

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062224\
 Data File : VU059421.D
 Acq On : 21 Jun 2024 21:00
 Operator : MD/SY
 Sample : P2962-01
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0T73

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: VU059421.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.592	82	94	108	rBV2	60900	95570	17.49%	1.811%
2	1.679	113	121	140	rVV	124486	159082	29.12%	3.014%
3	1.904	184	191	207	rVB	51812	75504	13.82%	1.431%
4	2.329	312	323	332	rBV3	9135	16759	3.07%	0.318%
5	2.557	380	394	406	rBV	96924	164219	30.06%	3.111%
6	2.624	406	415	440	rVB	86812	160276	29.33%	3.037%
7	2.785	455	465	480	rVB7	2554	5733	1.05%	0.109%
8	3.039	535	544	558	rBV8	3015	6229	1.14%	0.118%
9	3.190	577	591	607	rBV	9406	24017	4.40%	0.455%
10	4.438	960	979	994	rBV6	19410	63400	11.60%	1.201%
11	4.621	1022	1036	1058	rBV	91028	238050	43.57%	4.510%
12	5.055	1154	1171	1194	rBV	108955	248316	45.45%	4.705%
13	5.718	1357	1377	1403	rBV2	204279	546389	100.00%	10.352%
14	6.245	1526	1541	1561	rBV	186632	375144	68.66%	7.108%
15	6.531	1619	1630	1643	rVB8	6218	14370	2.63%	0.272%
16	6.685	1661	1678	1696	rBV	133620	270447	49.50%	5.124%
17	6.885	1731	1740	1750	rBV5	6445	11192	2.05%	0.212%
18	7.123	1802	1814	1822	rBV5	6125	13787	2.52%	0.261%
19	7.563	1939	1951	1974	rBV	54361	102953	18.84%	1.951%
20	7.894	2040	2054	2072	rBV	231227	415164	75.98%	7.866%
21	7.965	2073	2076	2090	rVB6	5978	9961	1.82%	0.189%
22	8.177	2132	2142	2165	rBV2	35460	69655	12.75%	1.320%
23	8.631	2271	2283	2295	rBV	259729	505025	92.43%	9.569%
24	8.788	2324	2332	2342	rVB2	16162	26026	4.76%	0.493%
25	9.415	2515	2527	2550	rBV	273132	469354	85.90%	8.893%
26	9.650	2592	2600	2608	rBV2	8446	14498	2.65%	0.275%
27	10.135	2744	2751	2767	rVB4	5809	10822	1.98%	0.205%
28	10.235	2772	2782	2805	rBV	33616	65781	12.04%	1.246%
29	10.348	2810	2817	2835	rVB10	4183	10057	1.84%	0.191%
30	10.753	2929	2943	2960	rBV	112239	188658	34.53%	3.574%
31	10.862	2968	2977	2997	rVB5	12084	27956	5.12%	0.530%
32	11.576	3192	3199	3206	rBV6	3704	5919	1.08%	0.112%
33	11.811	3258	3272	3291	rBV	263634	444933	81.43%	8.430%
34	12.190	3378	3390	3407	rBV	238123	403043	73.76%	7.636%
35	12.894	3598	3609	3620	rBV7	6597	12722	2.33%	0.241%
36	14.100	3975	3984	3994	rBV4	3815	6977	1.28%	0.132%

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ClientSampleId :
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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

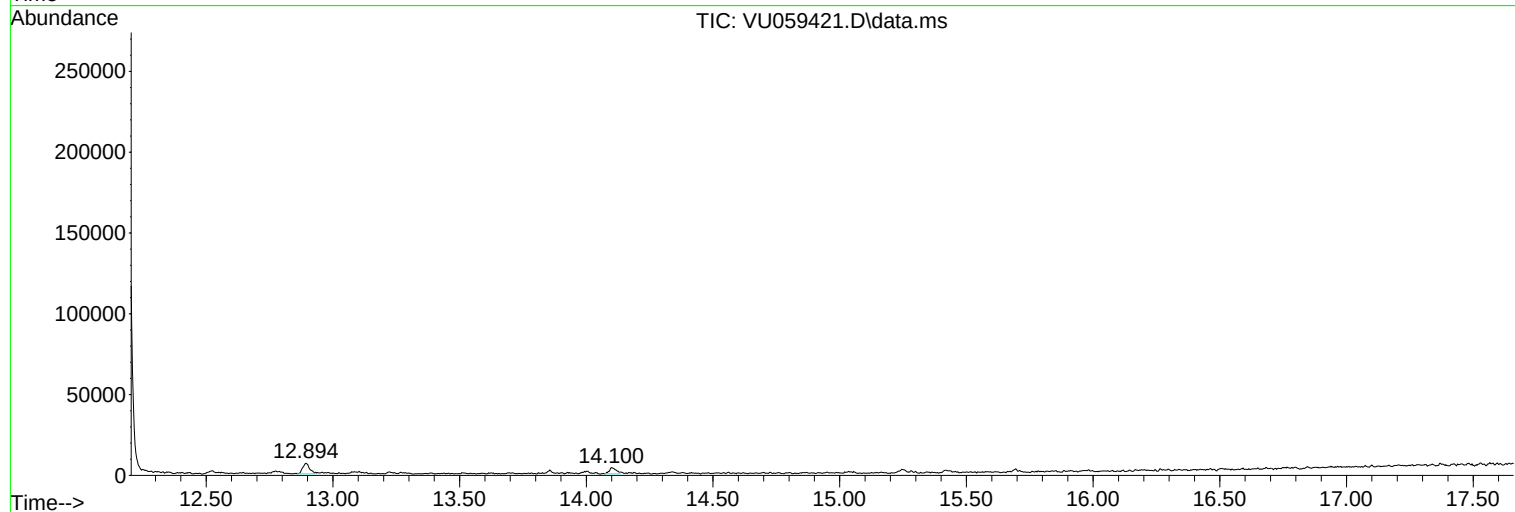
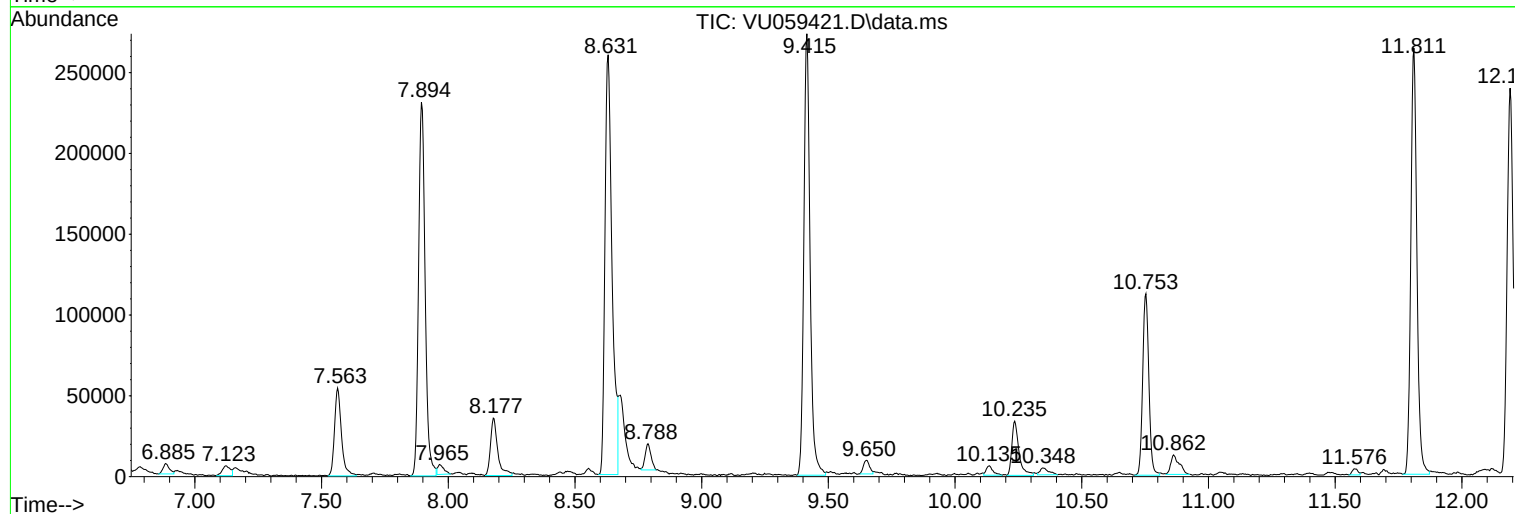
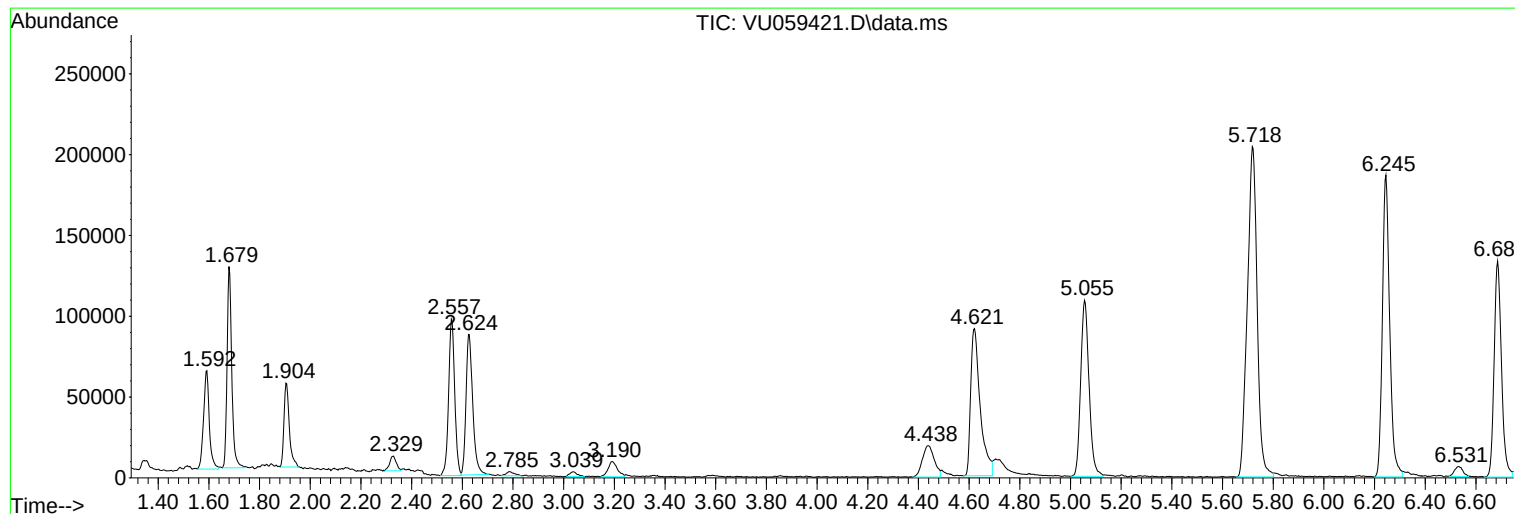
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

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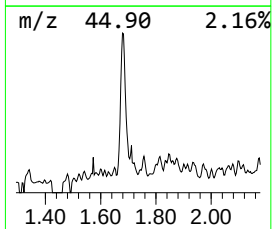
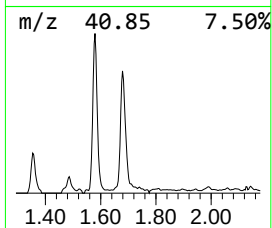
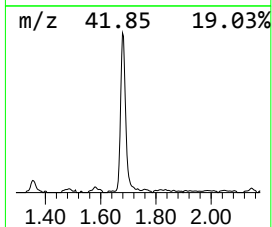
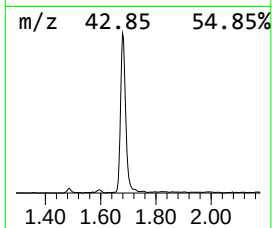
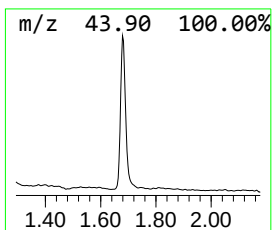
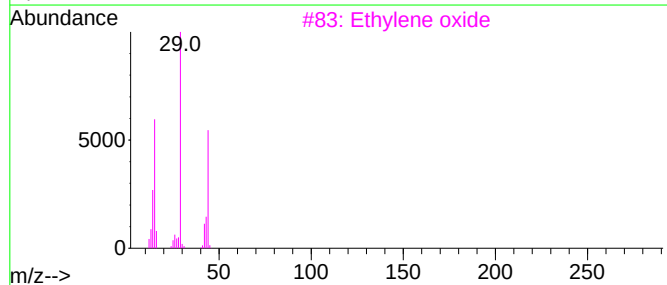
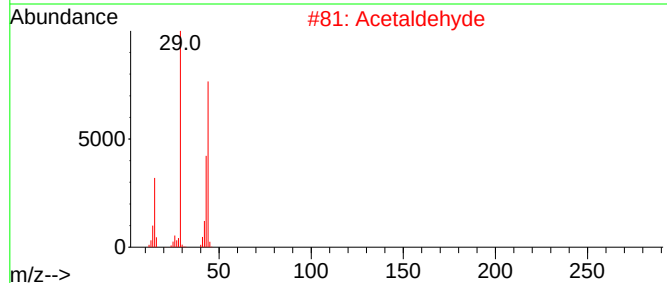
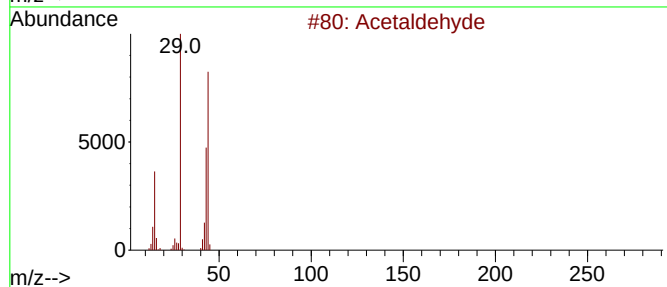
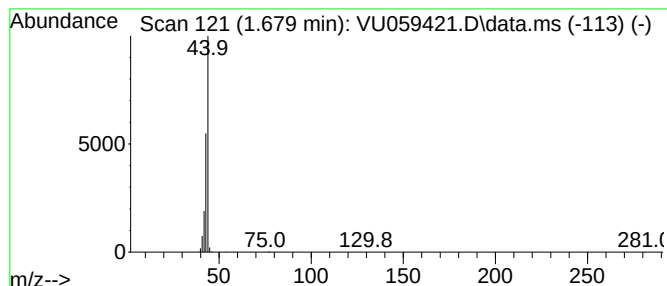
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.679	2.12 ug/L	159082	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			Propane	44	C3H8	000074-98-6	4



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Sample : P2962-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
COT73

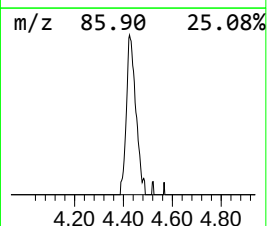
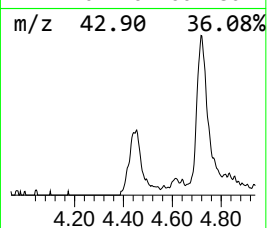
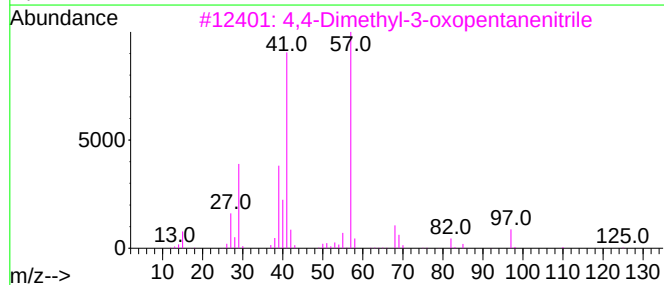
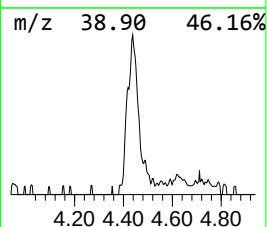
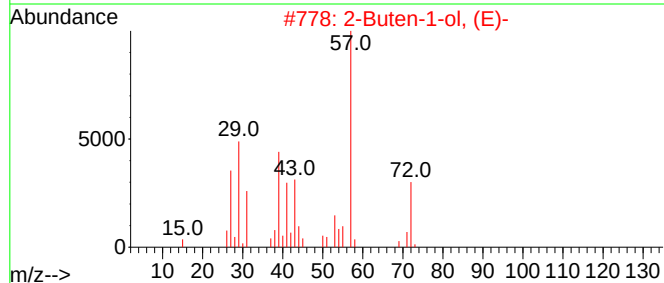
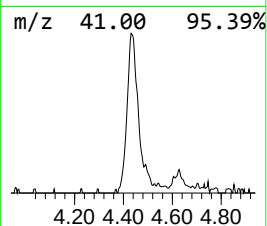
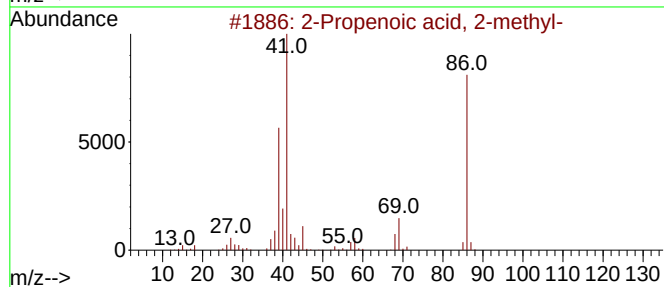
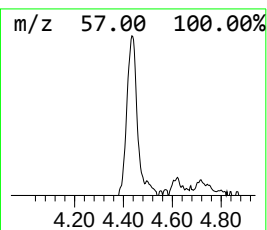
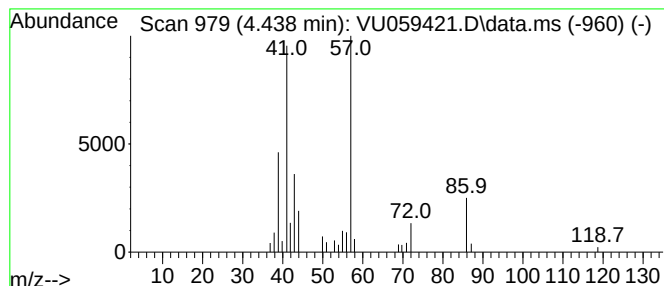
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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	0.85 ug/L	63400	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propenoic acid, 2-methyl-	86	C4H6O2	000079-41-4	47
2			2-Buten-1-ol, (E)-	72	C4H8O	000504-61-0	43
3			4,4-Dimethyl-3-oxopentanenitrile	125	C7H11NO	059997-51-2	38
4			2-Propenoic acid, 2-methyl-	86	C4H6O2	000079-41-4	38
5			2-Buten-1-ol	72	C4H8O	006117-91-5	37



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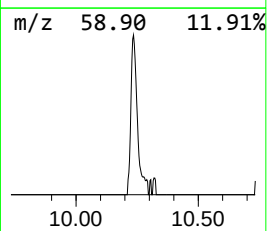
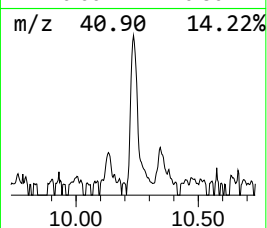
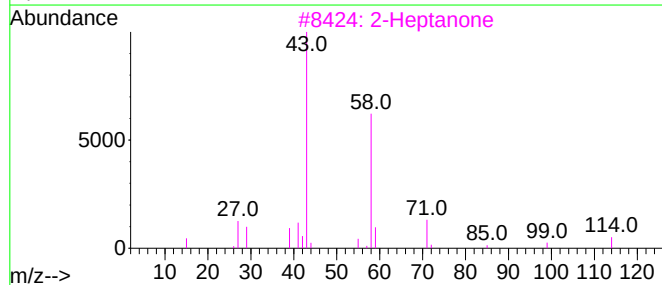
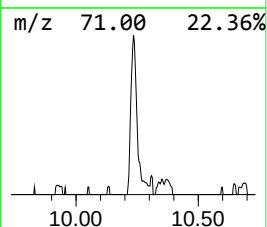
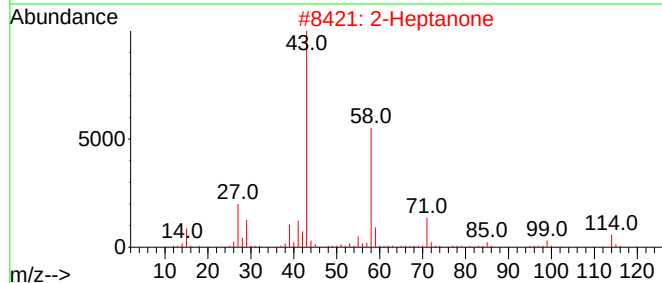
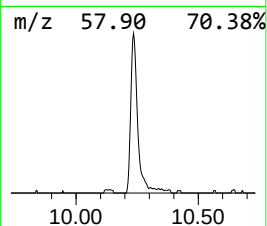
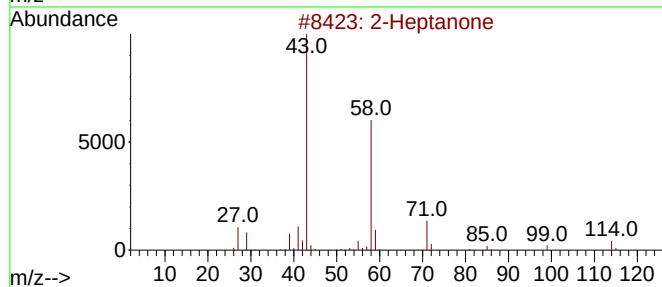
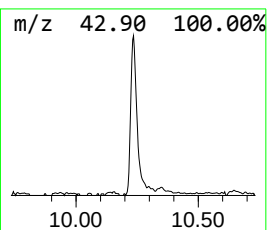
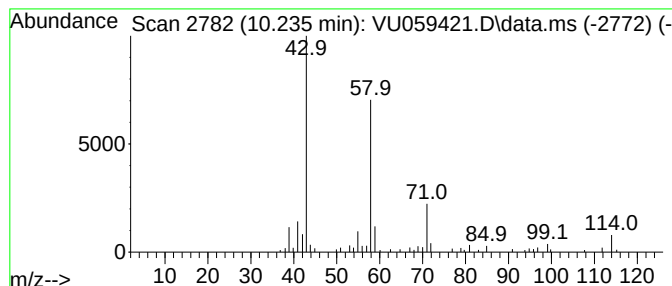
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
10.235	0.70 ug/L	65781	Chlorobenzene-d5	9.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone			114	C7H14O	000110-43-0	90
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	80
5	2-Heptanone			114	C7H14O	000110-43-0	76



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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	1.679	2.1	ug/L	159082	1	6.245	375144	5.0
unknown-02	4.438	0.8	ug/L	63400	1	6.245	375144	5.0
2-Heptanone	10.235	0.7	ug/L	65781	2	9.415	469354	5.0