

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100722\
 Data File : BG055103.D
 Acq On : 7 Oct 2022 17:36
 Operator : CG/JU
 Sample : N5031-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 5869-3

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: BG055103.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	9	14	30	rVB	548728	843644	45.11%	10.732%
2	5.379	350	356	364	rVB	54340	82343	4.40%	1.047%
3	5.849	430	436	445	rVB	140983	231696	12.39%	2.947%
4	7.459	702	710	718	rVB	93776	157515	8.42%	2.004%
5	8.335	852	859	871	rVB	77899	128252	6.86%	1.631%
6	9.504	1051	1058	1067	rBV	229571	397892	21.27%	5.061%
7	10.908	1291	1297	1306	rBV	12914	20454	1.09%	0.260%
8	11.167	1333	1341	1348	rBV	107428	187046	10.00%	2.379%
9	13.570	1743	1750	1757	rBV	632942	974607	52.11%	12.398%
10	14.939	1972	1983	1990	rBV	186159	294913	15.77%	3.751%
11	16.413	2227	2234	2243	rBV	655563	983110	52.56%	12.506%
12	17.671	2442	2448	2455	rBV	301151	448334	23.97%	5.703%
13	18.523	2588	2593	2602	rBV2	55331	81879	4.38%	1.042%
14	19.774	2803	2806	2816	rBV2	27088	41532	2.22%	0.528%
15	20.250	2880	2887	2892	rBV	1403882	1870369	100.00%	23.792%
16	21.566	3105	3111	3117	rBV2	40429	67324	3.60%	0.856%
17	21.966	3172	3179	3188	rVB	297536	514857	27.53%	6.549%
18	25.409	3753	3765	3781	rVB2	172632	535519	28.63%	6.812%

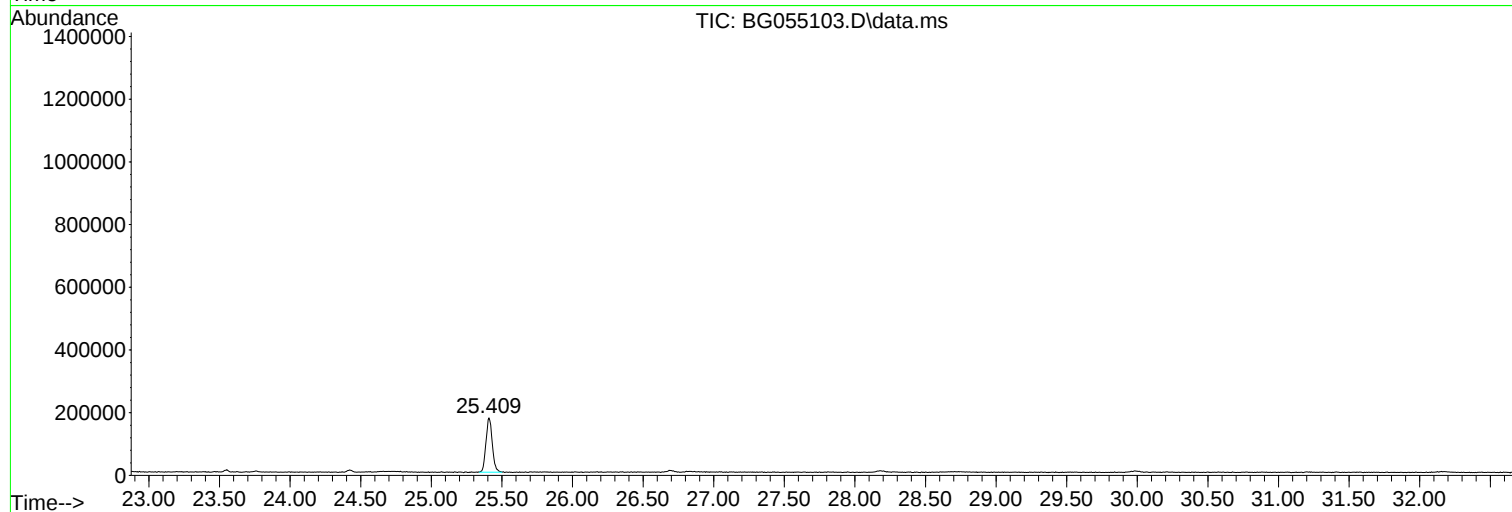
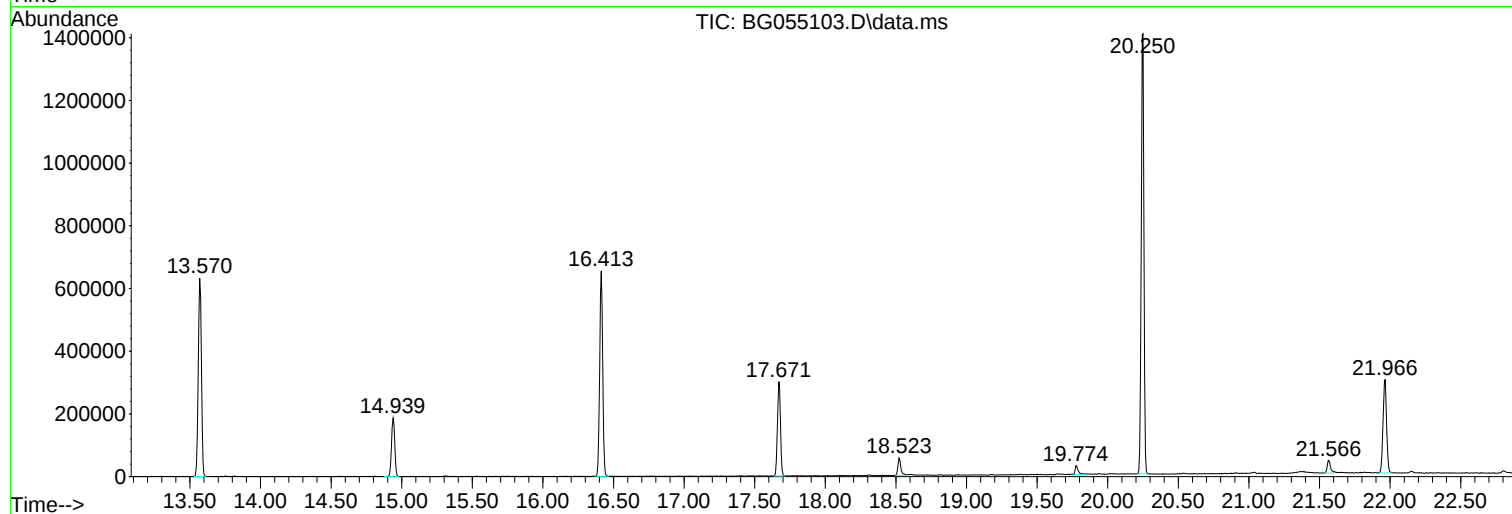
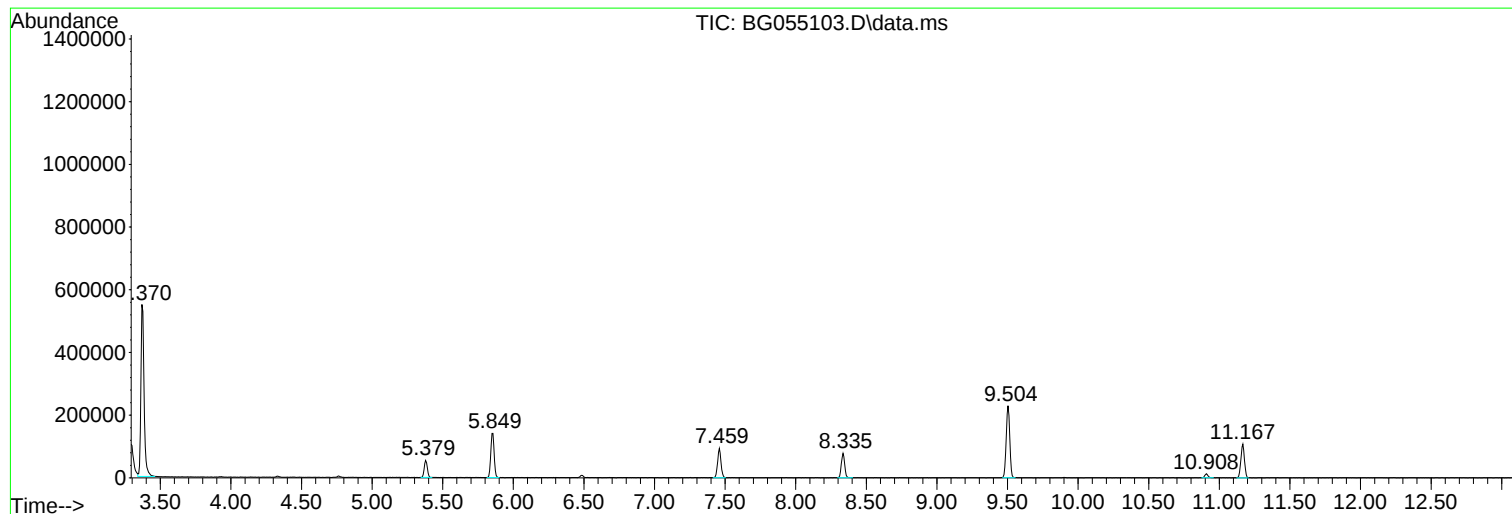
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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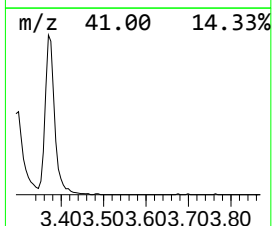
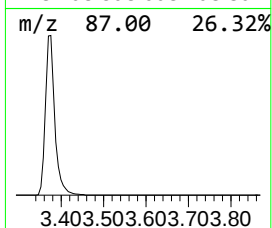
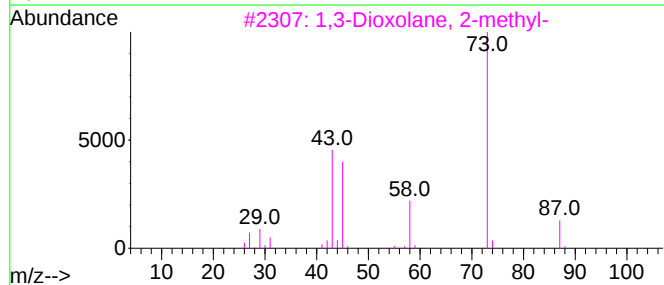
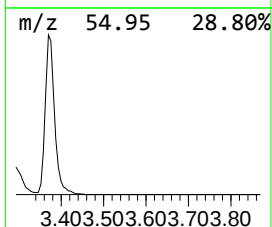
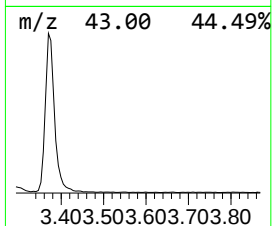
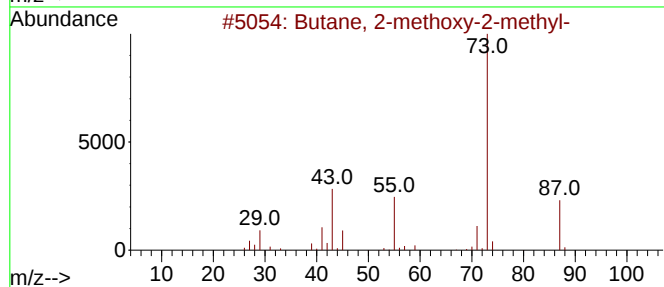
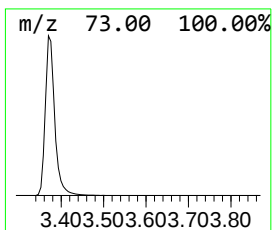
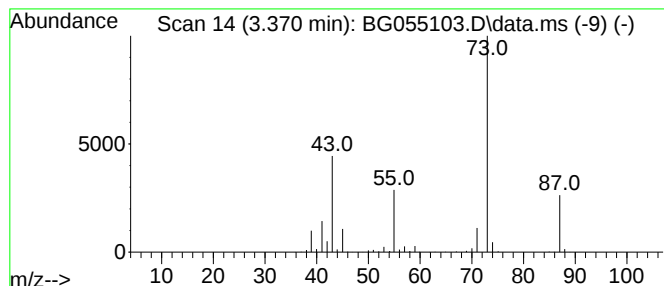
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.370	131.56 ng	843644	1,4-Dichlorobenzene-d4	8.335

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			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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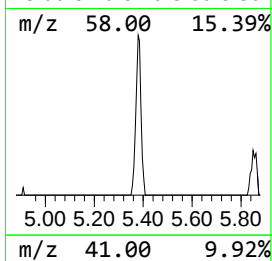
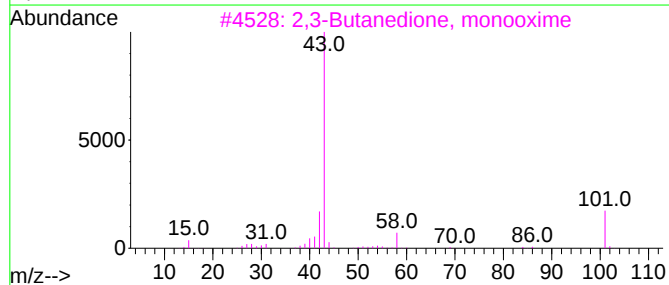
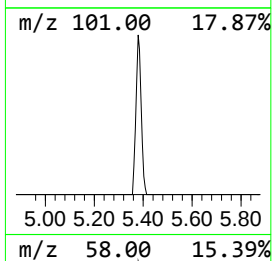
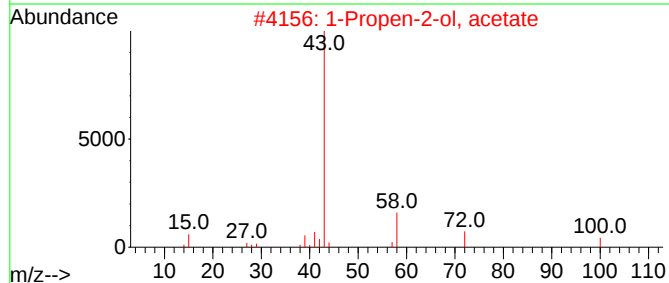
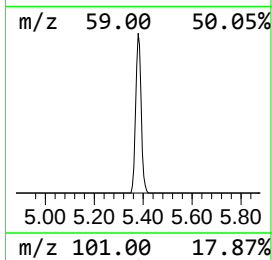
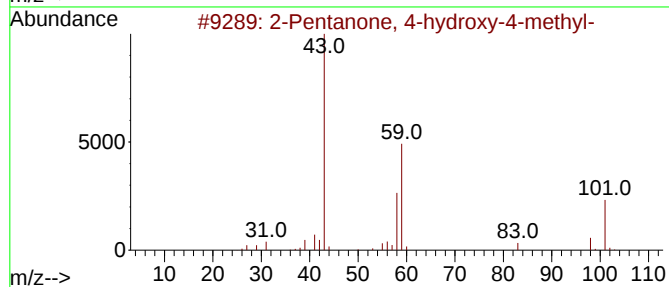
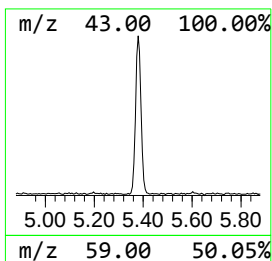
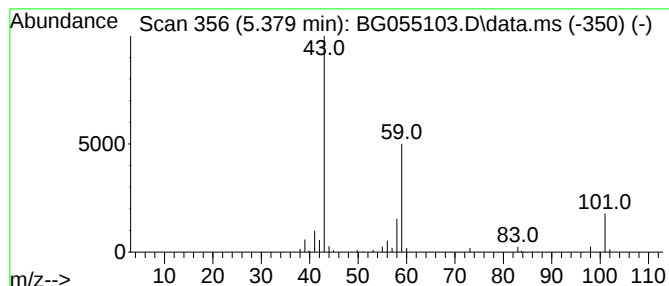
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.379	12.84 ng	82343	1,4-Dichlorobenzene-d4	8.335

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Acetamide, N-(cyanomethyl)-	98	C4H6N2O	004814-80-6	9



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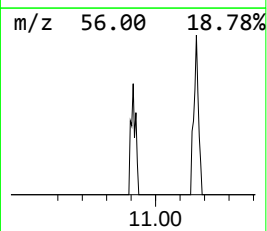
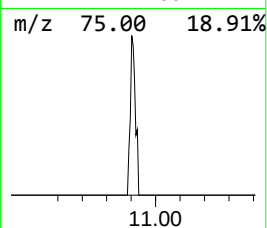
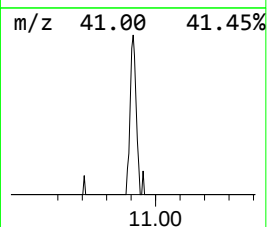
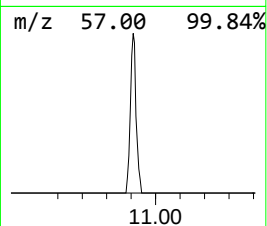
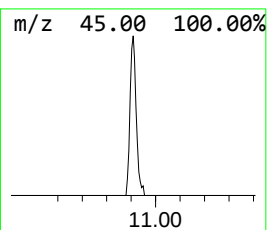
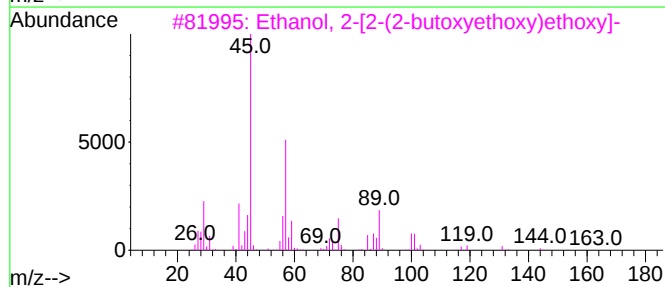
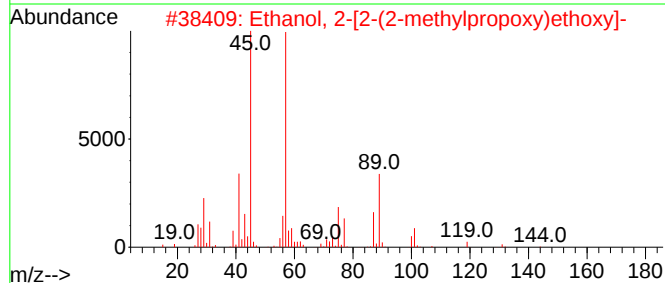
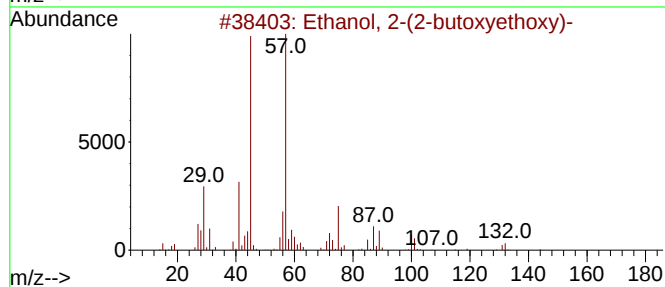
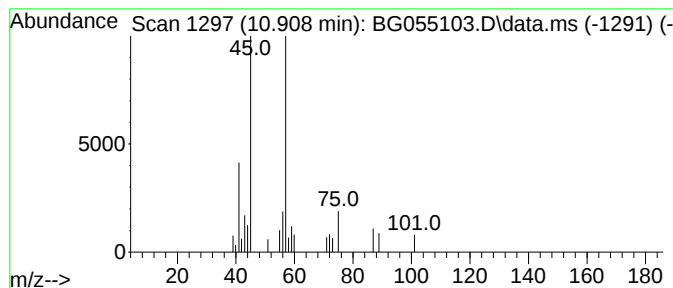
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.908	2.19 ng	20454	Naphthalene-d8	11.166

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
3			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	56
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
5			Ethylene glycol diglycidyl ether	174	C8H14O4	002224-15-9	39



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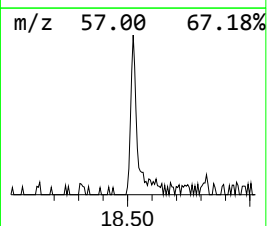
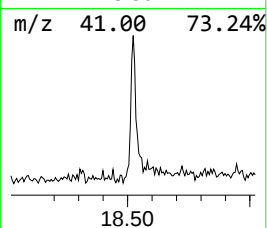
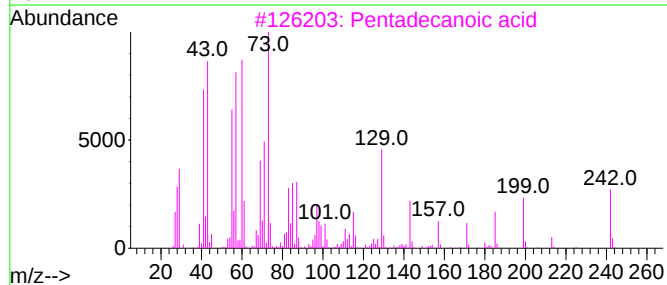
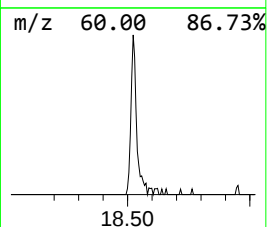
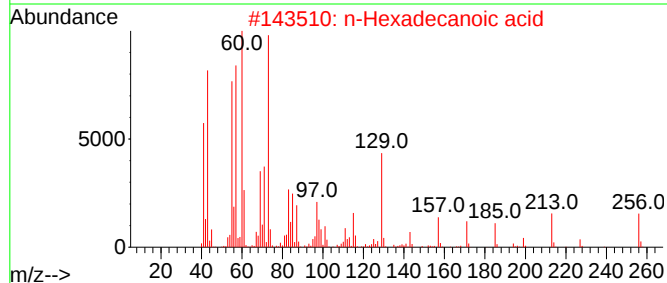
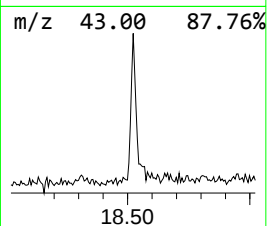
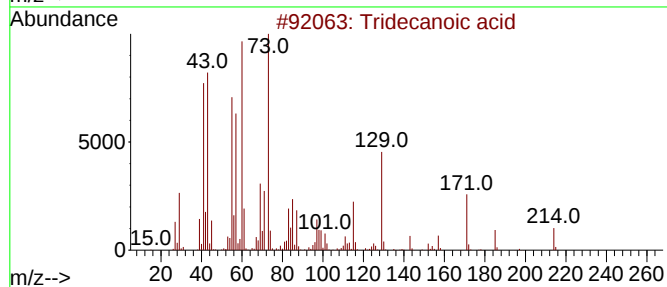
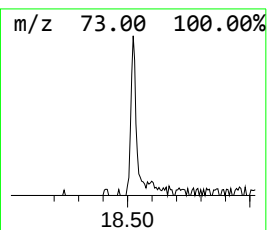
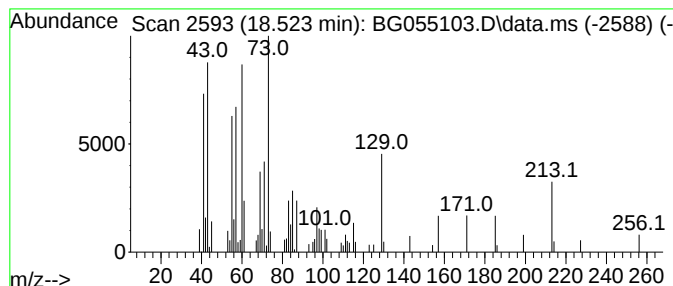
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.523	3.65 ng	81879	Phenanthrene-d10	17.671

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	91
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Undecanoic acid	186	C11H22O2	000112-37-8	76



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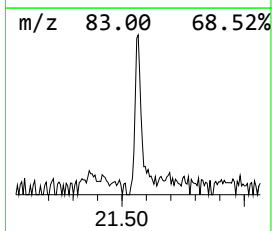
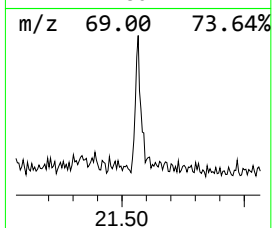
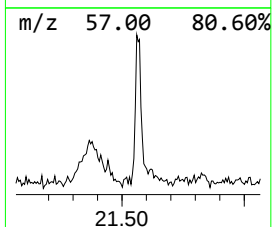
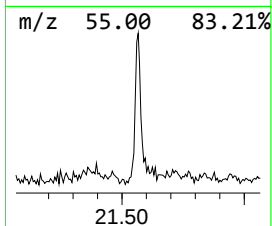
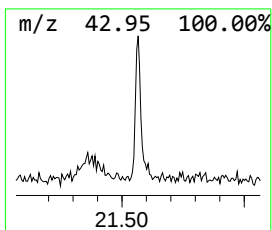
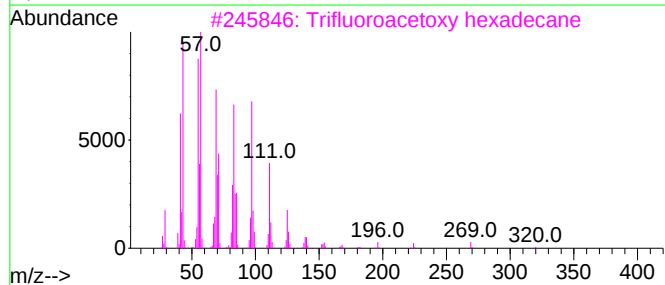
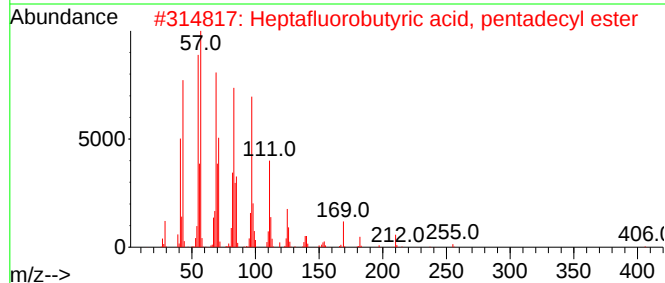
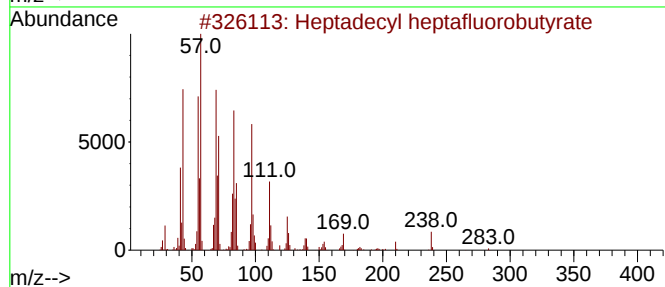
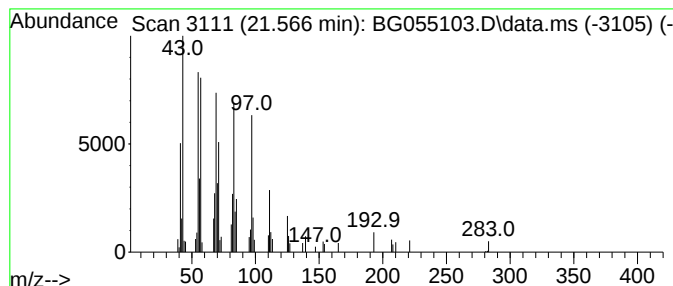
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.566	2.62 ng	67324	Chrysene-d12	21.966

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	95
2			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
4			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	90
5			1-Hexacosene	364	C26H52	018835-33-1	90



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.370	131.6	ng	843644	1	8.335	128252	20.0
2-Pentanone, 4-...	5.379	12.8	ng	82343	1	8.335	128252	20.0
Ethanol, 2-(2-b...	10.908	2.2	ng	20454	2	11.166	187046	20.0
Tridecanoic acid	18.523	3.6	ng	81879	4	17.671	448334	20.0
Heptadecyl hept...	21.566	2.6	ng	67324	5	21.966	514857	20.0