

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN103123\
 Data File : VN079745.D
 Acq On : 31 Oct 2023 15:43
 Operator : JC\MD
 Sample : 05107-17
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 1072

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: VN079745.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.447	414	424	430	rBV2	15995	47947	1.30%	0.211%
2	8.171	1045	1057	1062	rBV2	272143	674261	18.34%	2.963%
3	8.229	1062	1067	1079	rVB	376744	820000	22.31%	3.603%
4	8.582	1117	1127	1150	rBV2	293287	902963	24.56%	3.968%
5	8.841	1163	1171	1182	rVB3	13918	36845	1.00%	0.162%
6	9.106	1206	1216	1229	rBV	609980	1247114	33.92%	5.480%
7	10.571	1455	1465	1472	rBV	899916	1666667	45.34%	7.323%
8	10.635	1472	1476	1483	rVB	56954	102929	2.80%	0.452%
9	10.888	1511	1519	1530	rBV	75791	145615	3.96%	0.640%
10	11.276	1576	1585	1590	rBV4	41699	100814	2.74%	0.443%
11	11.353	1590	1598	1617	rVB	1953540	3676200	100.00%	16.153%
12	11.870	1677	1686	1689	rBV	939959	1669718	45.42%	7.337%
13	11.912	1689	1693	1709	rVV	1042458	1931712	52.55%	8.488%
14	12.070	1709	1720	1730	rVB	156377	325515	8.85%	1.430%
15	12.212	1737	1744	1756	rBV2	349374	722838	19.66%	3.176%
16	12.312	1756	1761	1764	rVV3	43538	75889	2.06%	0.333%
17	12.353	1764	1768	1772	rVV	144851	267053	7.26%	1.173%
18	12.400	1772	1776	1785	rVB	276219	473958	12.89%	2.083%
19	12.576	1797	1806	1812	rBV2	123433	241681	6.57%	1.062%
20	12.647	1812	1818	1822	rVV2	195896	400446	10.89%	1.760%
21	12.694	1822	1826	1838	rVB	209766	387771	10.55%	1.704%
22	12.853	1846	1853	1859	rBV	754377	1317932	35.85%	5.791%
23	12.900	1859	1861	1866	rVB3	45371	52349	1.42%	0.230%
24	12.982	1870	1875	1879	rBV7	32578	66761	1.82%	0.293%
25	13.017	1879	1881	1887	rVB3	37374	52523	1.43%	0.231%
26	13.082	1887	1892	1895	rBV2	73181	138277	3.76%	0.608%
27	13.129	1895	1900	1906	rVB	490123	835528	22.73%	3.671%
28	13.223	1912	1916	1920	rBV3	27009	40823	1.11%	0.179%
29	13.347	1930	1937	1938	rBV	37508	61929	1.68%	0.272%
30	13.423	1944	1950	1953	rBV	124023	225597	6.14%	0.991%
31	13.470	1953	1958	1971	rVB2	435495	990830	26.95%	4.354%
32	13.612	1979	1982	1987	rVB4	26677	41302	1.12%	0.181%
33	13.688	1987	1995	2002	rBV4	80435	250480	6.81%	1.101%
34	13.794	2007	2013	2025	rVB2	829467	1702025	46.30%	7.479%
35	13.906	2027	2032	2036	rBV	22997	45191	1.23%	0.199%
36	13.994	2042	2047	2053	rBV3	68702	161907	4.40%	0.711%

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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

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Title : SW846 8260

37	14.123	2064	2069	2075	rVB2	108743	205074	5.58%	0.901%
38	14.194	2075	2081	2086	rBV	98741	170121	4.63%	0.748%
39	14.241	2086	2089	2094	rVB5	32246	50564	1.38%	0.222%
40	14.582	2138	2147	2154	rVB9	26440	68610	1.87%	0.301%
41	14.764	2176	2178	2186	rVB5	27955	46197	1.26%	0.203%
42	15.041	2217	2225	2235	rVB4	65094	185947	5.06%	0.817%
43	15.211	2248	2254	2257	rBV4	22305	47009	1.28%	0.207%
44	15.605	2314	2321	2327	rBV4	38035	83154	2.26%	0.365%

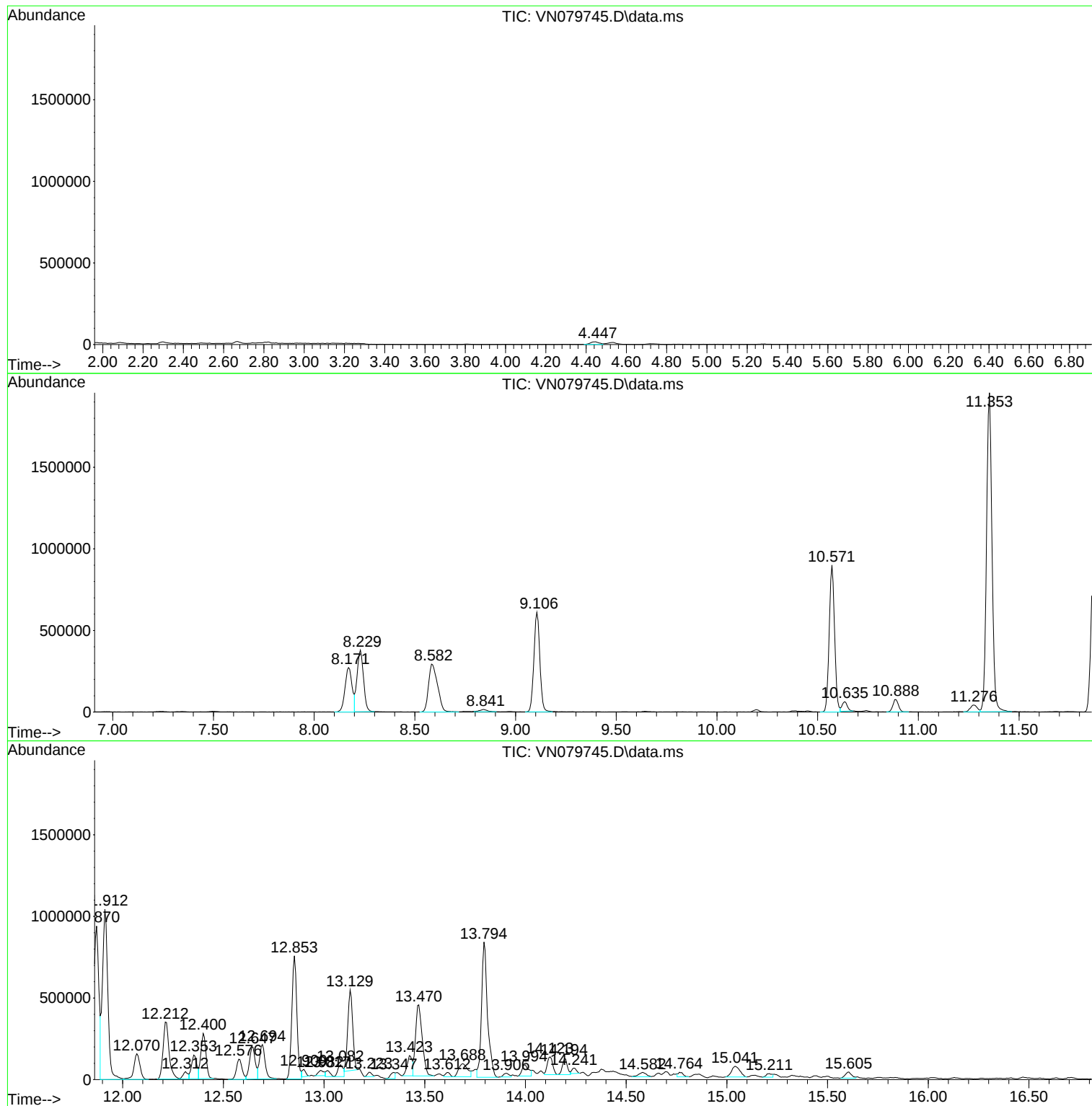
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103023W.M
Quant Title : SW846 8260

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



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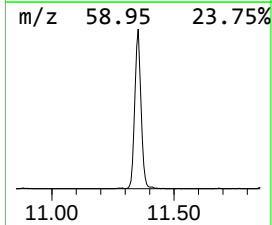
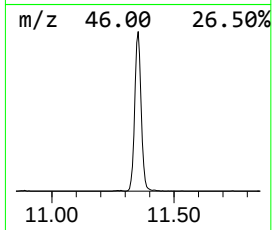
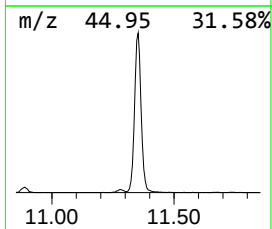
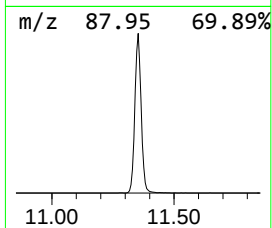
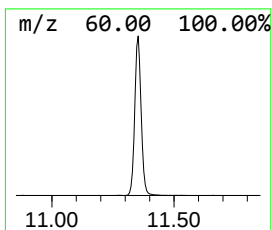
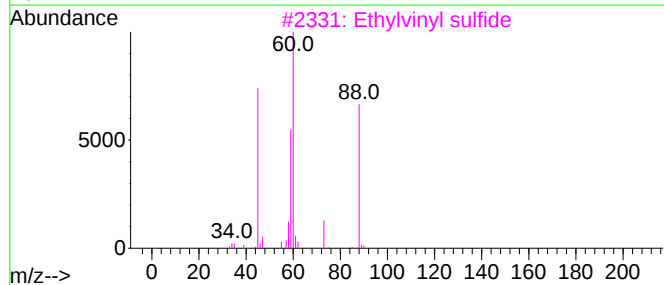
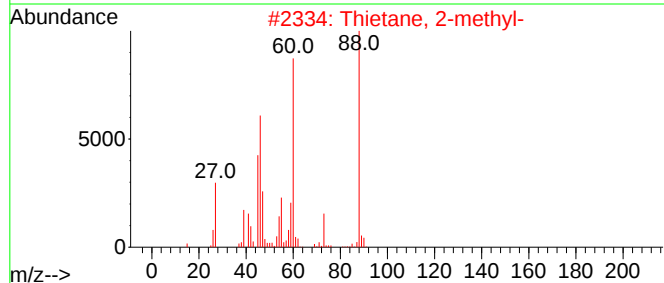
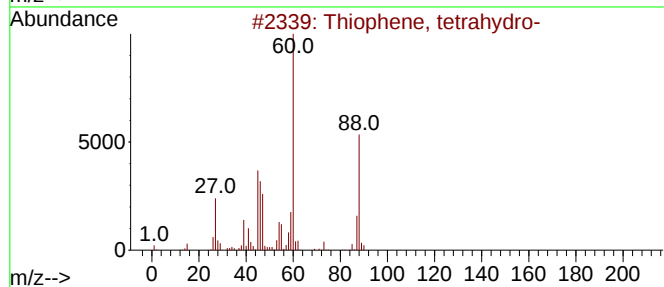
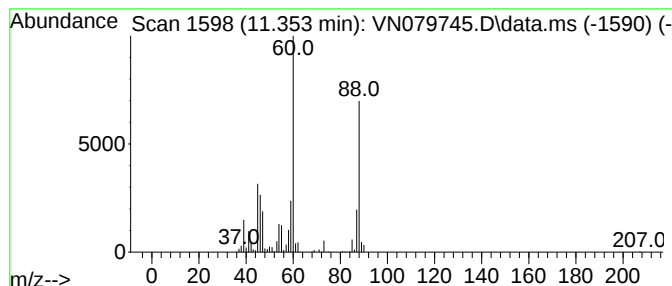
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103023W.M
Quant Title : SW846 8260

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

Peak Number 1 Thiophene, tetrahydro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.353	110.08 ug/l	3676200	Chlorobenzene-d5	11.870

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	64
3			Ethylvinyl sulfide	88	C4H8S	000627-50-9	40
4			1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	33
5			4-Bromobutyric acid	166	C4H7BrO2	002623-87-2	23



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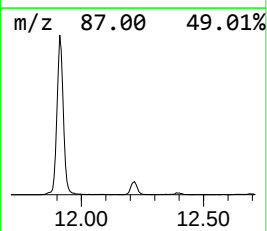
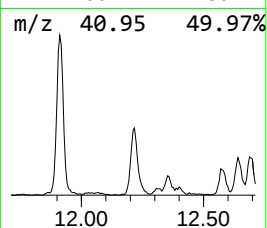
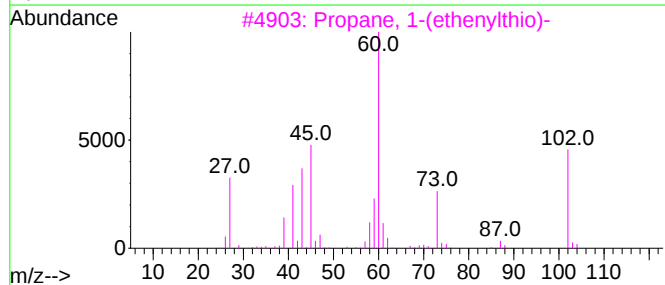
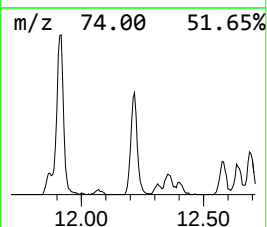
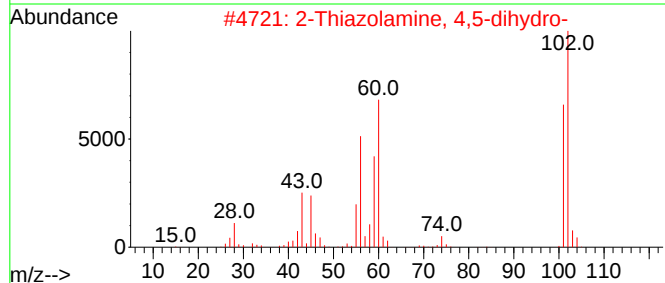
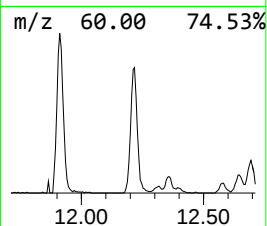
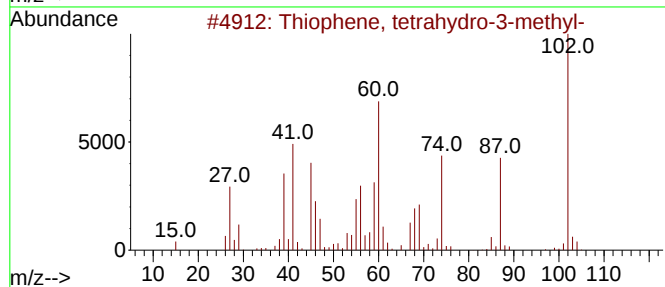
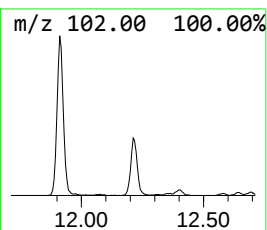
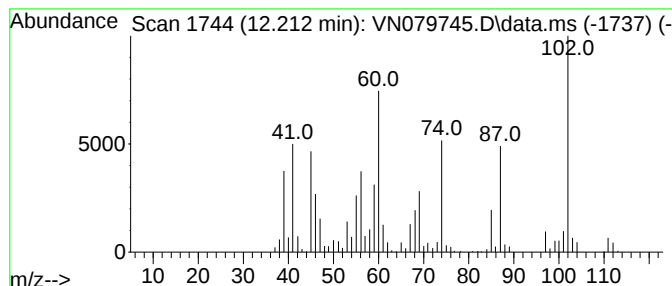
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.212	21.65 ug/l	722838	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	46
3	Propane, 1-(ethenylthio)-	102	C5H10S	016330-21-5	37
4	2-Methyl-3-(methylthio)-1-propene	102	C5H10S	052326-10-0	35
5	Butanoic acid, 2,2-dimethyl-3-ox...	144	C7H12O3	038923-57-8	27



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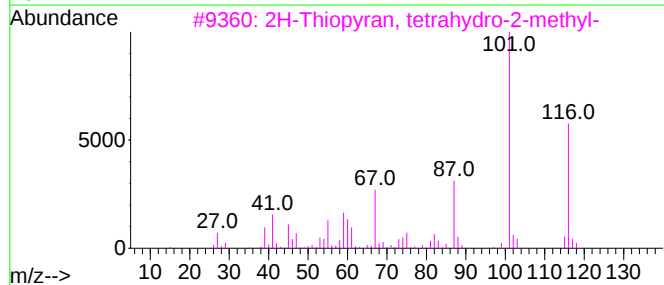
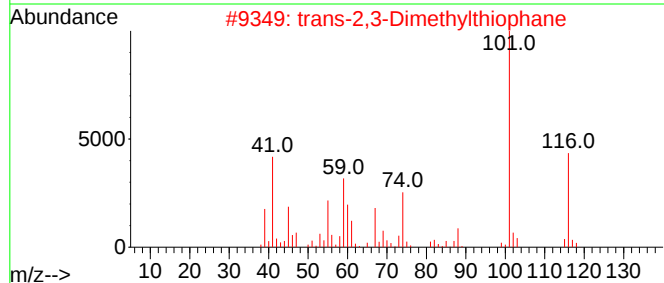
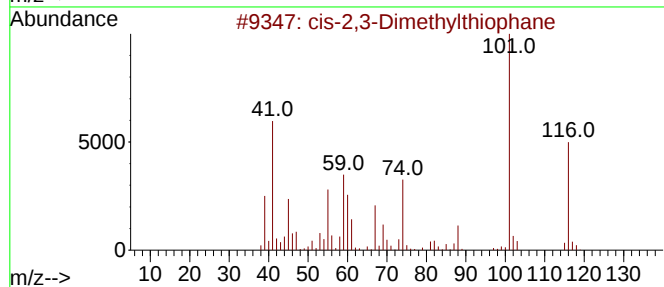
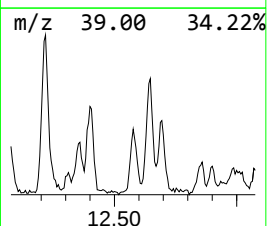
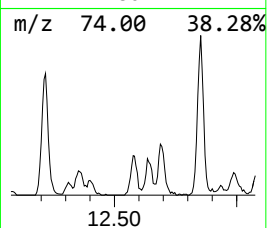
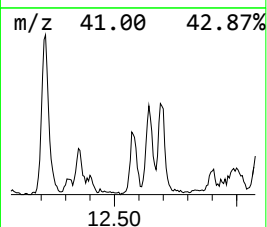
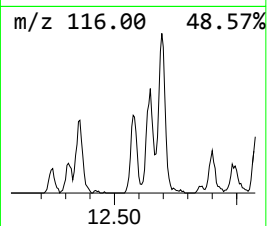
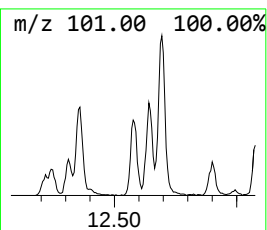
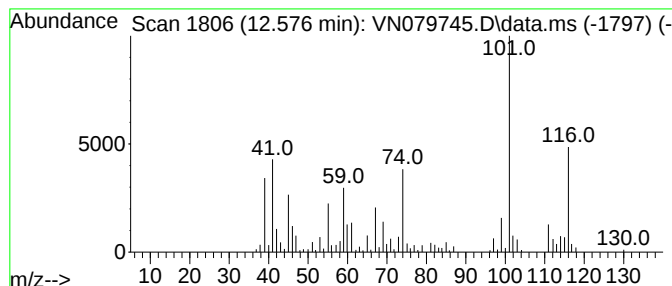
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.576	7.24 ug/l	241681	Chlorobenzene-d5	11.870

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	62
3			2H-Thiopyran, tetrahydro-2-methyl-	116	C6H12S	005161-16-0	58
4			Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-14-8	53
5			Thiazole, 4,5-dihydro-4-methyl-2...	116	C4H8N2S	010416-81-6	52



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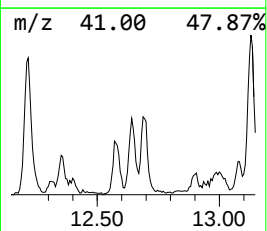
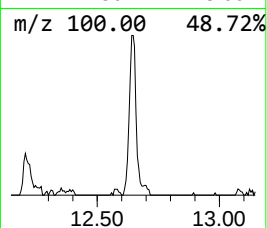
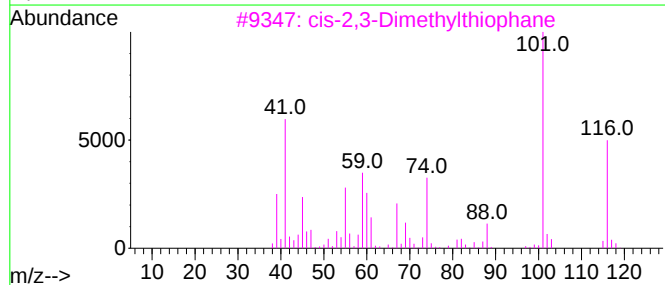
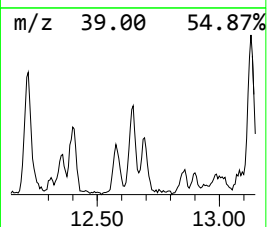
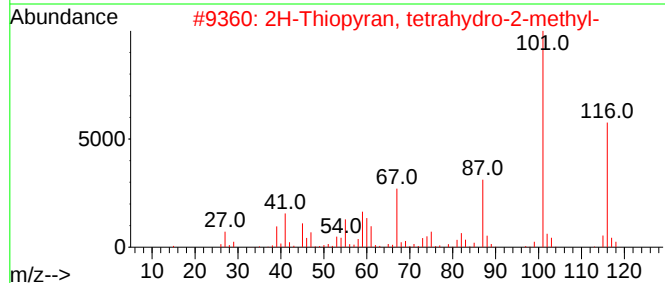
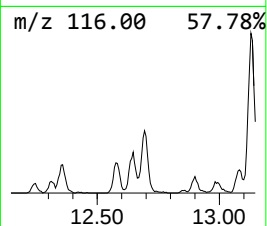
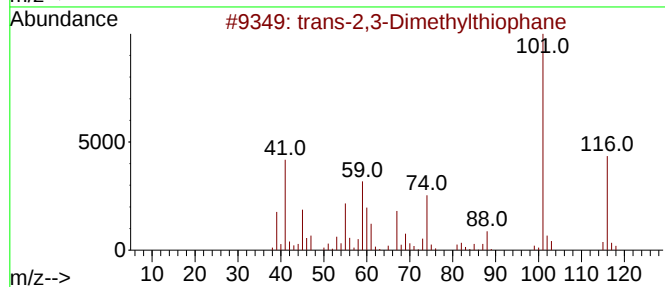
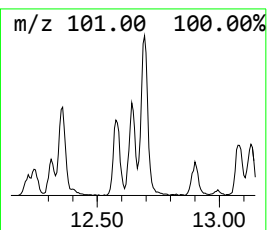
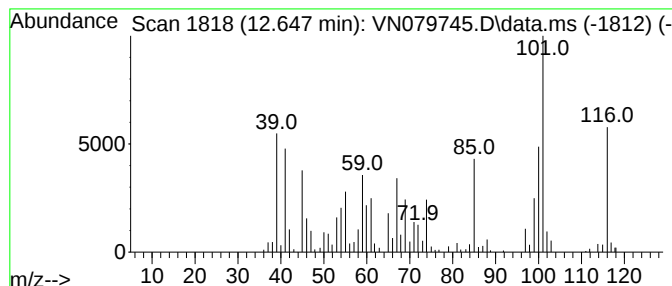
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.647	11.99 ug/l	400446	Chlorobenzene-d5	11.870	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	92
2	2H-Thiopyran, tetrahydro-2-methyl-	116	C6H12S	005161-16-0	60
3	cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	49
4	Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-13-7	43
5	Thiazole, 4,5-dihydro-4-methyl-2...	116	C4H8N2S	010416-81-6	43



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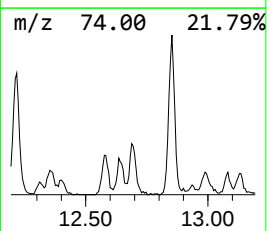
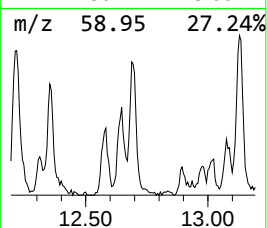
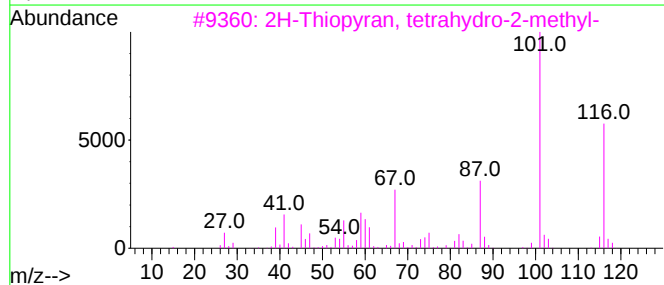
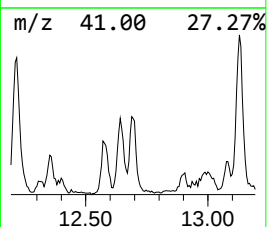
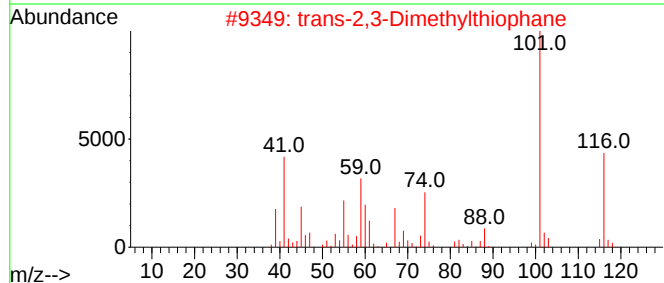
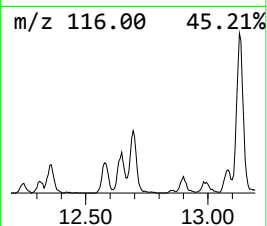
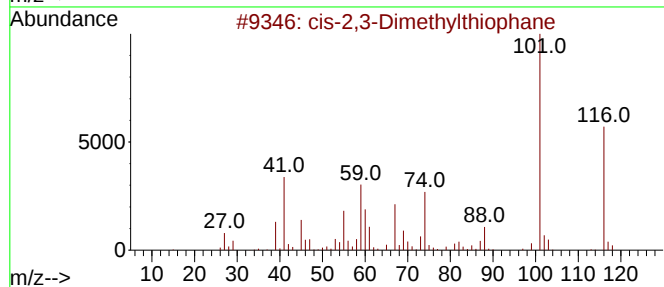
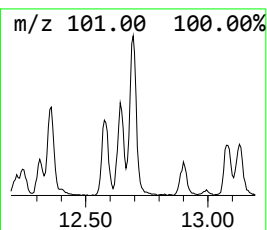
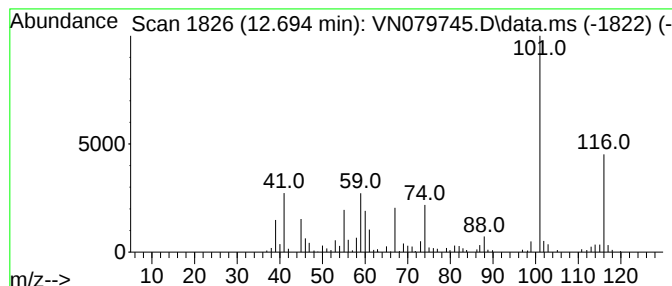
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Quant Title : SW846 8260

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

Peak Number 5 2H-Thiopyran, tetrahydro-2-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.694	11.61 ug/l	387771	Chlorobenzene-d5	11.870

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	97
2			trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	94
3			2H-Thiopyran, tetrahydro-2-methyl-	116	C6H12S	005161-16-0	68
4			Thiazole, 4,5-dihydro-4-methyl-2...	116	C4H8N2S	010416-81-6	58
5			Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-13-7	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN103123\
Data File : VN079745.D
Acq On : 31 Oct 2023 15:43
Operator : JC\MD
Sample : 05107-17
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1072

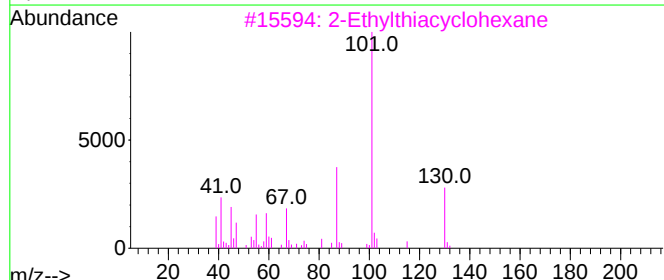
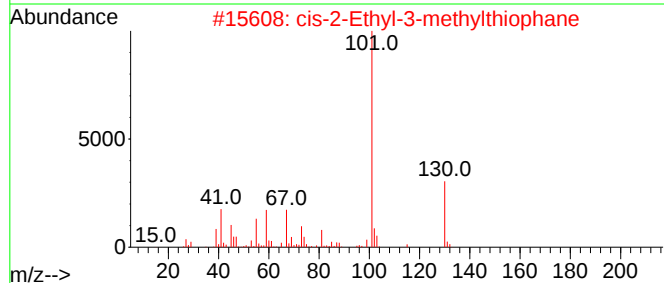
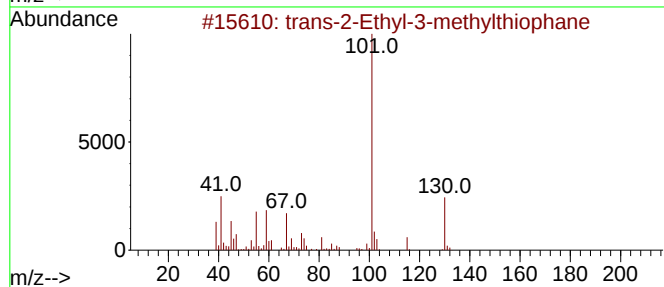
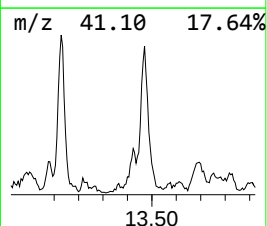
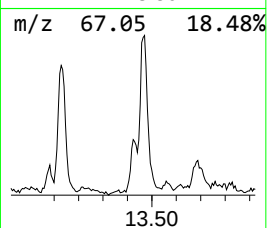
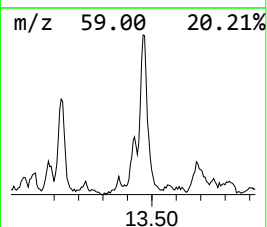
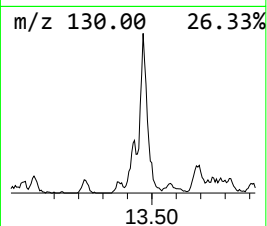
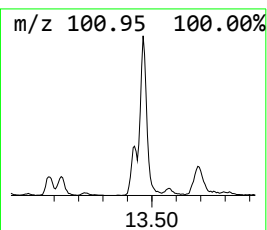
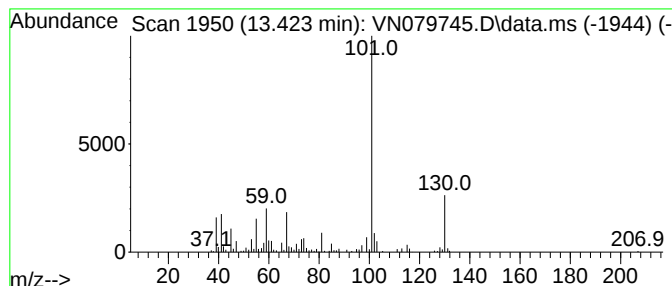
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.423	6.63 ug/l	225597	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	90
2			cis-2-Ethyl-3-methylthiophane	130	C7H14S	061568-37-4	86
3			2-Ethylthiacyclohexane	130	C7H14S	001613-52-1	83
4			cis-3-Methyl-2-n-propylthiophane	144	C8H16S	118068-76-1	59
5			Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN103123\
Data File : VN079745.D
Acq On : 31 Oct 2023 15:43
Operator : JC\MD
Sample : 05107-17
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1072

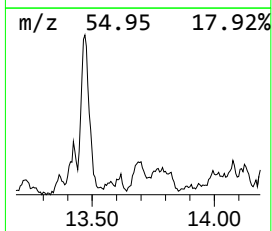
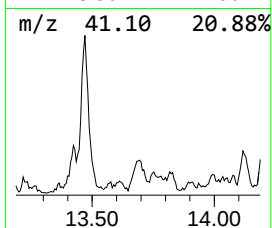
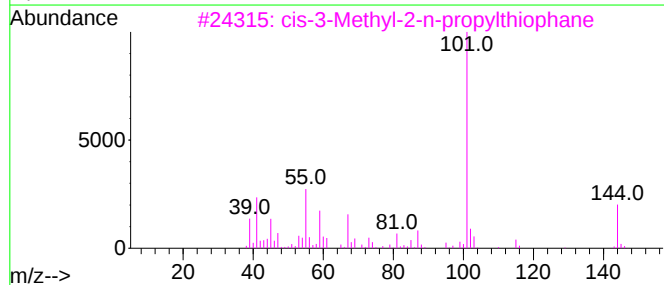
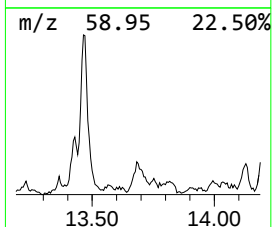
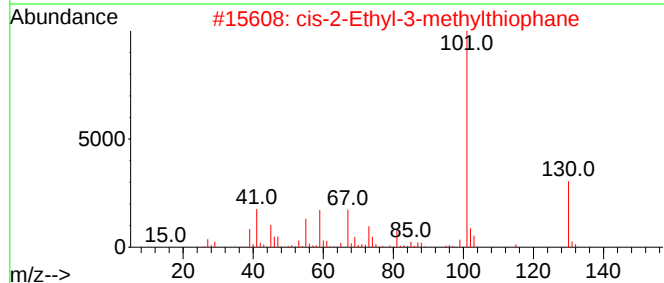
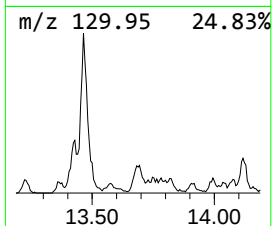
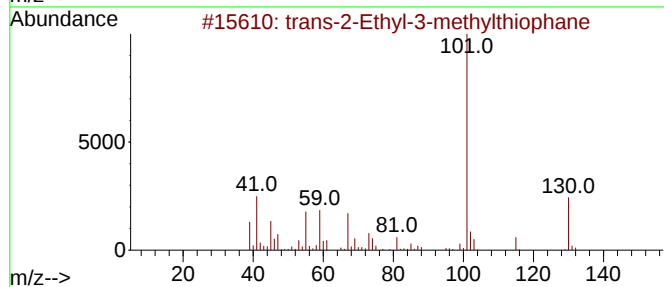
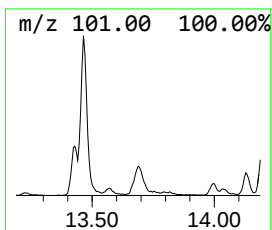
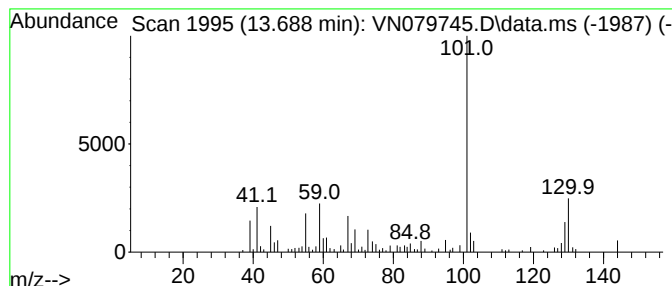
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Quant Title : SW846 8260

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

Peak Number 7 cis-2-Ethyl-3-methylthiophane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.688	7.36 ug/l	250480	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	94
2			cis-2-Ethyl-3-methylthiophane	130	C7H14S	061568-37-4	93
3			cis-3-Methyl-2-n-propylthiophane	144	C8H16S	118068-76-1	70
4			trans-3-Methyl-2-n-propylthiophane	144	C8H16S	118068-75-0	64
5			2-Ethylthiacyclohexane	130	C7H14S	001613-52-1	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN103123\
Data File : VN079745.D
Acq On : 31 Oct 2023 15:43
Operator : JC\MD
Sample : 05107-17
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1072

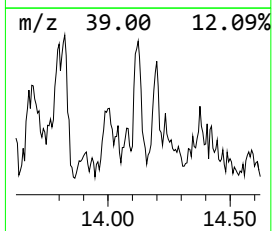
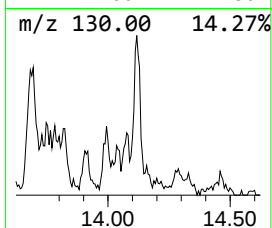
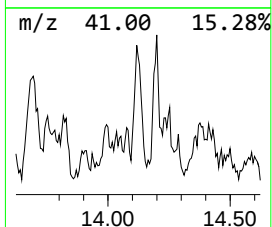
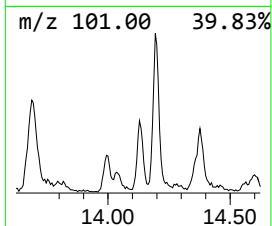
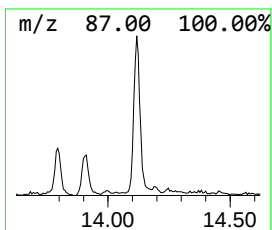
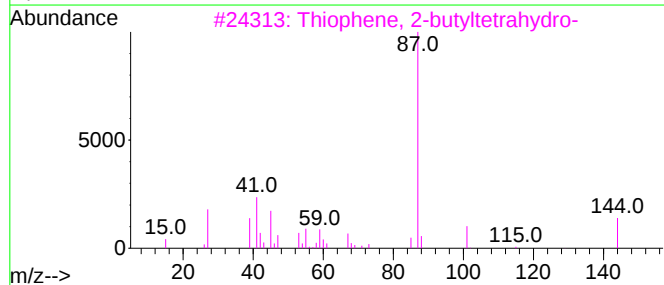
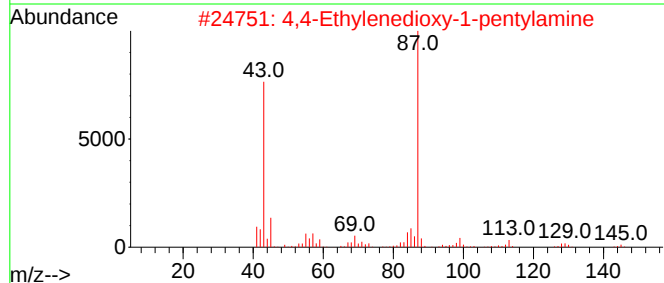
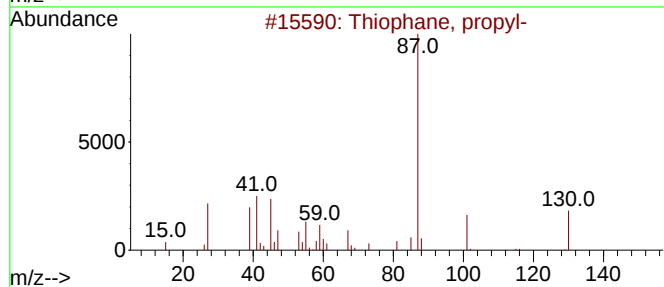
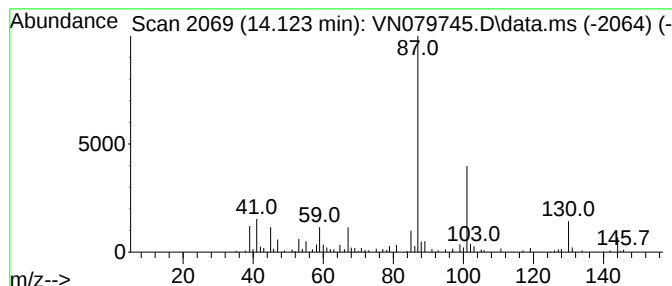
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Quant Title : SW846 8260

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

Peak Number 8 Thiophane, propyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.123	6.02 ug/l	205074	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophane, propyl-	130	C7H14S	001551-34-4	70
2			4,4-Ethylenedioxy-1-pentylamine	145	C7H15NO2	066442-97-5	43
3			Thiophene, 2-butyltetrahydro-	144	C8H16S	001613-49-6	43
4			Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	38
5			1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN103123\
Data File : VN079745.D
Acq On : 31 Oct 2023 15:43
Operator : JC\MD
Sample : 05107-17
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1072

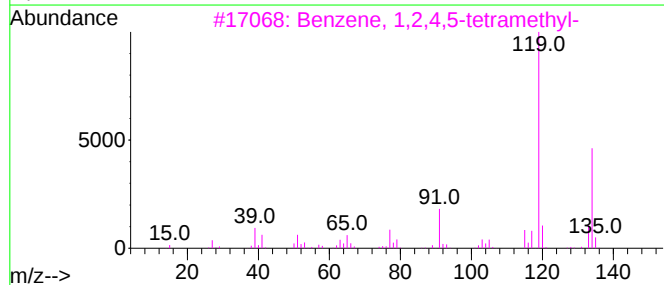
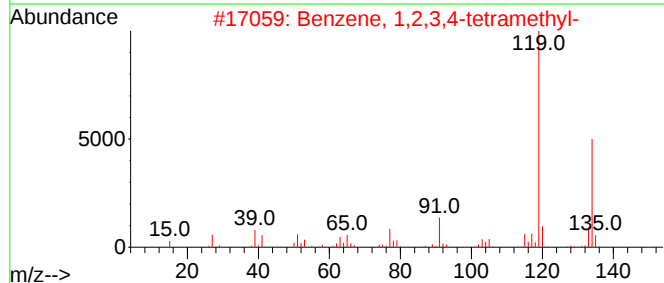
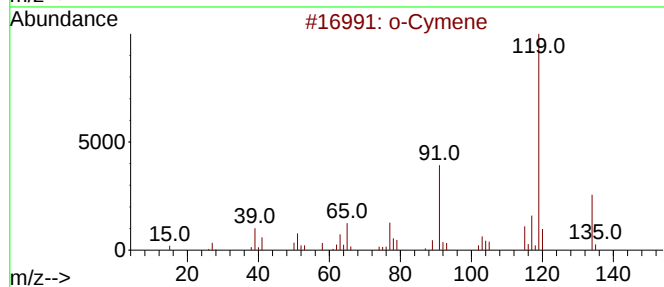
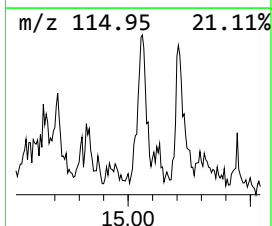
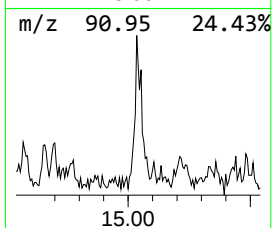
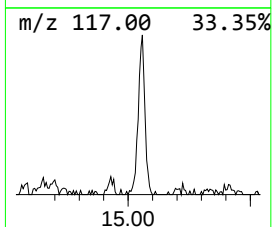
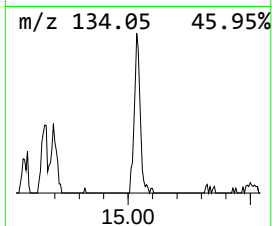
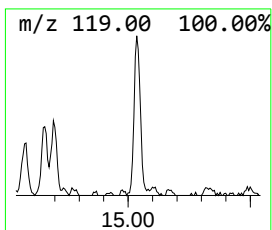
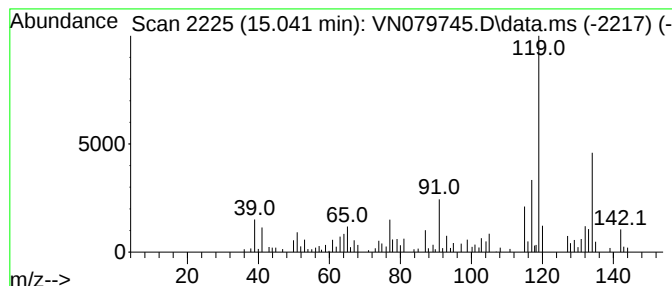
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Quant Title : SW846 8260

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

Peak Number 9 o-Cymene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.041	5.46 ug/l	185947	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	70
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	70
3			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	70
4			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	64
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN103123\
Data File : VN079745.D
Acq On : 31 Oct 2023 15:43
Operator : JC\MD
Sample : 05107-17
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1072

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...	12.212	21.6	ug/l	722838	3	11.870	1669720	50.0
cis-2,3-Dimethy...	12.576	7.2	ug/l	241681	3	11.870	1669720	50.0
trans-2,3-Dimet...	12.647	12.0	ug/l	400446	3	11.870	1669720	50.0
2H-Thiopyran, t...	12.694	11.6	ug/l	387771	3	11.870	1669720	50.0
trans-2-Ethyl-3...	13.423	6.6	ug/l	225597	4	13.794	1702030	50.0
cis-2-Ethyl-3-m...	13.688	7.4	ug/l	250480	4	13.794	1702030	50.0
Thiophane, propyl-	14.123	6.0	ug/l	205074	4	13.794	1702030	50.0
o-Cymene	15.041	5.5	ug/l	185947	4	13.794	1702030	50.0