

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121121\
 Data File : VU046296.D
 Acq On : 11 Dec 2021 18:50
 Operator : SY/MD
 Sample : M4983-18DL 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW5P8DL

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\SFAMULM112921WMA.M

Title : VOC Analysis

Signal : TIC: VU046296.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.475	37	42	60	rVB	71769	73278	11.92%	1.279%
2	1.600	75	81	94	rVB	68150	75289	12.24%	1.314%
3	1.916	172	179	192	rVB	55939	71513	11.63%	1.248%
4	2.221	271	274	278	rBV	380	281	0.05%	0.005%
5	2.272	285	290	291	rBV	226	204	0.03%	0.004%
6	2.575	371	384	405	rBV3	137819	263120	42.79%	4.593%
7	3.006	516	518	521	rBV	314	165	0.03%	0.003%
8	3.047	521	531	545	rBV	10467	19590	3.19%	0.342%
9	3.186	565	574	589	rBV2	1906	4538	0.74%	0.079%
10	3.276	598	602	605	rBV2	361	356	0.06%	0.006%
11	3.359	623	628	635	rVB5	1191	1944	0.32%	0.034%
12	3.475	661	664	666	rBV	289	177	0.03%	0.003%
13	3.633	710	713	715	rBV2	208	153	0.02%	0.003%
14	3.723	736	741	746	rBV	342	384	0.06%	0.007%
15	3.768	751	755	757	rBV	344	281	0.05%	0.005%
16	3.874	774	788	810	rVB2	36158	86646	14.09%	1.512%
17	3.980	819	821	824	rVB	372	210	0.03%	0.004%
18	4.006	824	829	832	rBV2	315	321	0.05%	0.006%
19	4.051	838	843	850	rVB	400	522	0.08%	0.009%
20	4.079	850	852	854	rBV	224	109	0.02%	0.002%
21	4.099	854	858	864	rBV2	467	483	0.08%	0.008%
22	4.192	885	887	890	rVB2	219	108	0.02%	0.002%
23	4.211	890	893	897	rBV2	434	283	0.05%	0.005%
24	4.234	898	900	903	rVB2	196	92	0.01%	0.002%
25	4.362	938	940	941	rBV	177	83	0.01%	0.001%
26	4.440	955	964	966	rBV2	304	431	0.07%	0.008%
27	4.530	988	992	996	rBV2	339	286	0.05%	0.005%
28	4.642	1011	1027	1056	rBV2	68944	249432	40.57%	4.354%
29	4.909	1107	1110	1112	rVB	134	76	0.01%	0.001%
30	4.928	1112	1116	1121	rBV	228	279	0.05%	0.005%
31	4.977	1127	1131	1134	rBV	348	263	0.04%	0.005%
32	4.993	1134	1136	1137	rBV	177	84	0.01%	0.001%
33	5.067	1143	1159	1183	rBV	111770	258035	41.96%	4.504%
34	5.198	1198	1200	1201	rBB	104	33	0.01%	0.001%
35	5.211	1201	1204	1210	rVB	272	214	0.03%	0.004%
36	5.240	1210	1213	1216	rBV	322	268	0.04%	0.005%

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 Title : VOC Analysis

37	5.321	1221	1238	1265	rBV	137665	310817	50.55%	5.425%
38	5.446	1275	1277	1279	rBV	176	111	0.02%	0.002%
39	5.507	1293	1296	1299	rVB	348	186	0.03%	0.003%
40	5.530	1300	1303	1304	rBV	164	100	0.02%	0.002%
41	5.542	1304	1307	1309	rVV	286	167	0.03%	0.003%
42	5.729	1342	1365	1394	rBV2	224004	614889	100.00%	10.733%
43	6.034	1457	1460	1463	rVB2	258	141	0.02%	0.002%
44	6.054	1463	1466	1468	rBV2	344	196	0.03%	0.003%
45	6.179	1500	1505	1508	rBV	322	278	0.05%	0.005%
46	6.253	1514	1528	1559	rBV	192246	364255	59.24%	6.358%
47	6.420	1573	1580	1582	rBV	365	336	0.05%	0.006%
48	6.546	1607	1619	1633	rBV3	28523	54335	8.84%	0.948%
49	6.694	1652	1665	1686	rBV	147206	283303	46.07%	4.945%
50	6.915	1731	1734	1737	rVB2	312	196	0.03%	0.003%
51	6.948	1741	1744	1746	rBV2	371	234	0.04%	0.004%
52	6.986	1753	1756	1758	rBV	442	322	0.05%	0.006%
53	7.115	1792	1796	1800	rBV	374	342	0.06%	0.006%
54	7.185	1811	1818	1821	rBV2	680	786	0.13%	0.014%
55	7.327	1857	1862	1866	rBV2	413	407	0.07%	0.007%
56	7.378	1875	1878	1880	rBV	273	182	0.03%	0.003%
57	7.439	1894	1897	1900	rBV	488	404	0.07%	0.007%
58	7.568	1925	1937	1957	rBV	79508	137799	22.41%	2.405%
59	7.684	1969	1973	1975	rBV2	794	574	0.09%	0.010%
60	7.716	1980	1983	1987	rBV2	336	326	0.05%	0.006%
61	7.832	2016	2019	2023	rBV	363	249	0.04%	0.004%
62	7.899	2027	2040	2057	rBV	261861	456582	74.25%	7.970%
63	8.111	2103	2106	2109	rBV	262	233	0.04%	0.004%
64	8.182	2117	2128	2143	rBV	56748	92333	15.02%	1.612%
65	8.401	2193	2196	2202	rVB4	1032	959	0.16%	0.017%
66	8.555	2234	2244	2257	rVB2	43651	73432	11.94%	1.282%
67	8.636	2257	2269	2294	rBV	225646	386540	62.86%	6.747%
68	8.787	2313	2316	2320	rVB	427	270	0.04%	0.005%
69	8.835	2325	2331	2333	rBV2	307	322	0.05%	0.006%
70	9.372	2493	2498	2500	rBV2	553	475	0.08%	0.008%
71	9.420	2500	2513	2531	rVV	291762	477935	77.73%	8.343%
72	9.764	2616	2620	2621	rBV	309	211	0.03%	0.004%
73	9.851	2644	2647	2649	rBV	328	204	0.03%	0.004%
74	9.893	2657	2660	2664	rBV	334	298	0.05%	0.005%
75	9.928	2668	2671	2673	rBV	281	209	0.03%	0.004%
76	10.089	2717	2721	2722	rBV2	425	302	0.05%	0.005%

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Peak Location: TOP

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Title : VOC Analysis

77	10.388	2811	2814	2816	rBV2	444	322	0.05%	0.006%
78	10.758	2917	2929	2949	rVB	239319	383651	62.39%	6.697%
79	10.867	2956	2963	2967	rBV	530	886	0.14%	0.015%
80	10.951	2987	2989	2991	rBV	233	122	0.02%	0.002%
81	11.198	3063	3066	3069	rBV2	299	276	0.04%	0.005%
82	11.407	3128	3131	3139	rVB2	476	546	0.09%	0.010%
83	11.459	3145	3147	3148	rBV	437	199	0.03%	0.003%
84	11.812	3245	3257	3276	rVB	314329	486525	79.12%	8.493%
85	12.060	3331	3334	3339	rVB	589	430	0.07%	0.008%
86	12.195	3364	3376	3390	rBV	307088	483229	78.59%	8.435%
87	12.336	3417	3420	3425	rBV	540	501	0.08%	0.009%
88	12.639	3512	3514	3520	rBV	322	350	0.06%	0.006%
89	13.121	3661	3664	3669	rBV	488	463	0.08%	0.008%
90	13.420	3754	3757	3759	rBV	392	293	0.05%	0.005%
91	13.754	3858	3861	3863	rBV	388	279	0.05%	0.005%

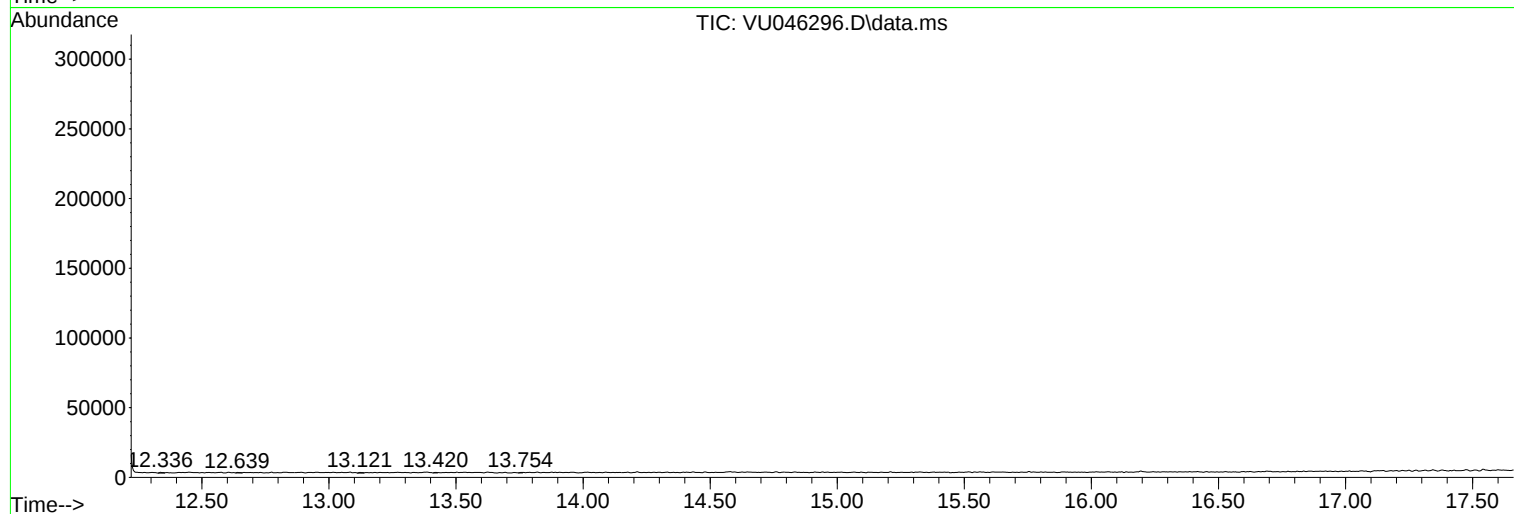
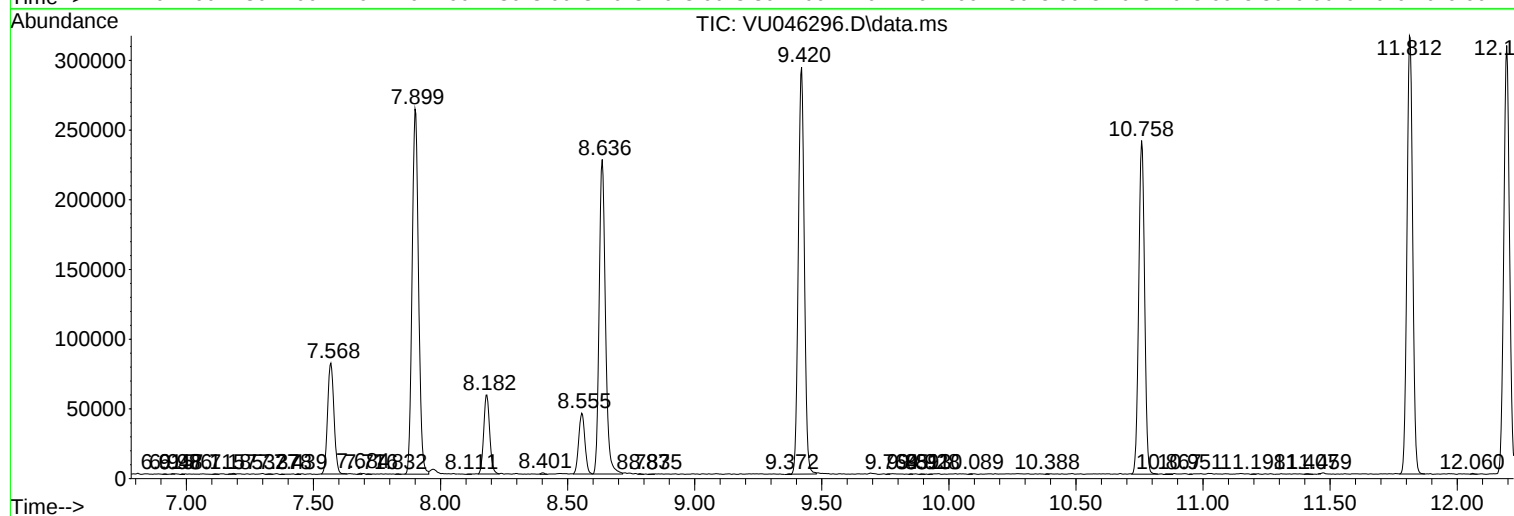
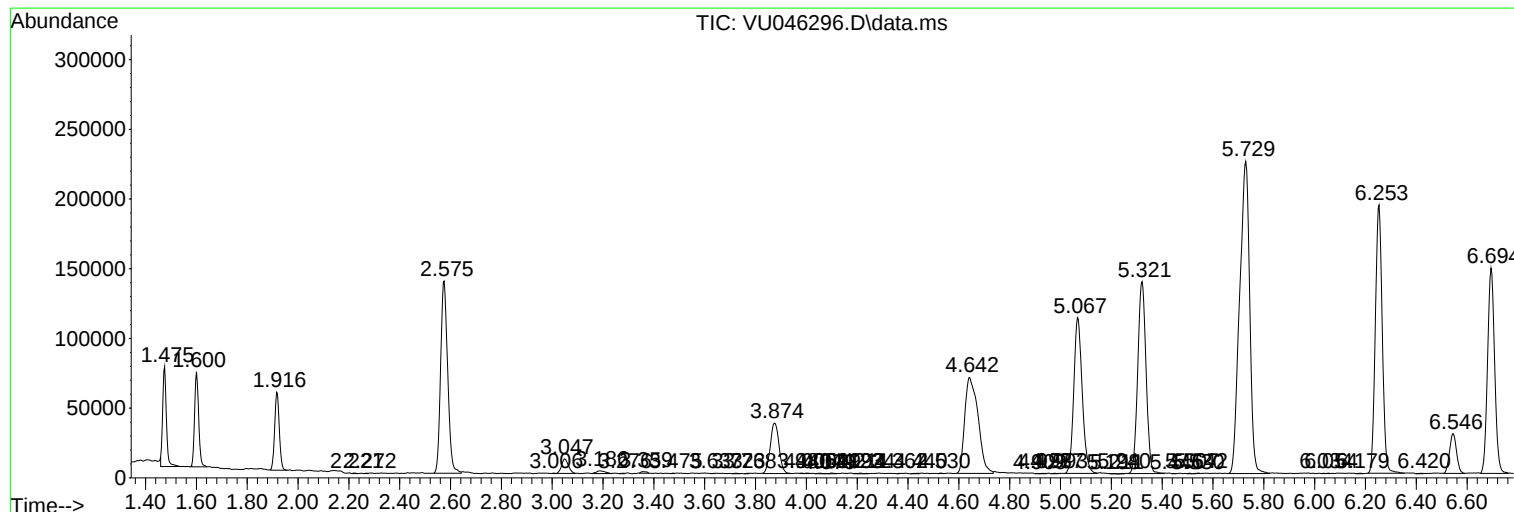
Sum of corrected areas: 5728843

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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



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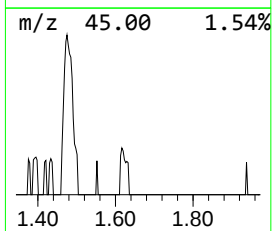
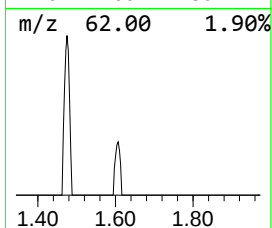
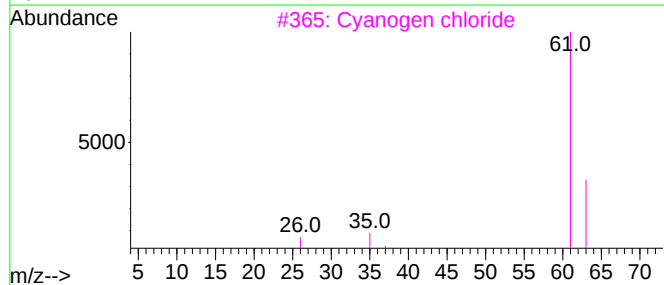
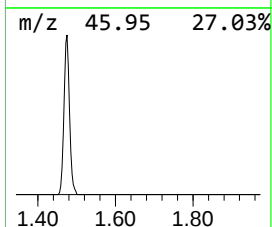
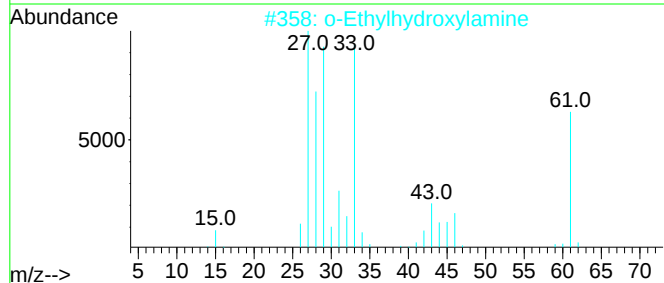
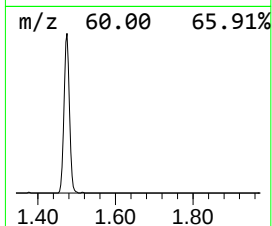
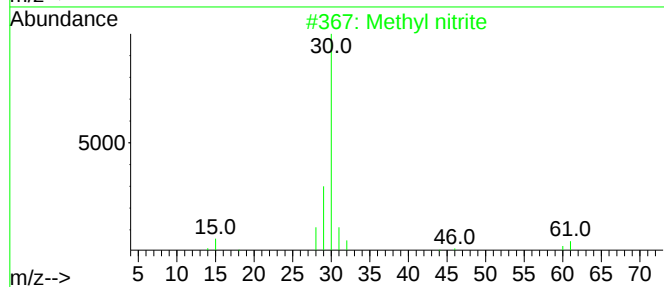
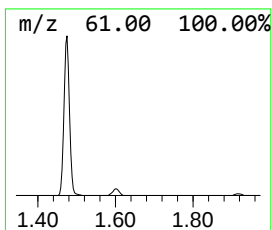
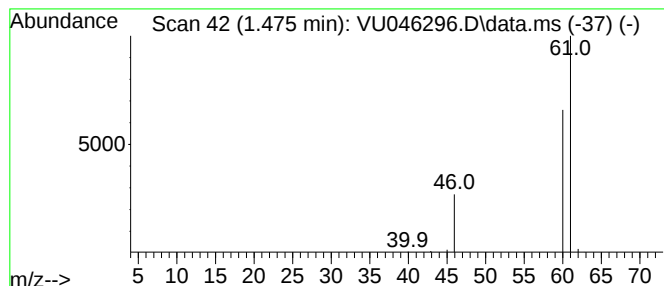
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.475	10.06 ug/L	73278	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl nitrite	61	CH3NO2	000624-91-9	5
2			o-Ethylhydroxylamine	61	C2H7NO	000624-86-2	4
3			Cyanogen chloride	61	CClN	000506-77-4	4
4			Trifluoroguanidine	113	CH2F3N3	037950-72-4	4
5			Cyanogen chloride	61	CClN	000506-77-4	4



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.475	10.1	ug/L	73278	1	6.253	364255	50.0