

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU050720\
 Data File : VU038053.D
 Acq On : 07 May 2020 20:51
 Operator : JC/MD
 Sample : L2527-16
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFSK3

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\SOMUTR050720WMA.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	309026	312451	20.20%	2.302%
2	1.610	74	84	96	rBV	224325	254030	16.42%	1.871%
3	1.928	175	183	198	rVB	174755	223102	14.42%	1.644%
4	2.591	376	389	401	rBV	298677	484866	31.34%	3.572%
5	2.652	401	408	420	rVB	16190	27913	1.80%	0.206%
6	2.784	438	449	467	rBV	54695	104207	6.74%	0.768%
7	3.218	570	584	600	rBV	22572	53127	3.43%	0.391%
8	3.391	626	638	656	rVB4	7313	18516	1.20%	0.136%
9	3.732	732	744	759	rVB3	9072	20813	1.35%	0.153%
10	4.568	989	1004	1017	rBV3	14706	34110	2.20%	0.251%
11	4.665	1018	1034	1068	rBV3	304315	816661	52.79%	6.016%
12	4.841	1075	1089	1111	rVB	174799	378598	24.47%	2.789%
13	5.102	1153	1170	1192	rBV3	254771	616105	39.83%	4.539%
14	5.423	1256	1270	1285	rVB5	14540	33381	2.16%	0.246%
15	5.758	1349	1374	1399	rBV2	531127	1363541	88.14%	10.045%
16	6.279	1521	1536	1562	rBV	457028	870806	56.29%	6.415%
17	6.719	1659	1673	1694	rBV	329352	640562	41.41%	4.719%
18	7.066	1768	1781	1801	rBV	160257	284641	18.40%	2.097%
19	7.590	1931	1944	1961	rBV	173391	295313	19.09%	2.176%
20	7.922	2028	2047	2078	rBV	648262	1180160	76.29%	8.694%
21	8.201	2122	2134	2153	rBV	103080	172333	11.14%	1.270%
22	8.655	2261	2275	2315	rBV	804365	1546939	100.00%	11.396%
23	9.436	2504	2518	2543	rBV	655060	1121062	72.47%	8.259%
24	10.770	2921	2933	2947	rBV	228827	367152	23.73%	2.705%
25	11.825	3248	3261	3278	rBV	682450	1077835	69.68%	7.940%
26	12.079	3331	3340	3355	rBV5	8751	17508	1.13%	0.129%
27	12.204	3366	3379	3395	rBV	609849	980662	63.39%	7.225%
28	17.378	4976	4988	5003	rBV2	145883	277662	17.95%	2.046%

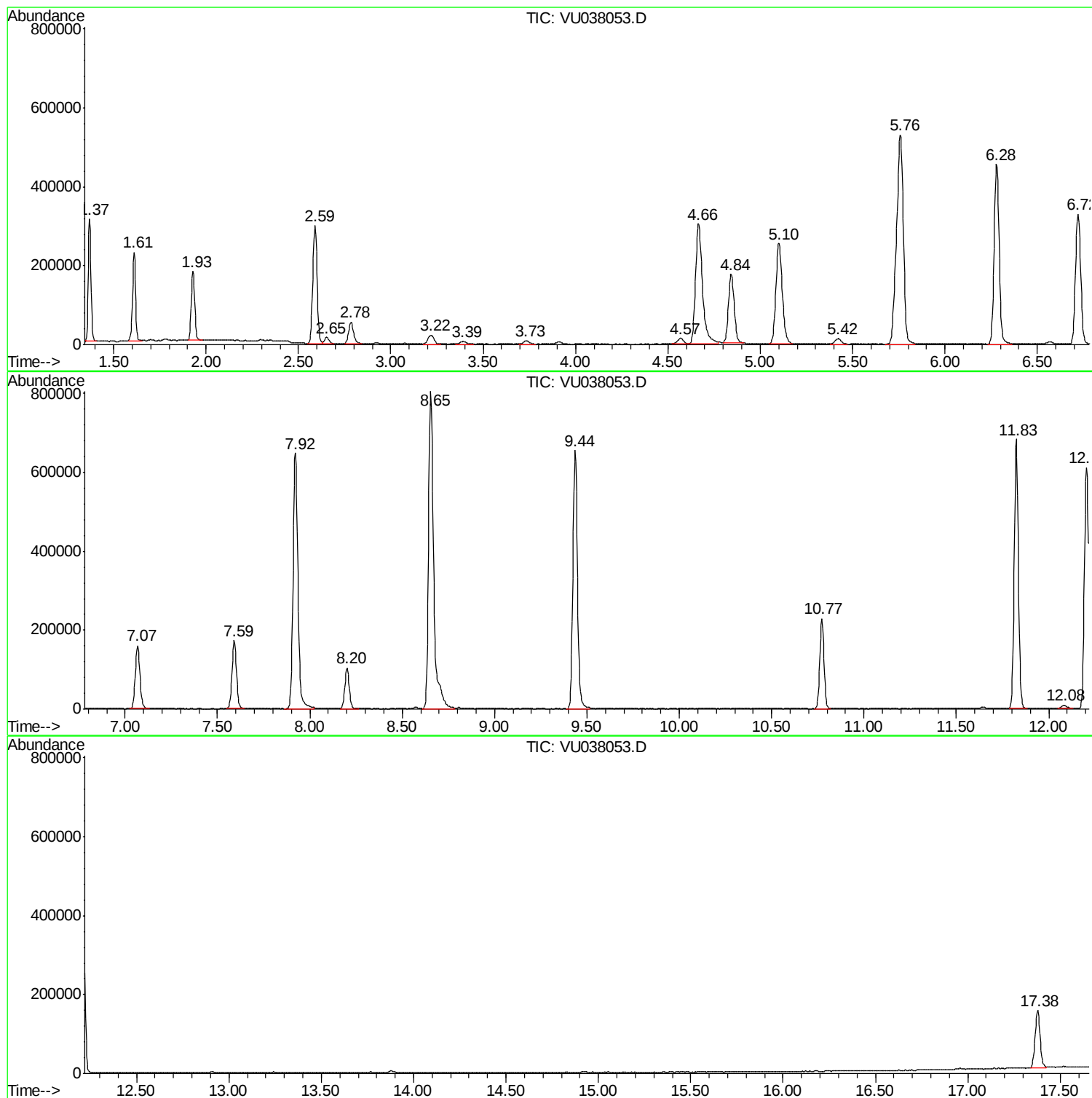
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ALS Vial : 1 Sample Multiplier: 1

Instrument :
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ClientSampleId :
BFSK3

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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



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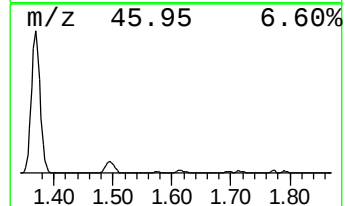
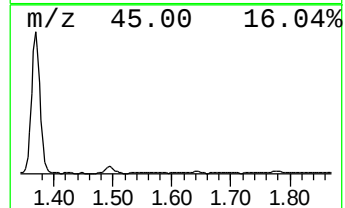
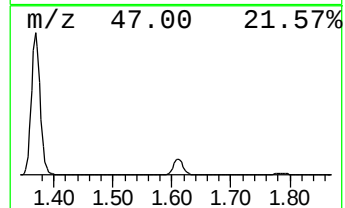
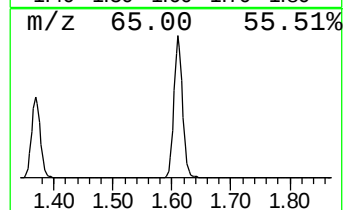
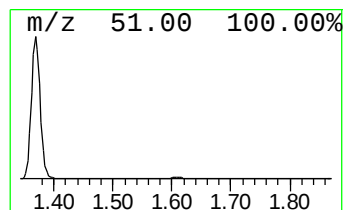
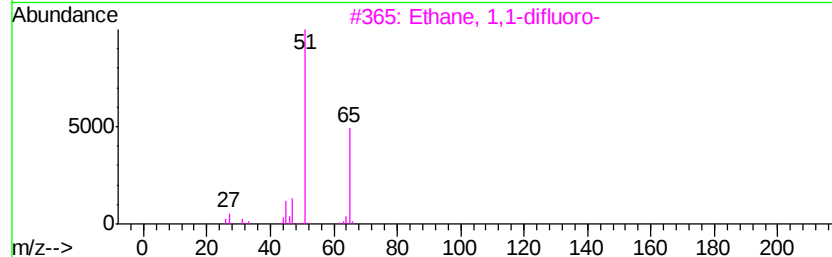
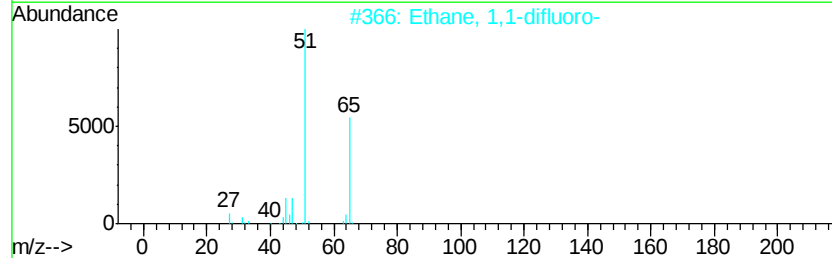
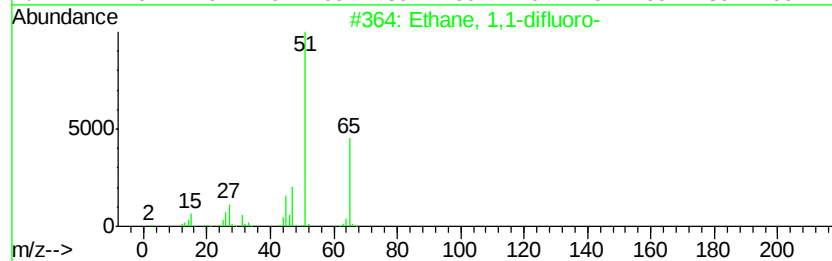
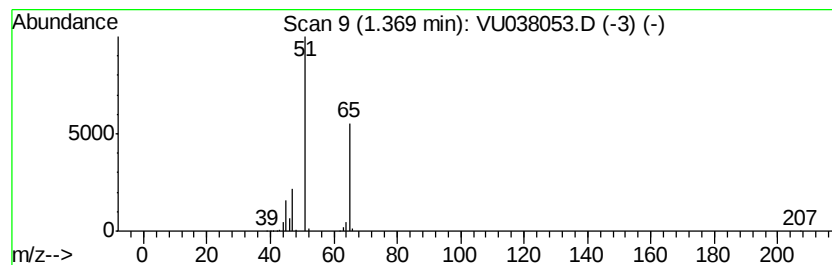
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Ethane, 1,1-difluoro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.37	1.79 ug/L	312451	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			Propiolonitrile	51	C3HN	001070-71-9	3
5			Propane, 2,2-difluoro-	80	C3H6F2	000420-45-1	2



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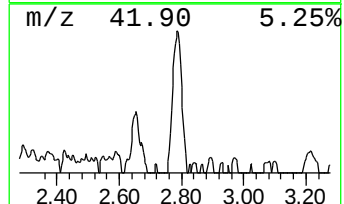
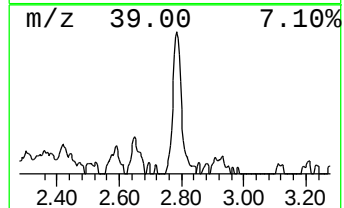
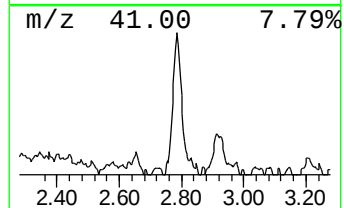
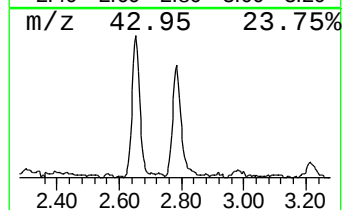
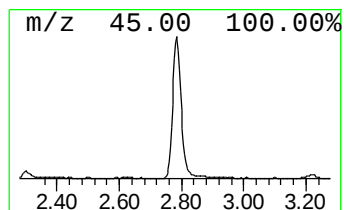
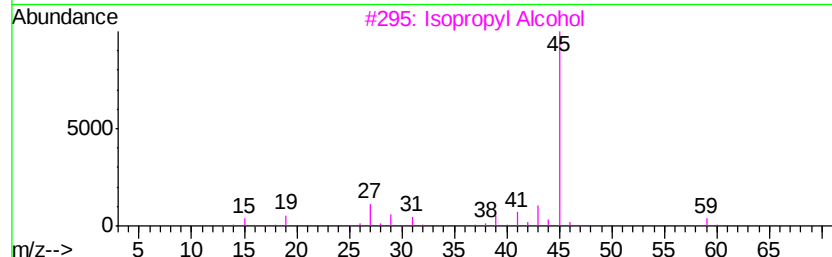
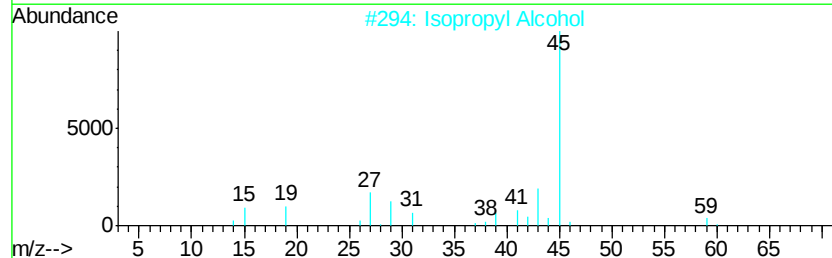
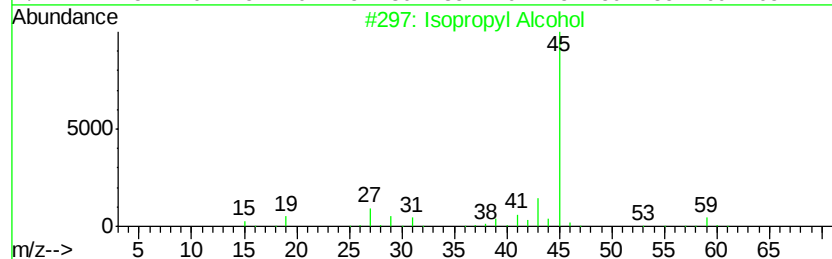
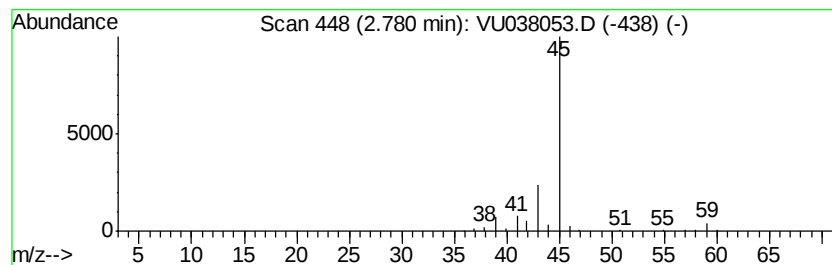
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 Isopropyl Alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.78	0.60 ug/L	104207	1,4-Difluorobenzene	6.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	86
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
5			Hydrazine, ethyl-	60	C2H8N2	000624-80-6	40



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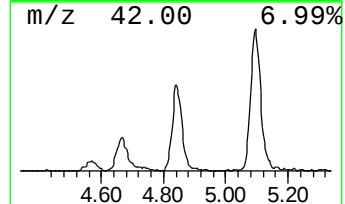
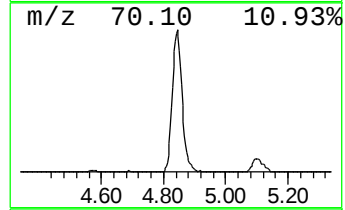
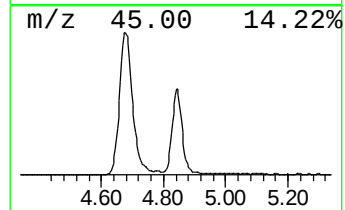
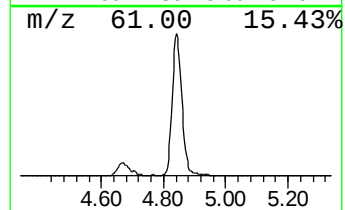
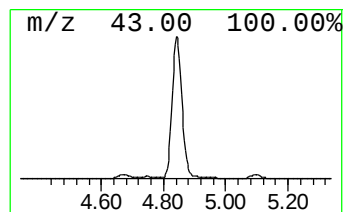
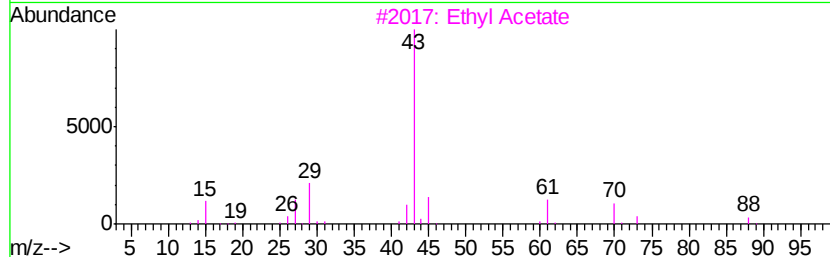
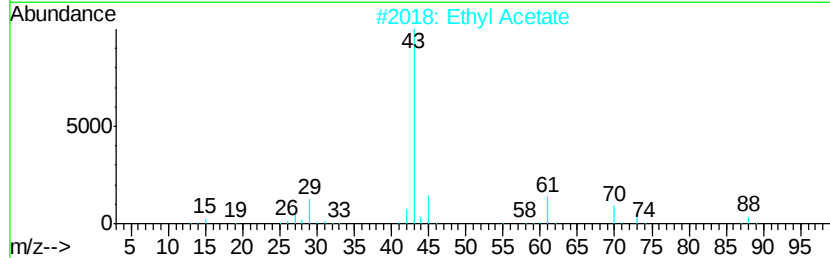
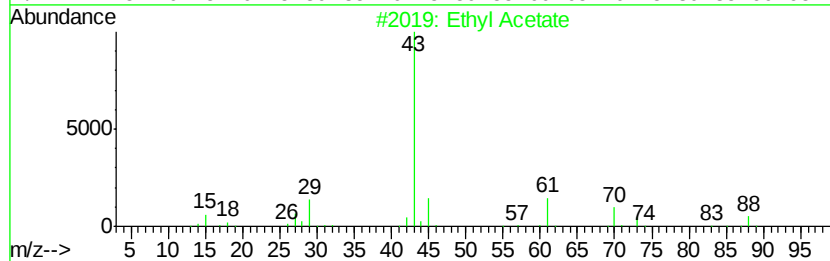
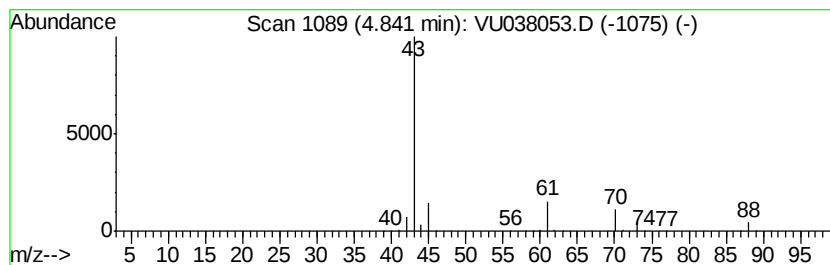
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 Ethyl Acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	2.17 ug/L	378598	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	86
3		Ethyl Acetate	88	C4H8O2	000141-78-6	86
4		Ethyl Acetate	88	C4H8O2	000141-78-6	83
5		CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	9



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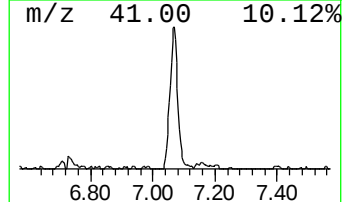
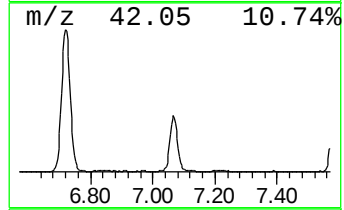
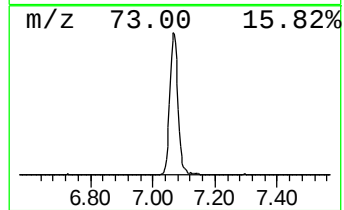
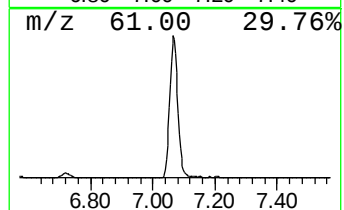
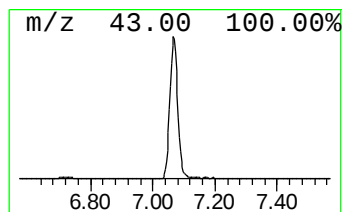
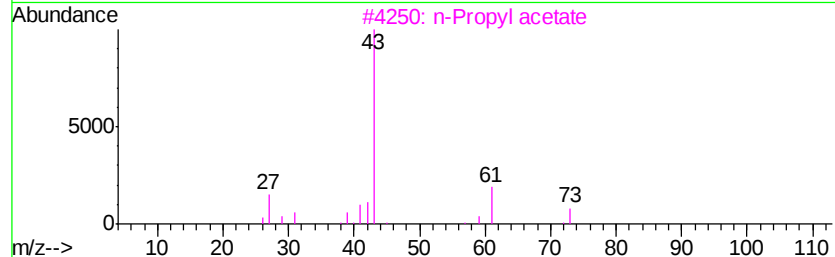
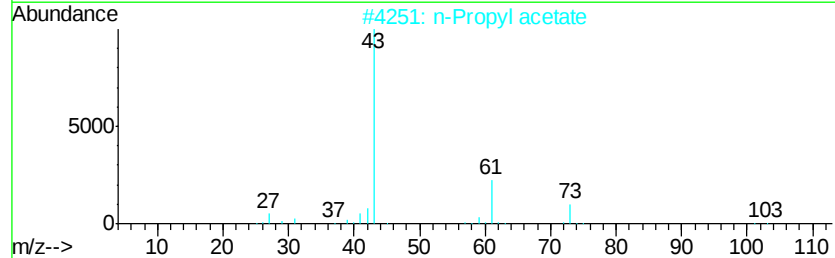
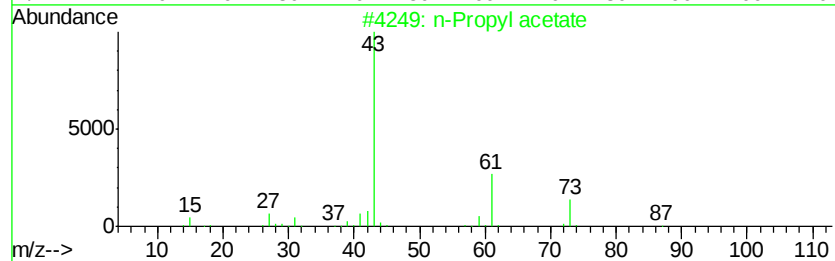
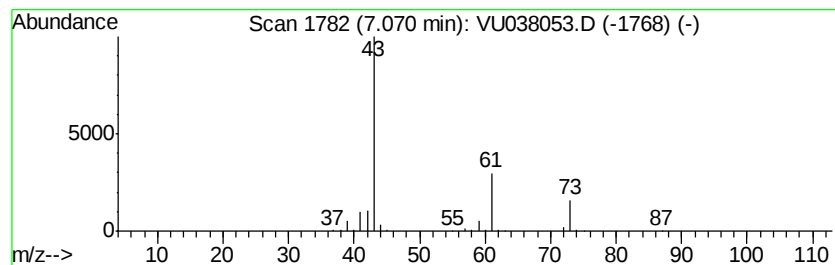
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Propyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.07	1.63 ug/L	284641	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	78		
3	n-Propyl acetate	102	C5H10O2	000109-60-4	72		
4	Isopropyl acetate	102	C5H10O2	000108-21-4	38		
5	Acetic acid, pentyl ester	130	C7H14O2	000628-63-7	9		



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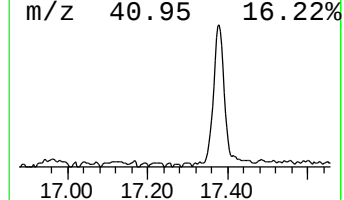
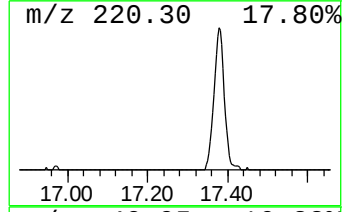
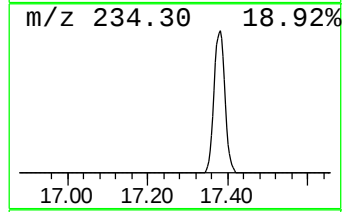
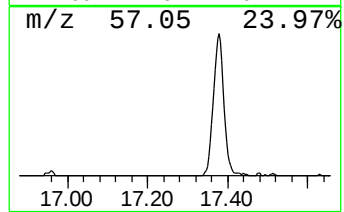
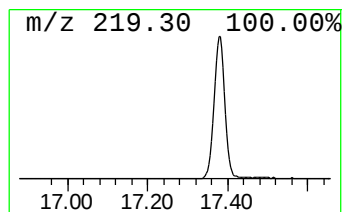
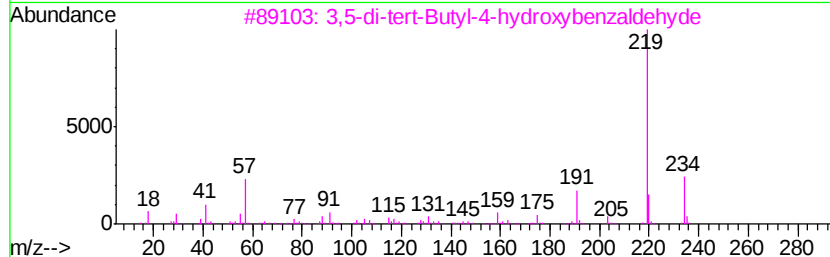
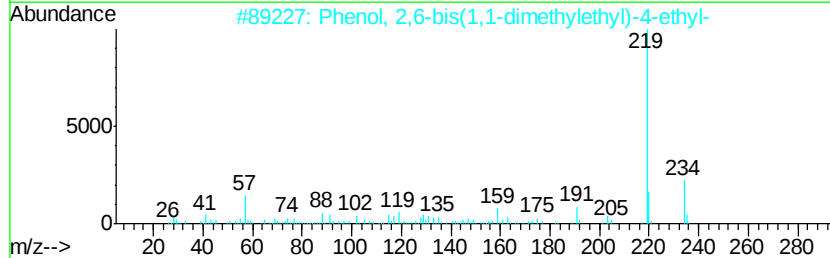
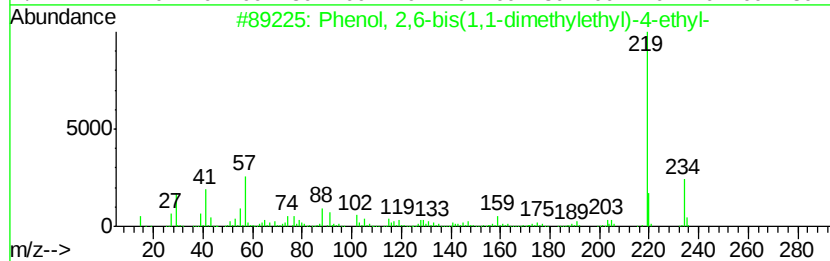
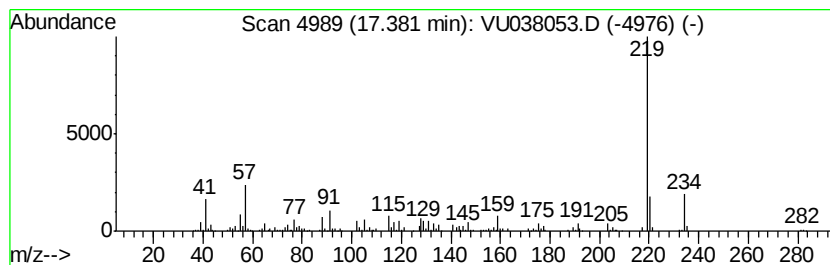
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.38	1.29 ug/L	277662	1,4-Dichlorobenzene-d4	11.82

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	94	
2	Phenol, 2,6-bis(1,1-dimethylethyl)-4-hydroxybenzoic acid	234	C16H26O	004130-42-1	91	
3	3,5-di-tert-Butyl-4-hydroxybenzoic acid	234	C15H22O2	001620-98-0	87	
4	Phenol, 2,6-bis(1,1-dimethylethyl)-4-hydroxybenzoic acid	234	C16H26O	004130-42-1	83	
5	3,5-Di-tert-butylbenzoic acid	234	C15H22O2	016225-26-6	80	



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethane, 1,1-diflu...	1.37	1.8	ug/L	312451	1	6.28	870806	5.0
Isopropyl Alcohol	2.78	0.6	ug/L	104207	1	6.28	870806	5.0
Ethyl Acetate	4.84	2.2	ug/L	378598	1	6.28	870806	5.0
n-Propyl acetate	7.07	1.6	ug/L	284641	1	6.28	870806	5.0
Phenol, 2,6-bis(1...	17.38	1.3	ug/L	277662	3	11.82	1077840	5.0