

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV110425\
 Data File : VV039314.D
 Acq On : 04 Nov 2025 14:56
 Operator : SY/MD
 Sample : Q3521-03
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 TANK-2025

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

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\82V100725W.M
 Title : SW846 8260

Signal : TIC: VV039314.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.204	41	51	96	rBV	6742980	20643560	100.00%	44.141%
2	2.002	291	299	326	rVB	203678	389475	1.89%	0.833%
3	2.117	328	335	360	rVB	384634	718265	3.48%	1.536%
4	2.262	373	380	401	rVB	192627	370733	1.80%	0.793%
5	3.879	873	883	909	rBV	103862	307088	1.49%	0.657%
6	4.503	1061	1077	1095	rBV2	535712	1427230	6.91%	3.052%
7	4.600	1096	1107	1146	rVB	689369	1900015	9.20%	4.063%
8	4.940	1201	1213	1232	rBV2	578971	1398864	6.78%	2.991%
9	5.532	1385	1397	1441	rBV	1124226	2593984	12.57%	5.547%
10	7.236	1915	1927	1949	rBV	1999973	3683229	17.84%	7.876%
11	8.773	2394	2405	2438	rBV	1907485	3259181	15.79%	6.969%
12	8.937	2446	2456	2482	rBV	396151	696199	3.37%	1.489%
13	10.001	2777	2787	2820	rVV	1739521	2856168	13.84%	6.107%
14	10.226	2844	2857	2874	rBV	408405	696648	3.37%	1.490%
15	11.172	3140	3151	3189	rVB2	2463474	3964438	19.20%	8.477%
16	12.879	3672	3682	3702	rBV	900754	1520435	7.37%	3.251%
17	13.210	3772	3785	3801	rBV7	125071	341847	1.66%	0.731%

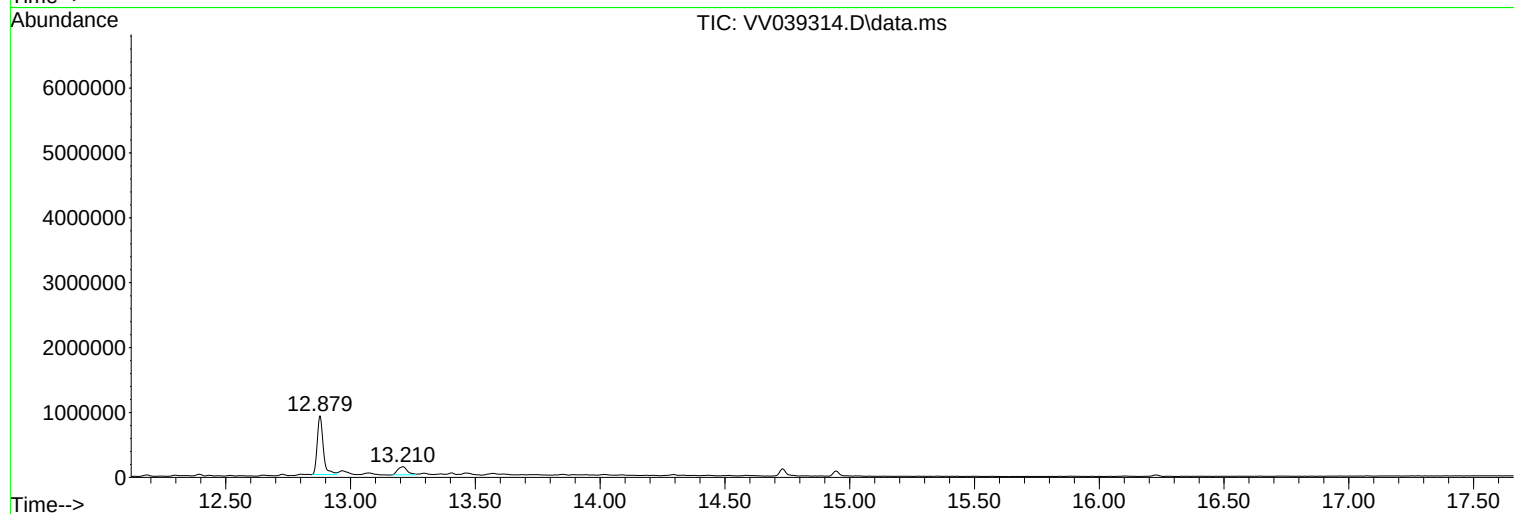
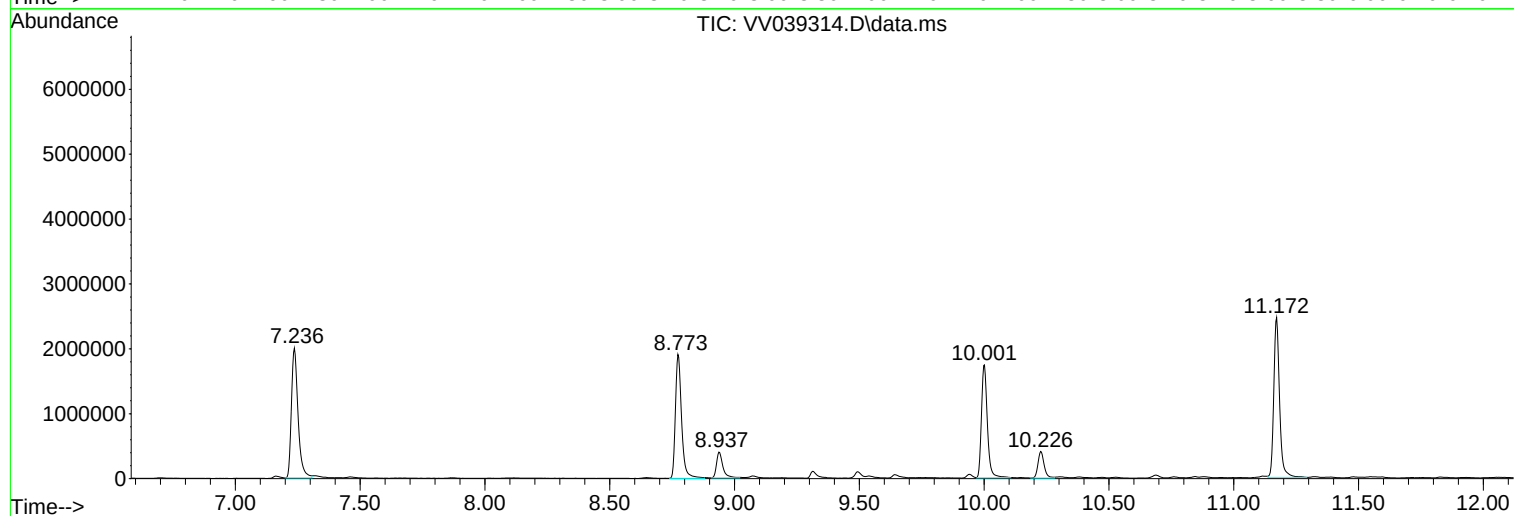
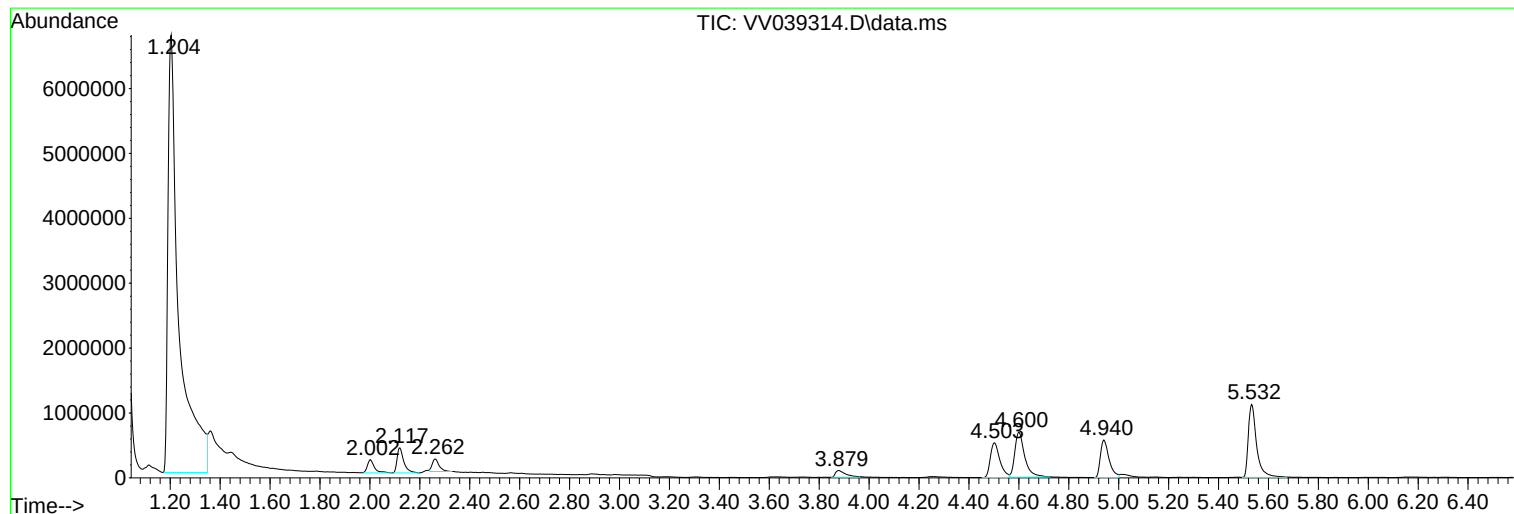
Sum of corrected areas: 46767359

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV110425\
Data File : VV039314.D
Acq On : 04 Nov 2025 14:56
Operator : SY/MD
Sample : Q3521-03
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
TANK-2025

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\82V100725W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV110425\
Data File : VV039314.D
Acq On : 04 Nov 2025 14:56
Operator : SY/MD
Sample : Q3521-03
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
TANK-2025

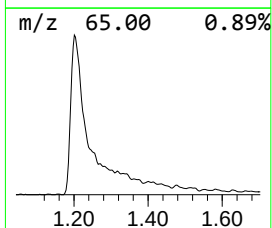
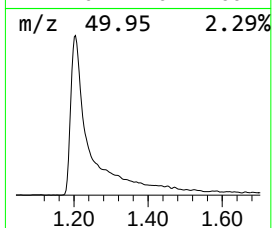
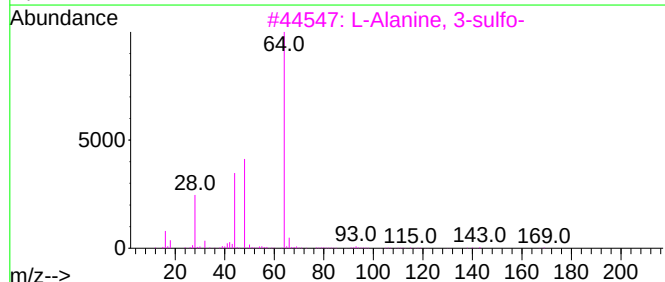
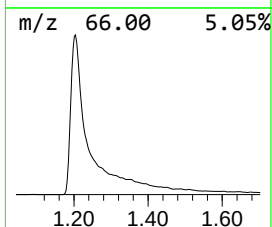
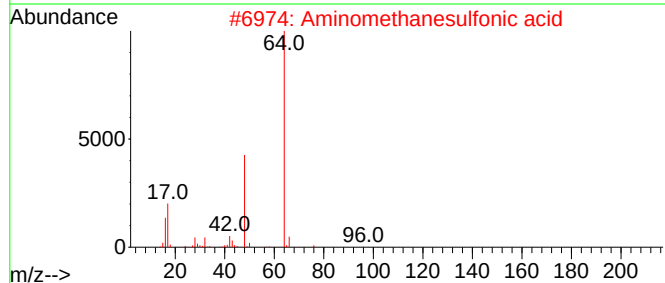
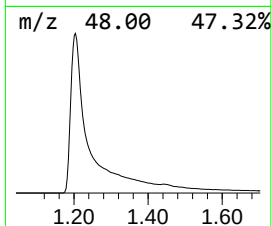
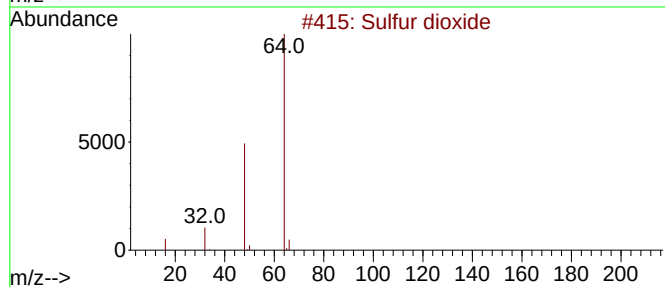
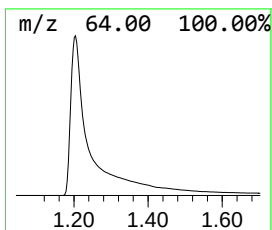
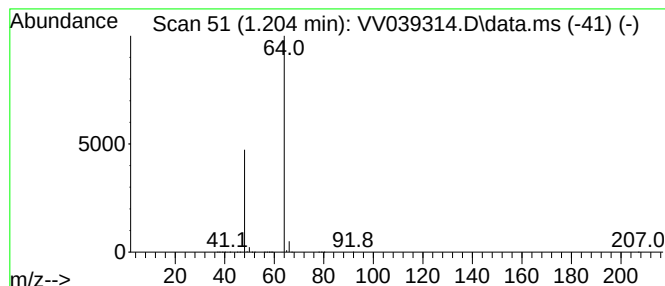
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\82V100725W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.204	543.25 ug/l	20643600	Pentafluorobenzene	4.600

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV110425\
Data File : VV039314.D
Acq On : 04 Nov 2025 14:56
Operator : SY/MD
Sample : Q3521-03
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
TANK-2025

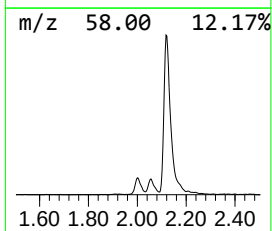
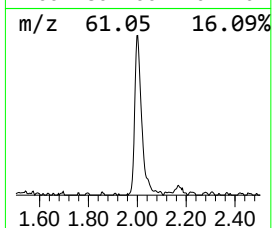
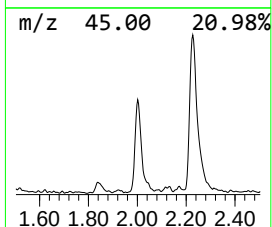
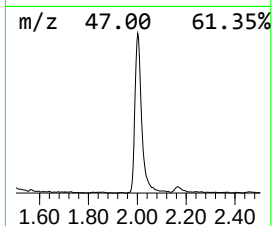
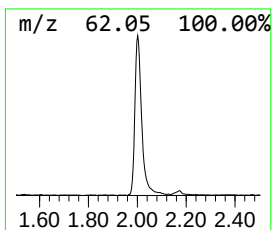
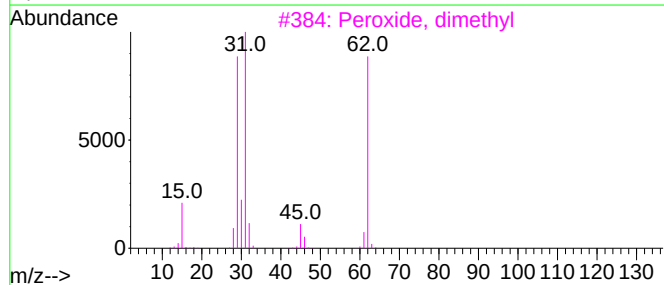
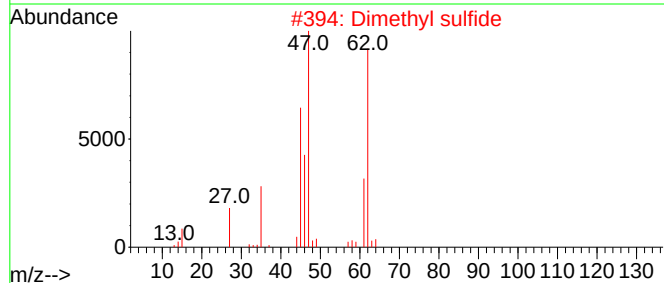
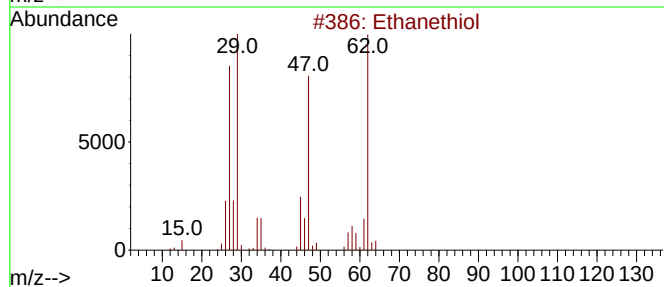
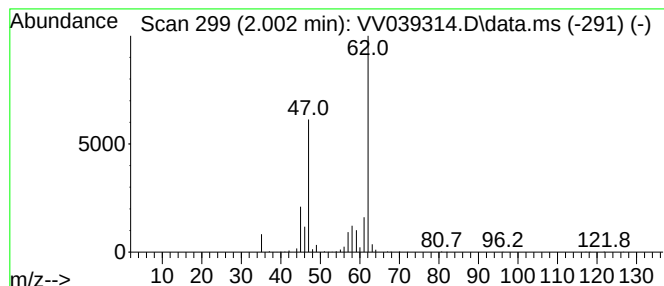
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\82V100725W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanethiol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.002	10.25 ug/l	389475	Pentafluorobenzene	4.600

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanethiol	62	C2H6S	000075-08-1	91
2			Dimethyl sulfide	62	C2H6S	000075-18-3	72
3			Peroxide, dimethyl	62	C2H6O2	000690-02-8	50
4			Ethene, chloro-	62	C2H3Cl	000075-01-4	45
5			Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	39



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV110425\
Data File : VV039314.D
Acq On : 04 Nov 2025 14:56
Operator : SY/MD
Sample : Q3521-03
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
TANK-2025

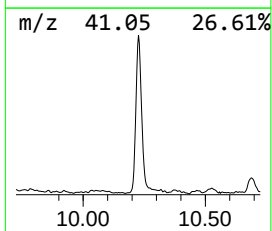
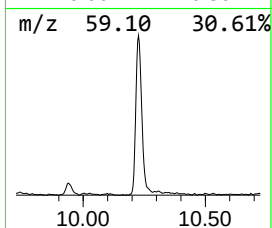
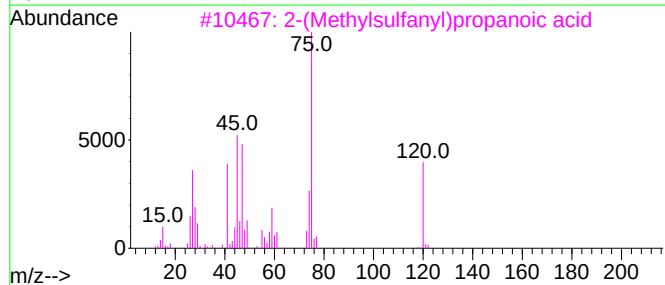
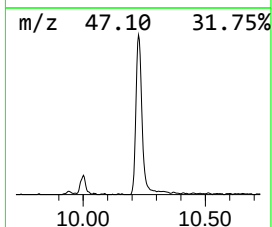
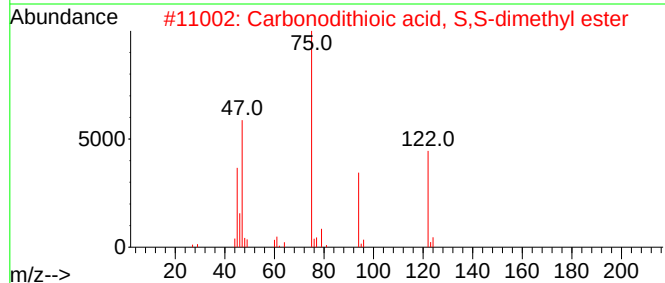
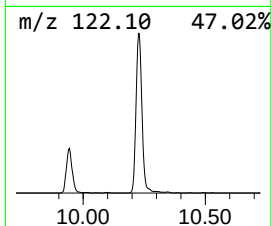
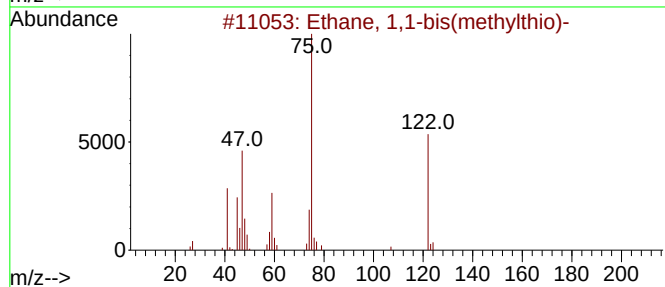
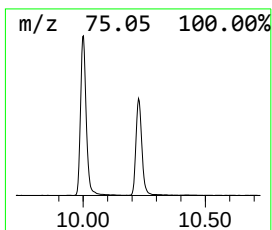
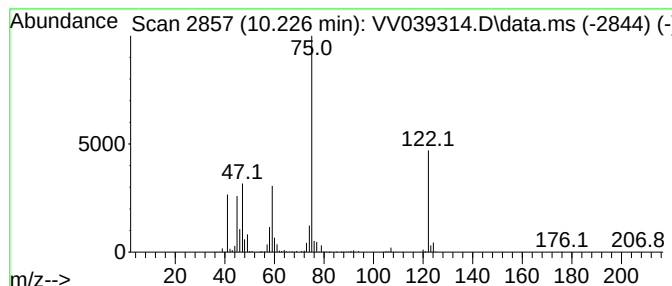
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\82V100725W.M
Quant Title : SW846 8260

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

Peak Number 3 Ethane, 1,1-bis(methylthio)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.226	8.79 ug/l	696648	1,4-Dichlorobenzene-d4	11.172

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1,1-bis(methylthio)-	122	C4H10S2	007379-30-8	91
2			Carbonodithioic acid, S,S-dimeth...	122	C3H6OS2	000868-84-8	72
3			2-(Methylsulfanyl)propanoic acid	120	C4H8O2S	080582-20-3	53
4			Ethane, 1,1,2-trimethoxy-	120	C5H12O3	024332-20-5	40
5			Ethanethioamide	75	C2H5NS	000062-55-5	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV110425\
Data File : VV039314.D
Acq On : 04 Nov 2025 14:56
Operator : SY/MD
Sample : Q3521-03
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
TANK-2025

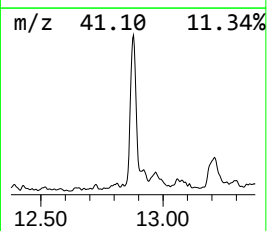
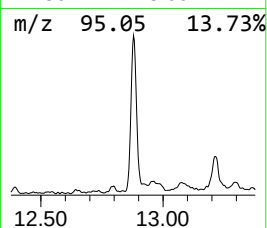
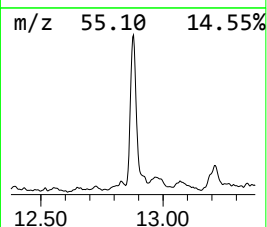
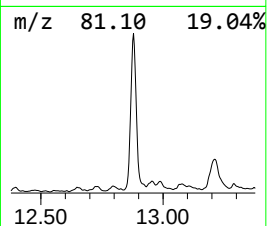
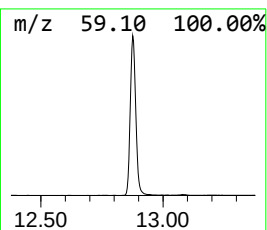
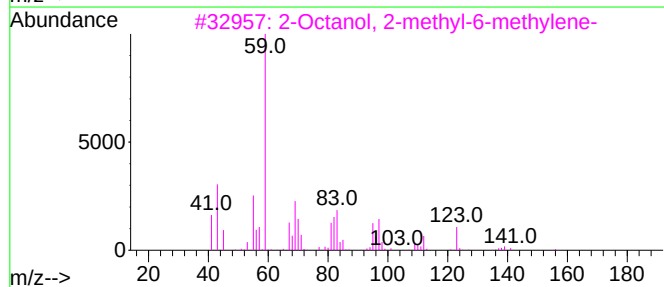
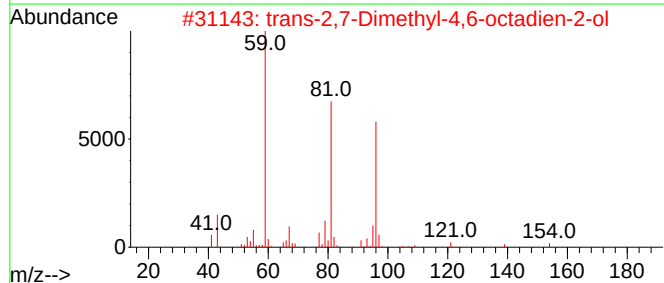
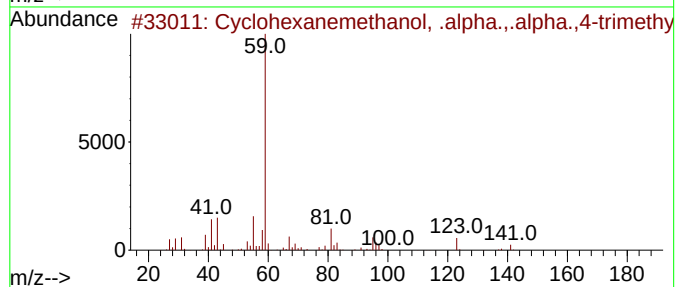
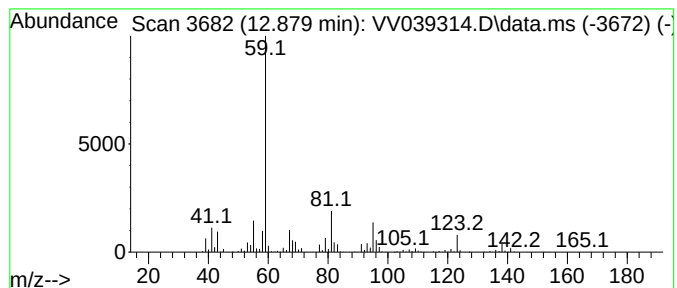
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\82V100725W.M
Quant Title : SW846 8260

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

Peak Number 4 Cyclohexanemethanol, .alpha... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.879	19.18 ug/l	1520440	1,4-Dichlorobenzene-d4	11.172

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	000498-81-7	72
2			trans-2,7-Dimethyl-4,6-octadien-...	154	C10H18O	1010281-69-5	40
3			2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	39
4			Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	007322-63-6	38
5			Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	005114-00-1	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV110425\
Data File : VV039314.D
Acq On : 04 Nov 2025 14:56
Operator : SY/MD
Sample : Q3521-03
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
TANK-2025

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\82V100725W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.204	543.3	ug/l	20643600	1	4.600	1900020	50.0
Ethanethiol	2.002	10.3	ug/l	389475	1	4.600	1900020	50.0
Ethane, 1,1-bis...	10.226	8.8	ug/l	696648	4	11.172	3964440	50.0
Cyclohexanemeth...	12.879	19.2	ug/l	1520440	4	11.172	3964440	50.0