LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060620\
Data File : VU038621.D
Acq On : 06 Jun 2020 16:53
Operator : SY/MD
Sample : L2910-14
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D31

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	18	rBV2	45570	44677	3.05%	0.349%
2	1.613	71	85	92	rBV	112209	146481	9.99%	1.145%
3	1.932	176	184	201	rVB	92453	126477	8.63%	0.988%
4	2.594	378	390	403	rBV	183910	305860	20.87%	2.390%
5	2.671	405	414	433	rVB	20535	52464	3.58%	0.410%
6	4.674	1020	1037	1076	rBV	191341	569777	38.88%	4.452%
7	4.845	1077	1090	1113	rVB2	71073	165272	11.28%	1.291%
8	5.102	1153	1170	1191	rBV	191482	420898	28.72%	3.289%
9	5.424	1255	1270	1286	rBV3	23058	50903	3.47%	0.398%
10	5.761	1349	1375	1389	rBV2	375772	986706	67.32%	7.709%
11	5.829	1392	1396	1410	rVB3	15979	26169	1.79%	0.204%
12	6.279	1521	1536	1555	rBV	365526	707010	48.24%	5.524%
13	6.597	1616	1635	1651	rBV2	38737	78397	5.35%	0.613%
14	6.719	1659	1673	1695	rBV	238064	468641	31.98%	3.662%
15	7.591	1931	1944	1960	rBV	126685	226051	15.42%	1.766%
16	7.922	2030	2047	2064	rBV	438356	770749	52.59%	6.022%
17	8.202	2121	2134	2152	rBV	73962	122678	8.37%	0.959%
18	8.439	2196	2208	2217	rBV2	18329	29378	2.00%	0.230%
19	8.655	2259	2275	2314	rBV	799556	1465619	100.00%	11.451%
20	9.436	2504	2518	2551	rBV	541908	923696	63.02%	7.217%
21	9.845	2633	2645	2669	rBV2	141203	250580	17.10%	1.958%
22	10.050	2693	2709	2723	rBV10	16741	35656	2.43%	0.279%
23	10.295	2773	2785	2796	rBV3	43841	74968	5.12%	0.586%
24	10.378	2799	2811	2821	rVV2	50633	91981	6.28%	0.719%
25	10.439	2821	2830	2846	rVB	64582	107227	7.32%	0.838%
26	10.664	2890	2900	2914	rVB2	40246	65796	4.49%	0.514%
27	10.771	2915	2933	2939	rBV	217140	381775	26.05%	2.983%
28	10.857	2954	2960	2968	rVV4	12076	16617	1.13%	0.130%
29	10.906	2968	2975	2977	rVV4	19041	22511	1.54%	0.176%
30	10.947	2978	2988	3007	rVB4	226482	494572	33.74%	3.864%
31	11.079	3018	3029	3038	rBV3	68095	113754	7.76%	0.889%
32	11.127	3038	3044	3057	rVB6	16067	29074	1.98%	0.227%
33	11.333	3097	3108	3118	rVV3	30579	49777	3.40%	0.389%
34	11.414	3118	3133	3148	rVB7	108501	270142	18.43%	2.111%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060620\
Data File : VU038621.D
Acq On : 06 Jun 2020 16:53
Operator : SY/MD
Sample : L2910-14
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D31

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	3161	3171	3181	rBV3	24985	40106	2.74%	0.313%
36	11.645	3195	3205	3219	rBV9	47737	130534	8.91%	1.020%
37	11.764	3238	3242	3248	rVB6	12901	14689	1.00%	0.115%
38	11.822	3248	3260	3273	rVB	616243	984272	67.16%	7.690%
39	12.025	3314	3323	3330	rBV5	30099	54676	3.73%	0.427%
40	12.079	3330	3340	3358	rVV5	72093	182081	12.42%	1.423%
41	12.205	3361	3379	3398	rVB	519296	952660	65.00%	7.443%
42	12.330	3409	3418	3421	rBV9	10120	14933	1.02%	0.117%
43	12.388	3429	3436	3440	rBV6	14656	21904	1.49%	0.171%
44	12.430	3442	3449	3456	rVV5	35855	60366	4.12%	0.472%
45	12.475	3458	3463	3478	rVB9	19269	35491	2.42%	0.277%
46	12.629	3499	3511	3518	rBV9	5991	15082	1.03%	0.118%
47	12.706	3519	3535	3549	rVB6	19188	56596	3.86%	0.442%
48	13.166	3673	3678	3690	rVB8	14443	25643	1.75%	0.200%
49	13.246	3694	3703	3712	rBV9	15046	25857	1.76%	0.202%
50	13.404	3744	3752	3767	rVB9	10321	22367	1.53%	0.175%
51	13.510	3776	3785	3790	rBV9	9176	15463	1.06%	0.121%
52	14.468	4071	4083	4091	rBV9	19316	40439	2.76%	0.316%
53	15.069	4259	4270	4282	rVB8	17491	31399	2.14%	0.245%
54	15.352	4349	4358	4370	rVB5	33533	58488	3.99%	0.457%
55	15.436	4376	4384	4389	rBV7	16392	25574	1.74%	0.200%
56	15.478	4390	4397	4410	rVB4	37781	67713	4.62%	0.529%
57	15.603	4426	4436	4445	rBV4	26288	46053	3.14%	0.360%
58	16.143	4595	4604	4619	rVB4	11162	24443	1.67%	0.191%
59	16.449	4690	4699	4709	rBV6	15185	26106	1.78%	0.204%
60	17.384	4979	4990	5004	rBV2	71605	133396	9.10%	1.042%

Sum of corrected areas: 12798664

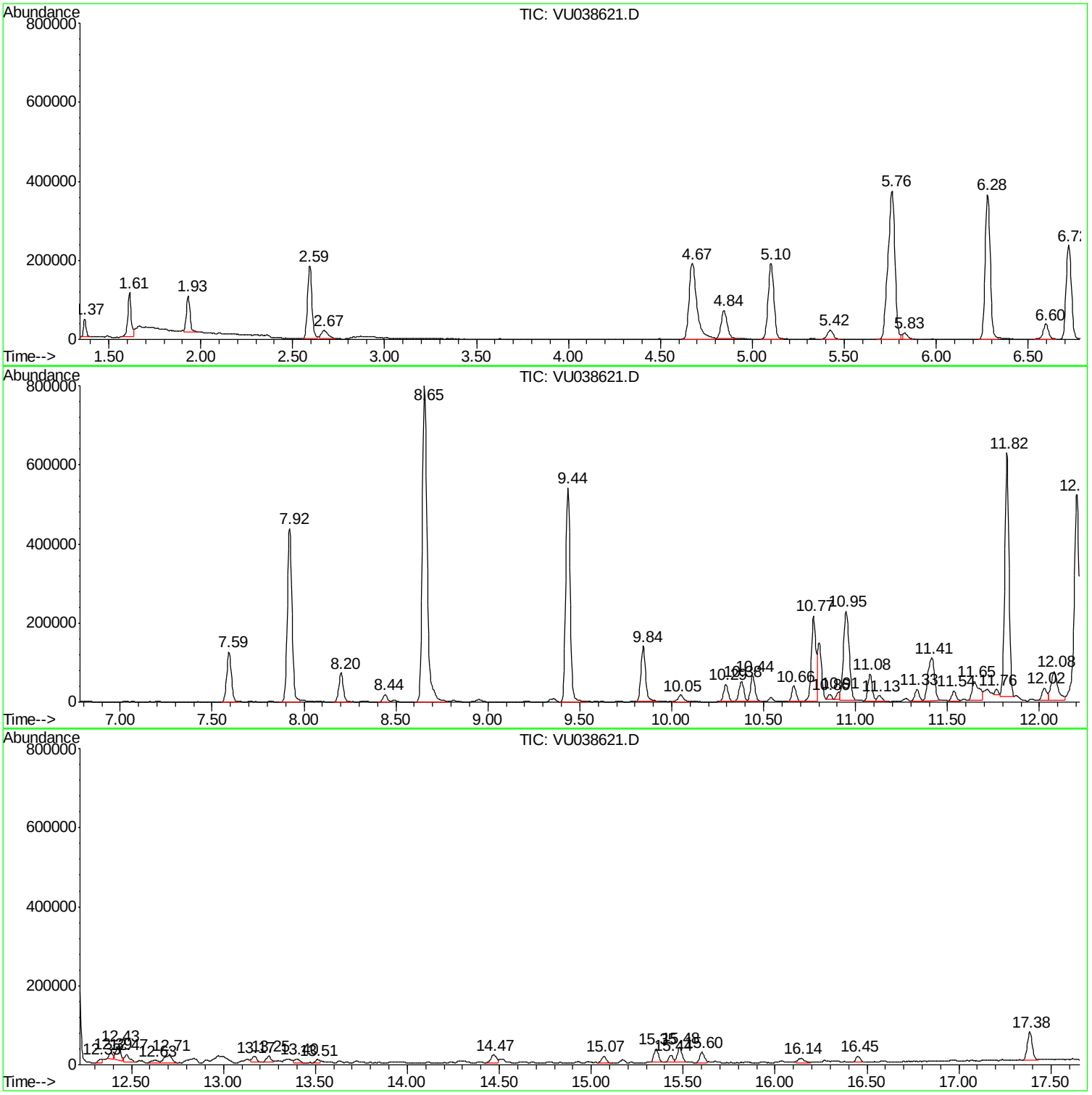
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060620\
Data File : VU038621.D
Acq On : 06 Jun 2020 16:53
Operator : SY/MD
Sample : L2910-14
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D31

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 : VU038621.D
Acq On : 06 Jun 2020 16:53
Operator : SY/MD
Sample : L2910-14
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D31

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

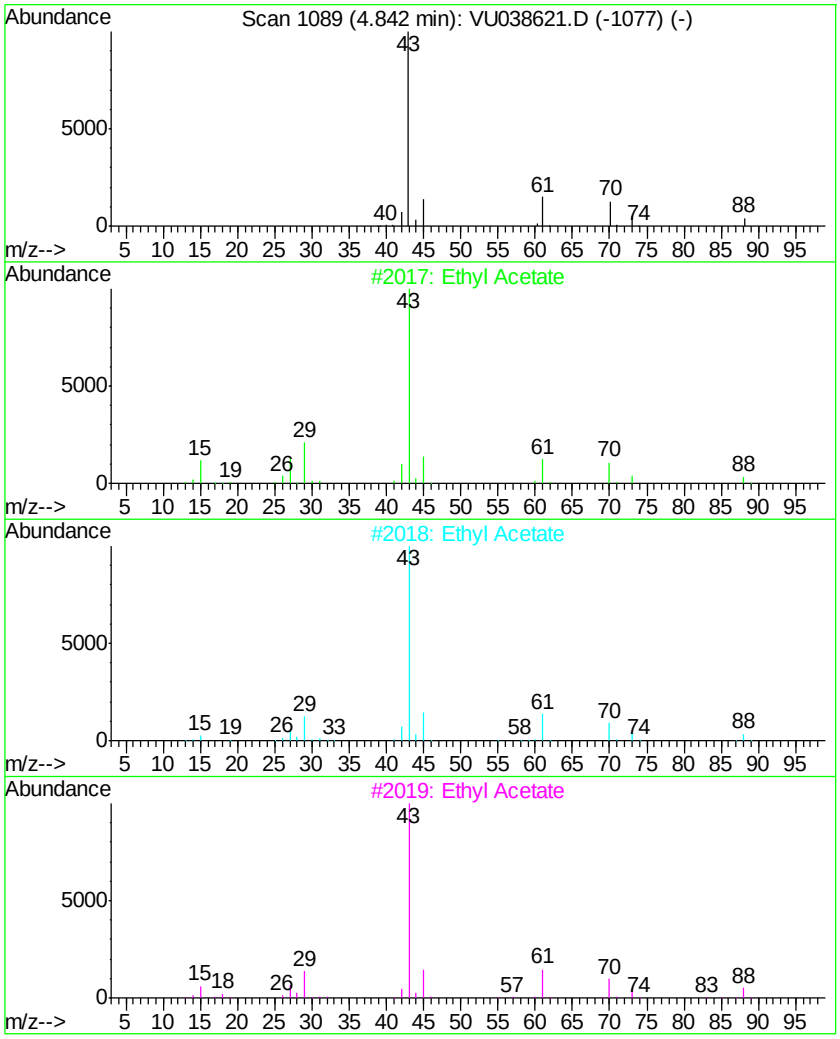
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

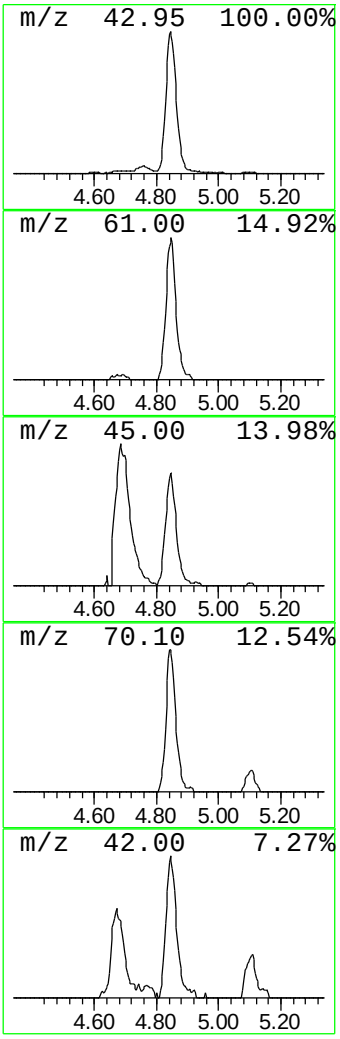
****

Peak Number 1 Ethyl Acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	1.17 ug/L	165272	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	90
3	Ethyl Acetate	88	C4H8O2	000141-78-6	90
4	Ethyl Acetate	88	C4H8O2	000141-78-6	83
5	CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	40





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU060620\
Data File : VU038621.D
Acq On : 06 Jun 2020 16:53
Operator : SY/MD
Sample : L2910-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D31

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

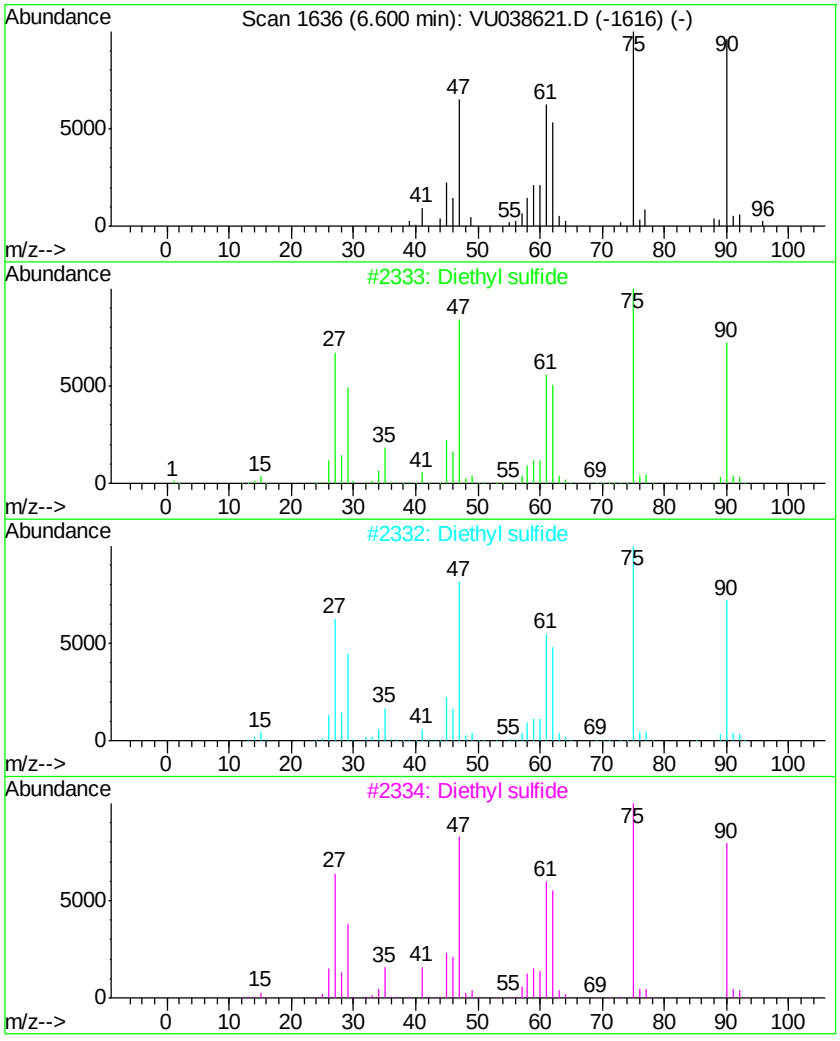
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

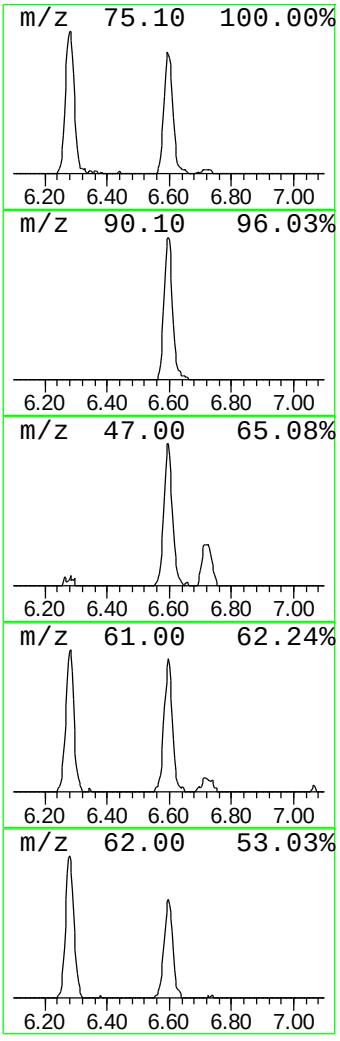
****

Peak Number 2 Diethyl sulfide Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	0.55 ug/L	78397	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyl sulfide	90	C4H10S	000352-93-2	91
2	Diethyl sulfide	90	C4H10S	000352-93-2	91
3	Diethyl sulfide	90	C4H10S	000352-93-2	91
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 U\DATA\VU060620\
Data File : VU038621.D
Acq On : 06 Jun 2020 16:53
Operator : SY/MD
Sample : L2910-14
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D31

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

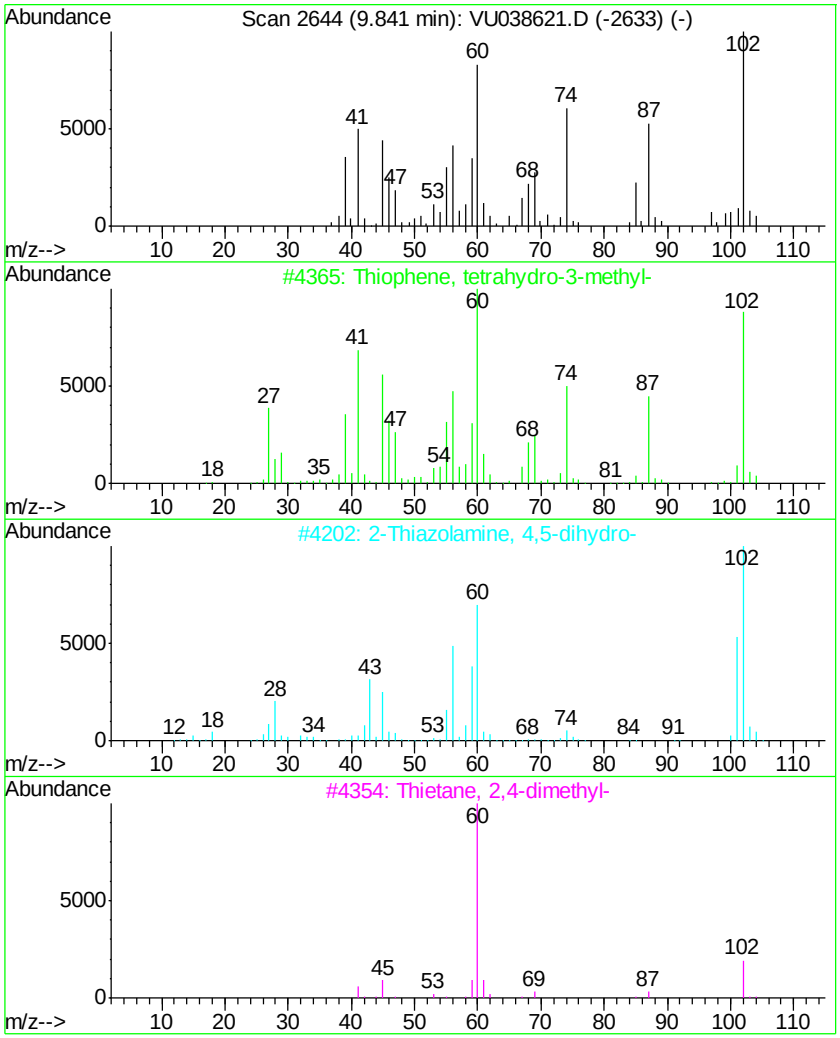
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

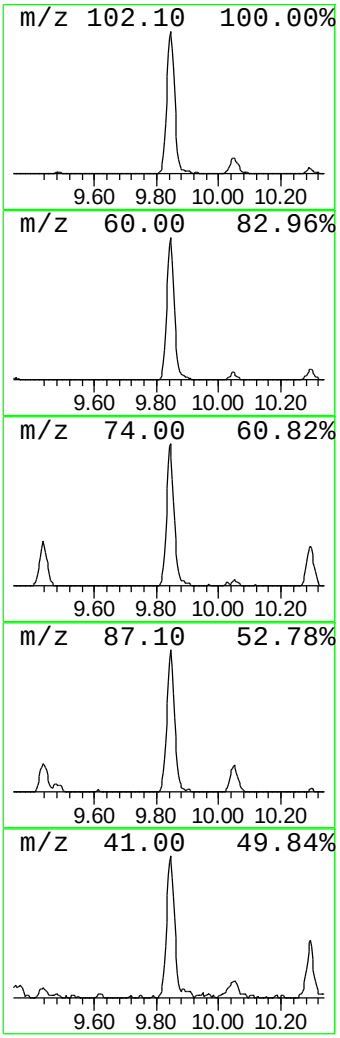
****

Peak Number 4 Thiophene, tetrahydro-3-met... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.84	1.36 ug/L	250580	Chlorobenzene-d5	9.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, tetrahydro-3-methyl-	102	C5H10S	004740-00-5	96
2	2-Thiazolamine, 4,5-dihydro-	102	C3H6N2S	001779-81-3	49
3	Thietane, 2,4-dimethyl-	102	C5H10S	043044-24-2	43
4	2-Thiazolamine, 4,5-dihydro-	102	C3H6N2S	001779-81-3	43
5	2-Thiazolamine, 4,5-dihydro-	102	C3H6N2S	001779-81-3	43





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU060620\
Data File : VU038621.D
Acq On : 06 Jun 2020 16:53
Operator : SY/MD
Sample : L2910-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D31

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

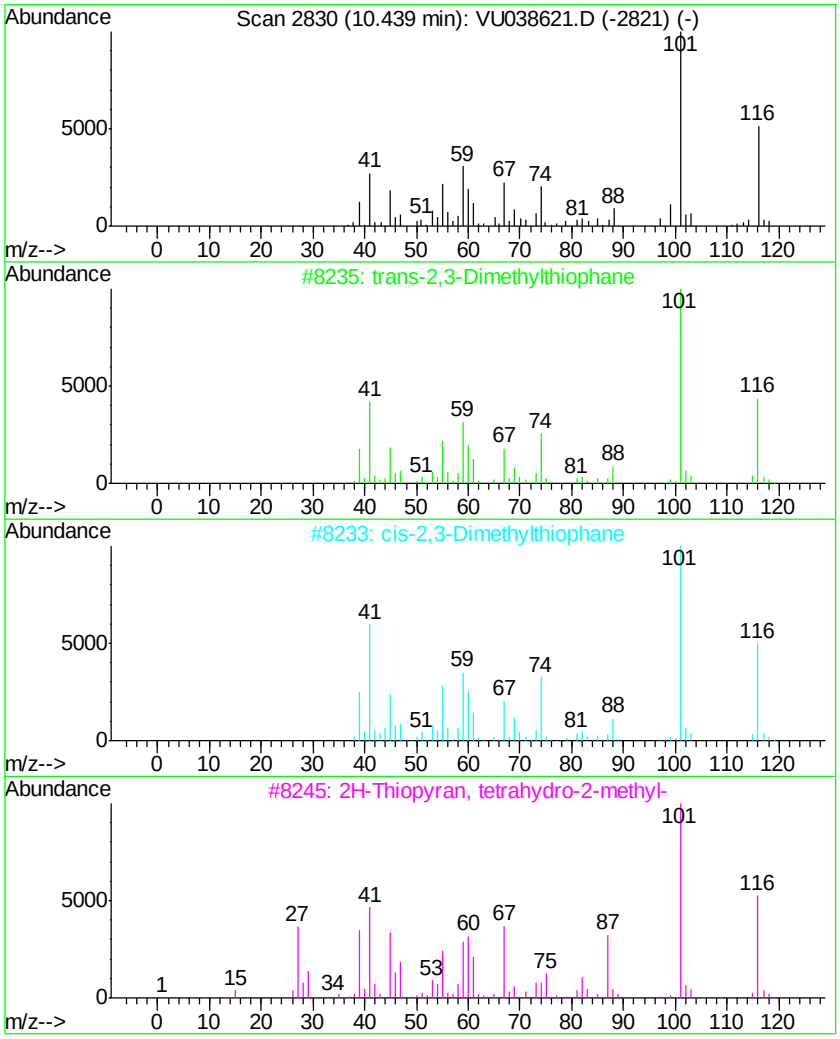
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

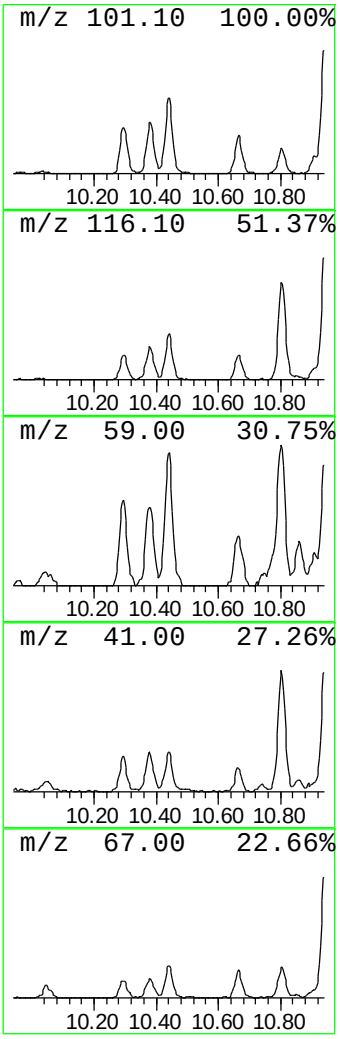
****

Peak Number 5 trans-2,3-Dimethylthiophane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.44	0.58 ug/L	107227	Chlorobenzene-d5	9.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	96
2	cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	93
3	2H-Thiopyran, tetrahydro-2-methyl-	116	C6H12S	005161-16-0	74
4	Thiazole, 4,5-dihydro-4-methyl-2...	116	C4H8N2S	010416-81-6	58
5	Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-14-8	53





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060620\
Data File : VU038621.D
Acq On : 06 Jun 2020 16:53
Operator : SY/MD
Sample : L2910-14
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D31

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

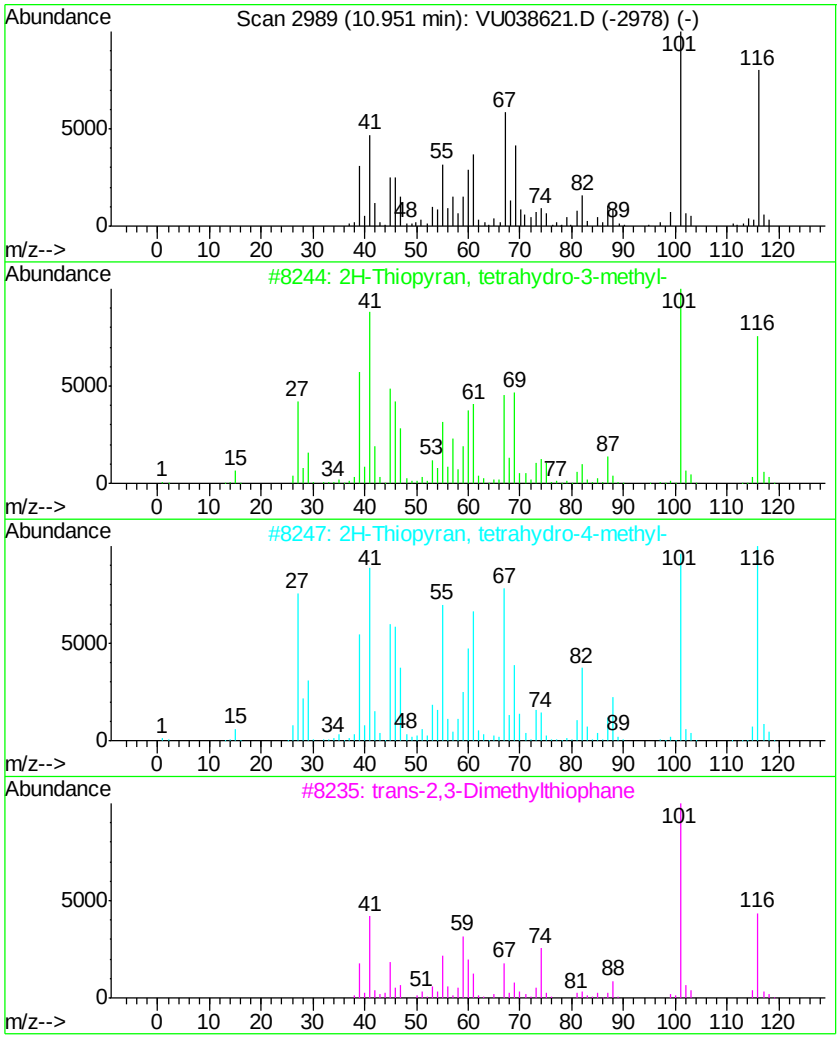
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

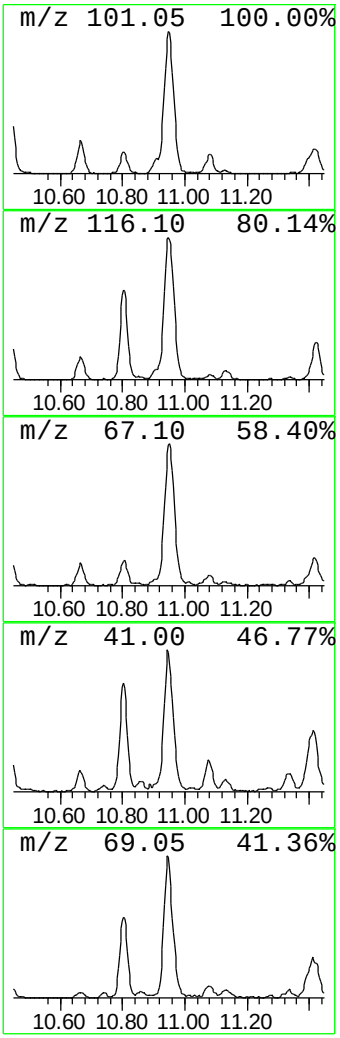
****

Peak Number 6 2H-Thiopyran, tetrahydro-3-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.95	2.51 ug/L	494572	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	64
4	Thiazole, 4,5-dihydro-4-methyl-2...	116	C4H8N2S	010416-81-6	50
5	Allylthiourea	116	C4H8N2S	000109-57-9	47





Library Search Compound Report

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Data File : VU038621.D
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Operator : SY/MD
Sample : L2910-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D31

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

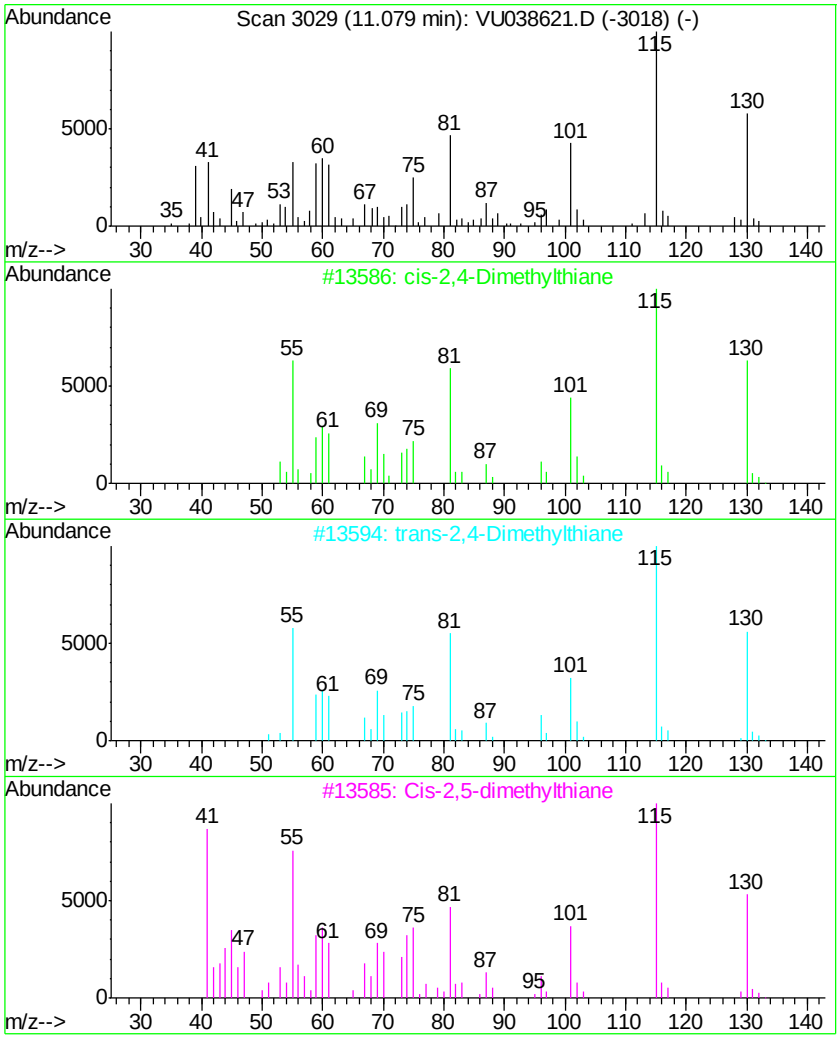
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

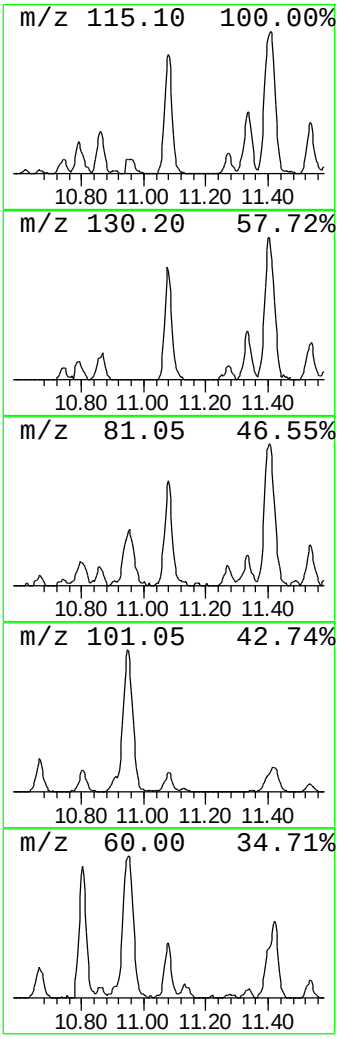
****

Peak Number 7 cis-2,4-Dimethylthiane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.08	0.58 ug/L	113754	1,4-Dichlorobenzene-d4	11.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-2,4-Dimethylthiane	130	C7H14S	061568-43-2	90
2	trans-2,4-Dimethylthiane	130	C7H14S	061568-42-1	83
3	Cis-2,5-dimethylthiane	130	C7H14S	1000215-06-6	72
4	Cis-2,3-dimethylthiane	130	C7H14S	1000215-06-5	40
5	1H-Phosphole, 2,3-dihydro-1,4-di...	130	C6H11OP	015450-68-7	38





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU060620\
Data File : VU038621.D
Acq On : 06 Jun 2020 16:53
Operator : SY/MD
Sample : L2910-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D31

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

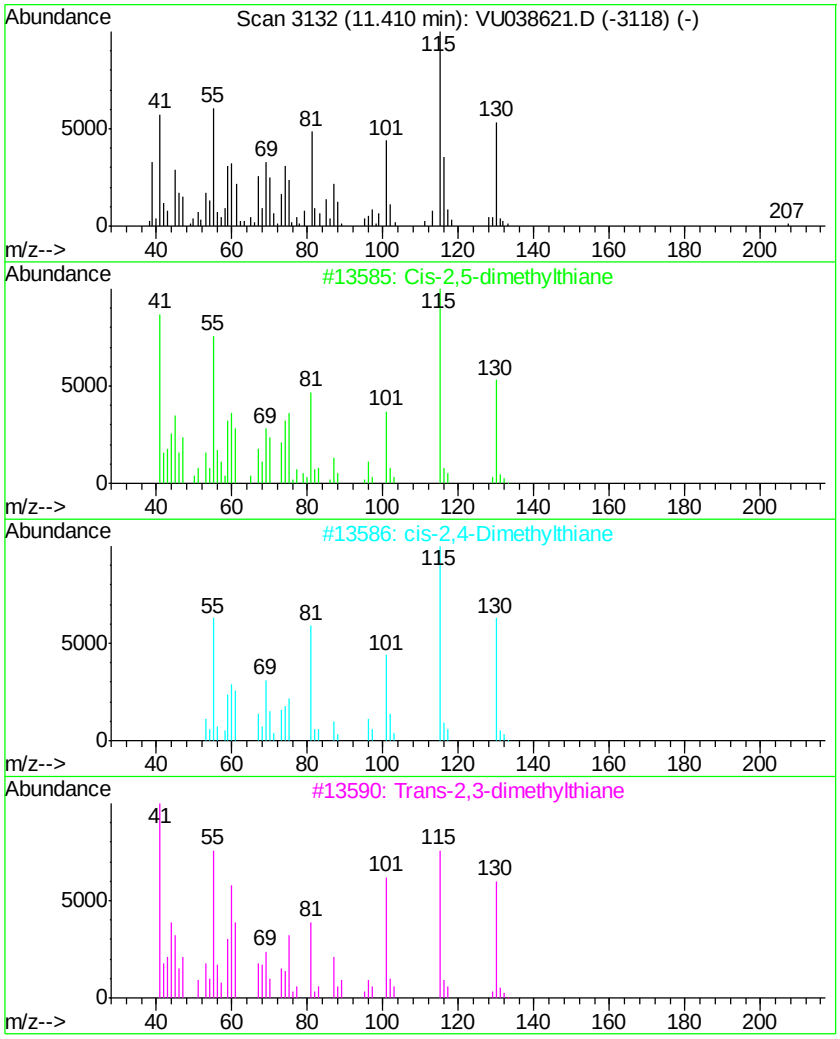
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

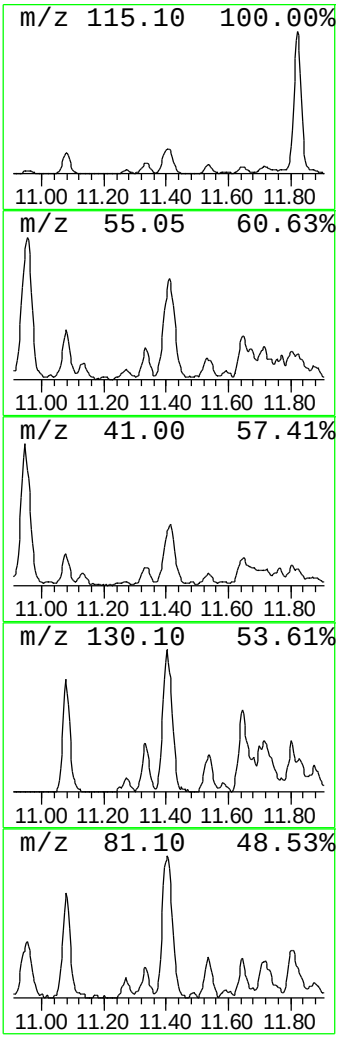
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.41	1.37 ug/L	270142	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	76
2	cis-2,4-Dimethylthiane	130	C7H14S	061568-43-2	70
3	Trans-2,3-dimethylthiane	130	C7H14S	1000215-06-9	64
4	trans-2,4-Dimethylthiane	130	C7H14S	061568-42-1	58
5	Trans-2,5-dimethylthiane	130	C7H14S	1000215-06-8	58





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Data File : VU038621.D
Acq On : 06 Jun 2020 16:53
Operator : SY/MD
Sample : L2910-14
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D31

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

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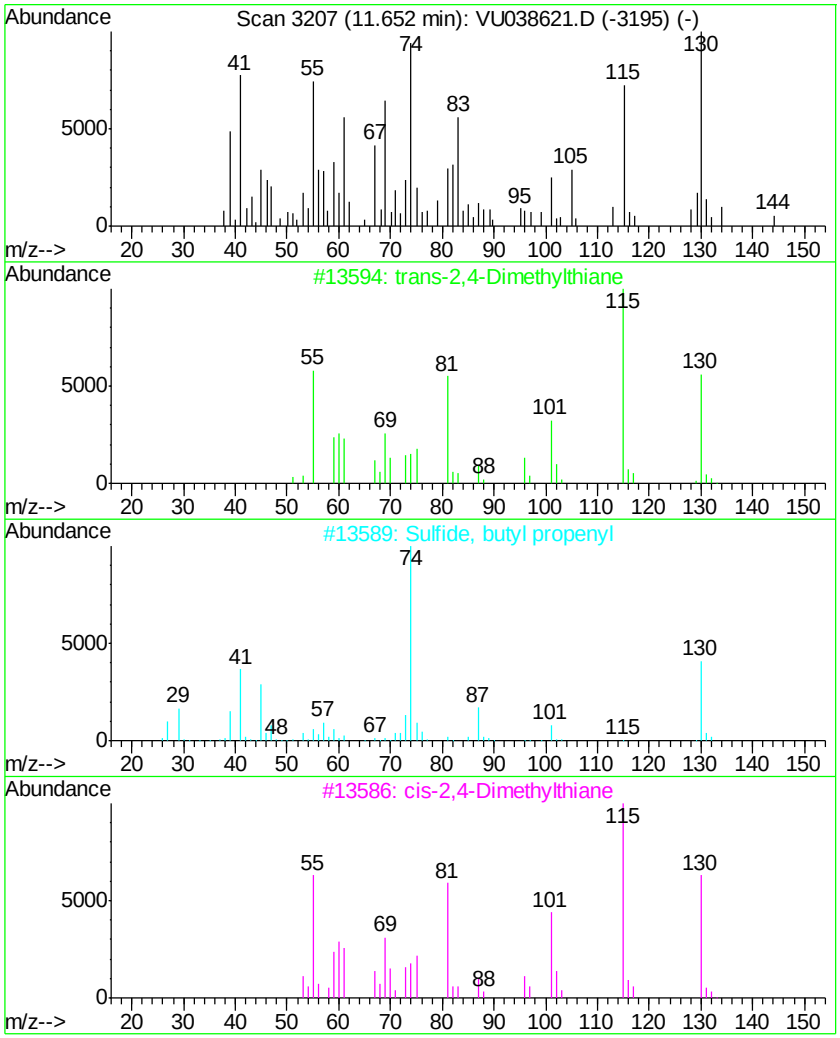
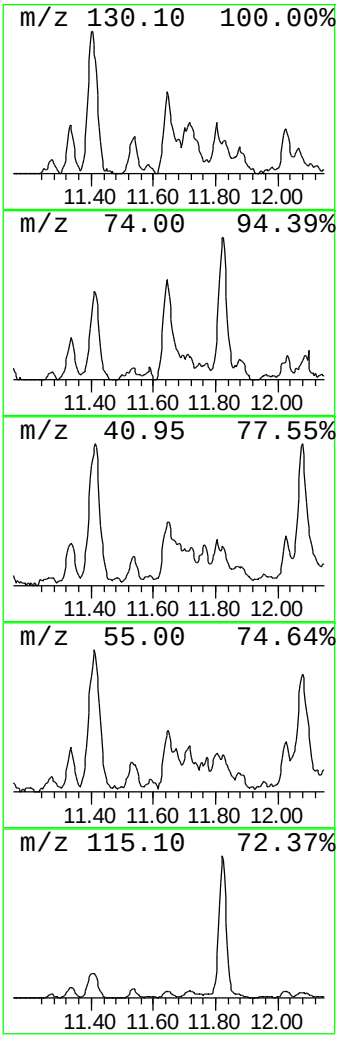
Peak Number 9 unknown-01 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.65	0.66 ug/L	130534	1,4-Dichlorobenzene-d4	11.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-2,4-Dimethylthiane	130	C7H14S	061568-42-1	42
2	Sulfide, butyl propenyl	130	C7H14S	024298-51-9	42
3	cis-2,4-Dimethylthiane	130	C7H14S	061568-43-2	38
4	1,3,2-Oxathiaborinane, 2-ethyl-	130	C5H11BOS	1000162-06-0	35
5	1,3,4-Thiadiazol-2-amine, 5-methyl-	115	C3H5N3S	000108-33-8	22





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060620\
Data File : VU038621.D
Acq On : 06 Jun 2020 16:53
Operator : SY/MD
Sample : L2910-14
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D31

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

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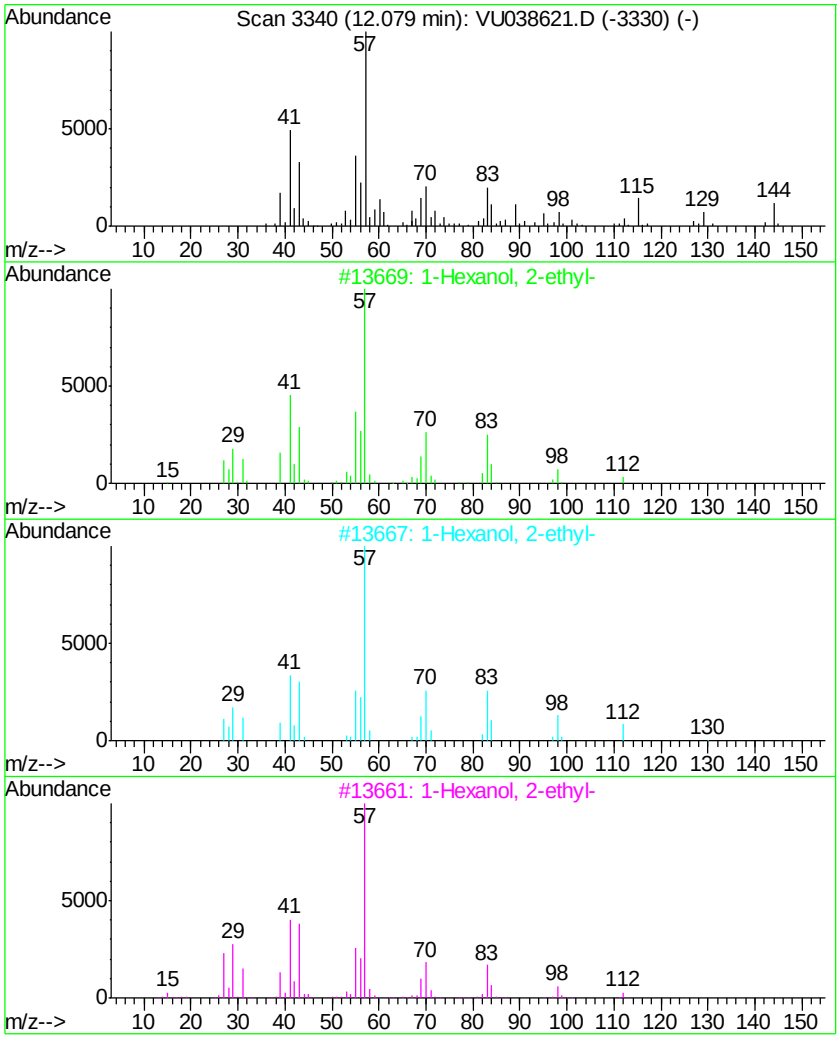
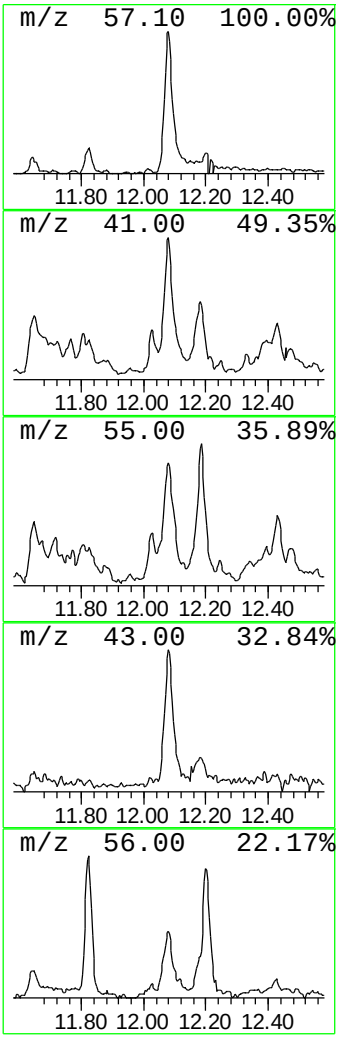
Peak Number 10 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.08	0.92 ug/L	182081	1,4-Dichlorobenzene-d4	11.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	52
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	50
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	50
4	1-Butoxy-2-ethylhexane	186	C12H26O	062625-25-6	47
5	2-Propyl-1-Pentanol, trifluoroac...	226	C10H17F3O2	1000365-19-7	43





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060620\
Data File : VU038621.D
Acq On : 06 Jun 2020 16:53
Operator : SY/MD
Sample : L2910-14
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D31

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

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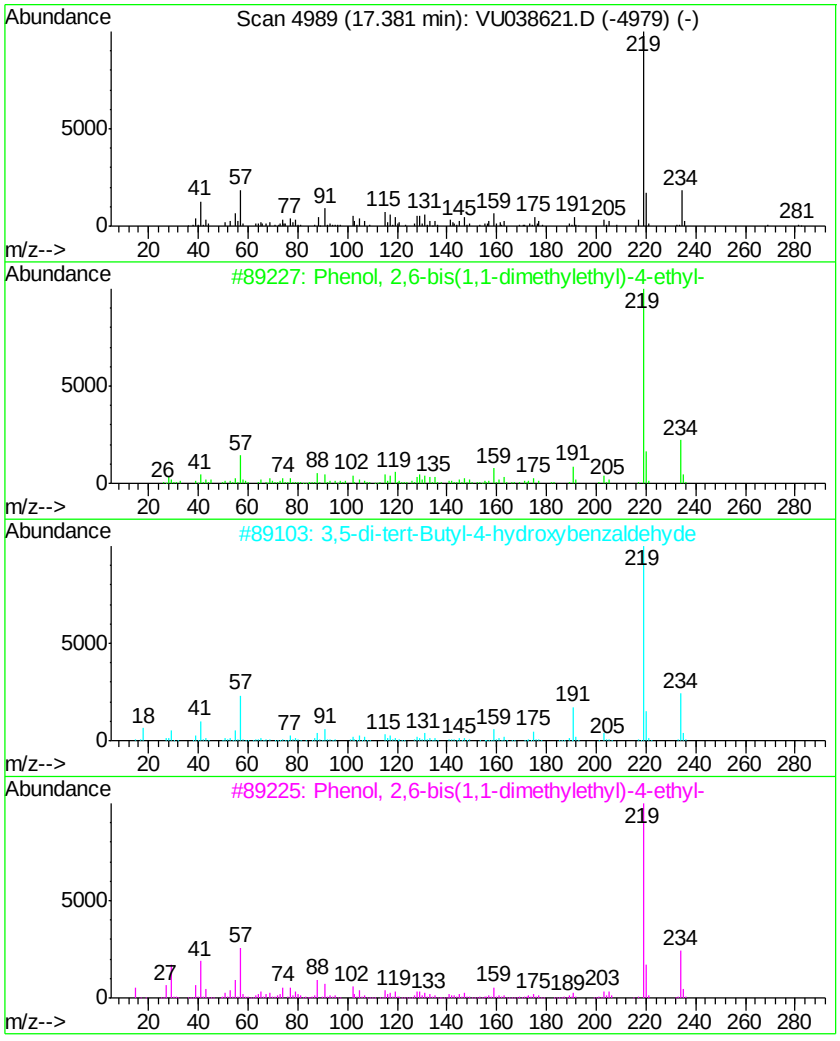
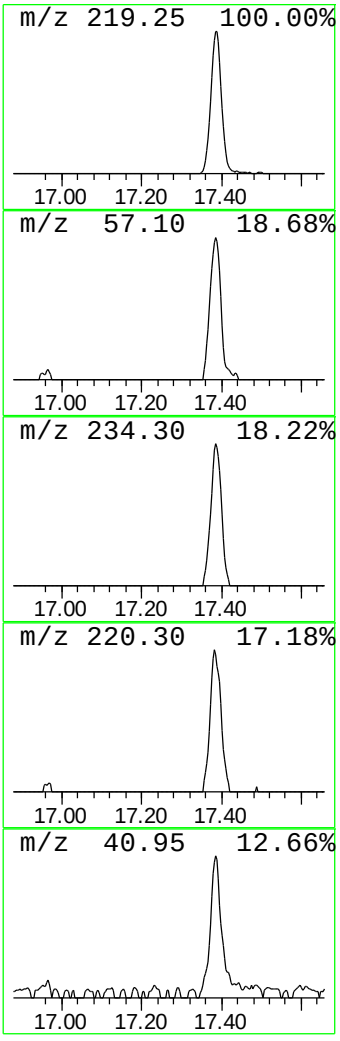
Peak Number 11 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.38	0.68 ug/L	133396	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	91
2	3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	90
3	Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	83
4	Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	83
5	4-tert-Butyl-2,6-diisopropylphenol	234	C16H26O	057354-65-1	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU060620\
Data File : VU038621.D
Acq On : 06 Jun 2020 16:53
Operator : SY/MD
Sample : L2910-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D31

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	1.2	ug/L	165272	1	6.28	707010	5.0
Diethyl sulfide	6.60	0.6	ug/L	78397	1	6.28	707010	5.0
Thiophene, tetrah...	9.84	1.4	ug/L	250580	2	9.44	923696	5.0
trans-2,3-Dimethy...	10.44	0.6	ug/L	107227	2	9.44	923696	5.0
2H-Thiopyran, tet...	10.95	2.5	ug/L	494572	3	11.82	984272	5.0
cis-2,4-Dimethylt...	11.08	0.6	ug/L	113754	3	11.82	984272	5.0
Cis-2,5-dimethylt...	11.41	1.4	ug/L	270142	3	11.82	984272	5.0
unknown-01	11.65	0.7	ug/L	130534	3	11.82	984272	5.0
1-Hexanol, 2-ethyl-	12.08	0.9	ug/L	182081	3	11.82	984272	5.0
Phenol, 2,6-bis(1...	17.38	0.7	ug/L	133396	3	11.82	984272	5.0