

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV062322\
 Data File : VV026542.D
 Acq On : 24 Jun 2022 09:53
 Operator : SY/MD
 Sample : N3401-17
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AG3

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_V\Method\SFAMVTR062322WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VV026542.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.314	76	85	95	rBV	108801	127645	14.59%	1.814%
2	1.574	160	166	190	rVB	105613	143091	16.36%	2.033%
3	2.111	324	333	349	rVB	196980	293254	33.52%	4.167%
4	2.207	349	363	366	rBV2	10773	20265	2.32%	0.288%
5	2.731	500	526	527	rBV4	18703	57010	6.52%	0.810%
6	3.690	804	824	863	rBV2	319345	874735	100.00%	12.431%
7	3.924	883	897	933	rBV2	36892	184826	21.13%	2.627%
8	4.352	1012	1030	1056	rBV	113728	288675	33.00%	4.102%
9	4.677	1119	1131	1149	rVB6	6939	18238	2.08%	0.259%
10	5.050	1231	1247	1281	rBV2	258050	632257	72.28%	8.985%
11	5.619	1412	1424	1449	rBV	221652	456351	52.17%	6.485%
12	6.069	1551	1564	1586	rBV	140207	294139	33.63%	4.180%
13	6.532	1691	1708	1719	rBV	394008	839920	96.02%	11.936%
14	6.989	1840	1850	1869	rBV	57298	110348	12.62%	1.568%
15	7.316	1940	1952	1975	rBV	306424	549084	62.77%	7.803%
16	7.625	2039	2048	2065	rBV2	30710	56191	6.42%	0.799%
17	8.091	2182	2193	2229	rBV2	165465	373113	42.65%	5.302%
18	8.252	2235	2243	2258	rVB8	5362	11139	1.27%	0.158%
19	8.850	2413	2429	2458	rBV	324075	532278	60.85%	7.564%
20	10.213	2841	2853	2872	rBV2	89852	143140	16.36%	2.034%
21	11.246	3163	3174	3194	rBV	288376	451797	51.65%	6.420%
22	11.535	3255	3264	3280	rBV3	10151	20358	2.33%	0.289%
23	11.622	3280	3291	3312	rVV	247594	388097	44.37%	5.515%
24	12.342	3507	3515	3526	rBV3	10713	15602	1.78%	0.222%
25	13.747	3942	3952	3966	rBV	39933	60886	6.96%	0.865%
26	15.110	4367	4376	4387	rBV3	14610	21194	2.42%	0.301%
27	16.178	4696	4708	4717	rBV2	43611	64157	7.33%	0.912%
28	16.226	4717	4723	4732	rVB8	6203	9154	1.05%	0.130%

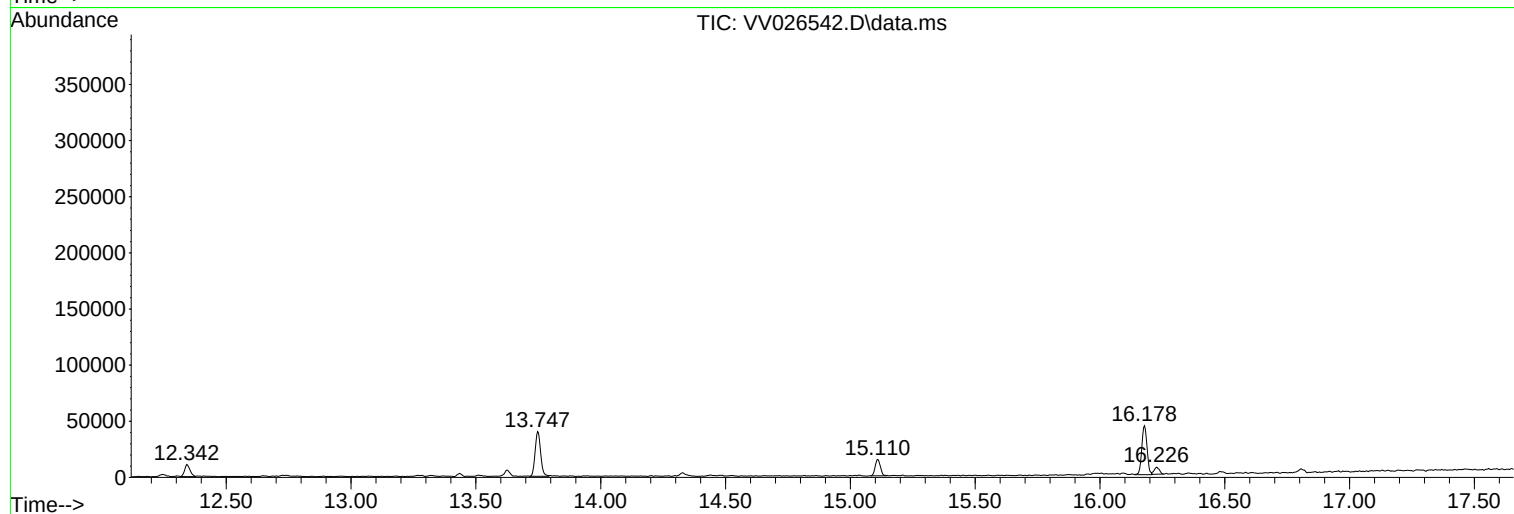
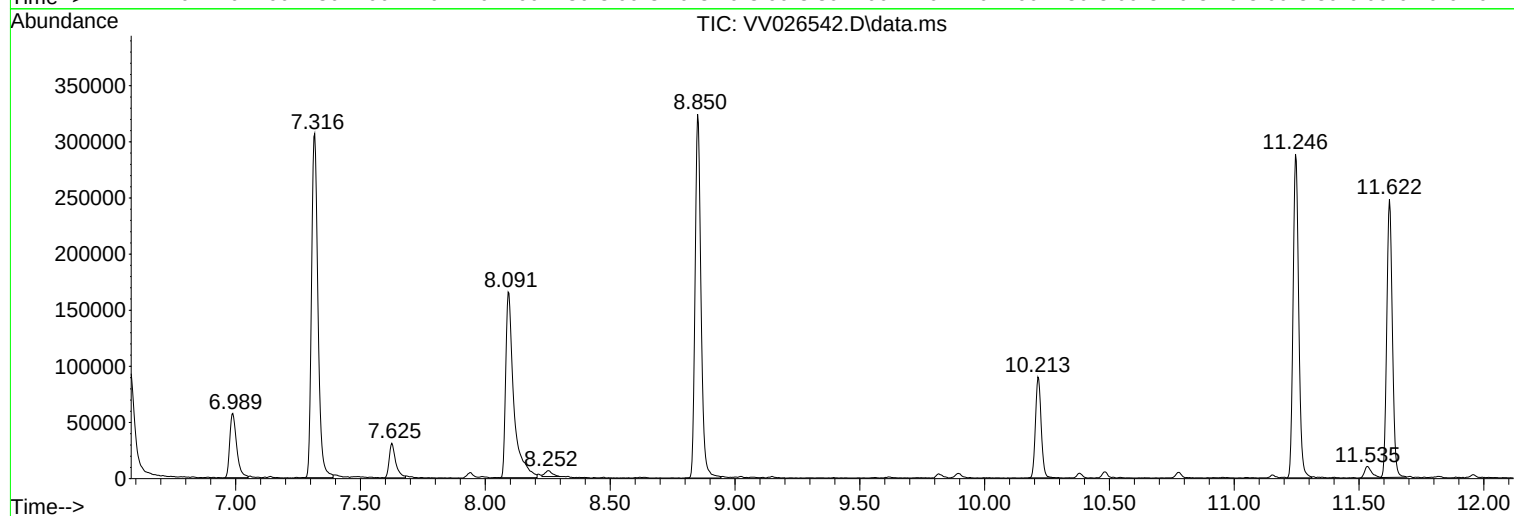
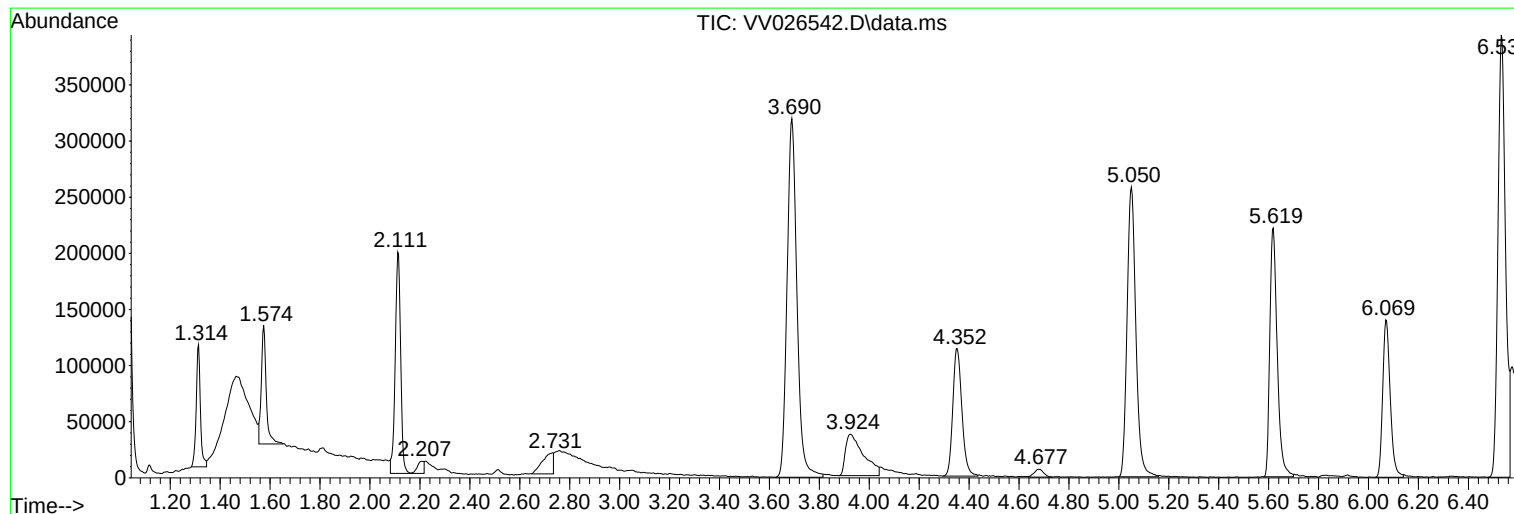
Sum of corrected areas: 7036944

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV062322\
Data File : VV026542.D
Acq On : 24 Jun 2022 09:53
Operator : SY/MD
Sample : N3401-17
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AG3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR062322WMA.M
Quant Title : TRACE VOA SFAM1.0

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV062322\
Data File : VV026542.D
Acq On : 24 Jun 2022 09:53
Operator : SY/MD
Sample : N3401-17
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AG3

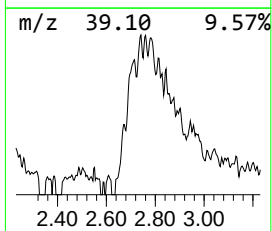
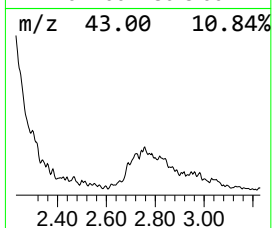
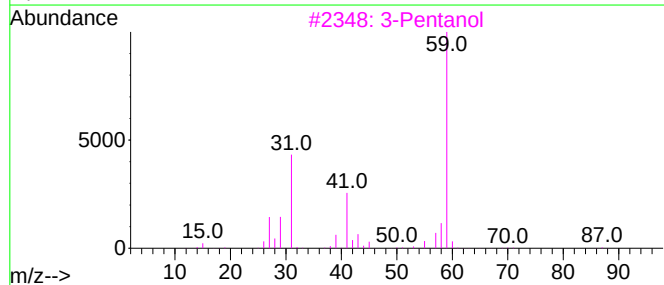
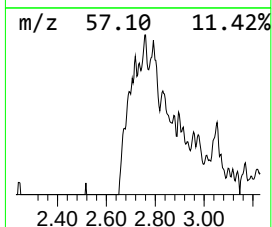
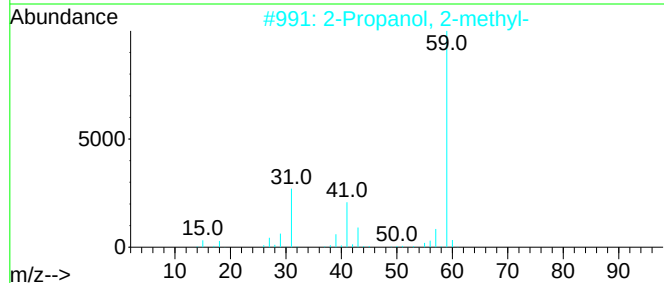
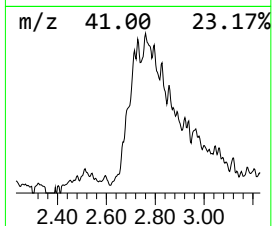
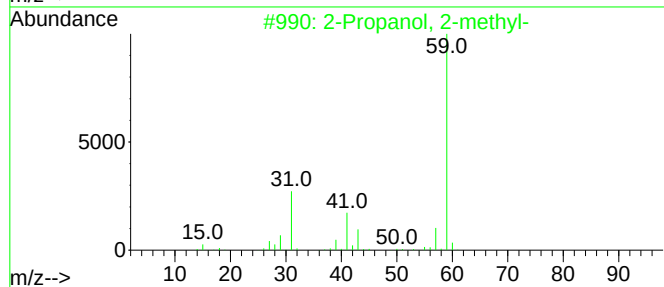
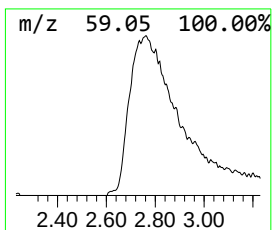
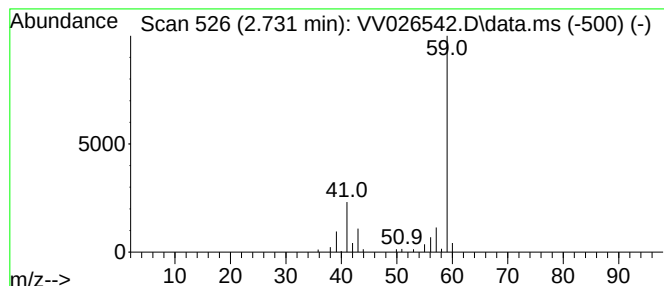
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR062322WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 2-Propanol, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.731	0.62 ug/L	57010	1,4-Difluorobenzene	5.619

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 2-methyl-		74	C4H10O	000075-65-0	78
2	2-Propanol, 2-methyl-		74	C4H10O	000075-65-0	64
3	3-Pentanol		88	C5H12O	000584-02-1	56
4	2-Propanol, 2-methyl-		74	C4H10O	000075-65-0	43
5	3-Pentanol		88	C5H12O	000584-02-1	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV062322\
Data File : VV026542.D
Acq On : 24 Jun 2022 09:53
Operator : SY/MD
Sample : N3401-17
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AG3

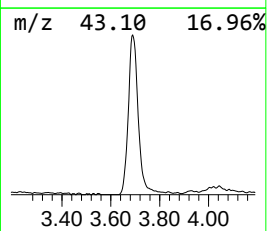
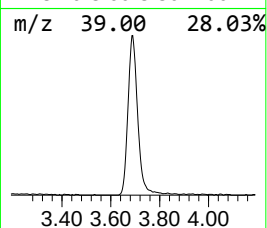
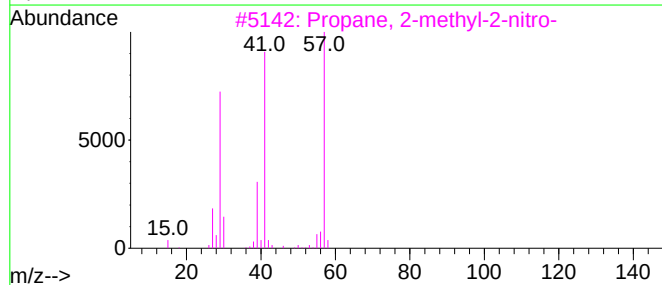
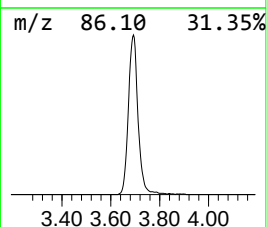
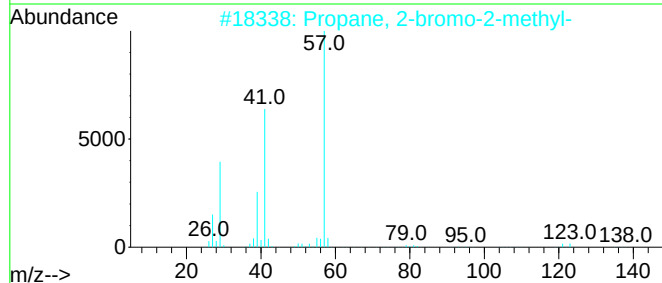
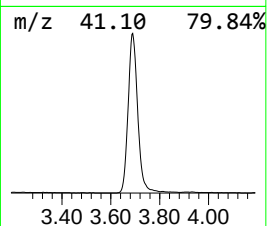
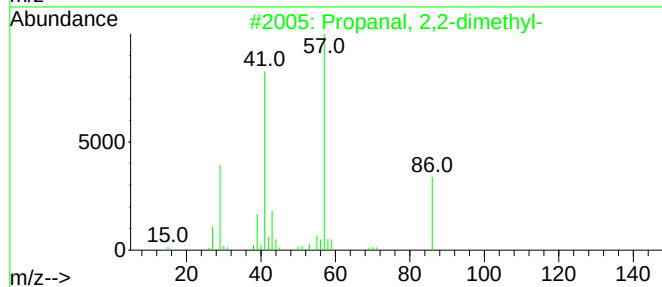
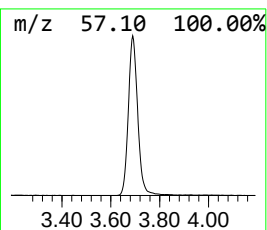
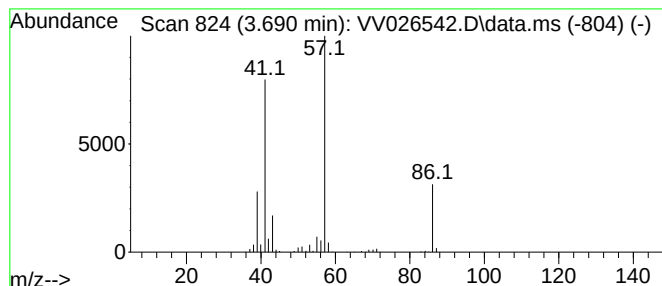
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR062322WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Propanal, 2,2-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.690	9.58 ug/L	874735	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	80
2			Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	59
3			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	53
4			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	43
5			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV062322\
Data File : VV026542.D
Acq On : 24 Jun 2022 09:53
Operator : SY/MD
Sample : N3401-17
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AG3

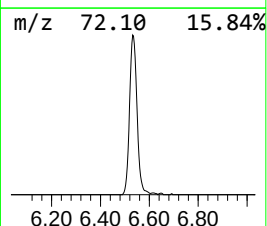
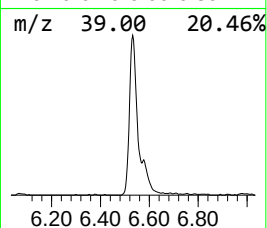
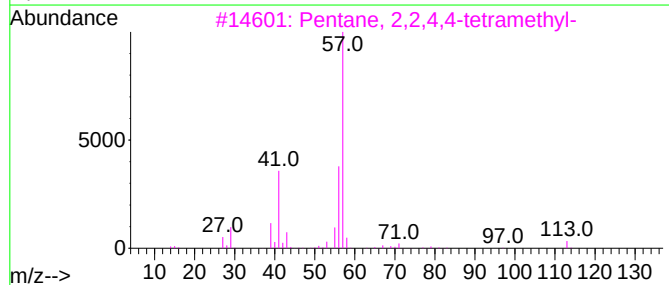
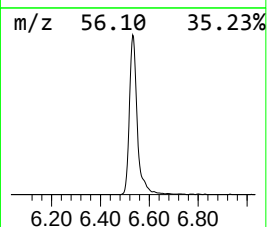
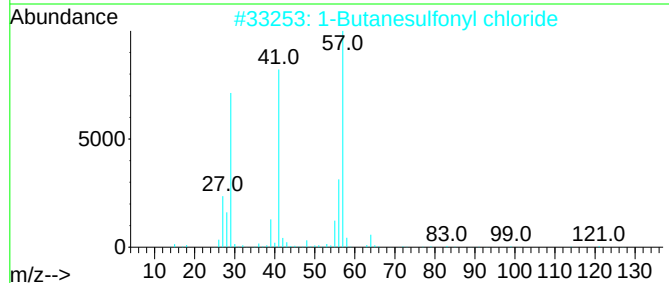
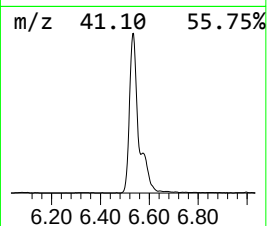
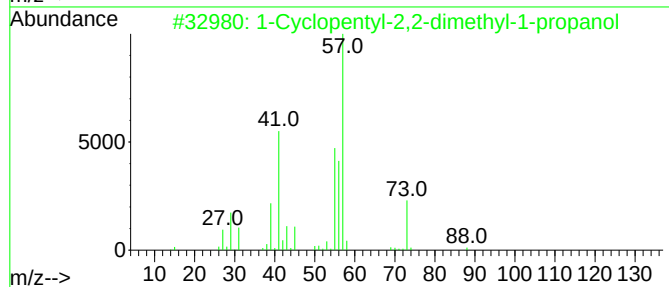
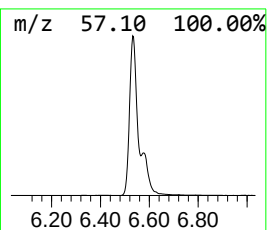
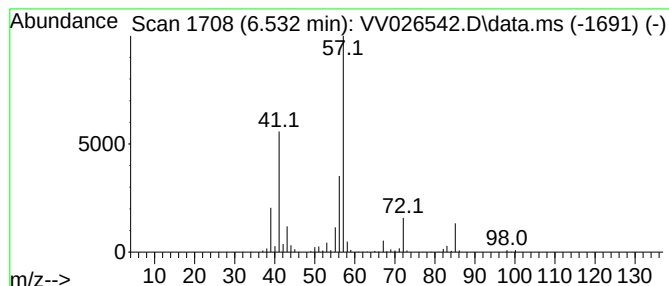
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR062322WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.532	9.20 ug/L	839920	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Cyclopentyl-2,2-dimethyl-1-pro...	156	C10H20O	337966-85-5	40
2			1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	40
3			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	40
4			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	40
5			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV062322\
Data File : VV026542.D
Acq On : 24 Jun 2022 09:53
Operator : SY/MD
Sample : N3401-17
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AG3

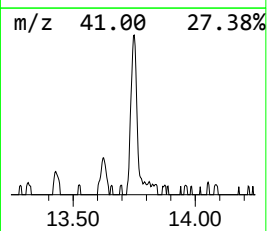
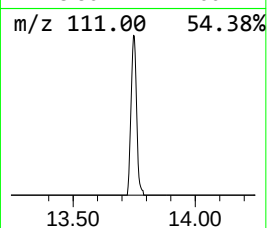
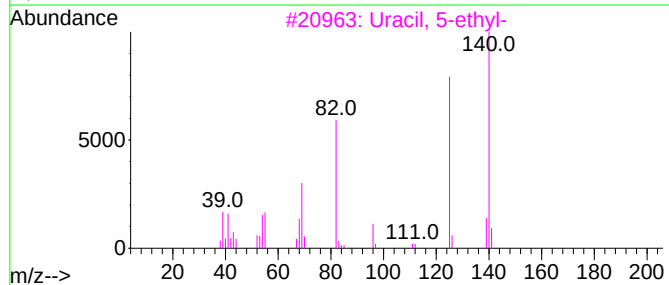
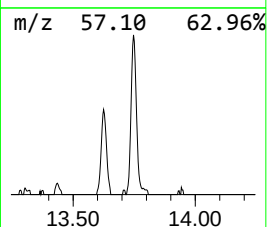
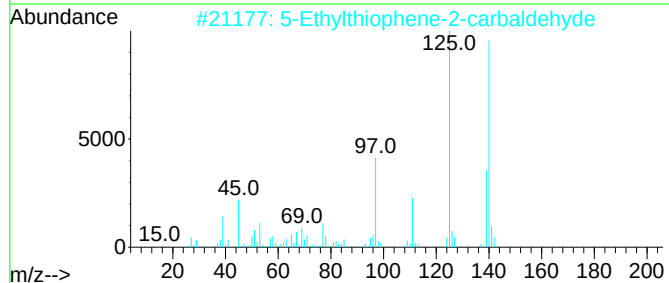
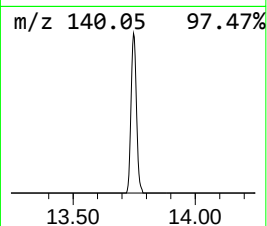
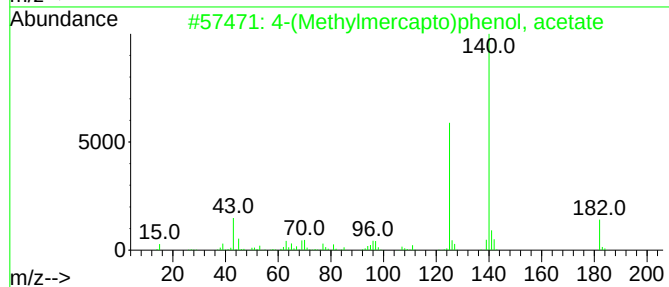
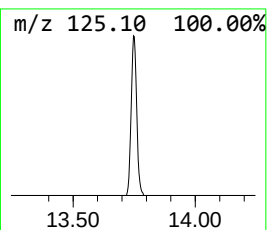
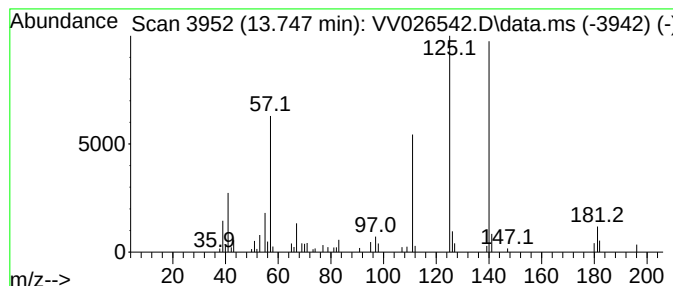
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR062322WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 4-(Methylmercapto)phenol, a... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.747	0.67 ug/L	60886	1,4-Dichlorobenzene-d4	11.246

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-(Methylmercapto)phenol, acetate	182	C9H10O2S	1000353-05-2	59
2			5-Ethylthiophene-2-carbaldehyde	140	C7H8OS	036880-33-8	59
3			Uracil, 5-ethyl-	140	C6H8N2O2	004212-49-1	53
4			Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	53
5			1,4-Benzenediol, 2-methoxy-	140	C7H8O3	000824-46-4	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV062322\
Data File : VV026542.D
Acq On : 24 Jun 2022 09:53
Operator : SY/MD
Sample : N3401-17
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AG3

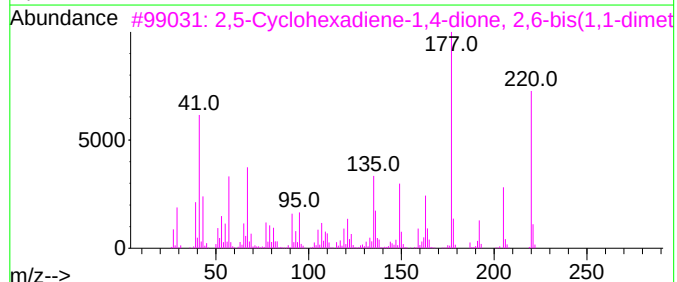
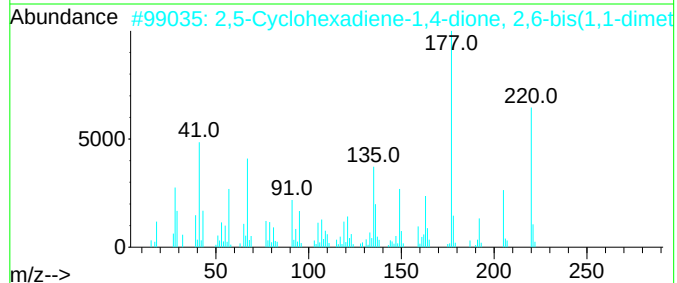
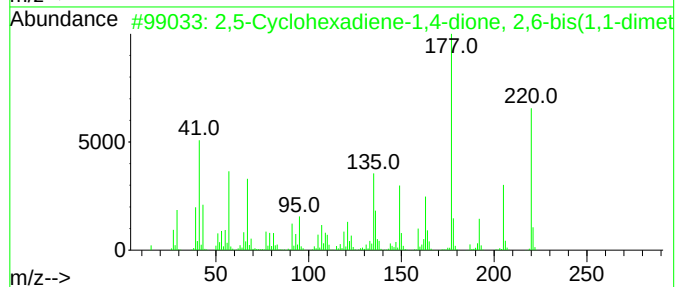
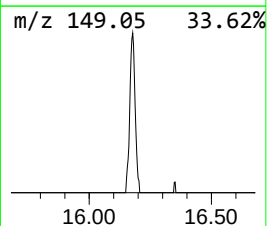
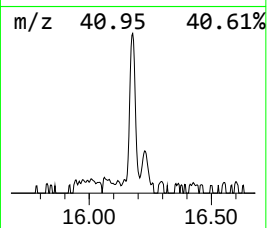
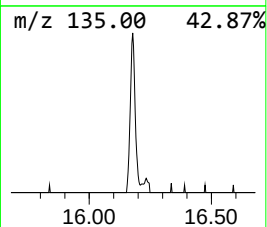
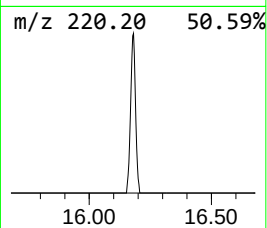
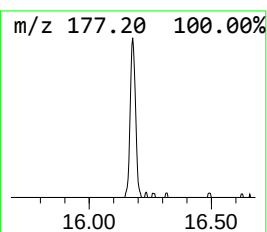
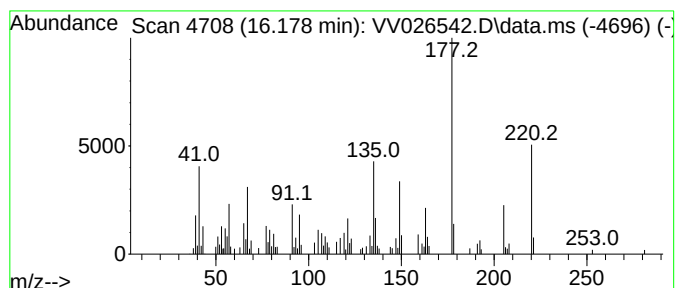
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR062322WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.178	0.71 ug/L	64157	1,4-Dichlorobenzene-d4	11.246

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	96
2			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	94
3			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	94
4			trans-.beta.-Ionone	192	C13H20O	000079-77-6	66
5			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV062322\
Data File : VV026542.D
Acq On : 24 Jun 2022 09:53
Operator : SY/MD
Sample : N3401-17
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AG3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR062322WMA.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
2-Propanol, 2-m...	2.731	0.6	ug/L	57010	1	5.619	456351	5.0
Propanal, 2,2-d...	3.690	9.6	ug/L	874735	1	5.619	456351	5.0
unknown-01	6.532	9.2	ug/L	839920	1	5.619	456351	5.0
4-(Methylmercap...	13.747	0.7	ug/L	60886	3	11.246	451797	5.0
2,5-Cyclohexadi...	16.178	0.7	ug/L	64157	3	11.246	451797	5.0