LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU053120\
Data File : VU038423.D
Acq On : 30 May 2020 19:06
Operator : JC/MD
Sample : L2787-02
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFX72

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	rVB	88052	87016	5.62%	0.729%
2	1.610	74	84	96	rBV	151959	180468	11.66%	1.512%
3	1.932	172	184	195	rBV	120105	154544	9.98%	1.295%
4	2.594	374	390	404	rBV	246593	411735	26.60%	3.451%
5	2.675	407	415	430	rVB2	11437	26212	1.69%	0.220%
6	3.395	622	639	655	rVB5	11993	26803	1.73%	0.225%
7	3.736	731	745	759	rVB3	12758	29084	1.88%	0.244%
8	4.572	989	1005	1020	rBV3	22781	54435	3.52%	0.456%
9	4.674	1020	1037	1075	rVV	211586	635051	41.02%	5.322%
10	4.845	1076	1090	1125	rVB	284854	649933	41.98%	5.447%
11	5.102	1150	1170	1198	rBV	261896	594775	38.42%	4.985%
12	5.420	1255	1269	1283	rBV6	10187	21432	1.38%	0.180%
13	5.761	1353	1375	1406	rBV2	445509	1161004	75.00%	9.730%
14	6.282	1522	1537	1578	rBV	382172	742031	47.93%	6.219%
15	6.723	1659	1674	1691	rBV	269539	523732	33.83%	4.389%
16	7.067	1768	1781	1805	rBV	232965	421329	27.22%	3.531%
17	7.591	1931	1944	1964	rBV	142311	250599	16.19%	2.100%
18	7.922	2033	2047	2063	rBV	521597	919981	59.43%	7.710%
19	7.993	2063	2069	2081	rVB2	14942	26052	1.68%	0.218%
20	8.202	2122	2134	2150	rVB	91374	153824	9.94%	1.289%
21	8.655	2258	2275	2312	rBV	826746	1548036	100.00%	12.974%
22	9.436	2504	2518	2551	rBV	548198	937875	60.58%	7.860%
23	10.771	2921	2933	2951	rBV	220013	351874	22.73%	2.949%
24	11.825	3248	3261	3278	rBV	580344	933676	60.31%	7.825%
25	12.082	3330	3341	3351	rBV5	11202	22917	1.48%	0.192%
26	12.205	3364	3379	3394	rBV	560253	890165	57.50%	7.460%
27	13.250	3693	3704	3715	rBV3	11197	16739	1.08%	0.140%
28	17.385	4979	4990	5005	rBV2	86666	160735	10.38%	1.347%

Sum of corrected areas: 11932057

LSC Report - Integrated Chromatogram

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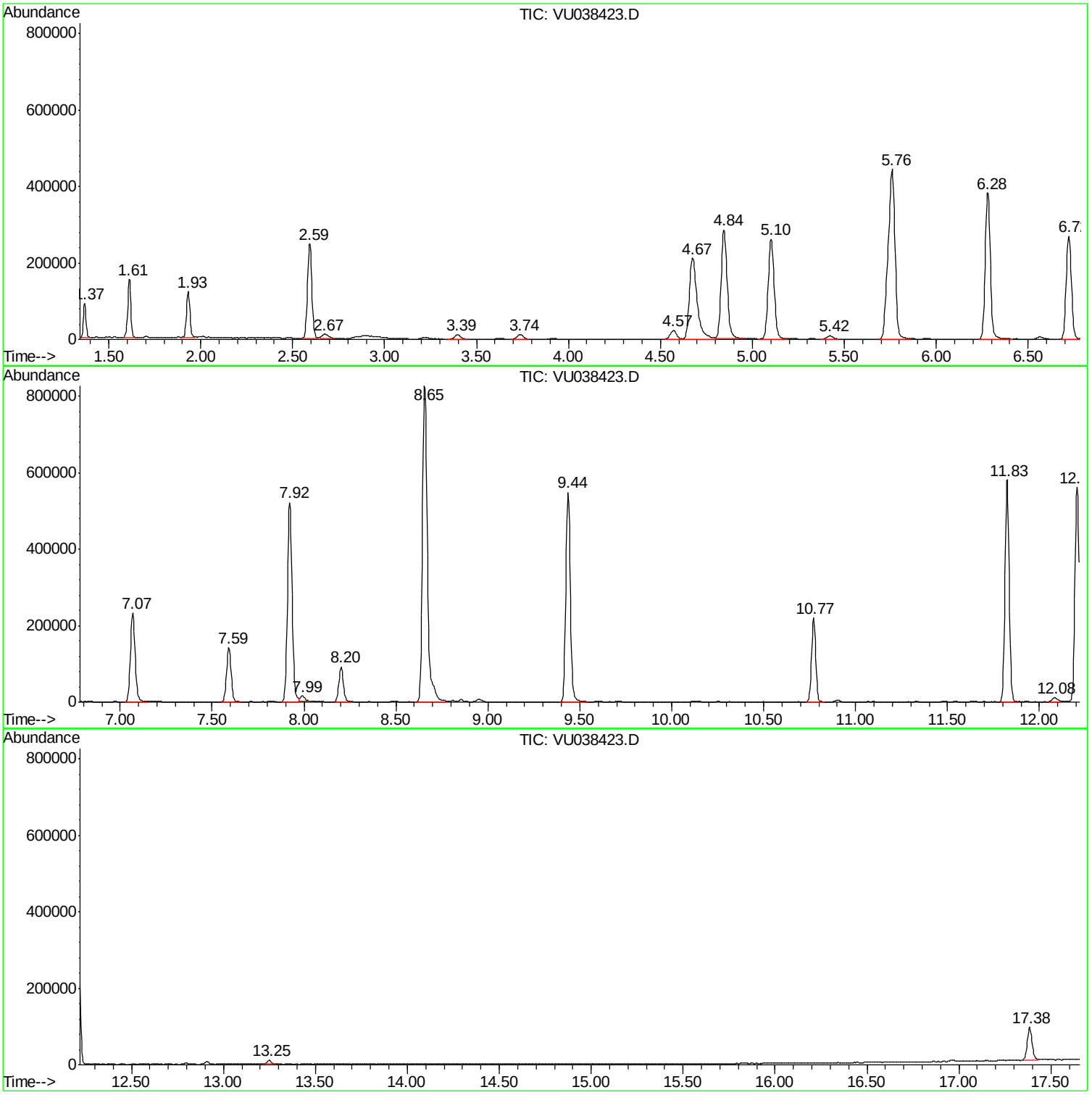
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFX72

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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Operator : JC/MD
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Instrument : MSVOA_U
ClientSampleId : BFX72

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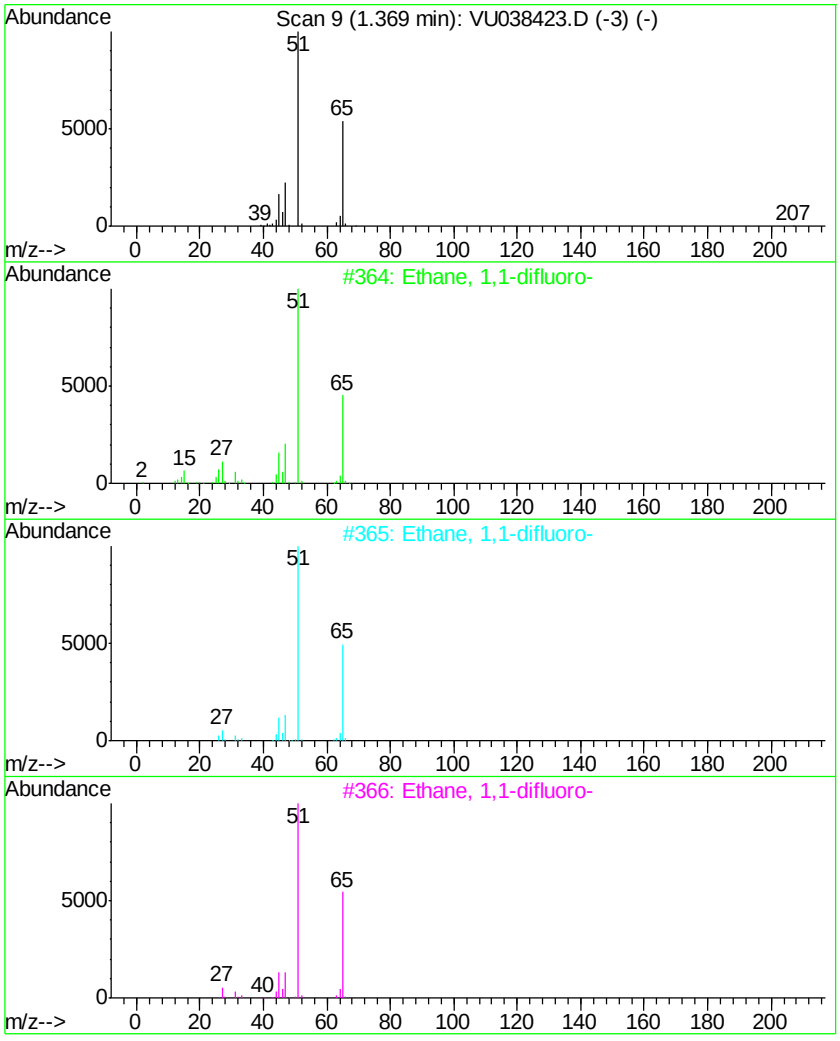
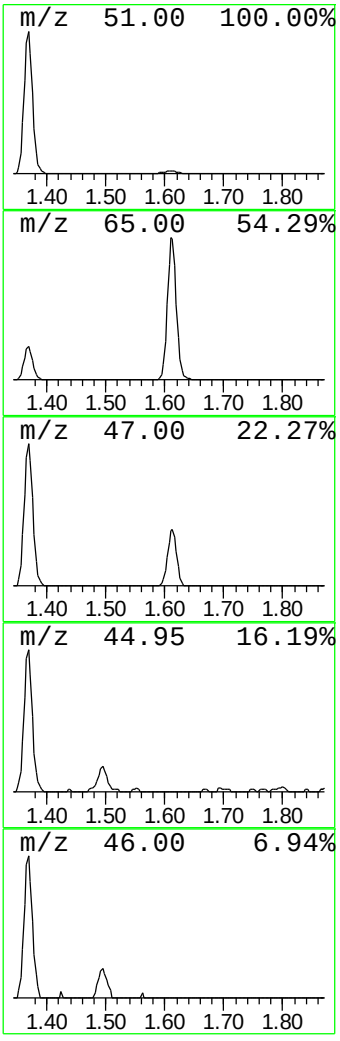
Peak Number 1 Ethane, 1,1-difluoro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.37	0.59 ug/L	87016	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





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ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFX72

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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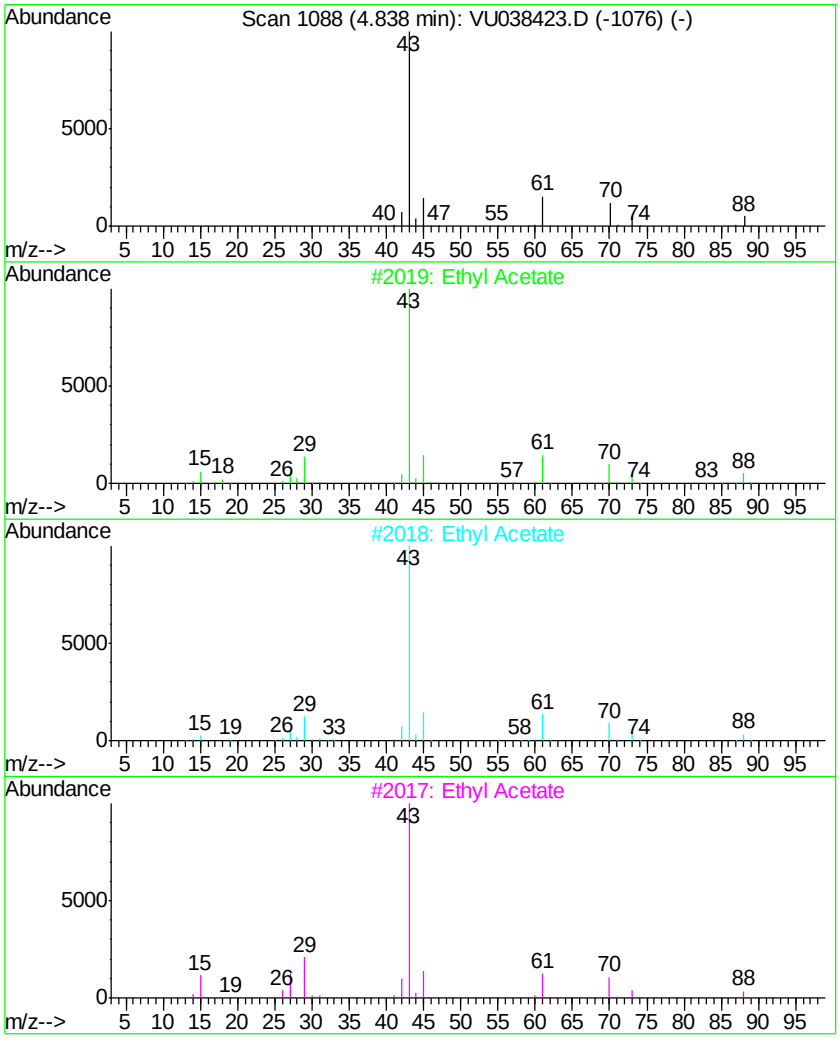
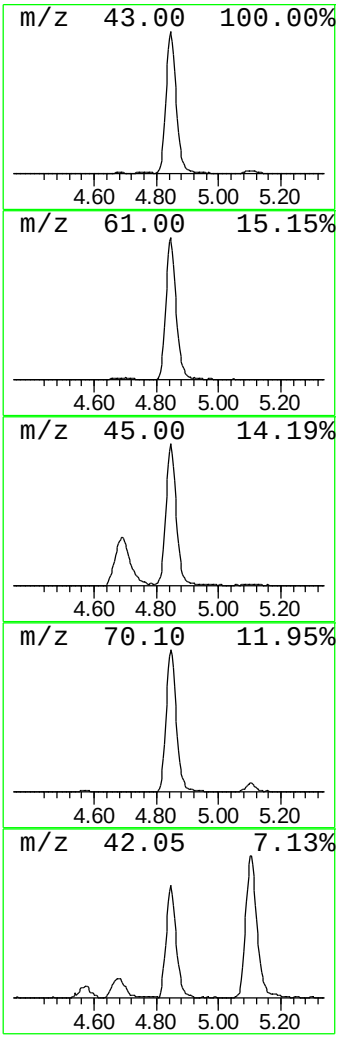
Peak Number 2 Ethyl Acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	4.38 ug/L	649933	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl Acetate	88	C4H8O2	000141-78-6	91
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	53





Library Search Compound Report

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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 : BFX72

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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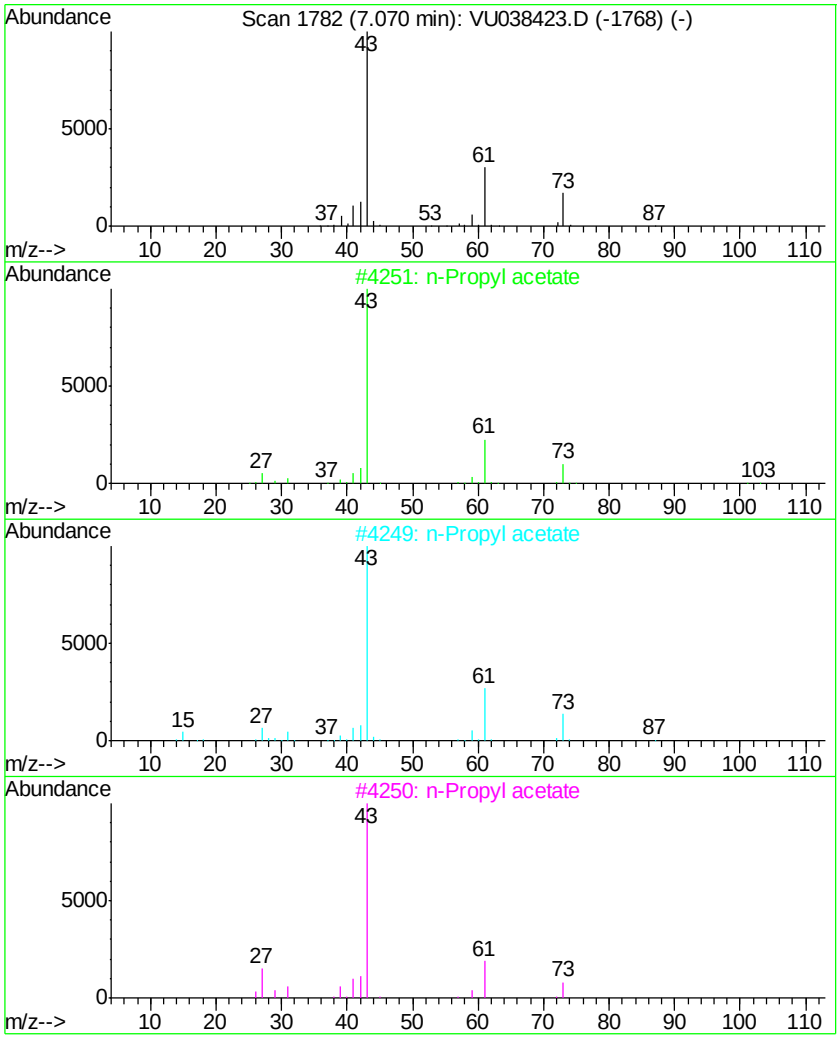
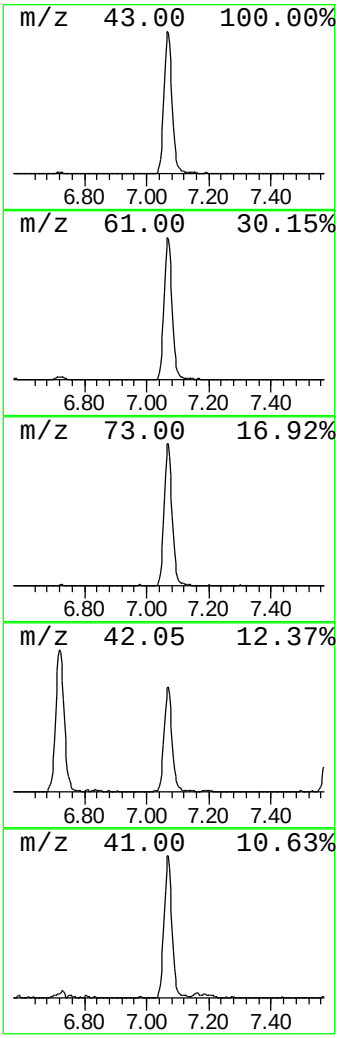
Peak Number 3 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.07	2.84 ug/L	421329	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	Isopropyl acetate	102	C5H10O2	000108-21-4	33





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ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFX72

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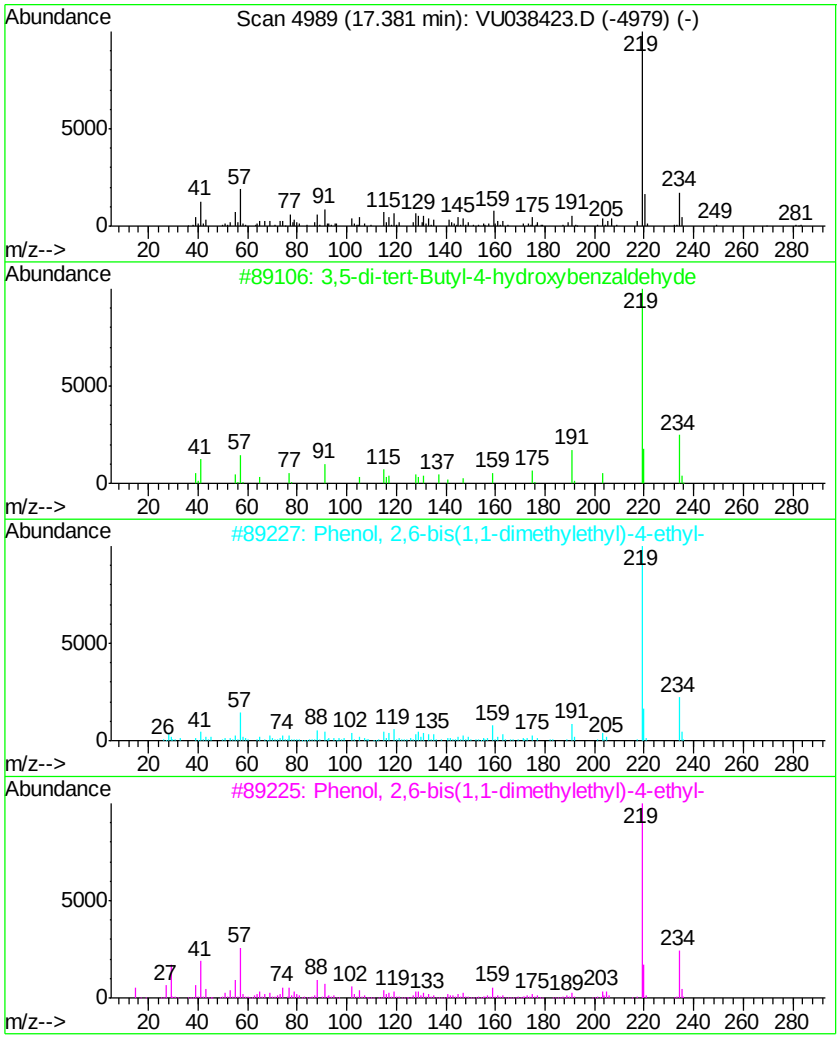
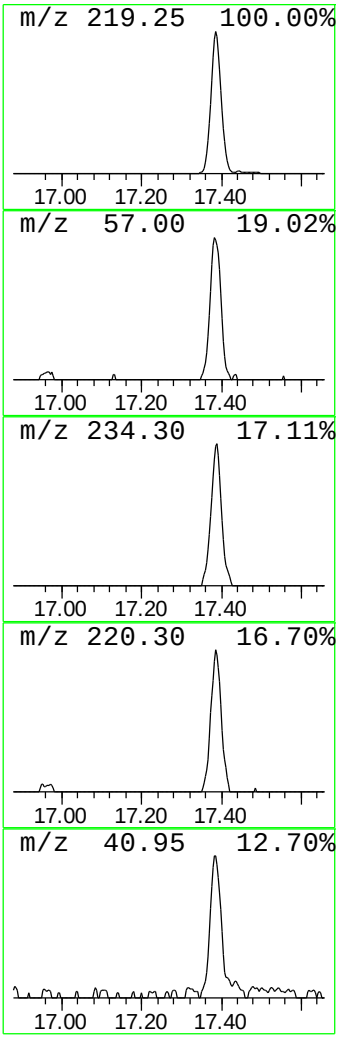
Peak Number 5 3,5-di-tert-Butyl-4-hydroxy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.38	0.86 ug/L	160735	1,4-Dichlorobenzene-d4	11.83

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	Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	91
4	3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	90
5	4-tert-Butyl-2,6-diisopropylphenol	234	C16H26O	057354-65-1	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU053120\
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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	87016	1	6.28	742031	5.0
Ethyl Acetate	4.84	4.4	ug/L	649933	1	6.28	742031	5.0
n-Propyl acetate	7.07	2.8	ug/L	421329	1	6.28	742031	5.0
3,5-di-tert-Butyl...	17.38	0.9	ug/L	160735	3	11.83	933676	5.0