

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU053120\
 Data File : VU038433.D
 Acq On : 30 May 2020 22:57
 Operator : JC/MD
 Sample : L2787-12
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFX94

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	18	rBV	85109	83288	5.18%	0.648%
2	1.613	75	85	97	rBV	148688	172854	10.76%	1.345%
3	1.932	175	184	195	rBV	118754	147516	9.18%	1.148%
4	2.594	376	390	404	rBV	250590	423121	26.34%	3.293%
5	2.671	404	414	428	rVB	12233	29559	1.84%	0.230%
6	2.855	449	471	472	rBV3	8320	18656	1.16%	0.145%
7	3.218	570	584	602	rBV2	7310	16198	1.01%	0.126%
8	3.398	627	640	656	rVB5	11478	25647	1.60%	0.200%
9	3.739	730	746	763	rBV3	10990	24061	1.50%	0.187%
10	3.912	781	800	816	rBV2	53214	125623	7.82%	0.978%
11	4.572	989	1005	1021	rBV4	18945	45899	2.86%	0.357%
12	4.674	1021	1037	1075	rVV2	229771	768992	47.86%	5.985%
13	4.848	1076	1091	1116	rVB	178587	403037	25.09%	3.137%
14	5.102	1151	1170	1194	rBV2	264350	651521	40.55%	5.071%
15	5.420	1256	1269	1283	rBV4	10970	23707	1.48%	0.185%
16	5.761	1353	1375	1398	rBV2	444323	1161741	72.31%	9.042%
17	6.282	1519	1537	1567	rBV	374139	725239	45.14%	5.644%
18	6.571	1611	1627	1651	rBV	542835	1017542	63.33%	7.919%
19	6.723	1658	1674	1692	rBV	269314	522940	32.55%	4.070%
20	7.067	1767	1781	1801	rBV	156859	281677	17.53%	2.192%
21	7.591	1931	1944	1966	rBV2	141905	251480	15.65%	1.957%
22	7.922	2033	2047	2064	rBV	523133	916164	57.02%	7.130%
23	8.202	2120	2134	2152	rBV	90069	152399	9.49%	1.186%
24	8.655	2262	2275	2316	rBV	878636	1606627	100.00%	12.504%
25	9.436	2504	2518	2541	rBV	538043	911562	56.74%	7.095%
26	10.771	2920	2933	2950	rVB	230172	362377	22.56%	2.820%
27	11.825	3245	3261	3275	rBV	567350	903801	56.25%	7.034%
28	12.079	3331	3340	3356	rBV5	9527	21538	1.34%	0.168%
29	12.205	3366	3379	3393	rBV	550359	885335	55.11%	6.891%
30	13.250	3695	3704	3716	rVB3	11171	16096	1.00%	0.125%
31	17.381	4979	4989	5005	rVB3	83999	152433	9.49%	1.186%

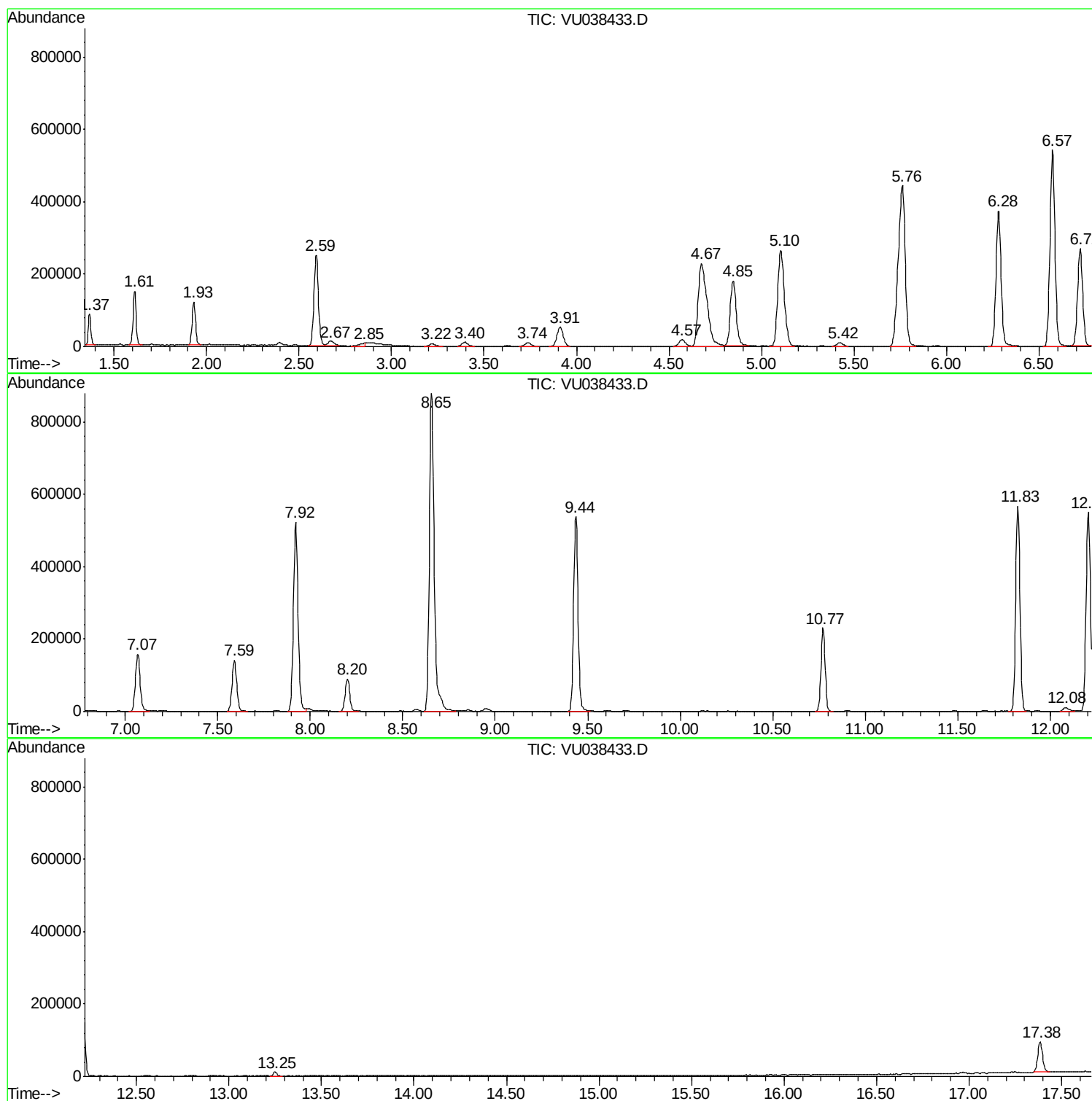
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

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



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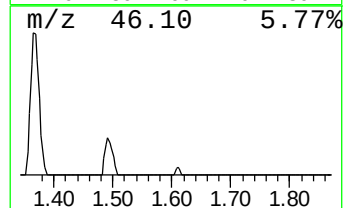
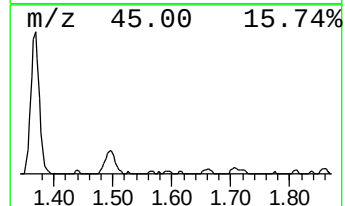
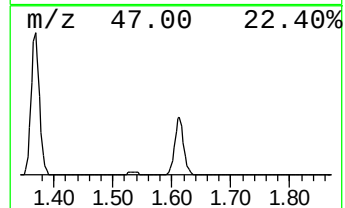
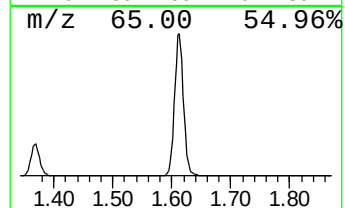
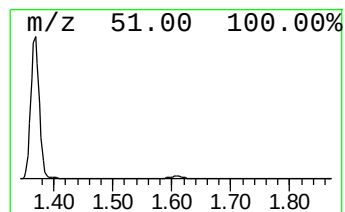
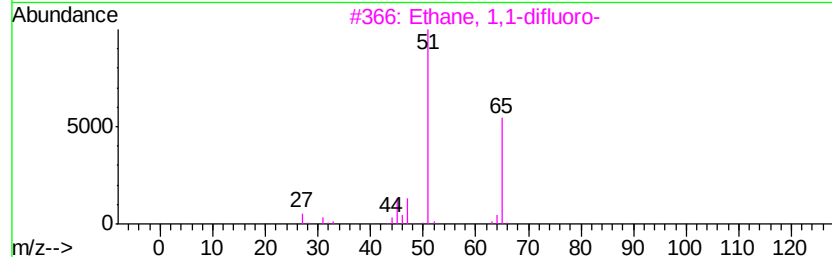
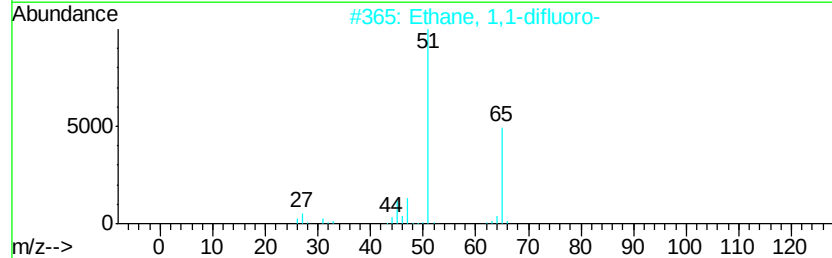
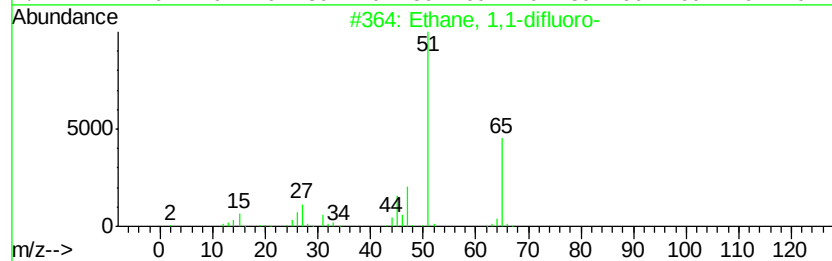
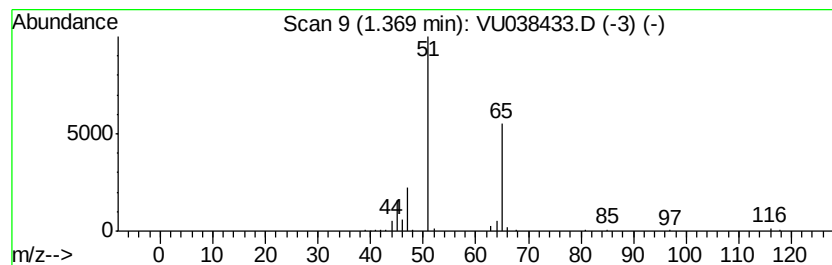
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.37	0.57 ug/L	83288	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		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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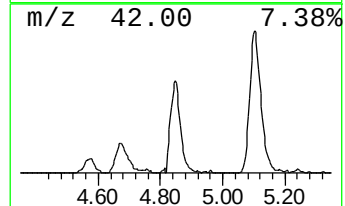
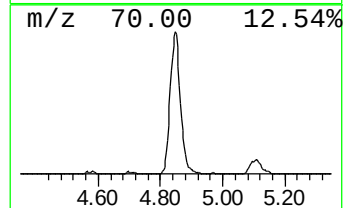
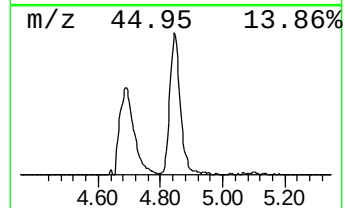
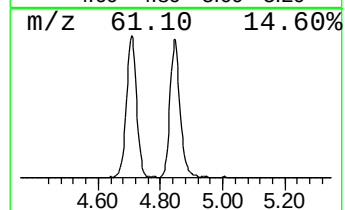
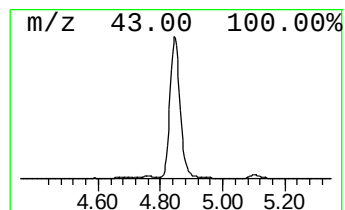
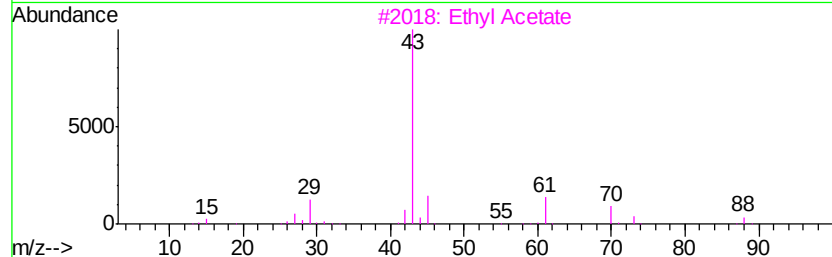
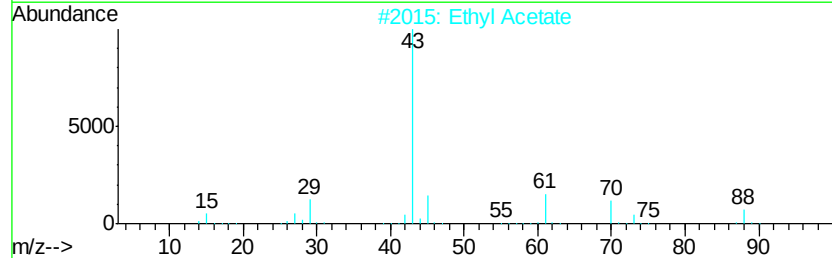
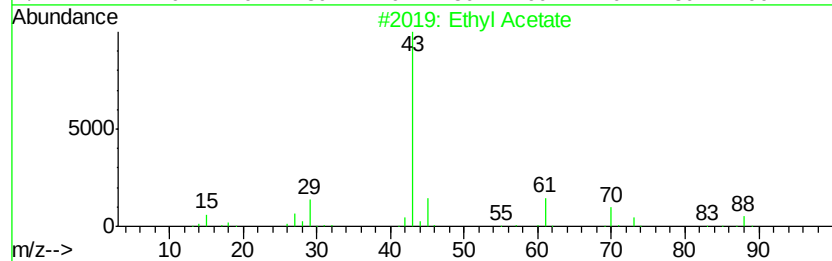
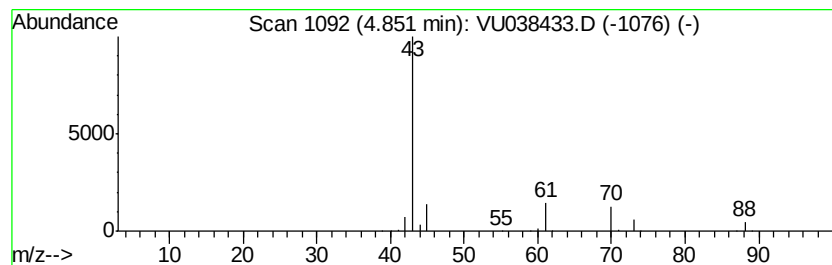
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

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.
4.85	2.78 ug/L	403037	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	86
3			Ethyl Acetate	88	C4H8O2	000141-78-6	86
4			Ethyl Acetate	88	C4H8O2	000141-78-6	86
5			(3-Methyl-oxiran-2-yl)-methanol	88	C4H8O2	1000194-22-9	9



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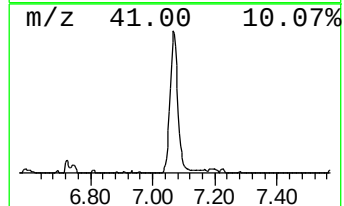
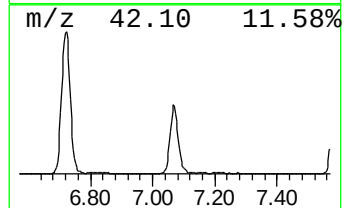
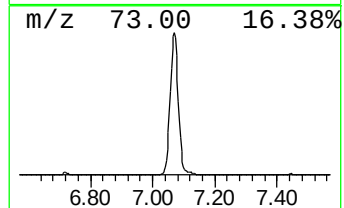
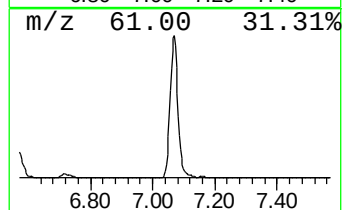
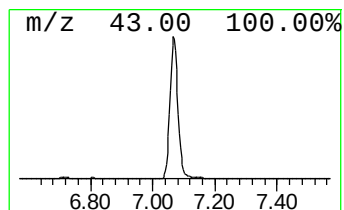
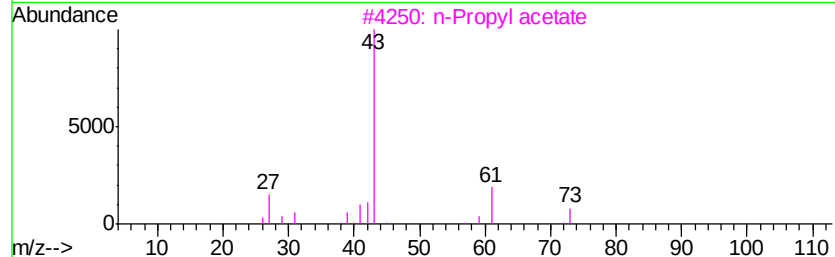
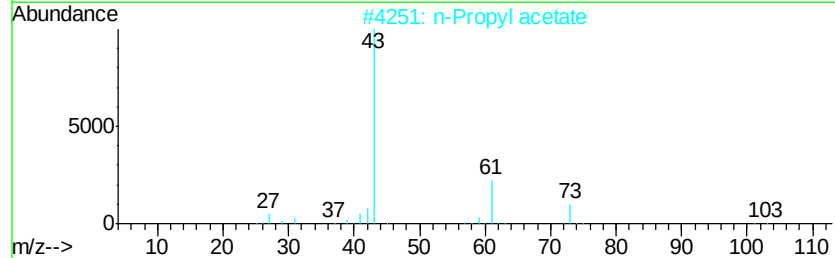
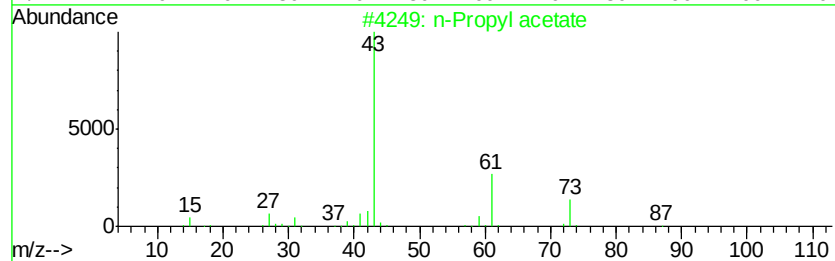
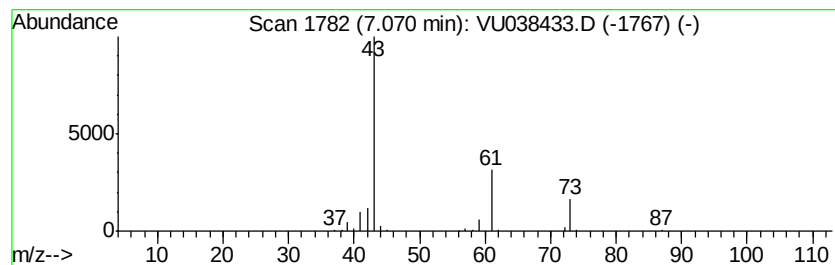
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.07	1.94 ug/L	281677	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	9
5		1-Butanamine	73	C4H11N	000109-73-9	7



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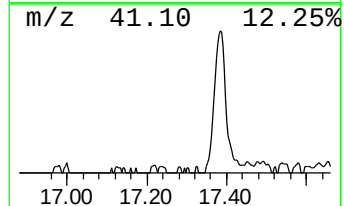
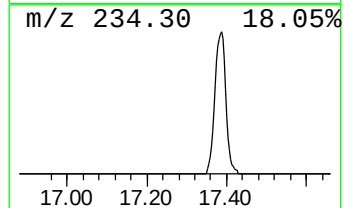
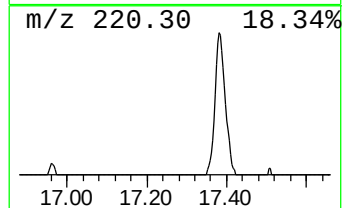
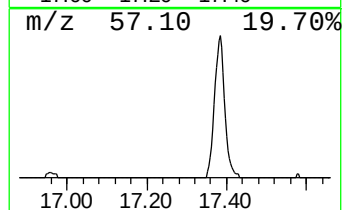
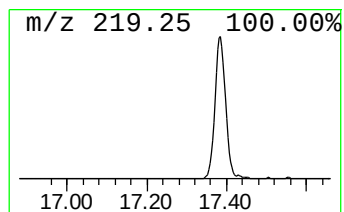
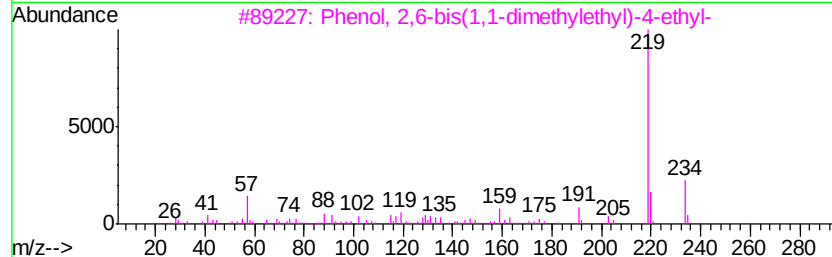
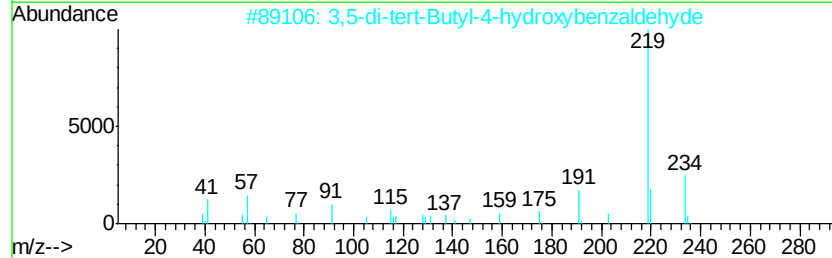
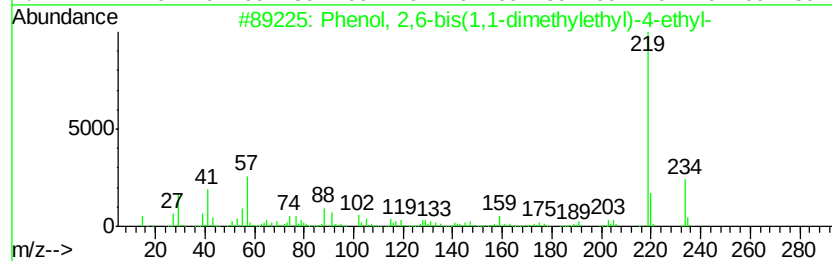
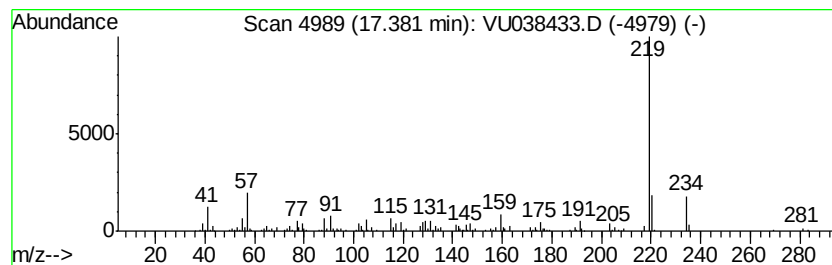
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Peak Number 5 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.38	0.84 ug/L	152433	1,4-Dichlorobenzene-d4	11.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, 2,6-bis(1,1-dimethylethyl)...	234	C16H26O	004130-42-1	91
2		3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	91
3		Phenol, 2,6-bis(1,1-dimethylethyl)...	234	C16H26O	004130-42-1	90
4		3,5-Di-tert-butylbenzoic acid	234	C15H22O2	016225-26-6	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, 1,1-diflu...	1.37	0.6	ug/L	83288	1	6.28	725239	5.0
Ethyl Acetate	4.85	2.8	ug/L	403037	1	6.28	725239	5.0
n-Propyl acetate	7.07	1.9	ug/L	281677	1	6.28	725239	5.0
Phenol, 2,6-bis(1...	17.38	0.8	ug/L	152433	3	11.83	903801	5.0