

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122322\
 Data File : VU052550.D
 Acq On : 23 Dec 2022 20:16
 Operator : JC/MD
 Sample : N6170-01
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 GBQB0

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\SFAMUTR122022WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU052550.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	25	rVB	2001156	1834138	13.52%	5.377%
2	1.591	69	78	95	rBV3	944167	1402994	10.34%	4.113%
3	1.735	116	123	138	rVB	163170	208598	1.54%	0.612%
4	1.912	164	178	193	rVV2	126247	200741	1.48%	0.589%
5	2.157	245	254	263	rBV	247312	345689	2.55%	1.013%
6	2.218	263	273	289	rVB3	187162	370177	2.73%	1.085%
7	2.417	323	335	344	rBV	95529	154221	1.14%	0.452%
8	2.568	367	382	396	rBV2	162680	292135	2.15%	0.856%
9	3.584	681	698	720	rVB4	77714	198851	1.47%	0.583%
10	4.661	1010	1033	1079	rBV2	344825	1126883	8.30%	3.304%
11	5.060	1140	1157	1179	rVB	150031	353238	2.60%	1.036%
12	5.722	1340	1363	1395	rBV2	304065	855129	6.30%	2.507%
13	6.247	1512	1526	1550	rBV	231309	469758	3.46%	1.377%
14	6.539	1600	1617	1651	rBV	7363906	13568809	100.00%	39.780%
15	6.687	1651	1663	1679	rVB	205173	396667	2.92%	1.163%
16	7.562	1921	1935	1945	rBV	94314	166617	1.23%	0.488%
17	7.893	2027	2038	2051	rBV	343321	590113	4.35%	1.730%
18	8.549	2228	2242	2257	rBV	5015805	8344122	61.49%	24.463%
19	8.632	2257	2268	2293	rVB	713754	1345169	9.91%	3.944%
20	9.414	2500	2511	2526	rBV	329000	536821	3.96%	1.574%
21	10.751	2916	2927	2944	rVB	187062	297969	2.20%	0.874%
22	11.806	3244	3255	3274	rBV	318115	506878	3.74%	1.486%
23	12.188	3362	3374	3393	rBV	342789	543704	4.01%	1.594%

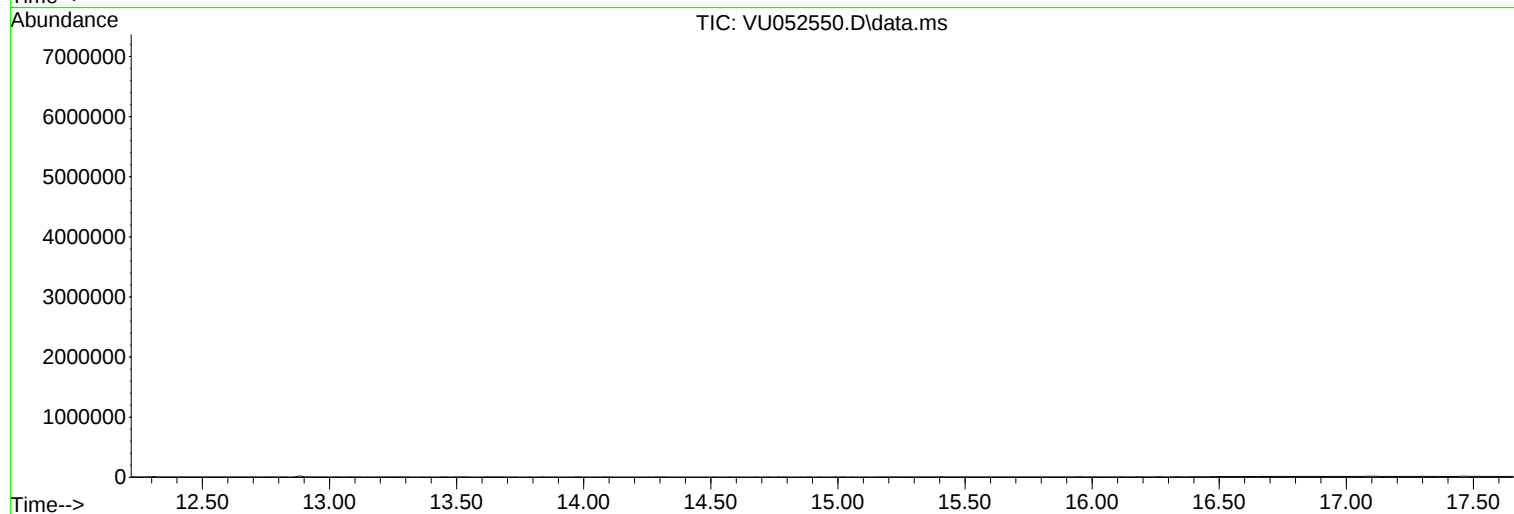
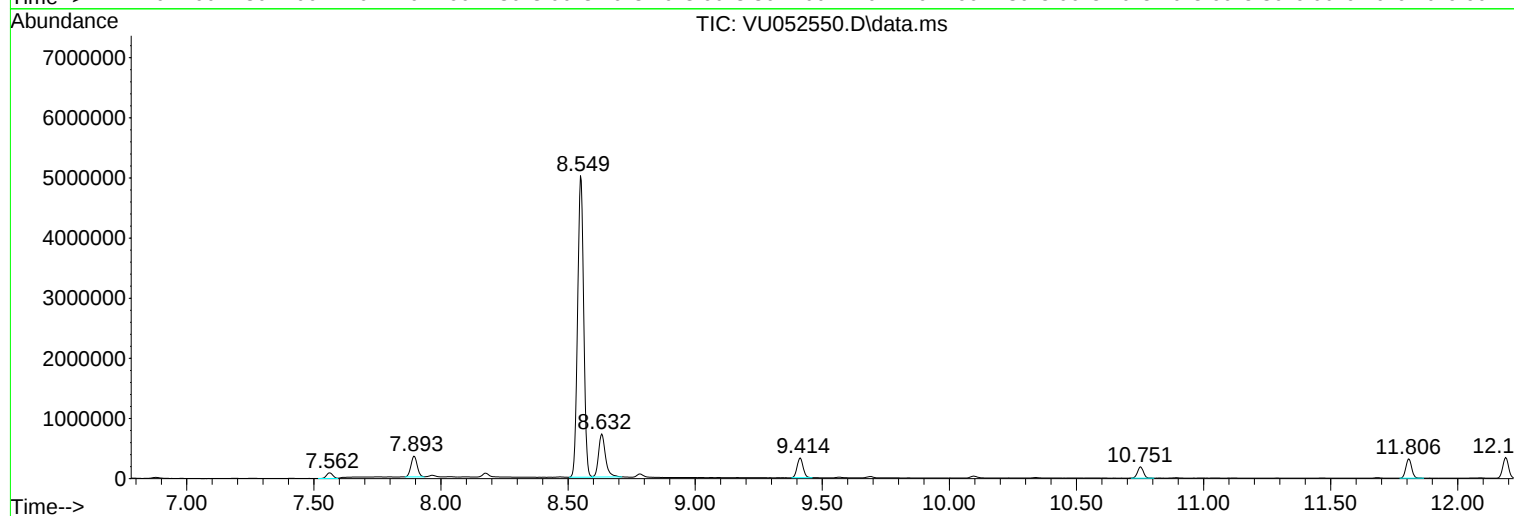
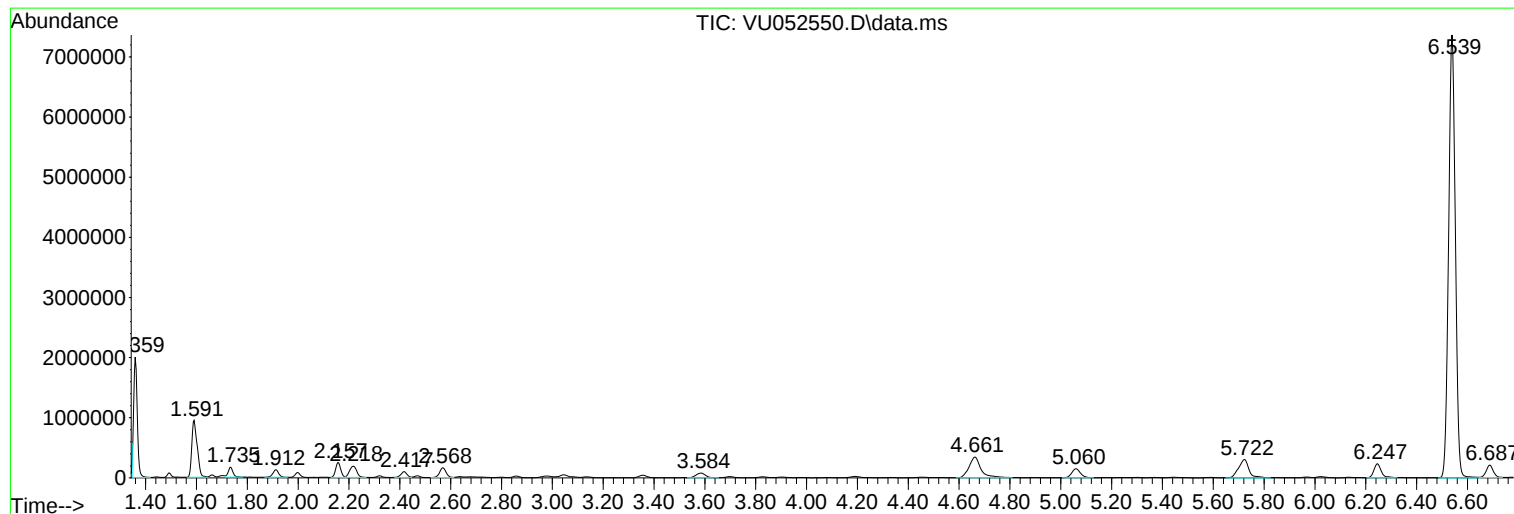
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Instrument :
MSVOA_U
ClientSampleId :
GBQB0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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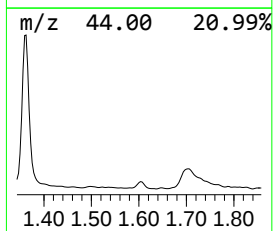
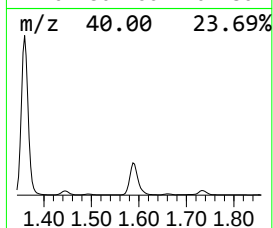
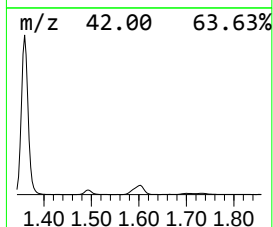
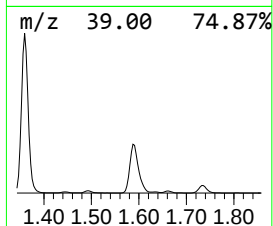
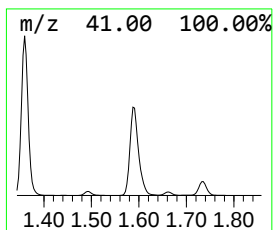
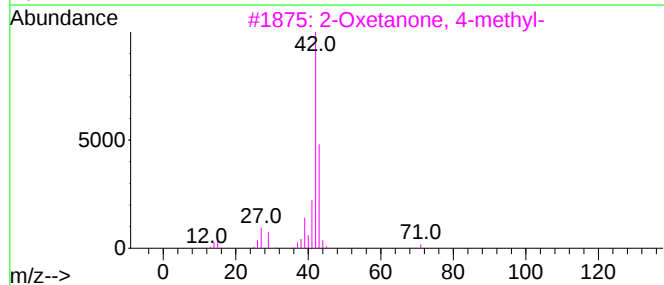
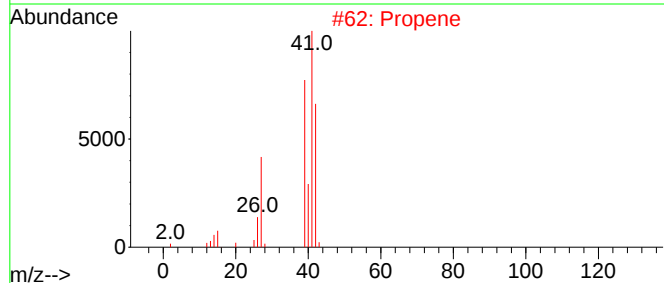
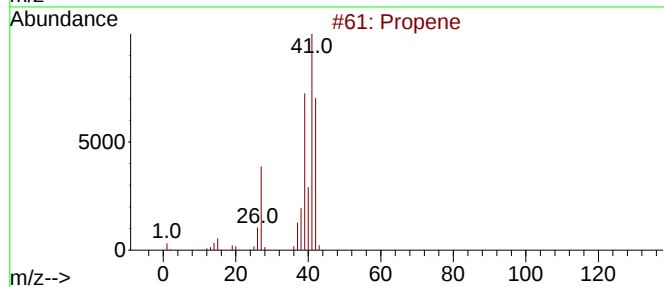
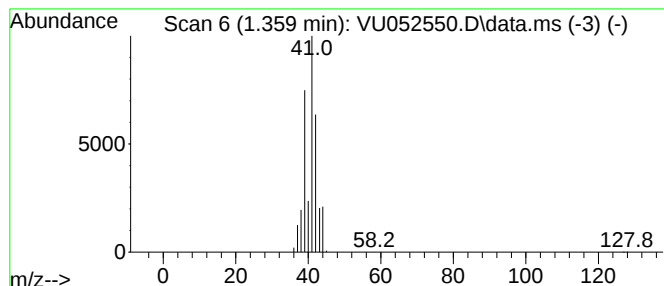
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Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.359	19.52 ug/L	1834140	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	90
2			Propene	42	C3H6	000115-07-1	42
3			2-Oxetanone, 4-methyl-	86	C4H6O2	003068-88-0	9
4			Cyclopropane	42	C3H6	000075-19-4	9
5			Cyclopropene	40	C3H4	002781-85-3	9



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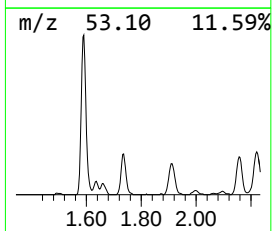
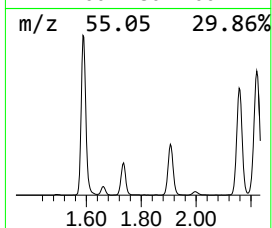
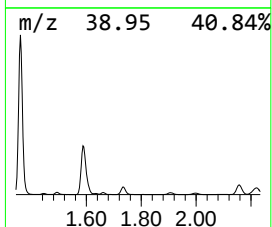
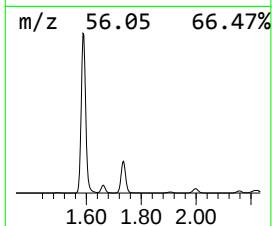
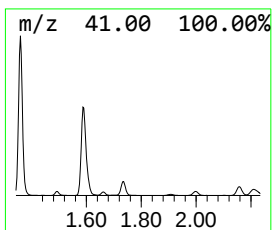
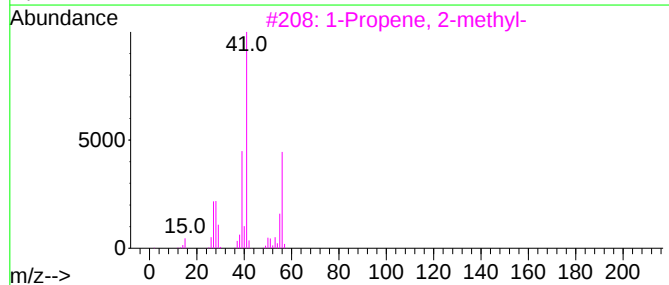
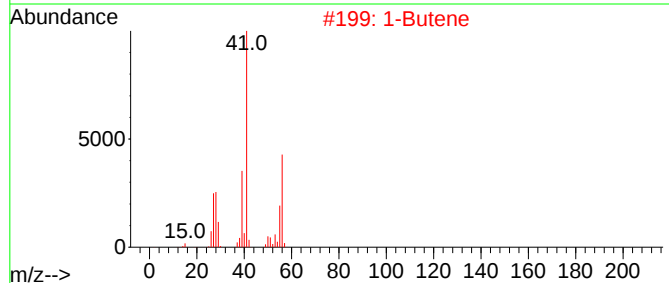
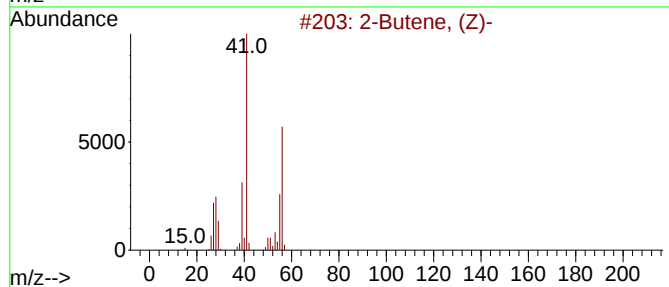
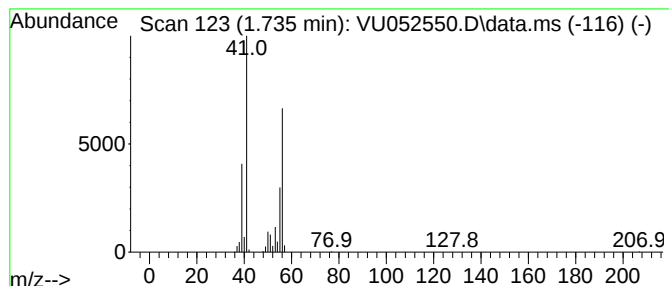
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.735	2.22 ug/L	208598	1,4-Difluorobenzene	6.247

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butene, (Z)-		56	C4H8	000590-18-1	83
2	1-Butene		56	C4H8	000106-98-9	83
3	1-Propene, 2-methyl-		56	C4H8	000115-11-7	83
4	1-Butene		56	C4H8	000106-98-9	83
5	1-Butene		56	C4H8	000106-98-9	80



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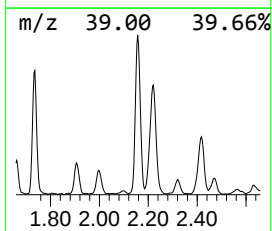
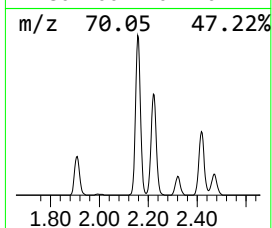
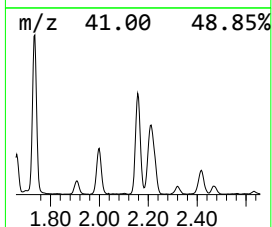
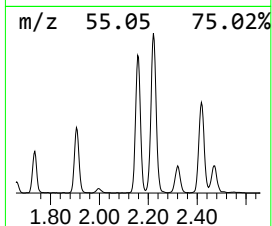
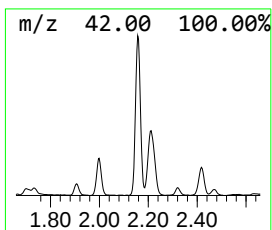
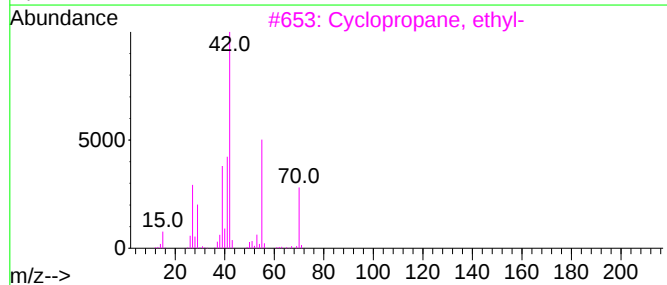
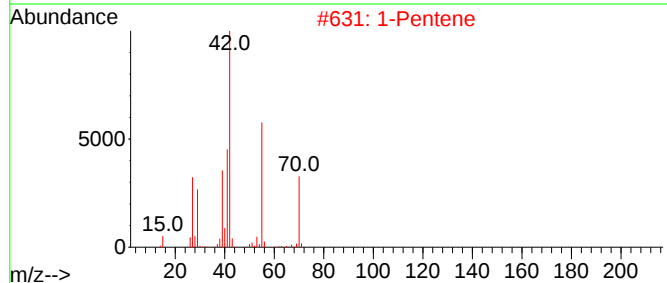
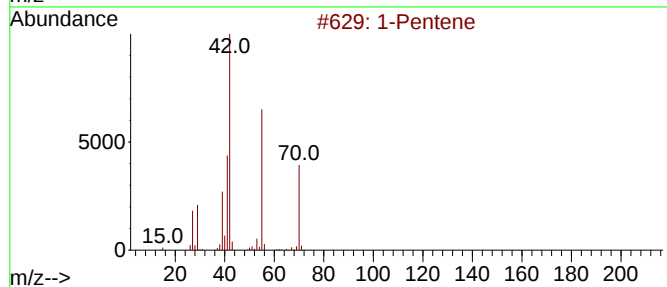
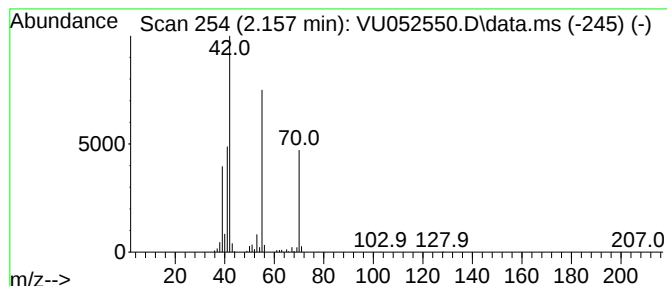
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Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.157	3.68 ug/L	345689	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentene	70	C5H10	000109-67-1	91
2			1-Pentene	70	C5H10	000109-67-1	76
3			Cyclopropane, ethyl-	70	C5H10	001191-96-4	68
4			Cyclobutane, methyl-	70	C5H10	000598-61-8	64
5			1-Pentene	70	C5H10	000109-67-1	64



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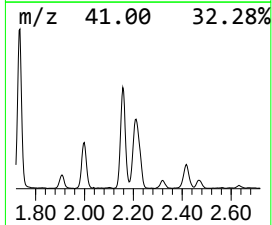
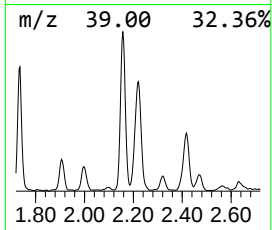
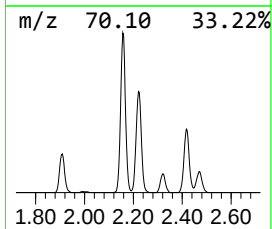
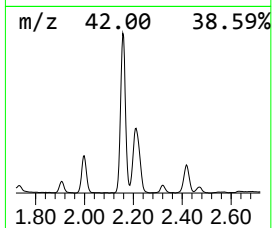
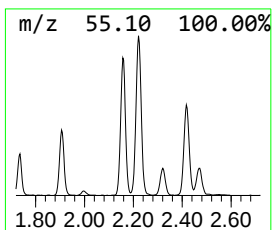
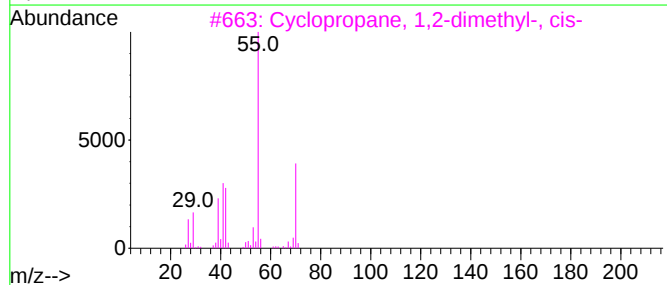
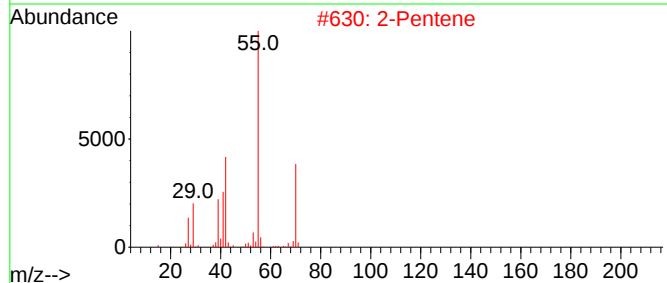
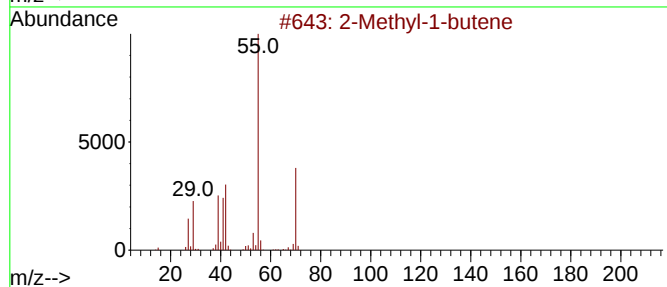
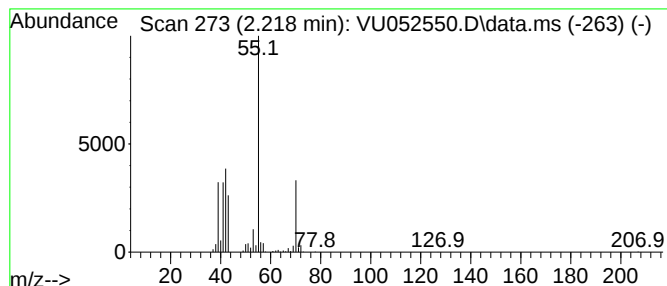
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Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.218	3.94 ug/L	370177	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyl-1-butene			70	C5H10	000563-46-2	90
2	2-Pentene			70	C5H10	000109-68-2	87
3	Cyclopropane, 1,2-dimethyl-, cis-			70	C5H10	000930-18-7	87
4	2-Pentene, (Z)-			70	C5H10	000627-20-3	87
5	2-Pentene, (E)-			70	C5H10	000646-04-8	87



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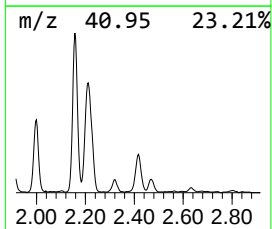
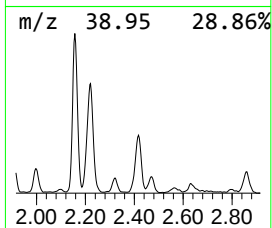
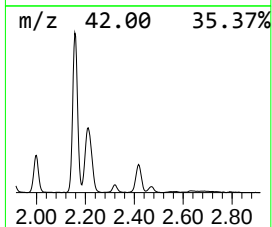
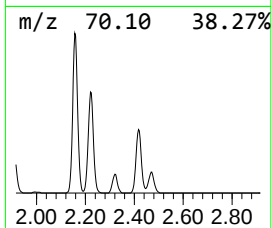
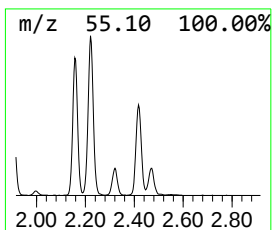
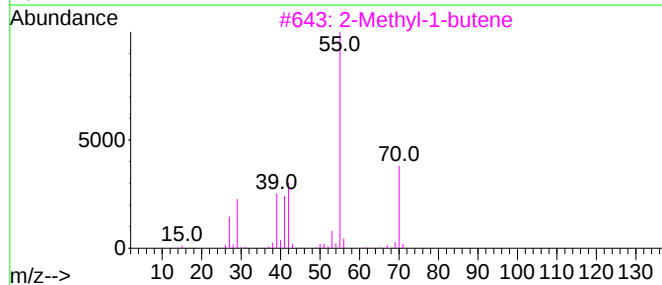
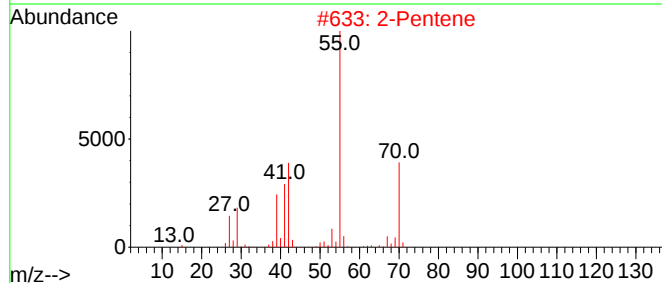
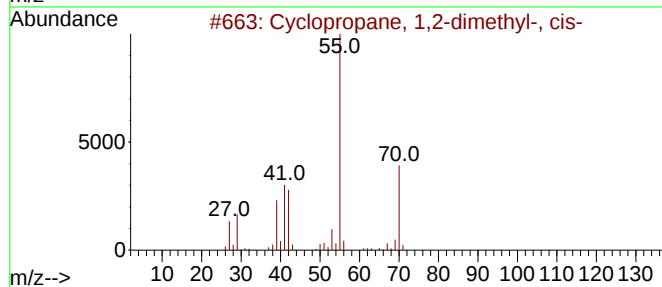
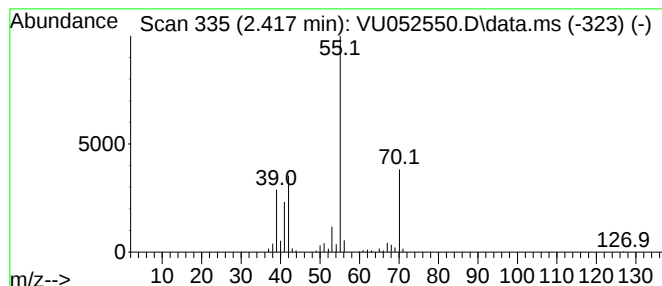
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 (DEL) Alkane: Cyclic2.417 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.417	1.64 ug/L	154221	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	91
2			2-Pentene	70	C5H10	000109-68-2	91
3			2-Methyl-1-butene	70	C5H10	000563-46-2	91
4			2-Pentene, (Z)-	70	C5H10	000627-20-3	90
5			2-Butene, 2-methyl-	70	C5H10	000513-35-9	90



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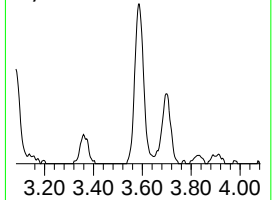
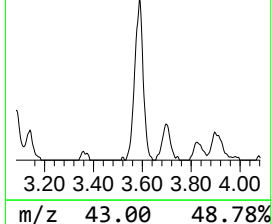
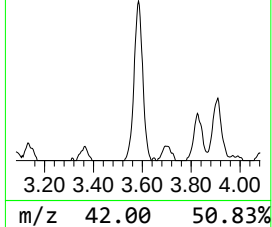
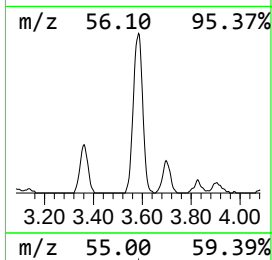
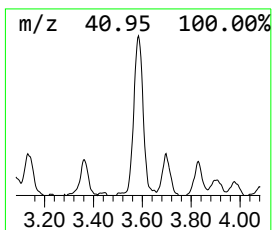
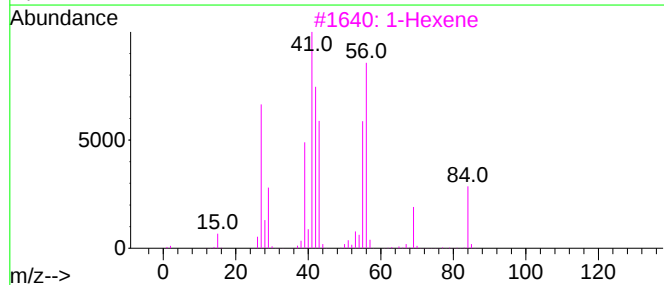
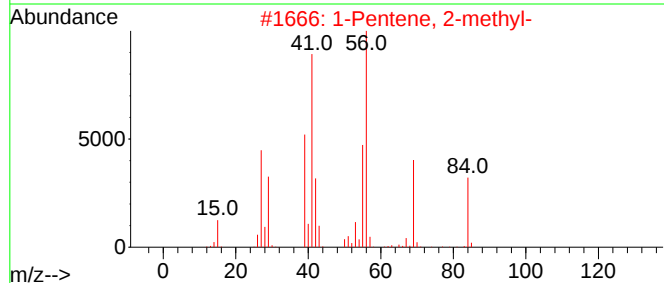
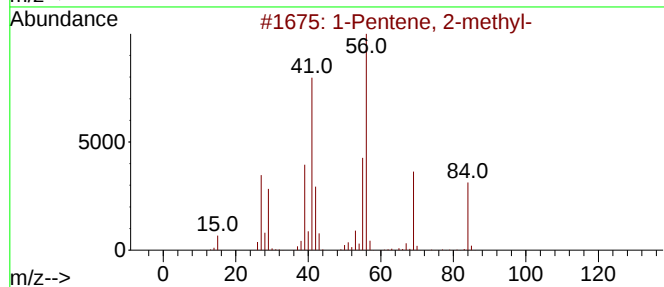
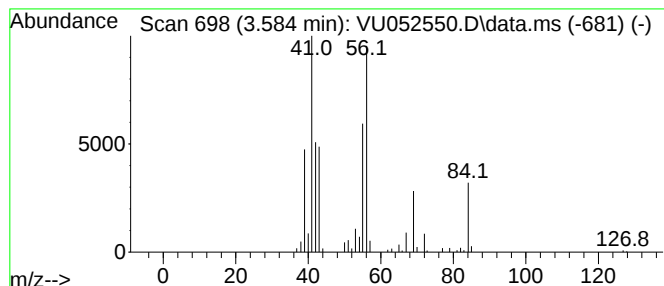
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.584	2.12 ug/L	198851	1,4-Difluorobenzene	6.247

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	87
2		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	87
3		1-Hexene	84	C6H12	000592-41-6	76
4		1-Hexene	84	C6H12	000592-41-6	70
5		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122322\
Data File : VU052550.D
Acq On : 23 Dec 2022 20:16
Operator : JC/MD
Sample : N6170-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQB0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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

					--Internal Standard--			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL) Alkane: S...	1.359	19.5	ug/L	1834140	1	6.247	469758	5.0
(DEL) Alkane: S...	1.735	2.2	ug/L	208598	1	6.247	469758	5.0
(DEL) Alkane: S...	2.157	3.7	ug/L	345689	1	6.247	469758	5.0
(DEL) Alkane: S...	2.218	3.9	ug/L	370177	1	6.247	469758	5.0
(DEL) Alkane: C...	2.417	1.6	ug/L	154221	1	6.247	469758	5.0
(DEL) Alkane: S...	3.584	2.1	ug/L	198851	1	6.247	469758	5.0