

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN103123\
 Data File : VN079758.D
 Acq On : 31 Oct 2023 20:55
 Operator : JC\MD
 Sample : 05107-19
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 26 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: VN079758.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	285163	717520	1.42%	0.416%
2	8.230	1062	1067	1078	rVB	418179	925215	1.83%	0.537%
3	8.606	1111	1131	1152	rBV3	1060578	2947763	5.84%	1.710%
4	9.106	1207	1216	1227	rBV	667797	1356747	2.69%	0.787%
5	10.571	1457	1465	1470	rBV	1020564	1853282	3.67%	1.075%
6	10.635	1470	1476	1488	rVB	1519622	2760005	5.46%	1.602%
7	10.888	1510	1519	1531	rBV	1191498	2184318	4.33%	1.267%
8	11.282	1576	1586	1590	rBV2	491005	1013102	2.01%	0.588%
9	11.353	1590	1598	1623	rVB	27629883	50504061	100.00%	29.306%
10	11.870	1678	1686	1688	rBV	1035145	1798905	3.56%	1.044%
11	11.912	1688	1693	1701	rVB	11358357	19743625	39.09%	11.456%
12	12.070	1709	1720	1729	rVB	889537	1755915	3.48%	1.019%
13	12.212	1733	1744	1756	rBV2	4487490	8842741	17.51%	5.131%
14	12.312	1756	1761	1764	rVV	431278	746151	1.48%	0.433%
15	12.353	1764	1768	1772	rVV	1227856	2187516	4.33%	1.269%
16	12.400	1772	1776	1783	rVB3	922955	1697171	3.36%	0.985%
17	12.576	1799	1806	1812	rBV	1336035	2453900	4.86%	1.424%
18	12.641	1812	1817	1822	rVV	2533095	4895330	9.69%	2.841%
19	12.694	1822	1826	1837	rVB	2090890	3621249	7.17%	2.101%
20	12.853	1845	1853	1857	rBV	913129	1624802	3.22%	0.943%
21	12.900	1857	1861	1865	rVB	344805	536790	1.06%	0.311%
22	12.988	1870	1876	1879	rBV4	336984	756226	1.50%	0.439%
23	13.082	1886	1892	1895	rBV	600008	1098338	2.17%	0.637%
24	13.129	1895	1900	1912	rVB	5018635	8906769	17.64%	5.168%
25	13.223	1912	1916	1921	rBV	299209	513210	1.02%	0.298%
26	13.365	1932	1940	1944	rBV3	241726	577199	1.14%	0.335%
27	13.423	1944	1950	1953	rVV	1205159	2313386	4.58%	1.342%
28	13.464	1953	1957	1968	rVB2	3641236	8000331	15.84%	4.642%
29	13.617	1978	1983	1986	rBV2	320319	578047	1.14%	0.335%
30	13.688	1986	1995	2003	rVV2	912566	2930199	5.80%	1.700%
31	13.794	2008	2013	2024	rVB2	1349873	3251809	6.44%	1.887%
32	14.029	2041	2053	2059	rBV4	1046927	4181303	8.28%	2.426%
33	14.123	2063	2069	2075	rVV2	1402317	3240293	6.42%	1.880%
34	14.188	2075	2080	2086	rVV2	965718	2244192	4.44%	1.302%
35	14.376	2102	2112	2117	rBV	414720	1210166	2.40%	0.702%
36	14.576	2138	2146	2155	rVB7	286838	1058490	2.10%	0.614%

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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	14.853	2186	2193	2202	rVB5	283364	846261	1.68%	0.491%
38	15.053	2216	2227	2236	rBV7	336846	1327043	2.63%	0.770%
39	15.641	2314	2327	2337	rBV2	6400387	14602505	28.91%	8.473%
40	15.747	2339	2345	2353	rVB	265346	533938	1.06%	0.310%

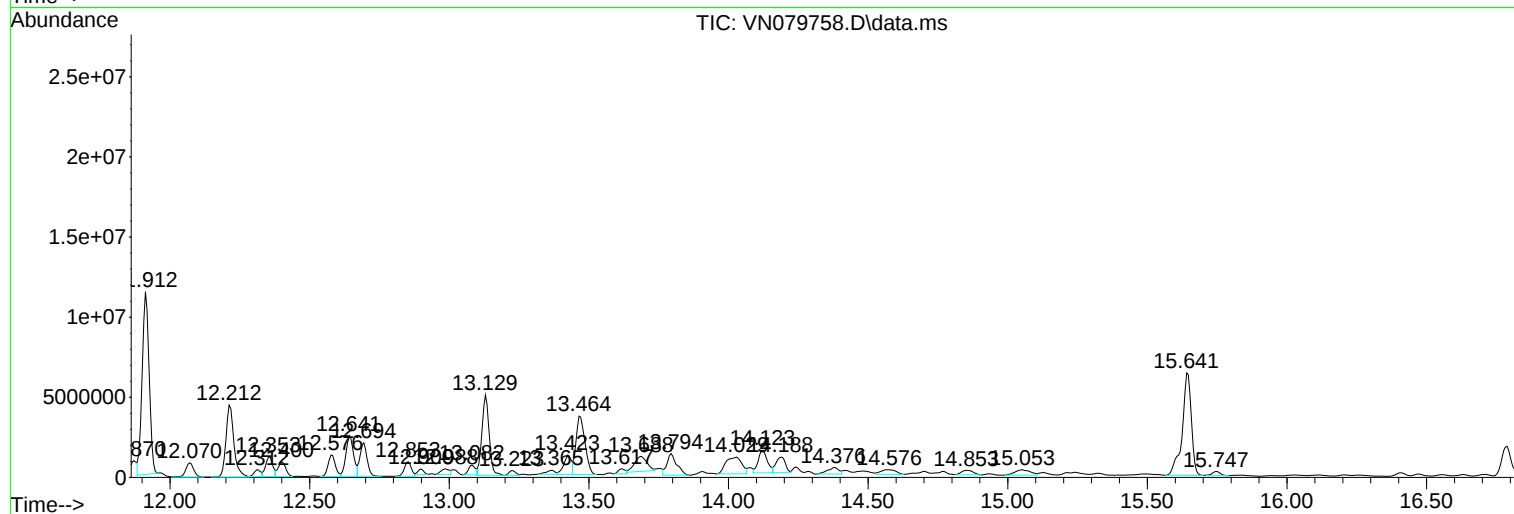
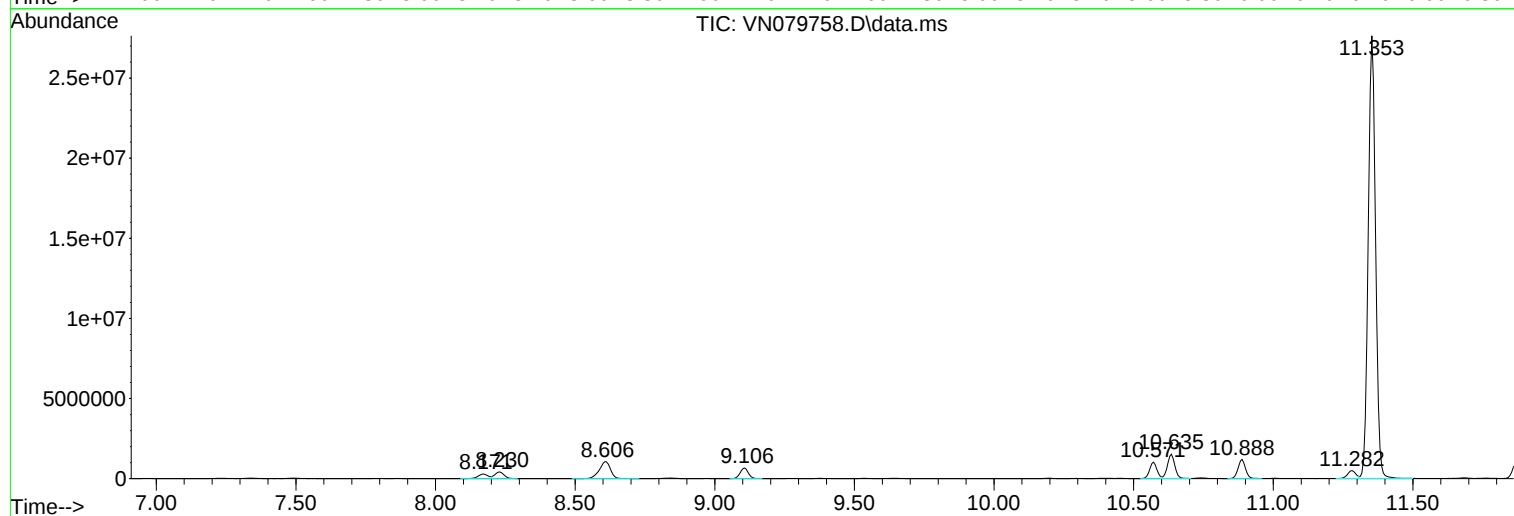
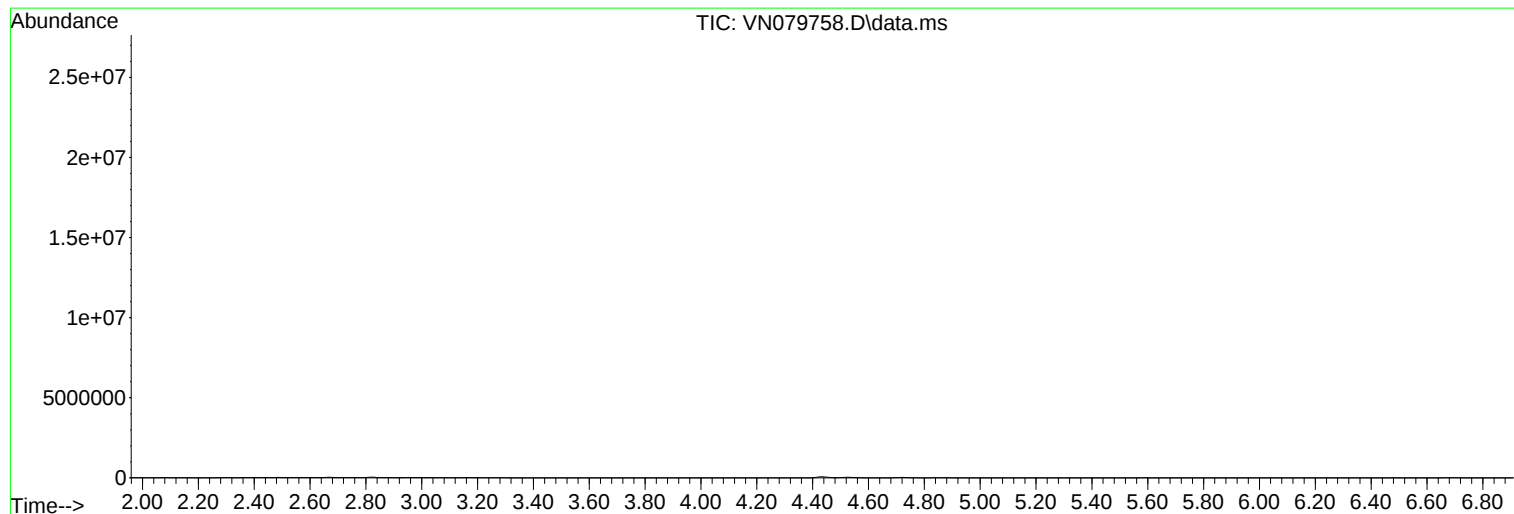
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103023W.M
Quant Title : SW846 8260

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



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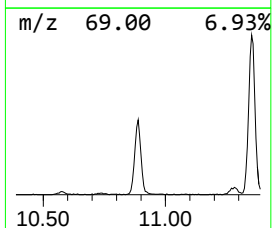
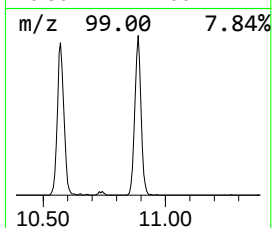
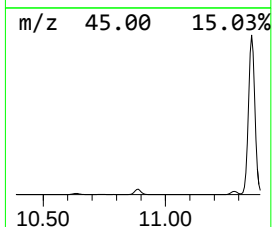
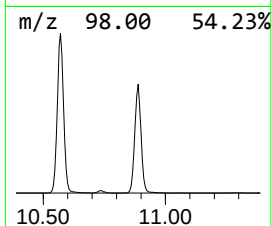
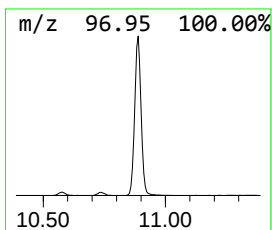
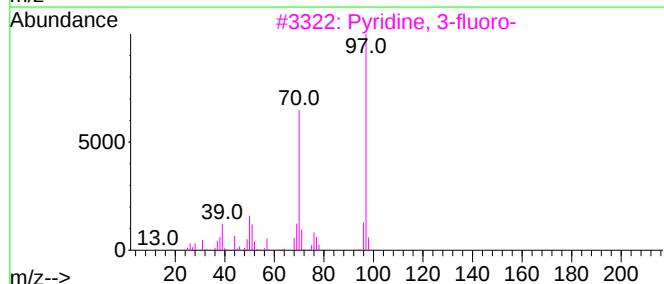
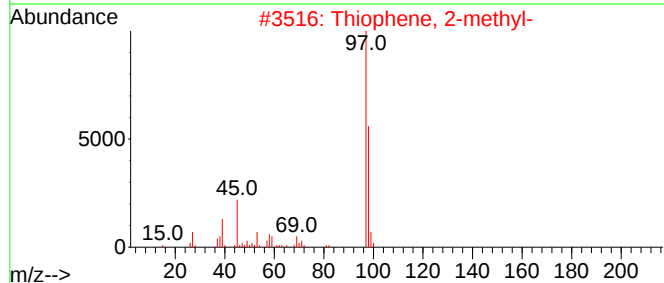
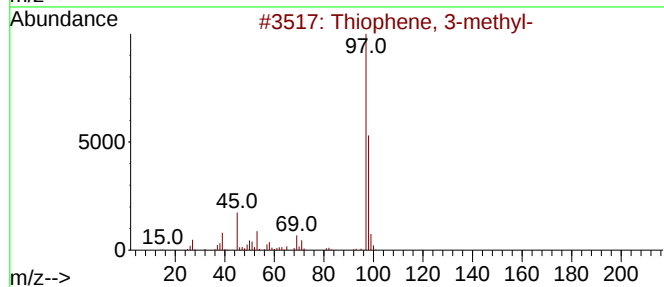
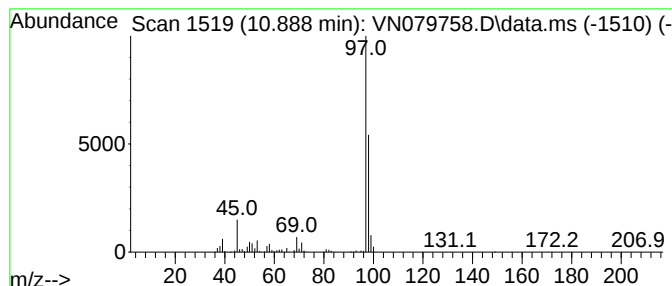
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103023W.M
Quant Title : SW846 8260

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

Peak Number 1 Thiophene, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.888	60.71 ug/l	2184320	Chlorobenzene-d5	11.871

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	91
3			Pyridine, 3-fluoro-	97	C5H4FN	000372-47-4	47
4			2-Fluoropyridine	97	C5H4FN	000372-48-5	47
5			Propennitrile, 3-ethoxy-2-(2-thi...	257	C10H11NO3S2	1000267-97-5	33



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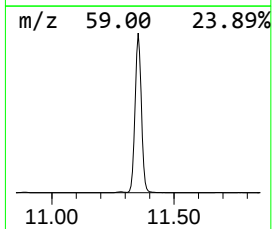
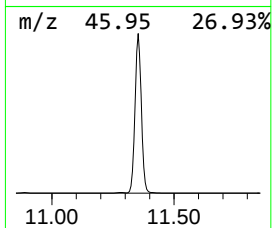
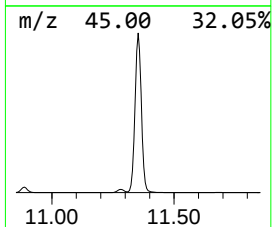
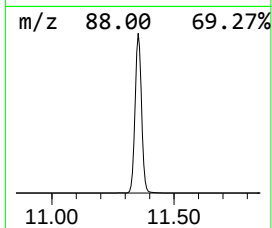
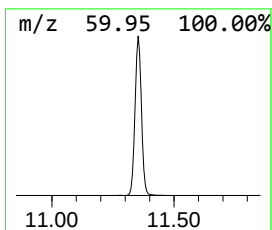
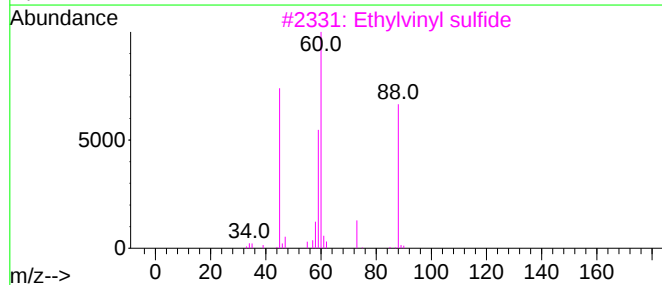
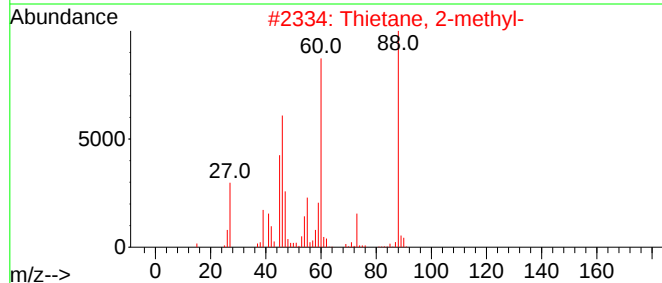
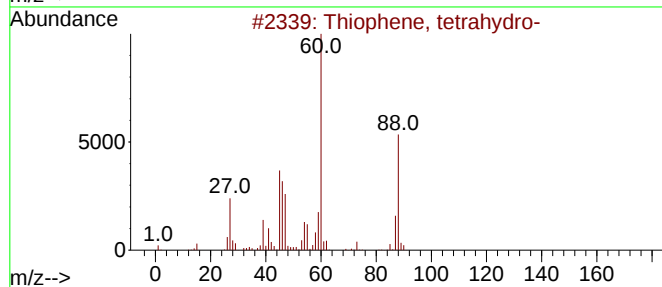
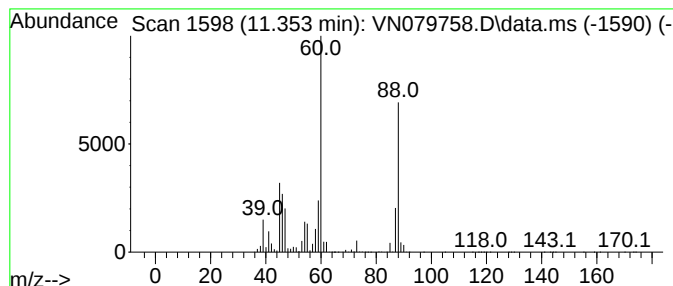
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Thiophene, tetrahydro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.353	1403.74 ug/l	50504100	Chlorobenzene-d5	11.871

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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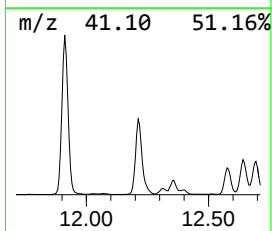
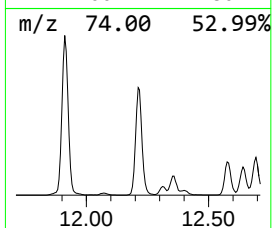
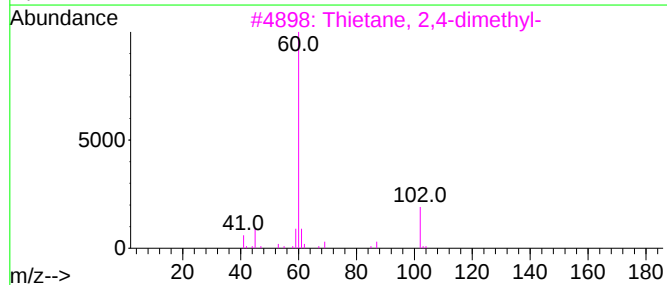
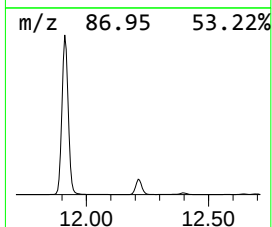
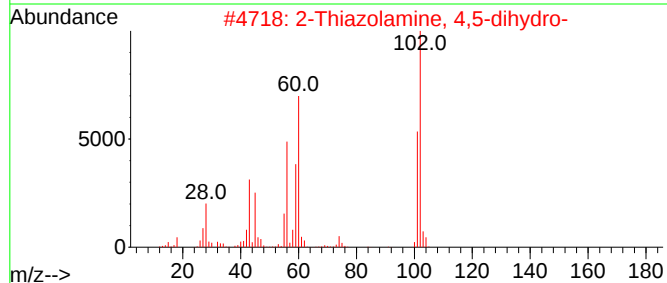
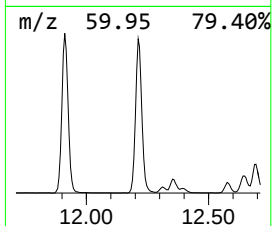
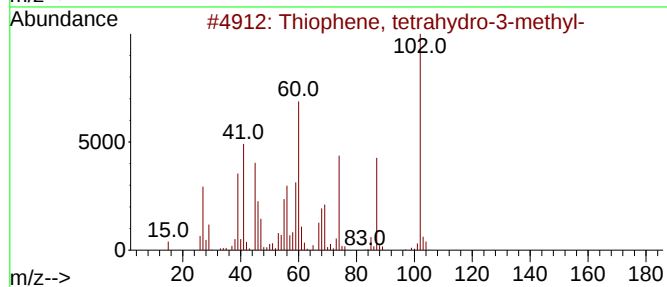
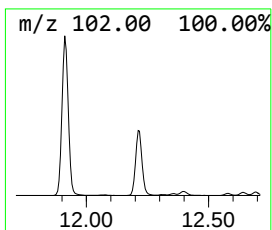
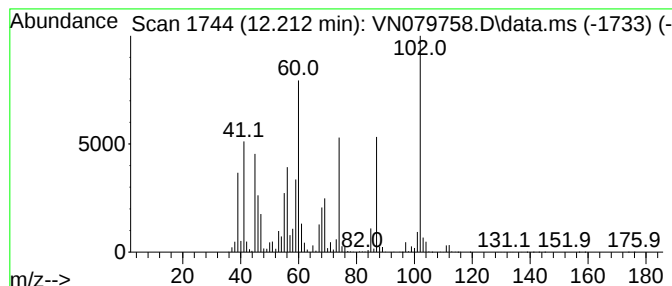
Instrument :
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Quant Title : SW846 8260

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.	
12.212	245.78 ug/l	8842740	Chlorobenzene-d5		11.871	
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	Thietane, 2,4-dimethyl-		102	C5H10S	043044-24-2	43
4	Thiophene, tetrahydro-2-methyl-		102	C5H10S	001795-09-1	43
5	1-Butene, 1-(methylthio)-, (Z)-		102	C5H10S	017414-15-2	38



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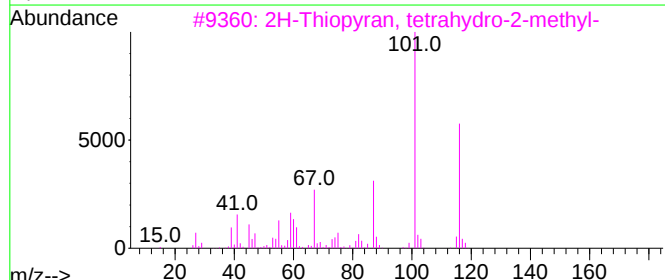
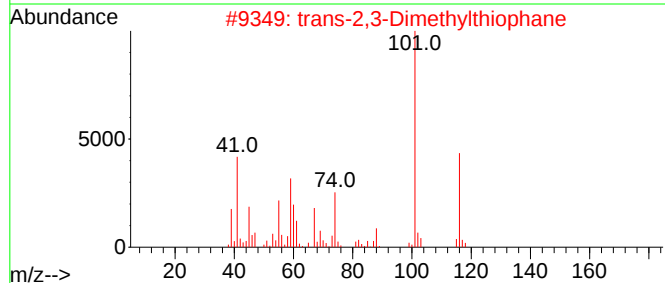
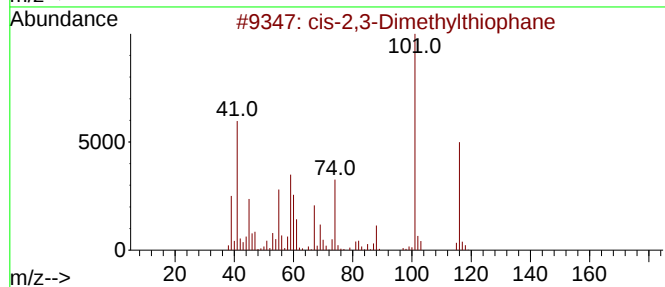
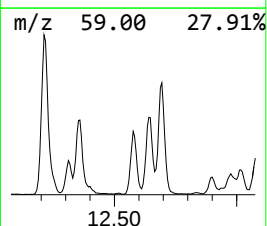
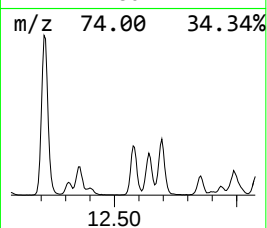
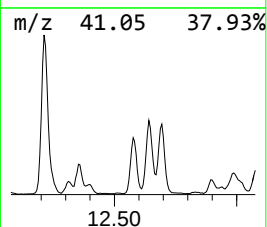
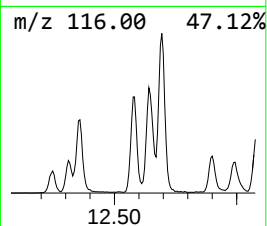
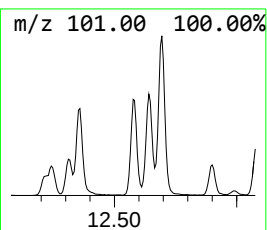
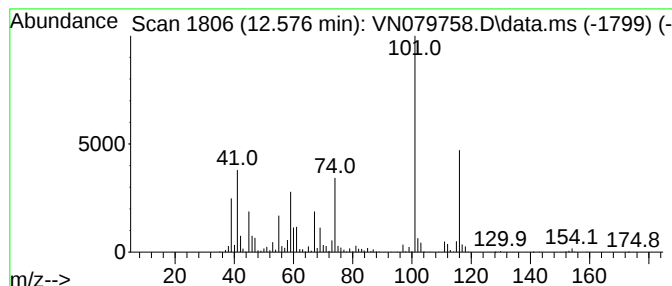
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 cis-2,3-Dimethylthiophane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.576	68.21 ug/l	2453900	Chlorobenzene-d5	11.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	93
2			trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	93
3			2H-Thiopyran, tetrahydro-2-methyl-	116	C6H12S	005161-16-0	81
4			Thiazole, 4,5-dihydro-4-methyl-2...	116	C4H8N2S	010416-81-6	81
5			Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-14-8	72



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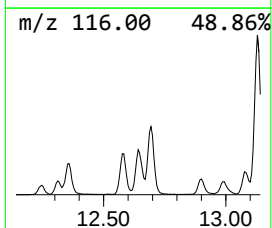
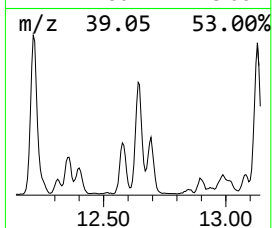
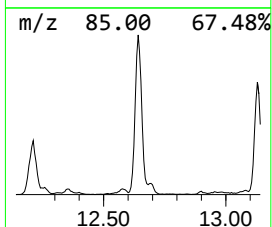
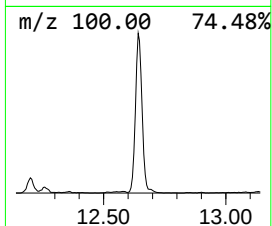
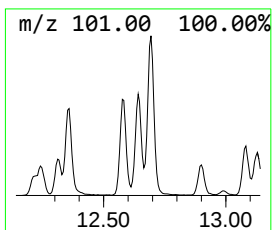
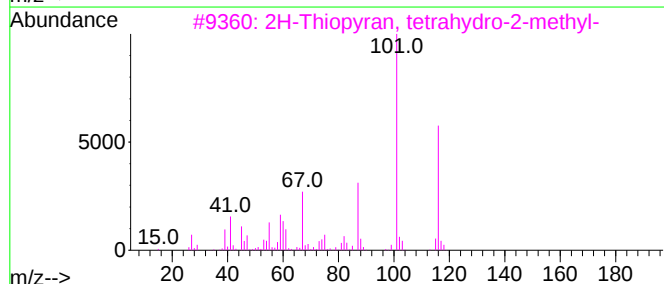
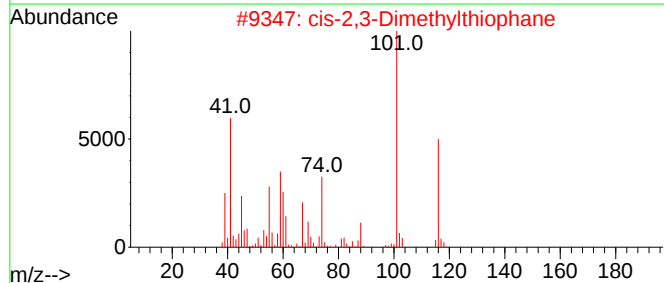
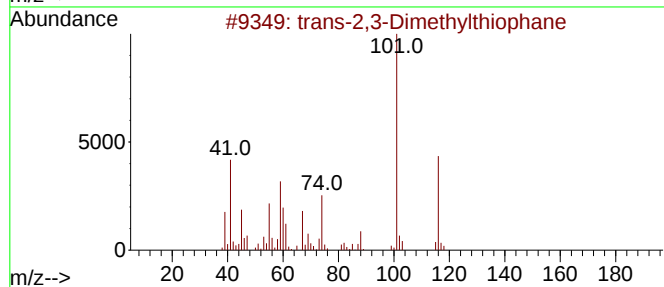
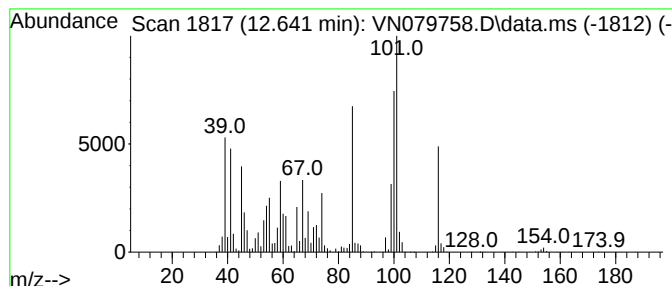
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.641	136.06 ug/l	4895330	Chlorobenzene-d5	11.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	50
2			cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	50
3			2H-Thiopyran, tetrahydro-2-methyl-	116	C6H12S	005161-16-0	45
4			Thiazole, 4,5-dihydro-4-methyl-2...	116	C4H8N2S	010416-81-6	43
5			Thiophene, 2,3-dihydro-5-methyl-	100	C5H8S	004610-02-0	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN103123\
Data File : VN079758.D
Acq On : 31 Oct 2023 20:55
Operator : JC\MD
Sample : 05107-19
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1051

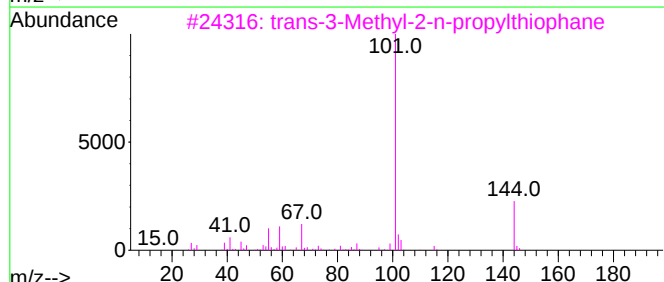
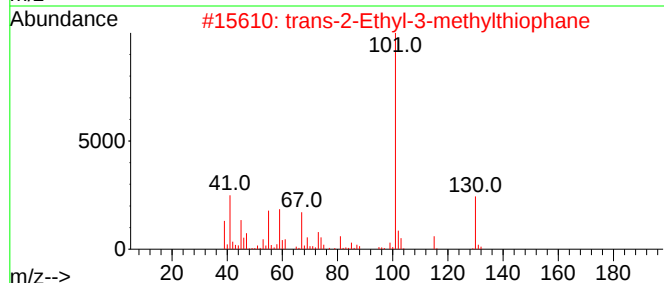
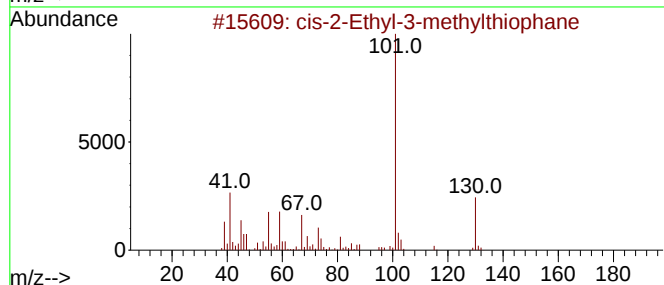
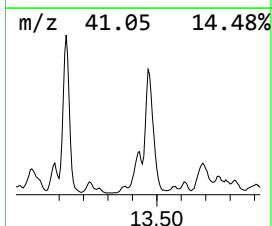
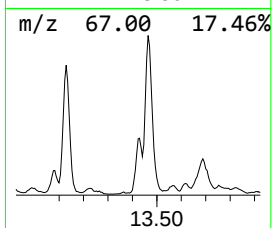
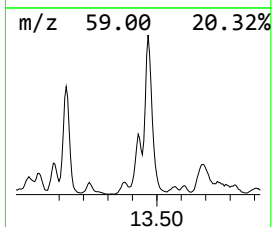
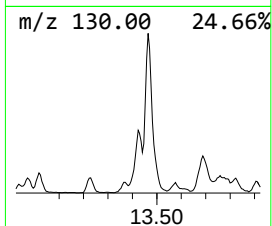
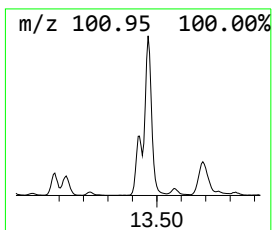
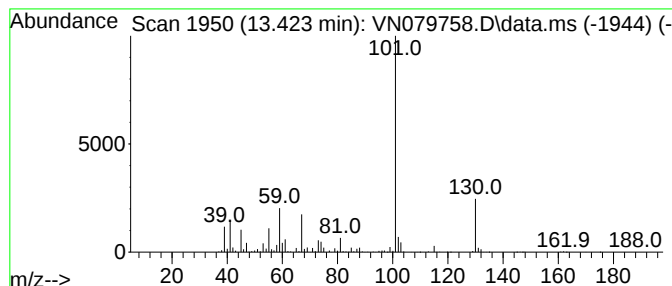
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Quant Title : SW846 8260

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

Peak Number 6 cis-2-Ethyl-3-methylthiophane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.423	35.57 ug/l	2313390	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	87
2			trans-2-Ethyl-3-methylthiophane	130	C7H14S	061568-36-3	87
3			trans-3-Methyl-2-n-propylthiophane	144	C8H16S	118068-75-0	80
4			2-Ethylthiacyclohexane	130	C7H14S	001613-52-1	78
5			2-n-Propylthiane	144	C8H16S	017912-23-1	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN103123\
Data File : VN079758.D
Acq On : 31 Oct 2023 20:55
Operator : JC\MD
Sample : 05107-19
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1051

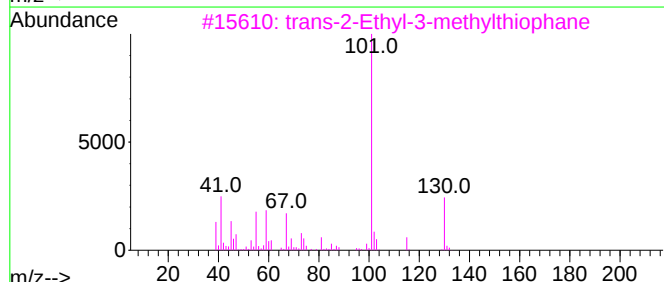
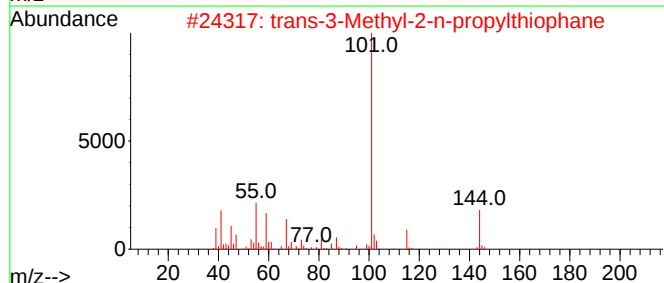
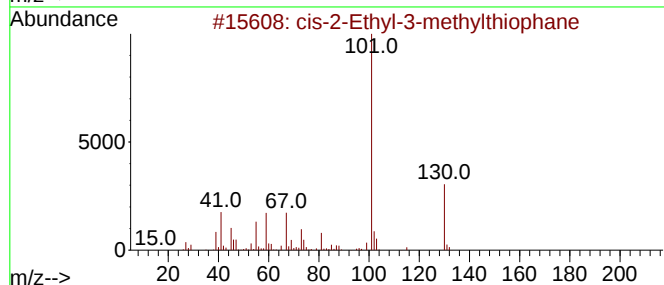
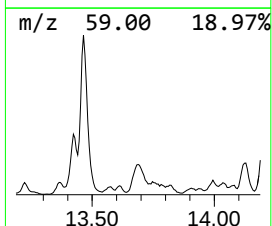
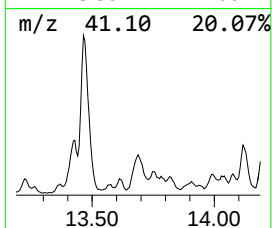
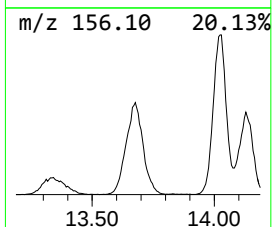
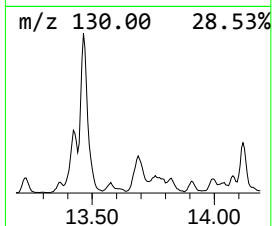
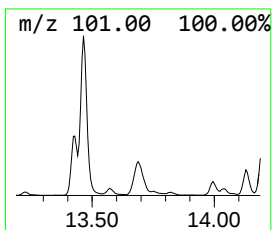
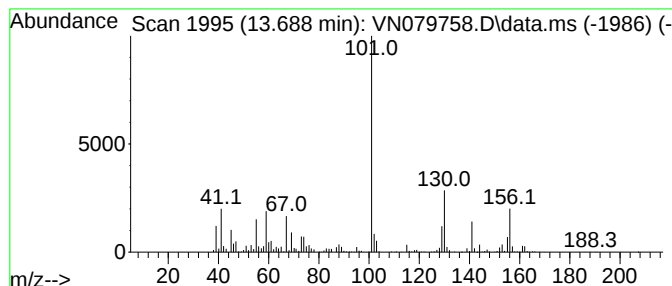
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Quant Title : SW846 8260

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

Peak Number 7 trans-3-Methyl-2-n-propylth... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.688	45.05 ug/l	2930200	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	70
2			trans-3-Methyl-2-n-propylthiophane	144	C8H16S	118068-75-0	55
3			trans-2-Ethyl-3-methylthiophane	130	C7H14S	061568-36-3	52
4			2-Ethylthiacyclohexane	130	C7H14S	001613-52-1	52
5			Dichloromethyldimethylsilyloxy...	212	C7H14Cl2OSi	1010283-10-2	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN103123\
Data File : VN079758.D
Acq On : 31 Oct 2023 20:55
Operator : JC\MD
Sample : 05107-19
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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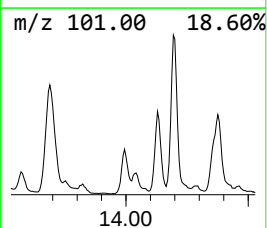
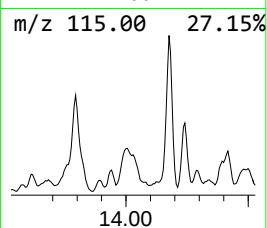
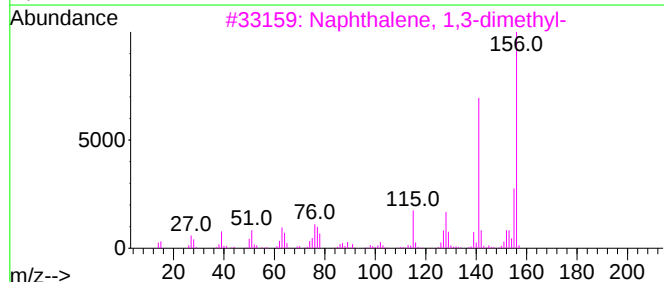
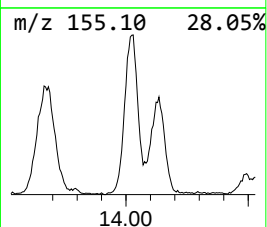
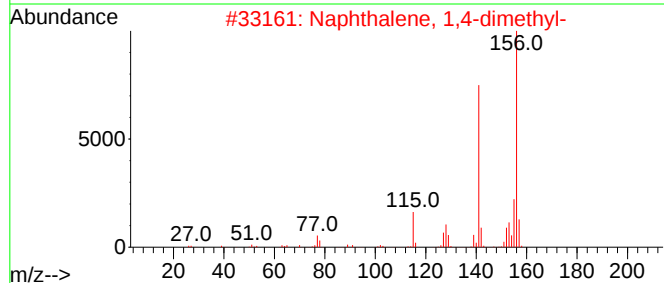
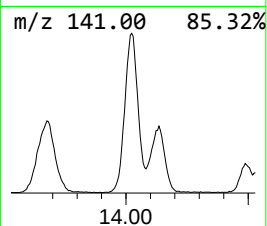
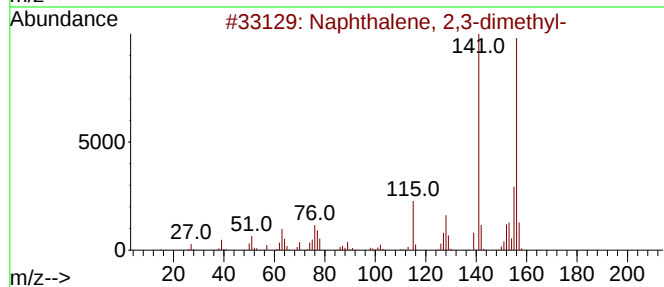
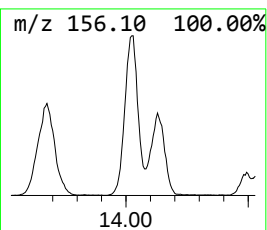
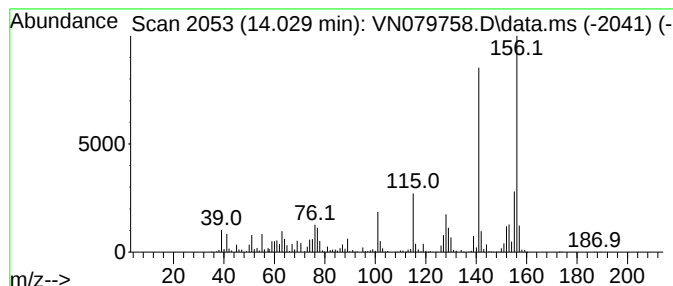
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Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.029	64.29 ug/l	4181300	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
3			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96
4			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	96
5			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN103123\
Data File : VN079758.D
Acq On : 31 Oct 2023 20:55
Operator : JC\MD
Sample : 05107-19
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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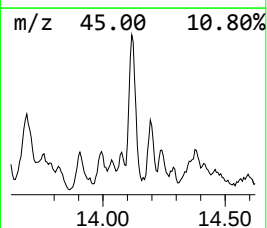
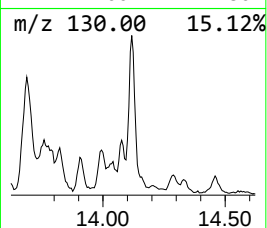
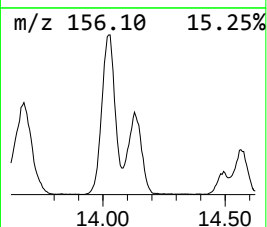
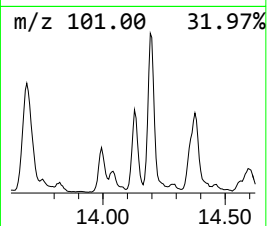
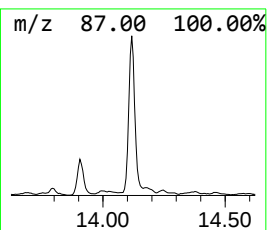
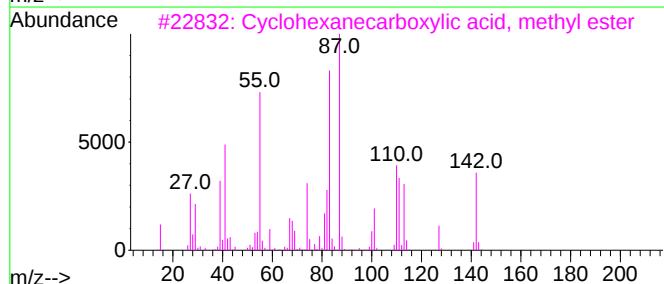
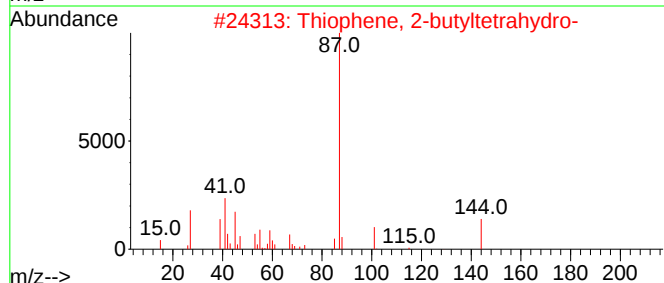
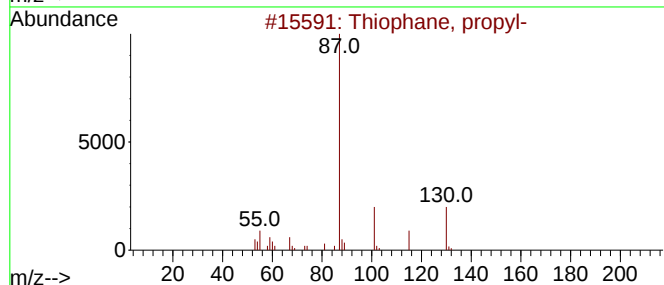
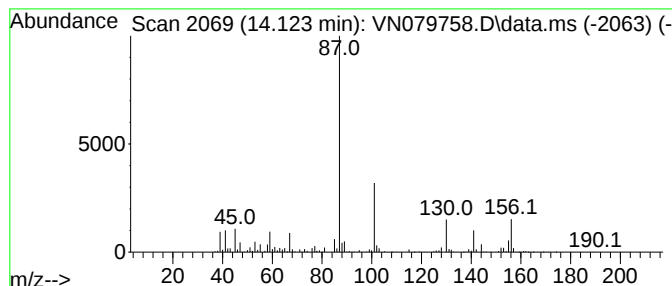
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Quant Title : SW846 8260

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

Peak Number 9 Thiophane, propyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.123	49.82 ug/l	3240290	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophane, propyl-	130	C7H14S	001551-34-4	58
2			Thiophene, 2-butyltetrahydro-	144	C8H16S	001613-49-6	50
3			Cyclohexanecarboxylic acid, meth...	142	C8H14O2	004630-82-4	47
4			Tetrahydrothiophene-2-carboxylic...	146	C6H10O2S	113990-87-7	47
5			Tetrahydrothiophene-2-carboxylic...	132	C5H8O2S	019418-11-2	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN103123\
Data File : VN079758.D
Acq On : 31 Oct 2023 20:55
Operator : JC\MD
Sample : 05107-19
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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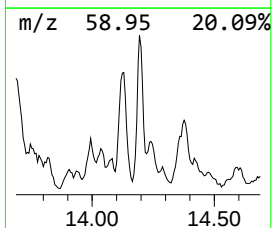
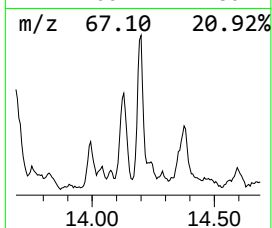
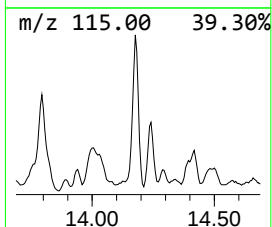
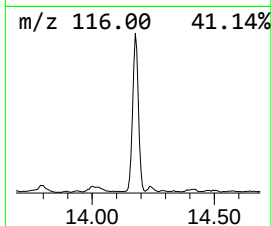
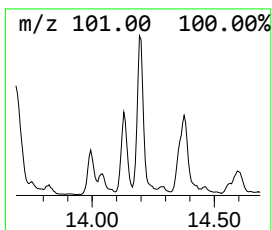
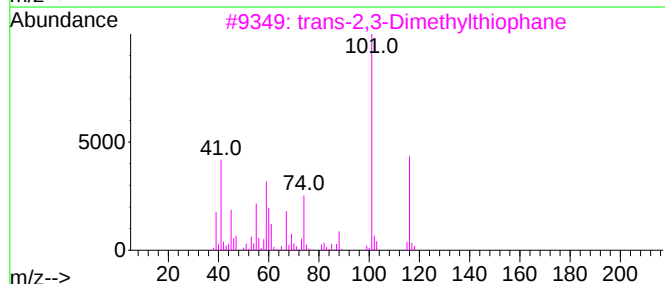
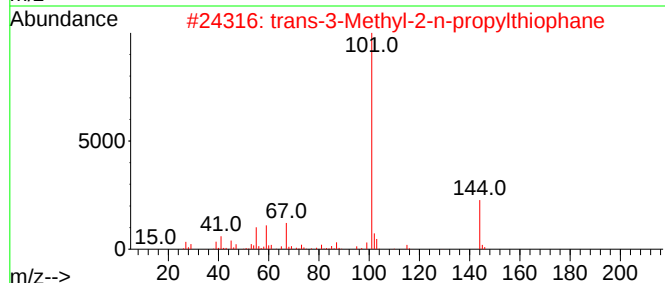
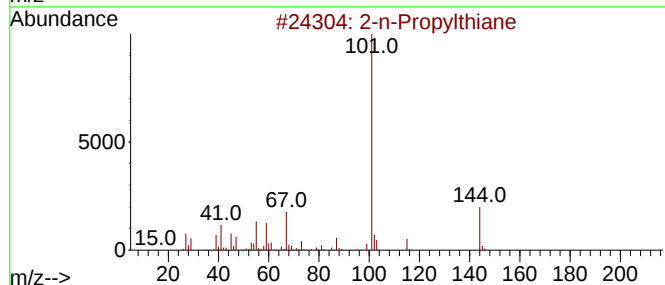
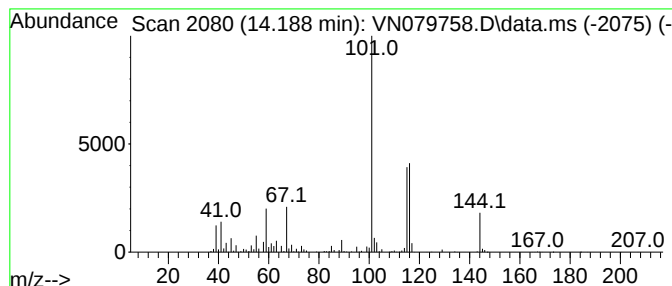
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Quant Title : SW846 8260

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

Peak Number 10 unknown14.188 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.188	34.51 ug/l	2244190	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-n-Propylthiane	144	C8H16S	017912-23-1	49
2			trans-3-Methyl-2-n-propylthiophane	144	C8H16S	118068-75-0	43
3			trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	40
4			Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-13-7	40
5			Thiazole, 4,5-dihydro-4-methyl-2...	116	C4H8N2S	010416-81-6	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN103123\
Data File : VN079758.D
Acq On : 31 Oct 2023 20:55
Operator : JC\MD
Sample : 05107-19
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 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\NIST0.L
TIC Integration Parameters: LSCINT.P

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					#	RT	Resp	Conc
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Thiophene, tetr...	11.353	1403.7	ug/l	50504100	3	11.871	1798910	50.0
Thiophene, tetr...	12.212	245.8	ug/l	8842740	3	11.871	1798910	50.0
cis-2,3-Dimethy...	12.576	68.2	ug/l	2453900	3	11.871	1798910	50.0
trans-2,3-Dimet...	12.641	136.1	ug/l	4895330	3	11.871	1798910	50.0
cis-2-Ethyl-3-m...	13.423	35.6	ug/l	2313390	4	13.794	3251810	50.0
trans-3-Methyl-...	13.688	45.0	ug/l	2930200	4	13.794	3251810	50.0
Naphthalene, 2,...	14.029	64.3	ug/l	4181300	4	13.794	3251810	50.0
Thiophane, propyl-	14.123	49.8	ug/l	3240290	4	13.794	3251810	50.0
unknown14.188	14.188	34.5	ug/l	2244190	4	13.794	3251810	50.0