

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112421\
 Data File : VU046003.D
 Acq On : 24 Nov 2021 18:38
 Operator : SY/MD
 Sample : M4722-07
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0G28

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\SFAMUTR111521WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU046003.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.363	3	7	21	rVB	110494	104905	15.70%	1.859%
2	1.491	37	47	53	rBV2	14107	16049	2.40%	0.284%
3	1.604	69	82	93	rBV4	166297	266107	39.82%	4.717%
4	1.662	94	100	110	rVB2	24516	29677	4.44%	0.526%
5	1.736	115	123	134	rVB2	25759	33498	5.01%	0.594%
6	1.916	168	179	193	rVB	34450	49236	7.37%	0.873%
7	1.999	197	205	213	rVB2	7877	10785	1.61%	0.191%
8	2.160	245	255	263	rVB3	7999	10819	1.62%	0.192%
9	2.208	263	270	280	rBV3	6465	10306	1.54%	0.183%
10	2.572	368	383	396	rBV	53992	86974	13.01%	1.542%
11	2.691	401	420	433	rBV4	7776	20401	3.05%	0.362%
12	2.800	441	454	469	rVB	142783	240549	36.00%	4.264%
13	3.051	520	532	551	rVB3	25906	54434	8.15%	0.965%
14	3.353	608	626	644	rBV2	9923	36921	5.52%	0.654%
15	3.707	722	736	749	rBV3	8511	18424	2.76%	0.327%
16	4.536	982	994	1008	rBV4	6350	14614	2.19%	0.259%
17	4.652	1013	1030	1069	rBV2	47385	218112	32.64%	3.866%
18	5.070	1140	1160	1184	rBV3	71616	204909	30.66%	3.632%
19	5.729	1344	1365	1375	rBV2	129743	343567	51.41%	6.090%
20	6.253	1514	1528	1547	rBV	106371	201239	30.11%	3.567%
21	6.694	1652	1665	1682	rVV	84474	164439	24.61%	2.915%
22	6.790	1682	1695	1708	rVB	5293	11889	1.78%	0.211%
23	7.568	1926	1937	1954	rBV	30247	52646	7.88%	0.933%
24	7.797	1994	2008	2028	rBV	59707	117398	17.57%	2.081%
25	7.899	2028	2040	2051	rVV	152062	267658	40.05%	4.744%
26	7.970	2051	2062	2096	rVB	372585	668263	100.00%	11.845%
27	8.179	2117	2127	2138	rBV2	19443	32132	4.81%	0.570%
28	8.639	2257	2270	2304	rBV	233053	490809	73.45%	8.700%
29	8.970	2363	2373	2386	rVB3	6143	10658	1.59%	0.189%
30	9.420	2500	2513	2532	rBV	152756	258616	38.70%	4.584%
31	9.571	2548	2560	2569	rBV	27318	45063	6.74%	0.799%
32	9.636	2569	2580	2589	rVV2	206670	339502	50.80%	6.018%
33	9.694	2589	2598	2615	rVV	114296	199107	29.79%	3.529%
34	9.777	2617	2624	2636	rVB2	6729	11055	1.65%	0.196%
35	9.919	2657	2668	2682	rVB4	4142	6870	1.03%	0.122%
36	10.102	2714	2725	2741	rBV	54573	90604	13.56%	1.606%

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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\SFAMUTR111521WMA.M
Title : TRACE VOA SFAM1.0

37	10.758	2918	2929	2945	rVB	75921	121771	18.22%	2.158%
38	10.999	2994	3004	3011	rBV3	5968	10456	1.56%	0.185%
39	11.468	3141	3150	3161	rBV2	8977	12518	1.87%	0.222%
40	11.812	3246	3257	3272	rVV	159199	252818	37.83%	4.481%
41	12.060	3322	3334	3364	rBV	102482	213551	31.96%	3.785%
42	12.195	3365	3376	3394	rVB	167775	276938	41.44%	4.909%
43	12.375	3423	3432	3447	rVB5	8747	15338	2.30%	0.272%

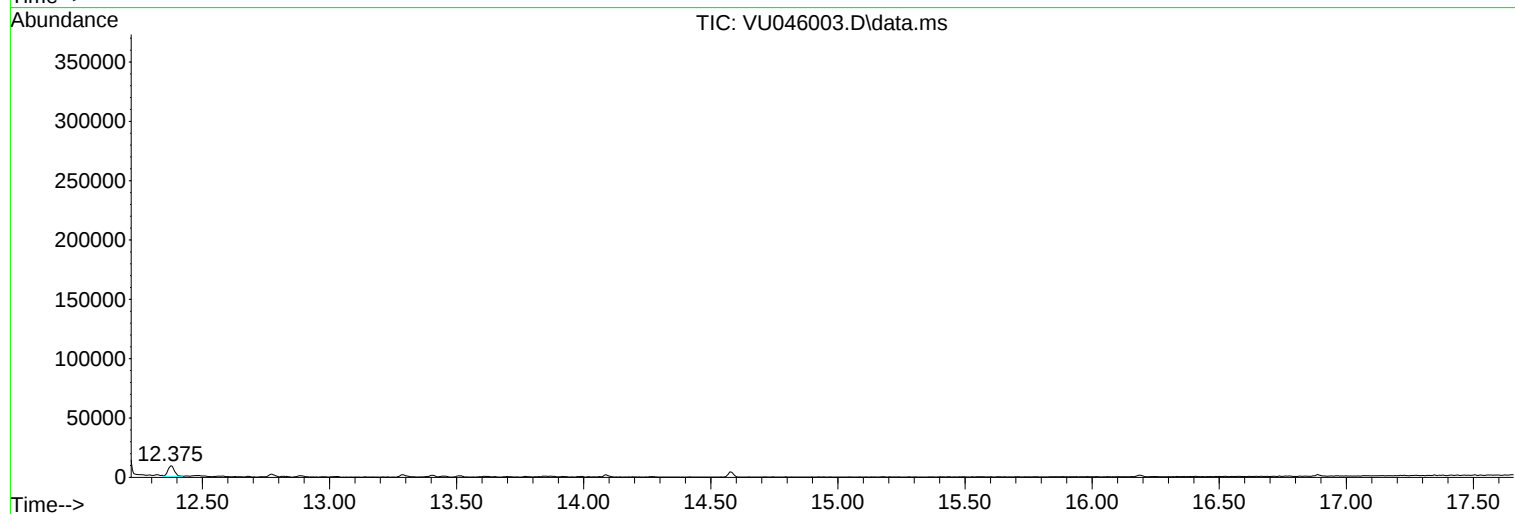
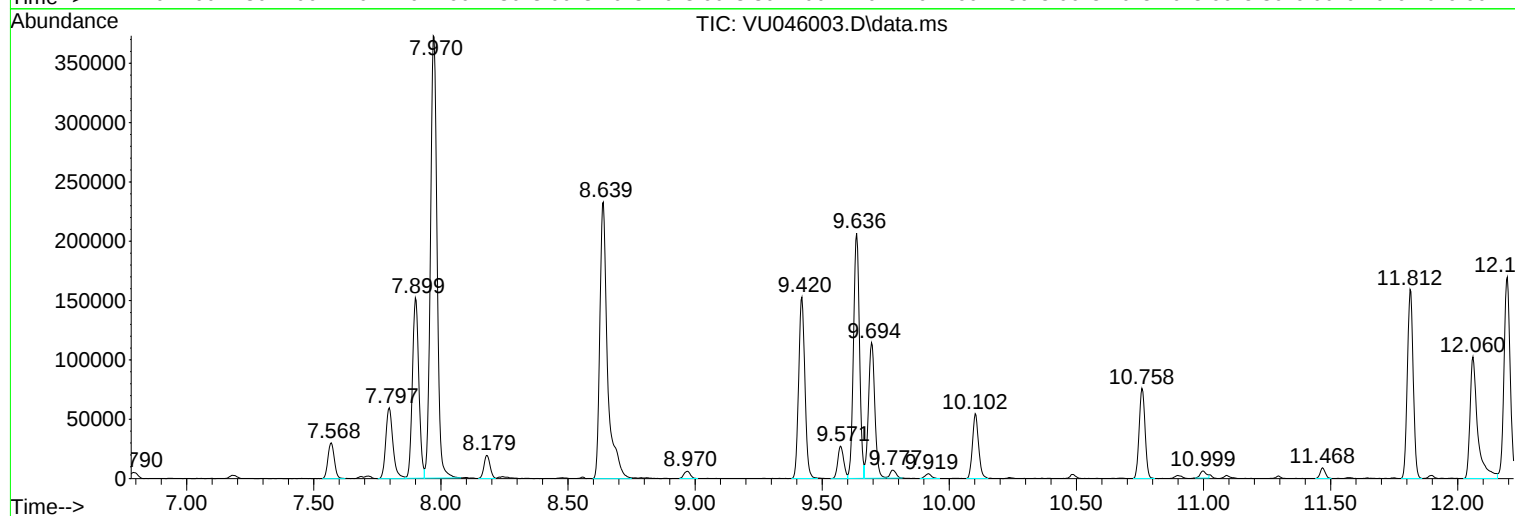
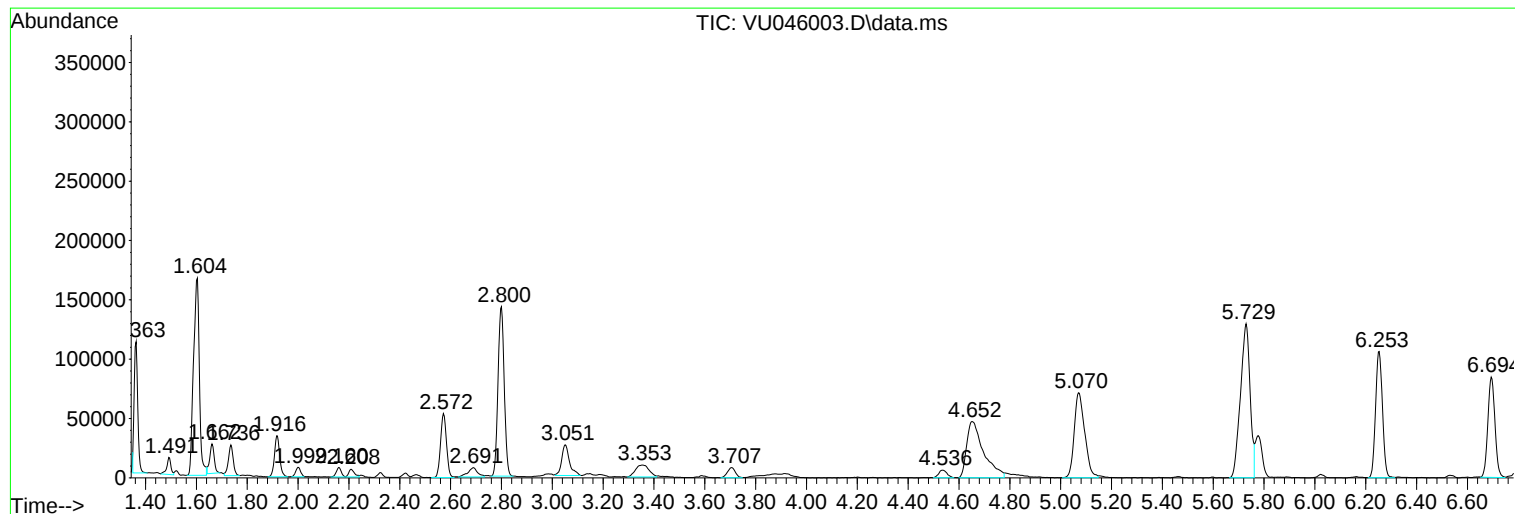
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111521WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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Misc : 25.0mL/MSVOA_U/WATER
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Instrument :
MSVOA_U
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C0G28

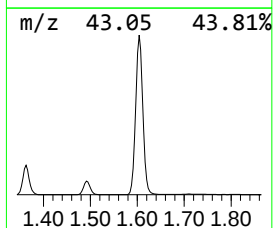
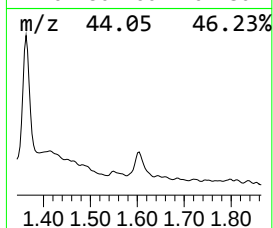
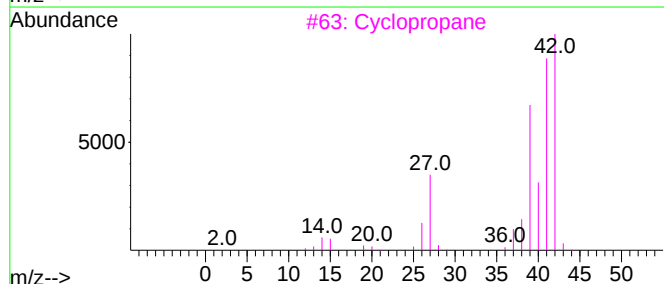
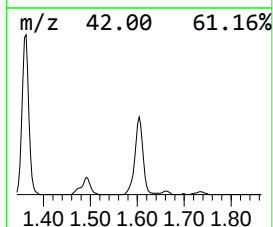
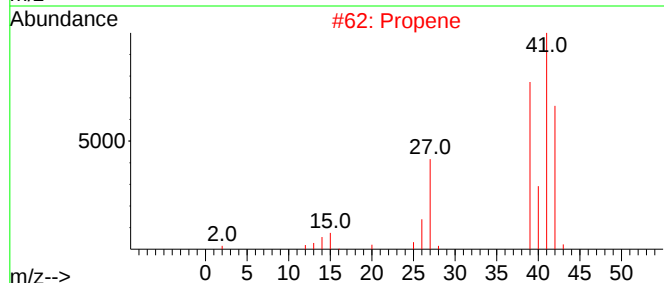
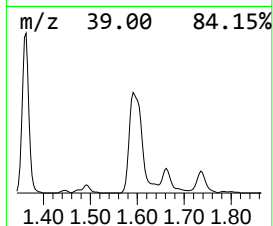
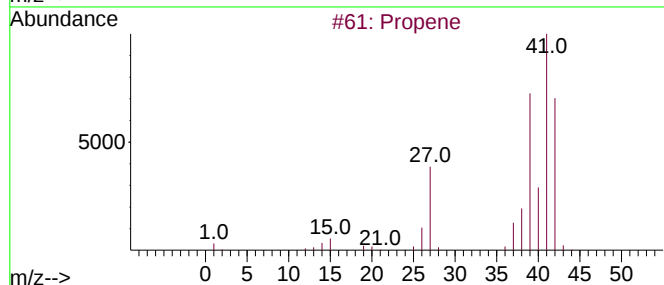
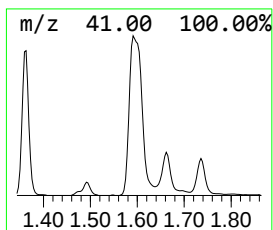
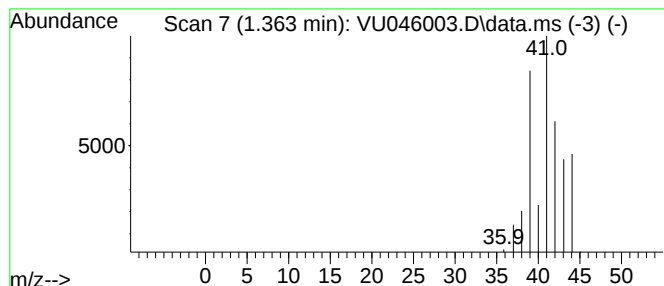
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.363	2.61 ug/L	104905	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	86
2			Propene	42	C3H6	000115-07-1	42
3			Cyclopropane	42	C3H6	000075-19-4	40
4			Cyclopropane	42	C3H6	000075-19-4	7
5			Cyclopropene	40	C3H4	002781-85-3	5



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Instrument :
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ClientSampleId :
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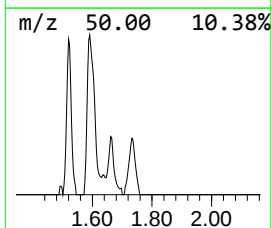
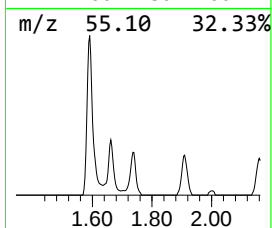
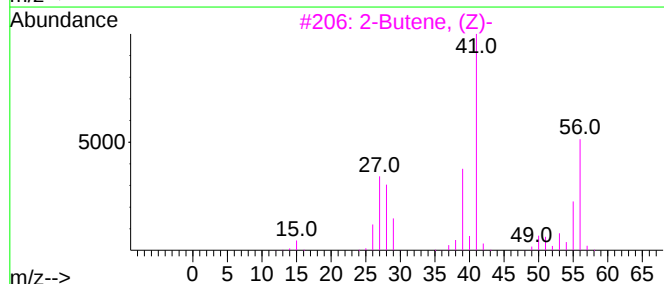
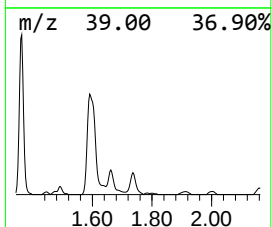
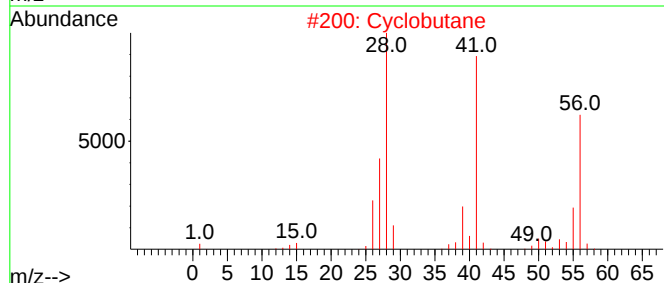
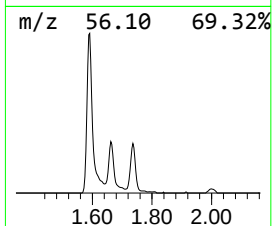
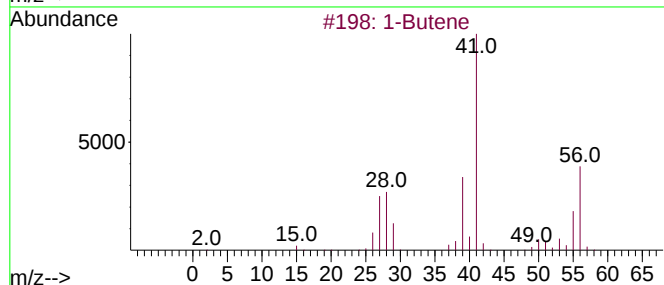
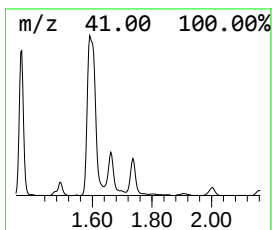
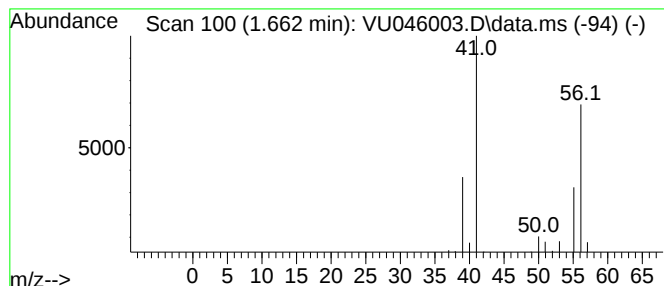
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111521WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.662	0.74 ug/L	29677	1,4-Difluorobenzene	6.253

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Butene	56	C4H8	000106-98-9	80
2		Cyclobutane	56	C4H8	000287-23-0	72
3		2-Butene, (Z)-	56	C4H8	000590-18-1	72
4		2-Butene, (E)-	56	C4H8	000624-64-6	72
5		1-Butene	56	C4H8	000106-98-9	72



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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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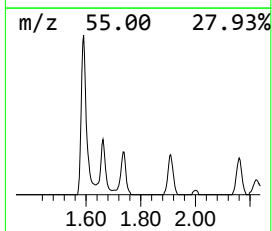
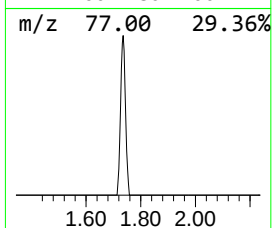
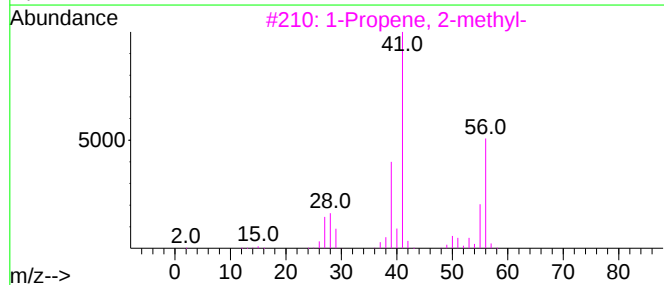
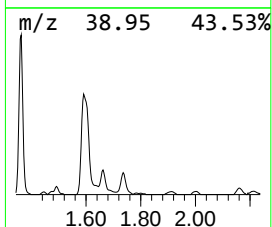
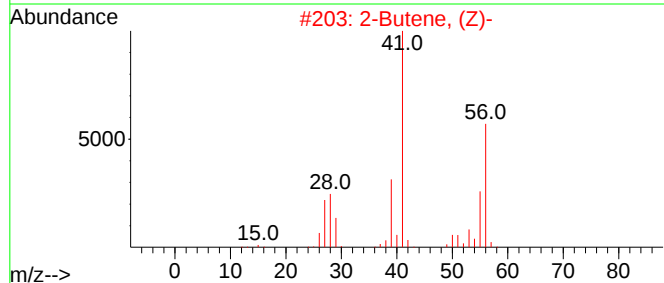
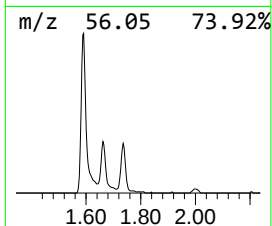
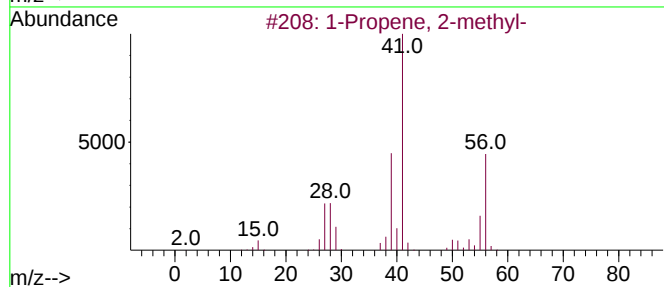
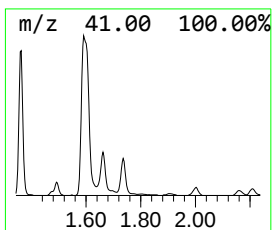
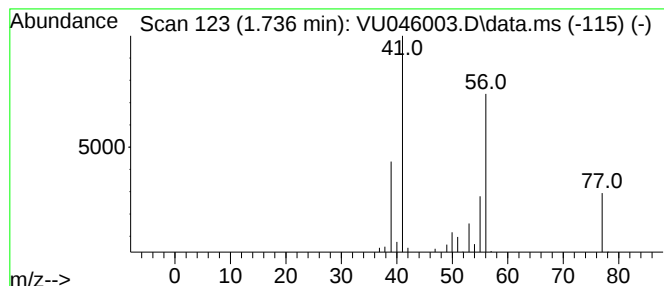
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111521WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.736	0.83 ug/L	33498	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-methyl-			56	C4H8	000115-11-7	64
2	2-Butene, (Z)-			56	C4H8	000590-18-1	64
3	1-Propene, 2-methyl-			56	C4H8	000115-11-7	64
4	2-Butene			56	C4H8	000107-01-7	62
5	2-Butene, (Z)-			56	C4H8	000590-18-1	58



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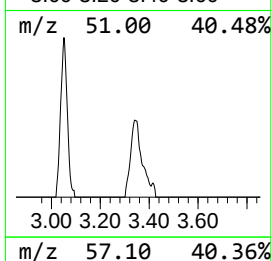
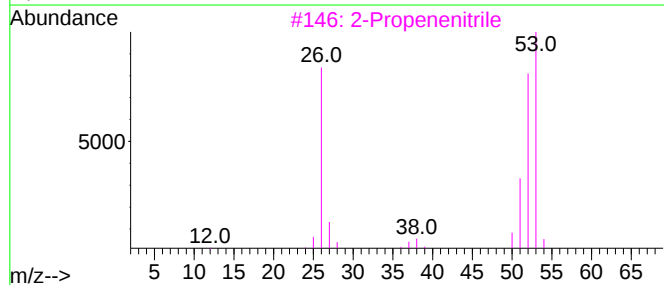
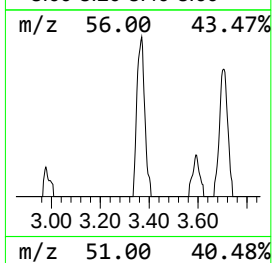
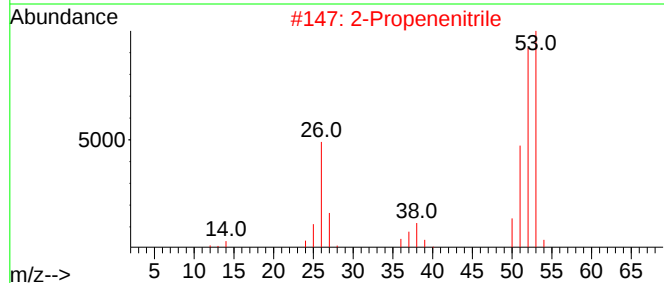
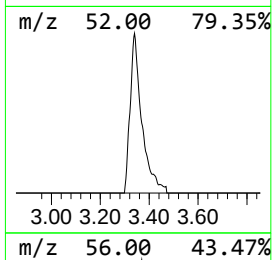
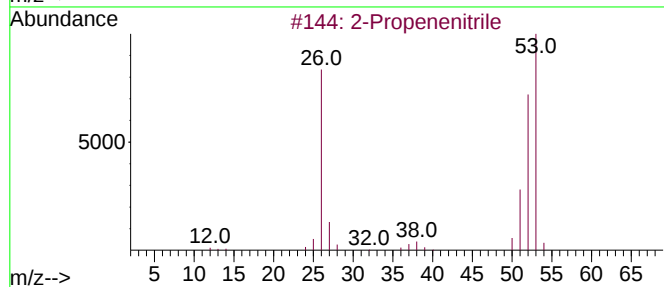
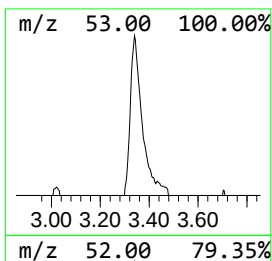
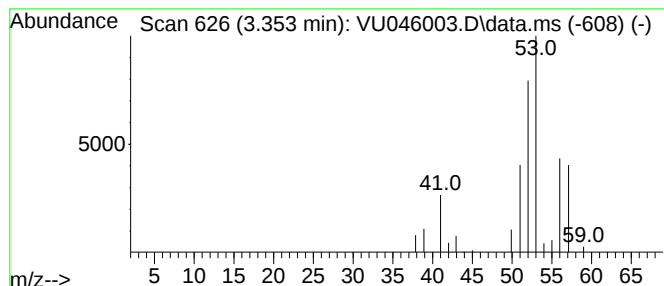
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111521WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 2-Propenenitrile Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.353	0.92 ug/L	36921	1,4-Difluorobenzene	6.253

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propenenitrile	53	C3H3N	000107-13-1	80
2		2-Propenenitrile	53	C3H3N	000107-13-1	80
3		2-Propenenitrile	53	C3H3N	000107-13-1	72
4		2-Propenenitrile	53	C3H3N	000107-13-1	72
5		1-Buten-3-yne	52	C4H4	000689-97-4	5



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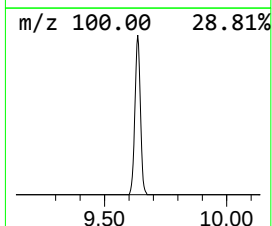
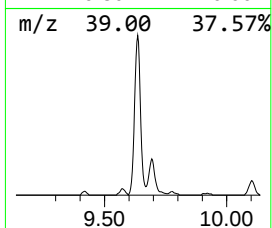
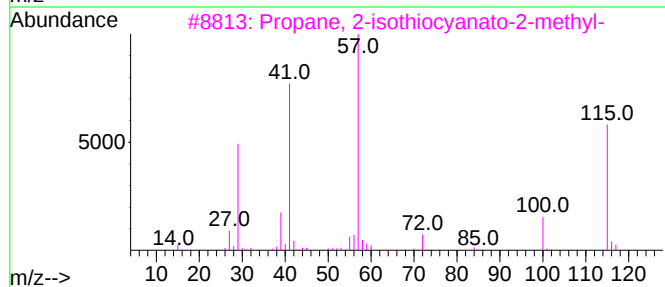
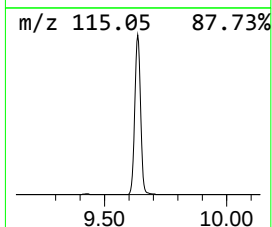
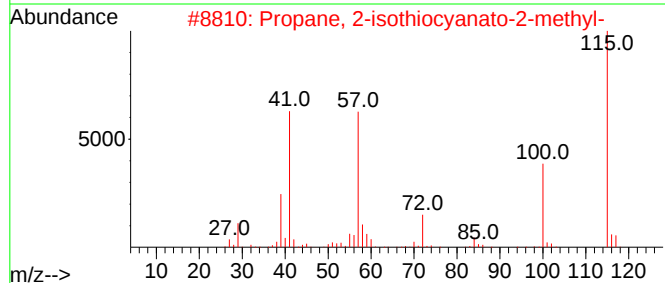
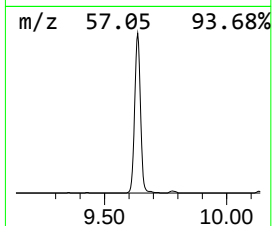
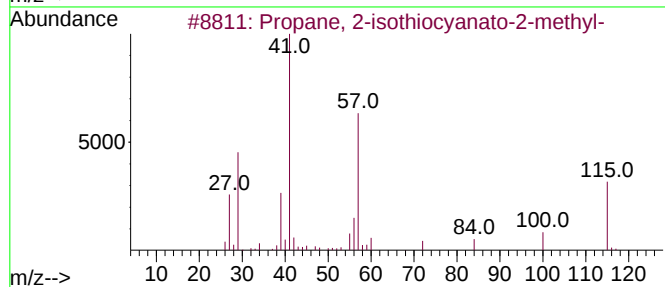
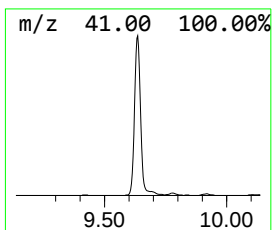
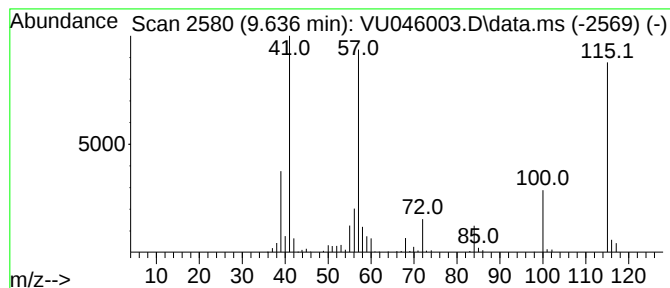
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 Propane, 2-isothiocyanato-2... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.636	6.56 ug/L	339502	Chlorobenzene-d5	9.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-isothiocyanato-2-methyl-	115	C5H9NS	000590-42-1	90
2			Propane, 2-isothiocyanato-2-methyl-	115	C5H9NS	000590-42-1	81
3			Propane, 2-isothiocyanato-2-methyl-	115	C5H9NS	000590-42-1	72
4			Butane, 2-isothiocyanato-	115	C5H9NS	004426-79-3	59
5			Isobutyl isothiocyanate	115	C5H9NS	000591-82-2	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112421\
Data File : VU046003.D
Acq On : 24 Nov 2021 18:38
Operator : SY/MD
Sample : M4722-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0G28

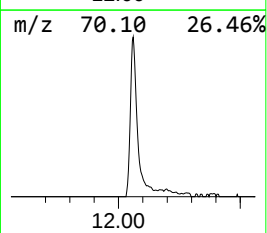
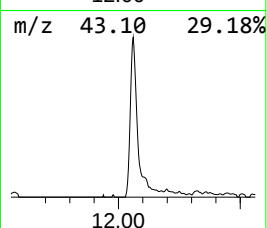
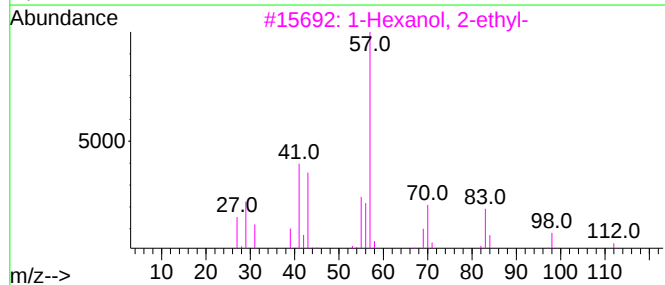
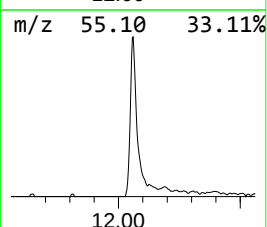
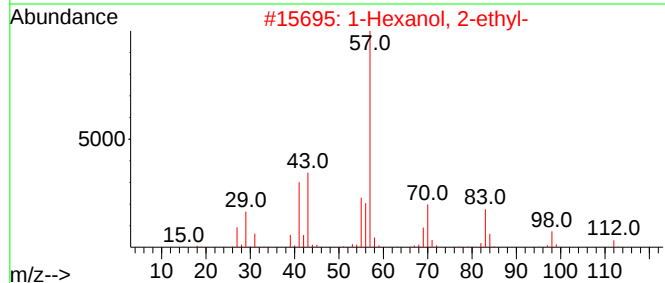
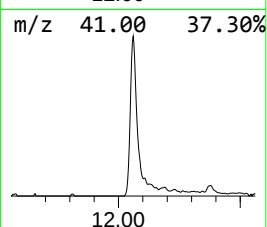
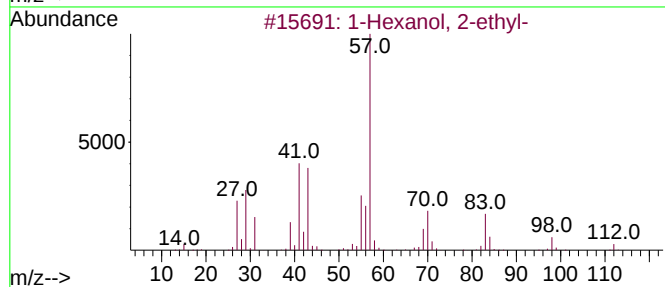
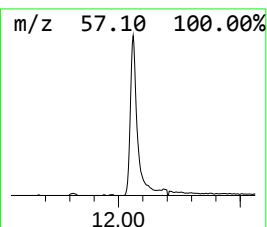
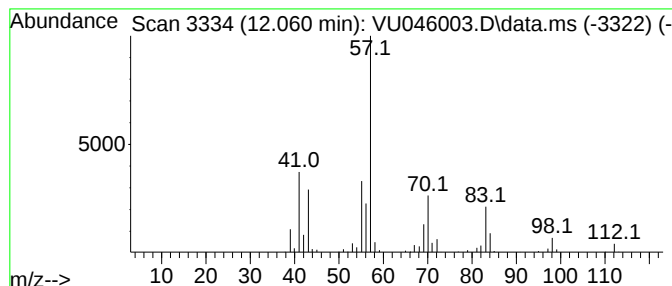
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.060	4.22 ug/L	213551	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
5			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112421\
 Data File : VU046003.D
 Acq On : 24 Nov 2021 18:38
 Operator : SY/MD
 Sample : M4722-07
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0G28

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111521WMA.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...	1.363	2.6	ug/L	104905	1	6.253	201239	5.0
(DEL) Alkane: S...	1.662	0.7	ug/L	29677	1	6.253	201239	5.0
(DEL) Alkane: S...	1.736	0.8	ug/L	33498	1	6.253	201239	5.0
2-Propenenitrile	3.353	0.9	ug/L	36921	1	6.253	201239	5.0
Propane, 2-isot...	9.636	6.6	ug/L	339502	2	9.420	258616	5.0
1-Hexanol, 2-et...	12.060	4.2	ug/L	213551	3	11.816	252818	5.0