

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU111523\
 Data File : VU056390.D
 Acq On : 16 Nov 2023 06:11
 Operator : MD/SY
 Sample : 05411-17
 Misc : 25mL/MSVOA_U/WATER
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0QK2

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\SFAMUTR111323WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU056390.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.464	45	54	65	rBV	148951	212215	19.97%	2.307%
2	1.518	65	71	84	rVV	56564	83626	7.87%	0.909%
3	1.583	84	91	103	rVB	51644	66521	6.26%	0.723%
4	1.686	118	123	131	rVB2	8699	11750	1.11%	0.128%
5	1.911	185	193	206	rVB	113133	155729	14.66%	1.693%
6	3.042	533	545	554	rBV3	10332	20423	1.92%	0.222%
7	4.621	1021	1036	1072	rBV	144226	393432	37.03%	4.277%
8	5.055	1155	1171	1206	rVB	225785	558460	52.56%	6.071%
9	5.521	1305	1316	1330	rVB3	6578	14353	1.35%	0.156%
10	5.721	1357	1378	1412	rBV2	345090	950169	89.42%	10.329%
11	6.245	1528	1541	1572	rBV	341776	670451	63.10%	7.289%
12	6.528	1619	1629	1642	rVB9	7023	15813	1.49%	0.172%
13	6.685	1664	1678	1696	rBV	264002	523439	49.26%	5.690%
14	7.100	1794	1807	1821	rBV4	18461	35098	3.30%	0.382%
15	7.795	2012	2023	2039	rBV3	40231	74436	7.01%	0.809%
16	8.184	2135	2144	2156	rBV4	6517	11330	1.07%	0.123%
17	8.631	2271	2283	2317	rBV	557537	1062572	100.00%	11.551%
18	8.801	2324	2336	2348	rVB10	18302	41851	3.94%	0.455%
19	9.412	2514	2526	2542	rBV	596028	1028536	96.80%	11.181%
20	9.486	2543	2549	2569	rVV3	30548	56467	5.31%	0.614%
21	10.341	2805	2815	2835	rBV3	40506	72784	6.85%	0.791%
22	10.457	2843	2851	2863	rBV3	5962	12709	1.20%	0.138%
23	10.750	2928	2942	2959	rBV	189402	313794	29.53%	3.411%
24	10.926	2985	2997	3017	rVB	253590	427134	40.20%	4.643%
25	11.042	3021	3033	3051	rBV2	153026	258787	24.35%	2.813%
26	11.807	3259	3271	3296	rBV	515573	851719	80.16%	9.259%
27	12.061	3340	3350	3361	rBV3	51781	115198	10.84%	1.252%
28	12.187	3377	3389	3411	rBV	509119	879785	82.80%	9.564%
29	12.286	3412	3420	3434	rVB4	24553	41823	3.94%	0.455%
30	12.885	3597	3606	3617	rBV6	10855	16849	1.59%	0.183%
31	13.100	3660	3673	3688	rVB3	76389	172946	16.28%	1.880%
32	13.360	3744	3754	3762	rBV8	8301	13882	1.31%	0.151%
33	13.524	3796	3805	3820	rBV4	18262	34582	3.25%	0.376%

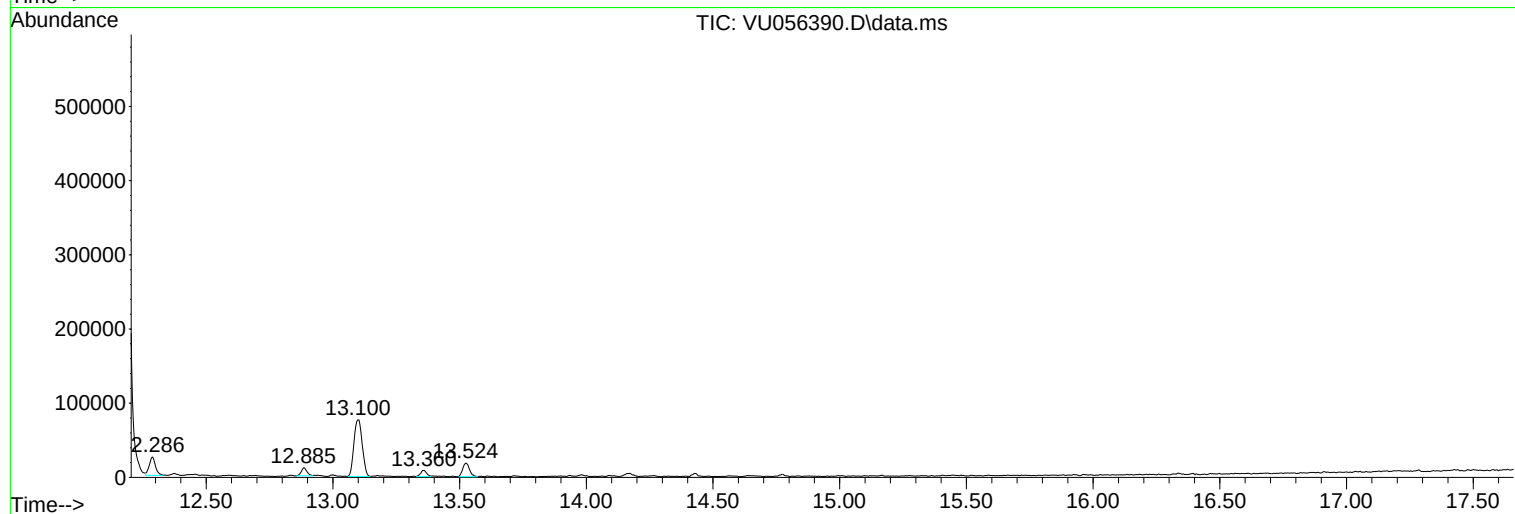
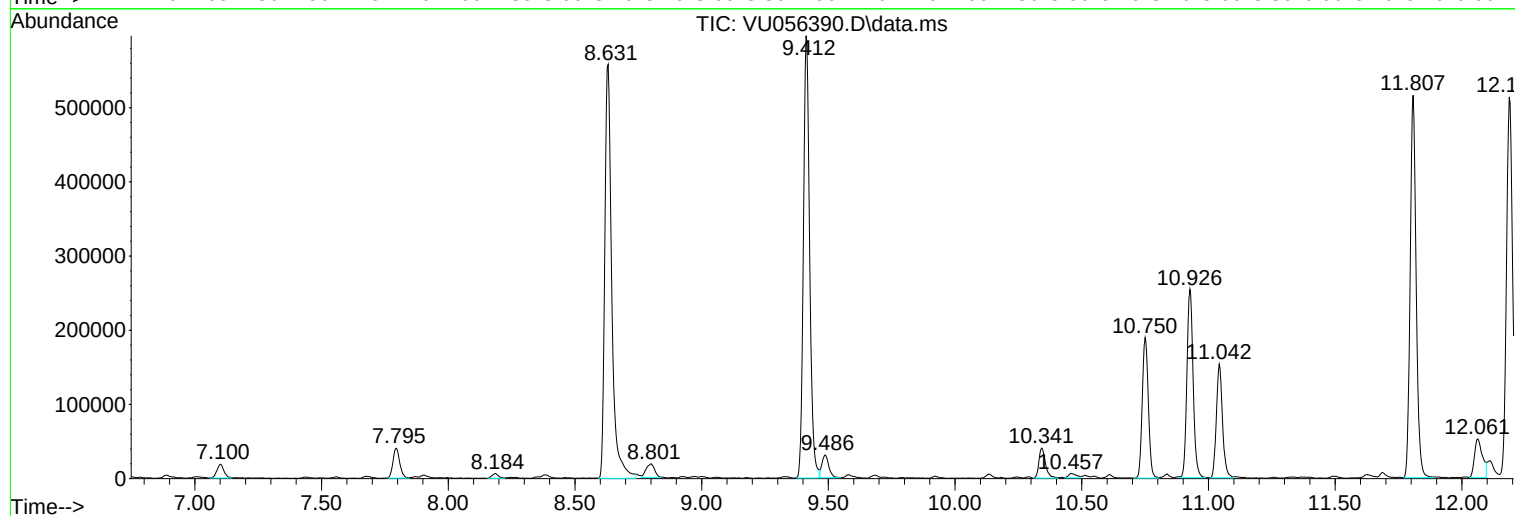
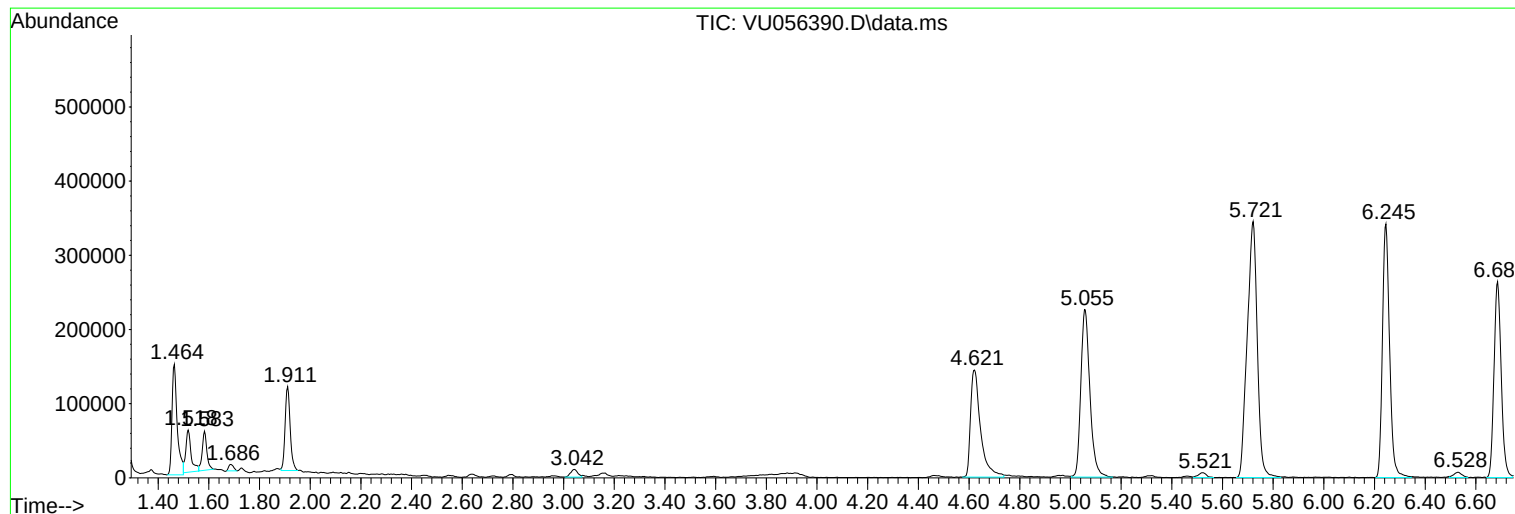
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Instrument :
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ClientSampleId :
C0QK2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111323WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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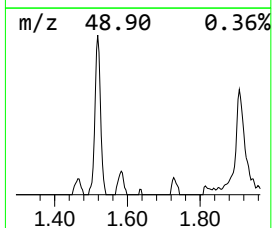
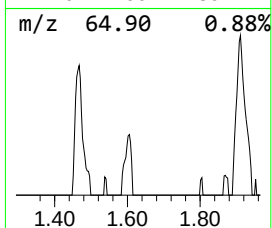
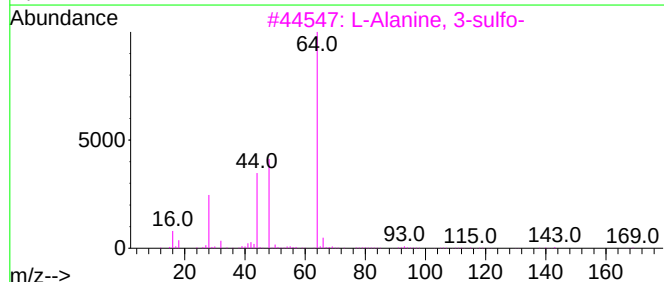
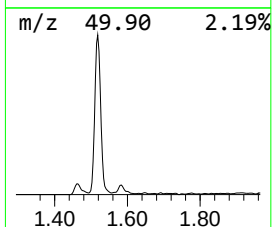
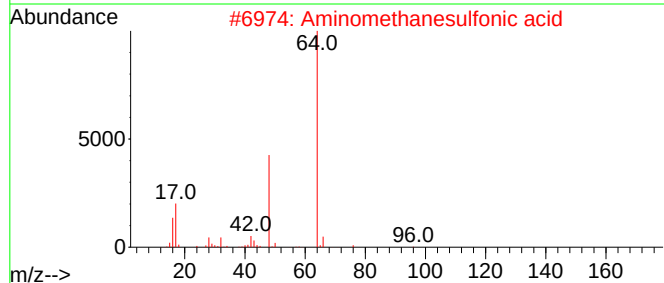
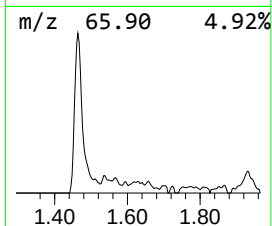
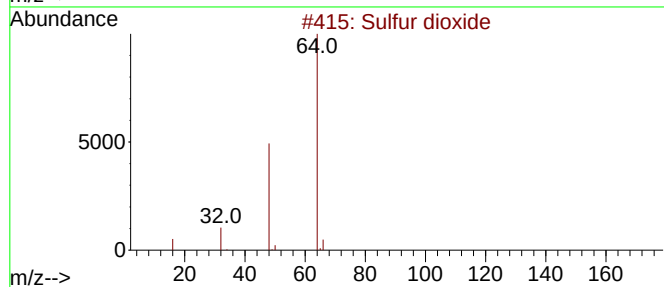
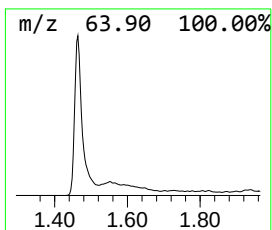
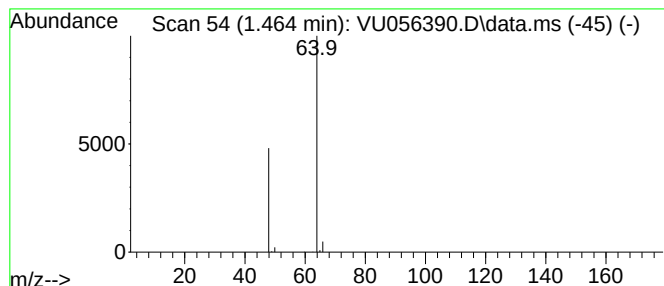
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.464	1.58 ug/L	212215	1,4-Difluorobenzene	6.245

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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Sulfur dioxide	64	O2S	007446-09-5	5



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ClientSampleId :
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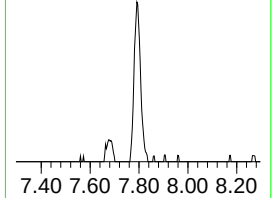
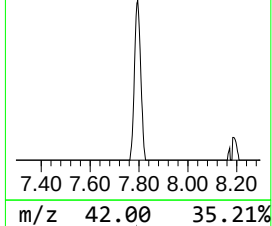
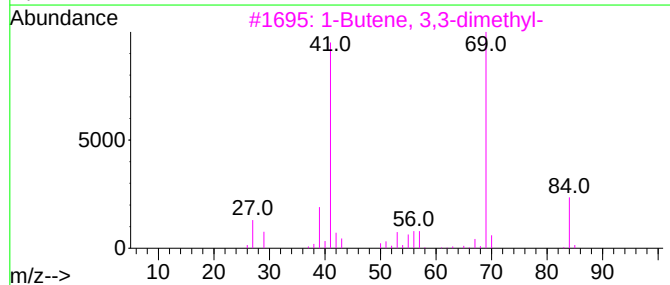
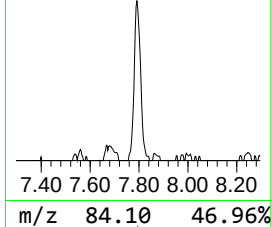
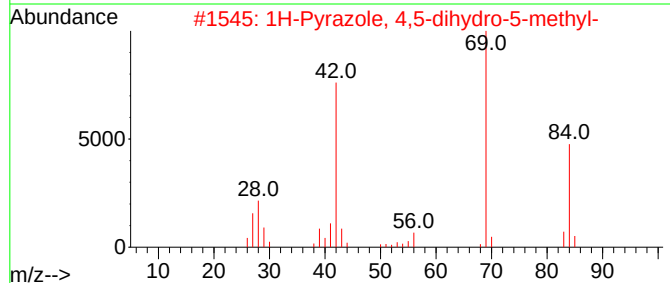
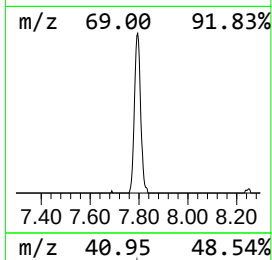
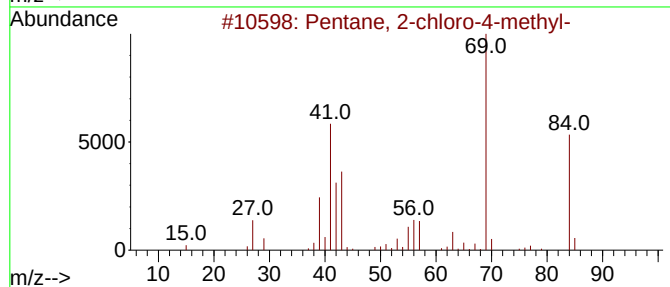
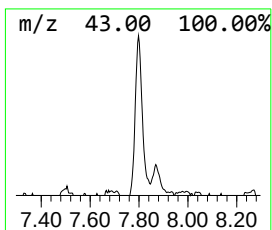
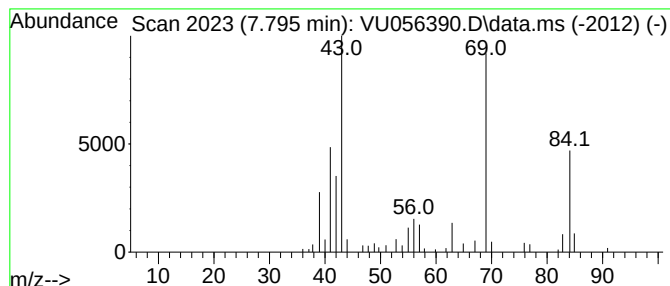
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111323WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Pentane, 2-chloro-4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.795	0.56 ug/L	74436	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-chloro-4-methyl-	120	C6H13Cl	025346-32-1	90
2			1H-Pyrazole, 4,5-dihydro-5-methyl-	84	C4H8N2	001568-20-3	64
3			1-Butene, 3,3-dimethyl-	84	C6H12	000558-37-2	58
4			Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	53
5			3-Buten-2-one, 3-methyl-	84	C5H8O	000814-78-8	53



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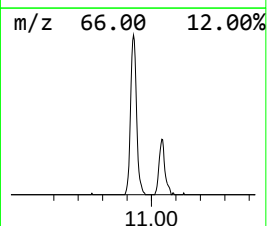
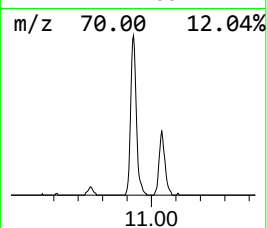
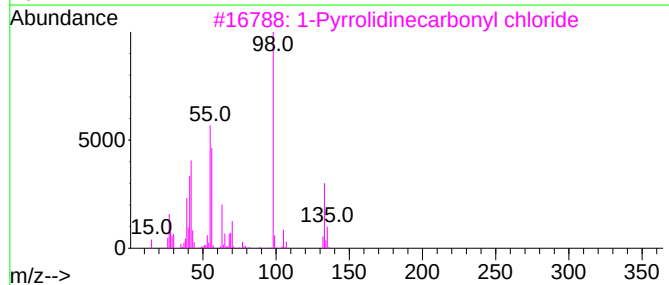
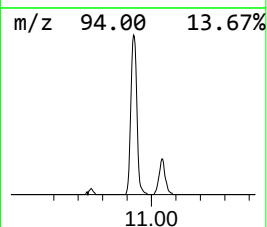
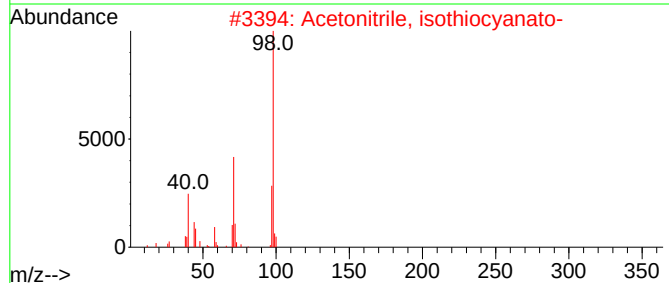
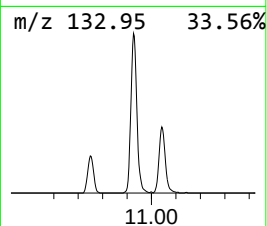
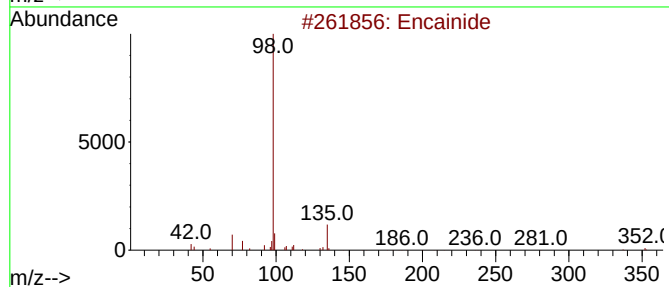
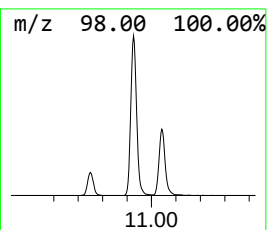
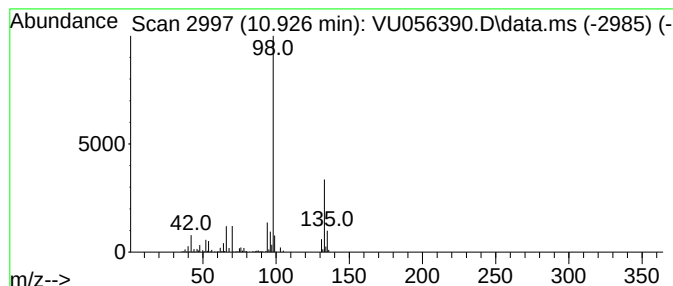
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111323WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Encainide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.926	2.51 ug/L	427134	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Encainide	352	C22H28N2O2	037612-13-8	50
2			Acetonitrile, isothiocyanato-	98	C3H2N2S	032772-75-1	37
3			1-Pyrrolidinecarbonyl chloride	133	C5H8ClNO	001192-63-8	36
4			Benzamide, 3-methyl-N-[2-(1-pipe...	246	C15H22N2O	339241-69-9	28
5			2-Benzyl-1-methylpiperidine	189	C13H19N	031414-56-9	25



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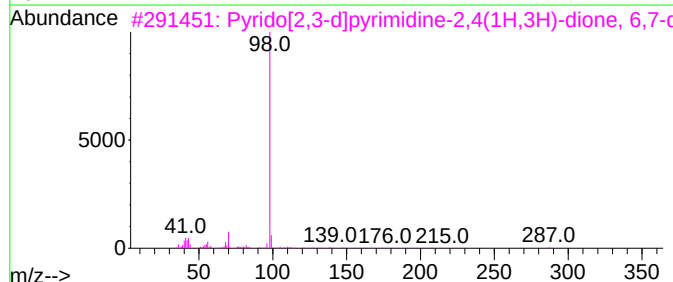
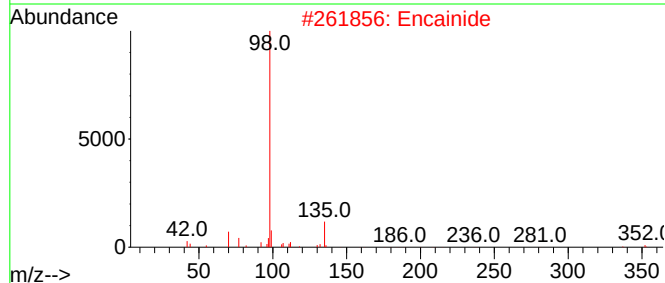
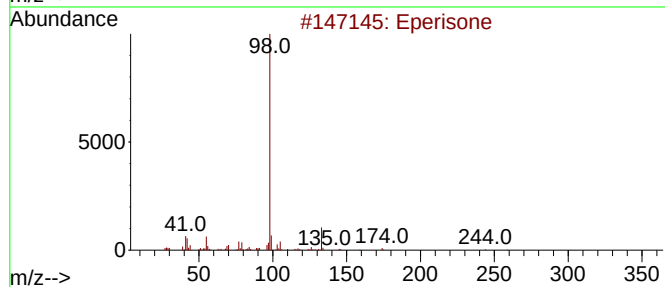
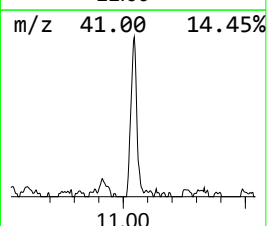
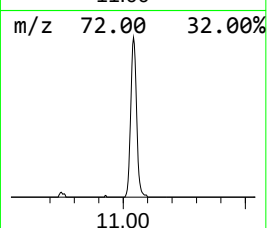
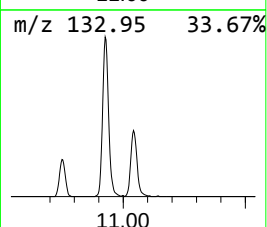
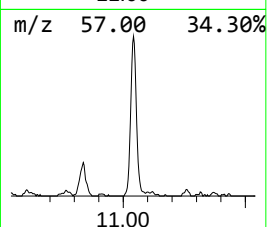
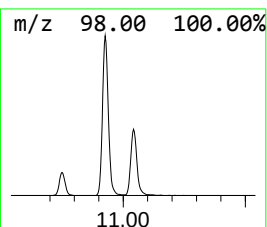
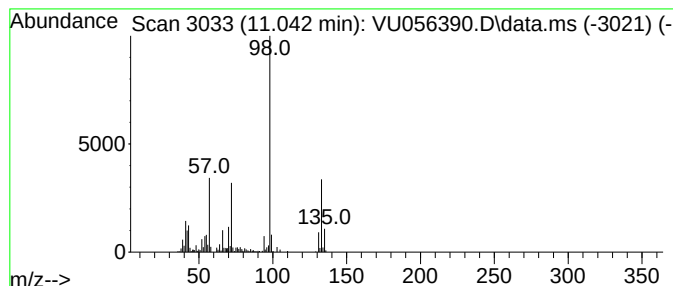
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.042	1.52 ug/L	258787	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eperisone	259	C17H25NO	064840-90-0	47
2			Encainide	352	C22H28N2O2	037612-13-8	43
3			Pyrido[2,3-d]pyrimidine-2,4(1H,3...)	385	C16H21Cl2N5O2	1000265-65-2	43
4			3H-Pyrazol-3-one, 1,2-dihydro-5-...	98	C4H6N2O	004344-87-0	43
5			.alpha.-Methyl-1-piperidineethanol	143	C8H17NO	000934-90-7	43



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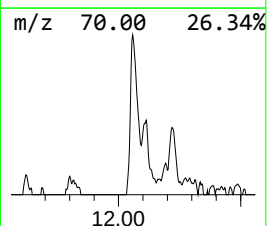
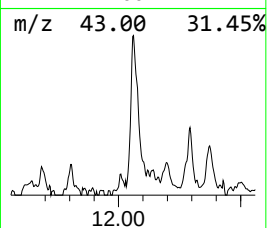
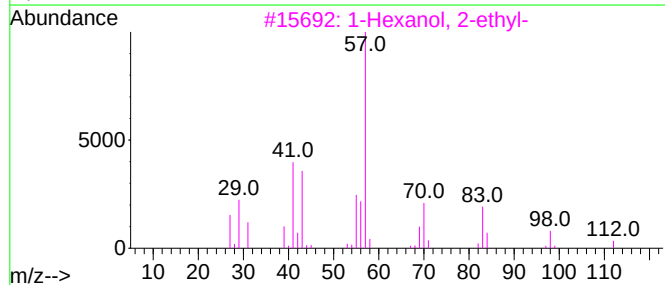
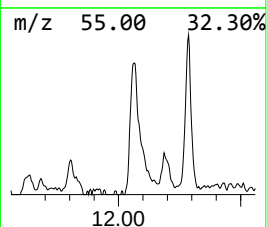
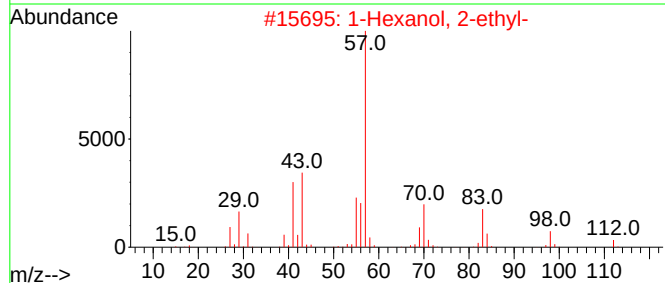
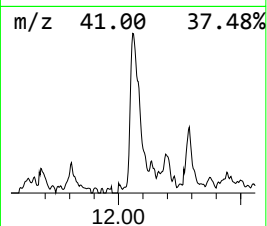
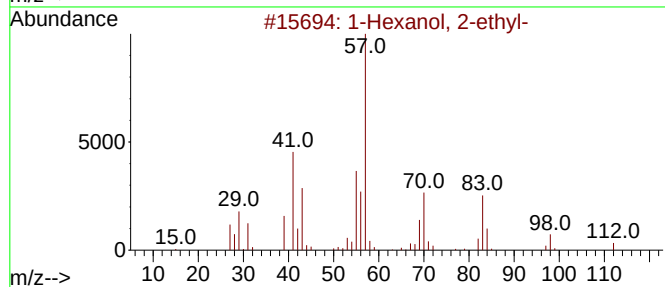
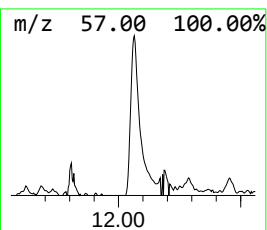
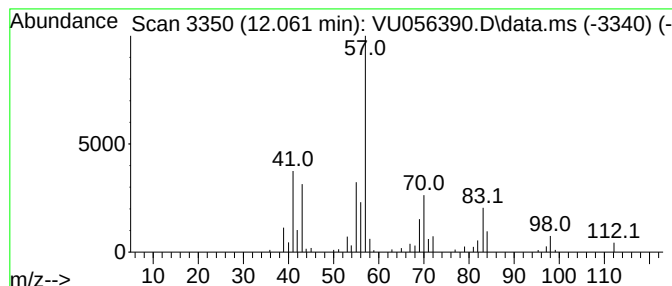
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.061	0.68 ug/L	115198	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	90
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	83
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
4	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	64
5	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	64



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ClientSampleId :
C0QK2

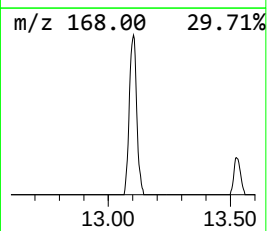
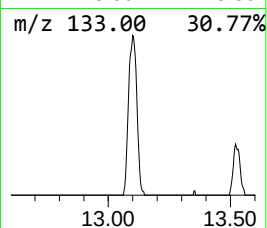
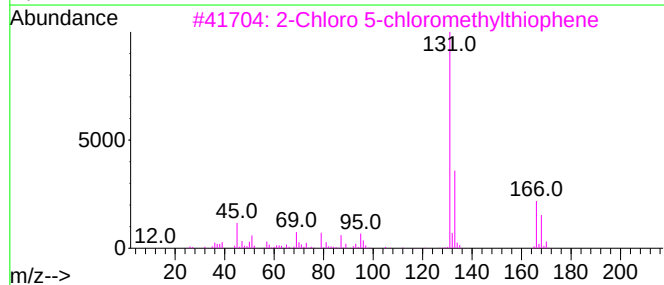
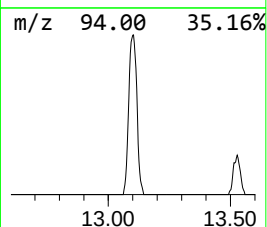
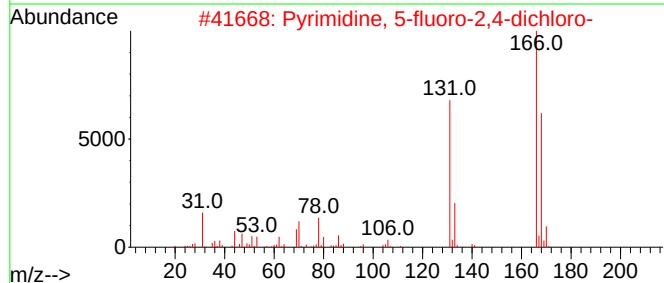
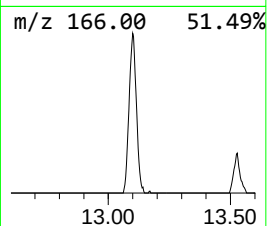
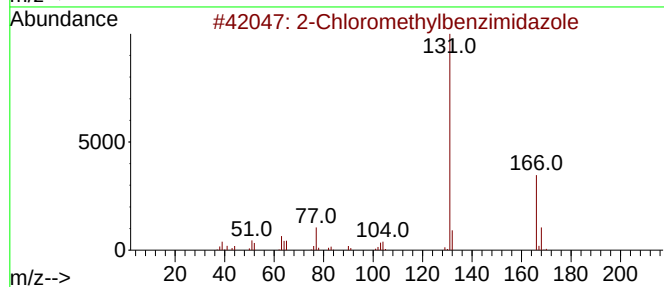
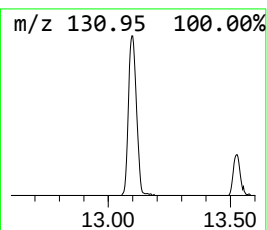
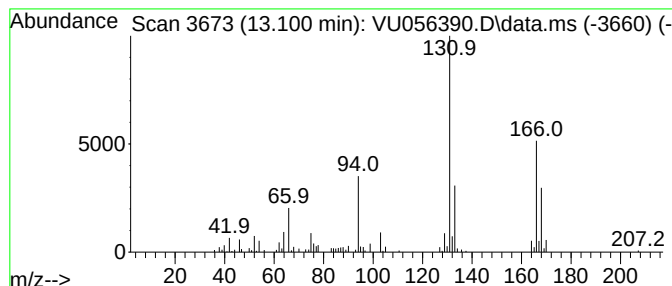
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	1.02 ug/L	172946	1,4-Dichlorobenzene-d4	11.807

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Chloromethylbenzimidazole	166	C8H7ClN2	004857-04-9	38
2		Pyrimidine, 5-fluoro-2,4-dichloro-	166	C4HC12FN2	002927-71-1	37
3		2-Chloro 5-chloromethylthiophene	166	C5H4Cl2S	023784-96-5	35
4		2-Chloromethylbenzimidazole	166	C8H7ClN2	004857-04-9	35
5		4,6-Dichloro-2-fluoropyrimidine	166	C4HC12FN2	003824-45-1	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU111523\
Data File : VU056390.D
Acq On : 16 Nov 2023 06:11
Operator : MD/SY
Sample : 05411-17
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0QK2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111323WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.464	1.6	ug/L	212215	1	6.245	670451	5.0
Pentane, 2-chlo...	7.795	0.6	ug/L	74436	1	6.245	670451	5.0
Encainide	10.926	2.5	ug/L	427134	3	11.807	851719	5.0
unknown-01	11.042	1.5	ug/L	258787	3	11.807	851719	5.0
1-Hexanol, 2-et...	12.061	0.7	ug/L	115198	3	11.807	851719	5.0
unknown-02	13.100	1.0	ug/L	172946	3	11.807	851719	5.0