

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071824\
 Data File : VU060067.D
 Acq On : 19 Jul 2024 17:54
 Operator : MD/SY
 Sample : P3298-21
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHAY8

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\SFAMUTR071824WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU060067.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	14	26	38	rBV4	3151	6572	1.36%	0.130%
2	1.596	83	95	106	rBV	45659	61206	12.67%	1.214%
3	1.686	114	123	152	rBV	284740	441640	91.45%	8.761%
4	1.911	184	193	208	rVB	39586	54168	11.22%	1.075%
5	2.560	381	395	407	rBV2	68131	118606	24.56%	2.353%
6	2.637	407	419	458	rVV	138046	408855	84.66%	8.111%
7	3.197	574	593	598	rBV3	7222	20141	4.17%	0.400%
8	4.435	954	978	1011	rBV5	55577	167327	34.65%	3.319%
9	4.628	1024	1038	1059	rBV2	66672	210152	43.51%	4.169%
10	4.817	1089	1097	1113	rVB3	5613	14394	2.98%	0.286%
11	5.055	1156	1171	1196	rBV	89702	208340	43.14%	4.133%
12	5.718	1358	1377	1402	rBV2	146247	388991	80.55%	7.717%
13	6.242	1528	1540	1561	rBV	140835	279165	57.80%	5.538%
14	6.685	1662	1678	1698	rBV2	92028	191388	39.63%	3.797%
15	6.779	1698	1707	1722	rVB3	8073	18859	3.91%	0.374%
16	6.878	1730	1738	1750	rBV3	14571	27607	5.72%	0.548%
17	7.119	1801	1813	1821	rBV3	15187	30715	6.36%	0.609%
18	7.560	1935	1950	1967	rBV2	43906	78357	16.22%	1.554%
19	7.894	2041	2054	2071	rBV	169117	297346	61.57%	5.899%
20	8.174	2132	2141	2156	rBV2	26212	45917	9.51%	0.911%
21	8.467	2222	2232	2245	rVB2	7683	17182	3.56%	0.341%
22	8.550	2246	2258	2272	rVB2	35925	61214	12.68%	1.214%
23	8.627	2272	2282	2321	rBV	228203	482943	100.00%	9.581%
24	8.782	2321	2330	2349	rVB3	36623	65129	13.49%	1.292%
25	9.412	2512	2526	2554	rBV	207714	352710	73.03%	6.997%
26	9.643	2591	2598	2607	rBV4	4365	7221	1.50%	0.143%
27	10.132	2744	2750	2763	rVB3	4294	7084	1.47%	0.141%
28	10.232	2770	2781	2802	rBV	51005	89997	18.64%	1.785%
29	10.341	2808	2815	2825	rVB5	3914	7032	1.46%	0.140%
30	10.750	2930	2942	2958	rBV	89350	143699	29.75%	2.851%
31	10.888	2969	2985	2996	rVB3	18900	36588	7.58%	0.726%
32	11.685	3223	3233	3249	rVB4	5863	10230	2.12%	0.203%
33	11.807	3260	3271	3288	rBV	205849	334032	69.17%	6.627%
34	12.068	3341	3352	3364	rBV8	7236	18142	3.76%	0.360%
35	12.187	3378	3389	3411	rBV	176381	295323	61.15%	5.859%
36	12.772	3560	3571	3582	rBV5	7340	12474	2.58%	0.247%

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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\SFAMUTR071824WMA.M
Title : TRACE VOA SFAM1.0

37	12.885	3596	3606	3621	rBV7	11933	20597	4.26%	0.409%
38	14.569	4118	4130	4140	rBV	5889	9428	1.95%	0.187%

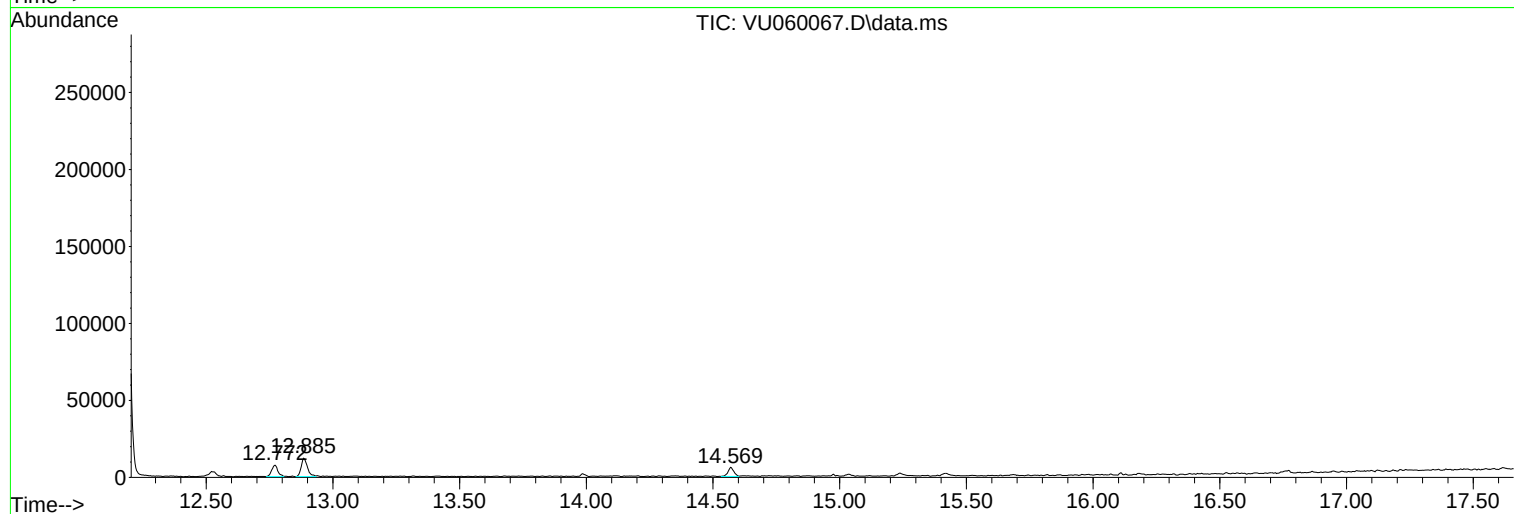
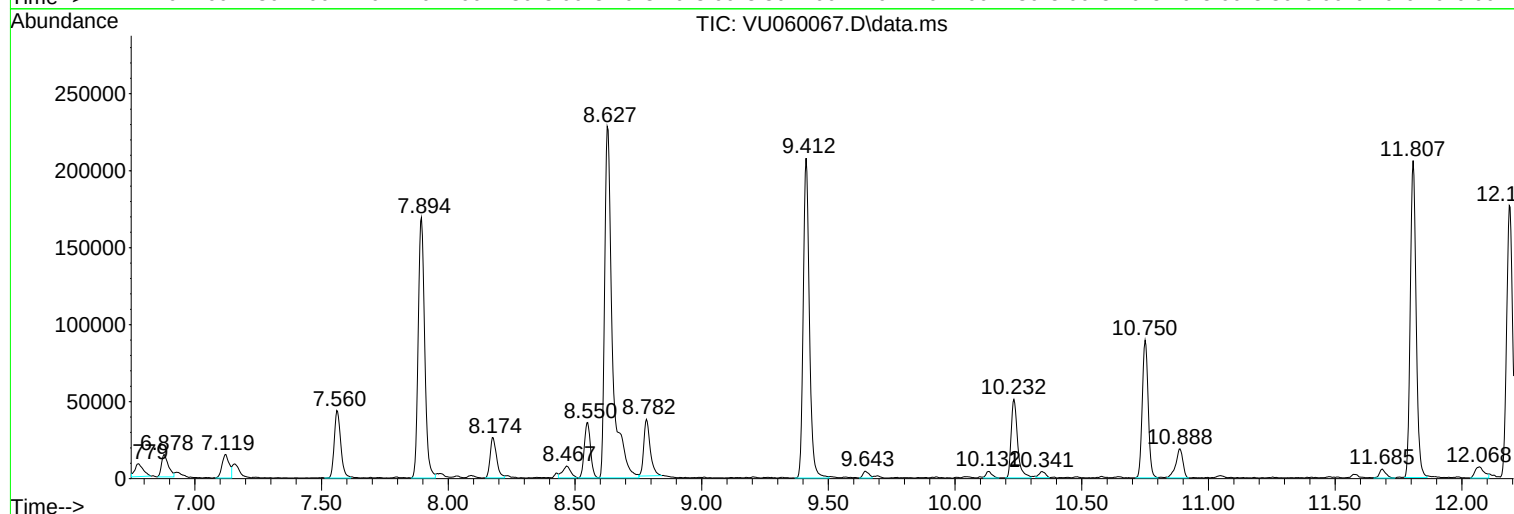
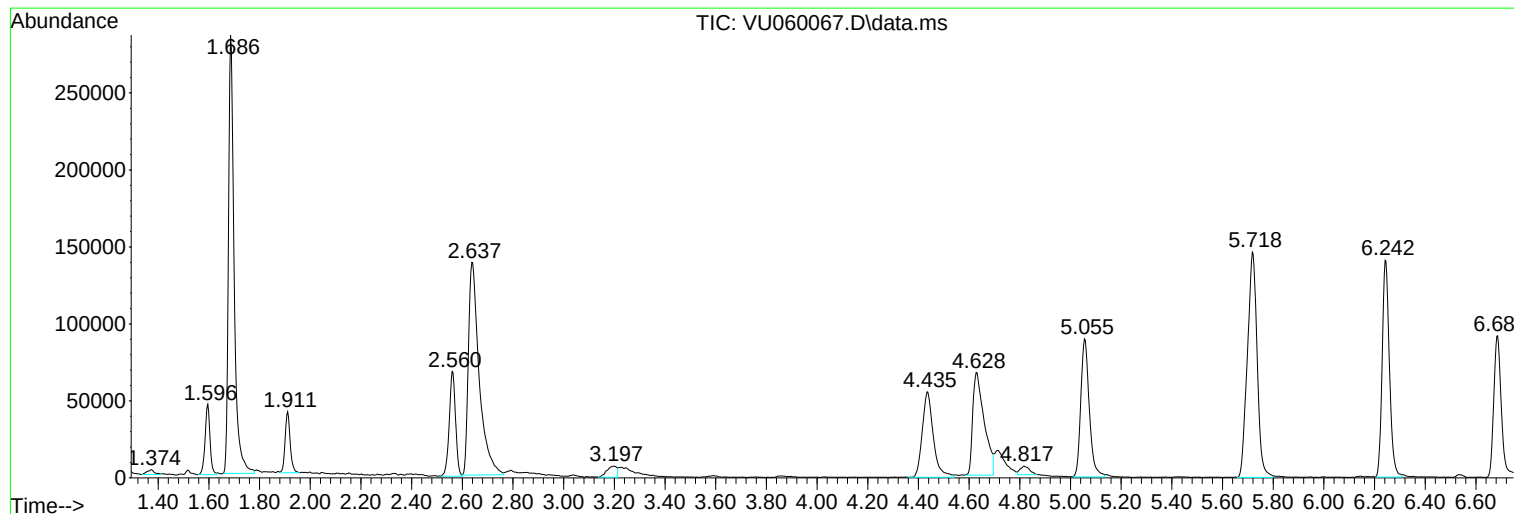
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR071824WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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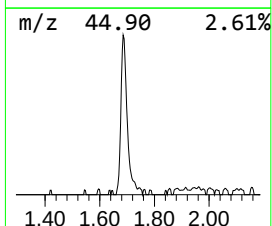
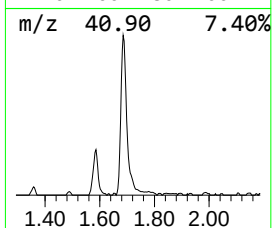
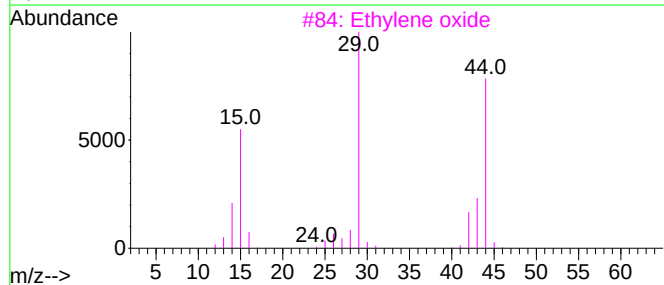
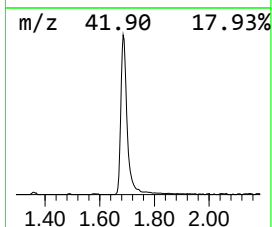
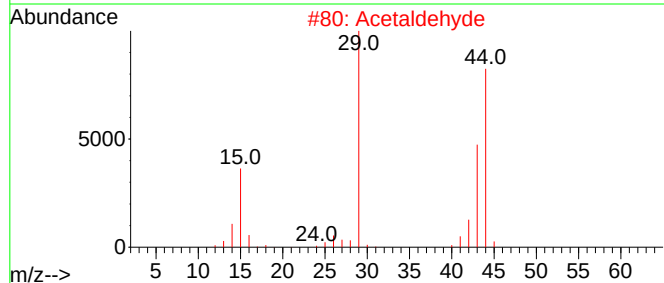
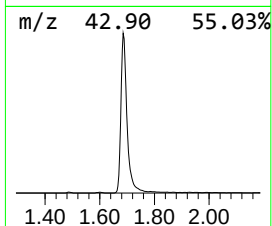
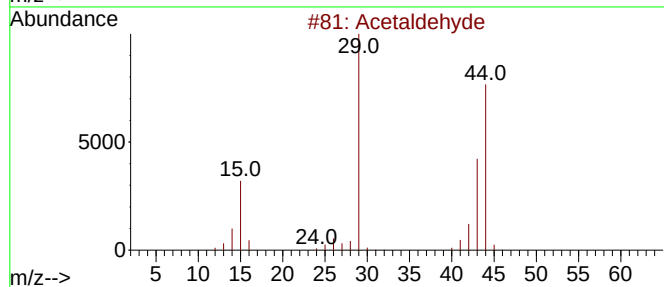
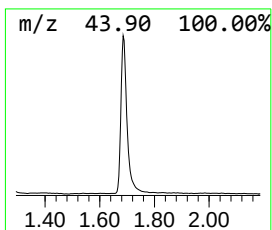
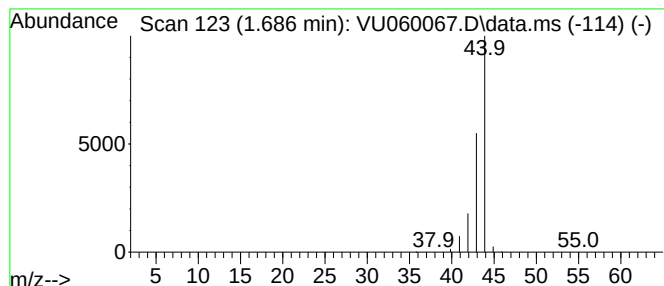
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.686	7.91 ug/L	441640	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	74
2			Acetaldehyde	44	C2H4O	000075-07-0	74
3			Ethylene oxide	44	C2H4O	000075-21-8	5
4			Ethylene oxide	44	C2H4O	000075-21-8	5
5			Ethylene oxide	44	C2H4O	000075-21-8	5



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Instrument :
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ClientSampleId :
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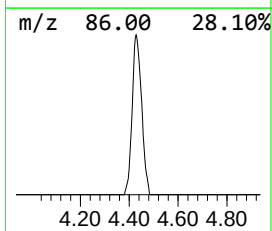
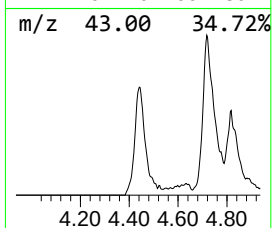
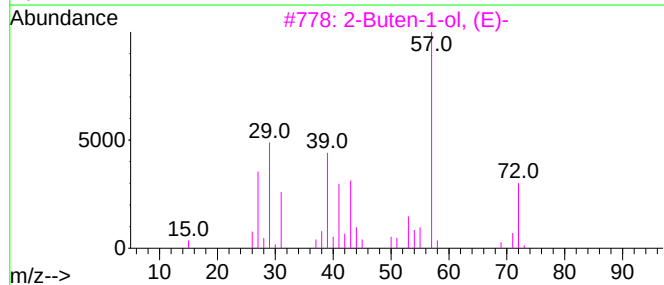
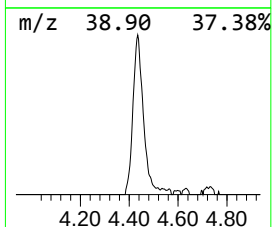
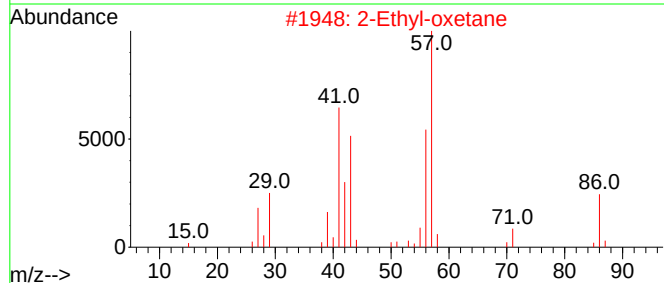
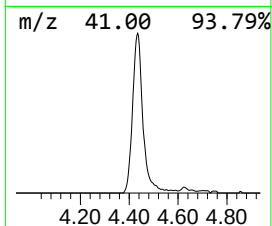
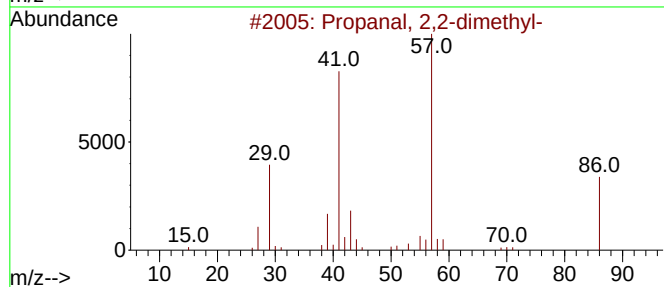
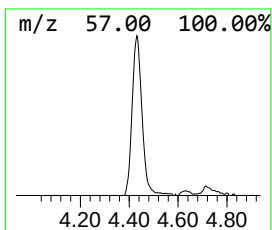
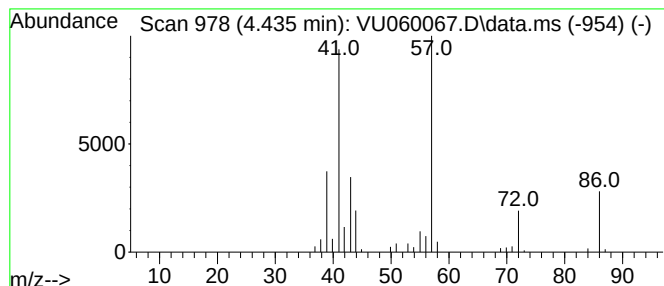
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR071824WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.435	3.00 ug/L	167327	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	49
2			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	35
3			2-Buten-1-ol, (E)-	72	C4H8O	000504-61-0	30
4			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	27
5			Propane, 1-bromo-2-methyl-	136	C4H9Br	000078-77-3	25



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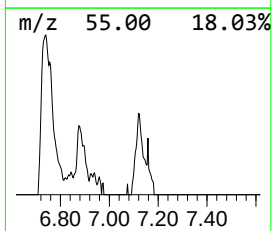
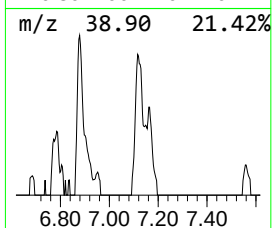
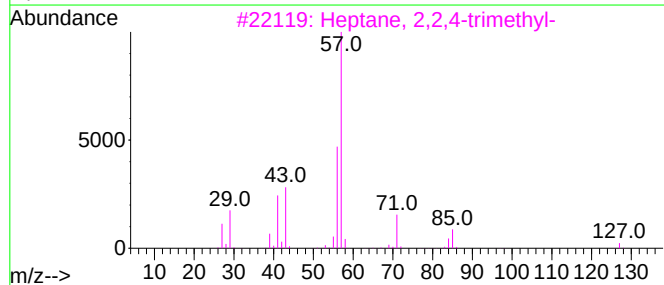
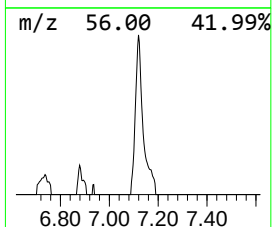
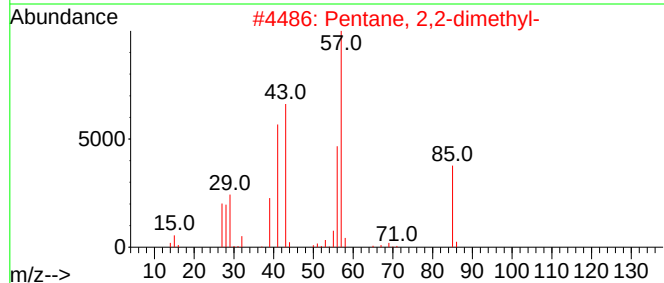
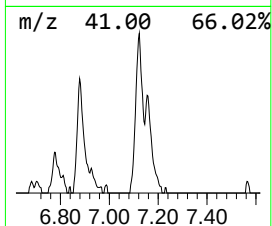
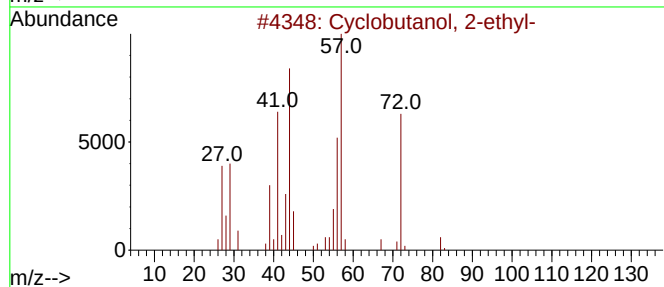
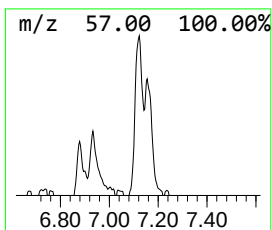
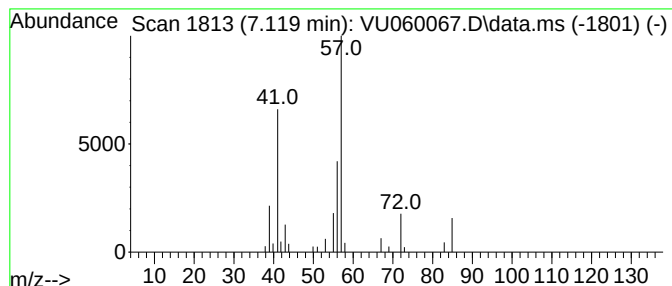
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR071824WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 unknown-02 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.119	0.55 ug/L	30715	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclobutanol, 2-ethyl-	100	C6H12O	035301-43-0	42
2			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	42
3			Heptane, 2,2,4-trimethyl-	142	C10H22	014720-74-2	36
4			2-Butene, (Z)-	56	C4H8	000590-18-1	35
5			Cyclobutane	56	C4H8	000287-23-0	35



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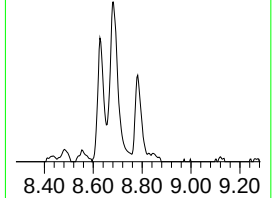
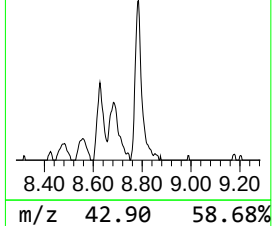
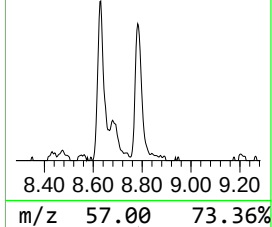
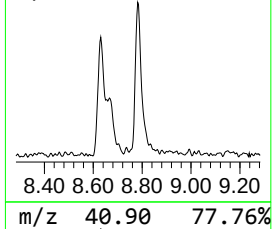
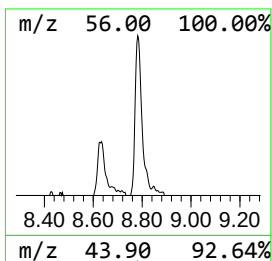
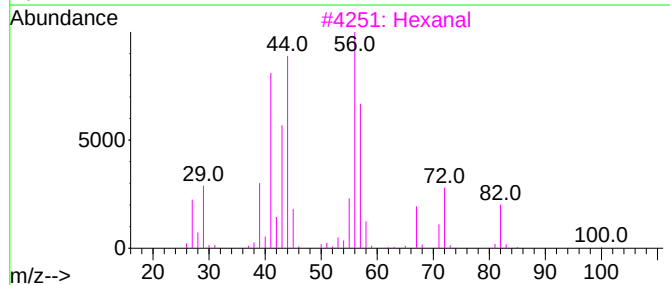
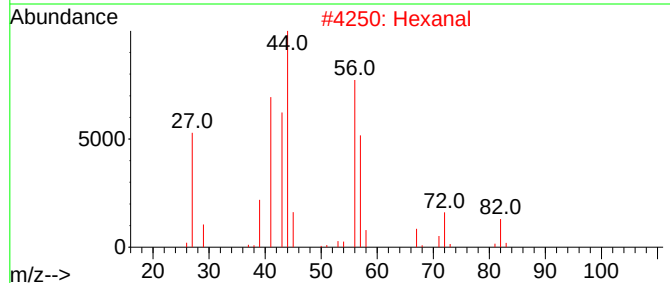
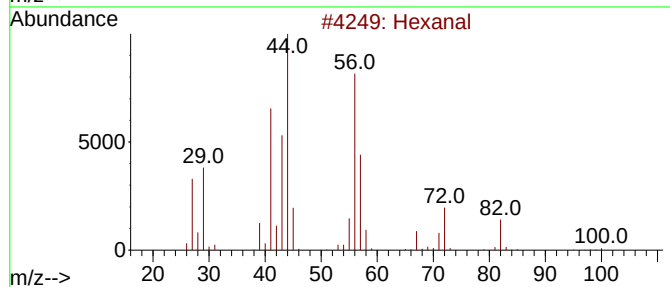
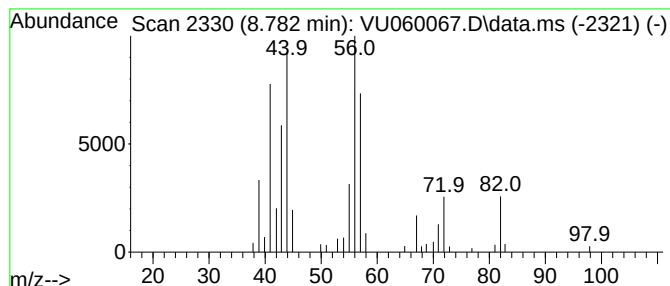
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR071824WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Hexanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.782	0.92 ug/L	65129	Chlorobenzene-d5	9.412

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	78
2	Hexanal			100	C6H12O	000066-25-1	78
3	Hexanal			100	C6H12O	000066-25-1	72
4	Hexanal			100	C6H12O	000066-25-1	64
5	Hexanal			100	C6H12O	000066-25-1	64



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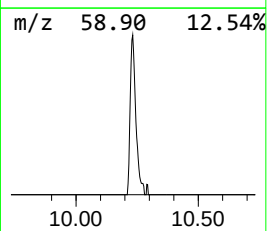
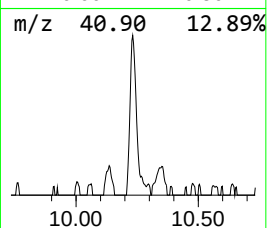
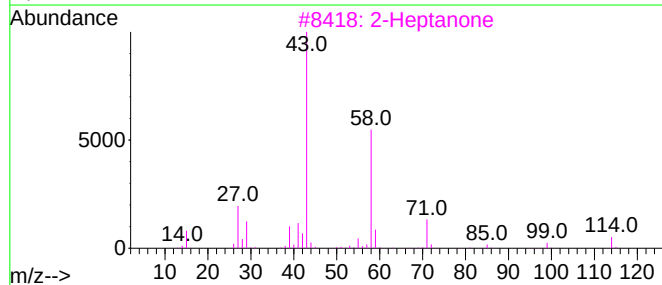
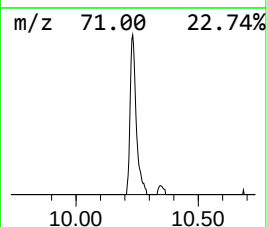
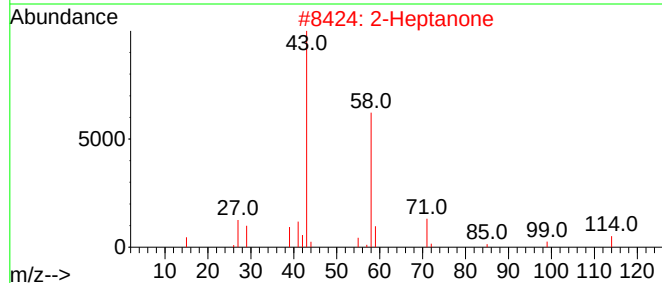
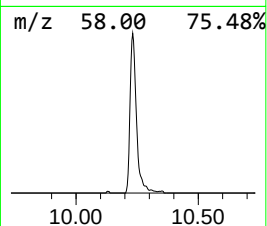
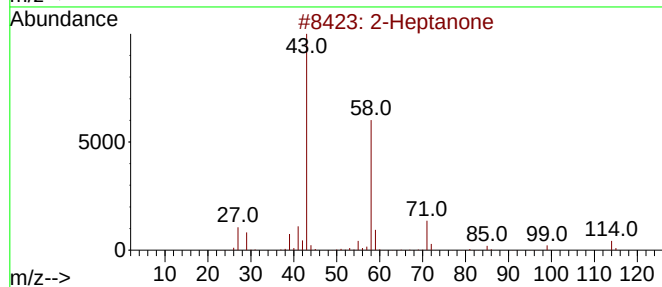
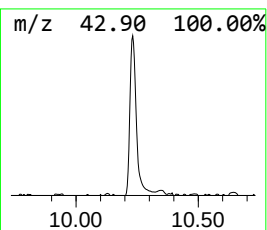
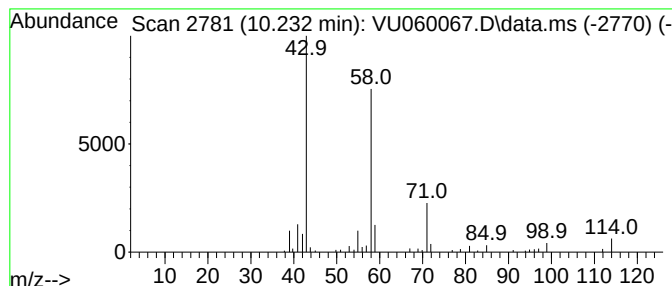
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR071824WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 2-Heptanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.232	1.28 ug/L	89997	Chlorobenzene-d5	9.412

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptanone	114	C7H14O	000110-43-0	91
2			2-Heptanone	114	C7H14O	000110-43-0	91
3			2-Heptanone	114	C7H14O	000110-43-0	91
4			2-Heptanone	114	C7H14O	000110-43-0	80
5			2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071824\
Data File : VU060067.D
Acq On : 19 Jul 2024 17:54
Operator : MD/SY
Sample : P3298-21
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHAY8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR071824WMA.M
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
Acetaldehyde	1.686	7.9	ug/L	441640	1	6.242	279165	5.0
unknown-01	4.435	3.0	ug/L	167327	1	6.242	279165	5.0
unknown-02	7.119	0.6	ug/L	30715	1	6.242	279165	5.0
Hexanal	8.782	0.9	ug/L	65129	2	9.412	352710	5.0
2-Heptanone	10.232	1.3	ug/L	89997	2	9.412	352710	5.0