

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122222\
 Data File : VU052512.D
 Acq On : 22 Dec 2022 23:39
 Operator : JC/MD
 Sample : N6170-06
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 GBQB3

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: VU052512.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	26	rVB	995926	903887	11.10%	3.577%
2	1.591	69	78	89	rBV3	452959	738322	9.07%	2.922%
3	1.732	116	122	139	rVB	69688	87574	1.08%	0.347%
4	1.912	164	178	193	rVV2	103932	157339	1.93%	0.623%
5	2.157	244	254	262	rBV	108655	153038	1.88%	0.606%
6	2.215	262	272	289	rVB4	93319	192443	2.36%	0.762%
7	2.568	366	382	395	rBV	158341	265446	3.26%	1.051%
8	3.353	606	626	650	rBV	138971	285760	3.51%	1.131%
9	3.584	683	698	720	rVB4	38713	96509	1.19%	0.382%
10	4.661	1011	1033	1079	rBV2	513033	1534339	18.85%	6.073%
11	5.060	1141	1157	1182	rVB	142466	333802	4.10%	1.321%
12	5.722	1341	1363	1394	rBV2	294294	821023	10.08%	3.249%
13	6.247	1513	1526	1552	rBV	217993	431935	5.31%	1.710%
14	6.539	1601	1617	1650	rBV	3696055	6892659	84.66%	27.280%
15	6.687	1650	1663	1679	rVB	193861	374623	4.60%	1.483%
16	7.562	1922	1935	1954	rBV	88793	162893	2.00%	0.645%
17	7.896	2026	2039	2053	rBV	326484	571085	7.01%	2.260%
18	8.176	2115	2126	2146	rBV	56599	99994	1.23%	0.396%
19	8.549	2228	2242	2257	rBV	4909800	8141447	100.00%	32.222%
20	8.632	2257	2268	2305	rVB	642269	1253451	15.40%	4.961%
21	9.414	2492	2511	2532	rBV	310381	527573	6.48%	2.088%
22	10.751	2912	2927	2943	rBV	168735	274666	3.37%	1.087%
23	11.809	3244	3256	3273	rBV	291342	460973	5.66%	1.824%
24	12.188	3362	3374	3397	rBV	311245	505798	6.21%	2.002%

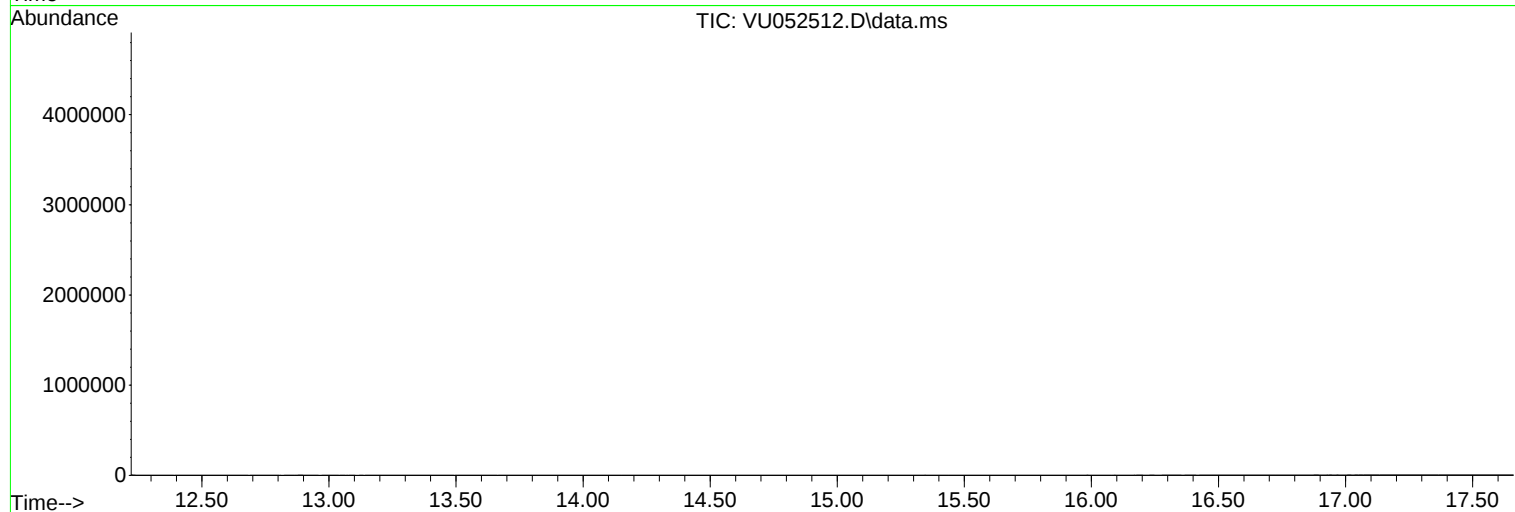
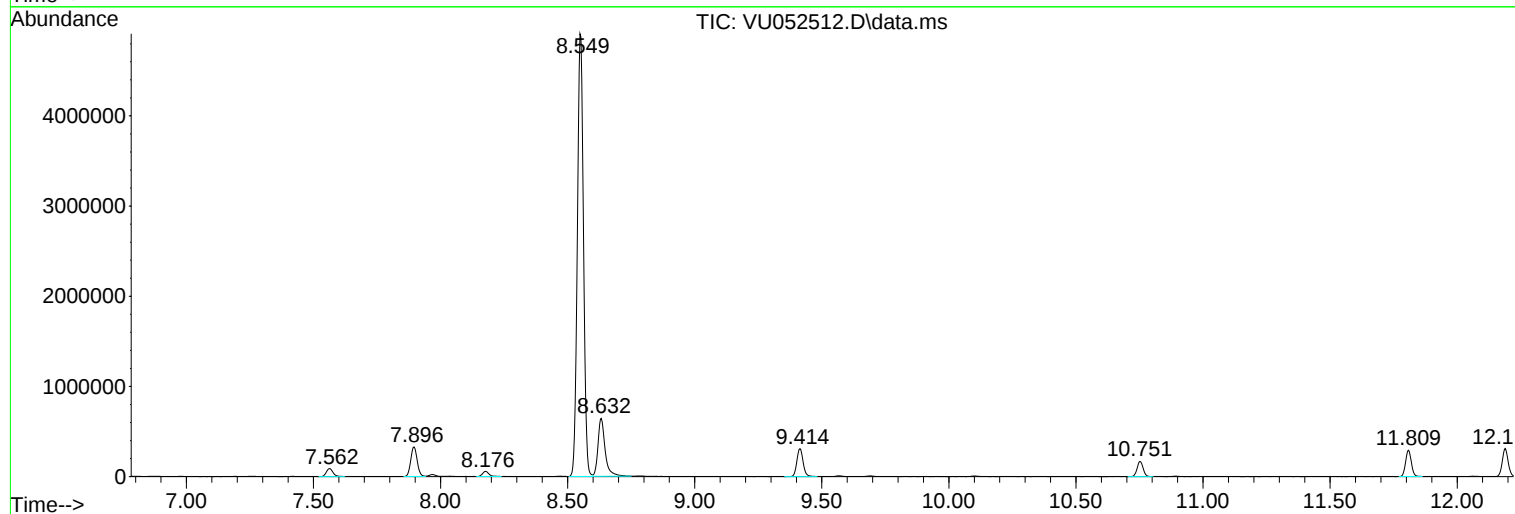
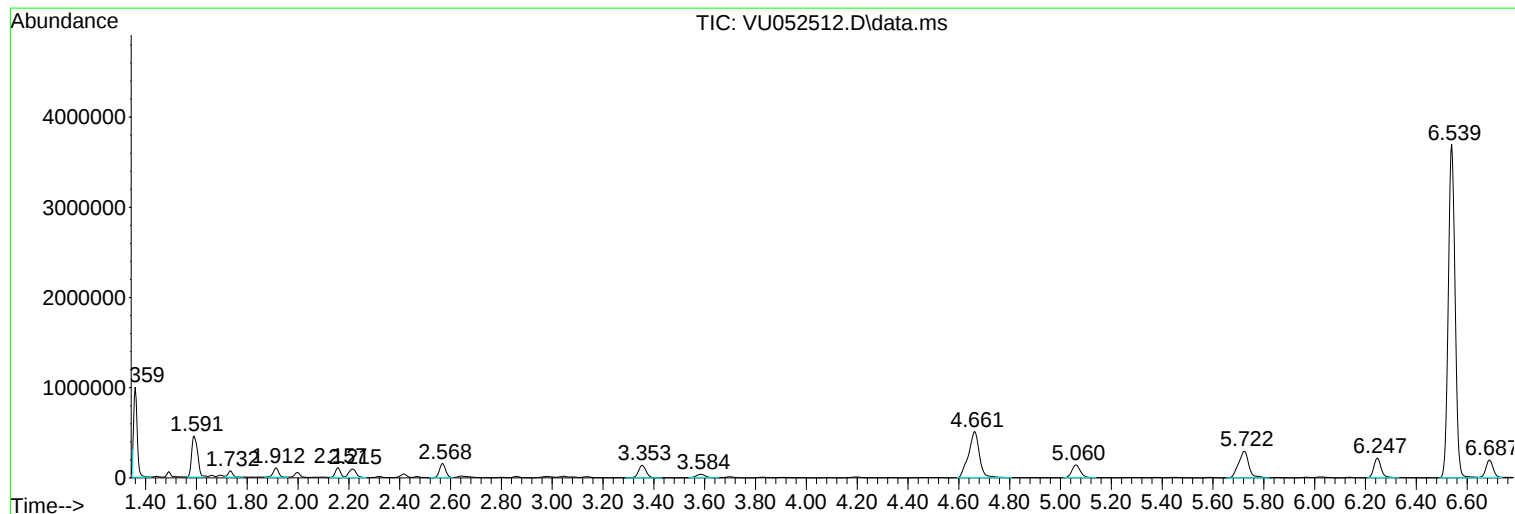
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ALS Vial : 34 Sample Multiplier: 1

Instrument :
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ClientSampleId :
GBQB3

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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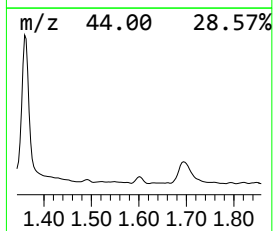
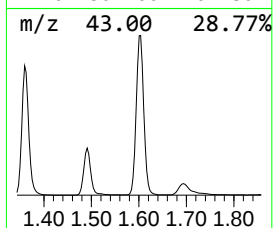
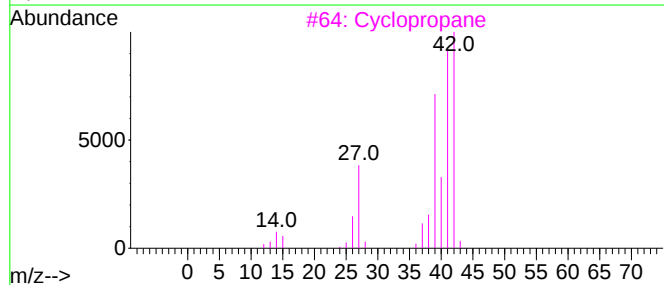
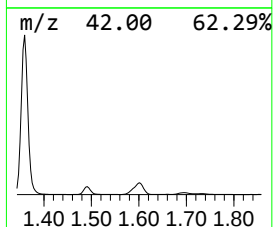
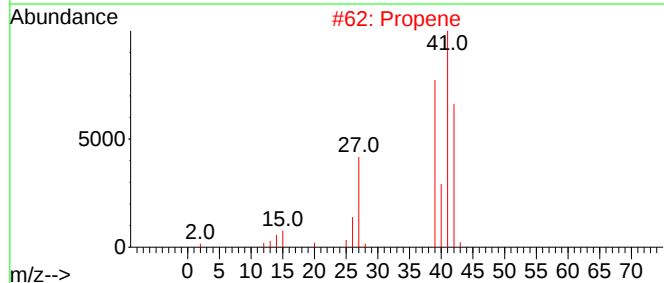
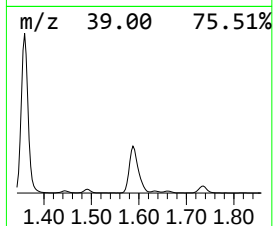
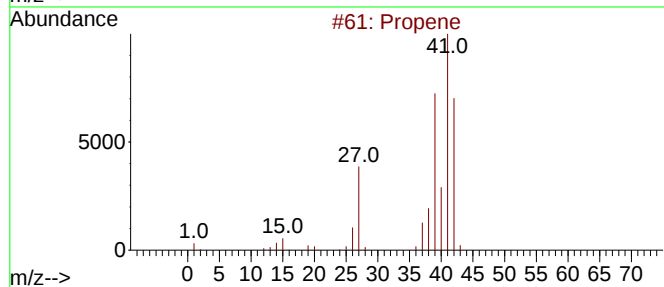
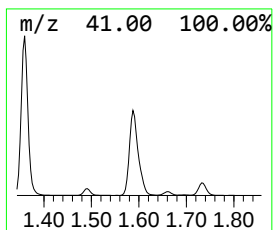
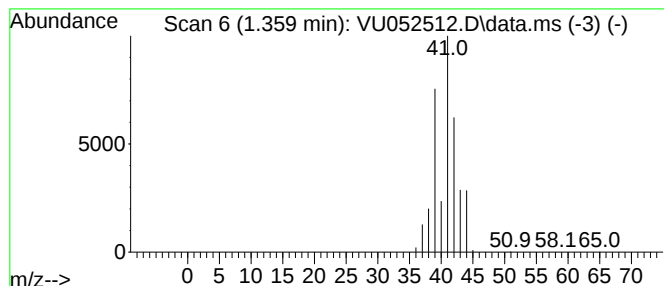
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Quant Title : TRACE VOA SFAM1.0

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	10.46 ug/L	903887	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			Cyclopropane	42	C3H6	000075-19-4	9
4			Cyclopropene	40	C3H4	002781-85-3	9
5			Cyclopropane	42	C3H6	000075-19-4	7



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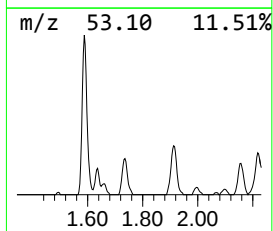
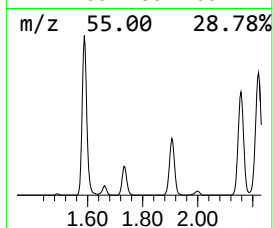
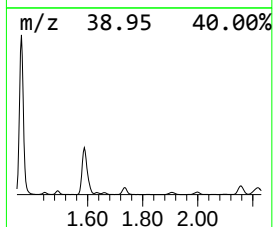
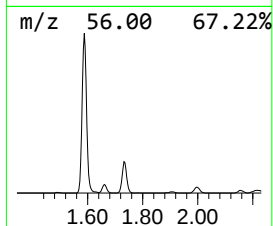
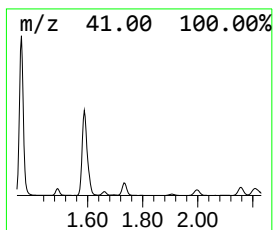
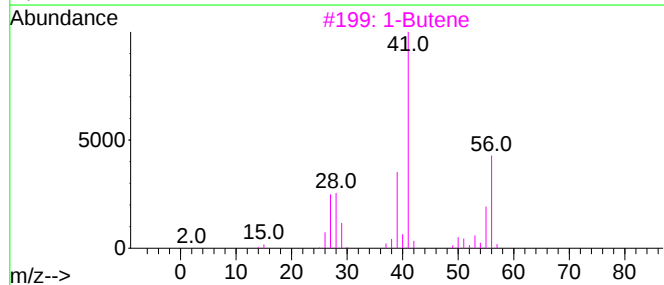
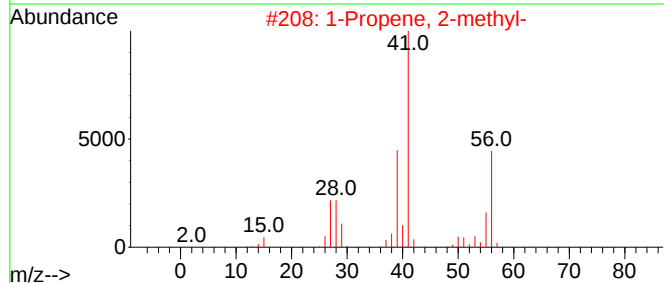
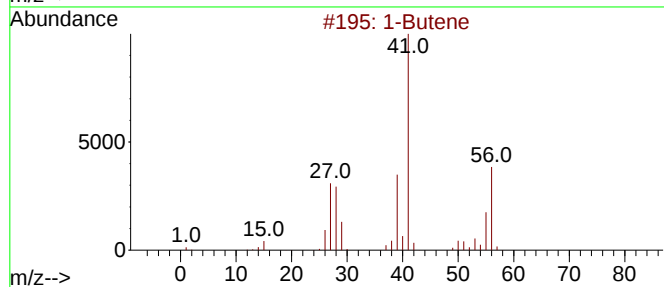
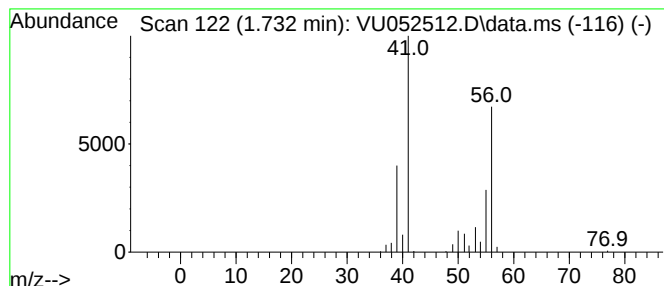
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.732	1.01 ug/L	87574	1,4-Difluorobenzene	6.247

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Butene	56	C4H8	000106-98-9	80
2		1-Propene, 2-methyl-	56	C4H8	000115-11-7	80
3		1-Butene	56	C4H8	000106-98-9	80
4		2-Butene, (Z)-	56	C4H8	000590-18-1	80
5		2-Butene, (Z)-	56	C4H8	000590-18-1	74



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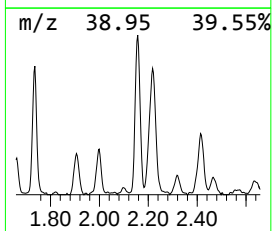
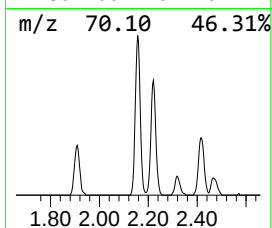
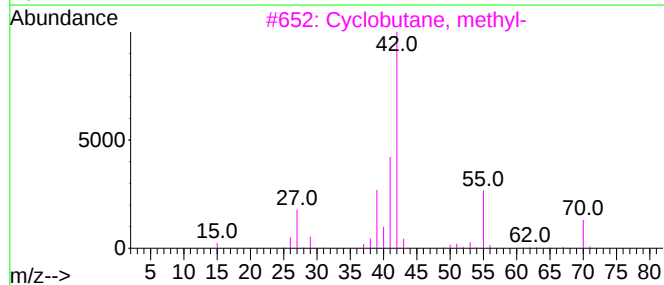
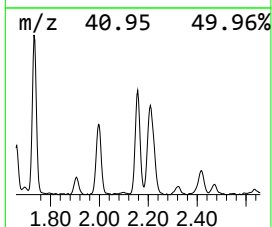
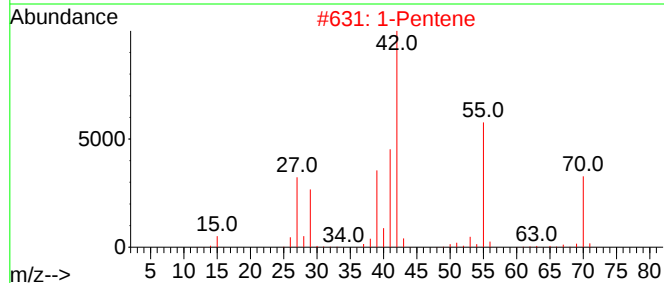
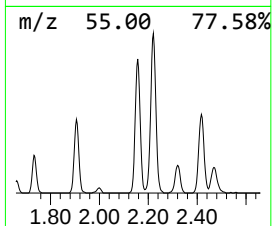
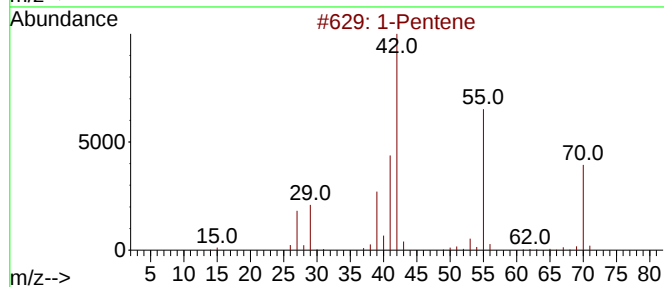
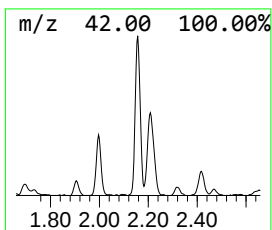
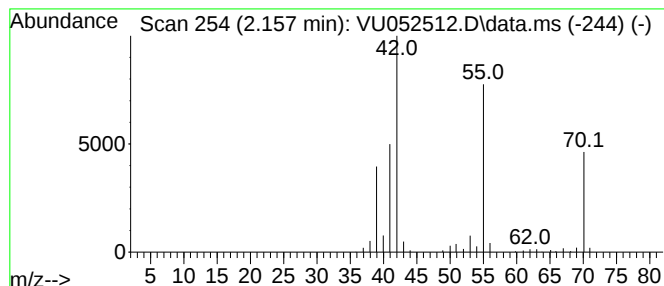
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.157	1.77 ug/L	153038	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene			70	C5H10	000109-67-1	81
2	1-Pentene			70	C5H10	000109-67-1	76
3	Cyclobutane, methyl-			70	C5H10	000598-61-8	74
4	Cyclopropane, ethyl-			70	C5H10	001191-96-4	68
5	Cyclopropane, ethyl-			70	C5H10	001191-96-4	64



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQB3

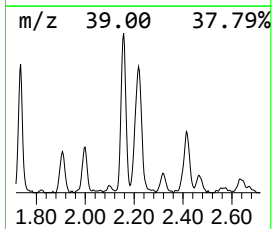
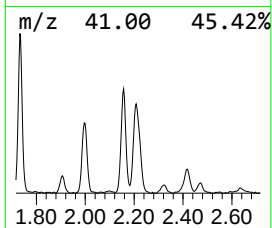
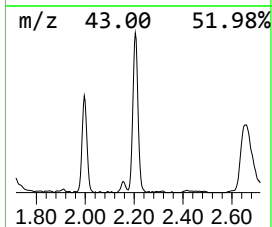
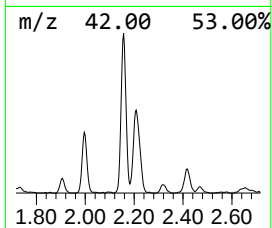
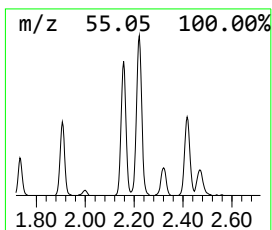
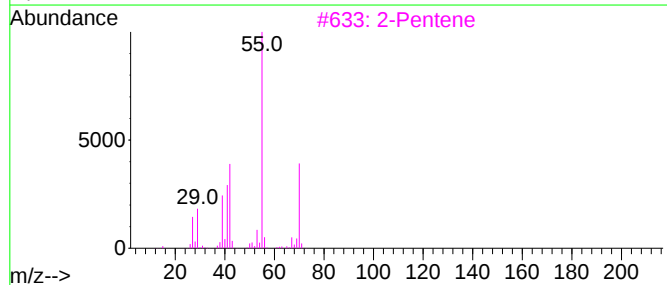
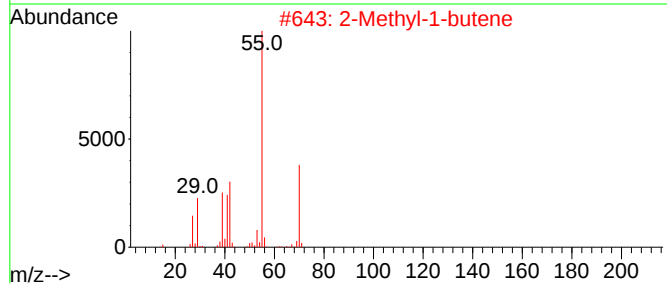
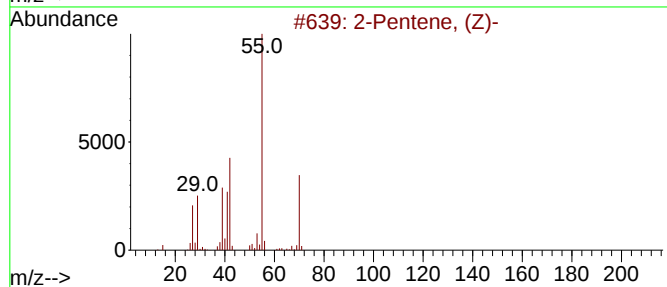
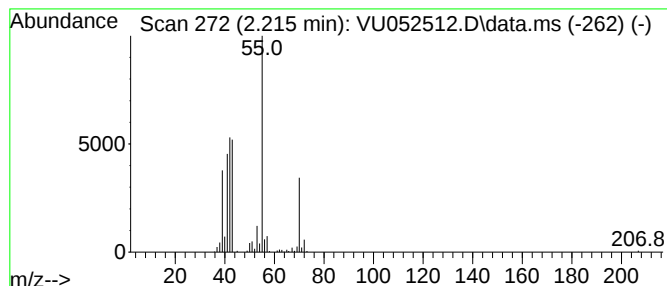
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Quant Title : TRACE VOA SFAM1.0

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.
2.215	2.23 ug/L	192443	1,4-Difluorobenzene	6.247

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentene, (Z)-	70	C5H10	000627-20-3	90
2		2-Methyl-1-butene	70	C5H10	000563-46-2	87
3		2-Pentene	70	C5H10	000109-68-2	86
4		2-Pentene, (Z)-	70	C5H10	000627-20-3	83
5		2-Pentene, (E)-	70	C5H10	000646-04-8	83



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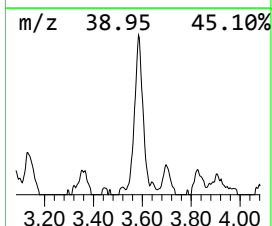
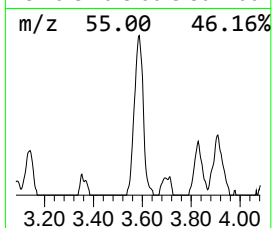
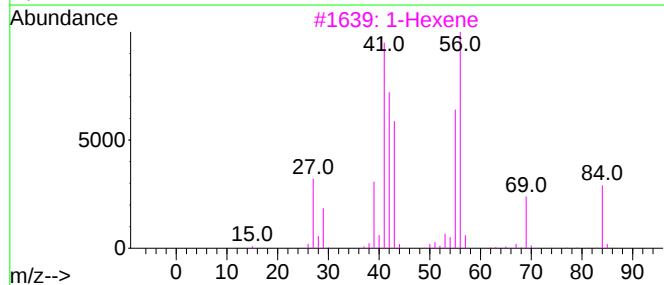
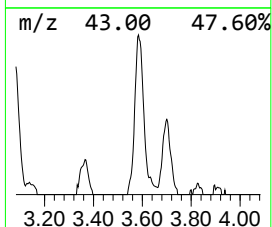
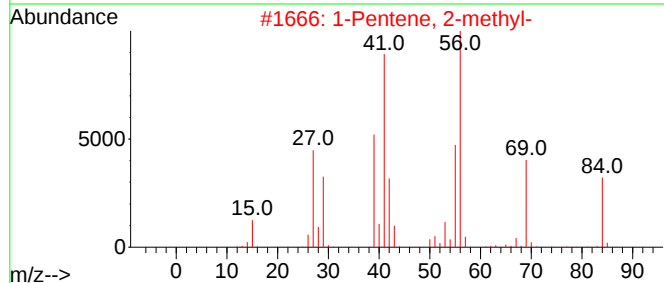
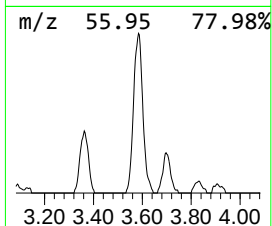
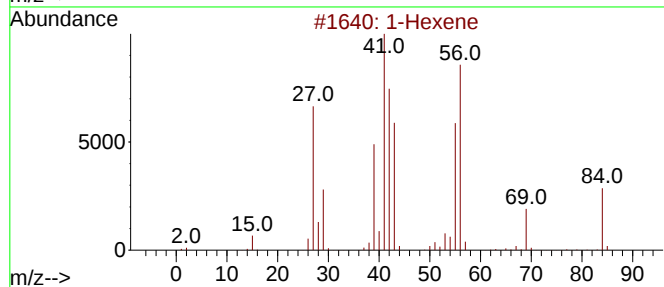
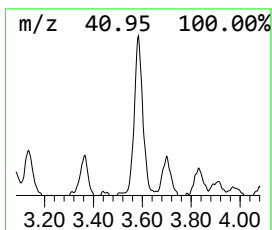
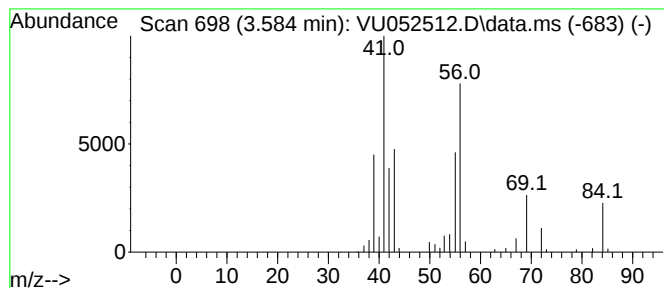
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.584	1.12 ug/L	96509	1,4-Difluorobenzene	6.247

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexene	84	C6H12	000592-41-6	81
2		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	74
3		1-Hexene	84	C6H12	000592-41-6	64
4		Cyclohexane	84	C6H12	000110-82-7	59
5		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	59



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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	10.5	ug/L	903887	1	6.247	431935 5.0
(DEL)	Alkane: S...	1.732	1.0	ug/L	87574	1	6.247	431935 5.0
(DEL)	Alkane: S...	2.157	1.8	ug/L	153038	1	6.247	431935 5.0
(DEL)	Alkane: S...	2.215	2.2	ug/L	192443	1	6.247	431935 5.0
(DEL)	Alkane: S...	3.584	1.1	ug/L	96509	1	6.247	431935 5.0