LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU053120\
Data File : VU038425.D
Acq On : 30 May 2020 19:52
Operator : JC/MD
Sample : L2787-04
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFX74

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	16	rVB	88565	84613	5.16%	0.671%
2	1.613	73	85	95	rBV	157881	183870	11.20%	1.457%
3	1.932	175	184	197	rVB	119192	153699	9.36%	1.218%
4	2.594	377	390	405	rBV	256369	423922	25.83%	3.360%
5	3.221	571	585	601	rBV2	13124	28983	1.77%	0.230%
6	3.398	627	640	655	rVB4	10788	23680	1.44%	0.188%
7	3.739	729	746	760	rBV4	12194	29534	1.80%	0.234%
8	4.568	990	1004	1021	rVB3	19613	46691	2.84%	0.370%
9	4.681	1021	1039	1076	rBV3	210779	737945	44.96%	5.850%
10	4.848	1076	1091	1121	rVB	219963	531161	32.36%	4.210%
11	5.105	1154	1171	1202	rBV3	270996	696677	42.45%	5.522%
12	5.420	1256	1269	1283	rBV4	9404	21468	1.31%	0.170%
13	5.761	1353	1375	1405	rBV2	447336	1187185	72.33%	9.411%
14	6.279	1519	1536	1559	rBV	395056	761636	46.40%	6.037%
15	6.571	1611	1627	1643	rBV	225981	426612	25.99%	3.382%
16	6.723	1658	1674	1692	rBV	276710	540965	32.96%	4.288%
17	7.070	1767	1782	1805	rBV	183441	339981	20.71%	2.695%
18	7.591	1930	1944	1959	rBV2	144550	256107	15.60%	2.030%
19	7.922	2032	2047	2064	rBV	538221	939872	57.26%	7.450%
20	8.202	2122	2134	2150	rBV	92975	156548	9.54%	1.241%
21	8.575	2237	2250	2261	rBV4	15226	25725	1.57%	0.204%
22	8.658	2261	2276	2314	rBV	877342	1641315	100.00%	13.010%
23	9.436	2503	2518	2537	rBV	576568	963298	58.69%	7.636%
24	10.771	2921	2933	2953	rBV	225779	371163	22.61%	2.942%
25	11.825	3248	3261	3282	rVB	603052	949672	57.86%	7.528%
26	12.082	3328	3341	3351	rBV6	10806	19544	1.19%	0.155%
27	12.205	3366	3379	3398	rVB	555891	898172	54.72%	7.120%
28	17.388	4979	4991	5004	rBV2	94172	175456	10.69%	1.391%

Sum of corrected areas: 12615494

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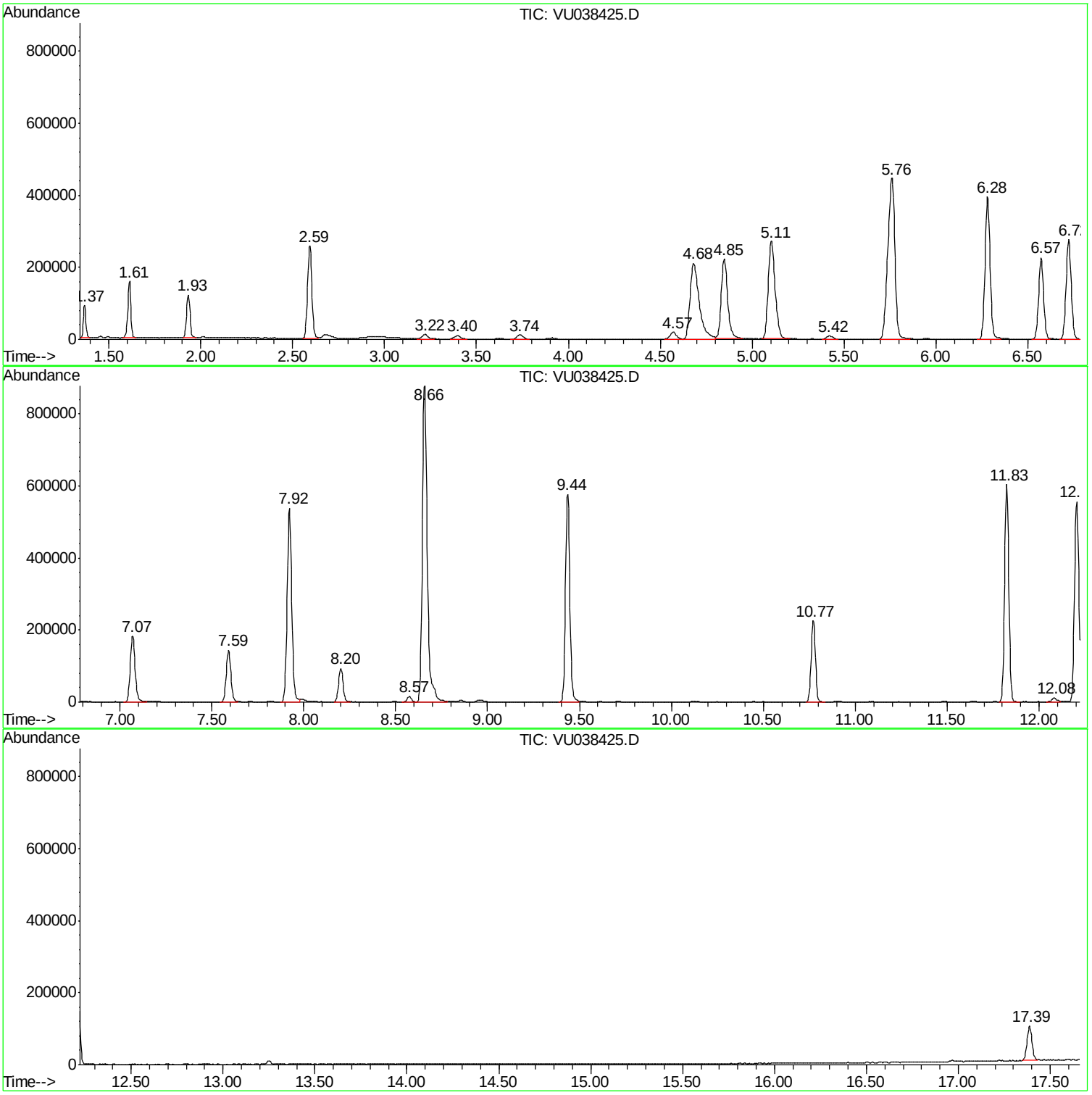
Instrument :
MSVOA_U
ClientSampleId :
BFX74

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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Quant Title : TRACE VOA SOM01.0

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

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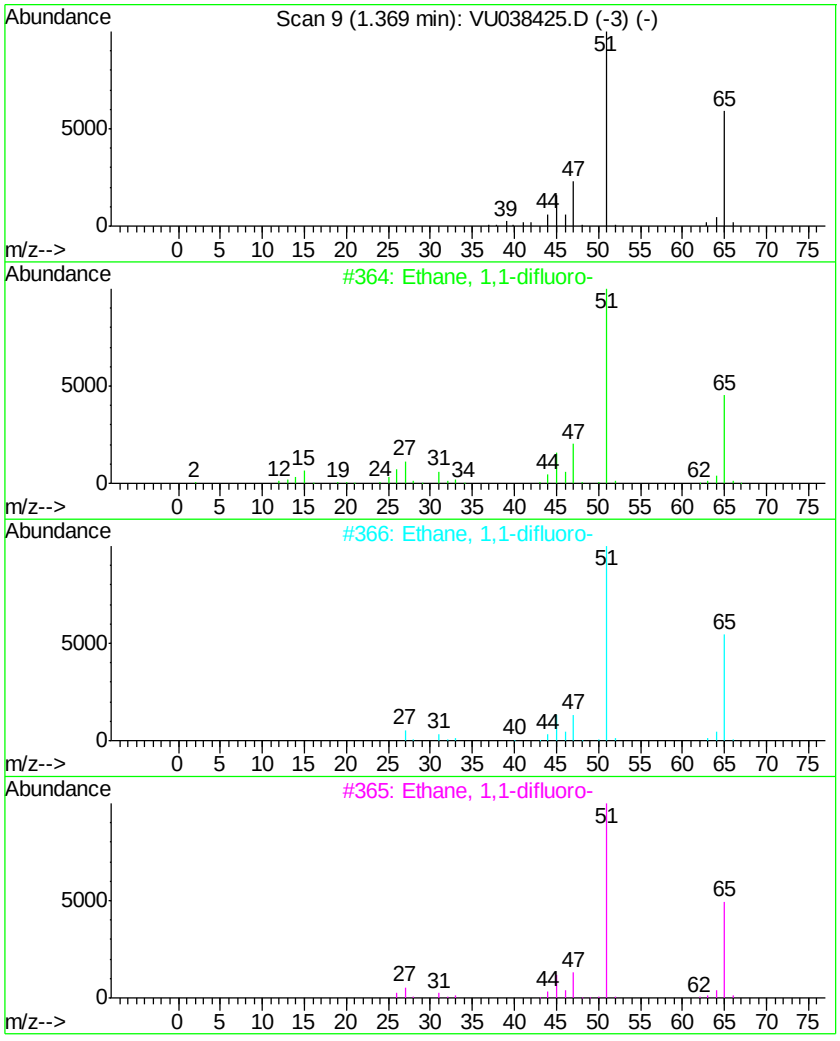
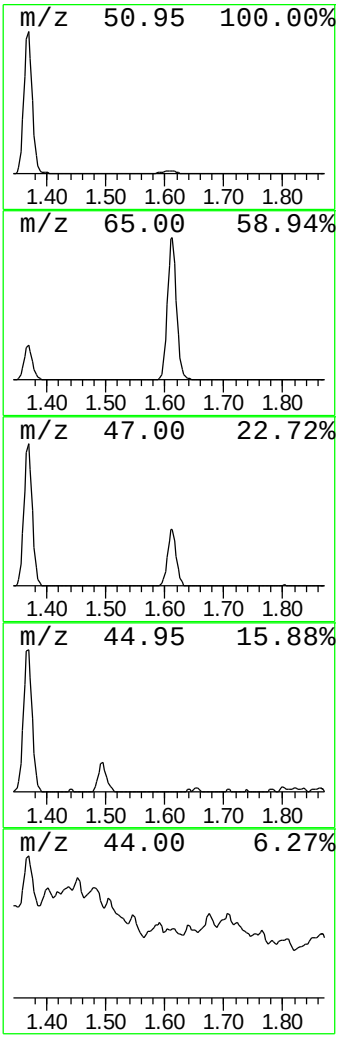
Peak Number 1 Ethane, 1,1-difluoro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.37	0.56 ug/L	84613	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	Propane, 2,2-difluoro-	80	C3H6F2	000420-45-1	4
5	Propiolonitrile	51	C3HN	001070-71-9	3





Library Search Compound Report

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Instrument : MSVOA_U
ClientSampleId : BFX74

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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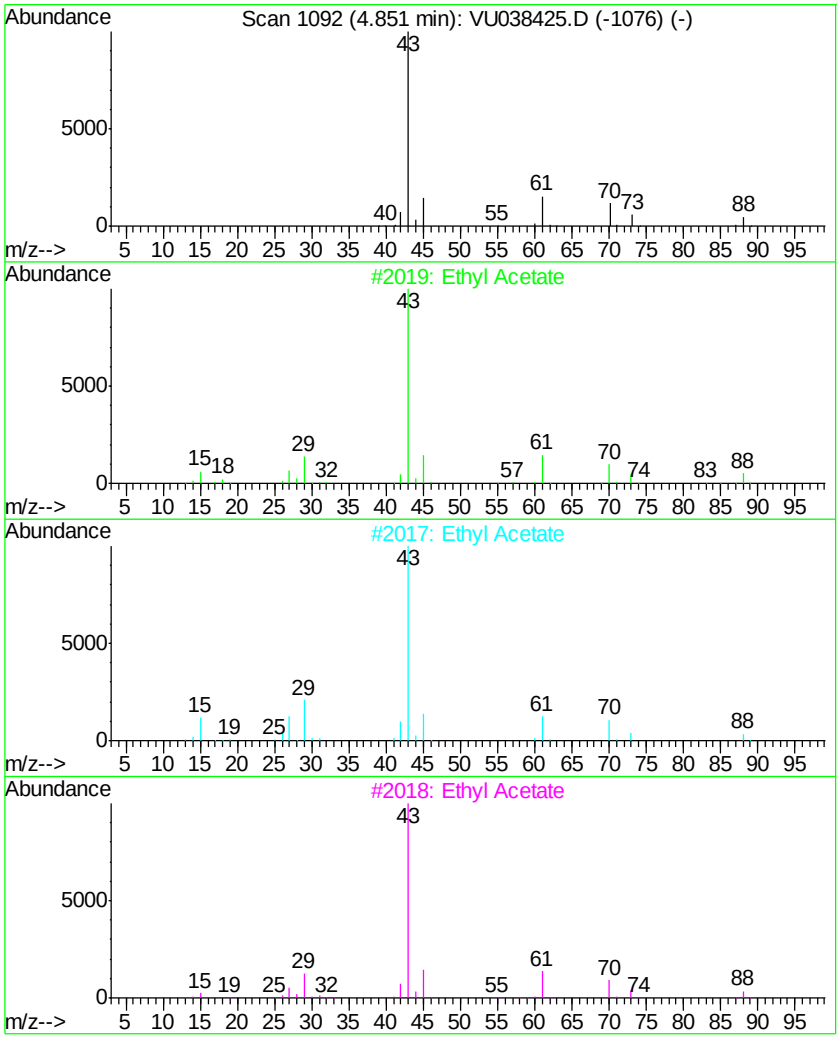
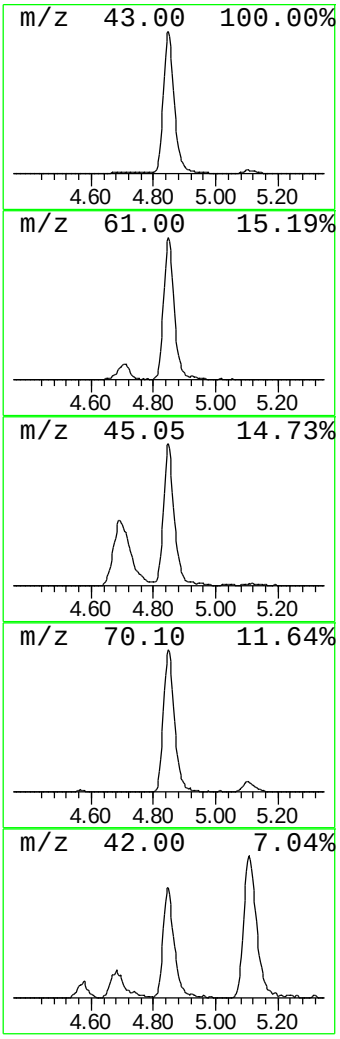
Peak Number 2 Ethyl Acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	3.49 ug/L	531161	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





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Operator : JC/MD
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Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFX74

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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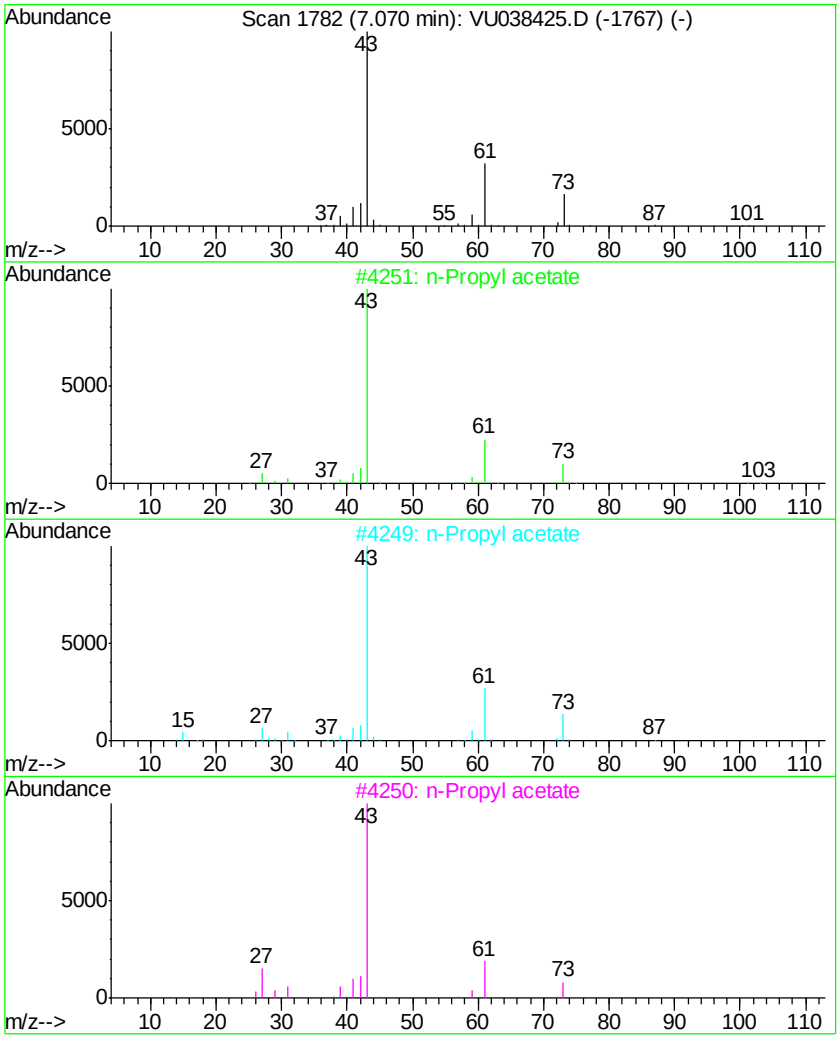
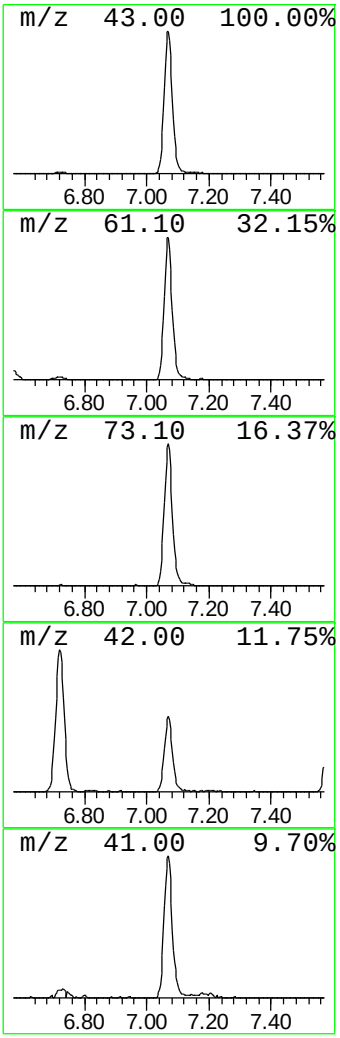
Peak Number 3 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.07	2.23 ug/L	339981	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	Isobutylamine	73	C4H11N	000078-81-9	9





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Instrument : MSVOA_U
ClientSampleId : BFX74

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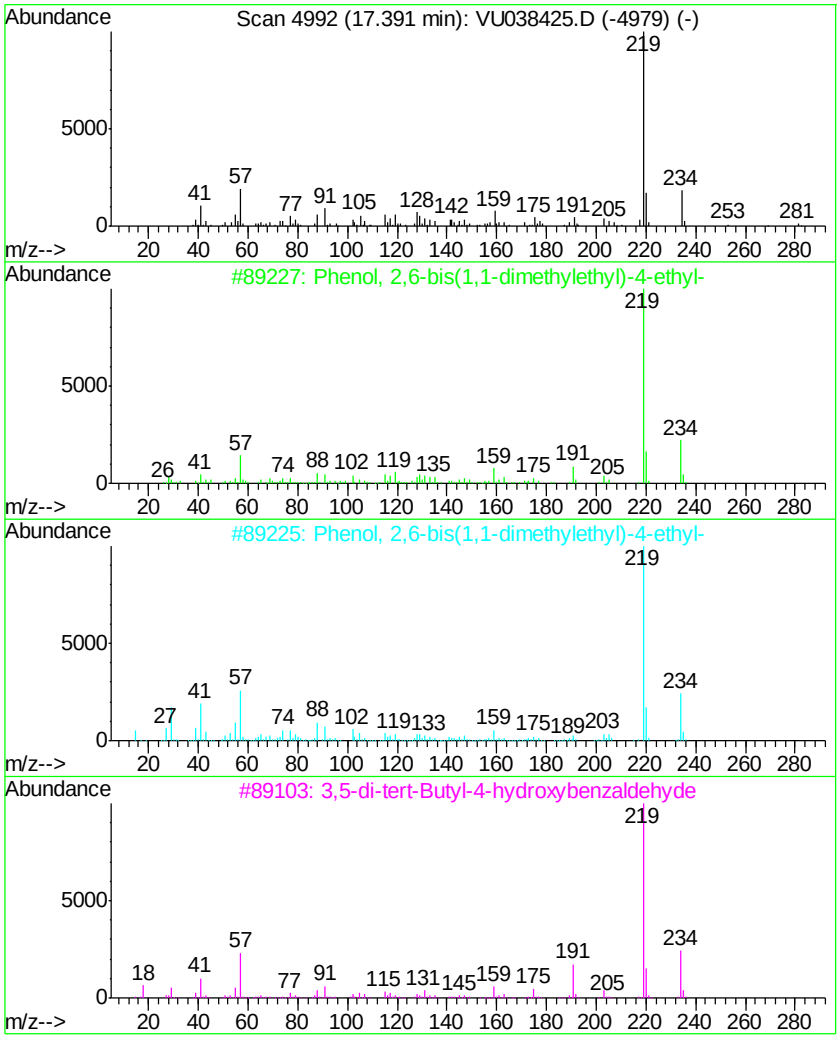
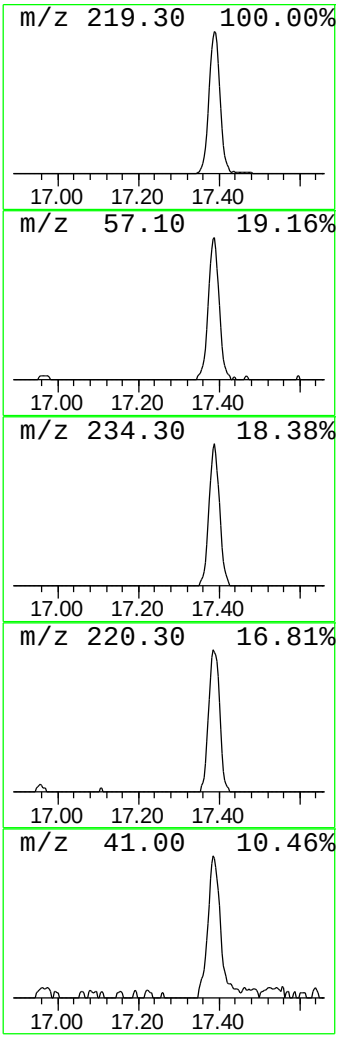
Peak Number 5 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.39	0.92 ug/L	175456	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	90
3	3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	87
4	3,5-Di-tert-butylbenzoic acid	234	C15H22O2	016225-26-6	86
5	4-tert-Butyl-2,6-diisopropylphenol	234	C16H26O	057354-65-1	86





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	0.6	ug/L	84613	1	6.28	761636	5.0
Ethyl Acetate	4.85	3.5	ug/L	531161	1	6.28	761636	5.0
n-Propyl acetate	7.07	2.2	ug/L	339981	1	6.28	761636	5.0
Phenol, 2,6-bis(1...	17.39	0.9	ug/L	175456	3	11.83	949672	5.0