

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100422\
 Data File : BG055066.D
 Acq On : 4 Oct 2022 16:52
 Operator : CG/JU
 Sample : N4909-02
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PE-5

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-BG100322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055066.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.382	11	16	32	rVB	380932	613894	24.71%	4.803%
2	4.774	248	253	260	rBV	42860	64546	2.60%	0.505%
3	5.391	351	358	370	rBV	644574	1027238	41.36%	8.038%
4	5.861	431	438	449	rBV	614073	1009582	40.64%	7.900%
5	6.496	540	546	553	rVB	44767	70134	2.82%	0.549%
6	7.471	703	712	725	rBV	664981	1151320	46.35%	9.009%
7	8.346	853	861	867	rBV	109635	189640	7.63%	1.484%
8	9.516	1051	1060	1070	rBV	393859	687358	27.67%	5.378%
9	11.173	1335	1342	1350	rBV	161968	284511	11.45%	2.226%
10	13.581	1745	1752	1762	rVB	1141833	1732806	69.76%	13.559%
11	14.950	1978	1985	1992	rBV	265367	412770	16.62%	3.230%
12	16.425	2229	2236	2249	rBV	869141	1297251	52.23%	10.151%
13	17.683	2443	2450	2456	rBV	332473	485677	19.55%	3.800%
14	17.788	2464	2468	2473	rBV	20330	28237	1.14%	0.221%
15	18.534	2590	2595	2602	rBV2	51319	70746	2.85%	0.554%
16	19.792	2805	2809	2813	rBV2	25659	31914	1.28%	0.250%
17	20.262	2882	2889	2895	rVB	1899328	2483925	100.00%	19.436%
18	21.578	3109	3113	3121	rVB	48891	76524	3.08%	0.599%
19	21.977	3174	3181	3188	rBV	290296	522074	21.02%	4.085%
20	25.438	3760	3770	3779	rBV2	170013	540011	21.74%	4.225%

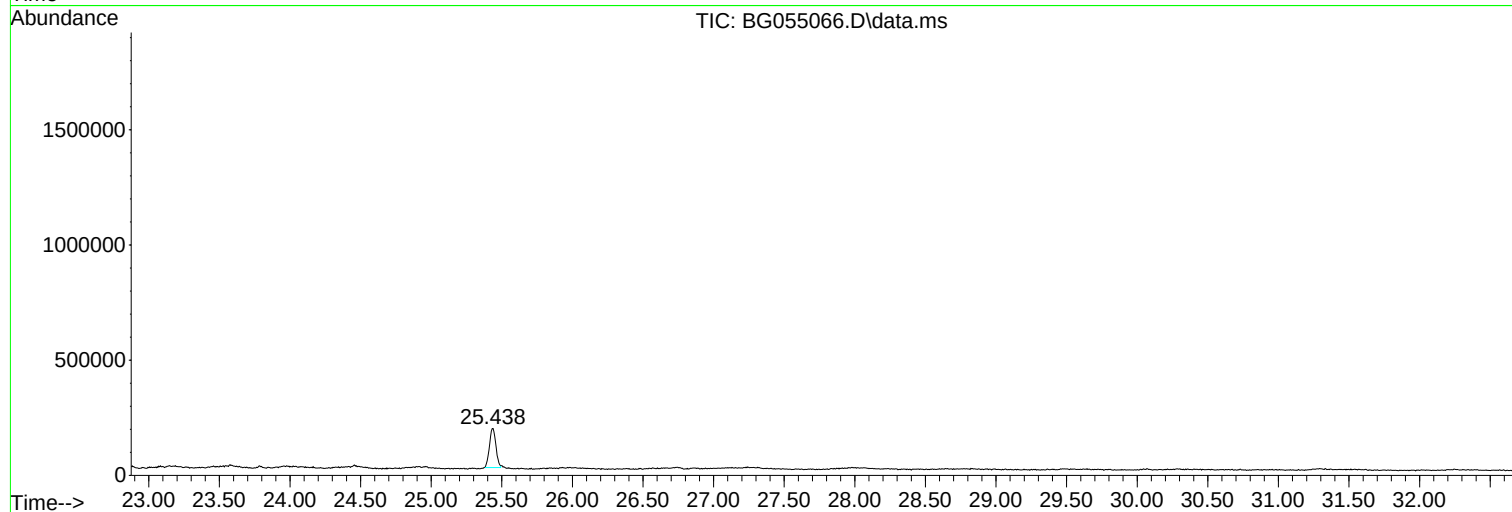
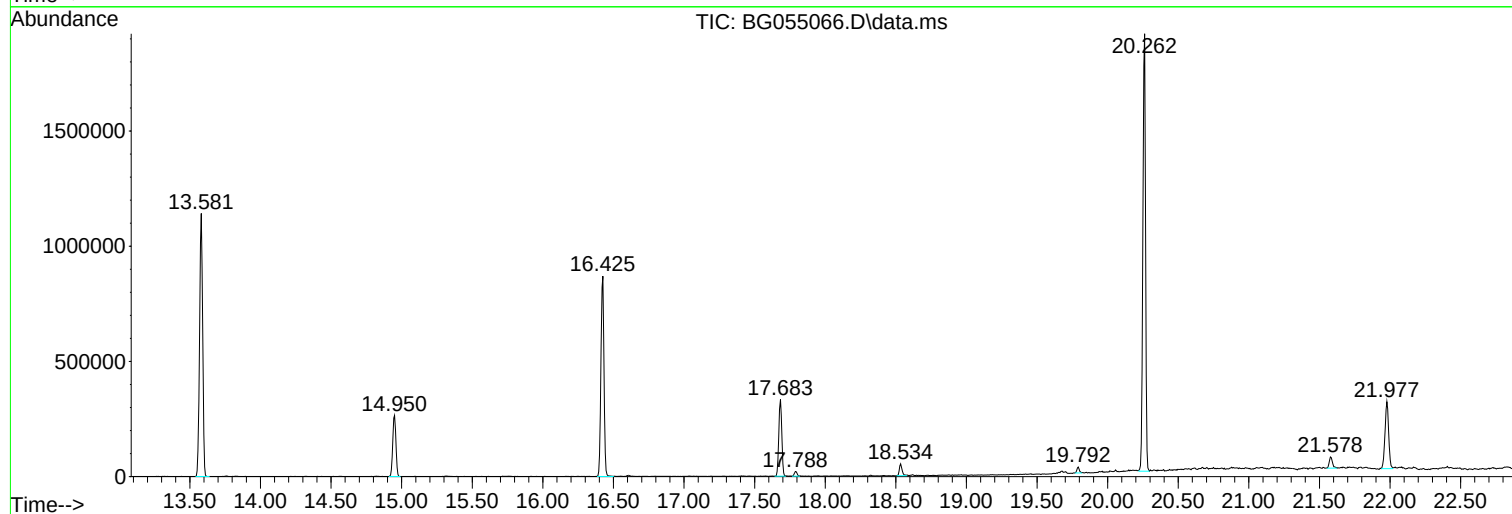
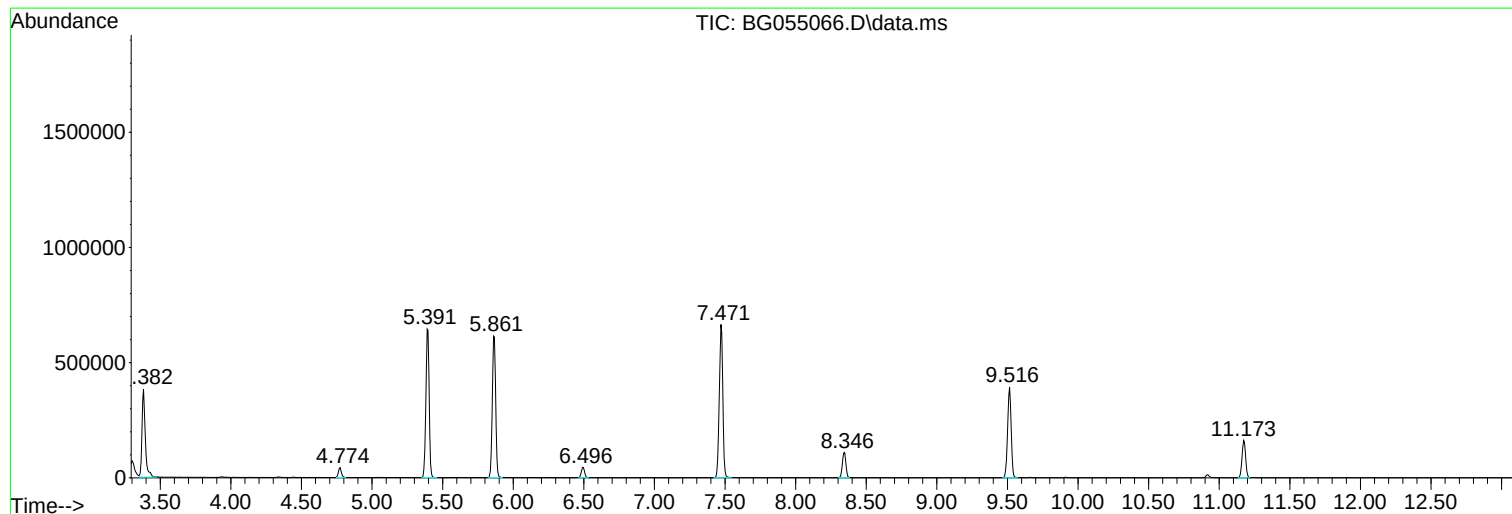
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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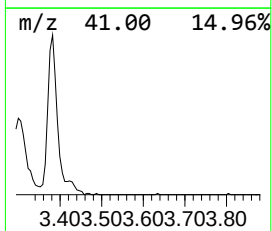
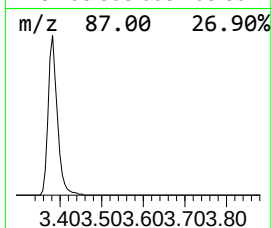
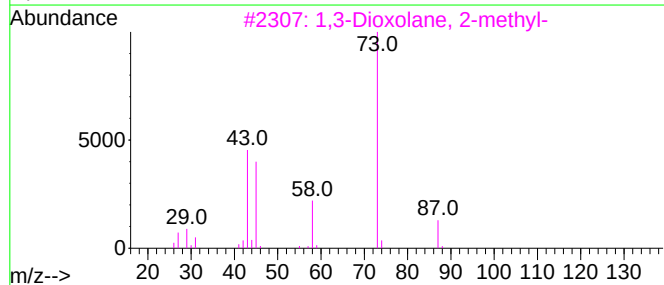
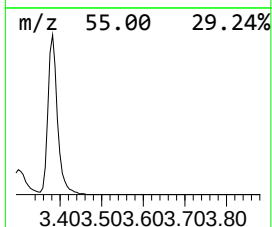
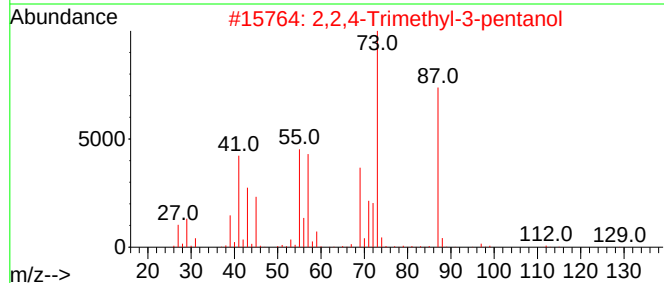
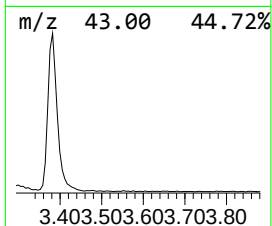
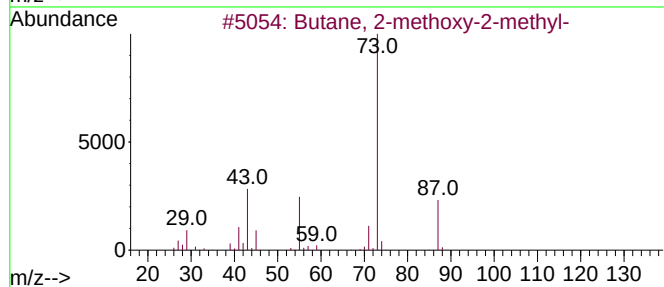
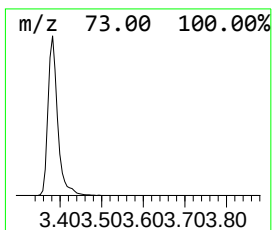
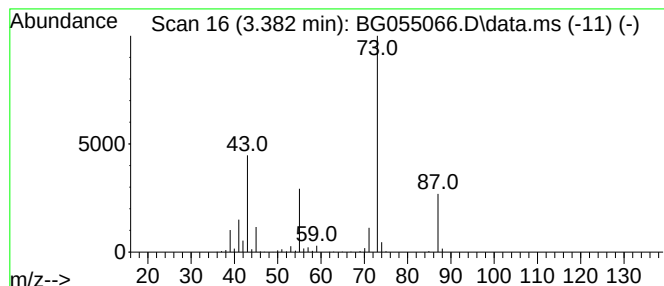
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.382	64.74 ng	613894	1,4-Dichlorobenzene-d4	8.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	23
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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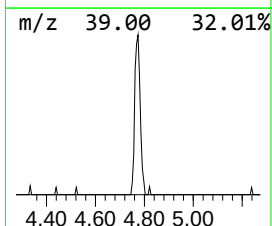
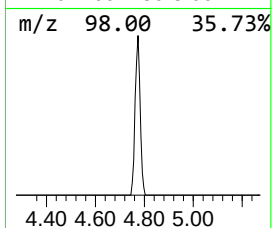
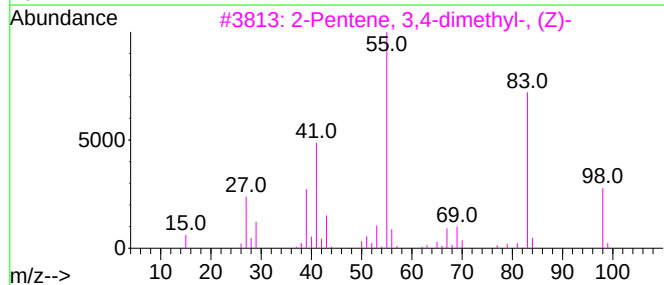
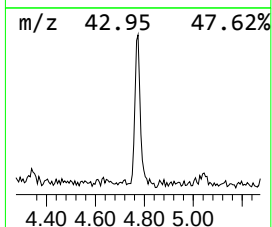
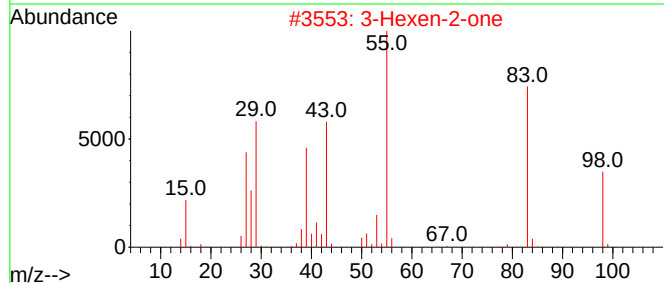
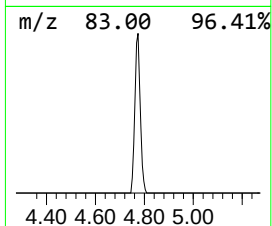
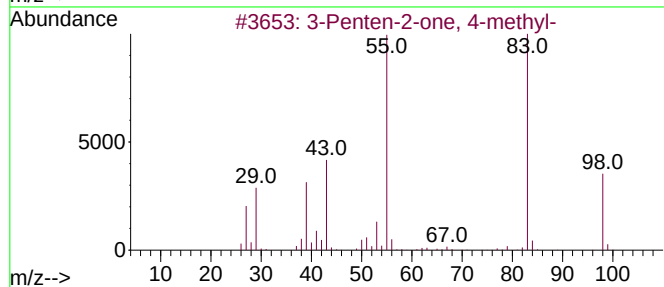
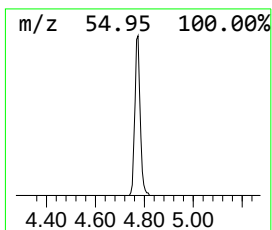
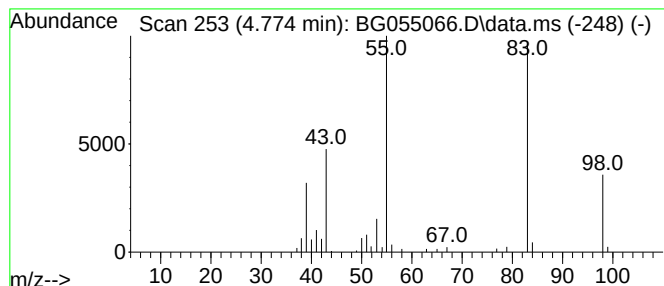
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.774	6.81 ng	64546	1,4-Dichlorobenzene-d4	8.346

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
5		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78



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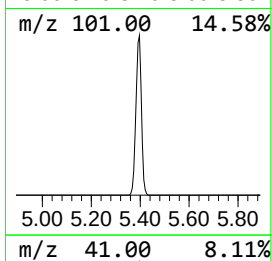
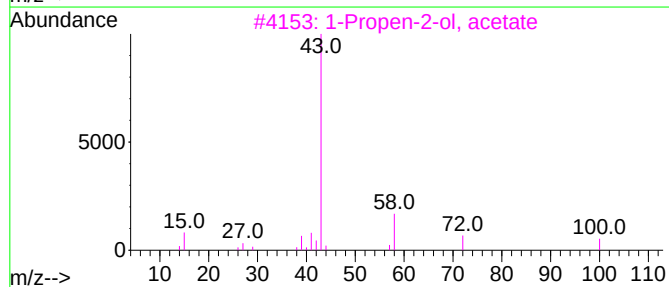
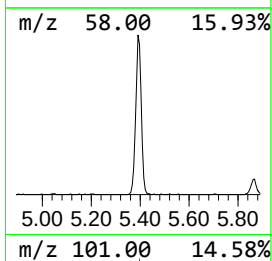
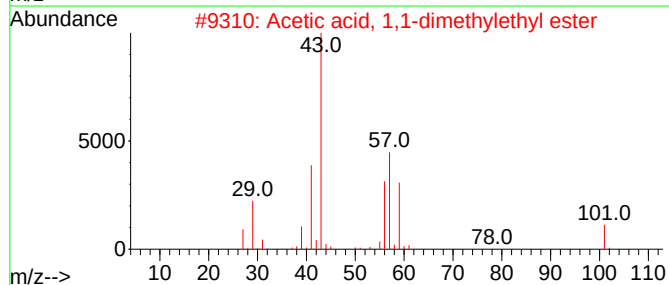
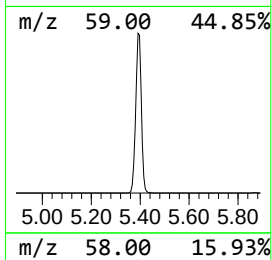
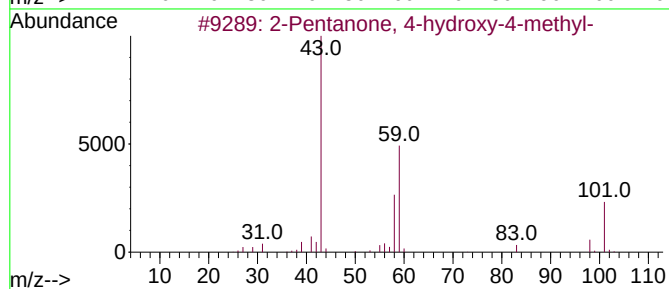
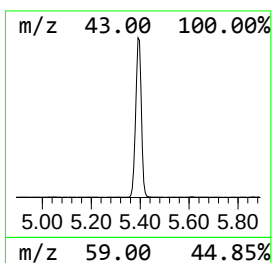
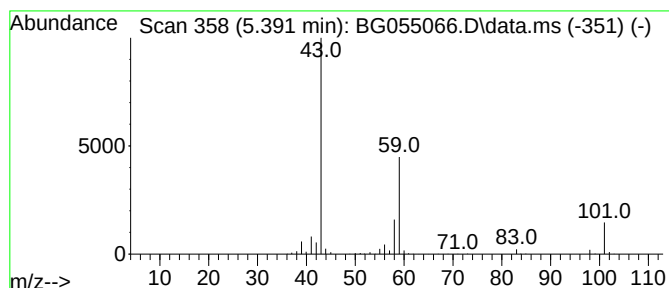
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.391	108.34 ng	1027240	1,4-Dichlorobenzene-d4	8.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4			Acetone	58	C3H6O	000067-64-1	12
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10



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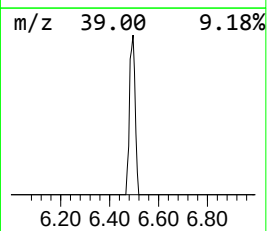
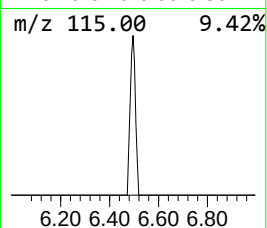
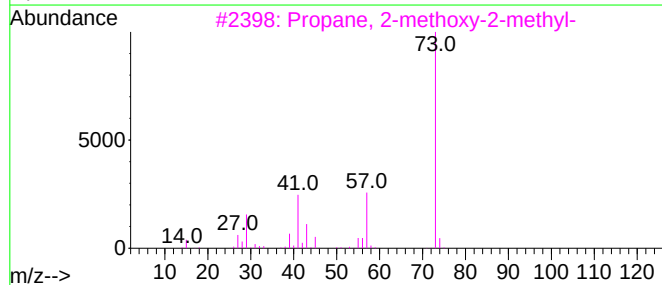
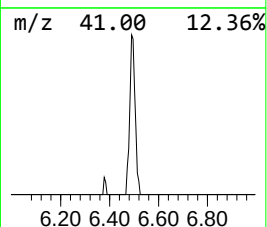
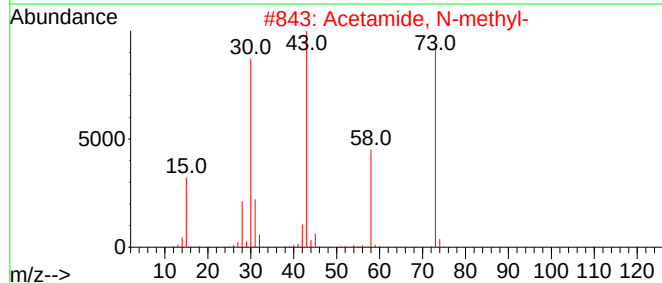
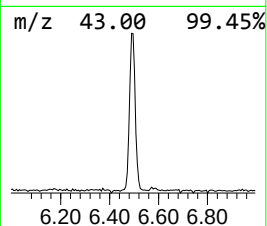
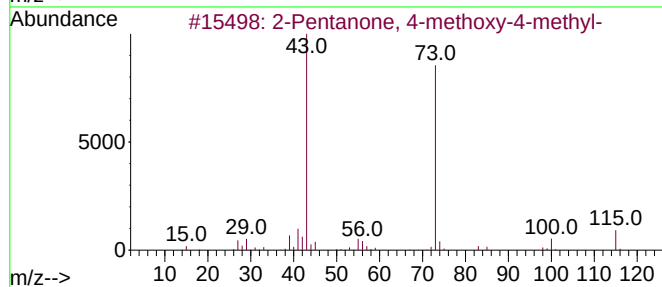
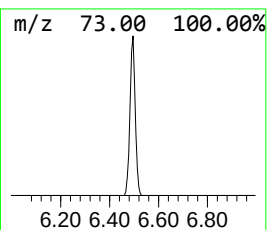
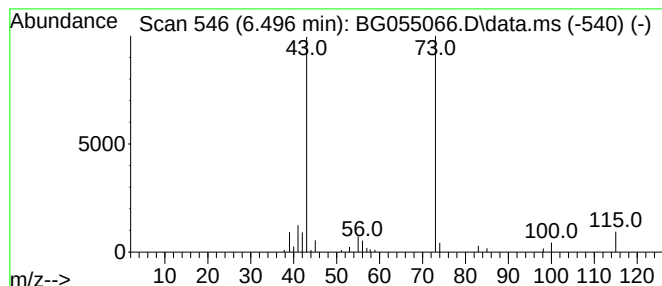
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.496	7.40 ng	70134	1,4-Dichlorobenzene-d4	8.346

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	90
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	50
3		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	17
4		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
5		Hexane, 2-methyl-	100	C7H16	000591-76-4	9



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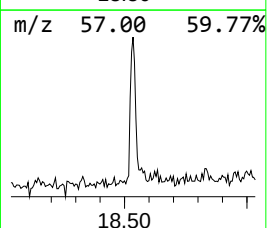
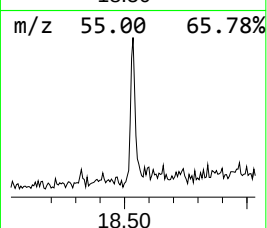
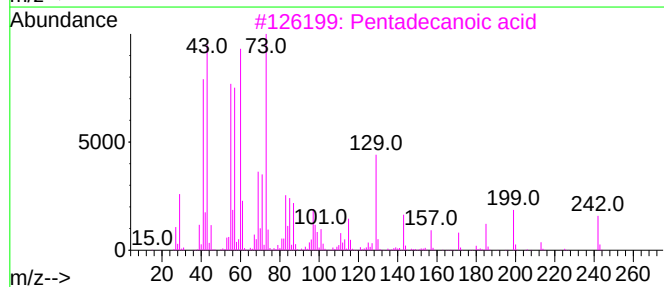
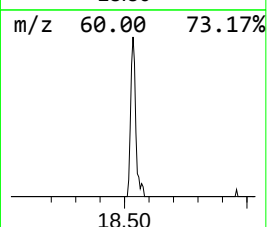
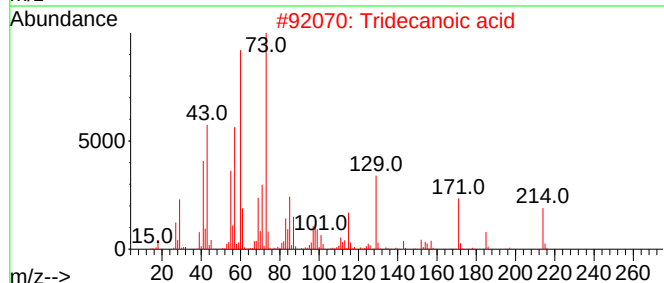
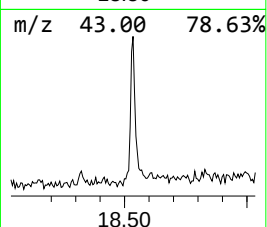
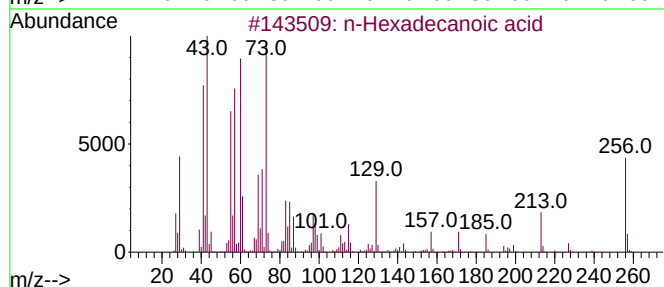
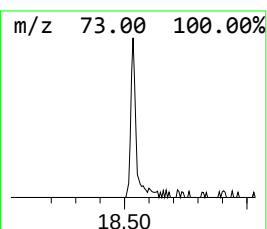
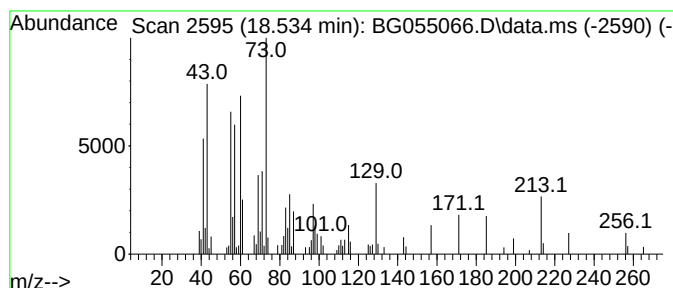
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.535	2.91 ng	70746	Phenanthrene-d10	17.683

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	76
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18



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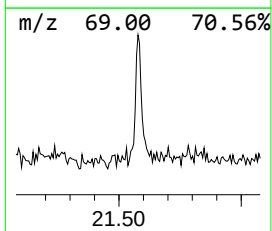
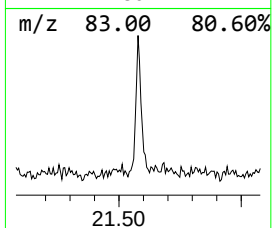
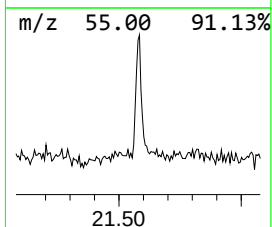
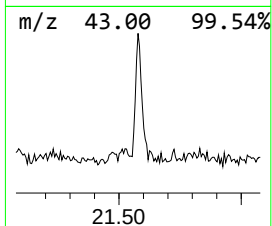
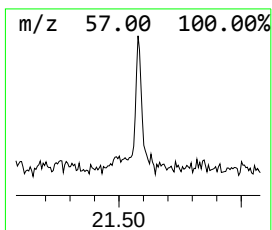
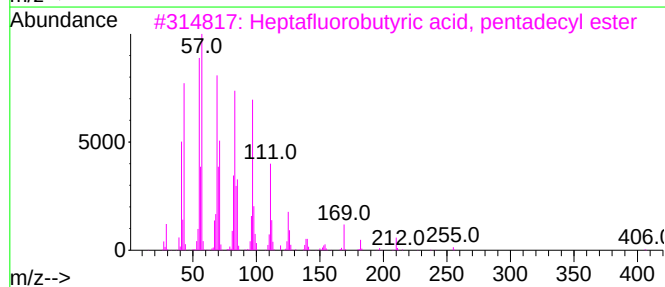
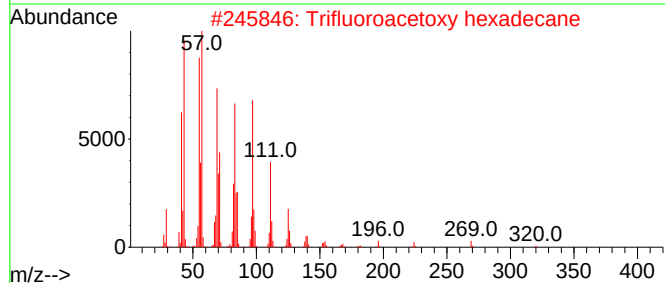
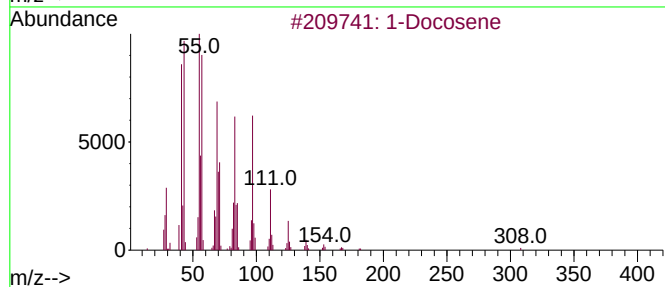
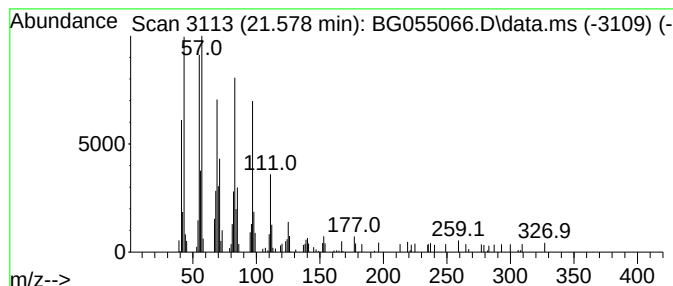
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.578	2.93 ng	76524	Chrysene-d12	21.977

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene		308	C22H44	001599-67-3	98
2	Trifluoroacetoxy hexadecane		338	C18H33F3O2	006222-03-3	93
3	Heptafluorobutyric acid, pentade...		424	C19H31F7O2	959261-23-5	93
4	Trichloroacetic acid, hexadecyl ...		386	C18H33Cl3O2	074339-54-1	93
5	Octadecyl trifluoroacetate		366	C20H37F3O2	079392-43-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100422\
Data File : BG055066.D
Acq On : 4 Oct 2022 16:52
Operator : CG/JU
Sample : N4909-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PE-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.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...	3.382	64.7	ng	613894	1	8.346	189640	20.0
3-Penten-2-one,...	4.774	6.8	ng	64546	1	8.346	189640	20.0
2-Pentanone, 4-...	5.391	108.3	ng	1027240	1	8.346	189640	20.0
2-Pentanone, 4-...	6.496	7.4	ng	70134	1	8.346	189640	20.0
n-Hexadecanoic ...	18.535	2.9	ng	70746	4	17.683	485677	20.0
1-Docosene	21.578	2.9	ng	76524	5	21.977	522074	20.0