LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060620\
Data File : VU038644.D
Acq On : 07 Jun 2020 02:53
Operator : SY/MD
Sample : L2911-07
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D32

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	42231	43167	2.68%	0.310%
2	1.613	71	85	93	rBV	148861	179376	11.14%	1.288%
3	1.932	176	184	198	rVB	117670	151544	9.41%	1.088%
4	2.591	377	389	402	rBV	249483	408803	25.39%	2.935%
5	2.668	402	413	441	rVB2	49135	123796	7.69%	0.889%
6	2.858	449	472	474	rBV	16503	45461	2.82%	0.326%
7	4.671	1018	1036	1076	rBV	224750	648013	40.25%	4.653%
8	4.845	1076	1090	1111	rVB	64300	146979	9.13%	1.055%
9	5.102	1153	1170	1191	rBV	220687	483477	30.03%	3.472%
10	5.427	1255	1271	1285	rVB3	16920	39113	2.43%	0.281%
11	5.761	1351	1375	1392	rBV2	451200	1175882	73.04%	8.443%
12	6.279	1521	1536	1569	rBV	401480	774952	48.14%	5.564%
13	6.597	1614	1635	1651	rVB5	22315	48716	3.03%	0.350%
14	6.723	1658	1674	1692	rBV	276658	545331	33.88%	3.916%
15	7.591	1929	1944	1962	rBV	142245	253413	15.74%	1.820%
16	7.922	2031	2047	2077	rBV	540598	956642	59.43%	6.869%
17	8.202	2120	2134	2149	rBV	88687	149793	9.30%	1.076%
18	8.443	2199	2209	2219	rBV4	10897	18481	1.15%	0.133%
19	8.655	2261	2275	2308	rBV	879189	1609820	100.00%	11.559%
20	8.944	2351	2365	2380	rBV2	10321	20646	1.28%	0.148%
21	9.436	2504	2518	2544	rBV	568712	976024	60.63%	7.008%
22	9.845	2634	2645	2667	rBV2	82391	146140	9.08%	1.049%
23	10.295	2774	2785	2796	rVB4	10776	17610	1.09%	0.126%
24	10.378	2796	2811	2821	rBV6	13726	26105	1.62%	0.187%
25	10.439	2821	2830	2843	rVB2	25980	42417	2.63%	0.305%
26	10.539	2851	2861	2872	rBV3	9844	17280	1.07%	0.124%
27	10.771	2914	2933	2939	rBV	237266	397748	24.71%	2.856%
28	10.947	2967	2988	3005	rBV3	146611	322053	20.01%	2.312%
29	11.336	3097	3109	3118	rBV3	37218	60402	3.75%	0.434%
30	11.401	3118	3129	3149	rVB8	97492	259680	16.13%	1.865%
31	11.648	3193	3206	3221	rBV7	48077	114924	7.14%	0.825%
32	11.729	3221	3231	3232	rBV8	11157	16548	1.03%	0.119%
33	11.767	3237	3243	3249	rVV5	29939	48485	3.01%	0.348%
34	11.822	3249	3260	3272	rVB	645234	1031069	64.05%	7.403%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060620\
Data File : VU038644.D
Acq On : 07 Jun 2020 02:53
Operator : SY/MD
Sample : L2911-07
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D32

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	12.025	3312	3323	3330	rBV3	38303	67189	4.17%	0.482%
36	12.082	3330	3341	3355	rVV5	75035	167793	10.42%	1.205%
37	12.201	3358	3378	3399	rVB	618790	1198235	74.43%	8.604%
38	12.394	3429	3438	3442	rBV6	21947	37158	2.31%	0.267%
39	12.426	3443	3448	3456	rVV4	40606	71971	4.47%	0.517%
40	12.475	3457	3463	3479	rVB8	29326	60325	3.75%	0.433%
41	12.629	3499	3511	3515	rBV10	12350	22605	1.40%	0.162%
42	12.684	3517	3528	3533	rBV10	23833	50559	3.14%	0.363%
43	12.822	3561	3571	3591	rVB9	26473	71202	4.42%	0.511%
44	12.970	3604	3617	3618	rBV10	10323	19052	1.18%	0.137%
45	13.166	3670	3678	3691	rVB5	43774	75977	4.72%	0.546%
46	13.246	3696	3703	3711	rVB3	16739	26011	1.62%	0.187%
47	13.510	3777	3785	3794	rBV3	10199	19178	1.19%	0.138%
48	14.278	4016	4024	4031	rBV10	13769	24923	1.55%	0.179%
49	14.471	4069	4084	4090	rBV10	16721	32951	2.05%	0.237%
50	14.513	4093	4097	4108	rVB10	11286	17424	1.08%	0.125%
51	15.069	4261	4270	4284	rVB3	48093	83496	5.19%	0.600%
52	15.169	4294	4301	4310	rBV9	9964	17088	1.06%	0.123%
53	15.349	4349	4357	4370	rVB7	46062	91373	5.68%	0.656%
54	15.436	4375	4384	4391	rVV7	28076	51260	3.18%	0.368%
55	15.478	4391	4397	4409	rVB4	28028	51403	3.19%	0.369%
56	15.603	4425	4436	4448	rBV3	37003	67554	4.20%	0.485%
57	16.034	4562	4570	4581	rBV8	24858	42281	2.63%	0.304%
58	16.137	4597	4602	4613	rVB10	10495	17340	1.08%	0.125%
59	16.452	4691	4700	4712	rVB3	21378	36072	2.24%	0.259%
60	17.388	4980	4991	5006	rVB2	104489	206687	12.84%	1.484%

Sum of corrected areas: 13926997

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060620\
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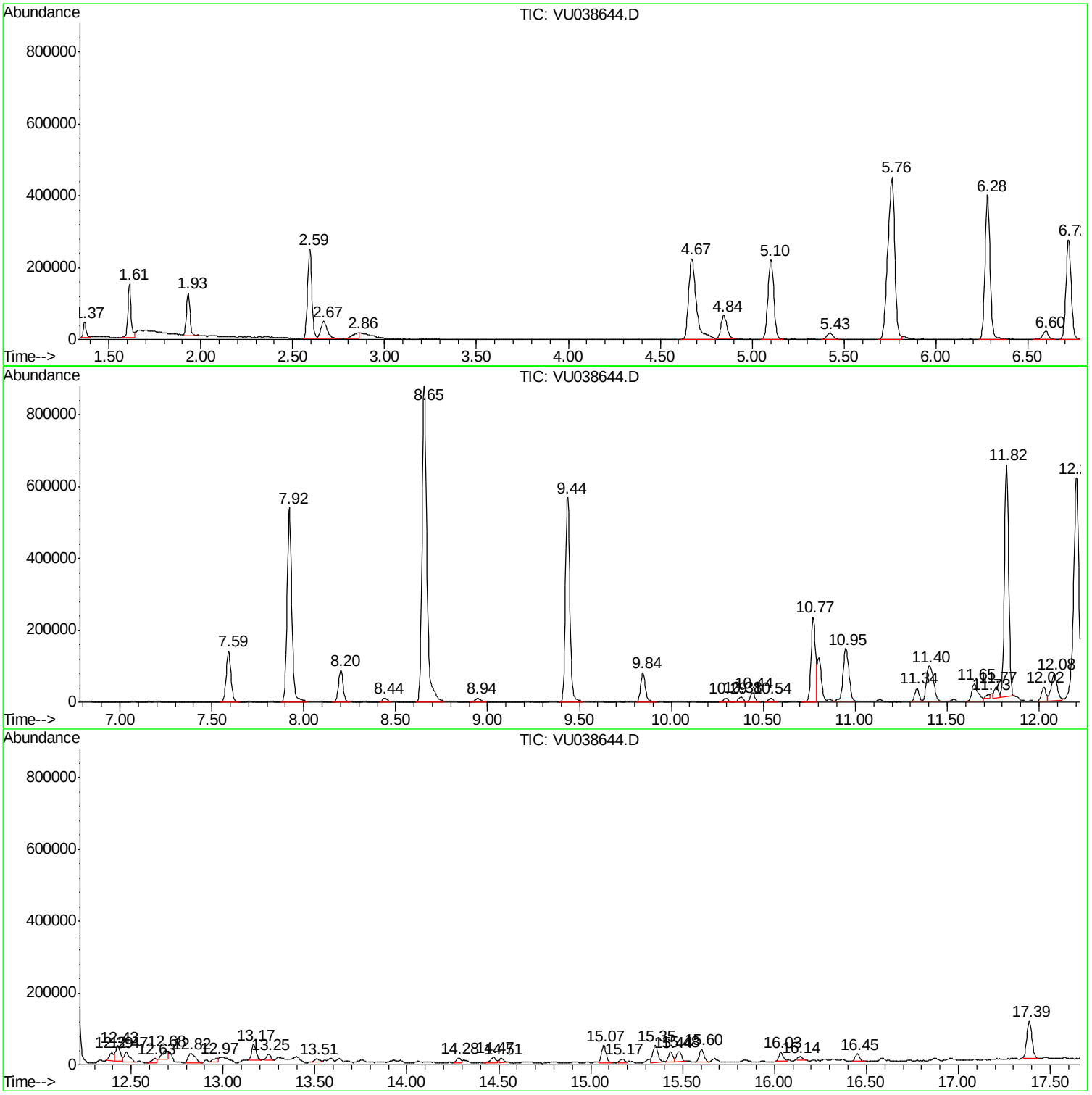
Acq On : 07 Jun 2020 02:53
Operator : SY/MD
Sample : L2911-07
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D32

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060620\
Data File : VU038644.D
Acq On : 07 Jun 2020 02:53
Operator : SY/MD
Sample : L2911-07
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D32

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

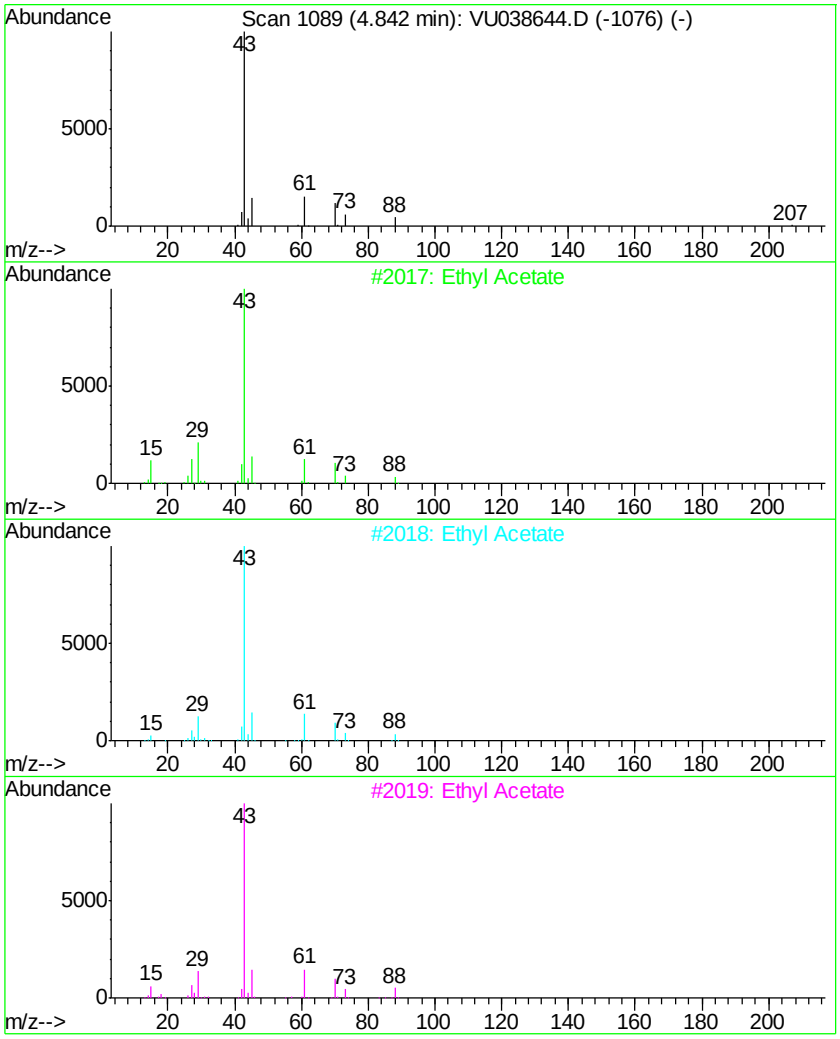
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

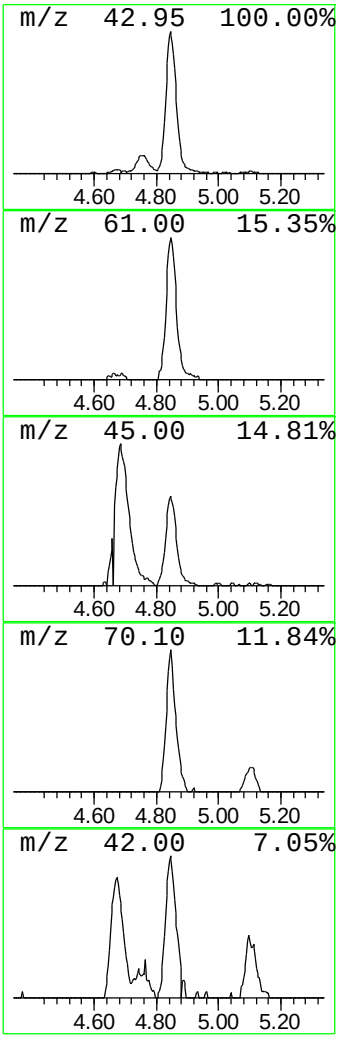
****

Peak Number 1 Ethyl Acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	0.95 ug/L	146979	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	86
4	Ethyl Acetate	88	C4H8O2	000141-78-6	78
5	CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	33





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060620\
Data File : VU038644.D
Acq On : 07 Jun 2020 02:53
Operator : SY/MD
Sample : L2911-07
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D32

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

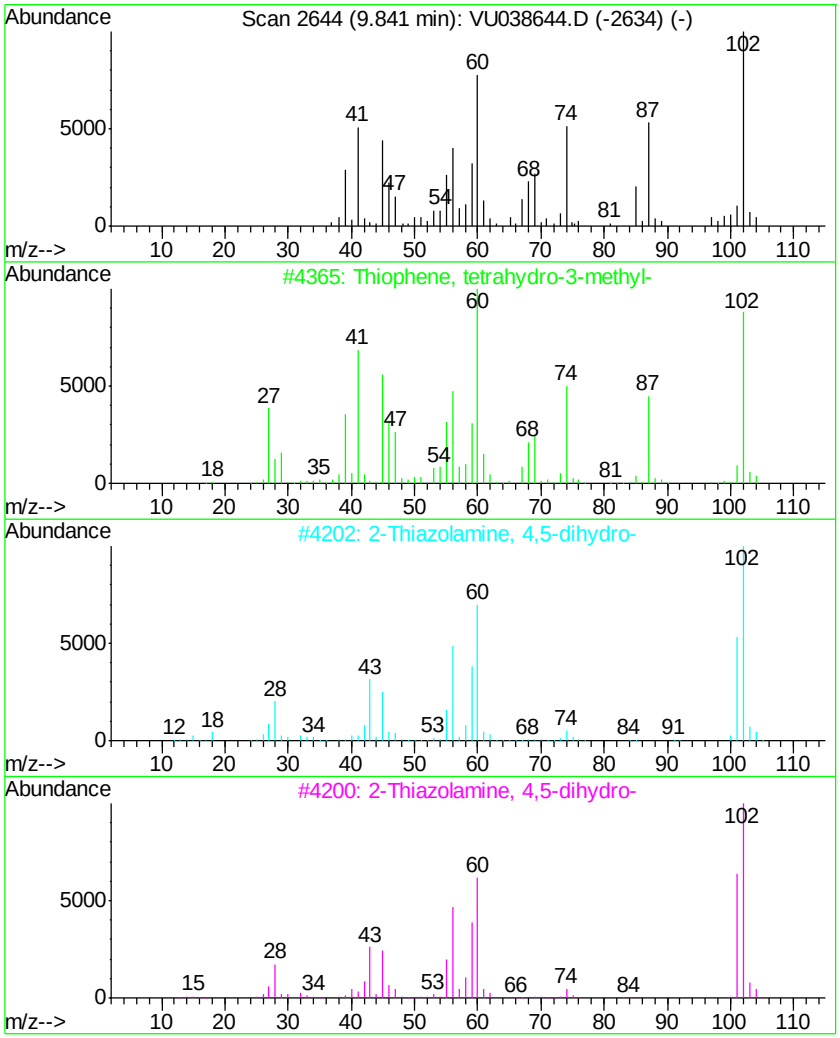
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

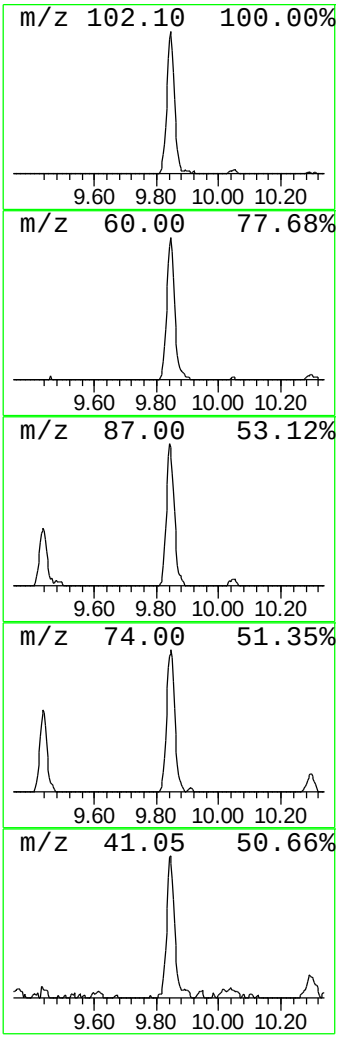
****

Peak Number 3 Thiophene, tetrahydro-3-met... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.84	0.75 ug/L	146140	Chlorobenzene-d5	9.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, tetrahydro-3-methyl-	102	C5H10S	004740-00-5	87
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	2-Thiazolamine, 4,5-dihydro-	102	C3H6N2S	001779-81-3	37
5	Propane, 1-(ethenylthio)-	102	C5H10S	016330-21-5	32





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU060620\
Data File : VU038644.D
Acq On : 07 Jun 2020 02:53
Operator : SY/MD
Sample : L2911-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D32

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

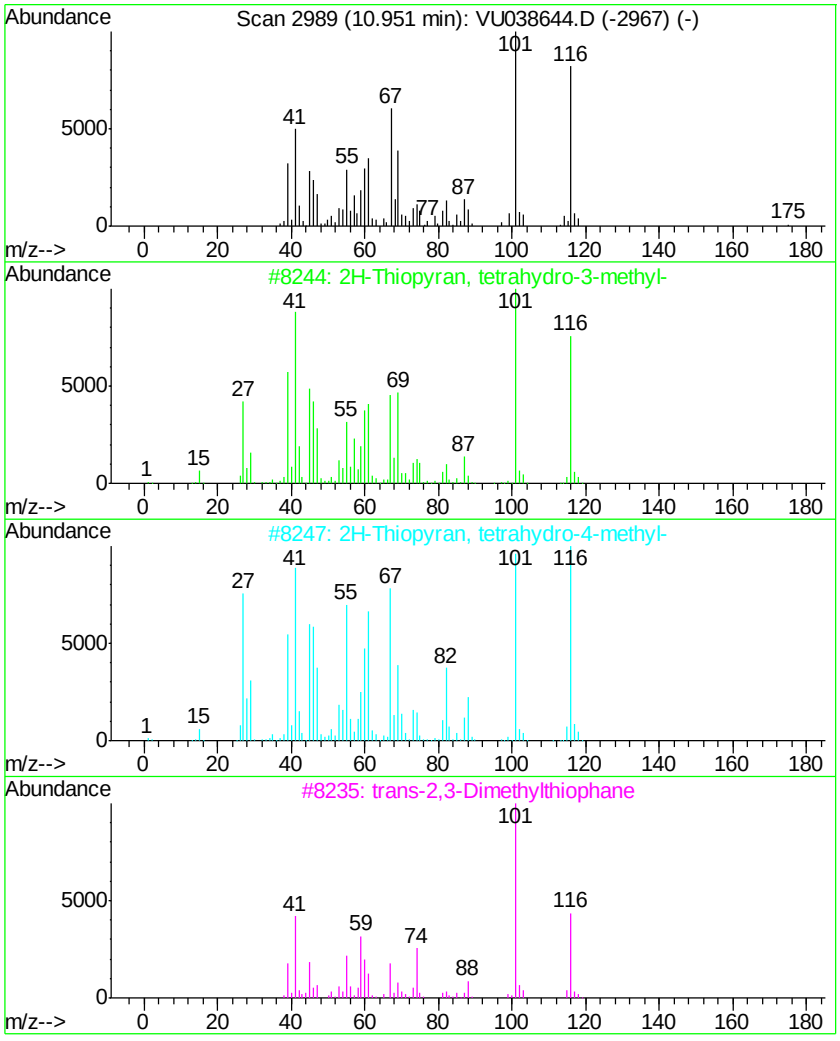
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

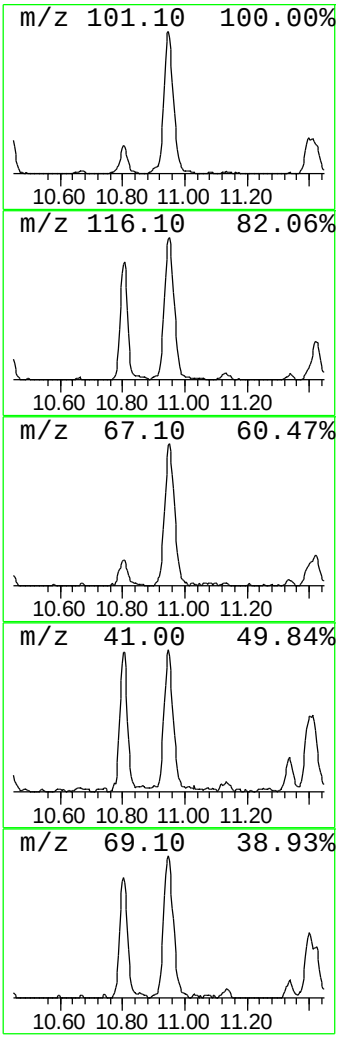
****

Peak Number 4 2H-Thiopyran, tetrahydro-3-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.95	1.56 ug/L	322053	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Thiopyran, tetrahydro-3-methyl-	116	C6H12S	005258-50-4	96
2	2H-Thiopyran, tetrahydro-4-methyl-	116	C6H12S	005161-17-1	94
3	trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	59
4	4-Imidazolidinone, 2-thioxo-	116	C3H4N2OS	000503-87-7	46
5	2H-Thiopyran-3(4H)-one, dihydro-	116	C5H8OS	019090-03-0	43





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU060620\
Data File : VU038644.D
Acq On : 07 Jun 2020 02:53
Operator : SY/MD
Sample : L2911-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D32

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

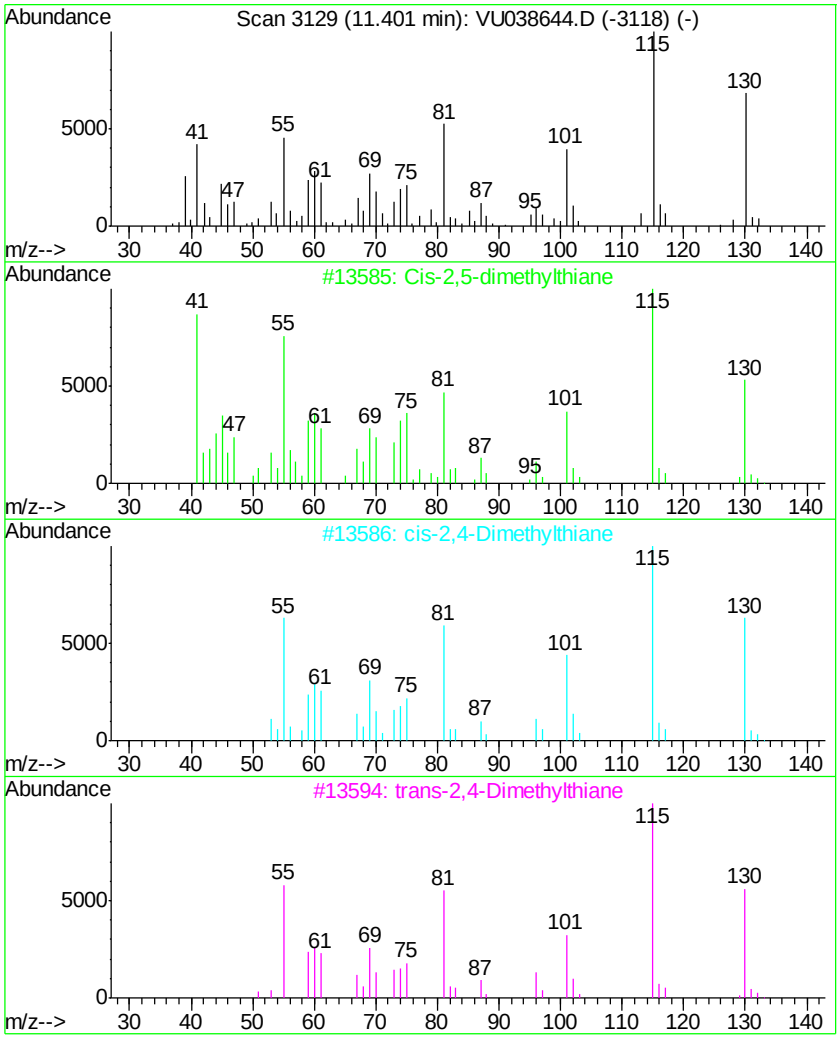
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

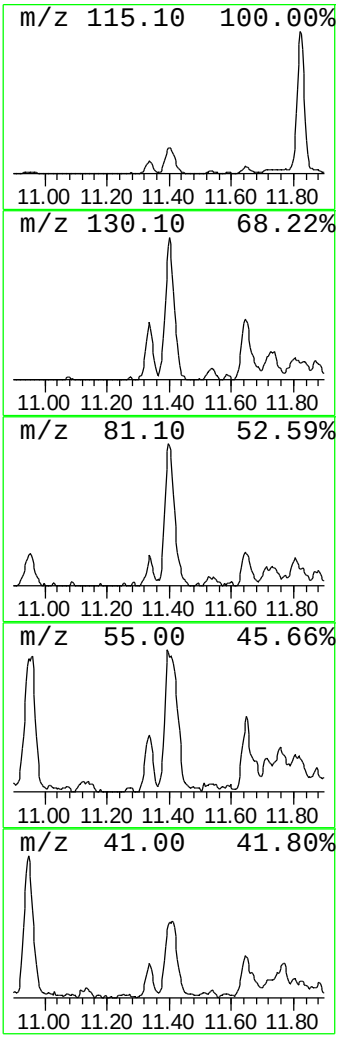
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.40	1.26 ug/L	259680	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cis-2,5-dimethylthiane	130	C7H14S	1000215-06-6	96
2	cis-2,4-Dimethylthiane	130	C7H14S	061568-43-2	95
3	trans-2,4-Dimethylthiane	130	C7H14S	061568-42-1	95
4	Cis-2,3-dimethylthiane	130	C7H14S	1000215-06-5	50
5	4-Ethylthiane	130	C7H14S	040324-31-0	47





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU060620\
Data File : VU038644.D
Acq On : 07 Jun 2020 02:53
Operator : SY/MD
Sample : L2911-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D32

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

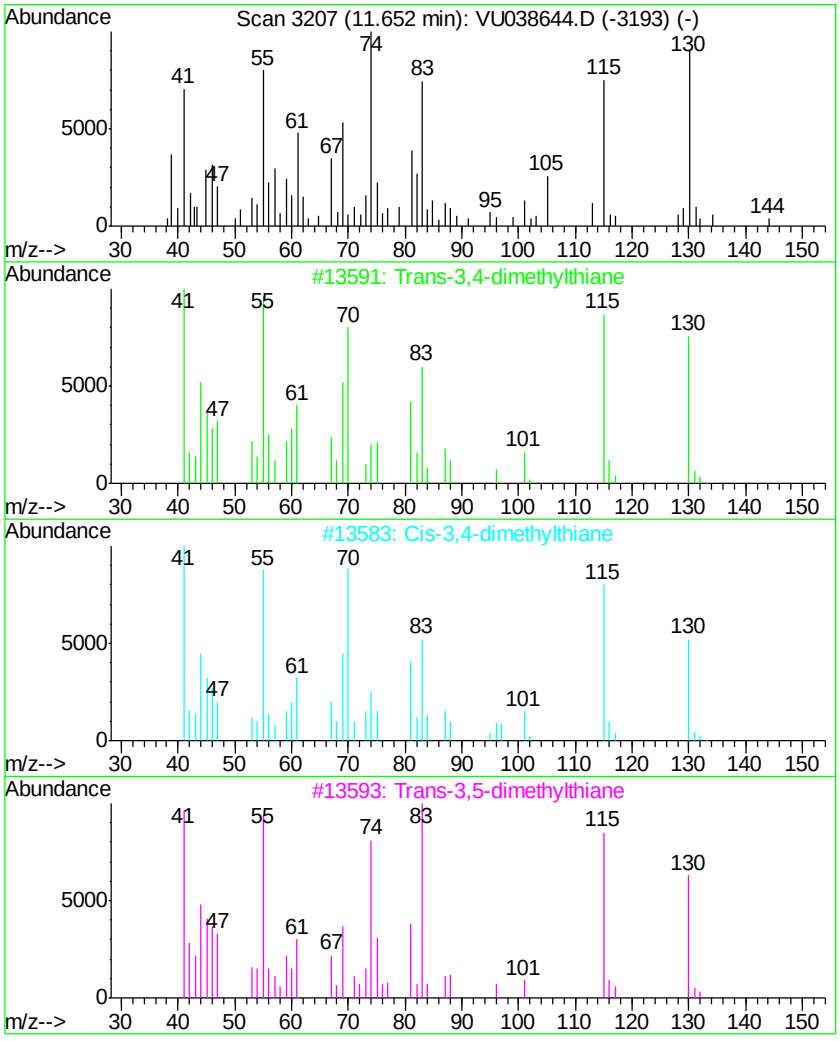
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

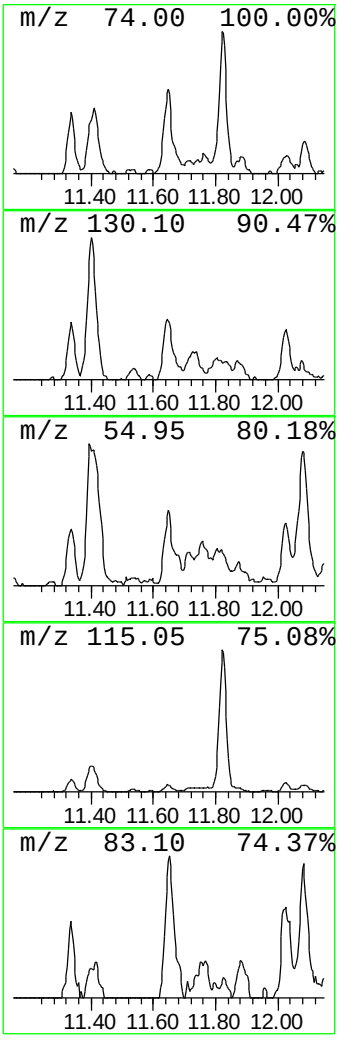
****

Peak Number 6 Trans-3,4-dimethylthiane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.65	0.56 ug/L	114924	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trans-3,4-dimethylthiane	130	C7H14S	1000215-07-1	55
2	Cis-3,4-dimethylthiane	130	C7H14S	1000215-07-0	41
3	Trans-3,5-dimethylthiane	130	C7H14S	1000215-06-7	38
4	1,3-Diazacycloheptane-2-thione	130	C5H10N2S	005700-04-9	38
5	1,3,4-Thiadiazol-2-amine, 5-methyl-	115	C3H5N3S	000108-33-8	35





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Operator : SY/MD
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ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D32

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

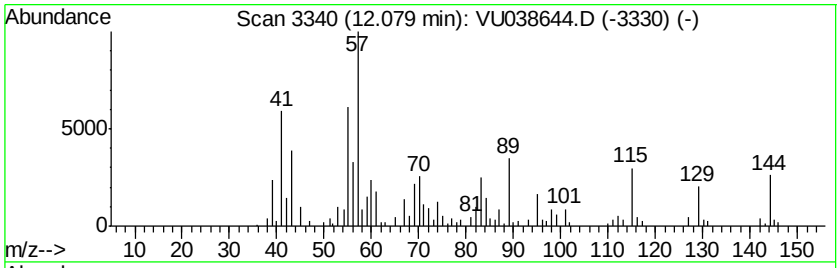
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

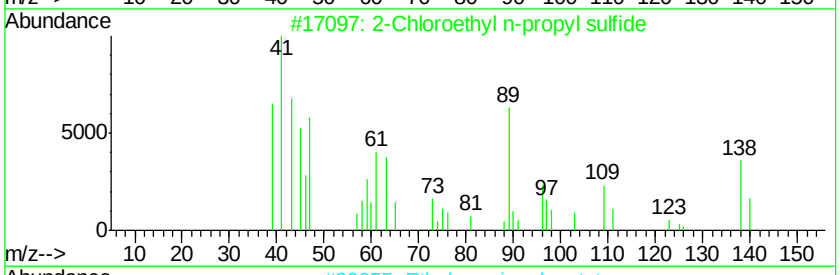
****

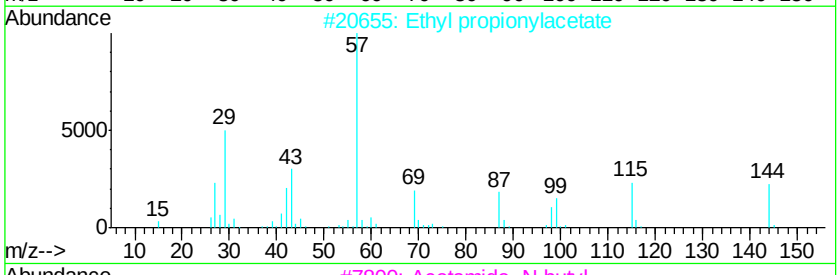
Peak Number 7 unknown-01 Concentration Rank 6

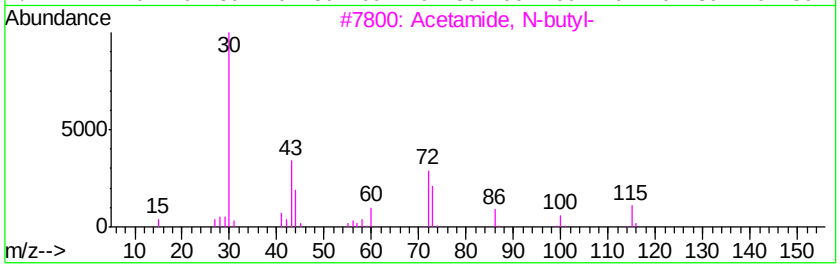
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.08	0.81 ug/L	167793	1,4-Dichlorobenzene-d4	11.83

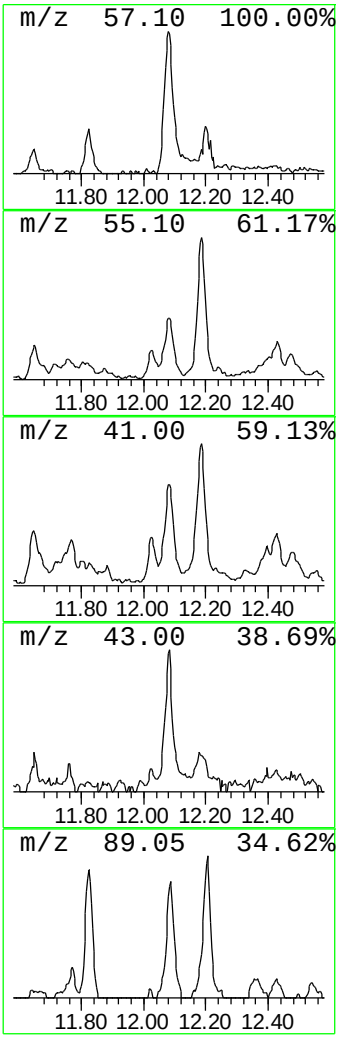
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chloroethyl n-propyl sulfide	138	C5H11ClS	004303-42-8	12
2	Ethyl propionylacetate	144	C7H12O3	004949-44-4	10
3	Acetamide, N-butyl-	115	C6H13NO	001119-49-9	9
4	N-Methylpivalamide	115	C6H13NO	006830-83-7	9
5	Butane, 1-(2-methoxyethoxy)-	132	C7H16O2	013343-98-1	9











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Data File : VU038644.D
Acq On : 07 Jun 2020 02:53
Operator : SY/MD
Sample : L2911-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D32

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

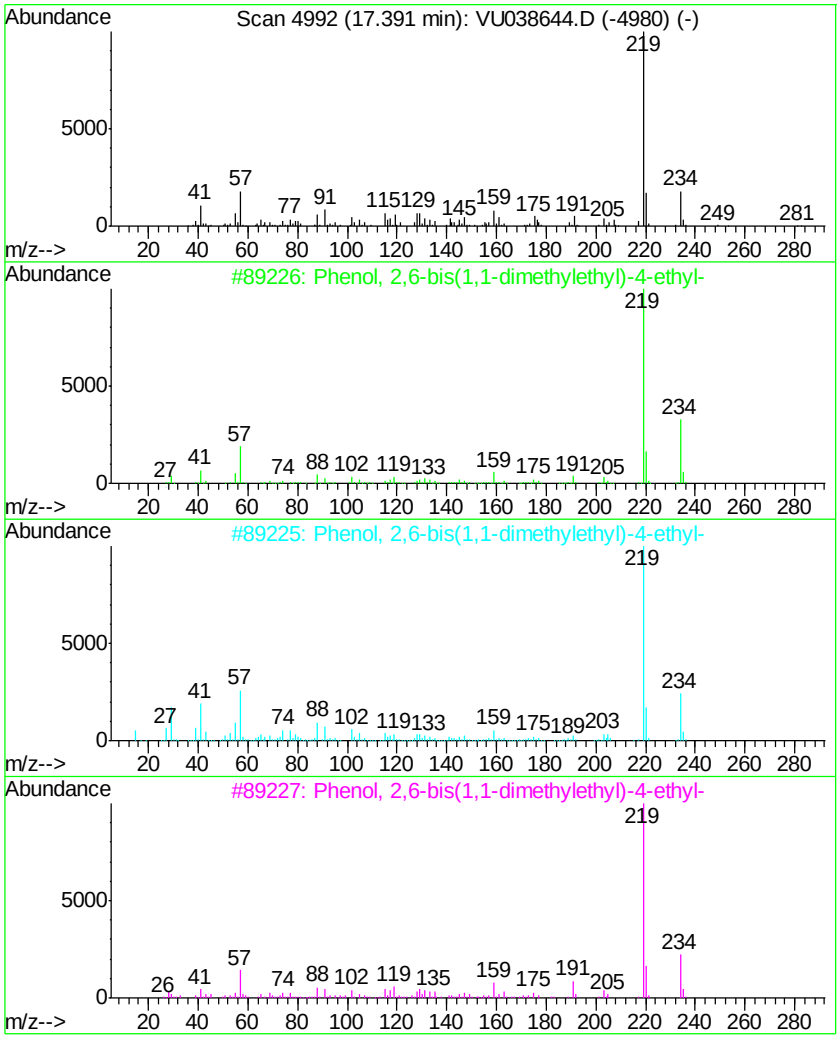
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

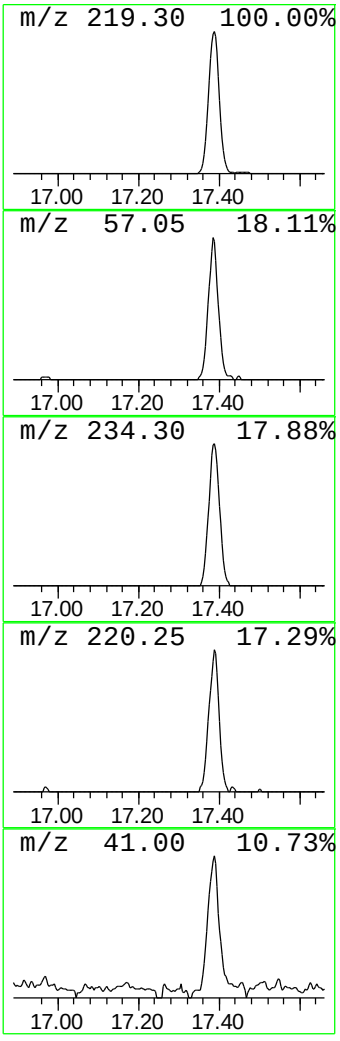
****

Peak Number 8 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.39	1.00 ug/L	206687	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	95
2	Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	94
3	Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	90
4	3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	87
5	3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU060620\
Data File : VU038644.D
Acq On : 07 Jun 2020 02:53
Operator : SY/MD
Sample : L2911-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D32

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	0.9	ug/L	146979	1	6.28	774952	5.0
Thiophene, tetrah...	9.84	0.8	ug/L	146140	2	9.44	976024	5.0
2H-Thiopyran, tet...	10.95	1.6	ug/L	322053	3	11.83	1031070	5.0
Cis-2,5-dimethylt...	11.40	1.3	ug/L	259680	3	11.83	1031070	5.0
Trans-3,4-dimethy...	11.65	0.6	ug/L	114924	3	11.83	1031070	5.0
unknown-01	12.08	0.8	ug/L	167793	3	11.83	1031070	5.0
Phenol, 2,6-bis(1...	17.39	1.0	ug/L	206687	3	11.83	1031070	5.0