LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU053120\
Data File : VU038436.D
Acq On : 31 May 2020 00:52
Operator : JC/MD
Sample : L2787-13
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFX95

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	17	rVB	77716	76469	5.04%	0.655%
2	1.611	74	84	96	rBV	144431	167491	11.04%	1.434%
3	1.932	175	184	198	rVB	114378	146347	9.64%	1.253%
4	2.591	376	389	407	rBV	239254	399904	26.35%	3.425%
5	3.218	572	584	601	rVB	8145	18555	1.22%	0.159%
6	3.395	623	639	653	rVB2	9669	21708	1.43%	0.186%
7	3.739	732	746	757	rBV5	10615	23382	1.54%	0.200%
8	4.569	990	1004	1020	rBV3	18017	43029	2.84%	0.369%
9	4.684	1020	1040	1077	rBV	173941	673403	44.38%	5.767%
10	4.848	1077	1091	1120	rVB2	154776	394766	26.02%	3.381%
11	5.102	1153	1170	1205	rBV	238417	574399	37.85%	4.919%
12	5.758	1349	1374	1403	rBV2	421732	1116026	73.55%	9.558%
13	6.279	1521	1536	1571	rBV	381380	748680	49.34%	6.412%
14	6.572	1614	1627	1643	rBV4	27433	56265	3.71%	0.482%
15	6.720	1658	1673	1693	rBV	262551	504334	33.24%	4.319%
16	7.070	1766	1782	1805	rBV	153567	288773	19.03%	2.473%
17	7.591	1931	1944	1963	rBV	133651	236980	15.62%	2.030%
18	7.922	2033	2047	2065	rBV	502109	885518	58.36%	7.584%
19	8.202	2121	2134	2150	rBV2	84722	145023	9.56%	1.242%
20	8.575	2237	2250	2263	rBV	241185	413507	27.25%	3.542%
21	8.658	2263	2276	2307	rVB	799118	1517379	100.00%	12.996%
22	9.437	2505	2518	2555	rVB	549453	937689	61.80%	8.031%
23	10.771	2917	2933	2951	rBV	216841	347018	22.87%	2.972%
24	11.822	3248	3260	3277	rBV	588210	936116	61.69%	8.017%
25	12.080	3329	3340	3359	rBV3	8890	19923	1.31%	0.171%
26	12.205	3366	3379	3392	rBV	527959	847888	55.88%	7.262%
27	13.250	3694	3704	3713	rVB8	11728	16895	1.11%	0.145%
28	17.388	4980	4991	5011	rVB	64039	118553	7.81%	1.015%

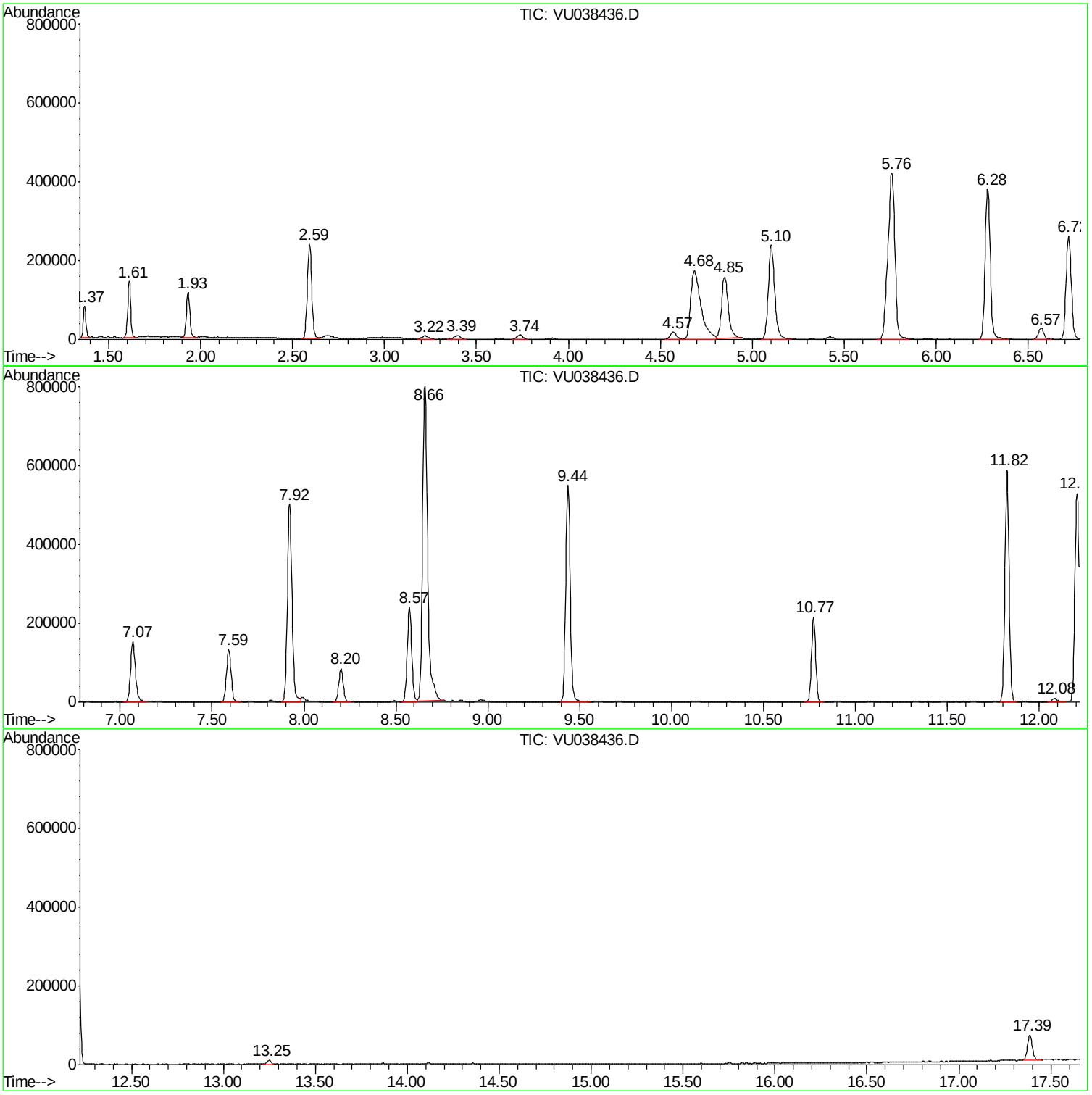
Sum of corrected areas: 11676020

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU053120\
Data File : VU038436.D
Acq On : 31 May 2020 00:52
Operator : JC/MD
Sample : L2787-13
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFX95

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\VU053120\
Data File : VU038436.D
Acq On : 31 May 2020 00:52
Operator : JC/MD
Sample : L2787-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFX95

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

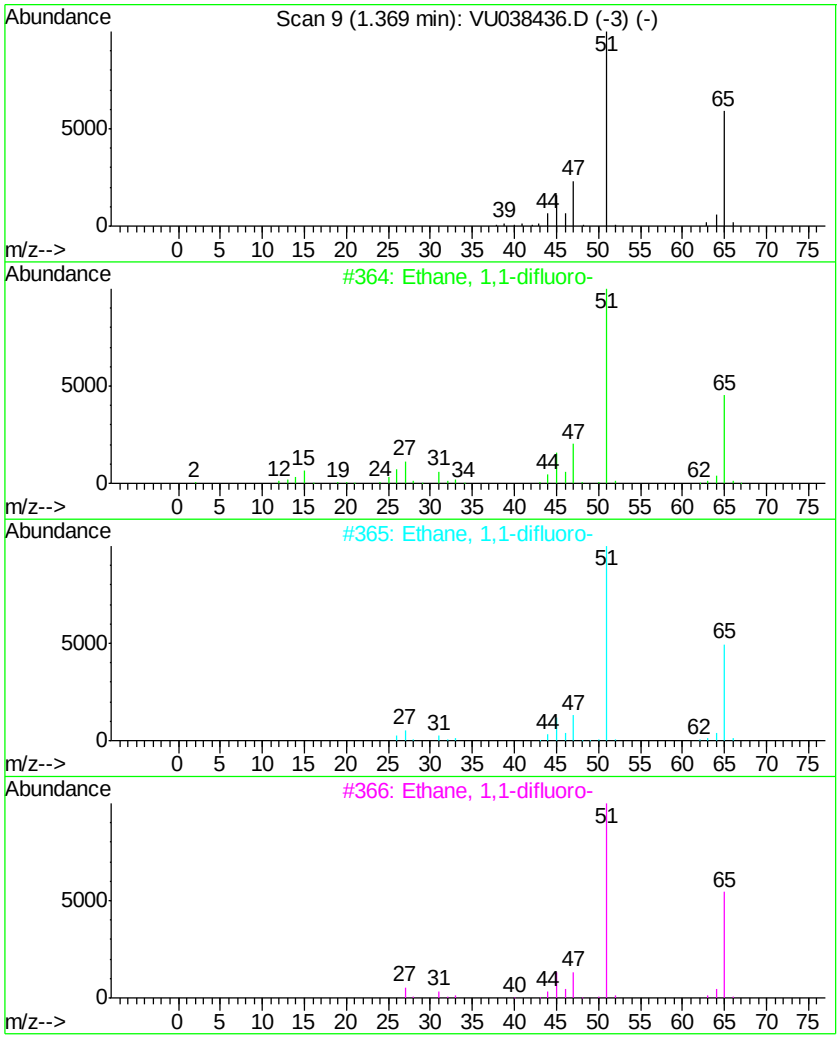
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

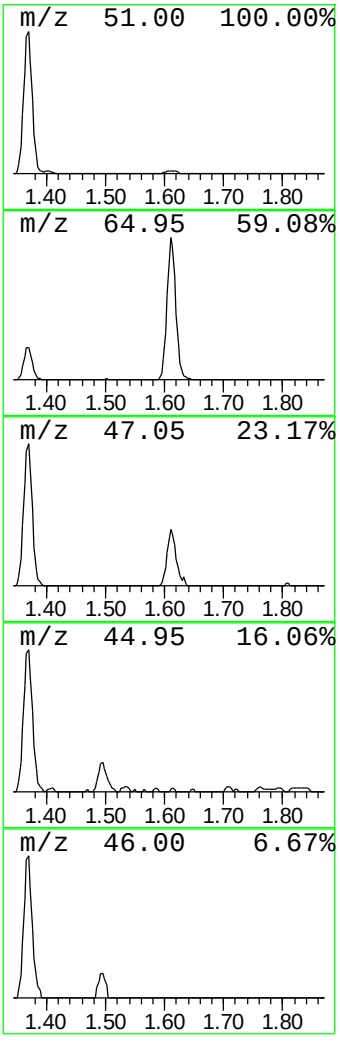
****

Peak Number 1 Ethane, 1,1-difluoro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.37	0.51 ug/L	76469	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	91
2	Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	90
3	Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	74
4	Propiolonitrile	51	C3HN	001070-71-9	3
5	Propane, 2,2-difluoro-	80	C3H6F2	000420-45-1	2





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU053120\
Data File : VU038436.D
Acq On : 31 May 2020 00:52
Operator : JC/MD
Sample : L2787-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFX95

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

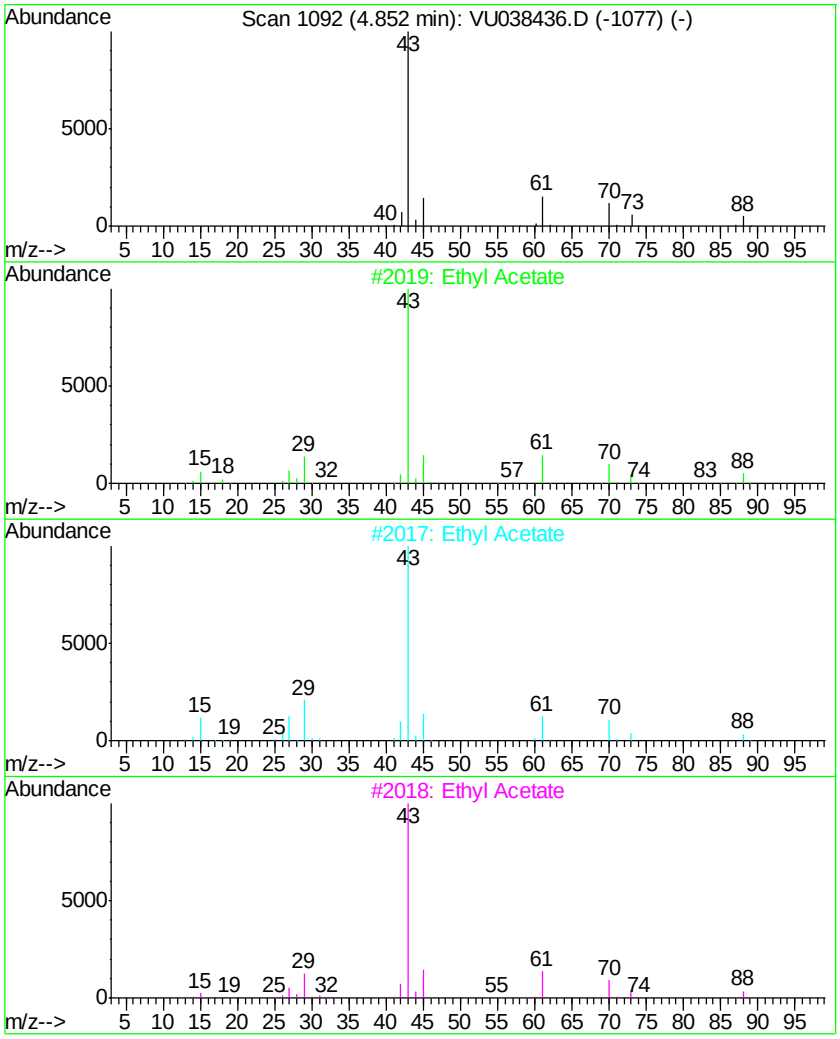
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

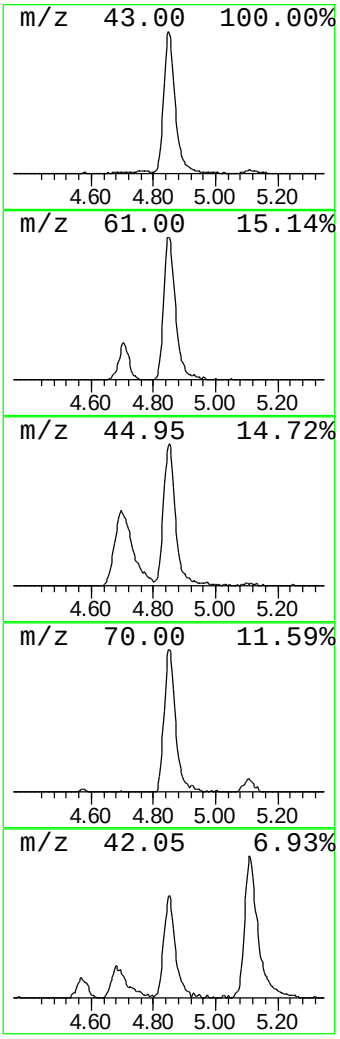
****

Peak Number 2 Ethyl Acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	2.64 ug/L	394766	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	86
4	Ethyl Acetate	88	C4H8O2	000141-78-6	86
5	CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	40





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU053120\
Data File : VU038436.D
Acq On : 31 May 2020 00:52
Operator : JC/MD
Sample : L2787-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFX95

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

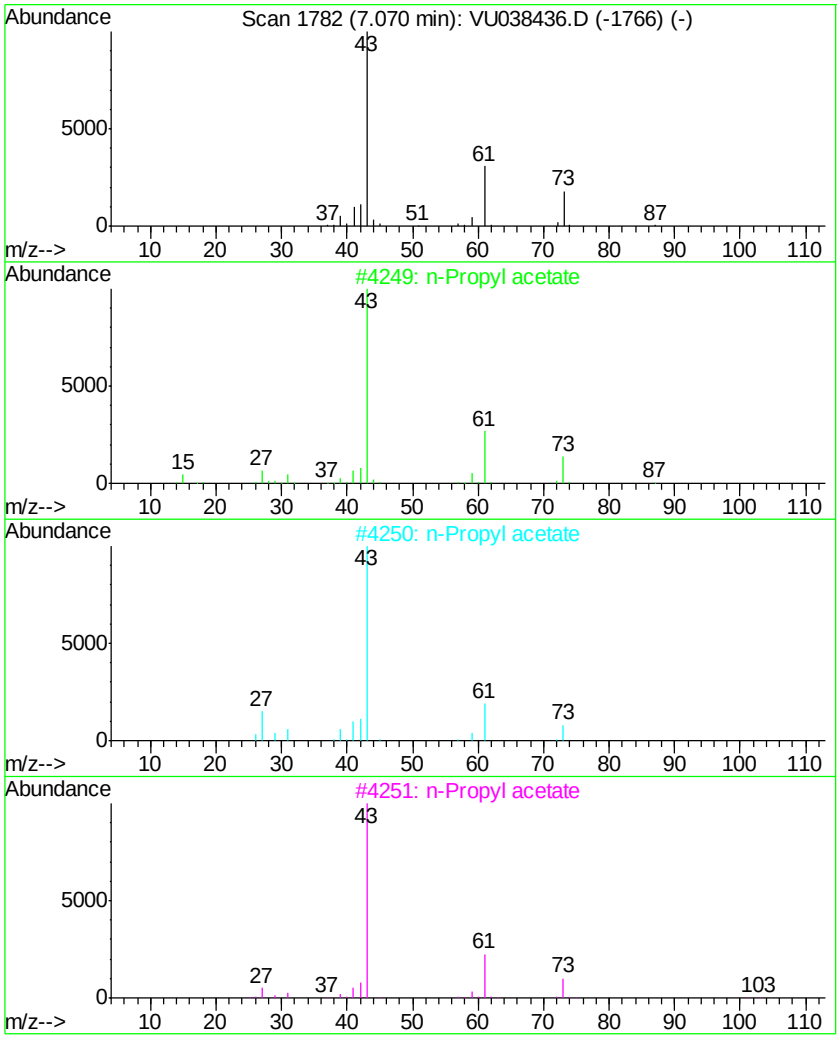
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

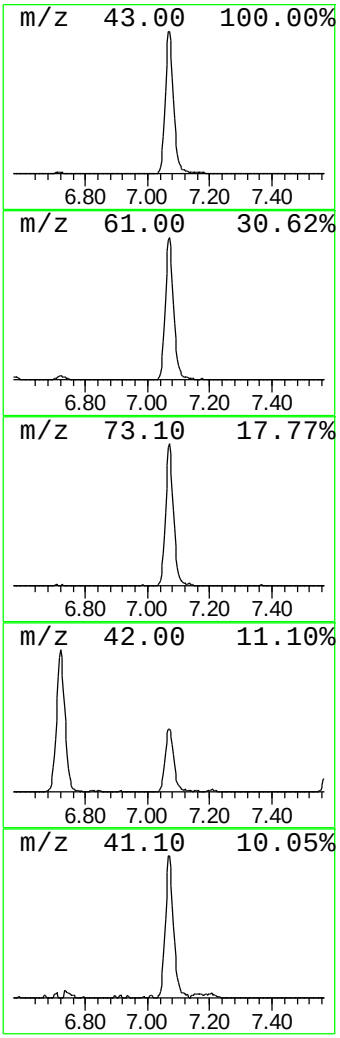
****

Peak Number 3 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.07	1.93 ug/L	288773	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	78
2	n-Propyl acetate	102	C5H10O2	000109-60-4	64
3	n-Propyl acetate	102	C5H10O2	000109-60-4	40
4	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	36
5	Isopropyl acetate	102	C5H10O2	000108-21-4	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU053120\
Data File : VU038436.D
Acq On : 31 May 2020 00:52
Operator : JC/MD
Sample : L2787-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFX95

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

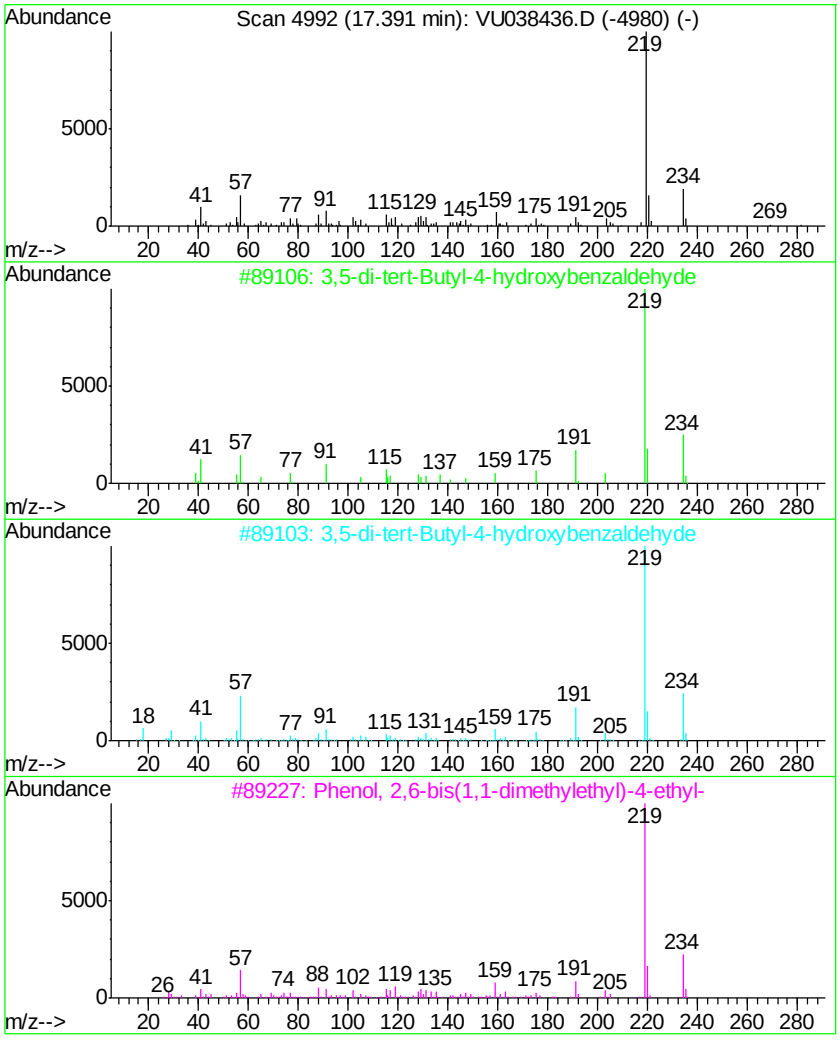
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

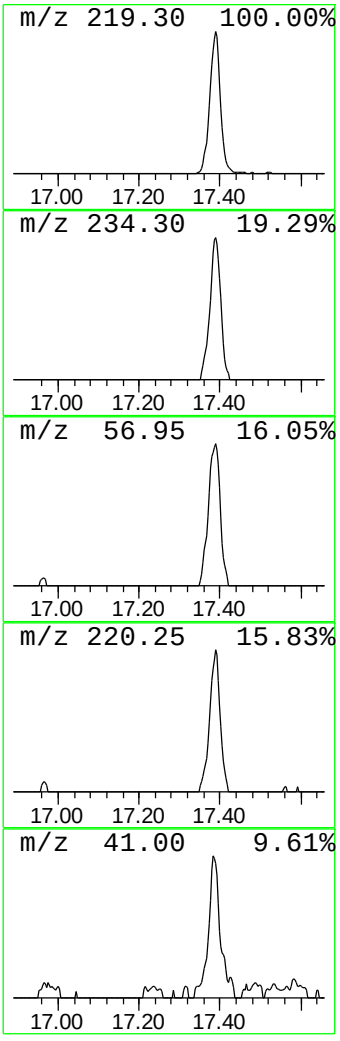
****

Peak Number 5 3,5-di-tert-Butyl-4-hydroxy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.39	0.63 ug/L	118553	1,4-Dichlorobenzene-d4	11.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	94
2	3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	94
3	Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	93
4	Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	93
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\VU053120\
Data File : VU038436.D
Acq On : 31 May 2020 00:52
Operator : JC/MD
Sample : L2787-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFX95

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
Ethane, 1,1-diflu...	1.37	0.5	ug/L	76469	1	6.28	748680	5.0
Ethyl Acetate	4.85	2.6	ug/L	394766	1	6.28	748680	5.0
n-Propyl acetate	7.07	1.9	ug/L	288773	1	6.28	748680	5.0
3,5-di-tert-Butyl...	17.39	0.6	ug/L	118553	3	11.82	936116	5.0