

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081321\
 Data File : BG049838.D
 Acq On : 13 Aug 2021 17:17
 Operator : CG/JU
 Sample : M3343-07
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20210558-COM-31

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-BG080321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049838.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.138	12	17	23	rBV	83161	149661	10.46%	1.940%
2	3.185	23	25	34	rVB5	13222	19254	1.35%	0.250%
3	5.112	348	353	363	rBV	22010	39340	2.75%	0.510%
4	5.588	423	434	445	rBV	403765	662584	46.31%	8.588%
5	7.197	700	708	720	rBV	407096	713163	49.84%	9.244%
6	8.032	844	850	858	rVB	102203	178824	12.50%	2.318%
7	9.201	1040	1049	1061	rVB	246187	456282	31.89%	5.914%
8	10.616	1284	1290	1304	rBV2	27565	66309	4.63%	0.859%
9	10.851	1323	1330	1338	rVB	136530	246240	17.21%	3.192%
10	13.301	1741	1747	1757	rBV	565463	914874	63.94%	11.859%
11	14.687	1976	1983	1991	rVB	224546	353078	24.68%	4.577%
12	16.179	2231	2237	2248	rBV	589221	956608	66.85%	12.400%
13	17.437	2445	2451	2458	rBV	295142	453281	31.68%	5.875%
14	18.089	2559	2562	2567	rBV3	12484	16217	1.13%	0.210%
15	19.258	2757	2761	2766	rVB3	39857	46423	3.24%	0.602%
16	19.393	2779	2784	2787	rVB6	13278	16943	1.18%	0.220%
17	20.045	2890	2895	2902	rVB	1087938	1430893	100.00%	18.547%
18	21.361	3114	3119	3126	rBV8	19646	50024	3.50%	0.648%
19	21.425	3129	3130	3136	rVB5	11507	17523	1.22%	0.227%
20	21.719	3174	3180	3188	rBV2	275456	451488	31.55%	5.852%
21	24.997	3728	3738	3750	rVB	158569	475831	33.25%	6.168%

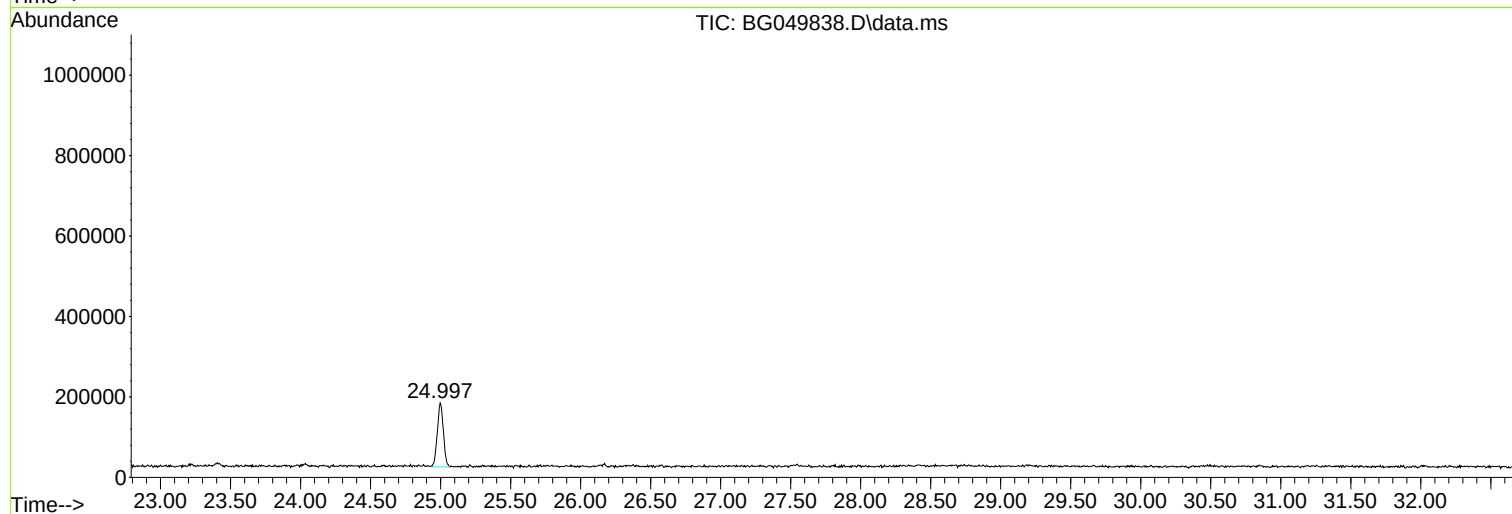
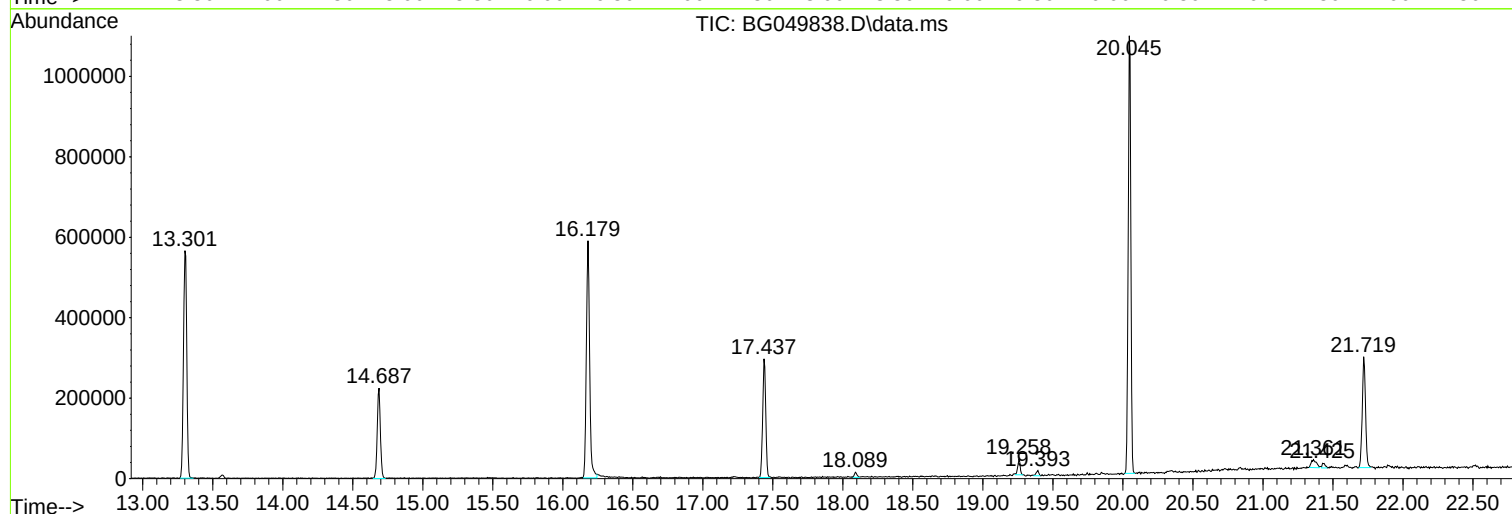
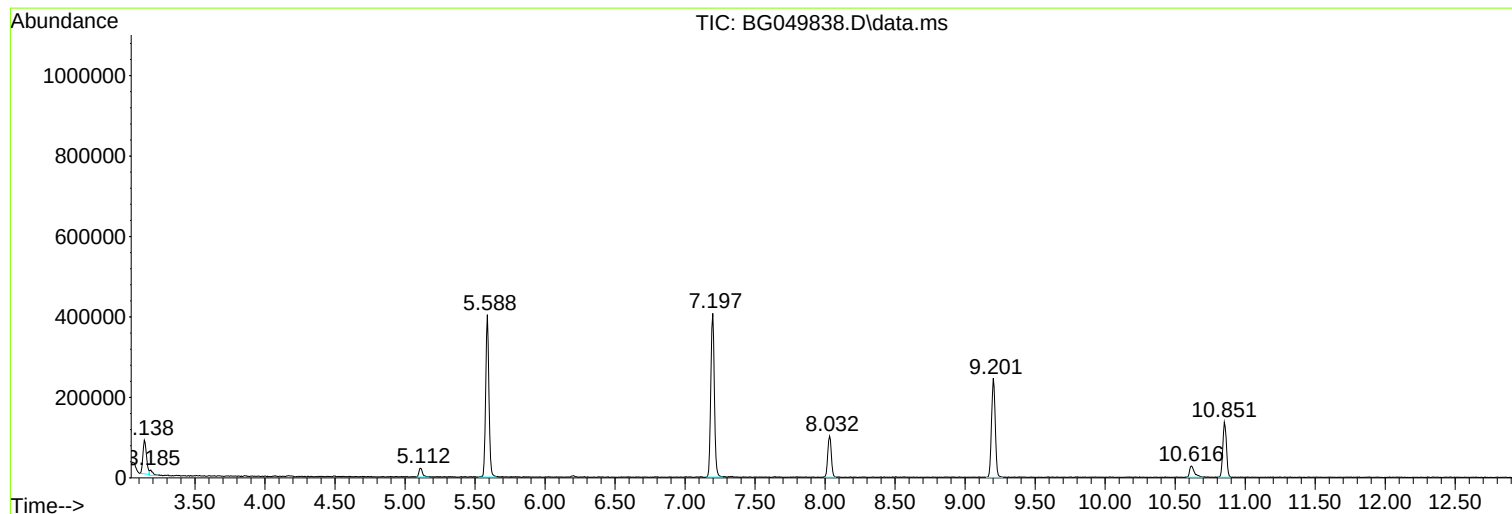
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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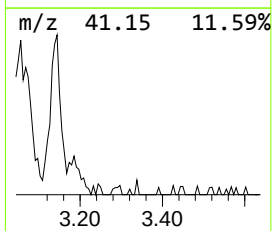
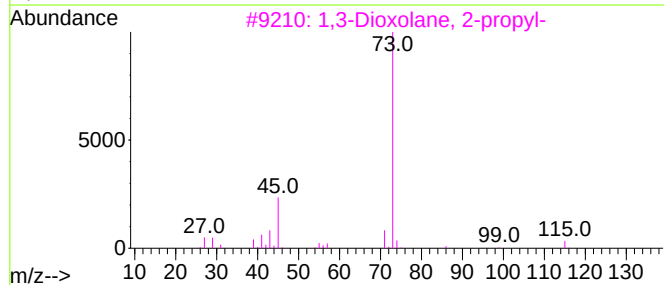
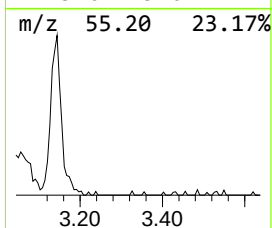
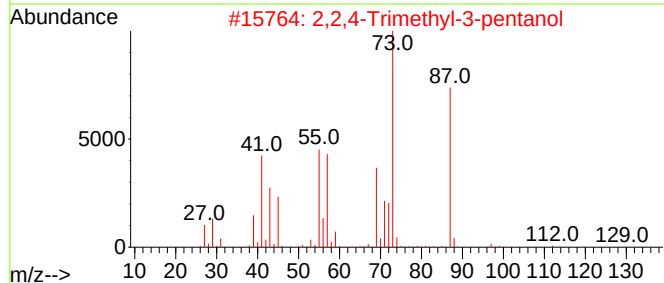
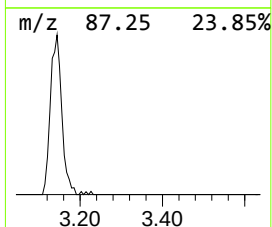
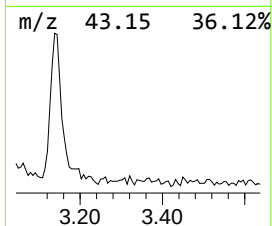
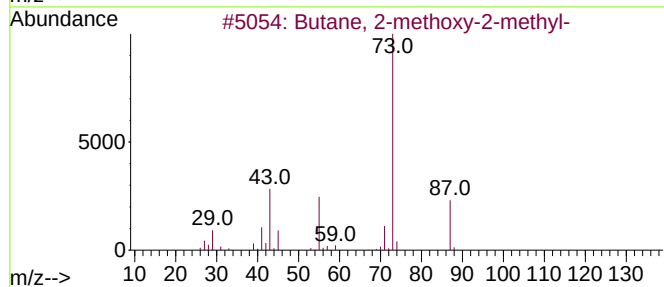
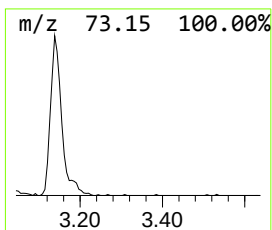
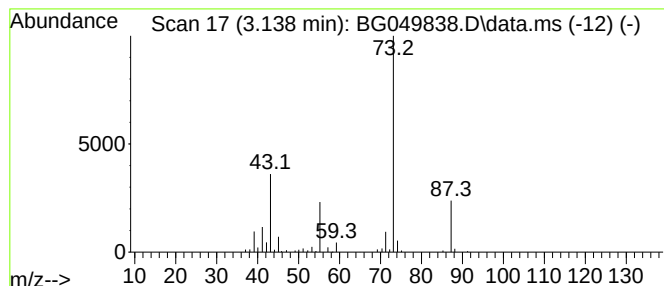
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.138	16.74 ng	149661	1,4-Dichlorobenzene-d4	8.032

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
4			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	16
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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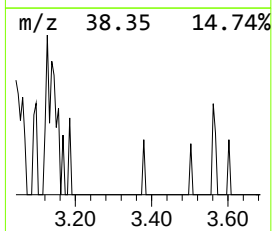
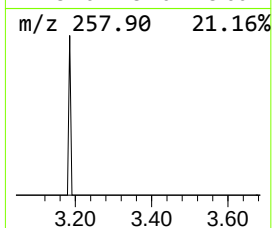
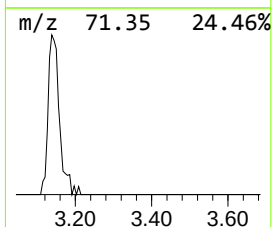
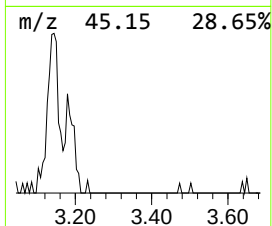
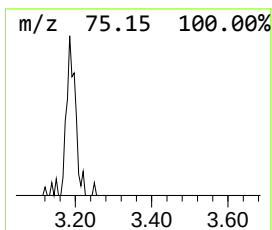
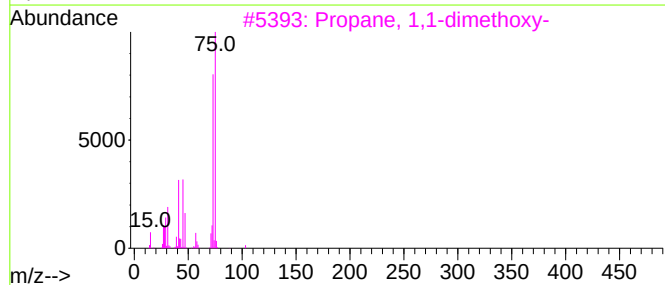
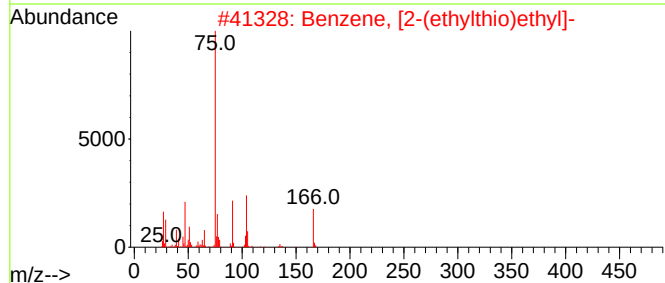
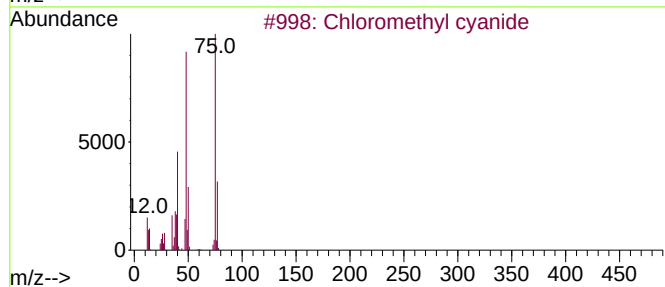
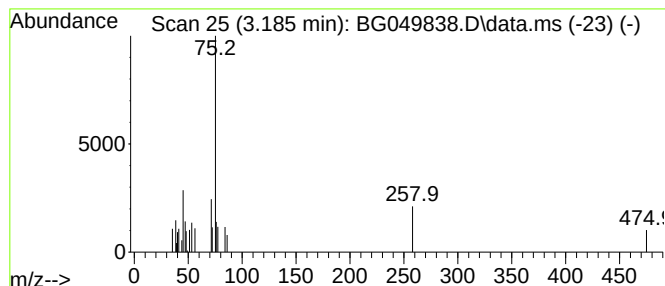
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown3.185 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.185	2.15 ng	19254	1,4-Dichlorobenzene-d4	8.032

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Chloromethyl cyanide	75	C2H2ClN	000107-14-2	38
2			Benzene, [2-(ethylthio)ethyl]-	166	C10H14S	022914-08-5	17
3			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	9
4			Methacrolein, dimethyl acetal	116	C6H12O2	1000458-49-1	9
5			Acetic acid, TMS derivative	132	C5H12O2Si	002754-27-0	9



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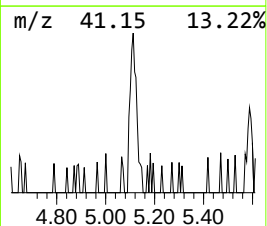
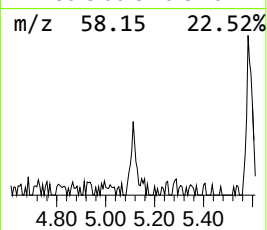
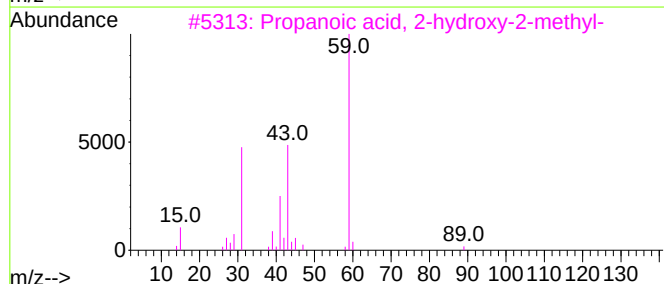
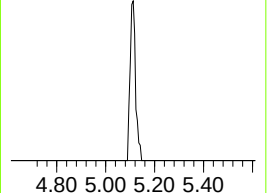
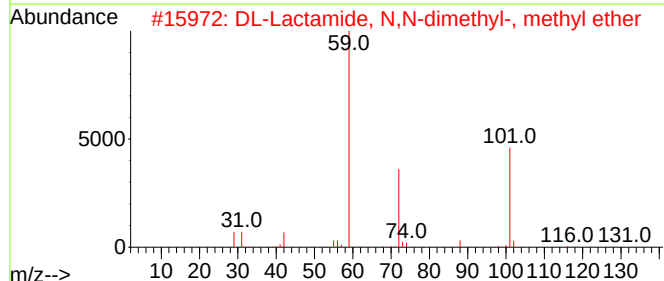
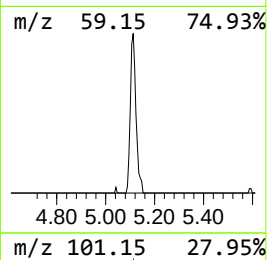
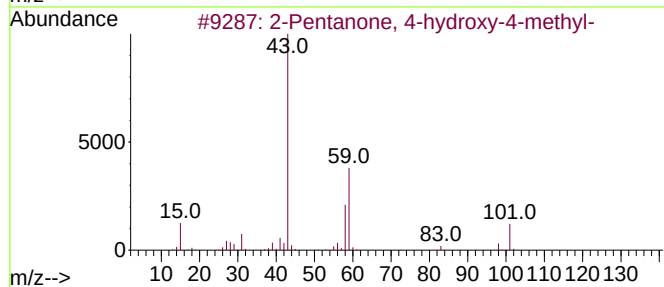
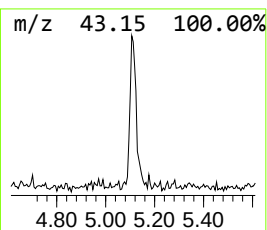
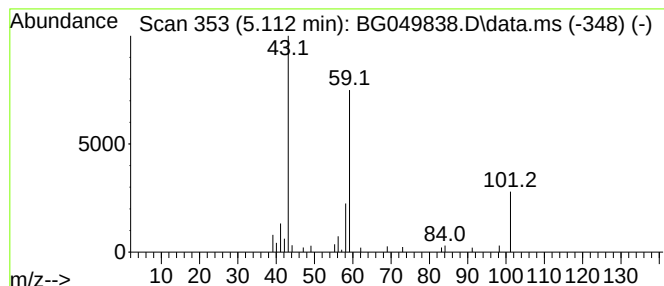
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.112	4.40 ng	39340	1,4-Dichlorobenzene-d4	8.032

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		DL-Lactamide, N,N-dimethyl-, met...	131	C6H13NO2	1000452-57-0	33
3		Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	25
4		Acetone	58	C3H6O	000067-64-1	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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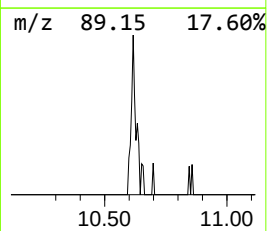
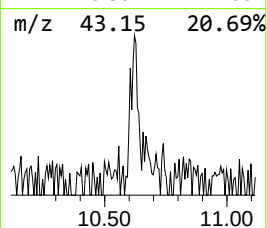
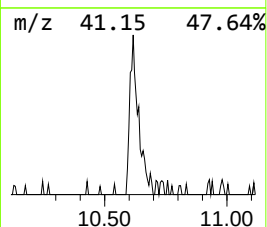
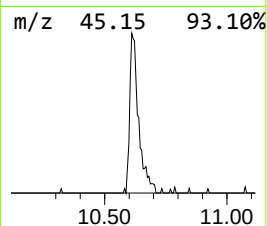
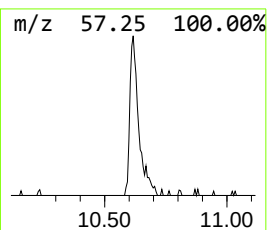
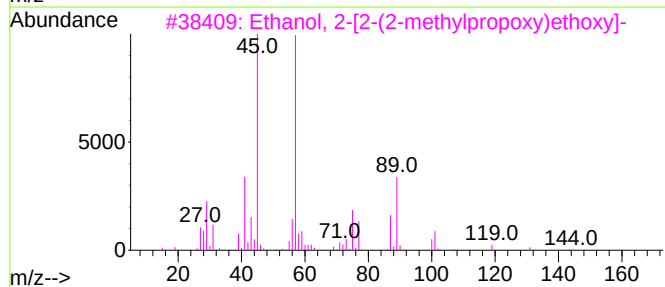
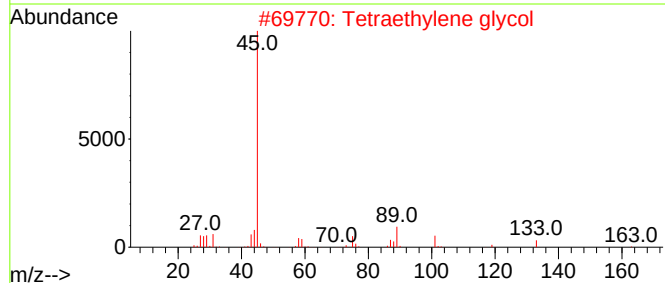
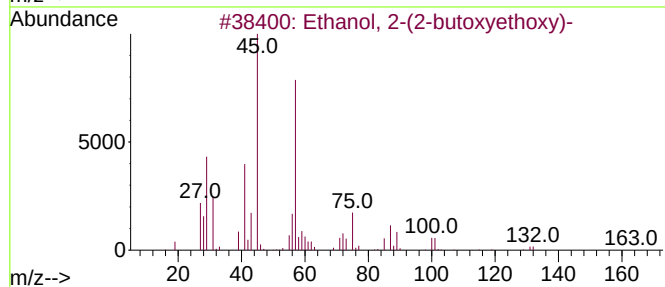
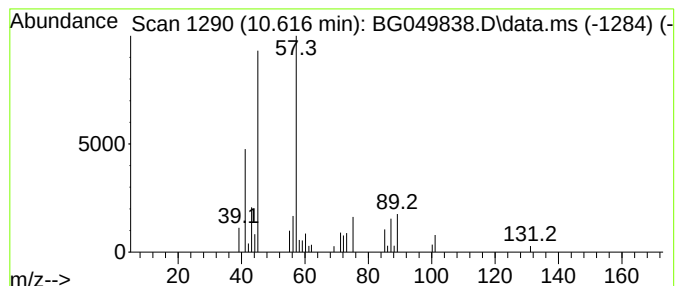
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Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.616	5.39 ng	66309	Naphthalene-d8	10.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	64
2			Tetraethylene glycol	194	C8H18O5	000112-60-7	50
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
4			Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	47
5			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	45



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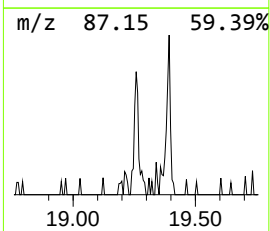
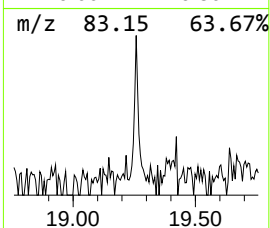
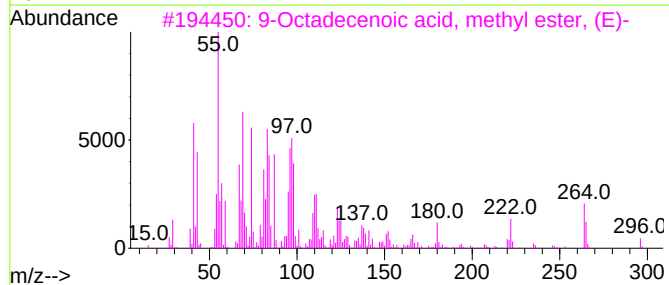
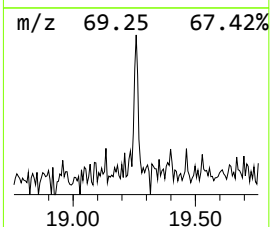
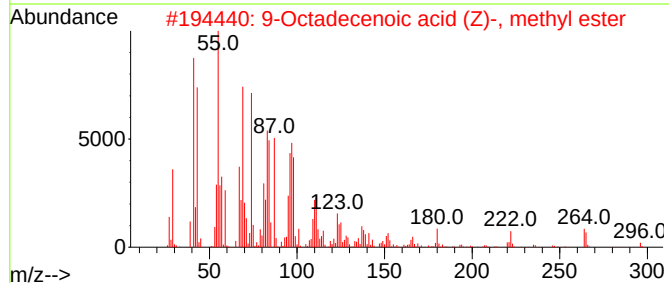
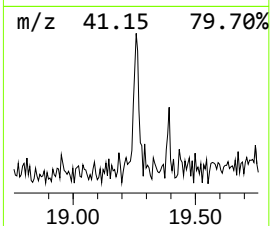
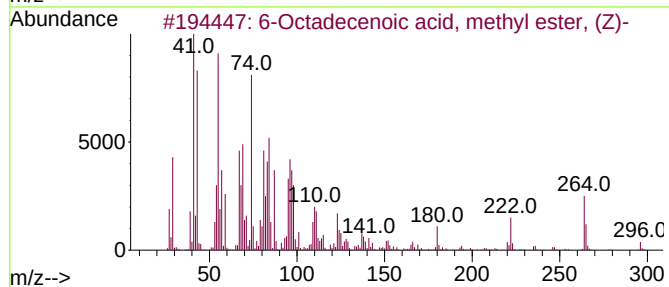
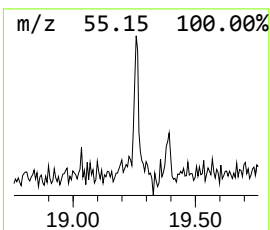
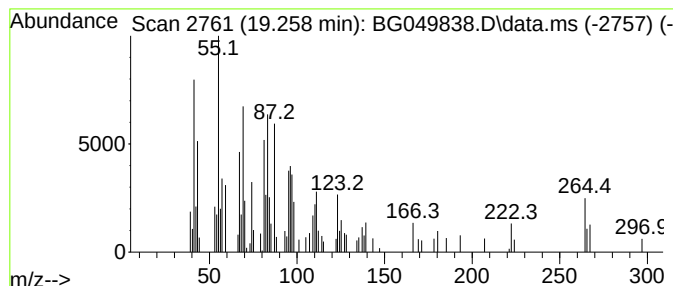
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Peak Number 5 6-Octadecenoic acid, methyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.258	2.05 ng	46423	Phenanthrene-d10	17.436	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	64
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	62
3	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	58
4	7-Octadecenoic acid, methyl ester	296	C19H36O2	057396-98-2	58
5	9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	58



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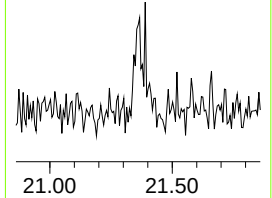
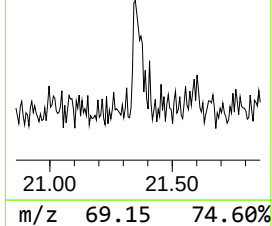
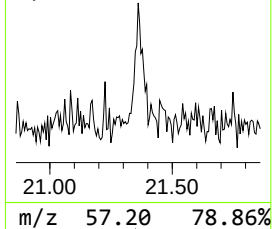
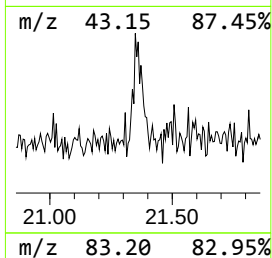
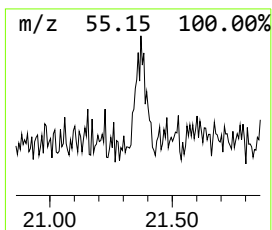
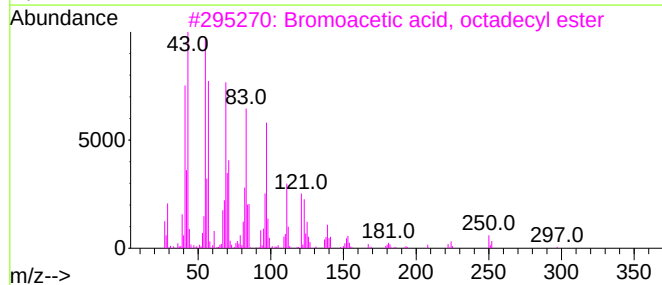
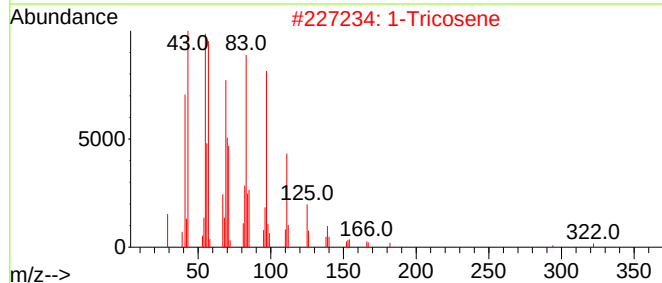
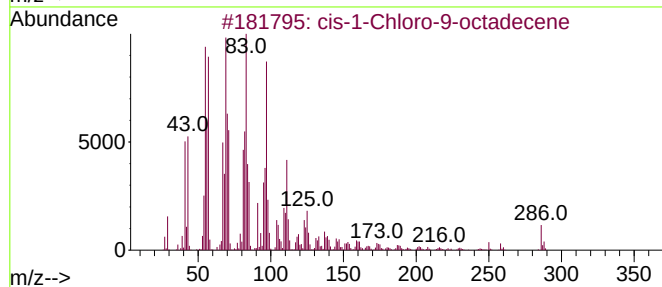
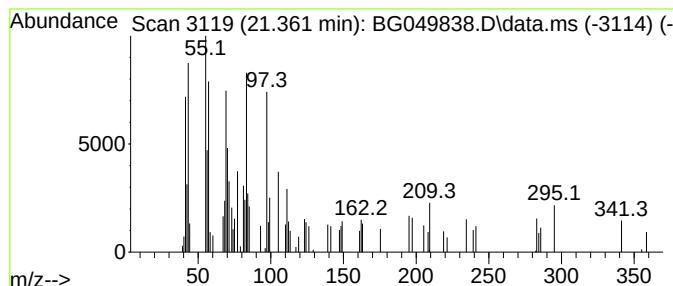
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 cis-1-Chloro-9-octadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.361	2.22 ng	50024	Chrysene-d12	21.719

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-1-Chloro-9-octadecene	286	C18H35Cl	016507-61-2	89
2			1-Tricosene	322	C23H46	018835-32-0	70
3			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	62
4			9-Eicosene, (E)-	280	C20H40	074685-29-3	60
5			5-Octadecene, (E)-	252	C18H36	007206-21-5	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081321\
Data File : BG049838.D
Acq On : 13 Aug 2021 17:17
Operator : CG/JU
Sample : M3343-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20210558-COM-31

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.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
Butane, 2-metho...	3.138	16.7	ng	149661	1	8.032	178824	20.0
unknown3.185	3.185	2.1	ng	19254	1	8.032	178824	20.0
2-Pentanone, 4-...	5.112	4.4	ng	39340	1	8.032	178824	20.0
Ethanol, 2-(2-b...	10.616	5.4	ng	66309	2	10.851	246240	20.0
6-Octadecenoic ...	19.258	2.0	ng	46423	4	17.436	453281	20.0
cis-1-Chloro-9-...	21.361	2.2	ng	50024	5	21.719	451488	20.0