

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062824\
 Data File : VU059567.D
 Acq On : 27 Jun 2024 17:13
 Operator : MD/SY
 Sample : P3026-05
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0TB5

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: VU059567.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.355	12	20	31	rVB2	7606	9698	1.86%	0.191%
2	1.596	84	95	111	rBV2	57939	82796	15.92%	1.630%
3	1.683	113	122	138	rBV	137456	177751	34.17%	3.499%
4	1.908	184	192	209	rBV	52370	72076	13.86%	1.419%
5	2.326	305	322	337	rBV5	6925	14817	2.85%	0.292%
6	2.560	378	395	405	rBV	100673	167425	32.19%	3.296%
7	2.622	405	414	437	rVB	111182	209825	40.34%	4.130%
8	2.782	451	464	481	rVB3	6011	14096	2.71%	0.277%
9	3.036	534	543	557	rVB2	4662	9418	1.81%	0.185%
10	3.184	574	589	607	rBV3	12854	31231	6.00%	0.615%
11	4.438	961	979	1012	rBV6	20155	66953	12.87%	1.318%
12	4.618	1019	1035	1056	rBV	85395	224728	43.21%	4.424%
13	5.056	1155	1171	1192	rBV	103029	228596	43.95%	4.500%
14	5.718	1355	1377	1401	rBV2	200068	520124	100.00%	10.239%
15	6.245	1526	1541	1569	rBV	177266	353110	67.89%	6.951%
16	6.683	1664	1677	1695	rBV	123375	243623	46.84%	4.796%
17	6.776	1698	1706	1728	rVB	6236	13076	2.51%	0.257%
18	6.882	1731	1739	1749	rBV3	8593	15051	2.89%	0.296%
19	7.123	1801	1814	1820	rBV5	4832	9872	1.90%	0.194%
20	7.560	1938	1950	1969	rBV2	52568	94964	18.26%	1.869%
21	7.895	2041	2054	2072	rBV	229768	410929	79.01%	8.089%
22	8.178	2131	2142	2158	rBV	33569	58130	11.18%	1.144%
23	8.628	2271	2282	2295	rBV	258354	484658	93.18%	9.541%
24	8.785	2322	2331	2359	rVB2	20498	39891	7.67%	0.785%
25	9.412	2514	2526	2555	rBV	260597	448982	86.32%	8.838%
26	9.647	2590	2599	2607	rBV3	6495	10872	2.09%	0.214%
27	10.129	2734	2749	2760	rBV5	6160	10453	2.01%	0.206%
28	10.232	2771	2781	2797	rBV	38698	66305	12.75%	1.305%
29	10.345	2808	2816	2829	rVB5	4065	7059	1.36%	0.139%
30	10.750	2931	2942	2958	rBV2	106203	174211	33.49%	3.429%
31	10.862	2966	2977	2982	rBV2	8405	13305	2.56%	0.262%
32	11.573	3188	3198	3210	rBV4	3937	7186	1.38%	0.141%
33	11.808	3260	3271	3289	rBV	252084	408270	78.49%	8.037%
34	12.187	3377	3389	3410	rBV	221341	372360	71.59%	7.330%
35	12.888	3601	3607	3621	rVB6	5390	8066	1.55%	0.159%

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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

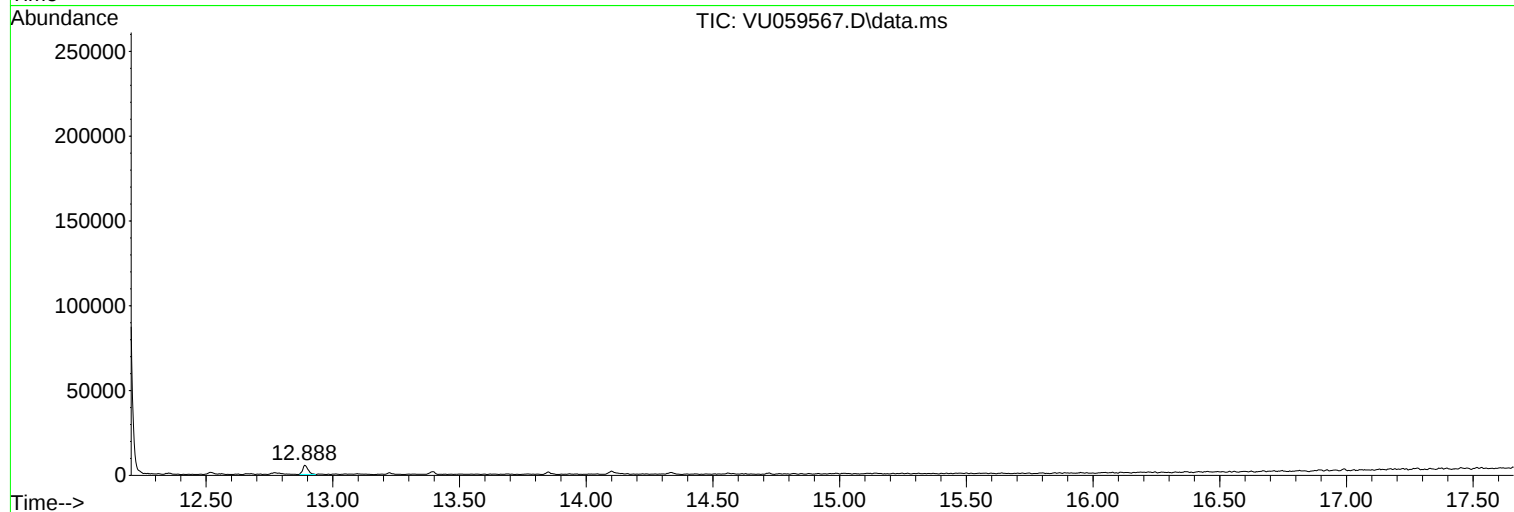
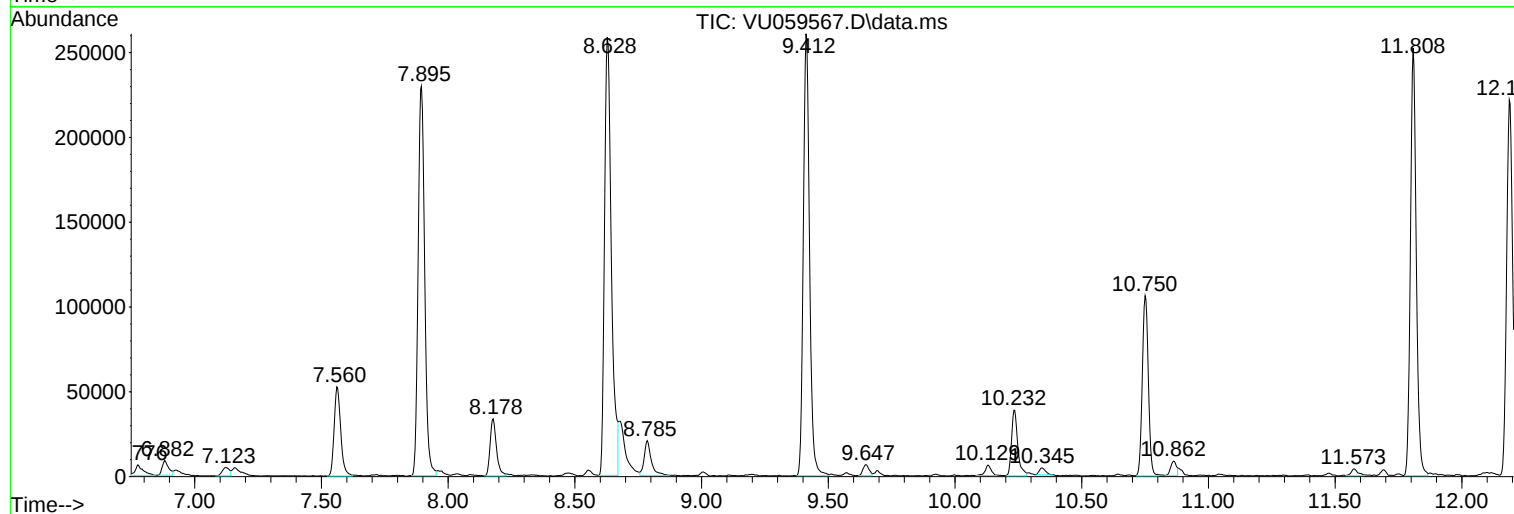
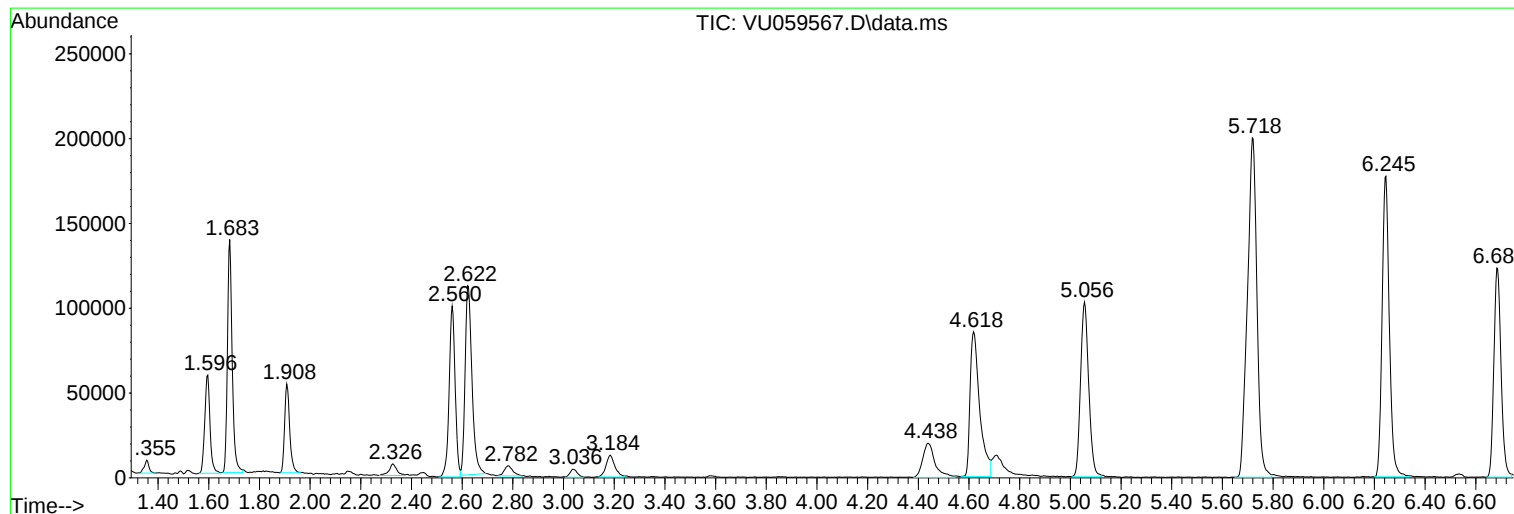
Sum of corrected areas: 5079907

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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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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0TB5

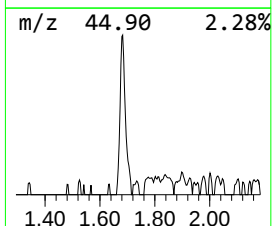
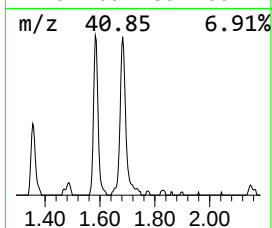
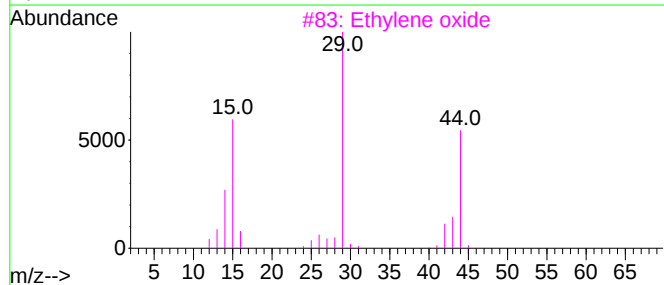
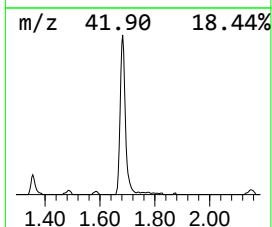
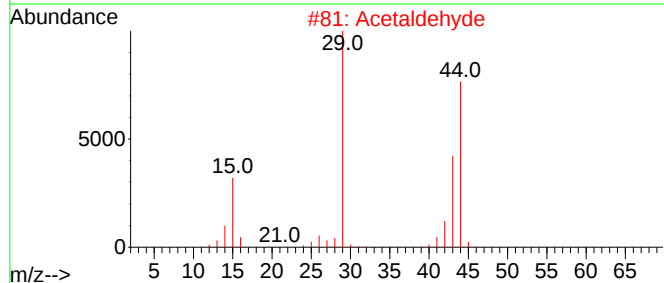
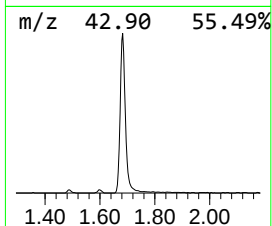
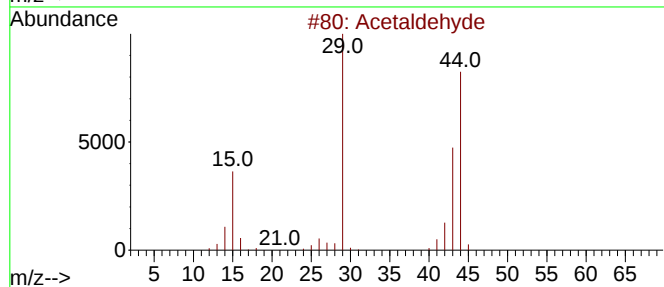
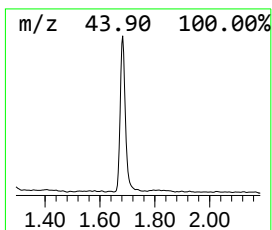
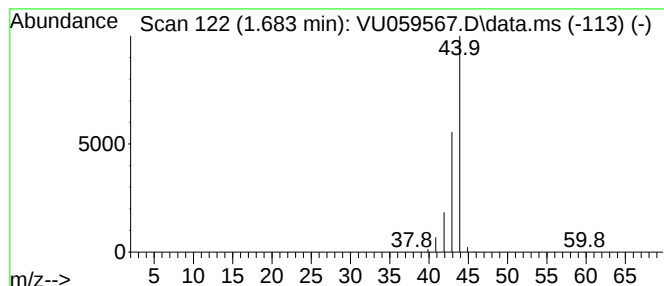
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.683	2.52 ug/L	177751	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	9
2			Acetaldehyde	44	C2H4O	000075-07-0	9
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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Sample : P3026-05
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0TB5

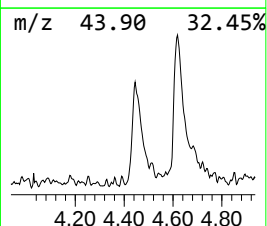
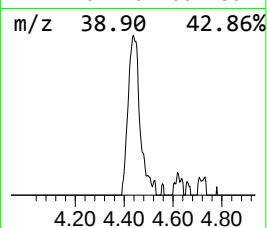
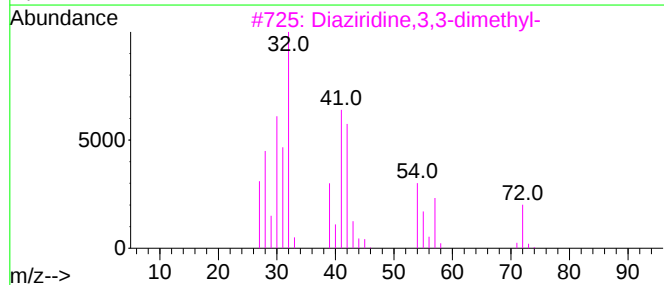
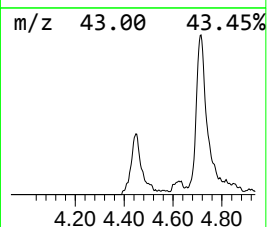
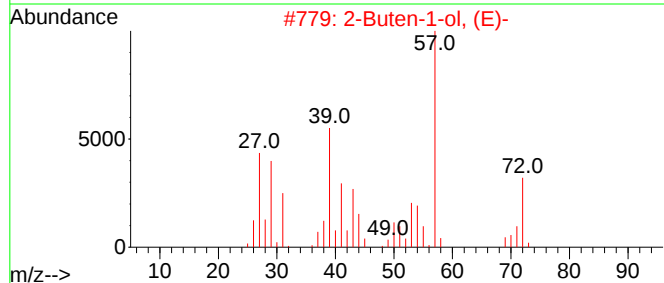
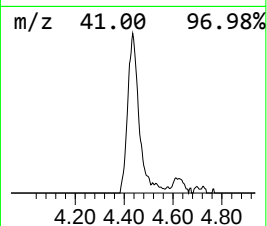
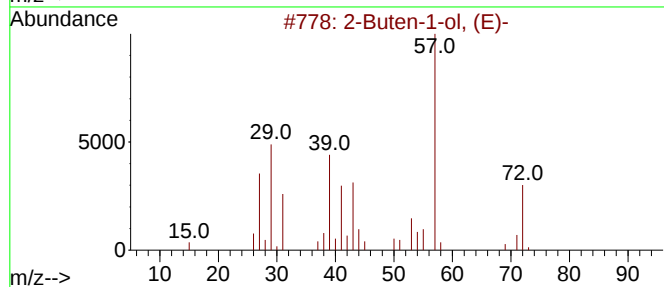
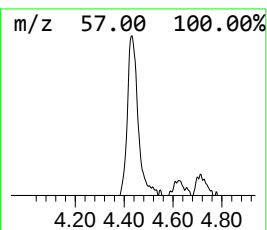
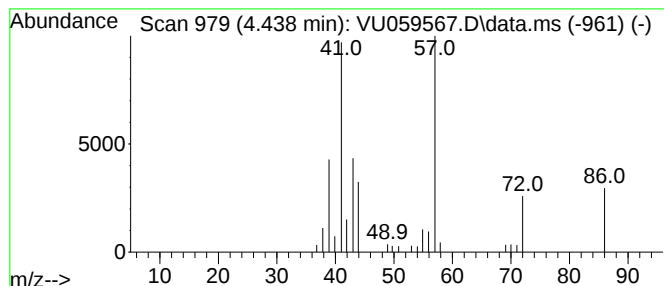
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 unknown-02 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.438	0.95 ug/L	66953	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Buten-1-ol, (E)-			72	C4H8O	000504-61-0	46
2	2-Buten-1-ol, (E)-			72	C4H8O	000504-61-0	46
3	Diaziridine,3,3-dimethyl-			72	C3H8N2	004901-76-2	43
4	2-Propen-1-ol, 2-methyl-			72	C4H8O	000513-42-8	43
5	Propane, 2-methyl-2-nitro-			103	C4H9NO2	000594-70-7	37



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ALS Vial : 6 Sample Multiplier: 1

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MSVOA_U
ClientSampleId :
C0TB5

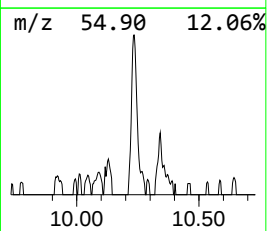
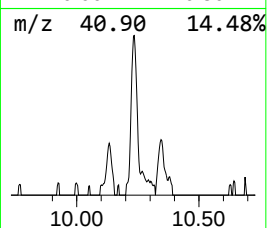
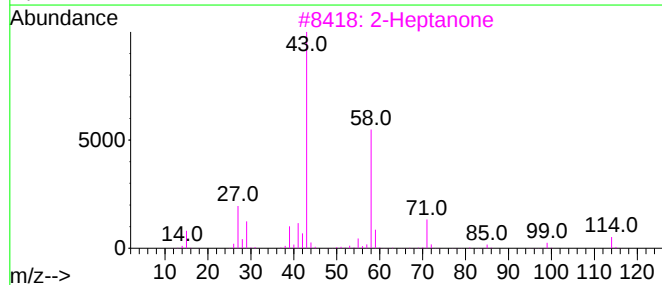
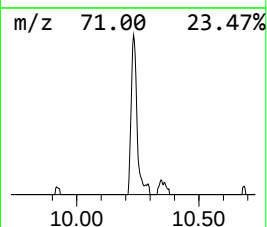
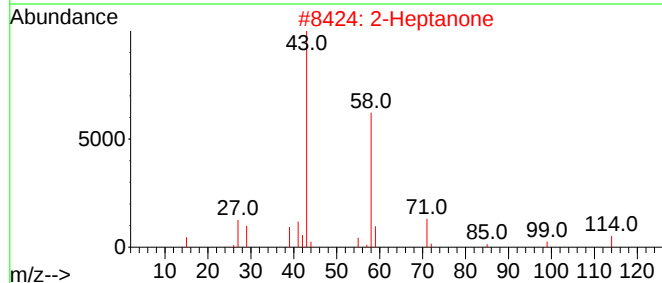
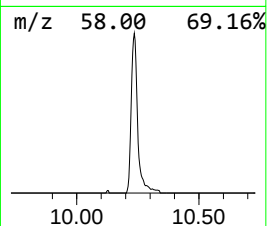
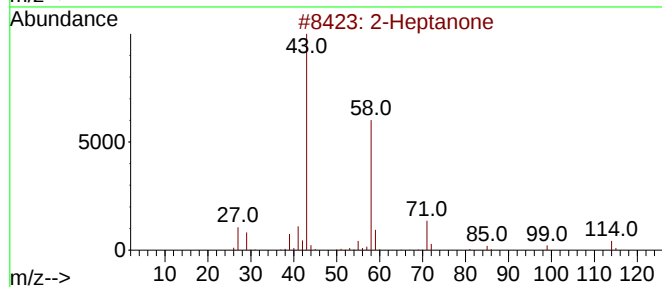
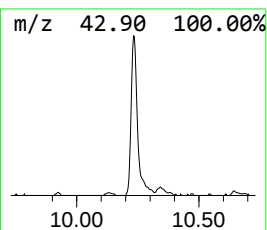
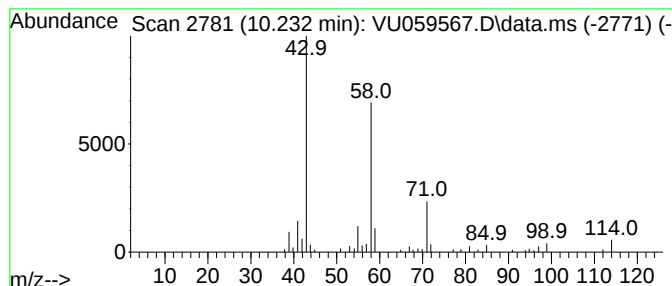
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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	0.74 ug/L	66305	Chlorobenzene-d5	9.412

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone			114	C7H14O	000110-43-0	87
2	2-Heptanone			114	C7H14O	000110-43-0	87
3	2-Heptanone			114	C7H14O	000110-43-0	87
4	2-Heptanone			114	C7H14O	000110-43-0	86
5	2-Hexanone, 4-methyl-			114	C7H14O	000105-42-0	59



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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.683	2.5	ug/L	177751	1	6.245	353110	5.0
unknown-02	4.438	0.9	ug/L	66953	1	6.245	353110	5.0
2-Heptanone	10.232	0.7	ug/L	66305	2	9.412	448982	5.0