

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062524\
 Data File : VU059519.D
 Acq On : 26 Jun 2024 11:58
 Operator : MD/SY
 Sample : P2987-10
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 69 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0T97

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\SFAMUTR061724WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU059519.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.354	11	20	27	rBV3	5181	7495	1.51%	0.161%
2	1.596	85	95	111	rBV2	55894	75512	15.26%	1.622%
3	1.682	113	122	136	rBV	123146	162693	32.88%	3.494%
4	1.908	183	192	209	rVB	49785	69231	13.99%	1.487%
5	2.329	311	323	333	rBV4	6318	12456	2.52%	0.268%
6	2.560	379	395	406	rBV	92625	153768	31.08%	3.303%
7	2.625	406	415	451	rVB	92262	187403	37.87%	4.025%
8	3.039	535	544	557	rBV4	3263	6193	1.25%	0.133%
9	3.187	578	590	607	rBV3	7652	20401	4.12%	0.438%
10	4.435	959	978	996	rBV6	20073	60207	12.17%	1.293%
11	4.618	1023	1035	1057	rBV	67720	181060	36.59%	3.889%
12	5.055	1154	1171	1193	rBV	93069	208753	42.19%	4.484%
13	5.718	1359	1377	1405	rBV2	180916	475004	96.00%	10.202%
14	6.242	1523	1540	1565	rBV	156727	314519	63.56%	6.755%
15	6.682	1663	1677	1698	rBV	112081	222293	44.93%	4.774%
16	6.779	1698	1707	1721	rVB5	4593	10354	2.09%	0.222%
17	6.882	1731	1739	1749	rBV4	6678	12807	2.59%	0.275%
18	7.120	1802	1813	1820	rBV6	4433	9080	1.84%	0.195%
19	7.158	1820	1825	1835	rVB3	3644	6048	1.22%	0.130%
20	7.560	1938	1950	1972	rBV2	47286	83619	16.90%	1.796%
21	7.891	2040	2053	2071	rBV	213483	373864	75.56%	8.030%
22	8.174	2127	2141	2155	rBV	29406	51644	10.44%	1.109%
23	8.554	2247	2259	2270	rBV8	3144	5198	1.05%	0.112%
24	8.627	2270	2282	2322	rVV	237630	494805	100.00%	10.627%
25	8.785	2322	2331	2347	rVB2	17774	31294	6.32%	0.672%
26	9.412	2514	2526	2560	rBV	238182	406471	82.15%	8.730%
27	9.644	2590	2598	2608	rBV2	8047	13457	2.72%	0.289%
28	10.132	2743	2750	2762	rVB3	4765	7794	1.58%	0.167%
29	10.232	2771	2781	2799	rBV2	38513	66591	13.46%	1.430%
30	10.344	2806	2816	2829	rVB7	4313	6992	1.41%	0.150%
31	10.750	2929	2942	2957	rBV	96404	157561	31.84%	3.384%
32	10.859	2967	2976	2982	rBV3	11637	17954	3.63%	0.386%
33	11.576	3187	3199	3206	rBV5	4011	6958	1.41%	0.149%
34	11.807	3258	3271	3289	rBV	230135	370601	74.90%	7.960%
35	12.068	3342	3352	3361	rBV8	6162	14348	2.90%	0.308%
36	12.187	3378	3389	3405	rBV	207804	342645	69.25%	7.359%

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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\SFAMUTR061724WMA.M
Title : TRACE VOA SFAM1.0

37	12.888	3598	3607	3618	rBV4	5511	8952	1.81%	0.192%
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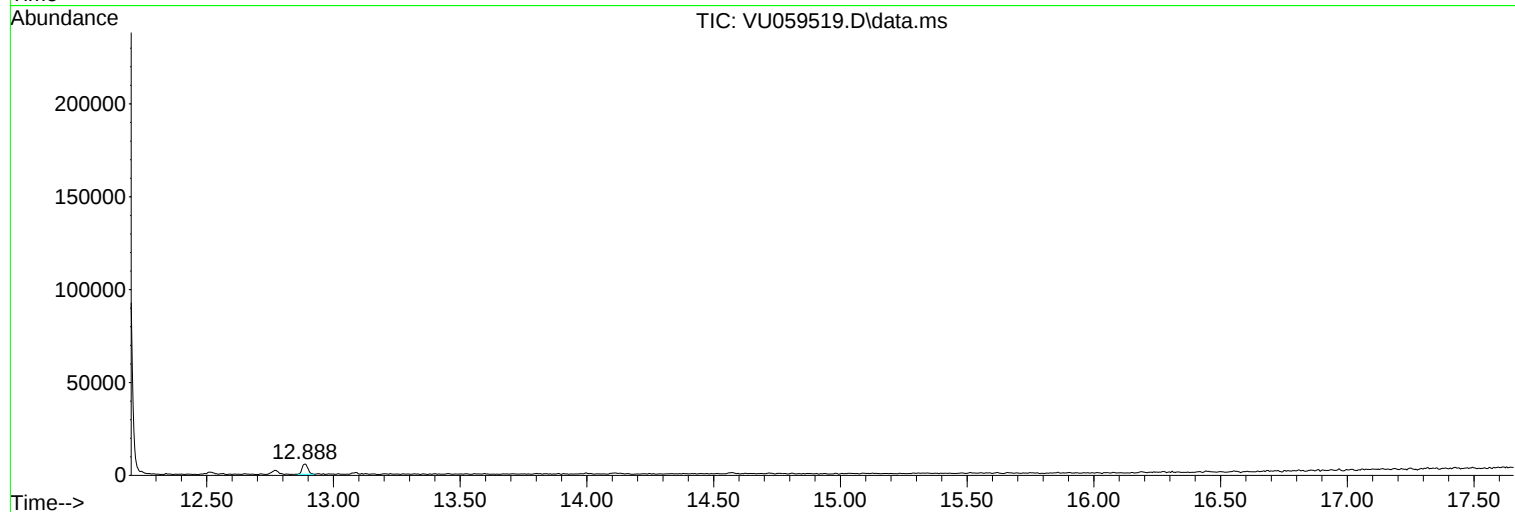
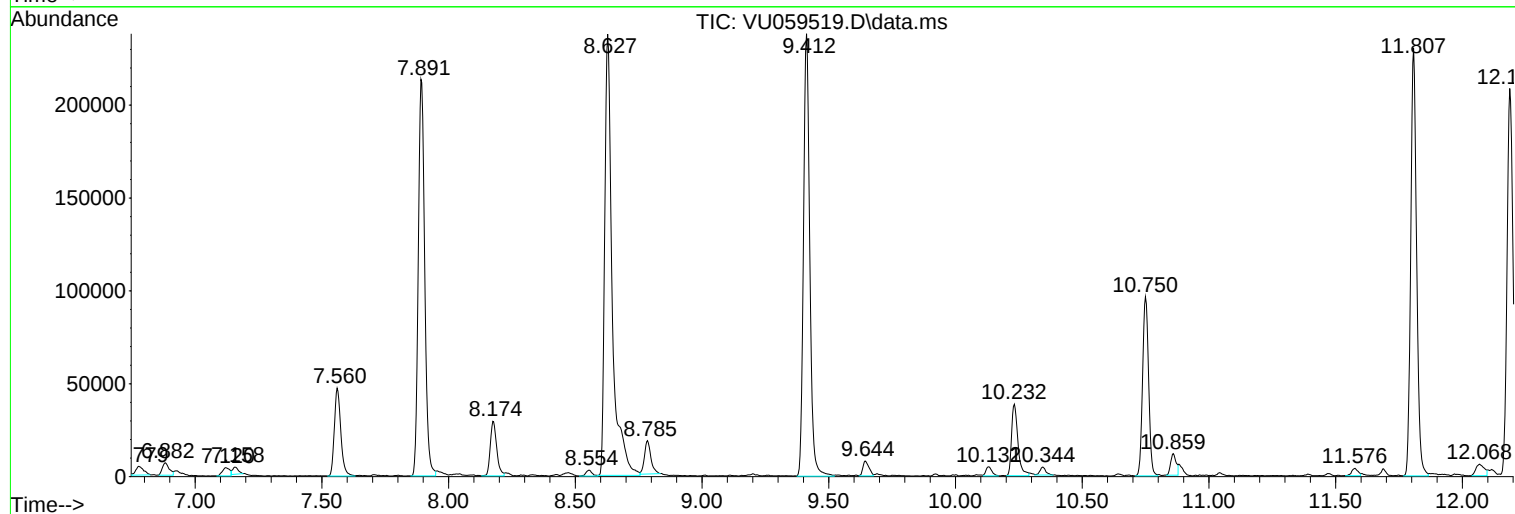
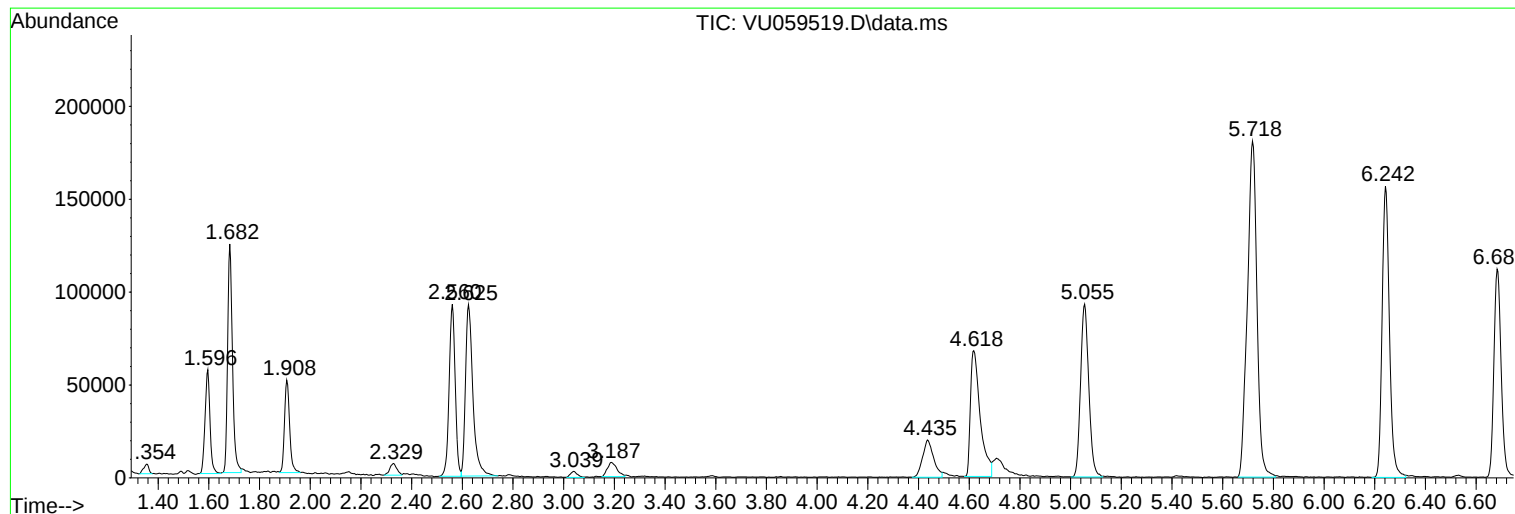
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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Instrument :
MSVOA_U
ClientSampleId :
COT97

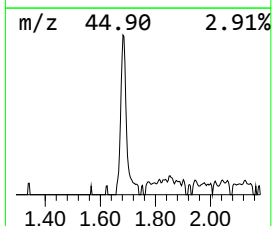
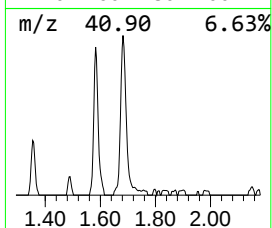
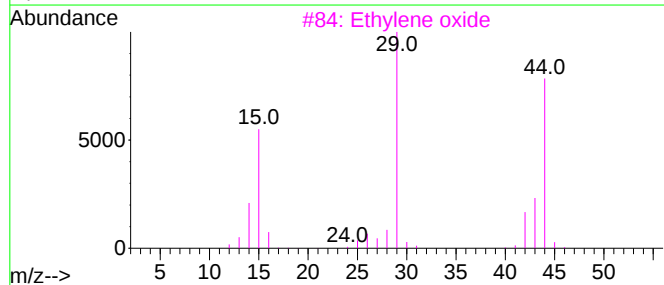
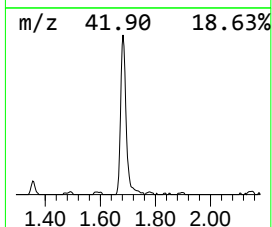
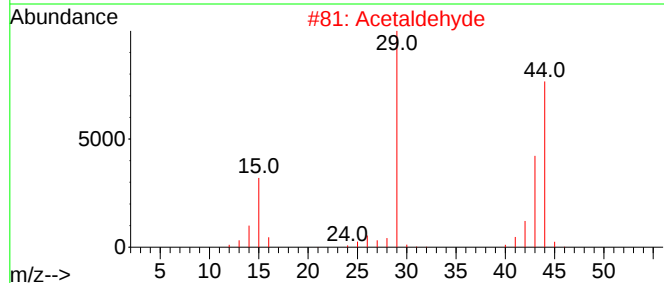
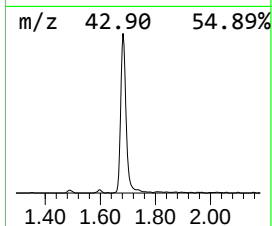
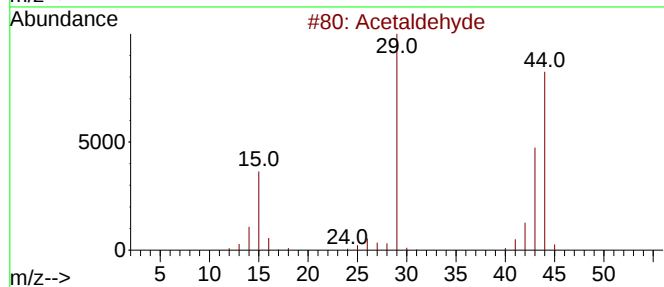
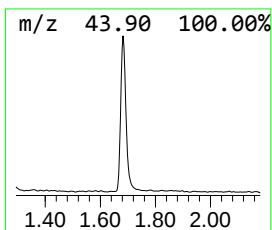
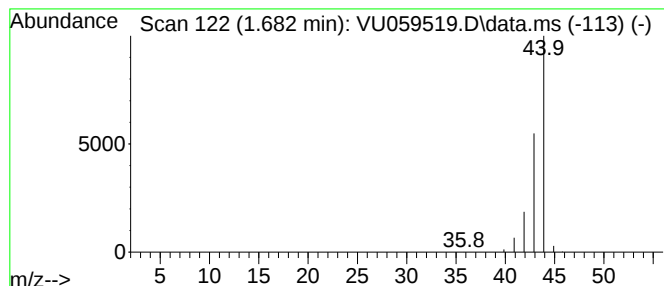
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
1.682	2.59 ug/L	162693	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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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 69 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0T97

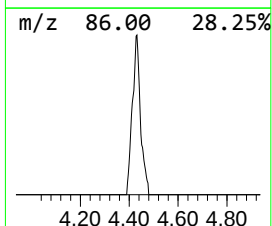
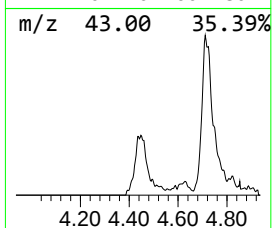
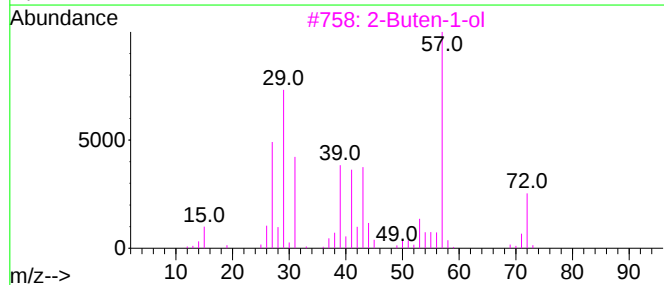
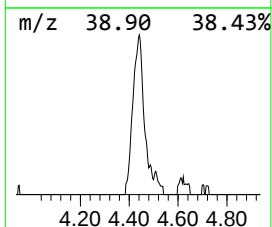
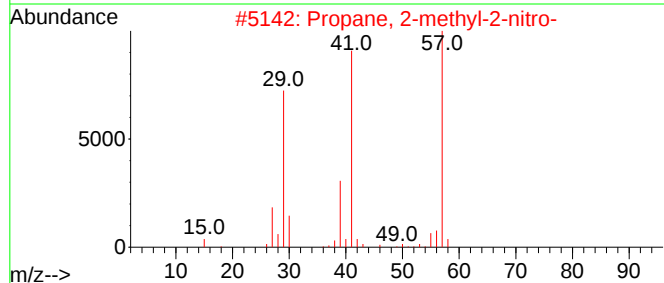
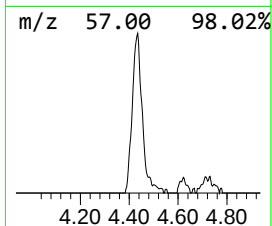
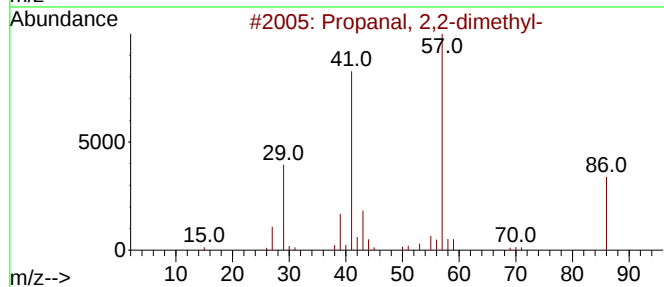
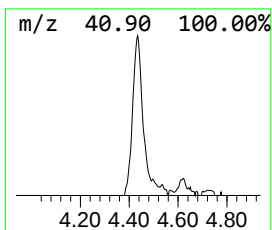
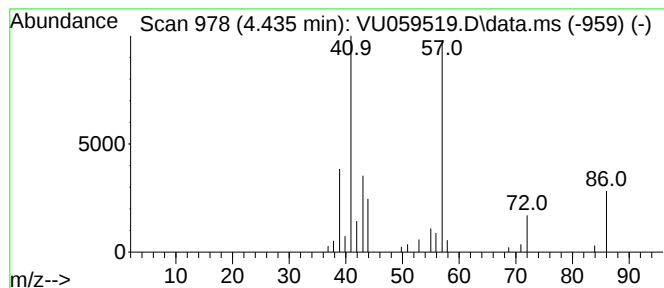
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.435	0.96 ug/L	60207	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	38
2			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	28
3			2-Buten-1-ol	72	C4H8O	006117-91-5	25
4			Butanal, 2-methyl-	86	C5H10O	000096-17-3	16
5			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	16



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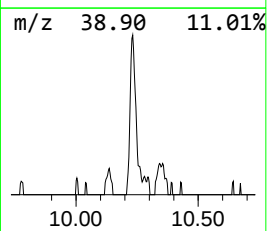
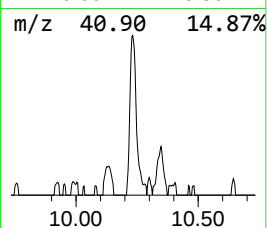
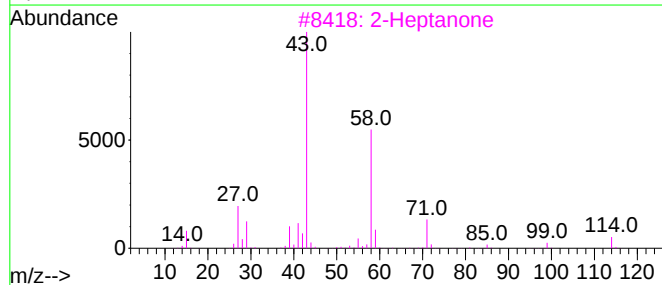
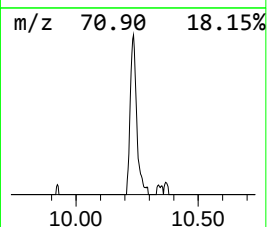
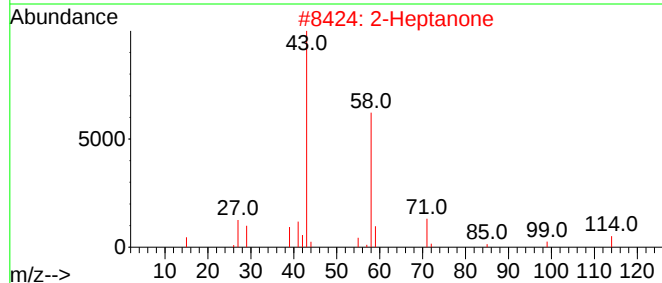
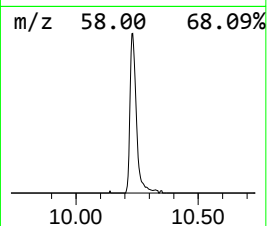
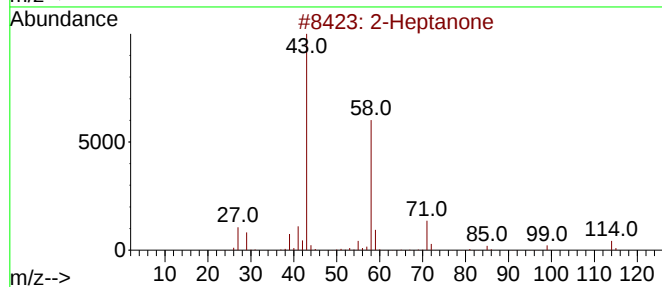
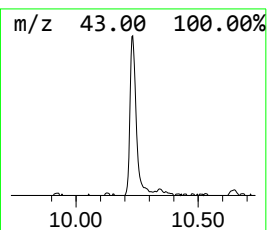
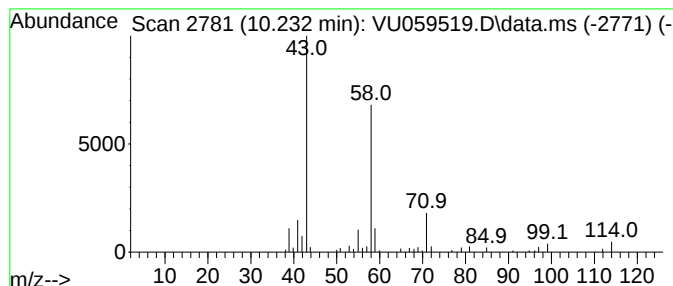
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 2-Heptanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.232	0.82 ug/L	66591	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	90
5	2-Hexanone, 5-methyl-			114	C7H14O	000110-12-3	78



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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
Acetaldehyde	1.682	2.6	ug/L	162693	1	6.242	314519	5.0
unknown-01	4.435	1.0	ug/L	60207	1	6.242	314519	5.0
2-Heptanone	10.232	0.8	ug/L	66591	2	9.412	406471	5.0