

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU103122\
 Data File : VU051642.D
 Acq On : 01 Nov 2022 04:31
 Operator : JC/MD
 Sample : N5319-06
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHAF1

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.1

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:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU051642.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.472	32	41	59	rBV	132937	259246	23.88%	3.786%
2	1.597	74	80	89	rBV	74868	90977	8.38%	1.329%
3	1.909	169	177	196	rVB	85867	116936	10.77%	1.708%
4	2.565	369	381	393	rBV	100056	159472	14.69%	2.329%
5	2.633	393	402	420	rVB3	13017	27531	2.54%	0.402%
6	2.781	434	448	474	rBV	23126	65660	6.05%	0.959%
7	3.044	519	530	542	rBV	16925	31472	2.90%	0.460%
8	3.581	683	697	715	rBV2	29456	71242	6.56%	1.040%
9	4.623	1009	1021	1049	rBV	188516	481312	44.33%	7.029%
10	5.067	1142	1159	1197	rBV2	183435	539665	49.71%	7.881%
11	5.723	1341	1363	1399	rBV2	277832	773075	71.21%	11.289%
12	6.247	1513	1526	1546	rBV	188978	361428	33.29%	5.278%
13	6.690	1650	1664	1684	rBV	206887	404954	37.30%	5.913%
14	7.157	1799	1809	1816	rBV6	5713	10890	1.00%	0.159%
15	7.565	1925	1936	1952	rBV2	54196	97062	8.94%	1.417%
16	7.713	1969	1982	2001	rBV2	61706	120767	11.12%	1.764%
17	7.896	2026	2039	2054	rBV	239147	414570	38.19%	6.054%
18	7.970	2054	2062	2074	rVB2	19321	33921	3.12%	0.495%
19	8.179	2113	2127	2145	rBV2	36835	63461	5.85%	0.927%
20	8.632	2253	2268	2296	rBV2	561458	1085632	100.00%	15.853%
21	8.787	2308	2316	2330	rVB5	12084	22384	2.06%	0.327%
22	9.417	2499	2512	2529	rBV	282808	479586	44.18%	7.003%
23	9.690	2585	2597	2609	rBV6	11455	22001	2.03%	0.321%
24	10.754	2913	2928	2949	rBV	193992	311086	28.65%	4.543%
25	10.893	2959	2971	2980	rBV3	6811	11050	1.02%	0.161%
26	11.812	3245	3257	3278	rBV	219143	362570	33.40%	5.295%
27	12.060	3326	3334	3350	rBV6	6418	13224	1.22%	0.193%
28	12.192	3362	3375	3397	rBV	232143	385560	35.51%	5.630%
29	12.886	3583	3591	3603	rBV5	12607	20197	1.86%	0.295%
30	16.767	4790	4798	4806	rBV9	7760	11030	1.02%	0.161%

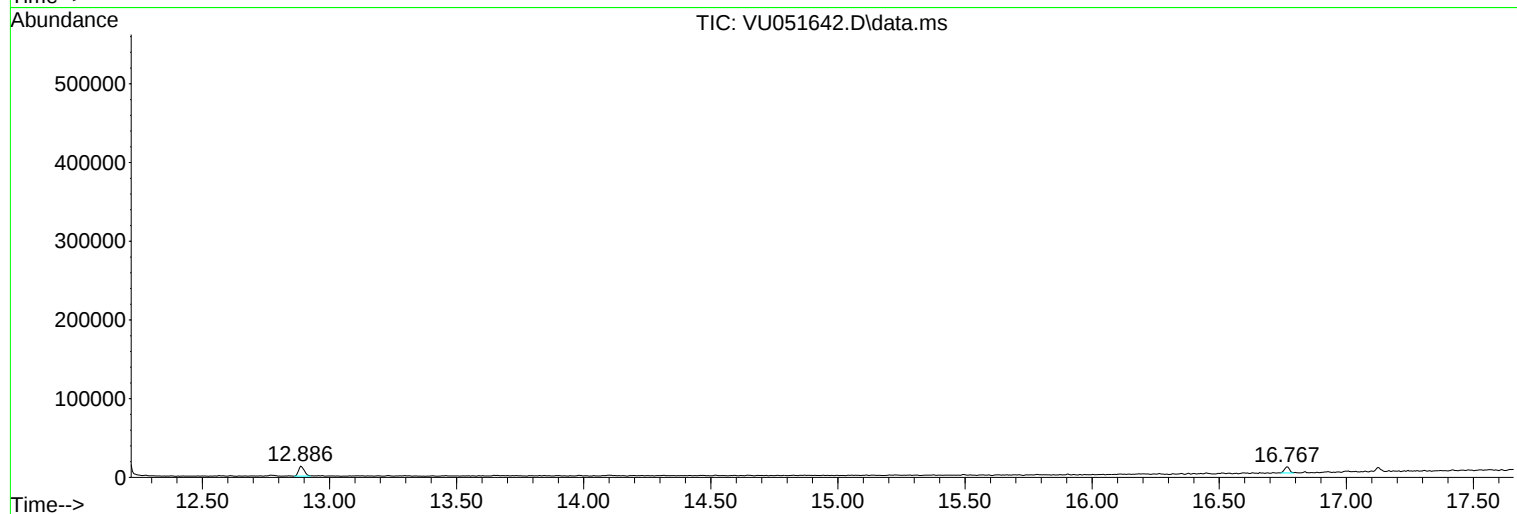
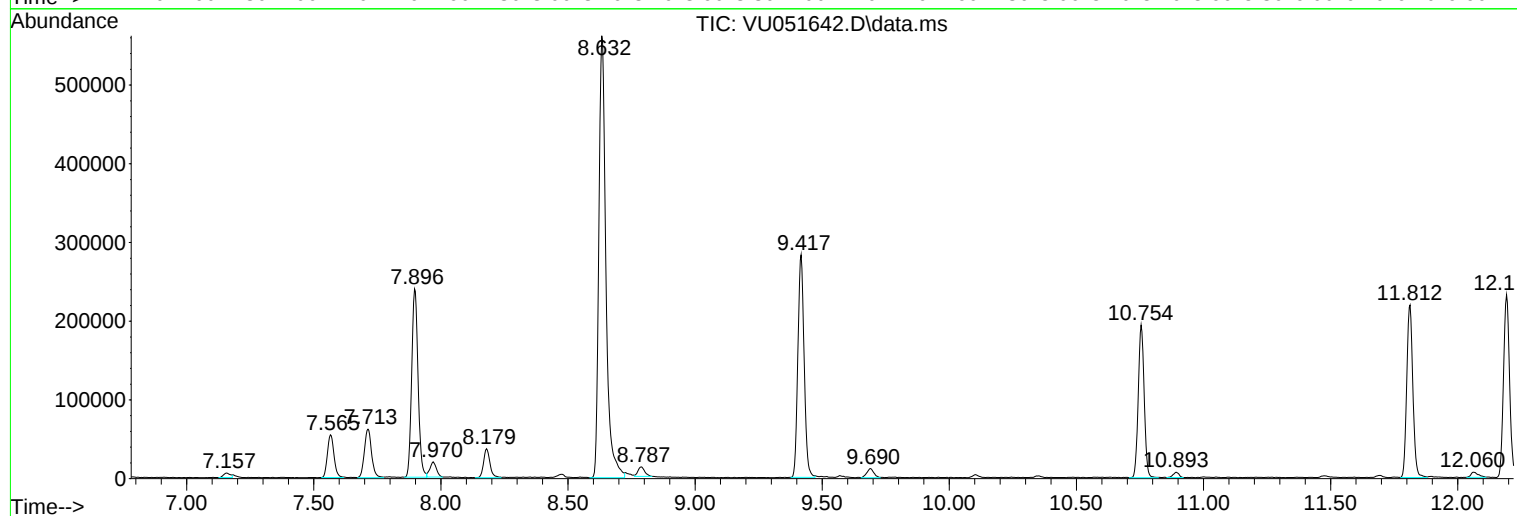
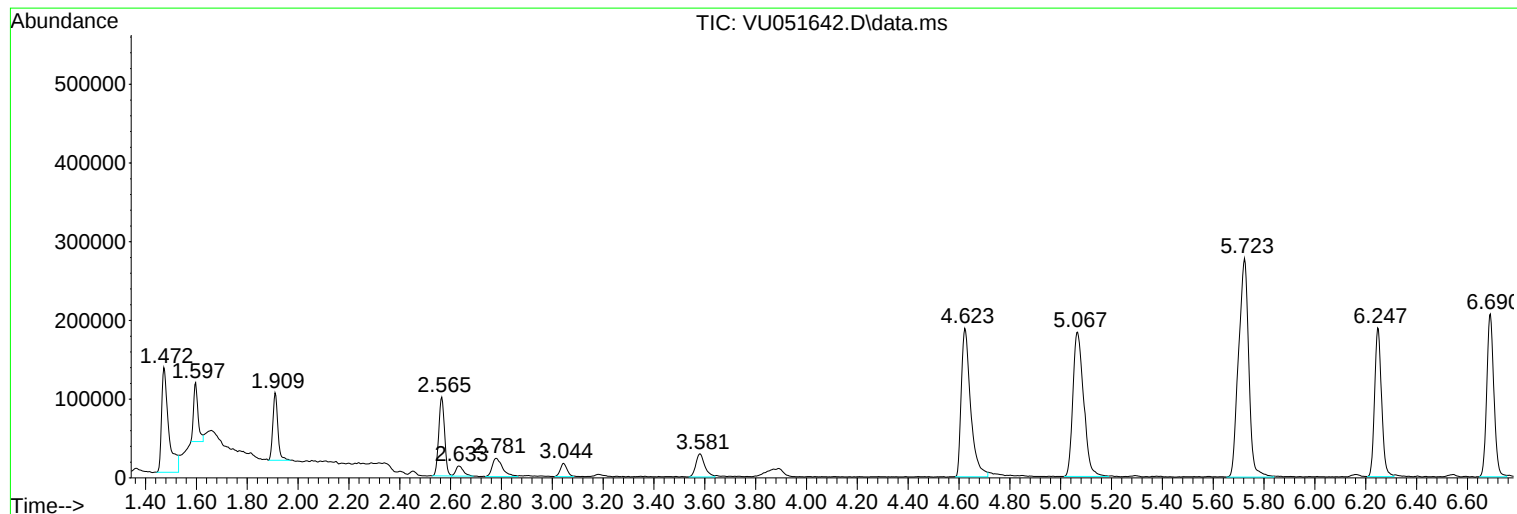
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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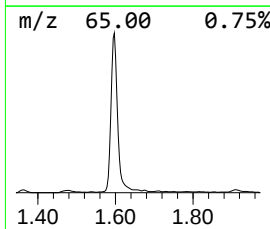
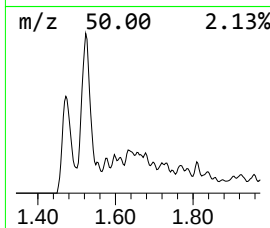
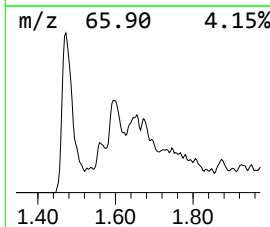
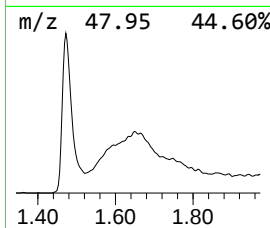
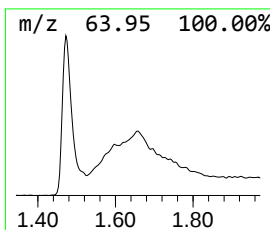
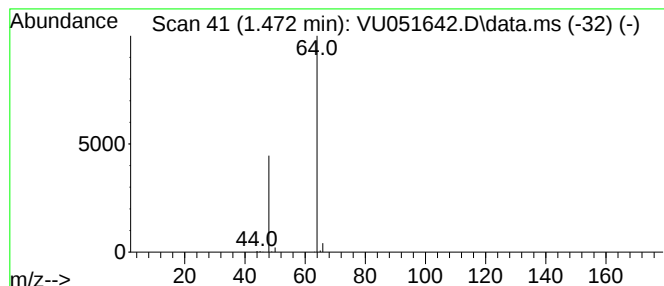
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.472	3.59 ug/L	259246	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Sulfur dioxide	64	O2S	007446-09-5	5
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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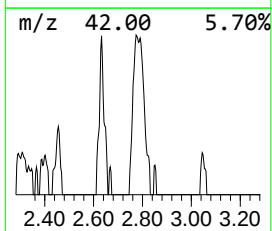
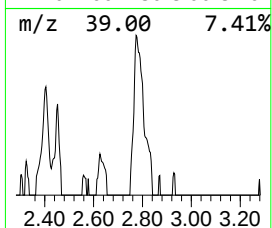
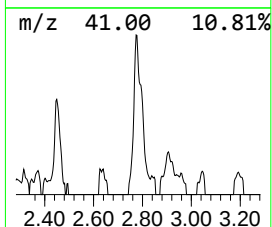
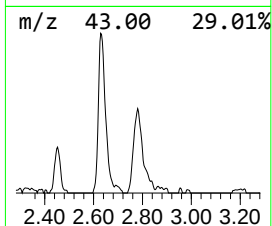
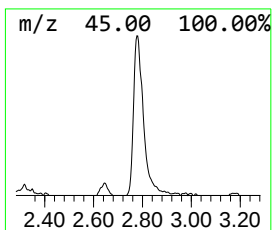
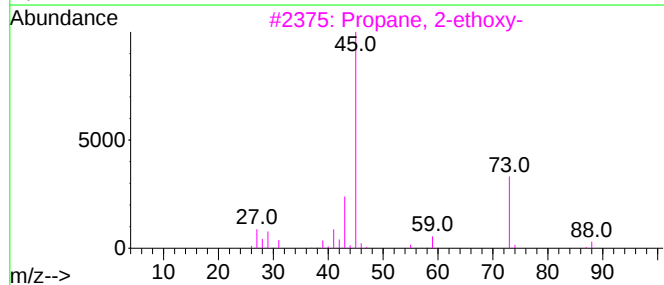
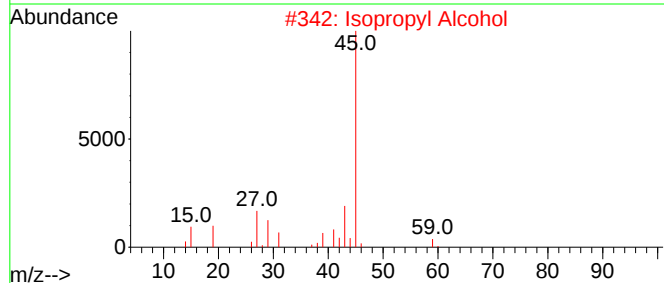
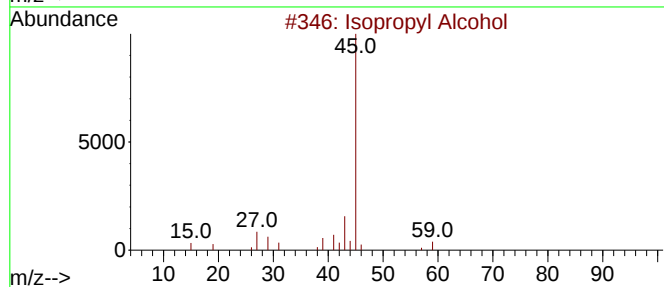
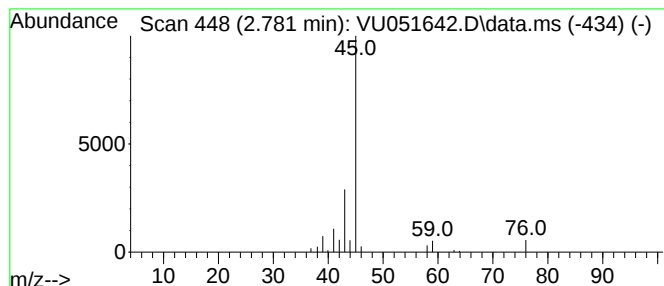
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Isopropyl Alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.781	0.91 ug/L	65660	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	43
3			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	40
4			Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	40
5			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	40



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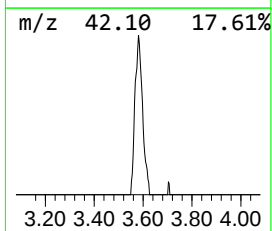
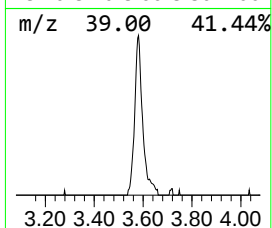
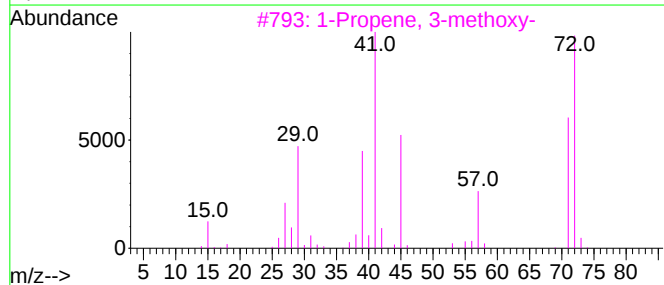
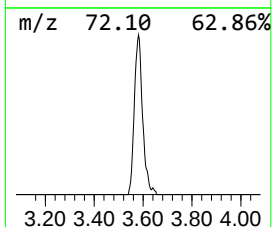
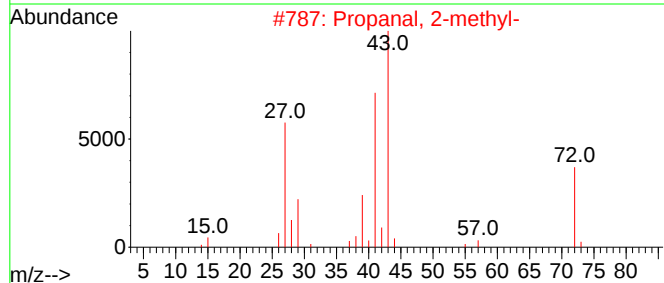
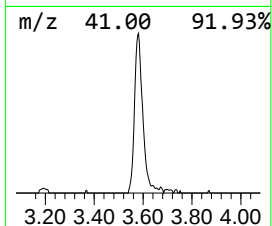
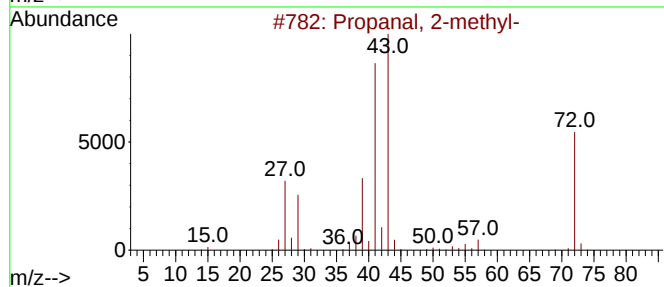
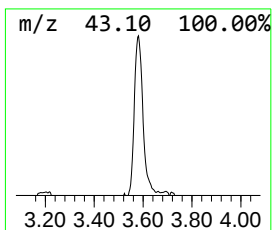
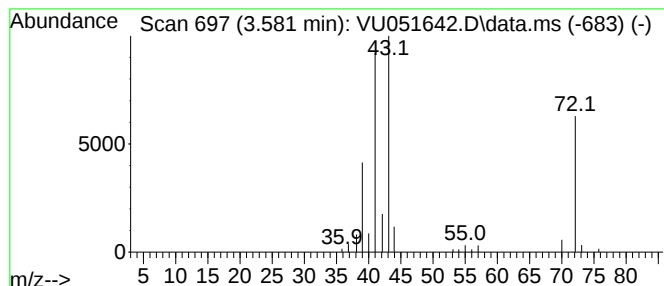
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Propanal, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.581	0.99 ug/L	71242	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal, 2-methyl-			72	C4H8O	000078-84-2	78
2	Propanal, 2-methyl-			72	C4H8O	000078-84-2	64
3	1-Propene, 3-methoxy-			72	C4H8O	000627-40-7	59
4	Propanal, 2-methyl-			72	C4H8O	000078-84-2	58
5	Butanal			72	C4H8O	000123-72-8	56



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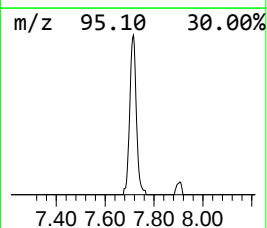
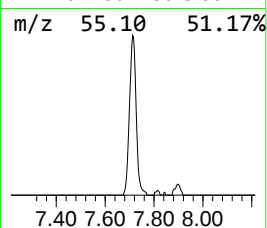
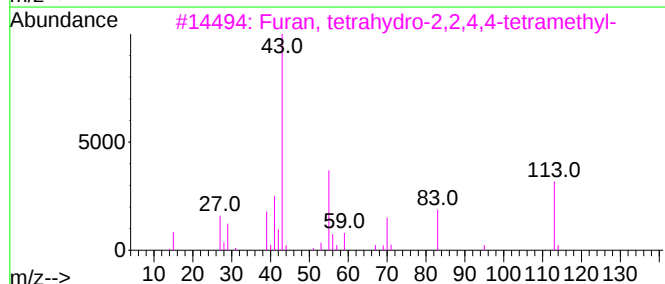
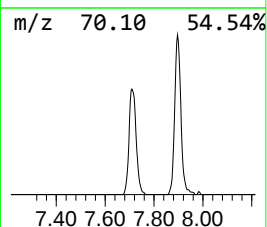
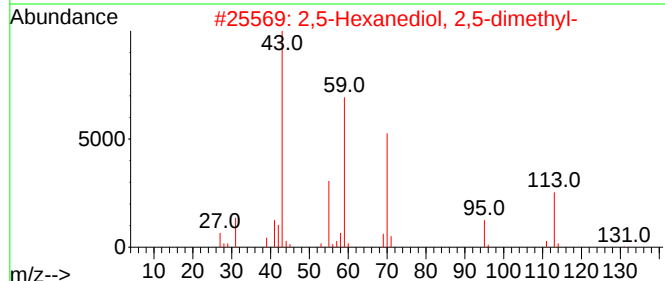
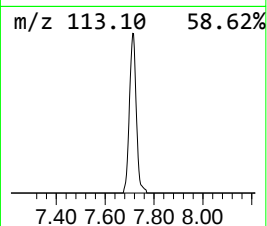
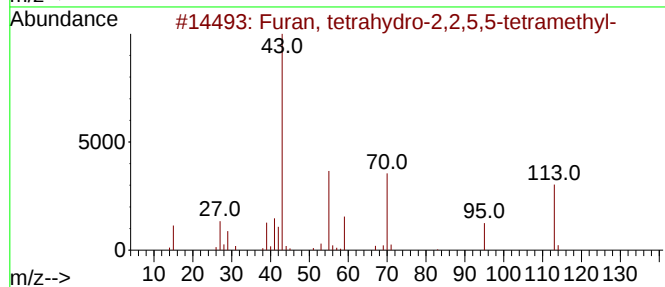
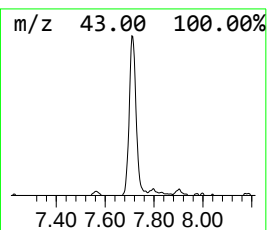
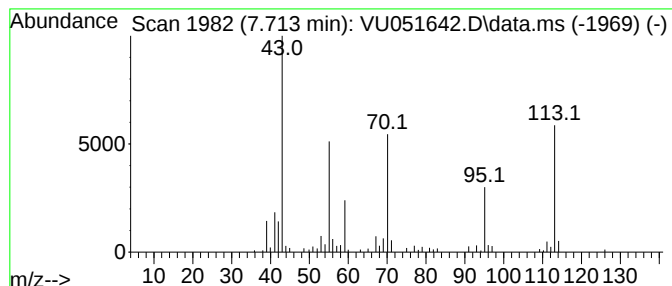
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Furan, tetrahydro-2,2,5,5-t... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.713	1.67 ug/L	120767	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	83
2			2,5-Hexanediol, 2,5-dimethyl-	146	C8H18O2	000110-03-2	59
3			Furan, tetrahydro-2,2,4,4-tetram...	128	C8H16O	003358-28-9	53
4			Pyrrolidine, 1-acetyl-	113	C6H11NO	004030-18-6	53
5			Pyrrolidine, 1-acetyl-	113	C6H11NO	004030-18-6	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.472	3.6	ug/L	259246	1	6.250	361428	5.0
Isopropyl Alcohol	2.781	0.9	ug/L	65660	1	6.250	361428	5.0
Propanal, 2-met...	3.581	1.0	ug/L	71242	1	6.250	361428	5.0
Furan, tetrahyd...	7.713	1.7	ug/L	120767	1	6.250	361428	5.0