LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU053120\
Data File : VU038442.D
Acq On : 31 May 2020 03:10
Operator : JC/MD
Sample : L2787-19
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXA6

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	rVB	101752	99986	6.32%	0.879%
2	1.610	74	84	101	rVB	142724	168223	10.63%	1.479%
3	1.932	175	184	197	rBV	118803	148512	9.38%	1.306%
4	2.591	377	389	406	rBV	233632	389594	24.62%	3.426%
5	3.218	572	584	599	rVB2	8519	19681	1.24%	0.173%
6	3.398	626	640	654	rVB4	12789	30534	1.93%	0.269%
7	3.736	730	745	759	rBV3	13912	30784	1.95%	0.271%
8	4.568	990	1004	1020	rBV2	21242	50599	3.20%	0.445%
9	4.681	1021	1039	1075	rBV	194183	668114	42.22%	5.876%
10	4.848	1077	1091	1116	rVB	149000	365848	23.12%	3.217%
11	5.102	1154	1170	1198	rBV3	252171	596939	37.72%	5.250%
12	5.424	1259	1270	1285	rVB4	10497	22954	1.45%	0.202%
13	5.758	1350	1374	1403	rBV3	427598	1125402	71.12%	9.897%
14	6.279	1520	1536	1571	rBV	372140	721307	45.58%	6.344%
15	6.568	1614	1626	1638	rVB7	8121	16584	1.05%	0.146%
16	6.719	1659	1673	1693	rBV	261114	510887	32.28%	4.493%
17	7.070	1768	1782	1801	rBV	166181	303625	19.19%	2.670%
18	7.591	1930	1944	1963	rBV	136013	237595	15.01%	2.090%
19	7.922	2031	2047	2072	rBV	504499	893432	56.46%	7.857%
20	8.202	2121	2134	2148	rBV	87039	147340	9.31%	1.296%
21	8.658	2256	2276	2311	rBV	842869	1582501	100.00%	13.917%
22	8.957	2359	2369	2387	rVB4	6690	16422	1.04%	0.144%
23	9.436	2505	2518	2540	rBV	549164	917245	57.96%	8.067%
24	10.771	2921	2933	2951	rVB	224110	359562	22.72%	3.162%
25	11.822	3247	3260	3276	rBV	580594	917244	57.96%	8.067%
26	12.083	3327	3341	3354	rBV4	8177	16531	1.04%	0.145%
27	12.205	3367	3379	3394	rVB	532643	855110	54.04%	7.520%
28	17.385	4978	4990	5003	rBV2	84837	158141	9.99%	1.391%

Sum of corrected areas: 11370696

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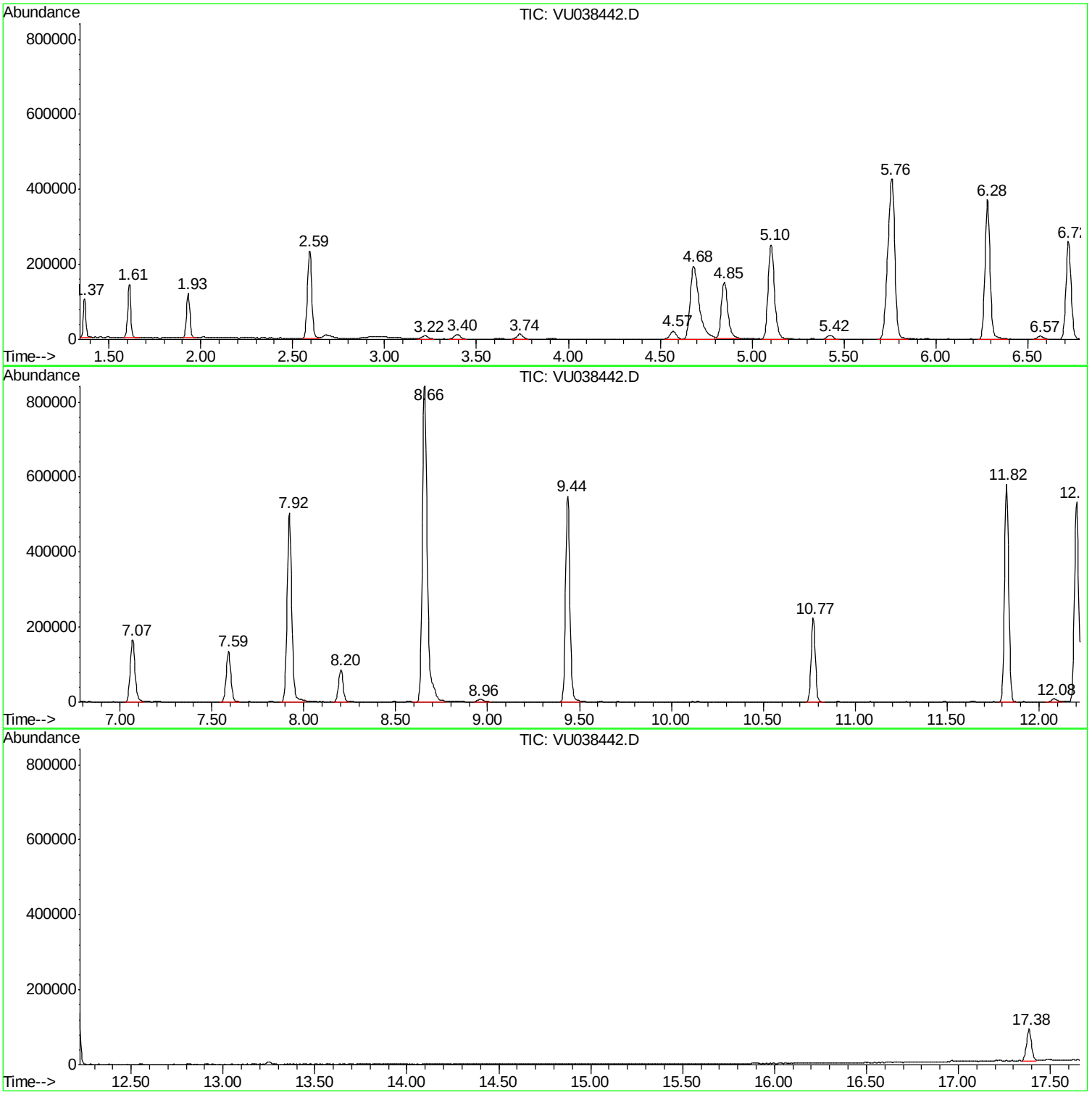
ClientSampleId : BFXA6

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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TIC Integration Parameters: LSCINT.P

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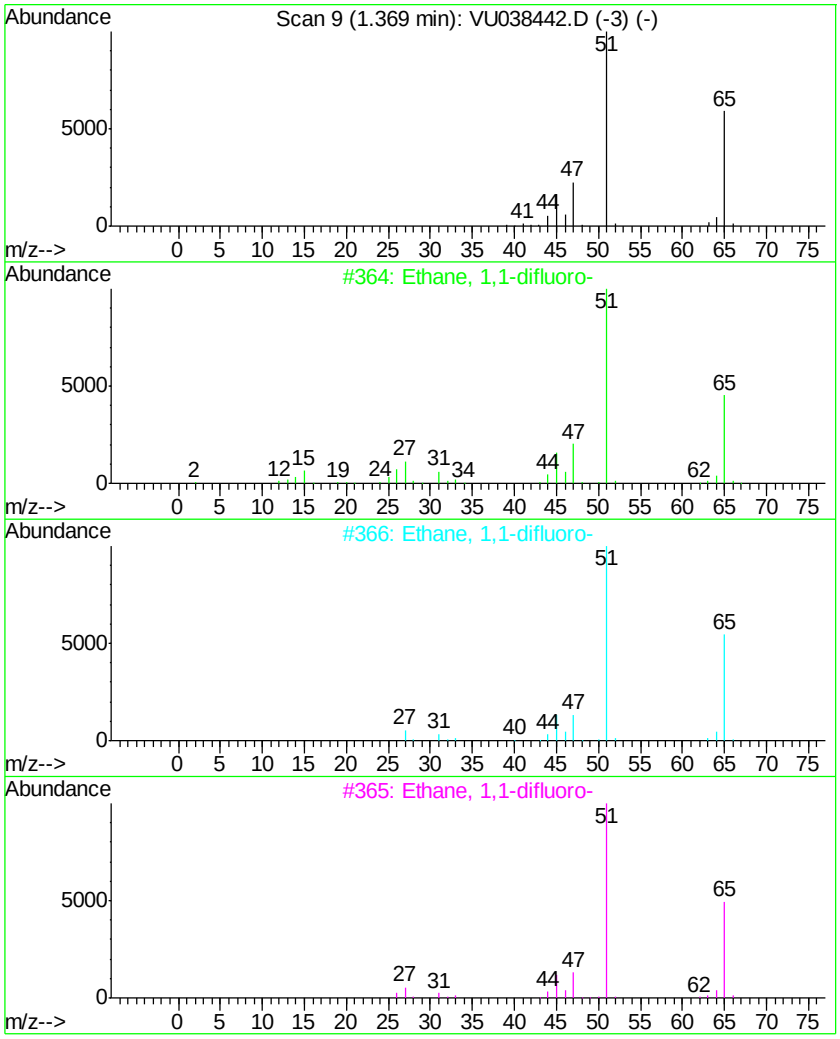
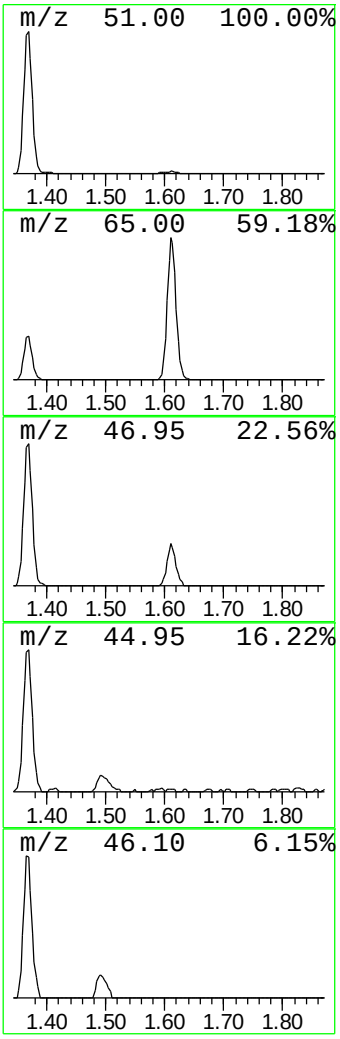
Peak Number 1 Ethane, 1,1-difluoro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.37	0.69 ug/L	99986	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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ClientSampleId : BFXA6

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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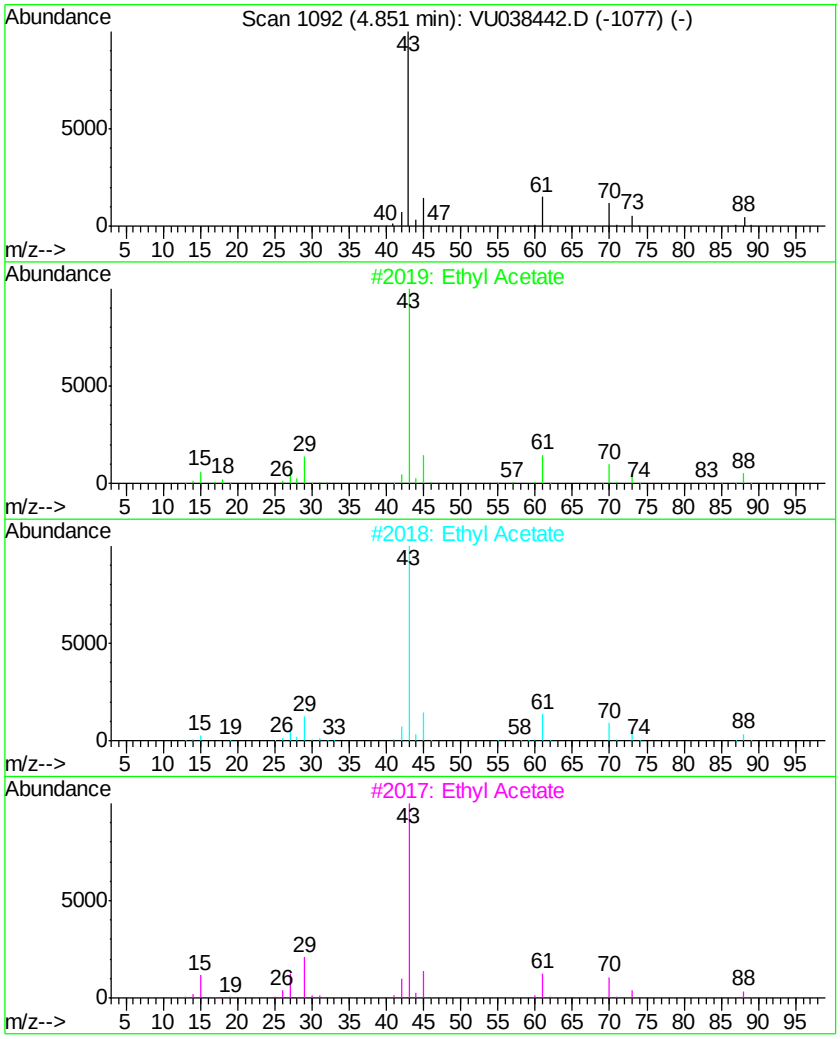
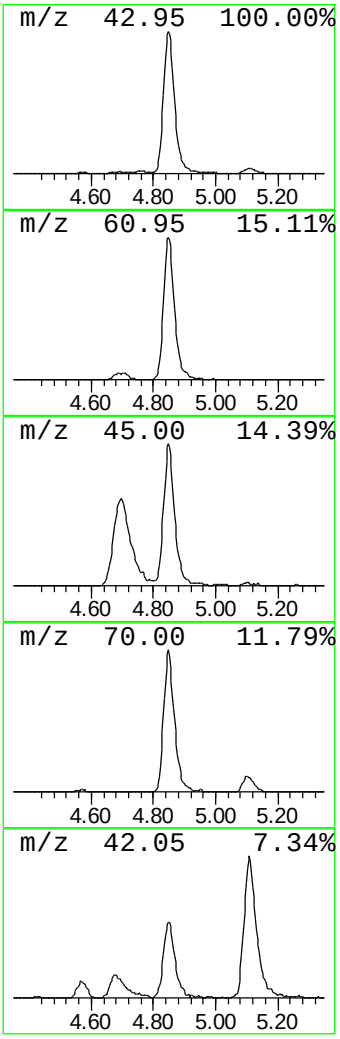
Peak Number 2 Ethyl Acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	2.54 ug/L	365848	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	64
5	CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	40





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ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXA6

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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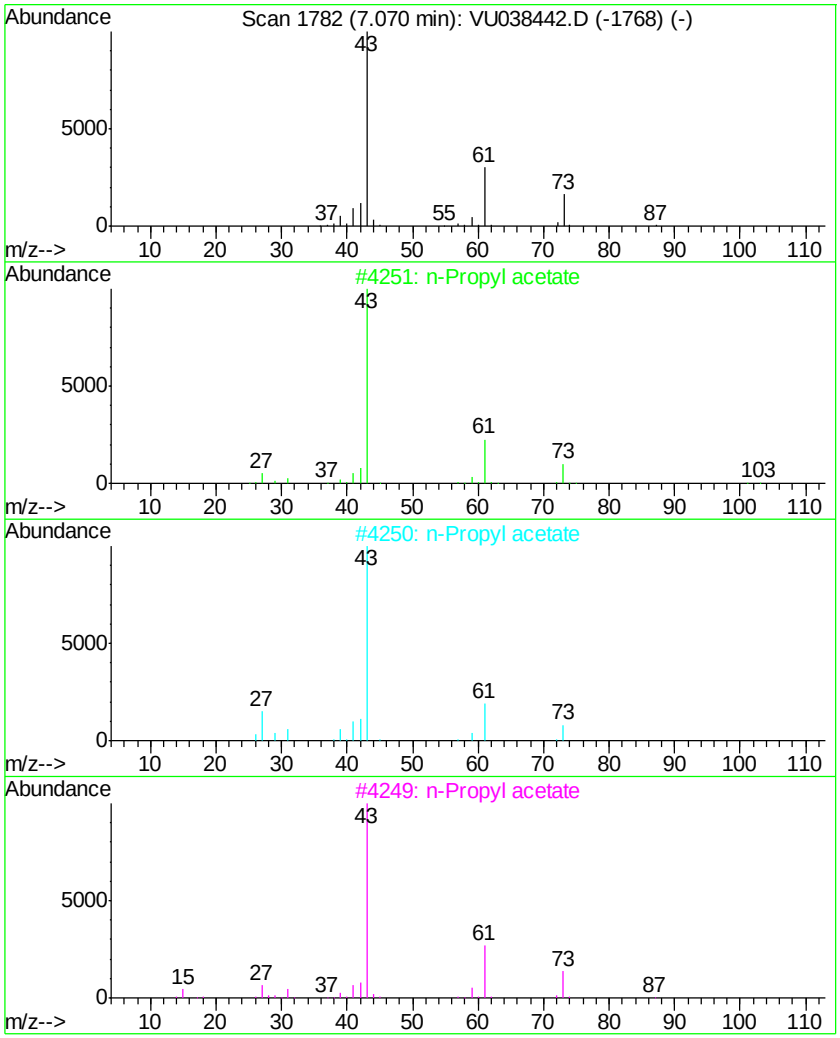
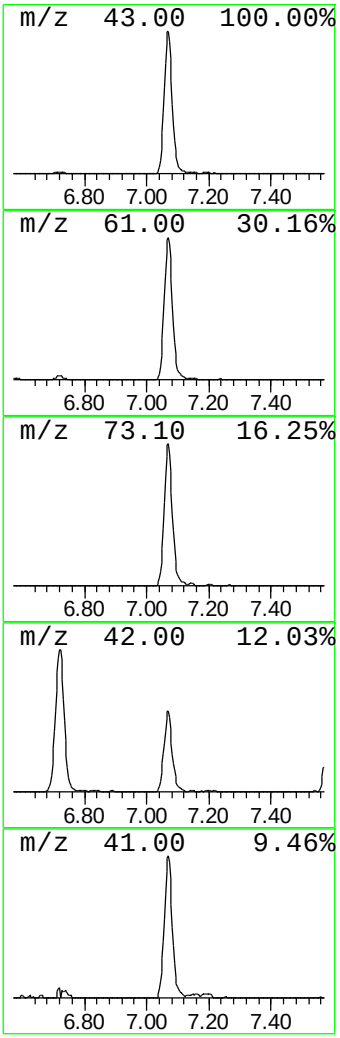
Peak Number 3 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.07	2.10 ug/L	303625	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	36
5	Isobutylamine	73	C4H11N	000078-81-9	9





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ClientSampleId : BFXA6

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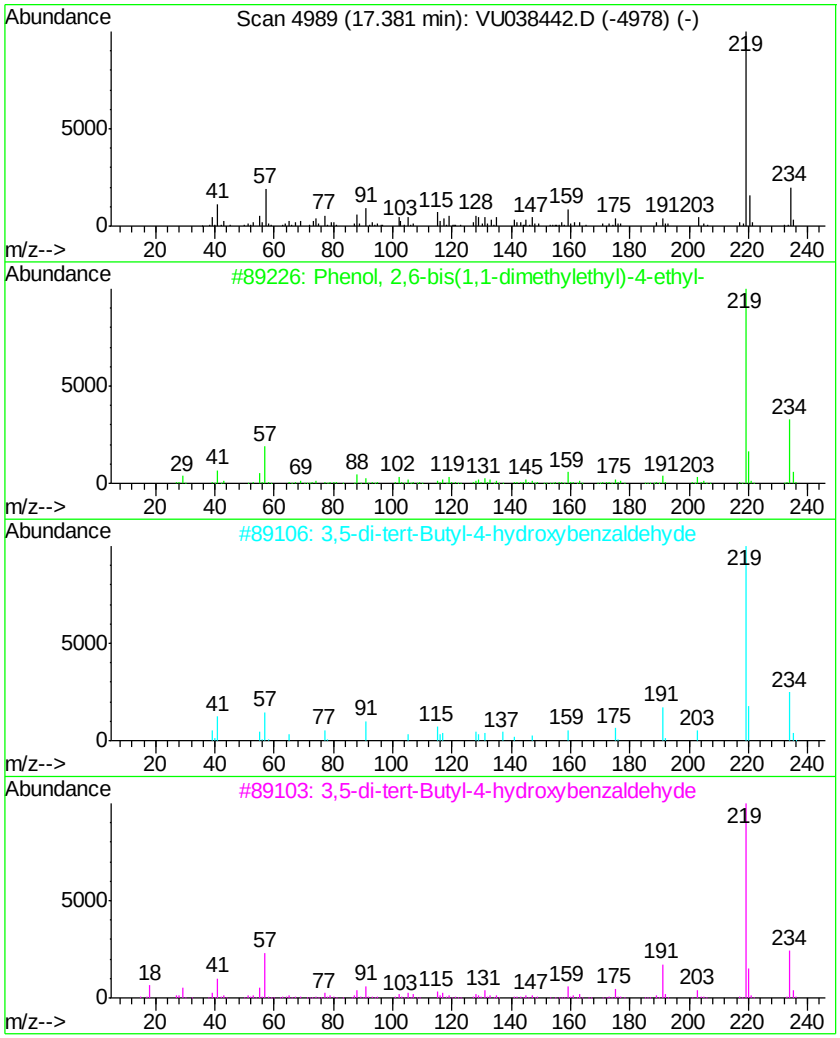
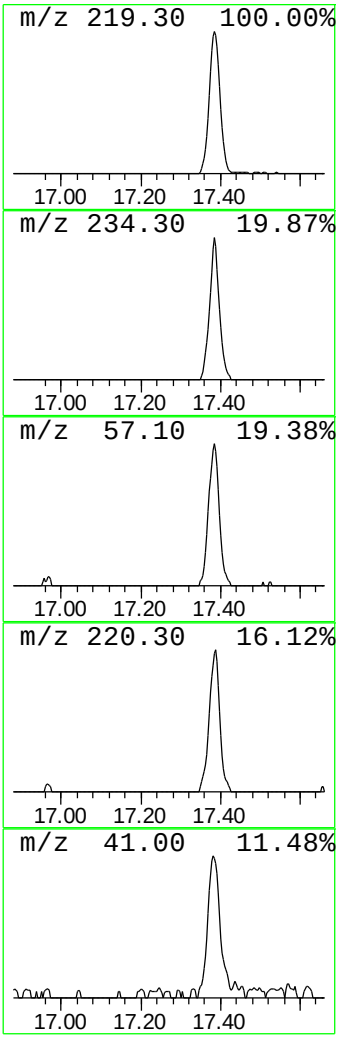
Peak Number 5 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.38	0.86 ug/L	158141	1,4-Dichlorobenzene-d4	11.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	94
2	3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	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	93
5	Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	91





Tentatively Identified Compound (LSC) summary

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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	0.7	ug/L	99986	1	6.28	721307	5.0
Ethyl Acetate	4.85	2.5	ug/L	365848	1	6.28	721307	5.0
n-Propyl acetate	7.07	2.1	ug/L	303625	1	6.28	721307	5.0
Phenol, 2,6-bis(1...	17.38	0.9	ug/L	158141	3	11.82	917244	5.0