

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV060820\
 Data File : VV016662.D
 Acq On : 08 Jun 2020 16:13
 Operator : SY/MD
 Sample : L2861-16
 Misc : 5.0mL/MSVOA V/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 F9E61

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	1.113	3	7	12	rVB2	15035	12464	0.82%	0.083%
2	1.222	37	41	51	rVB2	25581	24175	1.58%	0.161%
3	1.315	63	70	79	rVB	189253	189903	12.42%	1.266%
4	1.560	139	146	159	rVB	124607	156019	10.20%	1.040%
5	1.939	262	264	267	rBV5	1868	1125	0.07%	0.008%
6	2.116	310	319	333	rBV	301492	449379	29.39%	2.996%
7	2.293	367	374	375	rBV5	3636	3861	0.25%	0.026%
8	2.367	395	397	401	rBV4	1509	1071	0.07%	0.007%
9	2.399	404	407	414	rVV7	1721	1921	0.13%	0.013%
10	2.502	435	439	442	rBV6	3496	3543	0.23%	0.024%
11	2.614	472	474	477	rVB4	2177	1087	0.07%	0.007%
12	2.637	479	481	486	rVV6	2212	2141	0.14%	0.014%
13	2.659	486	488	493	rVB5	1788	1505	0.10%	0.010%
14	2.814	531	536	538	rBV5	1352	1307	0.09%	0.009%
15	2.849	543	547	551	rVB6	1920	1666	0.11%	0.011%
16	2.923	566	570	573	rBV5	1892	1802	0.12%	0.012%
17	3.180	647	650	652	rBV2	1875	1476	0.10%	0.010%
18	3.196	652	655	656	rBV4	2640	1234	0.08%	0.008%
19	3.418	720	724	727	rVV4	1815	1563	0.10%	0.010%
20	3.450	732	734	739	rVB5	1928	1492	0.10%	0.010%
21	3.486	743	745	750	rVB5	1411	1041	0.07%	0.007%
22	3.512	750	753	757	rBV5	1412	1261	0.08%	0.008%
23	3.534	757	760	763	rBV5	1264	1080	0.07%	0.007%
24	3.675	799	804	807	rBV6	1694	1444	0.09%	0.010%
25	3.798	840	842	845	rVB4	1740	1047	0.07%	0.007%
26	3.823	845	850	851	rBV5	1616	1475	0.10%	0.010%
27	3.894	861	872	900	rBV	115439	310669	20.32%	2.072%
28	4.373	1005	1021	1042	rBV	243562	594873	38.91%	3.967%
29	4.579	1082	1085	1089	rBV5	1692	1412	0.09%	0.009%
30	4.640	1099	1104	1106	rVV6	1123	1028	0.07%	0.007%
31	4.698	1118	1122	1123	rBV2	1864	1234	0.08%	0.008%
32	5.071	1219	1238	1253	rBV2	593965	1529020	100.00%	10.195%
33	5.155	1253	1264	1287	rVB2	289787	627955	41.07%	4.187%
34	5.524	1375	1379	1381	rBV4	1843	1460	0.10%	0.010%

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 Title : VOC Analysis

35	5.640	1400	1415	1443	rBV	442241	888112	58.08%	5.922%
36	5.772	1453	1456	1460	rBV6	1550	1376	0.09%	0.009%
37	5.859	1479	1483	1484	rBV3	2138	1501	0.10%	0.010%
38	5.897	1492	1495	1497	rBV4	1890	1241	0.08%	0.008%
39	5.933	1497	1506	1507	rVV7	8244	10864	0.71%	0.072%
40	5.968	1510	1517	1535	rVB3	32448	66127	4.32%	0.441%
41	6.093	1543	1556	1578	rBV	338989	681478	44.57%	4.544%
42	6.335	1626	1631	1633	rBV5	1483	1367	0.09%	0.009%
43	6.653	1725	1730	1737	rBV9	2218	2625	0.17%	0.018%
44	6.727	1748	1753	1756	rBV7	2399	2180	0.14%	0.015%
45	6.798	1772	1775	1777	rVV3	2592	1598	0.10%	0.011%
46	6.830	1777	1785	1795	rVV4	9839	17566	1.15%	0.117%
47	6.868	1795	1797	1802	rVV5	1754	1481	0.10%	0.010%
48	7.007	1825	1840	1858	rBV	223941	416908	27.27%	2.780%
49	7.161	1878	1888	1891	rBV9	4027	6546	0.43%	0.044%
50	7.264	1917	1920	1923	rBV4	1536	1074	0.07%	0.007%
51	7.338	1924	1943	1962	rBV	706262	1227482	80.28%	8.185%
52	7.605	2022	2026	2027	rBV3	3332	2162	0.14%	0.014%
53	7.640	2028	2037	2056	rVB	137095	232130	15.18%	1.548%
54	7.962	2131	2137	2139	rBV6	2903	2912	0.19%	0.019%
55	8.000	2145	2149	2157	rVB10	2358	2643	0.17%	0.018%
56	8.106	2172	2182	2212	rBV	405621	749728	49.03%	4.999%
57	8.241	2216	2224	2237	rVB4	16177	30643	2.00%	0.204%
58	8.354	2252	2259	2266	rVB4	6174	8919	0.58%	0.059%
59	8.598	2333	2335	2339	rVB5	1809	1060	0.07%	0.007%
60	8.662	2352	2355	2356	rBV3	2441	1396	0.09%	0.009%
61	8.794	2385	2396	2400	rBV8	7425	11410	0.75%	0.076%
62	8.875	2409	2421	2431	rBV	669806	1074618	70.28%	7.165%
63	9.039	2467	2472	2475	rBV6	4061	3986	0.26%	0.027%
64	9.283	2531	2548	2557	rBV	358382	600955	39.30%	4.007%
65	9.405	2577	2586	2597	rBV	144902	231651	15.15%	1.545%
66	9.469	2597	2606	2630	rVB2	131081	237019	15.50%	1.580%
67	9.650	2657	2662	2663	rBV5	2267	1929	0.13%	0.013%
68	9.740	2676	2690	2703	rBV2	126112	234454	15.33%	1.563%
69	9.826	2706	2717	2726	rVV2	146290	271150	17.73%	1.808%
70	9.884	2727	2735	2755	rVB	180363	303033	19.82%	2.021%
71	10.106	2796	2804	2819	rVB4	47042	83652	5.47%	0.558%

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72	10.186	2822	2829	2831	rBV4	11651	13390	0.88%	0.089%
73	10.238	2834	2845	2859	rVB	539477	892171	58.35%	5.949%
74	10.347	2873	2879	2885	rBV2	37429	55917	3.66%	0.373%
75	10.524	2927	2934	2943	rBV4	32958	54691	3.58%	0.365%
76	10.717	2986	2994	3004	rBV6	20801	38836	2.54%	0.259%
77	10.797	3008	3019	3027	rVV7	25404	60595	3.96%	0.404%
78	10.981	3070	3076	3083	rBV3	14546	19063	1.25%	0.127%
79	11.270	3152	3166	3179	rBV	724206	1125519	73.61%	7.505%
80	11.553	3247	3254	3266	rVB2	50440	87412	5.72%	0.583%
81	11.646	3272	3283	3303	rVB	781764	1228957	80.38%	8.195%
82	12.273	3471	3478	3479	rBV6	4664	5587	0.37%	0.037%
83	12.521	3548	3555	3565	rBV6	8349	15347	1.00%	0.102%
84	13.170	3754	3757	3758	rBV3	2825	1652	0.11%	0.011%
85	13.235	3774	3777	3780	rBV4	3380	2790	0.18%	0.019%
86	13.289	3791	3794	3799	rVB6	2579	1987	0.13%	0.013%
87	13.331	3801	3807	3808	rBV6	4537	4423	0.29%	0.029%
88	13.649	3902	3906	3911	rBV2	4546	4986	0.33%	0.033%
89	13.781	3944	3947	3949	rBV3	2702	1729	0.11%	0.012%
90	13.868	3966	3974	3982	rBV3	5322	9682	0.63%	0.065%
91	14.096	4042	4045	4049	rVB5	2025	1287	0.08%	0.009%
92	14.280	4099	4102	4104	rBV3	1653	1020	0.07%	0.007%
93	14.315	4107	4113	4116	rBV8	4960	6136	0.40%	0.041%
94	14.858	4275	4282	4289	rVB8	4260	7084	0.46%	0.047%
95	15.003	4323	4327	4328	rBV4	2617	1595	0.10%	0.011%
96	15.074	4347	4349	4354	rVB4	2194	1649	0.11%	0.011%
97	15.141	4368	4370	4377	rBV9	1826	1296	0.08%	0.009%
98	15.453	4463	4467	4470	rBV5	1533	1343	0.09%	0.009%
99	15.530	4487	4491	4493	rBV5	1473	1143	0.07%	0.008%
100	15.726	4549	4552	4553	rBV3	1946	1130	0.07%	0.008%

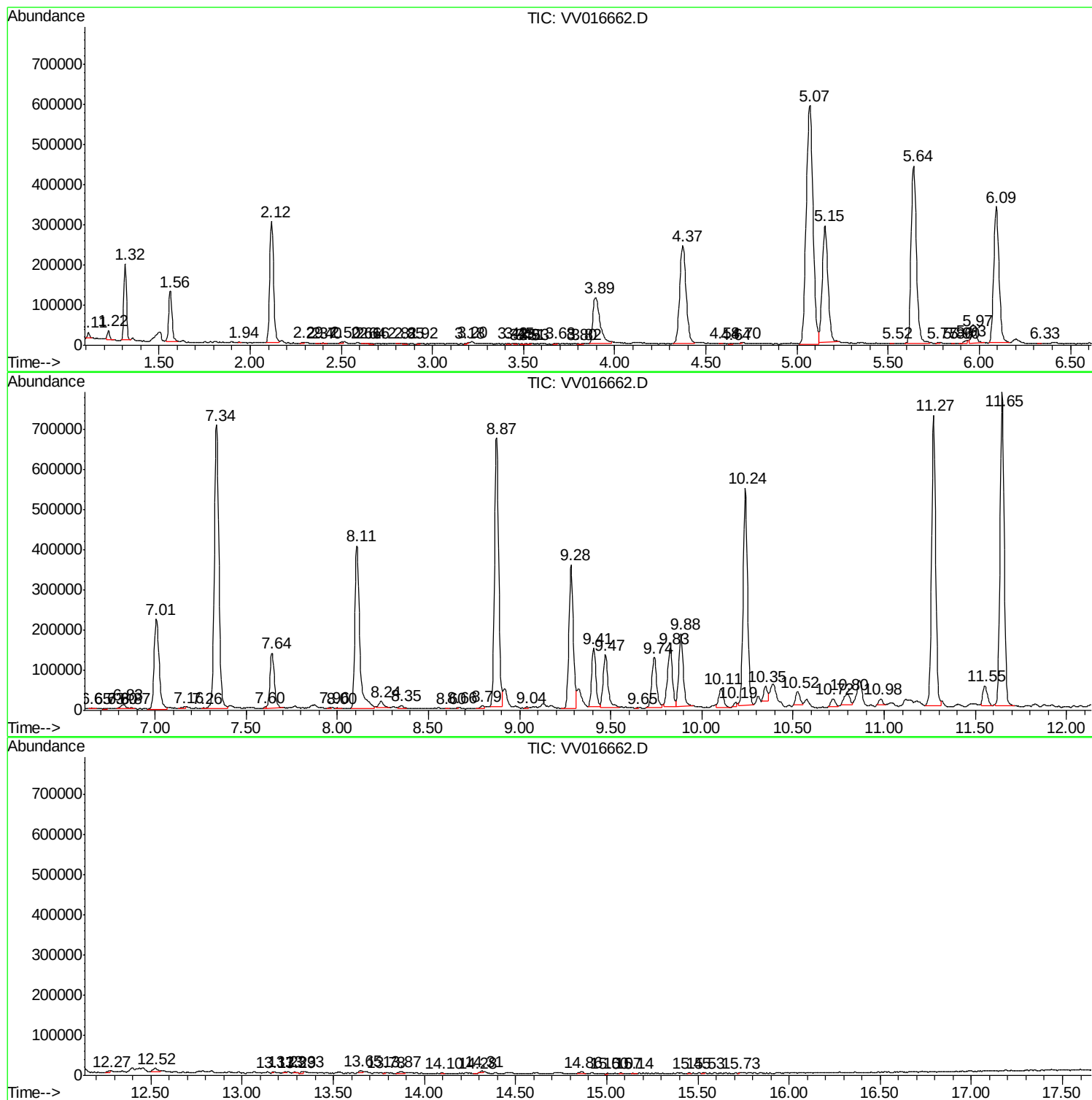
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MSVOA_V
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060820WMA.M
Quant Title : VOC Analysis

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



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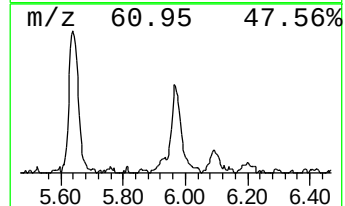
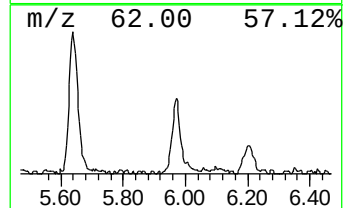
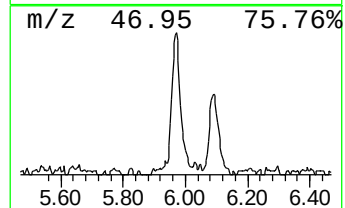
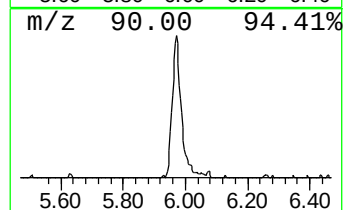
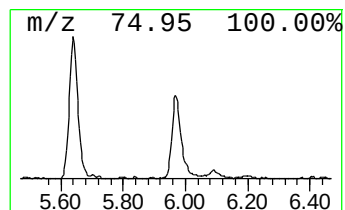
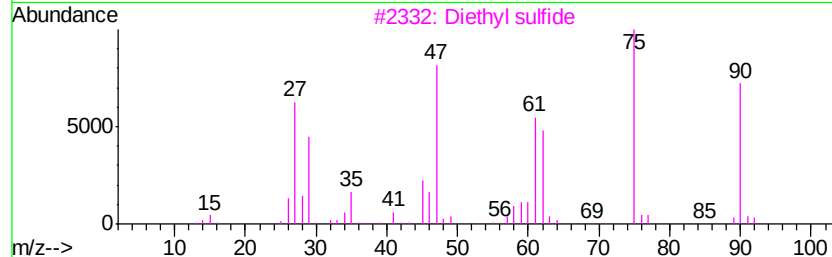
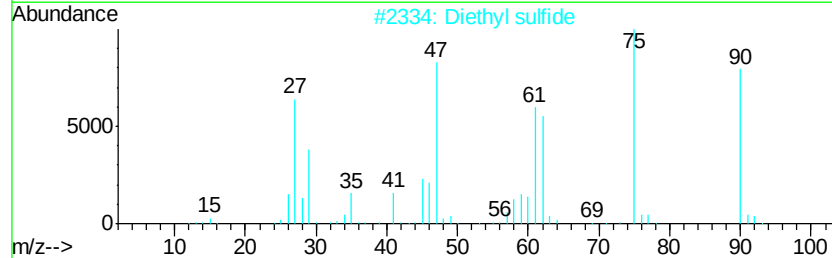
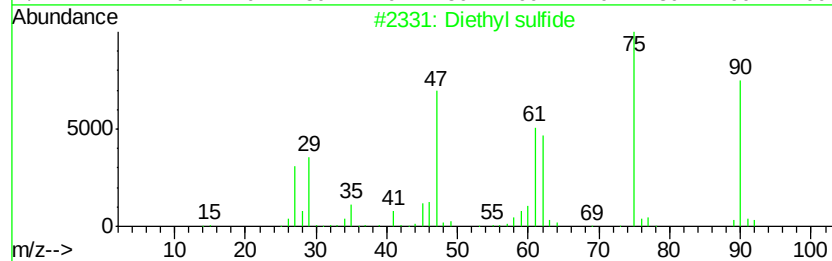
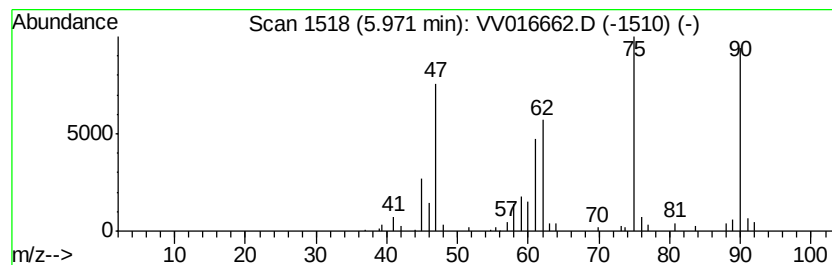
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060820WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Diethyl sulfide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.97	3.72 ug/L	66127	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Diethyl sulfide	90	C4H10S	000352-93-2	94
2		Diethyl sulfide	90	C4H10S	000352-93-2	94
3		Diethyl sulfide	90	C4H10S	000352-93-2	91
4		Diethyl sulfide	90	C4H10S	000352-93-2	91
5		3-Thietanol	90	C3H6OS	010304-16-2	37



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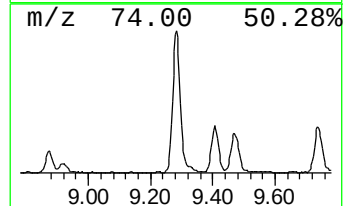
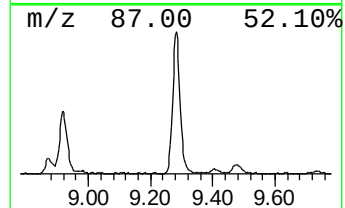
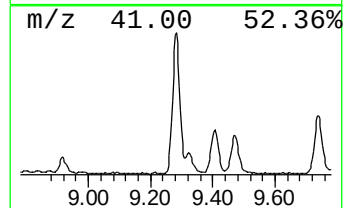
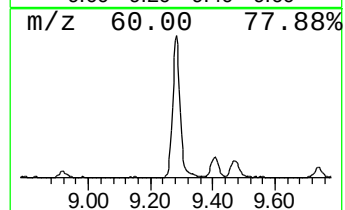
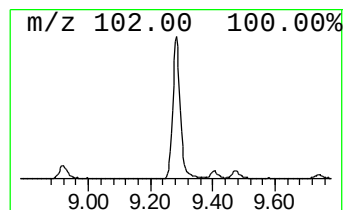
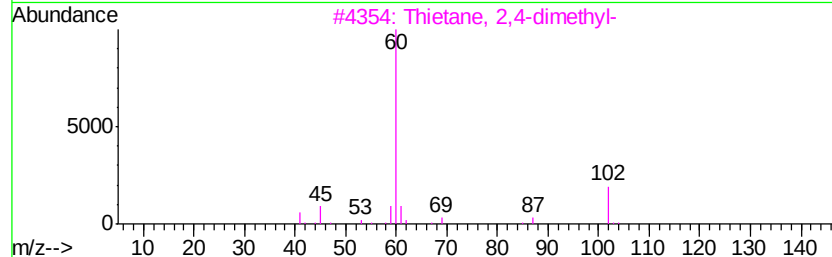
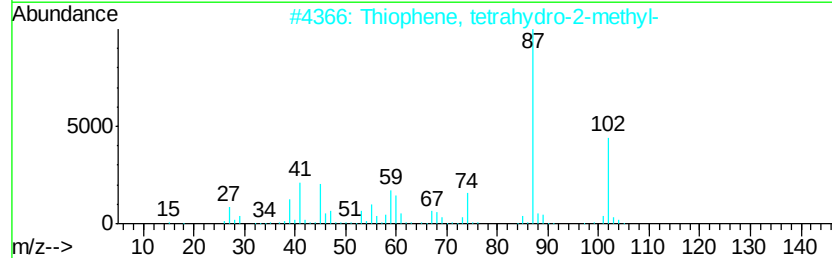
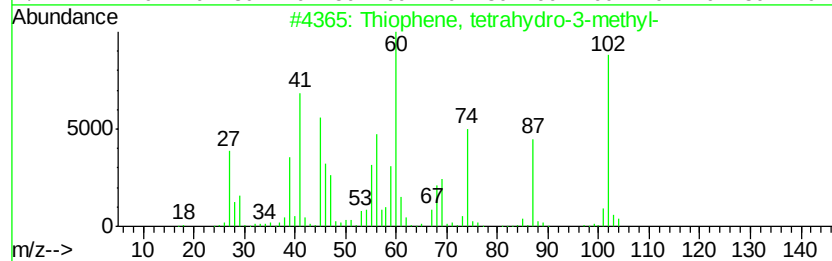
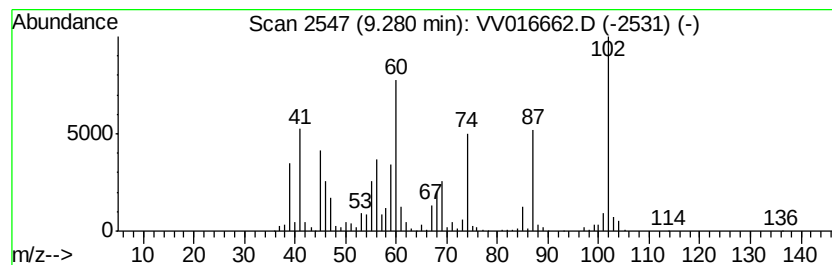
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Thiophene, tetrahydro-3-met... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.28	27.96 ug/L	600955	Chlorobenzene-d5	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Thiophene, tetrahydro-3-methyl-	102	C5H10S	004740-00-5	96
2		Thiophene, tetrahydro-2-methyl-	102	C5H10S	001795-09-1	49
3		Thietane, 2,4-dimethyl-	102	C5H10S	043044-24-2	47
4		Thiophene, tetrahydro-2-methyl-	102	C5H10S	001795-09-1	47
5		2H-Thiopyran, tetrahydro-	102	C5H10S	001613-51-0	43



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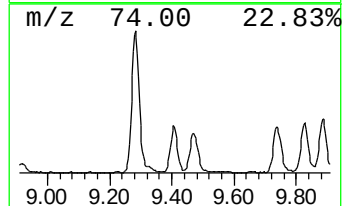
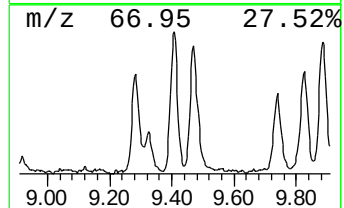
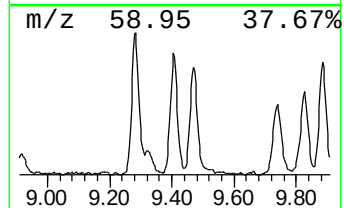
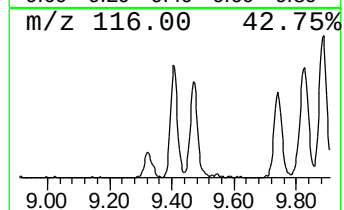
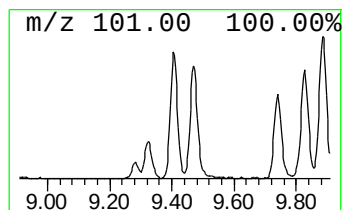
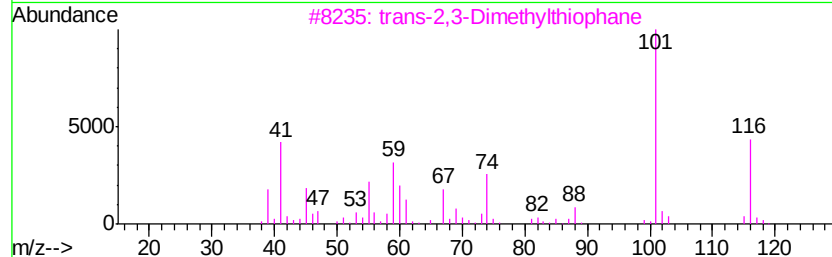
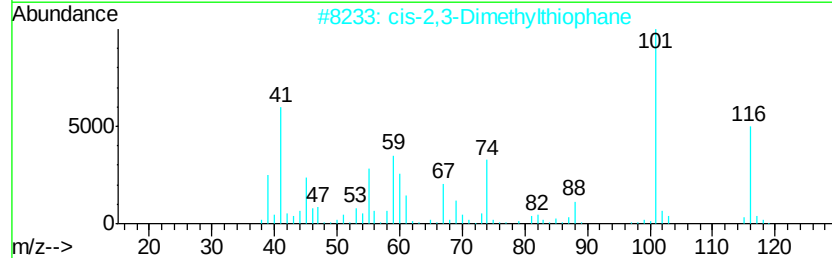
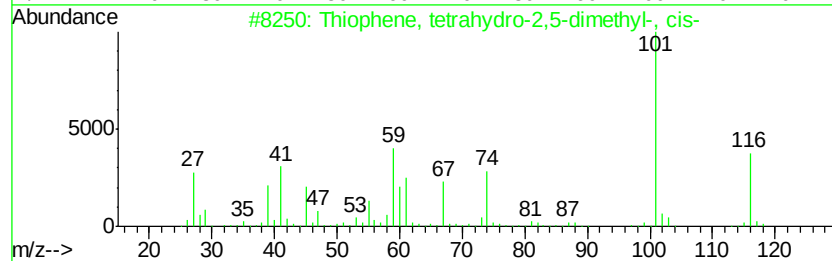
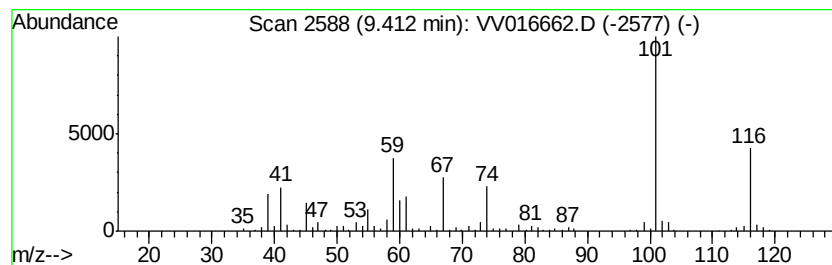
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Peak Number 4 Thiophene, tetrahydro-2,5-d... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.41	10.78 ug/L	231651	Chlorobenzene-d5	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-13-7	91
2		cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	81
3		trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	81
4		Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-14-8	74
5		Thiazole, 4,5-dihydro-4-methyl-2...	116	C4H8N2S	010416-81-6	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV060820\
Data File : VV016662.D
Acq On : 08 Jun 2020 16:13
Operator : SY/MD
Sample : L2861-16
Misc : 5.0mL/MSVOA V/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
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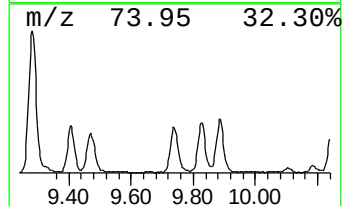
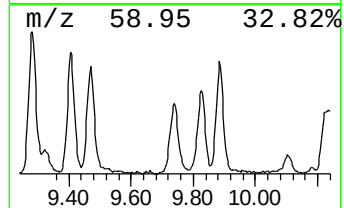
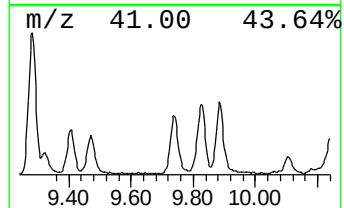
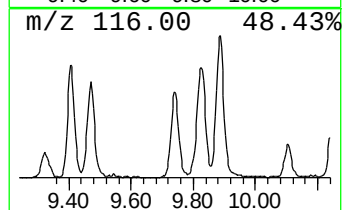
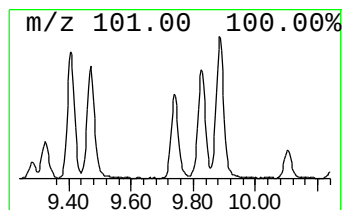
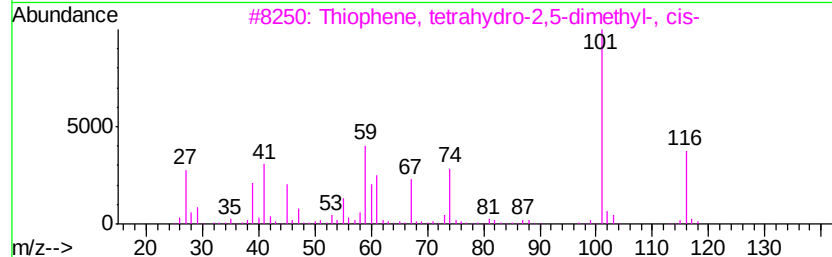
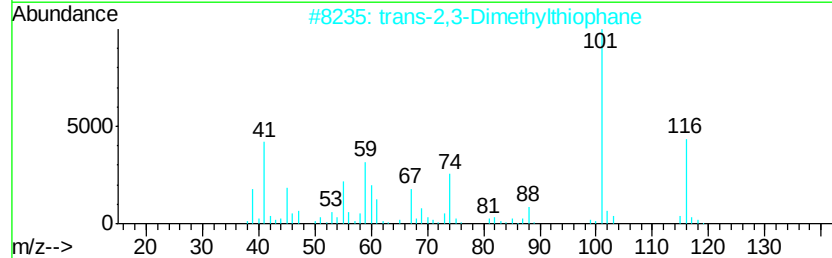
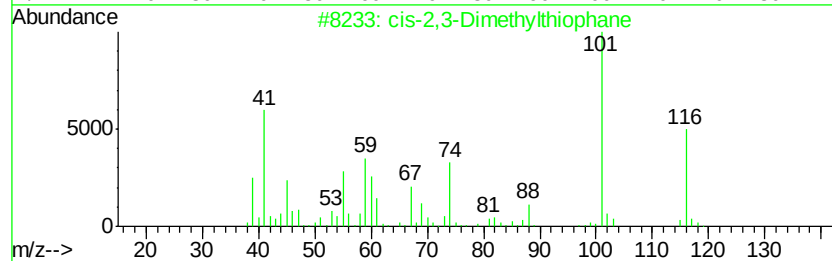
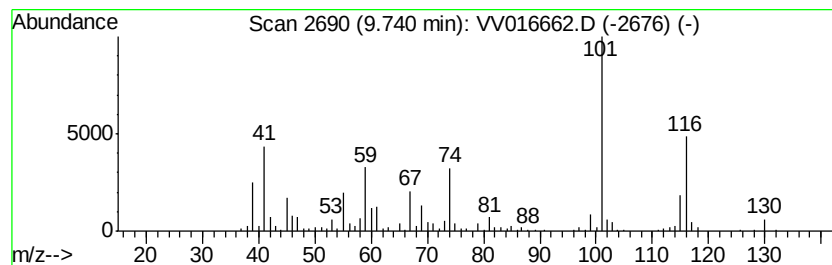
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.74	10.91 ug/L	234454	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	005161-13-7	80
4		Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-14-8	72
5		Thiazole, 4,5-dihydro-4-methyl-2...	116	C4H8N2S	010416-81-6	68



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV060820\
Data File : VV016662.D
Acq On : 08 Jun 2020 16:13
Operator : SY/MD
Sample : L2861-16
Misc : 5.0mL/MSVOA V/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F9E61

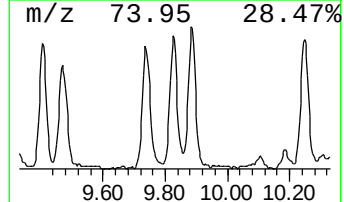
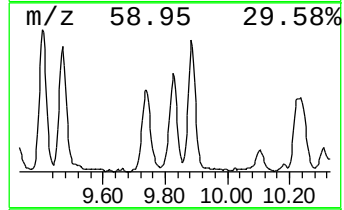
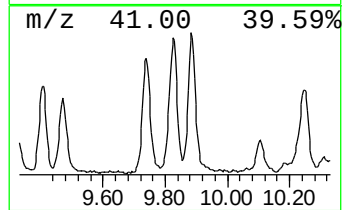
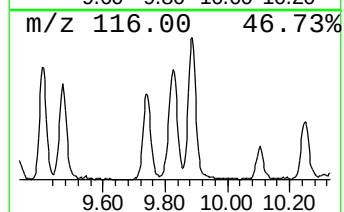
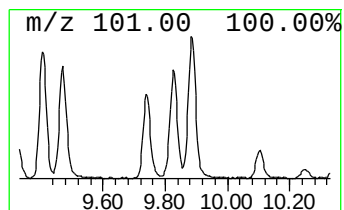
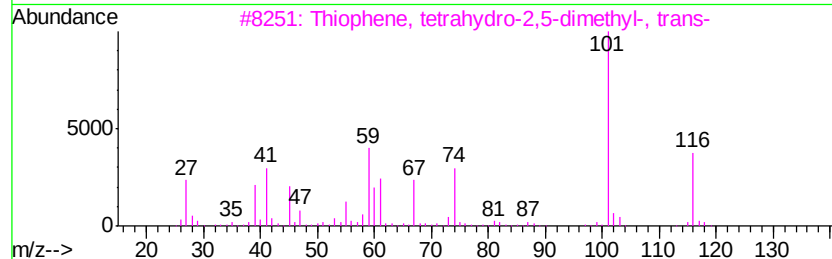
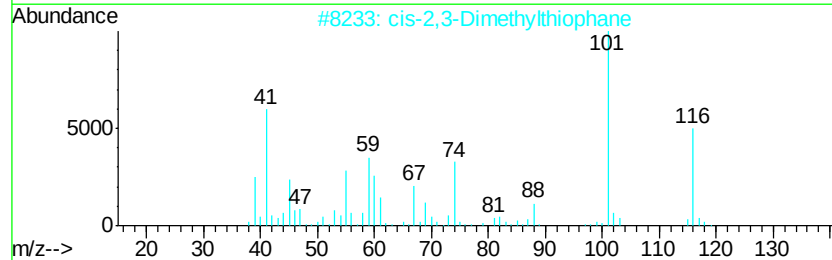
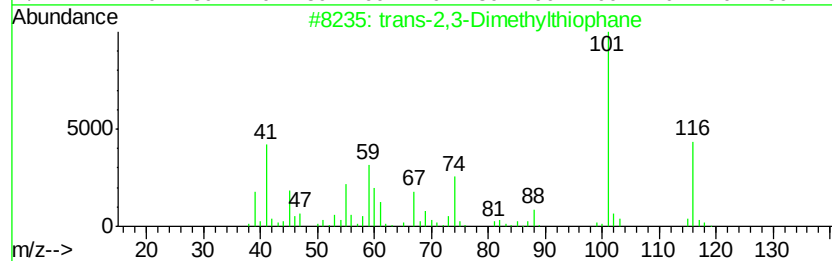
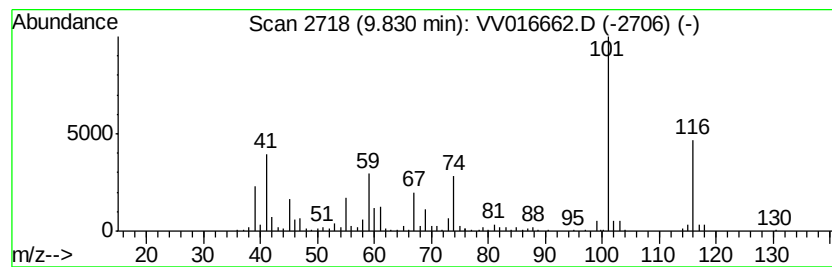
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Quant Title : VOC Analysis

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

Peak Number 7 trans-2,3-Dimethylthiophane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.83	12.62 ug/L	271150	Chlorobenzene-d5	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	94
2		cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	94
3		Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-14-8	91
4		Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-13-7	91
5		2H-Thiopyran, tetrahydro-2-methyl-	116	C6H12S	005161-16-0	87



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV060820\
Data File : VV016662.D
Acq On : 08 Jun 2020 16:13
Operator : SY/MD
Sample : L2861-16
Misc : 5.0mL/MSVOA V/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
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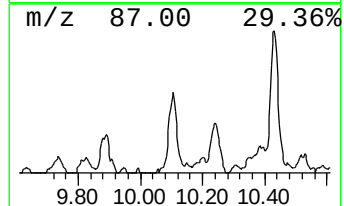
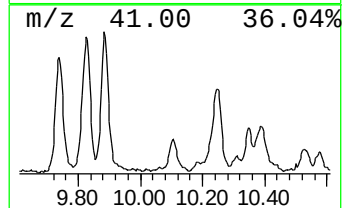
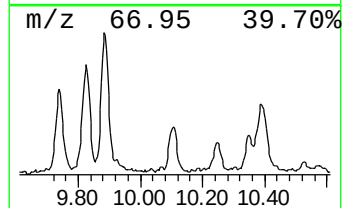
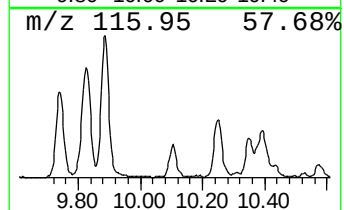
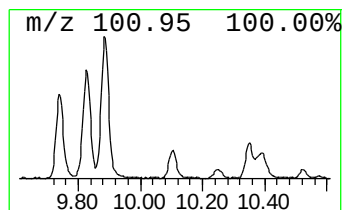
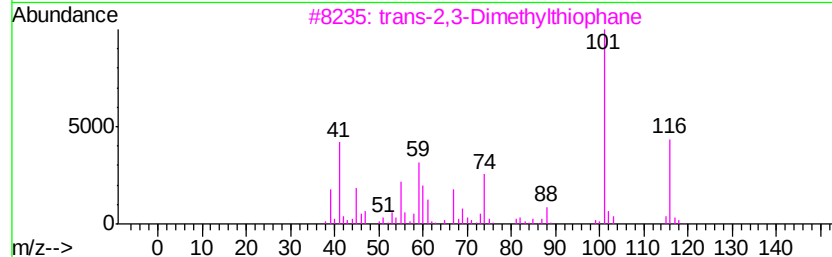
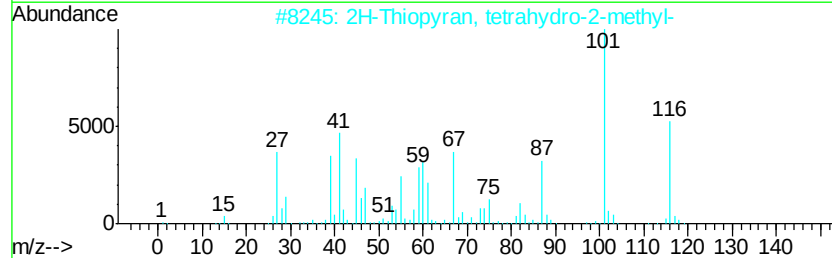
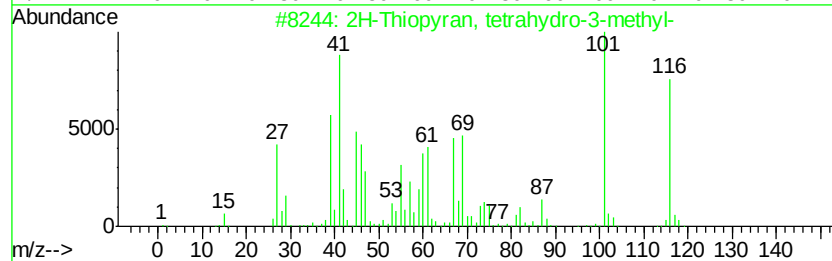
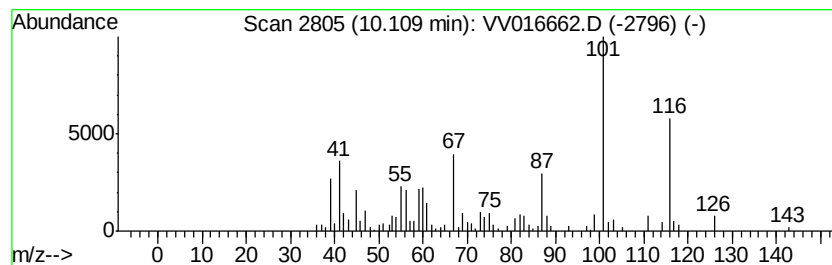
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Quant Title : VOC Analysis

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

Peak Number 9 2H-Thiopyran, tetrahydro-3-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.11	3.72 ug/L	83652	1,4-Dichlorobenzene-d4	11.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2H-Thiopyran, tetrahydro-3-methyl-	116	C6H12S	005258-50-4	87
2		2H-Thiopyran, tetrahydro-2-methyl-	116	C6H12S	005161-16-0	72
3		trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	68
4		Thiazole, 4,5-dihydro-4-methyl-2...	116	C4H8N2S	010416-81-6	52
5		Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-14-8	45



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV060820\
Data File : VV016662.D
Acq On : 08 Jun 2020 16:13
Operator : SY/MD
Sample : L2861-16
Misc : 5.0mL/MSVOA V/WATER
ALS Vial : 18 Sample Multiplier: 1

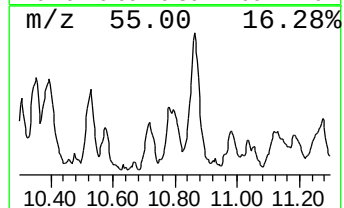
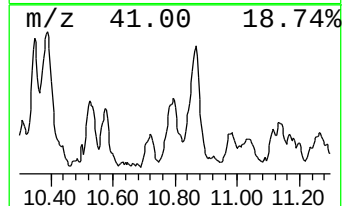
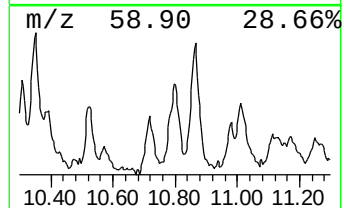
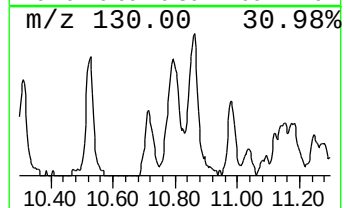
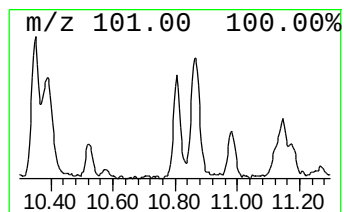
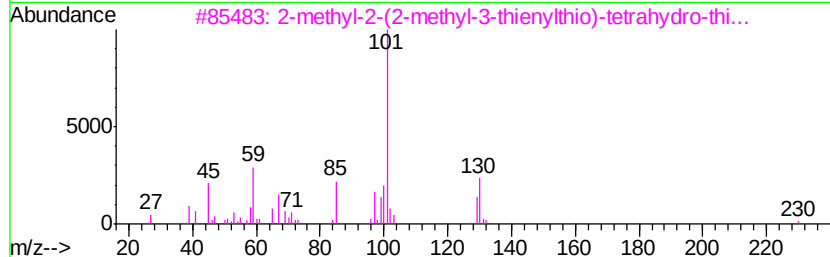
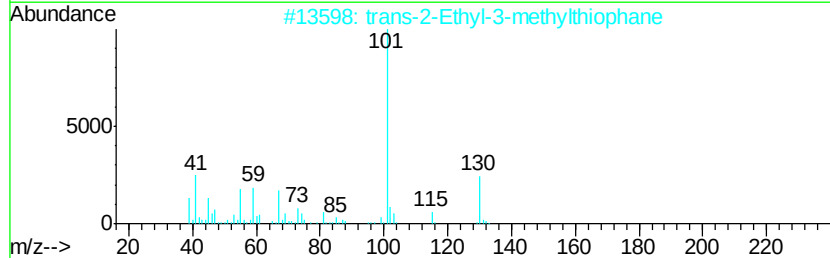
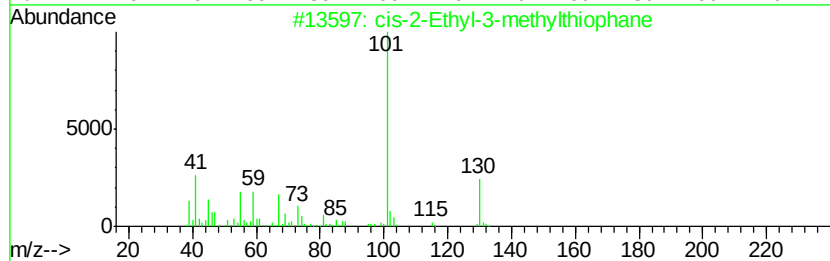
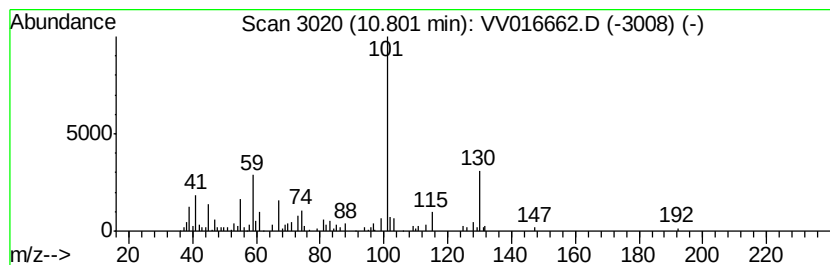
Instrument :
MSVOA_V
ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060820WMA.M
Quant Title : VOC Analysis

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

Peak Number 10 cis-2-Ethyl-3-methylthiophane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	2.69 ug/L	60595	1,4-Dichlorobenzene-d4	11.27
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		cis-2-Ethyl-3-methylthiophane	130 C7H14S	061568-37-4 53
2		trans-2-Ethyl-3-methylthiophane	130 C7H14S	061568-36-3 50
3		2-methyl-2-(2-methyl-3-thienylthio)-tetrahydro-thi...	230 C10H14S3	1000365-97-2 47
4		Thiophene, tetrahydro-2,5-dimeth...	116 C6H12S	005161-13-7 43
5		1,2,4-Thiadiazole, 5-amino-	101 C2H3N3S	007552-07-0 43



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV060820\
Data File : VV016662.D
Acq On : 08 Jun 2020 16:13
Operator : SY/MD
Sample : L2861-16
Misc : 5.0mL/MSVOA V/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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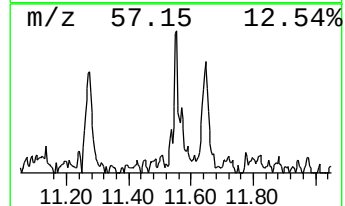
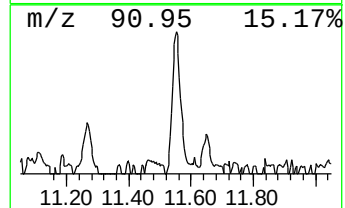
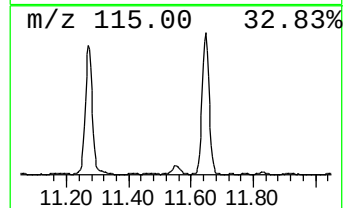
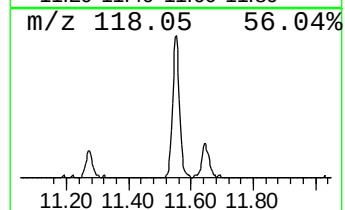
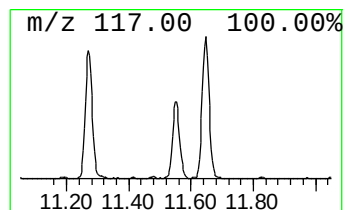
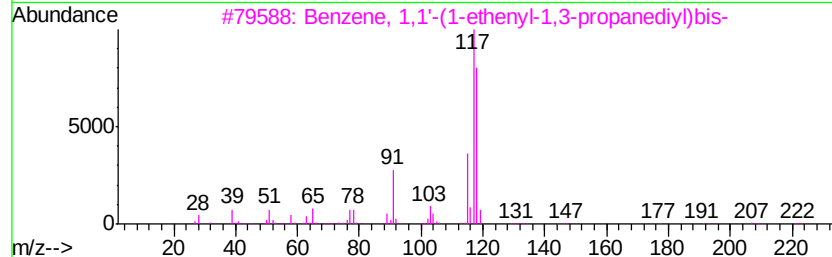
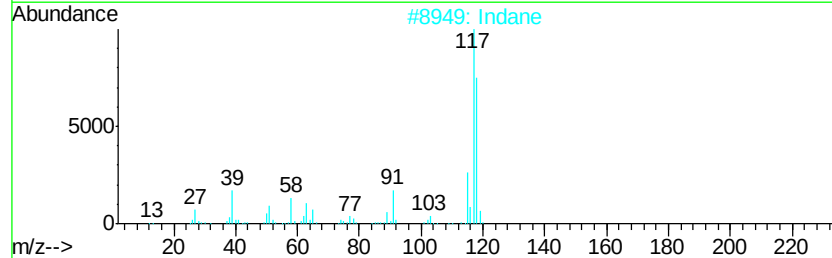
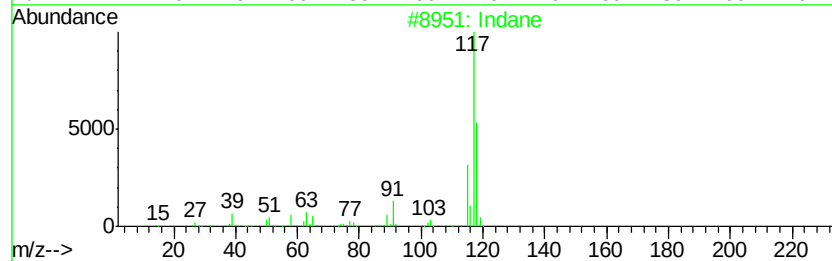
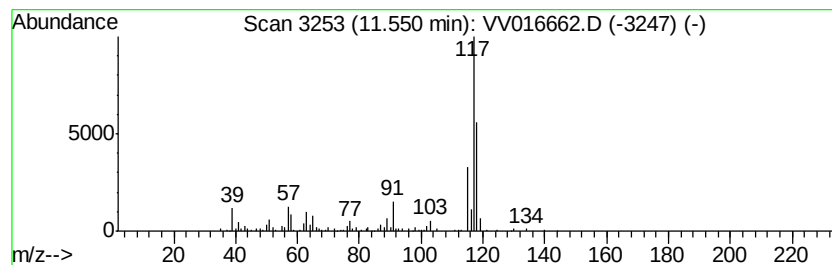
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Quant Title : VOC Analysis

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

Peak Number 11 Indane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.55	3.88 ug/L	87412	1,4-Dichlorobenzene-d4	11.27

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane			118	C9H10	000496-11-7	94
2	Indane			118	C9H10	000496-11-7	91
3	Benzene, 1,1'-(1-ethenvl-1,3-pro...			222	C17H18	061141-97-7	90
4	Indane			118	C9H10	000496-11-7	87
5	Benzene, 2-propenyl-			118	C9H10	000300-57-2	87



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV060820\
Data File : VV016662.D
Acq On : 08 Jun 2020 16:13
Operator : SY/MD
Sample : L2861-16
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F9E61

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
Diethyl sulfide	5.97	3.7	ug/L	66127	1	5.64	888112	50.0
Thiophene, tetrahydro	9.28	28.0	ug/L	600955	2	8.87	1074620	50.0
Thiophene, tetrahydro	9.41	10.8	ug/L	231651	2	8.87	1074620	50.0
cis-2,3-Dimethyltetrahydro	9.74	10.9	ug/L	234454	2	8.87	1074620	50.0
trans-2,3-Dimethyltetrahydro	9.83	12.6	ug/L	271150	2	8.87	1074620	50.0
2H-Thiopyran, tetrahydro	10.11	3.7	ug/L	83652	3	11.27	1125520	50.0
cis-2-Ethyl-3-methyltetrahydro	10.80	2.7	ug/L	60595	3	11.27	1125520	50.0
Indane	11.55	3.9	ug/L	87412	3	11.27	1125520	50.0