LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU053120\
Data File : VU038437.D
Acq On : 31 May 2020 01:15
Operator : JC/MD
Sample : L2787-14
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFX96

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	rBV	80299	77485	5.12%	0.711%
2	1.613	75	85	95	rBV	143296	160724	10.62%	1.474%
3	1.932	176	184	199	rVB	112733	143325	9.47%	1.315%
4	2.594	375	390	404	rBV	229086	385696	25.47%	3.538%
5	2.675	405	415	435	rVB	13104	34764	2.30%	0.319%
6	2.877	453	478	479	rBV8	11820	36024	2.38%	0.330%
7	3.218	571	584	595	rBV	10576	24111	1.59%	0.221%
8	3.398	627	640	652	rBV4	8323	17408	1.15%	0.160%
9	3.736	731	745	759	rBV4	9217	21172	1.40%	0.194%
10	4.572	985	1005	1020	rBV3	13721	31985	2.11%	0.293%
11	4.674	1020	1037	1074	rBV	222621	654683	43.24%	6.006%
12	4.845	1076	1090	1112	rVB2	113138	260073	17.18%	2.386%
13	5.102	1154	1170	1201	rVB2	234354	530068	35.01%	4.863%
14	5.424	1256	1270	1286	rVB6	10644	24071	1.59%	0.221%
15	5.761	1352	1375	1394	rBV2	417848	1100304	72.67%	10.094%
16	6.279	1521	1536	1570	rBV	366871	710819	46.95%	6.521%
17	6.568	1613	1626	1639	rBV6	9941	20708	1.37%	0.190%
18	6.719	1658	1673	1691	rBV	254154	498383	32.92%	4.572%
19	7.067	1769	1781	1798	rBV	113030	201549	13.31%	1.849%
20	7.591	1930	1944	1962	rBV	135526	234905	15.51%	2.155%
21	7.922	2030	2047	2066	rBV	495742	868435	57.36%	7.967%
22	8.202	2119	2134	2149	rBV2	84842	143635	9.49%	1.318%
23	8.575	2239	2250	2262	rBV	48462	83440	5.51%	0.765%
24	8.655	2262	2275	2304	rBV	836516	1514054	100.00%	13.890%
25	8.948	2349	2366	2381	rBV4	8146	18037	1.19%	0.165%
26	9.436	2502	2518	2546	rBV	534979	902336	59.60%	8.278%
27	10.771	2920	2933	2947	rBV	216087	344695	22.77%	3.162%
28	11.825	3248	3261	3275	rBV	575481	896976	59.24%	8.229%
29	12.205	3365	3379	3395	rBV	522509	836759	55.27%	7.676%
30	17.385	4978	4990	5004	rBV3	66029	123917	8.18%	1.137%

Sum of corrected areas: 10900541

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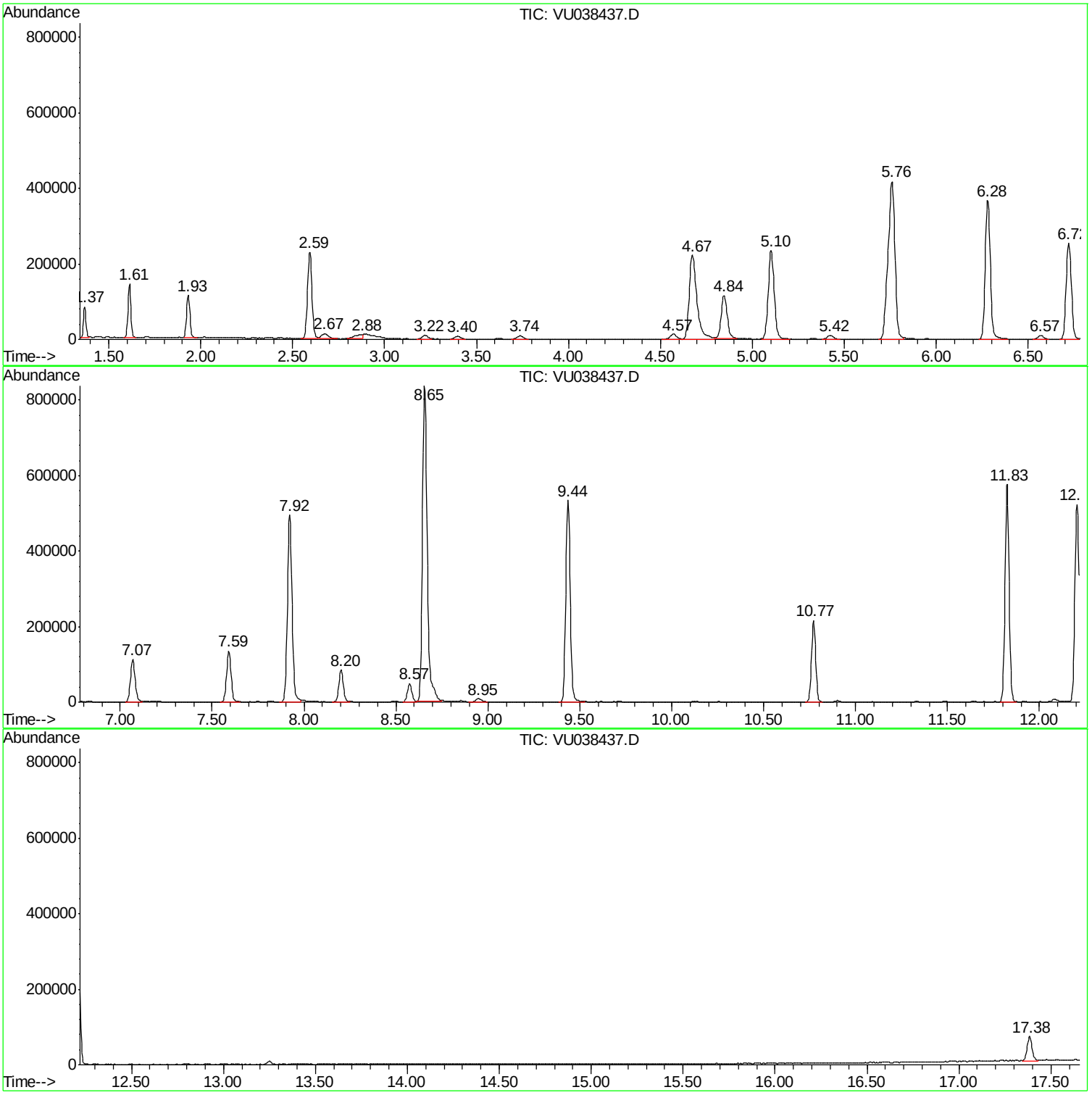
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFX96

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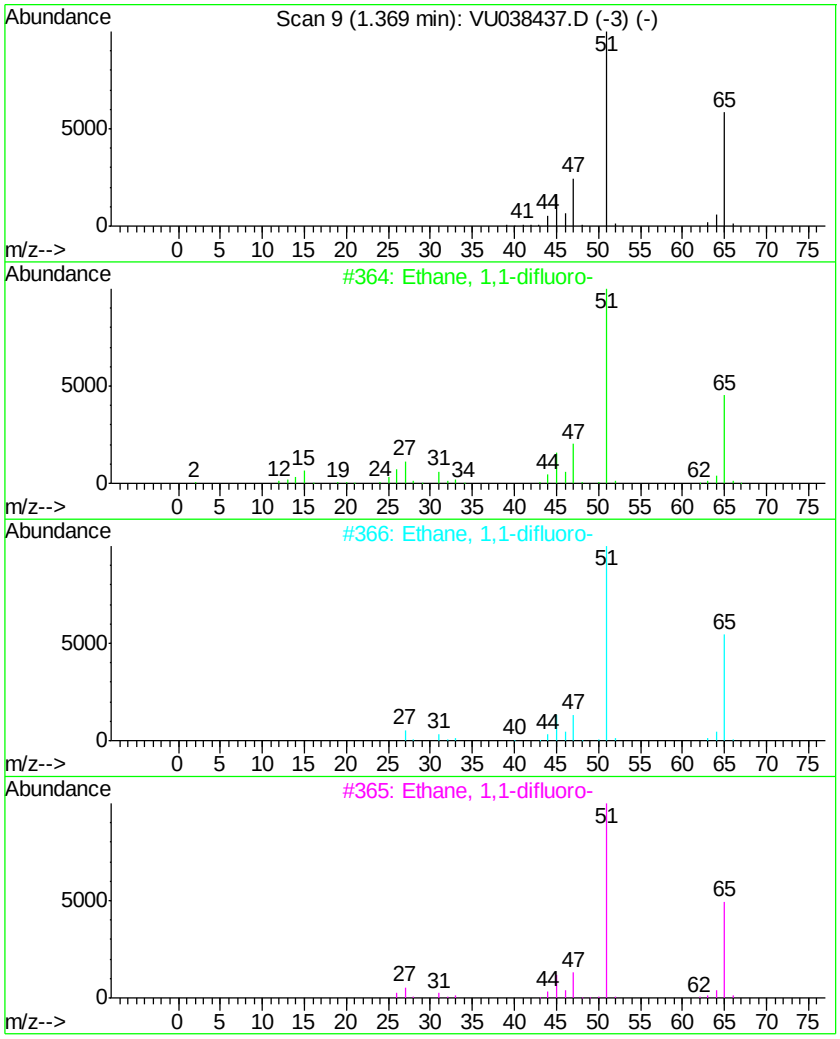
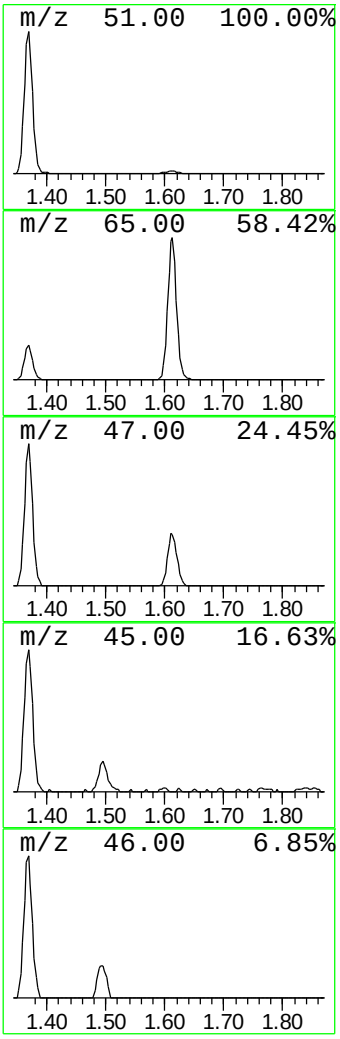
Peak Number 1 Ethane, 1,1-difluoro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.37	0.55 ug/L	77485	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





Library Search Compound Report

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Instrument : MSVOA_U
ClientSampleId : BFX96

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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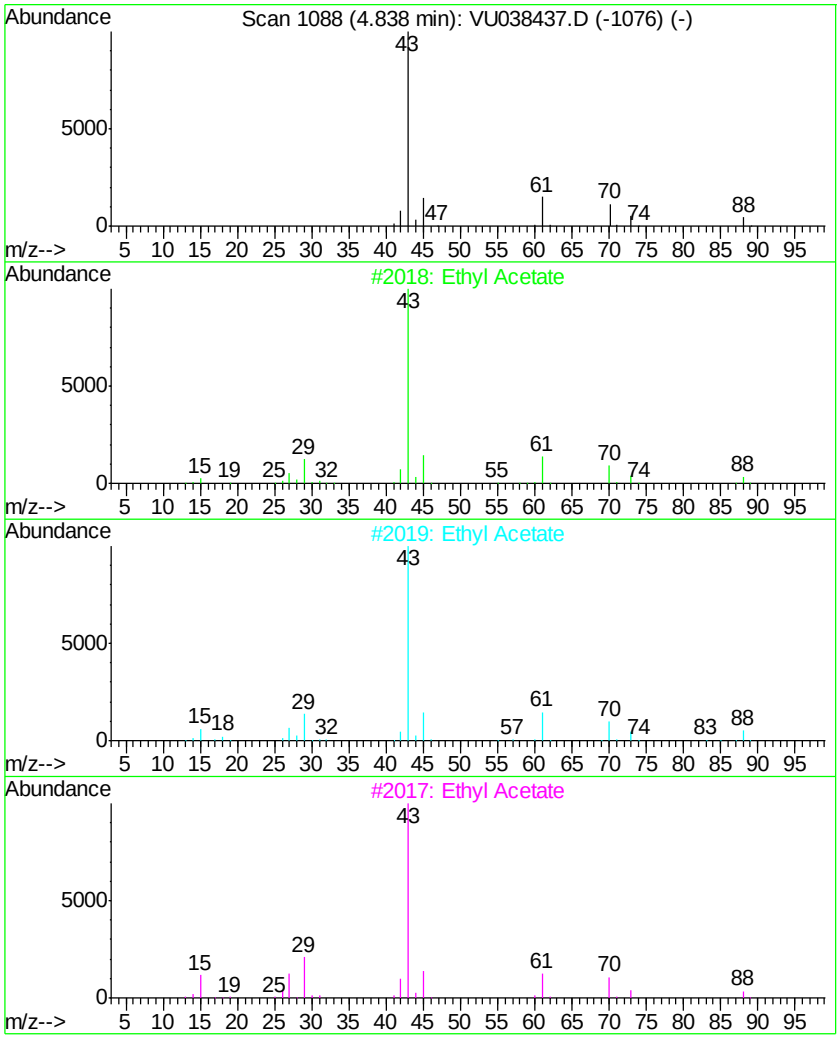
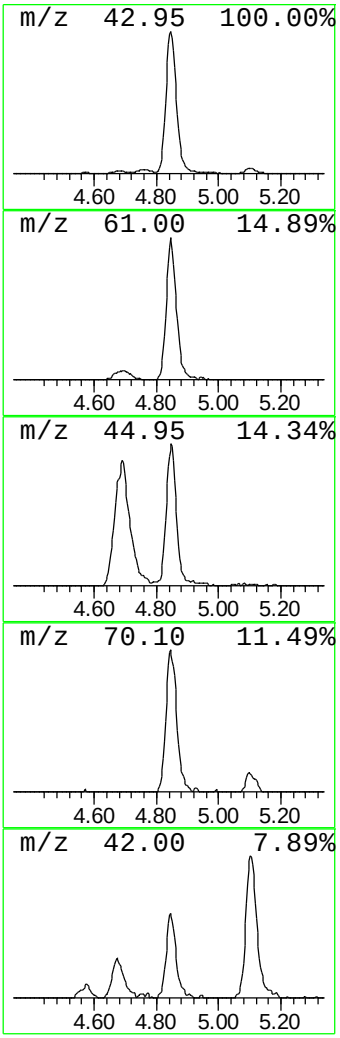
Peak Number 2 Ethyl Acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	1.83 ug/L	260073	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	78
5	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	28





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ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFX96

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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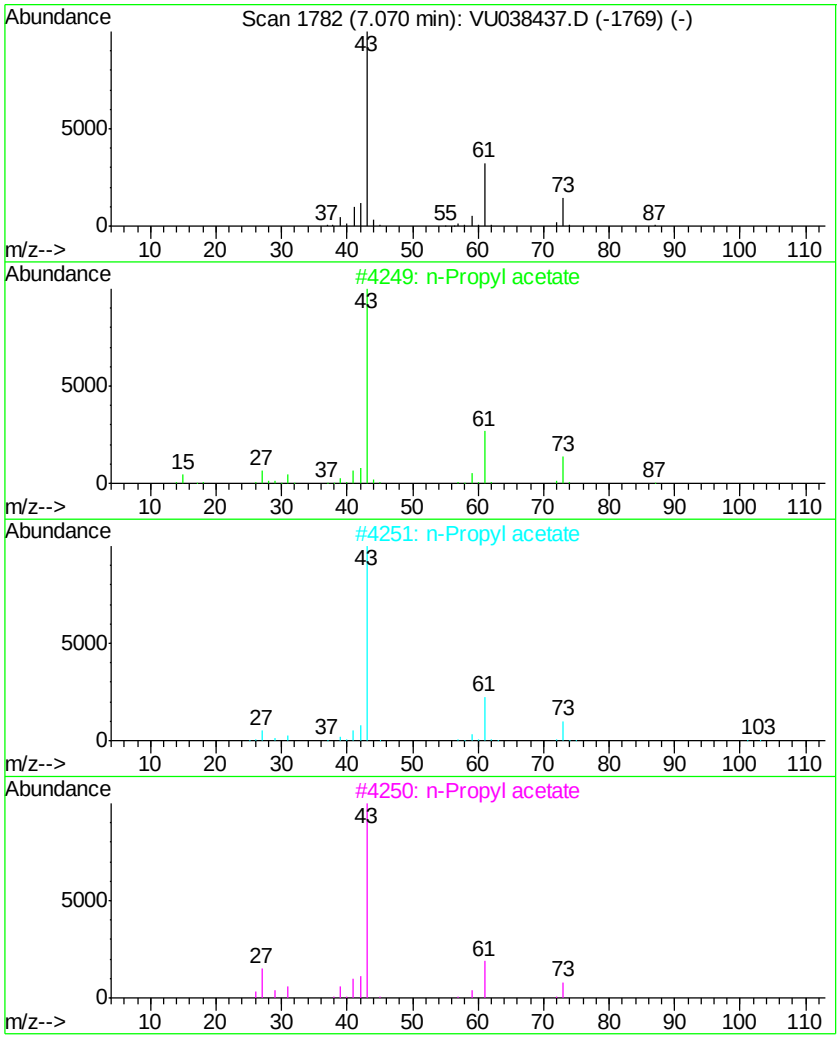
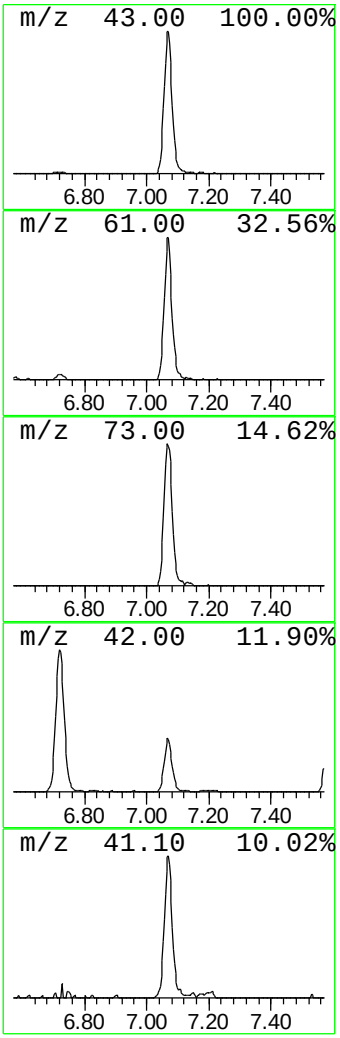
Peak Number 3 n-Propyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.07	1.42 ug/L	201549	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	83
3	n-Propyl acetate	102	C5H10O2	000109-60-4	78
4	Isopropyl acetate	102	C5H10O2	000108-21-4	36
5	1-Butanamine	73	C4H11N	000109-73-9	9





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Instrument : MSVOA_U
ClientSampleId : BFX96

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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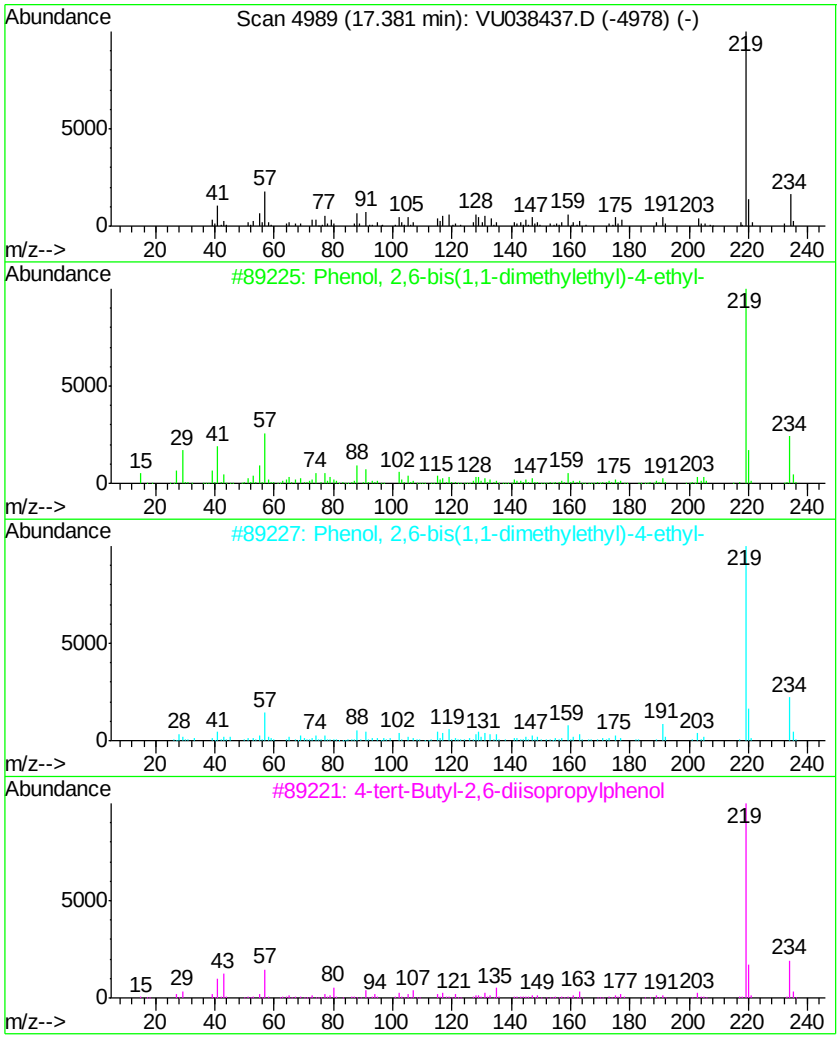
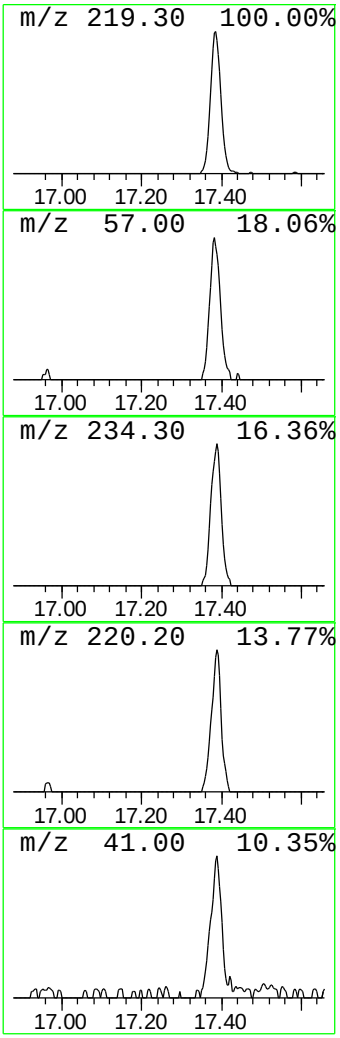
Peak Number 5 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.38	0.69 ug/L	123917	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	91
2	Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	87
3	4-tert-Butyl-2,6-diisopropylphenol	234	C16H26O	057354-65-1	83
4	3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	83
5	3,5-Di-tert-butylbenzoic acid	234	C15H22O2	016225-26-6	80





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethane, 1,1-diflu...	1.37	0.6	ug/L	77485	1	6.28	710819	5.0
Ethyl Acetate	4.84	1.8	ug/L	260073	1	6.28	710819	5.0
n-Propyl acetate	7.07	1.4	ug/L	201549	1	6.28	710819	5.0
Phenol, 2,6-bis(1...	17.38	0.7	ug/L	123917	3	11.83	896976	5.0