

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN103123\
 Data File : VN079746.D
 Acq On : 31 Oct 2023 16:07
 Operator : JC\MD
 Sample : 05107-19
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 1051

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_N\methods\82N103023W.M
 Title : SW846 8260

Signal : TIC: VN079746.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.171	1043	1057	1062	rBV	285525	711781	1.54%	0.462%
2	8.229	1062	1067	1079	rVB	391212	860567	1.86%	0.559%
3	8.606	1113	1131	1146	rBV2	1060401	2920945	6.32%	1.897%
4	9.106	1207	1216	1228	rBV	632268	1304310	2.82%	0.847%
5	10.571	1456	1465	1470	rBV	987210	1782492	3.86%	1.158%
6	10.635	1470	1476	1488	rVB	1532984	2799835	6.06%	1.818%
7	10.888	1507	1519	1534	rBV	1435507	2627005	5.69%	1.706%
8	11.282	1576	1586	1590	rBV2	467668	1003284	2.17%	0.652%
9	11.353	1590	1598	1621	rVB	25052780	46204390	100.00%	30.007%
10	11.870	1678	1686	1688	rBV	1042787	1800938	3.90%	1.170%
11	11.912	1688	1693	1700	rVV	10685987	18944441	41.00%	12.303%
12	12.070	1709	1720	1729	rVB	964739	1892984	4.10%	1.229%
13	12.212	1731	1744	1756	rBV2	4188172	8154619	17.65%	5.296%
14	12.312	1756	1761	1764	rVV	396605	678418	1.47%	0.441%
15	12.353	1764	1768	1772	rVV	1223404	2168433	4.69%	1.408%
16	12.400	1772	1776	1784	rVB2	984794	1780706	3.85%	1.156%
17	12.576	1799	1806	1812	rBV	1238394	2264502	4.90%	1.471%
18	12.641	1812	1817	1822	rVV	2236535	4285985	9.28%	2.784%
19	12.694	1822	1826	1844	rVB	1877977	3320730	7.19%	2.157%
20	12.853	1844	1853	1857	rBV	937221	1676709	3.63%	1.089%
21	12.900	1857	1861	1865	rVB	337395	483661	1.05%	0.314%
22	12.988	1870	1876	1879	rBV4	301621	671764	1.45%	0.436%
23	13.082	1886	1892	1895	rBV	552185	1010115	2.19%	0.656%
24	13.129	1895	1900	1911	rVB	4689559	8342216	18.06%	5.418%
25	13.364	1931	1940	1944	rBV4	251728	614539	1.33%	0.399%
26	13.423	1944	1950	1953	rVV	1139221	2178542	4.72%	1.415%
27	13.470	1953	1958	1969	rVB2	3382588	7601022	16.45%	4.936%
28	13.688	1987	1995	2003	rBV	626121	1985925	4.30%	1.290%
29	13.794	2008	2013	2024	rVB2	1329597	3113120	6.74%	2.022%
30	13.994	2041	2047	2052	rBV2	473898	1006096	2.18%	0.653%
31	14.117	2064	2068	2074	rVB2	917461	1543101	3.34%	1.002%
32	14.188	2074	2080	2086	rBV2	820471	1770702	3.83%	1.150%
33	14.241	2086	2089	2094	rVB2	312236	462764	1.00%	0.301%
34	14.382	2101	2113	2117	rBV	388225	1161697	2.51%	0.754%
35	14.853	2187	2193	2202	rVB5	170353	497366	1.08%	0.323%
36	15.047	2216	2226	2235	rBV8	277672	956012	2.07%	0.621%

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Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 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_N\methods\82N103023W.M
Title : SW846 8260

37	15.641	2313	2327	2337	rBV2	5819918	13394829	28.99%	8.699%
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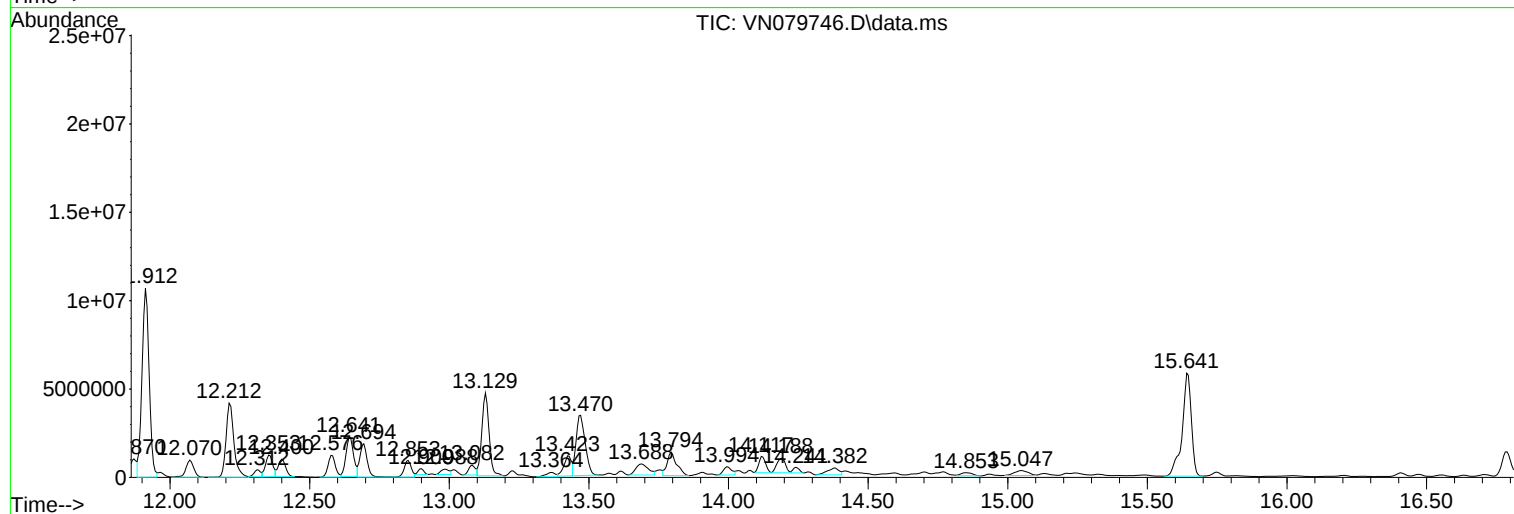
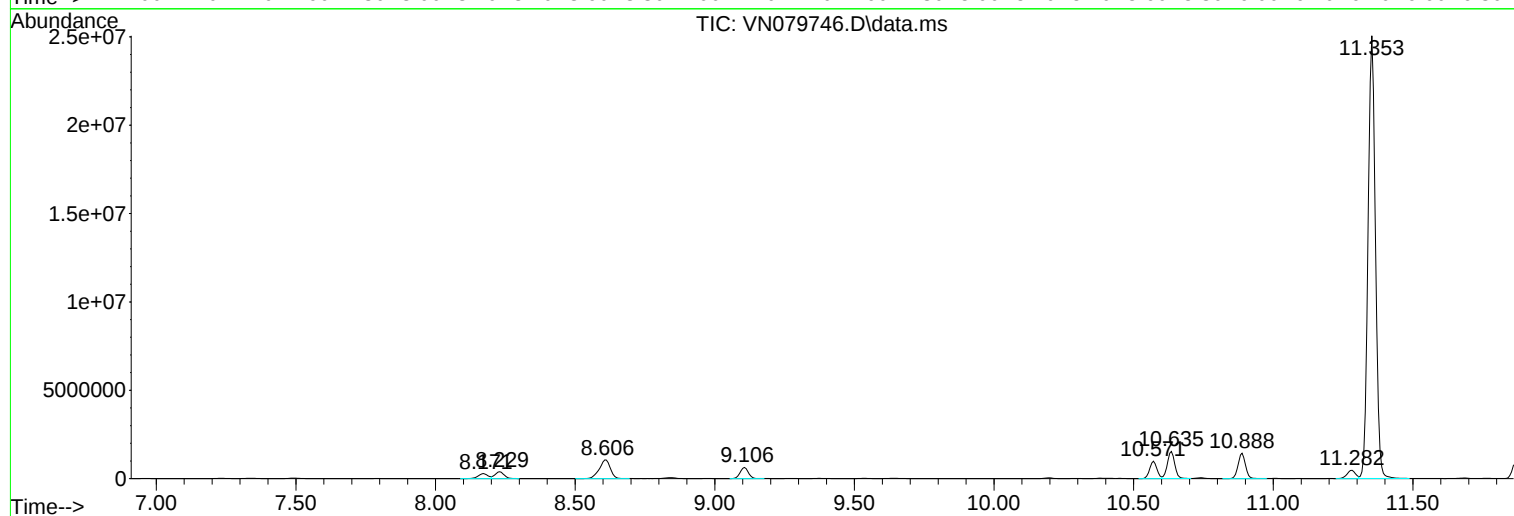
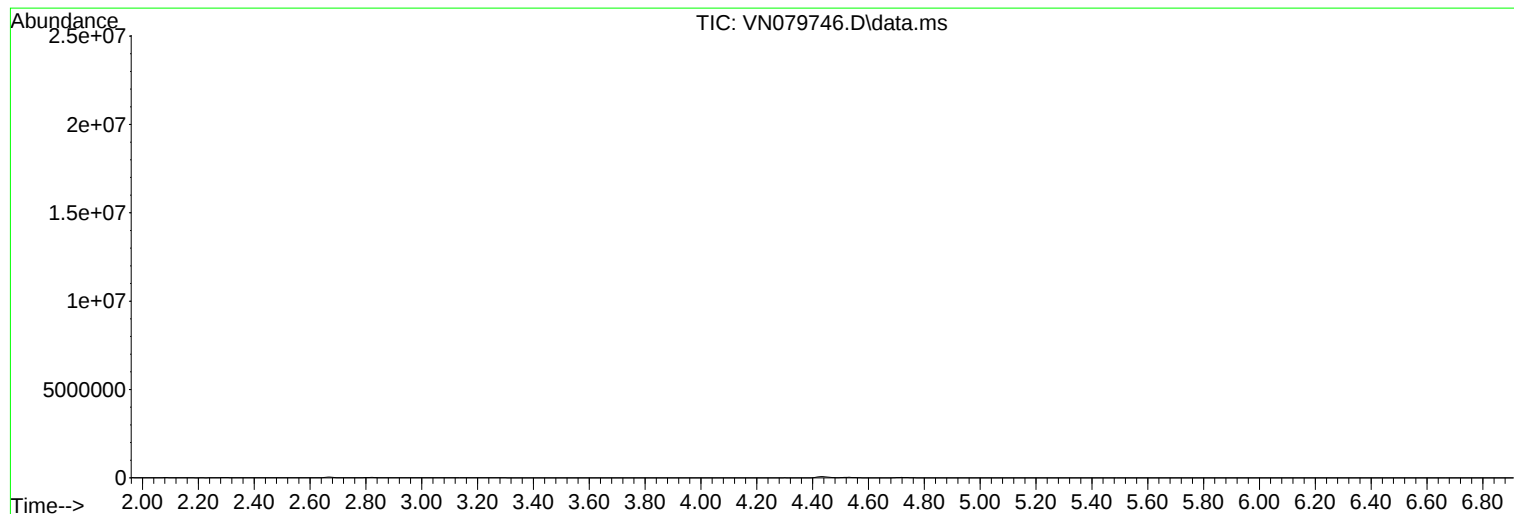
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103023W.M
Quant Title : SW846 8260

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



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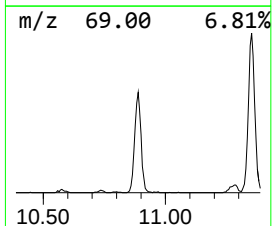
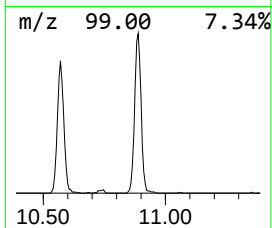
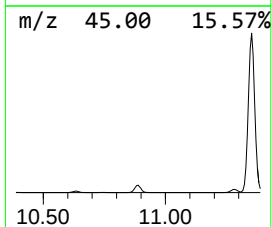
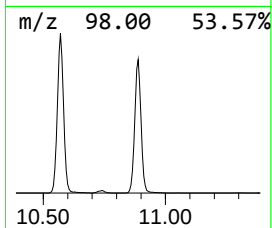
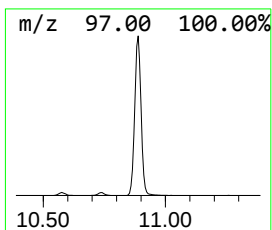
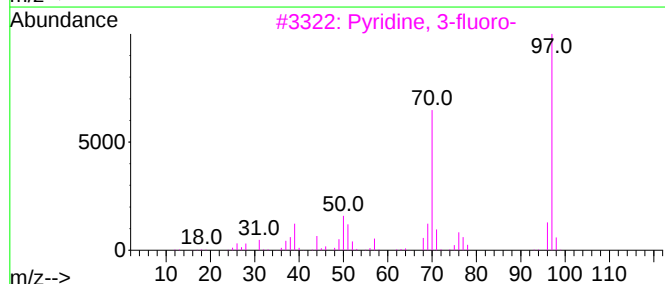
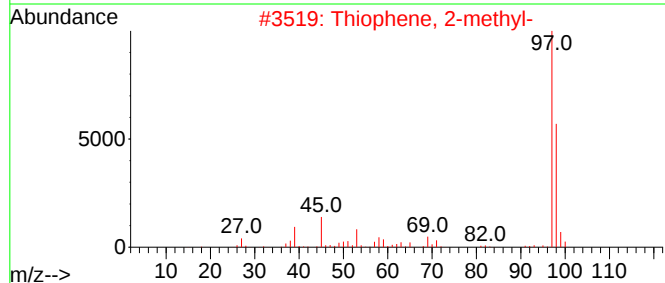
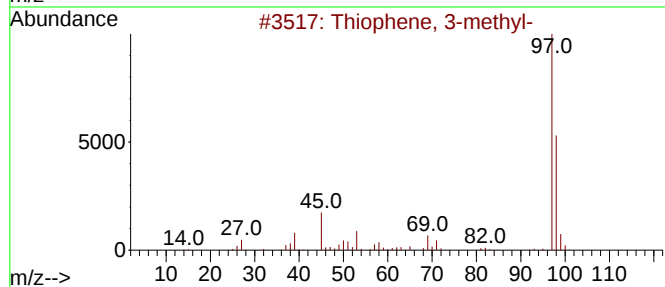
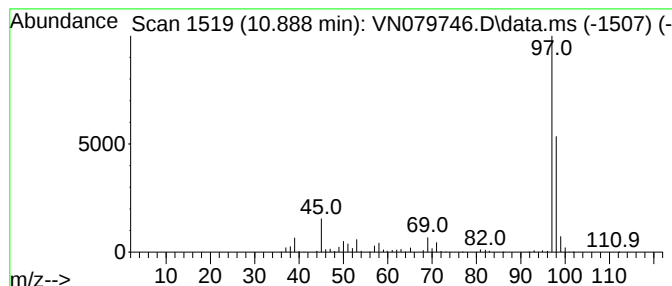
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103023W.M
Quant Title : SW846 8260

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

Peak Number 1 Thiophene, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.888	72.93 ug/l	2627010	Chlorobenzene-d5	11.870

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, 3-methyl-	98	C5H6S	000616-44-4	95
2			Thiophene, 2-methyl-	98	C5H6S	000554-14-3	90
3			Pyridine, 3-fluoro-	97	C5H4FN	000372-47-4	47
4			Propennitrile, 3-ethoxy-2-(2-thi...	257	C10H11NO3S2	1000267-97-5	28
5			4-Methyl-2-pyrazolin-5-one	98	C4H6N2O	013315-23-6	25



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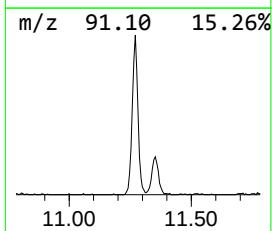
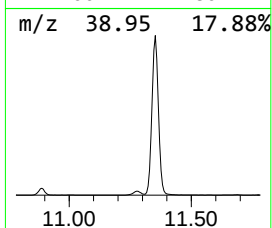
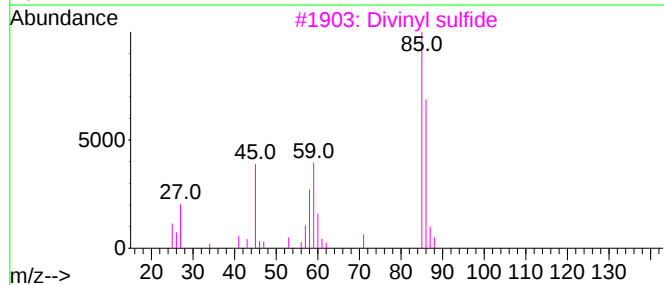
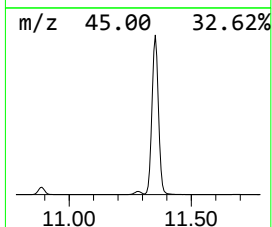
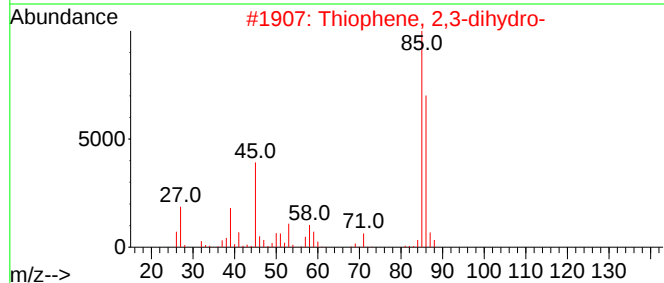
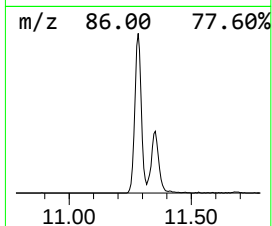
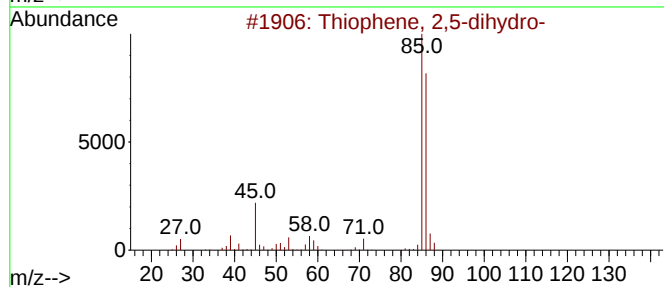
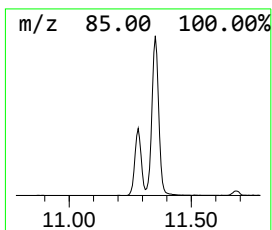
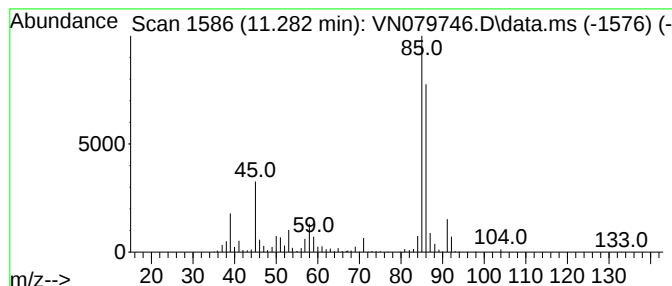
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103023W.M
Quant Title : SW846 8260

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

Peak Number 2 Thiophene, 2,5-dihydro- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.282	27.85 ug/l	1003280	Chlorobenzene-d5	11.870

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, 2,5-dihydro-	86	C4H6S	001708-32-3	93
2			Thiophene, 2,3-dihydro-	86	C4H6S	001120-59-8	90
3			Divinyl sulfide	86	C4H6S	000627-51-0	80
4			N-Aminopyrrolidine	86	C4H10N2	016596-41-1	45
5			9-Acetylhydrazono-2,7-bis-[2-(di...	466	C27H38N4O3	1000111-05-8	32



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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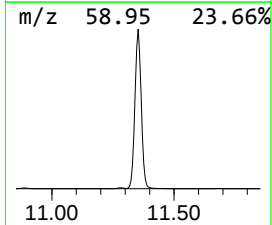
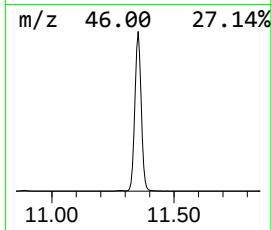
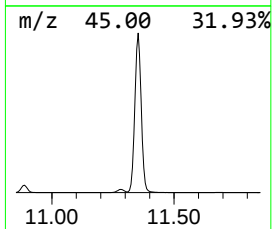
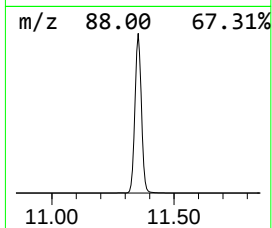
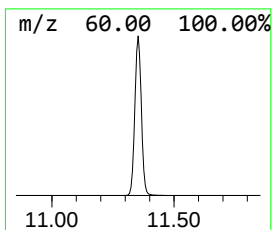
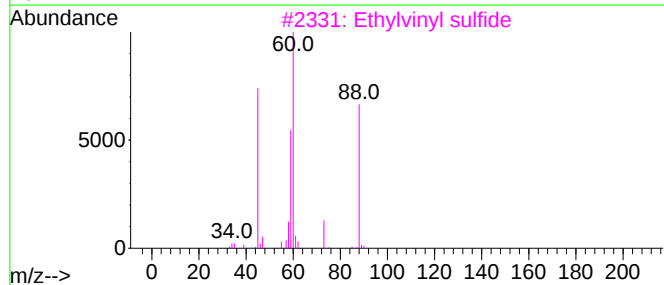
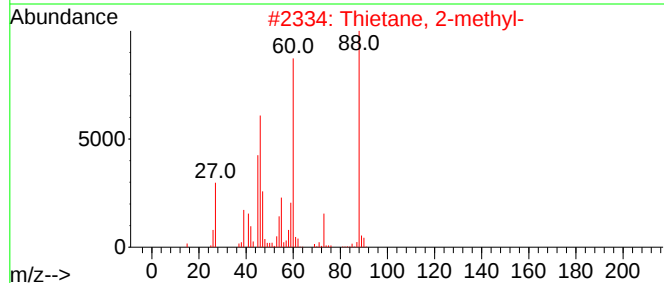
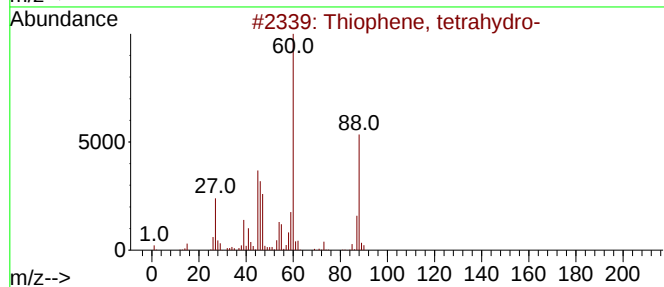
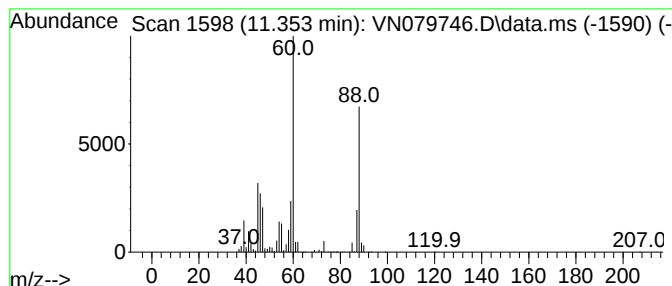
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103023W.M
Quant Title : SW846 8260

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

Peak Number 3 Thiophene, tetrahydro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.353	1282.79 ug/l	46204400	Chlorobenzene-d5	11.870

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, tetrahydro-	88	C4H8S	000110-01-0	97
2			Thietane, 2-methyl-	88	C4H8S	017837-41-1	74
3			Ethylvinyl sulfide	88	C4H8S	000627-50-9	38
4			1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	33
5			Ethanol, 2-mercapto-	78	C2H6OS	000060-24-2	23



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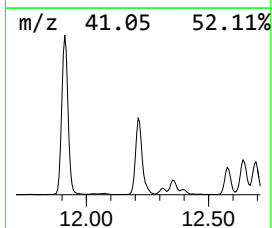
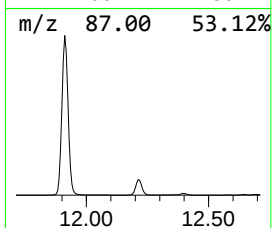
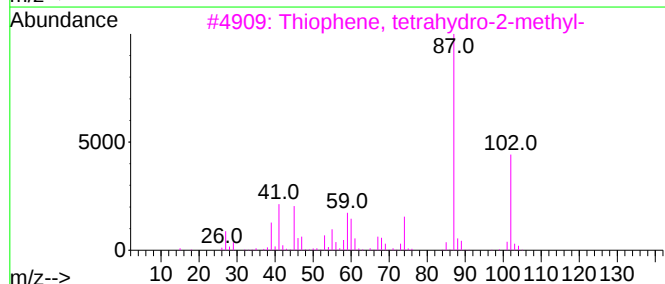
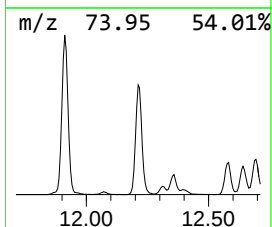
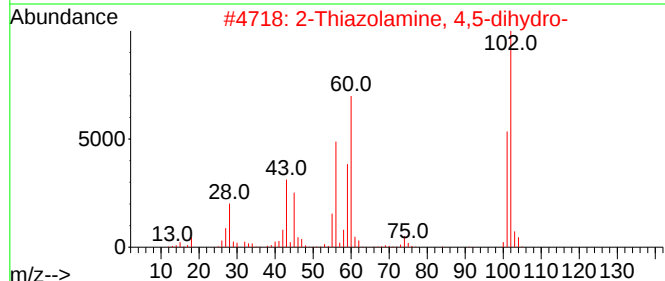
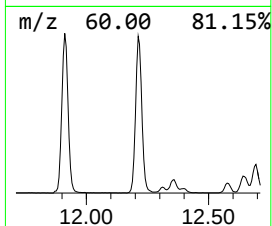
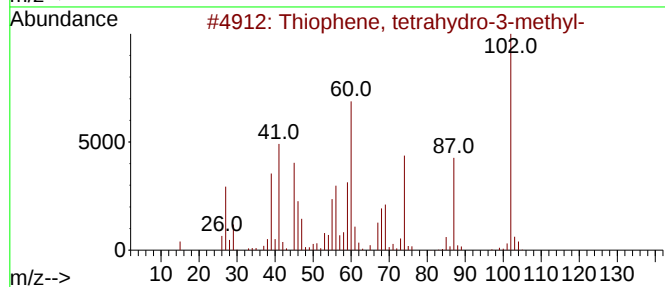
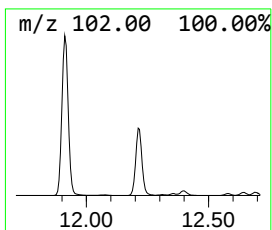
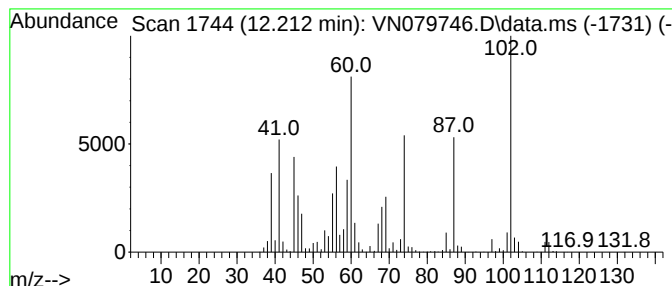
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Thiophene, tetrahydro-3-met... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.212	226.40 ug/l	8154620	Chlorobenzene-d5	11.870	
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	52
3	Thiophene, tetrahydro-2-methyl-	102	C5H10S	001795-09-1	43
4	Thietane, 2,4-dimethyl-	102	C5H10S	043044-24-2	43
5	1-Butene, 1-(methylthio)-, (Z)-	102	C5H10S	017414-15-2	38



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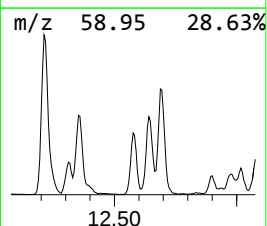
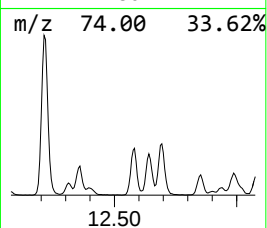
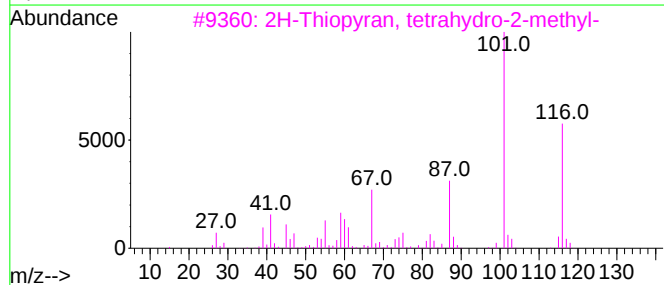
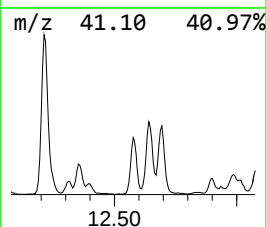
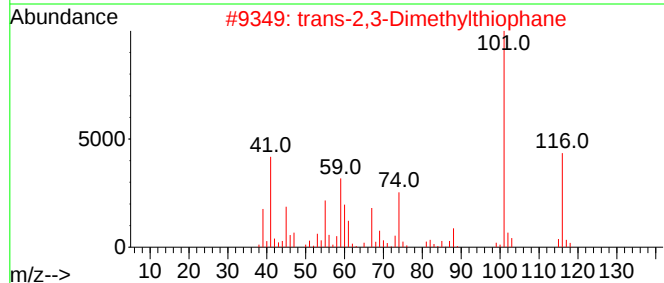
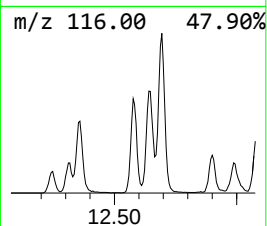
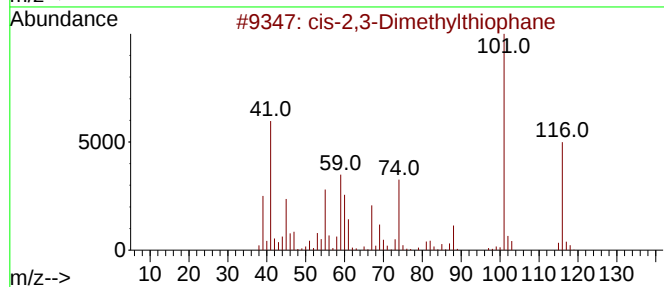
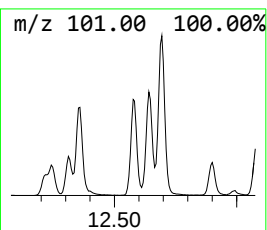
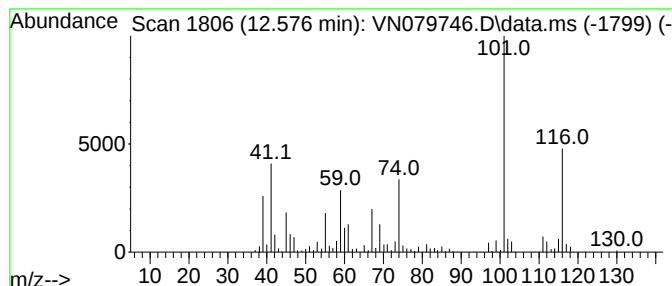
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.576	62.87 ug/l	2264500	Chlorobenzene-d5	11.870

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	95
2			trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	94
3			2H-Thiopyran, tetrahydro-2-methyl-	116	C6H12S	005161-16-0	87
4			Thiazole, 4,5-dihydro-4-methyl-2...	116	C4H8N2S	010416-81-6	68
5			Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-13-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN103123\
Data File : VN079746.D
Acq On : 31 Oct 2023 16:07
Operator : JC\MD
Sample : 05107-19
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1051

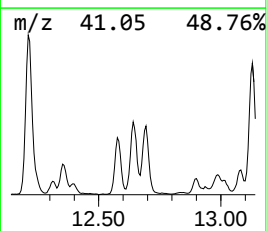
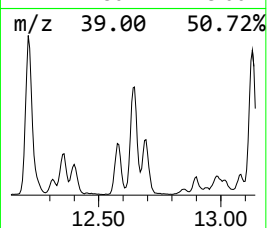
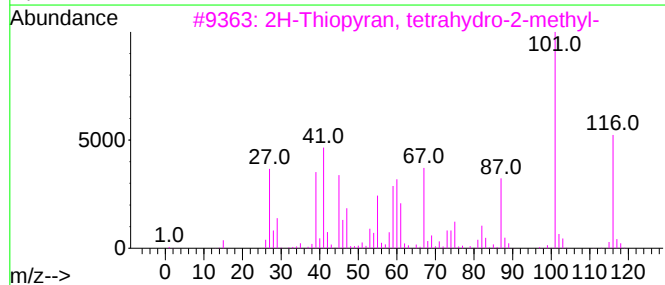
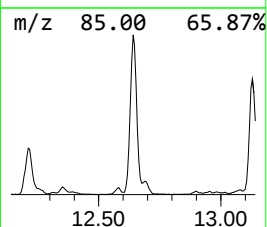
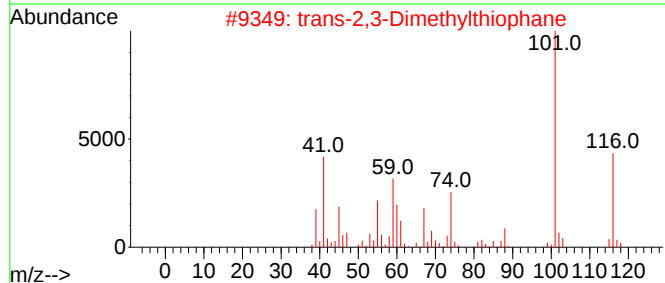
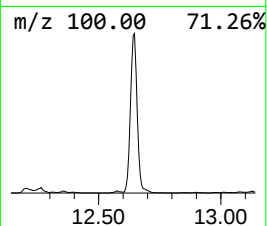
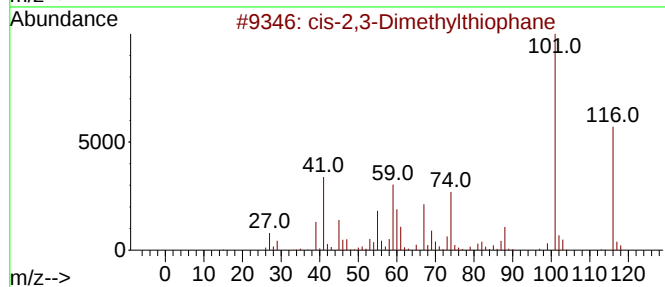
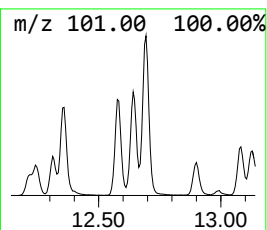
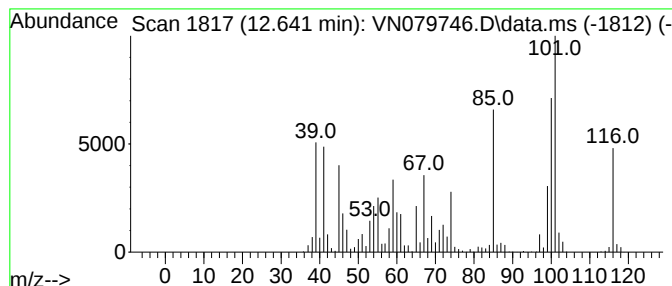
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Quant Title : SW846 8260

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

Peak Number 6 trans-2,3-Dimethylthiophane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.641	118.99 ug/l	4285990	Chlorobenzene-d5	11.870

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	55
2			trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	55
3			2H-Thiopyran, tetrahydro-2-methyl-	116	C6H12S	005161-16-0	52
4			Thiazole, 4,5-dihydro-4-methyl-2...	116	C4H8N2S	010416-81-6	49
5			Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN103123\
Data File : VN079746.D
Acq On : 31 Oct 2023 16:07
Operator : JC\MD
Sample : 05107-19
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1051

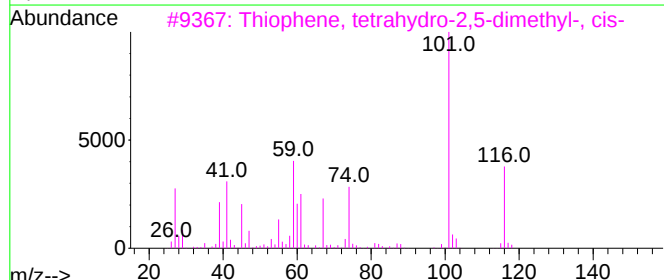
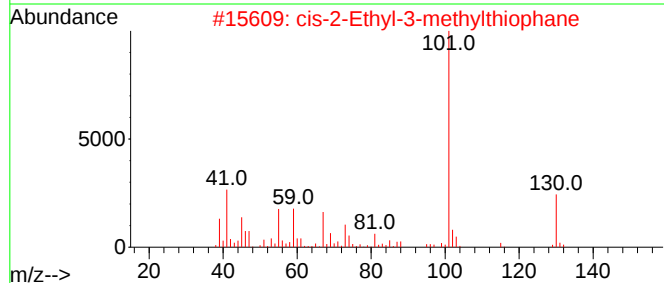
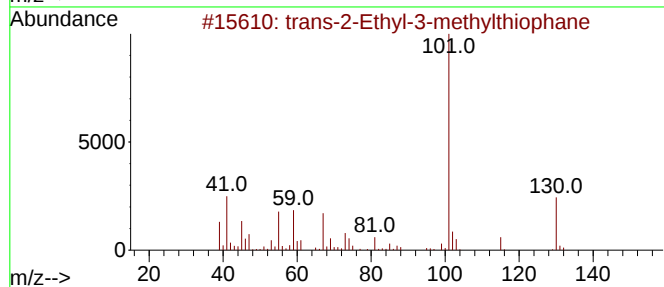
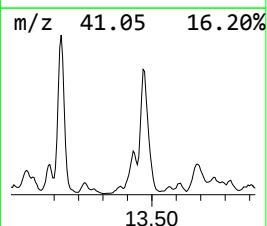
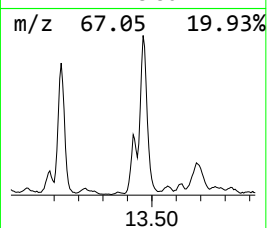
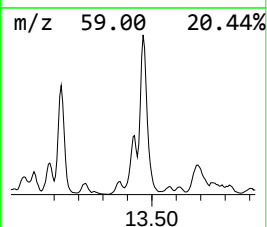
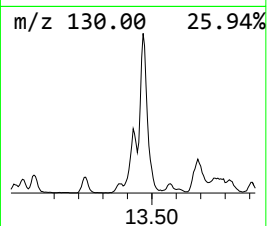
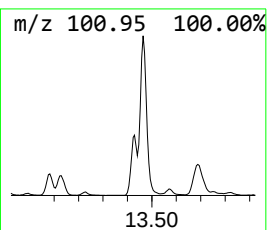
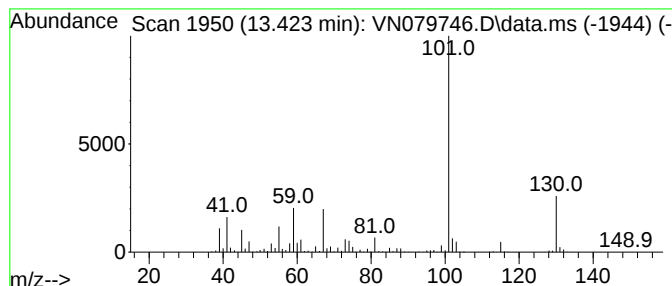
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Quant Title : SW846 8260

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

Peak Number 7 trans-2-Ethyl-3-methylthiop... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.423	34.99 ug/l	2178540	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-2-Ethyl-3-methylthiophane	130	C7H14S	061568-36-3	78
2			cis-2-Ethyl-3-methylthiophane	130	C7H14S	061568-37-4	78
3			Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-13-7	50
4			cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	50
5			Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN103123\
Data File : VN079746.D
Acq On : 31 Oct 2023 16:07
Operator : JC\MD
Sample : 05107-19
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1051

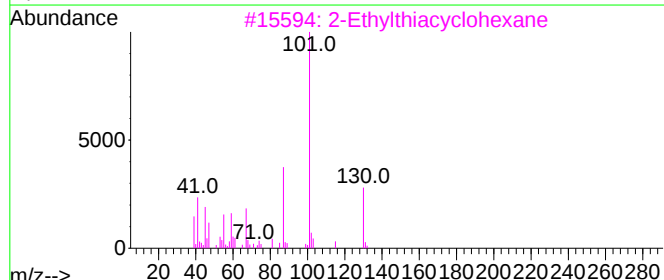
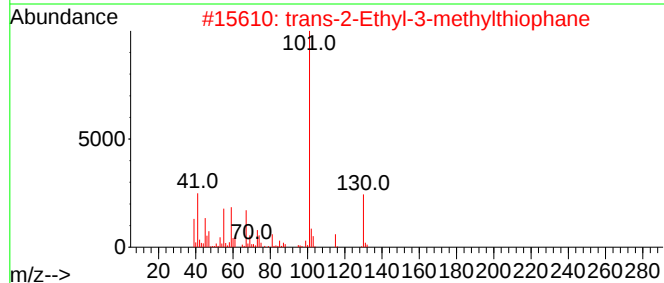
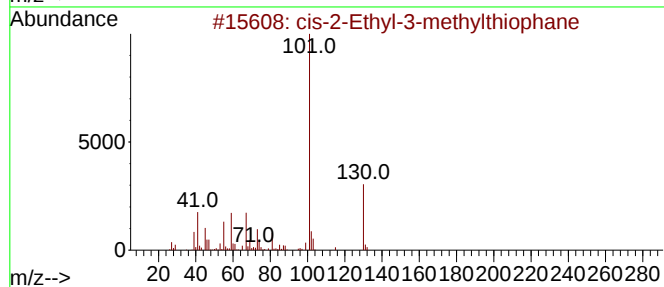
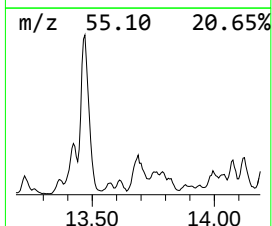
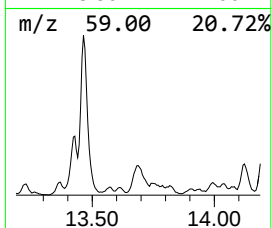
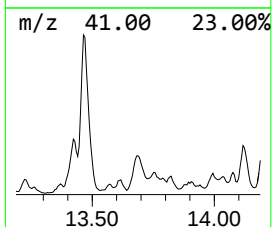
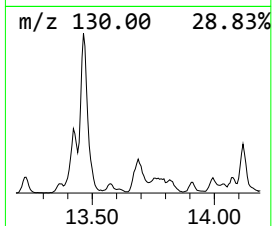
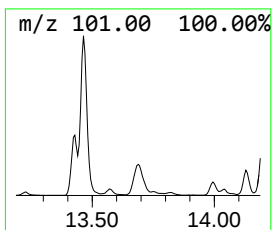
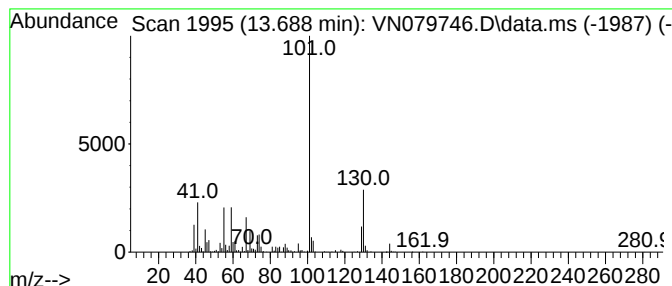
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Quant Title : SW846 8260

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

Peak Number 8 cis-2-Ethyl-3-methylthiophane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.688	31.90 ug/l	1985930	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-2-Ethyl-3-methylthiophane	130	C7H14S	061568-37-4	81
2			trans-2-Ethyl-3-methylthiophane	130	C7H14S	061568-36-3	72
3			2-Ethylthiacyclohexane	130	C7H14S	001613-52-1	68
4			trans-3-Methyl-2-n-propylthiophane	144	C8H16S	118068-75-0	64
5			2-n-Propylthiane	144	C8H16S	017912-23-1	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN103123\
Data File : VN079746.D
Acq On : 31 Oct 2023 16:07
Operator : JC\MD
Sample : 05107-19
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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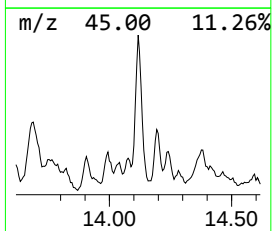
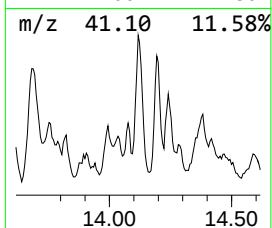
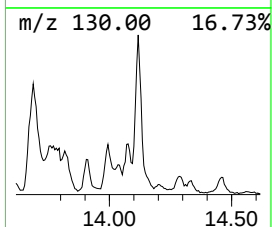
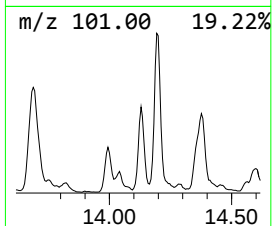
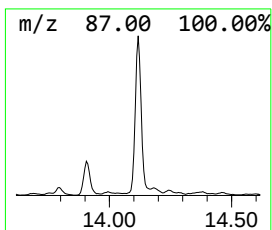
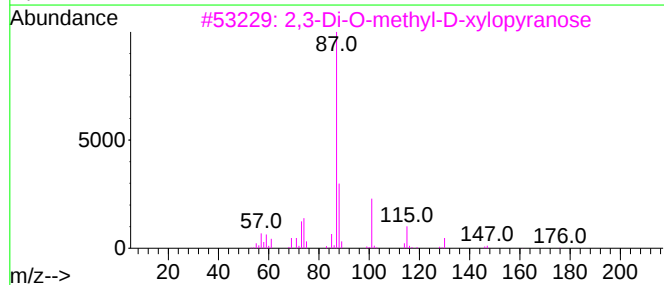
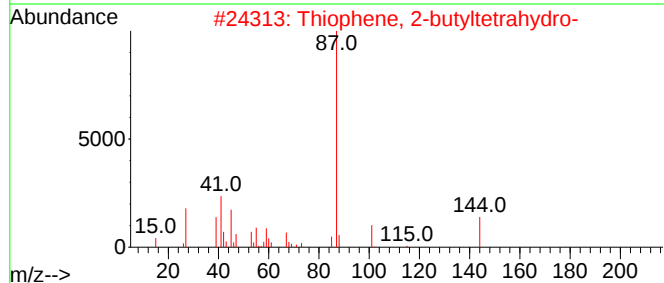
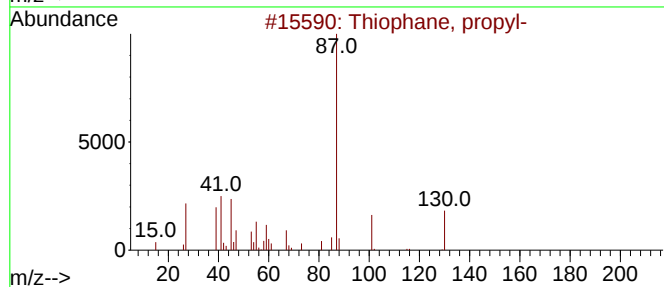
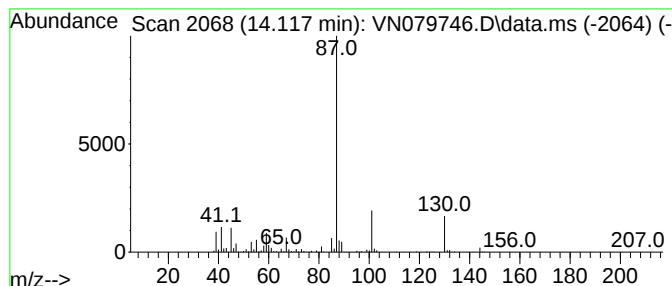
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Quant Title : SW846 8260

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

Peak Number 9 Thiophane, propyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.117	24.78 ug/l	1543100	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophane, propyl-	130	C7H14S	001551-34-4	91
2			Thiophene, 2-butyltetrahydro-	144	C8H16S	001613-49-6	81
3			2,3-Di-O-methyl-D-xylopyranose	178	C7H14O5	018186-26-0	64
4			Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	50
5			Cyclohexanecarboxylic acid, meth...	142	C8H14O2	004630-82-4	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN103123\
Data File : VN079746.D
Acq On : 31 Oct 2023 16:07
Operator : JC\MD
Sample : 05107-19
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1051

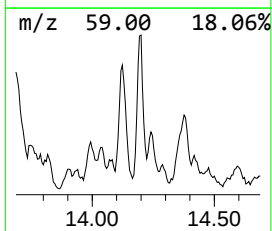
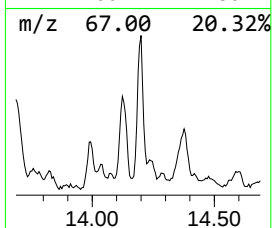
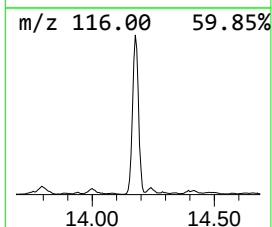
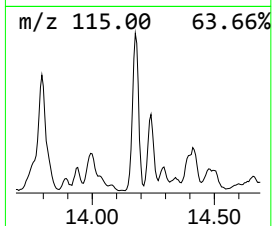
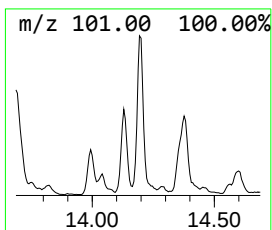
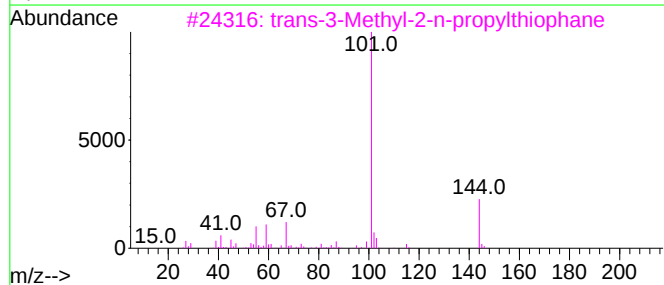
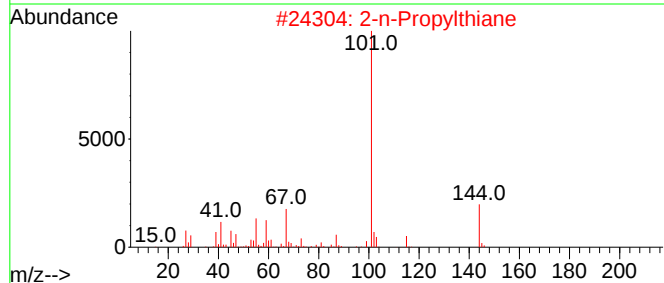
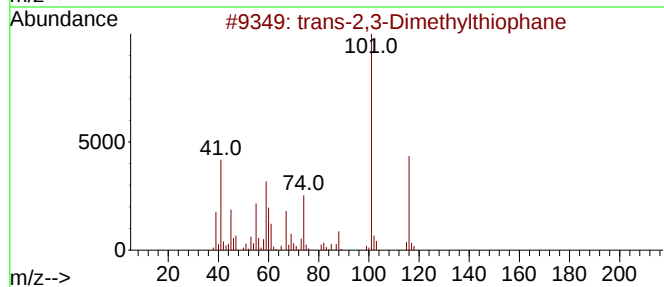
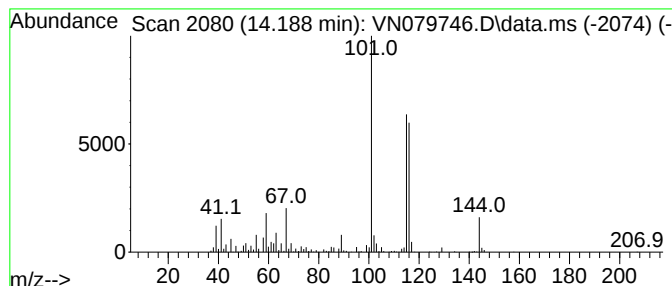
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Quant Title : SW846 8260

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

Peak Number 10 unknown14.188 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.188	28.44 ug/l	1770700	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	50
2			2-n-Propylthiane	144	C8H16S	017912-23-1	49
3			trans-3-Methyl-2-n-propylthiophane	144	C8H16S	118068-75-0	43
4			Benzene, 1-propynyl-	116	C9H8	000673-32-5	42
5			Indene	116	C9H8	000095-13-6	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN103123\
Data File : VN079746.D
Acq On : 31 Oct 2023 16:07
Operator : JC\MD
Sample : 05107-19
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1051

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103023W.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
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Thiophene, 2,5-...	11.282	27.9	ug/l	1003280	3	11.870	1800940	50.0
Thiophene, tetr...	11.353	1282.8	ug/l	46204400	3	11.870	1800940	50.0
Thiophene, tetr...	12.212	226.4	ug/l	8154620	3	11.870	1800940	50.0
cis-2,3-Dimethy...	12.576	62.9	ug/l	2264500	3	11.870	1800940	50.0
trans-2,3-Dimet...	12.641	119.0	ug/l	4285990	3	11.870	1800940	50.0
trans-2-Ethyl-3...	13.423	35.0	ug/l	2178540	4	13.794	3113120	50.0
cis-2-Ethyl-3-m...	13.688	31.9	ug/l	1985930	4	13.794	3113120	50.0
Thiophane, propyl-	14.117	24.8	ug/l	1543100	4	13.794	3113120	50.0
unknown14.188	14.188	28.4	ug/l	1770700	4	13.794	3113120	50.0