

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU050720\
 Data File : VU038054.D
 Acq On : 07 May 2020 21:13
 Operator : JC/MD
 Sample : L2527-17
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFSK4

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	137815	138002	9.06%	1.012%
2	1.610	75	84	98	rBV	222867	248469	16.32%	1.823%
3	1.928	175	183	197	rVB	175221	223577	14.68%	1.640%
4	2.591	376	389	401	rBV	292781	475873	31.25%	3.491%
5	2.652	401	408	425	rVB	27790	49049	3.22%	0.360%
6	2.784	435	449	468	rBV	65650	122293	8.03%	0.897%
7	3.218	570	584	599	rVB2	22627	52271	3.43%	0.384%
8	3.398	624	640	656	rBV4	17011	39908	2.62%	0.293%
9	3.735	727	745	765	rBV3	24697	55892	3.67%	0.410%
10	4.568	990	1004	1018	rBV3	22807	57927	3.80%	0.425%
11	4.665	1018	1034	1072	rBV3	299935	825599	54.22%	6.057%
12	4.841	1076	1089	1111	rVB	167983	362445	23.81%	2.659%
13	5.099	1153	1169	1195	rBV3	274048	652205	42.84%	4.785%
14	5.420	1257	1269	1282	rVB6	7611	16430	1.08%	0.121%
15	5.758	1352	1374	1400	rBV2	529986	1372202	90.13%	10.068%
16	6.279	1522	1536	1562	rBV	456191	875930	57.53%	6.427%
17	6.571	1613	1627	1644	rVB2	61068	119956	7.88%	0.880%
18	6.719	1657	1673	1691	rBV	327757	638029	41.91%	4.681%
19	7.066	1766	1781	1802	rBV	151962	265718	17.45%	1.950%
20	7.591	1930	1944	1960	rBV	166022	291810	19.17%	2.141%
21	7.922	2031	2047	2080	rBV	643285	1183550	77.73%	8.683%
22	8.198	2121	2133	2153	rBV2	100884	169145	11.11%	1.241%
23	8.571	2238	2249	2261	rBV	55923	95933	6.30%	0.704%
24	8.652	2261	2274	2317	rVV	778050	1522552	100.00%	11.171%
25	9.433	2504	2517	2540	rBV	647028	1120870	73.62%	8.224%
26	10.770	2921	2933	2951	rBV	228828	366451	24.07%	2.689%
27	11.822	3248	3260	3278	rBV	664785	1070983	70.34%	7.858%
28	12.079	3331	3340	3352	rBV4	8708	16655	1.09%	0.122%
29	12.204	3364	3379	3393	rBV	604173	977401	64.19%	7.171%
30	17.372	4975	4986	5004	rBV2	122231	222759	14.63%	1.634%

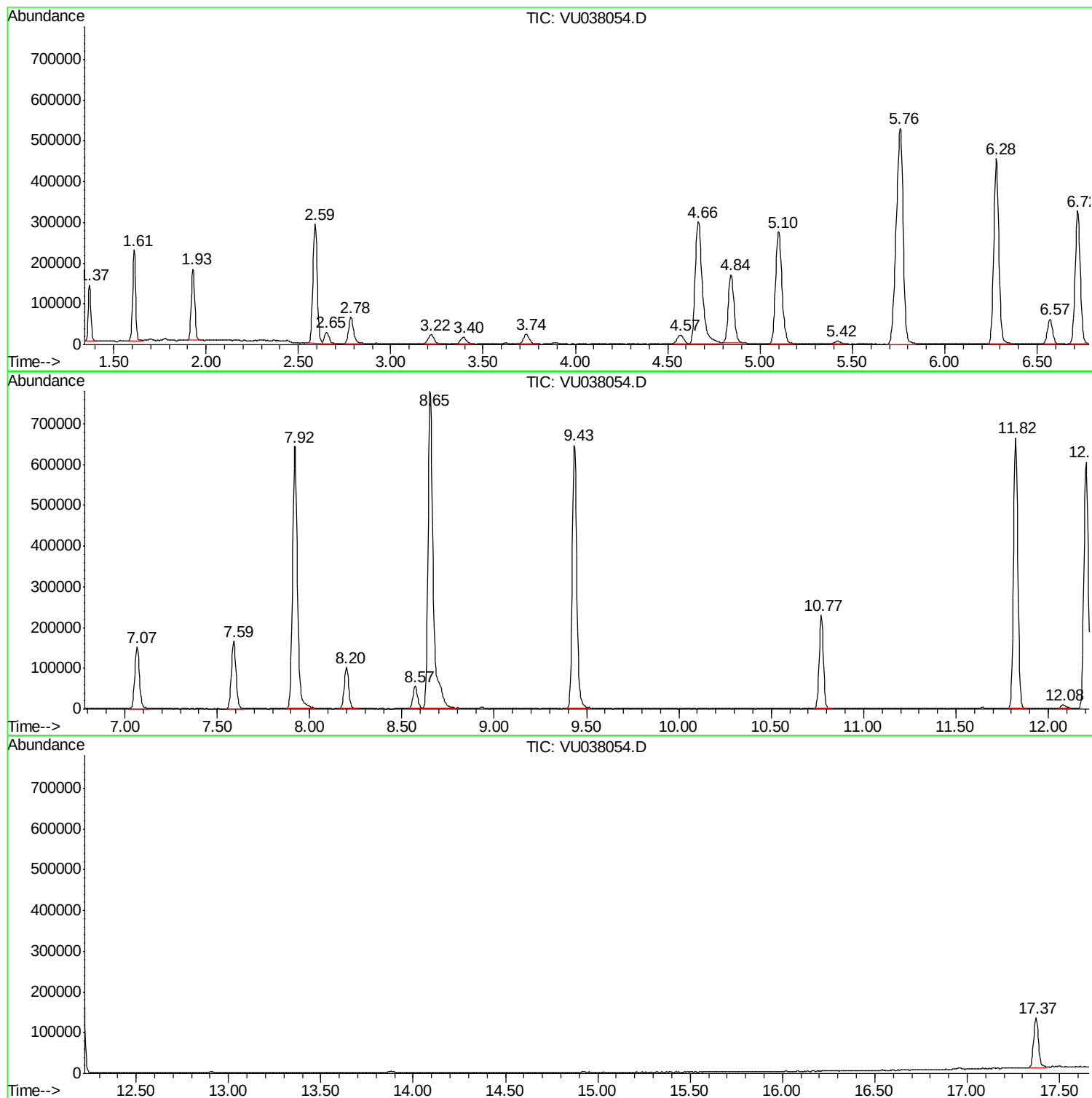
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ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFSK4

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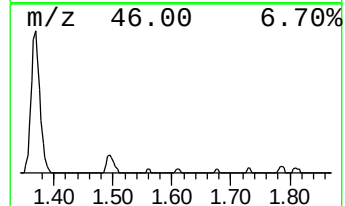
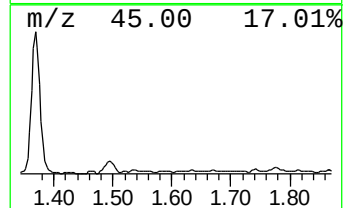
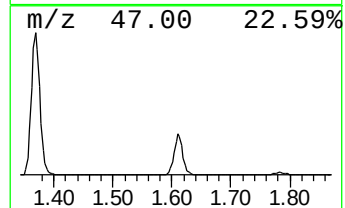
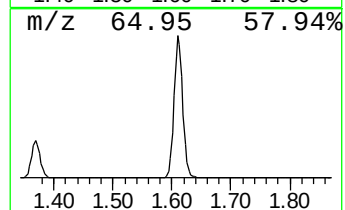
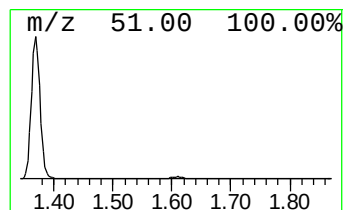
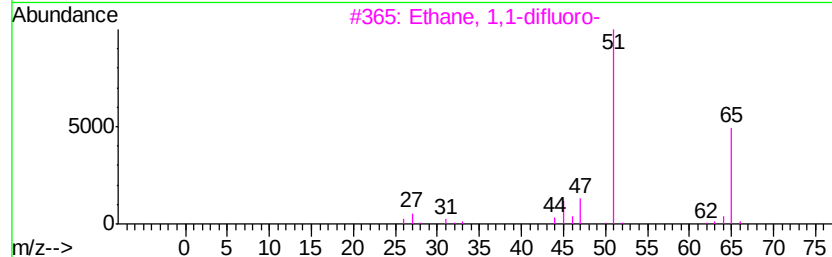
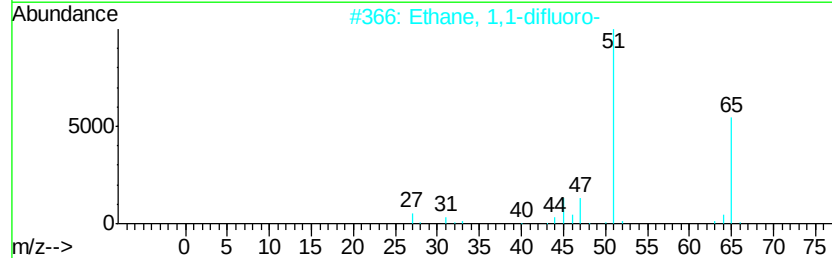
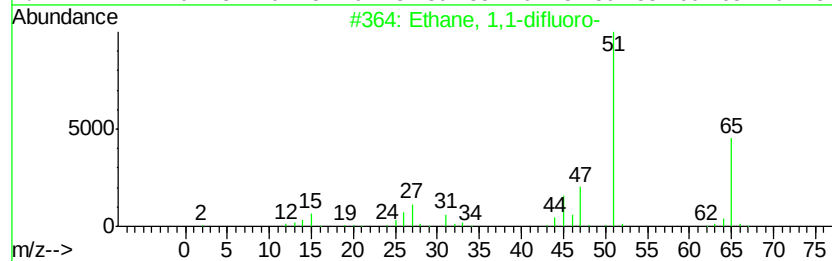
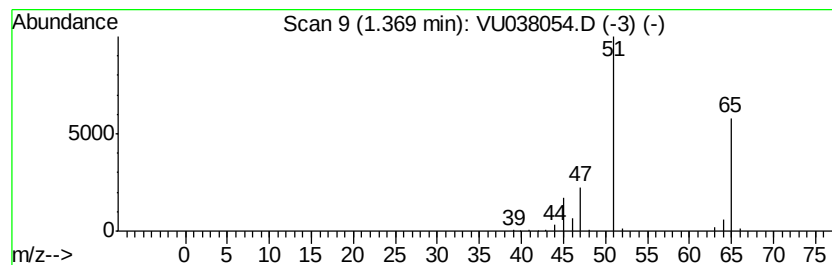
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.37	0.79 ug/L	138002	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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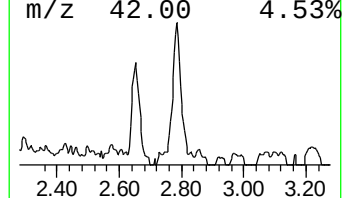
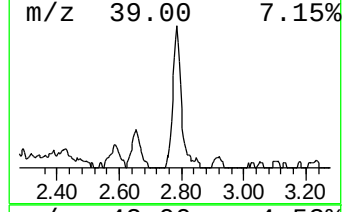
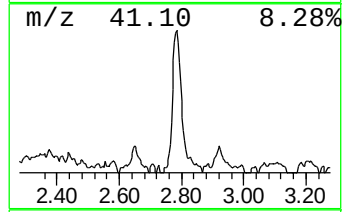
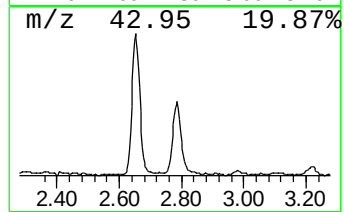
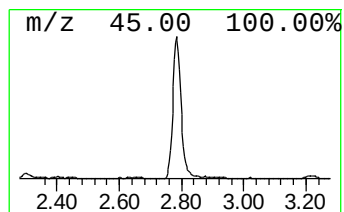
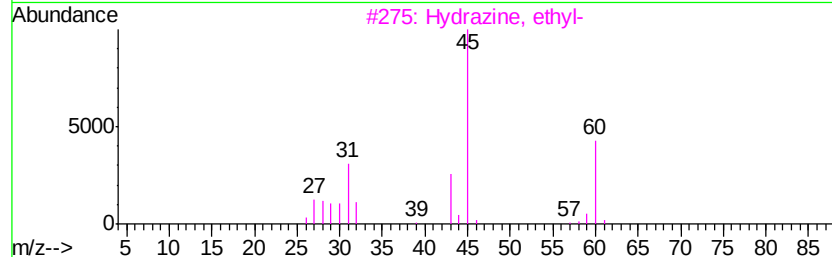
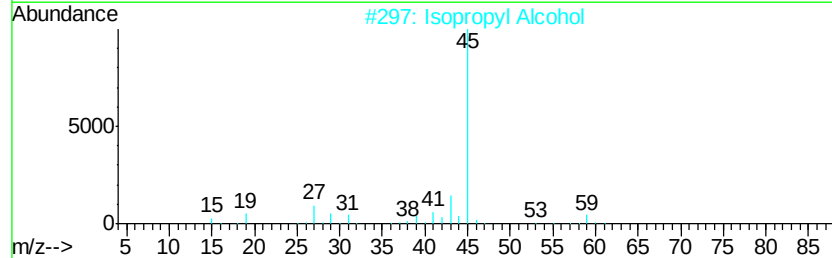
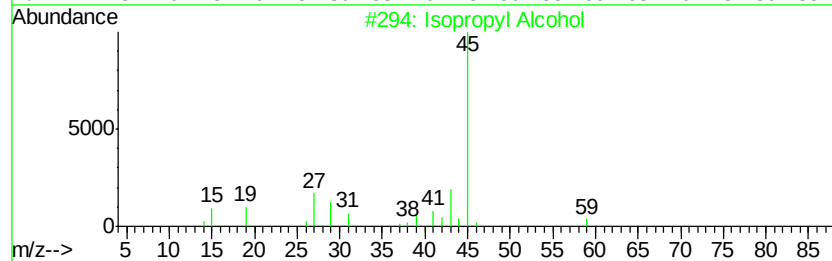
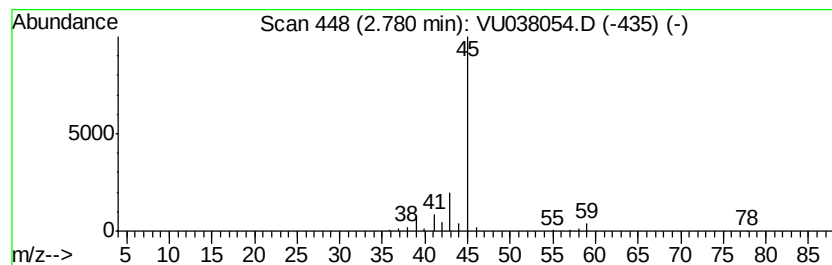
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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	0.70 ug/L	122293	1,4-Difluorobenzene	6.28

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isopropyl Alcohol	60	C3H8O	000067-63-0	64
2		Isopropyl Alcohol	60	C3H8O	000067-63-0	43
3		Hydrazine, ethyl-	60	C2H8N2	000624-80-6	40
4		(S)-(+)-2-Pentanol	88	C5H12O	026184-62-3	9
5		Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	9



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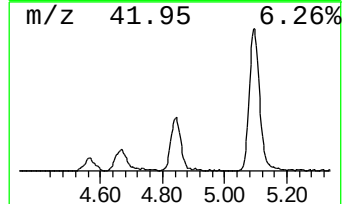
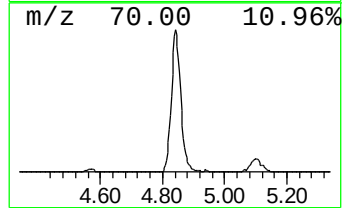
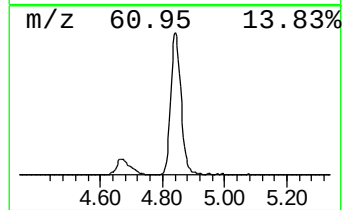
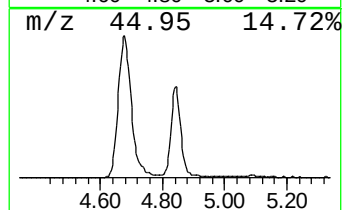
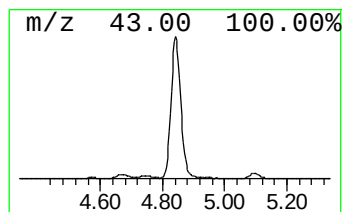
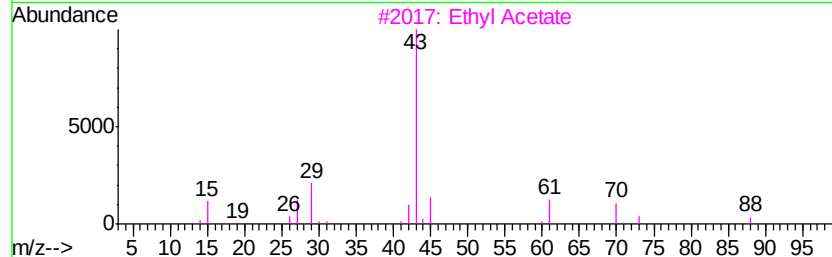
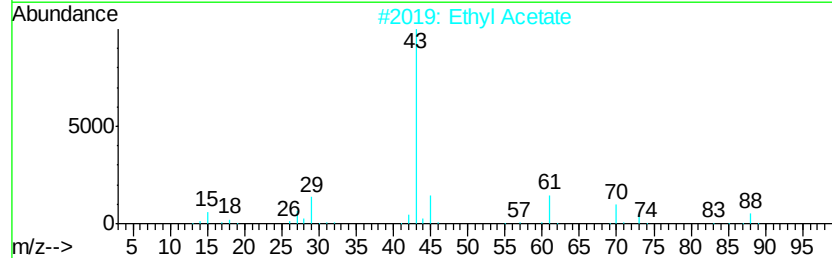
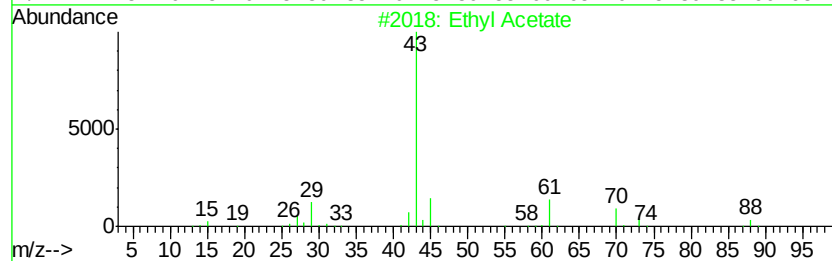
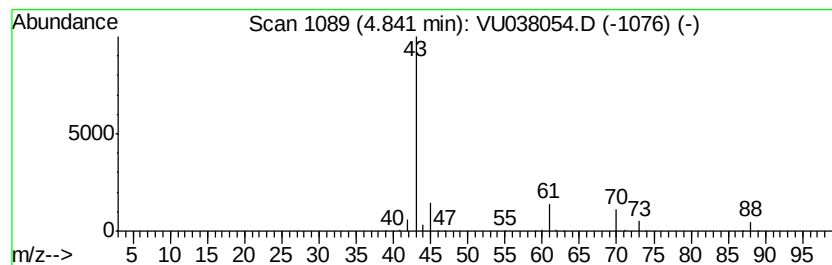
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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	2.07 ug/L	362445	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	64
4		Ethyl Acetate	88	C4H8O2	000141-78-6	59
5		CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	33



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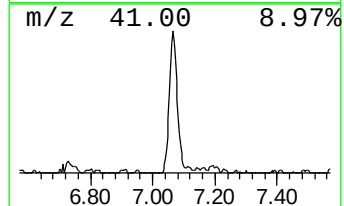
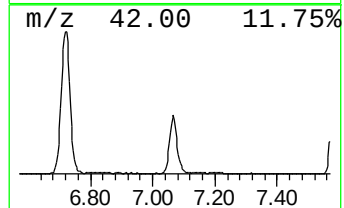
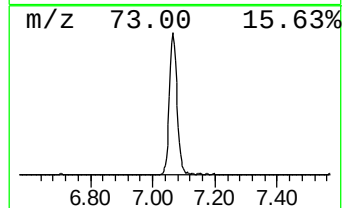
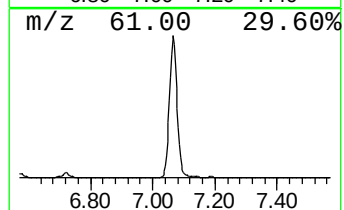
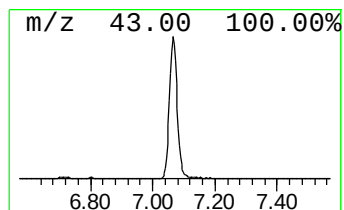
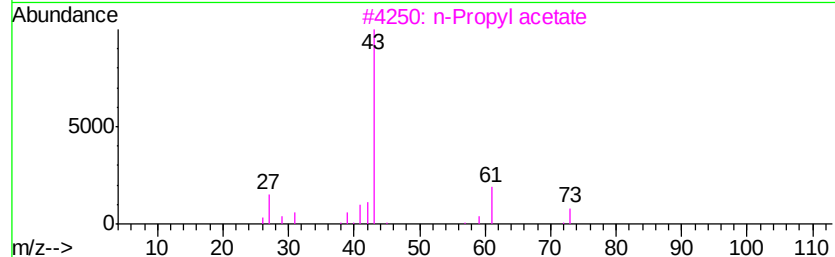
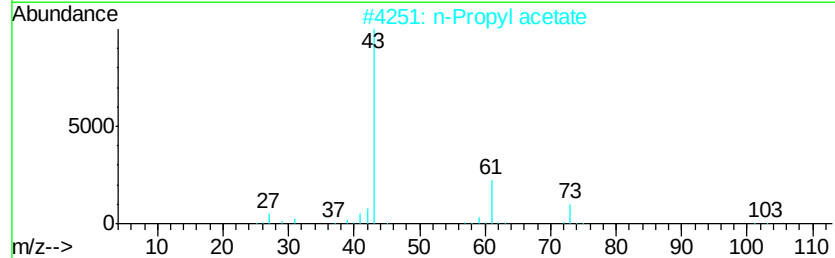
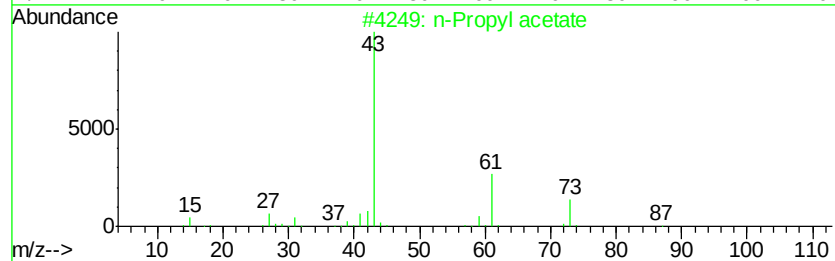
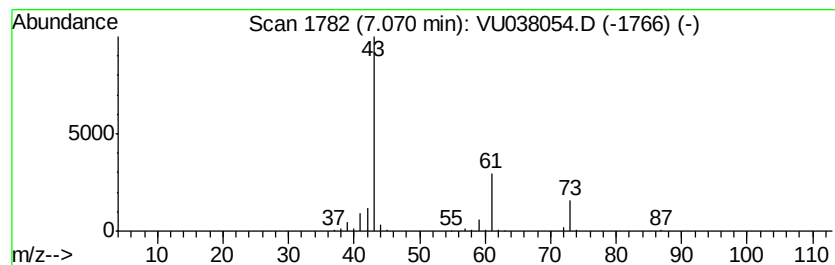
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Propyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.07	1.52 ug/L	265718	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	72
4		Isopropyl acetate	102	C5H10O2	000108-21-4	38
5		Isobutylamine	73	C4H11N	000078-81-9	9



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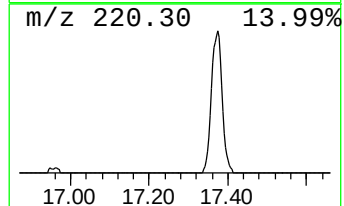
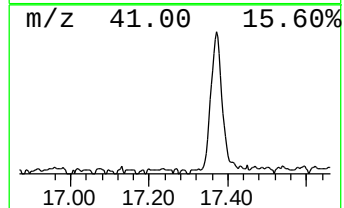
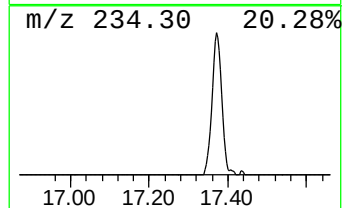
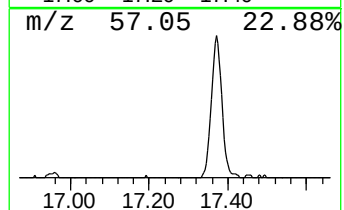
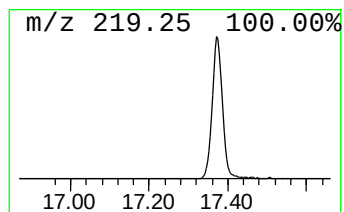
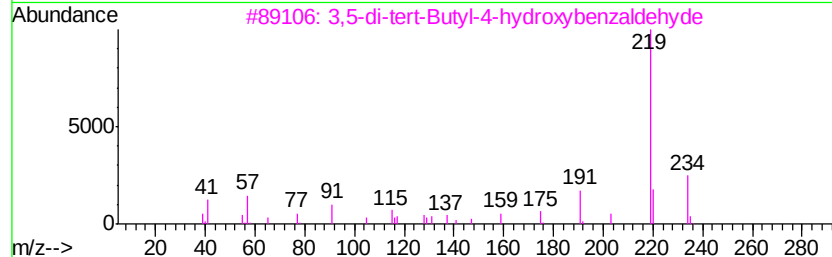
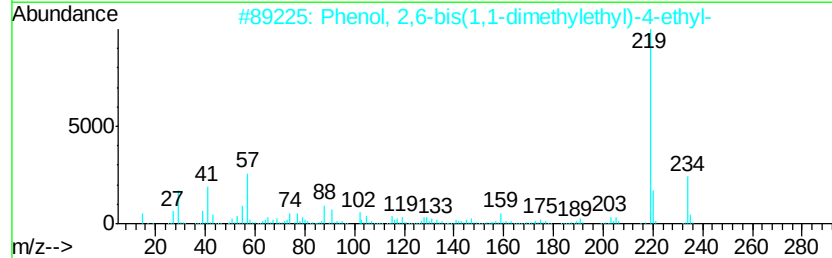
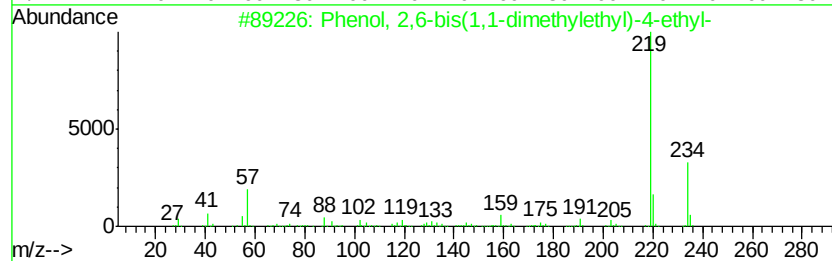
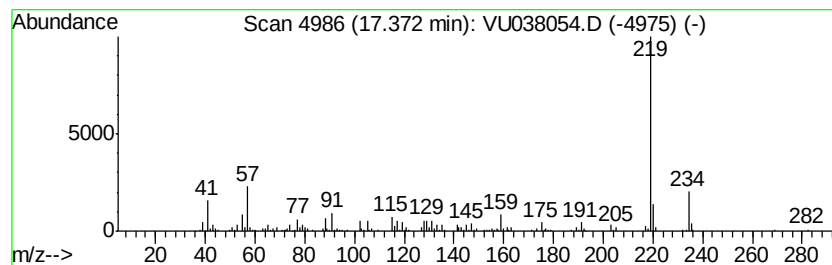
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Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.37	1.04 ug/L	222759	1,4-Dichlorobenzene-d4	11.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	96
2		Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	94
3		3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	94
4		Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	93
5		3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	93



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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	138002	1	6.28	875930	5.0
Isopropyl Alcohol	2.78	0.7	ug/L	122293	1	6.28	875930	5.0
Ethyl Acetate	4.84	2.1	ug/L	362445	1	6.28	875930	5.0
n-Propyl acetate	7.07	1.5	ug/L	265718	1	6.28	875930	5.0
Phenol, 2,6-bis(1...	17.37	1.0	ug/L	222759	3	11.82	1070980	5.0