

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100722\
 Data File : VU051282.D
 Acq On : 08 Oct 2022 19:21
 Operator : JC/MD
 Sample : N4873-13
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXZ58

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\SFAMUTR100722WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU051282.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.359	3	6	24	rVB	1934233	1815012	100.00%	17.141%
2	1.437	24	30	38	rVB	57364	58439	3.22%	0.552%
3	1.495	38	48	53	rBV	47316	53836	2.97%	0.508%
4	1.588	69	77	85	rBV2	705448	821109	45.24%	7.754%
5	1.633	85	91	96	rVV	605113	644640	35.52%	6.088%
6	1.659	96	99	111	rVB	142947	142816	7.87%	1.349%
7	1.729	113	121	129	rBV	128266	145138	8.00%	1.371%
8	1.877	160	167	171	rBV	39548	48761	2.69%	0.460%
9	1.909	171	177	195	rVB2	93569	136151	7.50%	1.286%
10	2.096	226	235	244	rBV	83156	113595	6.26%	1.073%
11	2.154	245	253	263	rVB	110555	150603	8.30%	1.422%
12	2.318	295	304	312	rBV	20748	29910	1.65%	0.282%
13	2.398	318	329	343	rBV2	63763	118043	6.50%	1.115%
14	2.565	369	381	393	rBV2	130022	226249	12.47%	2.137%
15	2.630	393	401	418	rVB3	43200	71924	3.96%	0.679%
16	2.755	425	440	446	rBV2	11889	21166	1.17%	0.200%
17	2.797	446	453	463	rVV4	24994	47047	2.59%	0.444%
18	2.858	464	472	489	rVB4	16203	34281	1.89%	0.324%
19	3.015	512	521	541	rVB5	14906	36124	1.99%	0.341%
20	3.591	683	700	711	rBV5	9888	22939	1.26%	0.217%
21	3.867	760	786	812	rVB	147735	375579	20.69%	3.547%
22	4.623	1008	1021	1058	rBV	111223	353218	19.46%	3.336%
23	5.064	1142	1158	1177	rBV	133201	298267	16.43%	2.817%
24	5.314	1213	1236	1255	rBV2	146533	340897	18.78%	3.219%
25	5.723	1340	1363	1398	rBV2	248150	696698	38.39%	6.579%
26	6.250	1512	1527	1545	rBV	209149	402217	22.16%	3.798%
27	6.543	1606	1618	1634	rBV2	53419	100680	5.55%	0.951%
28	6.690	1649	1664	1682	rBV	172690	338524	18.65%	3.197%
29	7.565	1925	1936	1951	rBV	68333	122144	6.73%	1.154%
30	7.896	2026	2039	2055	rBV	251062	438081	24.14%	4.137%
31	8.179	2116	2127	2147	rBV	44189	75910	4.18%	0.717%
32	8.552	2234	2243	2253	rBV2	24218	38868	2.14%	0.367%
33	8.633	2256	2268	2304	rBV2	292946	680626	37.50%	6.428%
34	9.417	2499	2512	2534	rBV	324202	555921	30.63%	5.250%
35	10.755	2916	2928	2952	rVB	138571	226843	12.50%	2.142%
36	11.812	3244	3257	3279	rBV	260847	422941	23.30%	3.994%

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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\SFAMUTR100722WMA.M
Title : TRACE VOA SFAM1.0

37	12.192	3363	3375	3393	rBV	232453	383751	21.14%	3.624%
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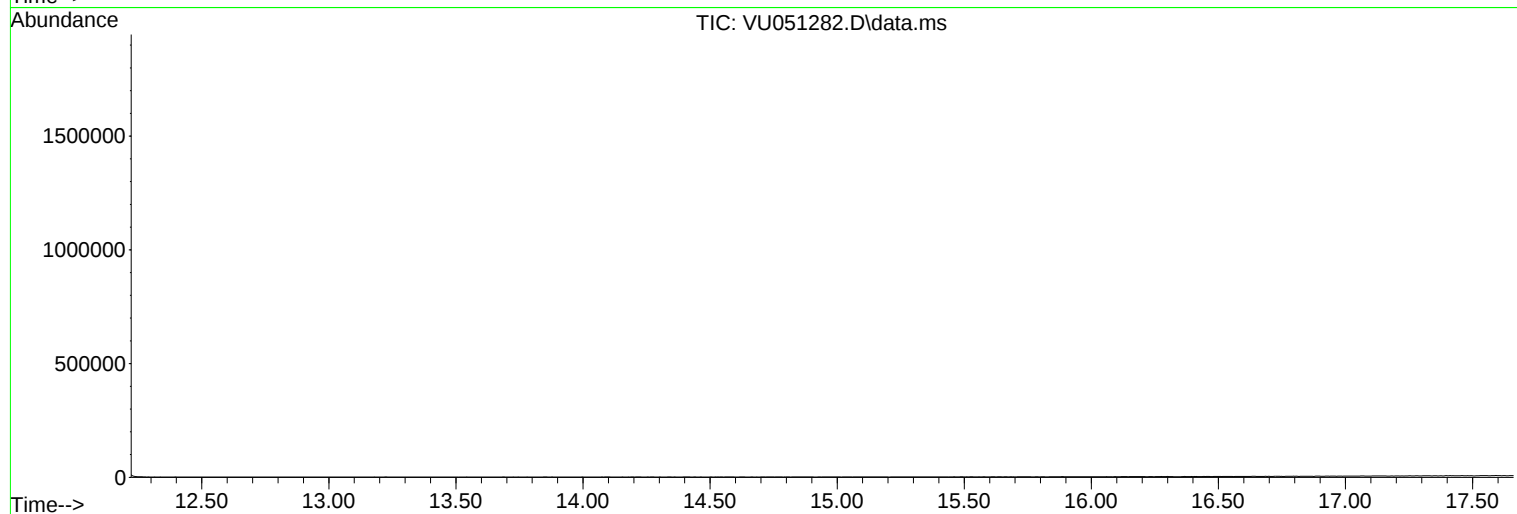
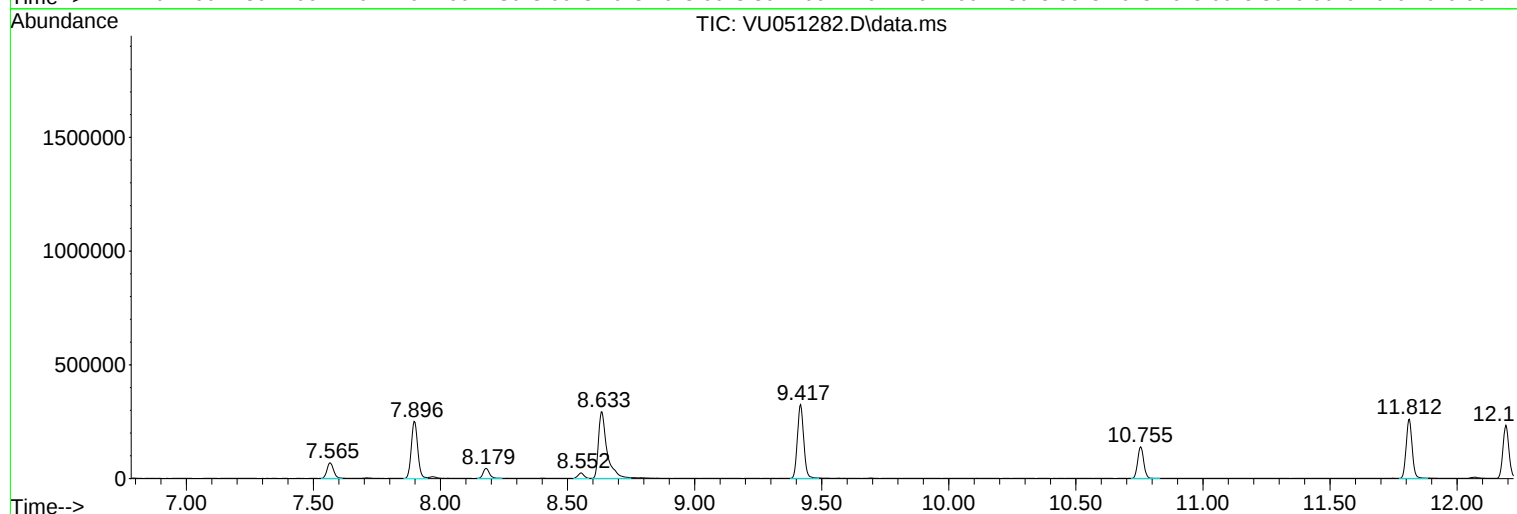
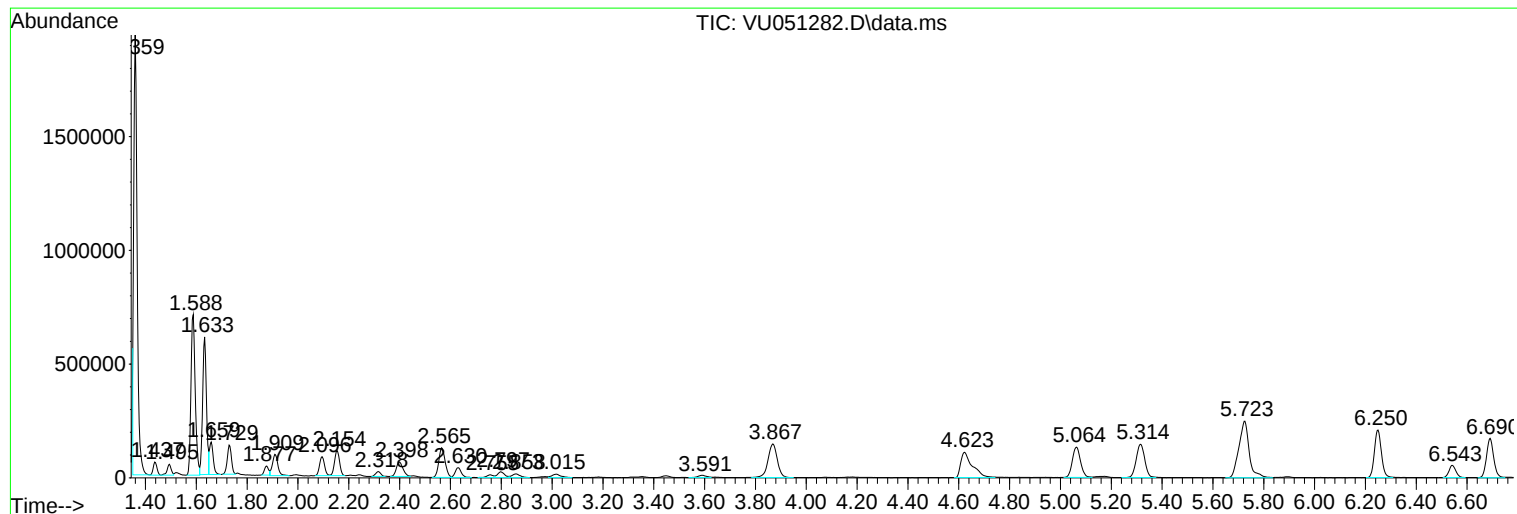
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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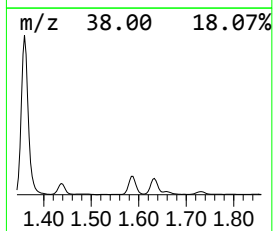
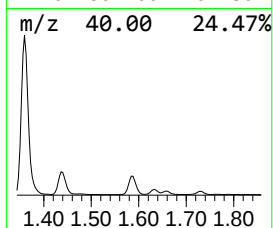
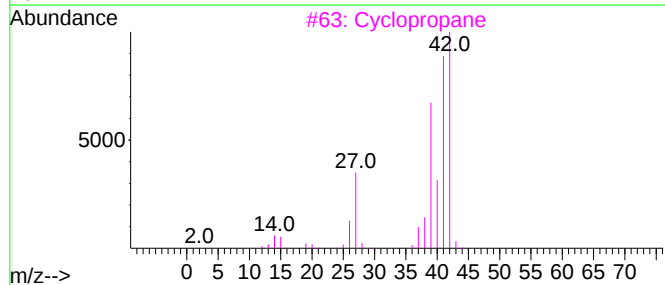
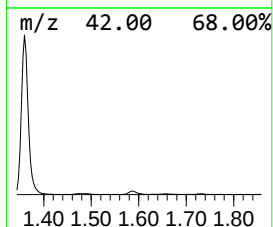
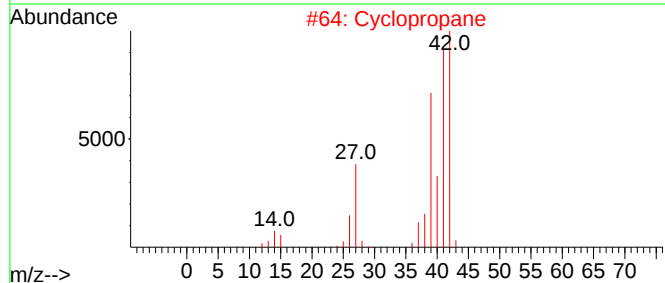
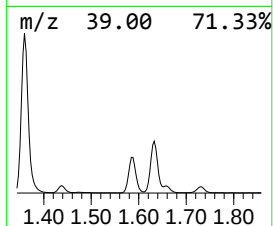
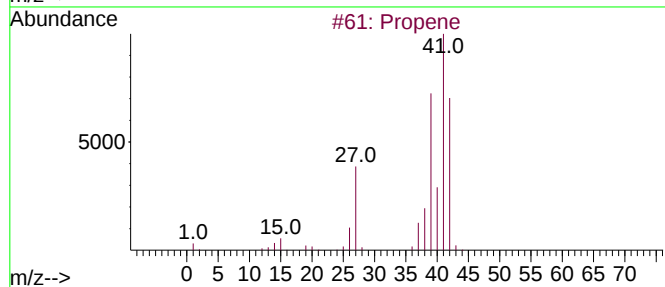
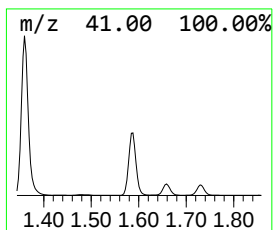
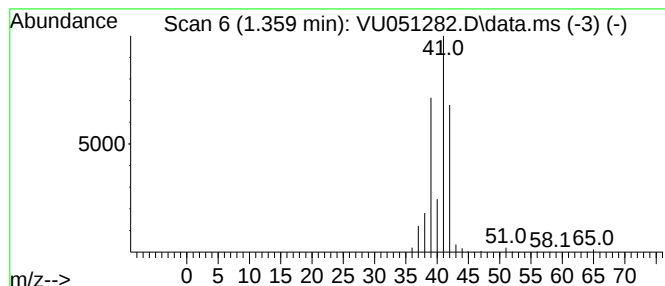
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.359	22.56 ug/L	1815010	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	86
2			Cyclopropane	42	C3H6	000075-19-4	80
3			Cyclopropane	42	C3H6	000075-19-4	72
4			Propene	42	C3H6	000115-07-1	47
5			Cyclopropane	42	C3H6	000075-19-4	37



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXZ58

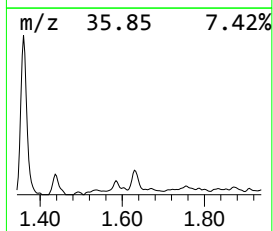
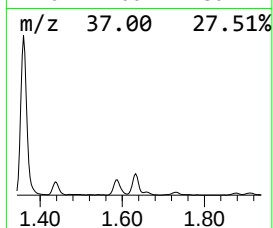
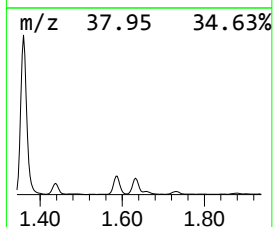
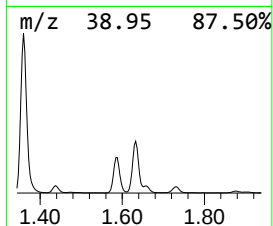
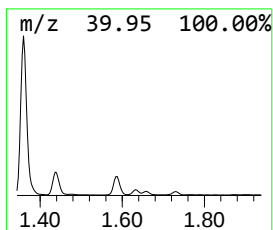
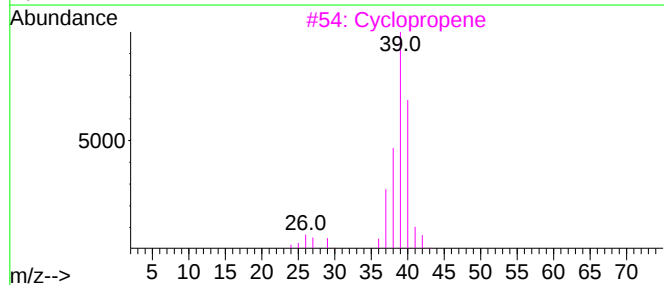
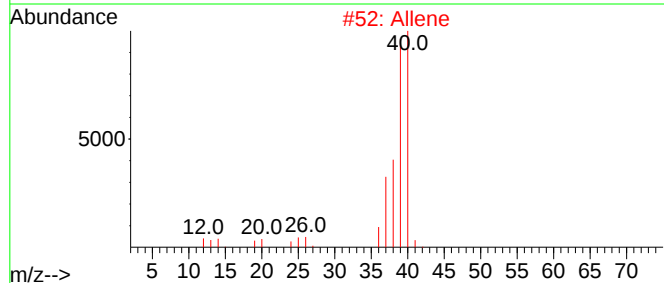
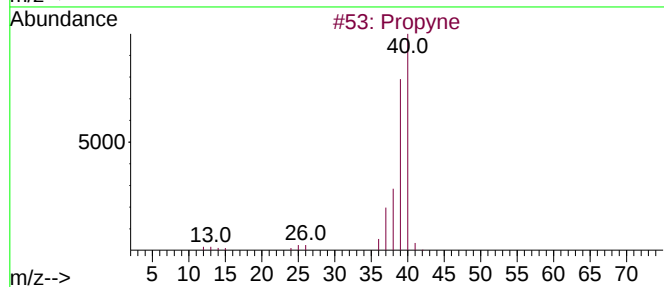
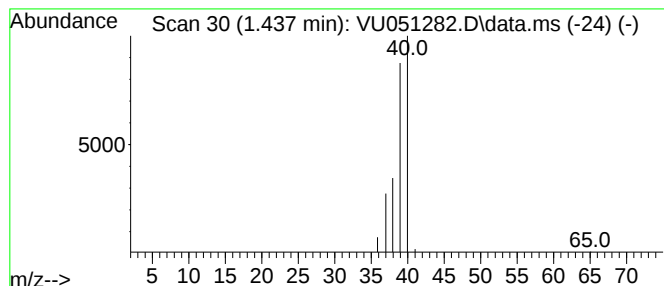
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Propyne Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.437	0.73 ug/L	58439	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propyne	40	C3H4	000074-99-7	90
2			Allene	40	C3H4	000463-49-0	83
3			Cyclopropene	40	C3H4	002781-85-3	43
4			Chloro(prop-2-yn-1-yloxy)methanone	118	C4H3ClO2	035718-08-2	2
5			Methylenecyclopropane	54	C4H6	006142-73-0	1



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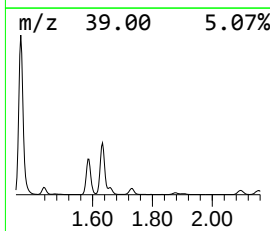
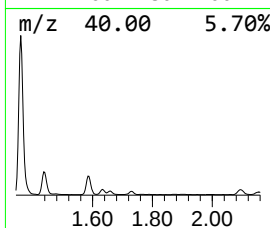
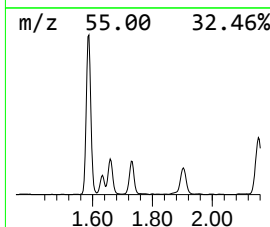
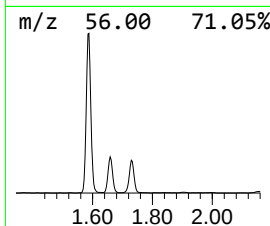
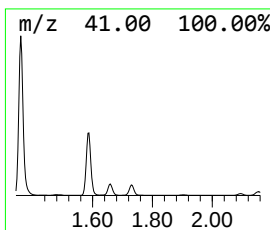
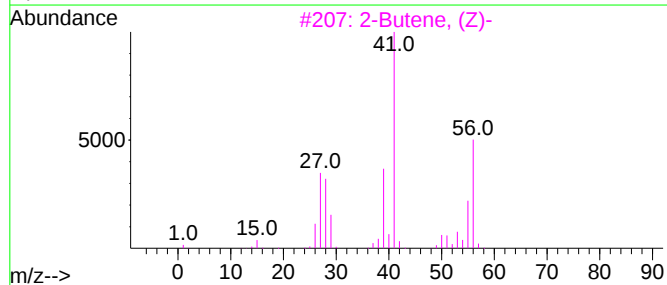
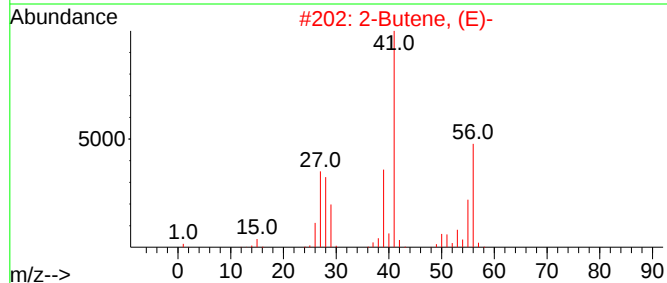
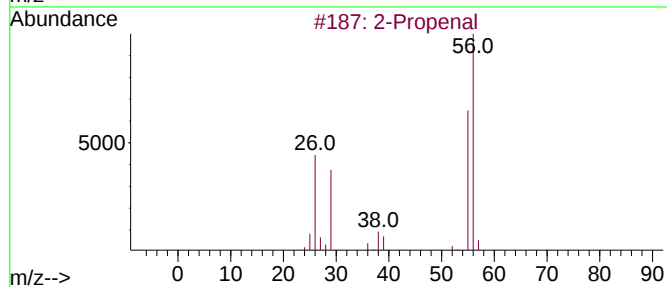
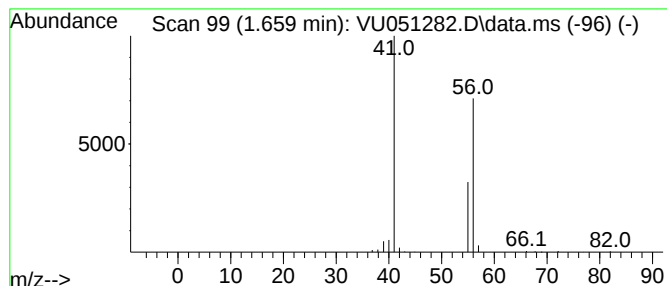
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.659	1.78 ug/L	142816	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenal			56	C3H4O	000107-02-8	33
2	2-Butene, (E)-			56	C4H8	000624-64-6	9
3	2-Butene, (Z)-			56	C4H8	000590-18-1	9
4	2-Butene			56	C4H8	000107-01-7	9
5	2-Butene, (Z)-			56	C4H8	000590-18-1	9



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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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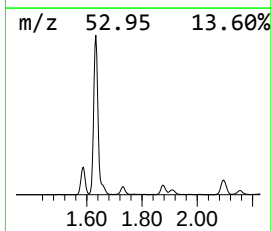
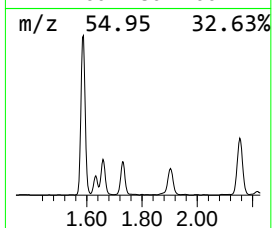
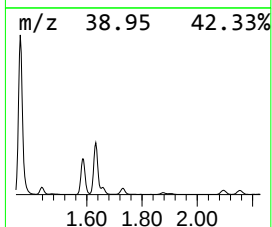
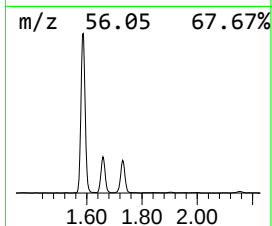
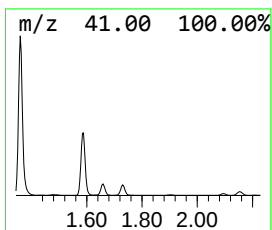
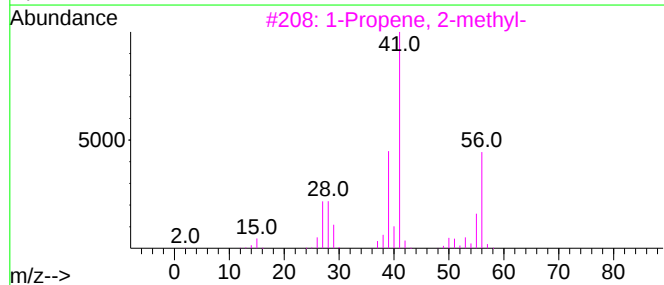
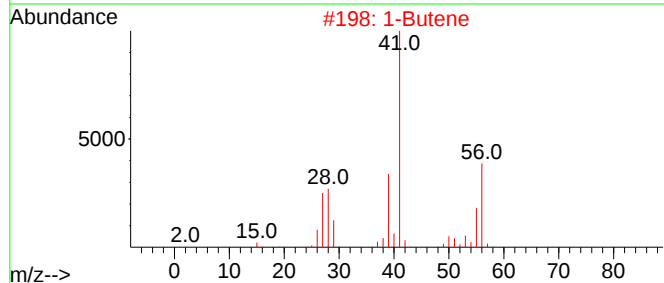
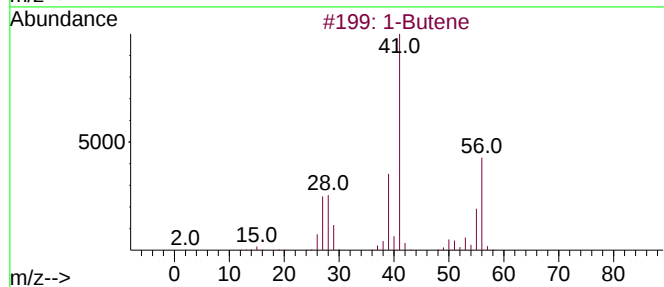
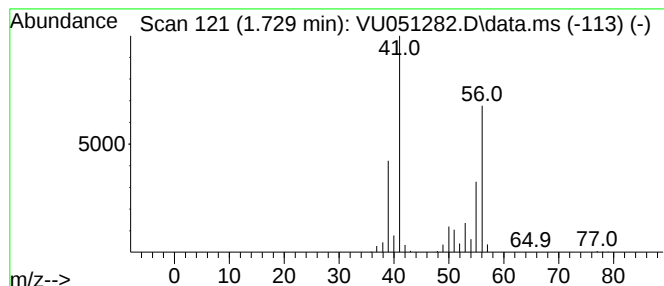
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.729	1.80 ug/L	145138	1,4-Difluorobenzene	6.250

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butene		56	C4H8	000106-98-9	87
2	1-Butene		56	C4H8	000106-98-9	83
3	1-Propene, 2-methyl-		56	C4H8	000115-11-7	72
4	1-Butene		56	C4H8	000106-98-9	72
5	2-Butene, (Z)-		56	C4H8	000590-18-1	68



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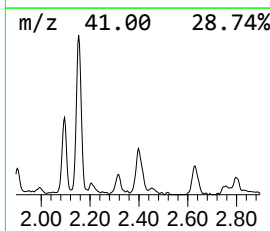
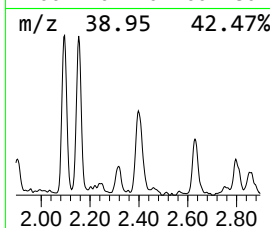
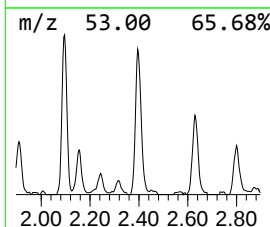
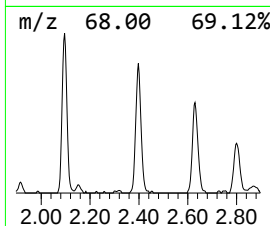
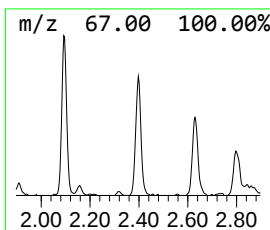
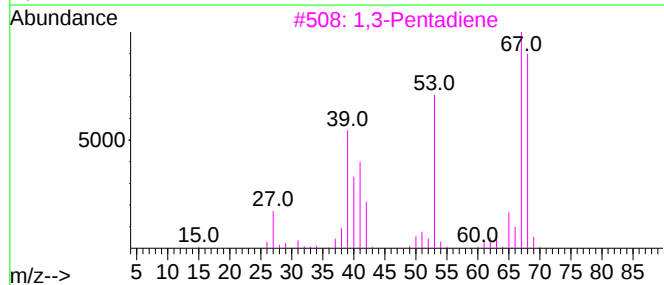
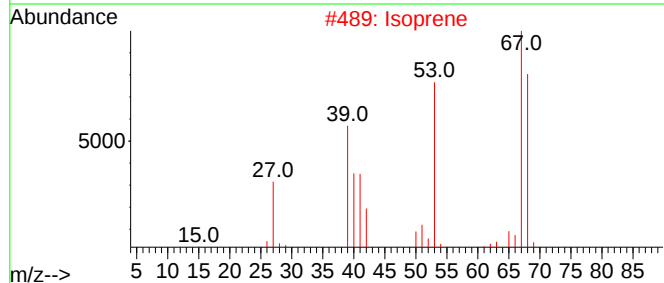
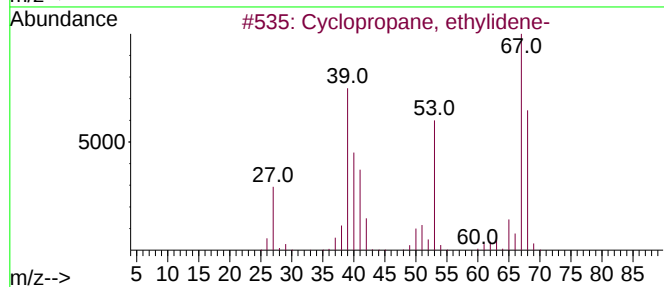
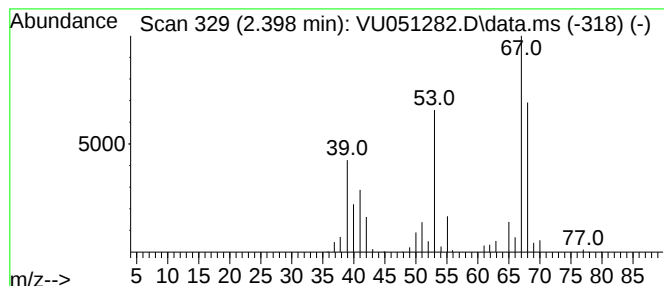
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Cyclopropane, ethylidene- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.398	1.47 ug/L	118043	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, ethylidene-	68	C5H8	018631-83-9	95
2			Isoprene	68	C5H8	000078-79-5	95
3			1,3-Pentadiene	68	C5H8	000504-60-9	95
4			1,3-Pentadiene, (Z)-	68	C5H8	001574-41-0	94
5			1,3-Pentadiene, (E)-	68	C5H8	002004-70-8	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100722\
Data File : VU051282.D
Acq On : 08 Oct 2022 19:21
Operator : JC/MD
Sample : N4873-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXZ58

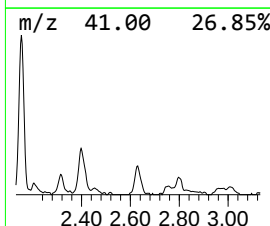
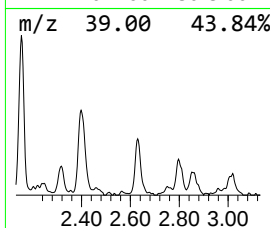
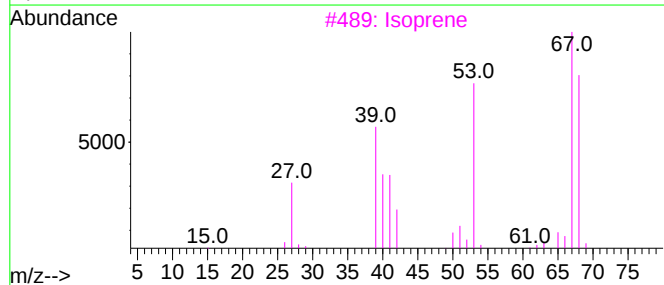
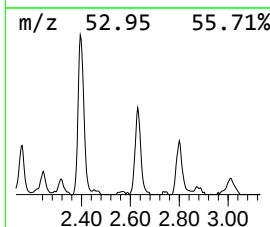
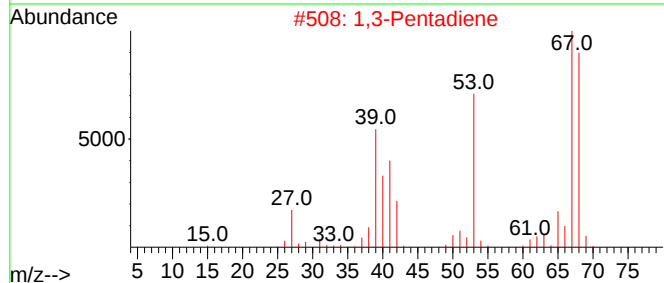
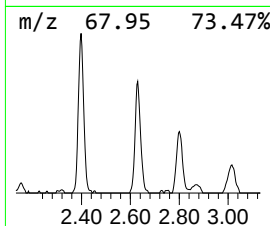
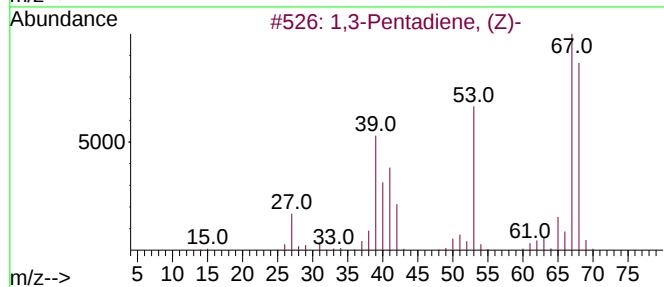
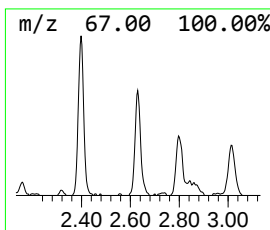
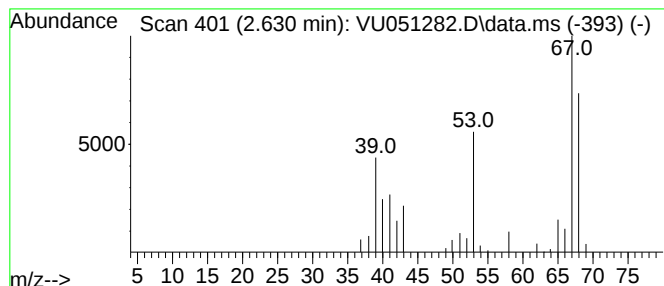
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 1,3-Pentadiene, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.630	0.89 ug/L	71924	1,4-Difluorobenzene	6.250

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Pentadiene, (Z)-	68	C5H8	001574-41-0	95
2		1,3-Pentadiene	68	C5H8	000504-60-9	95
3		Isoprene	68	C5H8	000078-79-5	94
4		1,3-Pentadiene, (E)-	68	C5H8	002004-70-8	94
5		1,3-Pentadiene, (Z)-	68	C5H8	001574-41-0	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100722\
Data File : VU051282.D
Acq On : 08 Oct 2022 19:21
Operator : JC/MD
Sample : N4873-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXZ58

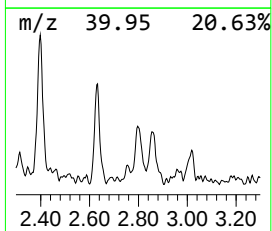
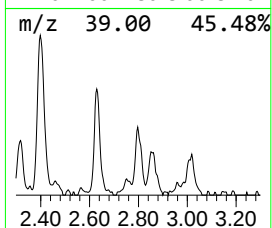
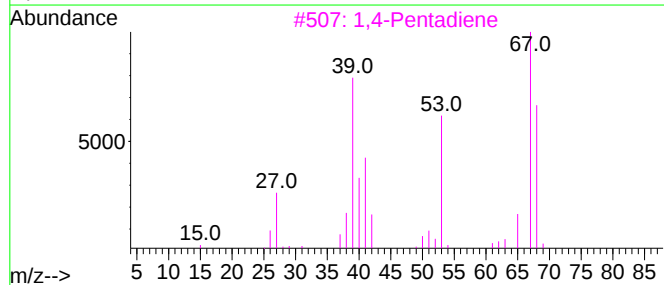
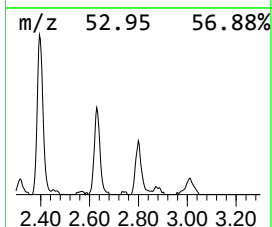
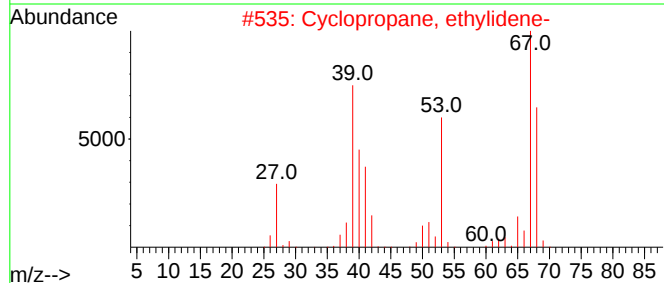
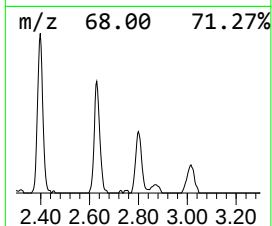
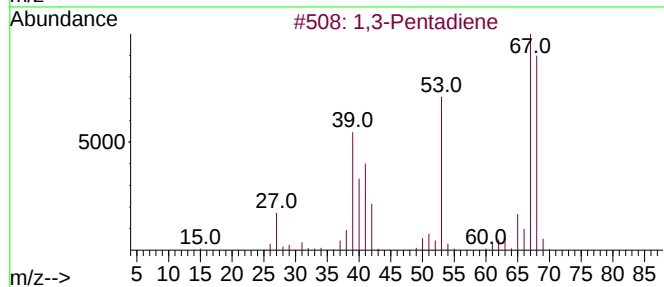
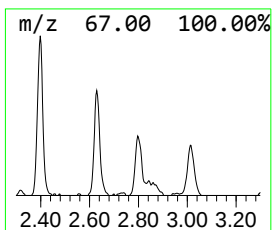
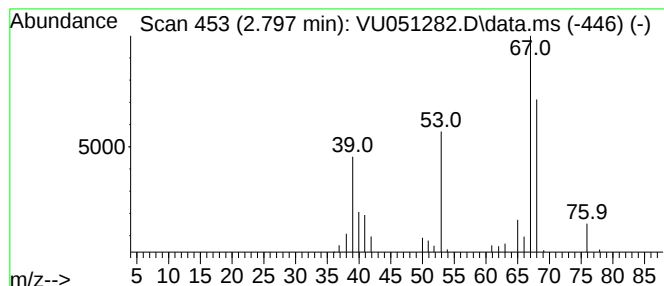
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 1,3-Pentadiene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.797	0.58 ug/L	47047	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Pentadiene	68	C5H8	000504-60-9	91
2			Cyclopropane, ethylidene-	68	C5H8	018631-83-9	91
3			1,4-Pentadiene	68	C5H8	000591-93-5	90
4			1,3-Pentadiene	68	C5H8	000504-60-9	90
5			1,3-Pentadiene, (E)-	68	C5H8	002004-70-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100722\
Data File : VU051282.D
Acq On : 08 Oct 2022 19:21
Operator : JC/MD
Sample : N4873-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXZ58

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	1.359	22.6	ug/L	1815010	1	6.250	402217	5.0
Propyne	1.437	0.7	ug/L	58439	1	6.250	402217	5.0
unknown-01	1.659	1.8	ug/L	142816	1	6.250	402217	5.0
(DEL) Alkane: S...	1.729	1.8	ug/L	145138	1	6.250	402217	5.0
Cyclopropane, e...	2.398	1.5	ug/L	118043	1	6.250	402217	5.0
1,3-Pentadiene,...	2.630	0.9	ug/L	71924	1	6.250	402217	5.0
1,3-Pentadiene	2.797	0.6	ug/L	47047	1	6.250	402217	5.0