LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060120\
Data File : VU038477.D
Acq On : 01 Jun 2020 17:37
Operator : JC/MD
Sample : L2789-15
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 2 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXA1

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	22	rVB	72239	71267	4.69%	0.684%
2	1.610	76	84	94	rBV	108301	122421	8.05%	1.174%
3	1.932	175	184	198	rVB	102059	131141	8.62%	1.258%
4	2.594	372	390	404	rBV	199946	337197	22.17%	3.235%
5	2.684	410	418	433	rVB2	6759	17244	1.13%	0.165%
6	4.568	992	1004	1021	rBV5	8010	18067	1.19%	0.173%
7	4.681	1021	1039	1076	rBV2	183080	624167	41.04%	5.987%
8	4.848	1077	1091	1119	rVB	125812	307348	20.21%	2.948%
9	5.102	1152	1170	1194	rBV	225185	509170	33.48%	4.884%
10	5.761	1353	1375	1404	rBV2	387504	1045158	68.72%	10.026%
11	6.279	1522	1536	1562	rBV	352555	684714	45.02%	6.568%
12	6.571	1611	1627	1639	rBV7	23410	47747	3.14%	0.458%
13	6.719	1658	1673	1695	rBV	245791	482806	31.74%	4.631%
14	7.070	1769	1782	1802	rBV	119286	212369	13.96%	2.037%
15	7.591	1932	1944	1965	rBV	127665	224713	14.77%	2.156%
16	7.922	2033	2047	2067	rBV	452051	809091	53.20%	7.761%
17	8.201	2122	2134	2150	rBV	82661	139887	9.20%	1.342%
18	8.571	2238	2249	2262	rBV3	19087	31547	2.07%	0.303%
19	8.658	2262	2276	2310	rBV	826752	1520939	100.00%	14.590%
20	8.960	2357	2370	2381	rBV4	6160	15711	1.03%	0.151%
21	9.436	2504	2518	2539	rBV	517618	872284	57.35%	8.367%
22	10.770	2918	2933	2951	rVB	216807	347478	22.85%	3.333%
23	11.822	3248	3260	3280	rBV	537719	843389	55.45%	8.090%
24	12.079	3329	3340	3357	rBV4	8280	17194	1.13%	0.165%
25	12.205	3366	3379	3395	rVB	512679	804738	52.91%	7.719%
26	17.384	4979	4990	5003	rBV2	100850	187022	12.30%	1.794%

Sum of corrected areas: 10424809

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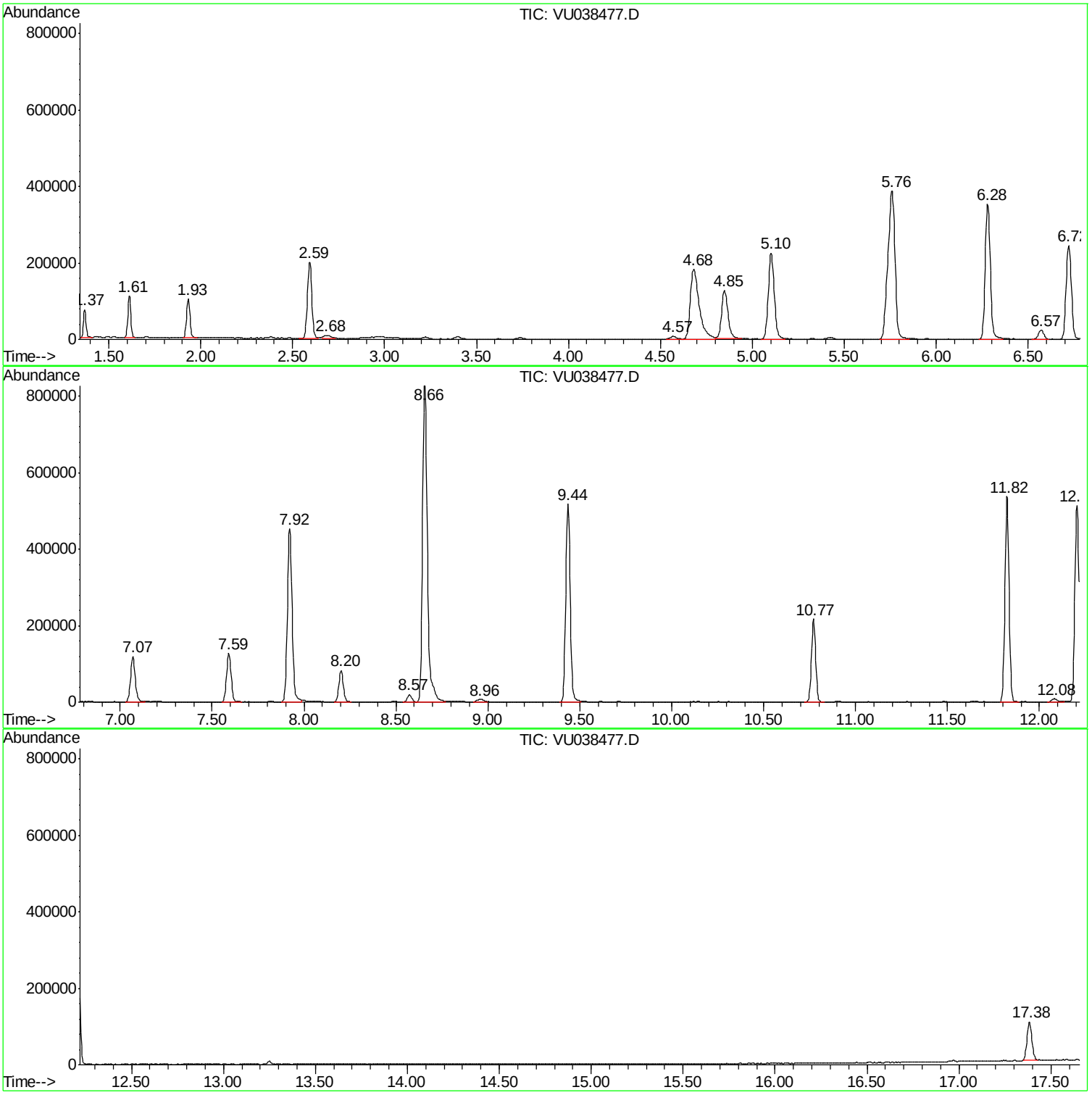
Instrument :
MSVOA_U
ClientSampleId :
BFXA1

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

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ClientSampleId : BFXA1

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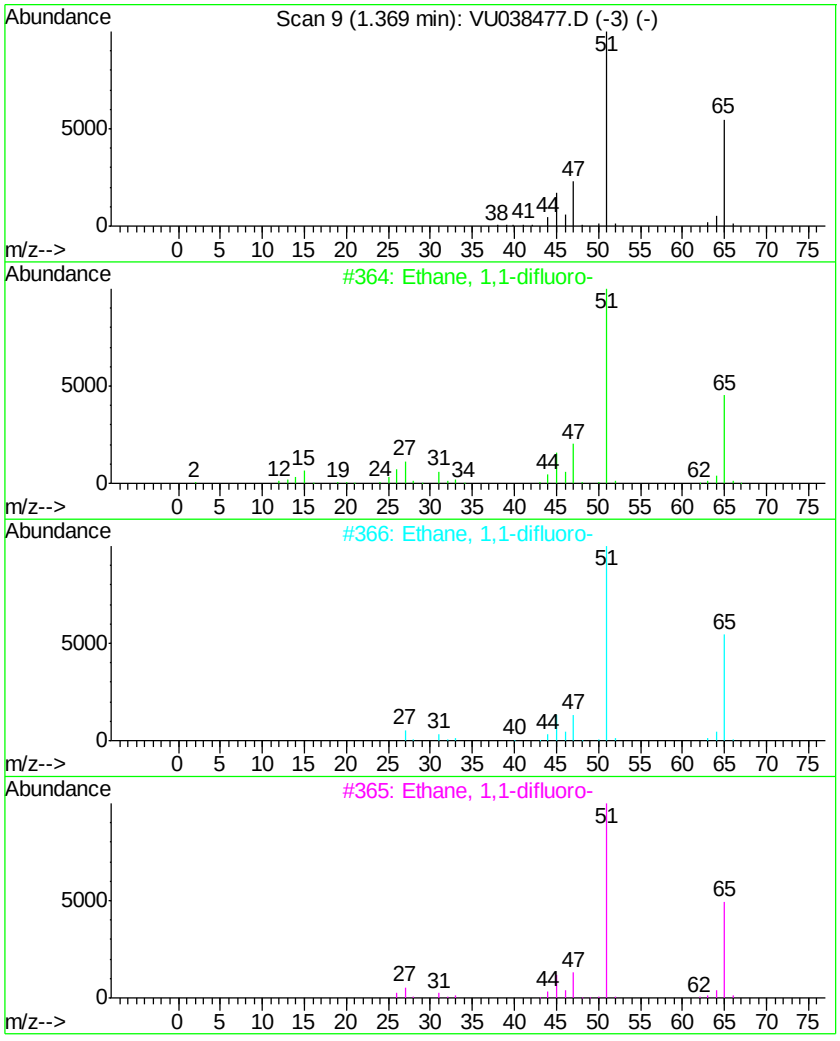
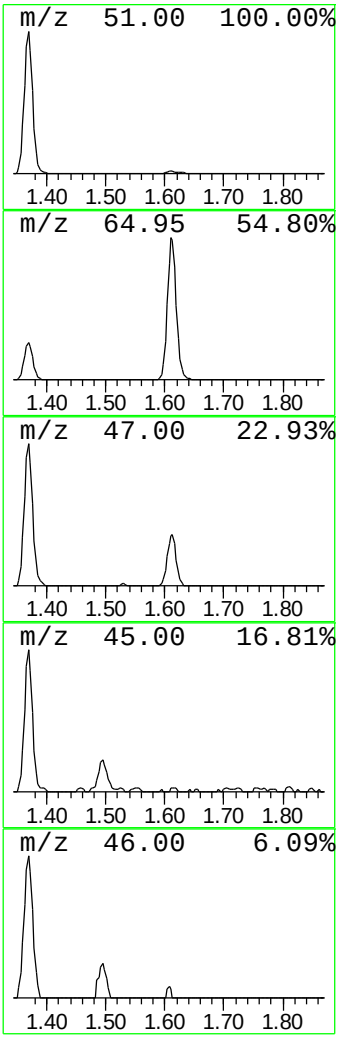
Peak Number 1 Ethane, 1,1-difluoro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.37	0.52 ug/L	71267	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	90
4	Propiolonitrile	51	C3HN	001070-71-9	3
5	Propane, 2,2-difluoro-	80	C3H6F2	000420-45-1	2





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ALS Vial : 2 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXA1

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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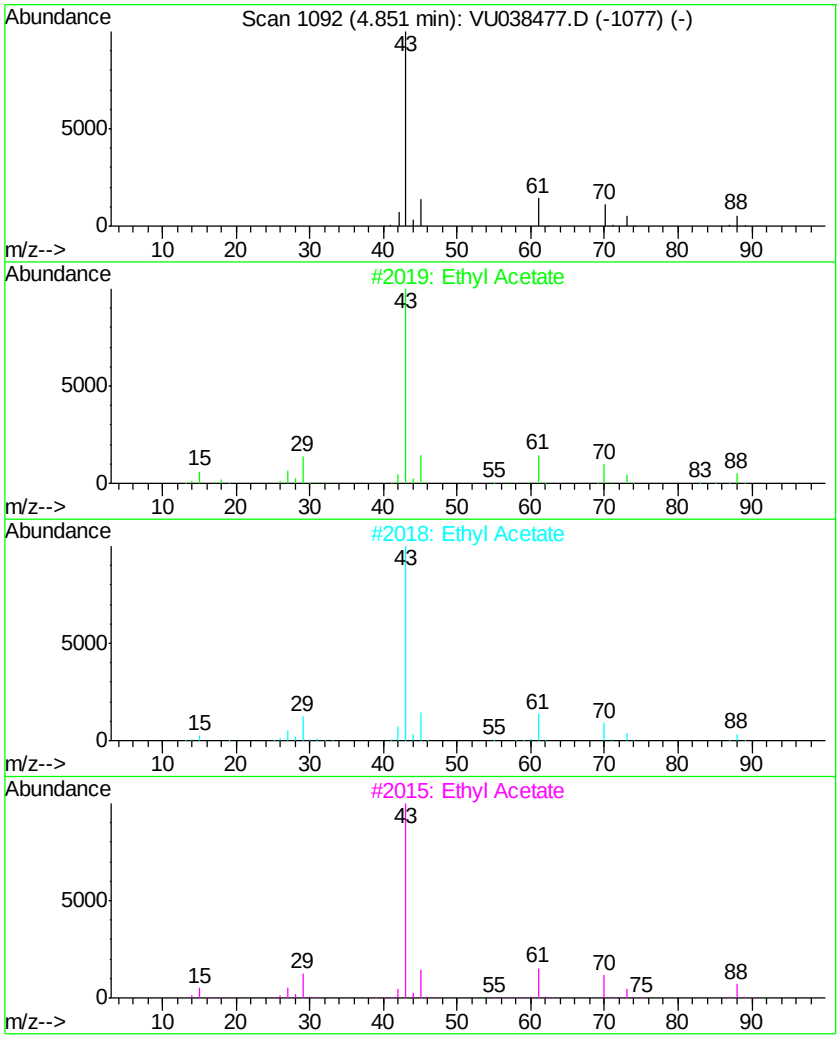
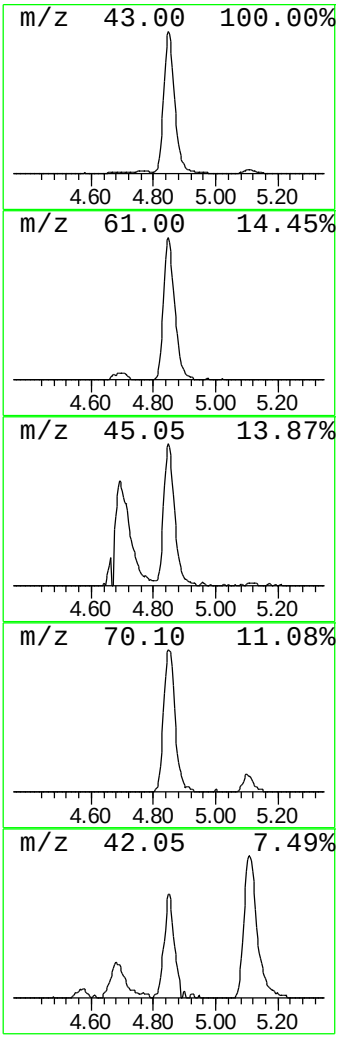
Peak Number 2 Ethyl Acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	2.24 ug/L	307348	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	33





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Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 2 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXA1

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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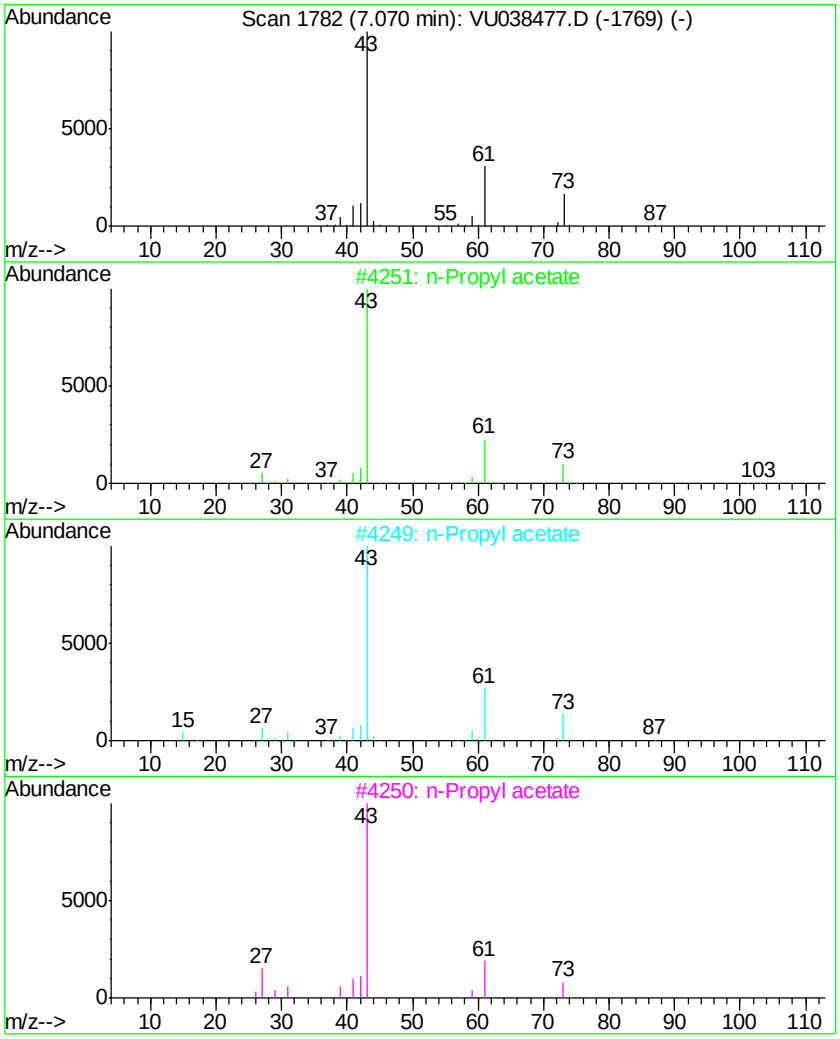
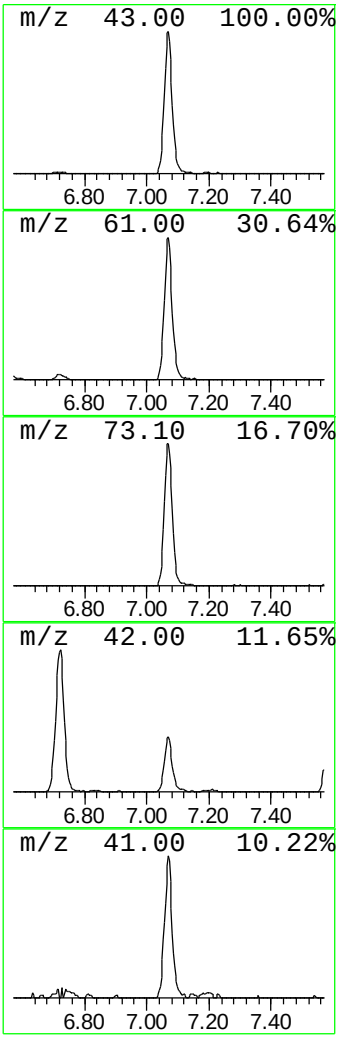
Peak Number 3 n-Propyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.07	1.55 ug/L	212369	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	n-Propyl acetate	102	C5H10O2	000109-60-4	78
3	n-Propyl acetate	102	C5H10O2	000109-60-4	78
4	Isopropyl acetate	102	C5H10O2	000108-21-4	9
5	Isobutyl acetate	116	C6H12O2	000110-19-0	9





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ALS Vial : 2 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXA1

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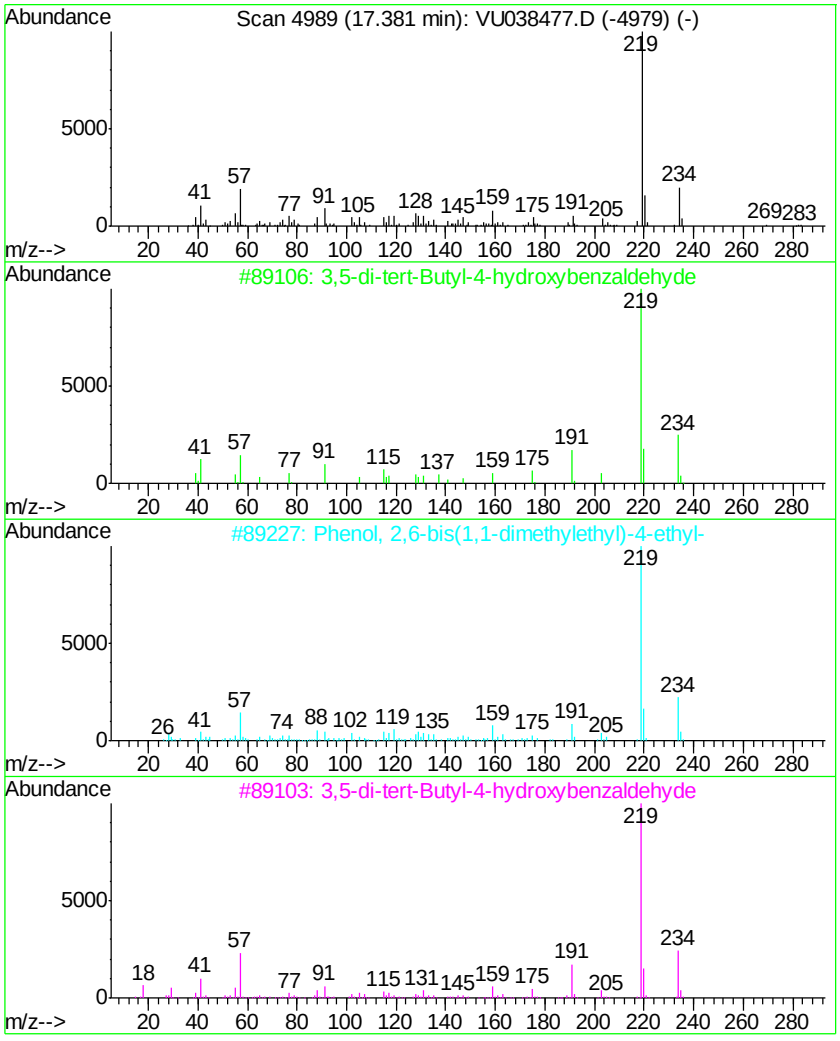
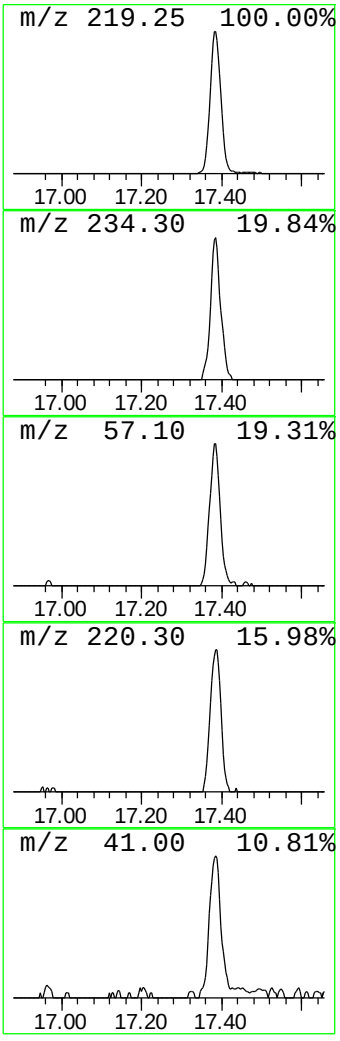
Peak Number 5 3,5-di-tert-Butyl-4-hydroxy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.38	1.11 ug/L	187022	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	Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	93
3	3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	93
4	Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	91
5	4-tert-Butyl-2,6-diisopropylphenol	234	C16H26O	057354-65-1	90





Tentatively Identified Compound (LSC) summary

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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	71267	1	6.28	684714	5.0
Ethyl Acetate	4.85	2.2	ug/L	307348	1	6.28	684714	5.0
n-Propyl acetate	7.07	1.6	ug/L	212369	1	6.28	684714	5.0
3,5-di-tert-Butyl...	17.38	1.1	ug/L	187022	3	11.82	843389	5.0