

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122722\
 Data File : VU052558.D
 Acq On : 27 Dec 2022 12:44
 Operator : JC/MD
 Sample : N6169-11
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 GBQA2

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: VU052558.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	23	rVB	761400	695553	54.40%	6.605%
2	1.491	40	47	55	rBV	50309	52654	4.12%	0.500%
3	1.591	69	78	94	rBV3	345389	585124	45.76%	5.556%
4	1.661	95	100	104	rVV	12966	14420	1.13%	0.137%
5	1.690	104	109	116	rVV	16104	23749	1.86%	0.226%
6	1.732	116	122	133	rVB	49796	60254	4.71%	0.572%
7	1.912	170	178	195	rVB2	86674	125197	9.79%	1.189%
8	1.996	196	204	217	rVB	45775	63570	4.97%	0.604%
9	2.157	244	254	262	rBV	81141	113354	8.87%	1.076%
10	2.215	262	272	292	rVB4	78471	162443	12.71%	1.543%
11	2.321	296	305	312	rBV2	9573	14602	1.14%	0.139%
12	2.417	323	335	344	rBV	29402	49602	3.88%	0.471%
13	2.469	344	351	366	rVB2	15514	24892	1.95%	0.236%
14	2.568	367	382	395	rBV	128674	216273	16.92%	2.054%
15	2.639	395	404	424	rVB2	13602	33373	2.61%	0.317%
16	2.861	463	473	487	rVB3	8232	14178	1.11%	0.135%
17	2.980	490	510	517	rBV7	9998	27830	2.18%	0.264%
18	3.044	522	530	538	rBV	13500	22015	1.72%	0.209%
19	3.353	610	626	643	rBV	206615	411854	32.21%	3.911%
20	3.581	682	697	715	rVB4	28972	72457	5.67%	0.688%
21	3.697	721	733	749	rVB4	10561	25343	1.98%	0.241%
22	4.195	875	888	899	rBV6	6490	15431	1.21%	0.147%
23	4.661	1008	1033	1072	rBV2	398010	1278575	100.00%	12.141%
24	5.060	1141	1157	1176	rVB	123923	281970	22.05%	2.678%
25	5.722	1338	1363	1395	rBV2	254776	701445	54.86%	6.661%
26	6.025	1448	1457	1471	rVB8	7496	16656	1.30%	0.158%
27	6.247	1512	1526	1549	rBV	201256	397763	31.11%	3.777%
28	6.539	1604	1617	1633	rBV	161720	306639	23.98%	2.912%
29	6.687	1649	1663	1682	rBV	171026	336595	26.33%	3.196%
30	7.562	1923	1935	1954	rBV2	78173	138435	10.83%	1.315%
31	7.893	2021	2038	2052	rBV	275012	475201	37.17%	4.512%
32	7.967	2052	2061	2069	rVB	14532	24376	1.91%	0.231%
33	8.176	2115	2126	2146	rBV	50275	89710	7.02%	0.852%
34	8.549	2229	2242	2255	rBV	572538	964116	75.41%	9.155%
35	8.629	2255	2267	2296	rVV	579083	1069412	83.64%	10.155%
36	9.414	2496	2511	2532	rBV	286348	476203	37.24%	4.522%

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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\SFAMUTR122022WMA.M
Title : TRACE VOA SFAM1.0

37	9.690	2584	2597	2608	rBV2	12767	20129	1.57%	0.191%
38	10.098	2712	2724	2738	rBV	15149	26322	2.06%	0.250%
39	10.751	2915	2927	2946	rBV	156522	250222	19.57%	2.376%
40	11.806	3244	3255	3270	rBV	257024	409360	32.02%	3.887%
41	12.188	3361	3374	3391	rBV	267213	443505	34.69%	4.212%

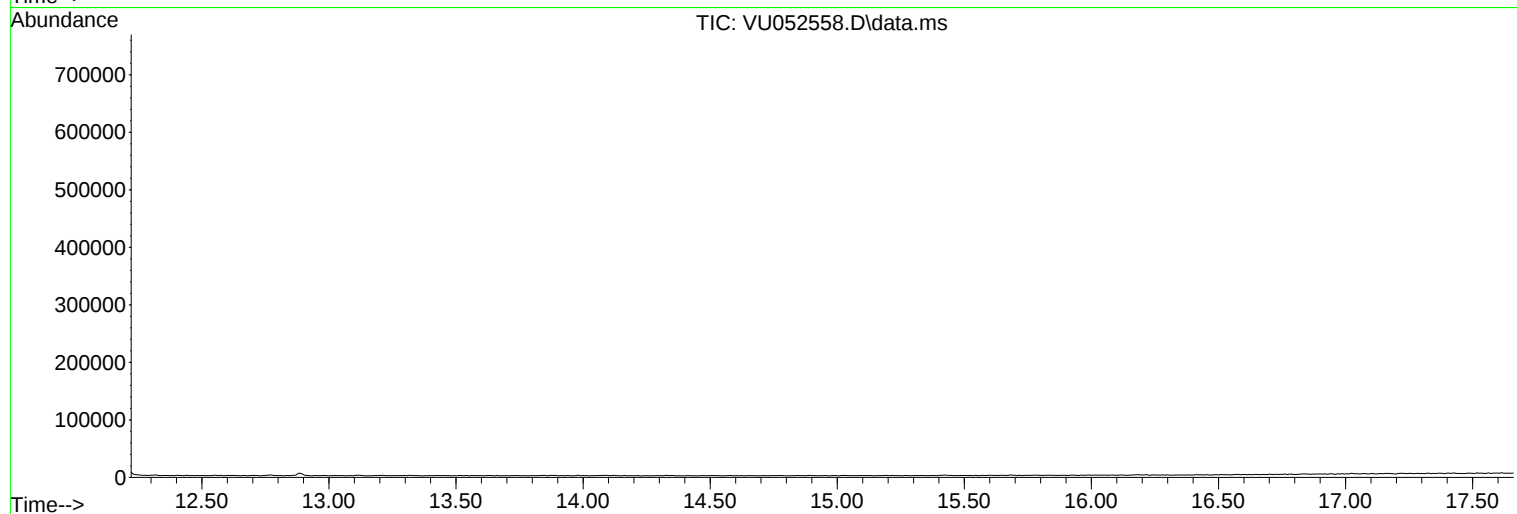
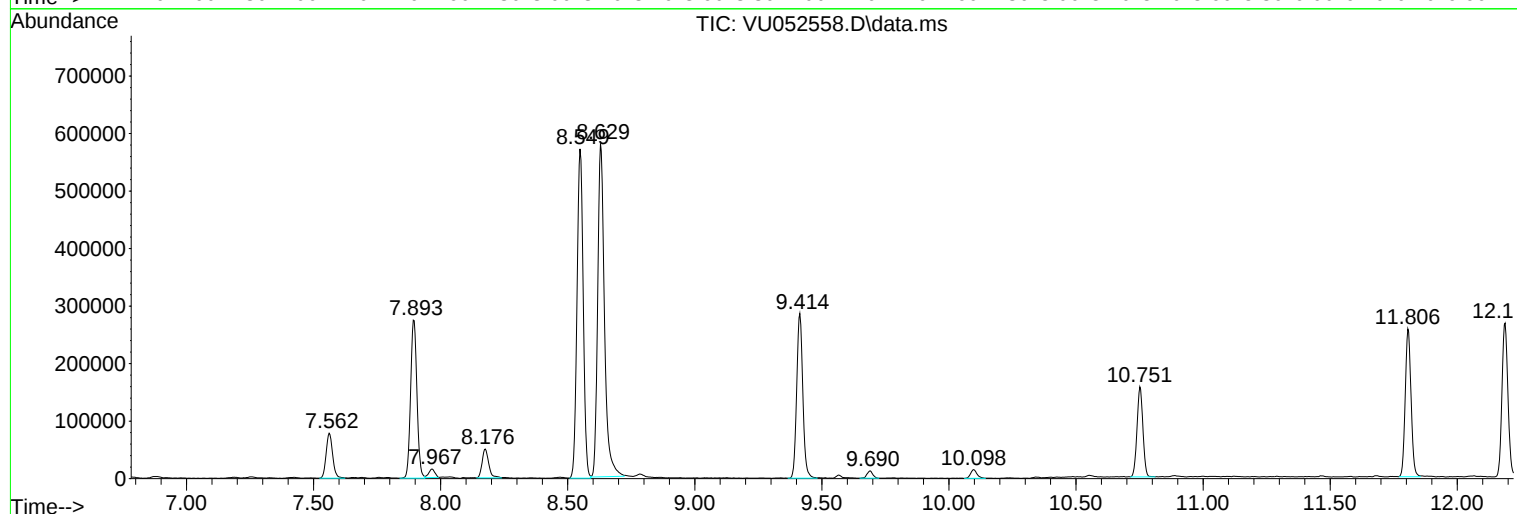
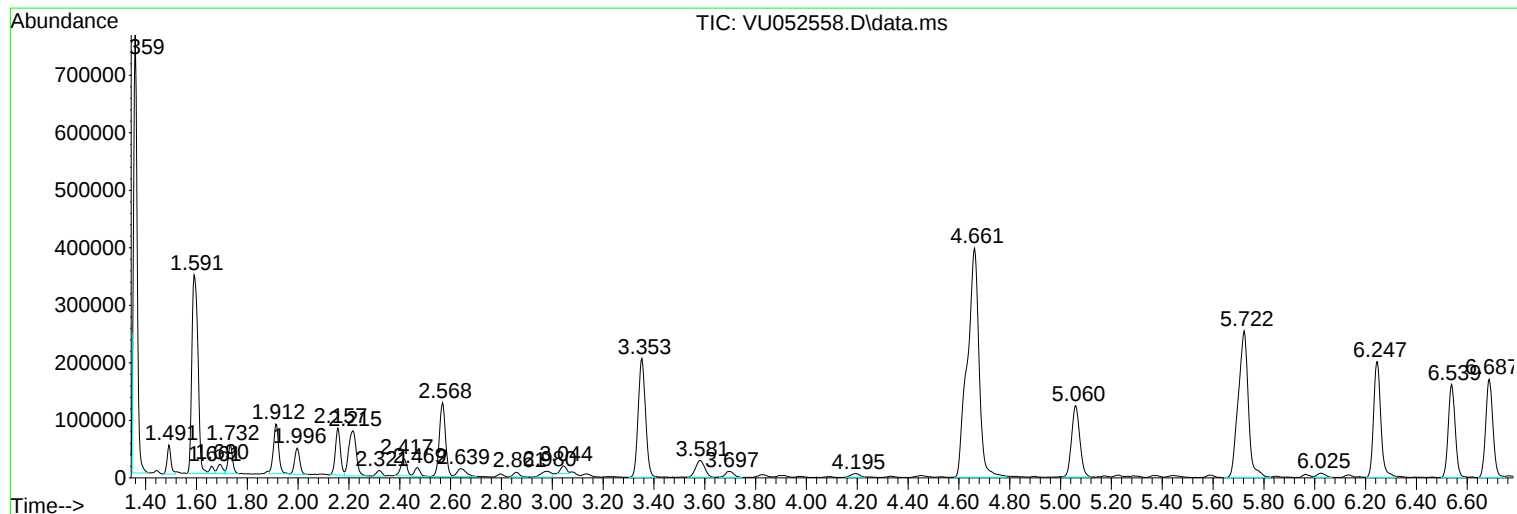
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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Instrument :
MSVOA_U
ClientSampleId :
GBQA2

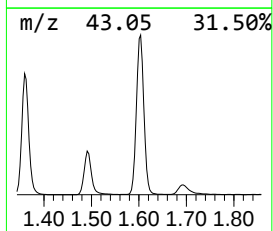
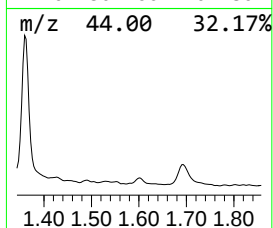
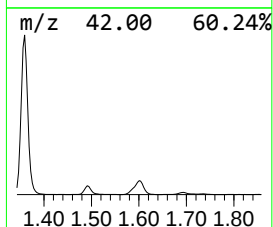
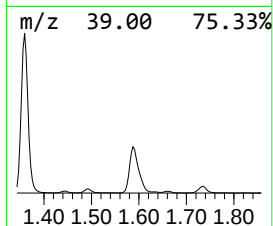
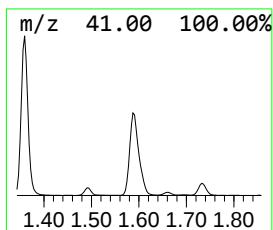
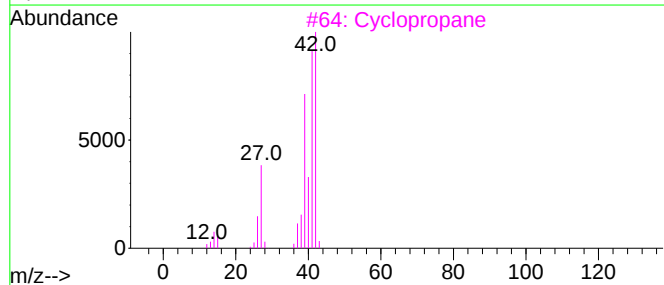
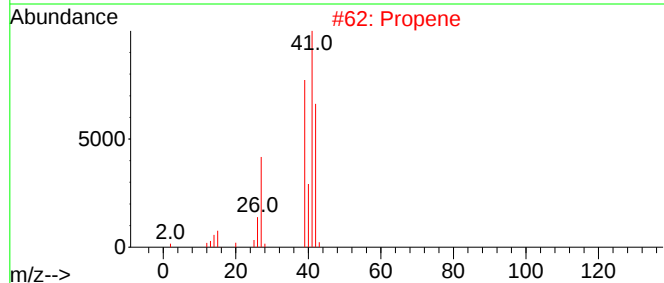
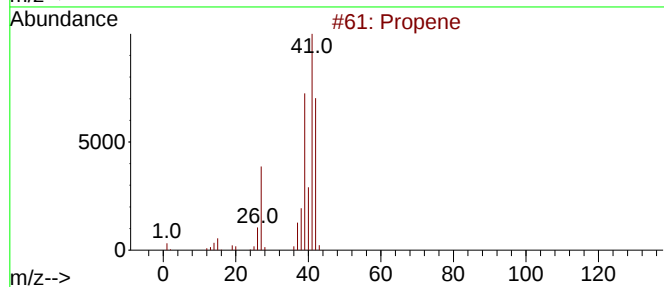
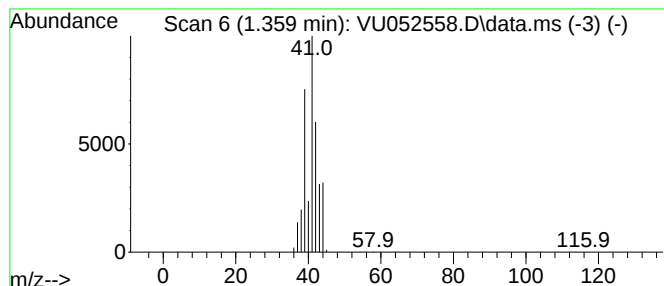
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Quant Title : TRACE VOA SFAM1.0

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	8.74 ug/L	695553	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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Instrument :
MSVOA_U
ClientSampleId :
GBQA2

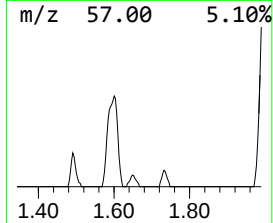
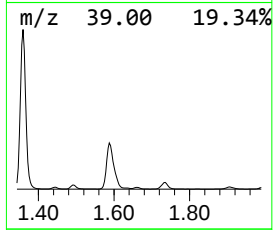
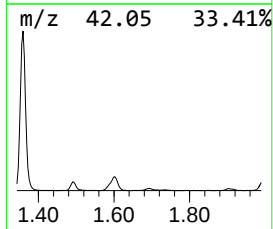
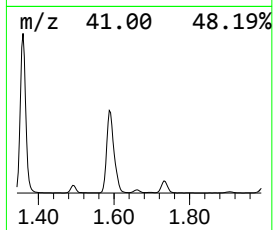
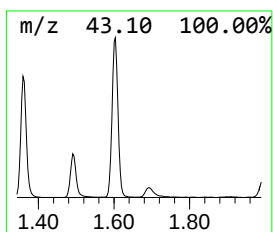
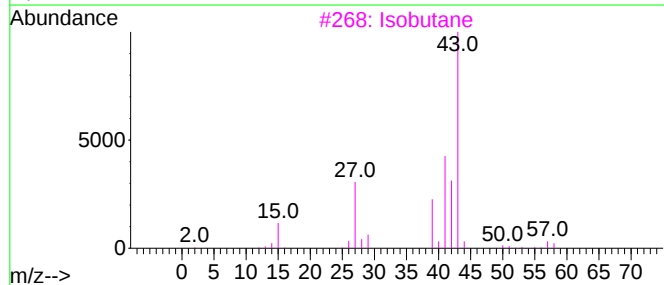
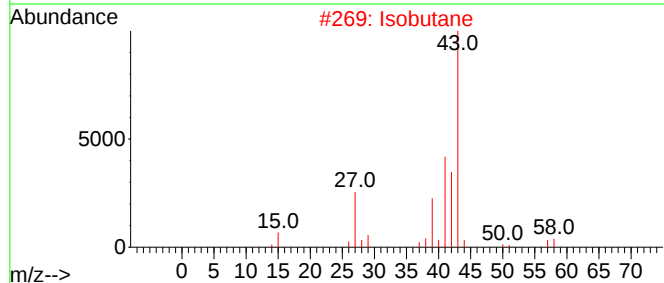
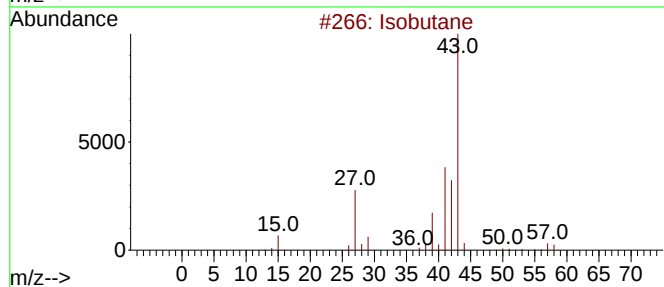
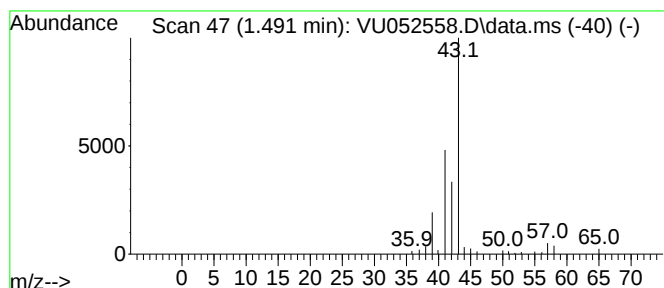
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.491	0.66 ug/L	52654	1,4-Difluorobenzene	6.247

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isobutane	58	C4H10	000075-28-5	72
2		Isobutane	58	C4H10	000075-28-5	64
3		Isobutane	58	C4H10	000075-28-5	64
4		Isobutane	58	C4H10	000075-28-5	64
5		Isobutane	58	C4H10	000075-28-5	42



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

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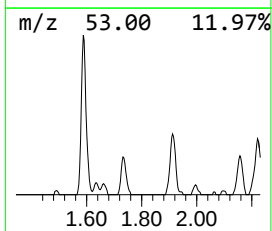
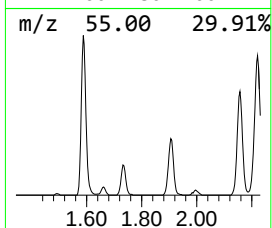
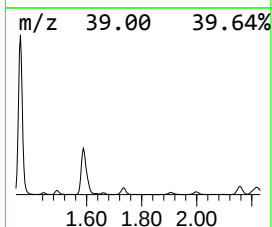
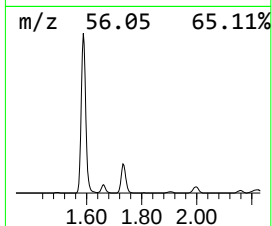
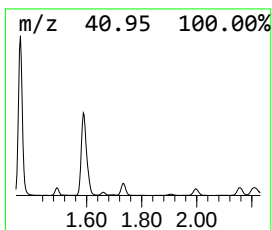
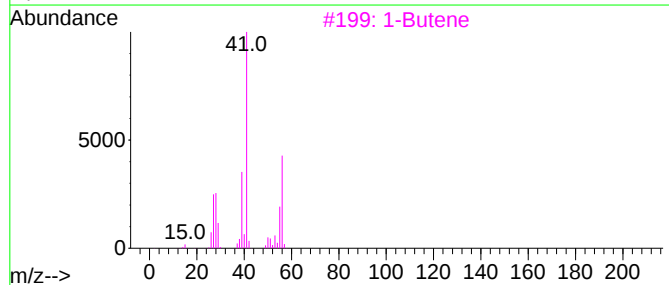
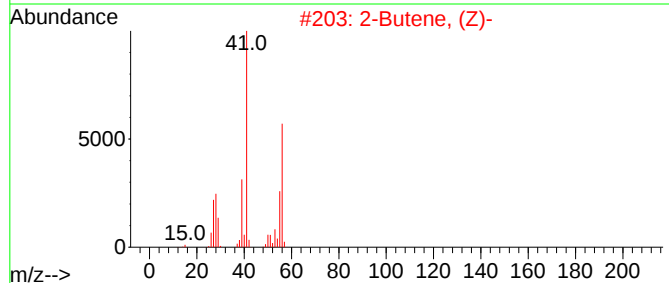
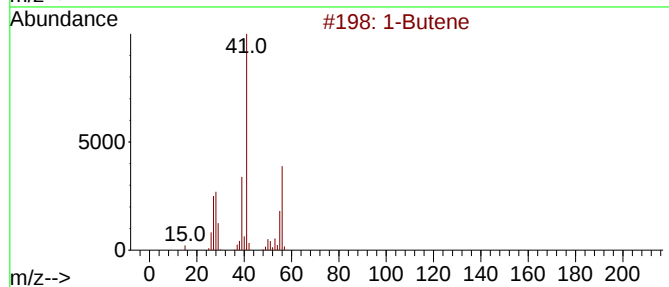
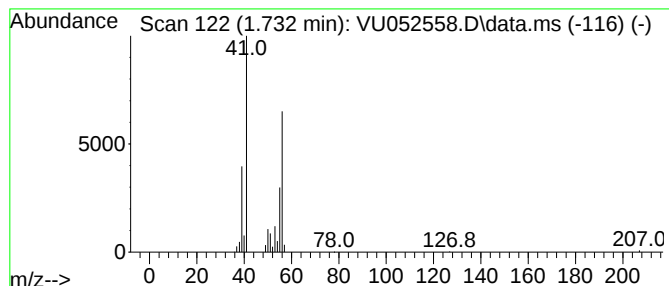
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.732	0.76 ug/L	60254	1,4-Difluorobenzene	6.247

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Butene	56	C4H8	000106-98-9	87
2		2-Butene, (Z)-	56	C4H8	000590-18-1	87
3		1-Butene	56	C4H8	000106-98-9	87
4		1-Butene	56	C4H8	000106-98-9	87
5		1-Propene, 2-methyl-	56	C4H8	000115-11-7	86



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Instrument :
MSVOA_U
ClientSampleId :
GBQA2

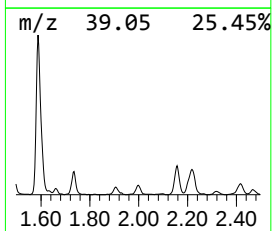
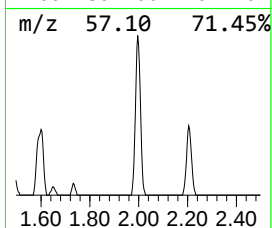
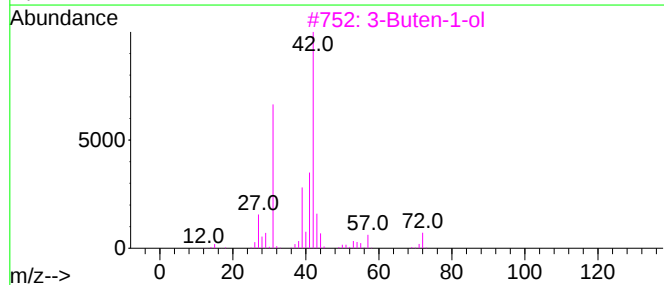
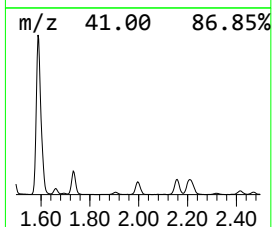
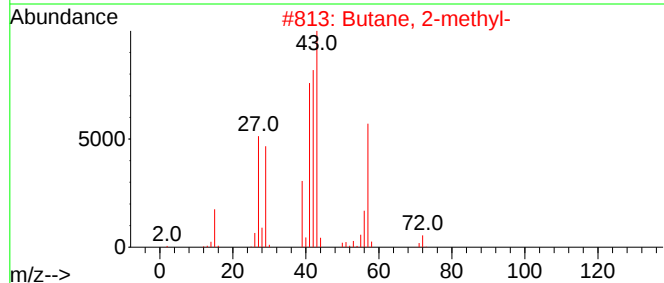
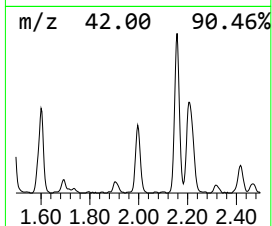
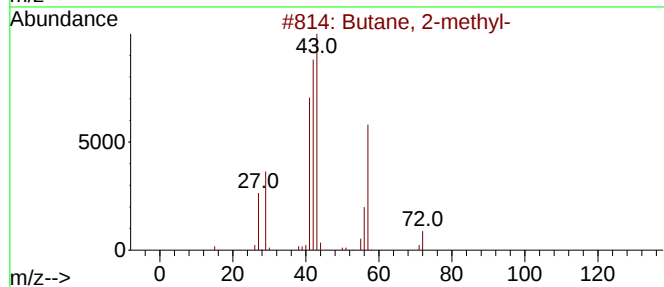
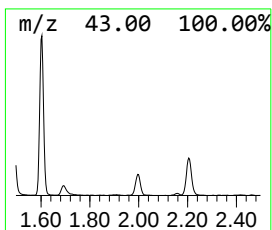
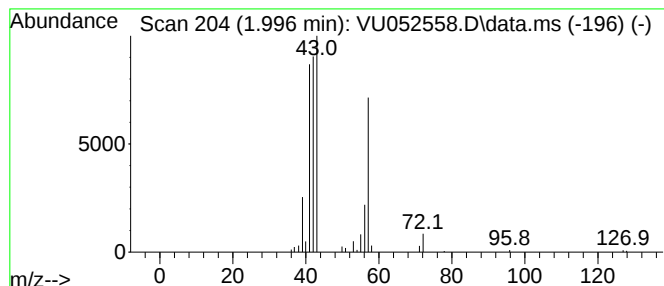
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.996	0.80 ug/L	63570	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-			72	C5H12	000078-78-4	90
2	Butane, 2-methyl-			72	C5H12	000078-78-4	90
3	3-Buten-1-ol			72	C4H8O	000627-27-0	47
4	1-Pentene, 4-methyl-			84	C6H12	000691-37-2	12
5	Butane, 1-isocyano-			83	C5H9N	002769-64-4	10



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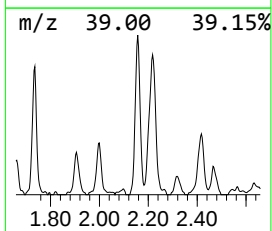
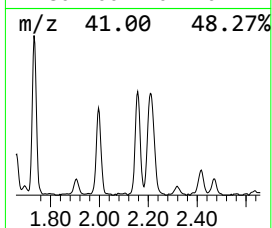
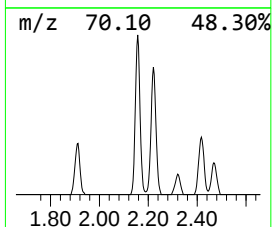
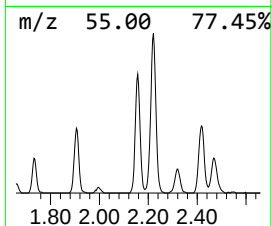
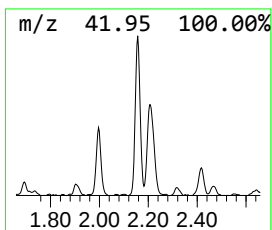
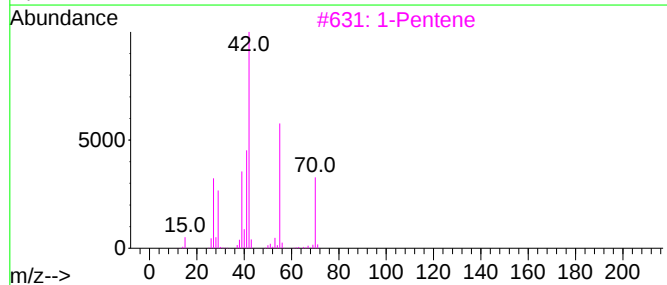
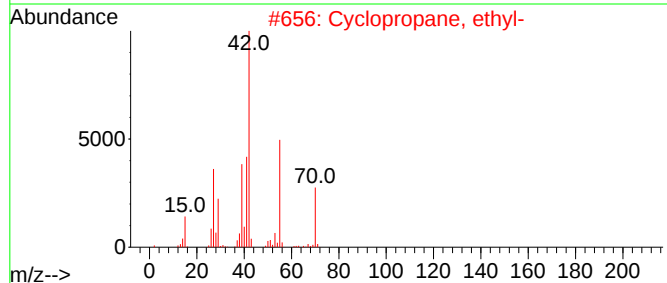
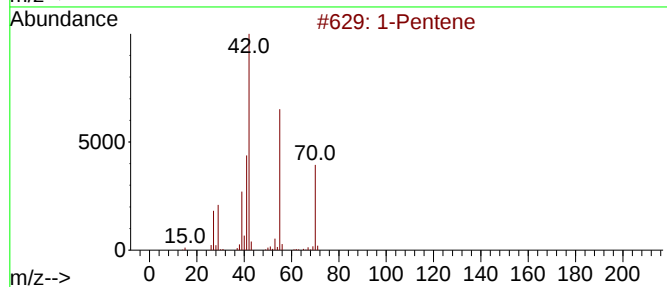
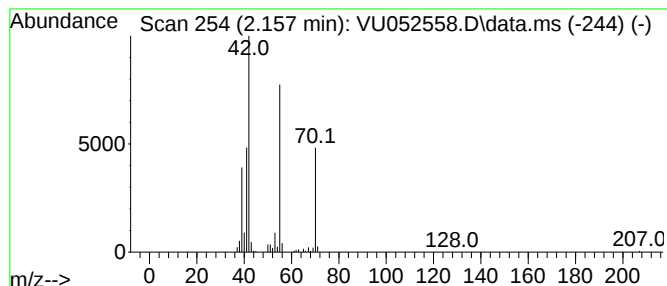
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.157	1.42 ug/L	113354	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentene	70	C5H10	000109-67-1	91
2			Cyclopropane, ethyl-	70	C5H10	001191-96-4	78
3			1-Pentene	70	C5H10	000109-67-1	76
4			Cyclopropane, ethyl-	70	C5H10	001191-96-4	68
5			Cyclobutane, methyl-	70	C5H10	000598-61-8	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122722\
Data File : VU052558.D
Acq On : 27 Dec 2022 12:44
Operator : JC/MD
Sample : N6169-11
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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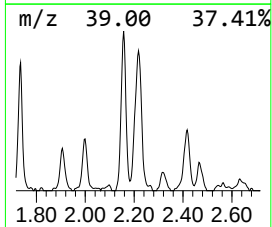
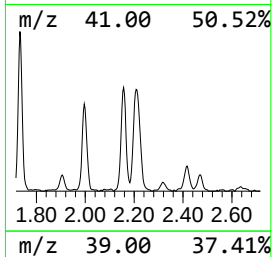
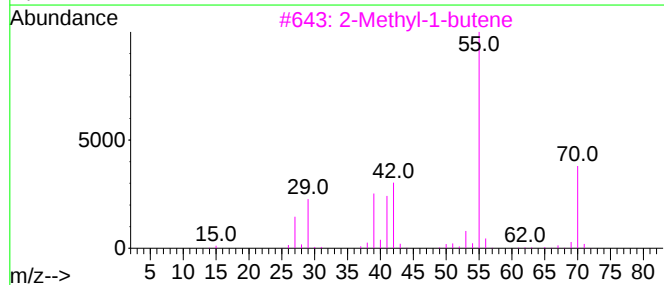
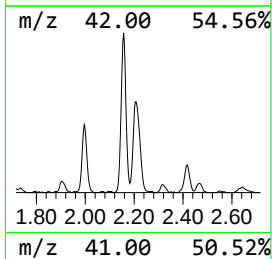
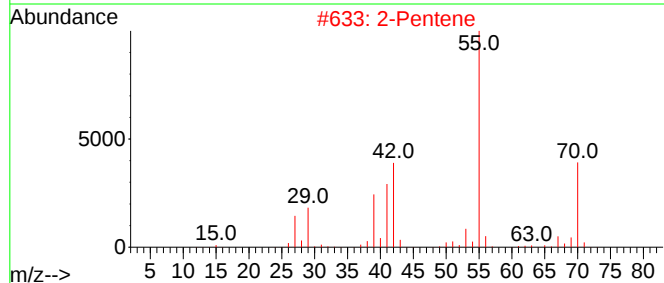
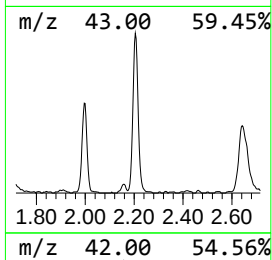
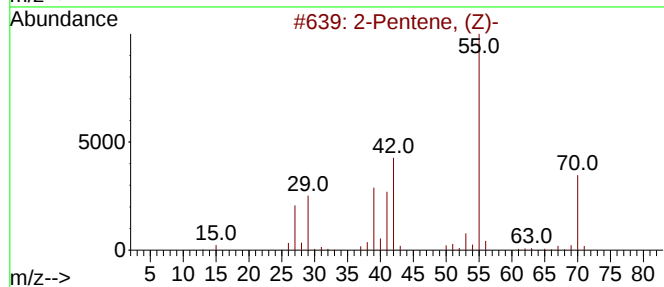
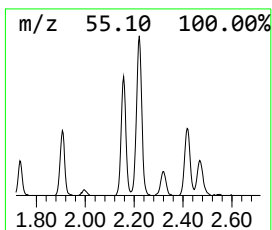
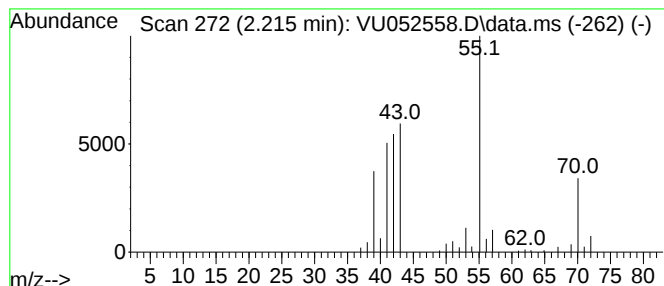
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Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.215	2.04 ug/L	162443	1,4-Difluorobenzene	6.247

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, (Z)-		70	C5H10	000627-20-3	87
2	2-Pentene		70	C5H10	000109-68-2	80
3	2-Methyl-1-butene		70	C5H10	000563-46-2	80
4	2-Pentene, (E)-		70	C5H10	000646-04-8	74
5	Cyclopropane, 1,2-dimethyl-, cis-		70	C5H10	000930-18-7	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122722\
Data File : VU052558.D
Acq On : 27 Dec 2022 12:44
Operator : JC/MD
Sample : N6169-11
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQA2

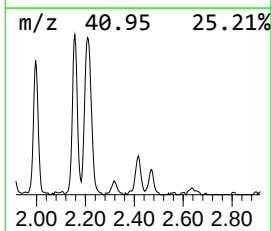
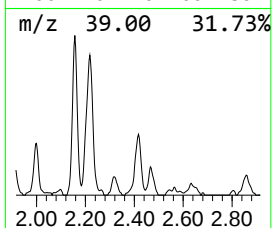
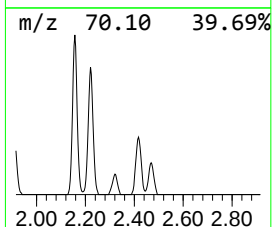
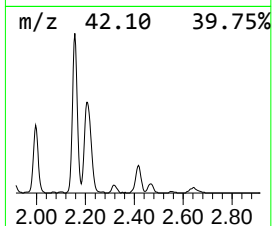
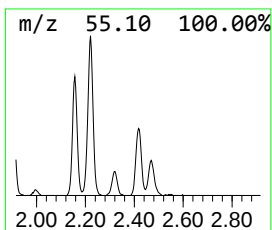
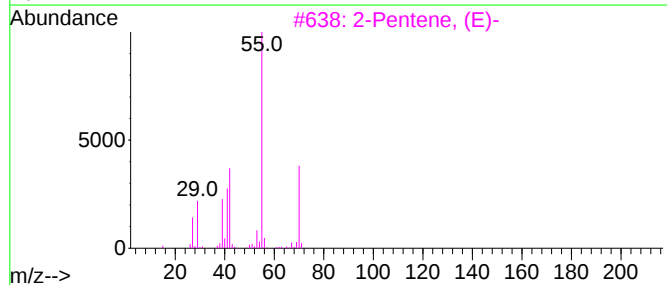
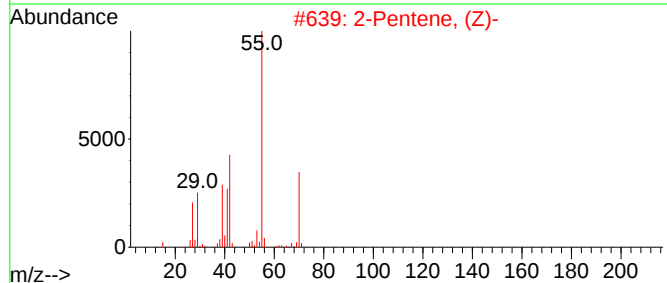
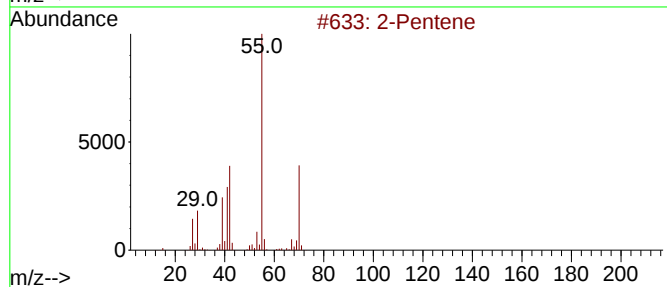
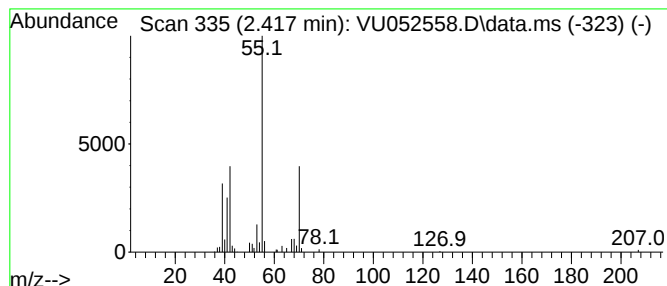
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.417	0.62 ug/L	49602	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene	70	C5H10	000109-68-2	91
2	2-Pentene, (Z)-	70	C5H10	000627-20-3	90
3	2-Pentene, (E)-	70	C5H10	000646-04-8	87
4	2-Methyl-1-butene	70	C5H10	000563-46-2	87
5	2-Pentene, (E)-	70	C5H10	000646-04-8	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122722\
Data File : VU052558.D
Acq On : 27 Dec 2022 12:44
Operator : JC/MD
Sample : N6169-11
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQA2

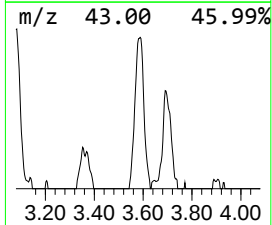
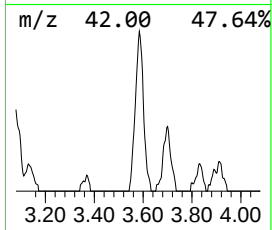
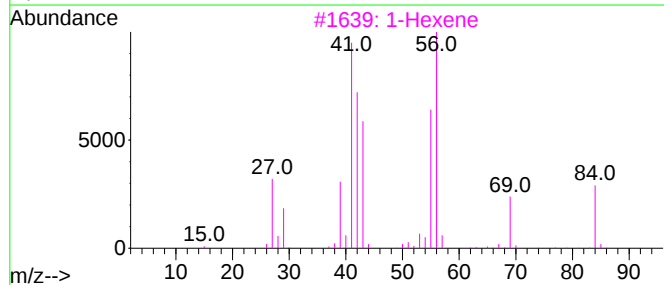
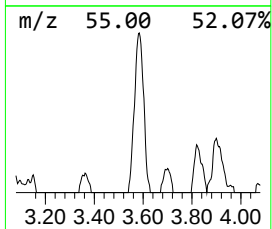
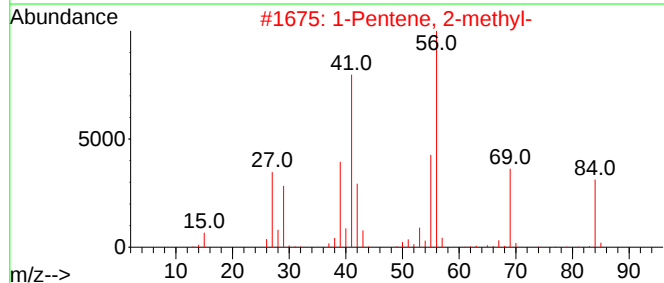
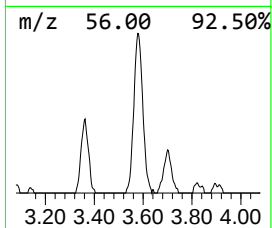
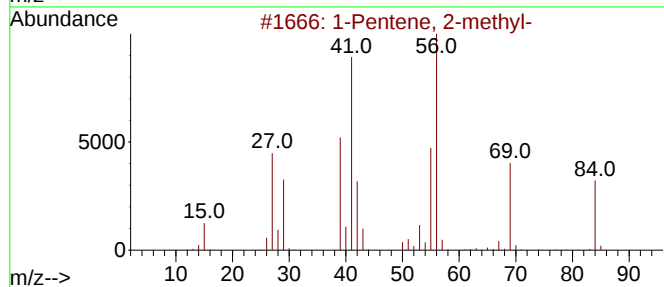
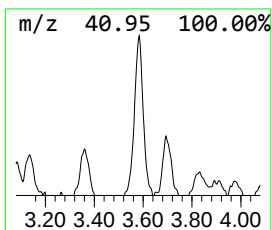
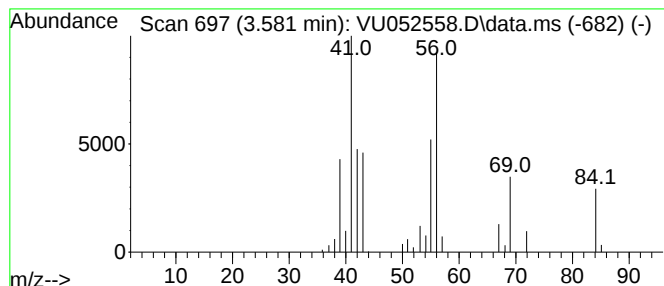
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.581	0.91 ug/L	72457	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	81
3		1-Hexene	84	C6H12	000592-41-6	58
4		1-Hexene	84	C6H12	000592-41-6	53
5		Cyclopentane, methyl-	84	C6H12	000096-37-7	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122722\
Data File : VU052558.D
Acq On : 27 Dec 2022 12:44
Operator : JC/MD
Sample : N6169-11
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQA2

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--			
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(DEL)	Alkane: S...	1.491	0.7	ug/L	52654	1	6.247	397763	5.0
(DEL)	Alkane: S...	1.732	0.8	ug/L	60254	1	6.247	397763	5.0
(DEL)	Alkane: S...	1.996	0.8	ug/L	63570	1	6.247	397763	5.0
(DEL)	Alkane: S...	2.157	1.4	ug/L	113354	1	6.247	397763	5.0
(DEL)	Alkane: S...	2.215	2.0	ug/L	162443	1	6.247	397763	5.0
(DEL)	Alkane: S...	2.417	0.6	ug/L	49602	1	6.247	397763	5.0
(DEL)	Alkane: S...	3.581	0.9	ug/L	72457	1	6.247	397763	5.0