

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101022\
 Data File : BG055117.D
 Acq On : 10 Oct 2022 18:04
 Operator : CG/JU
 Sample : N5054-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 510A-1

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: BG055117.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.370	8	14	33	rVB	755738	1234479	36.34%	8.999%
2	5.373	348	355	363	rBV	70794	106113	3.12%	0.774%
3	5.849	429	436	446	rVB	308977	496173	14.60%	3.617%
4	7.453	701	709	721	rBV	200959	343814	10.12%	2.506%
5	8.329	852	858	864	rBV	107279	184784	5.44%	1.347%
6	9.498	1048	1057	1066	rBV	404362	713004	20.99%	5.197%
7	10.902	1289	1296	1304	rBV	76088	122886	3.62%	0.896%
8	11.161	1332	1340	1347	rBV	144478	259602	7.64%	1.892%
9	12.013	1479	1485	1494	rBV	27510	47867	1.41%	0.349%
10	13.564	1742	1749	1756	rBV	1097464	1736281	51.11%	12.656%
11	14.375	1880	1887	1893	rBV	396458	559292	16.46%	4.077%
12	14.933	1974	1982	1989	rBV	245906	389135	11.45%	2.837%
13	16.408	2226	2233	2246	rBV	1060840	1590805	46.83%	11.596%
14	17.671	2442	2448	2456	rVB	371465	552770	16.27%	4.029%
15	18.517	2588	2592	2601	rBV2	29462	52328	1.54%	0.381%
16	18.605	2601	2607	2613	rVB	454496	569898	16.77%	4.154%
17	20.244	2880	2886	2892	rBV	2541371	3397317	100.00%	24.764%
18	21.560	3105	3110	3118	rBV2	36902	69860	2.06%	0.509%
19	21.960	3171	3178	3186	rVB	383404	636734	18.74%	4.641%
20	25.409	3752	3765	3779	rBV2	211378	655399	19.29%	4.777%

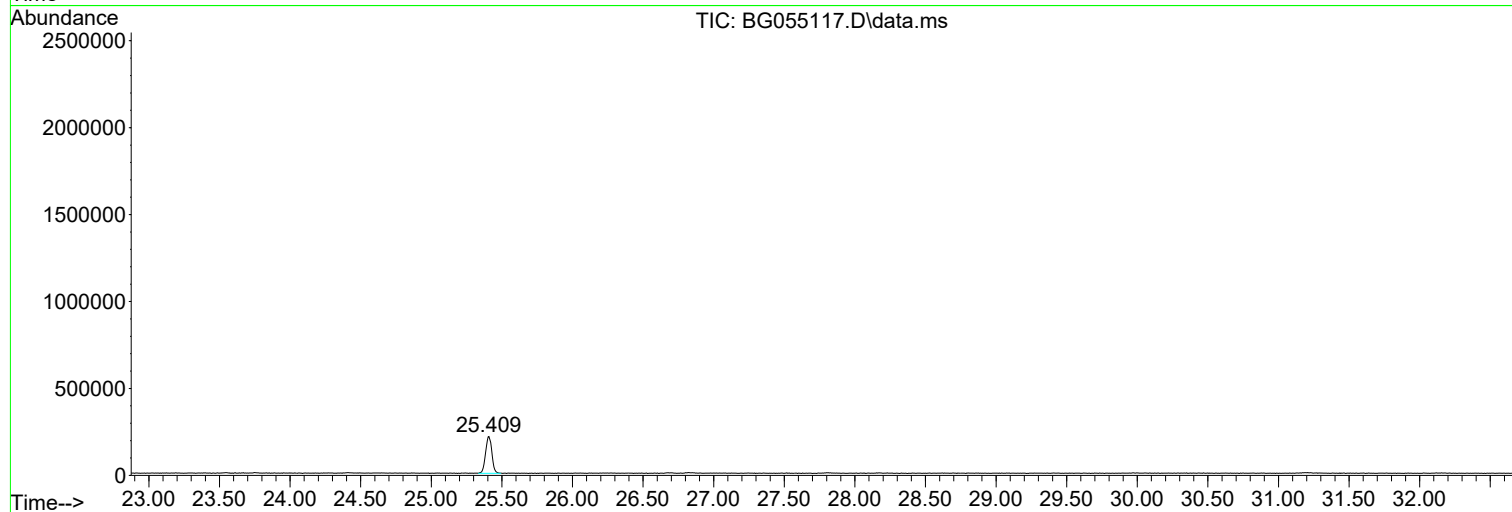
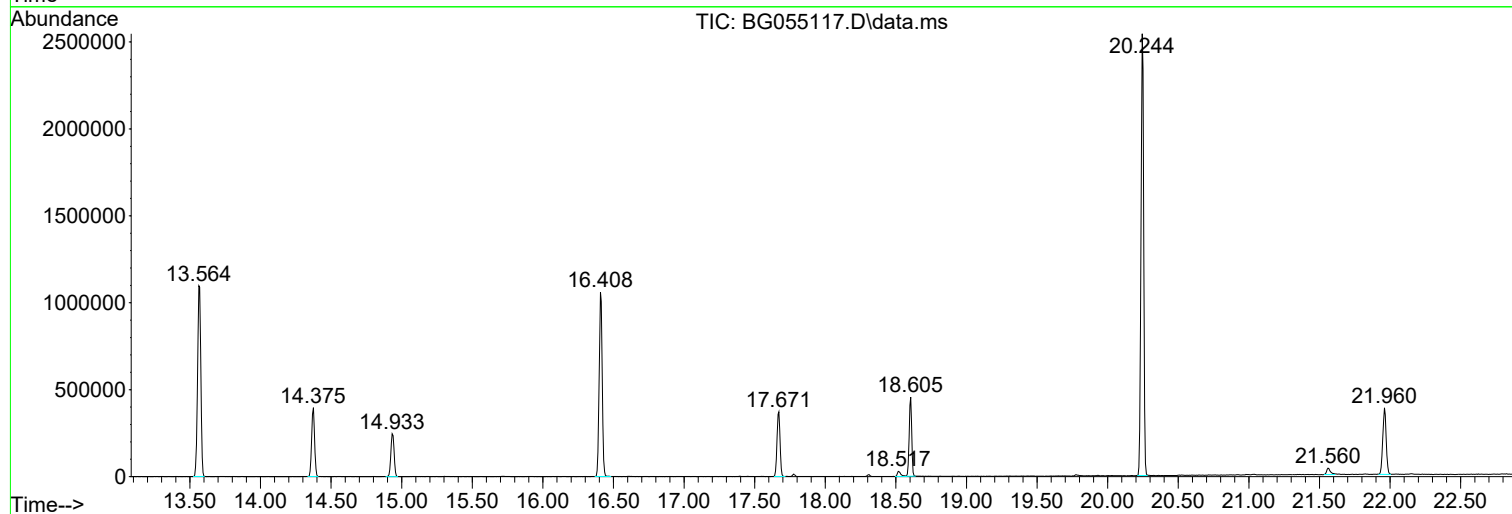
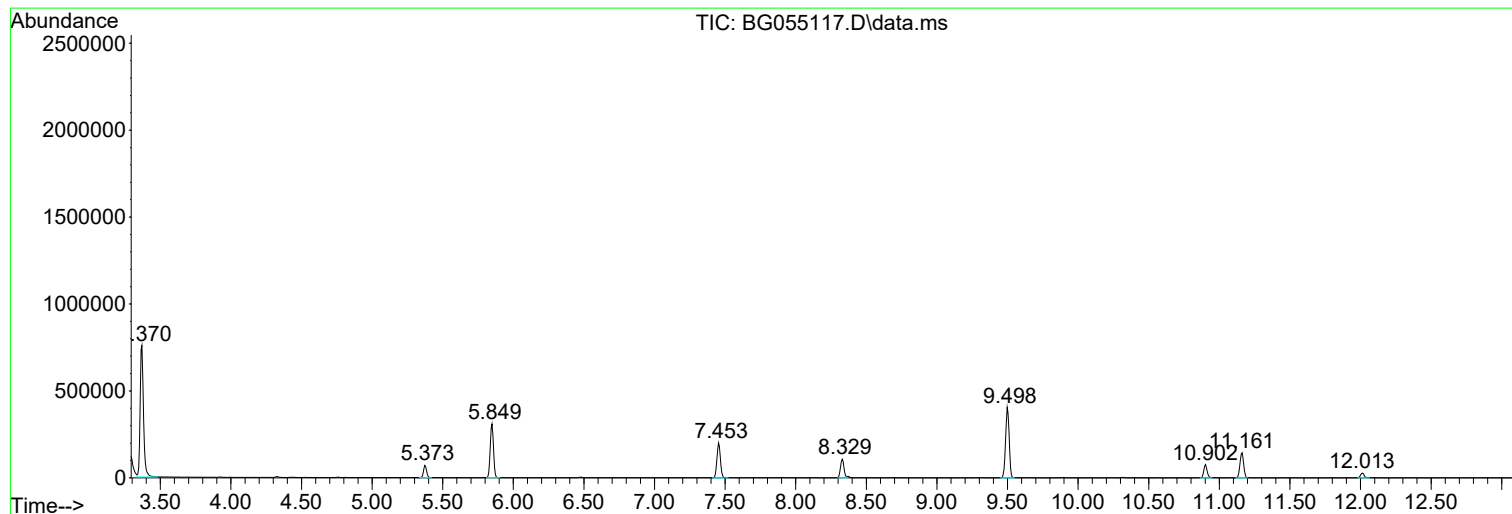
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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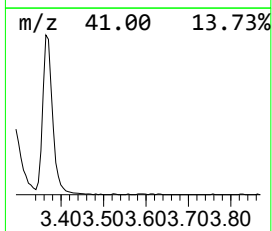
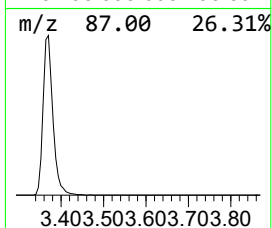
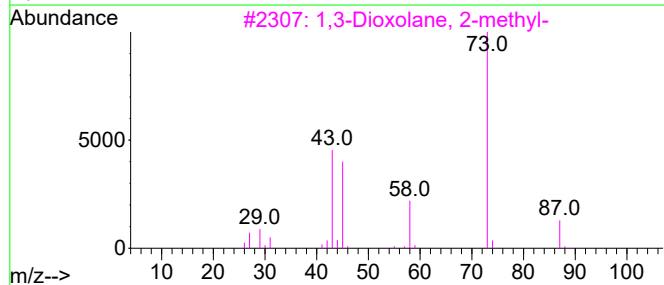
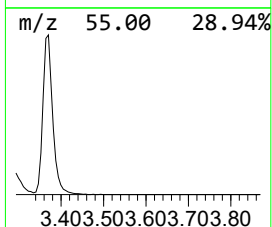
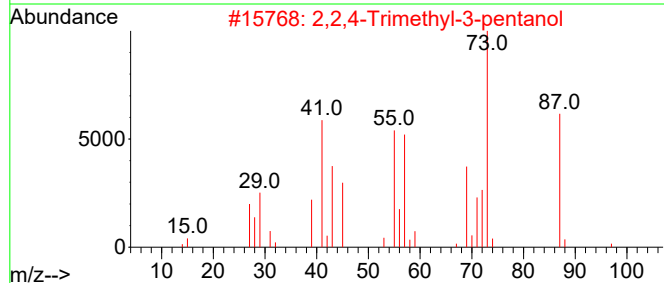
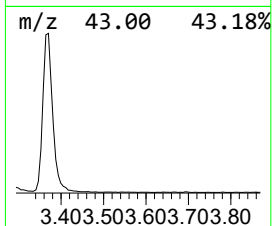
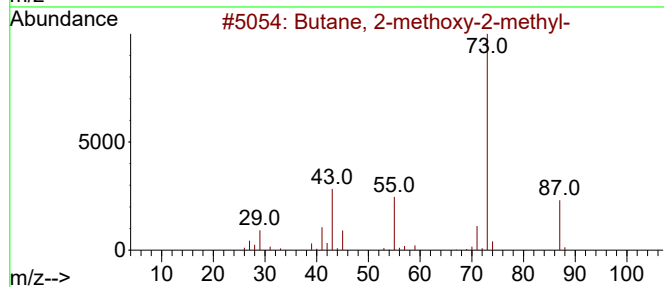
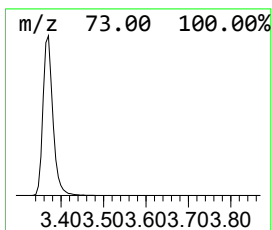
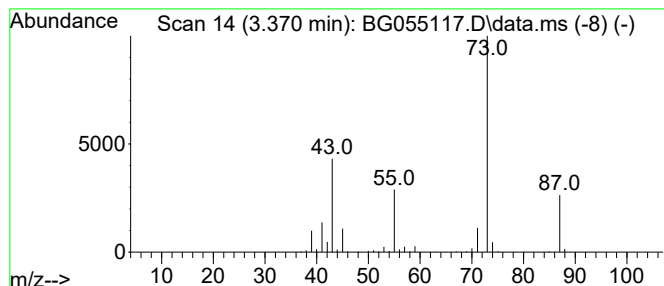
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.370	133.61 ng	1234480	1,4-Dichlorobenzene-d4	8.329

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			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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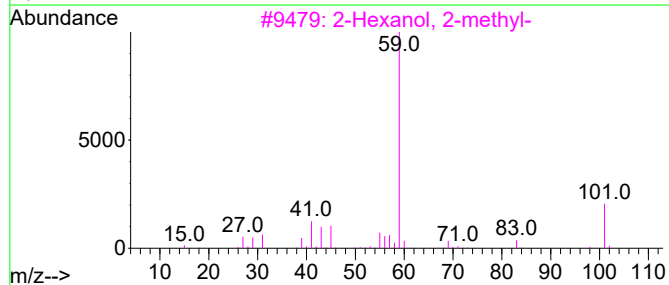
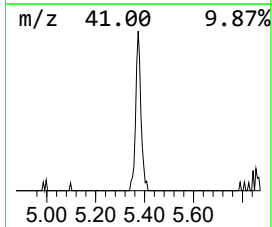
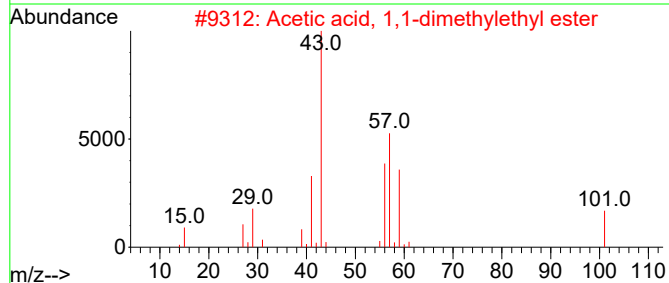
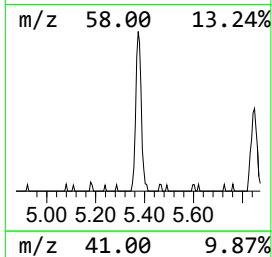
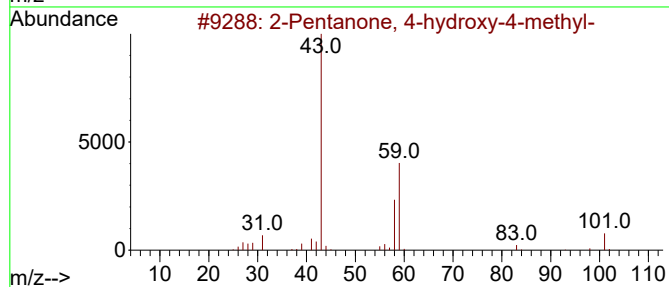
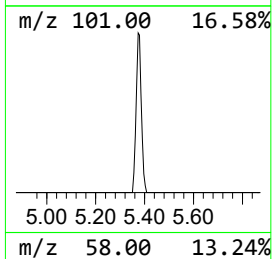
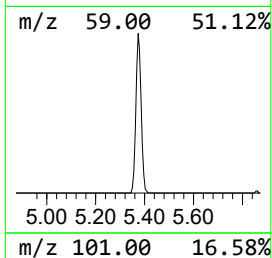
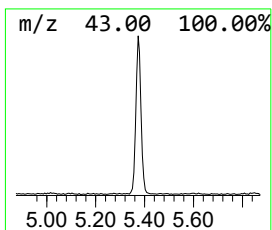
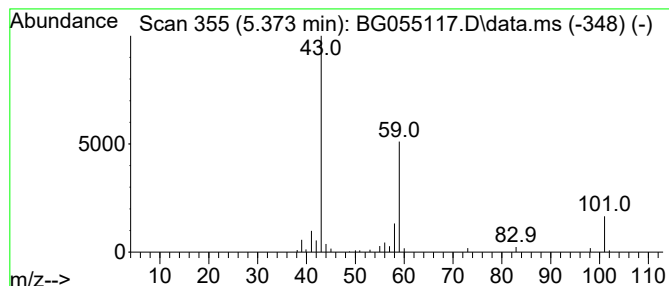
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.373	11.49 ng	106113	1,4-Dichlorobenzene-d4	8.329

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
4			3-Octanol	130	C8H18O	000589-98-0	33
5			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23



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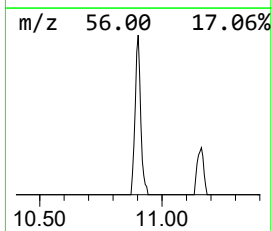
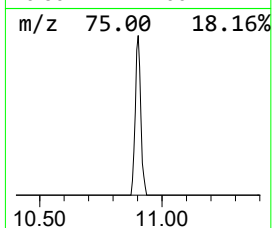
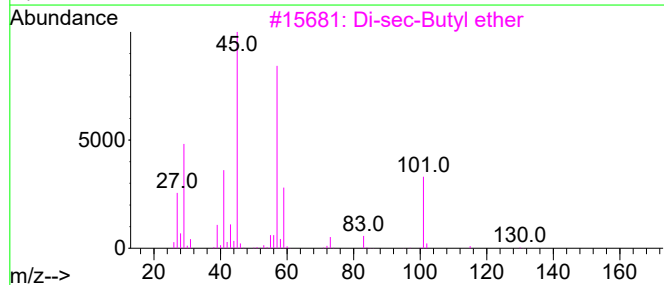
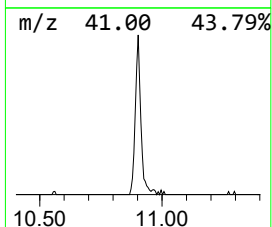
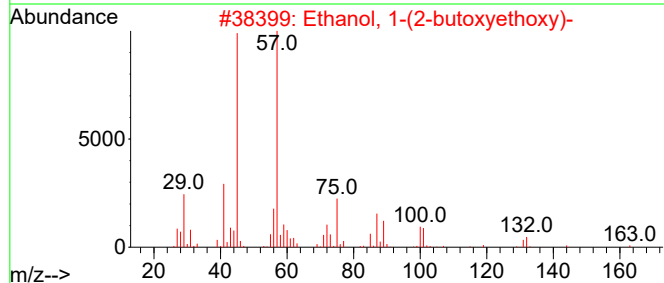
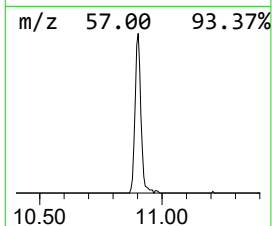
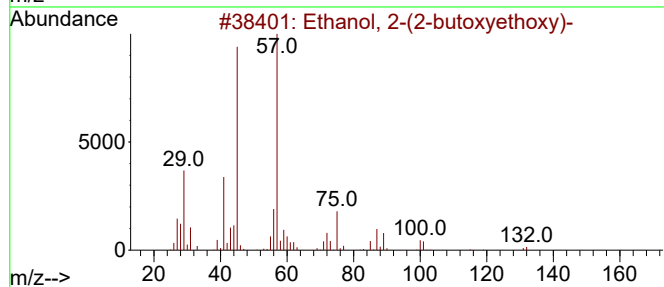
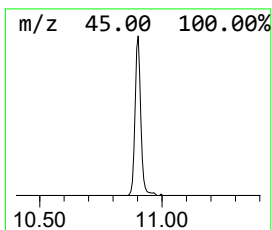
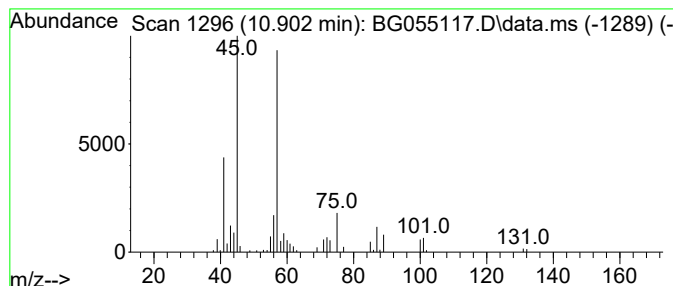
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.902	9.47 ng	122886	Naphthalene-d8	11.161

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Di-sec-Butyl ether	130	C8H18O	006863-58-7	59
4			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
5			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50



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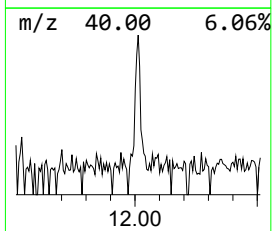
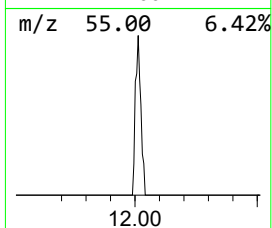
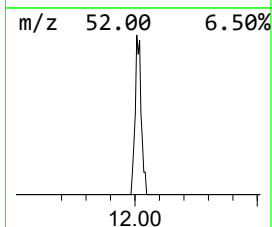
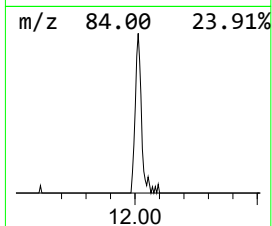
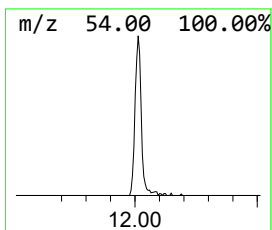
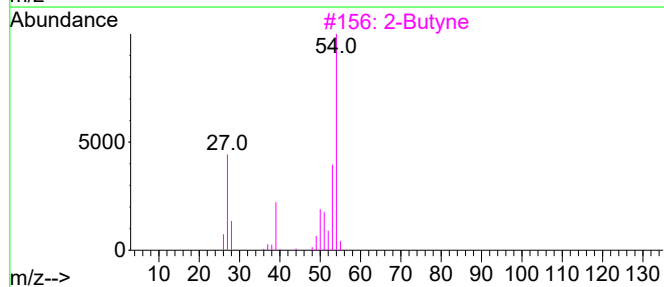
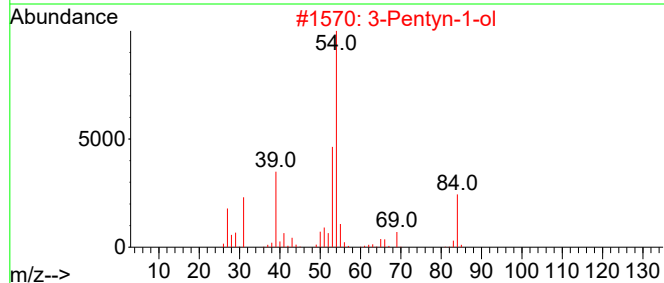
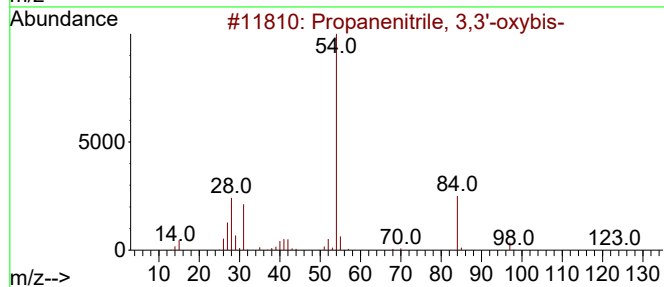
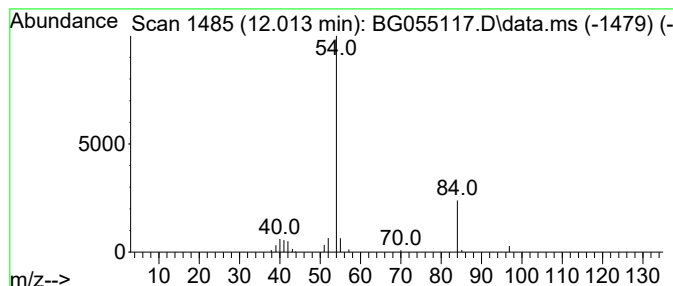
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Peak Number 4 Propanenitrile, 3,3'-oxybis- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.013	3.69 ng	47867	Naphthalene-d8	11.161

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanenitrile, 3,3'-oxybis-	124	C6H8N2O	001656-48-0	83
2			3-Pentyn-1-ol	84	C5H8O	010229-10-4	64
3			2-Butyne	54	C4H6	000503-17-3	5
4			1-Butyne	54	C4H6	000107-00-6	5
5			CH3OC(O)CN	85	C3H3NO2	017640-15-2	4



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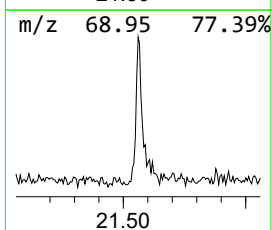
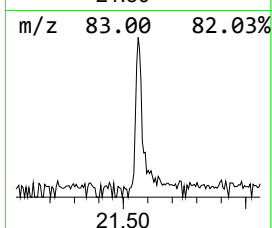
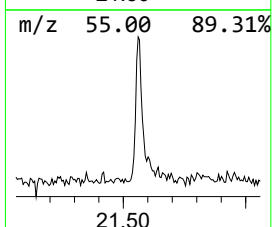
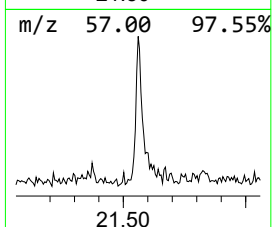
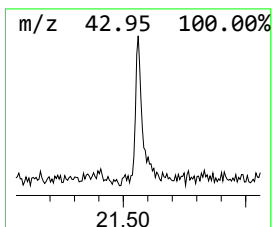
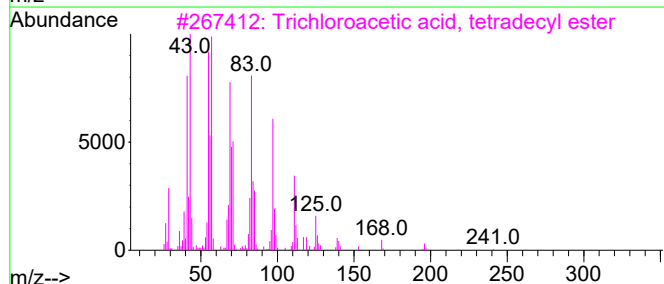
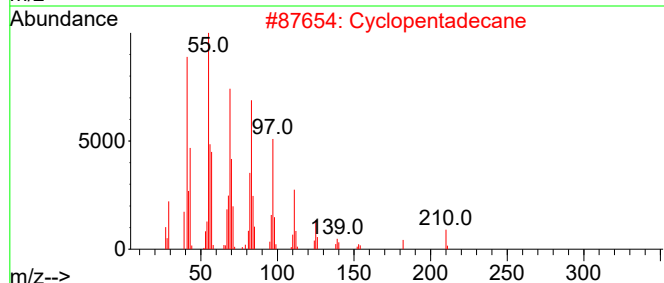
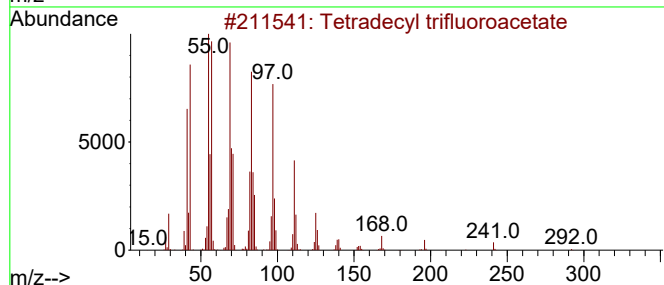
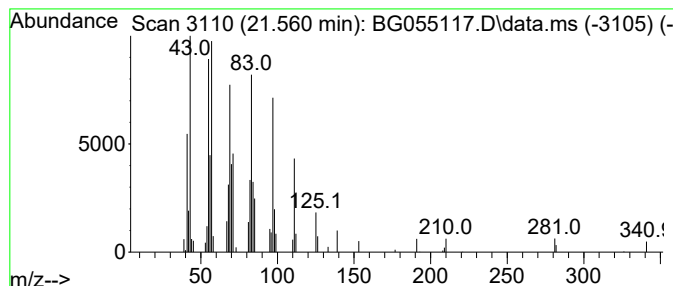
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tetradecyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.560	2.19 ng	69860	Chrysene-d12	21.960

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	94
2			Cyclopentadecane	210	C15H30	000295-48-7	93
3			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
4			Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	91
5			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.370	133.6	ng	1234480	1	8.329	184784	20.0
2-Pentanone, 4-...	5.373	11.5	ng	106113	1	8.329	184784	20.0
Ethanol, 2-(2-b...	10.902	9.5	ng	122886	2	11.161	259602	20.0
Propanenitrile,...	12.013	3.7	ng	47867	2	11.161	259602	20.0
Tetradecyl trif...	21.560	2.2	ng	69860	5	21.960	636734	20.0