LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV060520\
Data File : VV016544.D
Acq On : 05 Jun 2020 18:28
Operator : SY/MD
Sample : L2861-16
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : F9E61

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % 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_V\METHOD\SOMVLM060320WMA.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	15	rVB3	15687	14594	1.02%	0.104%
2	1.219	37	40	52	rVB2	22715	24855	1.74%	0.176%
3	1.312	62	69	78	rBV	208665	213246	14.97%	1.513%
4	1.560	139	146	159	rVB	127469	153416	10.77%	1.088%
5	2.116	309	319	332	rBV	289660	430040	30.18%	3.051%
6	2.486	427	434	437	rBV6	4826	5990	0.42%	0.042%
7	2.586	457	465	467	rBV6	4691	5885	0.41%	0.042%
8	2.643	479	483	486	rBV6	1540	1617	0.11%	0.011%
9	2.682	492	495	500	rVB6	1593	1398	0.10%	0.010%
10	2.762	515	520	522	rBV5	1474	1211	0.09%	0.009%
11	2.885	554	558	561	rBV4	1268	1113	0.08%	0.008%
12	2.971	581	585	588	rVV6	1260	1279	0.09%	0.009%
13	3.213	652	660	663	rBV6	4327	6497	0.46%	0.046%
14	3.772	830	834	835	rBV3	1809	1159	0.08%	0.008%
15	3.782	835	837	840	rVV4	1558	1229	0.09%	0.009%
16	3.894	862	872	904	rBV	110613	292104	20.50%	2.072%
17	4.106	936	938	942	rBV4	1682	1408	0.10%	0.010%
18	4.373	1000	1021	1041	rBV	229048	563727	39.57%	3.999%
19	4.634	1097	1102	1104	rBV5	1456	1120	0.08%	0.008%
20	4.701	1111	1123	1135	rVV8	11376	28612	2.01%	0.203%
21	4.942	1195	1198	1201	rBV3	1420	1209	0.08%	0.009%
22	5.068	1218	1237	1248	rBV2	555406	1424690	100.00%	10.108%
23	5.335	1317	1320	1322	rBV4	2016	1412	0.10%	0.010%
24	5.640	1402	1415	1443	rBV	507129	1008622	70.80%	7.156%
25	5.769	1453	1455	1462	rVV7	1368	1680	0.12%	0.012%
26	5.801	1462	1465	1472	rVB8	2177	2306	0.16%	0.016%
27	5.872	1484	1487	1491	rVB4	1829	1258	0.09%	0.009%
28	5.968	1507	1517	1530	rVV3	28519	55825	3.92%	0.396%
29	6.093	1543	1556	1578	rVV	317211	639907	44.92%	4.540%
30	6.338	1630	1632	1637	rVB4	1655	1121	0.08%	0.008%
31	6.399	1644	1651	1653	rBV7	2262	2227	0.16%	0.016%
32	6.582	1705	1708	1711	rBV2	1456	1211	0.09%	0.009%
33	6.647	1726	1728	1732	rVV6	1580	1262	0.09%	0.009%
34	6.772	1763	1767	1770	rBV4	1328	1117	0.08%	0.008%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV060520\
Data File : VV016544.D
Acq On : 05 Jun 2020 18:28
Operator : SY/MD
Sample : L2861-16
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : F9E61

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % 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_V\METHOD\SOMVLM060320WMA.M
Title : VOC Analysis

35	6.827	1774	1784	1793	rVB	12447	21691	1.52%	0.154%
36	7.007	1828	1840	1857	rBV	191931	358915	25.19%	2.546%
37	7.171	1880	1891	1900	rBV	4301	10430	0.73%	0.074%
38	7.338	1926	1943	1957	rVV	662260	1166773	81.90%	8.278%
39	7.412	1959	1966	1982	rVB	43148	77736	5.46%	0.552%
40	7.598	2022	2024	2025	rVV2	2576	1106	0.08%	0.008%
41	7.640	2028	2037	2055	rVB	120891	202197	14.19%	1.435%
42	7.872	2100	2109	2123	rVB9	8116	19078	1.34%	0.135%
43	7.952	2129	2134	2135	rBV4	1412	1218	0.09%	0.009%
44	8.106	2172	2182	2206	rBV	419775	715698	50.24%	5.078%
45	8.238	2216	2223	2236	rVB2	21916	36028	2.53%	0.256%
46	8.515	2303	2309	2311	rBV8	2044	2036	0.14%	0.014%
47	8.663	2352	2355	2357	rVV3	1613	1111	0.08%	0.008%
48	8.794	2388	2396	2401	rBV3	5377	9627	0.68%	0.068%
49	8.872	2409	2420	2431	rBV	754359	1212725	85.12%	8.604%
50	9.036	2462	2471	2484	rBV	48446	78640	5.52%	0.558%
51	9.129	2496	2500	2502	rBV4	4597	4075	0.29%	0.029%
52	9.164	2504	2511	2528	rVB2	28999	53415	3.75%	0.379%
53	9.283	2536	2548	2557	rBV	302916	506038	35.52%	3.590%
54	9.405	2577	2586	2597	rBV	116160	185312	13.01%	1.315%
55	9.470	2597	2606	2620	rVV	99248	171289	12.02%	1.215%
56	9.566	2630	2636	2652	rVB3	18274	29352	2.06%	0.208%
57	9.740	2678	2690	2702	rVV3	98817	180691	12.68%	1.282%
58	9.826	2705	2717	2726	rVV	122642	224638	15.77%	1.594%
59	9.884	2726	2735	2753	rVB	141636	240271	16.86%	1.705%
60	10.103	2788	2803	2818	rVB4	41354	78205	5.49%	0.555%
61	10.190	2822	2830	2833	rBV8	8750	13732	0.96%	0.097%
62	10.238	2834	2845	2859	rVB	493102	809498	56.82%	5.743%
63	10.309	2860	2867	2872	rBV3	17435	24190	1.70%	0.172%
64	10.351	2874	2880	2885	rBV3	28504	40038	2.81%	0.284%
65	10.524	2928	2934	2944	rBV4	22171	34443	2.42%	0.244%
66	10.717	2984	2994	3003	rBV8	18129	37889	2.66%	0.269%
67	11.119	3112	3119	3124	rBV8	11439	20230	1.42%	0.144%
68	11.270	3152	3166	3187	rBV	803334	1259000	88.37%	8.932%
69	11.553	3246	3254	3264	rBV2	37584	61844	4.34%	0.439%
70	11.646	3272	3283	3304	rVB	725707	1137057	79.81%	8.067%
71	11.759	3315	3318	3319	rBV3	2483	1517	0.11%	0.011%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV060520\
Data File : VV016544.D
Acq On : 05 Jun 2020 18:28
Operator : SY/MD
Sample : L2861-16
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : F9E61

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % 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_V\METHOD\SOMVLM060320WMA.M
Title : VOC Analysis

72	12.116	3423	3429	3430	rBV5	3855	4074	0.29%	0.029%
73	12.254	3469	3472	3473	rBV3	2611	1645	0.12%	0.012%
74	12.341	3497	3499	3503	rBV5	2655	1474	0.10%	0.010%
75	12.518	3549	3554	3568	rVB5	7118	13703	0.96%	0.097%
76	12.756	3621	3628	3631	rBV8	3635	4613	0.32%	0.033%
77	13.068	3716	3725	3727	rBV7	4488	6096	0.43%	0.043%
78	13.251	3772	3782	3785	rBV7	3598	5477	0.38%	0.039%
79	13.334	3804	3808	3811	rBV6	1836	1565	0.11%	0.011%
80	13.527	3860	3868	3879	rVB	26612	42591	2.99%	0.302%
81	13.601	3888	3891	3895	rVB6	1782	1480	0.10%	0.011%
82	13.649	3897	3906	3918	rVV	11837	20828	1.46%	0.148%
83	13.778	3940	3946	3947	rBV5	1715	1594	0.11%	0.011%
84	13.855	3965	3970	3971	rBV4	2409	1771	0.12%	0.013%
85	13.984	4008	4010	4015	rVB5	1781	1140	0.08%	0.008%
86	14.167	4062	4067	4072	rBV9	2576	2533	0.18%	0.018%
87	14.193	4072	4075	4078	rBV4	2238	1781	0.13%	0.013%
88	14.318	4103	4114	4119	rBV4	7779	12886	0.90%	0.091%
89	14.412	4141	4143	4148	rVB5	2208	1459	0.10%	0.010%
90	14.460	4155	4158	4165	rVB8	2194	2154	0.15%	0.015%
91	14.598	4199	4201	4204	rBV3	2053	1314	0.09%	0.009%
92	14.656	4215	4219	4220	rBV3	3296	2000	0.14%	0.014%
93	14.846	4268	4278	4293	rVB9	14749	31989	2.25%	0.227%
94	14.907	4293	4297	4300	rBV6	1542	1432	0.10%	0.010%
95	14.942	4306	4308	4312	rBV4	1571	1167	0.08%	0.008%
96	15.026	4332	4334	4340	rVB5	1617	1129	0.08%	0.008%
97	15.321	4424	4426	4429	rBV3	1720	1161	0.08%	0.008%
98	15.649	4524	4528	4530	rBV4	1648	1385	0.10%	0.010%
99	15.688	4538	4540	4543	rBV3	1845	1299	0.09%	0.009%
100	15.778	4566	4568	4573	rBV5	1599	1213	0.09%	0.009%

Sum of corrected areas: 14095033

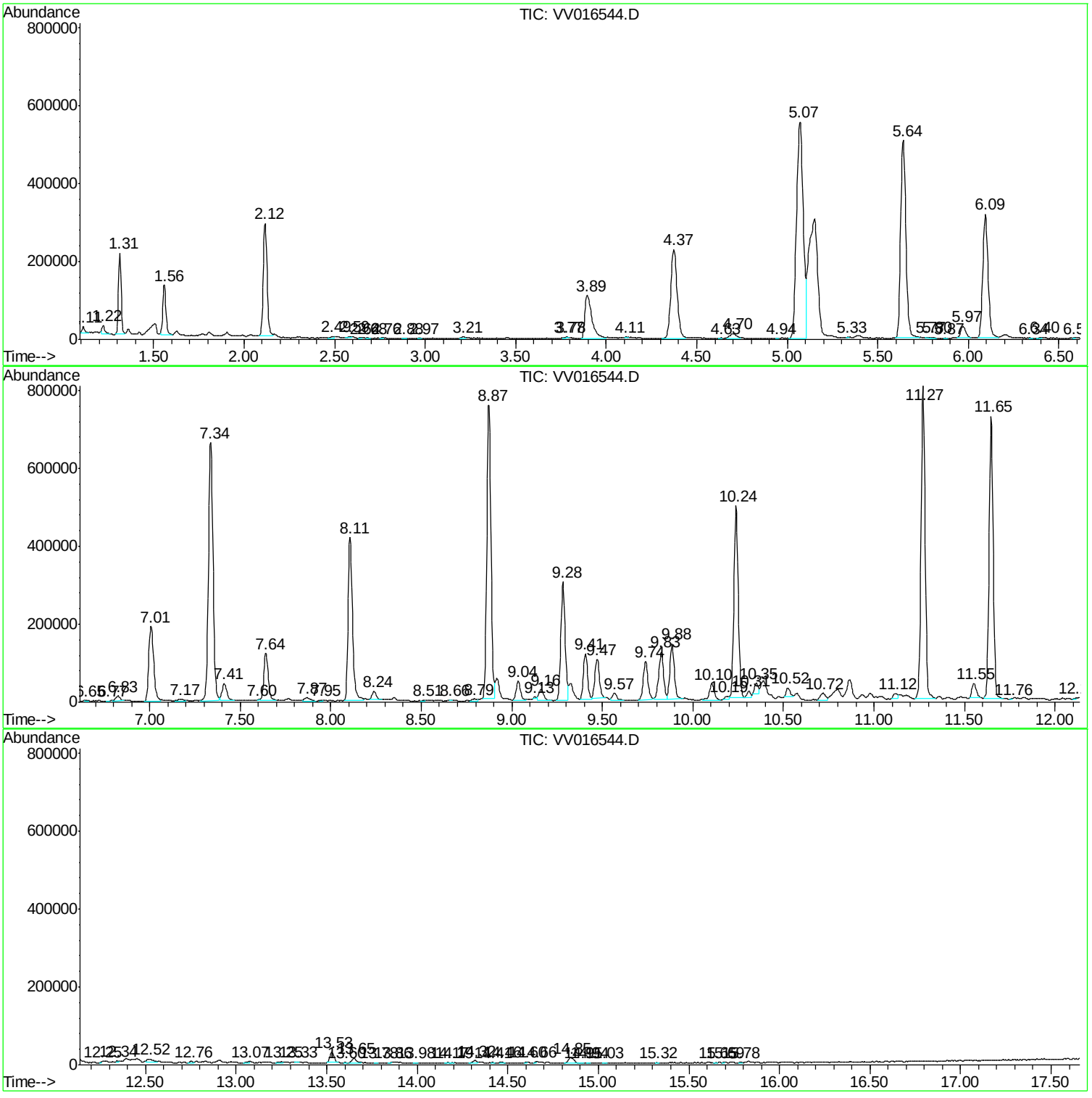
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV060520\
Data File : VV016544.D
Acq On : 05 Jun 2020 18:28
Operator : SY/MD
Sample : L2861-16
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : F9E61

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060320WMA.M
Quant Title : VOC Analysis

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV060520\
Data File : VV016544.D
Acq On : 05 Jun 2020 18:28
Operator : SY/MD
Sample : L2861-16
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : F9E61

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060320WMA.M
Quant Title : VOC Analysis

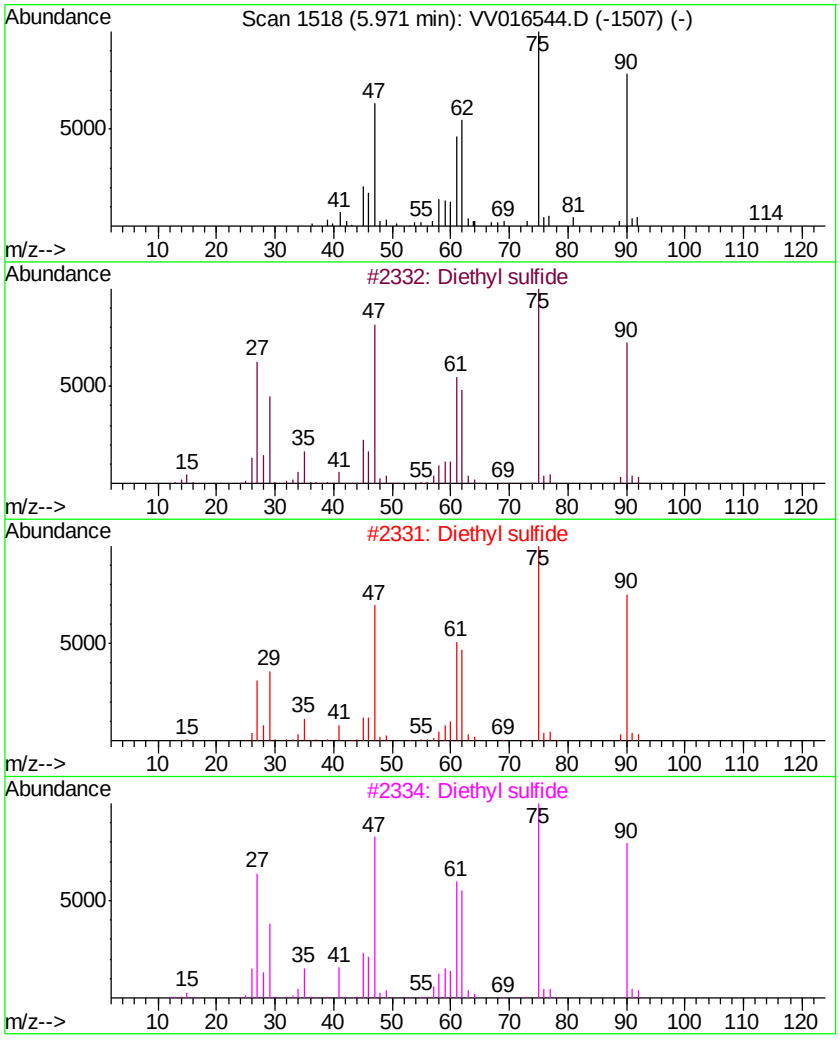
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

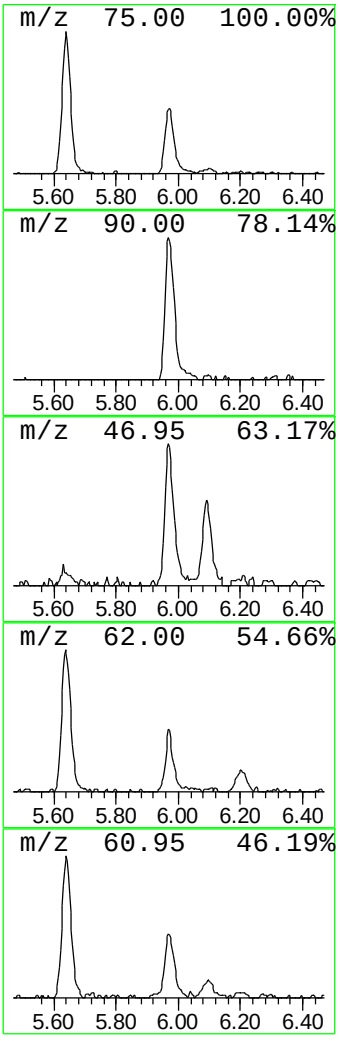
****

Peak Number 1 Diethyl sulfide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.97	2.77 ug/L	55825	1,4-Difluorobenzene	5.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyl sulfide	90	C4H10S	000352-93-2	97
2	Diethyl sulfide	90	C4H10S	000352-93-2	96
3	Diethyl sulfide	90	C4H10S	000352-93-2	94
4	Diethyl sulfide	90	C4H10S	000352-93-2	91
5	Propane, 2-(methylthio)-	90	C4H10S	001551-21-9	38





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV060520\
Data File : VV016544.D
Acq On : 05 Jun 2020 18:28
Operator : SY/MD
Sample : L2861-16
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : F9E61

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060320WMA.M
Quant Title : VOC Analysis

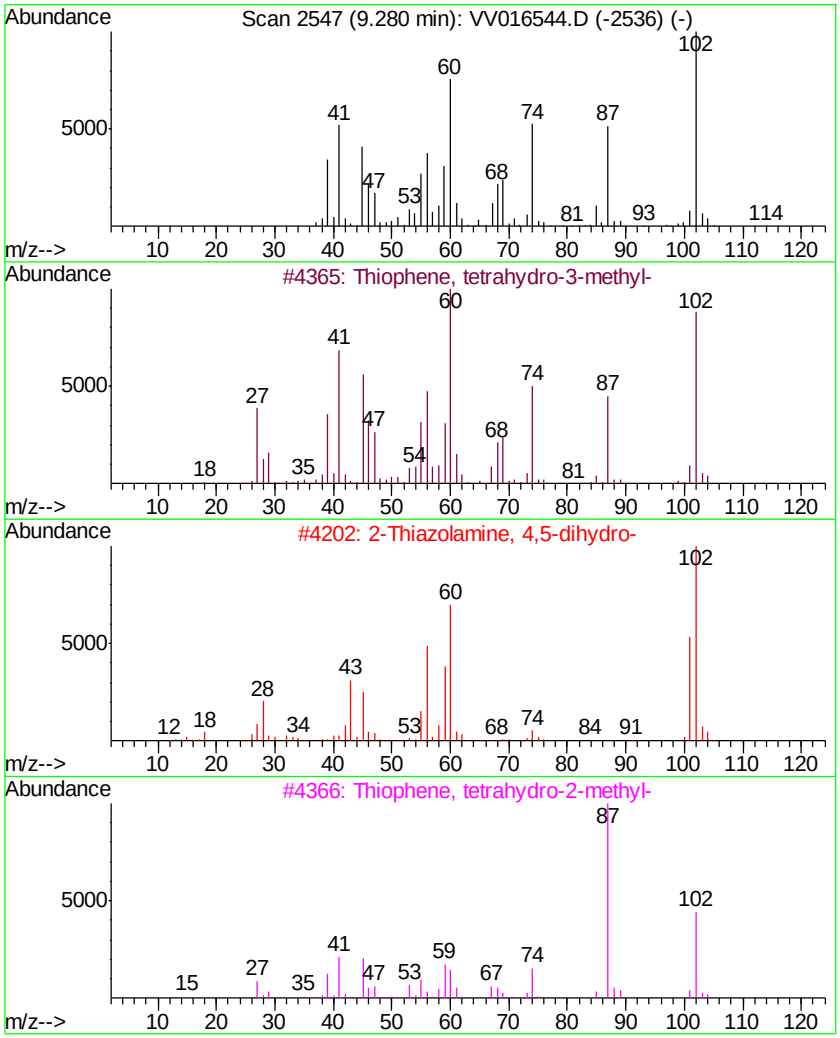
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

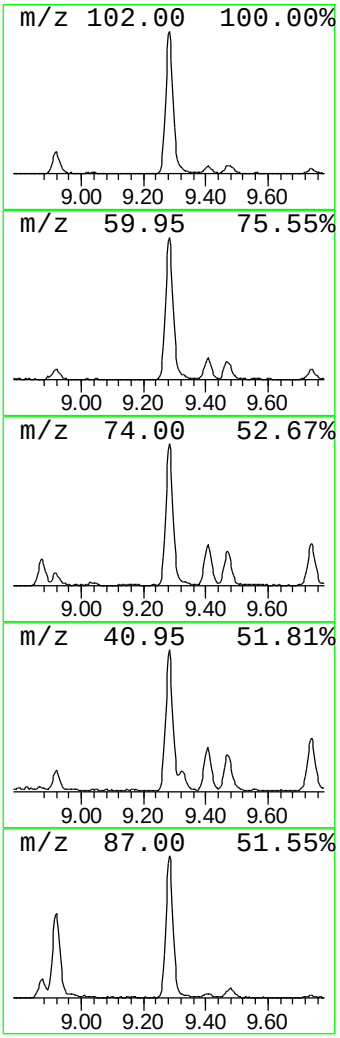
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.28	20.86 ug/L	506038	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	2-Thiazolamine, 4,5-dihydro-	102	C3H6N2S	001779-81-3	52
3	Thiophene, tetrahydro-2-methyl-	102	C5H10S	001795-09-1	43
4	2-Thiazolamine, 4,5-dihydro-	102	C3H6N2S	001779-81-3	43
5	1-Butene, 1-(methylthio)-, (Z)-	102	C5H10S	017414-15-2	41





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV060520\
Data File : VV016544.D
Acq On : 05 Jun 2020 18:28
Operator : SY/MD
Sample : L2861-16
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : F9E61

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060320WMA.M
Quant Title : VOC Analysis

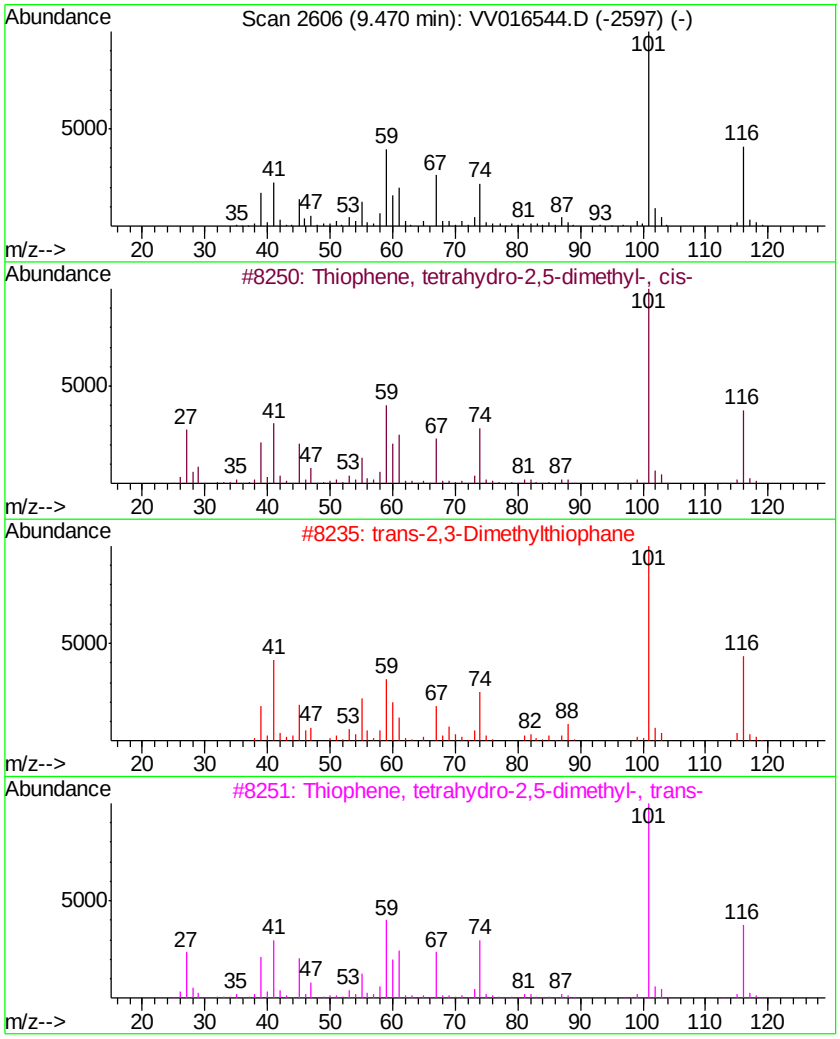
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

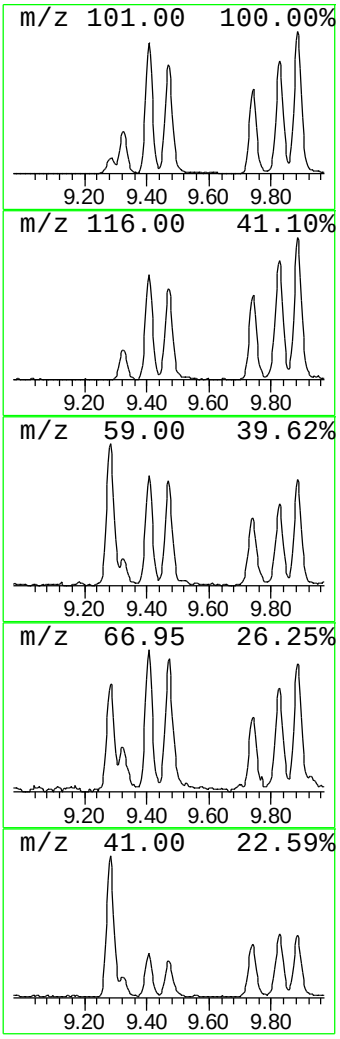
****

Peak Number 5 trans-2,3-Dimethylthiophane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.47	7.06 ug/L	171289	Chlorobenzene-d5	8.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-13-7	90
2	trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	90
3	Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-14-8	87
4	cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	74
5	2H-Thiopyran, tetrahydro-2-methyl-	116	C6H12S	005161-16-0	64





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV060520\
Data File : VV016544.D
Acq On : 05 Jun 2020 18:28
Operator : SY/MD
Sample : L2861-16
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : F9E61

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060320WMA.M
Quant Title : VOC Analysis

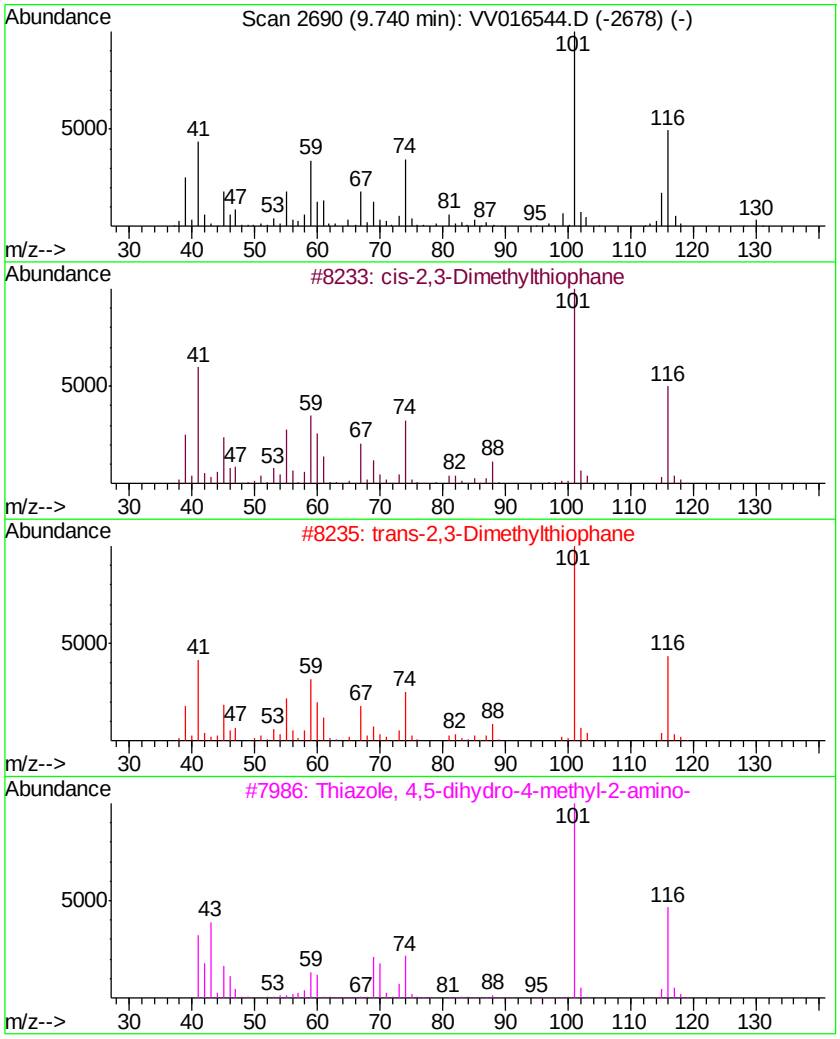
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

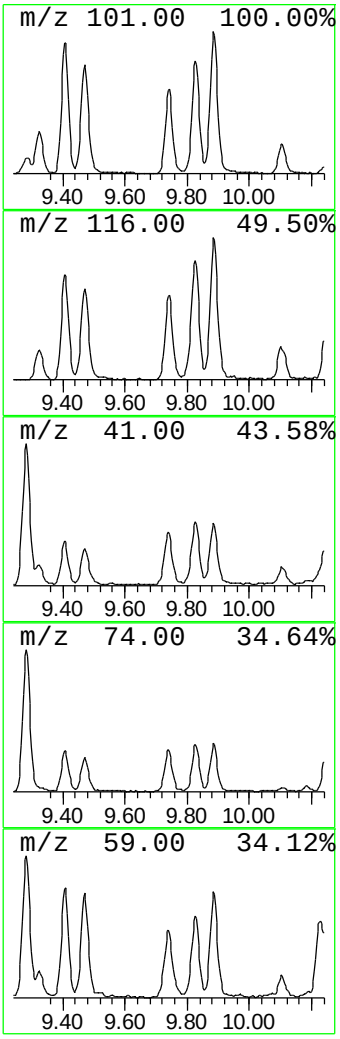
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.74	7.45 ug/L	180691	Chlorobenzene-d5	8.87

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	93
3	Thiazole, 4,5-dihydro-4-methyl-2...	116	C4H8N2S	010416-81-6	80
4	Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-14-8	64
5	Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-13-7	59





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV060520\
Data File : VV016544.D
Acq On : 05 Jun 2020 18:28
Operator : SY/MD
Sample : L2861-16
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : F9E61

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060320WMA.M
Quant Title : VOC Analysis

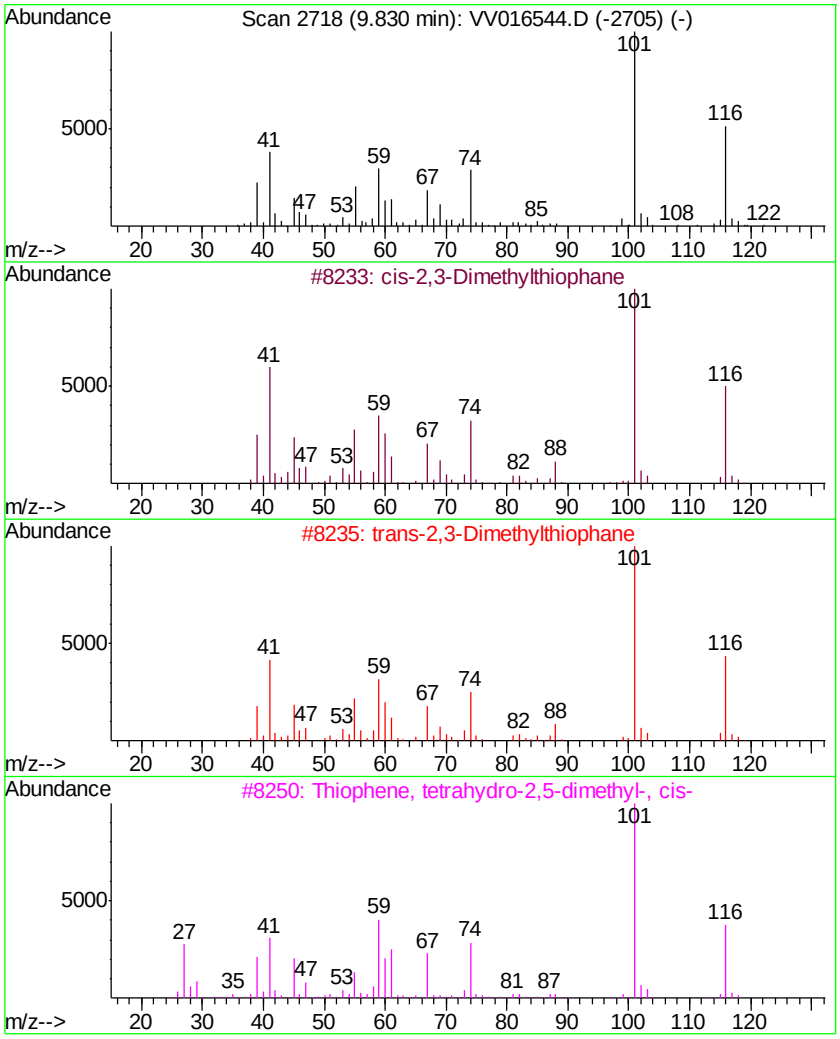
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

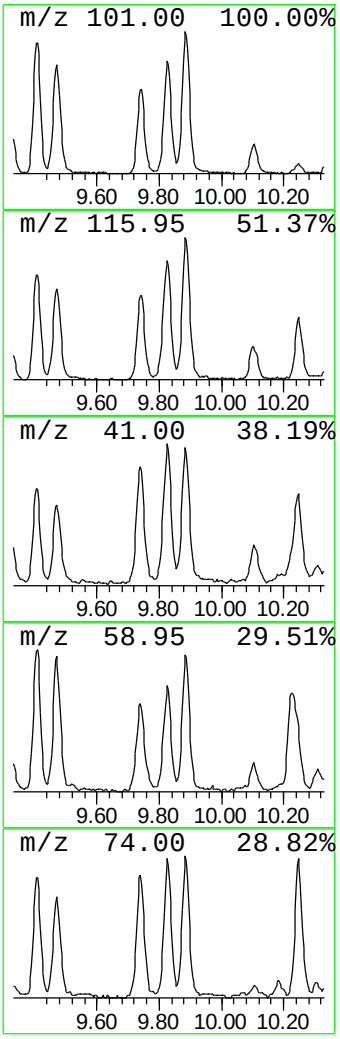
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.83	9.26 ug/L	224638	Chlorobenzene-d5	8.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	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	91
4	Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-14-8	91
5	2H-Thiopyran, tetrahydro-2-methyl-	116	C6H12S	005161-16-0	83





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV060520\
Data File : VV016544.D
Acq On : 05 Jun 2020 18:28
Operator : SY/MD
Sample : L2861-16
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : F9E61

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060320WMA.M
Quant Title : VOC Analysis

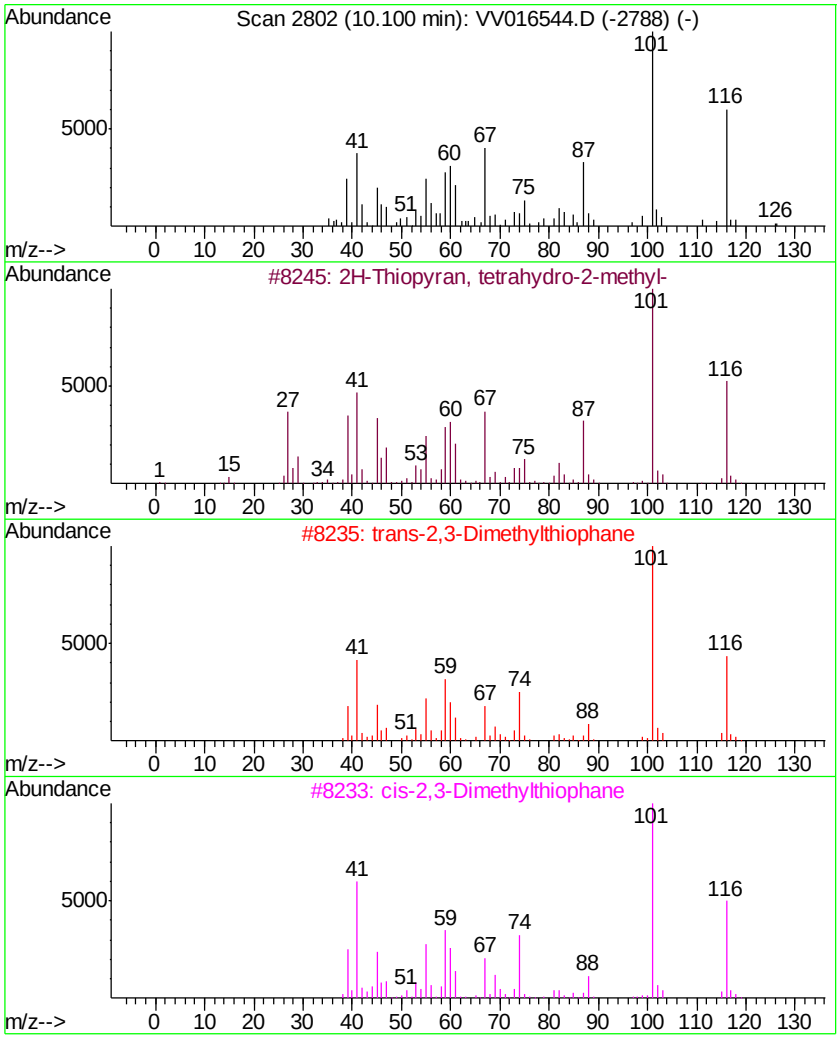
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

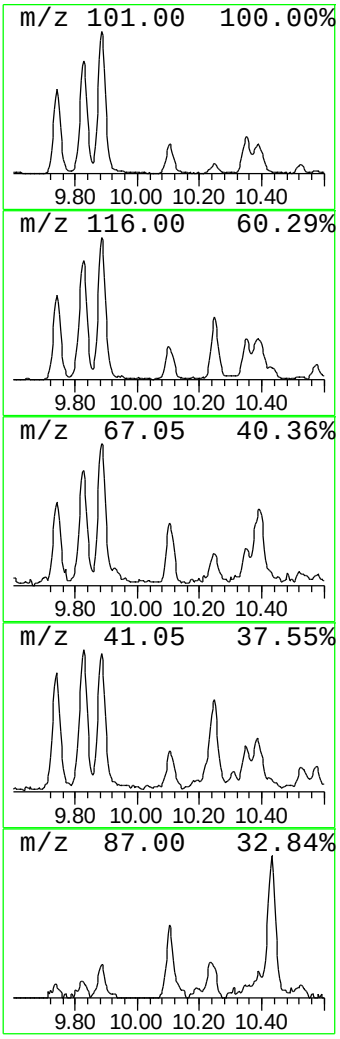
****

Peak Number 9 2H-Thiopyran, tetrahydro-2-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.10	3.11 ug/L	78205	1,4-Dichlorobenzene-d4	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Thiopyran, tetrahydro-2-methyl-	116	C6H12S	005161-16-0	95
2	trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	70
3	cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	70
4	1,2,4-Thiadiazole, 5-amino-	101	C2H3N3S	007552-07-0	43
5	Thiazole, 4,5-dihydro-4-methyl-2...	116	C4H8N2S	010416-81-6	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV060520\
Data File : VV016544.D
Acq On : 05 Jun 2020 18:28
Operator : SY/MD
Sample : L2861-16
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : F9E61

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060320WMA.M
Quant Title : VOC Analysis

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Diethyl sulfide	5.97	2.8	ug/L	55825	1	5.64	1008620	50.0
Thiophene, tetrah...	9.28	20.9	ug/L	506038	2	8.87	1212730	50.0
trans-2,3-Dimethy...	9.47	7.1	ug/L	171289	2	8.87	1212730	50.0
cis-2,3-Dimethylt...	9.74	7.5	ug/L	180691	2	8.87	1212730	50.0
Thiophene, tetrah...	9.83	9.3	ug/L	224638	2	8.87	1212730	50.0
2H-Thiopyran, tet...	10.10	3.1	ug/L	78205	3	11.27	1259000	50.0