

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV061120\
 Data File : VV016842.D
 Acq On : 11 Jun 2020 21:36
 Operator : SY/MD
 Sample : L2915-19
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 F9E65

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	1.110	4	6	16	rVB7	7639	7016	0.51%	0.061%
2	1.315	63	70	79	rBV	179629	177538	12.96%	1.533%
3	1.563	139	147	159	rVB	121906	148583	10.84%	1.283%
4	1.949	264	267	271	rBV6	1798	1570	0.11%	0.014%
5	1.984	275	278	279	rBV3	1913	1132	0.08%	0.010%
6	2.036	292	294	297	rBV4	1561	1104	0.08%	0.010%
7	2.116	309	319	334	rBV	280925	422433	30.83%	3.647%
8	2.264	362	365	367	rBV5	1627	1133	0.08%	0.010%
9	2.441	417	420	423	rBV4	1708	1162	0.08%	0.010%
10	2.505	435	440	442	rBV4	3237	2869	0.21%	0.025%
11	2.762	514	520	522	rBV6	2033	1577	0.12%	0.014%
12	2.881	554	557	560	rVB5	1219	895	0.07%	0.008%
13	2.914	565	567	570	rVB3	1629	954	0.07%	0.008%
14	2.939	570	575	576	rBV4	1375	1067	0.08%	0.009%
15	2.991	588	591	593	rBV4	1583	967	0.07%	0.008%
16	3.129	629	634	636	rBV4	1780	1408	0.10%	0.012%
17	3.148	636	640	643	rBV5	1147	889	0.06%	0.008%
18	3.190	651	653	656	rBV3	1526	1005	0.07%	0.009%
19	3.364	705	707	710	rBV3	1614	907	0.07%	0.008%
20	3.569	766	771	774	rBV7	1486	1370	0.10%	0.012%
21	3.679	798	805	807	rBV8	1786	2428	0.18%	0.021%
22	3.894	861	872	897	rBV	104672	273589	19.96%	2.362%
23	4.048	918	920	926	rBV6	1965	1846	0.13%	0.016%
24	4.286	991	994	1003	rVB10	1368	1701	0.12%	0.015%
25	4.373	1003	1021	1048	rBV	223329	555298	40.52%	4.794%
26	4.614	1089	1096	1099	rBV8	1433	1978	0.14%	0.017%
27	4.685	1110	1118	1120	rBV9	3041	3843	0.28%	0.033%
28	4.968	1197	1206	1220	rVB9	6912	16244	1.19%	0.140%
29	5.068	1220	1237	1261	rBV2	531904	1370379	100.00%	11.830%
30	5.232	1286	1288	1290	rBV3	1354	901	0.07%	0.008%
31	5.280	1301	1303	1307	rVB5	1460	1064	0.08%	0.009%
32	5.328	1314	1318	1320	rBV5	1876	1445	0.11%	0.012%
33	5.444	1351	1354	1357	rVB5	2069	1407	0.10%	0.012%
34	5.463	1357	1360	1363	rBV4	1518	1116	0.08%	0.010%

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

35	5.582	1393	1397	1401	rVB7	2088	1743	0.13%	0.015%
36	5.640	1401	1415	1439	rBV	439040	869425	63.44%	7.505%
37	5.823	1467	1472	1473	rBV4	2456	1596	0.12%	0.014%
38	5.929	1495	1505	1512	rBV7	13237	26217	1.91%	0.226%
39	6.093	1539	1556	1580	rBV	309574	630460	46.01%	5.442%
40	6.383	1640	1646	1649	rBV8	2286	2386	0.17%	0.021%
41	6.405	1651	1653	1656	rBV3	1526	1178	0.09%	0.010%
42	6.495	1675	1681	1684	rBV6	2874	3149	0.23%	0.027%
43	6.560	1696	1701	1704	rBV6	1243	976	0.07%	0.008%
44	6.611	1715	1717	1720	rBV4	1140	941	0.07%	0.008%
45	6.650	1725	1729	1731	rBV4	3108	2204	0.16%	0.019%
46	6.823	1779	1783	1785	rVV4	1916	1508	0.11%	0.013%
47	6.884	1800	1802	1806	rVB4	1772	1065	0.08%	0.009%
48	6.904	1806	1808	1812	rBV4	1850	1504	0.11%	0.013%
49	7.007	1826	1840	1855	rBV	188296	338480	24.70%	2.922%
50	7.232	1905	1910	1911	rBV5	1774	1476	0.11%	0.013%
51	7.338	1930	1943	1961	rBV	632307	1094581	79.87%	9.449%
52	7.463	1980	1982	1989	rVB7	4233	4213	0.31%	0.036%
53	7.560	2008	2012	2014	rVV5	1473	1099	0.08%	0.009%
54	7.640	2025	2037	2057	rBV	124694	226005	16.49%	1.951%
55	7.765	2066	2076	2087	rBV5	13392	25106	1.83%	0.217%
56	8.106	2171	2182	2218	rBV	319399	615066	44.88%	5.309%
57	8.421	2277	2280	2284	rBV6	1623	1333	0.10%	0.012%
58	8.495	2301	2303	2307	rVB5	1344	1045	0.08%	0.009%
59	8.531	2312	2314	2319	rVB5	1446	1039	0.08%	0.009%
60	8.611	2335	2339	2342	rVB5	1645	1053	0.08%	0.009%
61	8.656	2346	2353	2355	rBV8	5186	5352	0.39%	0.046%
62	8.791	2389	2395	2405	rBV7	6037	9168	0.67%	0.079%
63	8.871	2408	2420	2439	rBV	648990	1043605	76.15%	9.009%
64	9.068	2478	2481	2486	rVB5	1517	1072	0.08%	0.009%
65	9.122	2494	2498	2499	rBV4	1723	1200	0.09%	0.010%
66	9.193	2517	2520	2525	rBV7	1626	1490	0.11%	0.013%
67	9.283	2537	2548	2555	rBV6	19119	35461	2.59%	0.306%
68	9.646	2657	2661	2662	rBV3	3145	2050	0.15%	0.018%
69	9.736	2674	2689	2699	rBV4	44166	90403	6.60%	0.780%
70	9.826	2707	2717	2726	rBV3	32552	57524	4.20%	0.497%
71	9.884	2728	2735	2753	rVB2	40148	70689	5.16%	0.610%

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72	10.026	2774	2779	2780	rBV4	1417	1460	0.11%	0.013%
73	10.071	2786	2793	2798	rBV6	5382	7413	0.54%	0.064%
74	10.183	2821	2828	2834	rBV8	12469	19748	1.44%	0.170%
75	10.238	2834	2845	2858	rVB	448635	709217	51.75%	6.122%
76	10.309	2860	2867	2875	rVV3	25021	36840	2.69%	0.318%
77	10.482	2911	2921	2925	rBV8	11974	20120	1.47%	0.174%
78	10.524	2927	2934	2943	rVB3	28268	43631	3.18%	0.377%
79	10.650	2969	2973	2977	rBV8	2979	2244	0.16%	0.019%
80	10.720	2982	2995	3004	rBV9	13709	28587	2.09%	0.247%
81	10.785	3005	3015	3025	rVV3	36451	68613	5.01%	0.592%
82	10.849	3026	3035	3055	rVB9	34862	94500	6.90%	0.816%
83	10.977	3064	3075	3083	rBV5	17634	33574	2.45%	0.290%
84	11.116	3112	3118	3131	rVB5	29455	46088	3.36%	0.398%
85	11.270	3156	3166	3191	rVB	716615	1132333	82.63%	9.775%
86	11.646	3273	3283	3303	rVB	710013	1135126	82.83%	9.799%
87	12.508	3549	3551	3554	rBV3	2229	1712	0.12%	0.015%
88	12.929	3680	3682	3684	rBV3	2803	1726	0.13%	0.015%
89	14.357	4122	4126	4127	rBV3	1414	925	0.07%	0.008%
90	14.421	4144	4146	4149	rBV3	1353	883	0.06%	0.008%
91	14.460	4153	4158	4162	rBV8	3054	3296	0.24%	0.028%
92	14.720	4235	4239	4241	rBV4	3892	3108	0.23%	0.027%
93	15.074	4346	4349	4353	rVB5	1644	1085	0.08%	0.009%
94	15.199	4382	4388	4390	rBV7	2510	2913	0.21%	0.025%
95	15.466	4469	4471	4475	rVB4	2094	1141	0.08%	0.010%
96	15.662	4529	4532	4537	rBV6	1400	1310	0.10%	0.011%
97	15.723	4548	4551	4552	rBV3	1994	1091	0.08%	0.009%
98	15.733	4552	4554	4558	rVB4	1791	1143	0.08%	0.010%
99	15.778	4564	4568	4571	rBV6	1969	1639	0.12%	0.014%
100	15.839	4585	4587	4593	rVB5	1745	1171	0.09%	0.010%

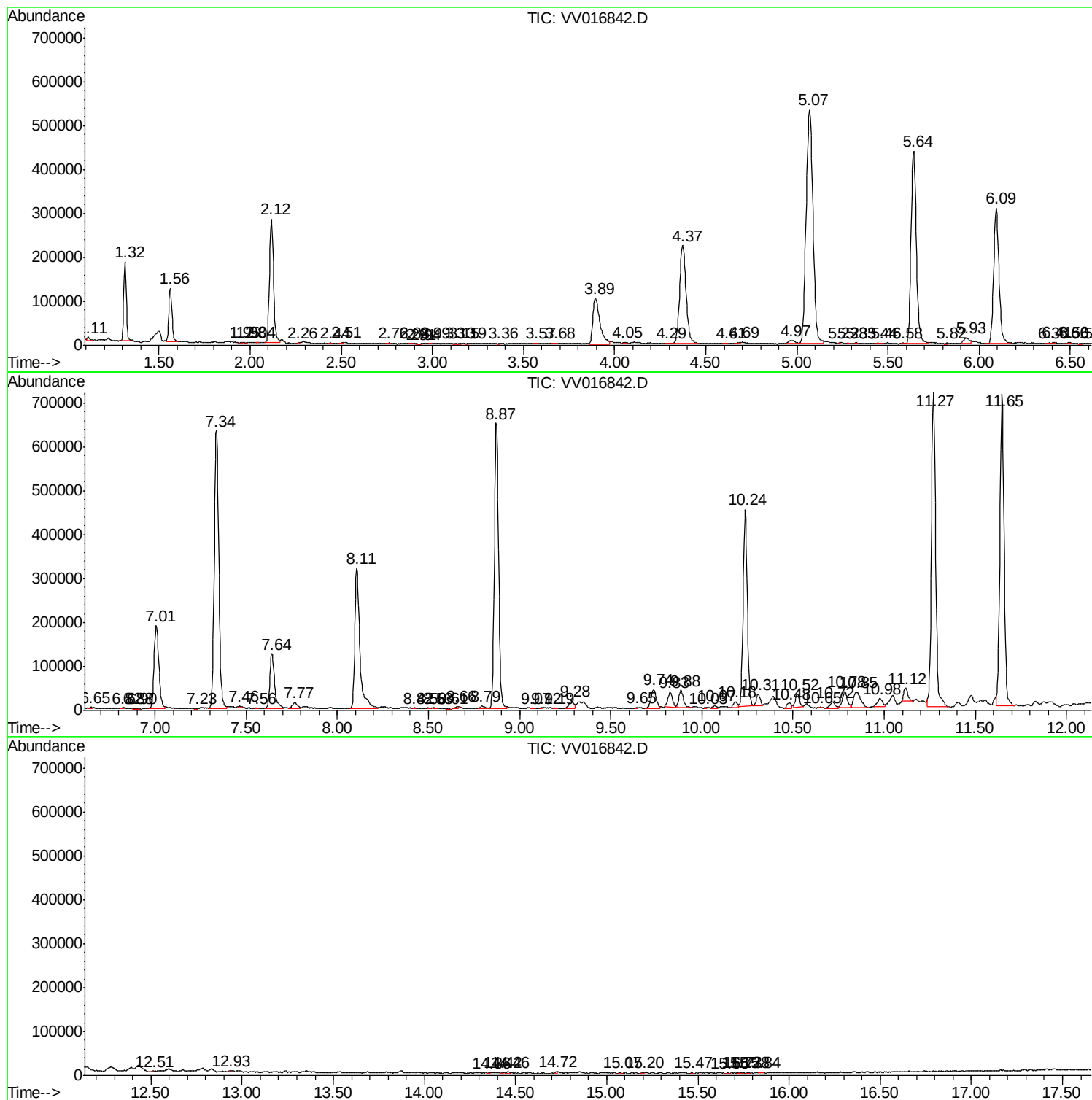
Sum of corrected areas: 11584317

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Instrument :
MSVOA_V
ClientSampled :
F9E65

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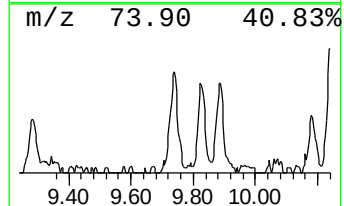
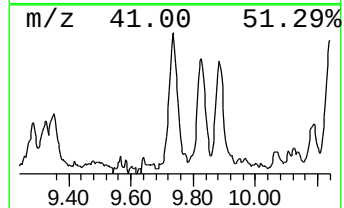
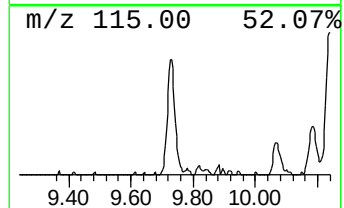
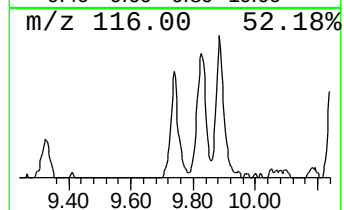
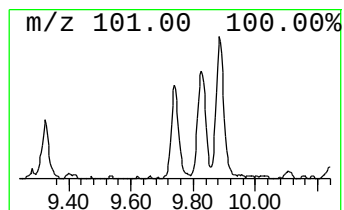
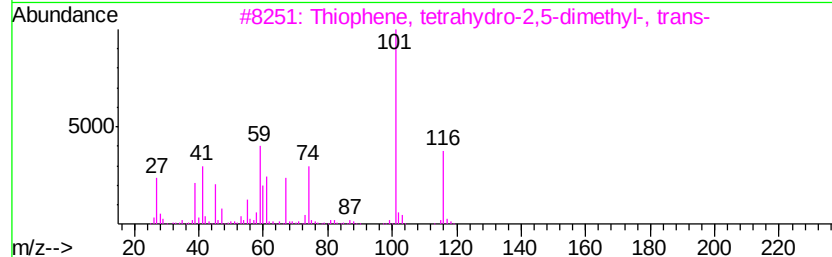
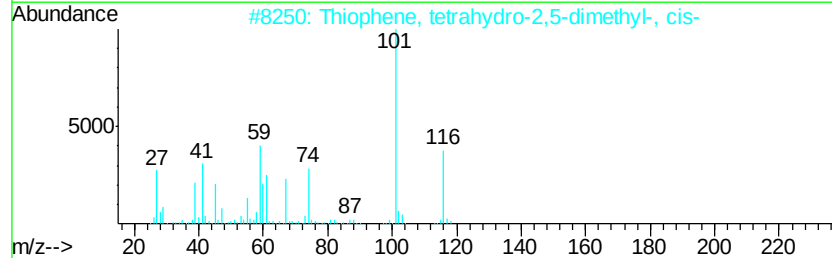
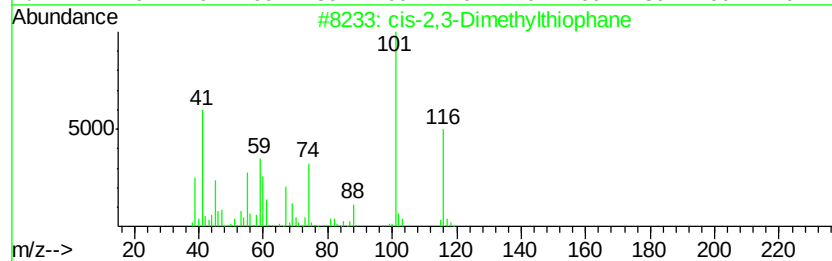
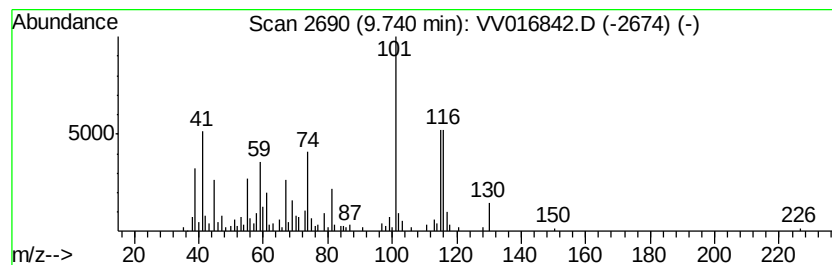
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060820WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.74	4.33 ug/L	90403	Chlorobenzene-d5	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	58
2		Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-13-7	52
3		Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-14-8	47
4		Thiazole, 4,5-dihydro-4-methyl-2...	116	C4H8N2S	010416-81-6	43
5		trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	38



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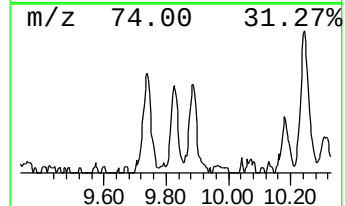
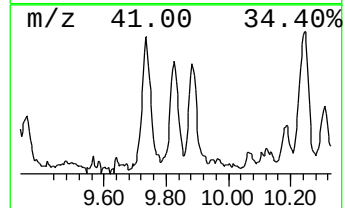
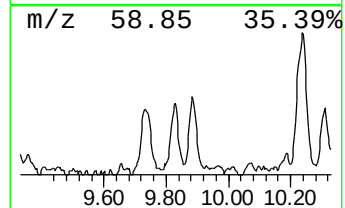
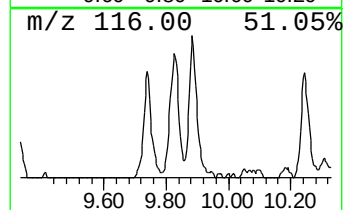
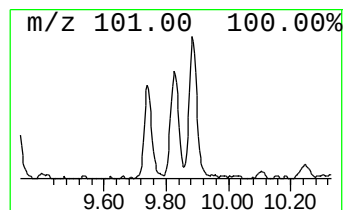
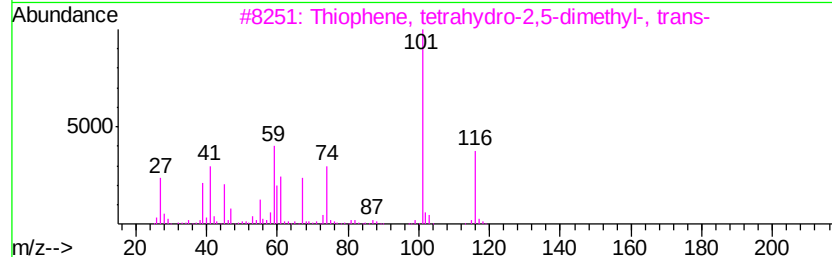
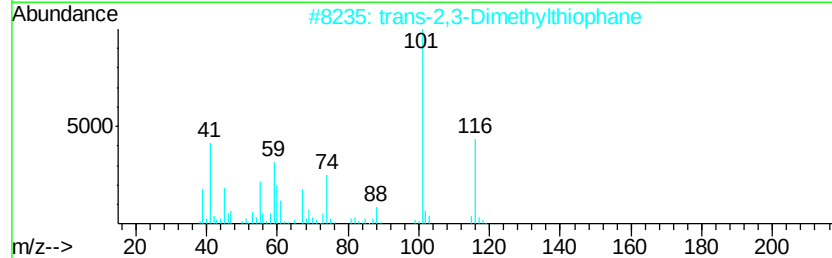
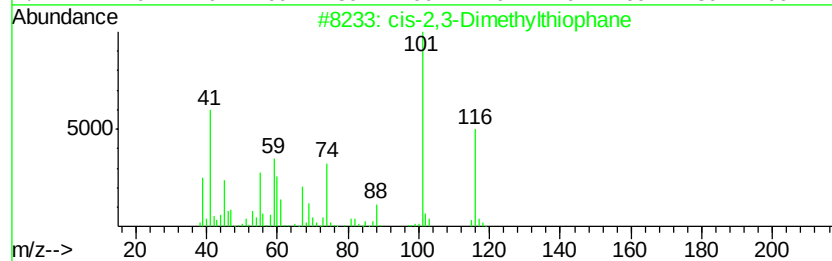
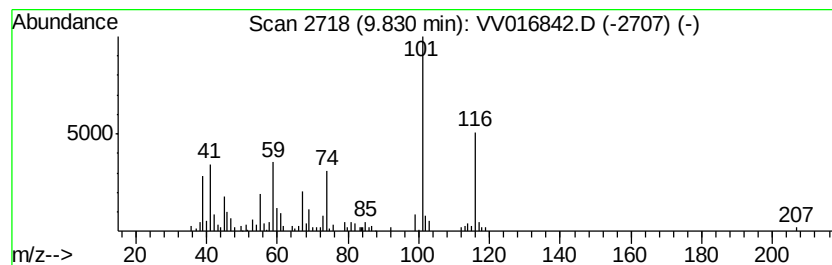
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060820WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Thiazole, 4,5-dihydro-4-met... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.83	2.76 ug/L	57524	Chlorobenzene-d5	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	91
2		trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	87
3		Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-14-8	80
4		Thiazole, 4,5-dihydro-4-methyl-2...	116	C4H8N2S	010416-81-6	74
5		Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-13-7	72



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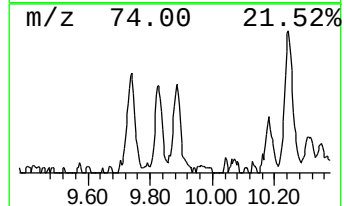
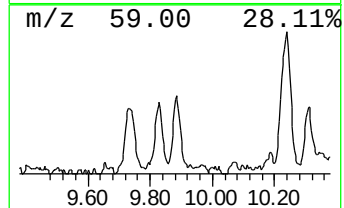
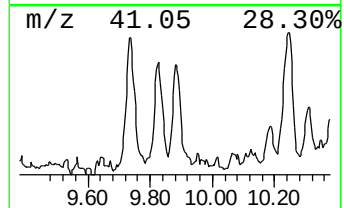
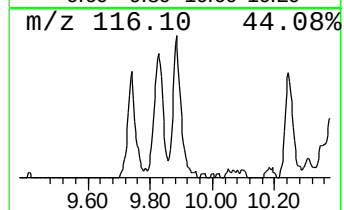
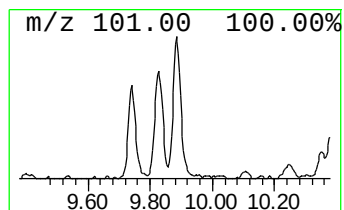
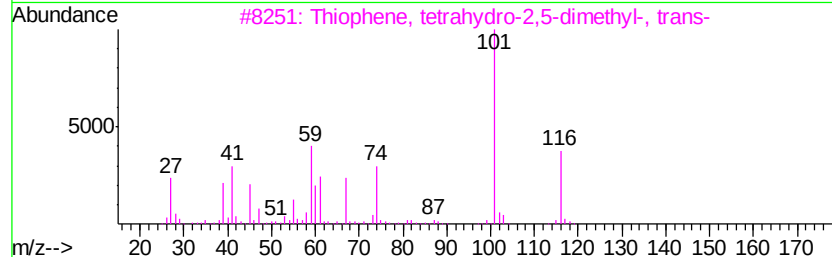
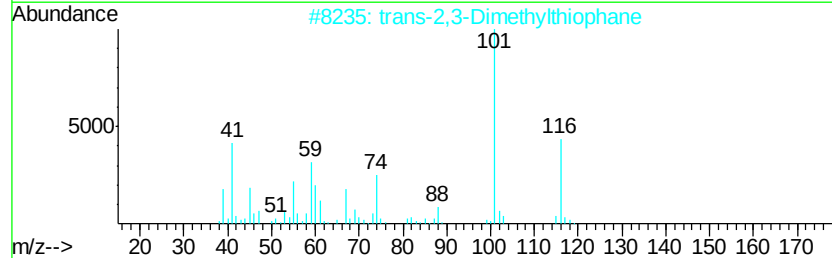
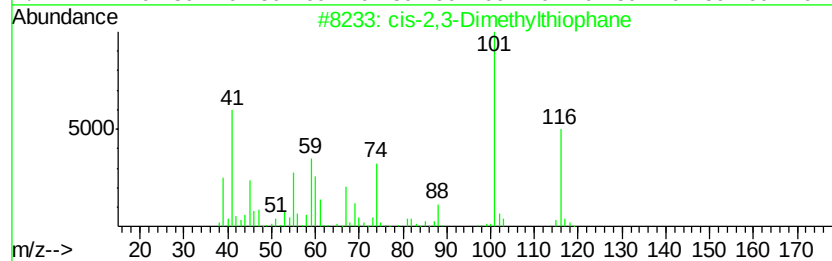
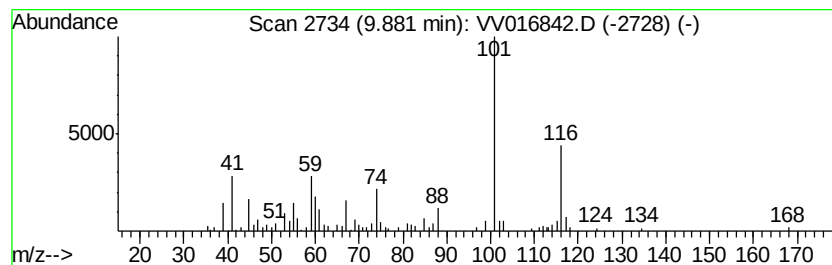
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Quant Title : VOC Analysis

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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.88	3.39 ug/L	70689	Chlorobenzene-d5	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	94
2		trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	94
3		Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-14-8	87
4		Thiazole, 4,5-dihydro-4-methyl-2...	116	C4H8N2S	010416-81-6	81
5		Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-13-7	72



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_V\DATA\VV061120\
Data File : VV016842.D
Acq On : 11 Jun 2020 21:36
Operator : SY/MD
Sample : L2915-19
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampled :
F9E65

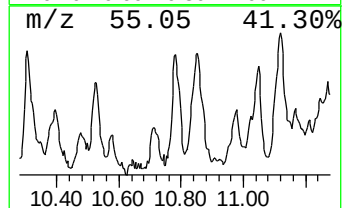
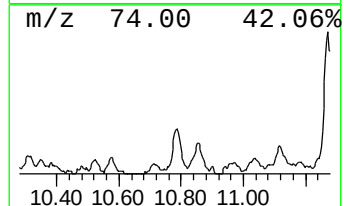
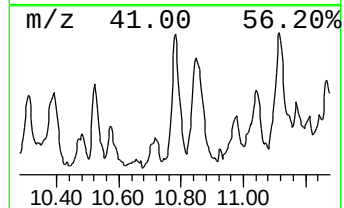
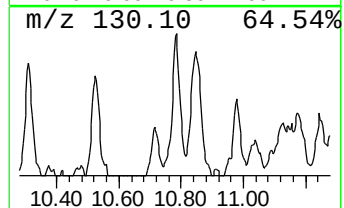
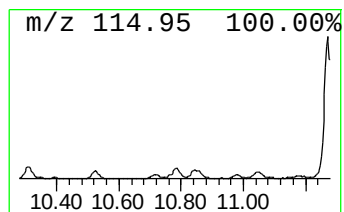
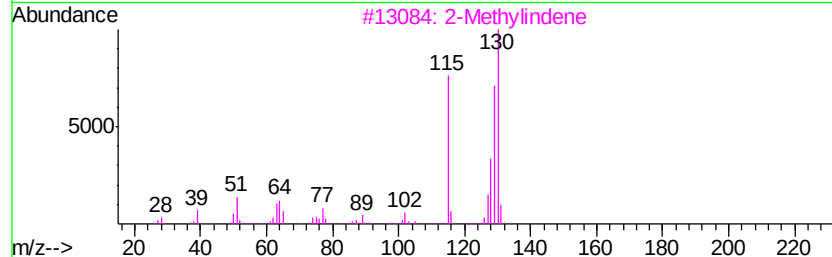
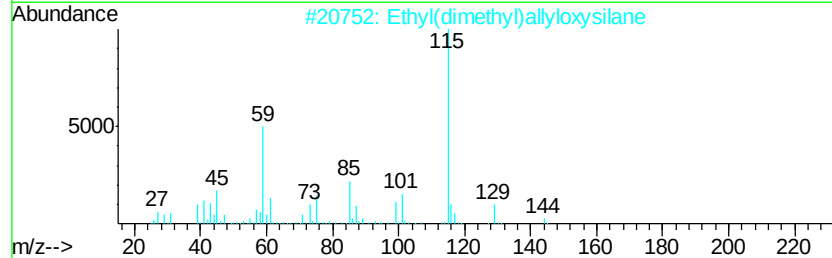
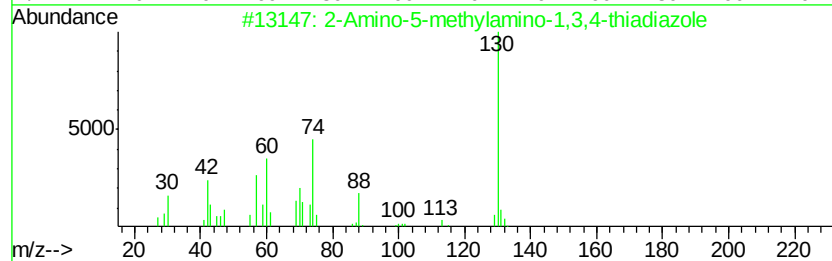
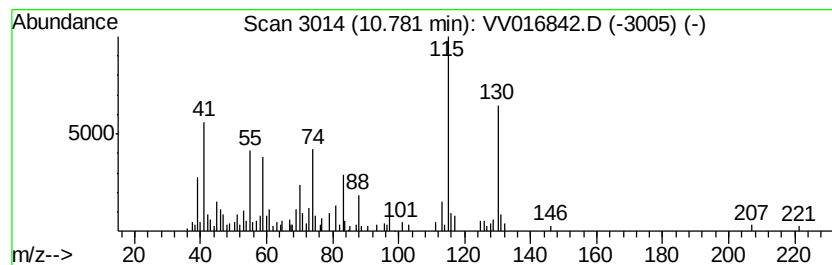
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Quant Title : VOC Analysis

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

Peak Number 5 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.78	3.03 ug/L	68613	1,4-Dichlorobenzene-d4	11.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Amino-5-methylamino-1,3,4-thia...	130	C3H6N4S	033151-04-1	41
2		Ethyl(dimethyl)allyloxysilane	144	C7H16OSi	1000278-59-3	35
3		2-Methylindene	130	C10H10	002177-47-1	30
4		Thiophene, 2-(methylthio)-	130	C5H6S2	005780-36-9	30
5		Thiophene, 2-(methylthio)-	130	C5H6S2	005780-36-9	27



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_V\DATA\VV061120\
Data File : VV016842.D
Acq On : 11 Jun 2020 21:36
Operator : SY/MD
Sample : L2915-19
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 33 Sample Multiplier: 1

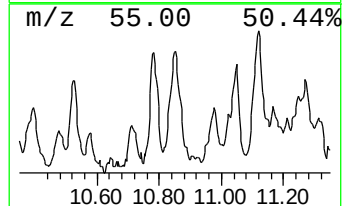
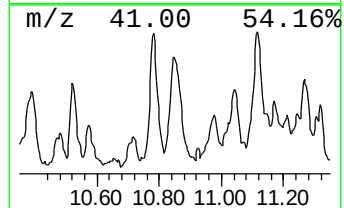
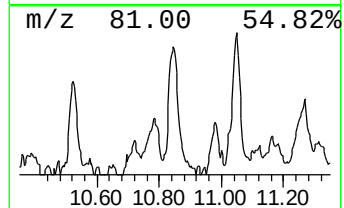
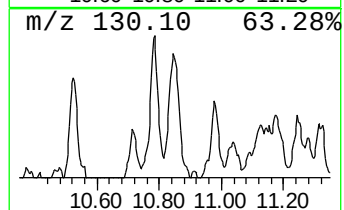
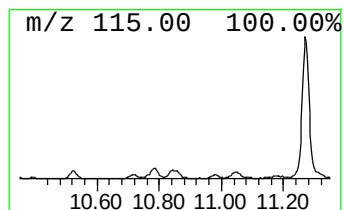
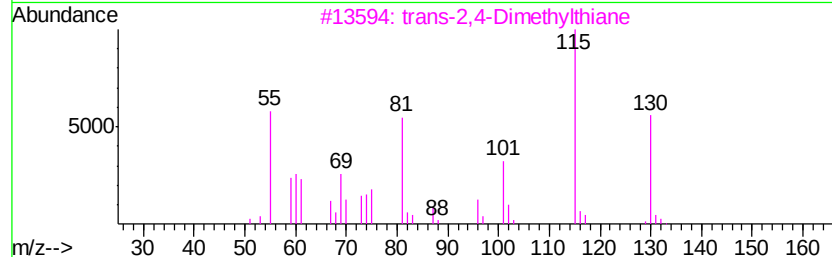
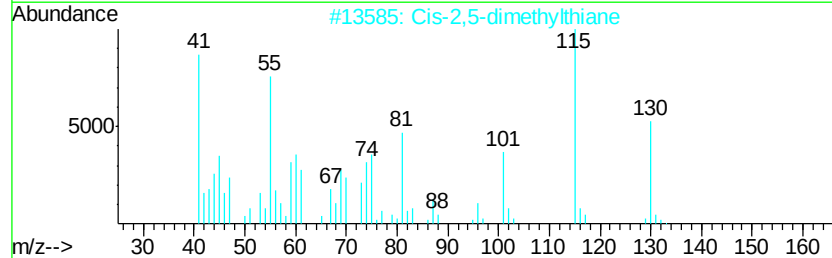
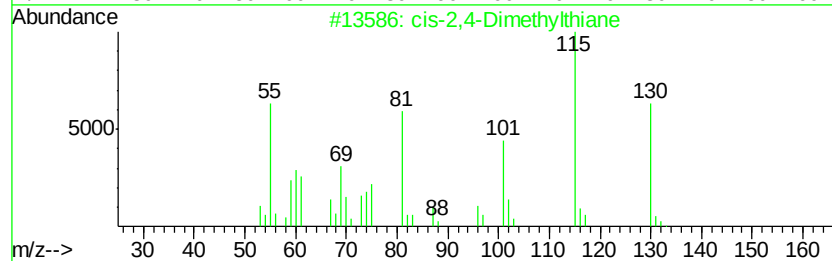
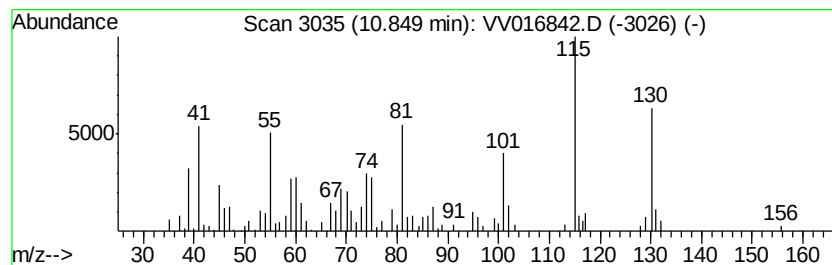
Instrument :
MSVOA_V
ClientSampleId :
F9E65

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 6 cis-2,4-Dimethylthiane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.85	4.17 ug/L	94500	1,4-Dichlorobenzene-d4	11.27
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		cis-2,4-Dimethylthiane	130 C7H14S	061568-43-2 90
2		Cis-2,5-dimethylthiane	130 C7H14S	1000215-06-6 90
3		trans-2,4-Dimethylthiane	130 C7H14S	061568-42-1 86
4		Trans-2,5-dimethylthiane	130 C7H14S	1000215-06-8 72
5		Cis-2,3-dimethylthiane	130 C7H14S	1000215-06-5 52



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV061120\
Data File : VV016842.D
Acq On : 11 Jun 2020 21:36
Operator : SY/MD
Sample : L2915-19
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F9E65

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

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
cis-2,3-Dimethylt...	9.74	4.3	ug/L	90403	2	8.87	1043610	50.0
Thiazole, 4,5-dih...	9.83	2.8	ug/L	57524	2	8.87	1043610	50.0
trans-2,3-Dimethy...	9.88	3.4	ug/L	70689	2	8.87	1043610	50.0
unknown-01	10.78	3.0	ug/L	68613	3	11.27	1132330	50.0
cis-2,4-Dimethylt...	10.85	4.2	ug/L	94500	3	11.27	1132330	50.0