

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061121\
 Data File : BF124276.D
 Acq On : 11 Jun 2021 23:23
 Operator : JU/CG
 Sample : M2625-14
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 18-B12(190-194)

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_F\METHODS\8270-BF060321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124276.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	14	17	23	rBB2	18471	22053	2.25%	0.329%
2	5.051	500	504	509	rBV	64993	74934	7.65%	1.117%
3	5.469	571	575	585	rBV	919641	815975	83.31%	12.162%
4	6.481	742	747	750	rBV	956985	802180	81.90%	11.956%
5	6.840	804	808	811	rBV	246612	193485	19.76%	2.884%
6	7.404	899	904	907	rBV	615339	542592	55.40%	8.087%
7	8.022	1006	1009	1018	rBV	114542	112965	11.53%	1.684%
8	8.122	1022	1026	1029	rBV	300332	243666	24.88%	3.632%
9	9.198	1205	1209	1212	rBV	1286623	979405	100.00%	14.598%
10	9.875	1321	1324	1328	rBV	346150	302309	30.87%	4.506%
11	10.669	1455	1459	1471	rBB	908378	761778	77.78%	11.354%
12	11.363	1574	1577	1581	rBV	358654	331193	33.82%	4.936%
13	11.892	1664	1667	1670	rBV	26612	23104	2.36%	0.344%
14	12.951	1843	1847	1850	rBV	1104452	934957	95.46%	13.935%
15	13.851	1994	2000	2002	rBV3	12226	15746	1.61%	0.235%
16	13.874	2002	2004	2011	rVB5	10379	19101	1.95%	0.285%
17	14.010	2023	2027	2030	rBV	257621	216225	22.08%	3.223%
18	14.168	2050	2054	2057	rBV4	13175	12937	1.32%	0.193%
19	15.121	2211	2216	2219	rBV4	10132	12596	1.29%	0.188%
20	15.486	2273	2278	2284	rBV	208066	252866	25.82%	3.769%
21	16.451	2434	2442	2447	rBV8	9559	26736	2.73%	0.398%
22	18.056	2713	2715	2722	rVB7	7142	12474	1.27%	0.186%

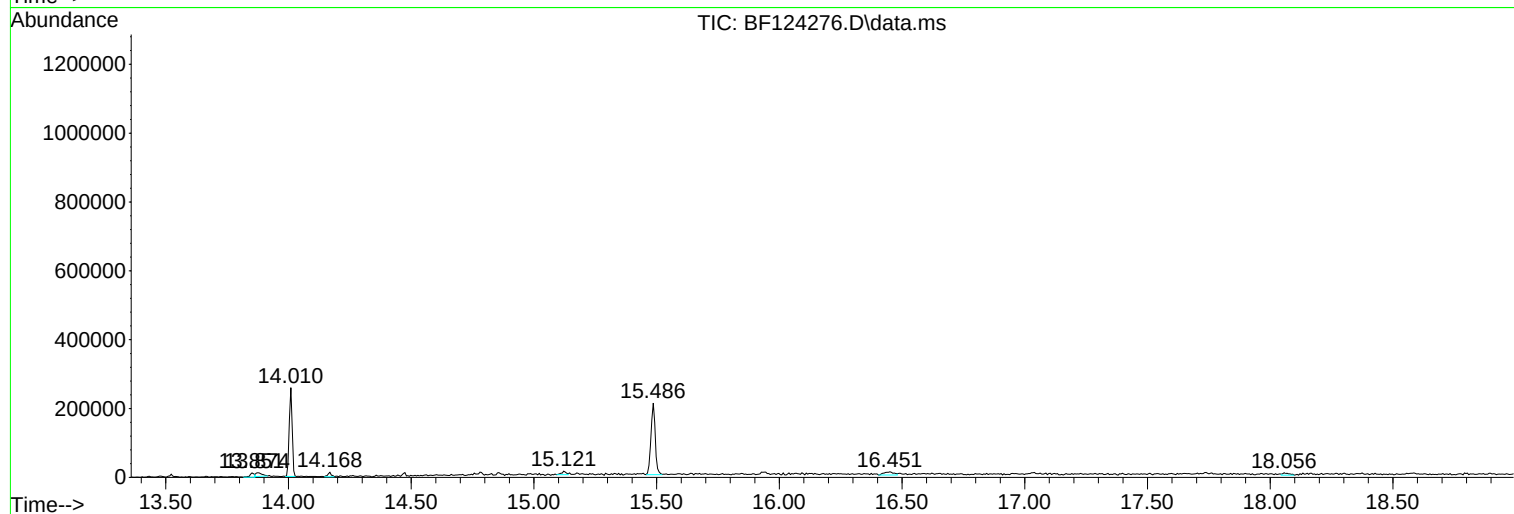
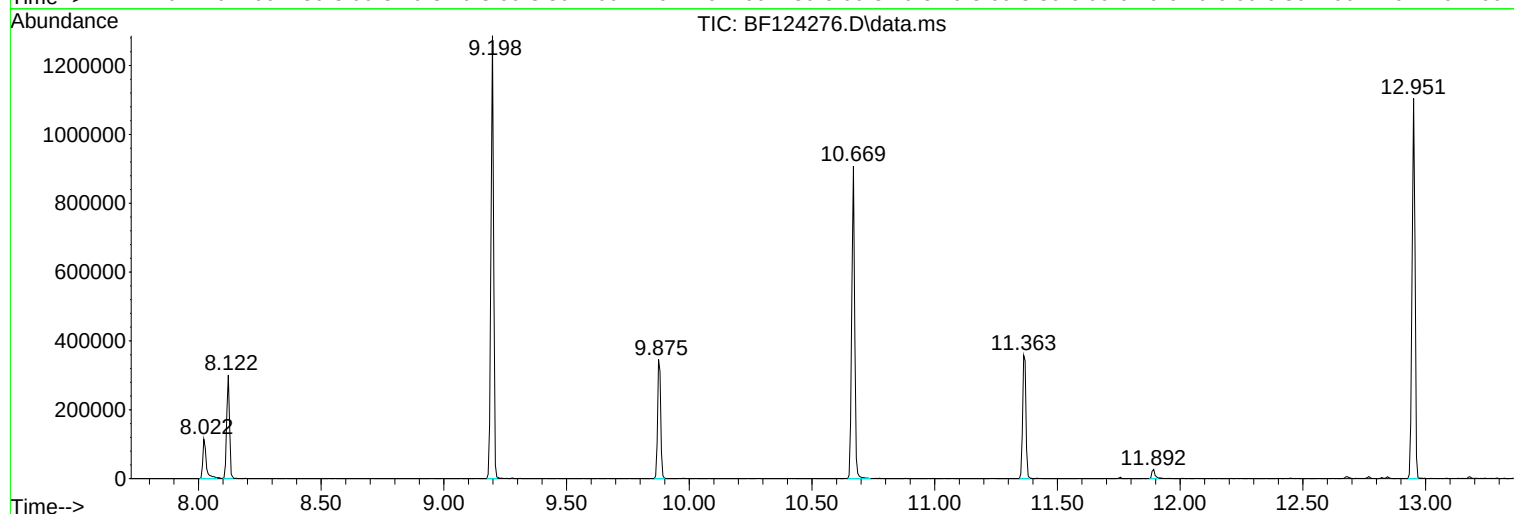
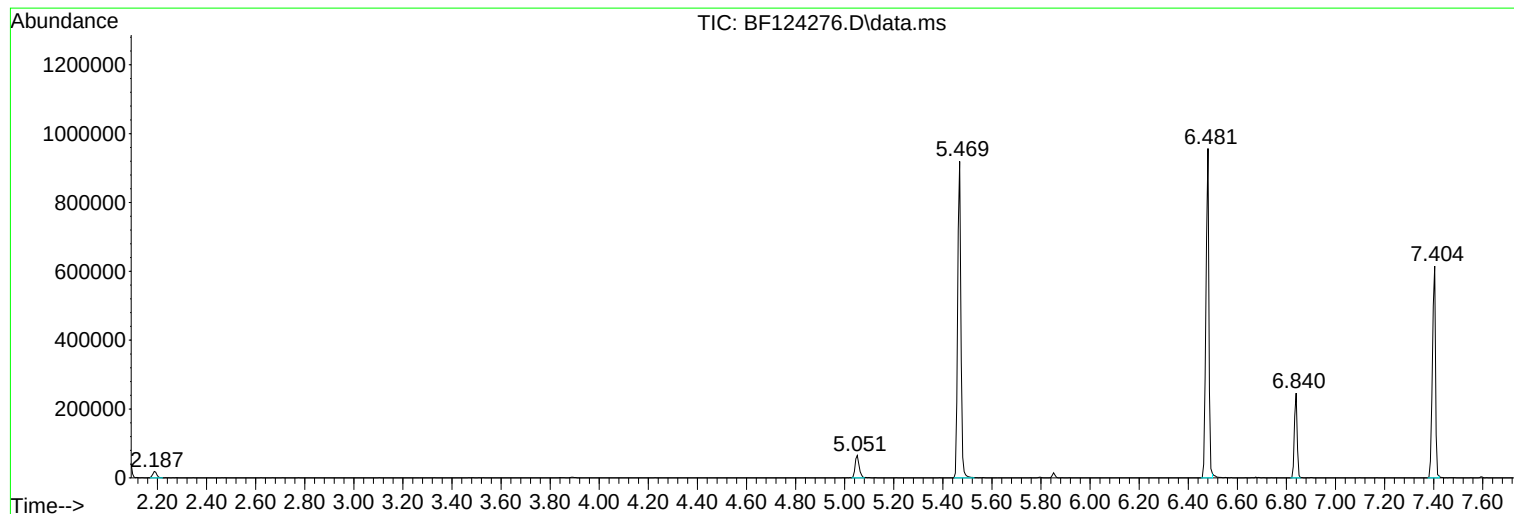
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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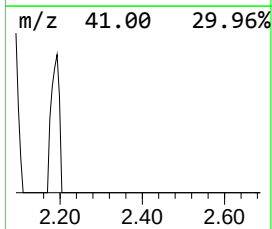
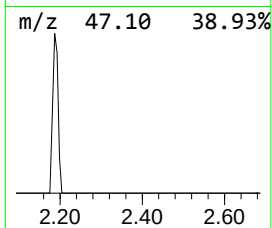
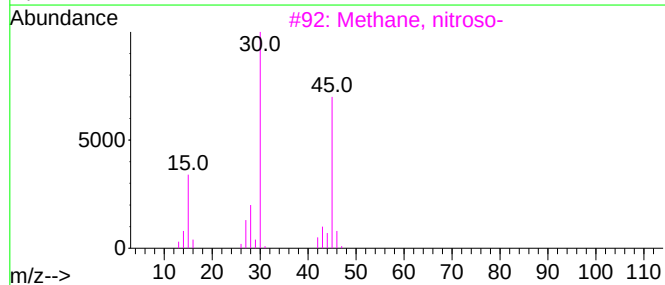
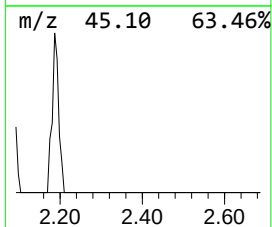
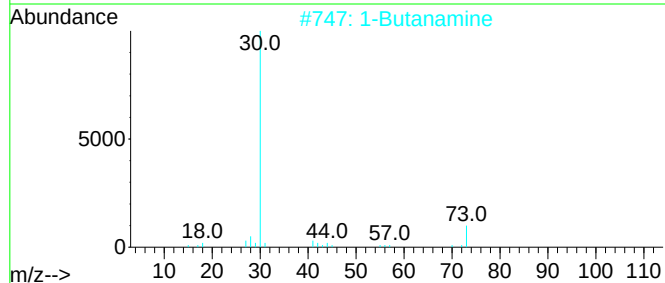
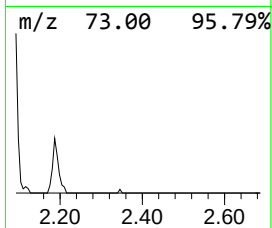
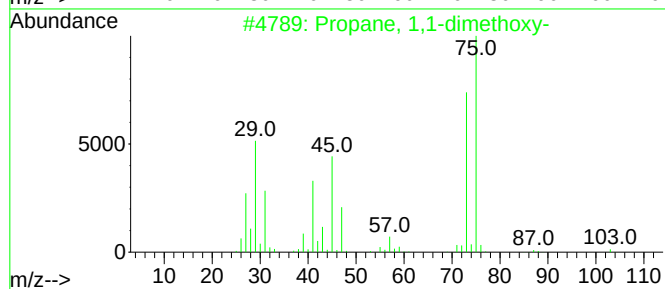
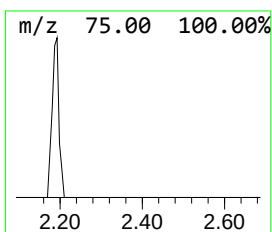
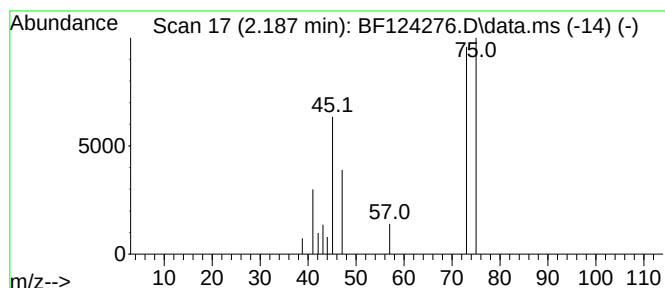
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown2.187 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.187	2.28 ng	22053	1,4-Dichlorobenzene-d4	6.840

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	9
2			1-Butanamine	73	C4H11N	000109-73-9	5
3			Methane, nitroso-	45	CH3NO	000865-40-7	4
4			Glycine	75	C2H5NO2	000056-40-6	4
5			Isobutylamine	73	C4H11N	000078-81-9	4



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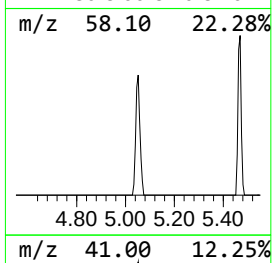
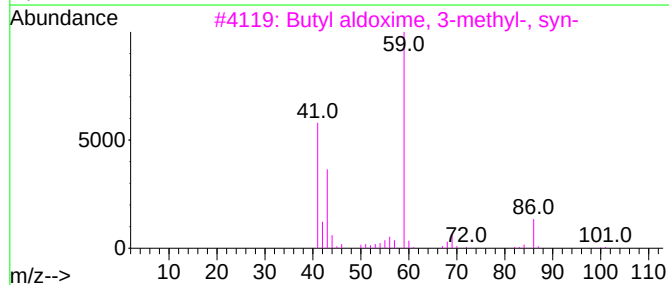
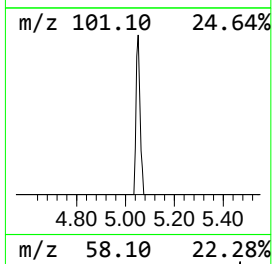
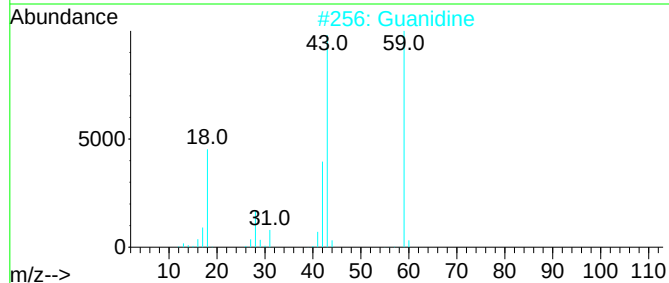
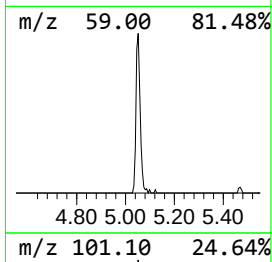
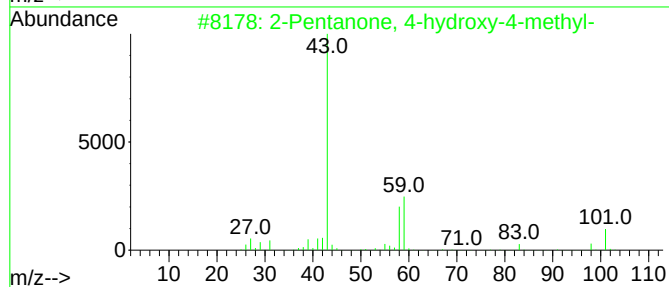
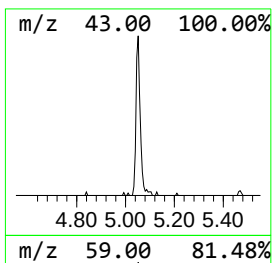
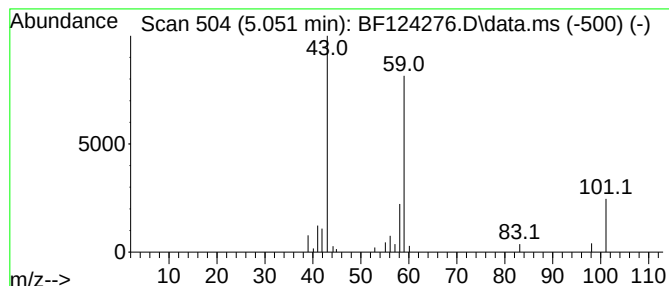
Instrument :
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ClientSampleId :
18-B12(190-194)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.
5.051	7.75 ng	74934	1,4-Dichlorobenzene-d4			6.840
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	64
2	Guanidine		59	CH5N3	000113-00-8	47
3	Butyl aldoxime, 3-methyl-, syn-		101	C5H11NO	005780-40-5	25
4	5-Hexen-2-one		98	C6H10O	000109-49-9	9
5	Acetone		58	C3H6O	000067-64-1	9



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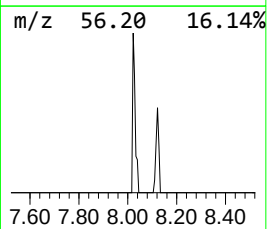
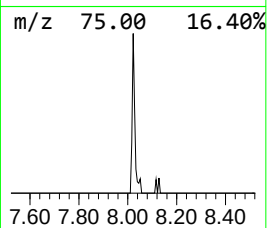
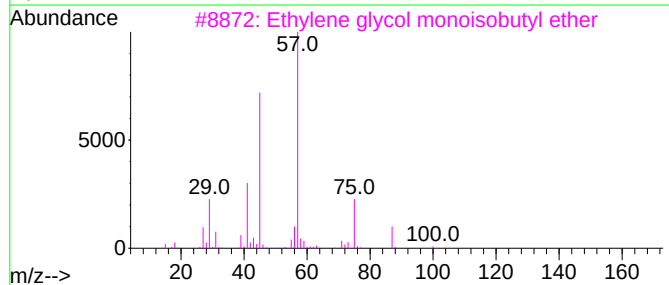
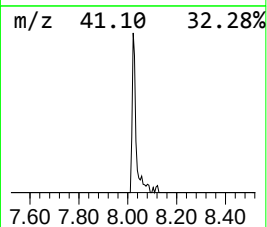
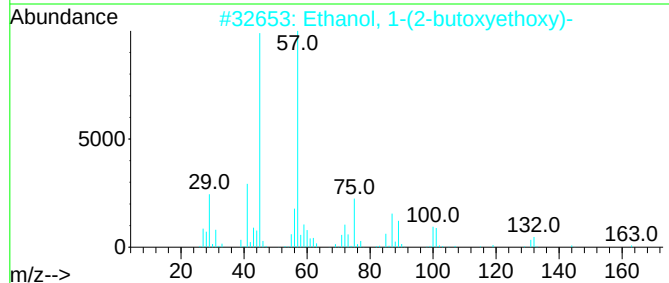
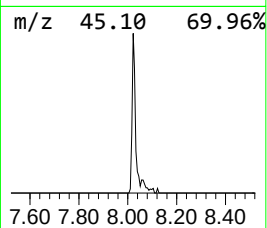
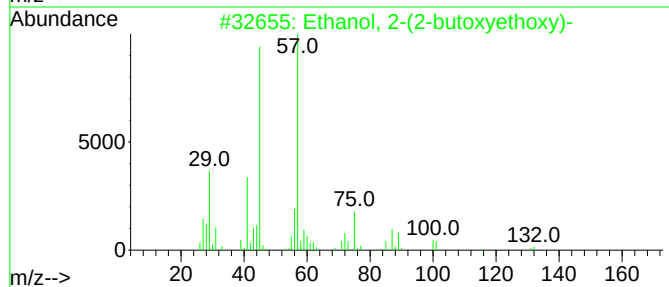
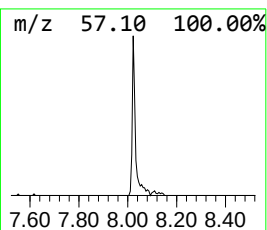
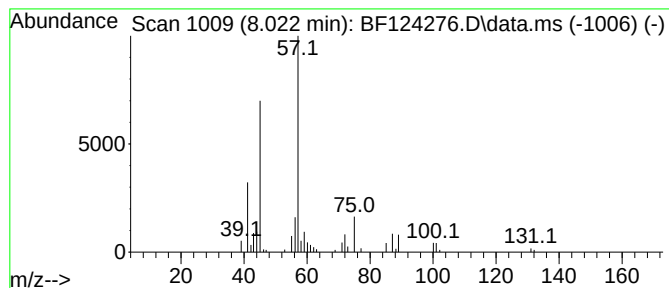
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Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.022	9.27 ng	112965	Naphthalene-d8	8.122

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	86
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	64
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	53
4			Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	50
5			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	45



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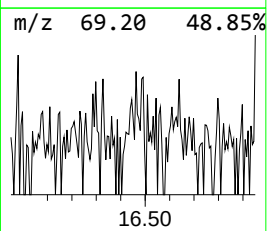
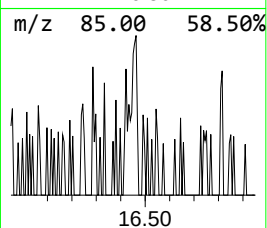
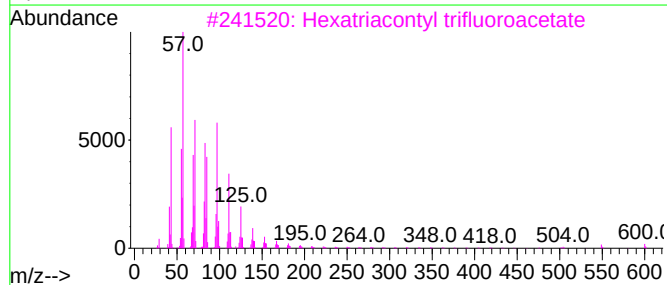
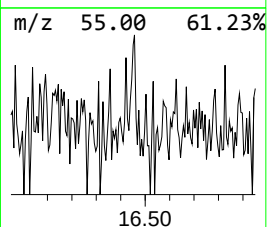
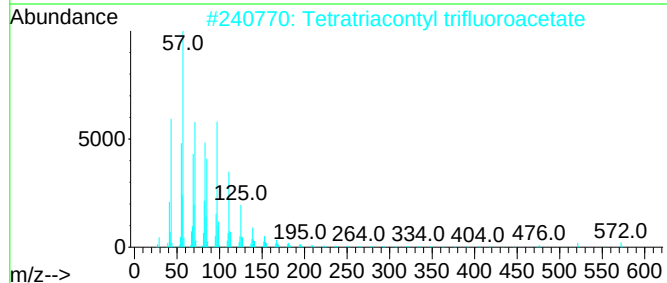
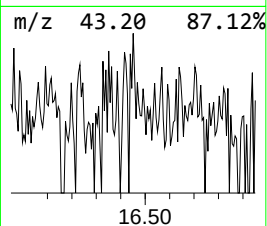
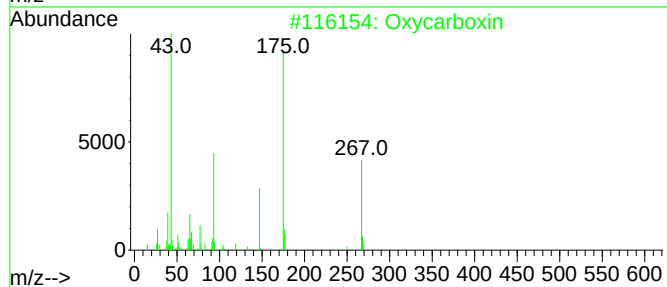
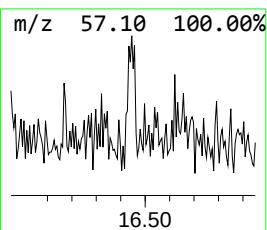
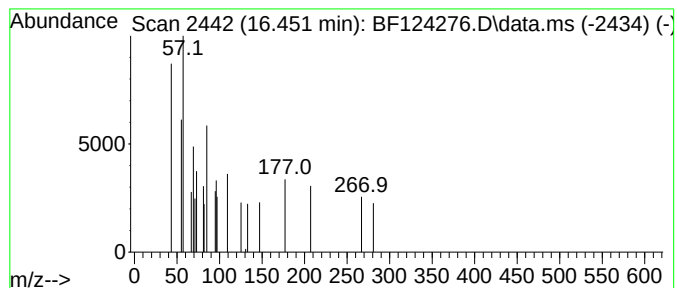
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 unknown16.451 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.451	2.11 ng	26736	Perylene-d12	15.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxycarboxin	267	C12H13NO4S	005259-88-1	9
2			Tetratriacontyl trifluoroacetate	591	C36H69F3O2	1000351-75-3	9
3			Hexatriacontyl trifluoroacetate	619	C38H73F3O2	1000351-88-6	9
4			Dotriacontyl trifluoroacetate	562	C34H65F3O2	1000351-75-4	9
5			Oxiranecarboxaldehyde, 3-methyl-...	168	C10H16O2	016996-12-6	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.187	2.187	2.3	ng	22053	1	6.840	193485	20.0
2-Pentanone, 4-...	5.051	7.8	ng	74934	1	6.840	193485	20.0
Ethanol, 2-(2-b...	8.022	9.3	ng	112965	2	8.122	243666	20.0
unknown16.451	16.451	2.1	ng	26736	6	15.486	252866	20.0