

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011123\
 Data File : BG056256.D
 Acq On : 11 Jan 2023 18:43
 Operator : CG/JU
 Sample : 01055-03
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MH-F

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-BG122722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056256.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.331	3	7	22	rVB	455418	707521	18.28%	4.763%
2	4.959	278	284	293	rVB	79957	138093	3.57%	0.930%
3	5.352	346	351	358	rVB	50127	75221	1.94%	0.506%
4	5.834	424	433	444	rVB	319696	524793	13.56%	3.533%
5	7.444	700	707	719	rBV	201679	346506	8.95%	2.333%
6	8.167	823	830	840	rBV2	36727	62499	1.62%	0.421%
7	8.314	848	855	863	rVB	125792	215314	5.56%	1.449%
8	9.489	1047	1055	1064	rBV	422746	763124	19.72%	5.137%
9	11.146	1329	1337	1344	rBV	168222	300990	7.78%	2.026%
10	13.555	1739	1747	1754	rBV	1726268	2540921	65.66%	17.105%
11	14.924	1974	1980	1991	rVB	320786	519648	13.43%	3.498%
12	16.404	2224	2232	2242	rBV	1271545	1954236	50.50%	13.156%
13	17.662	2437	2446	2457	rVB	488873	734589	18.98%	4.945%
14	18.508	2585	2590	2598	rBV2	98041	149126	3.85%	1.004%
15	19.765	2799	2804	2812	rBV	63865	103388	2.67%	0.696%
16	20.241	2879	2885	2890	rBV	2948564	3869583	100.00%	26.049%
17	21.539	3101	3106	3120	rBV	38524	94224	2.43%	0.634%
18	21.951	3170	3176	3185	rVB2	453109	825928	21.34%	5.560%
19	23.707	3470	3475	3480	rBV4	20194	39503	1.02%	0.266%
20	25.394	3750	3762	3776	rBV2	295910	889636	22.99%	5.989%

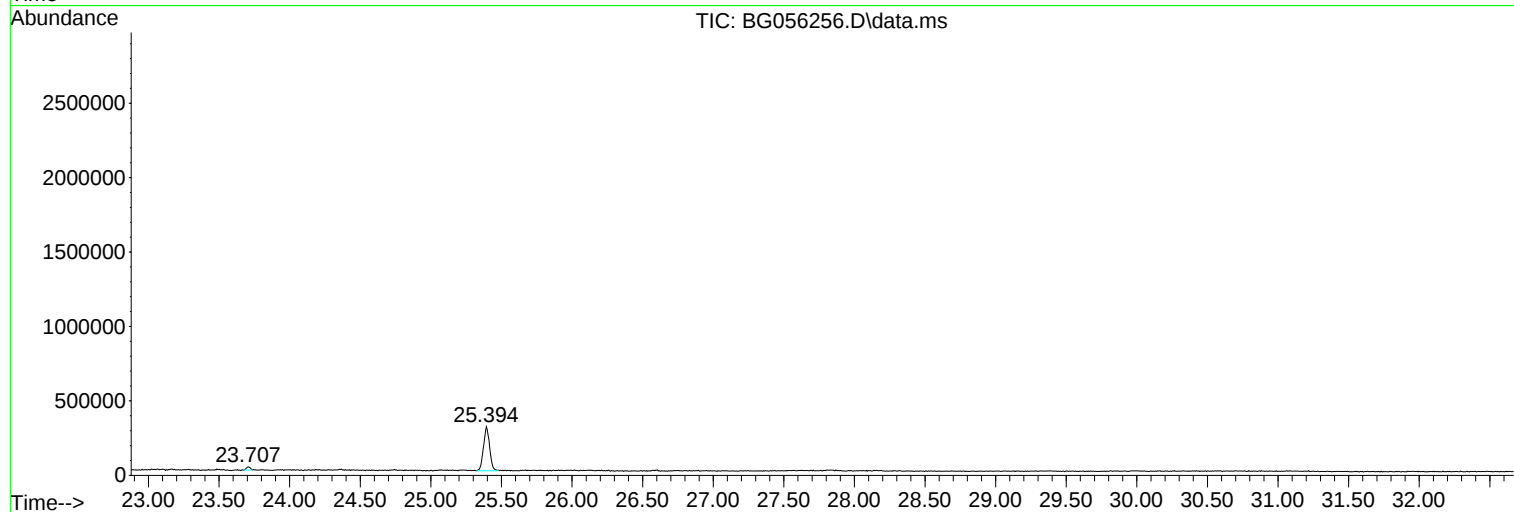
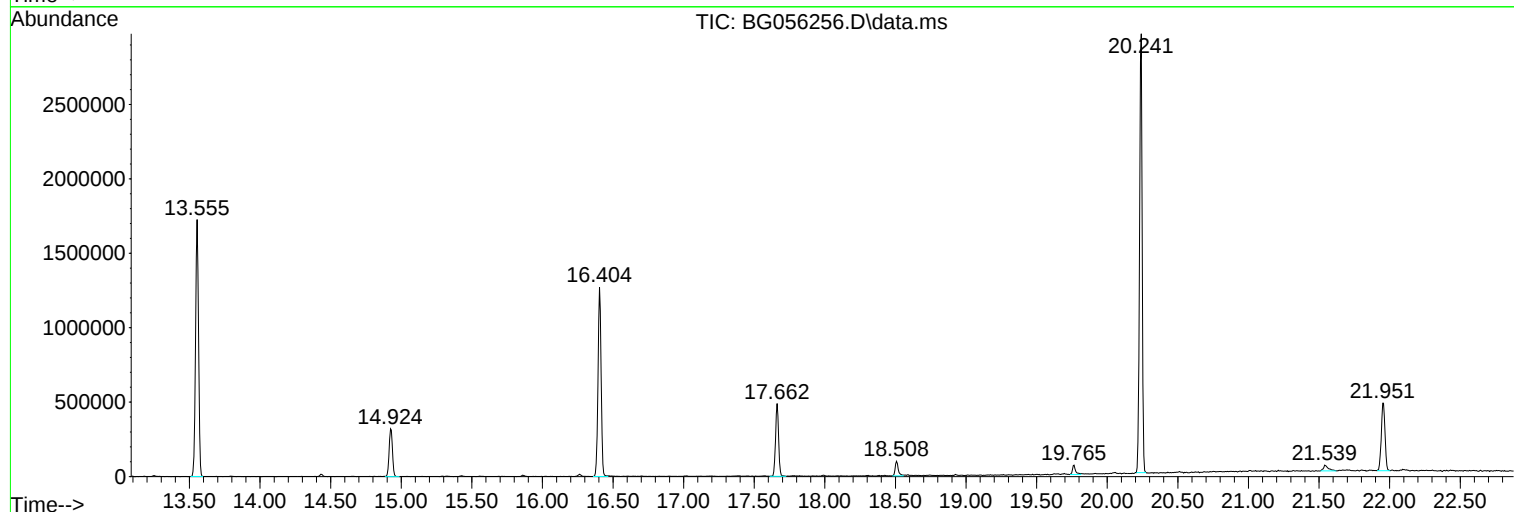
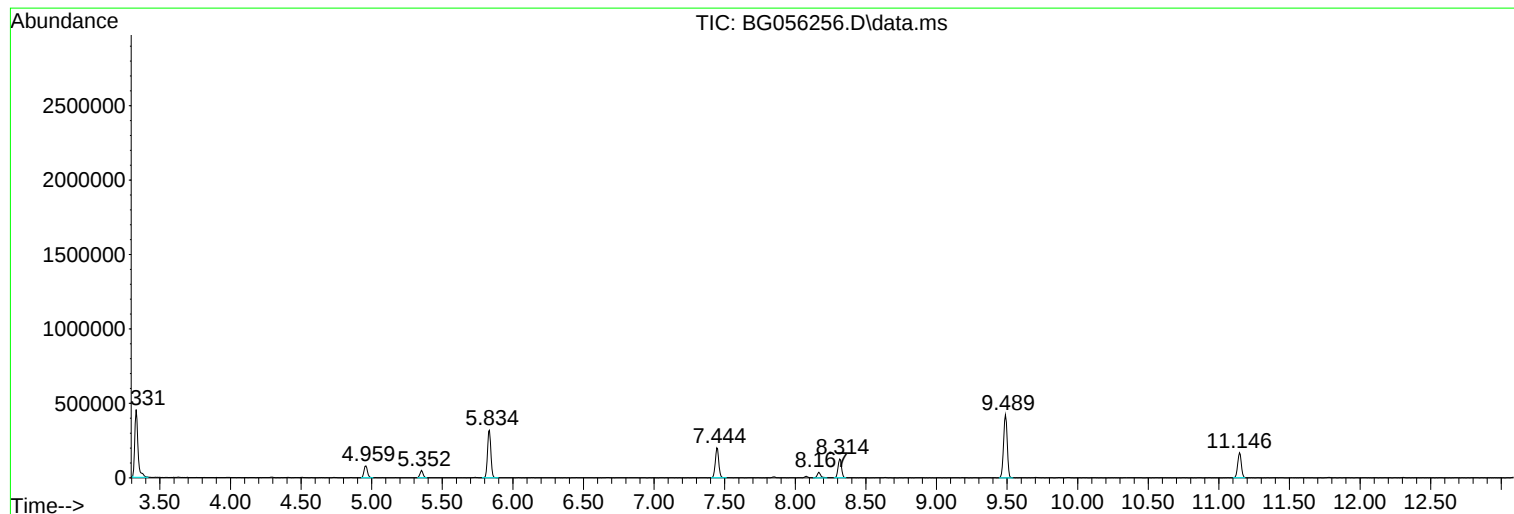
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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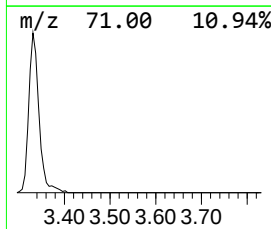
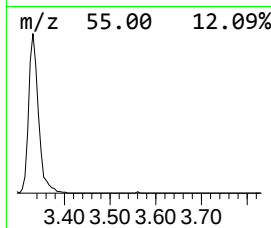
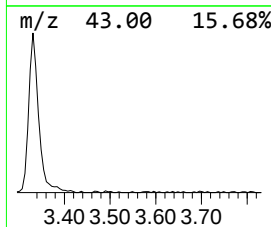
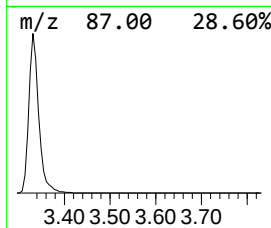
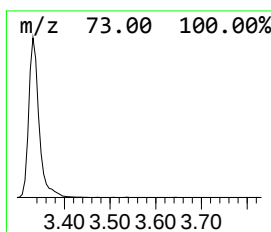
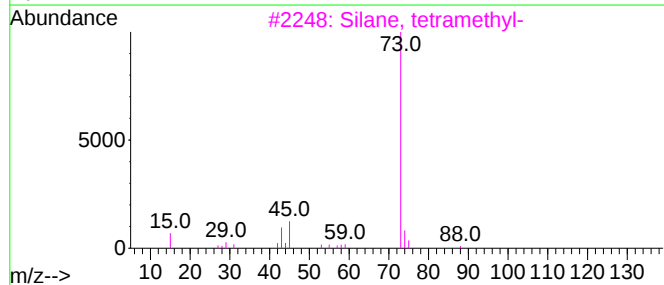
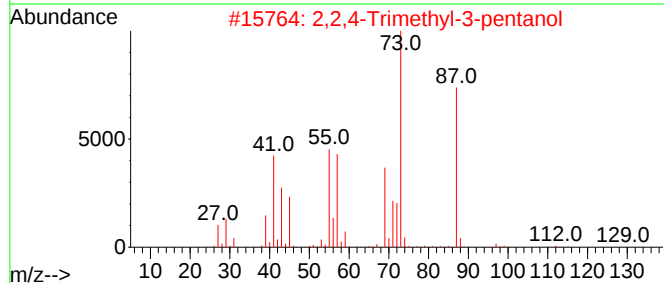
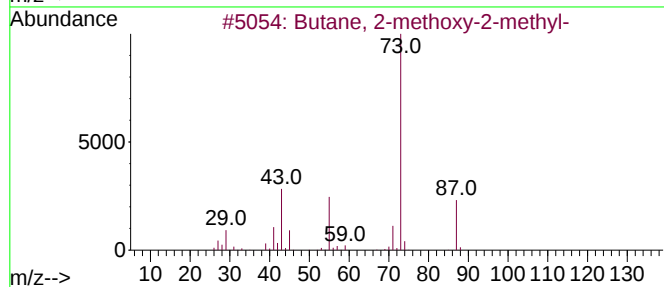
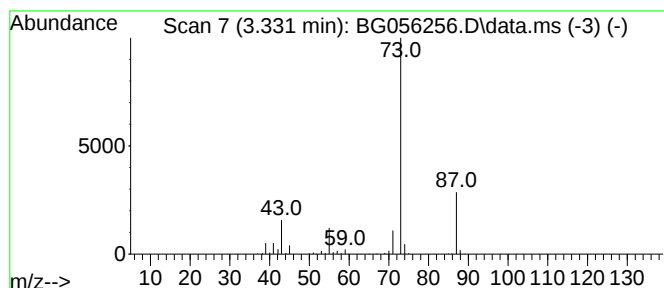
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.331	65.72 ng	707521	1,4-Dichlorobenzene-d4	8.314

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	74
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5			N-Ethylformamide	73	C3H7NO	000627-45-2	7



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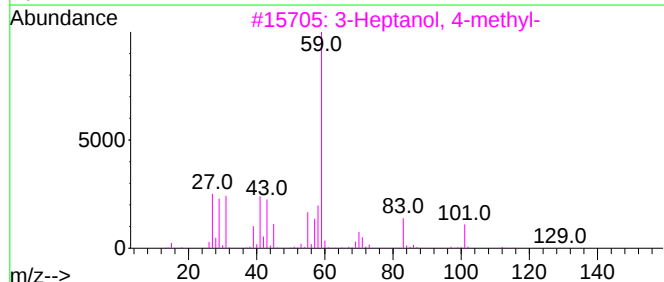
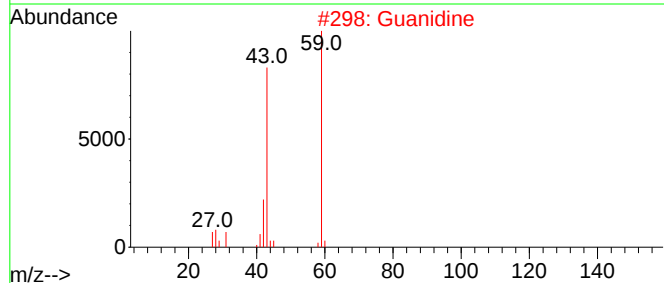
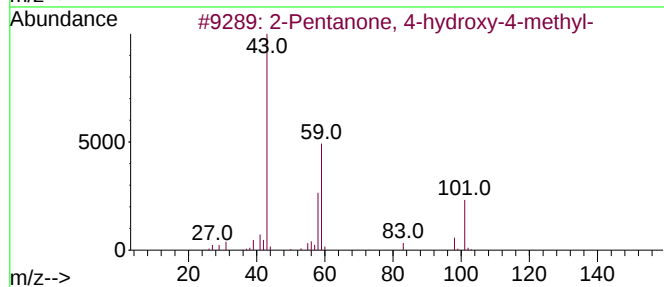
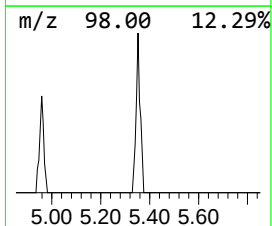
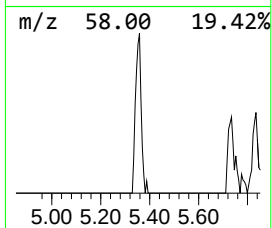
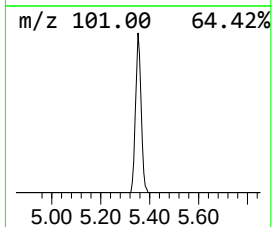
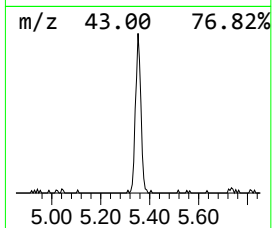
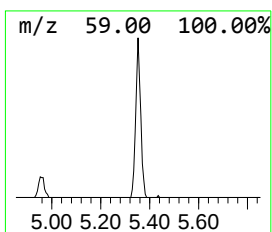
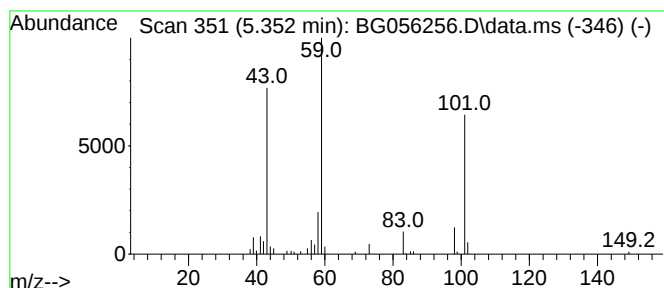
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.352	6.99 ng	75221	1,4-Dichlorobenzene-d4	8.314

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Guanidine	59	CH5N3	000113-00-8	43
3		3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	28
4		6-Nitrohexan-2-ol	147	C6H13NO3	062224-53-7	25
5		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25



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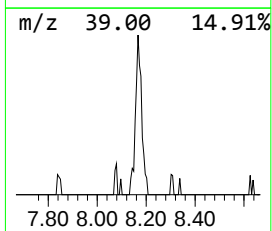
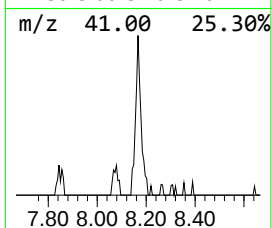
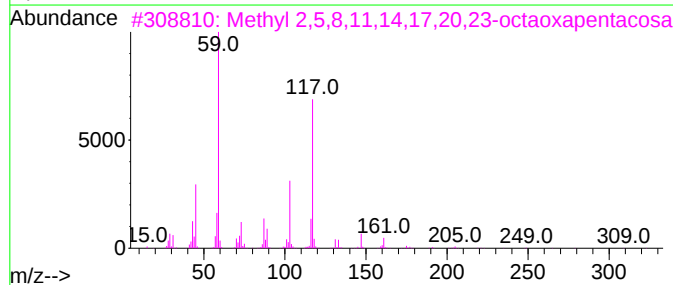
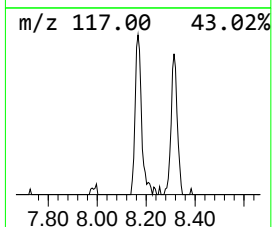
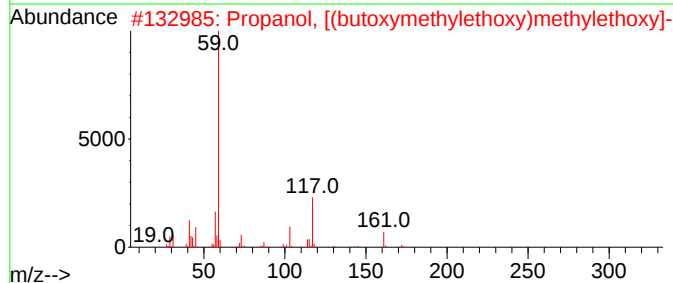
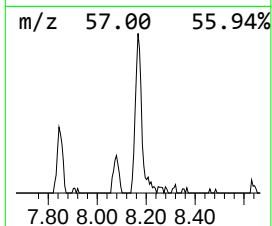
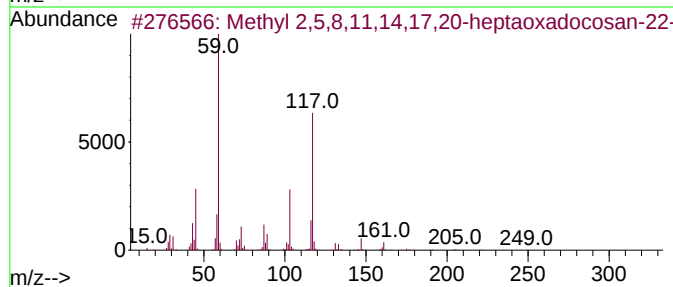
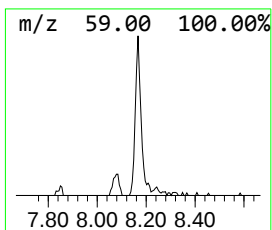
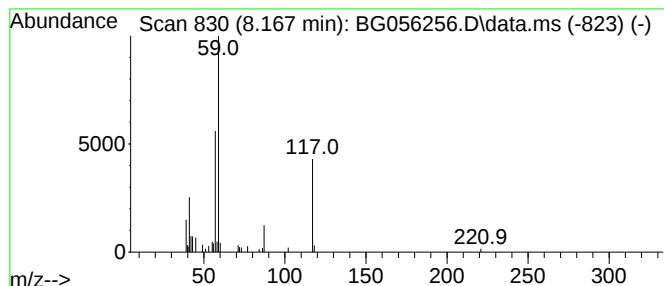
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Methyl 2,5,8,11,14,17,20-he... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.167	5.81 ng	62499	1,4-Dichlorobenzene-d4	8.314

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl 2,5,8,11,14,17,20-heptaox...	368	C16H32O9	1010366-81-3	78
2			Propanol, [(butoxymethylethoxy)m...	248	C13H28O4	055934-93-5	72
3			Methyl 2,5,8,11,14,17,20,23-octa...	412	C18H36O10	1000366-81-2	64
4			Methyl 2,5,8,11,14,17,20,23,26-n...	456	C20H40O11	1000366-81-1	64
5			Methyl 2,5,8,11-tetraoxatridecan...	236	C10H20O6	1000366-78-2	64



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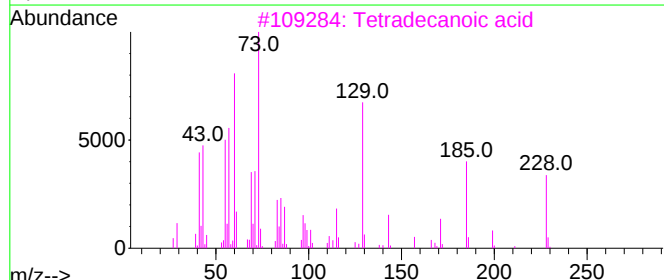
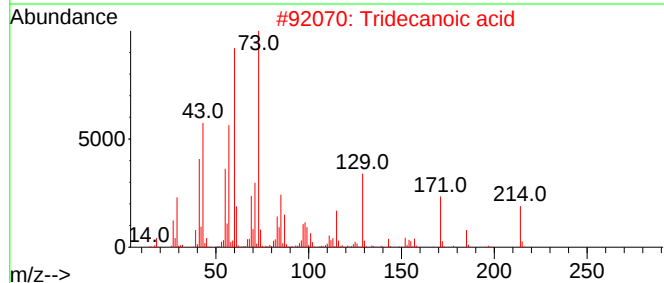
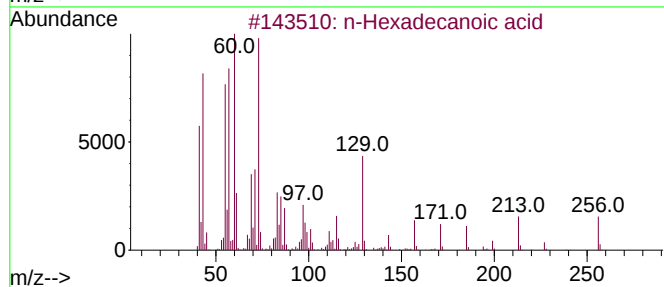
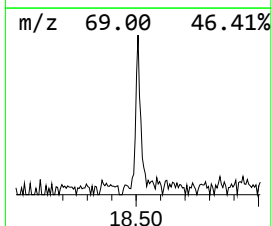
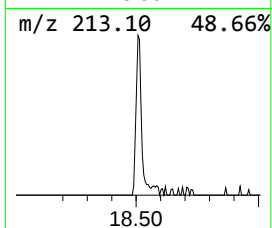
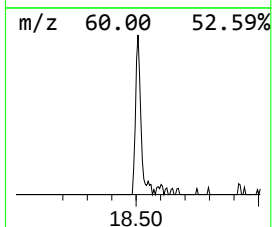
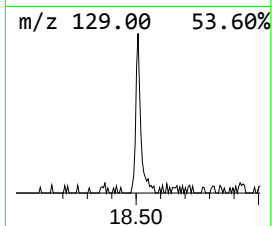
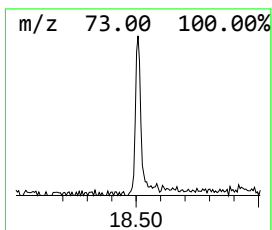
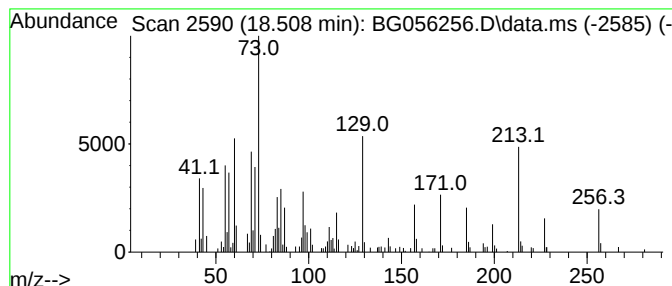
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.508	4.06 ng	149126	Phenanthrene-d10	17.662	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	55
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	55
4	Dodecanoic acid	200	C12H24O2	000143-07-7	53
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	27



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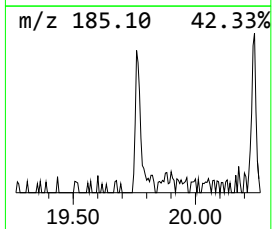
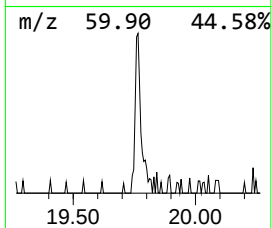
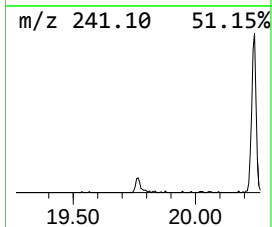
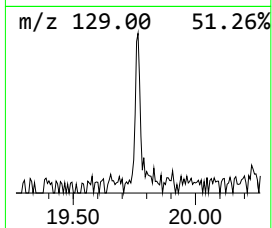
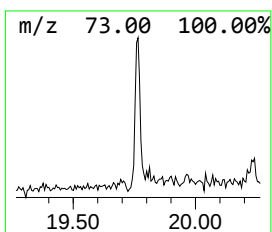
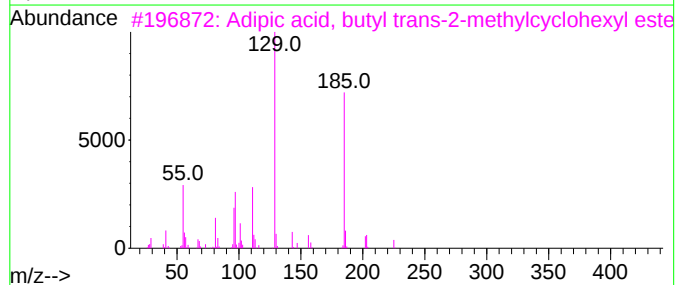
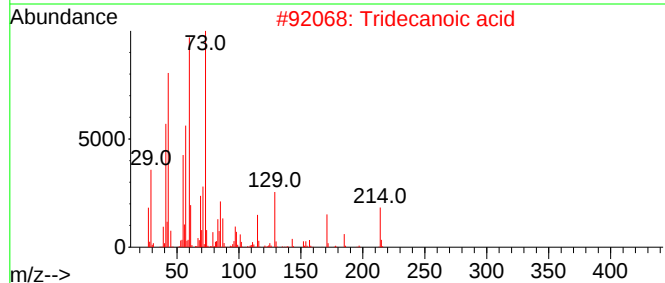
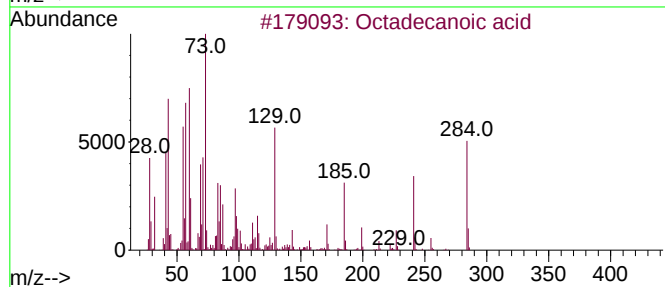
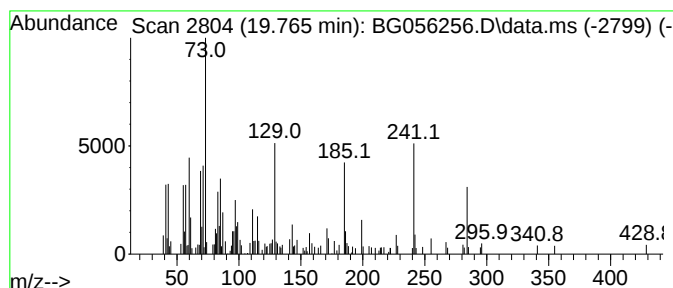
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.765	2.81 ng	103388	Phenanthrene-d10		17.662	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octadecanoic acid		284	C18H36O2	000057-11-4	93
2	Tridecanoic acid		214	C13H26O2	000638-53-9	38
3	Adipic acid, butyl trans-2-methy...		298	C17H30O4	1000324-74-6	35
4	Adipic acid, butyl 2-methylpent-...		286	C16H30O4	1010353-55-8	27
5	Adipic acid, butyl cycloheptyl e...		298	C17H30O4	1000324-71-6	27



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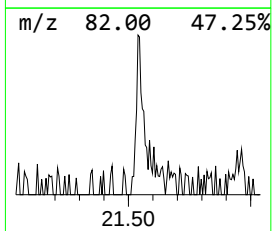
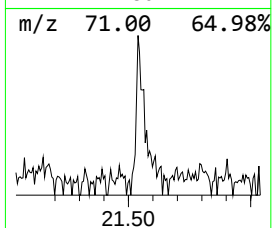
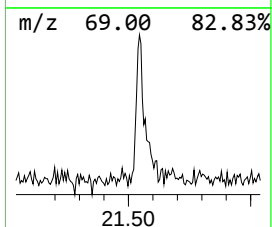
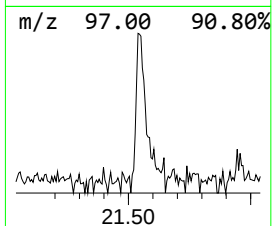
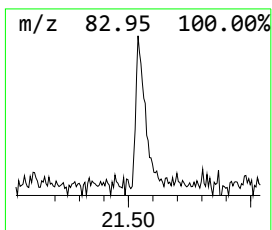
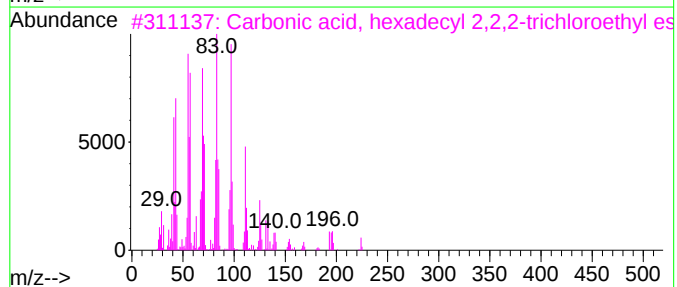
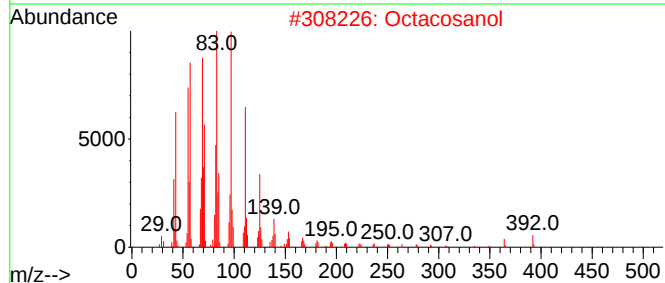
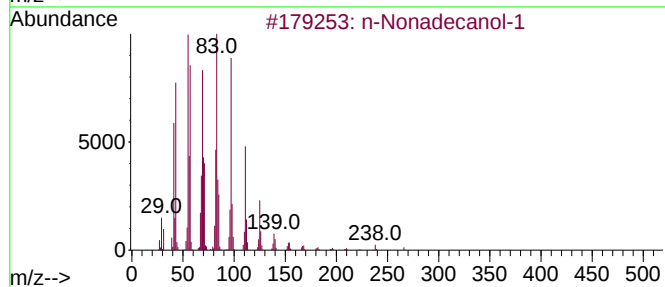
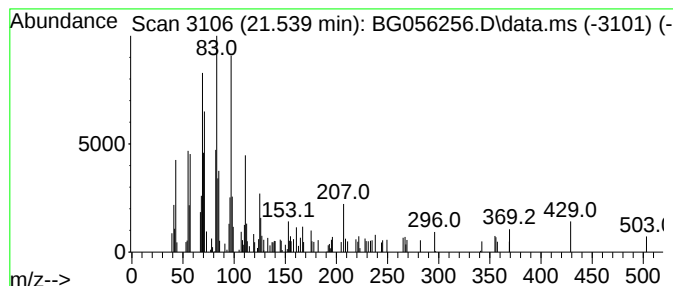
Instrument :
BNA_G
ClientSampleId :
MH-F

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Nonadecanol-1 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.539	2.28 ng	94224	Chrysene-d12	21.951	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	87
2	Octacosanol	410	C28H58O	000557-61-9	83
3	Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	72
4	Chloroacetic acid, pentadecyl ester	304	C17H33ClO2	070301-47-2	72
5	Carbonic acid, tetradecyl 2,2,2-...	388	C17H31Cl3O3	1000314-56-0	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011123\
Data File : BG056256.D
Acq On : 11 Jan 2023 18:43
Operator : CG/JU
Sample : 01055-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-F

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.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...	3.331	65.7	ng	707521	1	8.314	215314	20.0
2-Pentanone, 4-...	5.352	7.0	ng	75221	1	8.314	215314	20.0
Methyl 2,5,8,11...	8.167	5.8	ng	62499	1	8.314	215314	20.0
n-Hexadecanoic ...	18.508	4.1	ng	149126	4	17.662	734589	20.0
Octadecanoic acid	19.765	2.8	ng	103388	4	17.662	734589	20.0
n-Nonadecanol-1	21.539	2.3	ng	94224	5	21.951	825928	20.0