

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082923\
 Data File : VU054947.D
 Acq On : 29 Aug 2023 11:24
 Operator : MD/SY
 Sample : 04173-19
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AM3

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\SFAMUTR082823WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU054947.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.596	85	95	109	rVV	41695	56163	8.08%	0.951%
2	1.686	117	123	132	rBV	14102	18428	2.65%	0.312%
3	1.911	185	193	209	rVB	52451	68254	9.82%	1.155%
4	2.348	306	329	335	rBV3	17879	65269	9.39%	1.105%
5	2.564	383	396	408	rBV	83932	138721	19.95%	2.348%
6	2.631	408	417	440	rVB	37959	82790	11.91%	1.401%
7	2.795	453	468	517	rBV2	48141	210774	30.31%	3.567%
8	3.039	534	544	558	rBV3	8551	16182	2.33%	0.274%
9	3.133	564	573	581	rBV4	8680	14965	2.15%	0.253%
10	3.197	582	593	617	rVB4	15058	49505	7.12%	0.838%
11	3.361	631	644	657	rBV2	8495	19144	2.75%	0.324%
12	4.499	983	998	1019	rVB2	49870	125354	18.03%	2.122%
13	4.628	1023	1038	1058	rBV	102917	284698	40.95%	4.819%
14	5.062	1157	1173	1196	rBV	111070	248367	35.72%	4.204%
15	5.724	1359	1379	1404	rBV3	204626	554854	79.80%	9.391%
16	6.248	1529	1542	1561	rBV	220796	429086	61.71%	7.262%
17	6.528	1621	1629	1640	rVB9	3772	7461	1.07%	0.126%
18	6.689	1664	1679	1699	rBV2	140668	284343	40.90%	4.813%
19	7.165	1802	1827	1844	rBV5	8814	31408	4.52%	0.532%
20	7.567	1940	1952	1971	rBV2	59454	109819	15.79%	1.859%
21	7.711	1985	1997	2009	rBV6	5757	11448	1.65%	0.194%
22	7.898	2041	2055	2070	rBV	253029	454671	65.39%	7.695%
23	7.968	2070	2077	2091	rVB2	13523	26295	3.78%	0.445%
24	8.181	2133	2143	2160	rBV2	35111	61242	8.81%	1.037%
25	8.473	2223	2234	2249	rVB5	4374	8525	1.23%	0.144%
26	8.634	2271	2284	2319	rBV2	314971	695293	100.00%	11.768%
27	9.415	2515	2527	2546	rBV	306819	532214	76.55%	9.008%
28	9.698	2604	2615	2624	rBV2	5140	9127	1.31%	0.154%
29	10.753	2931	2943	2959	rBV	111935	188300	27.08%	3.187%
30	10.888	2977	2985	2996	rBV4	9812	15373	2.21%	0.260%
31	11.811	3258	3272	3290	rBV	351964	572933	82.40%	9.697%
32	12.065	3341	3351	3361	rBV4	9481	17312	2.49%	0.293%
33	12.193	3378	3391	3406	rBV	283646	468902	67.44%	7.936%
34	12.888	3599	3607	3622	rBV7	6912	12146	1.75%	0.206%
35	14.315	4043	4051	4061	rVB5	4448	7746	1.11%	0.131%
36	15.692	4470	4479	4486	rBV8	8187	11284	1.62%	0.191%

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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\SFAMUTR082823WMA.M
Title : TRACE VOA SFAM1.0

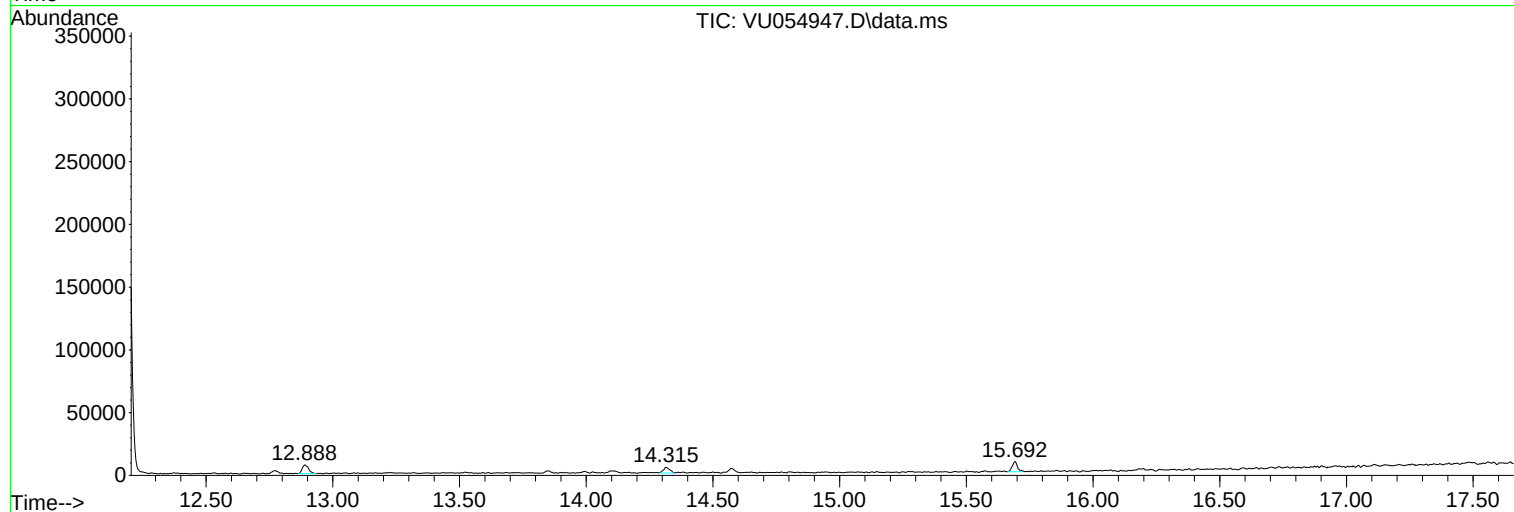
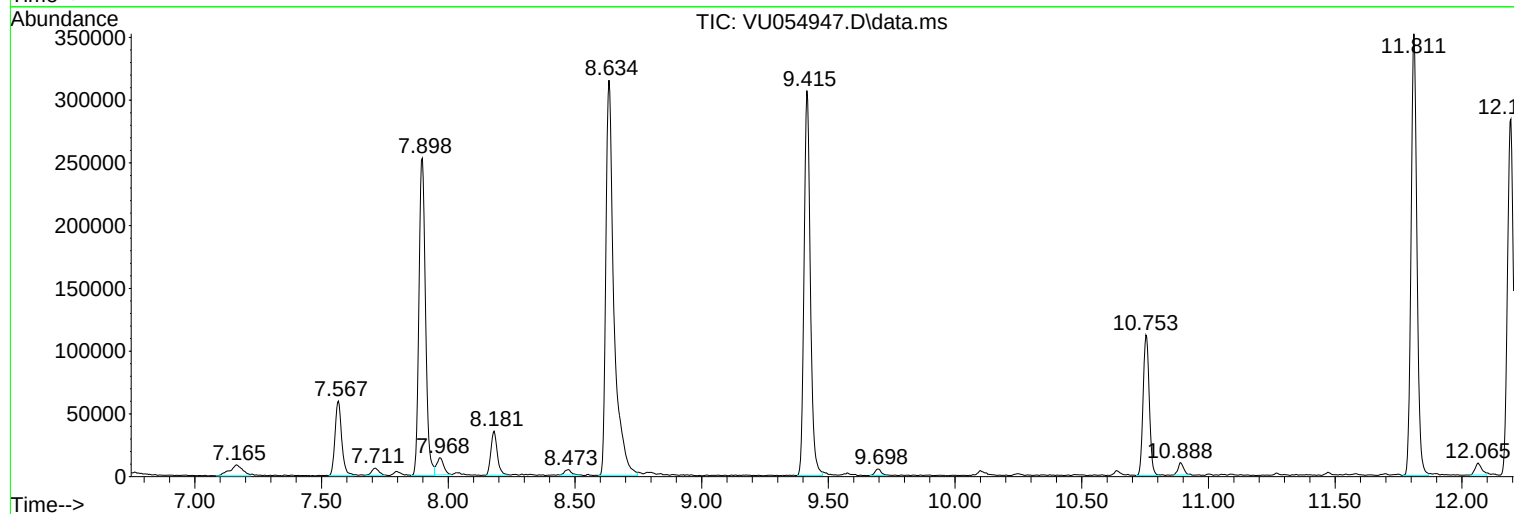
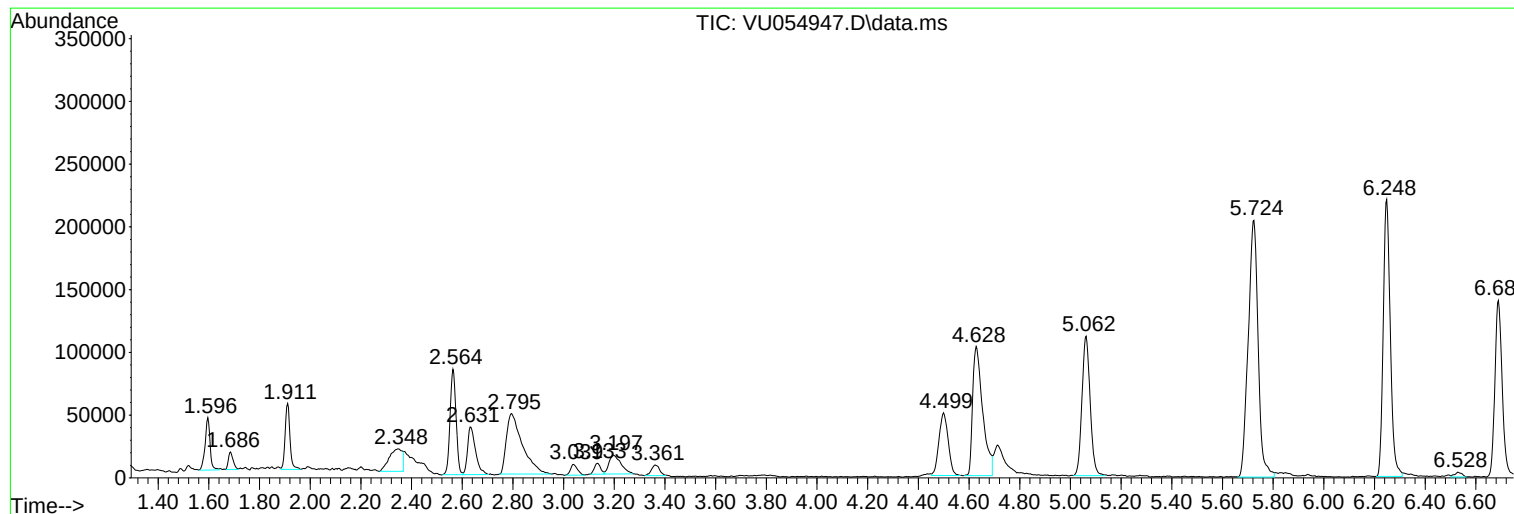
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR082823WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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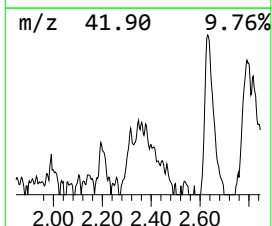
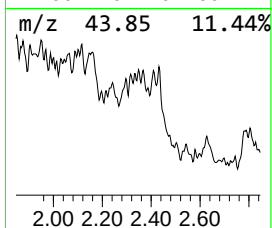
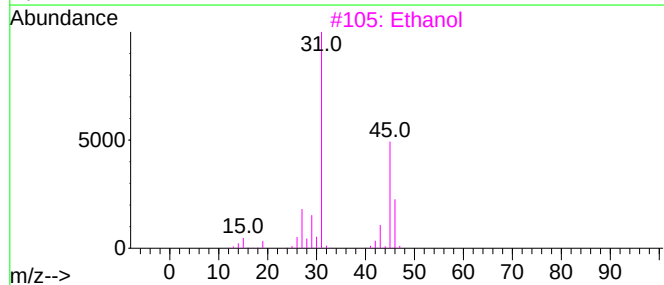
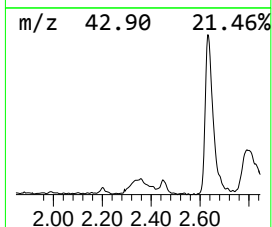
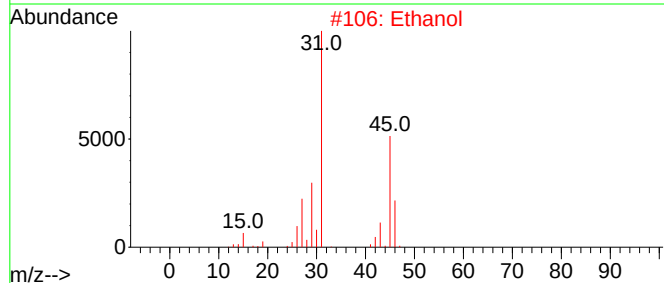
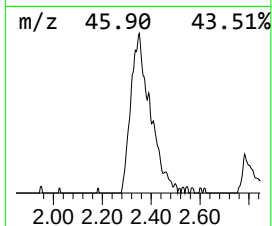
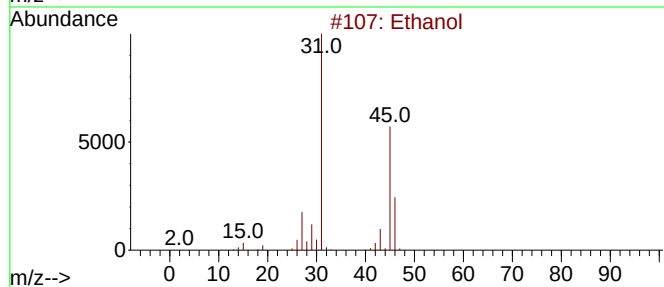
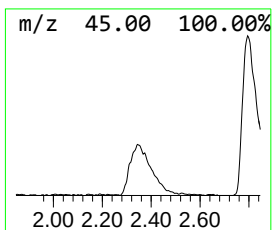
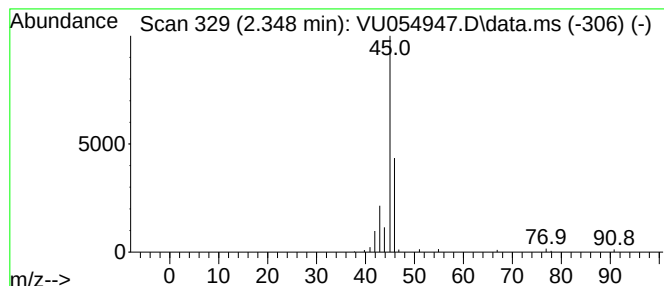
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Ethanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.348	0.76 ug/L	65269	1,4-Difluorobenzene	6.248

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	56
2	Ethanol			46	C2H6O	000064-17-5	56
3	Ethanol			46	C2H6O	000064-17-5	40
4	Dimethyl ether			46	C2H6O	000115-10-6	9
5	Dimethyl ether			46	C2H6O	000115-10-6	9



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ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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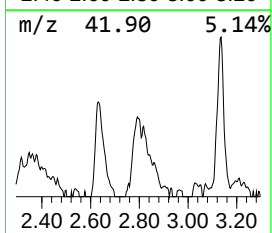
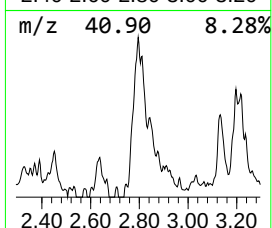
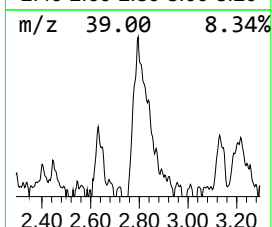
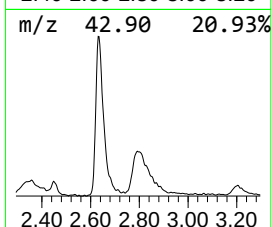
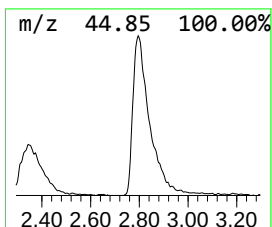
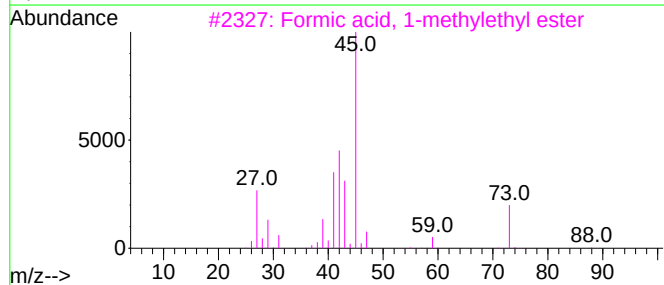
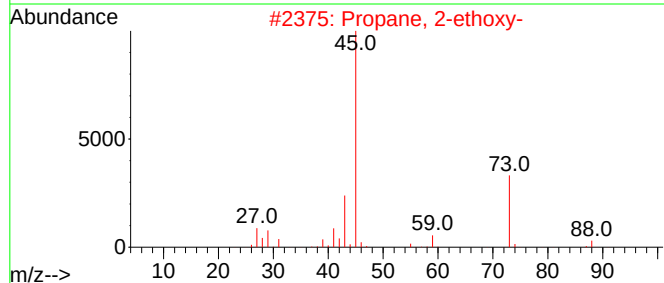
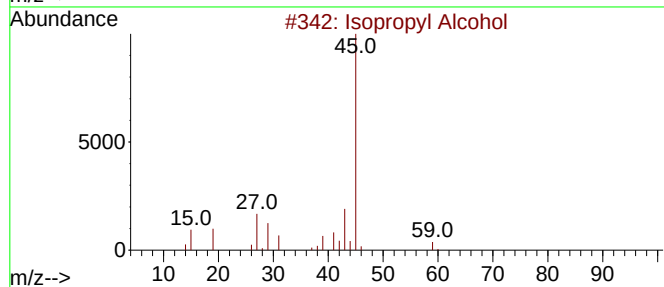
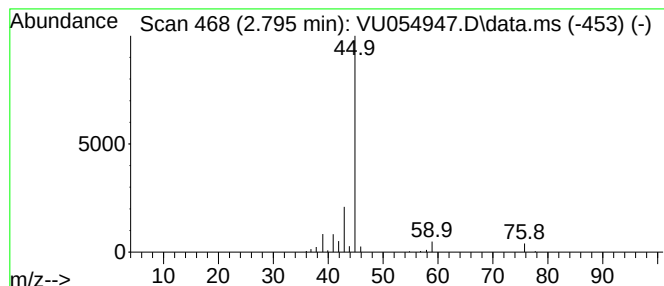
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR082823WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.795	2.46 ug/L	210774	1,4-Difluorobenzene	6.248

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	43
2			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	43
3			Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	40
4			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	40
5			(R)-(-)-2-Pentanol	88	C5H12O	031087-44-2	9



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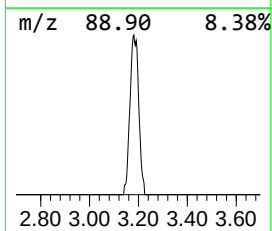
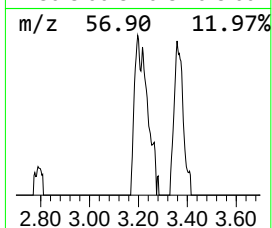
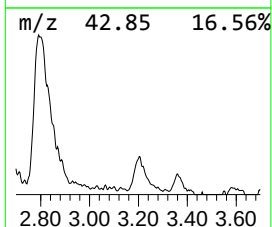
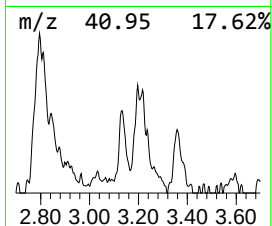
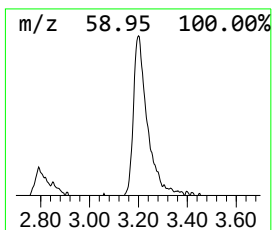
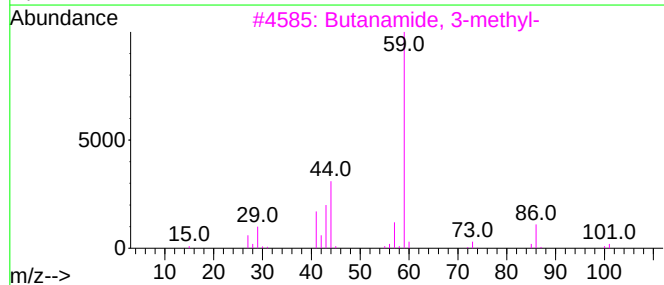
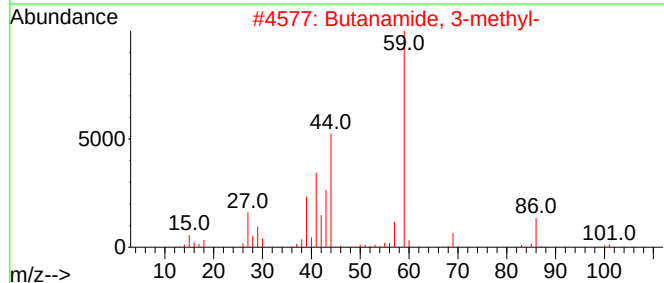
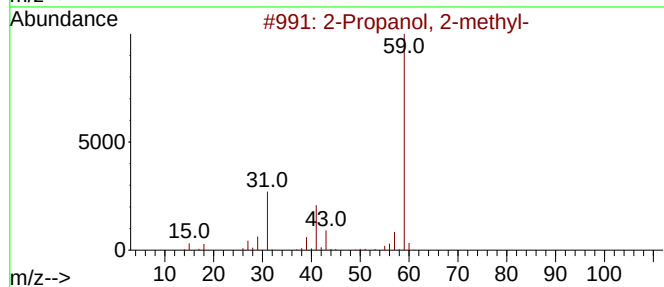
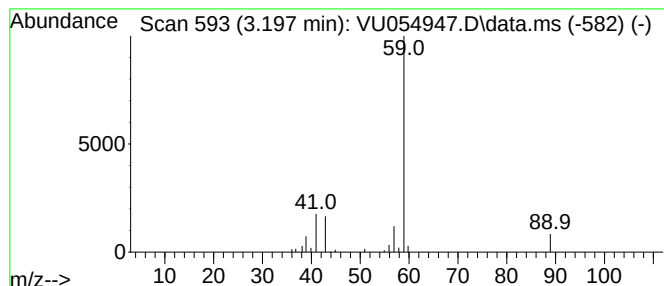
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR082823WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 unknown-02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.197	0.58 ug/L	49505	1,4-Difluorobenzene	6.248

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	40
2	Butanamide, 3-methyl-			101	C5H11NO	000541-46-8	9
3	Butanamide, 3-methyl-			101	C5H11NO	000541-46-8	9
4	Propane, 2-ethoxy-2-methyl-			102	C6H14O	000637-92-3	9
5	Guanidine			59	CH5N3	000113-00-8	7



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Instrument :
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ClientSampleId :
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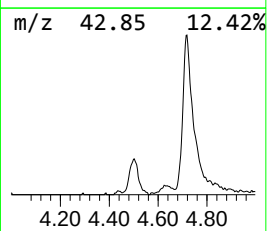
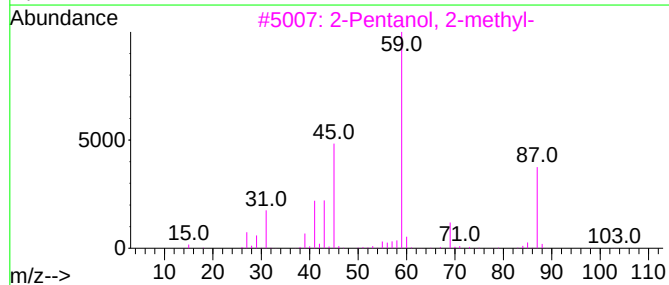
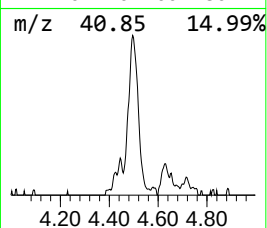
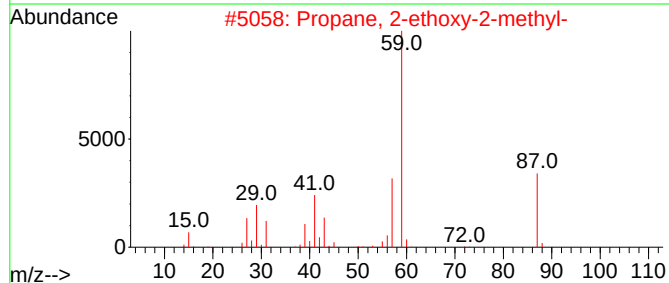
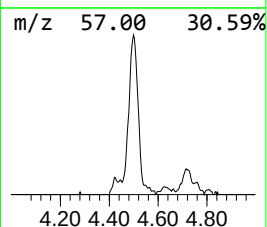
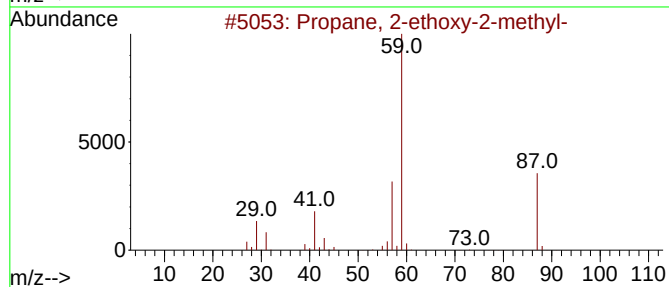
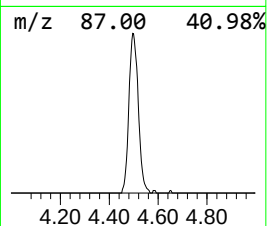
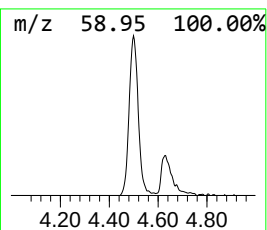
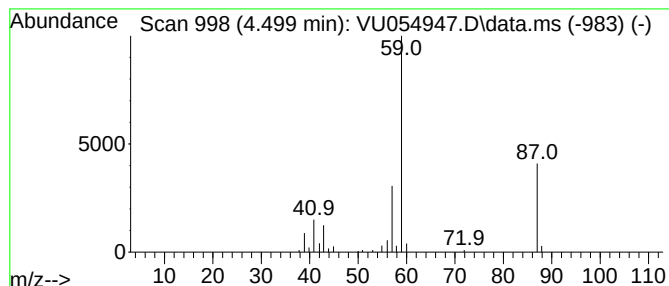
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Propane, 2-ethoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.499	1.46 ug/L	125354	1,4-Difluorobenzene	6.248

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	83
2			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	64
3			2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	64
4			DL-Lactamide, N,O-dimethyl-	117	C5H11NO2	1000452-56-3	56
5			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	50



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol	2.348	0.8	ug/L	65269	1	6.248	429086	5.0
unknown-01	2.795	2.5	ug/L	210774	1	6.248	429086	5.0
unknown-02	3.197	0.6	ug/L	49505	1	6.248	429086	5.0
Propane, 2-etho...	4.499	1.5	ug/L	125354	1	6.248	429086	5.0