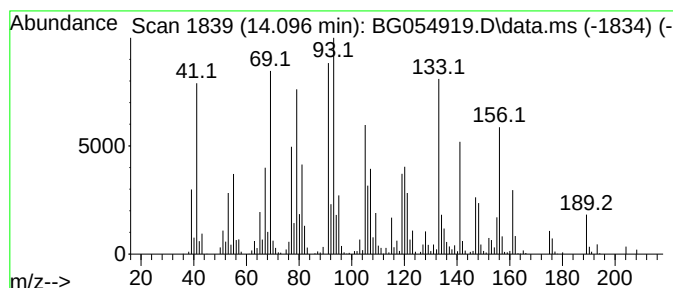
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Peak Number 5 Caryophyllene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.096	19.25 ng	483218	Acenaphthene-d10	14.778

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Caryophyllene	204	C15H24	000087-44-5	91
2			Bicyclo[5.2.0]nonane, 2-methylen...	204	C15H24	242794-76-9	86
3			Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	68
4			Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	013877-93-5	60
5			(+)-2-Carene, 4-.alpha.-isopropo...	176	C13H20	1000151-26-0	30



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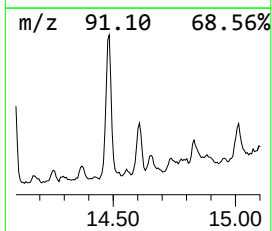
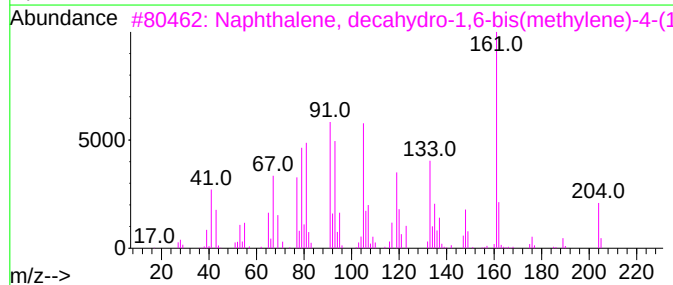
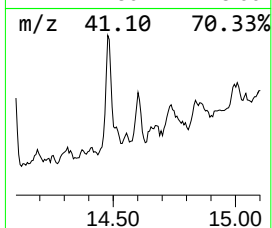
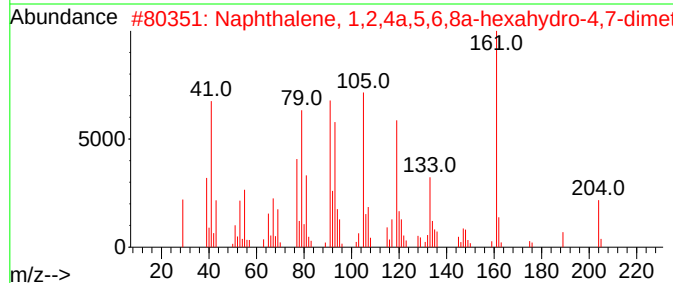
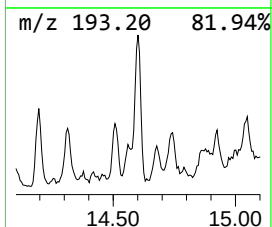
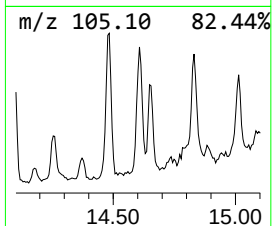
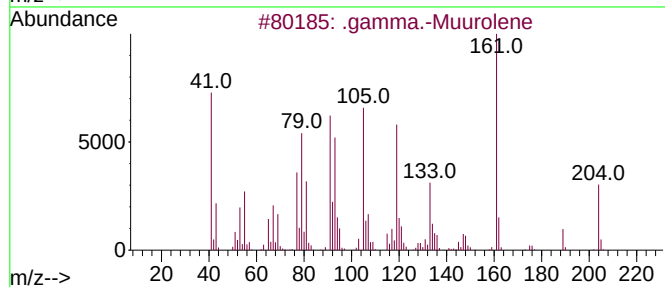
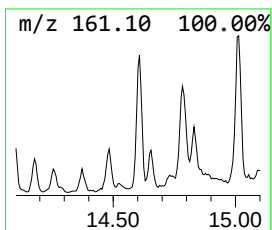
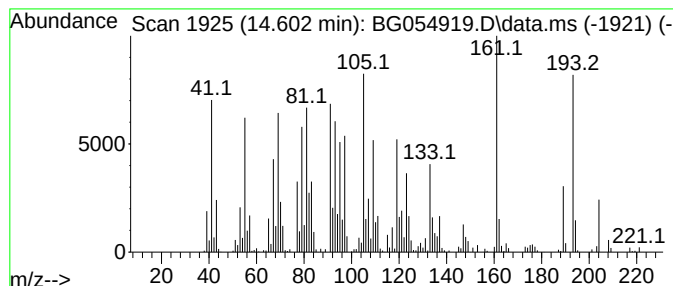
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 .gamma.-Muurolene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.602	11.99 ng	300900	Acenaphthene-d10	14.778

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.gamma.-Muurolene	204	C15H24	030021-74-0	95
2		Naphthalene, 1,2,4a,5,6,8a-hexah...	204	C15H24	000483-75-0	95
3		Naphthalene, decahydro-1,6-bis(m...	204	C15H24	030021-46-6	81
4		Longifolene	204	C15H24	000475-20-7	70
5		(S,1Z,6Z)-8-Isopropyl-1-methyl-5...	204	C15H24	317819-80-0	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091222\
Data File : BG054919.D
Acq On : 12 Sep 2022 23:49
Operator : CG/JU
Sample : N4562-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CHRT-2046

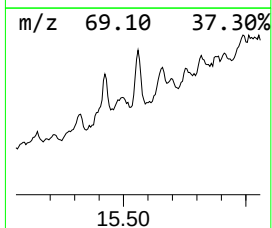
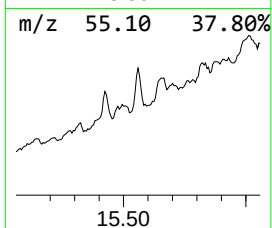
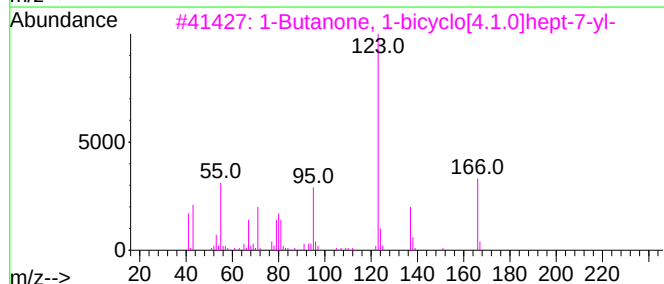
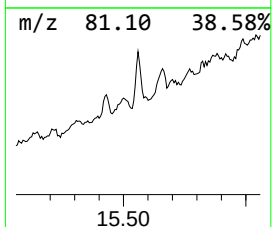
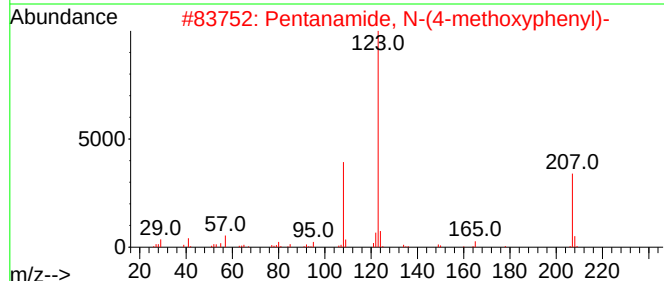
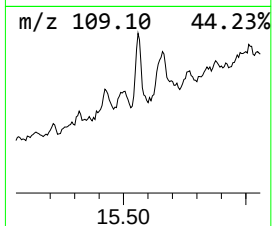
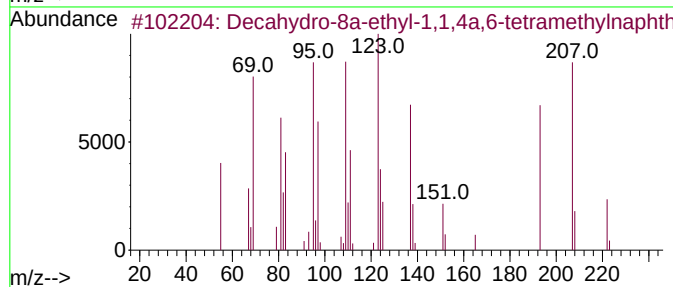
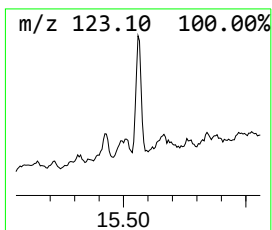
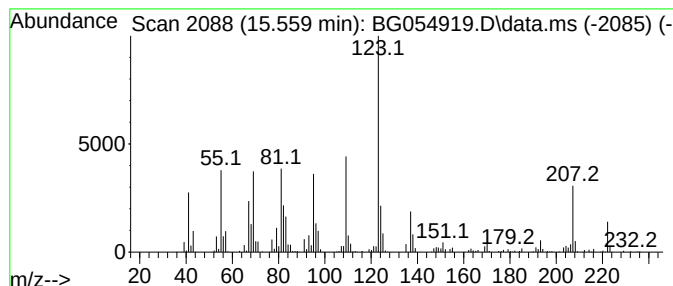
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown15.559 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.559	16.16 ng	405724	Acenaphthene-d10	14.778

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-8a-ethyl-1,1,4a,6-tetr...	222	C16H30	1000100-23-6	45
2			Pentanamide, N-(4-methoxyphenyl)-	207	C12H17NO2	1000306-89-3	43
3			1-Butanone, 1-bicyclo[4.1.0]hept...	166	C11H18O	054764-62-4	43
4			4-Fluoro-N-(1H-tetrazol-5-yl)ben...	207	C8H6FN5O	1000306-76-6	38
5			2-Amino-4-acetamino anisole	180	C9H12N2O2	006375-47-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091222\
Data File : BG054919.D
Acq On : 12 Sep 2022 23:49
Operator : CG/JU
Sample : N4562-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CHRT-2046

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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
2-Pentanone, 4-...	5.207	7.5	ng	100885	1	8.144	267369	20.0
endo-Borneol	10.736	5.0	ng	95647	2	10.970	384890	20.0
Decahydro-1,1,4...	13.562	3.1	ng	77744	3	14.778	502039	20.0
Cyclohexane, 1-...	13.644	5.0	ng	126275	3	14.778	502039	20.0
Caryophyllene	14.096	19.3	ng	483218	3	14.778	502039	20.0
.gamma.-Muurolene	14.602	12.0	ng	300900	3	14.778	502039	20.0
unknown15.559	15.559	16.2	ng	405724	3	14.778	502039	20.0