

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072424\
 Data File : VU060166.D
 Acq On : 24 Jul 2024 20:14
 Operator : MD/SY
 Sample : P3344-15
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHJC0

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: VU060166.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.596	84	95	111	rBV	136171	176145	9.89%	1.316%
2	1.686	113	123	159	rBV	921880	1440492	80.85%	10.760%
3	1.908	184	192	213	rVB	109245	149850	8.41%	1.119%
4	2.560	379	395	407	rBV2	208153	371201	20.83%	2.773%
5	2.641	407	420	466	rVV	569227	1781754	100.00%	13.309%
6	3.232	575	604	605	rBV5	23035	68005	3.82%	0.508%
7	4.435	955	978	1009	rBV4	154574	435747	24.46%	3.255%
8	4.625	1025	1037	1054	rBV	151846	437349	24.55%	3.267%
9	4.708	1056	1063	1091	rVB	65868	185158	10.39%	1.383%
10	5.056	1155	1171	1198	rBV	204217	463257	26.00%	3.460%
11	5.718	1355	1377	1406	rBV2	394402	1026422	57.61%	7.667%
12	6.242	1524	1540	1571	rBV	379538	760128	42.66%	5.678%
13	6.682	1651	1677	1696	rBV2	249604	524024	29.41%	3.914%
14	6.769	1697	1704	1727	rVB	38995	85516	4.80%	0.639%
15	6.875	1727	1737	1748	rBV3	49658	96250	5.40%	0.719%
16	7.120	1801	1813	1819	rBV2	30081	58002	3.26%	0.433%
17	7.560	1936	1950	1972	rBV2	107399	198113	11.12%	1.480%
18	7.891	2039	2053	2086	rBV	464973	828808	46.52%	6.191%
19	8.174	2131	2141	2154	rBV	70107	123399	6.93%	0.922%
20	8.422	2204	2218	2228	rBV2	14132	26595	1.49%	0.199%
21	8.628	2270	2282	2294	rBV	586012	1074306	60.29%	8.025%
22	8.782	2321	2330	2349	rVB2	52733	91681	5.15%	0.685%
23	9.412	2513	2526	2547	rBV	551195	927428	52.05%	6.927%
24	9.647	2589	2599	2608	rBV4	11245	19859	1.11%	0.148%
25	10.232	2770	2781	2807	rBV	96328	171361	9.62%	1.280%
26	10.750	2930	2942	2955	rBV	205255	325887	18.29%	2.434%
27	10.859	2966	2976	2994	rVB4	11233	23412	1.31%	0.175%
28	11.808	3258	3271	3289	rBV	510975	821103	46.08%	6.133%
29	12.187	3377	3389	3410	rBV	426596	696571	39.09%	5.203%

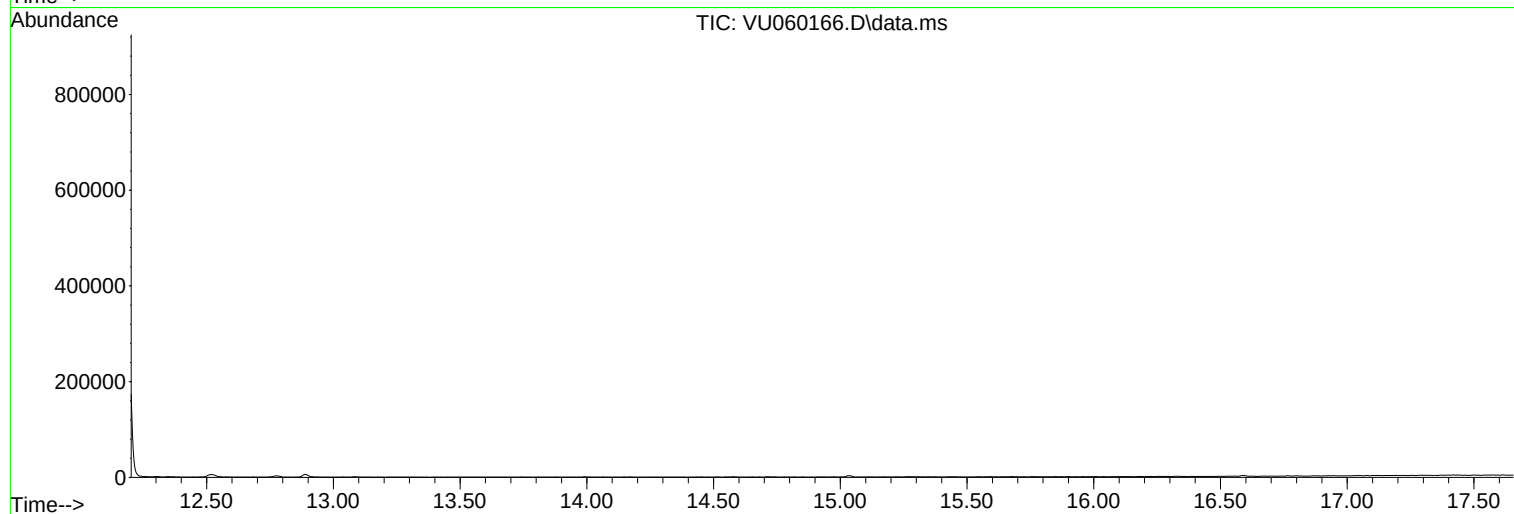
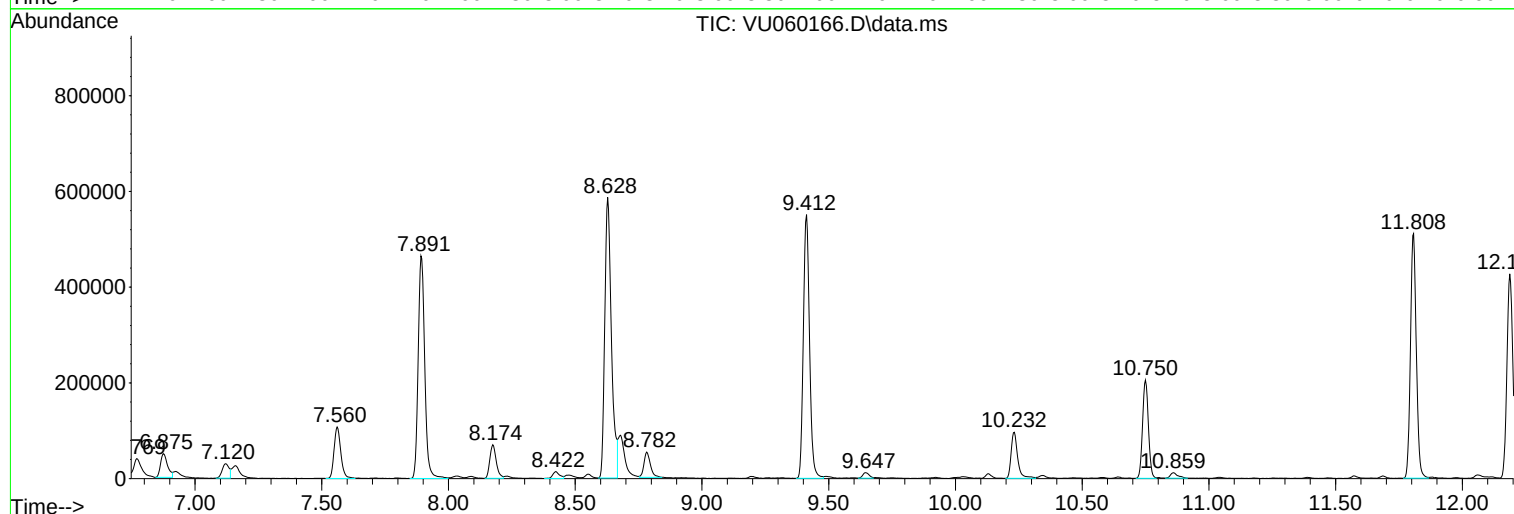
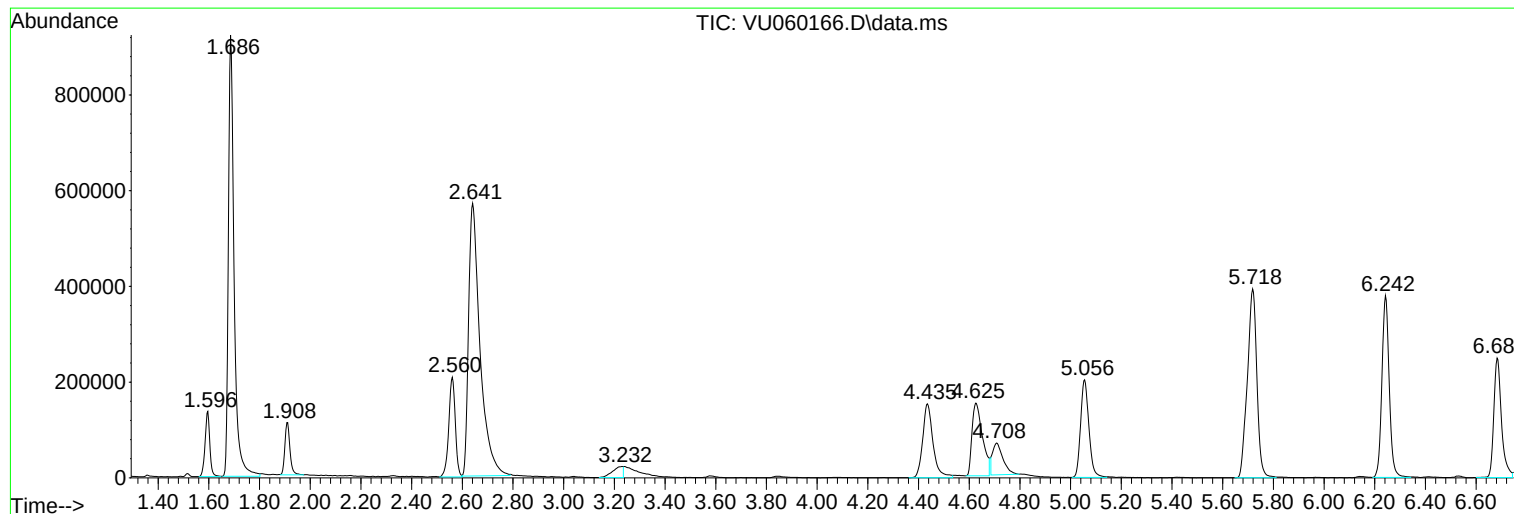
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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHJC0

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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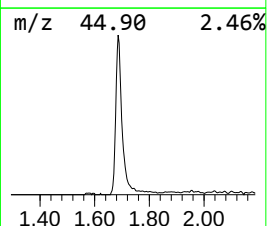
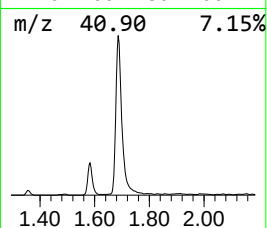
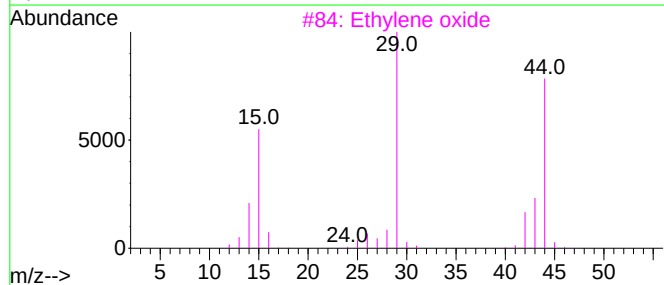
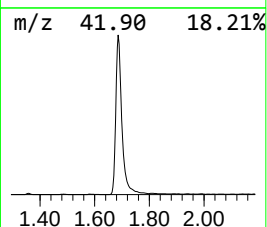
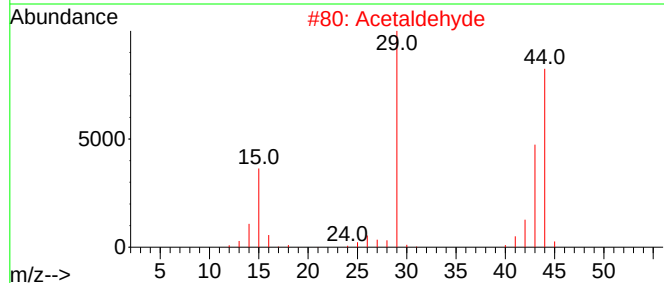
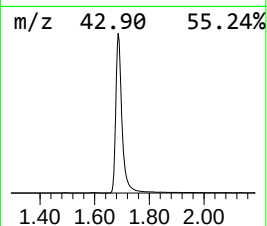
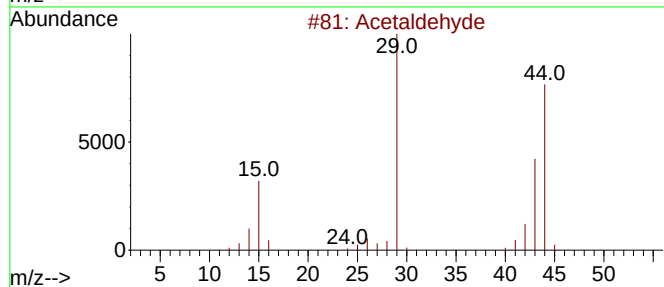
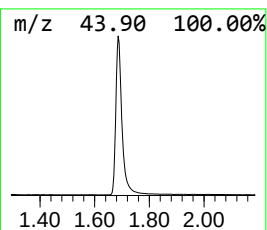
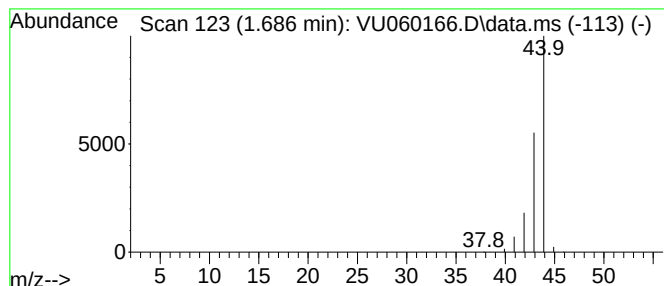
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.686	9.48 ug/L	1440490	1,4-Difluorobenzene	6.242

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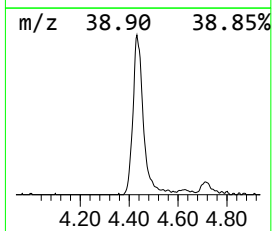
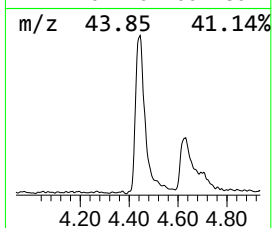
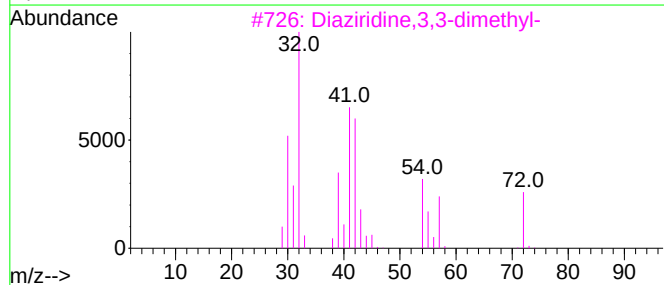
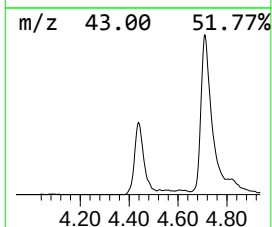
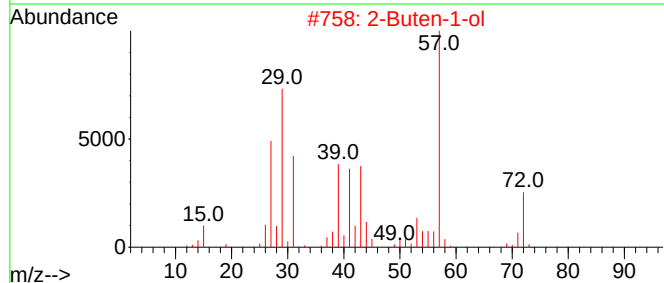
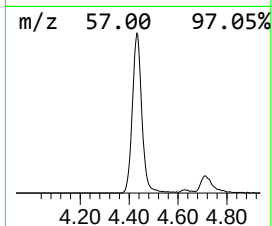
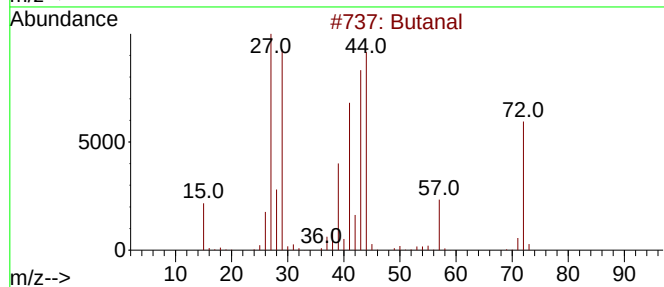
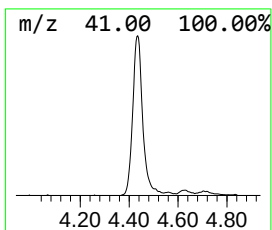
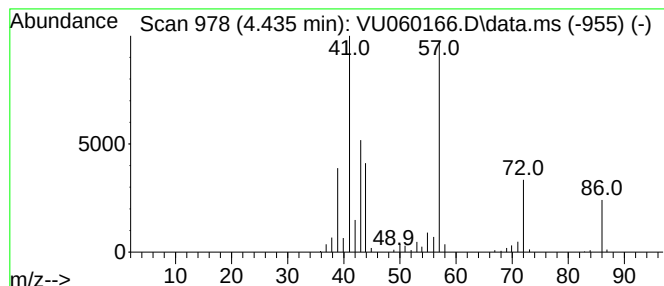
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR071824WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.435	2.87 ug/L	435747	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	43
2			2-Buten-1-ol	72	C4H8O	006117-91-5	43
3			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
4			2-Buten-1-ol, (E)-	72	C4H8O	000504-61-0	38
5			di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	32



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

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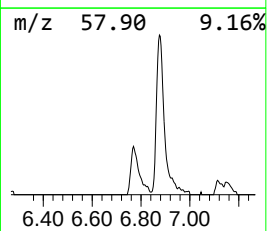
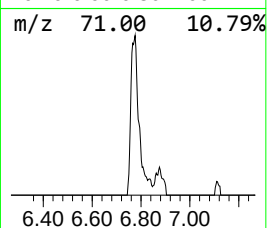
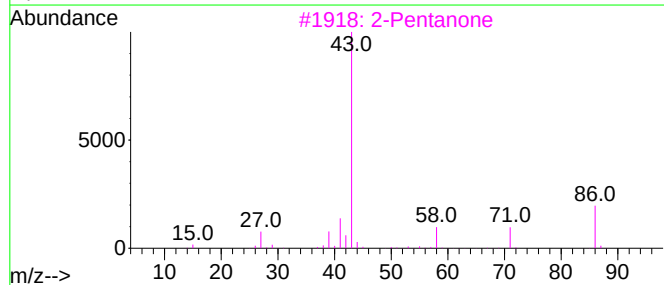
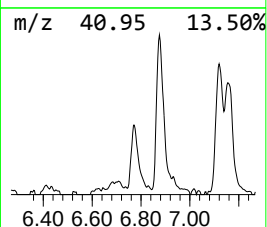
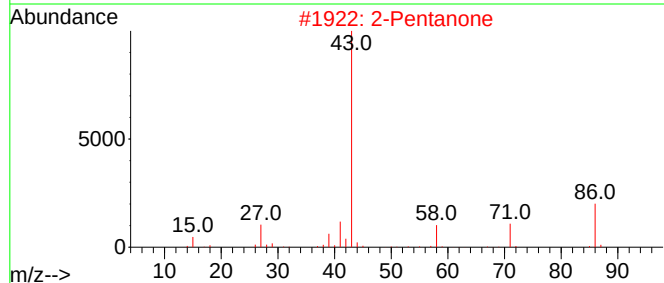
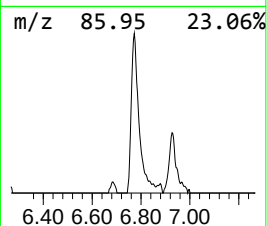
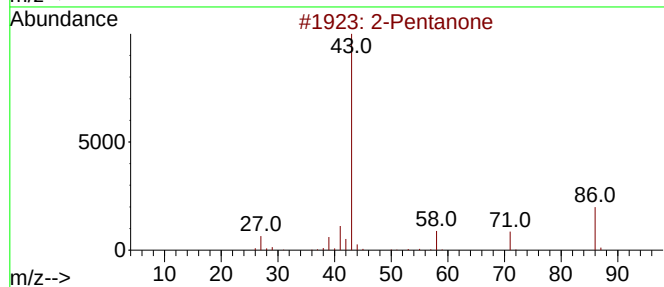
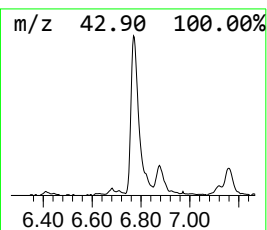
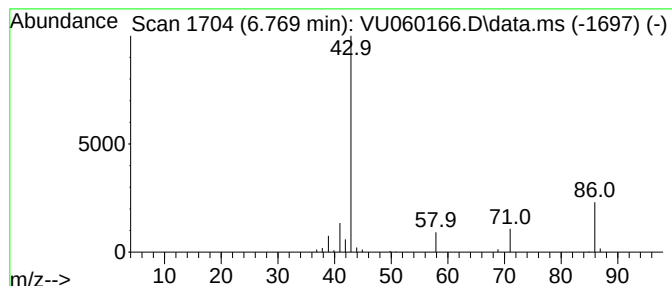
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR071824WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 2-Pentanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.769	0.56 ug/L	85516	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone			86	C5H10O	000107-87-9	86
2	2-Pentanone			86	C5H10O	000107-87-9	86
3	2-Pentanone			86	C5H10O	000107-87-9	86
4	2-Pentanone			86	C5H10O	000107-87-9	80
5	2-Butanone, 3-methyl-			86	C5H10O	000563-80-4	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072424\
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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHJC0

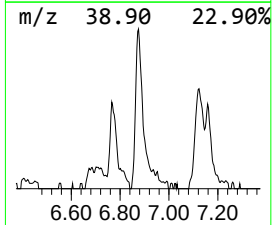
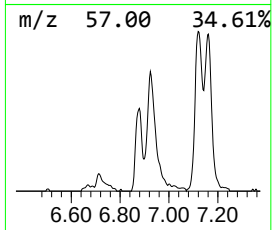
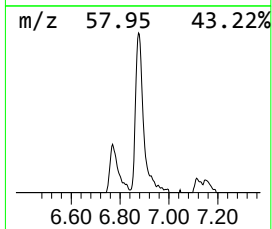
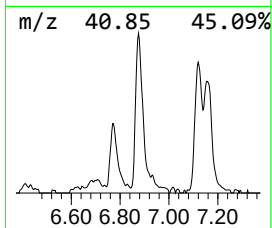
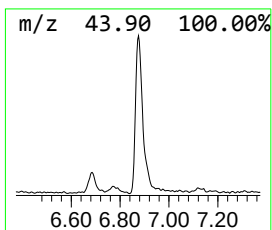
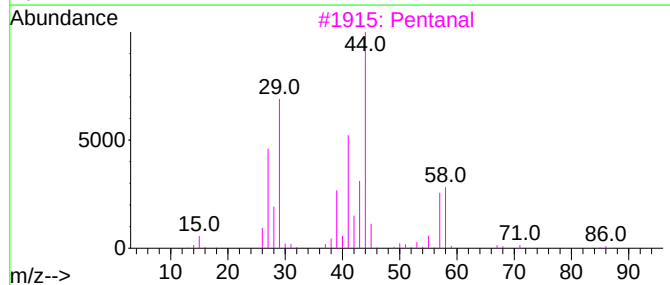
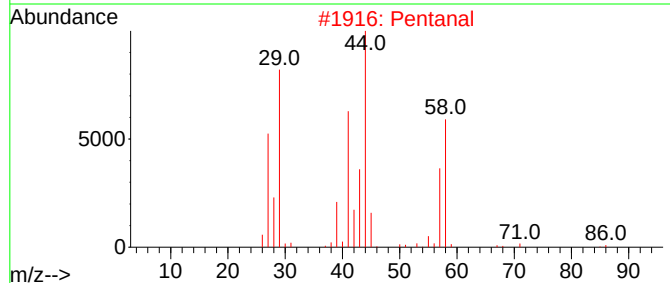
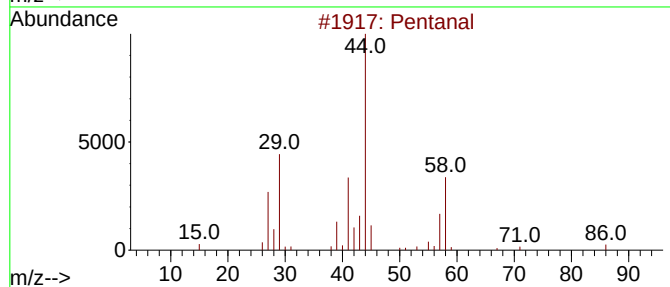
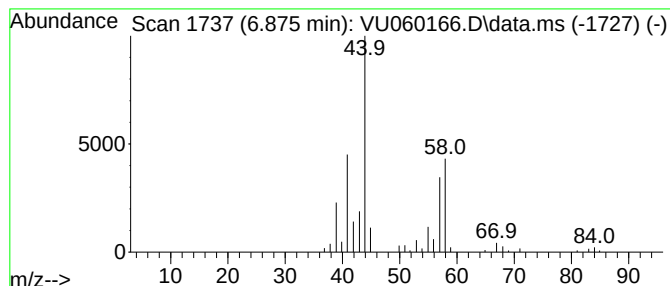
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR071824WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Pentanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.875	0.63 ug/L	96250	1,4-Difluorobenzene	6.242

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal	86	C5H10O	000110-62-3	74
2	Pentanal	86	C5H10O	000110-62-3	72
3	Pentanal	86	C5H10O	000110-62-3	64
4	Cyclopropyl carbinol	72	C4H8O	002516-33-8	40
5	2-Propanamine	59	C3H9N	000075-31-0	9



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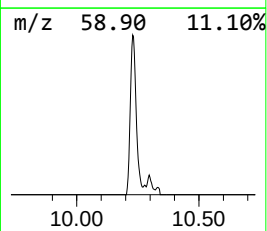
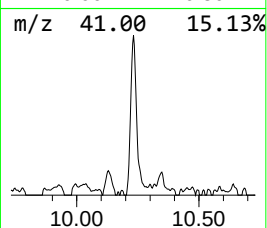
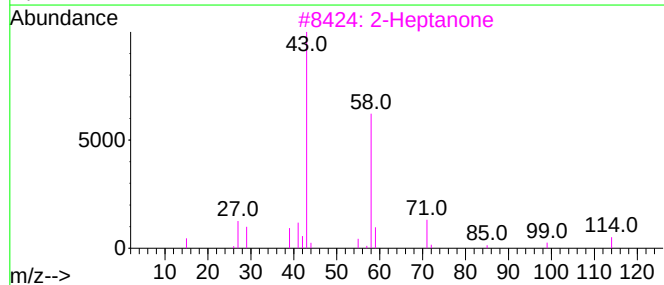
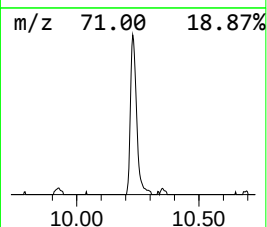
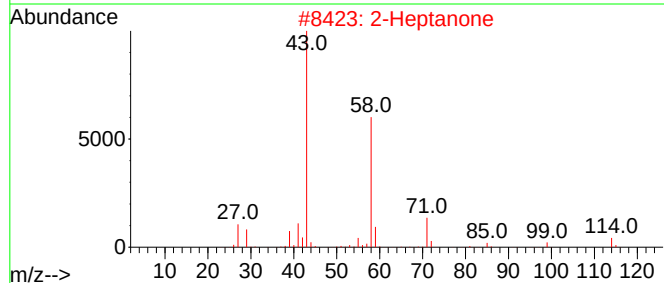
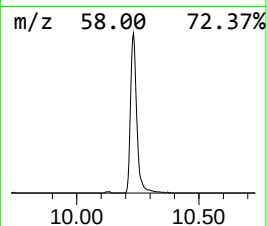
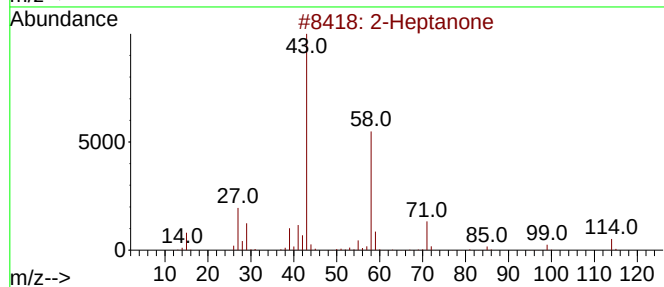
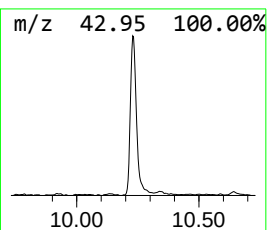
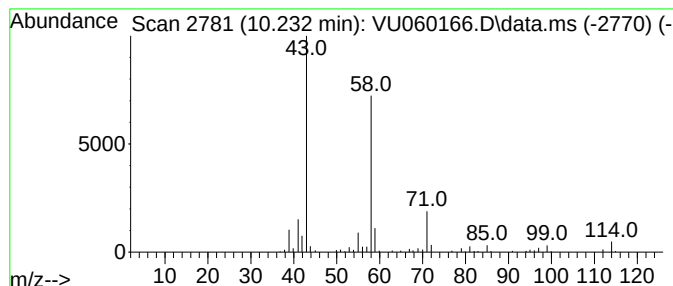
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 2-Heptanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.232	0.92 ug/L	171361	Chlorobenzene-d5	9.412

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	90
3			2-Heptanone	114	C7H14O	000110-43-0	90
4			2-Heptanone	114	C7H14O	000110-43-0	86
5			2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.686	9.5	ug/L	1440490	1	6.242	760128	5.0
unknown-02	4.435	2.9	ug/L	435747	1	6.242	760128	5.0
2-Pentanone	6.769	0.6	ug/L	85516	1	6.242	760128	5.0
Pentanal	6.875	0.6	ug/L	96250	1	6.242	760128	5.0
2-Heptanone	10.232	0.9	ug/L	171361	2	9.412	927428	5.0