

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092321\
 Data File : VU044787.D
 Acq On : 23 Sep 2021 16:13
 Operator : SY/MD
 Sample : M3873-08
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW7X8

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
 Title : VOC Analysis

Signal : TIC: VU044787.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.491	42	47	62	rBV6	8254	18544	0.59%	0.129%
2	1.601	74	81	93	rBV	213139	257440	8.15%	1.796%
3	1.912	170	178	194	rVB	145348	195368	6.19%	1.363%
4	1.993	197	203	215	rVB	48908	67133	2.13%	0.468%
5	2.205	264	269	283	rVB2	10994	15415	0.49%	0.108%
6	2.572	370	383	399	rBV	276288	466685	14.78%	3.255%
7	2.784	434	449	474	rBV	11535	37586	1.19%	0.262%
8	3.047	525	531	538	rBV4	2500	4042	0.13%	0.028%
9	3.147	555	562	566	rBV4	673	1237	0.04%	0.009%
10	3.195	567	577	600	rVB2	6619	18338	0.58%	0.128%
11	3.295	605	608	609	rBV	146	98	0.00%	0.001%
12	3.308	609	612	615	rVB2	261	120	0.00%	0.001%
13	3.359	615	628	643	rBV3	38047	77914	2.47%	0.543%
14	3.584	692	698	701	rBV2	145	160	0.01%	0.001%
15	3.848	777	780	782	rBV	115	80	0.00%	0.001%
16	4.125	861	866	868	rBV2	258	215	0.01%	0.001%
17	4.314	922	925	929	rVB	137	119	0.00%	0.001%
18	4.401	948	952	957	rBV2	131	141	0.00%	0.001%
19	4.427	957	960	961	rBV	347	184	0.01%	0.001%
20	4.465	970	972	976	rVB2	134	83	0.00%	0.001%
21	4.536	983	994	1005	rVB4	3147	6696	0.21%	0.047%
22	4.671	1009	1036	1071	rBV2	1243327	3156925	100.00%	22.020%
23	5.070	1144	1160	1179	rBV	233304	504767	15.99%	3.521%
24	5.298	1225	1231	1235	rVV4	680	846	0.03%	0.006%
25	5.324	1237	1239	1242	rVB3	417	219	0.01%	0.002%
26	5.385	1249	1258	1270	rBV5	958	1803	0.06%	0.013%
27	5.469	1277	1284	1287	rBV3	624	893	0.03%	0.006%
28	5.530	1300	1303	1308	rBV	194	218	0.01%	0.002%
29	5.555	1308	1311	1317	rVB2	126	136	0.00%	0.001%
30	5.613	1327	1329	1333	rVB2	166	88	0.00%	0.001%
31	5.649	1335	1340	1343	rBV2	224	247	0.01%	0.002%
32	5.729	1343	1365	1397	rBV2	486805	1317435	41.73%	9.189%
33	6.173	1500	1503	1509	rVB3	307	334	0.01%	0.002%
34	6.253	1513	1528	1551	rBV	354832	662925	21.00%	4.624%
35	6.546	1604	1619	1650	rBV	822286	1545157	48.95%	10.778%
36	6.697	1652	1666	1688	rVB	310458	605366	19.18%	4.223%

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 Title : VOC Analysis

37	6.838	1708	1710	1711	rBV2	342	145	0.00%	0.001%
38	6.906	1729	1731	1734	rBV2	280	191	0.01%	0.001%
39	6.977	1750	1753	1756	rBV	210	191	0.01%	0.001%
40	7.047	1769	1775	1785	rVB3	649	1004	0.03%	0.007%
41	7.186	1809	1818	1830	rVV7	1444	2404	0.08%	0.017%
42	7.378	1876	1878	1880	rVB	176	73	0.00%	0.001%
43	7.465	1898	1905	1908	rBV	225	340	0.01%	0.002%
44	7.507	1912	1918	1921	rBV	143	170	0.01%	0.001%
45	7.571	1925	1938	1957	rBV	161124	283236	8.97%	1.976%
46	7.742	1989	1991	1994	rBV	194	128	0.00%	0.001%
47	7.758	1994	1996	1998	rVB2	280	136	0.00%	0.001%
48	7.774	1998	2001	2004	rBV3	221	153	0.00%	0.001%
49	7.841	2020	2022	2025	rVB2	191	104	0.00%	0.001%
50	7.903	2025	2041	2056	rBV	564545	964268	30.54%	6.726%
51	7.973	2058	2063	2081	rVB2	9188	15665	0.50%	0.109%
52	8.182	2116	2128	2151	rBV	111667	189644	6.01%	1.323%
53	8.391	2191	2193	2196	rBV2	163	69	0.00%	0.000%
54	8.478	2213	2220	2227	rBV2	724	1046	0.03%	0.007%
55	8.565	2245	2247	2250	rVB3	191	110	0.00%	0.001%
56	8.584	2250	2253	2255	rBV	151	66	0.00%	0.000%
57	8.639	2256	2270	2314	rBV	480835	852253	27.00%	5.945%
58	8.928	2359	2360	2364	rBV2	144	104	0.00%	0.001%
59	9.066	2397	2403	2407	rBV2	200	232	0.01%	0.002%
60	9.301	2473	2476	2479	rVB2	151	86	0.00%	0.001%
61	9.420	2500	2513	2529	rBV	498588	819072	25.95%	5.713%
62	9.549	2550	2553	2556	rBV2	286	182	0.01%	0.001%
63	9.600	2567	2569	2574	rVB	135	89	0.00%	0.001%
64	9.626	2575	2577	2579	rBV	204	83	0.00%	0.001%
65	9.693	2591	2598	2604	rVB2	729	1086	0.03%	0.008%
66	9.722	2604	2607	2609	rBV2	160	106	0.00%	0.001%
67	10.108	2724	2727	2731	rVB	326	253	0.01%	0.002%
68	10.189	2749	2752	2754	rBV2	225	143	0.00%	0.001%
69	10.674	2896	2903	2911	rBV5	2525	3736	0.12%	0.026%
70	10.761	2917	2930	2951	rBV	422568	669763	21.22%	4.672%
71	10.931	2981	2983	2984	rBV	248	82	0.00%	0.001%
72	11.066	3022	3025	3028	rBV	175	145	0.00%	0.001%
73	11.121	3037	3042	3046	rVB4	447	366	0.01%	0.003%
74	11.144	3047	3049	3051	rVV2	262	113	0.00%	0.001%
75	11.156	3051	3053	3054	rVB	260	85	0.00%	0.001%
76	11.288	3092	3094	3098	rBV	162	99	0.00%	0.001%

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77	11.340	3108	3110	3116	rVB2	289	177	0.01%	0.001%
78	11.462	3141	3148	3158	rVB5	1763	2495	0.08%	0.017%
79	11.581	3181	3185	3189	rBV2	288	294	0.01%	0.002%
80	11.700	3217	3222	3228	rVB2	1063	1111	0.04%	0.008%
81	11.816	3245	3258	3274	rBV	454061	725200	22.97%	5.058%
82	11.944	3293	3298	3301	rBV3	772	778	0.02%	0.005%
83	12.063	3333	3335	3336	rBV3	486	228	0.01%	0.002%
84	12.124	3349	3354	3357	rBV2	377	370	0.01%	0.003%
85	12.198	3360	3377	3392	rBV	517914	829963	26.29%	5.789%
86	12.423	3443	3447	3451	rBV2	209	186	0.01%	0.001%
87	12.446	3451	3454	3459	rVB2	281	244	0.01%	0.002%
88	12.484	3462	3466	3469	rVB3	243	185	0.01%	0.001%
89	12.529	3478	3480	3481	rBV	282	134	0.00%	0.001%
90	12.594	3498	3500	3504	rBV2	223	166	0.01%	0.001%
91	12.635	3510	3513	3519	rVB3	319	236	0.01%	0.002%
92	12.680	3519	3527	3531	rBV2	337	426	0.01%	0.003%
93	13.147	3670	3672	3673	rBV2	201	94	0.00%	0.001%
94	14.086	3960	3964	3965	rBV2	396	311	0.01%	0.002%
95	14.240	4010	4012	4015	rBB2	246	114	0.00%	0.001%
96	14.333	4038	4041	4045	rVB2	439	282	0.01%	0.002%
97	14.561	4109	4112	4116	rVB2	345	251	0.01%	0.002%
98	14.931	4225	4227	4229	rBV3	331	192	0.01%	0.001%
99	15.034	4256	4259	4262	rBV3	347	270	0.01%	0.002%
100	15.131	4286	4289	4296	rBV3	487	559	0.02%	0.004%

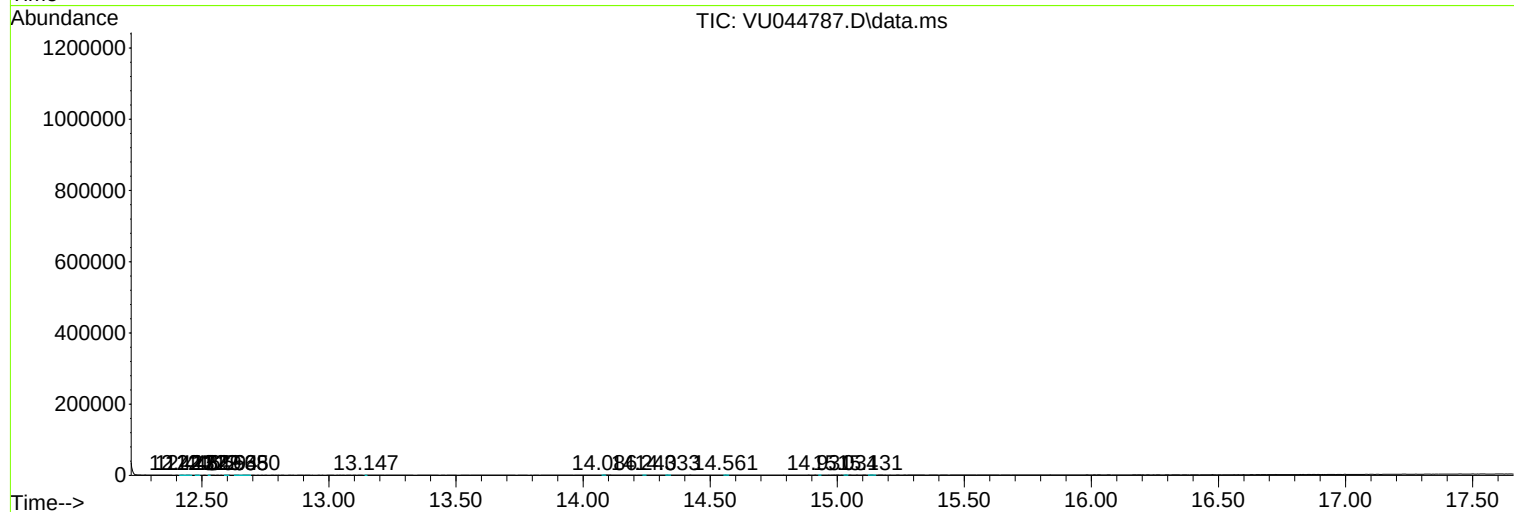
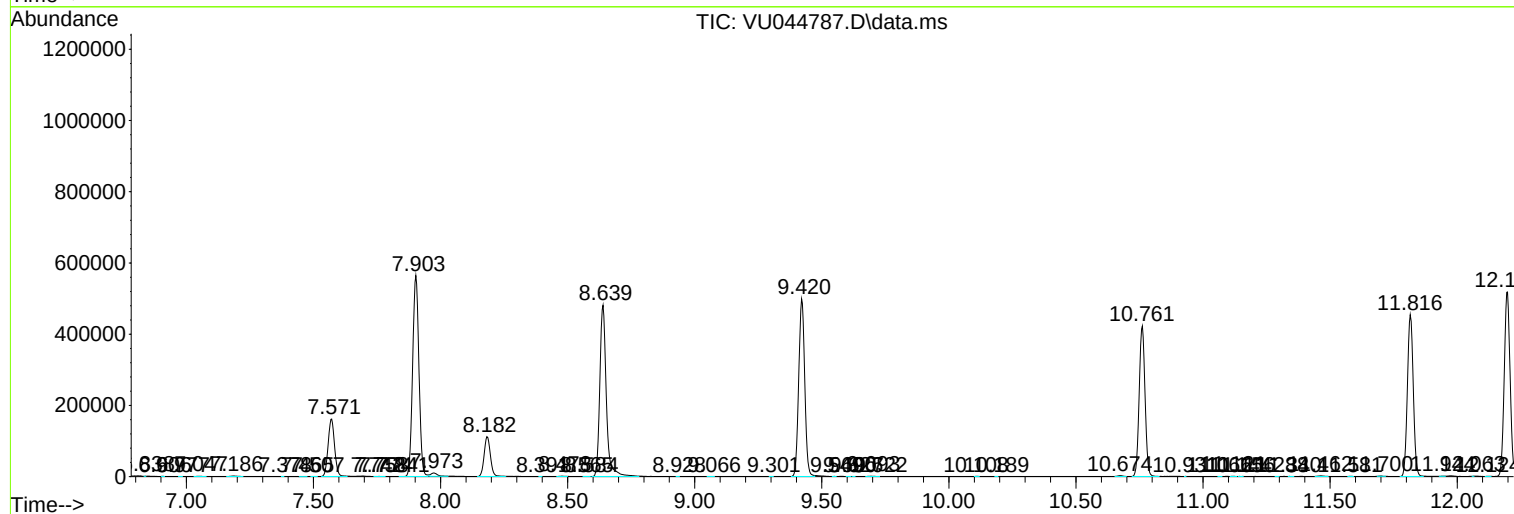
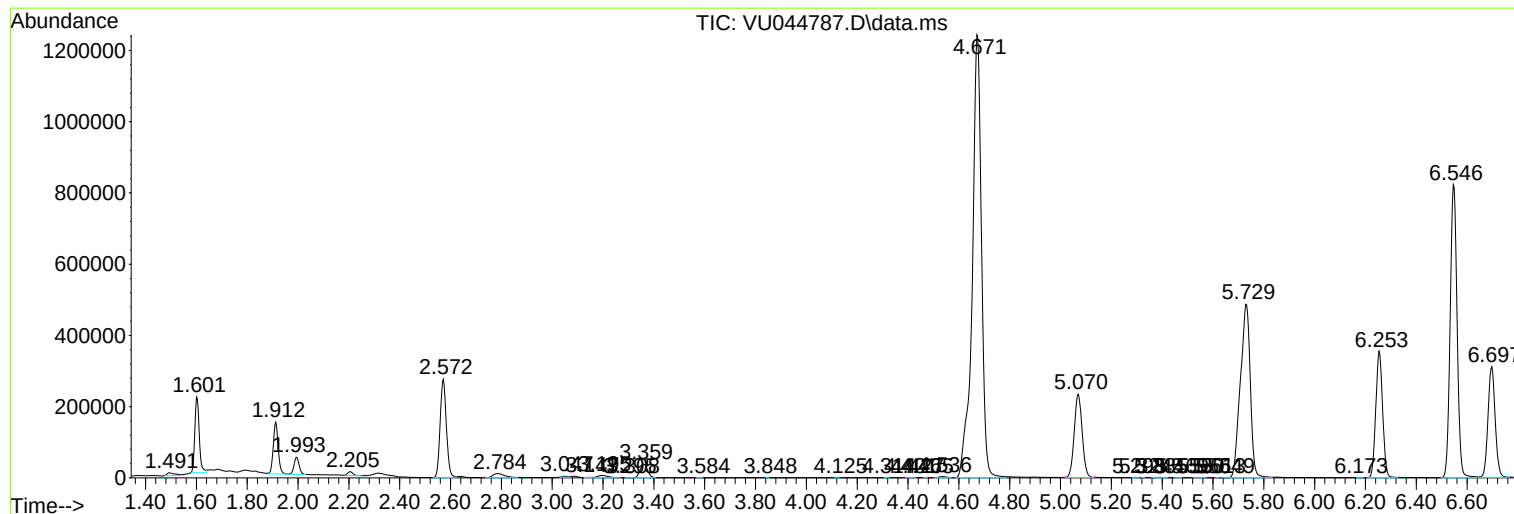
Sum of corrected areas: 14336444

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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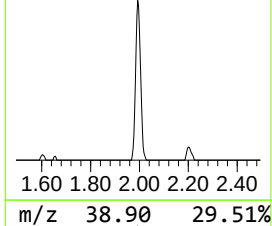
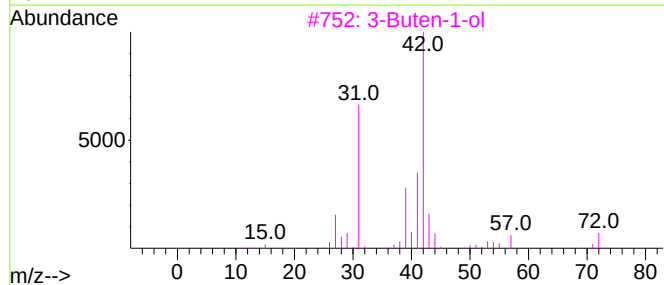
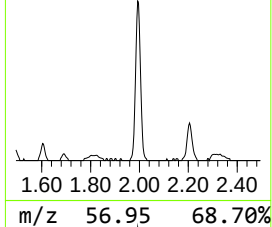
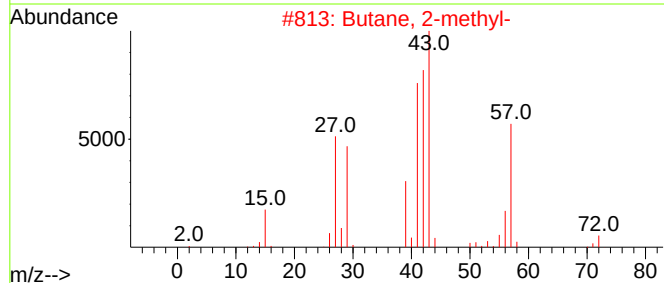
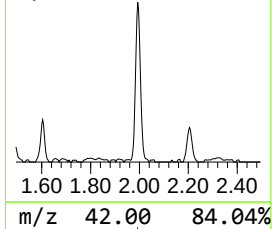
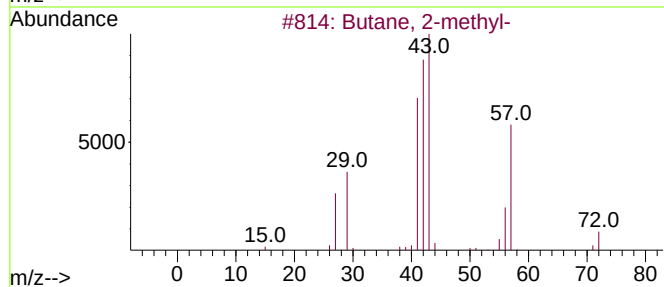
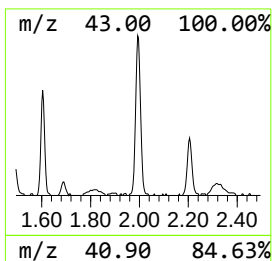
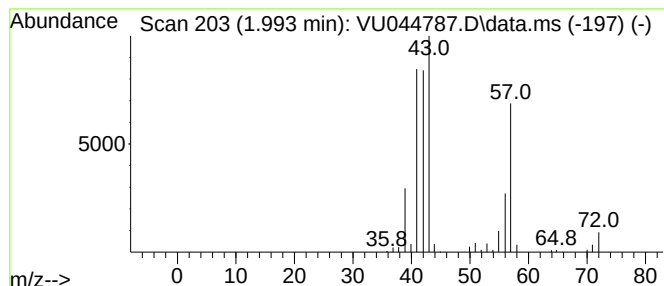
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.993	5.06 ug/L	67133	1,4-Difluorobenzene	6.253

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methyl-	72	C5H12	000078-78-4	87
2		Butane, 2-methyl-	72	C5H12	000078-78-4	80
3		3-Buten-1-ol	72	C4H8O	000627-27-0	38
4		Pentane	72	C5H12	000109-66-0	38
5		Oxirane, trimethyl-	86	C5H10O	005076-19-7	36



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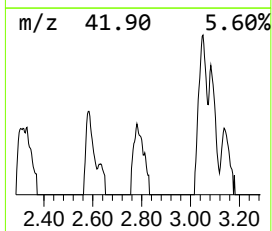
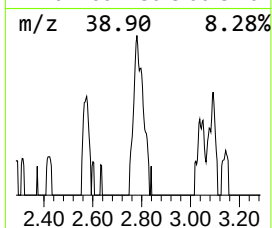
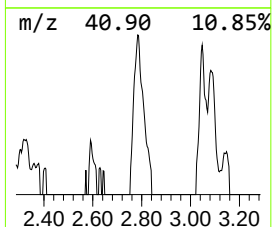
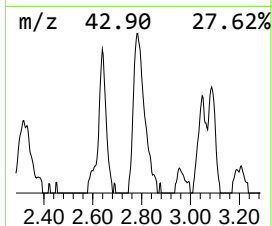
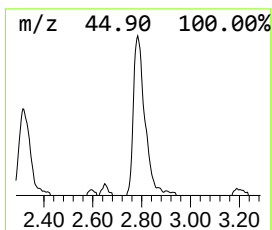
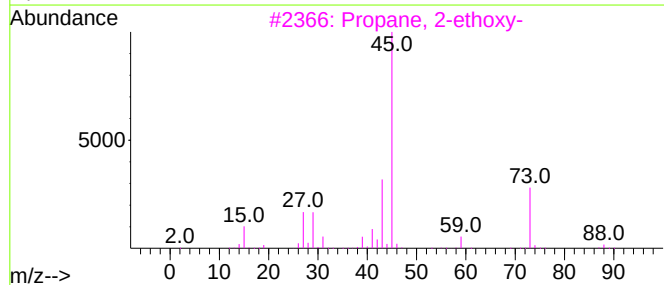
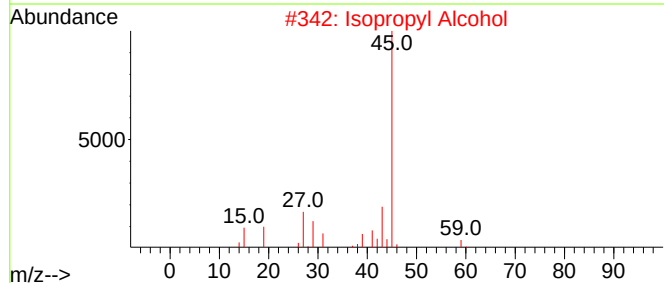
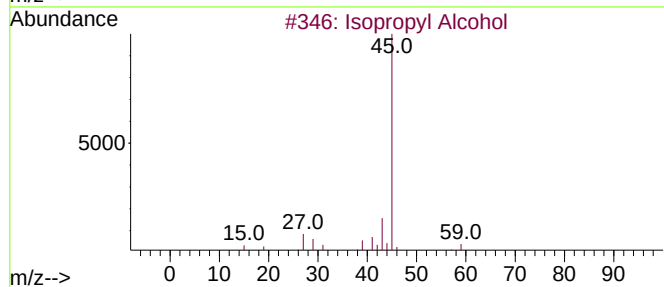
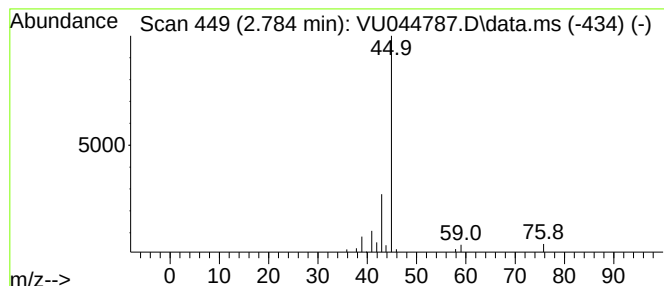
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Isopropyl Alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.784	2.83 ug/L	37586	1,4-Difluorobenzene	6.253

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	64
3			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	43
4			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	43
5			Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	9



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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	1.993	5.1	ug/L	67133	1	6.253	662925	50.0
Isopropyl Alcohol	2.784	2.8	ug/L	37586	1	6.253	662925	50.0