LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060520\
Data File : VU038606.D
Acq On : 06 Jun 2020 08:10
Operator : SY/MD
Sample : L2910-13
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D30

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	1.359	3	6	15	rVB	70198	66497	4.08%	0.406%
2	1.601	72	81	90	rBV	147504	172428	10.58%	1.052%
3	1.919	173	180	193	rVB	151950	193052	11.84%	1.178%
4	2.578	370	385	399	rBV	277539	463874	28.46%	2.831%
5	2.662	400	411	441	rVB2	26806	83780	5.14%	0.511%
6	2.810	446	457	463	rBV2	12786	23675	1.45%	0.144%
7	4.662	1015	1033	1071	rBV	259465	822762	50.48%	5.021%
8	4.835	1074	1087	1117	rVB	122488	303477	18.62%	1.852%
9	5.092	1149	1167	1188	rBV	268404	600558	36.84%	3.665%
10	5.417	1252	1268	1288	rVB3	79439	181881	11.16%	1.110%
11	5.752	1350	1372	1387	rBV3	534567	1422985	87.30%	8.684%
12	6.276	1518	1535	1574	rBV	510753	1037371	63.64%	6.331%
13	6.559	1609	1623	1624	rBV2	22382	32575	2.00%	0.199%
14	6.594	1626	1634	1654	rVB2	49961	106615	6.54%	0.651%
15	6.716	1659	1672	1692	rVB	334692	665613	40.84%	4.062%
16	7.591	1931	1944	1961	rBV	159749	290896	17.85%	1.775%
17	7.922	2028	2047	2082	rBV	567222	1091809	66.98%	6.663%
18	8.202	2121	2134	2152	rBV	92598	159760	9.80%	0.975%
19	8.443	2198	2209	2224	rBV5	17171	33586	2.06%	0.205%
20	8.658	2261	2276	2290	rBV2	854289	1629981	100.00%	9.947%
21	9.439	2505	2519	2549	rBV	714109	1293056	79.33%	7.891%
22	9.848	2633	2646	2673	rBV2	163178	319727	19.62%	1.951%
23	10.054	2695	2710	2725	rBV8	28987	61976	3.80%	0.378%
24	10.298	2773	2786	2799	rBV4	34793	65290	4.01%	0.398%
25	10.382	2799	2812	2822	rBV2	50371	95879	5.88%	0.585%
26	10.446	2822	2832	2847	rVB3	61200	108438	6.65%	0.662%
27	10.668	2891	2901	2916	rBV2	38502	68382	4.20%	0.417%
28	10.774	2916	2934	2940	rBV	226047	394209	24.18%	2.406%
29	10.864	2957	2962	2970	rVB3	13202	17255	1.06%	0.105%
30	10.954	2970	2990	3013	rVB4	221958	515935	31.65%	3.149%
31	11.083	3020	3030	3041	rBV3	60287	103263	6.34%	0.630%
32	11.137	3041	3047	3058	rVB5	15928	25672	1.57%	0.157%
33	11.340	3099	3110	3119	rVV2	29403	49044	3.01%	0.299%
34	11.417	3119	3134	3151	rBV6	106670	281278	17.26%	1.717%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060520\
Data File : VU038606.D
Acq On : 06 Jun 2020 08:10
Operator : SY/MD
Sample : L2910-13
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D30

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	11.539	3162	3172	3182	rVB4	25903	40540	2.49%	0.247%
36	11.652	3197	3207	3212	rBV6	44487	80604	4.95%	0.492%
37	11.828	3250	3262	3276	rVB	814811	1316173	80.75%	8.032%
38	12.028	3315	3324	3331	rBV6	29758	52872	3.24%	0.323%
39	12.086	3332	3342	3359	rVV4	77873	197089	12.09%	1.203%
40	12.208	3362	3380	3402	rVB	662084	1208482	74.14%	7.375%
41	12.433	3444	3450	3458	rVB6	31071	45575	2.80%	0.278%
42	12.481	3459	3465	3480	rVB6	18977	37766	2.32%	0.230%
43	12.697	3524	3532	3534	rBV8	13579	17594	1.08%	0.107%
44	12.828	3559	3573	3575	rBV9	11220	21405	1.31%	0.131%
45	13.176	3677	3681	3696	rVB9	13405	23356	1.43%	0.143%
46	13.256	3696	3706	3716	rBV7	19810	37345	2.29%	0.228%
47	14.484	4075	4088	4096	rBV4	18070	36148	2.22%	0.221%
48	15.089	4264	4276	4285	rBV9	14350	28148	1.73%	0.172%
49	15.372	4354	4364	4376	rBV3	30725	54523	3.35%	0.333%
50	15.452	4380	4389	4395	rBV6	16509	30068	1.84%	0.183%
51	15.497	4396	4403	4417	rVB3	36694	64028	3.93%	0.391%
52	15.626	4430	4443	4453	rBV4	25674	48002	2.94%	0.293%
53	16.169	4600	4612	4624	rVB4	12449	27957	1.72%	0.171%
54	17.430	4991	5004	5018	rBV2	106667	236085	14.48%	1.441%

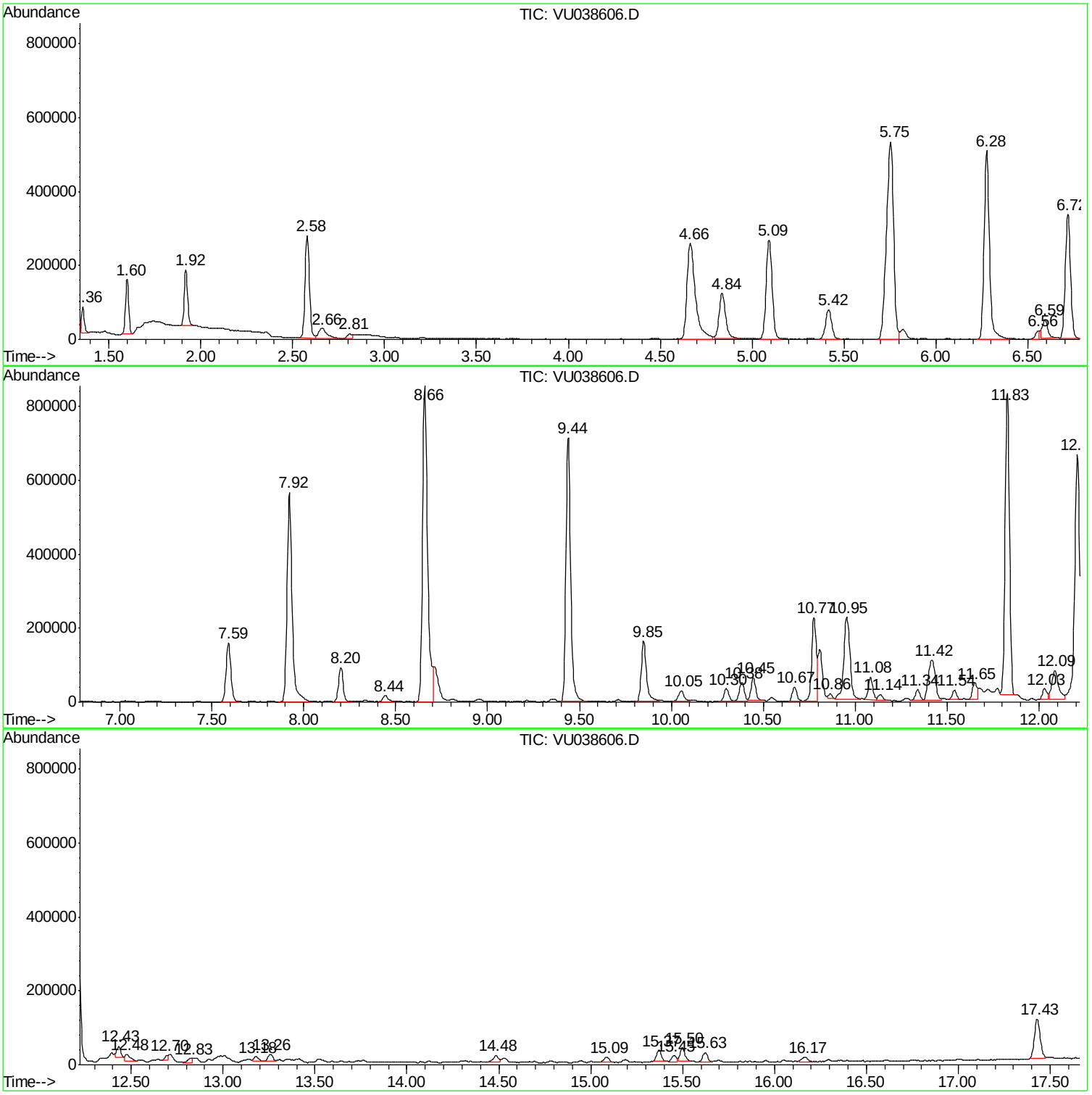
Sum of corrected areas: 16386339

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060520\
Data File : VU038606.D
Acq On : 06 Jun 2020 08:10
Operator : SY/MD
Sample : L2910-13
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F9D30

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\VU060520\
Data File : VU038606.D
Acq On : 06 Jun 2020 08:10
Operator : SY/MD
Sample : L2910-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D30

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

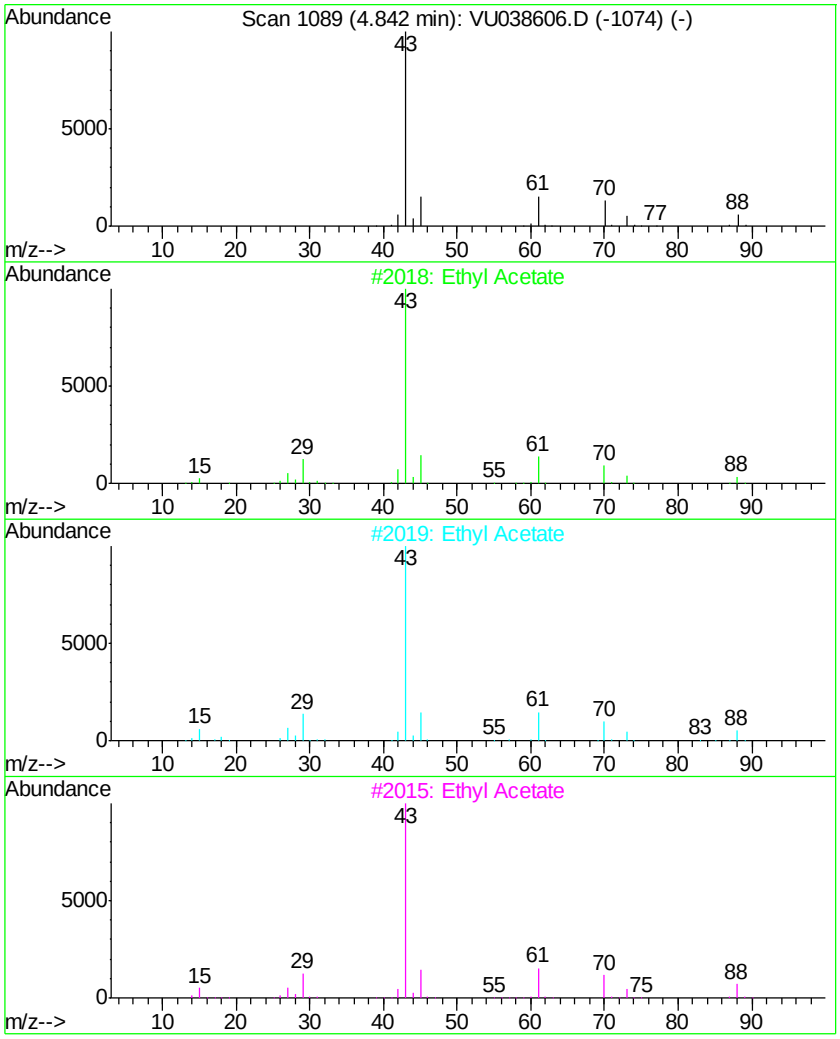
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

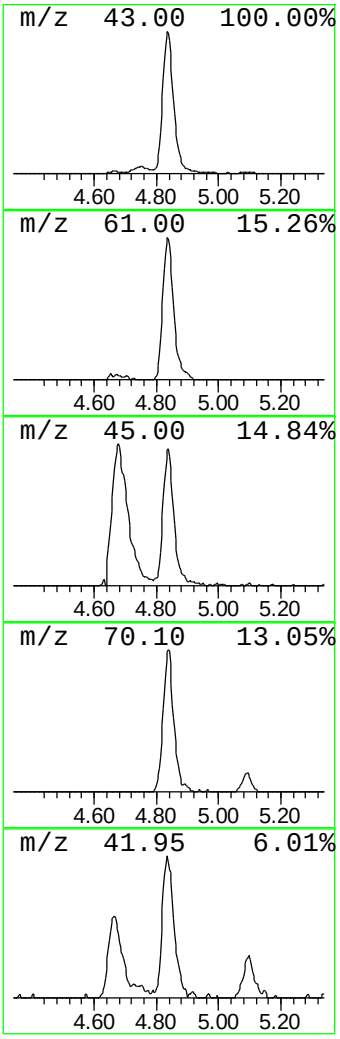
****

Peak Number 1 Ethyl Acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	1.46 ug/L	303477	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	40





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU060520\
Data File : VU038606.D
Acq On : 06 Jun 2020 08:10
Operator : SY/MD
Sample : L2910-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D30

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

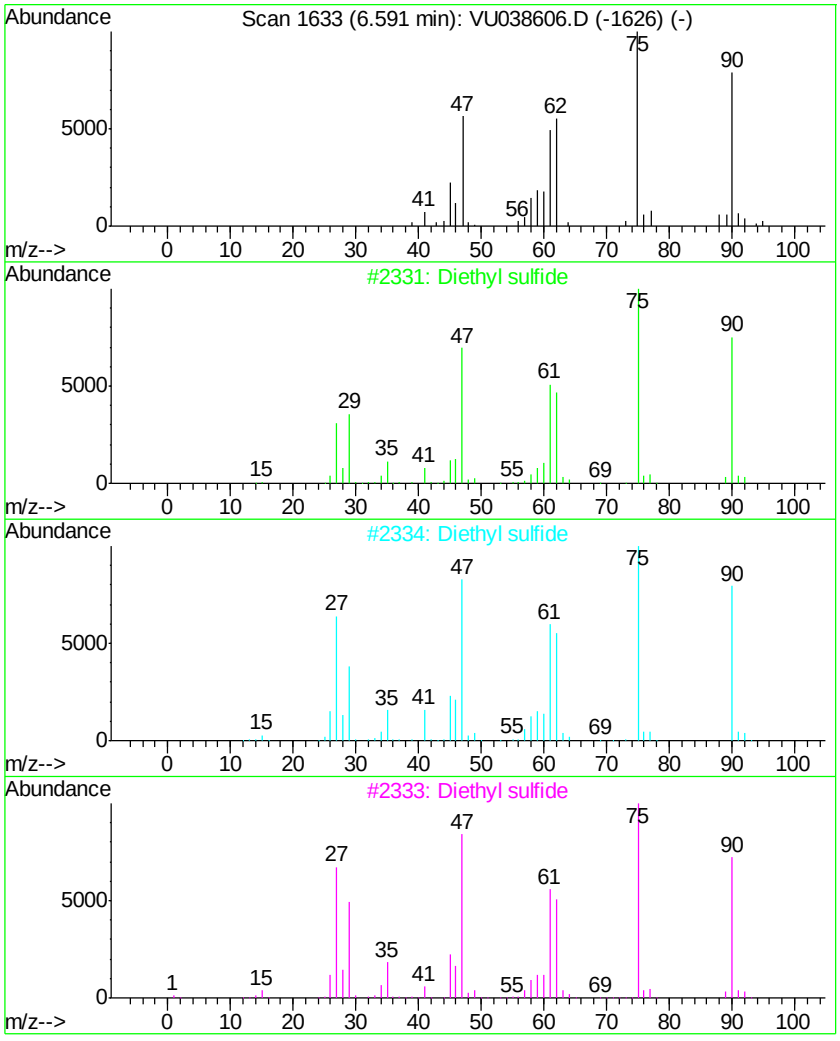
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

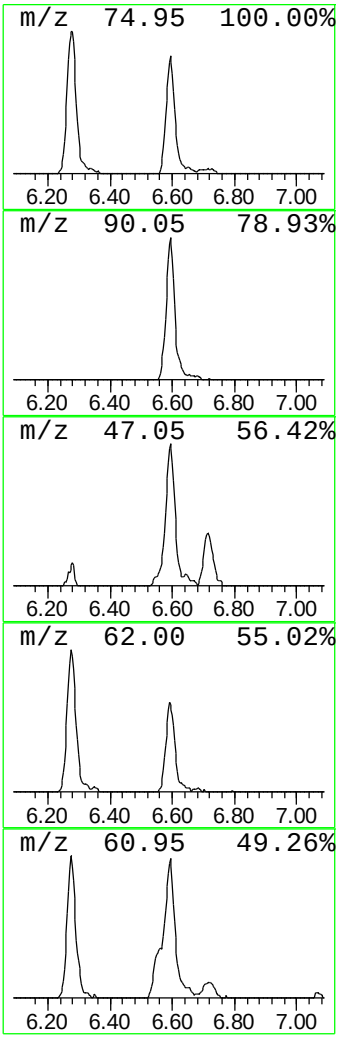
****

Peak Number 2 Diethyl sulfide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	0.51 ug/L	106615	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyl sulfide	90	C4H10S	000352-93-2	94
2	Diethyl sulfide	90	C4H10S	000352-93-2	91
3	Diethyl sulfide	90	C4H10S	000352-93-2	90
4	Diethyl sulfide	90	C4H10S	000352-93-2	90
5	Propane, 2-(methylthio)-	90	C4H10S	001551-21-9	50





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU060520\
Data File : VU038606.D
Acq On : 06 Jun 2020 08:10
Operator : SY/MD
Sample : L2910-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D30

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

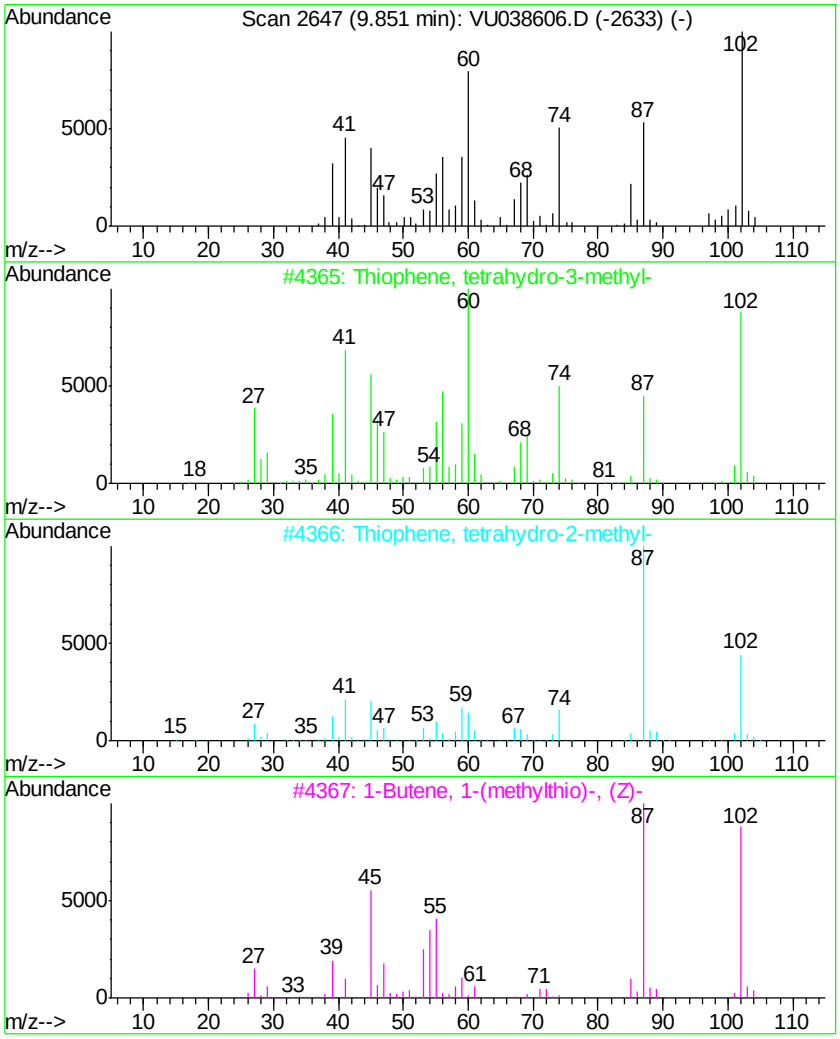
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

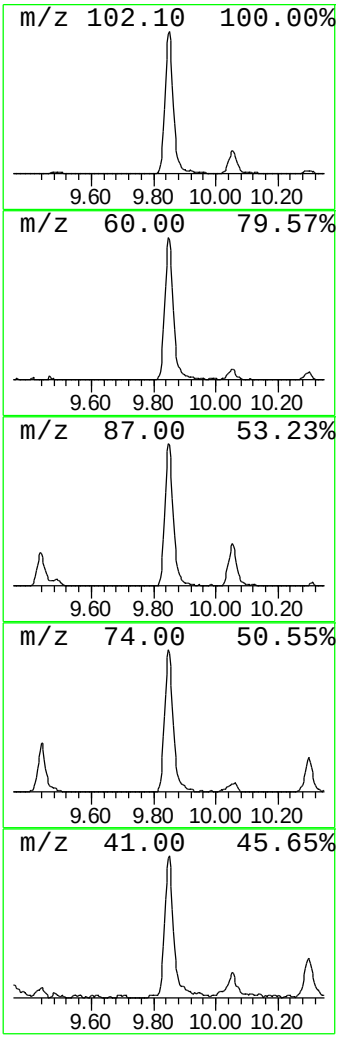
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.85	1.24 ug/L	319727	Chlorobenzene-d5	9.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, tetrahydro-3-methyl-	102	C5H10S	004740-00-5	97
2	Thiophene, tetrahydro-2-methyl-	102	C5H10S	001795-09-1	47
3	1-Butene, 1-(methylthio)-, (Z)-	102	C5H10S	017414-15-2	43
4	Thietane, 2,4-dimethyl-	102	C5H10S	043044-24-2	43
5	2-Methyl-3-(methylthio)-1-propene	102	C5H10S	052326-10-0	38





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU060520\
Data File : VU038606.D
Acq On : 06 Jun 2020 08:10
Operator : SY/MD
Sample : L2910-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D30

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

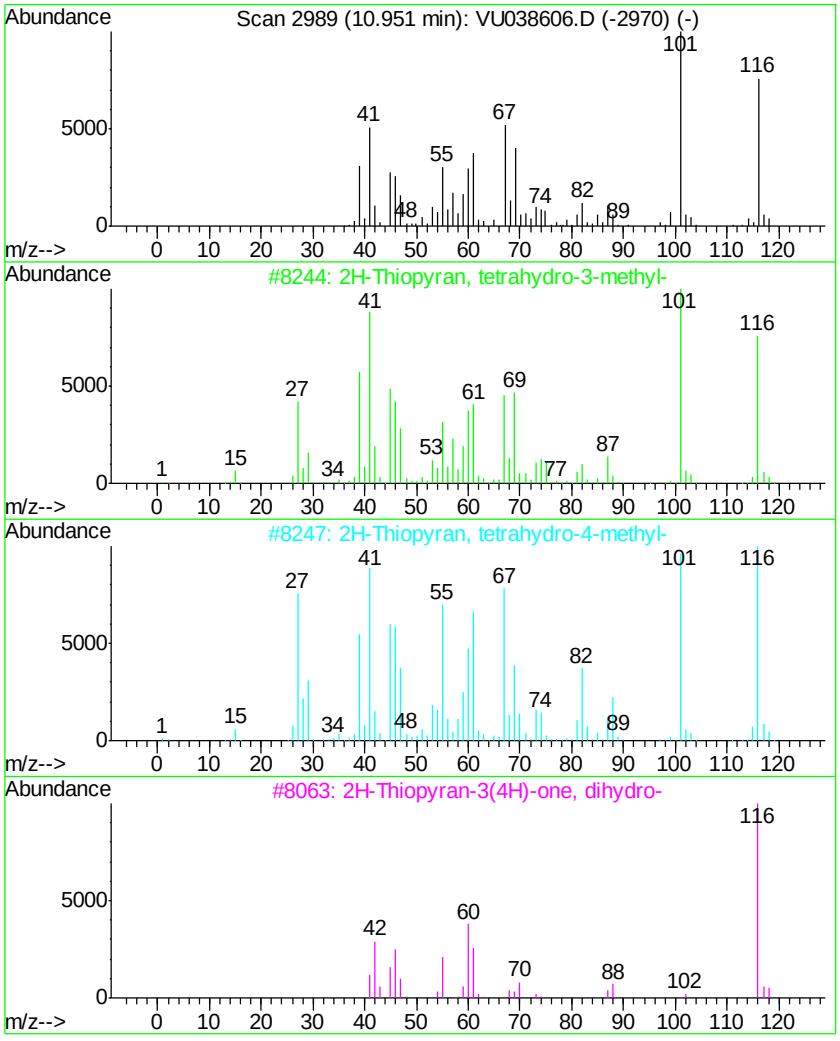
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

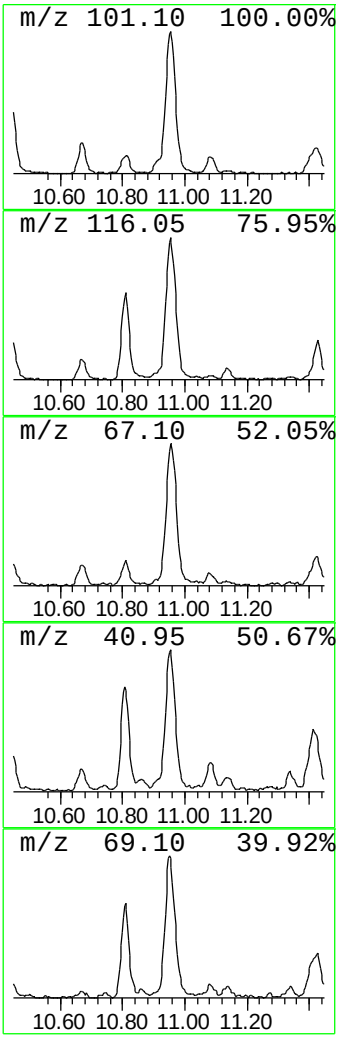
****

Peak Number 5 2H-Thiopyran, tetrahydro-3-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.95	1.96 ug/L	515935	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	94
2	2H-Thiopyran, tetrahydro-4-methyl-	116	C6H12S	005161-17-1	94
3	2H-Thiopyran-3(4H)-one, dihydro-	116	C5H8OS	019090-03-0	45
4	Cyclopentanethiol, 2-methyl-, tr...	116	C6H12S	001638-93-3	38
5	cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	38





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060520\
Data File : VU038606.D
Acq On : 06 Jun 2020 08:10
Operator : SY/MD
Sample : L2910-13
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D30

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

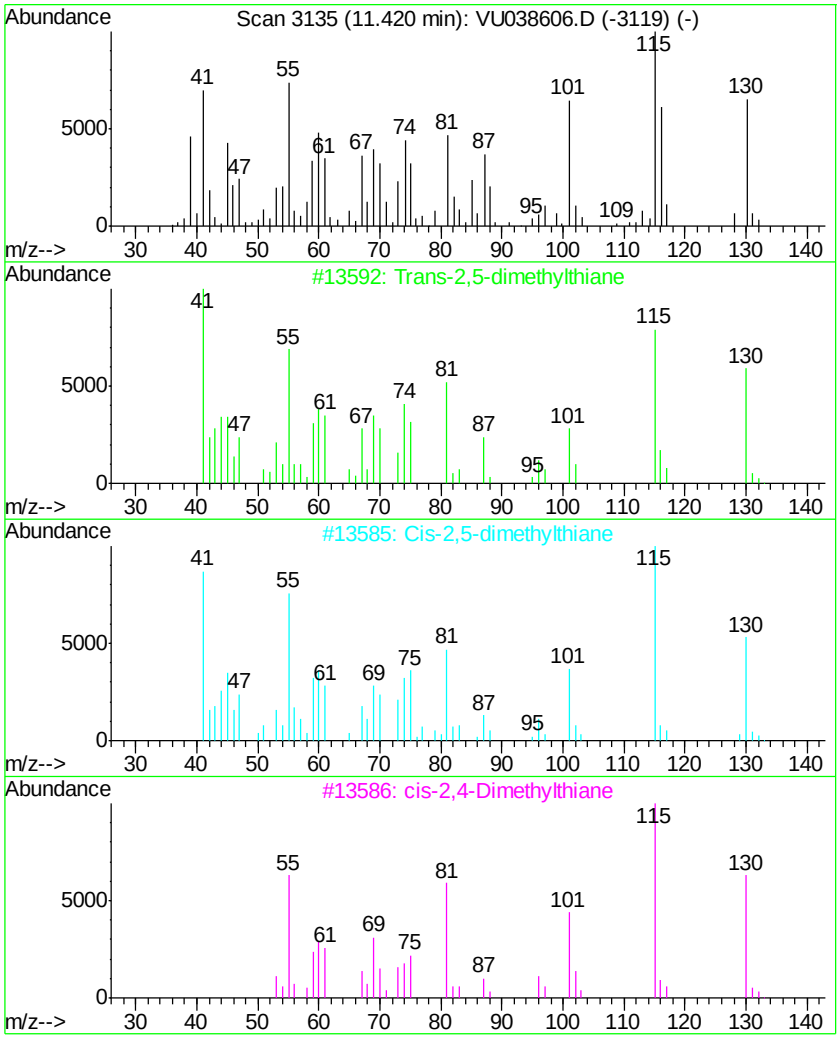
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

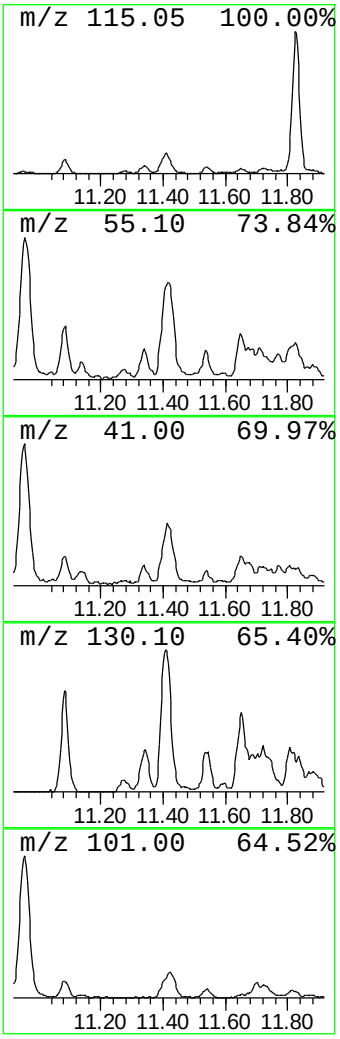
****

Peak Number 6 Trans-2,5-dimethylthiane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.42	1.07 ug/L	281278	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trans-2,5-dimethylthiane	130	C7H14S	1000215-06-8	91
2	Cis-2,5-dimethylthiane	130	C7H14S	1000215-06-6	90
3	cis-2,4-Dimethylthiane	130	C7H14S	061568-43-2	89
4	trans-2,4-Dimethylthiane	130	C7H14S	061568-42-1	60
5	Trans-2,3-dimethylthiane	130	C7H14S	1000215-06-9	60





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU060520\
Data File : VU038606.D
Acq On : 06 Jun 2020 08:10
Operator : SY/MD
Sample : L2910-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D30

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

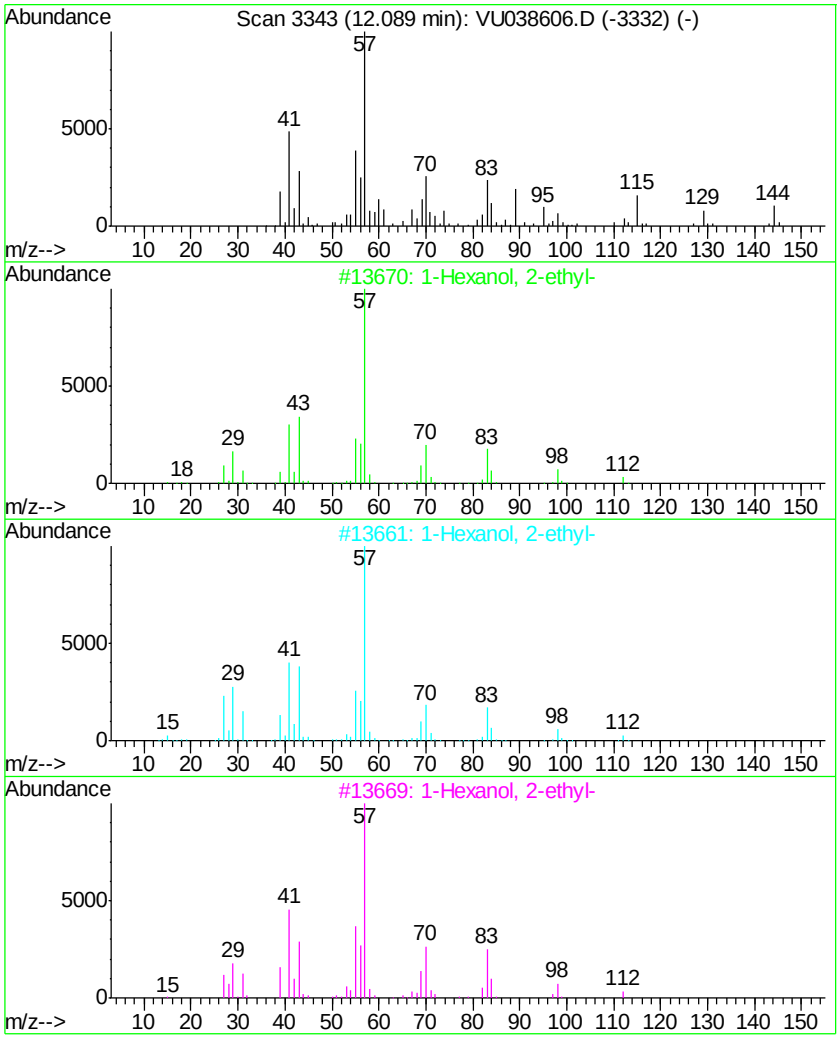
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

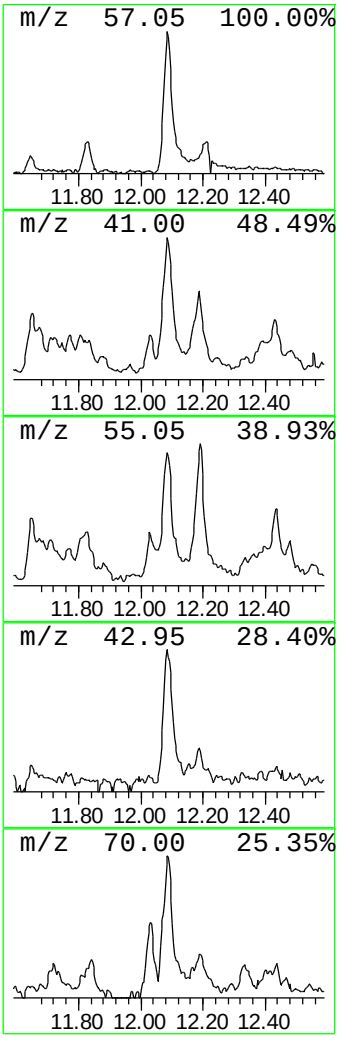
****

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.09	0.75 ug/L	197089	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	53
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	53
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	53
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	42
5	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	38





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060520\
Data File : VU038606.D
Acq On : 06 Jun 2020 08:10
Operator : SY/MD
Sample : L2910-13
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D30

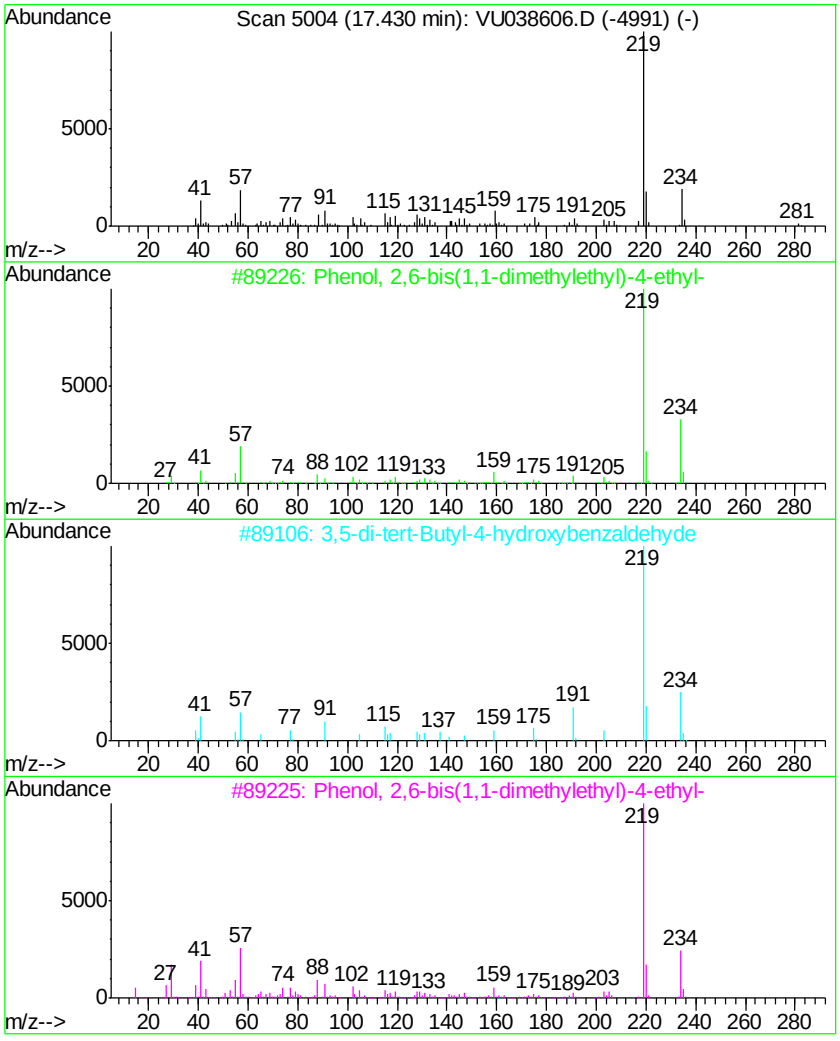
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

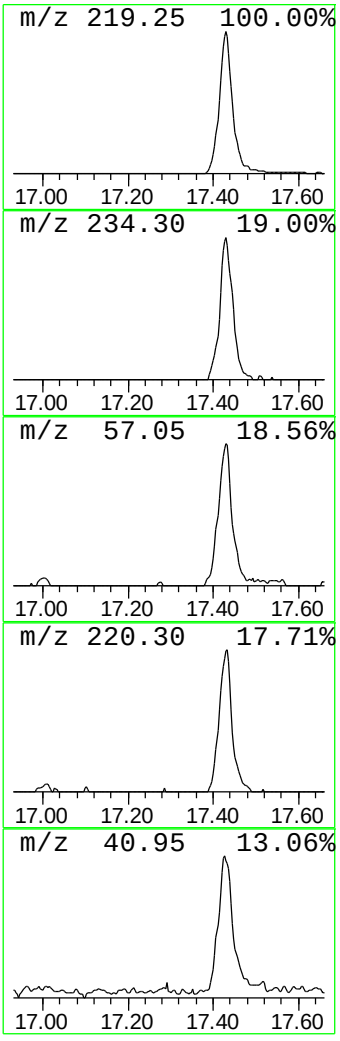
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.43	0.90 ug/L	236085	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	97
2	3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	95
3	Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	94
4	3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	91
5	Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU060520\
Data File : VU038606.D
Acq On : 06 Jun 2020 08:10
Operator : SY/MD
Sample : L2910-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9D30

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	303477	1	6.28	1037370	5.0
Diethyl sulfide	6.59	0.5	ug/L	106615	1	6.28	1037370	5.0
Thiophene, tetrah...	9.85	1.2	ug/L	319727	2	9.44	1293060	5.0
2H-Thiopyran, tet...	10.95	2.0	ug/L	515935	3	11.83	1316170	5.0
Trans-2,5-dimethy...	11.42	1.1	ug/L	281278	3	11.83	1316170	5.0
1-Hexanol, 2-ethyl-	12.09	0.8	ug/L	197089	3	11.83	1316170	5.0
Phenol, 2,6-bis(1...	17.43	0.9	ug/L	236085	3	11.83	1316170	5.0