

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060120\
 Data File : VU038467.D
 Acq On : 01 Jun 2020 13:47
 Operator : JC/MD
 Sample : L2789-05
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 2 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFX78

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

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	rBV	83342	80200	5.03%	0.690%
2	1.610	72	84	94	rBV2	130162	204462	12.83%	1.759%
3	1.932	175	184	199	rBV	108349	140056	8.79%	1.205%
4	2.594	375	390	405	rBV	219212	376321	23.61%	3.237%
5	2.883	451	480	483	rBV2	8134	24304	1.53%	0.209%
6	3.221	570	585	600	rVB	11635	25829	1.62%	0.222%
7	3.398	626	640	655	rVB4	16140	35822	2.25%	0.308%
8	3.735	729	745	767	rBV2	15661	36555	2.29%	0.314%
9	4.571	987	1005	1021	rBV3	28142	67156	4.21%	0.578%
10	4.681	1021	1039	1076	rBV2	223115	723869	45.42%	6.227%
11	4.845	1076	1090	1123	rVB	170117	408721	25.65%	3.516%
12	5.102	1154	1170	1194	rBV2	249221	571450	35.86%	4.916%
13	5.423	1256	1270	1286	rVB7	8377	19925	1.25%	0.171%
14	5.761	1352	1375	1406	rBV2	424144	1131359	70.99%	9.732%
15	6.282	1522	1537	1561	rBV	356964	695482	43.64%	5.983%
16	6.571	1613	1627	1643	rBV2	85579	167472	10.51%	1.441%
17	6.722	1657	1674	1694	rBV	264686	516304	32.40%	4.441%
18	7.066	1767	1781	1807	rBV	184843	333985	20.96%	2.873%
19	7.590	1928	1944	1958	rBV	139467	245777	15.42%	2.114%
20	7.922	2033	2047	2063	rBV	493022	866486	54.37%	7.454%
21	7.989	2064	2068	2082	rVB3	12930	22342	1.40%	0.192%
22	8.201	2121	2134	2149	rBV2	89652	151803	9.53%	1.306%
23	8.655	2262	2275	2306	rBV	868793	1593671	100.00%	13.709%
24	8.957	2356	2369	2386	rBV5	11068	26376	1.66%	0.227%
25	9.436	2504	2518	2545	rBV	518453	878279	55.11%	7.555%
26	10.770	2921	2933	2947	rBV	231048	364988	22.90%	3.140%
27	11.822	3248	3260	3279	rBV	542811	857452	53.80%	7.376%
28	12.082	3330	3341	3354	rBV4	8718	18180	1.14%	0.156%
29	12.204	3363	3379	3395	rBV	540648	861305	54.05%	7.409%
30	17.388	4980	4991	5003	rBV2	95734	179212	11.25%	1.542%

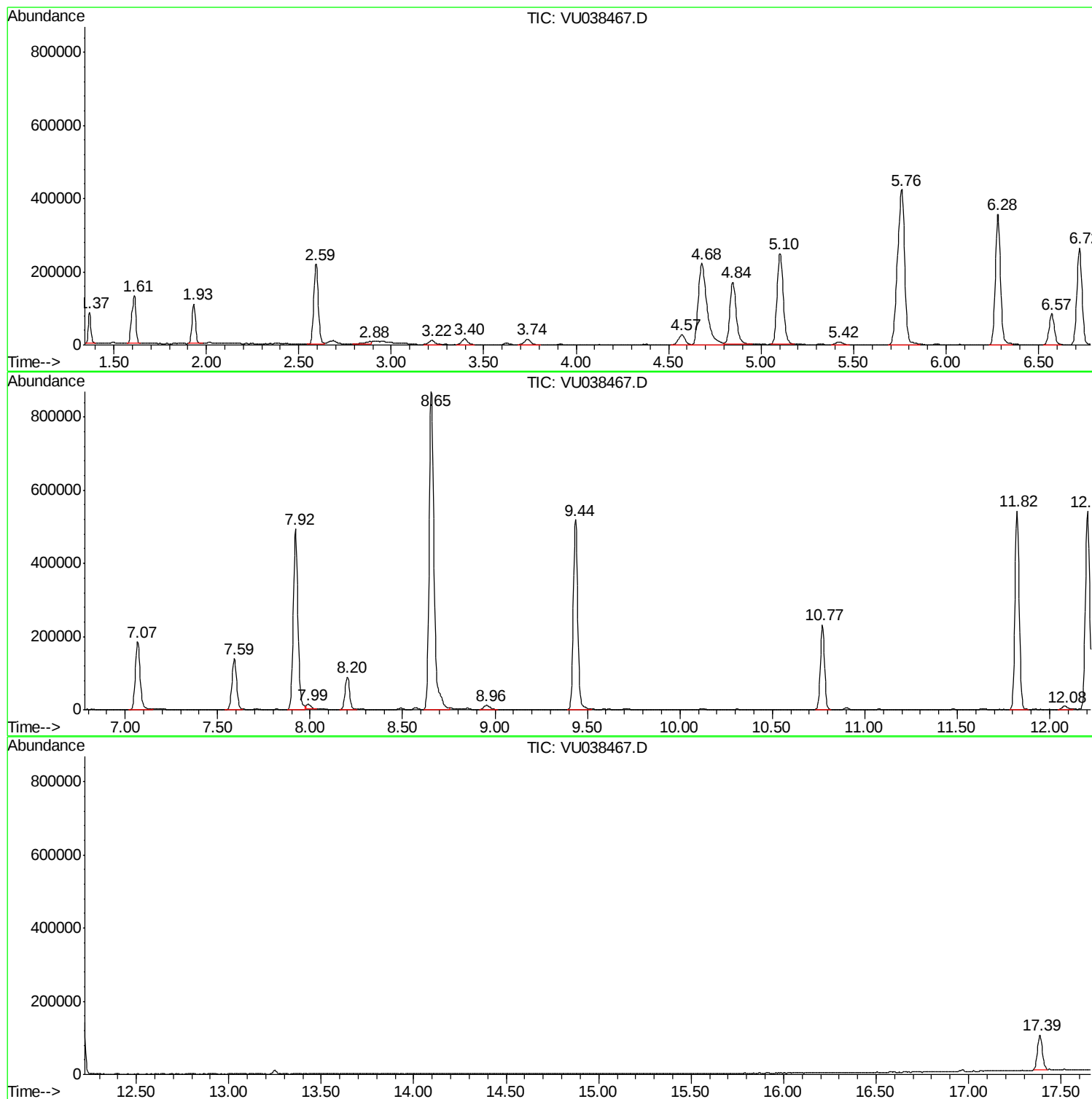
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ClientSampleId :
BFX78

Quant Method : Z:\V0ASRV\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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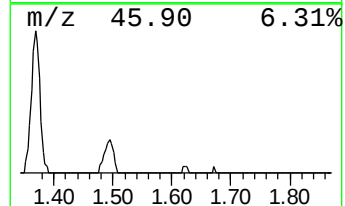
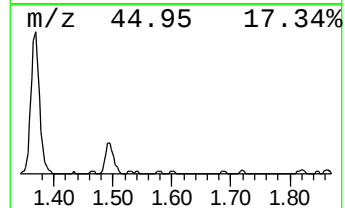
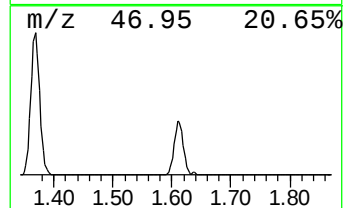
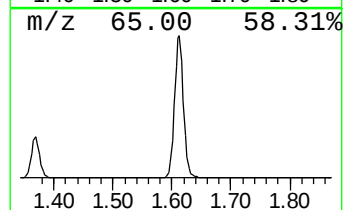
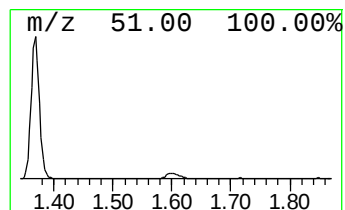
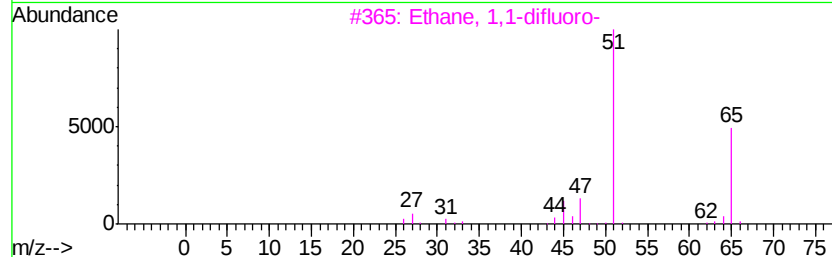
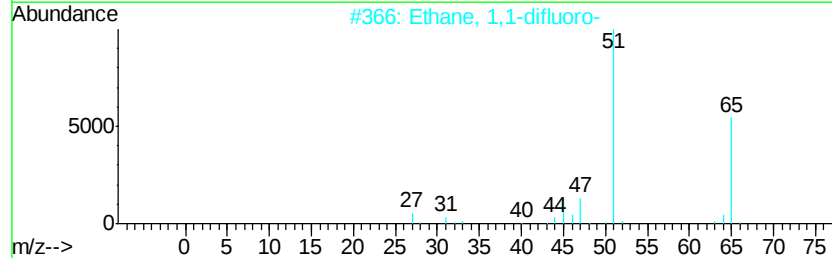
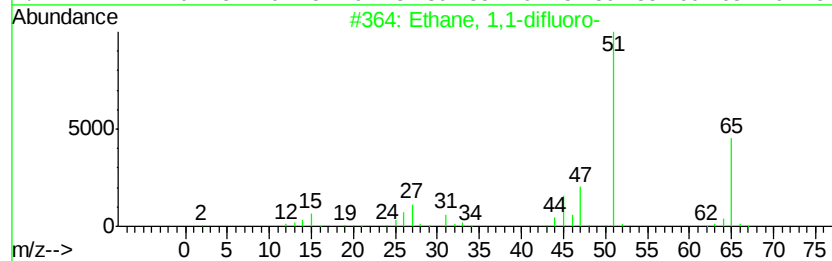
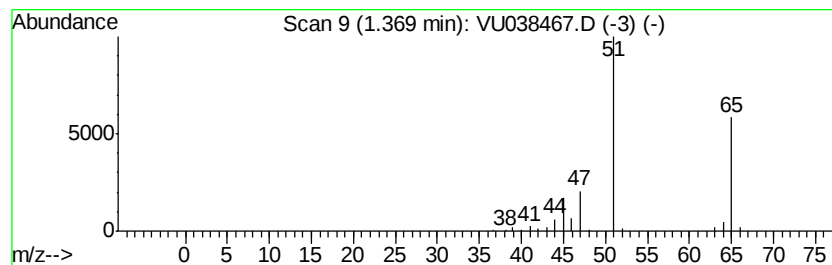
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.37	0.58 ug/L	80200	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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



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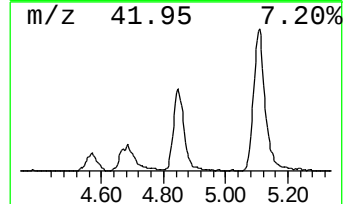
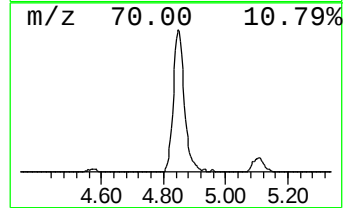
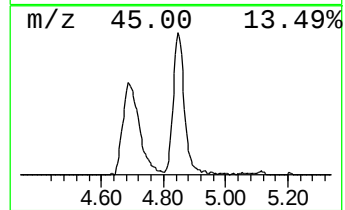
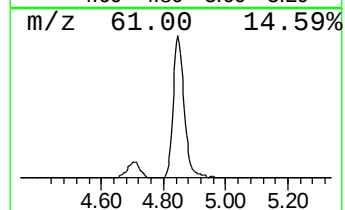
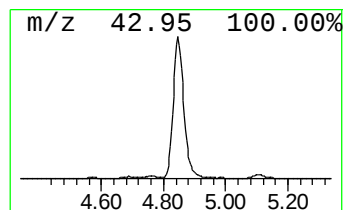
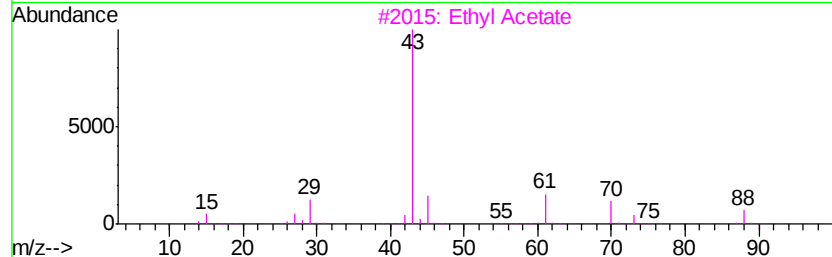
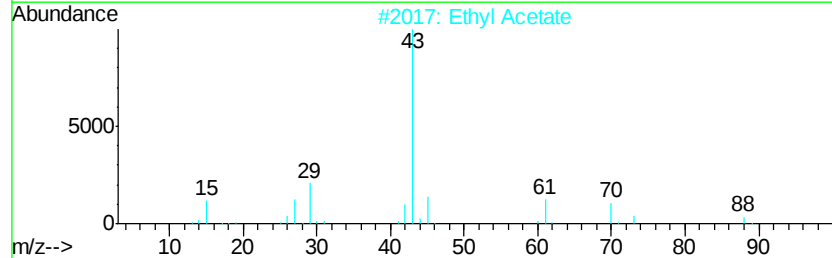
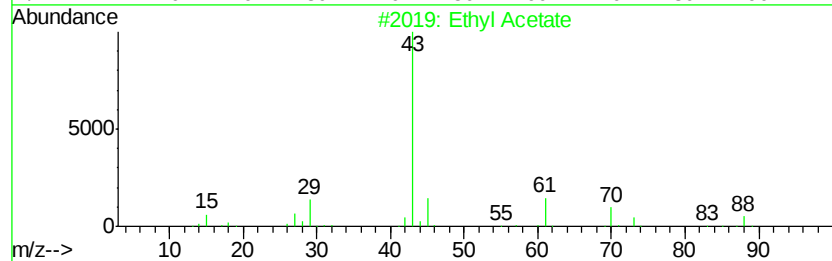
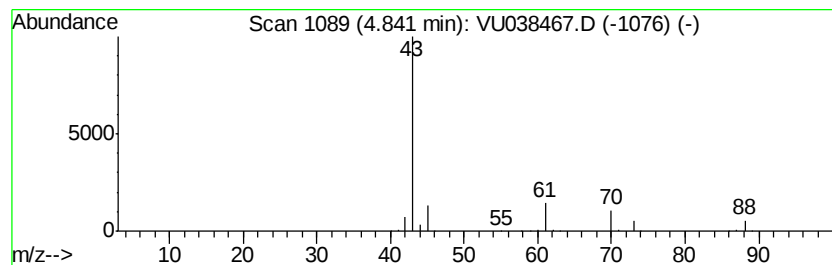
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 Ethyl Acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	2.94 ug/L	408721	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethyl Acetate	88	C4H8O2	000141-78-6	86
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	33



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ALS Vial : 2 Sample Multiplier: 1

Instrument :
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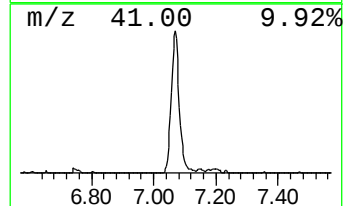
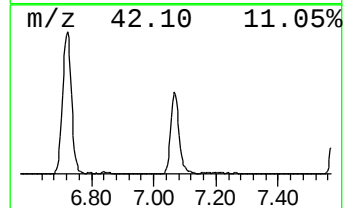
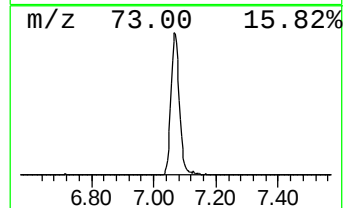
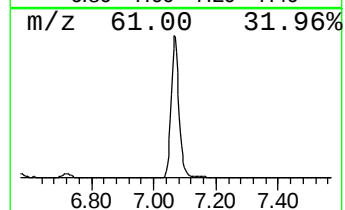
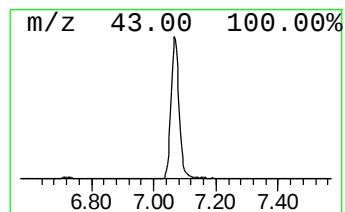
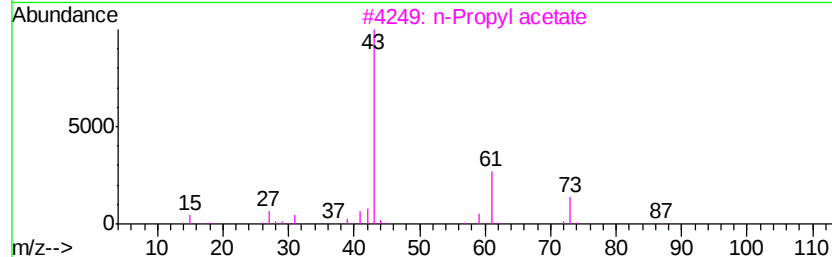
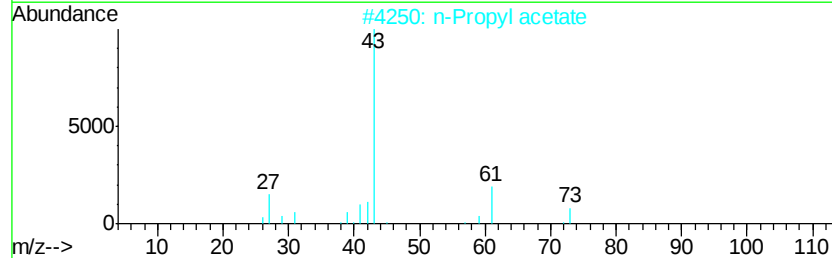
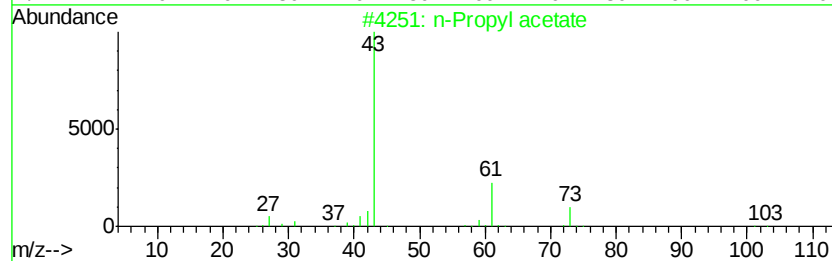
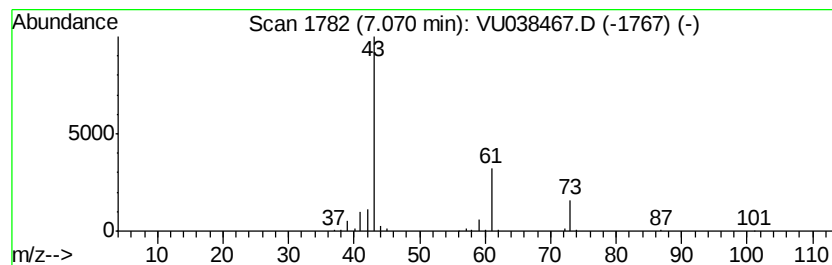
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.07	2.40 ug/L	333985	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		Isopropyl acetate	102	C5H10O2	000108-21-4	33



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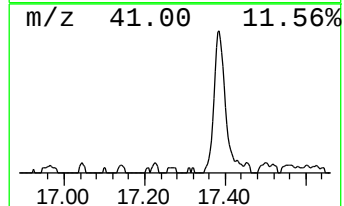
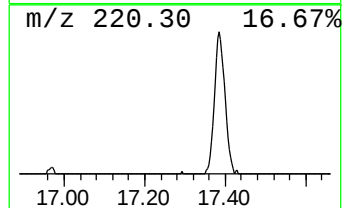
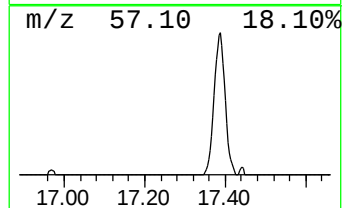
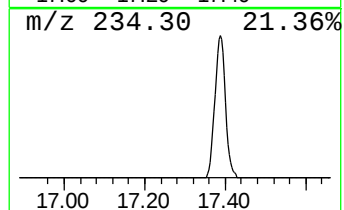
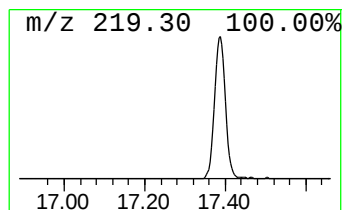
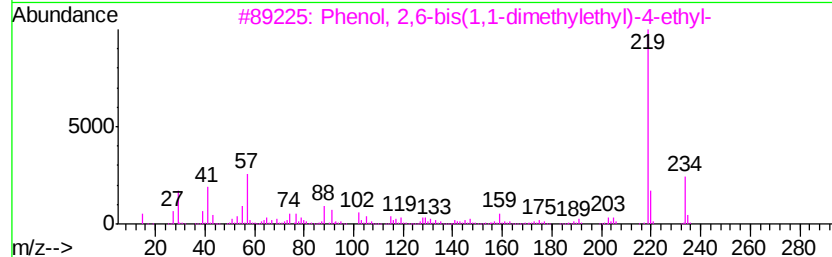
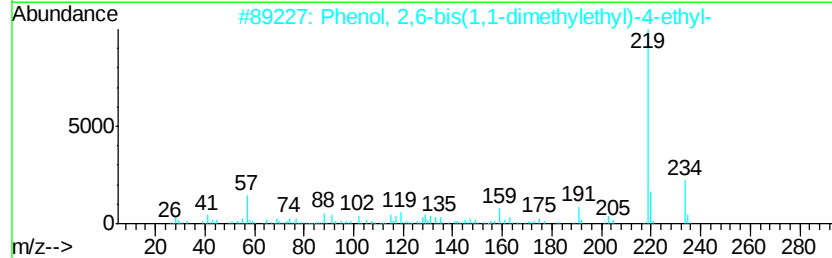
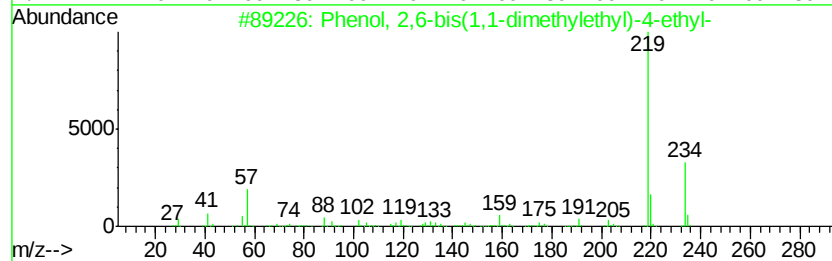
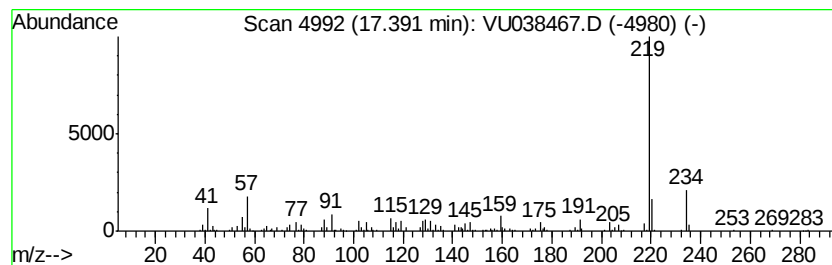
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Peak Number 5 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.39	1.05 ug/L	179212	1,4-Dichlorobenzene-d4	11.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, 2,6-bis(1,1-dimethylethyl)...	234	C16H26O	004130-42-1	94
2		Phenol, 2,6-bis(1,1-dimethylethyl)...	234	C16H26O	004130-42-1	91
3		Phenol, 2,6-bis(1,1-dimethylethyl)...	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	86



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethane, 1,1-diflu...	1.37	0.6	ug/L	80200	1	6.28	695482	5.0
Ethyl Acetate	4.84	2.9	ug/L	408721	1	6.28	695482	5.0
n-Propyl acetate	7.07	2.4	ug/L	333985	1	6.28	695482	5.0
Phenol, 2,6-bis(1...	17.39	1.1	ug/L	179212	3	11.82	857452	5.0