LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU053120\
Data File : VU038456.D
Acq On : 31 May 2020 08:32
Operator : JC/MD
Sample : L2788-18
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXC6

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	18	rVB	116852	113565	6.88%	0.905%
2	1.613	74	85	93	rBV	136139	155830	9.45%	1.242%
3	1.932	175	184	200	rVB	113893	147061	8.91%	1.172%
4	2.594	377	390	407	rBV	244730	417027	25.28%	3.323%
5	2.681	408	417	439	rVB2	8463	28022	1.70%	0.223%
6	3.218	570	584	603	rVB	10439	24313	1.47%	0.194%
7	3.395	624	639	652	rBV4	12612	28205	1.71%	0.225%
8	3.736	732	745	758	rBV6	8924	20368	1.23%	0.162%
9	4.572	989	1005	1021	rVB2	18653	45525	2.76%	0.363%
10	4.681	1021	1039	1077	rBV	203425	731384	44.33%	5.828%
11	4.848	1077	1091	1114	rVB	139809	336798	20.41%	2.684%
12	5.102	1152	1170	1194	rBV4	258892	656337	39.78%	5.230%
13	5.424	1256	1270	1284	rBV7	10595	23331	1.41%	0.186%
14	5.758	1352	1374	1398	rBV2	422409	1130766	68.54%	9.011%
15	6.282	1521	1537	1571	rBV	374076	725489	43.97%	5.781%
16	6.571	1612	1627	1652	rBV	557579	1046197	63.41%	8.337%
17	6.719	1659	1673	1692	rBV	265022	512967	31.09%	4.088%
18	7.070	1767	1782	1807	rBV	165712	299765	18.17%	2.389%
19	7.591	1930	1944	1960	rBV	134419	234215	14.20%	1.866%
20	7.922	2033	2047	2074	rBV	504070	890683	53.99%	7.098%
21	8.202	2119	2134	2153	rBV	85846	145950	8.85%	1.163%
22	8.575	2236	2250	2262	rBV3	19163	32447	1.97%	0.259%
23	8.655	2262	2275	2307	rBV	894162	1649829	100.00%	13.147%
24	8.960	2356	2370	2384	rBV3	7394	17353	1.05%	0.138%
25	9.436	2504	2518	2541	rBV	536628	904321	54.81%	7.206%
26	10.771	2918	2933	2950	rBV	231791	371278	22.50%	2.959%
27	11.822	3247	3260	3277	rBV	566783	898062	54.43%	7.157%
28	12.205	3365	3379	3398	rVB	546953	869512	52.70%	6.929%
29	17.385	4980	4990	5005	rVB3	52267	92199	5.59%	0.735%

Sum of corrected areas: 12548799

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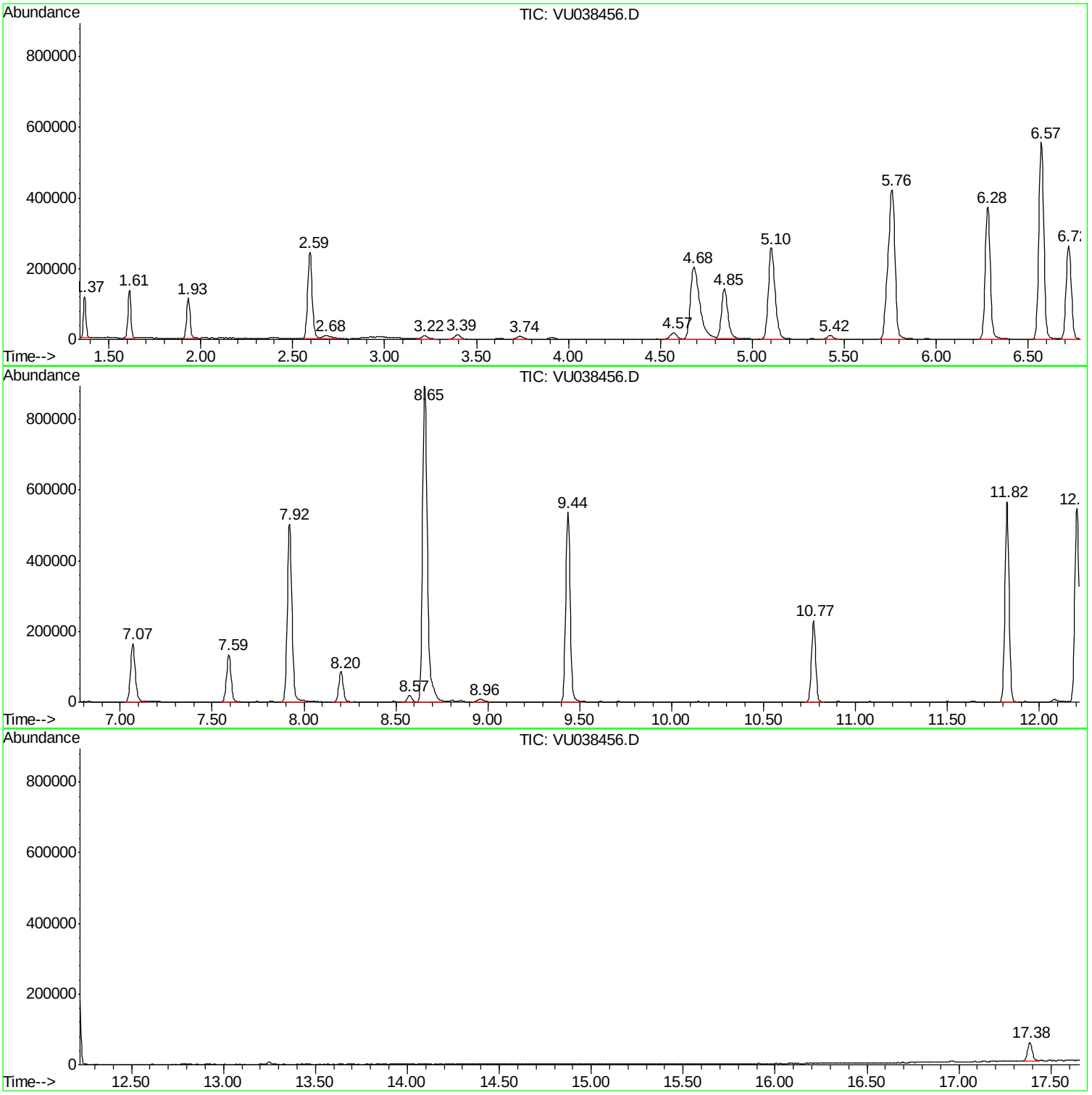
ClientSampleId : BFXC6

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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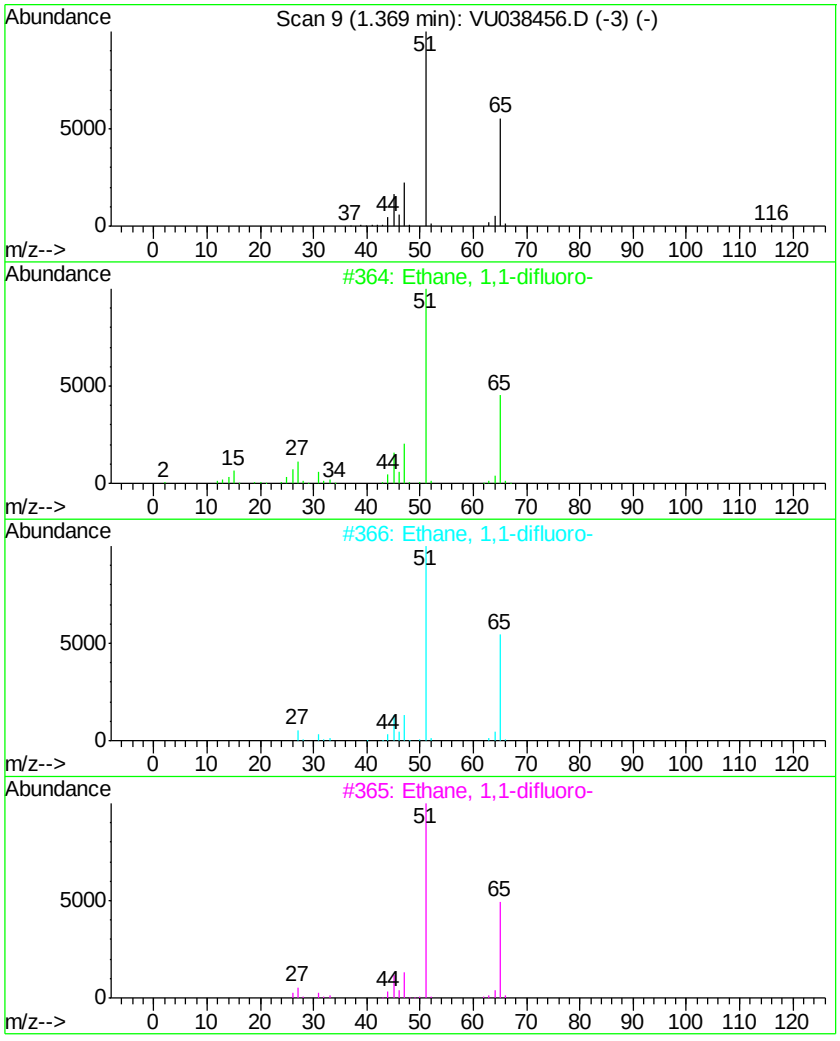
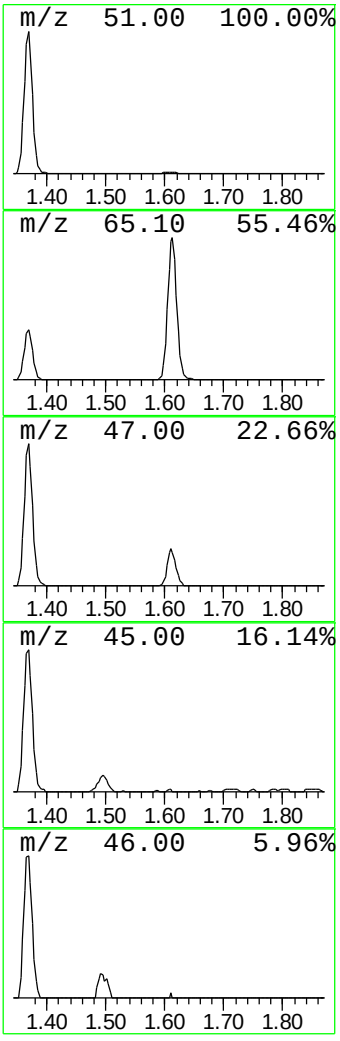
Peak Number 1 Ethane, 1,1-difluoro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.37	0.78 ug/L	113565	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	Ethane, 1-chloro-1,1-difluoro-	100	C2H3ClF2	000075-68-3	12
5	Ethane, 1-chloro-1,1-difluoro-	100	C2H3ClF2	000075-68-3	10





Library Search Compound Report

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Instrument : MSVOA_U
ClientSampleId : BFXC6

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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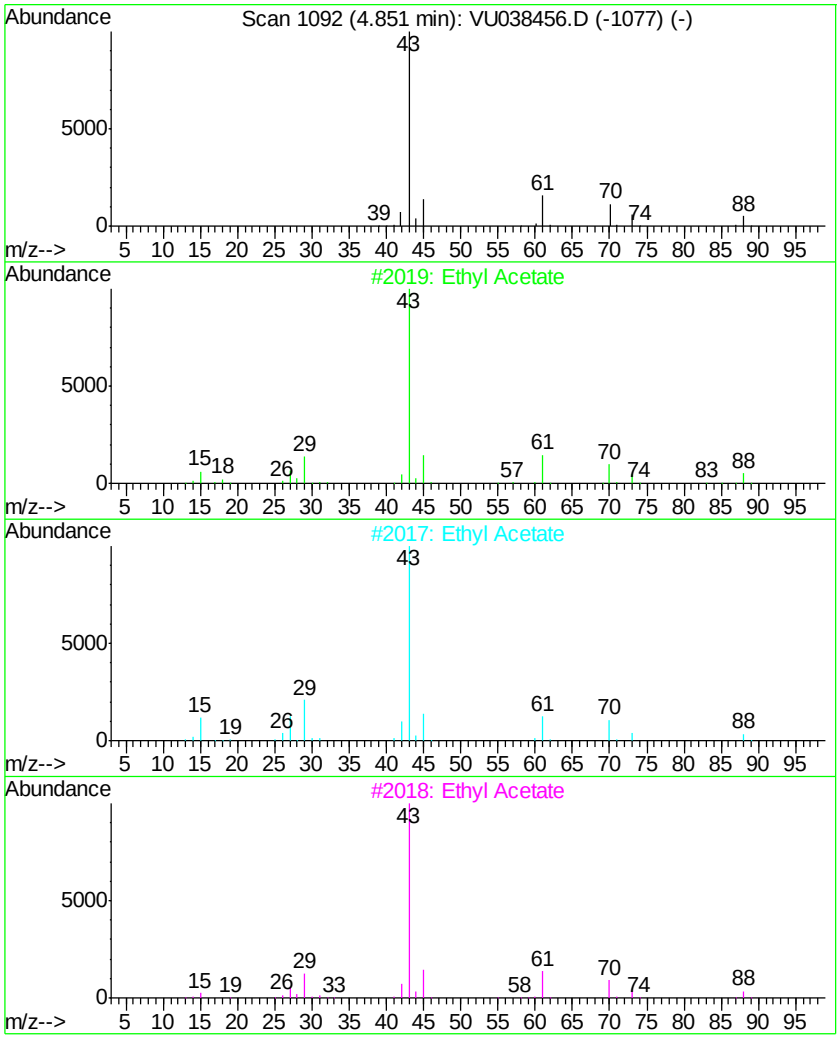
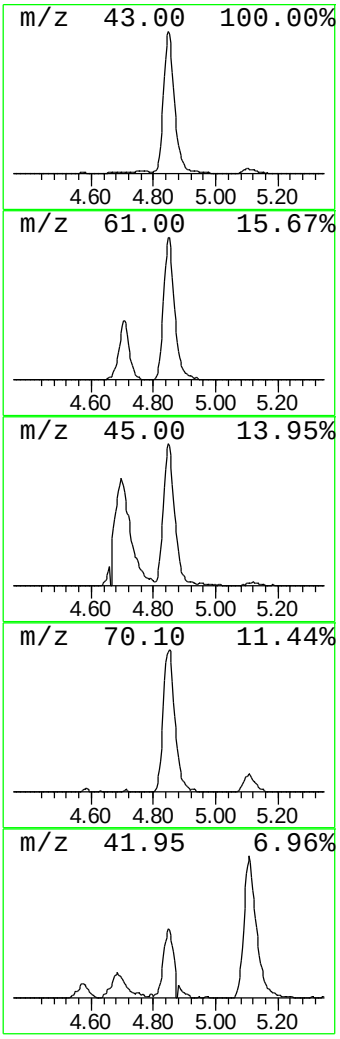
Peak Number 2 Ethyl Acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	2.32 ug/L	336798	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	64
5	CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	33





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ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXC6

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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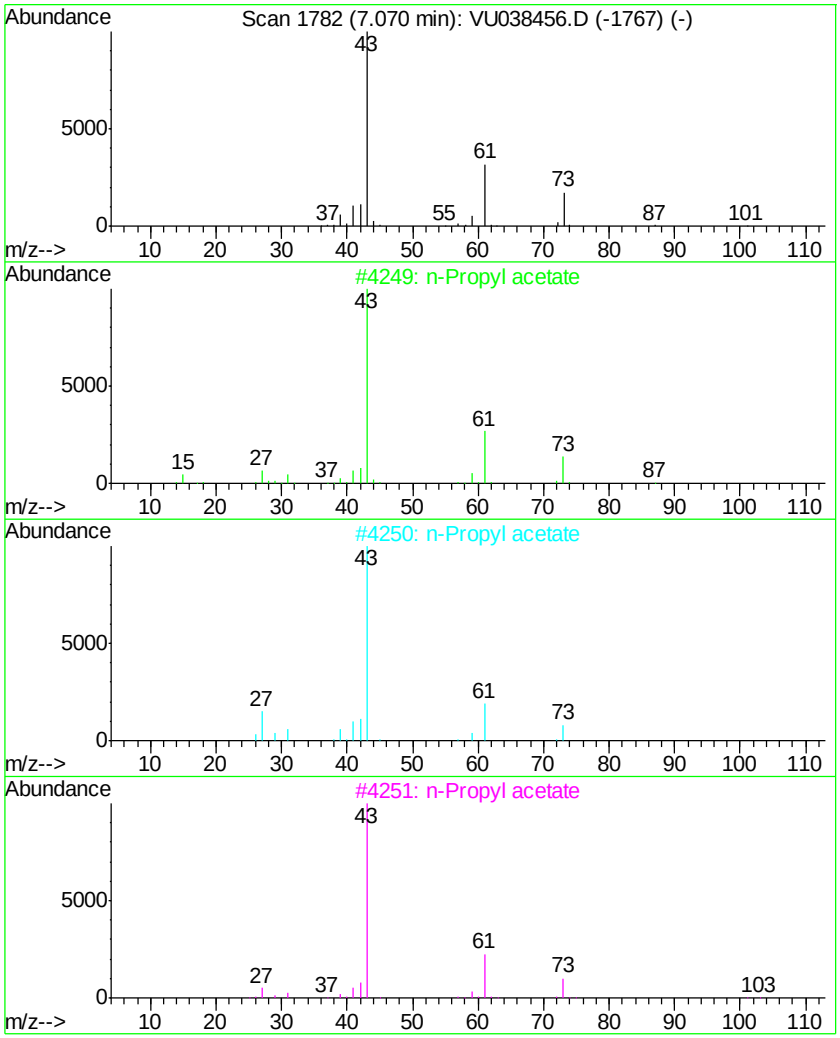
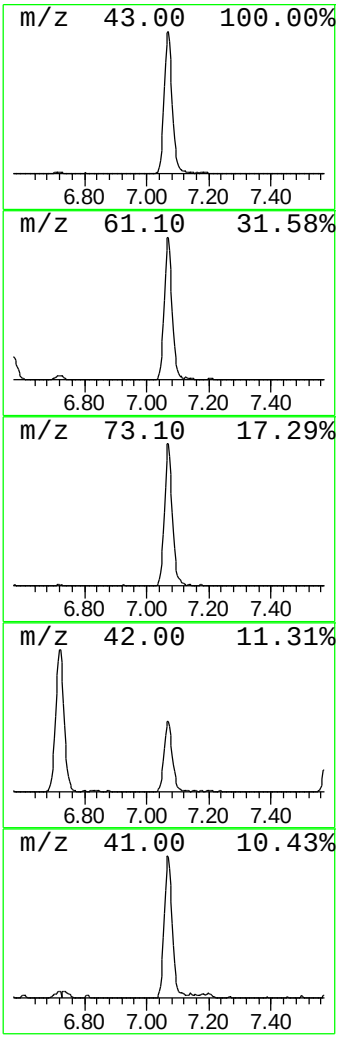
Peak Number 3 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.07	2.07 ug/L	299765	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	40
4	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	36
5	Isobutylamine	73	C4H11N	000078-81-9	9





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ClientSampleId : BFXC6

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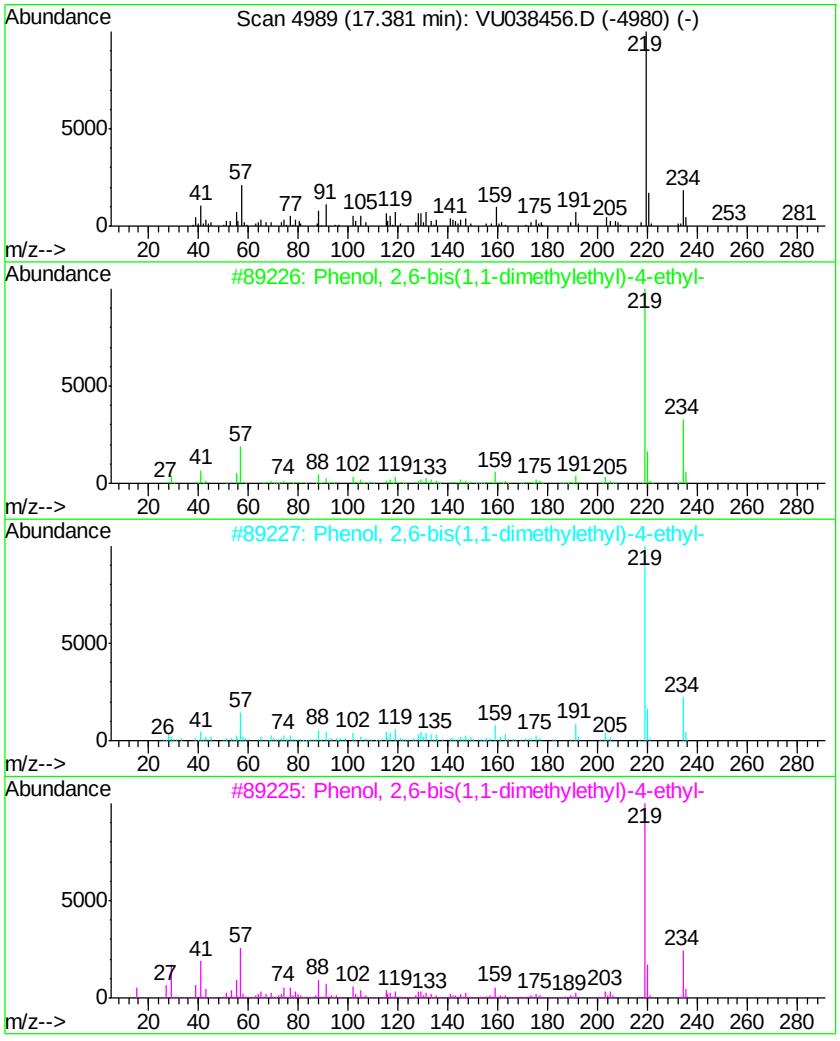
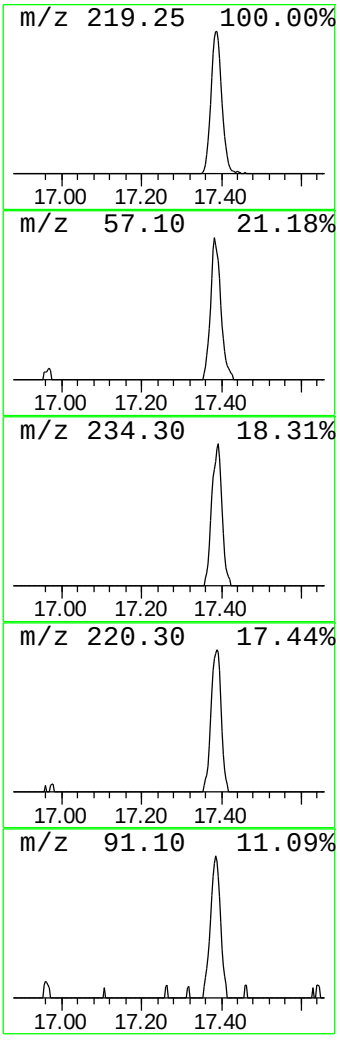
Peak Number 5 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.38	0.51 ug/L	92199	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	97
2	Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	95
3	Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	90
4	3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	87
5	3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	87





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethane, 1,1-diflu...	1.37	0.8	ug/L	113565	1	6.28	725489	5.0
Ethyl Acetate	4.85	2.3	ug/L	336798	1	6.28	725489	5.0
n-Propyl acetate	7.07	2.1	ug/L	299765	1	6.28	725489	5.0
Phenol, 2,6-bis(1...	17.38	0.5	ug/L	92199	3	11.83	898062	5.0