LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060620\
Data File : VU038622.D
Acq On : 06 Jun 2020 17:16
Operator : SY/MD
Sample : L2910-15
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D36

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 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_U\METHOD\SOMUTR053120WMA.M
Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.369	3	9	19	rBV	40996	42950	2.87%	0.324%
2	1.613	73	85	93	rBV	103980	130957	8.74%	0.987%
3	1.665	95	101	108	rVV2	25208	34362	2.29%	0.259%
4	1.932	176	184	197	rVB	87878	111845	7.47%	0.843%
5	2.591	378	389	406	rBV	182641	308748	20.61%	2.327%
6	2.674	406	415	434	rVB	11165	29065	1.94%	0.219%
7	4.674	1020	1037	1074	rBV	200166	584670	39.03%	4.407%
8	4.845	1077	1090	1115	rVB2	93172	216133	14.43%	1.629%
9	5.102	1150	1170	1187	rBV	192301	422492	28.20%	3.184%
10	5.423	1251	1270	1288	rBV2	22715	50760	3.39%	0.383%
11	5.758	1353	1374	1388	rBV2	374180	995216	66.43%	7.501%
12	5.829	1389	1396	1421	rVB	39290	78716	5.25%	0.593%
13	6.279	1520	1536	1557	rBV	374918	715718	47.77%	5.395%
14	6.594	1621	1634	1647	rVB4	22851	43880	2.93%	0.331%
15	6.722	1655	1674	1691	rBV	241939	470862	31.43%	3.549%
16	6.822	1691	1705	1720	rVB3	23398	46010	3.07%	0.347%
17	7.591	1930	1944	1963	rBV2	129772	233910	15.61%	1.763%
18	7.922	2028	2047	2064	rBV	447928	783654	52.31%	5.907%
19	8.201	2120	2134	2147	rBV2	78506	132371	8.84%	0.998%
20	8.439	2199	2208	2217	rBV5	9181	16022	1.07%	0.121%
21	8.655	2260	2275	2306	rBV	825952	1498130	100.00%	11.292%
22	9.436	2504	2518	2550	rBV	543368	916870	61.20%	6.911%
23	9.844	2632	2645	2656	rBV	226130	401491	26.80%	3.026%
24	10.295	2771	2785	2797	rBV4	57503	105419	7.04%	0.795%
25	10.378	2797	2811	2821	rVV3	93931	171129	11.42%	1.290%
26	10.439	2821	2830	2849	rVV	111709	197782	13.20%	1.491%
27	10.770	2914	2933	2938	rBV	232001	421735	28.15%	3.179%
28	10.860	2954	2961	2968	rVB2	29317	39687	2.65%	0.299%
29	10.906	2968	2975	2979	rVV6	24570	36085	2.41%	0.272%
30	10.951	2979	2989	3006	rVB6	203367	450189	30.05%	3.393%
31	11.131	3037	3045	3057	rVB6	19025	31820	2.12%	0.240%
32	11.272	3079	3089	3098	rBV6	14561	27053	1.81%	0.204%
33	11.336	3099	3109	3118	rVV2	53444	89430	5.97%	0.674%
34	11.414	3118	3133	3149	rVB6	138948	367985	24.56%	2.774%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060620\
Data File : VU038622.D
Acq On : 06 Jun 2020 17:16
Operator : SY/MD
Sample : L2910-15
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D36

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 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_U\METHOD\SOMUTR053120WMA.M
Title : TRACE VOA SOM01.0

35	11.536	3160	3171	3180	rBV	27977	44305	2.96%	0.334%
36	11.590	3180	3188	3196	rBV7	12034	20706	1.38%	0.156%
37	11.648	3196	3206	3211	rBV6	43584	80947	5.40%	0.610%
38	11.822	3248	3260	3271	rBV	630362	999835	66.74%	7.536%
39	12.024	3312	3323	3330	rVV5	35668	68522	4.57%	0.516%
40	12.082	3331	3341	3355	rVV4	70993	169170	11.29%	1.275%
41	12.201	3359	3378	3399	rVB	540895	1063806	71.01%	8.018%
42	12.391	3430	3437	3442	rBV8	14309	23099	1.54%	0.174%
43	12.430	3443	3449	3457	rVB6	29357	44908	3.00%	0.338%
44	12.687	3522	3529	3533	rBV8	15148	23225	1.55%	0.175%
45	12.828	3559	3573	3576	rBV10	13381	26686	1.78%	0.201%
46	12.970	3606	3617	3620	rBV10	12163	21697	1.45%	0.164%
47	13.166	3672	3678	3692	rVB10	23565	44243	2.95%	0.333%
48	14.278	4014	4024	4036	rBV10	8855	18755	1.25%	0.141%
49	14.468	4075	4083	4091	rBV10	10161	16830	1.12%	0.127%
50	15.073	4258	4271	4282	rVB8	19601	35389	2.36%	0.267%
51	15.352	4348	4358	4368	rBV8	25355	42312	2.82%	0.319%
52	15.436	4375	4384	4390	rBV8	12367	21587	1.44%	0.163%
53	15.481	4390	4398	4411	rVB3	25388	45730	3.05%	0.345%
54	15.603	4427	4436	4448	rBV3	20583	34031	2.27%	0.256%
55	17.384	4979	4990	5007	rVB2	116600	218527	14.59%	1.647%

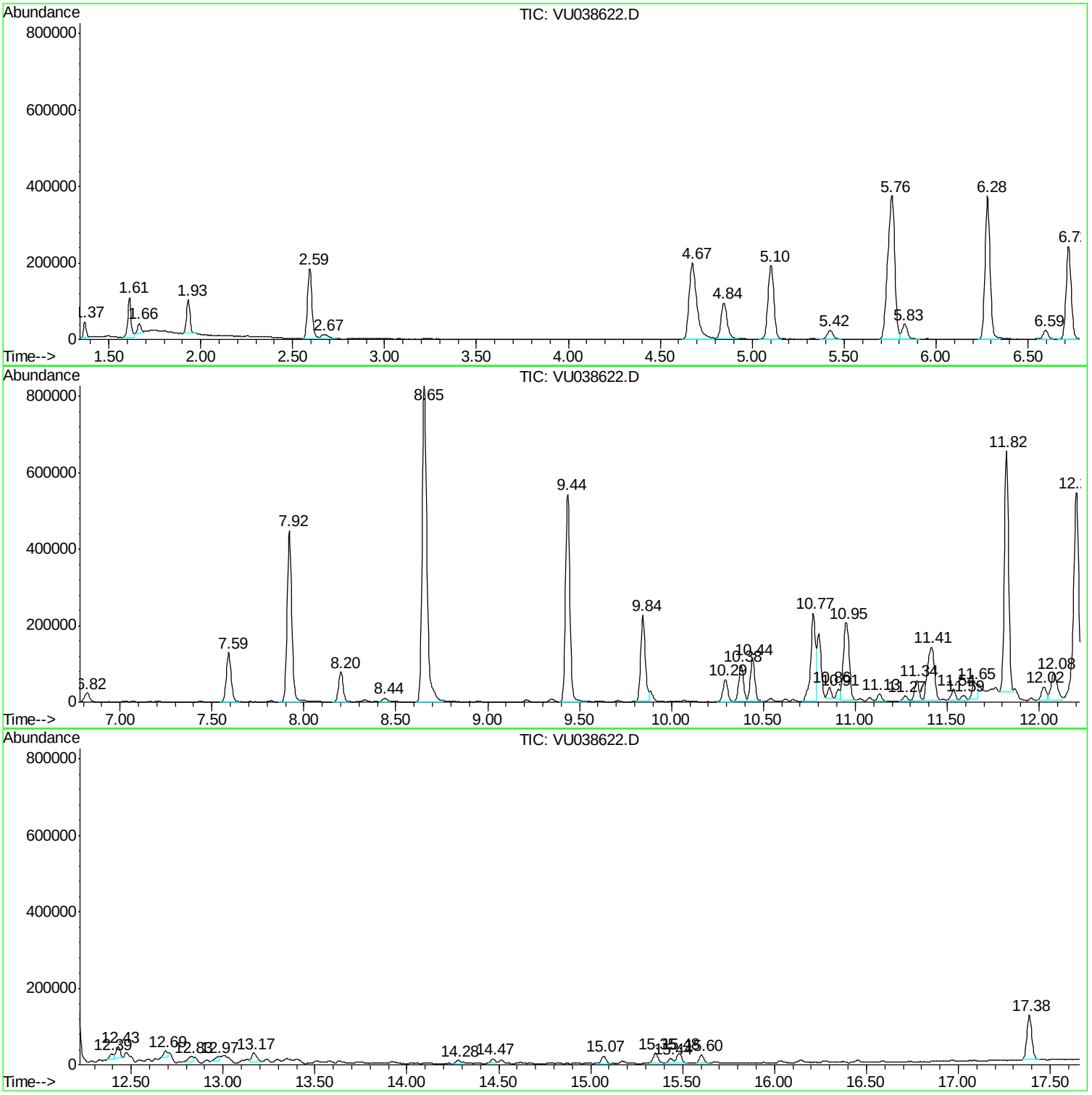
Sum of corrected areas: 13267456

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060620\
Data File : VU038622.D
Acq On : 06 Jun 2020 17:16
Operator : SY/MD
Sample : L2910-15
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D36

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060620\
Data File : VU038622.D
Acq On : 06 Jun 2020 17:16
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ClientSampleId : F9D36

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

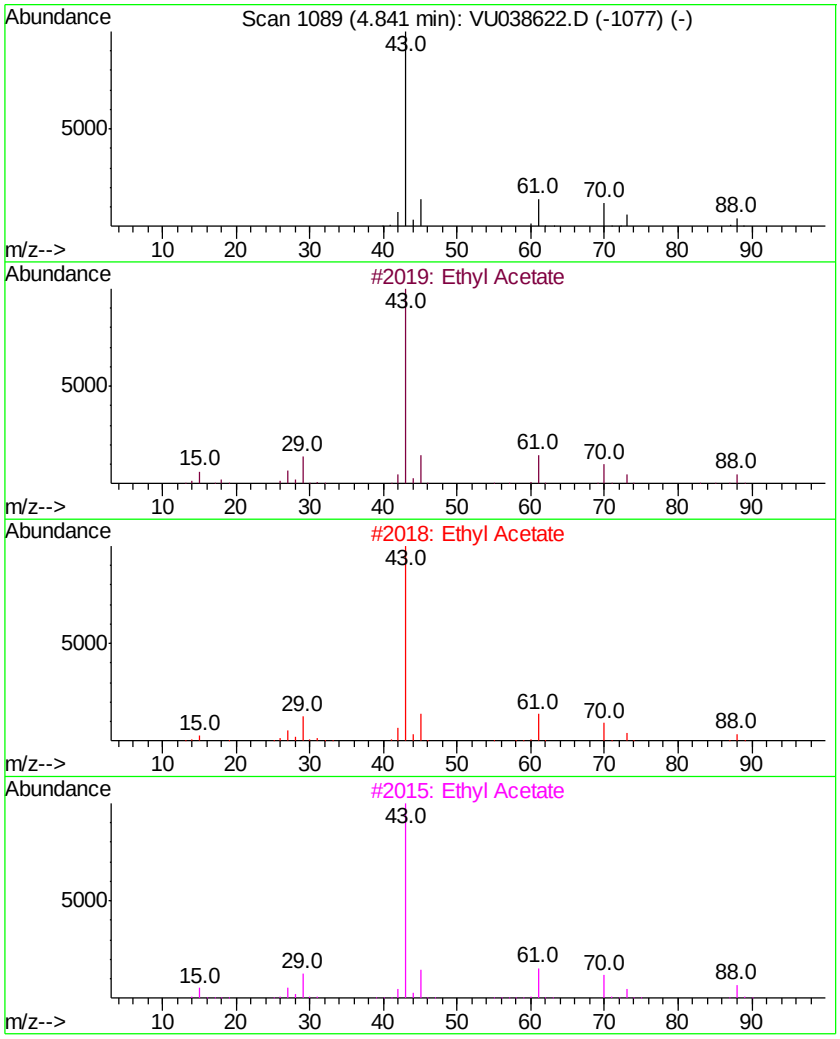
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

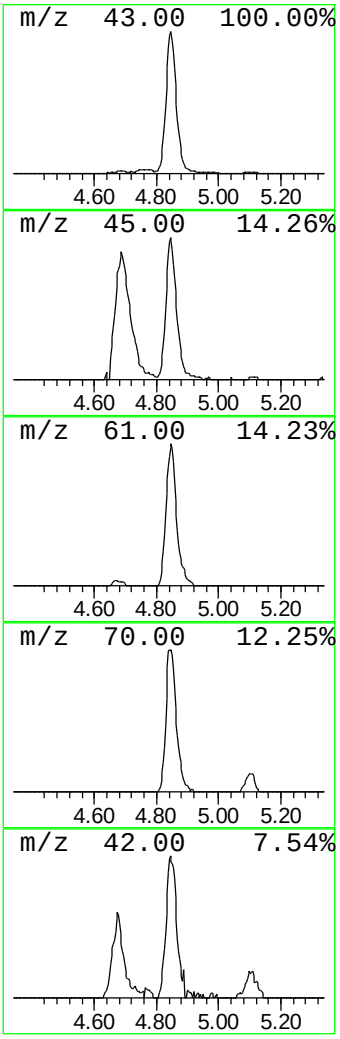
****

Peak Number 1 Ethyl Acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	1.51 ug/L	216133	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl Acetate	88	C4H8O2	000141-78-6	90
2	Ethyl Acetate	88	C4H8O2	000141-78-6	86
3	Ethyl Acetate	88	C4H8O2	000141-78-6	78
4	Ethyl Acetate	88	C4H8O2	000141-78-6	64
5	CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	40





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU060620\
Data File : VU038622.D
Acq On : 06 Jun 2020 17:16
Operator : SY/MD
Sample : L2910-15
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D36

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

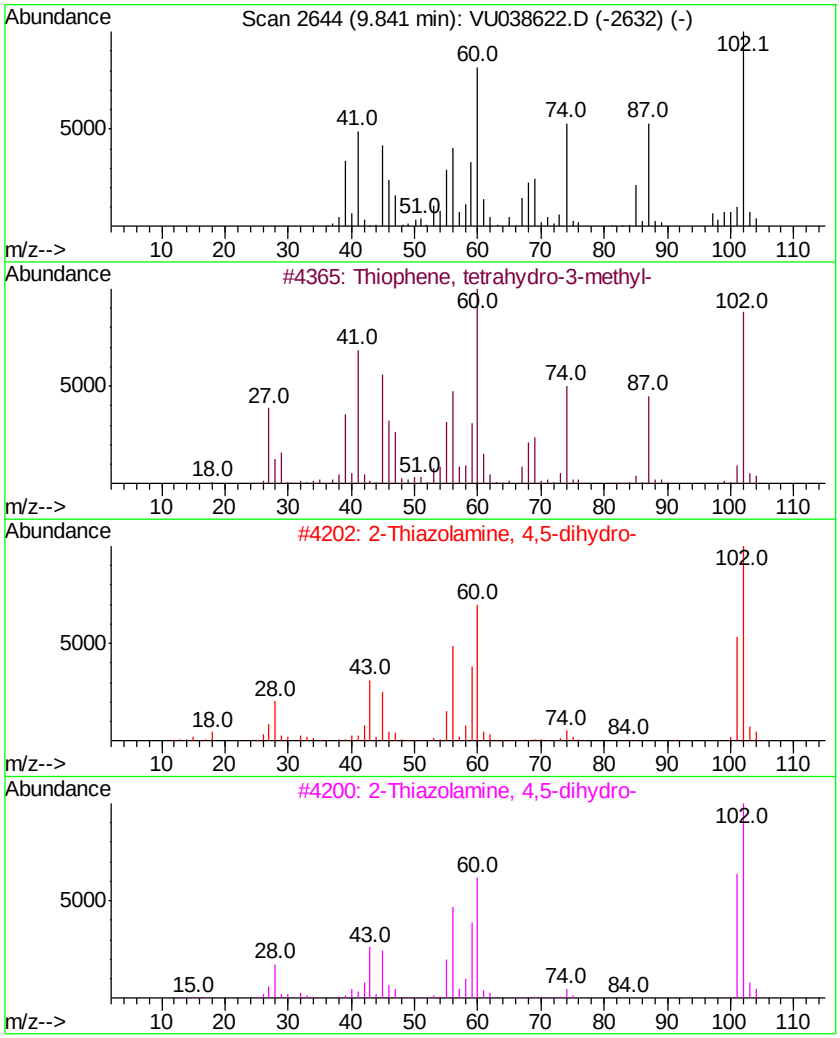
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

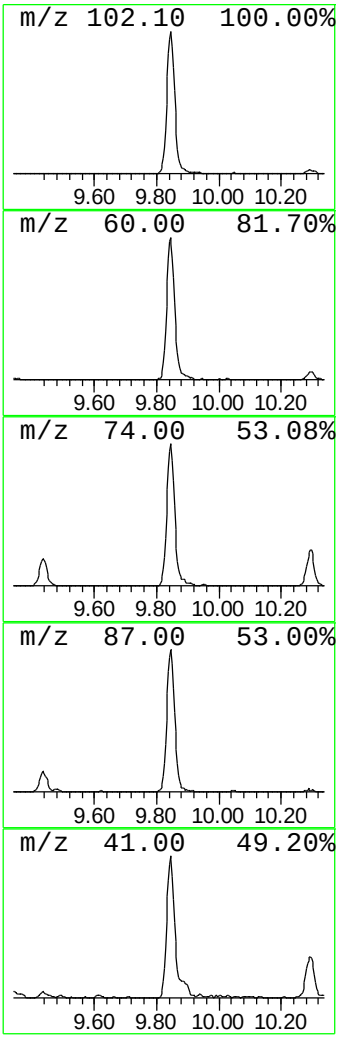
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.84	2.19 ug/L	401491	Chlorobenzene-d5	9.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, tetrahydro-3-methyl-	102	C5H10S	004740-00-5	94
2	2-Thiazolamine, 4,5-dihydro-	102	C3H6N2S	001779-81-3	49
3	2-Thiazolamine, 4,5-dihydro-	102	C3H6N2S	001779-81-3	43
4	Thietane, 2,4-dimethyl-	102	C5H10S	043044-24-2	38
5	Thiophene, tetrahydro-2-methyl-	102	C5H10S	001795-09-1	38





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU060620\
Data File : VU038622.D
Acq On : 06 Jun 2020 17:16
Operator : SY/MD
Sample : L2910-15
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D36

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

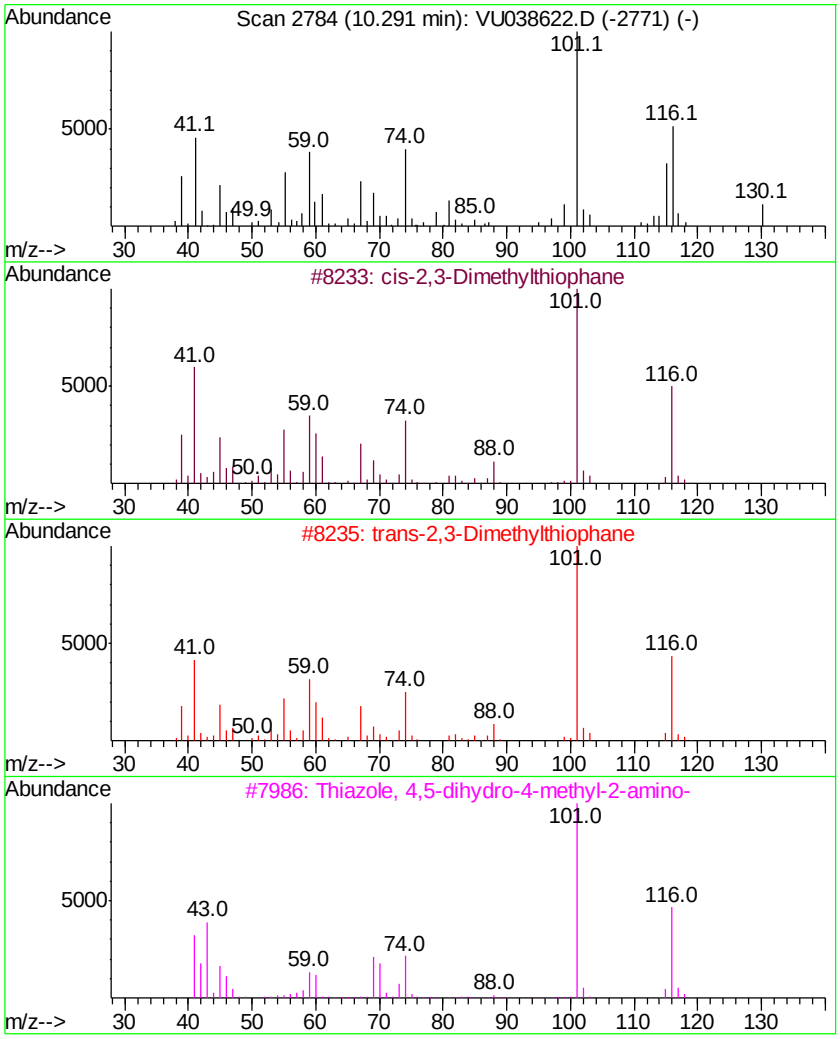
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

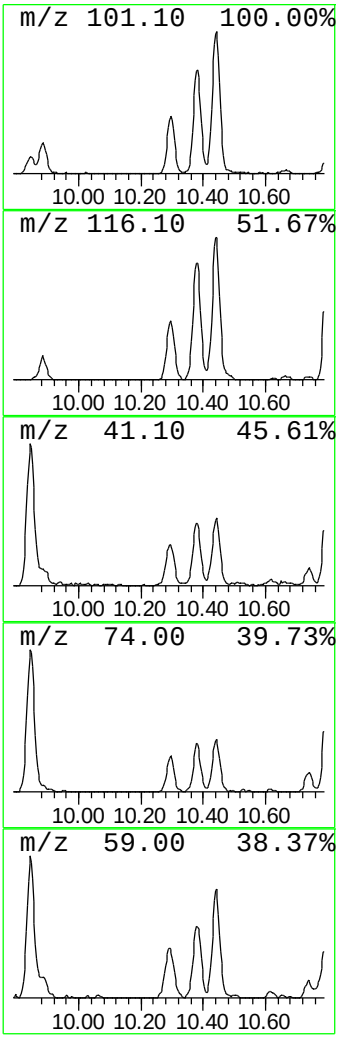
****

Peak Number 4 cis-2,3-Dimethylthiophane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.29	0.57 ug/L	105419	Chlorobenzene-d5	9.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	90
2	trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	89
3	Thiazole, 4,5-dihydro-4-methyl-2...	116	C4H8N2S	010416-81-6	49
4	trans-2-Ethyl-3-methylthiophane	130	C7H14S	061568-36-3	45
5	1,3,4-Thiadiazol-2-amine	101	C2H3N3S	004005-51-0	45





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060620\
Data File : VU038622.D
Acq On : 06 Jun 2020 17:16
Operator : SY/MD
Sample : L2910-15
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D36

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

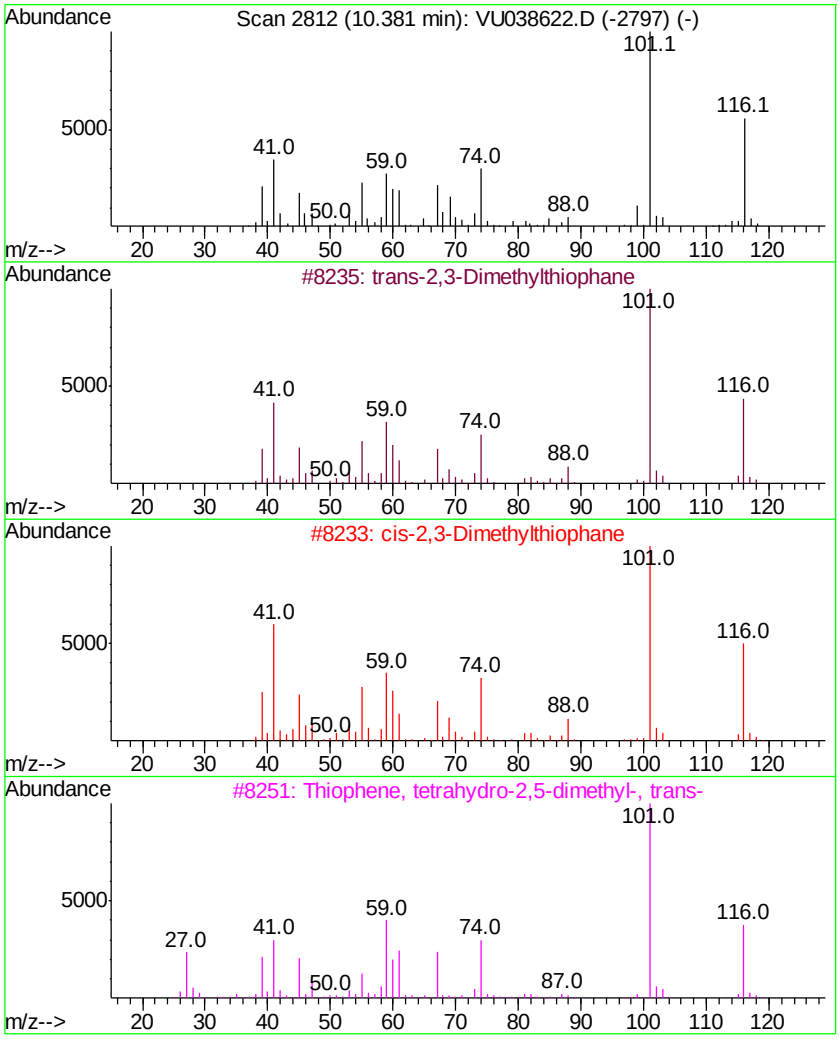
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

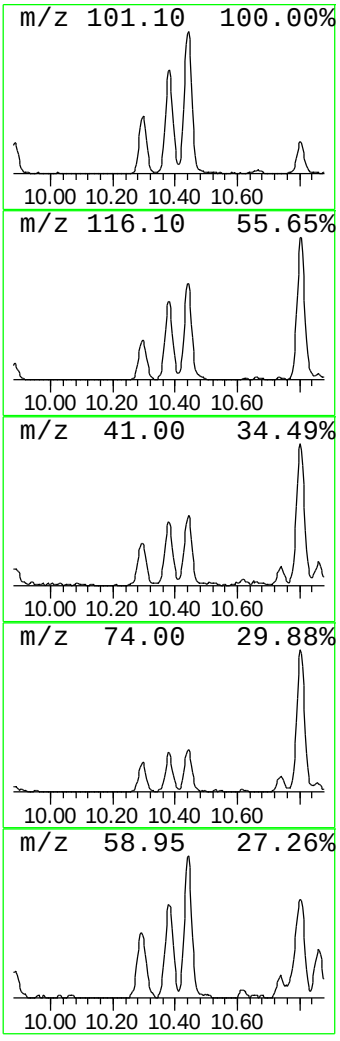
****

Peak Number 5 trans-2,3-Dimethylthiophane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.38	0.93 ug/L	171129	Chlorobenzene-d5	9.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	93
2	cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	93
3	Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-14-8	86
4	Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-13-7	64
5	2H-Thiopyran, tetrahydro-2-methyl-	116	C6H12S	005161-16-0	64





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Acq On : 06 Jun 2020 17:16
Operator : SY/MD
Sample : L2910-15
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D36

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

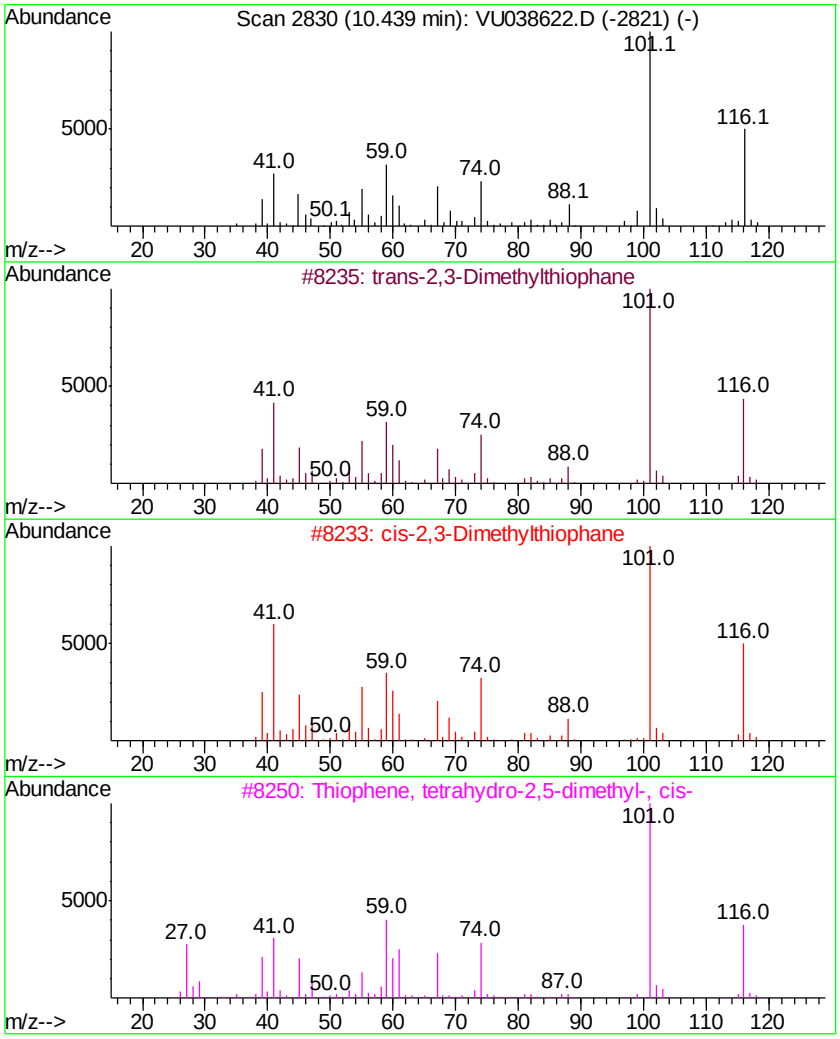
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

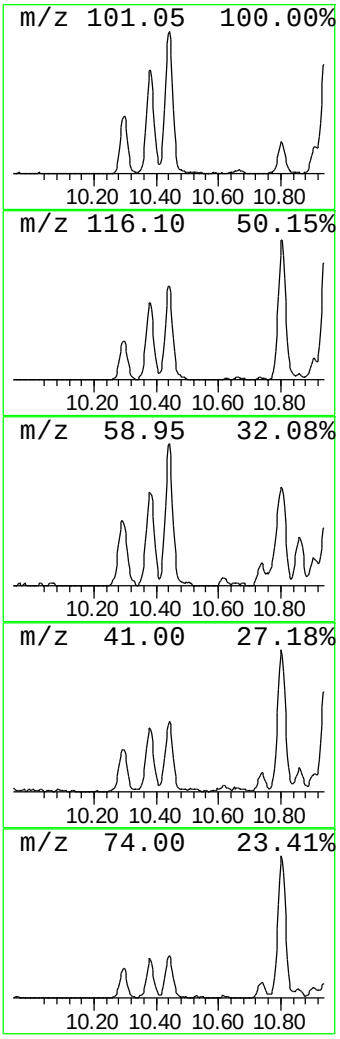
****

Peak Number 6 Thiazole, 4,5-dihydro-4-met... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.44	1.08 ug/L	197782	Chlorobenzene-d5	9.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	95
2	cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	93
3	Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-13-7	87
4	Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-14-8	87
5	Thiazole, 4,5-dihydro-4-methyl-2...	116	C4H8N2S	010416-81-6	64





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Sample : L2910-15
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D36

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

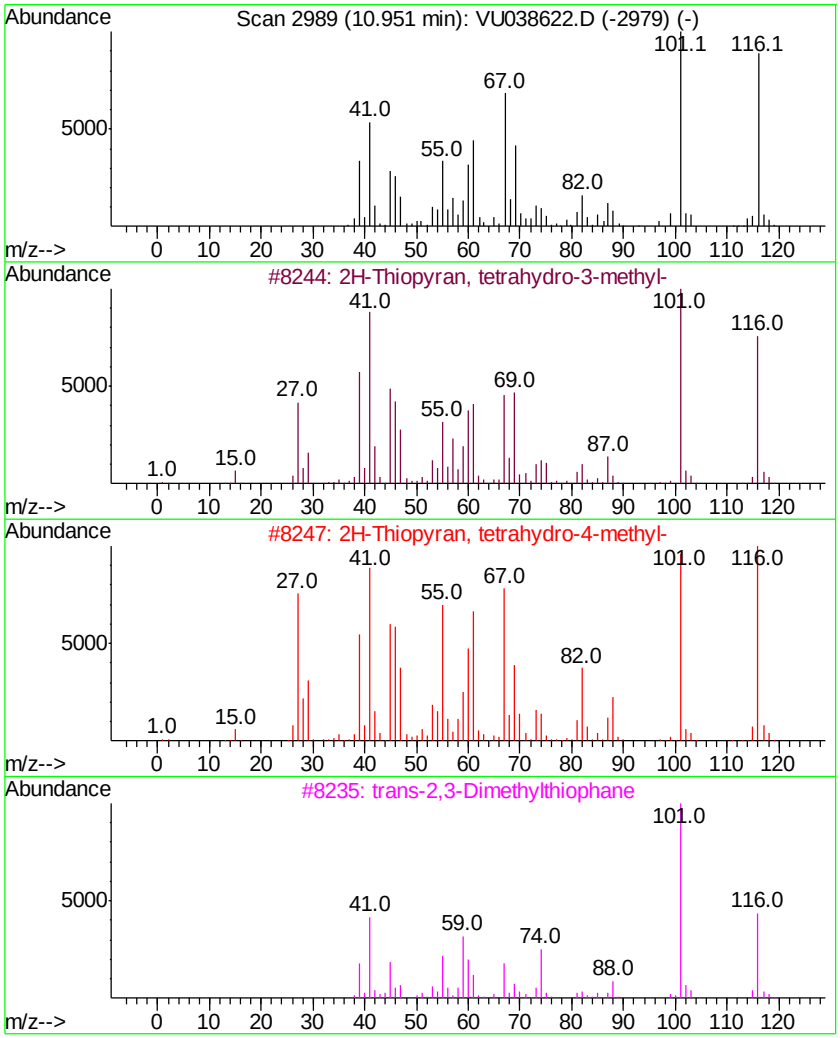
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

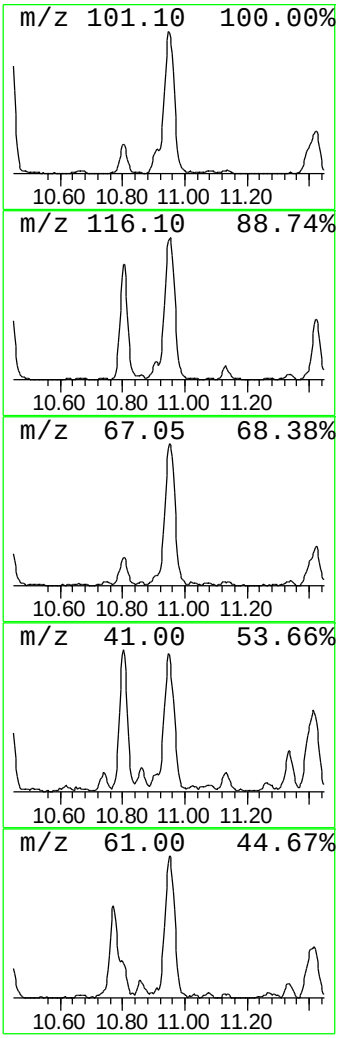
****

Peak Number 7 2H-Thiopyran, tetrahydro-3-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.95	2.25 ug/L	450189	1,4-Dichlorobenzene-d4	11.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Thiopyran, tetrahydro-3-methyl-	116	C6H12S	005258-50-4	94
2	2H-Thiopyran, tetrahydro-4-methyl-	116	C6H12S	005161-17-1	94
3	trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	50
4	2H-Thiopyran, tetrahydro-2-methyl-	116	C6H12S	005161-16-0	43
5	Allylthiourea	116	C4H8N2S	000109-57-9	43





Library Search Compound Report

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Data File : VU038622.D
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Operator : SY/MD
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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D36

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

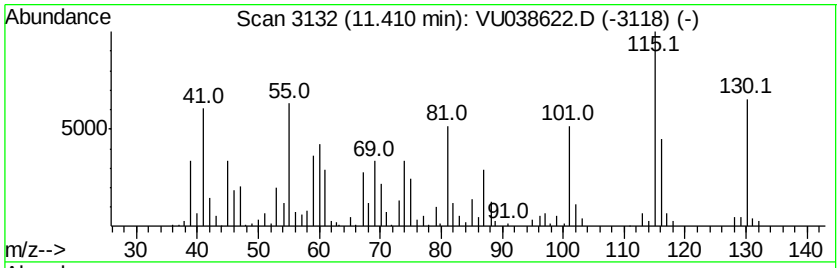
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

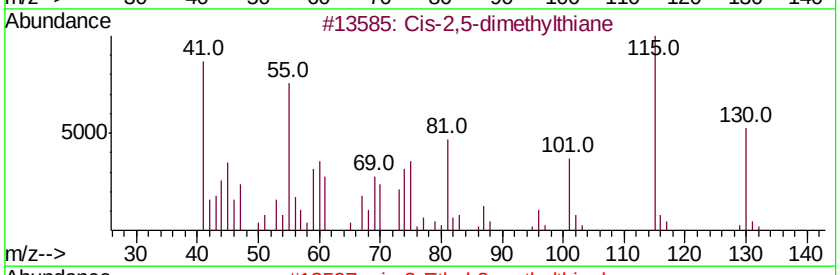
****

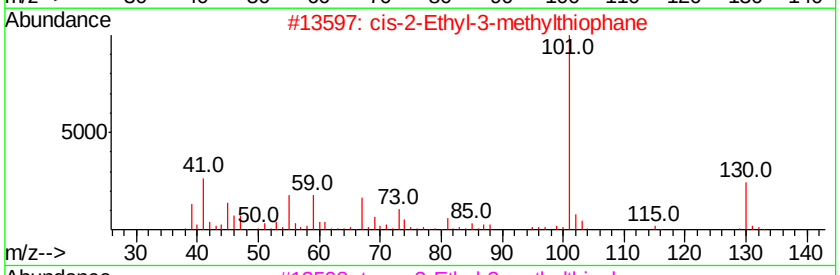
Peak Number 8 Cis-2,5-dimethylthiane Concentration Rank 3

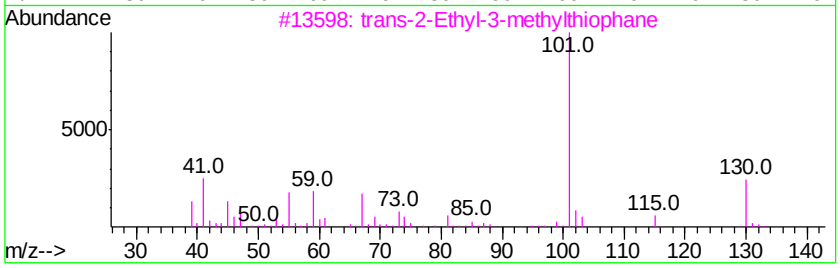
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.41	1.84 ug/L	367985	1,4-Dichlorobenzene-d4	11.82

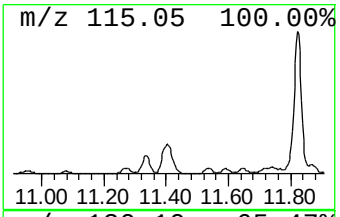
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cis-2,5-dimethylthiane	130	C7H14S	1000215-06-6	86
2	cis-2-Ethyl-3-methylthiophane	130	C7H14S	061568-37-4	83
3	trans-2-Ethyl-3-methylthiophane	130	C7H14S	061568-36-3	81
4	Trans-2,3-dimethylthiane	130	C7H14S	1000215-06-9	70
5	2H-Thiopyran, tetrahydro-2-methyl-	116	C6H12S	005161-16-0	64

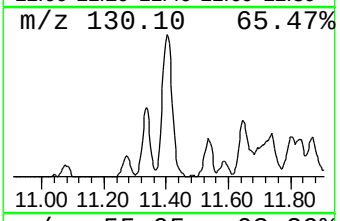


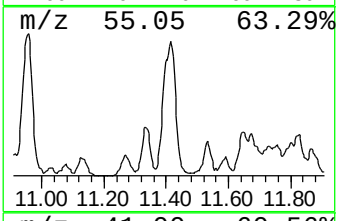


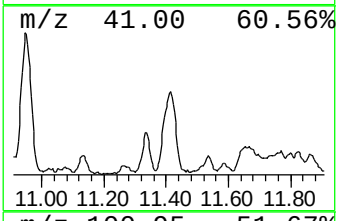


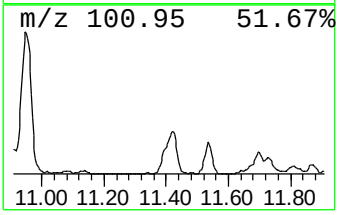












Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU060620\
Data File : VU038622.D
Acq On : 06 Jun 2020 17:16
Operator : SY/MD
Sample : L2910-15
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D36

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

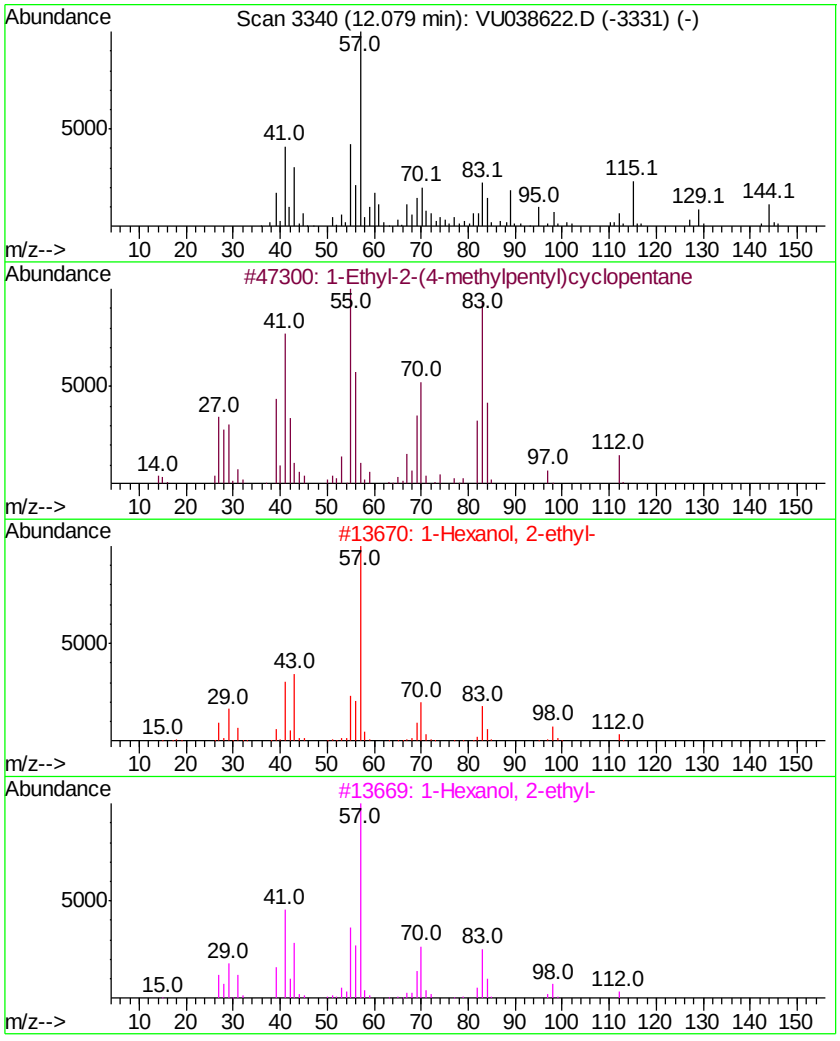
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

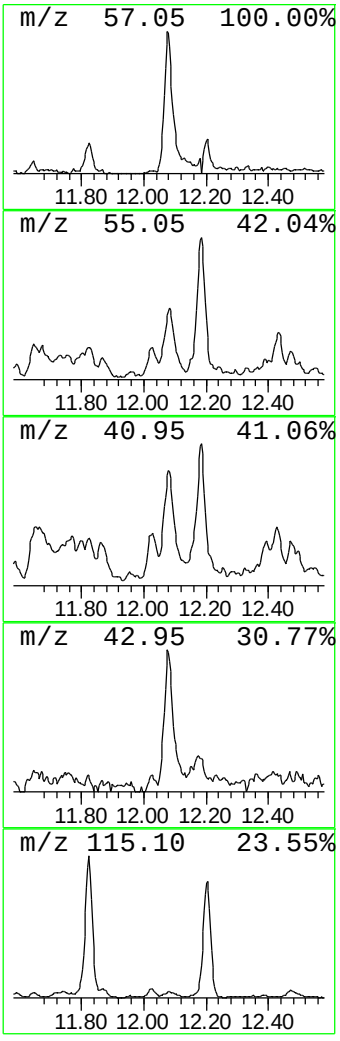
****

Peak Number 9 unknown-01 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.08	0.85 ug/L	169170	1,4-Dichlorobenzene-d4	11.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Ethyl-2-(4-methylpentyl)cyclop...	182	C13H26	219726-60-0	14
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	14
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	14
4	Ethyl propionylacetate	144	C7H12O3	004949-44-4	14
5	Cyclohexane, 1,2-dimethyl-, cis-	112	C8H16	002207-01-4	14





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060620\
Data File : VU038622.D
Acq On : 06 Jun 2020 17:16
Operator : SY/MD
Sample : L2910-15
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D36

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

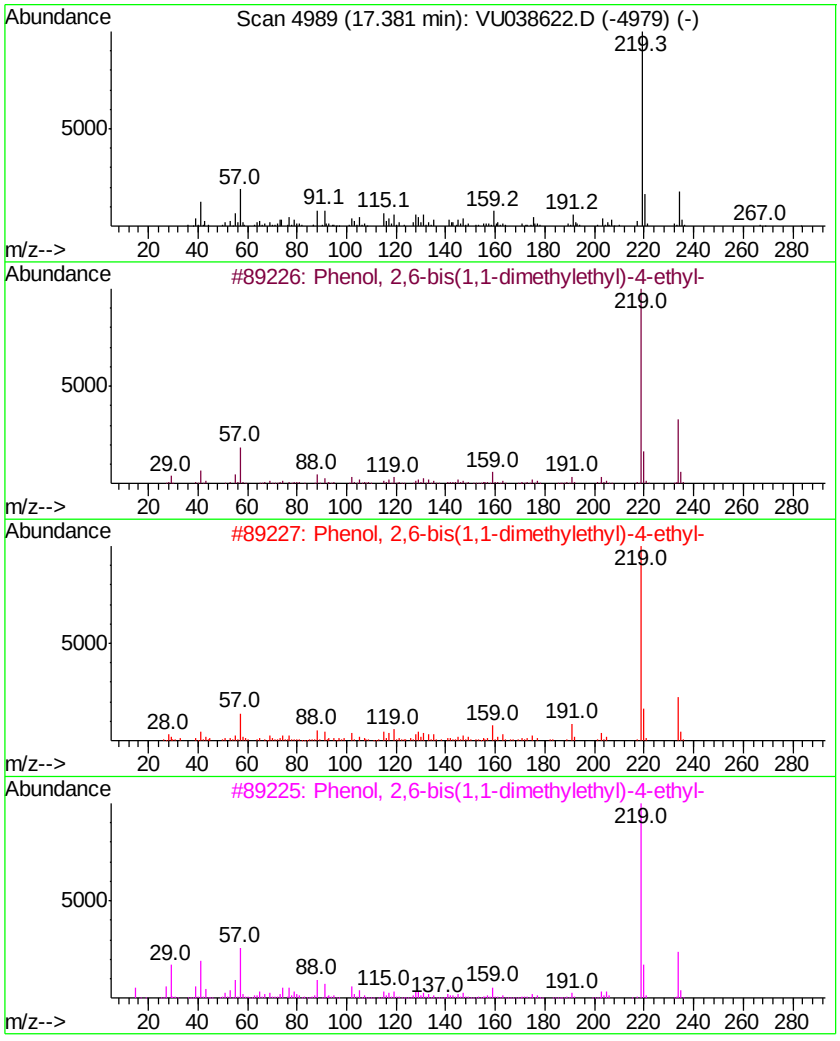
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

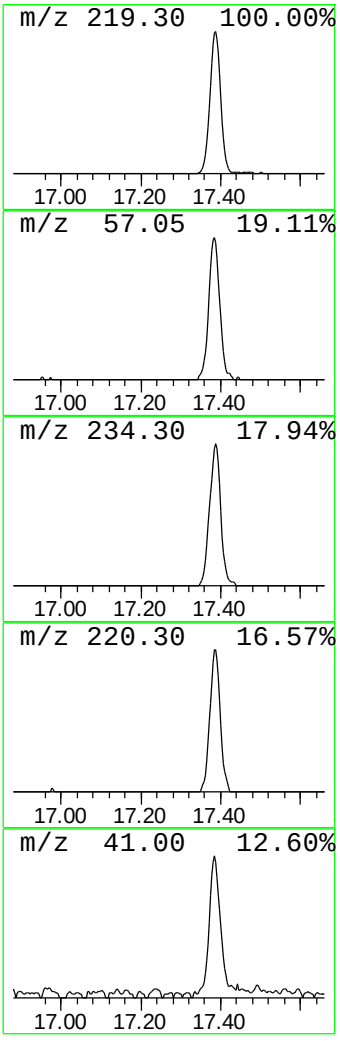
****

Peak Number 10 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.38	1.09 ug/L	218527	1,4-Dichlorobenzene-d4	11.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	94
2	Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	92
3	Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	91
4	3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	90
5	3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU060620\
Data File : VU038622.D
Acq On : 06 Jun 2020 17:16
Operator : SY/MD
Sample : L2910-15
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D36

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethyl Acetate	4.84	1.5	ug/L	216133	1	6.28	715718	5.0
Thiophene, tetrah...	9.84	2.2	ug/L	401491	2	9.44	916870	5.0
cis-2,3-Dimethylt...	10.29	0.6	ug/L	105419	2	9.44	916870	5.0
trans-2,3-Dimethy...	10.38	0.9	ug/L	171129	2	9.44	916870	5.0
Thiazole, 4,5-dih...	10.44	1.1	ug/L	197782	2	9.44	916870	5.0
2H-Thiopyran, tet...	10.95	2.3	ug/L	450189	3	11.82	999835	5.0
Cis-2,5-dimethylt...	11.41	1.8	ug/L	367985	3	11.82	999835	5.0
unknown-01	12.08	0.8	ug/L	169170	3	11.82	999835	5.0
Phenol, 2,6-bis(1...	17.38	1.1	ug/L	218527	3	11.82	999835	5.0