

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122322\
 Data File : VU052548.D
 Acq On : 23 Dec 2022 19:29
 Operator : JC/MD
 Sample : N6169-07
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 GBQA0

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: VU052548.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	28	rVB	471846	447387	18.81%	3.833%
2	1.494	41	48	53	rBV	37549	39695	1.67%	0.340%
3	1.591	69	78	93	rBV3	265689	453746	19.08%	3.888%
4	1.732	116	122	132	rVB	32826	40233	1.69%	0.345%
5	1.912	170	178	194	rVB2	88103	127231	5.35%	1.090%
6	1.996	196	204	214	rVB	46157	63343	2.66%	0.543%
7	2.157	245	254	262	rBV	64766	92712	3.90%	0.794%
8	2.215	262	272	290	rVB3	67473	139558	5.87%	1.196%
9	2.414	325	334	342	rBV	20792	33317	1.40%	0.285%
10	2.469	343	351	362	rVB2	21743	37230	1.57%	0.319%
11	2.568	371	382	398	rBV	137508	229248	9.64%	1.964%
12	2.858	463	472	486	rVB2	13465	25760	1.08%	0.221%
13	2.977	493	509	517	rBV7	9950	28146	1.18%	0.241%
14	3.044	519	530	550	rVV5	31356	87447	3.68%	0.749%
15	3.134	550	558	575	rVB3	10963	24566	1.03%	0.210%
16	3.353	609	626	650	rBV	913357	1813587	76.25%	15.540%
17	3.584	681	698	712	rVB6	26116	67897	2.85%	0.582%
18	4.665	1005	1034	1081	rBV2	933010	2378508	100.00%	20.381%
19	5.060	1142	1157	1178	rVB	131213	295637	12.43%	2.533%
20	5.372	1225	1254	1264	rBV2	56638	340832	14.33%	2.920%
21	5.723	1348	1363	1393	rVB2	269622	735104	30.91%	6.299%
22	6.243	1516	1525	1545	rVB	199918	382113	16.07%	3.274%
23	6.687	1653	1663	1677	rVB	176547	335623	14.11%	2.876%
24	7.562	1927	1935	1954	rVB	87618	162541	6.83%	1.393%
25	7.893	2028	2038	2054	rVB	300487	512962	21.57%	4.395%
26	8.176	2118	2126	2139	rVB	55243	92542	3.89%	0.793%
27	8.549	2236	2242	2254	rVB4	30592	50134	2.11%	0.430%
28	8.636	2258	2269	2306	rVV	391470	917878	38.59%	7.865%
29	9.414	2500	2511	2534	rVB	273125	467605	19.66%	4.007%
30	10.751	2917	2927	2941	rVB	162805	266106	11.19%	2.280%
31	11.806	3245	3255	3275	rVB	261643	419843	17.65%	3.597%
32	12.089	3337	3343	3353	rVB4	15523	24296	1.02%	0.208%
33	12.189	3363	3374	3390	rVB	295994	470220	19.77%	4.029%
34	17.455	5005	5012	5027	rBV4	39315	67444	2.84%	0.578%

Sum of corrected areas: 11670491

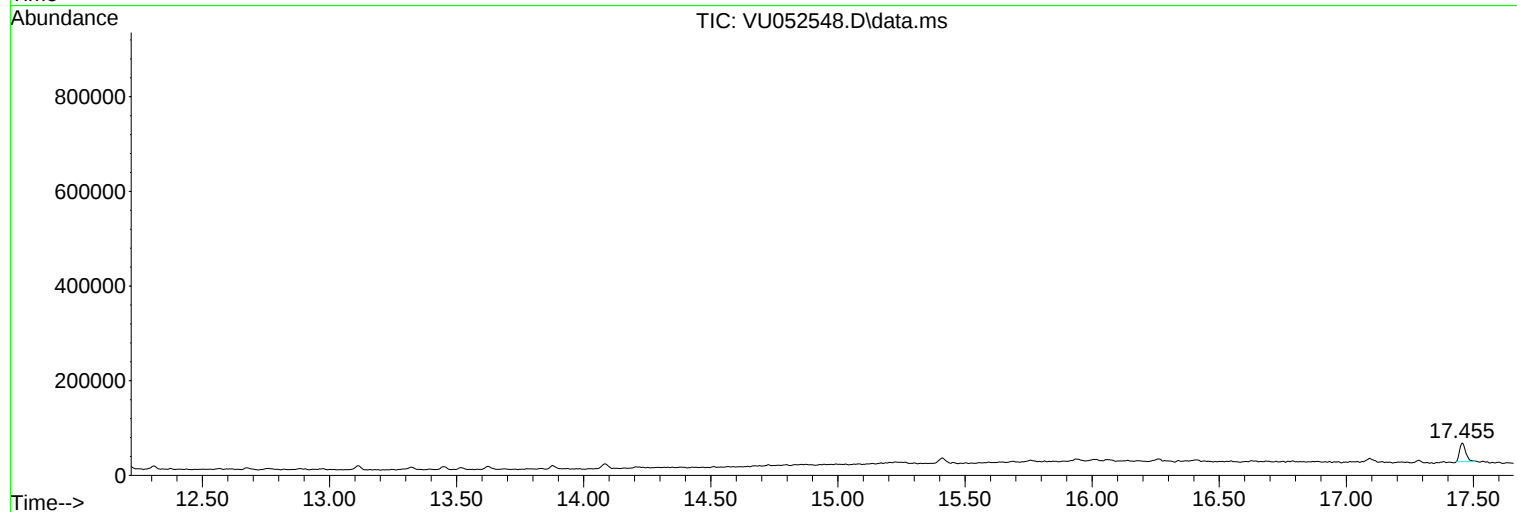
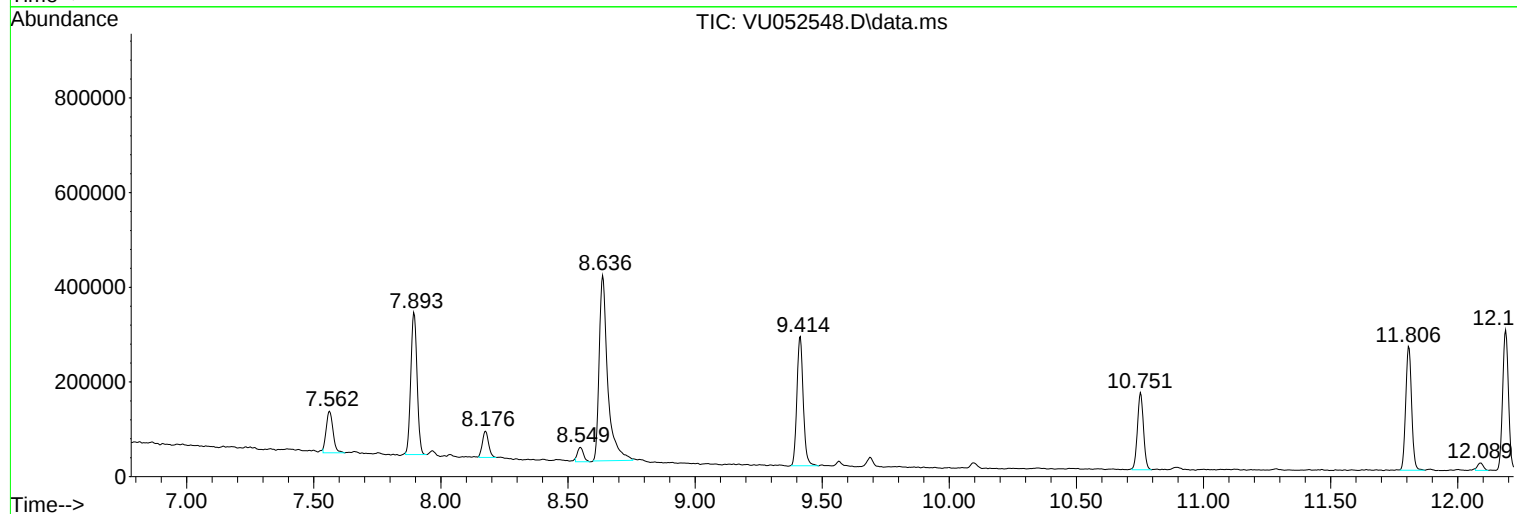
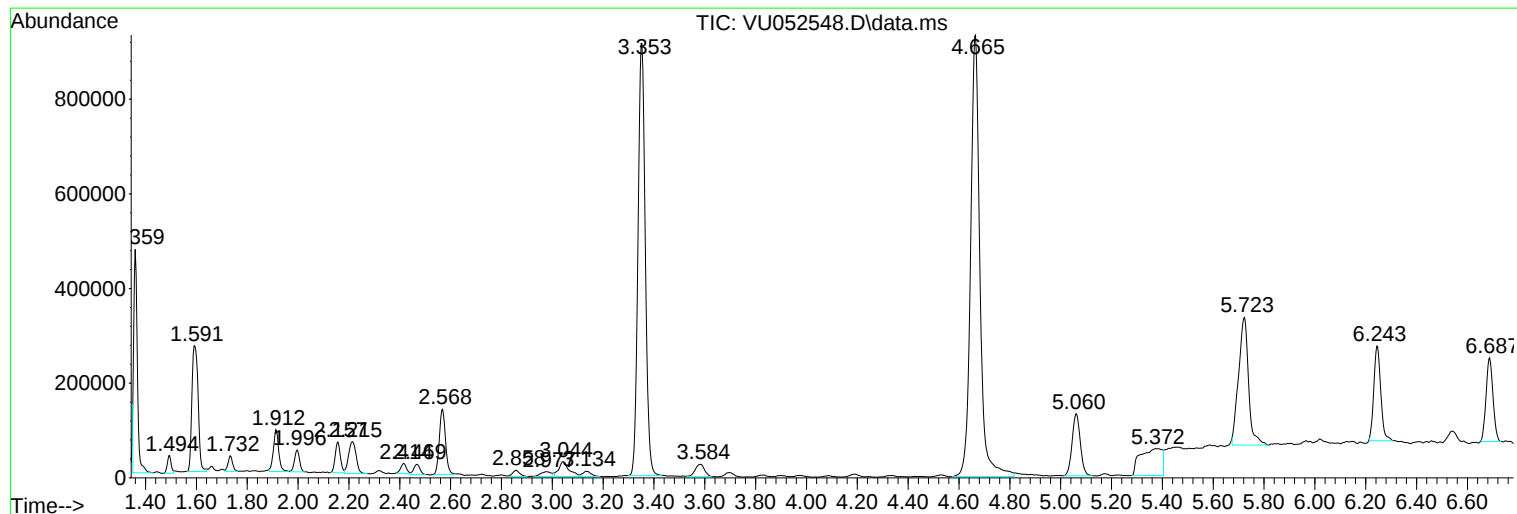
Instrument :
MSVOA_U
ClientSampleId :
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ClientSampleId :
GBQA0

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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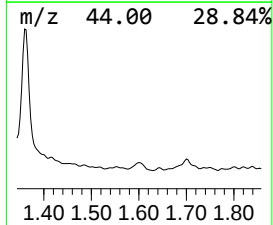
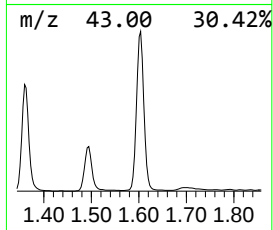
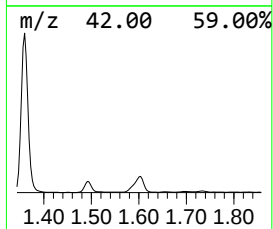
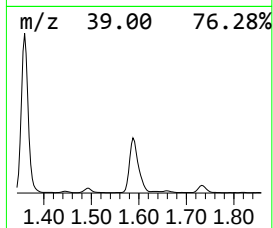
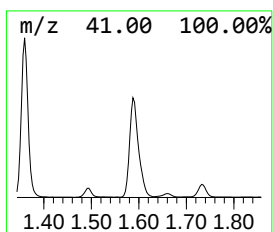
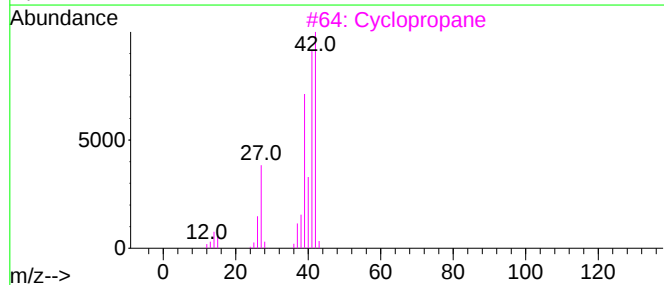
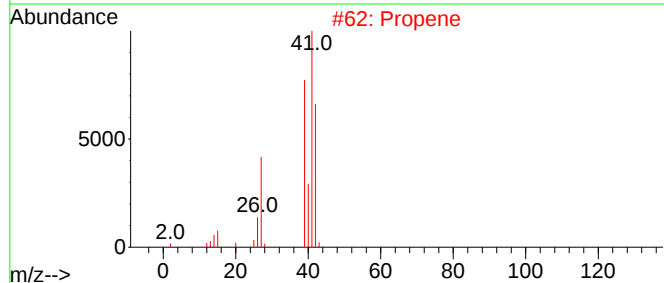
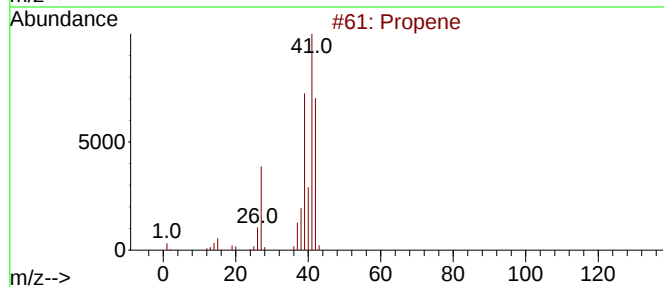
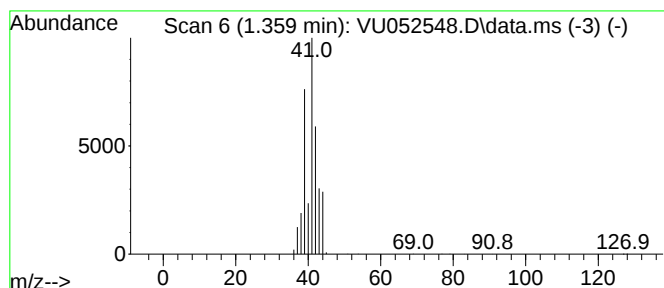
Instrument :
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ClientSampleId :
GBQA0

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
1.359	5.85 ug/L	447387	1,4-Difluorobenzene	6.243	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	86
2	Propene	42	C3H6	000115-07-1	50
3	Cyclopropane	42	C3H6	000075-19-4	10
4	Cyclopropane	42	C3H6	000075-19-4	8
5	Cyclopropane	42	C3H6	000075-19-4	4



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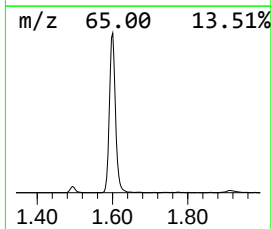
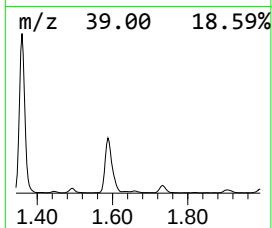
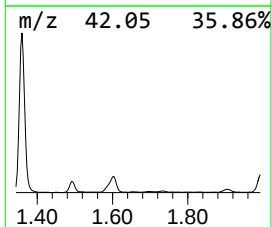
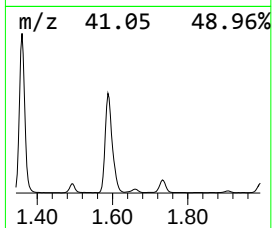
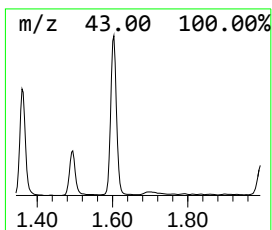
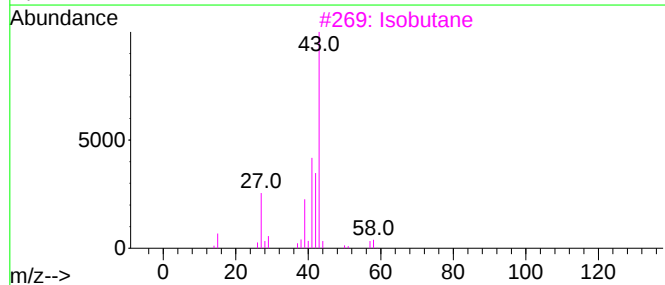
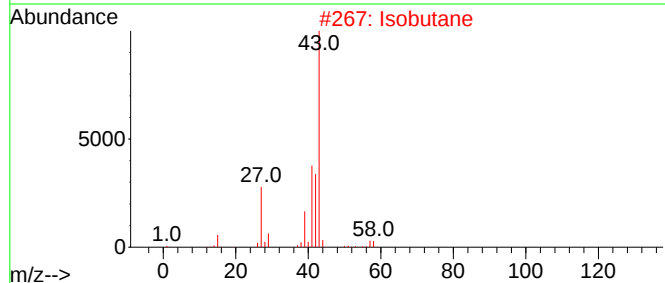
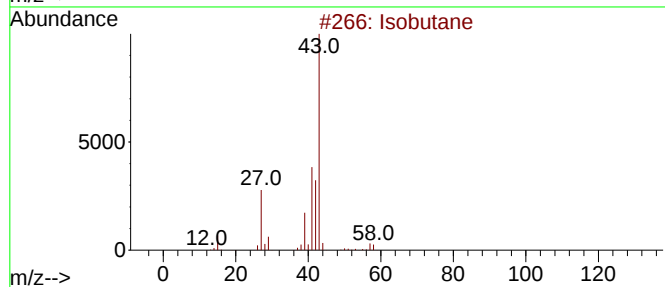
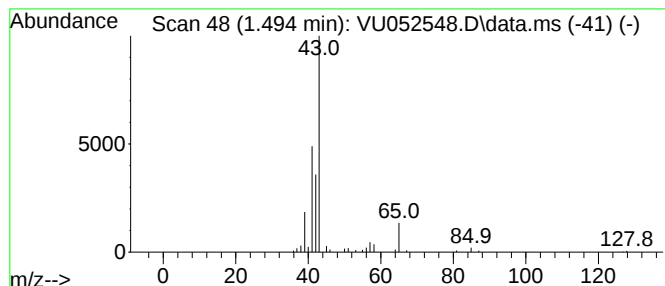
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.494	0.52 ug/L	39695	1,4-Difluorobenzene	6.243

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isobutane	58	C4H10	000075-28-5	59
2		Isobutane	58	C4H10	000075-28-5	59
3		Isobutane	58	C4H10	000075-28-5	45
4		Isobutane	58	C4H10	000075-28-5	45
5		Isobutane	58	C4H10	000075-28-5	40



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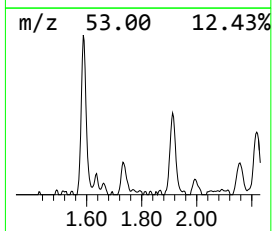
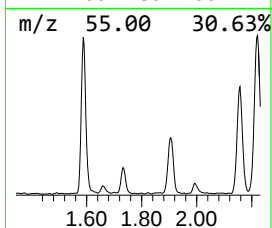
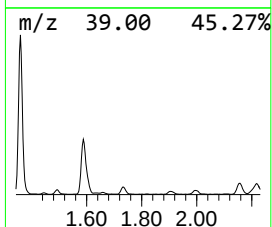
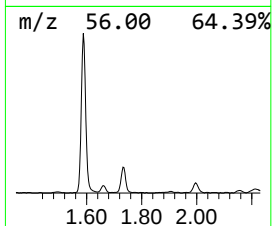
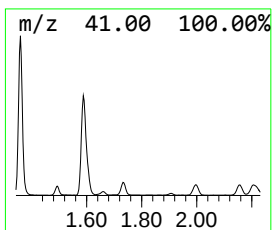
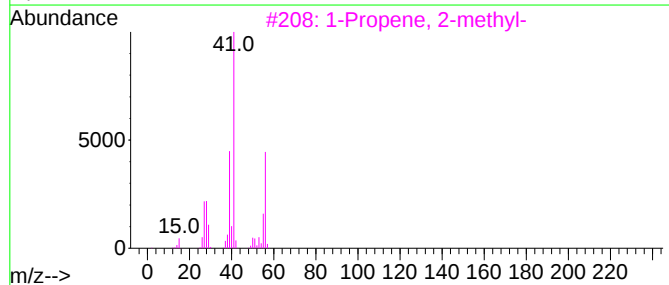
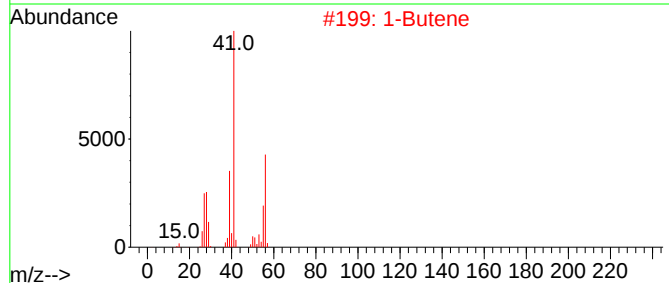
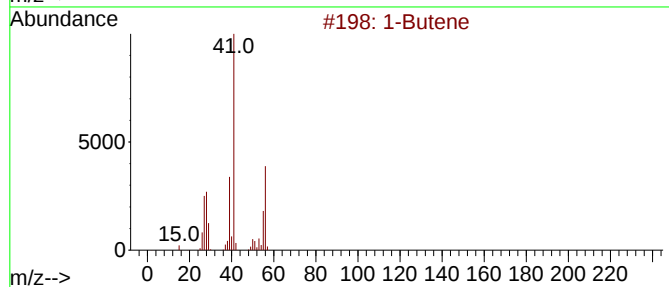
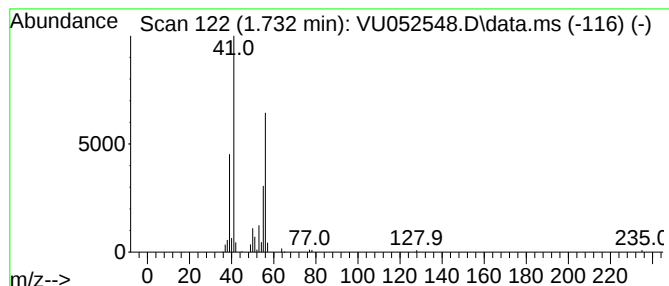
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.732	0.53 ug/L	40233	1,4-Difluorobenzene	6.243

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Butene	56	C4H8	000106-98-9	87
2		1-Butene	56	C4H8	000106-98-9	87
3		1-Propene, 2-methyl-	56	C4H8	000115-11-7	80
4		1-Butene	56	C4H8	000106-98-9	80
5		2-Butene, (Z)-	56	C4H8	000590-18-1	74



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MSVOA_U
ClientSampleId :
GBQA0

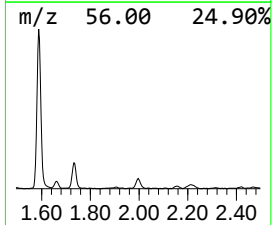
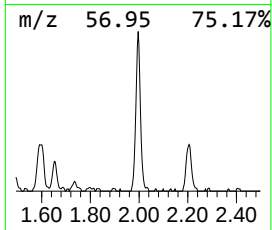
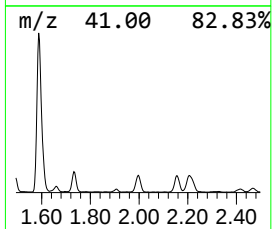
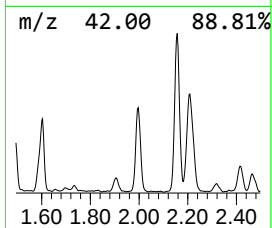
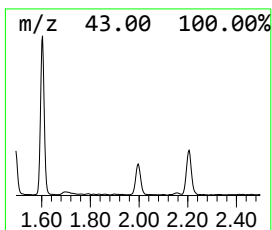
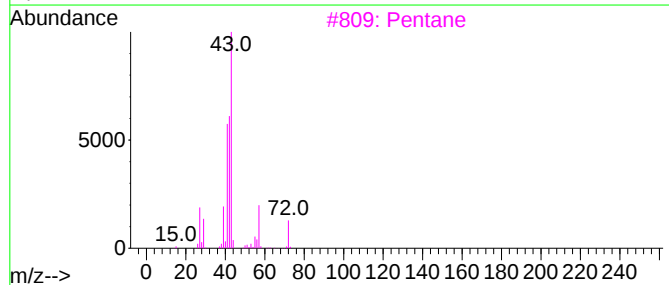
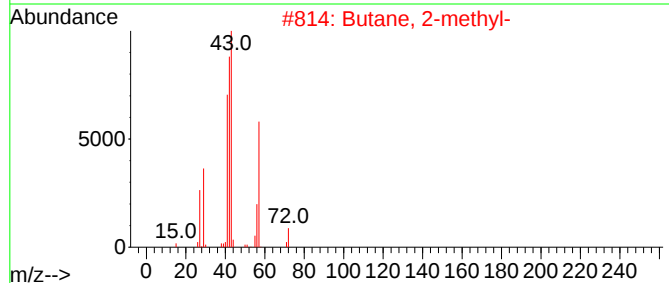
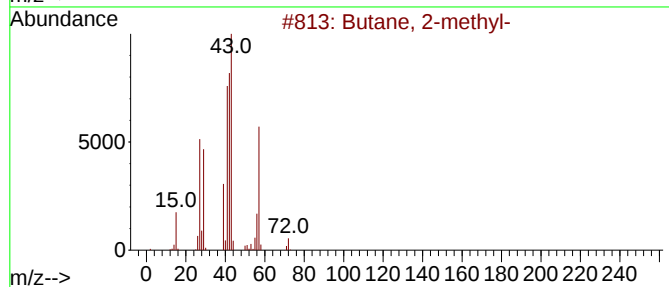
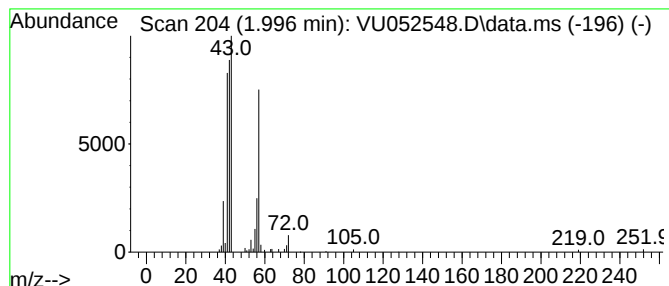
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.996	0.83 ug/L	63343	1,4-Difluorobenzene	6.243

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	86
3			Pentane	72	C5H12	000109-66-0	33
4			Butane, 1-isocyano-	83	C5H9N	002769-64-4	22
5			1-Butene	56	C4H8	000106-98-9	11



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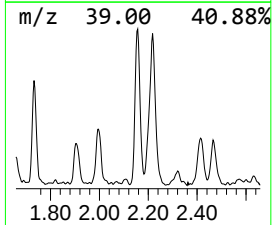
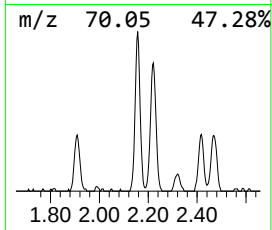
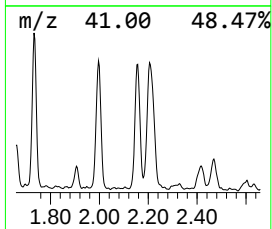
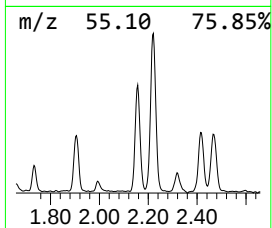
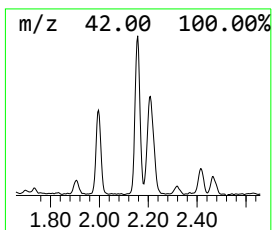
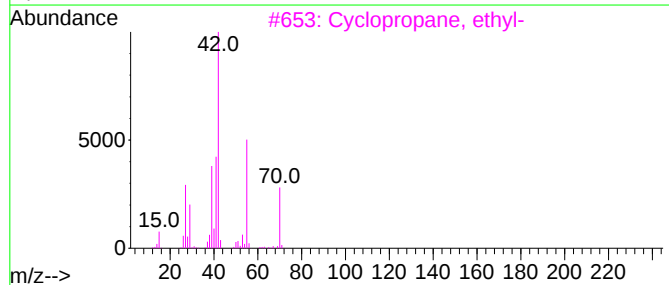
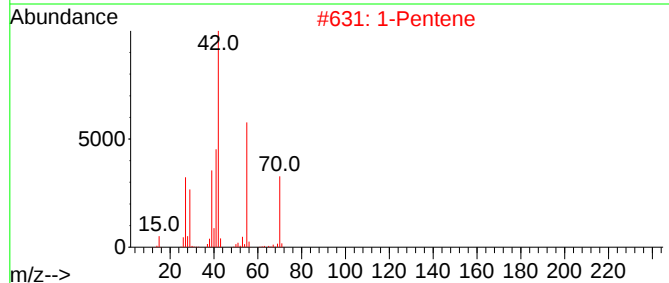
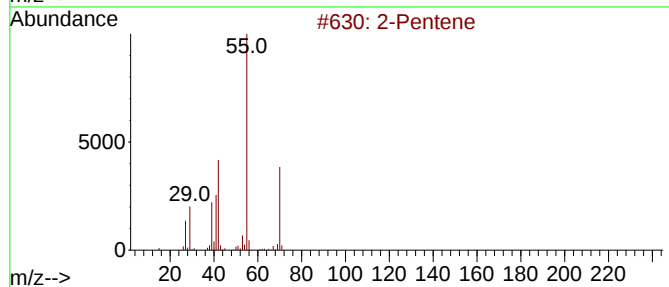
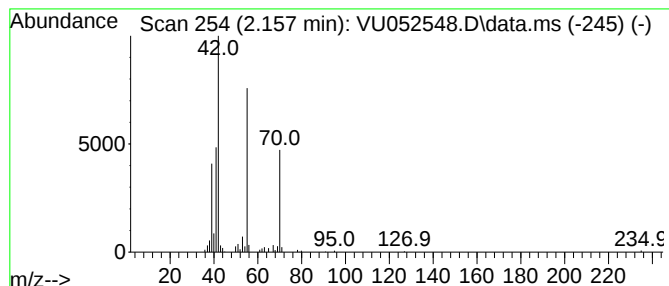
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST0.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.
2.157	1.21 ug/L	92712	1,4-Difluorobenzene	6.243

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentene	70	C5H10	000109-68-2	83
2		1-Pentene	70	C5H10	000109-67-1	68
3		Cyclopropane, ethyl-	70	C5H10	001191-96-4	68
4		1-Pentene	70	C5H10	000109-67-1	64
5		Cyclopropane, ethyl-	70	C5H10	001191-96-4	64



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GBQA0

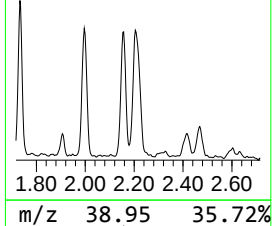
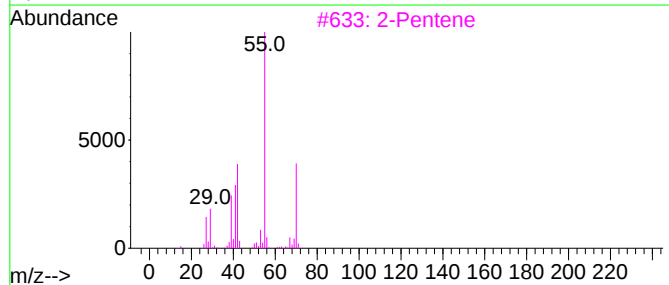
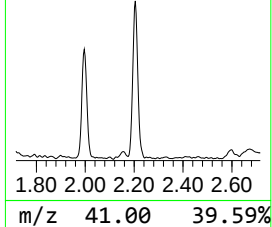
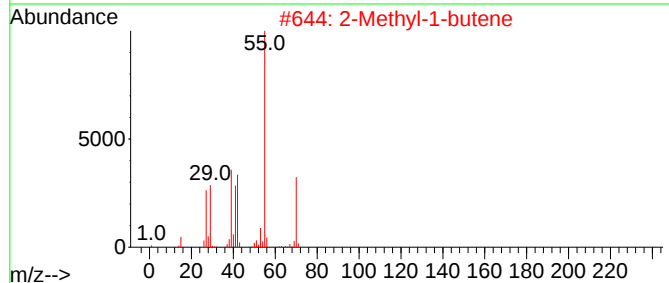
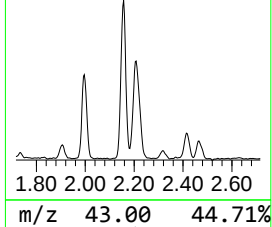
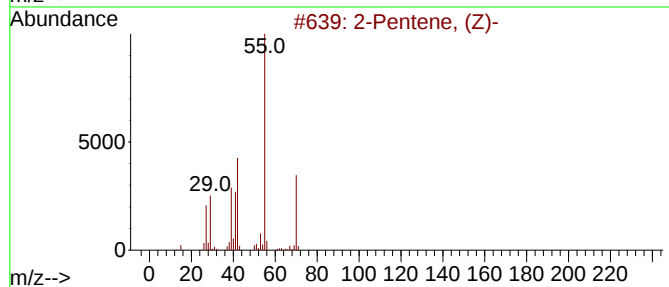
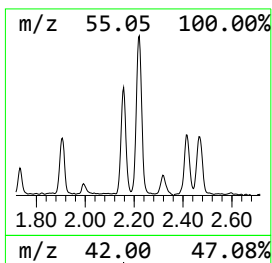
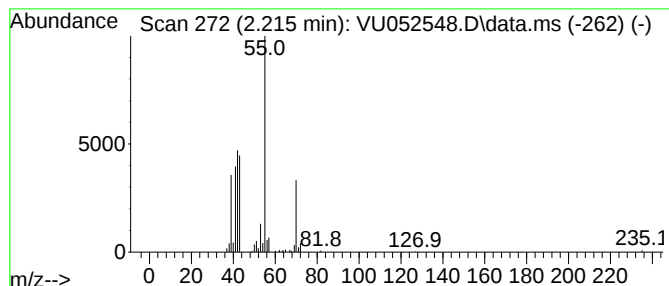
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Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.215	1.83 ug/L	139558	1,4-Difluorobenzene	6.243

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	87
4		2-Butene, 2-methyl-	70	C5H10	000513-35-9	86
5		Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122322\
Data File : VU052548.D
Acq On : 23 Dec 2022 19:29
Operator : JC/MD
Sample : N6169-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQA0

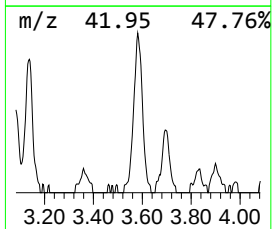
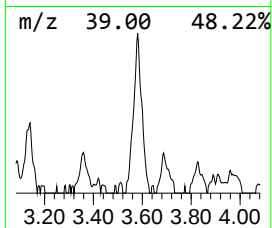
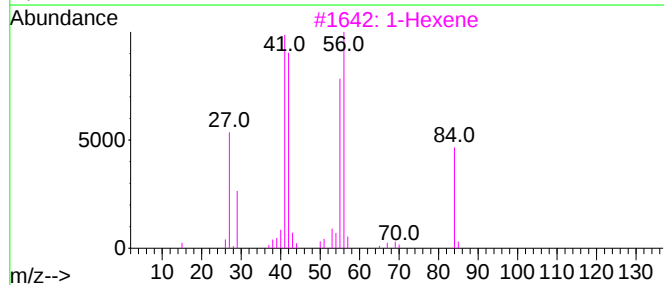
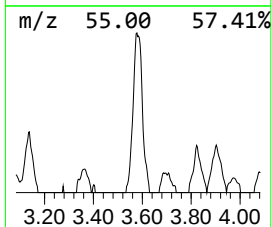
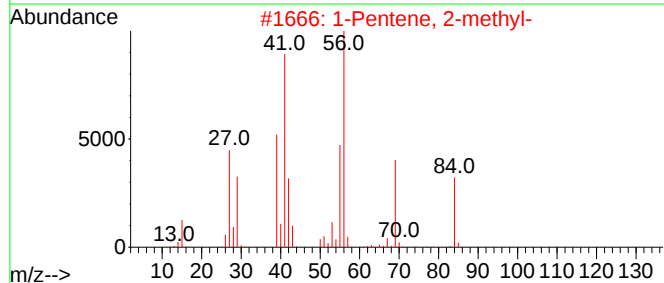
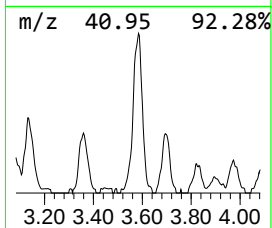
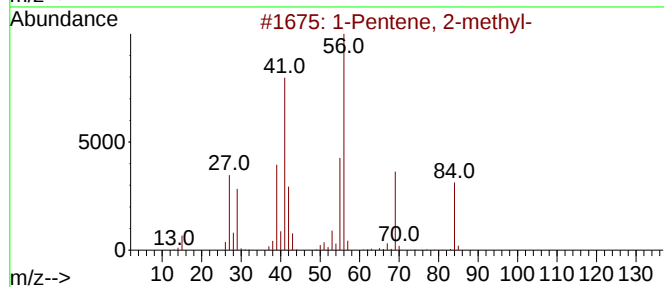
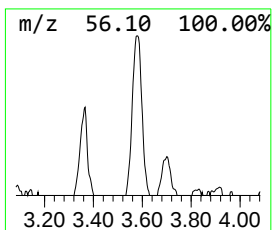
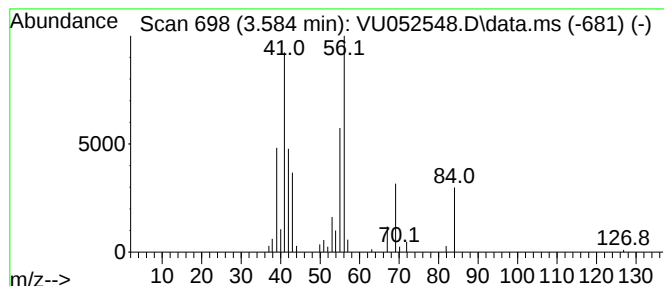
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.584	0.89 ug/L	67897	1,4-Difluorobenzene	6.243

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene, 2-methyl-		84	C6H12	000763-29-1	74
2	1-Pentene, 2-methyl-		84	C6H12	000763-29-1	72
3	1-Hexene		84	C6H12	000592-41-6	58
4	1-Hexene		84	C6H12	000592-41-6	53
5	1-Hexene		84	C6H12	000592-41-6	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122322\
Data File : VU052548.D
Acq On : 23 Dec 2022 19:29
Operator : JC/MD
Sample : N6169-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQA0

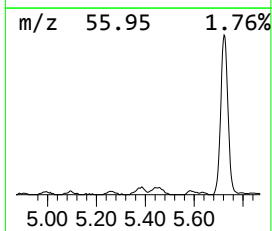
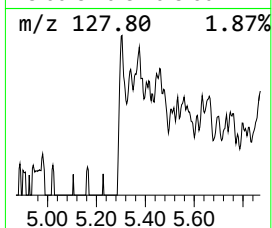
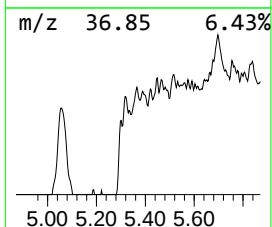
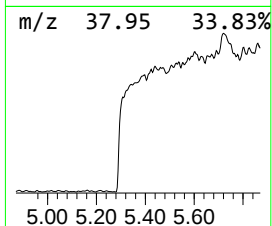
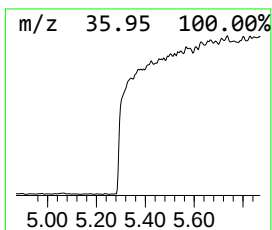
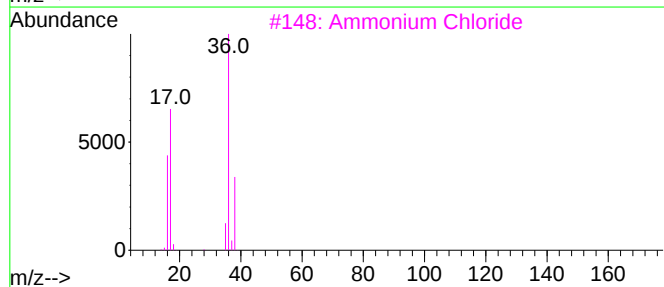
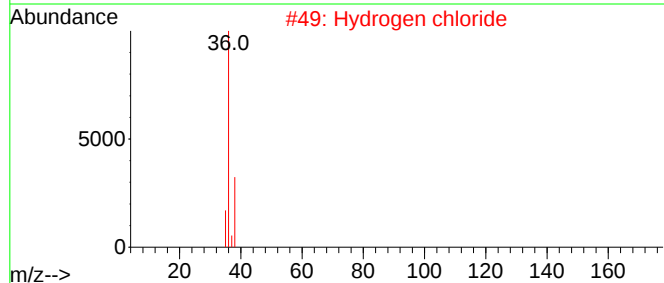
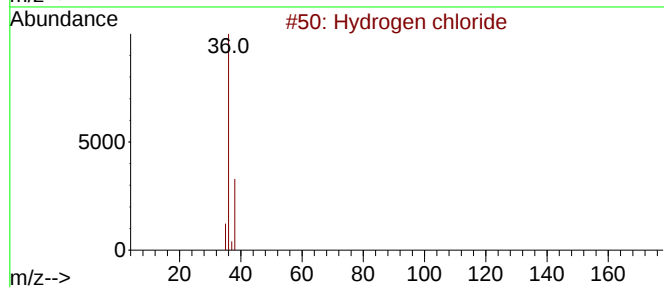
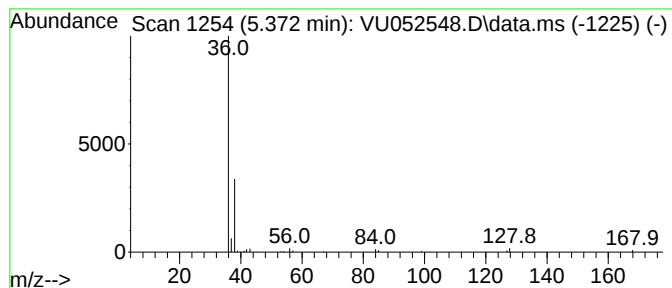
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.372	4.46 ug/L	340832	1,4-Difluorobenzene	6.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hydrogen chloride	36	ClH	007647-01-0	9
2			Hydrogen chloride	36	ClH	007647-01-0	9
3			Ammonium Chloride	53	ClH4N	012125-02-9	4
4			1H-Imidazole-1-ethanol, .alpha.-...	126	C6H10N2O	037788-55-9	2
5			Methanol-D4	36	CD4O	000811-98-3	2



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122322\
Data File : VU052548.D
Acq On : 23 Dec 2022 19:29
Operator : JC/MD
Sample : N6169-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

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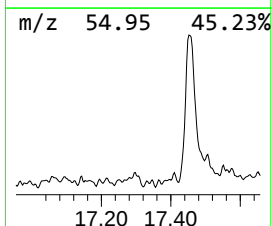
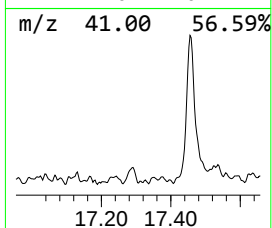
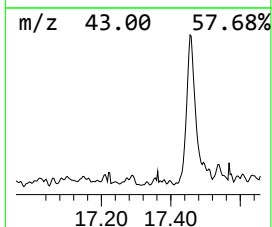
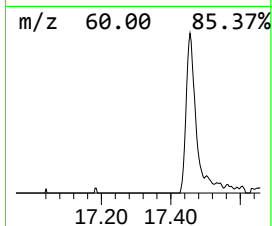
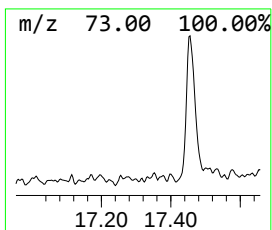
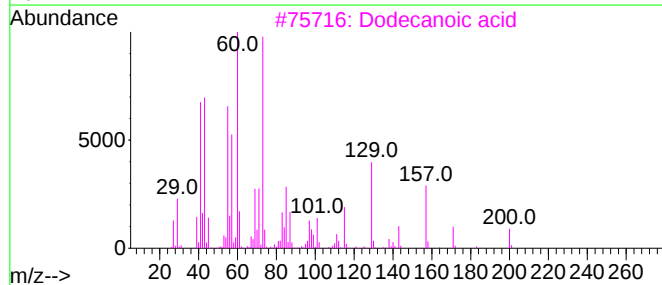
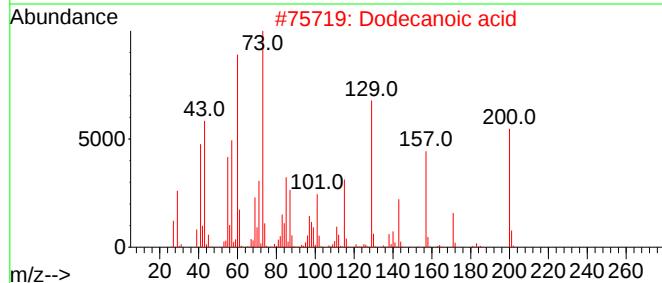
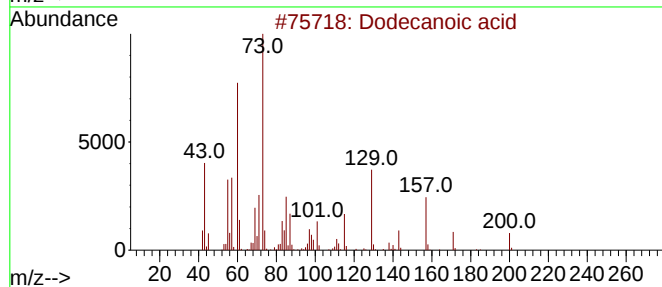
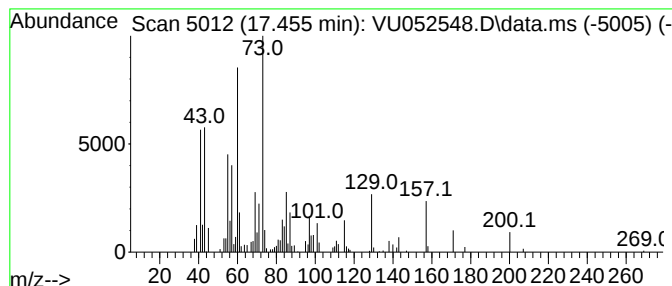
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 10 Dodecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.455	0.80 ug/L	67444	1,4-Dichlorobenzene-d4	11.806

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	97
2			Dodecanoic acid	200	C12H24O2	000143-07-7	96
3			Dodecanoic acid	200	C12H24O2	000143-07-7	96
4			Dodecanoic acid	200	C12H24O2	000143-07-7	95
5			Tridecanoic acid	214	C13H26O2	000638-53-9	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122322\
Data File : VU052548.D
Acq On : 23 Dec 2022 19:29
Operator : JC/MD
Sample : N6169-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 26 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

					--Internal Standard--			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL) Alkane: S...	1.359	5.8	ug/L	447387	1	6.243	382113	5.0
(DEL) Alkane: S...	1.494	0.5	ug/L	39695	1	6.243	382113	5.0
(DEL) Alkane: S...	1.732	0.5	ug/L	40233	1	6.243	382113	5.0
(DEL) Alkane: S...	1.996	0.8	ug/L	63343	1	6.243	382113	5.0
(DEL) Alkane: S...	2.157	1.2	ug/L	92712	1	6.243	382113	5.0
(DEL) Alkane: S...	2.215	1.8	ug/L	139558	1	6.243	382113	5.0
(DEL) Alkane: S...	3.584	0.9	ug/L	67897	1	6.243	382113	5.0
unknown-01	5.372	4.5	ug/L	340832	1	6.243	382113	5.0
Dodecanoic acid	17.455	0.8	ug/L	67444	3	11.806	419843	5.0