

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU053120\
 Data File : VU038447.D
 Acq On : 31 May 2020 05:05
 Operator : JC/MD
 Sample : L2788-09
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFXB3

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	17	rBV	53650	52481	3.26%	0.422%
2	1.613	75	85	94	rBV	150417	165231	10.26%	1.329%
3	1.932	176	184	197	rVB	116413	150598	9.35%	1.212%
4	2.395	315	328	339	rBV	80279	132761	8.24%	1.068%
5	2.594	377	390	404	rBV	248253	416117	25.84%	3.348%
6	2.684	407	418	447	rVB2	9269	35211	2.19%	0.283%
7	3.391	627	638	653	rVB6	14293	31730	1.97%	0.255%
8	3.735	734	745	765	rBV4	7480	16374	1.02%	0.132%
9	4.571	990	1005	1019	rBV5	11942	28063	1.74%	0.226%
10	4.697	1019	1044	1075	rBV3	235678	895608	55.62%	7.205%
11	4.848	1077	1091	1122	rVB	165457	421376	26.17%	3.390%
12	5.102	1150	1170	1203	rBV2	251042	590391	36.66%	4.750%
13	5.420	1257	1269	1285	rBV6	8883	19693	1.22%	0.158%
14	5.761	1353	1375	1405	rBV2	442139	1170372	72.68%	9.415%
15	6.282	1520	1537	1553	rBV	385747	743933	46.20%	5.985%
16	6.571	1613	1627	1650	rBV	209838	399976	24.84%	3.218%
17	6.719	1658	1673	1694	rBV	270910	532839	33.09%	4.287%
18	7.070	1767	1782	1800	rBV	144082	263272	16.35%	2.118%
19	7.591	1930	1944	1960	rBV	138151	243706	15.13%	1.961%
20	7.922	2032	2047	2069	rBV	515259	922134	57.27%	7.418%
21	8.201	2121	2134	2153	rBV	88583	150356	9.34%	1.210%
22	8.574	2238	2250	2263	rBV2	73696	128986	8.01%	1.038%
23	8.658	2263	2276	2315	rVB	872411	1610277	100.00%	12.954%
24	8.960	2357	2370	2391	rBV3	7638	19400	1.20%	0.156%
25	9.436	2505	2518	2550	rBV	550549	947204	58.82%	7.620%
26	10.771	2921	2933	2950	rVB	232396	368828	22.90%	2.967%
27	11.825	3248	3261	3280	rVB	584866	927600	57.60%	7.462%
28	12.079	3331	3340	3351	rBV4	8343	16436	1.02%	0.132%
29	12.205	3366	3379	3394	rBV	541757	881429	54.74%	7.091%
30	17.388	4979	4991	5009	rBV2	77684	147947	9.19%	1.190%

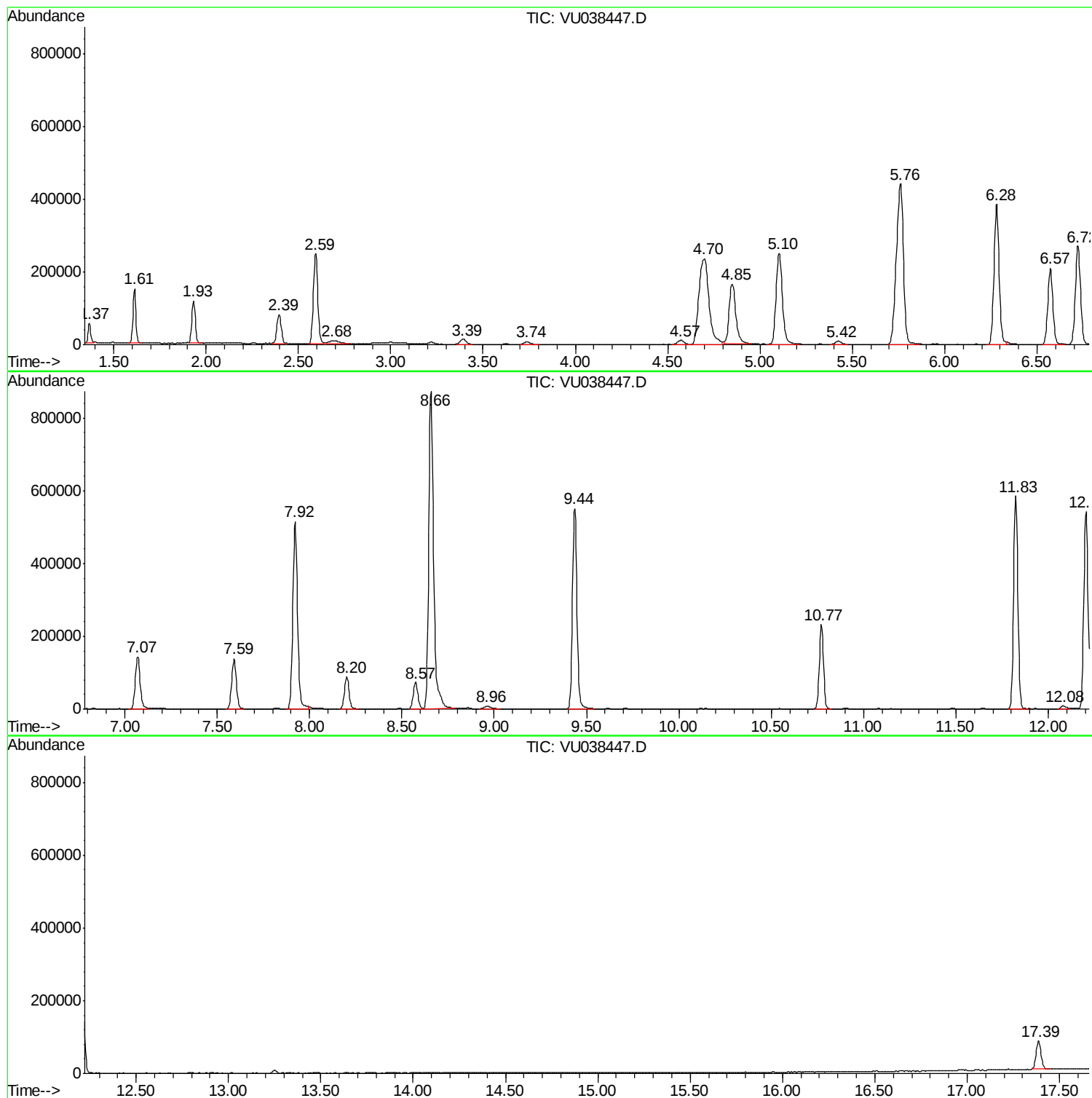
Sum of corrected areas: 12430329

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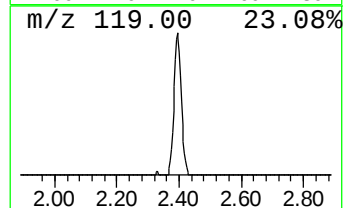
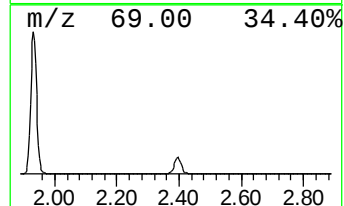
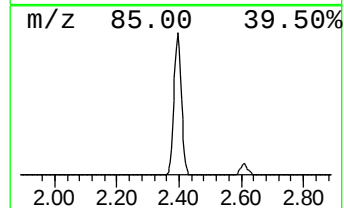
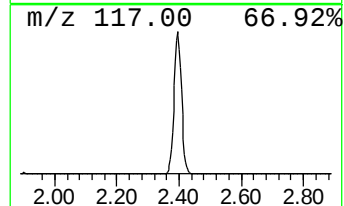
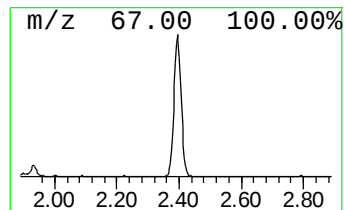
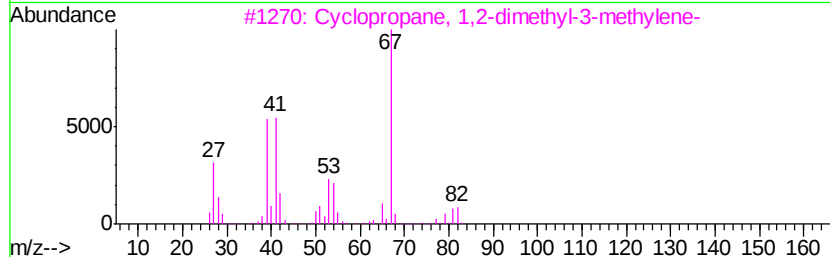
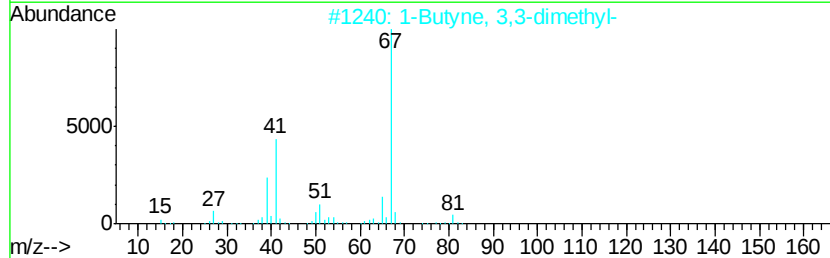
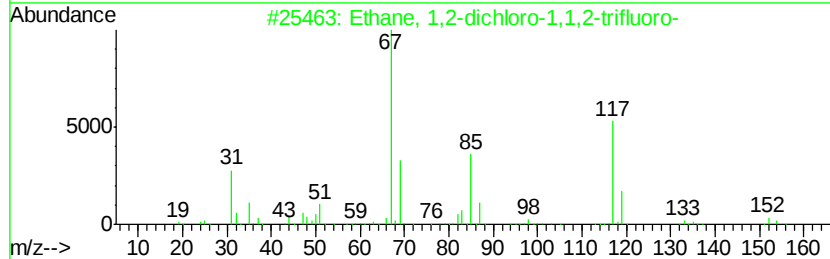
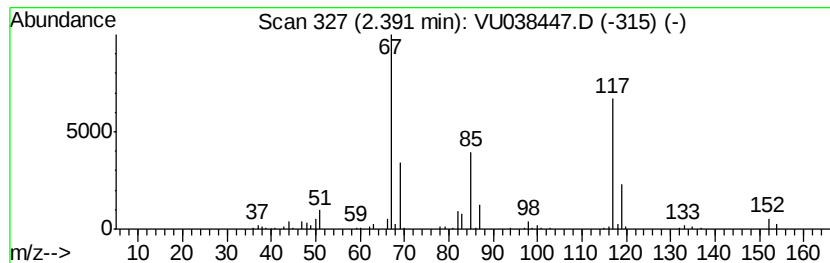
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Ethane, 1,2-dichloro-1,1,2-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.39	0.89 ug/L	132761	1,4-Difluorobenzene	6.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1,2-dichloro-1,1,2-trifl...	152	C2HCl2F3	000354-23-4	90
2			1-Butyne, 3,3-dimethyl-	82	C6H10	000917-92-0	12
3			Cyclopropane, 1,2-dimethyl-3-met...	82	C6H10	062338-02-7	9
4			1,4-Pentadiene, 3-methyl-	82	C6H10	001115-08-8	9
5			Methyl 2-butynoate	98	C5H6O2	023326-27-4	9



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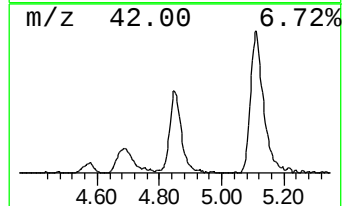
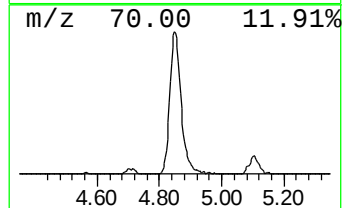
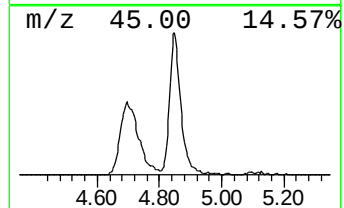
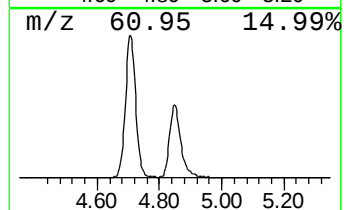
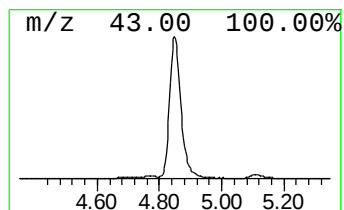
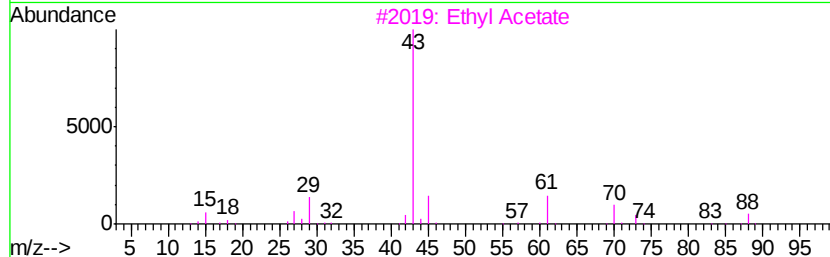
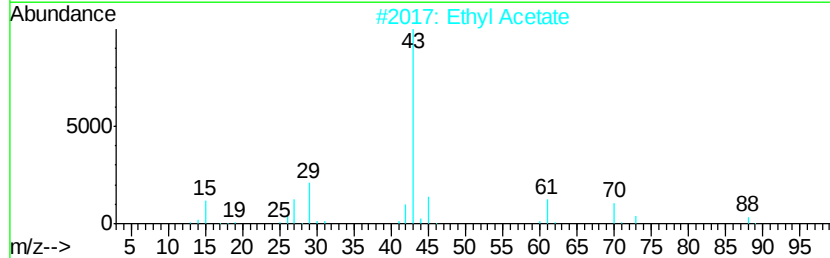
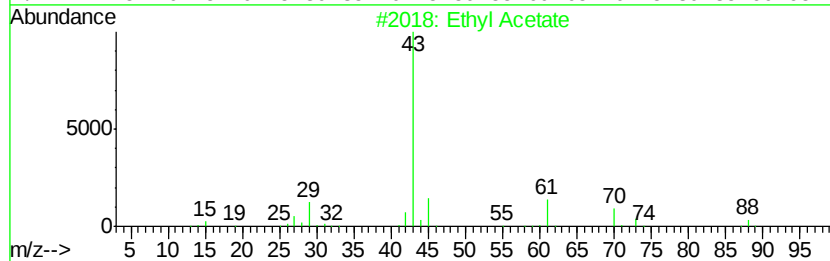
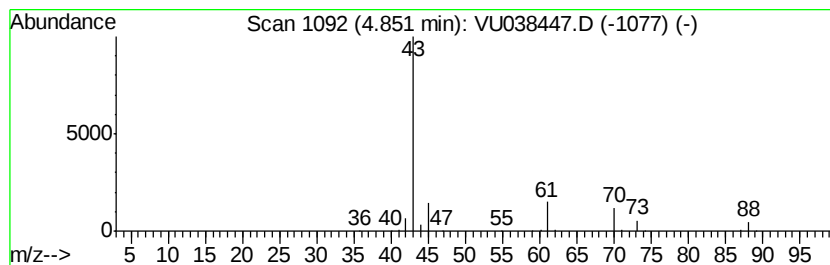
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Quant Title : TRACE VOA SOM01.0

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.
4.85	2.83 ug/L	421376	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	78
5		CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	40



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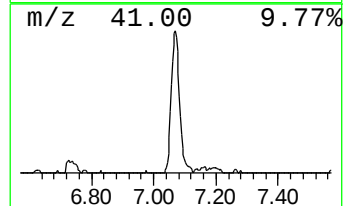
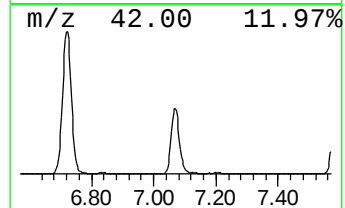
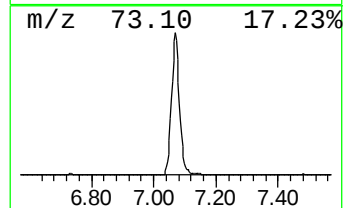
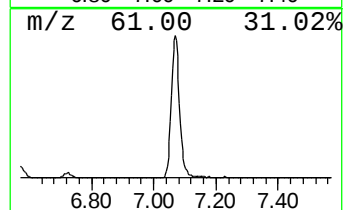
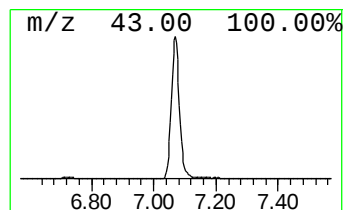
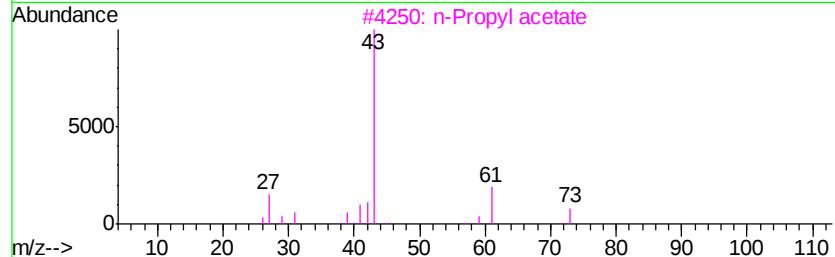
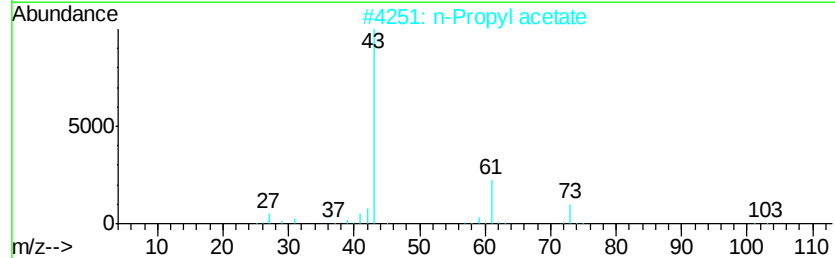
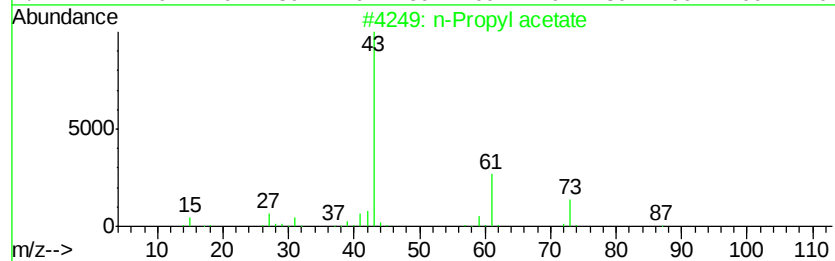
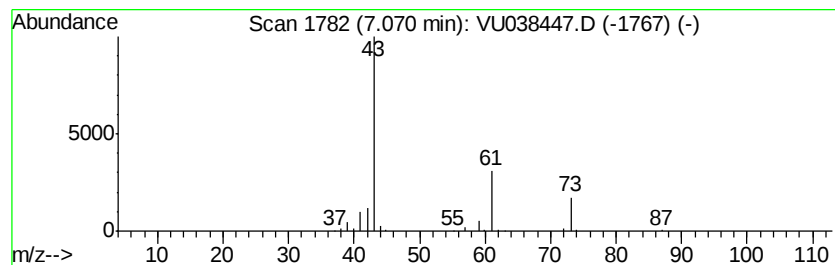
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Quant Title : TRACE VOA SOM01.0

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	1.77 ug/L	263272	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	83
3		n-Propyl acetate	102	C5H10O2	000109-60-4	78
4		Isopropyl acetate	102	C5H10O2	000108-21-4	9
5		1-Butanamine	73	C4H11N	000109-73-9	7



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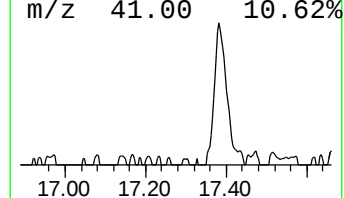
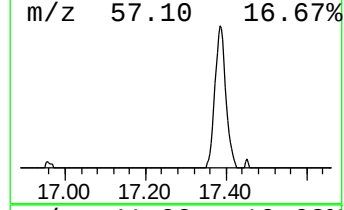
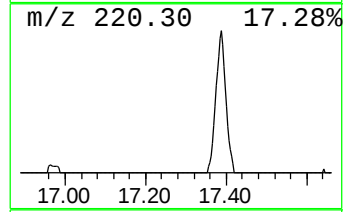
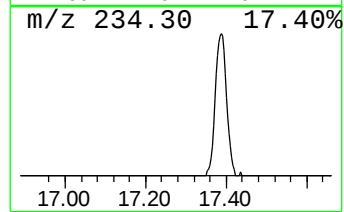
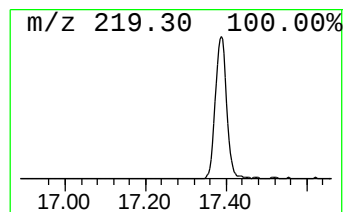
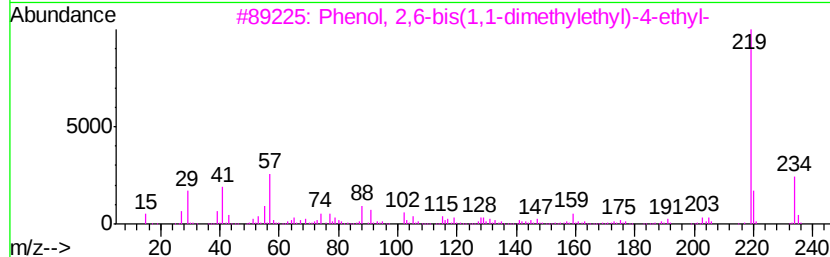
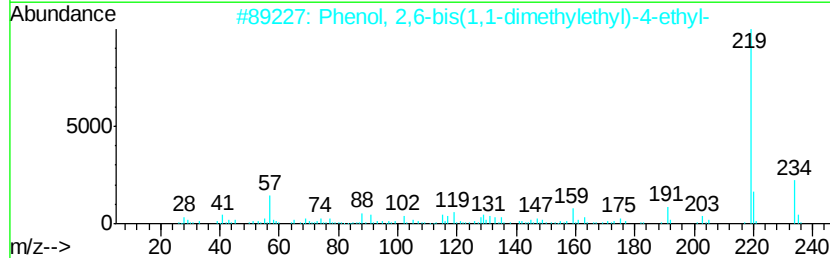
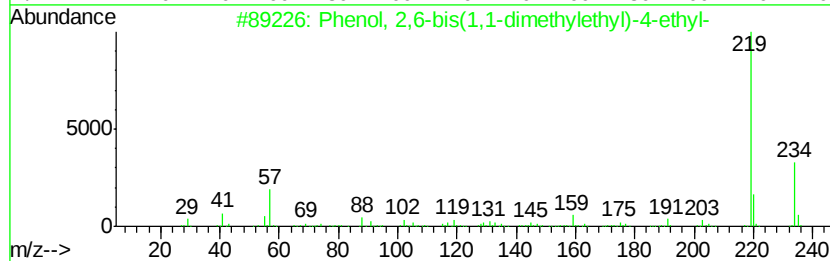
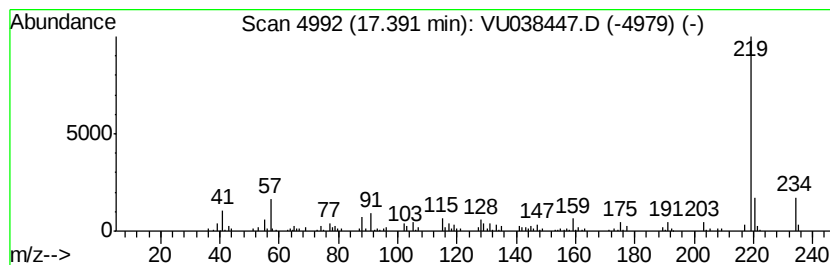
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.39	0.80 ug/L	147947	1,4-Dichlorobenzene-d4	11.83

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	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	4-tert-Butyl-2,6-diisopropylphenol	234	C16H26O	057354-65-1	87	
5	3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	87	



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethane, 1,2-dichl...	2.39	0.9	ug/L	132761	1	6.28	743933	5.0
Ethyl Acetate	4.85	2.8	ug/L	421376	1	6.28	743933	5.0
n-Propyl acetate	7.07	1.8	ug/L	263272	1	6.28	743933	5.0
Phenol, 2,6-bis(1...	17.39	0.8	ug/L	147947	3	11.83	927600	5.0