

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081721\
 Data File : VN068154.D
 Acq On : 17 Aug 2021 19:45
 Operator : JC/MD
 Sample : M3361-18 20X
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 41949

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\82N081721W.M
 Title : SW846 8260

Signal : TIC: VN068154.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	76	89	106	rBV	73232	109550	5.18%	0.756%
2	2.738	265	279	280	rBV4	19614	26564	1.26%	0.183%
3	3.693	621	635	652	rBV	29214	76232	3.60%	0.526%
4	8.024	2227	2250	2261	rBV2	282619	684850	32.36%	4.728%
5	8.088	2262	2274	2300	rVB	499499	1124414	53.13%	7.762%
6	8.440	2386	2405	2434	rBV3	290160	733533	34.66%	5.064%
7	8.971	2584	2603	2631	rBV	715787	1477252	69.80%	10.197%
8	10.446	3134	3153	3168	rBV	1124818	2116310	100.00%	14.609%
9	10.508	3168	3176	3196	rVB	71974	136694	6.46%	0.944%
10	10.762	3258	3271	3285	rBV	15214	26828	1.27%	0.185%
11	11.226	3426	3444	3462	rBV3	472317	895664	42.32%	6.183%
12	11.747	3621	3638	3648	rBV	1107465	1994115	94.23%	13.765%
13	11.950	3706	3714	3732	rVB	36314	69488	3.28%	0.480%
14	12.093	3739	3767	3792	rBV4	120270	264730	12.51%	1.827%
15	12.192	3792	3804	3810	rVV6	14946	25764	1.22%	0.178%
16	12.235	3811	3820	3829	rVV4	40514	74402	3.52%	0.514%
17	12.280	3830	3837	3855	rVB5	31552	61077	2.89%	0.422%
18	12.457	3890	3903	3915	rBV3	39006	70924	3.35%	0.490%
19	12.524	3915	3928	3937	rVV4	53135	100668	4.76%	0.695%
20	12.573	3937	3946	3963	rVB5	61674	112812	5.33%	0.779%
21	12.734	3989	4006	4033	rBV	876550	1560619	73.74%	10.773%
22	12.959	4081	4090	4096	rBV4	16979	26159	1.24%	0.181%
23	13.010	4097	4109	4123	rVB2	127792	226706	10.71%	1.565%
24	13.307	4206	4220	4226	rBV5	34213	58854	2.78%	0.406%
25	13.350	4226	4236	4267	rVB6	92144	240208	11.35%	1.658%
26	13.678	4342	4358	4380	rVB	999487	1753892	82.88%	12.107%
27	13.881	4421	4434	4442	rBV7	12838	24126	1.14%	0.167%
28	14.005	4469	4480	4492	rVB5	18261	32168	1.52%	0.222%
29	14.075	4492	4506	4517	rBV5	14314	28544	1.35%	0.197%
30	15.509	5022	5041	5057	rVB	168133	326263	15.42%	2.252%
31	16.622	5442	5456	5471	rVB3	13221	27078	1.28%	0.187%

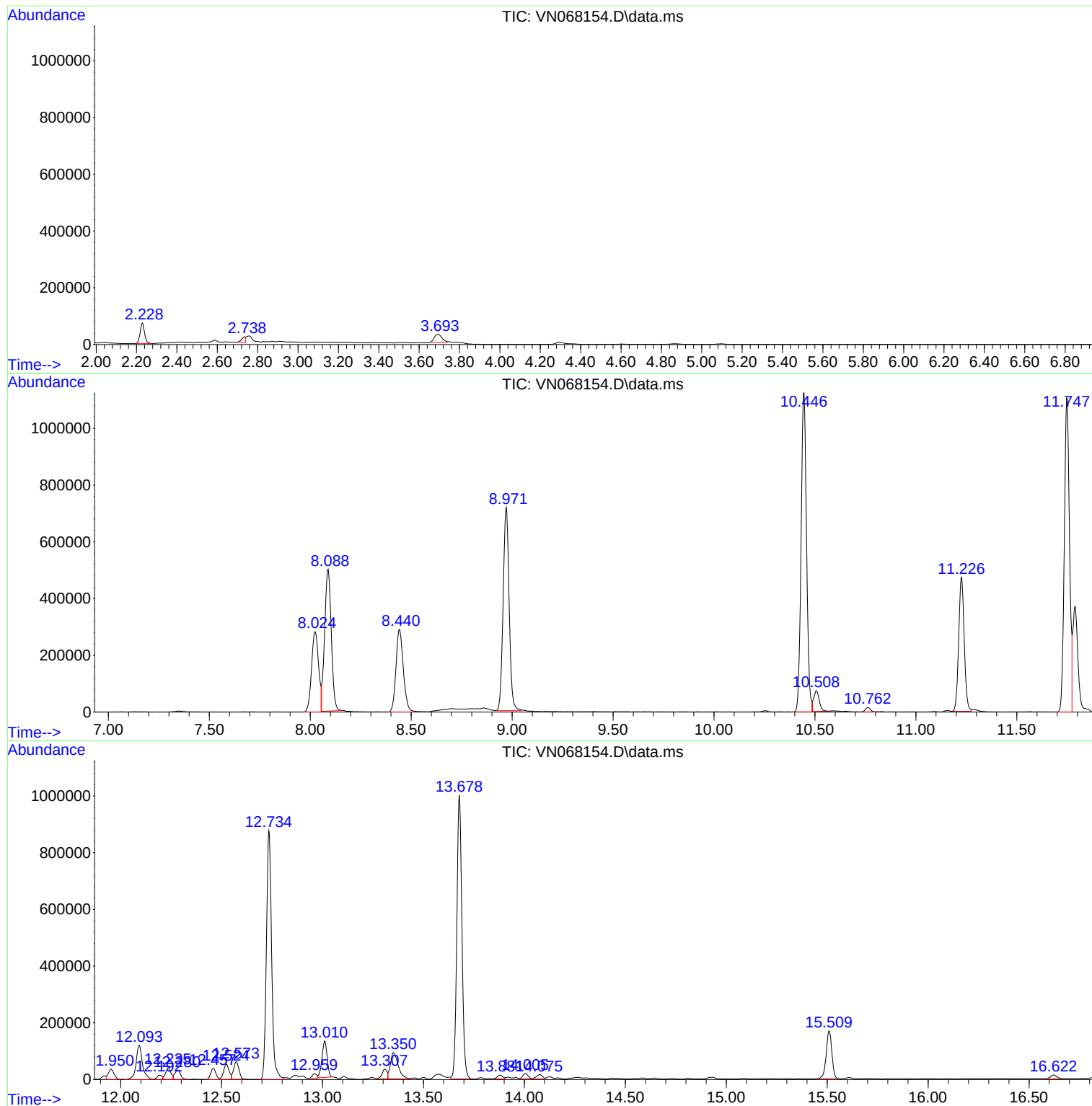
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081721W.M
Quant Title : SW846 8260

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



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Instrument :
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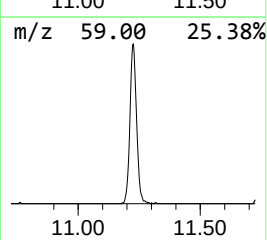
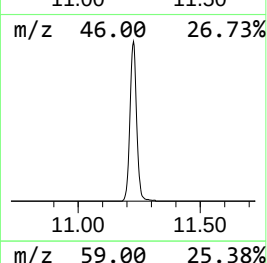
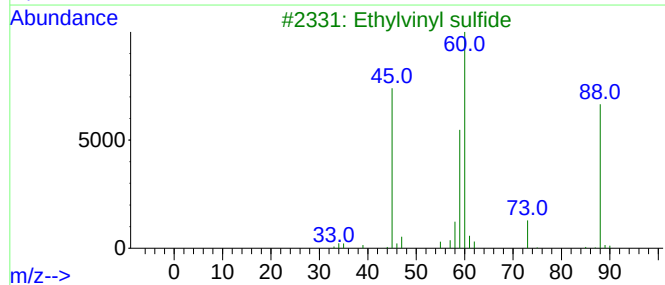
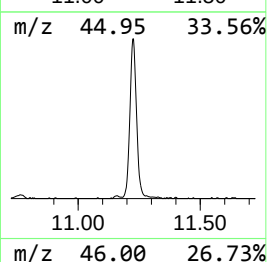
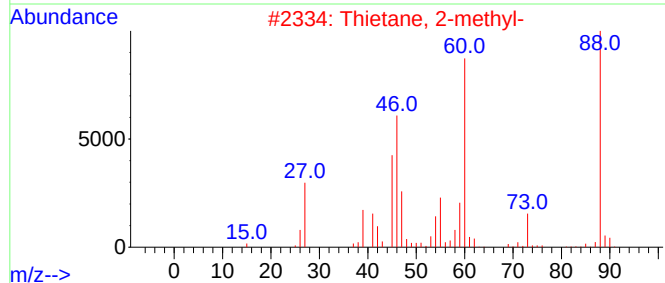
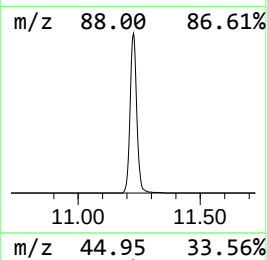
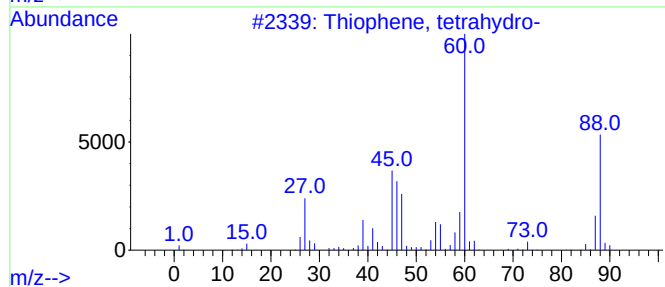
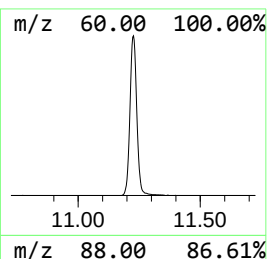
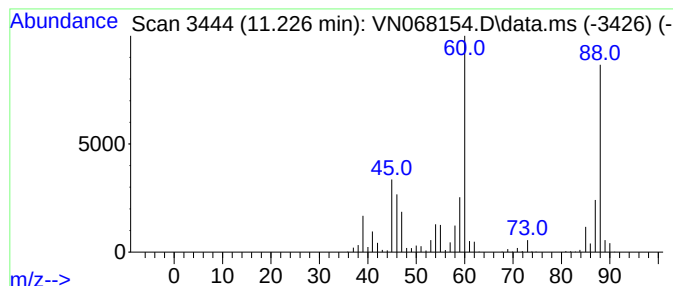
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081721W.M
Quant Title : SW846 8260

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.
11.226	22.46 ug/l	895664	Chlorobenzene-d5	11.747

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			2,2-Dimethylthiirane	88	C4H8S	003772-13-2	38
5			1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	36



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ClientSampled :
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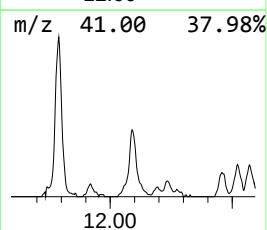
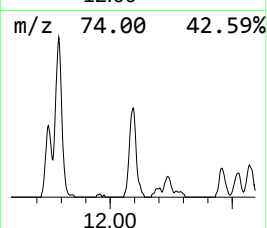
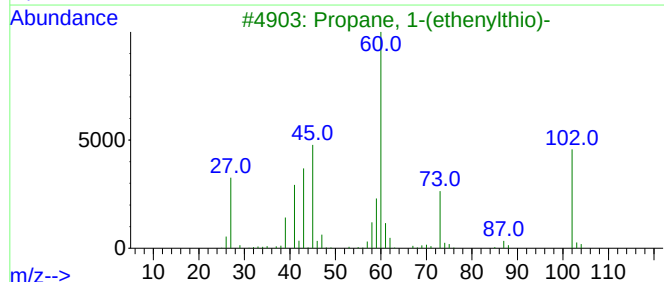
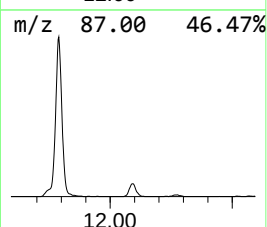
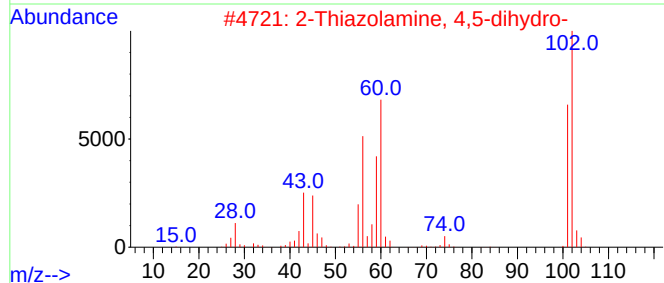
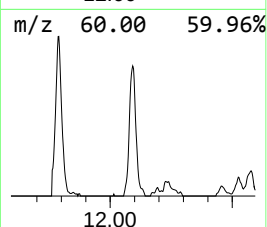
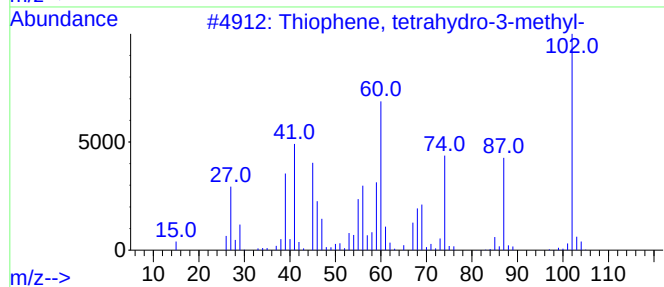
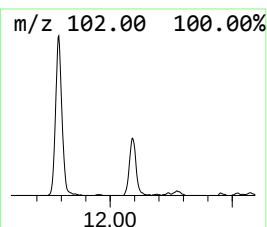
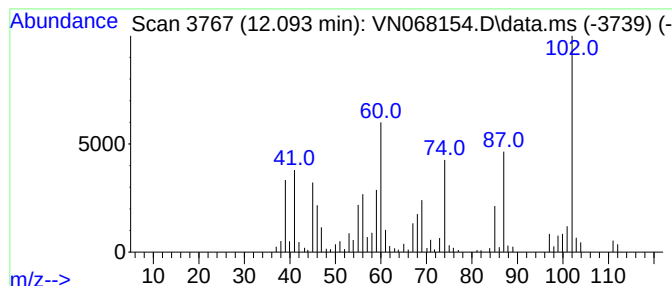
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081721W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.093	6.64 ug/l	264730	Chlorobenzene-d5	11.747

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	49
3			Propane, 1-(ethenylthio)-	102	C5H10S	016330-21-5	38
4			2H-Thiopyran, tetrahydro-	102	C5H10S	001613-51-0	37
5			2-Acetyl-2,3,5,6-tetrahydro-1,4-...	145	C6H11NOS	1000281-47-3	35



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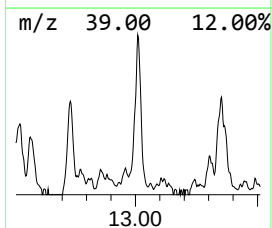
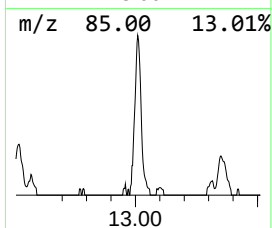
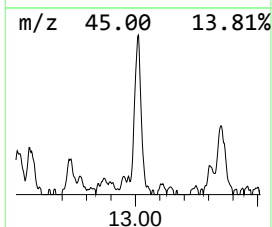
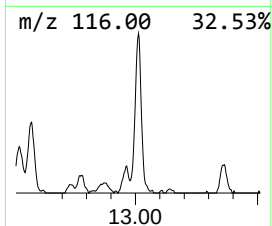
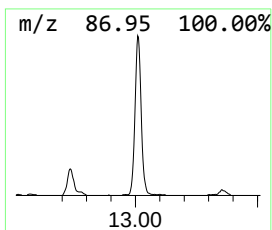
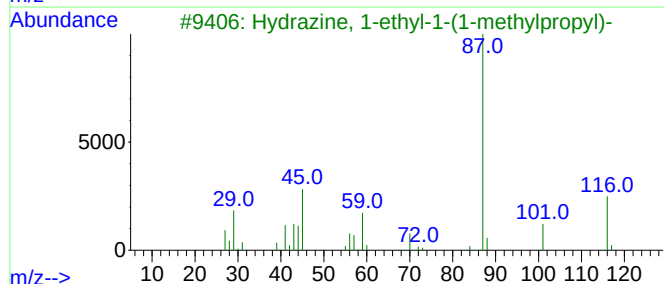
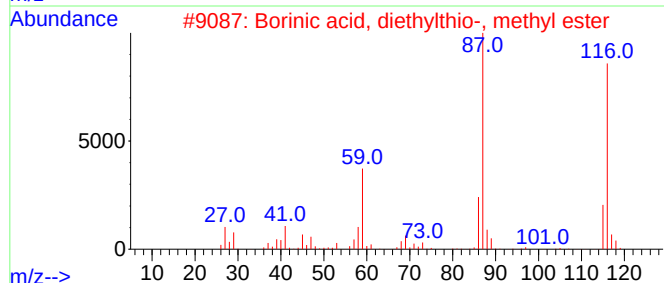
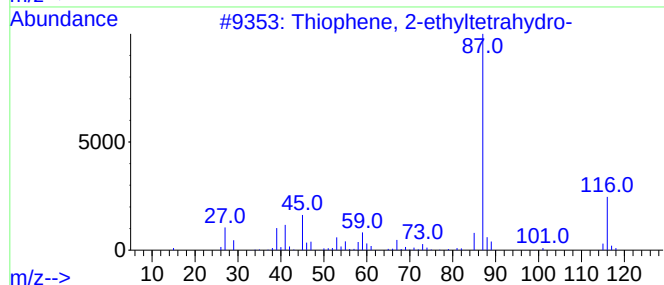
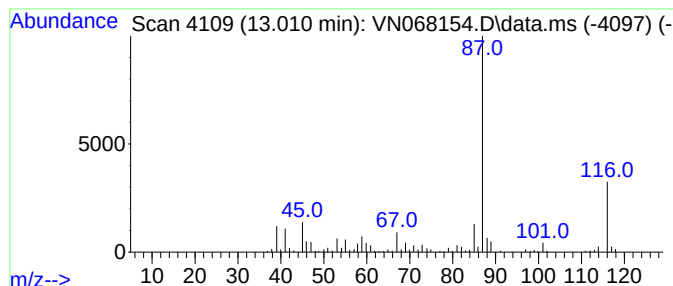
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Quant Title : SW846 8260

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

Peak Number 3 Thiophene, 2-ethyltetrahydro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.010	6.46 ug/l	226706	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	91
2			Borinic acid, diethylthio-, meth...	116	C5H13BS	092276-84-1	64
3			Hydrazine, 1-ethyl-1-(1-methylpr...	116	C6H16N2	020325-97-7	59
4			Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	53
5			Thiophene, tetrahydro-2-methyl-	102	C5H10S	001795-09-1	50



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ALS Vial : 23 Sample Multiplier: 1

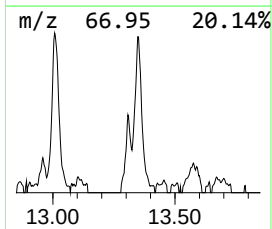
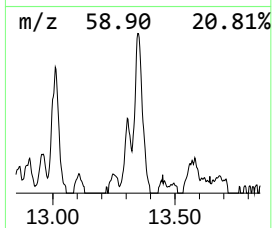
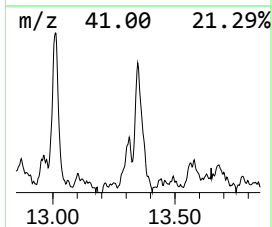
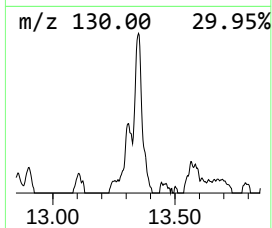
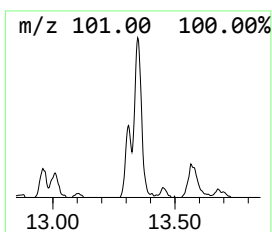
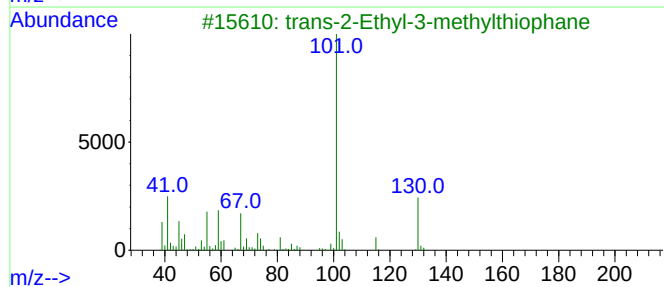
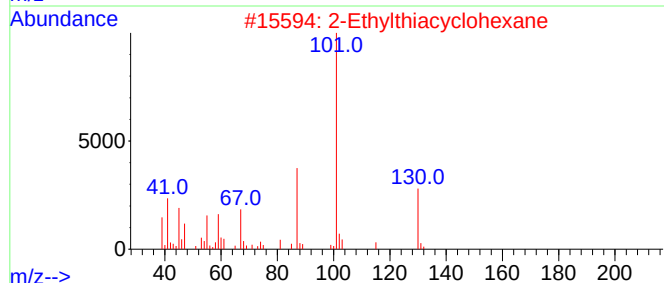
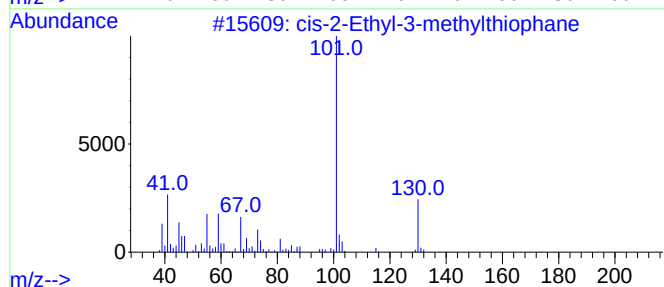
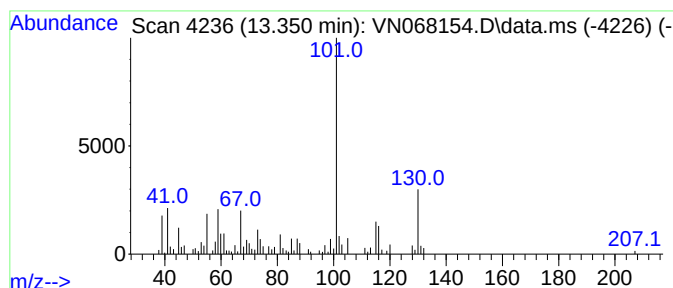
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 cis-2-Ethyl-3-methylthiophane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.350	6.85 ug/l	240208	1,4-Dichlorobenzene-d4		13.678	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	cis-2-Ethyl-3-methylthiophane		130	C7H14S	061568-37-4	87
2	2-Ethylthiacyclohexane		130	C7H14S	001613-52-1	83
3	trans-2-Ethyl-3-methylthiophane		130	C7H14S	061568-36-3	83
4	trans-3-Methyl-2-n-propylthiophane		144	C8H16S	118068-75-0	53
5	3-n-Butylthiane		158	C9H18S	018437-87-1	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Thiophene, tetr...	11.226	22.5	ug/l	895664	3	11.747	1994120	50.0
Thiophene, tetr...	12.093	6.6	ug/l	264730	3	11.747	1994120	50.0
Thiophene, 2-et...	13.010	6.5	ug/l	226706	4	13.678	1753890	50.0
cis-2-Ethyl-3-m...	13.350	6.8	ug/l	240208	4	13.678	1753890	50.0