

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110822\
 Data File : VU051777.D
 Acq On : 08 Nov 2022 12:24
 Operator : JC/MD
 Sample : N5493-09
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 H0AE3

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: VU051777.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	31	41	53	rBV	143155	255691	30.20%	3.415%
2	1.597	71	80	100	rVV	114343	154576	18.26%	2.064%
3	1.684	101	107	123	rVB	31291	44265	5.23%	0.591%
4	1.912	170	178	192	rVB	93948	122816	14.50%	1.640%
5	2.565	363	381	392	rBV	171695	282111	33.32%	3.768%
6	2.623	392	399	415	rVB	36624	62790	7.42%	0.839%
7	3.183	559	573	584	rBV3	8836	20340	2.40%	0.272%
8	3.829	753	774	790	rBV	7438	20397	2.41%	0.272%
9	4.436	942	963	986	rBV4	28799	79608	9.40%	1.063%
10	4.623	1008	1021	1042	rBV	124533	307578	36.33%	4.108%
11	5.063	1142	1158	1184	rBV	164210	372844	44.03%	4.979%
12	5.723	1343	1363	1394	rBV2	317079	846732	100.00%	11.308%
13	6.247	1513	1526	1547	rBV	260207	507859	59.98%	6.782%
14	6.690	1648	1664	1693	rBV	204009	404419	47.76%	5.401%
15	7.124	1784	1799	1826	rBV2	45022	111611	13.18%	1.491%
16	7.565	1923	1936	1962	rBV	91813	165099	19.50%	2.205%
17	7.896	2026	2039	2060	rBV	371884	655040	77.36%	8.748%
18	8.179	2116	2127	2148	rBV2	54776	96507	11.40%	1.289%
19	8.472	2209	2218	2236	rVB2	6599	12957	1.53%	0.173%
20	8.632	2256	2268	2300	rBV	403434	797103	94.14%	10.645%
21	8.787	2309	2316	2329	rVB7	8230	14503	1.71%	0.194%
22	9.417	2496	2512	2536	rBV	398854	676127	79.85%	9.030%
23	10.755	2915	2928	2944	rBV	164894	267400	31.58%	3.571%
24	10.890	2957	2970	2985	rVB2	12486	20895	2.47%	0.279%
25	11.478	3144	3153	3169	rBV4	4813	9214	1.09%	0.123%
26	11.809	3244	3256	3277	rBV	354344	569280	67.23%	7.603%
27	12.063	3324	3335	3355	rBV2	14927	28884	3.41%	0.386%
28	12.192	3362	3375	3393	rBV	350071	581217	68.64%	7.762%

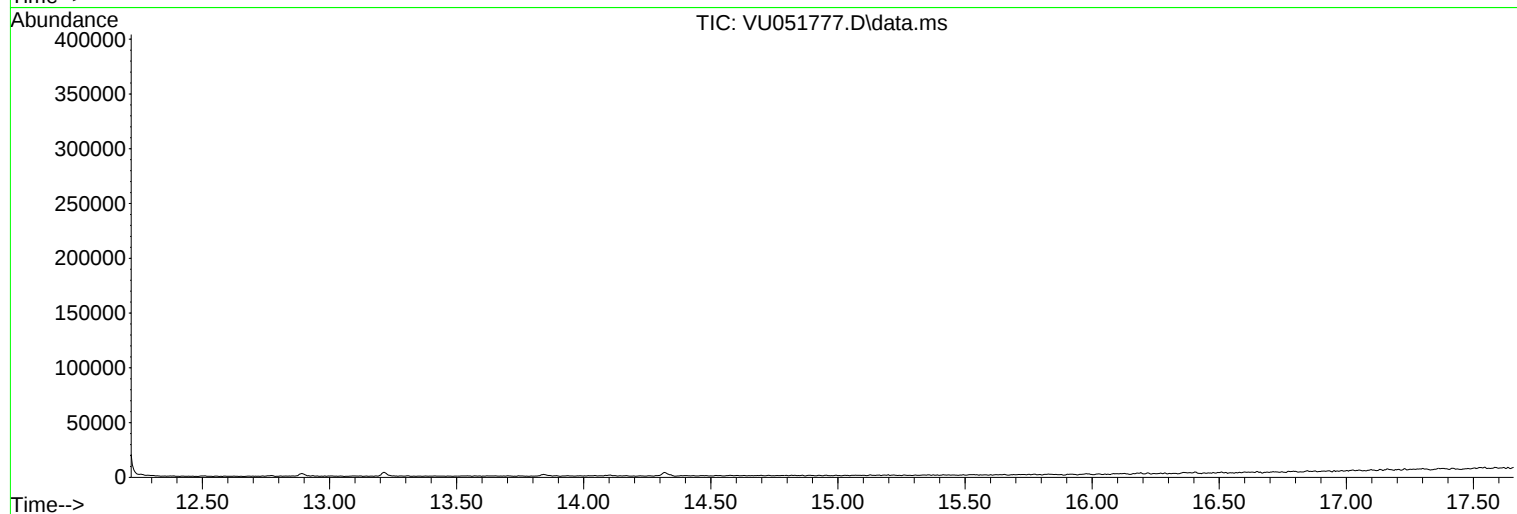
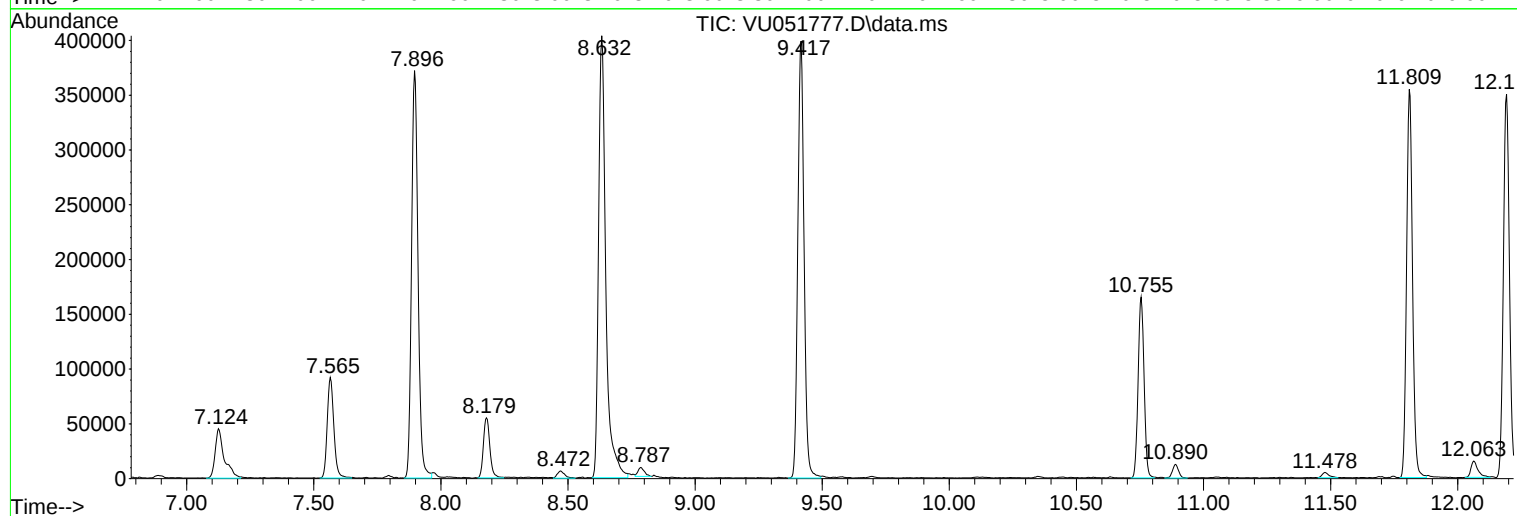
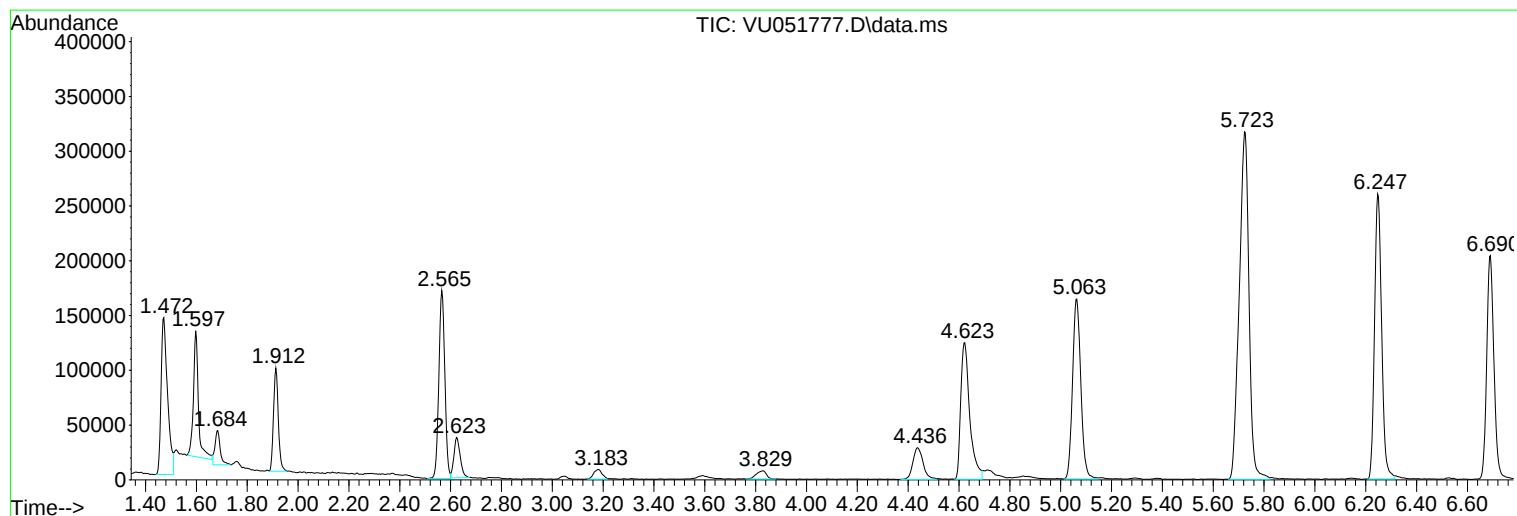
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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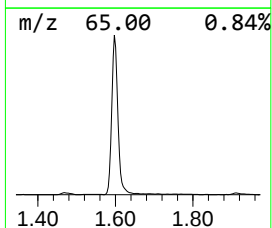
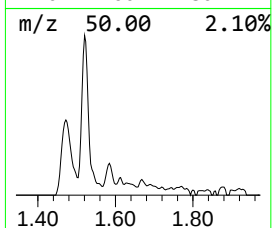
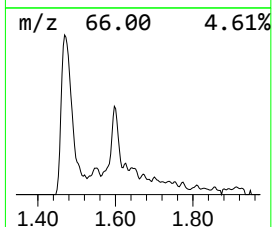
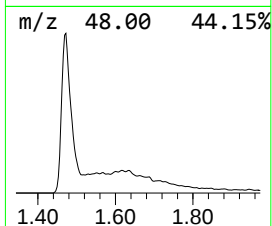
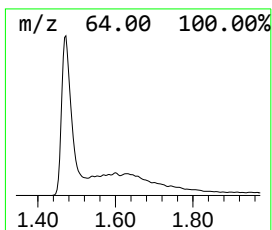
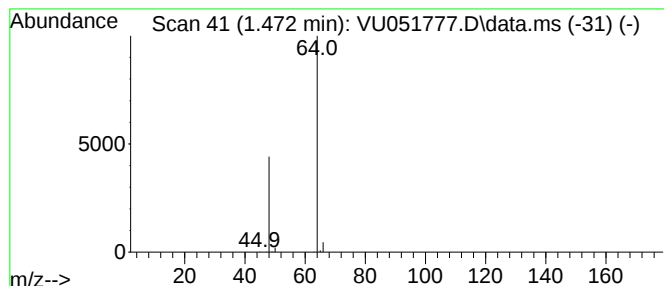
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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	2.52 ug/L	255691	1,4-Difluorobenzene	6.247

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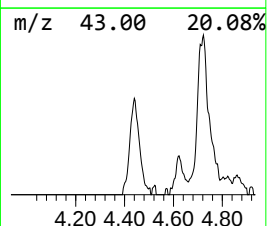
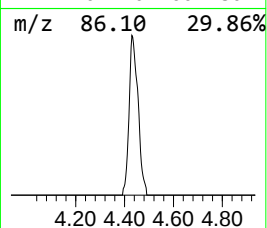
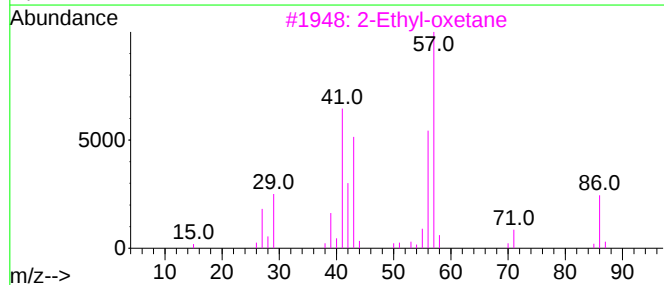
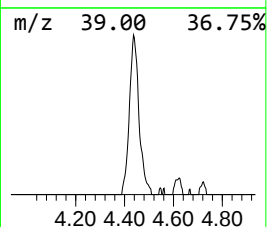
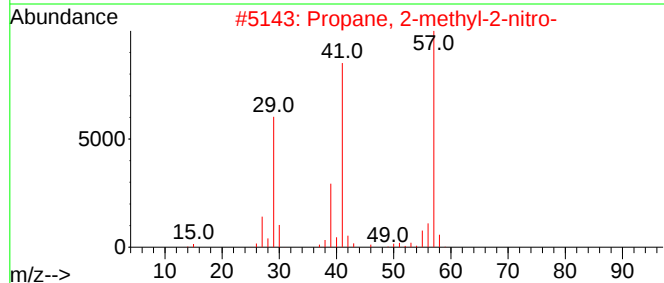
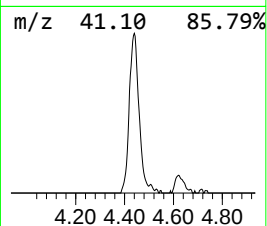
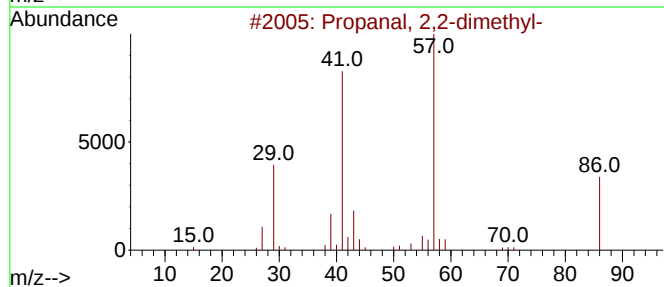
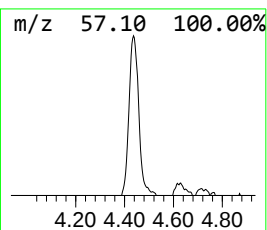
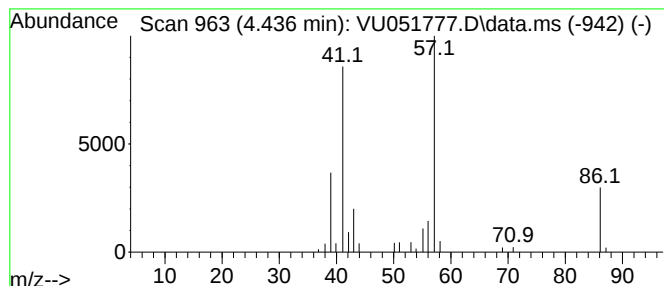
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Propanal, 2,2-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.436	0.78 ug/L	79608	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	64
2			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	59
3			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	47
4			3-Pentanone	86	C5H10O	000096-22-0	38
5			3-Heptanone, 5-ethyl-4-methyl-	156	C10H20O	027607-63-2	37



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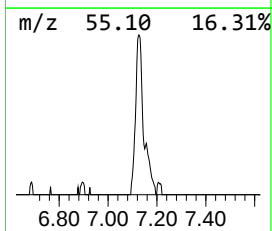
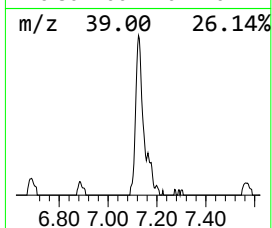
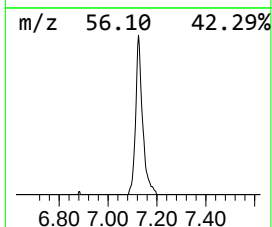
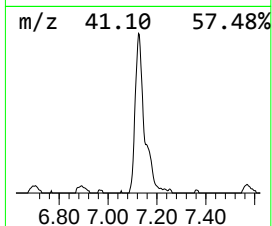
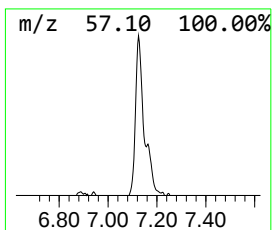
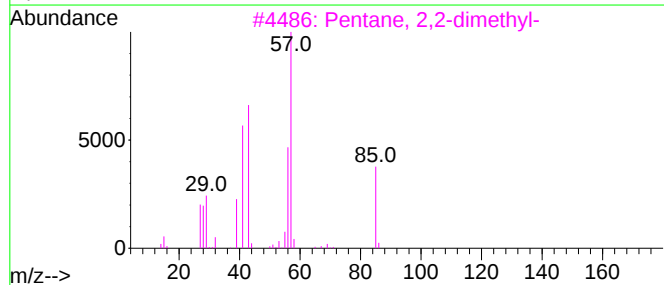
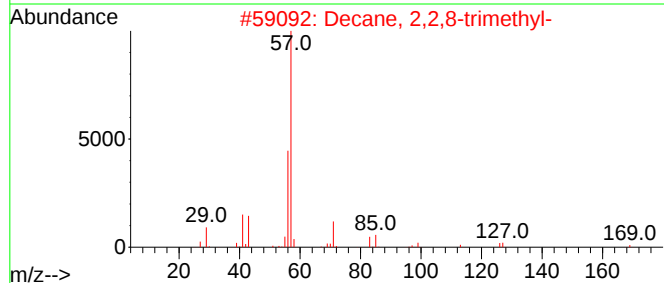
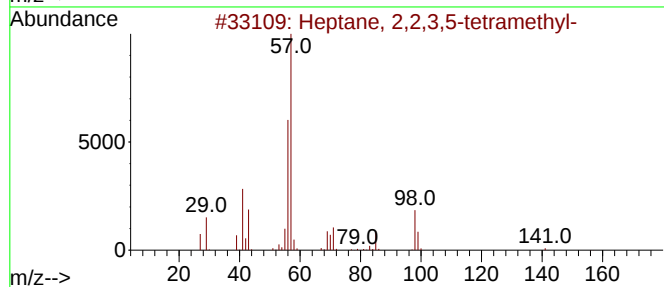
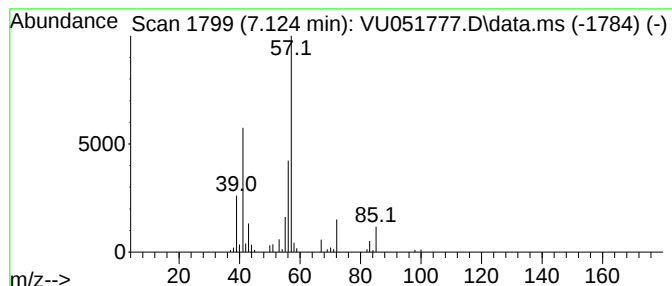
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.124	1.10 ug/L	111611	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 2,2,3,5-tetramethyl-	156	C11H24	061868-42-6	45
2			Decane, 2,2,8-trimethyl-	184	C13H28	062238-01-1	38
3			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	38
4			1-Hexene, 4-methyl-	98	C7H14	003769-23-1	37
5			Heptane, 2,2,4-trimethyl-	142	C10H22	014720-74-2	36



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Quant Title : TRACE VOA SFAM1.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.472	2.5	ug/L	255691	1	6.247	507859	5.0
Propanal, 2,2-d...	4.436	0.8	ug/L	79608	1	6.247	507859	5.0
(DEL) Alkane: S...	7.124	1.1	ug/L	111611	1	6.247	507859	5.0