

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU030520\
 Data File : VU037082.D
 Acq On : 05 Mar 2020 14:42
 Operator : JC/MD
 Sample : L1780-11
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0DG7

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % 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\SOMULM022420WMA.M
 Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.491	36	47	56	rBV	82898	197000	19.73%	2.530%
2	1.613	80	85	94	rVB	119416	122724	12.29%	1.576%
3	1.928	176	183	199	rVB	119030	160802	16.11%	2.065%
4	2.591	377	389	403	rBV	187512	304444	30.49%	3.910%
5	2.790	438	451	469	rBV	51110	95413	9.56%	1.225%
6	3.224	574	586	598	rBV2	3802	8417	0.84%	0.108%
7	3.430	645	650	653	rBV2	243	276	0.03%	0.004%
8	3.780	756	759	766	rVV2	164	233	0.02%	0.003%
9	3.903	791	797	801	rVB	266	334	0.03%	0.004%
10	3.935	801	807	809	rBV2	247	291	0.03%	0.004%
11	4.182	879	884	889	rBV	226	278	0.03%	0.004%
12	4.330	924	930	932	rBV2	287	330	0.03%	0.004%
13	4.469	968	973	977	rBV2	219	239	0.02%	0.003%
14	4.565	1000	1003	1006	rVV	247	199	0.02%	0.003%
15	4.668	1019	1035	1060	rBV	107443	251366	25.18%	3.228%
16	5.009	1138	1141	1146	rVB2	290	251	0.03%	0.003%
17	5.105	1154	1171	1194	rVV	174916	379252	37.98%	4.871%
18	5.221	1202	1207	1215	rVB2	377	450	0.05%	0.006%
19	5.324	1233	1239	1242	rBV2	601	714	0.07%	0.009%
20	5.407	1261	1265	1272	rVB2	454	561	0.06%	0.007%
21	5.494	1288	1292	1299	rBV2	200	269	0.03%	0.003%
22	5.761	1353	1375	1398	rBV2	378049	998459	100.00%	12.823%
23	6.031	1457	1459	1466	rVB2	220	262	0.03%	0.003%
24	6.076	1470	1473	1476	rVB	291	204	0.02%	0.003%
25	6.147	1491	1495	1497	rBV2	248	203	0.02%	0.003%
26	6.282	1521	1537	1562	rBV	338486	630022	63.10%	8.091%
27	6.562	1615	1624	1635	rBV7	2487	5353	0.54%	0.069%
28	6.722	1660	1674	1695	rVV2	238811	460994	46.17%	5.920%
29	6.832	1703	1708	1710	rBV3	390	416	0.04%	0.005%
30	6.890	1723	1726	1730	rVV2	261	249	0.02%	0.003%
31	6.976	1748	1753	1755	rBV2	241	223	0.02%	0.003%
32	7.073	1777	1783	1785	rBV2	258	259	0.03%	0.003%
33	7.208	1816	1825	1833	rBV5	2660	4179	0.42%	0.054%
34	7.475	1902	1908	1914	rVB2	181	304	0.03%	0.004%

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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM022420WMA.M
 Title : VOC Analysis

35	7.594	1932	1945	1964	rBV	118317	210255	21.06%	2.700%
36	7.713	1977	1982	1989	rVB4	1554	1909	0.19%	0.025%
37	7.745	1989	1992	2002	rVB3	557	766	0.08%	0.010%
38	7.877	2027	2033	2034	rBV2	191	209	0.02%	0.003%
39	7.925	2034	2048	2065	rBV	441741	768186	76.94%	9.866%
40	8.092	2097	2100	2108	rVB2	669	790	0.08%	0.010%
41	8.205	2123	2135	2149	rBV	81627	139071	13.93%	1.786%
42	8.427	2196	2204	2211	rVB2	264	453	0.05%	0.006%
43	8.494	2217	2225	2233	rVV3	773	1146	0.11%	0.015%
44	8.661	2263	2277	2319	rBV	268023	533939	53.48%	6.857%
45	9.169	2430	2435	2440	rBV2	267	322	0.03%	0.004%
46	9.388	2499	2503	2505	rBV	259	209	0.02%	0.003%
47	9.439	2505	2519	2540	rBV	458060	781384	78.26%	10.035%
48	9.578	2559	2562	2564	rBV	267	235	0.02%	0.003%
49	9.684	2592	2595	2601	rVB	261	289	0.03%	0.004%
50	9.713	2601	2604	2611	rVB2	307	366	0.04%	0.005%
51	9.774	2616	2623	2628	rBV2	319	504	0.05%	0.006%
52	9.873	2650	2654	2657	rVB2	205	215	0.02%	0.003%
53	10.208	2752	2758	2762	rBV2	268	347	0.03%	0.004%
54	10.308	2785	2789	2795	rBV2	224	295	0.03%	0.004%
55	10.545	2857	2863	2870	rBV2	230	366	0.04%	0.005%
56	10.687	2904	2907	2911	rVV	244	212	0.02%	0.003%
57	10.774	2922	2934	2951	rVV	312349	508380	50.92%	6.529%
58	10.873	2960	2965	2973	rBV2	272	473	0.05%	0.006%
59	10.915	2974	2978	2985	rVV2	358	443	0.04%	0.006%
60	10.970	2991	2995	3001	rVB2	230	301	0.03%	0.004%
61	11.050	3015	3020	3023	rVB	313	291	0.03%	0.004%
62	11.240	3075	3079	3085	rBV2	168	222	0.02%	0.003%
63	11.642	3198	3204	3205	rBV	234	249	0.02%	0.003%
64	11.684	3212	3217	3220	rBV2	274	265	0.03%	0.003%
65	11.764	3237	3242	3247	rBV3	383	430	0.04%	0.006%
66	11.828	3250	3262	3281	rVV	357711	596104	59.70%	7.656%
67	11.934	3292	3295	3303	rVB	392	392	0.04%	0.005%
68	12.073	3334	3338	3339	rVV	290	196	0.02%	0.003%
69	12.086	3339	3342	3346	rVV2	413	382	0.04%	0.005%
70	12.211	3367	3381	3398	rBV	361181	602295	60.32%	7.735%
71	12.645	3511	3516	3519	rBV2	271	229	0.02%	0.003%

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72	12.684	3524	3528	3533	rBV2	372	405	0.04%	0.005%
73	12.729	3539	3542	3545	rVB	326	224	0.02%	0.003%
74	12.777	3552	3557	3560	rBV	287	333	0.03%	0.004%
75	12.825	3567	3572	3575	rBV	255	285	0.03%	0.004%
76	12.941	3603	3608	3611	rBV	279	238	0.02%	0.003%
77	13.121	3661	3664	3667	rBV2	375	214	0.02%	0.003%
78	13.227	3692	3697	3700	rVV3	349	327	0.03%	0.004%
79	13.246	3700	3703	3708	rVB2	296	216	0.02%	0.003%
80	13.314	3721	3724	3727	rVB	393	269	0.03%	0.003%
81	13.336	3727	3731	3735	rBV2	259	203	0.02%	0.003%
82	13.359	3736	3738	3742	rVB2	388	239	0.02%	0.003%
83	13.468	3768	3772	3774	rBV2	238	252	0.03%	0.003%
84	13.484	3774	3777	3780	rVV2	295	201	0.02%	0.003%
85	13.526	3787	3790	3793	rBV2	246	201	0.02%	0.003%
86	13.648	3824	3828	3831	rVB2	317	256	0.03%	0.003%
87	13.851	3888	3891	3894	rBV2	363	275	0.03%	0.004%
88	13.870	3894	3897	3900	rBV2	389	385	0.04%	0.005%
89	13.992	3931	3935	3941	rVB2	352	408	0.04%	0.005%
90	14.021	3941	3944	3949	rBV	215	231	0.02%	0.003%
91	14.118	3972	3974	3977	rVB2	509	221	0.02%	0.003%
92	14.195	3994	3998	4000	rBV2	249	196	0.02%	0.003%
93	14.487	4086	4089	4092	rBV	483	396	0.04%	0.005%
94	14.732	4159	4165	4167	rBV2	239	305	0.03%	0.004%
95	14.915	4219	4222	4226	rBV2	447	427	0.04%	0.005%
96	14.957	4233	4235	4238	rBV	545	450	0.05%	0.006%
97	15.159	4295	4298	4302	rBV2	386	363	0.04%	0.005%
98	15.339	4351	4354	4359	rBV2	396	406	0.04%	0.005%
99	15.722	4467	4473	4478	rBV4	537	801	0.08%	0.010%
100	16.111	4591	4594	4599	rBV3	731	680	0.07%	0.009%

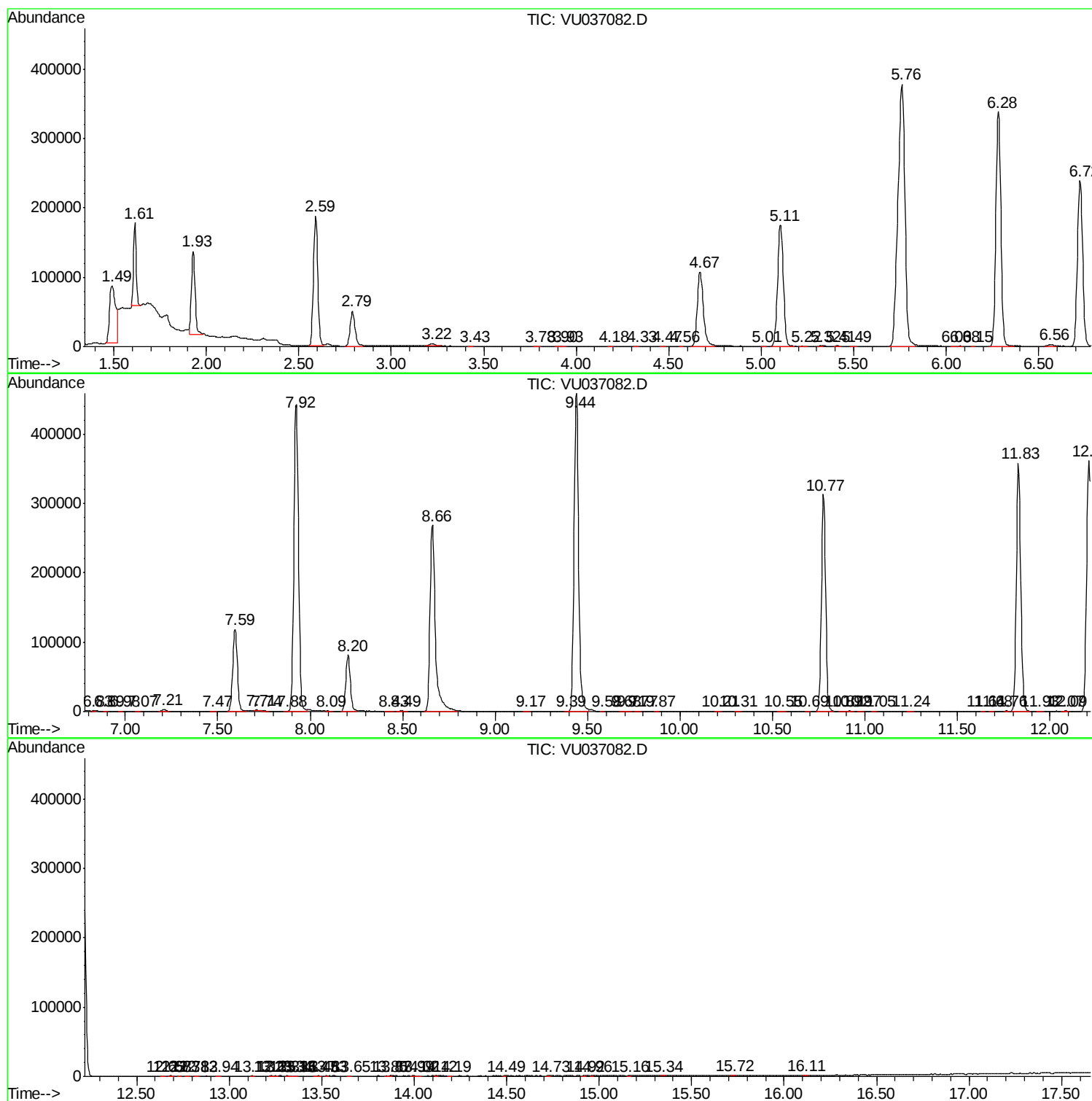
Sum of corrected areas: 7786497

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM022420WMA.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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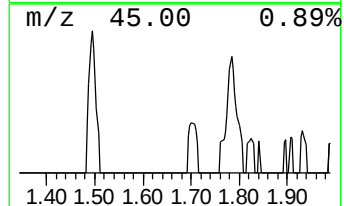
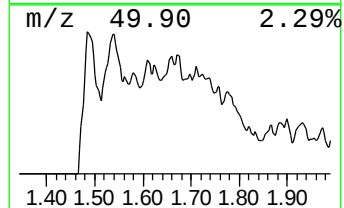
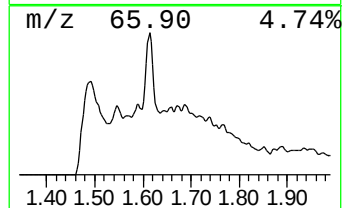
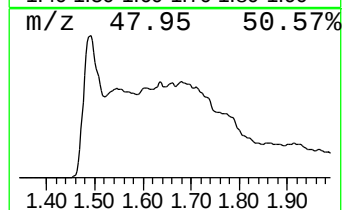
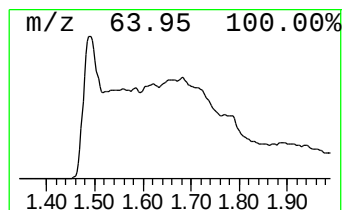
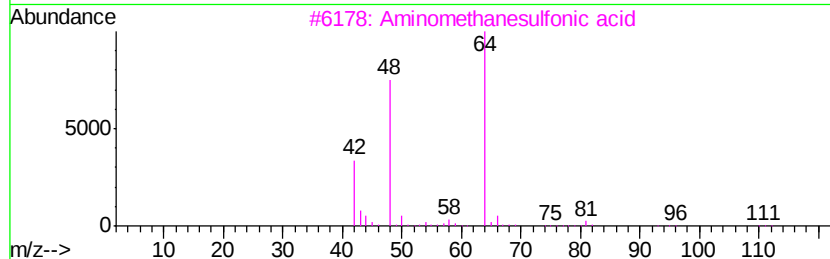
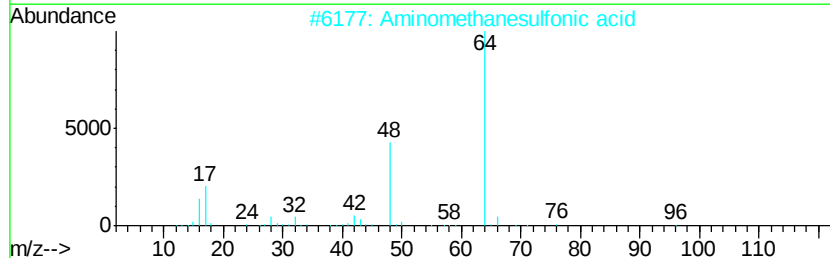
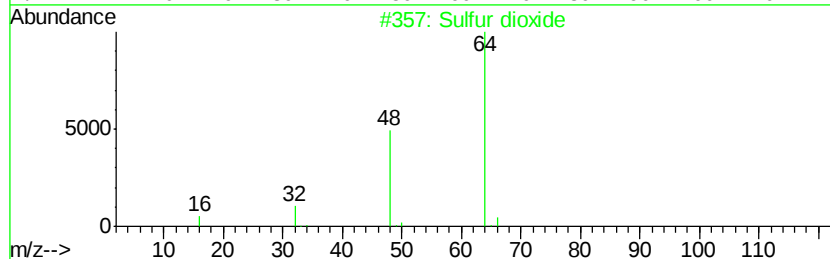
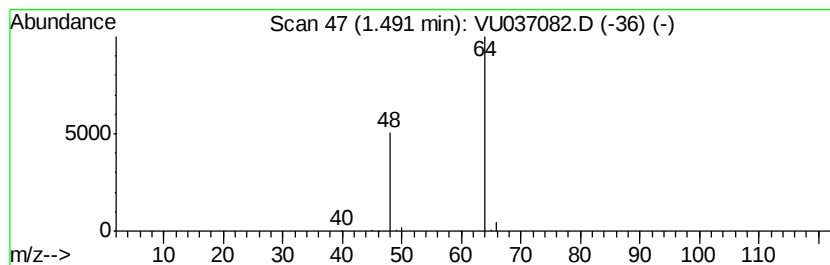
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM022420WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.49	15.63 ug/L	197000	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfur dioxide	64	O2S	007446-09-5	90
2		Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3		Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4		L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5		Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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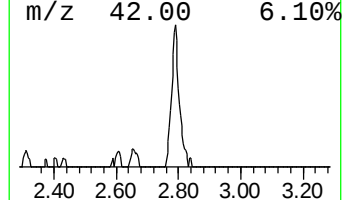
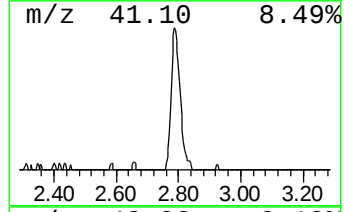
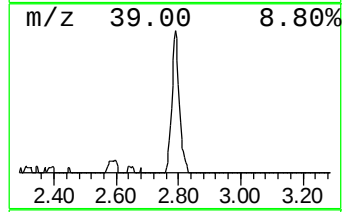
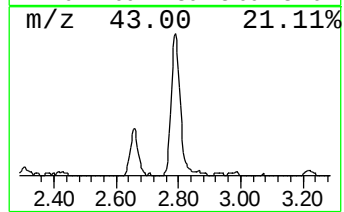
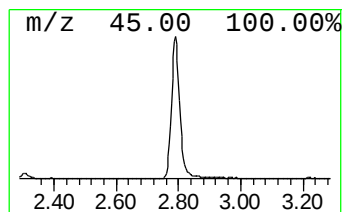
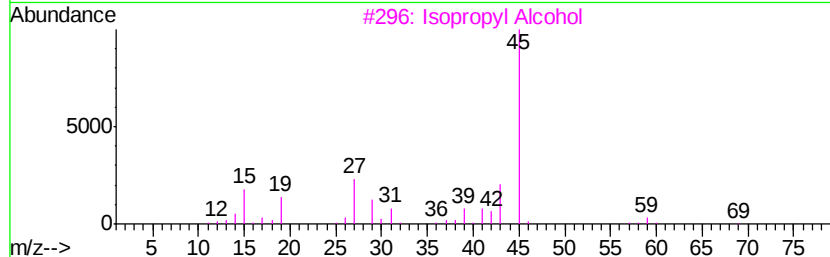
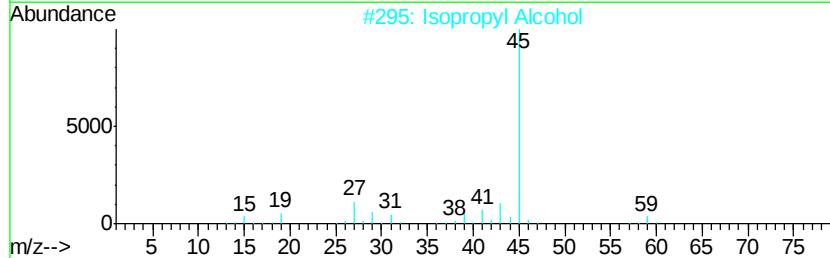
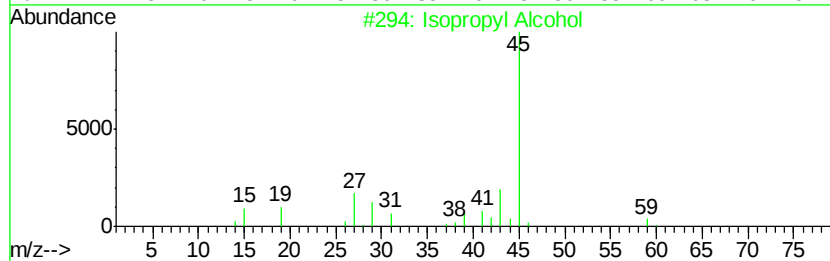
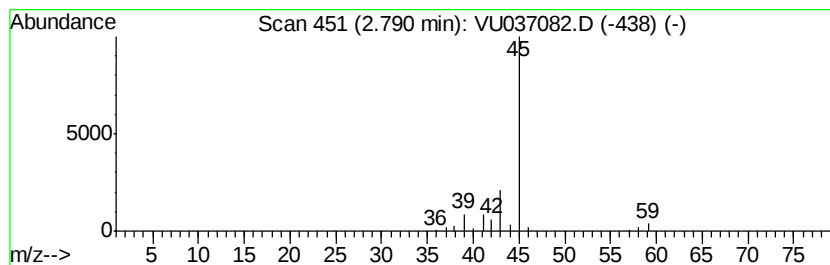
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Quant Title : VOC Analysis

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

Peak Number 2 Isopropyl Alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.79	7.57 ug/L	95413	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl Alcohol	60	C3H8O	000067-63-0	74
2		Isopropyl Alcohol	60	C3H8O	000067-63-0	9
3		Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4		Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5		Formamide	45	CH3NO	000075-12-7	4



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.49	15.6	ug/L	197000	1	6.28	630022	50.0
Isopropyl Alcohol	2.79	7.6	ug/L	95413	1	6.28	630022	50.0