

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU053120\
 Data File : VU038432.D
 Acq On : 30 May 2020 22:34
 Operator : JC/MD
 Sample : L2787-11
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFX93

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	20	rVB	117752	116442	7.15%	0.953%
2	1.613	73	85	94	rBV	149439	178180	10.94%	1.458%
3	1.932	175	184	196	rBV	113603	146202	8.98%	1.196%
4	2.398	321	329	341	rVB5	10287	18945	1.16%	0.155%
5	2.594	377	390	402	rBV	239509	401924	24.68%	3.289%
6	2.674	406	415	440	rVB2	10400	29963	1.84%	0.245%
7	3.395	626	639	653	rBV3	11657	25103	1.54%	0.205%
8	3.739	732	746	760	rVB3	11924	28069	1.72%	0.230%
9	3.912	782	800	816	rBV2	32445	74963	4.60%	0.613%
10	4.571	987	1005	1019	rBV2	21942	52187	3.20%	0.427%
11	4.678	1021	1038	1075	rVV	217124	696133	42.75%	5.696%
12	4.845	1076	1090	1117	rVB	211776	486936	29.90%	3.985%
13	5.102	1154	1170	1193	rBV2	252584	561076	34.45%	4.591%
14	5.761	1353	1375	1409	rBV2	432480	1146407	70.40%	9.381%
15	6.279	1519	1536	1563	rBV	368175	715443	43.93%	5.854%
16	6.571	1613	1627	1645	rBV2	247131	468490	28.77%	3.834%
17	6.719	1658	1673	1692	rBV	267193	524582	32.21%	4.293%
18	7.070	1766	1782	1799	rBV	207159	373046	22.91%	3.053%
19	7.591	1929	1944	1961	rBV	141780	247605	15.20%	2.026%
20	7.922	2030	2047	2063	rBV	514109	902622	55.43%	7.386%
21	7.989	2064	2068	2081	rVB3	9943	16939	1.04%	0.139%
22	8.202	2122	2134	2147	rBV2	89763	150437	9.24%	1.231%
23	8.655	2259	2275	2316	rBV	886525	1628482	100.00%	13.326%
24	8.954	2355	2368	2383	rBV3	7511	17156	1.05%	0.140%
25	9.436	2503	2518	2539	rBV	525619	892139	54.78%	7.300%
26	10.771	2920	2933	2950	rBV	227690	364585	22.39%	2.983%
27	11.825	3245	3261	3278	rBV	565631	894346	54.92%	7.318%
28	12.079	3330	3340	3352	rBV5	8468	17846	1.10%	0.146%
29	12.205	3366	3379	3398	rVB	548518	881763	54.15%	7.215%
30	17.384	4979	4990	5007	rBV2	87220	162564	9.98%	1.330%

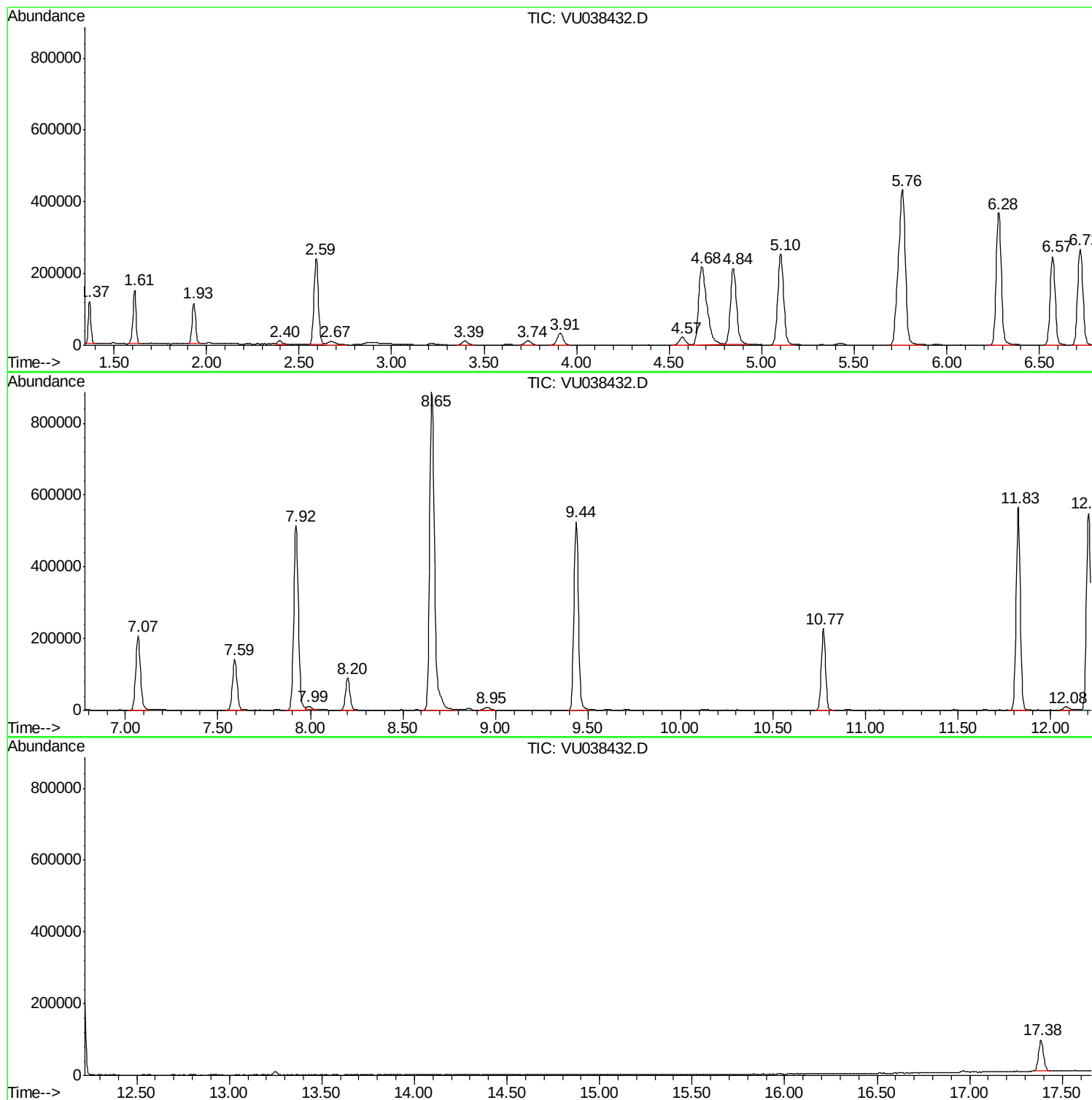
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

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



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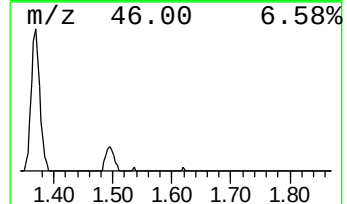
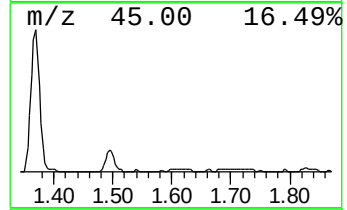
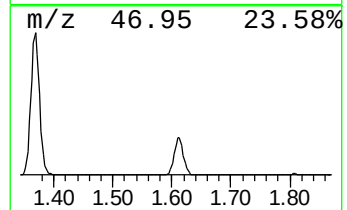
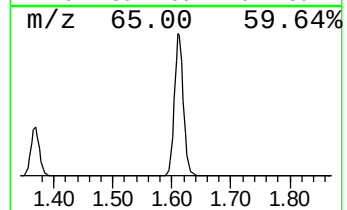
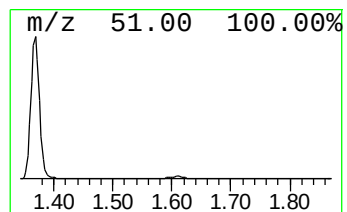
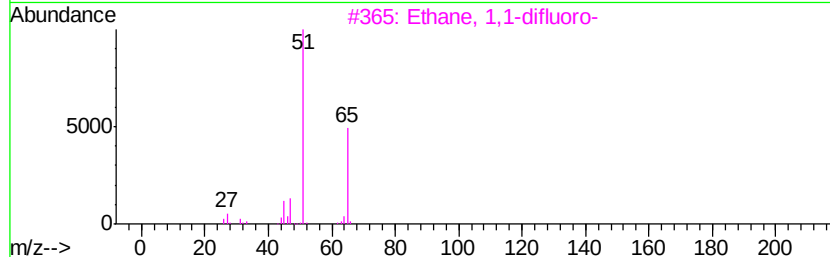
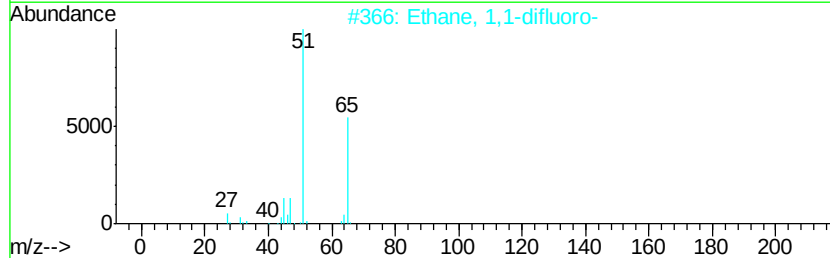
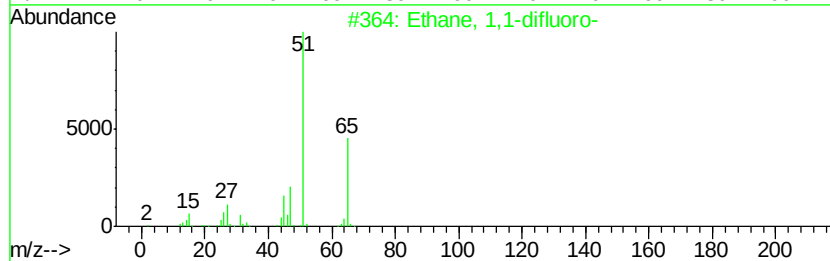
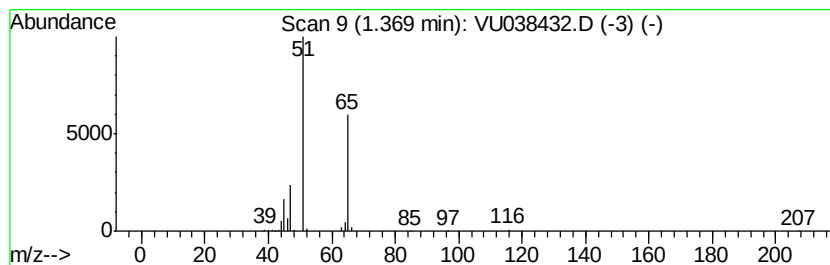
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Quant Title : TRACE VOA SOM01.0

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	0.81 ug/L	116442	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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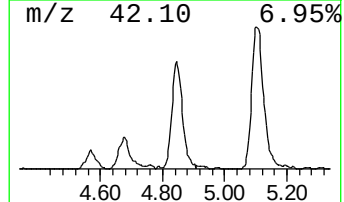
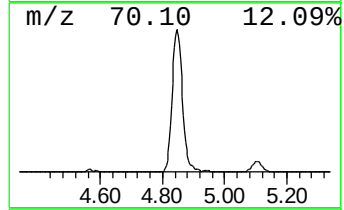
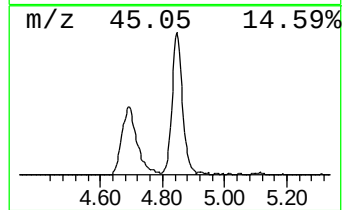
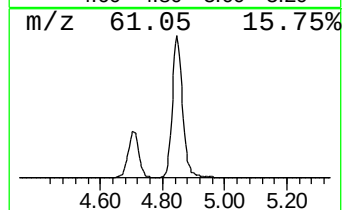
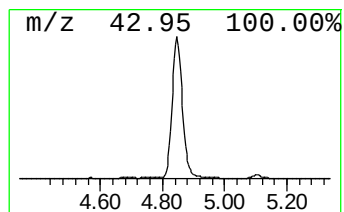
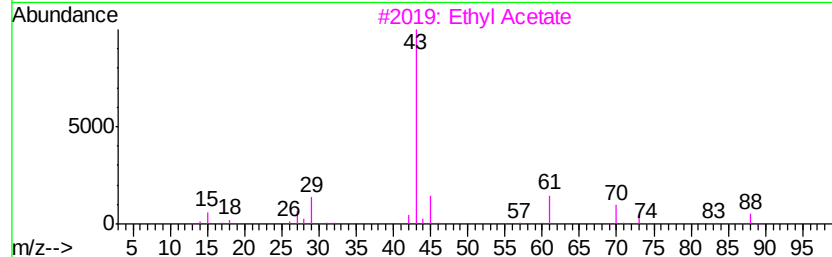
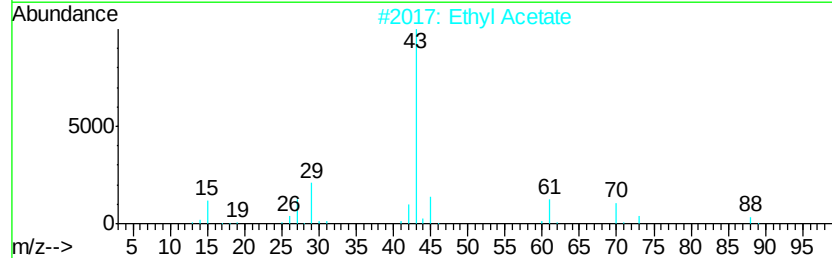
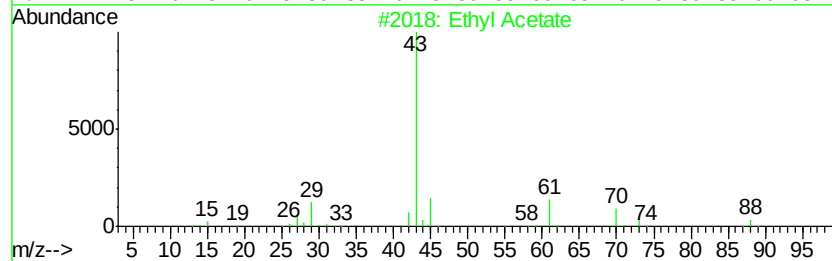
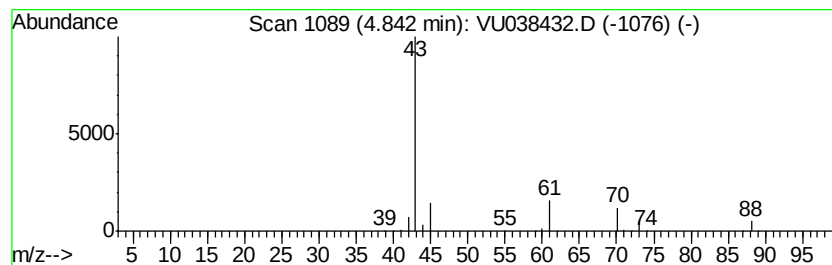
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Quant Title : TRACE VOA SOM01.0

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	3.40 ug/L	486936	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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	86
4		Ethyl Acetate	88	C4H8O2	000141-78-6	86
5		CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	40



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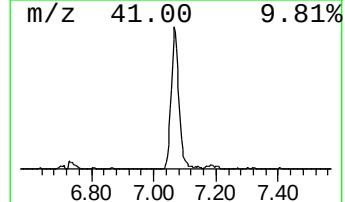
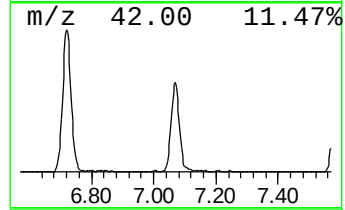
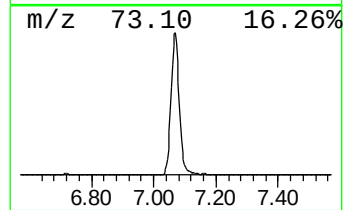
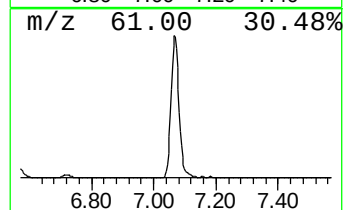
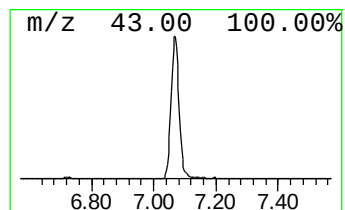
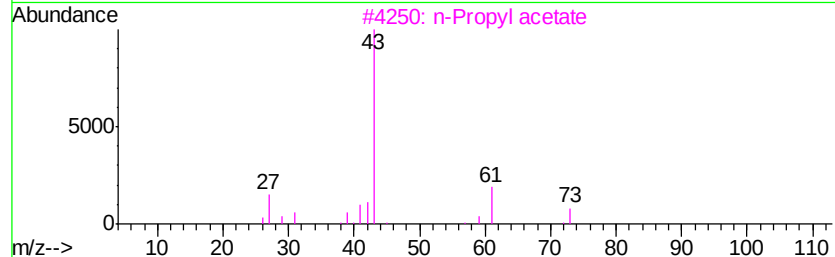
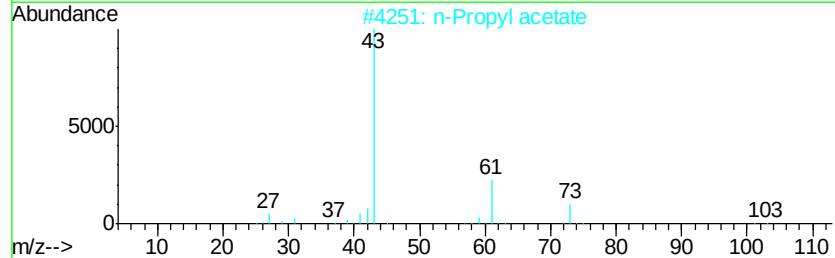
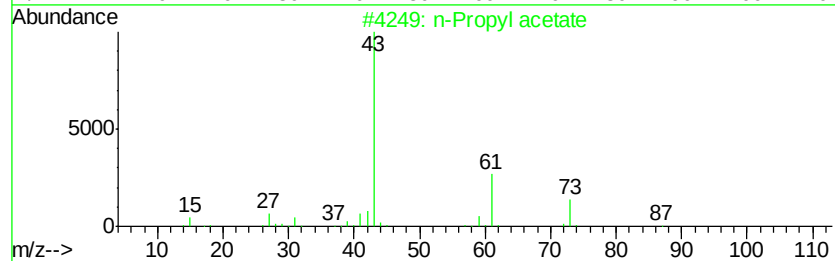
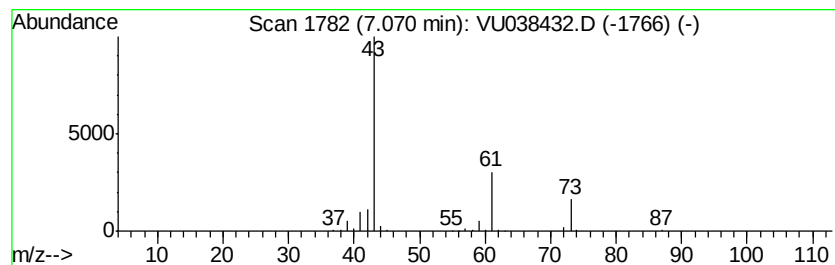
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Quant Title : TRACE VOA SOM01.0

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	2.61 ug/L	373046	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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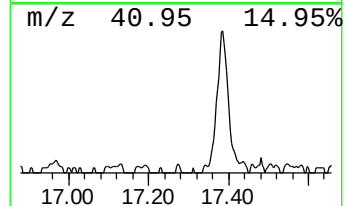
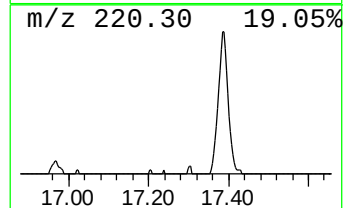
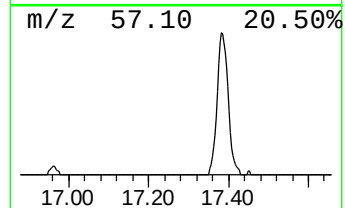
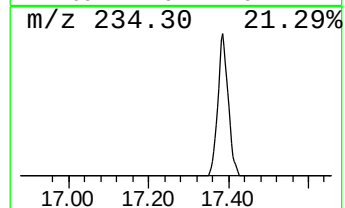
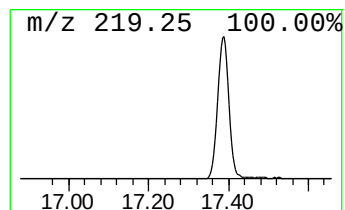
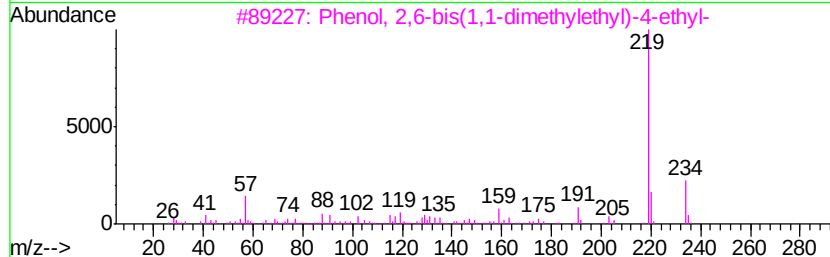
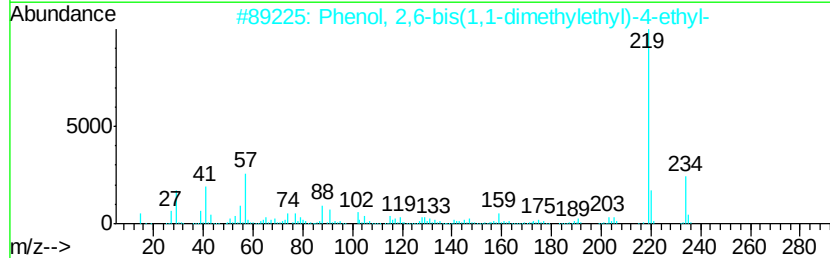
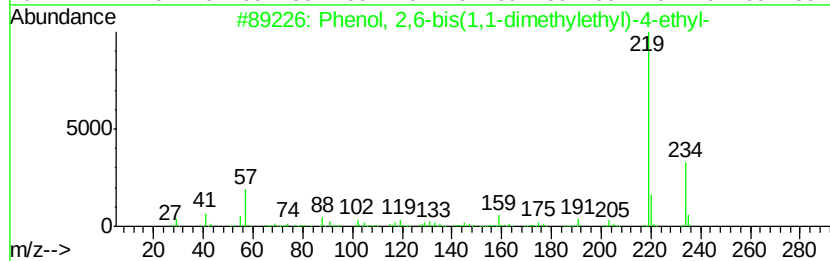
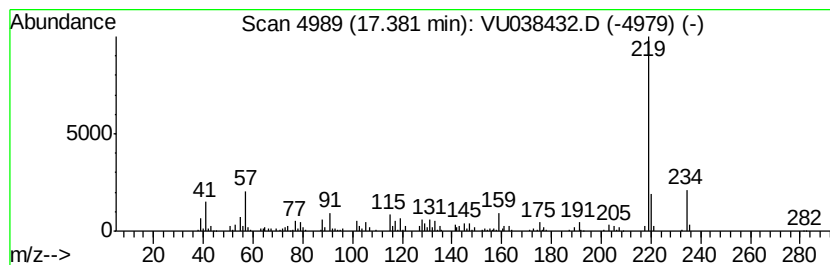
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Peak Number 5 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.38	0.91 ug/L	162564	1,4-Dichlorobenzene-d4	11.83

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-bis(1,1-dimethylethyl)-4-hydroxybenzoic acid	234	C16H26O	004130-42-1	95	
2	Phenol, 2,6-bis(1,1-dimethylethyl)-4-hydroxybenzoic acid	234	C16H26O	004130-42-1	93	
3	Phenol, 2,6-bis(1,1-dimethylethyl)-4-hydroxybenzoic acid	234	C16H26O	004130-42-1	90	
4	3,5-di-tert-Butyl-4-hydroxybenzoic acid	234	C15H22O2	001620-98-0	87	
5	4-tert-Butyl-2,6-diisopropylphenol	234	C16H26O	057354-65-1	83	



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethane, 1,1-diflu...	1.37	0.8	ug/L	116442	1	6.28	715443	5.0
Ethyl Acetate	4.84	3.4	ug/L	486936	1	6.28	715443	5.0
n-Propyl acetate	7.07	2.6	ug/L	373046	1	6.28	715443	5.0
Phenol, 2,6-bis(1...	17.38	0.9	ug/L	162564	3	11.83	894346	5.0