

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112023\
 Data File : VU056524.D
 Acq On : 20 Nov 2023 14:01
 Operator : MD/SY
 Sample : 05411-17RE
 Misc : 25mL/MSVOA_U/WATER
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0QK2RE

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: VU056524.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	87269	131263	14.74%	1.767%
2	1.518	65	71	83	rVV	81831	103636	11.64%	1.395%
3	1.583	85	91	104	rVB2	41122	52228	5.87%	0.703%
4	1.686	117	123	131	rBV	10638	14931	1.68%	0.201%
5	1.853	170	175	185	rBV3	9827	15082	1.69%	0.203%
6	1.907	185	192	211	rVB	60443	87947	9.88%	1.184%
7	2.563	381	396	408	rVB3	20857	39428	4.43%	0.531%
8	2.631	408	417	434	rVB	5398	11405	1.28%	0.154%
9	2.724	434	446	456	rBV3	5747	12205	1.37%	0.164%
10	3.039	533	544	556	rBV3	19658	38880	4.37%	0.523%
11	4.618	1022	1035	1071	rBV	120260	320622	36.01%	4.316%
12	4.955	1127	1140	1152	rBV7	6275	15506	1.74%	0.209%
13	5.058	1156	1172	1197	rBV2	157143	388744	43.66%	5.233%
14	5.521	1305	1316	1328	rVB5	4871	11928	1.34%	0.161%
15	5.721	1357	1378	1406	rBV2	247124	677428	76.08%	9.119%
16	6.245	1527	1541	1564	rBV	338086	663053	74.47%	8.925%
17	6.685	1663	1678	1700	rBV	184885	363714	40.85%	4.896%
18	6.888	1731	1741	1755	rBV5	6004	12571	1.41%	0.169%
19	7.100	1795	1807	1821	rBV4	17889	35606	4.00%	0.479%
20	7.560	1938	1950	1964	rBV4	19050	36834	4.14%	0.496%
21	7.795	2011	2023	2035	rBV3	27199	50660	5.69%	0.682%
22	7.901	2042	2056	2071	rVB5	8925	18381	2.06%	0.247%
23	8.180	2133	2143	2155	rBV3	15614	28726	3.23%	0.387%
24	8.627	2271	2282	2321	rBV	466057	885284	99.42%	11.917%
25	8.795	2323	2334	2353	rVB8	17966	46405	5.21%	0.625%
26	9.004	2392	2399	2407	rVB7	7386	11292	1.27%	0.152%
27	9.412	2512	2526	2542	rBV	508536	890422	100.00%	11.986%
28	9.486	2542	2549	2560	rVB	19909	37380	4.20%	0.503%
29	10.344	2805	2816	2830	rBV5	13823	25245	2.84%	0.340%
30	10.749	2931	2942	2960	rBV	149299	243275	27.32%	3.275%
31	10.885	2975	2984	2987	rVV3	14751	18517	2.08%	0.249%
32	10.926	2987	2997	3013	rVB2	196622	337233	37.87%	4.539%
33	11.042	3021	3033	3053	rBV	113978	190214	21.36%	2.560%
34	11.688	3224	3234	3245	rBV8	7790	12311	1.38%	0.166%
35	11.807	3259	3271	3294	rBV	500343	819448	92.03%	11.030%
36	12.058	3339	3349	3361	rBV2	50574	107938	12.12%	1.453%

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C0QK2RE

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

37	12.187	3377	3389	3411	rVV	345182	608115	68.30%	8.186%
38	12.286	3413	3420	3431	rVB4	21912	33310	3.74%	0.448%
39	12.884	3597	3606	3615	rBV7	10287	15824	1.78%	0.213%
40	13.357	3743	3753	3767	rBV4	9562	15940	1.79%	0.215%

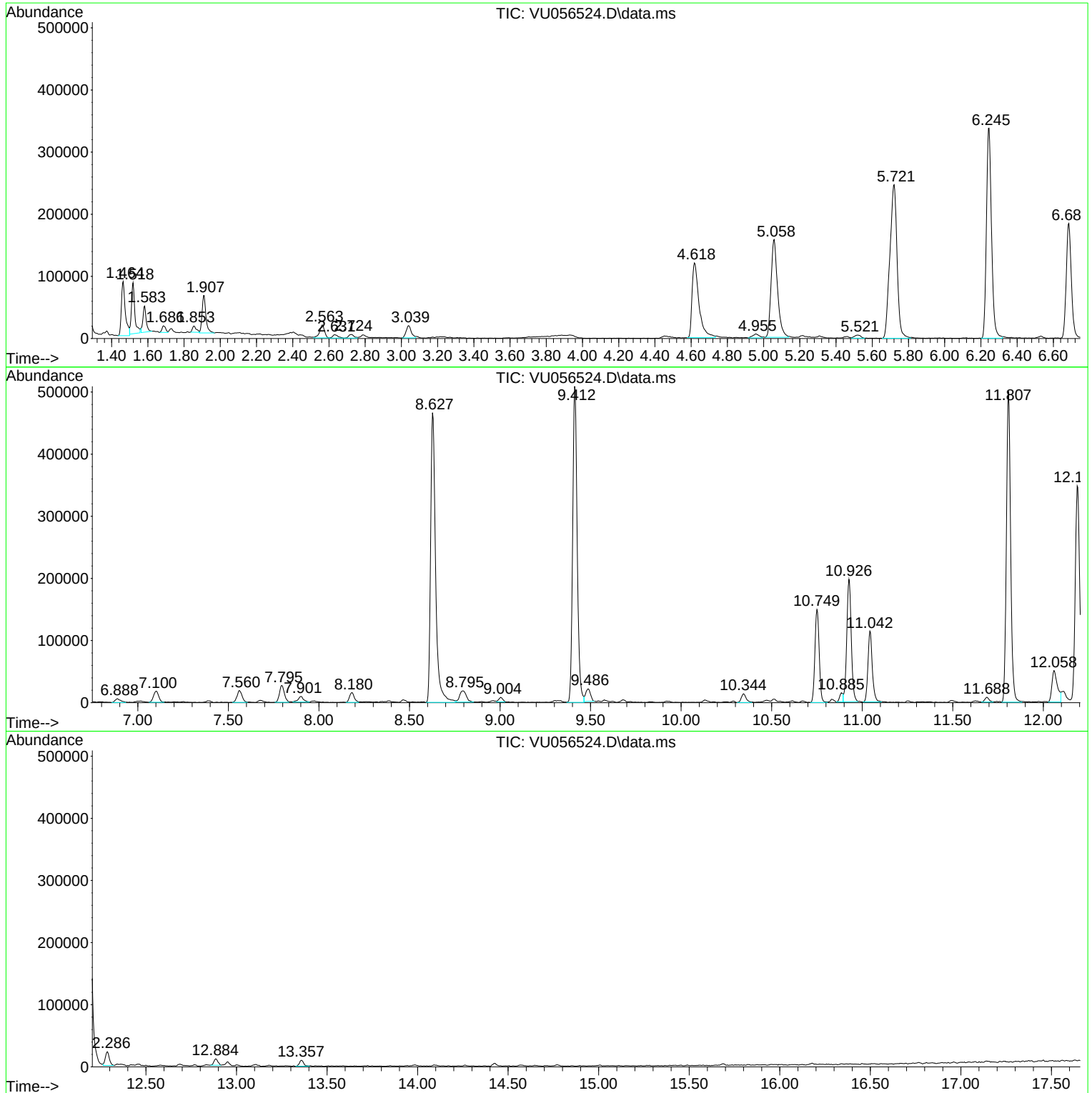
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111323WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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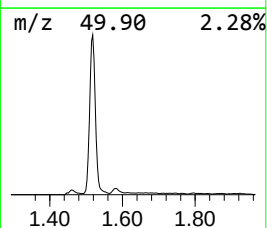
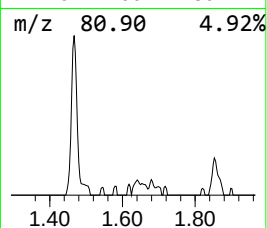
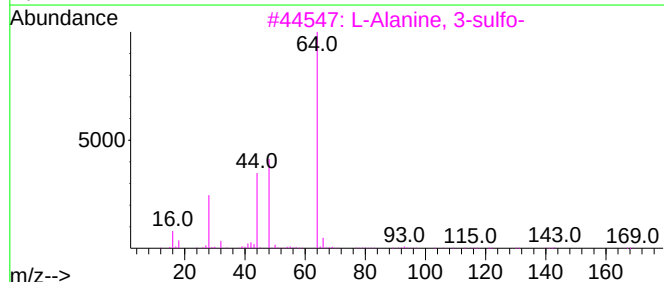
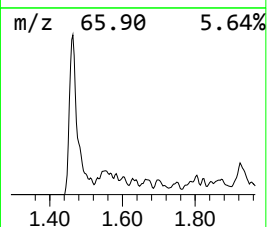
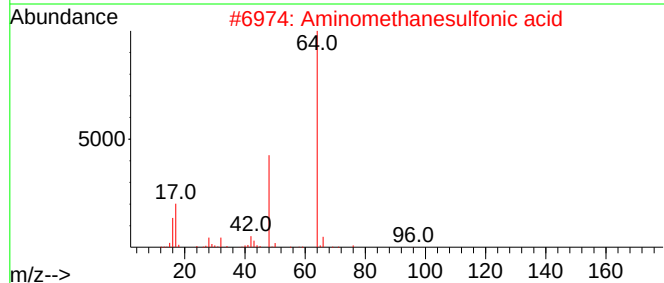
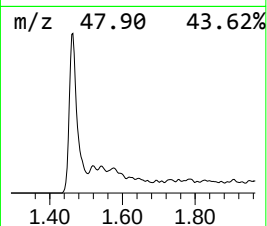
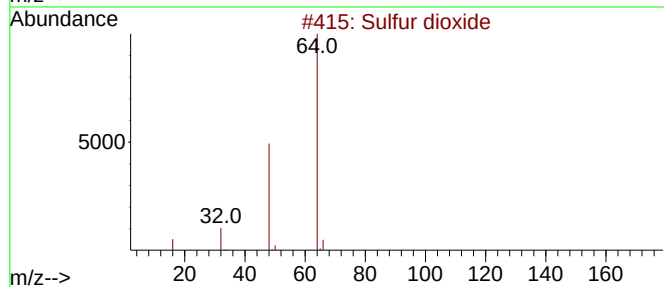
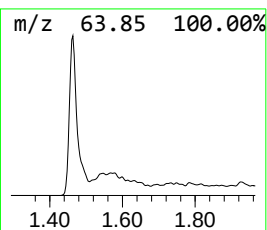
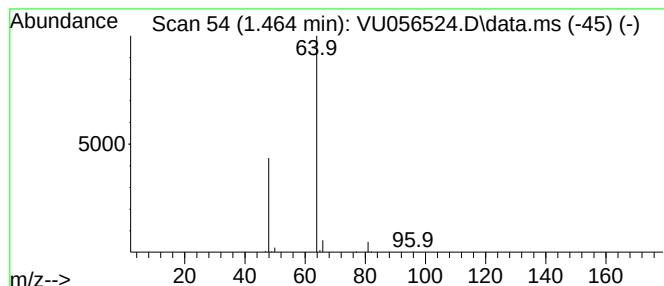
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.464	0.99 ug/L	131263	1,4-Difluorobenzene	6.242

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	64
4			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	64
5			(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	9



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Misc : 25mL/MSVOA_U/WATER
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Instrument :
MSVOA_U
ClientSampleId :
C0QK2RE

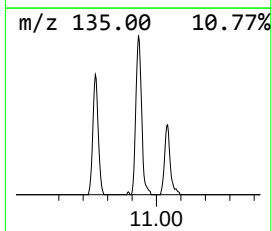
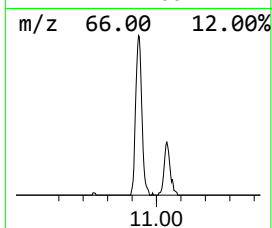
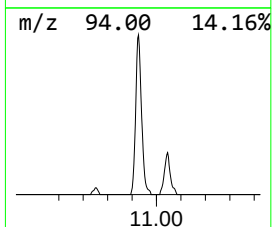
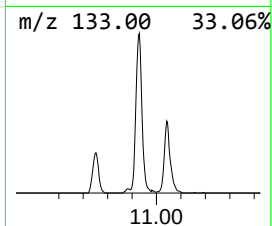
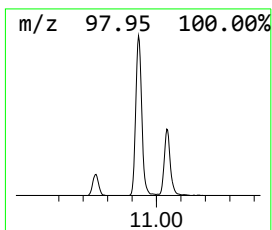
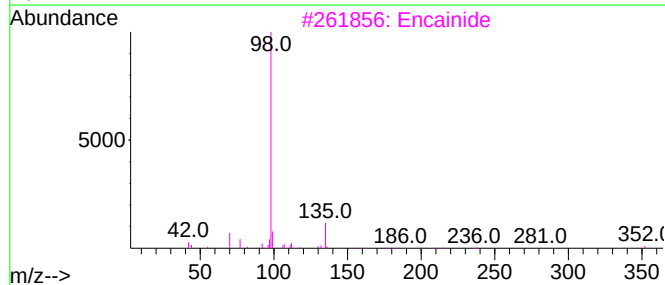
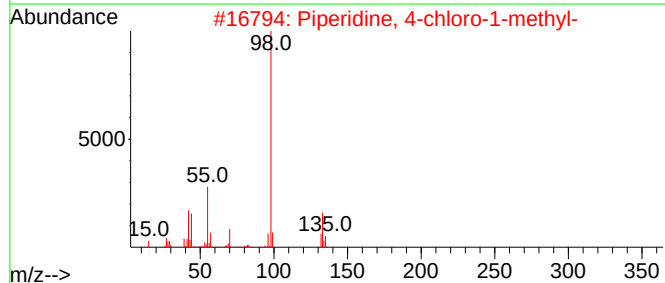
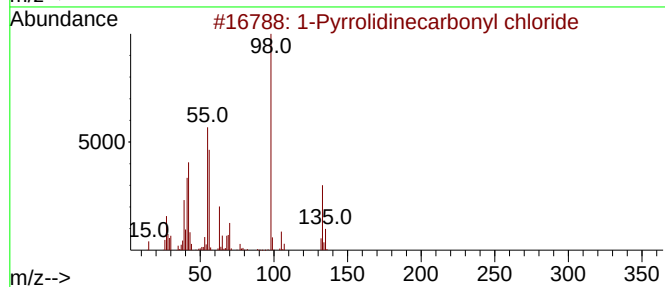
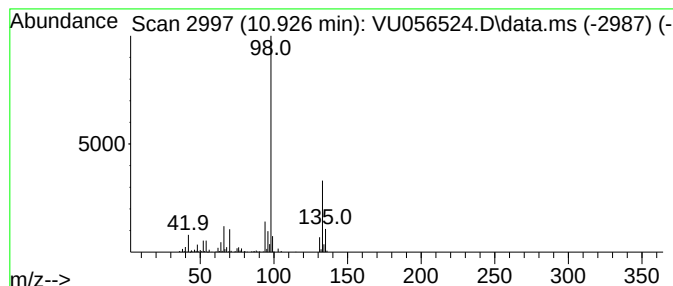
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111323WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 1-Pyrrolidinecarbonyl chloride Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.926	2.06 ug/L	337233	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pyrrolidinecarbonyl chloride	133	C5H8ClNO	001192-63-8	59
2			Piperidine, 4-chloro-1-methyl-	133	C6H12ClN	005570-77-4	45
3			Encainide	352	C22H28N2O2	037612-13-8	38
4			N-[(1-Ethyl-2-pyrrolidinyl)methy...	308	C17H29FN2Si	1000505-26-5	37
5			Acetonitrile, isothiocyanato-	98	C3H2N2S	032772-75-1	37



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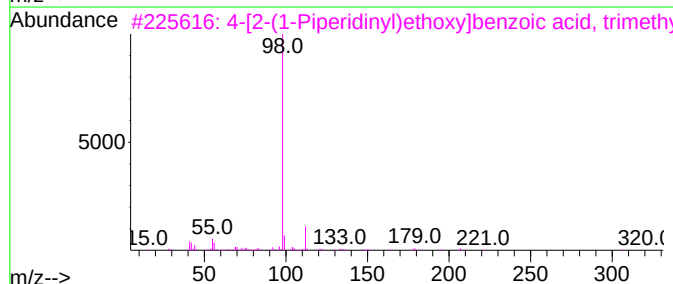
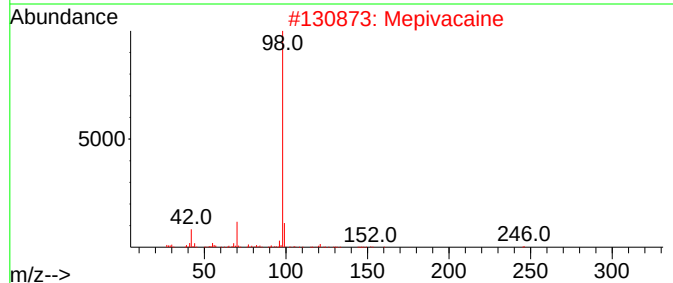
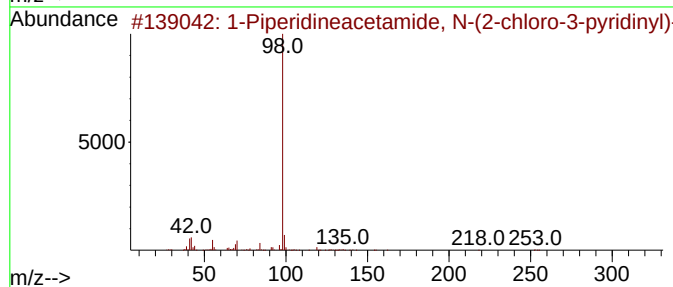
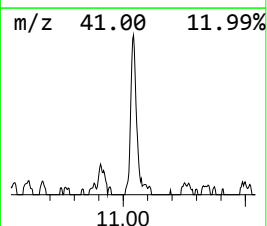
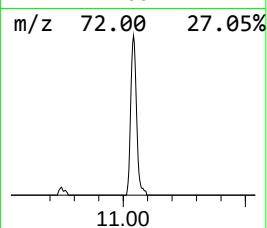
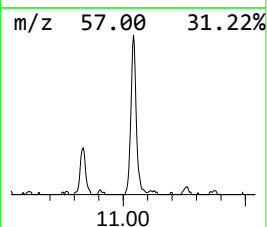
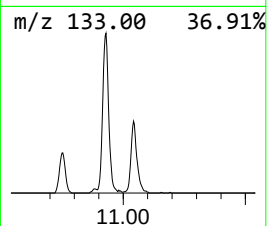
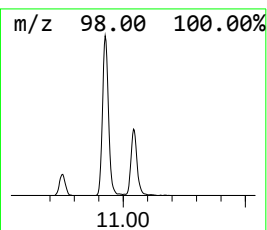
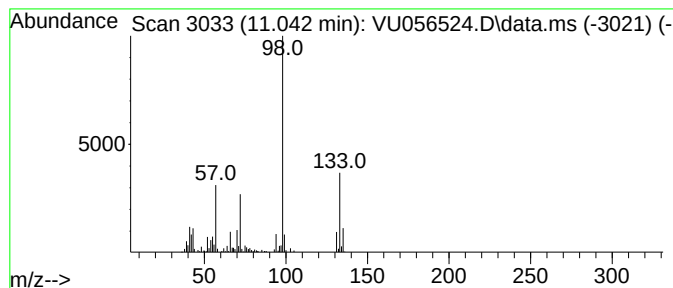
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111323WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.042	1.16 ug/L	190214	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Piperidineacetamide, N-(2-chlo...	253	C12H16ClN3O	329063-22-1	38
2			Mepivacaine	246	C15H22N2O	000096-88-8	38
3			4-[2-(1-Piperidinyl)ethoxy]benzo...	321	C17H27NO3Si	1000471-41-6	38
4			N-(1-Cyclopropyl-ethyl)-N-phenyl...	286	C18H26N2O	1000295-95-4	38
5			N-(4-Iodo-2-methyl-phenyl)-2-pip...	358	C14H19IN2O	247592-56-9	38



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ClientSampleId :
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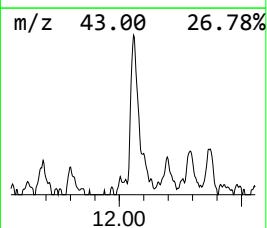
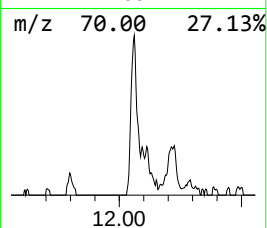
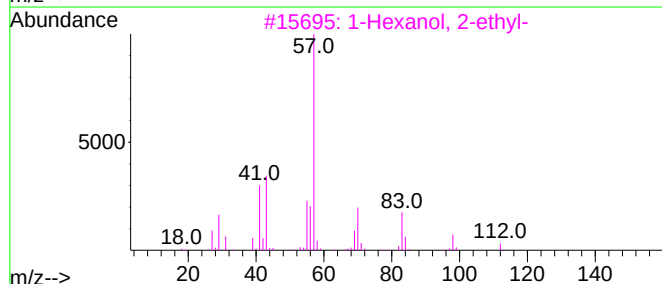
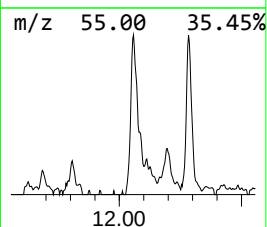
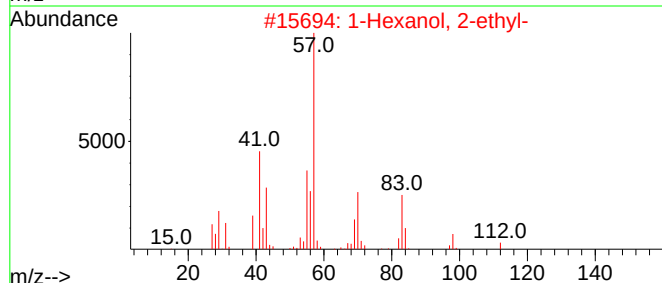
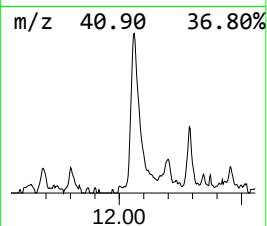
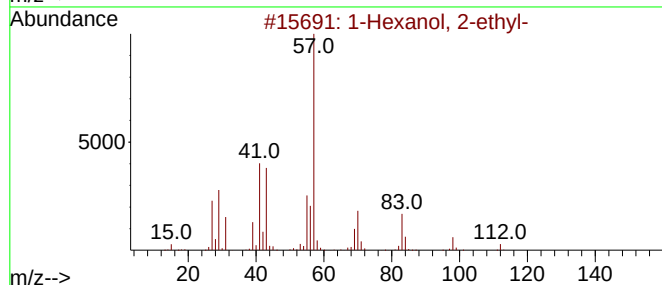
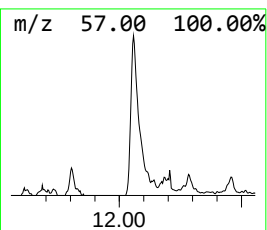
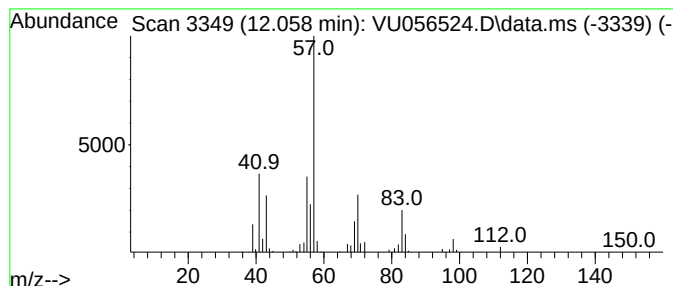
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.058	0.66 ug/L	107938	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	83
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	83
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	83
4	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
5	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72



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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	1.464	1.0	ug/L	131263	1	6.242	663053	5.0
1-Pyrrolidineca...	10.926	2.1	ug/L	337233	3	11.807	819448	5.0
unknown-01	11.042	1.2	ug/L	190214	3	11.807	819448	5.0
1-Hexanol, 2-et...	12.058	0.7	ug/L	107938	3	11.807	819448	5.0