

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
 Data File : BG055540.D
 Acq On : 10 Nov 2022 15:10
 Operator : CG/JU
 Sample : N5360-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20221112-COMP-11

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-BG110922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055540.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.329	3	7	13	rBV	257507	421025	13.87%	2.609%
2	3.370	13	14	24	rVB	34577	42687	1.41%	0.265%
3	5.327	340	347	357	rBV	153411	238558	7.86%	1.478%
4	5.797	420	427	438	rBV	1040130	1652540	54.46%	10.240%
5	7.407	691	701	710	rBV	964997	1723851	56.81%	10.682%
6	8.271	837	848	855	rBV	174718	296781	9.78%	1.839%
7	9.440	1037	1047	1056	rBV	562564	1003073	33.05%	6.216%
8	10.850	1281	1287	1295	rBV2	36451	60505	1.99%	0.375%
9	11.103	1322	1330	1339	rVB	220514	403209	13.29%	2.499%
10	13.517	1734	1741	1748	rBV	1257899	1931607	63.65%	11.969%
11	14.886	1968	1974	1982	rBV	349851	557717	18.38%	3.456%
12	16.367	2218	2226	2241	rBV	1221714	1867371	61.54%	11.571%
13	17.630	2433	2441	2447	rBV	477379	733636	24.18%	4.546%
14	17.742	2455	2460	2464	rBV3	29137	39519	1.30%	0.245%
15	18.494	2581	2588	2599	rBV2	54265	109064	3.59%	0.676%
16	20.215	2875	2881	2887	rVB	2374688	3034634	100.00%	18.804%
17	21.537	3101	3106	3115	rBV2	137892	220606	7.27%	1.367%
18	21.925	3165	3172	3179	rBV	490748	871035	28.70%	5.397%
19	22.119	3203	3205	3211	rVB3	28491	40499	1.33%	0.251%
20	25.351	3743	3755	3769	rBV2	284111	890117	29.33%	5.516%

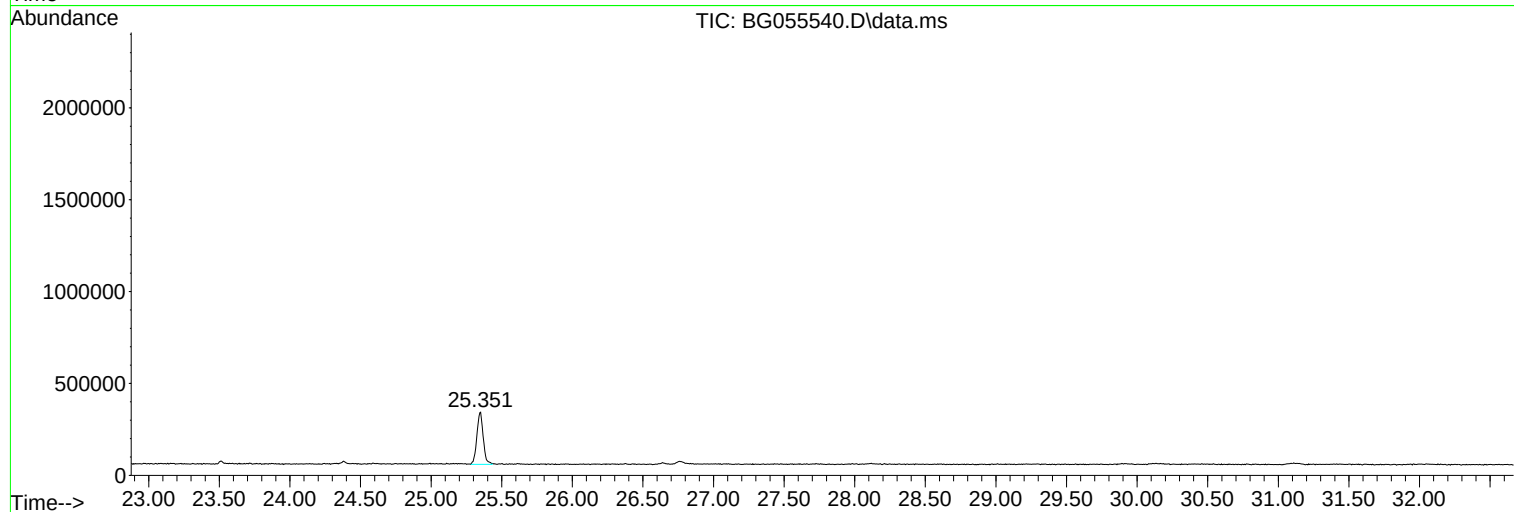
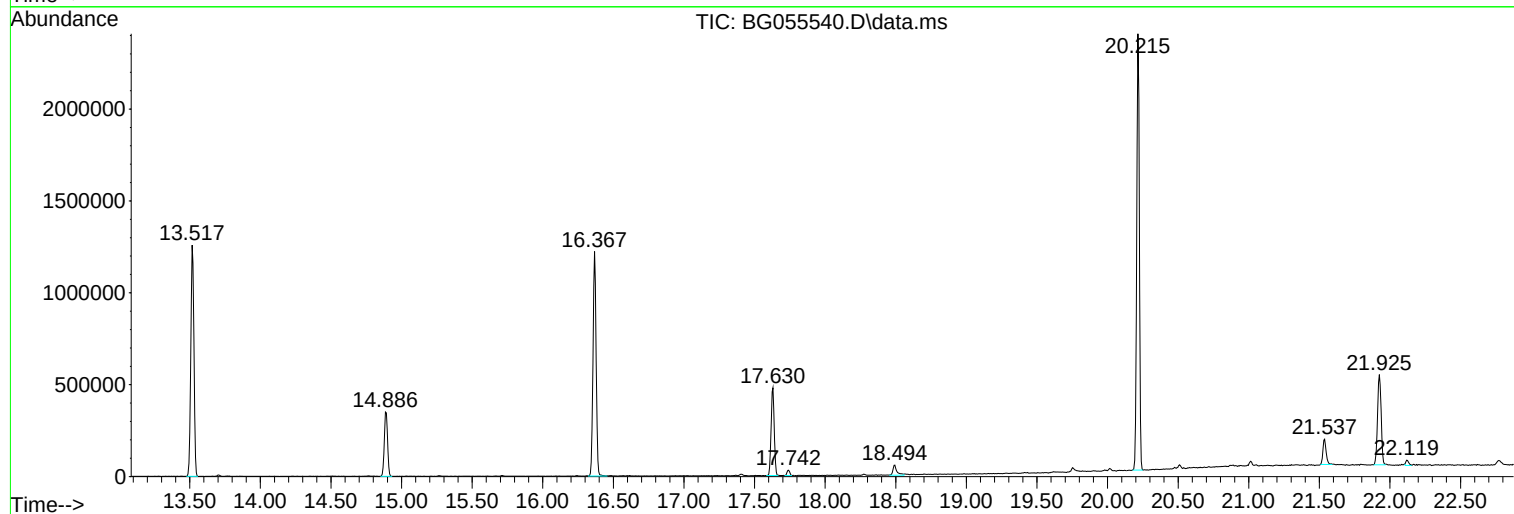
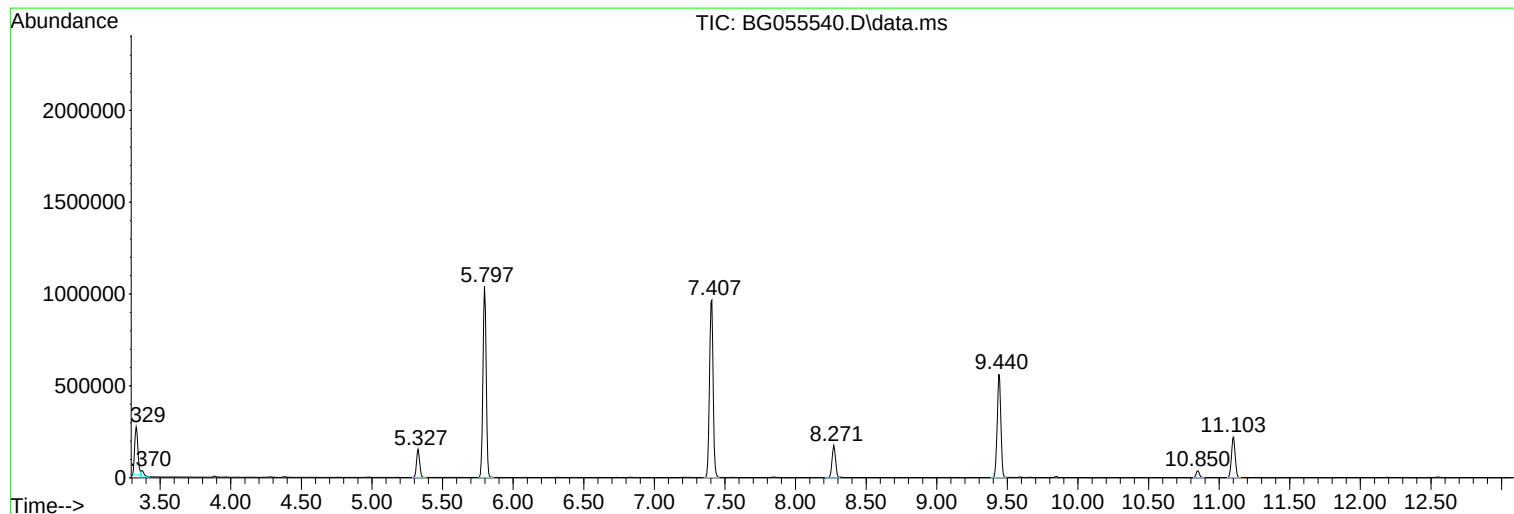
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Misc :
ALS Vial : 8 Sample Multiplier: 1

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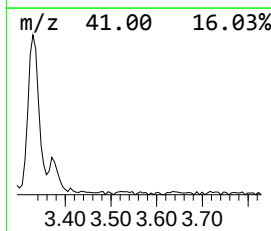
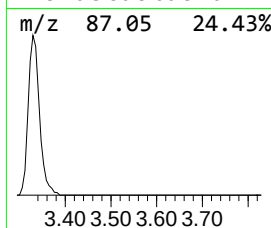
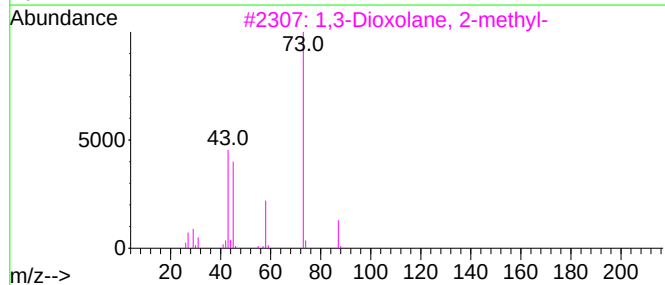
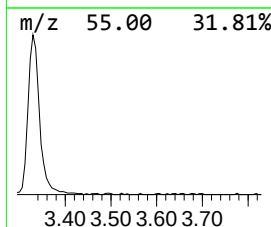
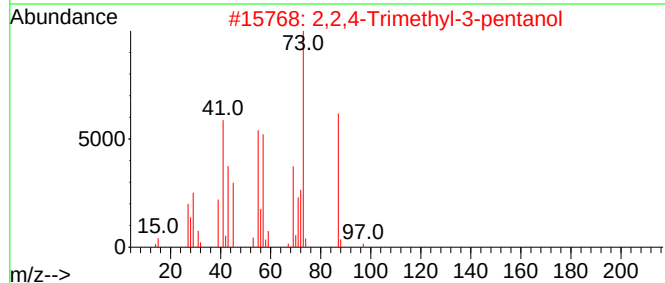
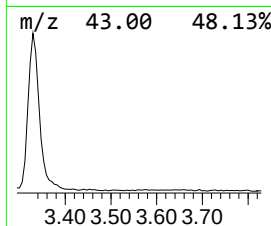
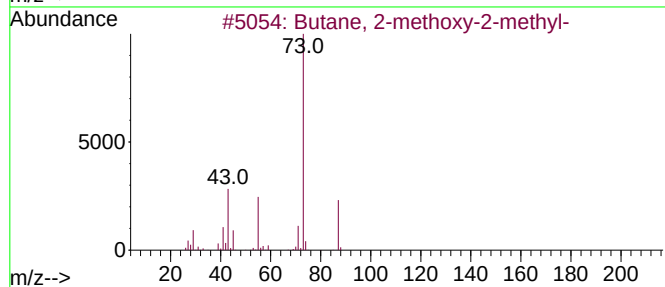
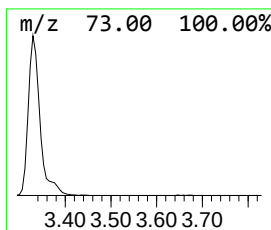
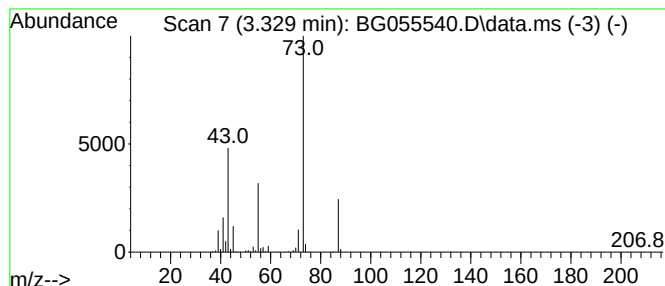
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.329	28.37 ng	421025	1,4-Dichlorobenzene-d4	8.271

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-methyl-	88	C4H8O2	000497-26-7	25
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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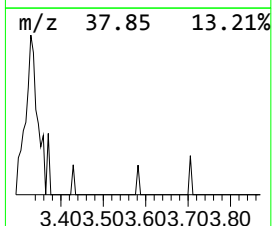
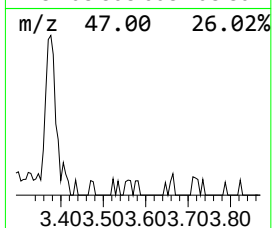
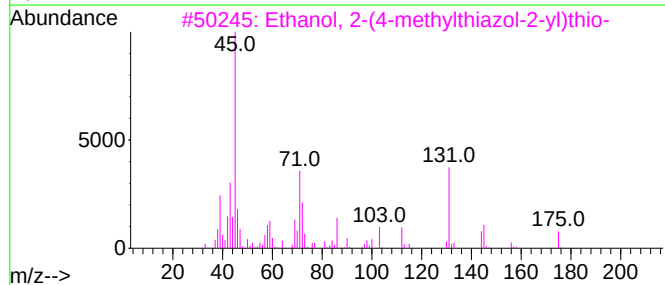
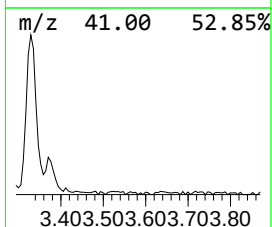
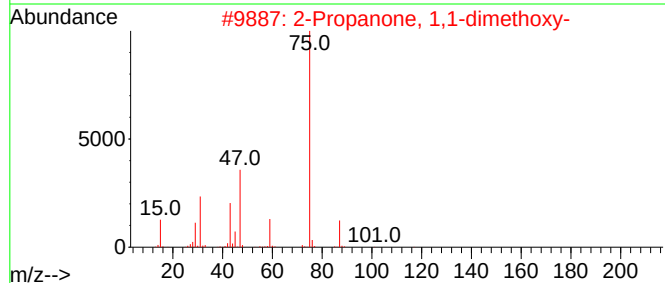
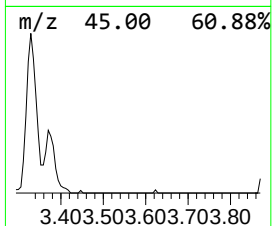
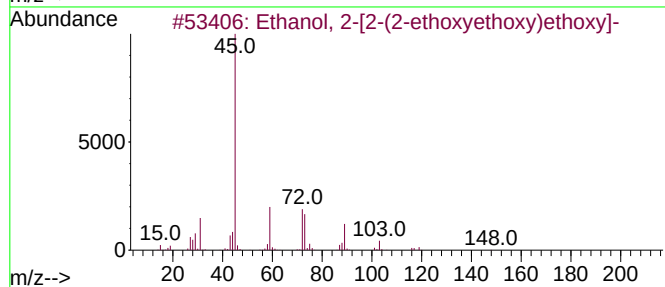
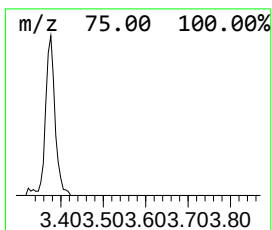
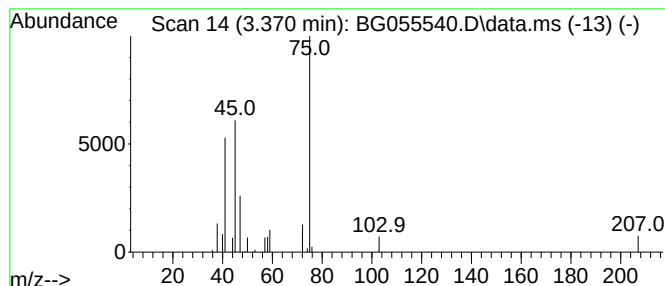
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown3.370 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.370	2.88 ng	42687	1,4-Dichlorobenzene-d4	8.271

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	9
2			2-Propanone, 1,1-dimethoxy-	118	C5H10O3	006342-56-9	9
3			Ethanol, 2-(4-methylthiazol-2-yl...	175	C6H9NOS2	040107-47-9	9
4			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	9
5			1,3-Octanediol	146	C8H18O2	023433-05-8	9



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ALS Vial : 8 Sample Multiplier: 1

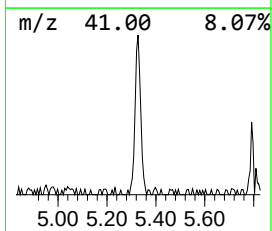
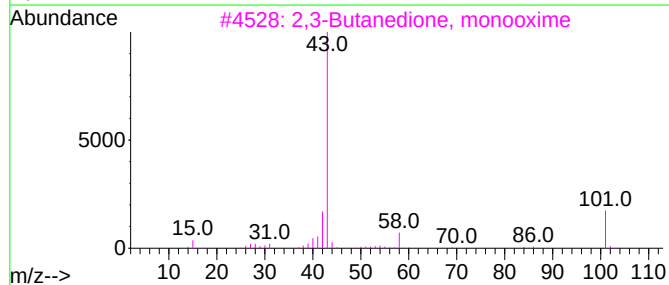
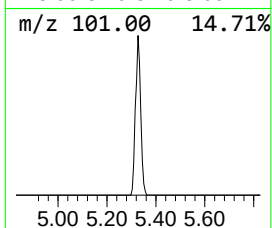
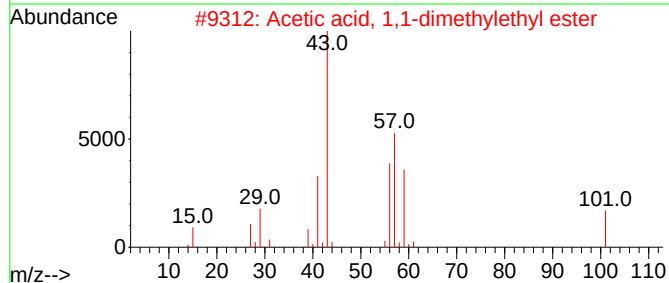
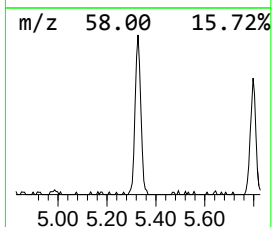
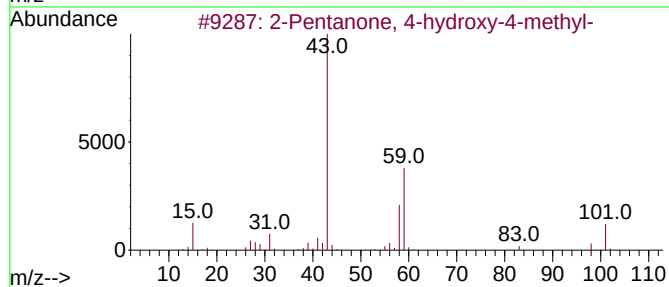
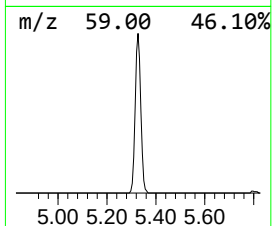
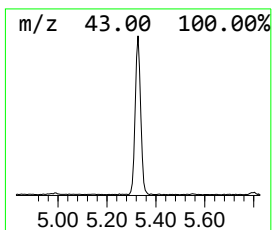
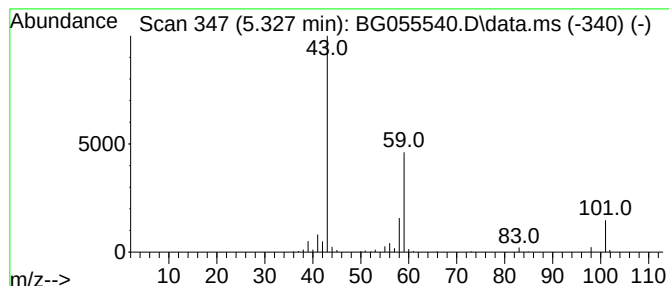
Instrument :
BNA_G
ClientSampleId :
20221112-COMP-11

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

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.327	16.08 ng	238558	1,4-Dichlorobenzene-d4			8.271
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...		116	C6H12O2	000540-88-5	38
3	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	27
4	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	12
5	Butane		58	C4H10	000106-97-8	9



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Misc :
ALS Vial : 8 Sample Multiplier: 1

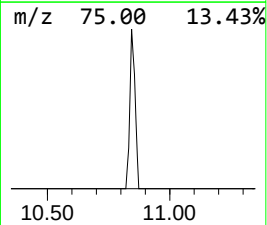
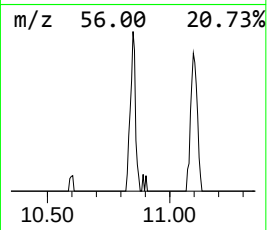
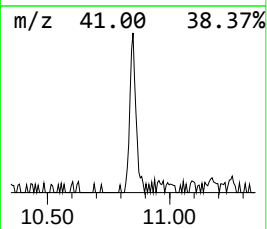
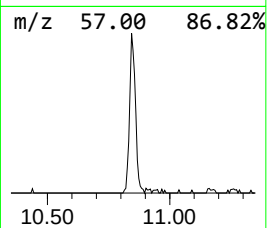
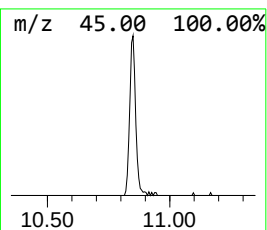
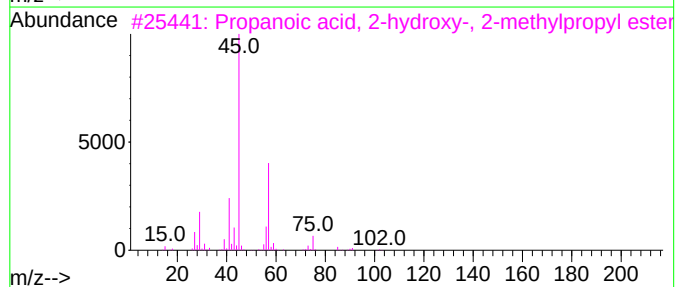
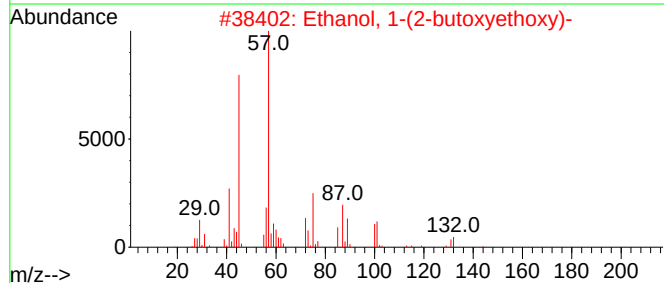
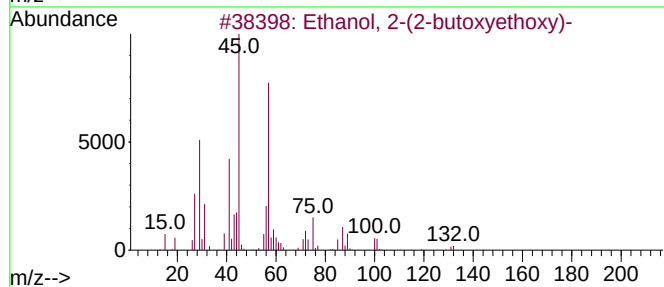
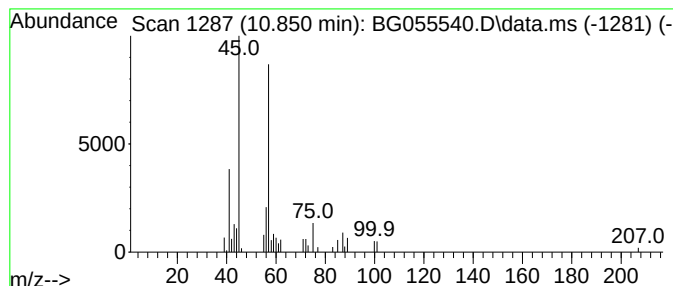
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.850	3.00 ng	60505	Naphthalene-d8	11.102	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	72
3	Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	59
4	Butane, 1,1'-[ethylidenebis(oxy)...	174	C10H22O2	000871-22-7	45
5	Acetaldehyde, di-sec-butyl acetal	174	C10H22O2	005314-41-0	42



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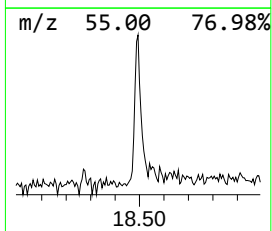
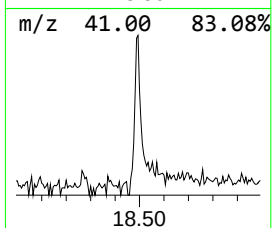
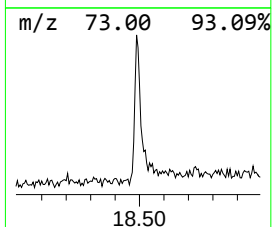
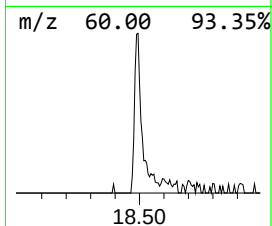
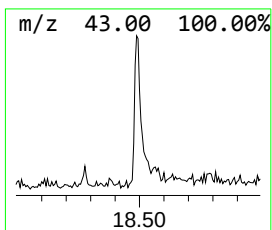
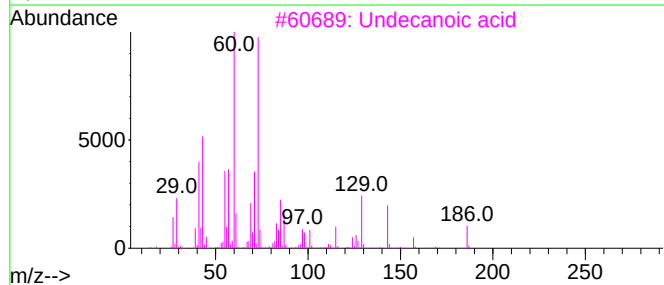
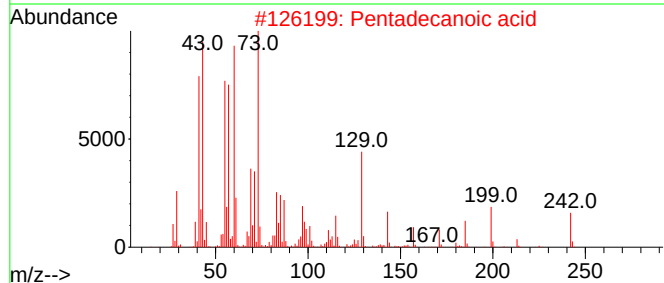
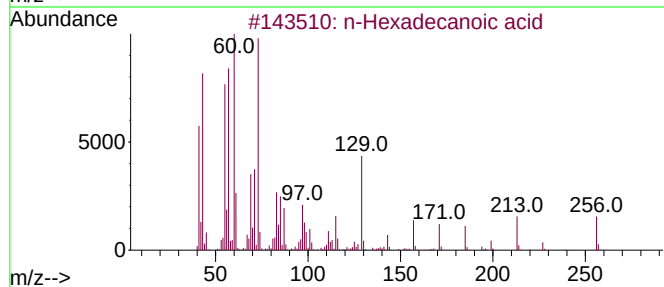
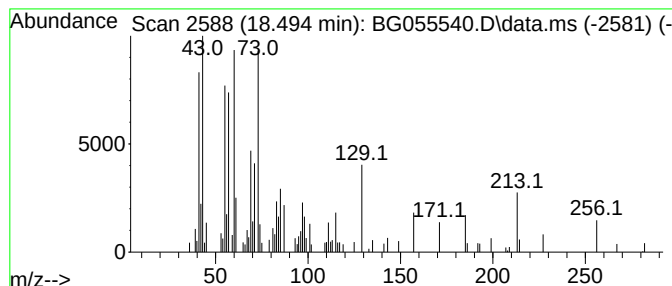
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.494	2.97 ng	109064	Phenanthrene-d10		17.630	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	87
3	Undecanoic acid		186	C11H22O2	000112-37-8	68
4	Tridecanoic acid		214	C13H26O2	000638-53-9	52
5	Dodecanoic acid		200	C12H24O2	000143-07-7	50



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ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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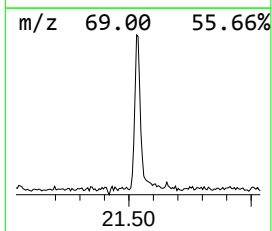
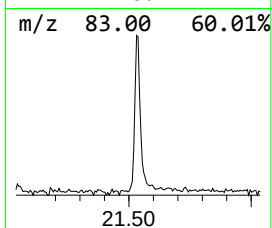
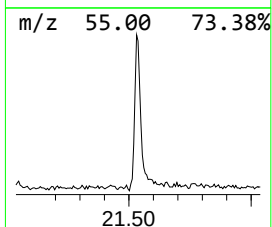
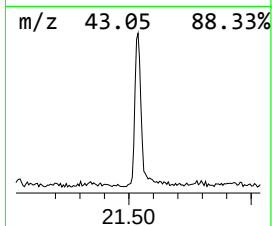
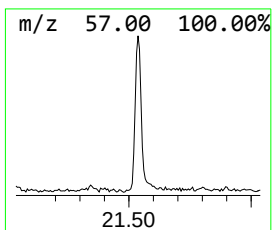
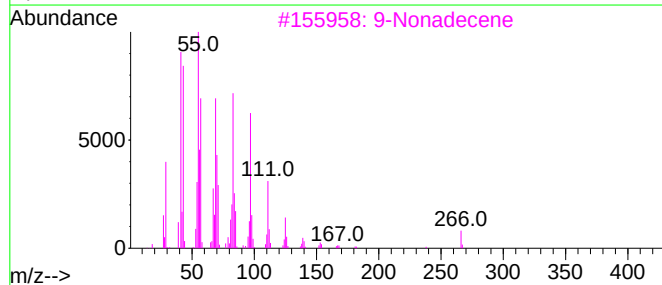
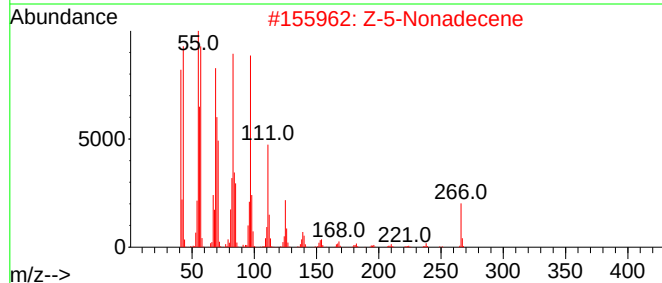
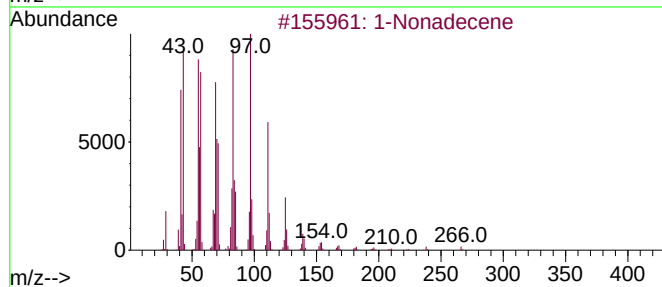
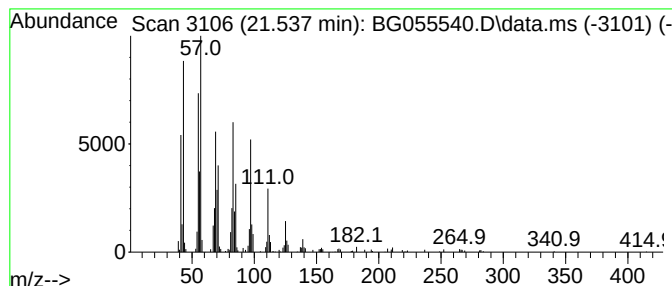
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Nonadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.537	5.07 ng	220606	Chrysene-d12	21.925

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Nonadecene	266	C19H38	018435-45-5	94
2			Z-5-Nonadecene	266	C19H38	1000131-11-8	93
3			9-Nonadecene	266	C19H38	031035-07-1	93
4			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
5			Nonadecyl heptafluorobutyrate	480	C23H39F7O2	1000351-83-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
Data File : BG055540.D
Acq On : 10 Nov 2022 15:10
Operator : CG/JU
Sample : N5360-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221112-COMP-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.329	28.4	ng	421025	1	8.271	296781	20.0
unknown3.370	3.370	2.9	ng	42687	1	8.271	296781	20.0
2-Pentanone, 4-...	5.327	16.1	ng	238558	1	8.271	296781	20.0
Ethanol, 2-(2-b...	10.850	3.0	ng	60505	2	11.102	403209	20.0
n-Hexadecanoic ...	18.494	3.0	ng	109064	4	17.630	733636	20.0
1-Nonadecene	21.537	5.1	ng	220606	5	21.925	871035	20.0