

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102723\
 Data File : VX038614.D
 Acq On : 27 Oct 2023 19:41
 Operator : JC/MD
 Sample : 05107-20 50X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1050

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_X\Method\82X100523W.M
 Title : SW846 8260

Signal : TIC: VX038614.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.385	693	705	722	rBV	165108	487855	6.98%	2.095%
2	5.550	722	732	747	rBV	227993	656601	9.40%	2.819%
3	5.958	787	799	807	rBV	166048	442888	6.34%	1.902%
4	6.043	807	813	829	rVB2	24002	71685	1.03%	0.308%
5	6.763	921	931	957	rBV	356233	872917	12.49%	3.748%
6	8.647	1234	1240	1247	rBV	857839	1352911	19.36%	5.809%
7	8.720	1247	1252	1261	rVB	47777	86450	1.24%	0.371%
8	9.012	1292	1300	1313	rBV	59858	94457	1.35%	0.406%
9	9.433	1363	1369	1372	rBV	102996	155244	2.22%	0.667%
10	9.488	1372	1378	1398	rVB	4845021	6986685	100.00%	30.001%
11	10.055	1465	1471	1474	rBV	866804	1217017	17.42%	5.226%
12	10.092	1474	1477	1491	rVB	1942466	2578375	36.90%	11.071%
13	10.402	1522	1528	1542	rBV2	814983	1433945	20.52%	6.157%
14	10.512	1542	1546	1550	rVB	62097	82816	1.19%	0.356%
15	10.567	1550	1555	1560	rBV2	139725	224383	3.21%	0.963%
16	10.787	1587	1591	1597	rVB	142637	195171	2.79%	0.838%
17	10.860	1597	1603	1608	rVV2	330508	626803	8.97%	2.691%
18	10.908	1608	1611	1625	rVB	281379	410014	5.87%	1.761%
19	11.079	1632	1639	1647	rBV	918272	1228467	17.58%	5.275%
20	11.201	1655	1659	1664	rBV2	64843	92814	1.33%	0.399%
21	11.286	1670	1673	1676	rBV	61863	88029	1.26%	0.378%
22	11.354	1679	1684	1690	rVV	536523	740759	10.60%	3.181%
23	11.652	1725	1733	1736	rBV	153793	224520	3.21%	0.964%
24	11.701	1736	1741	1747	rVB	406859	584014	8.36%	2.508%
25	12.024	1788	1794	1803	rVB	1057054	1389599	19.89%	5.967%
26	12.213	1816	1825	1835	rBV3	28823	109189	1.56%	0.469%
27	12.353	1844	1848	1855	rBV	116249	160208	2.29%	0.688%
28	12.420	1855	1859	1863	rBV2	75651	111819	1.60%	0.480%
29	13.780	2076	2082	2090	rVB2	275493	403778	5.78%	1.734%
30	14.633	2218	2222	2227	rVB	68516	87273	1.25%	0.375%
31	14.780	2241	2246	2251	rBV2	68230	91754	1.31%	0.394%

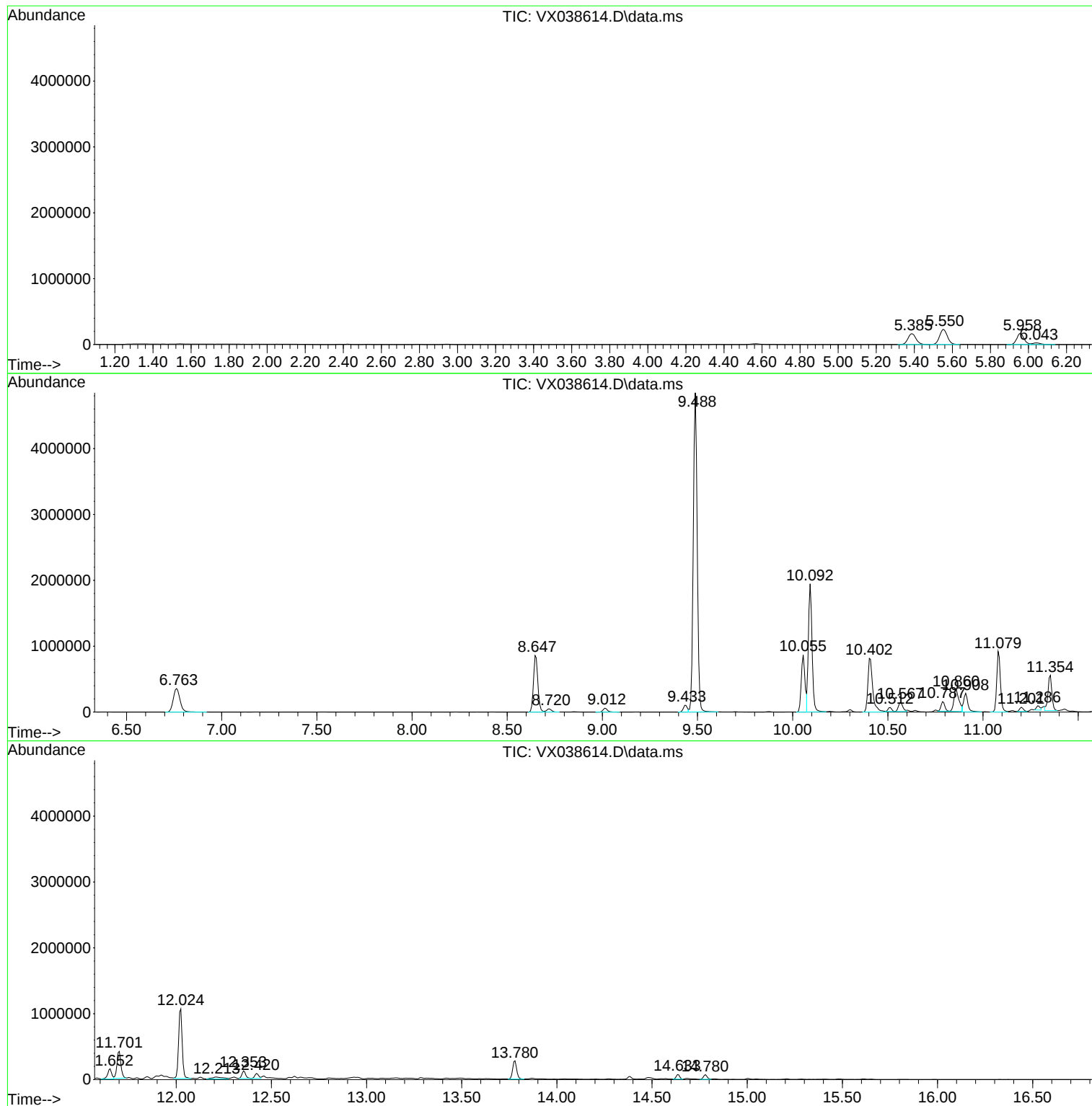
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ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1050

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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



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Instrument :
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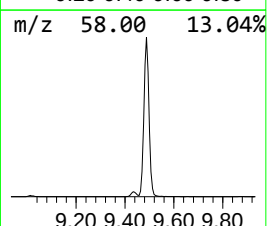
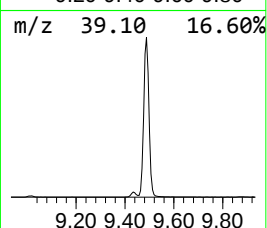
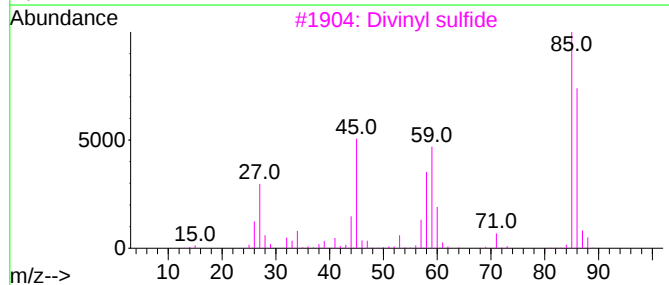
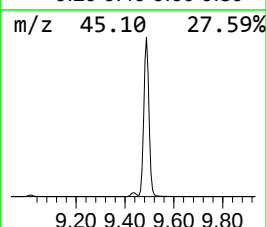
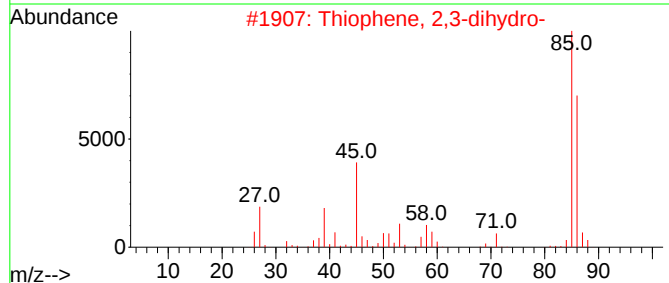
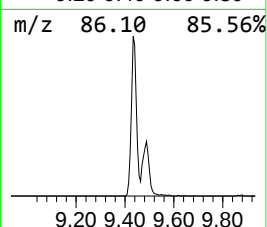
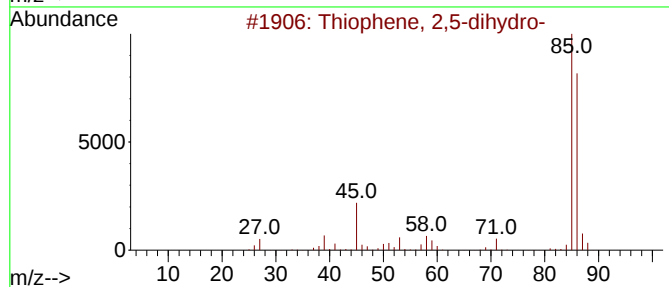
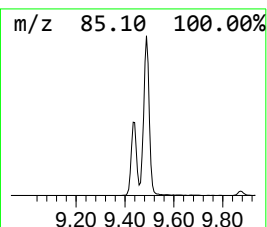
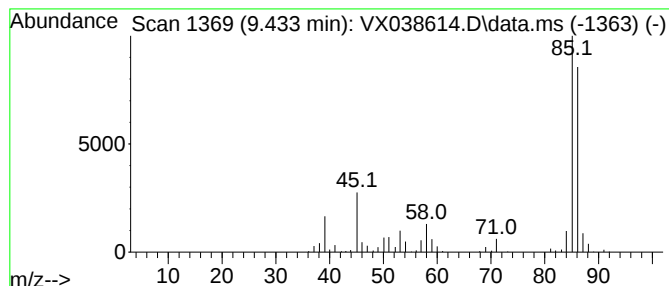
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 1 Thiophene, 2,5-dihydro- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.433	6.38 ug/l	155244	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, 2,5-dihydro-	86	C4H6S	001708-32-3	91
2			Thiophene, 2,3-dihydro-	86	C4H6S	001120-59-8	87
3			Divinyl sulfide	86	C4H6S	000627-51-0	64
4			N-Aminopyrrolidine	86	C4H10N2	016596-41-1	45
5			1-Propyne, 1-(methylthio)-	86	C4H6S	022174-51-2	32



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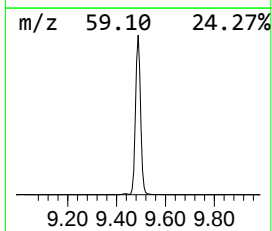
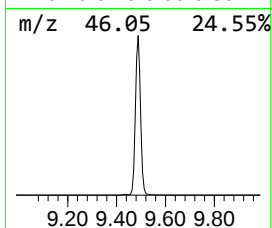
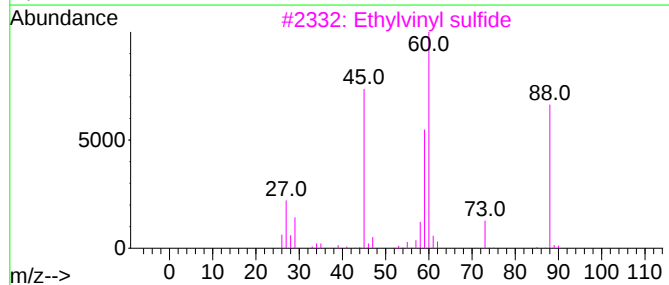
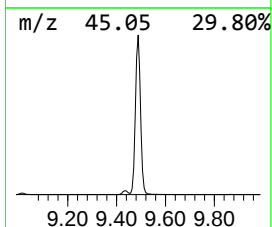
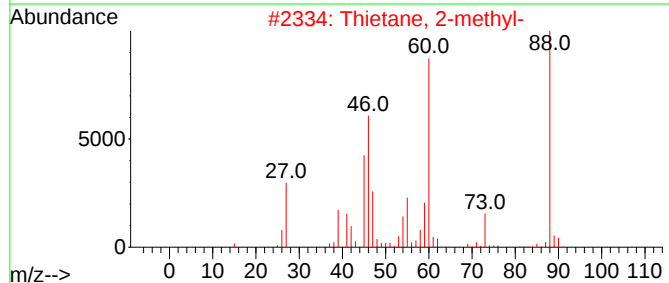
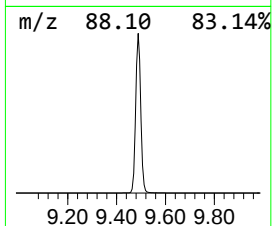
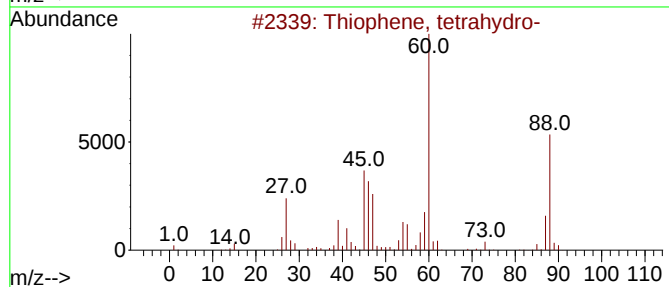
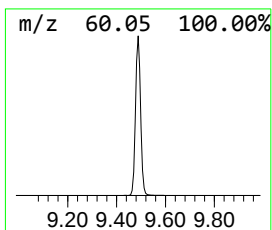
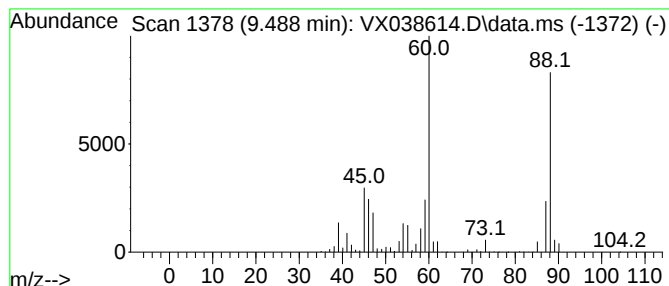
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 2 Thiophene, tetrahydro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.488	287.04 ug/l	6986690	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, tetrahydro-	88	C4H8S	000110-01-0	95
2			Thietane, 2-methyl-	88	C4H8S	017837-41-1	74
3			Ethylvinyl sulfide	88	C4H8S	000627-50-9	42
4			1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	36
5			Sulfide, allyl methyl	88	C4H8S	010152-76-8	35



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

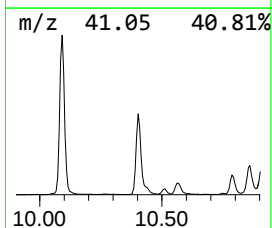
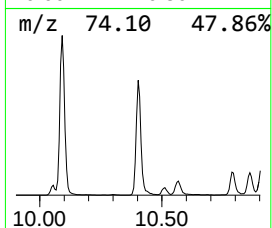
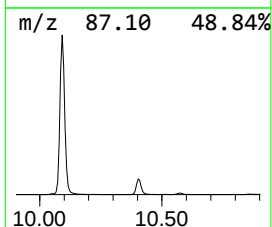
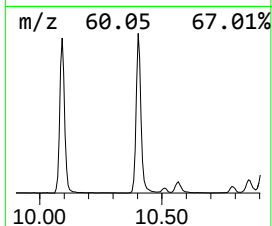
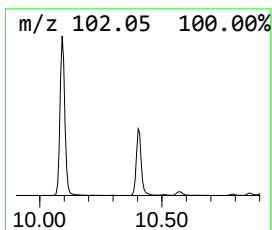
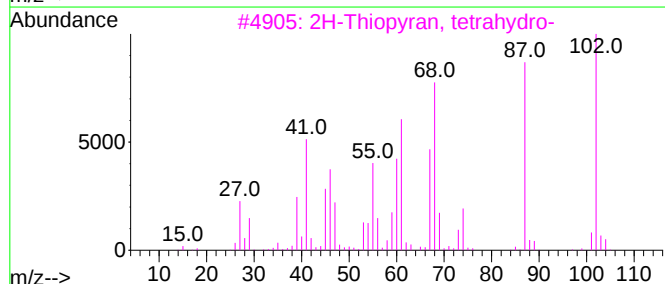
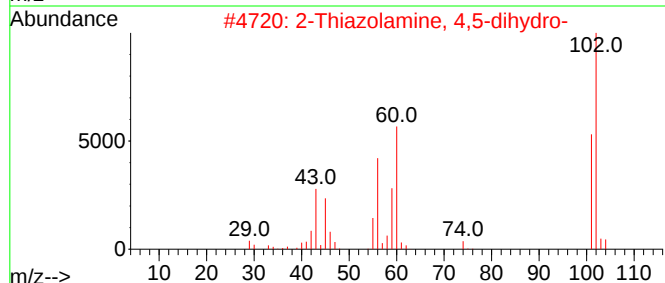
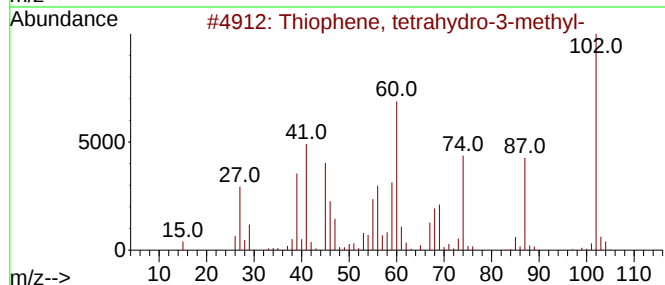
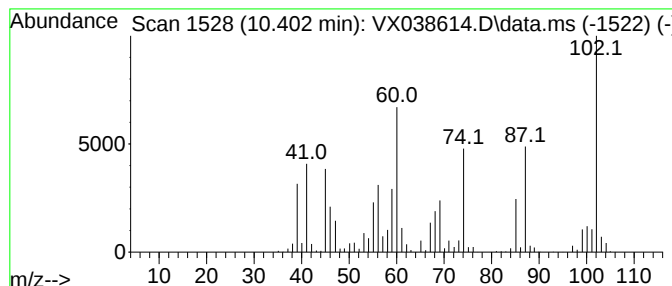
Instrument :
MSVOA_X
ClientSampleId :
1050

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 3 Thiophene, tetrahydro-3-met... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.403	58.91 ug/l	1433950	Chlorobenzene-d5	10.055	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, tetrahydro-3-methyl-	102	C5H10S	004740-00-5	98
2	2-Thiazolamine, 4,5-dihydro-	102	C3H6N2S	001779-81-3	38
3	2H-Thiopyran, tetrahydro-	102	C5H10S	001613-51-0	37
4	2-Acetyl-2,3,5,6-tetrahydro-1,4-...	145	C6H11NOS	1000281-47-3	27
5	Aziridine-2-carbothioamide	102	C3H6N2S	1000189-98-7	27



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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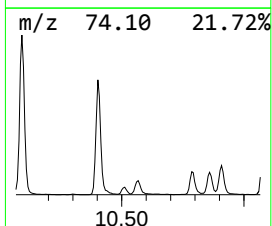
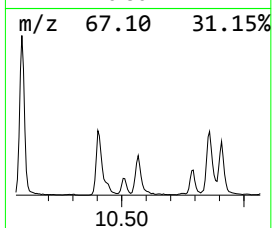
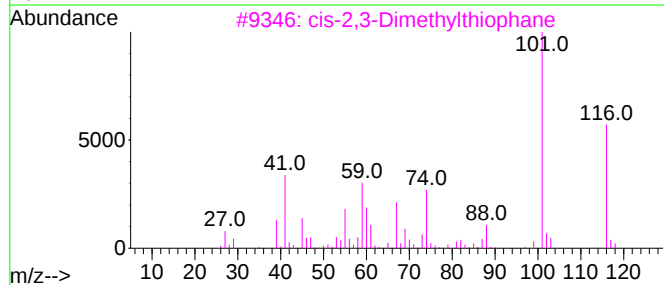
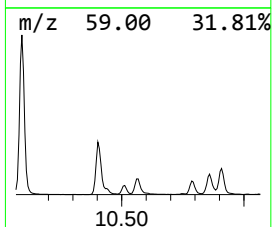
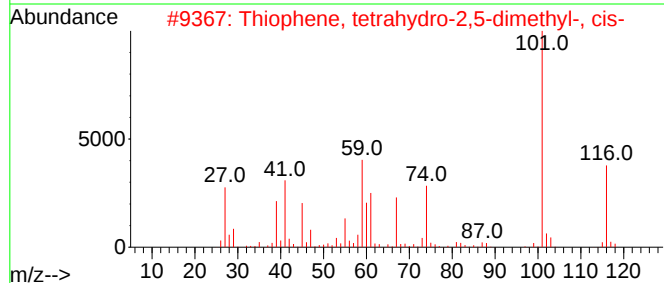
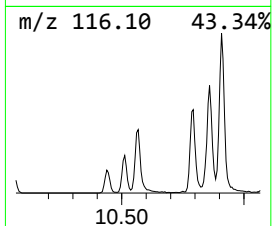
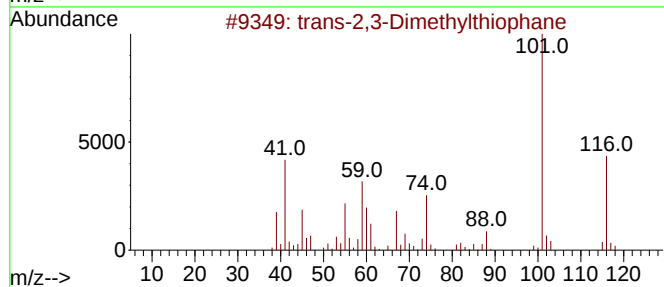
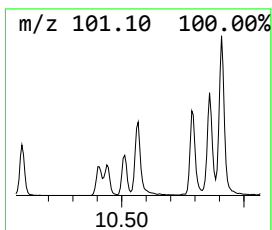
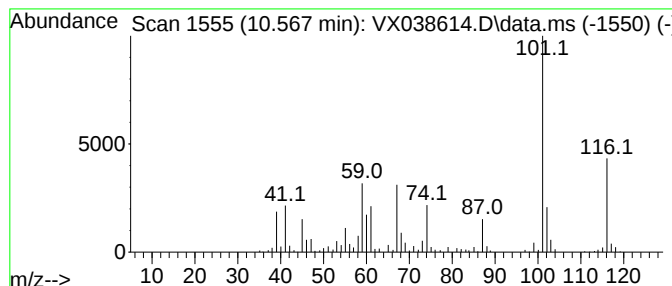
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 4 trans-2,3-Dimethylthiophane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.567	9.22 ug/l	224383	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	90
2			Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-13-7	87
3			cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	81
4			2H-Thiopyran, tetrahydro-2-methyl-	116	C6H12S	005161-16-0	64
5			Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-14-8	64



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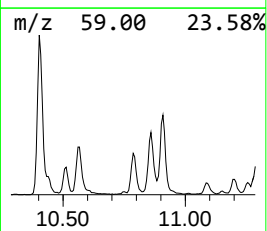
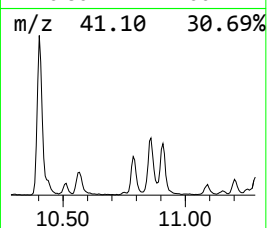
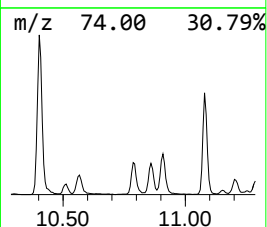
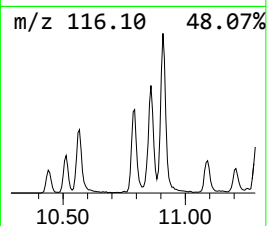
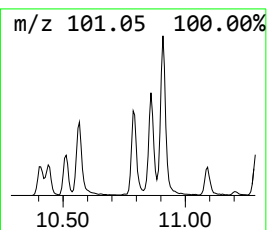
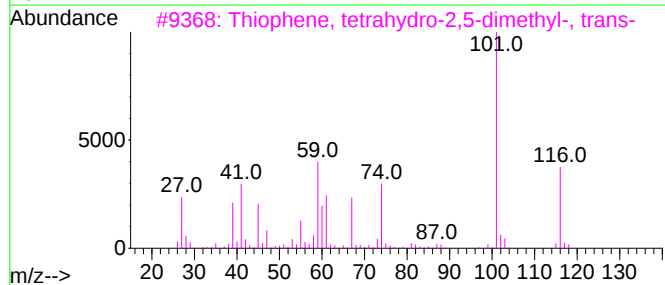
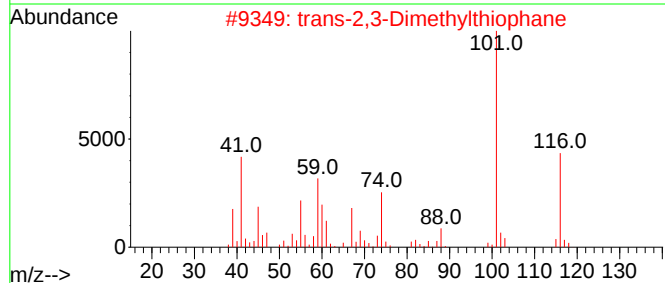
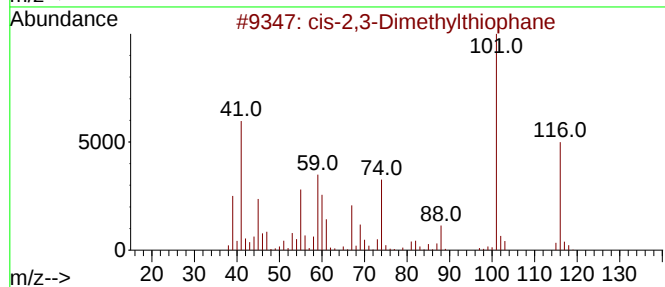
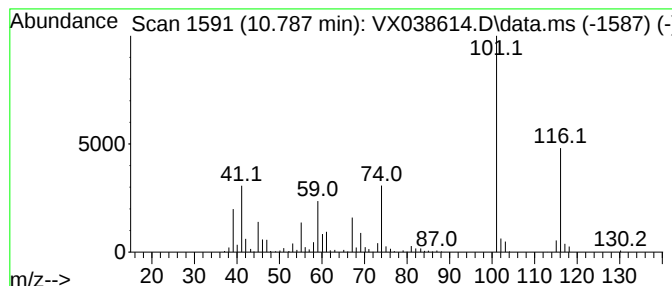
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 5 cis-2,3-Dimethylthiophane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.787	8.02 ug/l	195171	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	94
2			trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	93
3			Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-14-8	80
4			2H-Thiopyran, tetrahydro-2-methyl-	116	C6H12S	005161-16-0	60
5			Allylthiourea	116	C4H8N2S	000109-57-9	59



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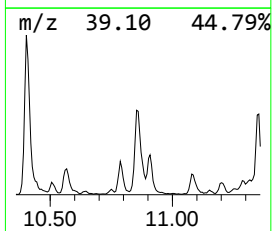
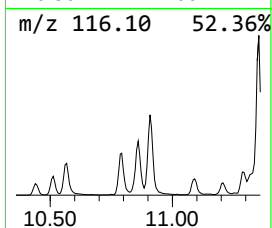
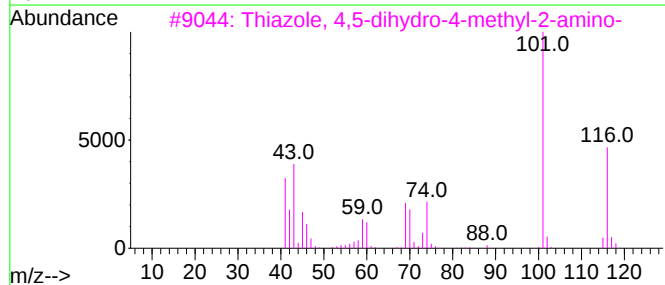
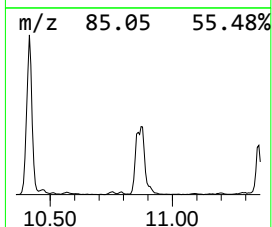
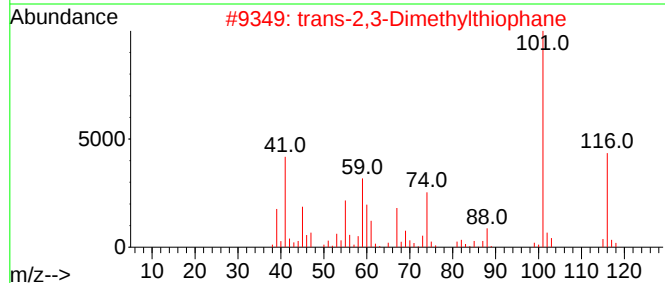
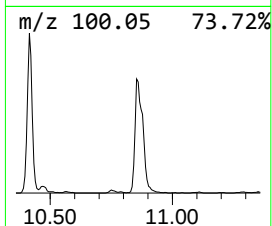
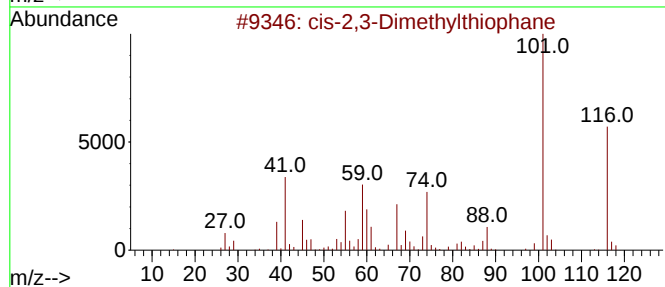
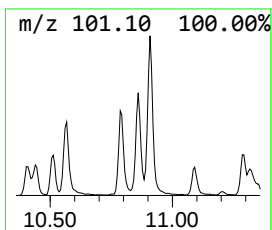
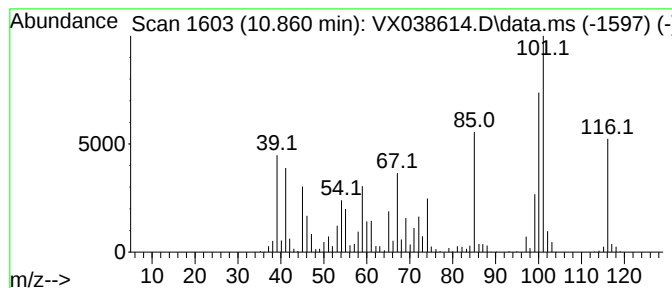
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 6 Thiazole, 4,5-dihydro-4-met... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.860	25.75 ug/l	626803	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	50
2			trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	50
3			Thiazole, 4,5-dihydro-4-methyl-2...	116	C4H8N2S	010416-81-6	50
4			2H-Thiopyran, tetrahydro-2-methyl-	116	C6H12S	005161-16-0	38
5			Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-14-8	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102723\
Data File : VX038614.D
Acq On : 27 Oct 2023 19:41
Operator : JC/MD
Sample : 05107-20 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1050

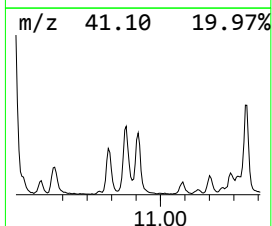
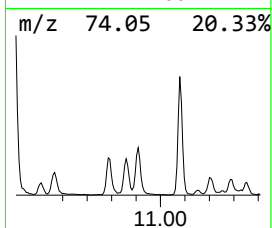
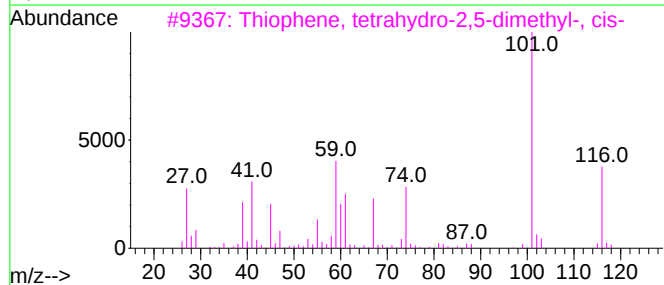
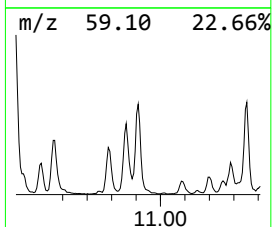
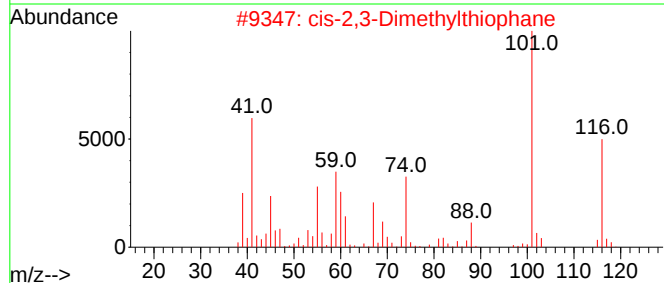
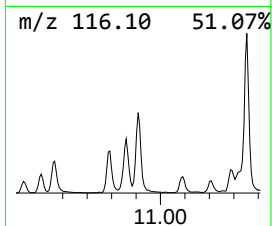
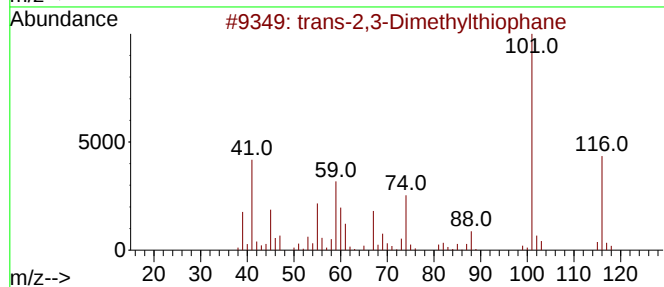
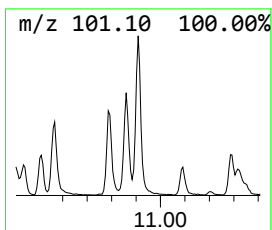
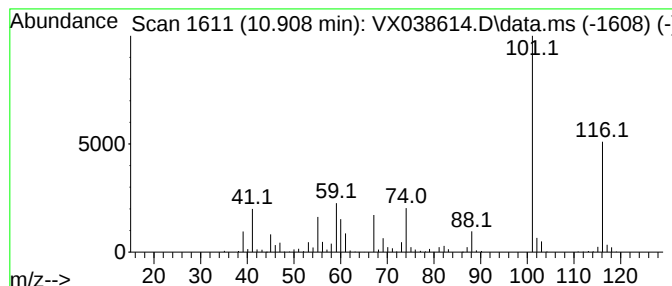
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Quant Title : SW846 8260

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

Peak Number 7 Thiophene, tetrahydro-2,5-d... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.909	16.84 ug/l	410014	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	96
2			cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	94
3			Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-13-7	90
4			Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-14-8	87
5			Thiazole, 4,5-dihydro-4-methyl-2...	116	C4H8N2S	010416-81-6	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102723\
Data File : VX038614.D
Acq On : 27 Oct 2023 19:41
Operator : JC/MD
Sample : 05107-20 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1050

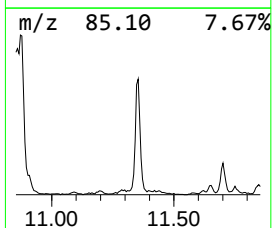
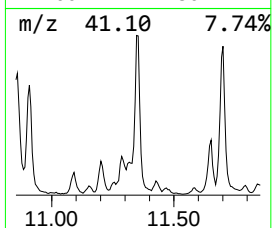
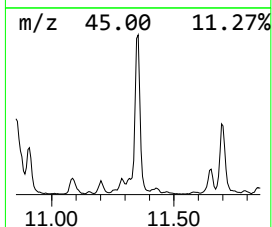
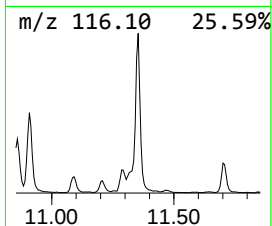
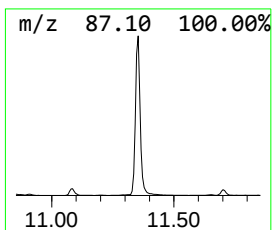
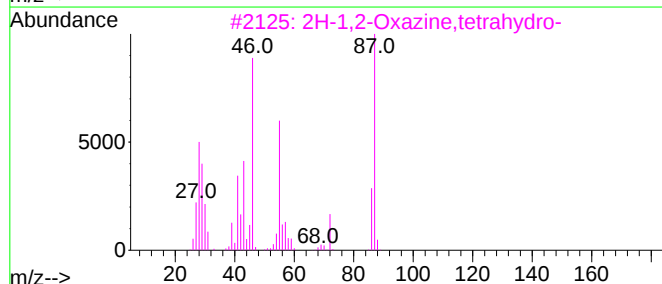
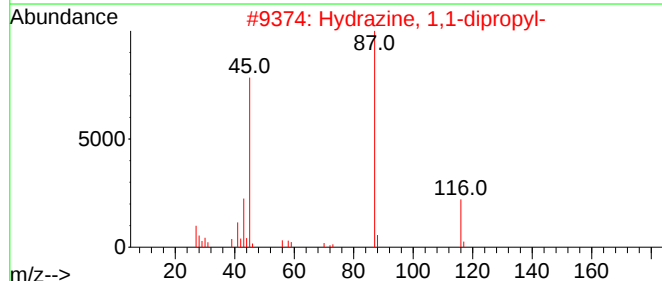
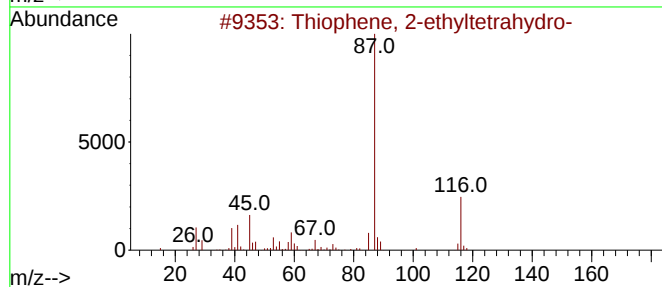
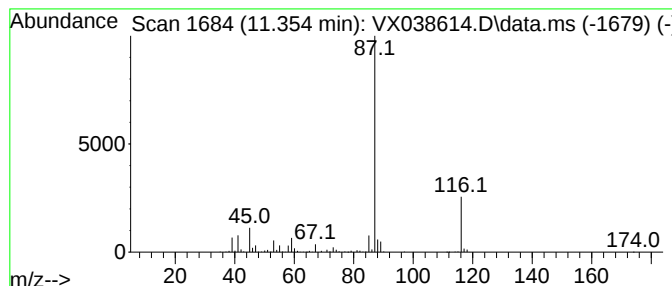
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 8 Thiophene, 2-ethyltetrahydro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.354	26.65 ug/l	740759	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	91
2			Hydrazine, 1,1-dipropyl-	116	C6H16N2	004986-50-9	64
3			2H-1,2-Oxazine,tetrahydro-	87	C4H9NO	036652-42-3	59
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102723\
Data File : VX038614.D
Acq On : 27 Oct 2023 19:41
Operator : JC/MD
Sample : 05107-20 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1050

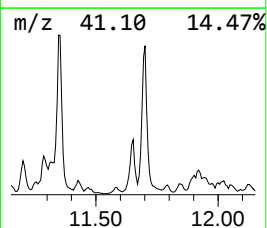
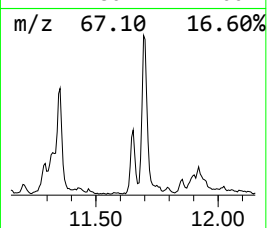
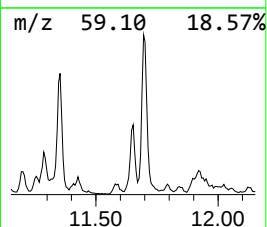
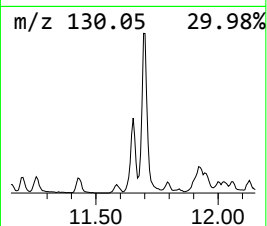
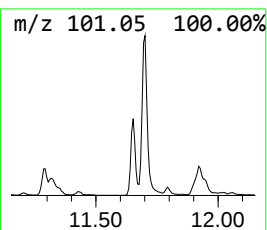
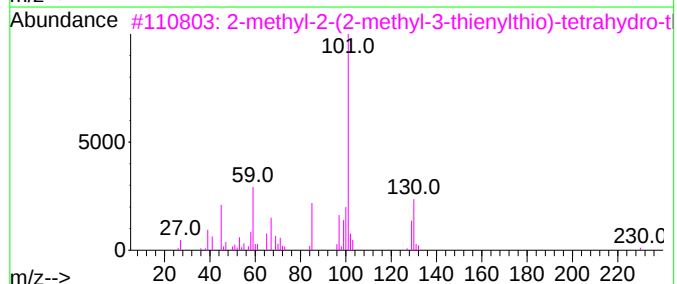
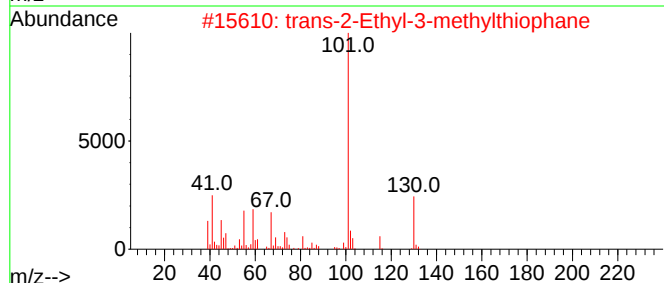
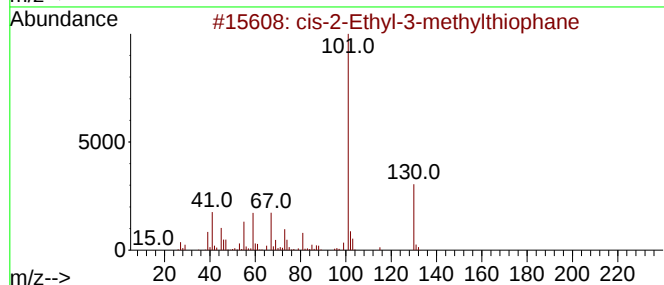
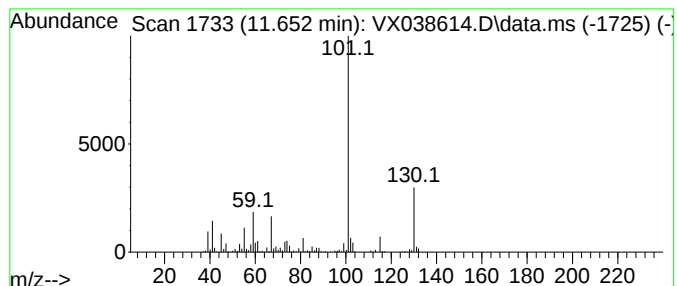
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 9 cis-2-Ethyl-3-methylthiophane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.652	8.08 ug/l	224520	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-2-Ethyl-3-methylthiophane	130	C7H14S	061568-37-4	93
2			trans-2-Ethyl-3-methylthiophane	130	C7H14S	061568-36-3	80
3			2-methyl-2-(2-methyl-3-thienylth...	230	C10H14S3	1000365-97-2	56
4			2-Amino-2-thiazoline-4-carboxyli...	146	C4H6N2O2S	002150-55-2	50
5			1,3-Dioxepane, 2-pentadecyl-	312	C20H40O2	041563-29-5	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102723\
Data File : VX038614.D
Acq On : 27 Oct 2023 19:41
Operator : JC/MD
Sample : 05107-20 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1050

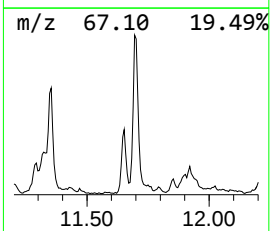
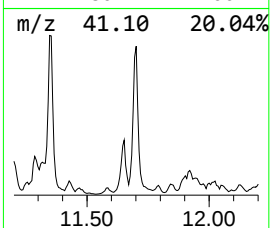
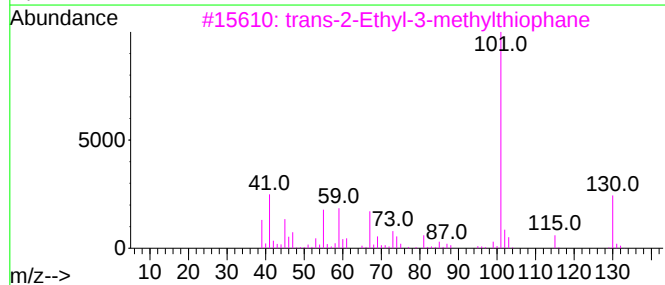
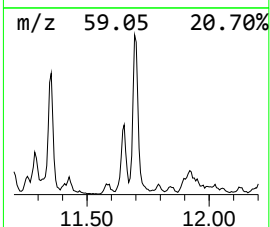
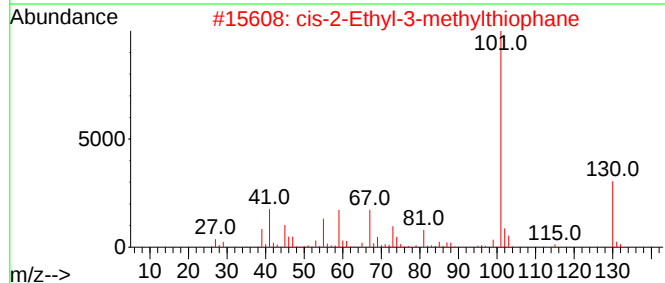
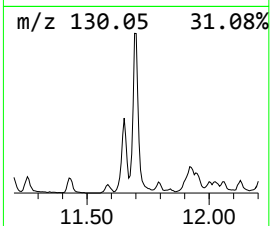
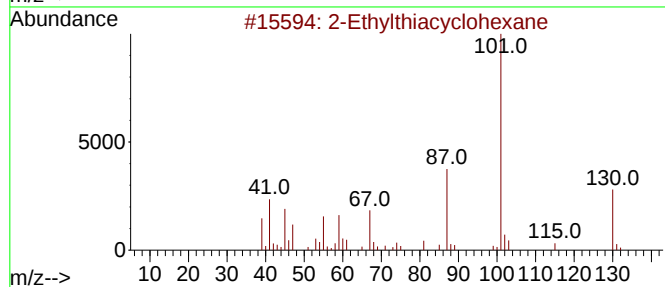
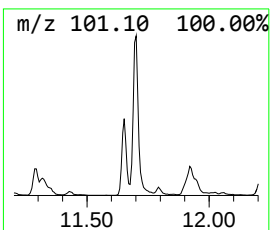
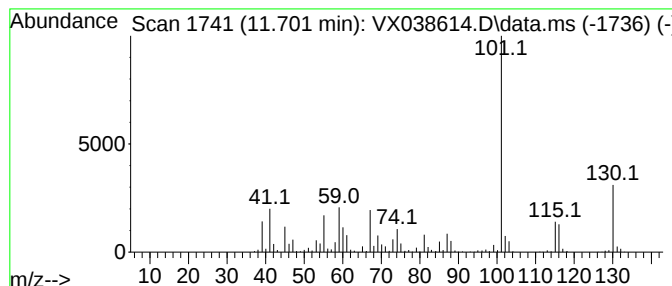
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 10 2-Ethylthiacyclohexane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.701	21.01 ug/l	584014	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Ethylthiacyclohexane	130	C7H14S	001613-52-1	74
2		cis-2-Ethyl-3-methylthiophane	130	C7H14S	061568-37-4	74
3		trans-2-Ethyl-3-methylthiophane	130	C7H14S	061568-36-3	64
4		3-Ethylthiane	130	C7H14S	061568-48-7	64
5		2H-Thiopyran, tetrahydro-2-methyl-	116	C6H12S	005161-16-0	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102723\
Data File : VX038614.D
Acq On : 27 Oct 2023 19:41
Operator : JC/MD
Sample : 05107-20 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1050

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.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
Thiophene, 2,5-...	9.433	6.4	ug/l	155244	3	10.055	1217020	50.0
Thiophene, tetr...	9.488	287.0	ug/l	6986690	3	10.055	1217020	50.0
Thiophene, tetr...	10.403	58.9	ug/l	1433950	3	10.055	1217020	50.0
trans-2,3-Dimet...	10.567	9.2	ug/l	224383	3	10.055	1217020	50.0
cis-2,3-Dimethy...	10.787	8.0	ug/l	195171	3	10.055	1217020	50.0
Thiazole, 4,5-d...	10.860	25.8	ug/l	626803	3	10.055	1217020	50.0
Thiophene, tetr...	10.909	16.8	ug/l	410014	3	10.055	1217020	50.0
Thiophene, 2-et...	11.354	26.6	ug/l	740759	4	12.024	1389600	50.0
cis-2-Ethyl-3-m...	11.652	8.1	ug/l	224520	4	12.024	1389600	50.0
2-Ethylthiacycl...	11.701	21.0	ug/l	584014	4	12.024	1389600	50.0