

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112321\
 Data File : VU045967.D
 Acq On : 23 Nov 2021 19:42
 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: VU045967.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	18	rVB	108495	102683	15.40%	1.763%
2	1.491	38	47	54	rBV	14079	14758	2.21%	0.253%
3	1.604	69	82	93	rBV3	167761	267236	40.07%	4.589%
4	1.662	94	100	110	rVB2	24982	30695	4.60%	0.527%
5	1.736	115	123	132	rVB	22237	28435	4.26%	0.488%
6	1.919	170	180	193	rVB	36877	52532	7.88%	0.902%
7	1.999	193	205	216	rVB	8052	11256	1.69%	0.193%
8	2.163	247	256	263	rBV2	7341	10311	1.55%	0.177%
9	2.211	263	271	279	rBV4	6101	10061	1.51%	0.173%
10	2.572	372	383	399	rBV	60122	97284	14.59%	1.671%
11	2.691	399	420	432	rBV2	8667	22178	3.33%	0.381%
12	2.800	441	454	474	rVB	143136	241502	36.21%	4.147%
13	3.051	520	532	554	rVB2	26297	57401	8.61%	0.986%
14	3.340	607	622	624	rBV2	8851	14575	2.19%	0.250%
15	3.707	724	736	749	rBV3	8458	18170	2.72%	0.312%
16	4.536	981	994	1007	rBV3	6689	14779	2.22%	0.254%
17	4.652	1011	1030	1074	rBV2	47647	219374	32.89%	3.767%
18	5.070	1136	1160	1198	rVB3	74647	218362	32.74%	3.750%
19	5.729	1344	1365	1375	rBV2	137104	363398	54.48%	6.240%
20	6.253	1511	1528	1544	rBV	108346	203009	30.44%	3.486%
21	6.694	1650	1665	1684	rBV	87785	170170	25.51%	2.922%
22	6.793	1684	1696	1709	rVB6	5377	10747	1.61%	0.185%
23	7.568	1925	1937	1953	rBV	32432	54399	8.16%	0.934%
24	7.796	1995	2008	2028	rBV	62977	125167	18.77%	2.149%
25	7.899	2028	2040	2051	rVV	163163	287681	43.13%	4.940%
26	7.970	2051	2062	2097	rVB	378468	666985	100.00%	11.453%
27	8.179	2117	2127	2140	rBV	20990	34296	5.14%	0.589%
28	8.636	2257	2269	2307	rBV	249005	525288	78.76%	9.020%
29	8.967	2361	2372	2382	rVB3	6624	10971	1.64%	0.188%
30	9.420	2500	2513	2531	rBV	156154	265658	39.83%	4.562%
31	9.571	2550	2560	2568	rBV	27728	43982	6.59%	0.755%
32	9.636	2568	2580	2589	rVV2	219098	355465	53.29%	6.104%
33	9.694	2589	2598	2615	rVV	113046	197374	29.59%	3.389%
34	9.780	2617	2625	2639	rVB2	7918	12804	1.92%	0.220%
35	9.919	2657	2668	2680	rBV5	4516	7665	1.15%	0.132%
36	10.102	2714	2725	2743	rBV	51678	88570	13.28%	1.521%

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37	10.758	2917	2929	2945	rVB	81189	130047	19.50%	2.233%
38	10.999	2987	3004	3010	rBV3	7348	12380	1.86%	0.213%
39	11.468	3140	3150	3161	rVB2	9188	12909	1.94%	0.222%
40	11.812	3245	3257	3272	rVB	160541	253471	38.00%	4.353%
41	12.060	3321	3334	3364	rBV	118748	247749	37.14%	4.254%
42	12.195	3364	3376	3394	rVB	174853	296317	44.43%	5.088%
43	12.375	3423	3432	3444	rVB4	8787	15392	2.31%	0.264%

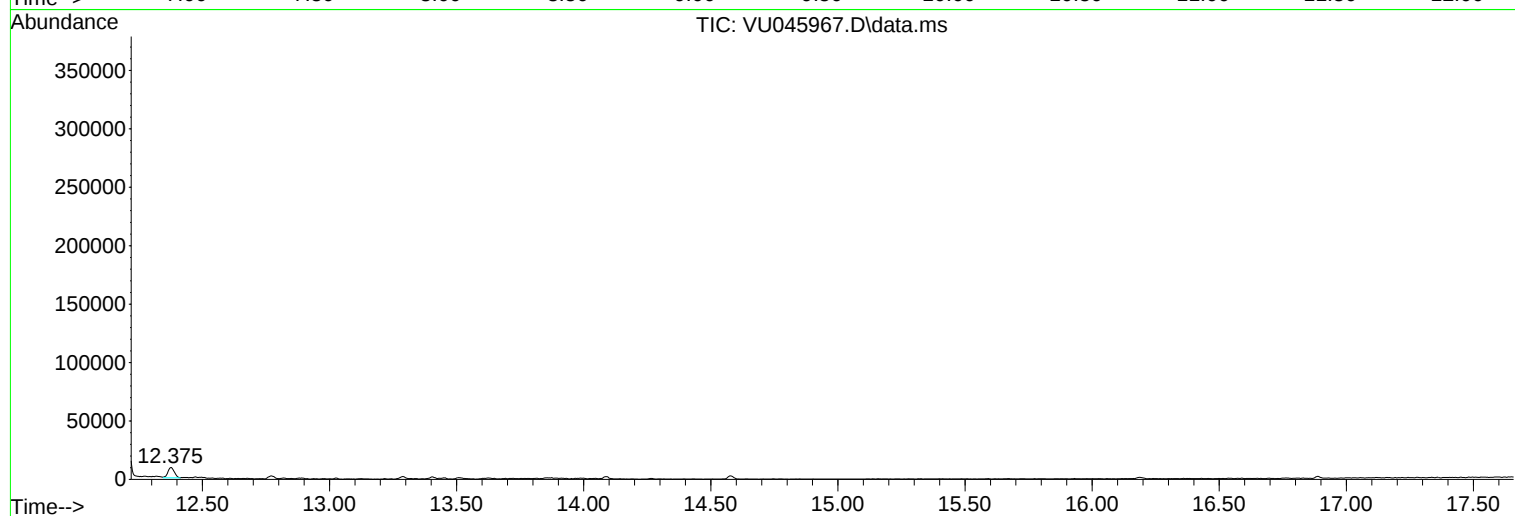
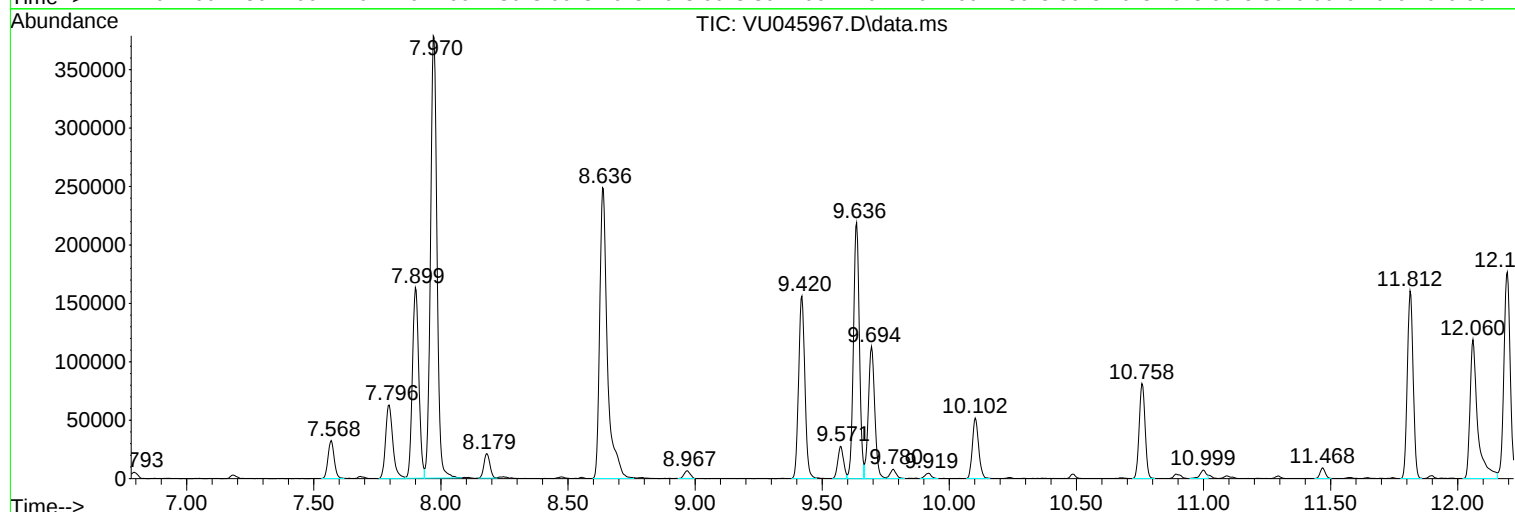
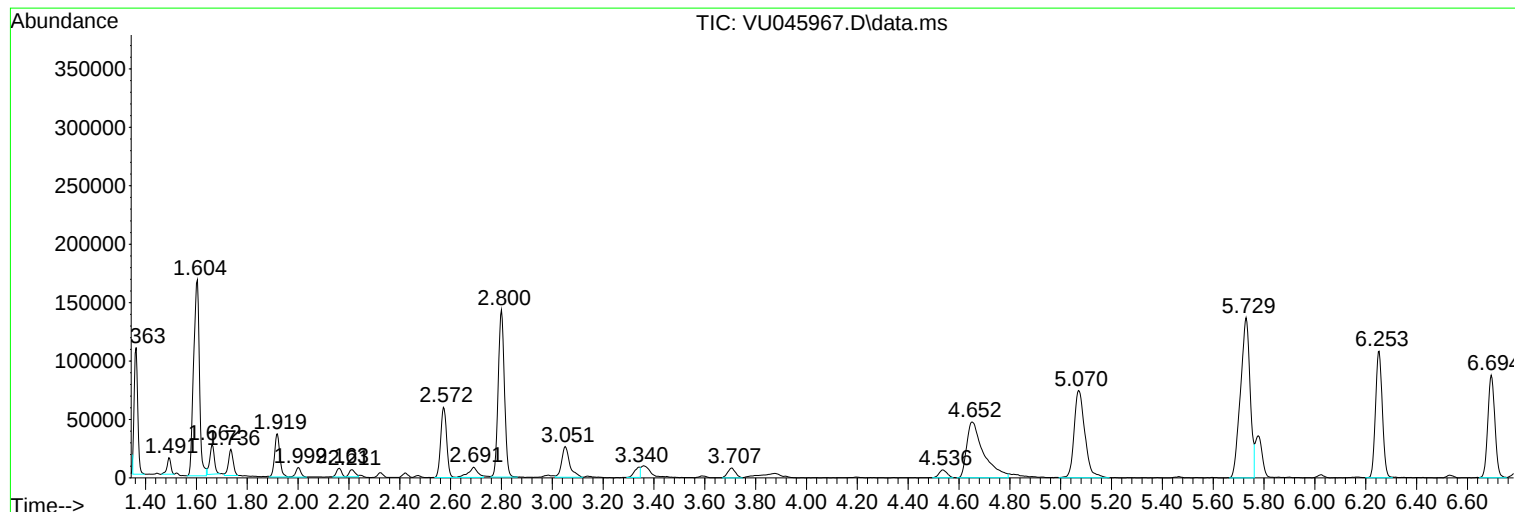
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111521WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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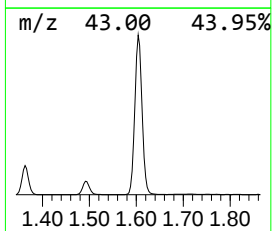
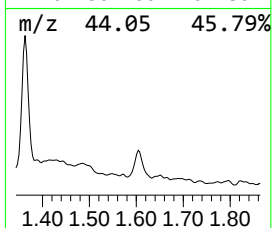
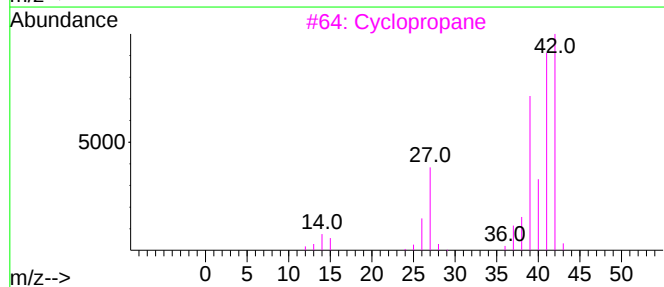
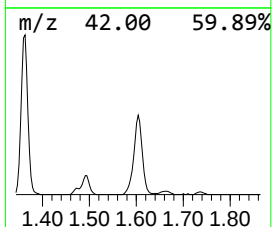
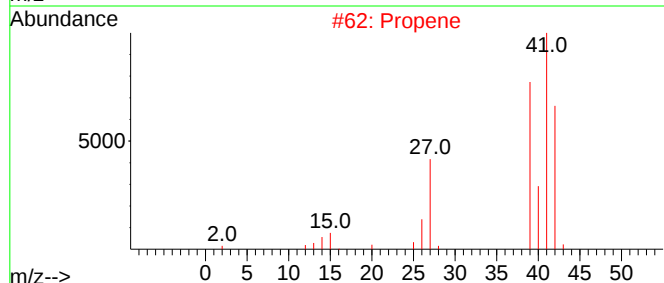
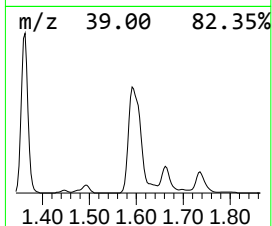
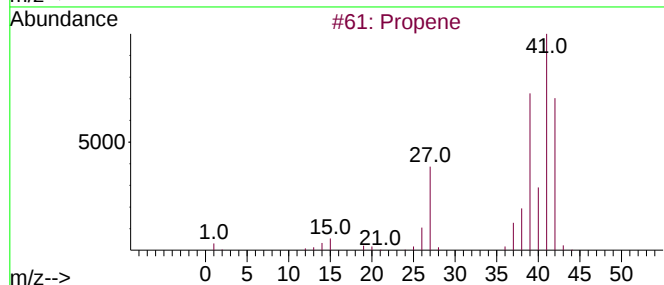
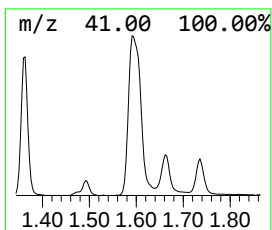
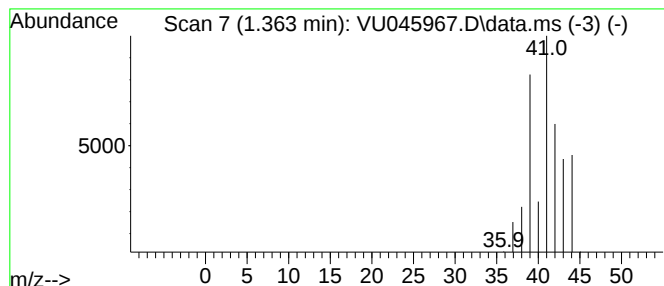
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Quant Title : TRACE VOA SFAM1.0

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	2.53 ug/L	102683	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	9
4		Cyclopropane	42	C3H6	000075-19-4	7
5		Cyclopropene	40	C3H4	002781-85-3	5



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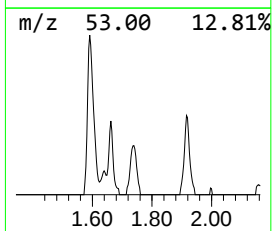
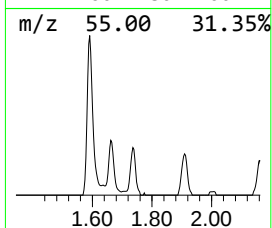
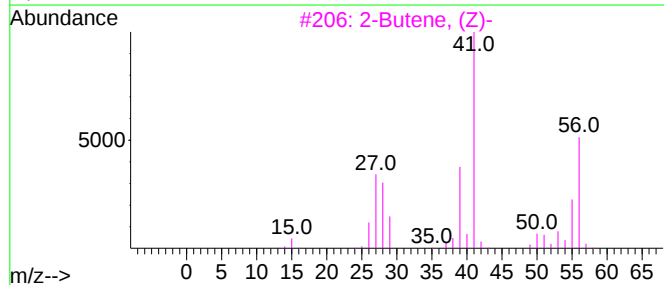
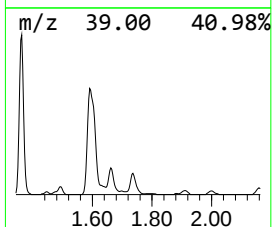
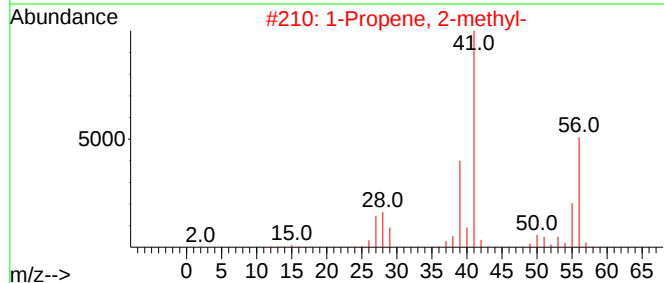
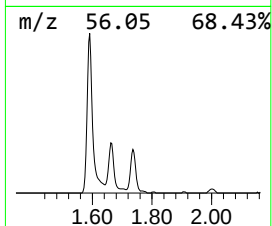
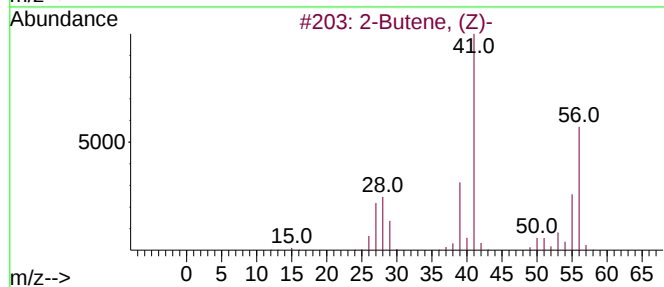
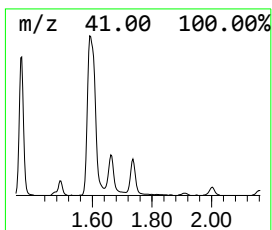
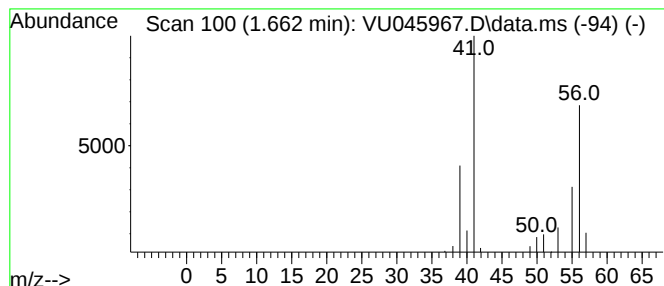
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111521WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.662	0.76 ug/L	30695	1,4-Difluorobenzene	6.253

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butene, (Z)-		56	C4H8	000590-18-1	72
2	1-Propene, 2-methyl-		56	C4H8	000115-11-7	72
3	2-Butene, (Z)-		56	C4H8	000590-18-1	64
4	2-Butene, (E)-		56	C4H8	000624-64-6	64
5	2-Butene, (E)-		56	C4H8	000624-64-6	59



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

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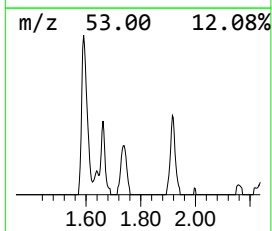
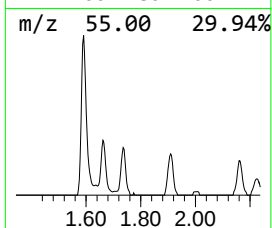
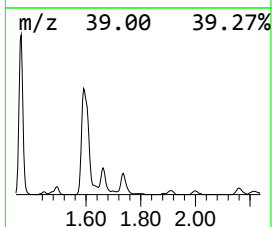
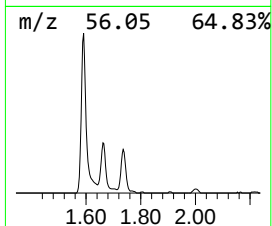
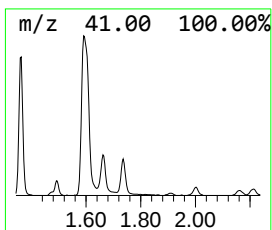
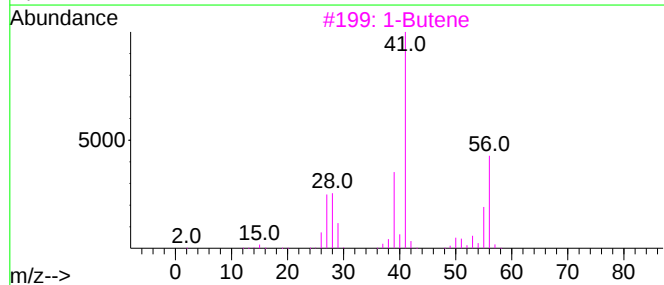
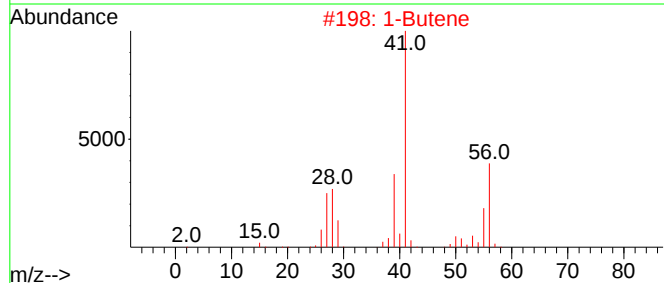
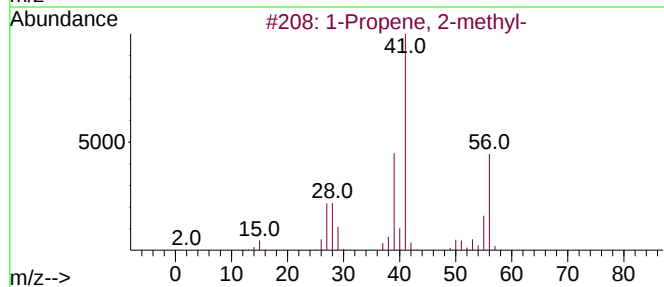
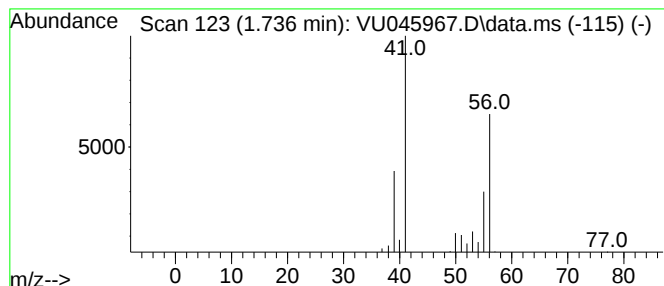
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111521WMA.M
Quant Title : TRACE VOA SFAM1.0

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	0.70 ug/L	28435	1,4-Difluorobenzene	6.253

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propene, 2-methyl-	56	C4H8	000115-11-7	80
2		1-Butene	56	C4H8	000106-98-9	80
3		1-Butene	56	C4H8	000106-98-9	80
4		2-Butene, (Z)-	56	C4H8	000590-18-1	80
5		1-Butene	56	C4H8	000106-98-9	80



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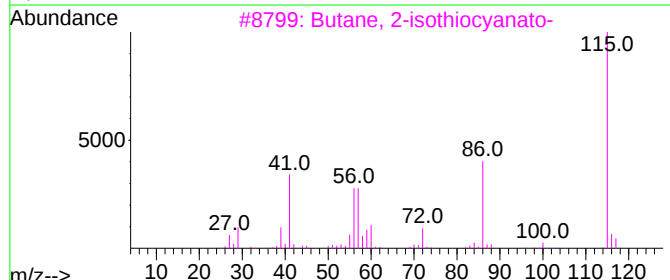
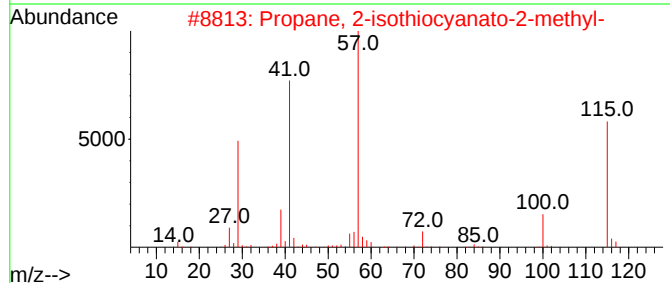
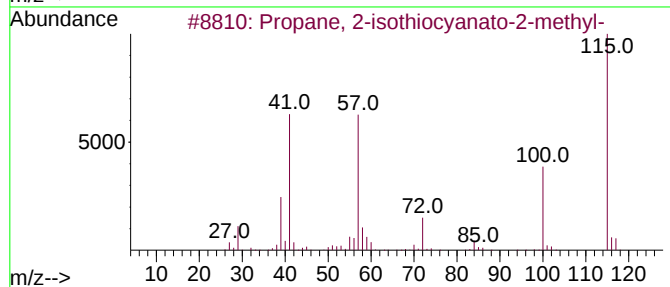
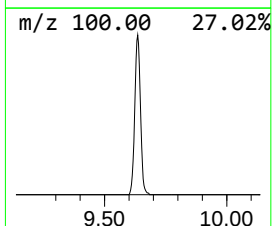
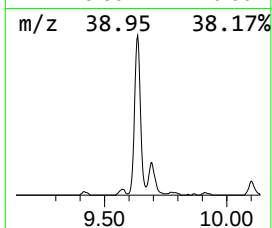
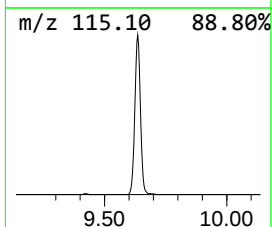
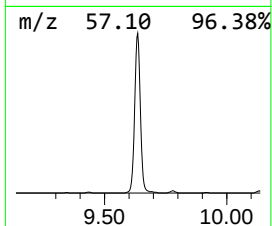
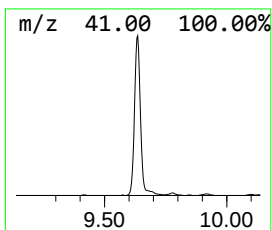
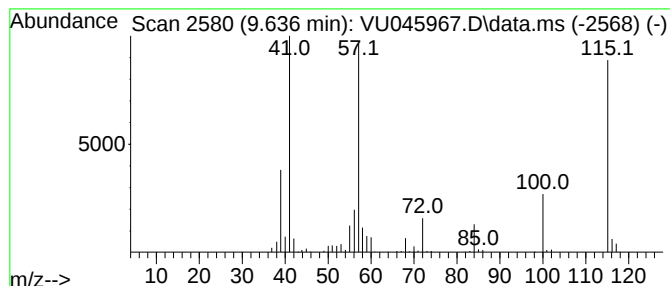
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Propane, 2-isothiocyanato-2... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.636	6.69 ug/L	355465	Chlorobenzene-d5	9.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-isothiocyanato-2-methyl-	115	C5H9NS	000590-42-1	70
2			Propane, 2-isothiocyanato-2-methyl-	115	C5H9NS	000590-42-1	53
3			Butane, 2-isothiocyanato-	115	C5H9NS	004426-79-3	47
4			Propane, 2-isothiocyanato-2-methyl-	115	C5H9NS	000590-42-1	43
5			Isobutyl isothiocyanate	115	C5H9NS	000591-82-2	43



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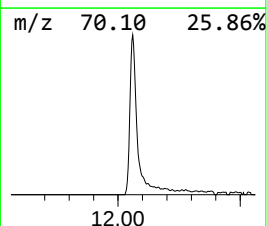
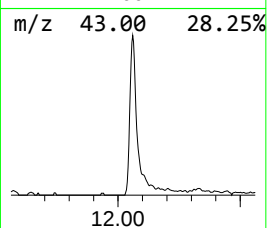
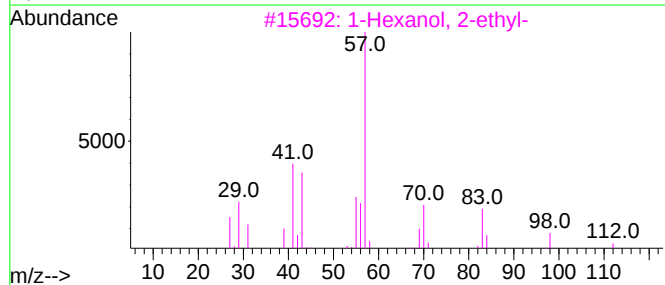
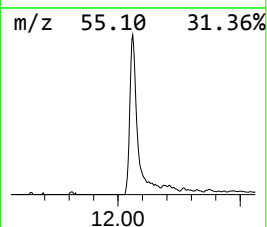
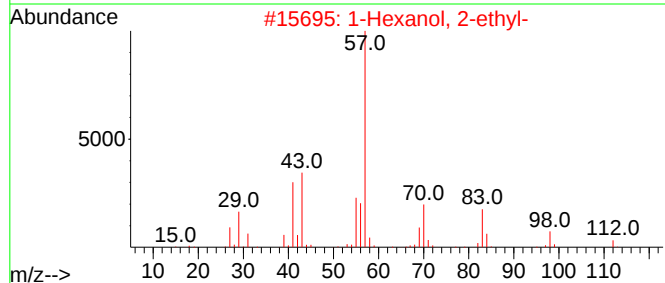
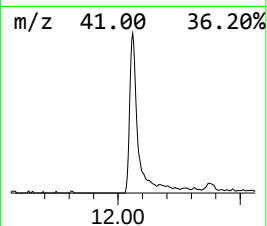
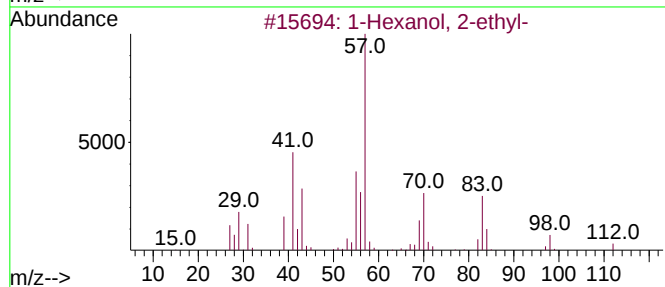
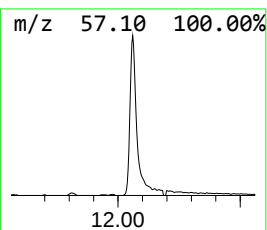
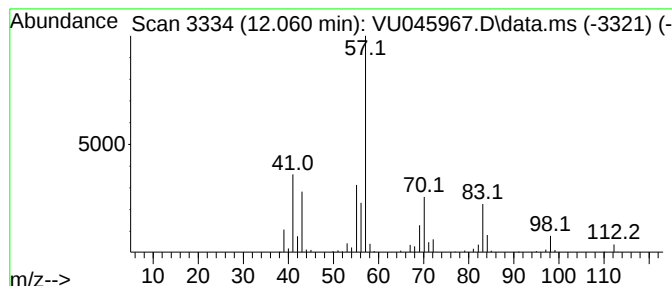
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111521WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.060	4.89 ug/L	247749	1,4-Dichlorobenzene-d4	11.812

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	90
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
5			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112321\
Data File : VU045967.D
Acq On : 23 Nov 2021 19:42
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\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	1.363	2.5	ug/L	102683	1	6.253	203009	5.0
(DEL) Alkane: S...	1.662	0.8	ug/L	30695	1	6.253	203009	5.0
(DEL) Alkane: S...	1.736	0.7	ug/L	28435	1	6.253	203009	5.0
Propane, 2-isot...	9.636	6.7	ug/L	355465	2	9.420	265658	5.0
1-Hexanol, 2-et...	12.060	4.9	ug/L	247749	3	11.812	253471	5.0