

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV061120\
 Data File : VV016844.D
 Acq On : 11 Jun 2020 22:24
 Operator : SY/MD
 Sample : L2914-15
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 F9E27

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060820WMA.M
 Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.312	63	69	79	rVB	192157	185376	14.68%	1.710%
2	1.557	139	145	157	rVB	116361	144569	11.45%	1.334%
3	2.116	310	319	333	rBV	270105	391294	30.99%	3.609%
4	2.852	545	548	550	rBV3	2023	1311	0.10%	0.012%
5	2.910	564	566	569	rBV4	1046	620	0.05%	0.006%
6	2.949	574	578	579	rBV4	1465	1155	0.09%	0.011%
7	3.119	629	631	632	rBV2	1134	451	0.04%	0.004%
8	3.151	638	641	643	rBV3	1559	749	0.06%	0.007%
9	3.206	652	658	659	rBV5	1867	1797	0.14%	0.017%
10	3.241	666	669	673	rVB4	1418	951	0.08%	0.009%
11	3.257	673	674	675	rBV	688	166	0.01%	0.002%
12	3.296	684	686	689	rVB4	1350	465	0.04%	0.004%
13	3.344	696	701	702	rBV3	1682	1235	0.10%	0.011%
14	3.376	708	711	716	rBV7	1721	1473	0.12%	0.014%
15	3.421	723	725	727	rBV3	997	500	0.04%	0.005%
16	3.463	736	738	740	rBV3	1325	705	0.06%	0.007%
17	3.524	755	757	758	rBV2	1375	497	0.04%	0.005%
18	3.534	758	760	763	rVV3	1194	871	0.07%	0.008%
19	3.566	767	770	774	rVB5	1076	670	0.05%	0.006%
20	3.585	774	776	778	rVB3	1023	455	0.04%	0.004%
21	3.605	780	782	783	rBV2	1136	416	0.03%	0.004%
22	3.634	789	791	794	rBV3	1063	464	0.04%	0.004%
23	3.698	809	811	814	rVB4	783	367	0.03%	0.003%
24	3.737	821	823	824	rBV2	836	334	0.03%	0.003%
25	3.859	857	861	862	rBV3	2131	1071	0.08%	0.010%
26	3.897	862	873	900	rVV	97651	261232	20.69%	2.410%
27	4.155	951	953	964	rVB9	2609	2882	0.23%	0.027%
28	4.370	999	1020	1044	rBV2	258608	707436	56.03%	6.526%
29	4.627	1097	1100	1103	rBV5	2051	1346	0.11%	0.012%
30	4.749	1136	1138	1140	rBV3	934	498	0.04%	0.005%
31	4.788	1148	1150	1152	rBV3	1400	814	0.06%	0.008%
32	4.827	1160	1162	1163	rBV2	981	326	0.03%	0.003%
33	4.839	1163	1166	1169	rBV4	1801	1205	0.10%	0.011%
34	4.904	1184	1186	1188	rBV3	1658	784	0.06%	0.007%

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35	4.968	1201	1206	1210	rBV6	2171	2801	0.22%	0.026%
36	5.068	1220	1237	1244	rBV2	526404	1262710	100.00%	11.648%
37	5.640	1402	1415	1437	rBV	417453	823422	65.21%	7.596%
38	5.820	1469	1471	1475	rVB4	2122	1340	0.11%	0.012%
39	5.843	1476	1478	1481	rBV4	1096	591	0.05%	0.005%
40	6.042	1538	1540	1543	rBV4	1228	1031	0.08%	0.010%
41	6.093	1543	1556	1577	rVV	295972	604082	47.84%	5.572%
42	6.457	1666	1669	1671	rBV4	1365	1005	0.08%	0.009%
43	6.489	1676	1679	1680	rVV3	1281	811	0.06%	0.007%
44	6.511	1684	1686	1688	rVV2	1184	564	0.04%	0.005%
45	6.537	1691	1694	1697	rVB5	1965	1053	0.08%	0.010%
46	6.640	1722	1726	1729	rBV6	1782	1428	0.11%	0.013%
47	6.753	1759	1761	1764	rBV2	1787	1173	0.09%	0.011%
48	6.798	1773	1775	1776	rBV2	1149	486	0.04%	0.004%
49	6.852	1790	1792	1793	rBB2	684	137	0.01%	0.001%
50	6.917	1811	1812	1815	rVB3	1699	608	0.05%	0.006%
51	6.962	1822	1826	1827	rBV3	758	549	0.04%	0.005%
52	7.007	1829	1840	1855	rVV	175529	314103	24.88%	2.897%
53	7.154	1885	1886	1889	rBV3	1660	1019	0.08%	0.009%
54	7.251	1913	1916	1917	rBV3	2020	827	0.07%	0.008%
55	7.338	1931	1943	1958	rBV	619075	1056146	83.64%	9.742%
56	7.640	2028	2037	2051	rBV	116295	192223	15.22%	1.773%
57	7.926	2123	2126	2128	rBV4	1920	1348	0.11%	0.012%
58	8.064	2168	2169	2171	rBV2	790	395	0.03%	0.004%
59	8.109	2172	2183	2209	rVV2	296702	590943	46.80%	5.451%
60	8.392	2269	2271	2274	rBV3	1837	1325	0.10%	0.012%
61	8.453	2288	2290	2296	rBV7	1188	1104	0.09%	0.010%
62	8.498	2302	2304	2306	rBV3	2113	944	0.07%	0.009%
63	8.563	2323	2324	2326	rVB	1124	307	0.02%	0.003%
64	8.617	2340	2341	2343	rBV2	1140	494	0.04%	0.005%
65	8.640	2346	2348	2350	rVB3	1613	587	0.05%	0.005%
66	8.662	2350	2355	2357	rBV4	2516	2436	0.19%	0.022%
67	8.733	2375	2377	2379	rBV3	1244	756	0.06%	0.007%
68	8.871	2409	2420	2448	rBV	620068	1027107	81.34%	9.474%
69	9.035	2462	2471	2483	rVB	68899	108371	8.58%	1.000%
70	9.283	2537	2548	2557	rBV	131804	230333	18.24%	2.125%
71	9.736	2680	2689	2700	rBV3	34960	62352	4.94%	0.575%

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72	10.238	2835	2845	2860	rVB	419806	677014	53.62%	6.245%
73	11.270	3156	3166	3189	rVB	667445	1040236	82.38%	9.596%
74	11.646	3272	3283	3302	rVB	706540	1092916	86.55%	10.082%
75	12.344	3498	3500	3505	rBV6	1441	896	0.07%	0.008%
76	13.128	3742	3744	3747	rBV4	2441	1799	0.14%	0.017%
77	13.219	3768	3772	3774	rBV5	1115	990	0.08%	0.009%
78	13.241	3777	3779	3780	rBV2	1348	445	0.04%	0.004%
79	13.276	3787	3790	3795	rBV6	2050	2305	0.18%	0.021%
80	13.521	3864	3866	3867	rBV2	2228	927	0.07%	0.009%
81	13.572	3880	3882	3885	rBV4	1661	660	0.05%	0.006%
82	13.656	3903	3908	3911	rVB6	2402	1948	0.15%	0.018%
83	14.042	4023	4028	4031	rBV7	1232	1228	0.10%	0.011%
84	14.302	4107	4109	4111	rBV3	1959	1150	0.09%	0.011%
85	14.399	4136	4139	4142	rBV4	1883	1392	0.11%	0.013%
86	14.431	4146	4149	4152	rBV4	1688	1404	0.11%	0.013%
87	14.495	4165	4169	4172	rBV5	1957	1540	0.12%	0.014%
88	14.952	4308	4311	4313	rBV4	1724	986	0.08%	0.009%
89	15.997	4633	4636	4638	rBV3	2100	1535	0.12%	0.014%

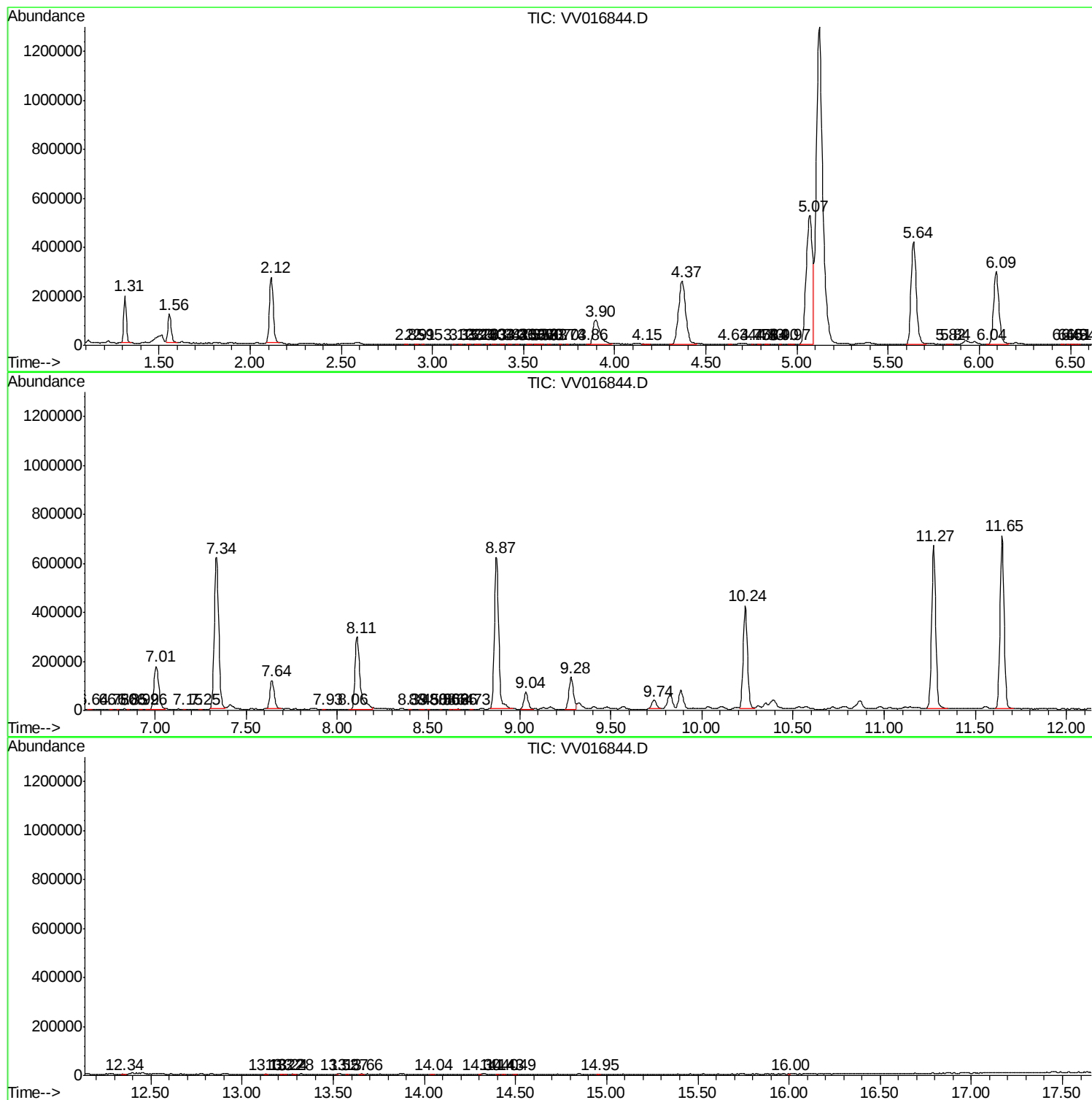
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060820WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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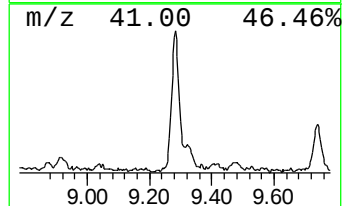
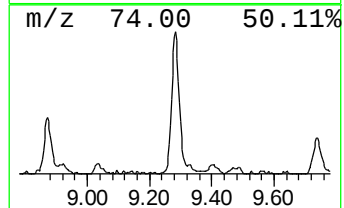
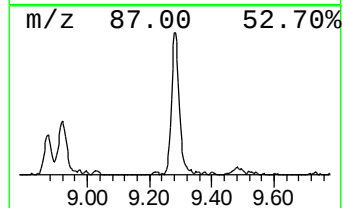
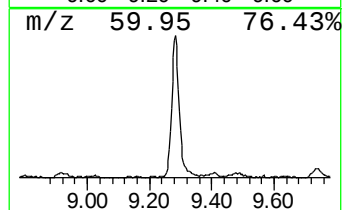
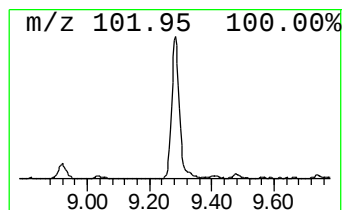
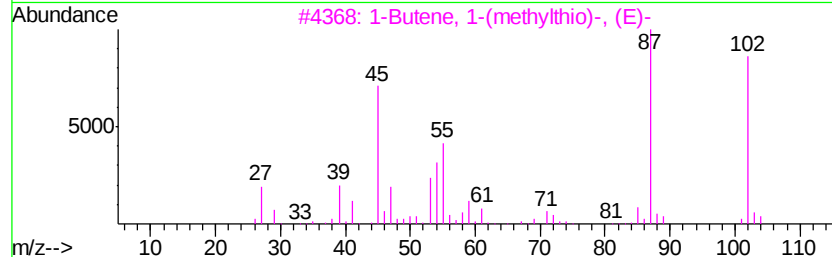
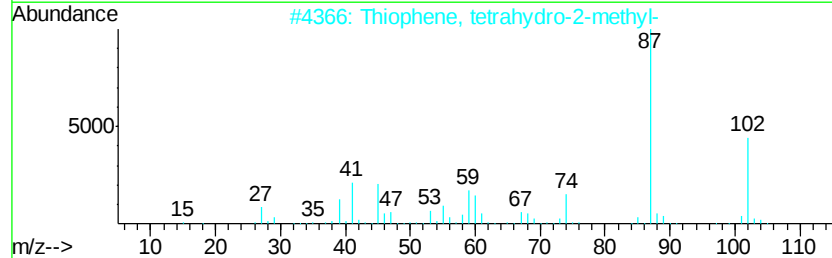
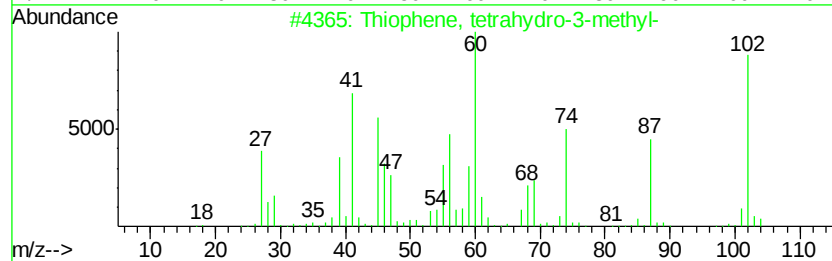
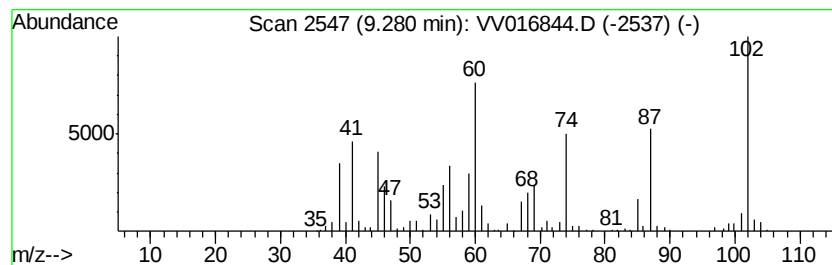
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060820WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.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.
9.28	11.21 ug/L	230333	Chlorobenzene-d5	8.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, tetrahydro-3-methyl-	102	C5H10S	004740-00-5	97
2			Thiophene, tetrahydro-2-methyl-	102	C5H10S	001795-09-1	46
3			1-Butene, 1-(methylthio)-, (E)-	102	C5H10S	017414-27-6	43
4			2H-Thiopyran, tetrahydro-	102	C5H10S	001613-51-0	37
5			Propane, 1-(ethenylthio)-	102	C5H10S	016330-21-5	37



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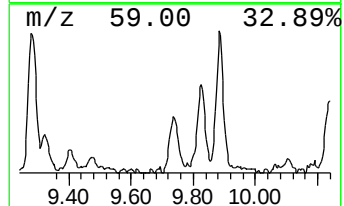
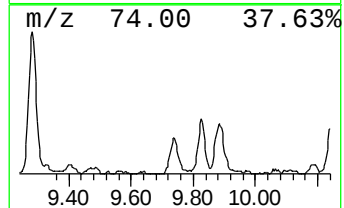
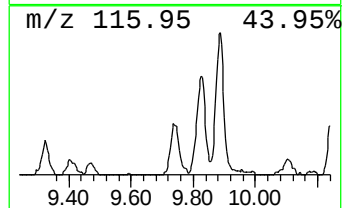
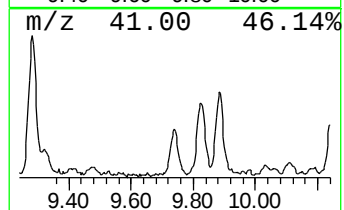
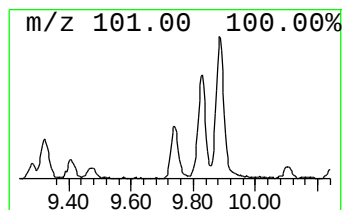
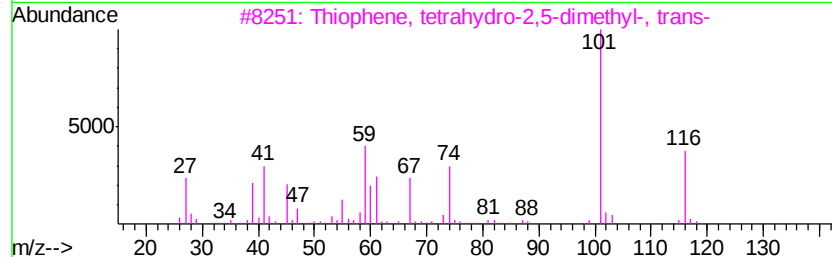
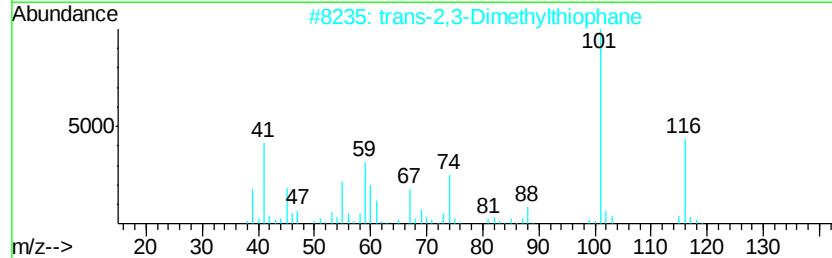
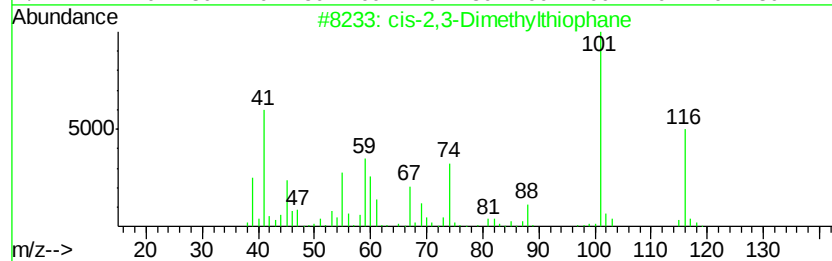
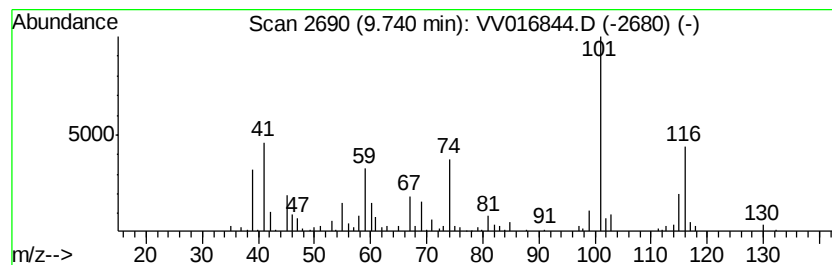
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 cis-2,3-Dimethylthiophane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.74	3.04 ug/L	62352	Chlorobenzene-d5	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	64
2		trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	62
3		Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-14-8	53
4		Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-13-7	53
5		Thiazole, 4,5-dihydro-4-methyl-2...	116	C4H8N2S	010416-81-6	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Thiophene, tetrah...	9.28	11.2	ug/L	230333	2	8.87	1027110	50.0
cis-2,3-Dimethylt...	9.74	3.0	ug/L	62352	2	8.87	1027110	50.0