

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121521\
 Data File : VU046390.D
 Acq On : 15 Dec 2021 12:29
 Operator : SY/MD
 Sample : M4997-02DL 5X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW5Q2DL

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: VU046390.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	35	42	54	rVB	64686	64061	13.10%	1.384%
2	1.604	74	82	102	rBV2	60331	75873	15.52%	1.639%
3	1.919	172	180	199	rBV	40463	57106	11.68%	1.234%
4	2.009	206	208	214	rBV2	427	289	0.06%	0.006%
5	2.327	305	307	311	rVB2	329	148	0.03%	0.003%
6	2.430	337	339	342	rVB	227	123	0.03%	0.003%
7	2.450	342	345	350	rVB	237	178	0.04%	0.004%
8	2.575	372	384	411	rBV	94072	157832	32.28%	3.410%
9	2.723	427	430	433	rVB	179	143	0.03%	0.003%
10	2.784	446	449	451	rBV	177	144	0.03%	0.003%
11	2.800	451	454	460	rVB	320	362	0.07%	0.008%
12	2.871	472	476	478	rBB	163	131	0.03%	0.003%
13	2.932	493	495	498	rBV	137	122	0.02%	0.003%
14	2.993	509	514	518	rBV	150	230	0.05%	0.005%
15	3.051	527	532	539	rVB3	580	773	0.16%	0.017%
16	3.105	544	549	551	rBB	157	148	0.03%	0.003%
17	3.189	566	575	585	rBB2	1017	1927	0.39%	0.042%
18	3.359	620	628	639	rBB2	3355	6016	1.23%	0.130%
19	3.459	657	659	663	rBB	141	121	0.02%	0.003%
20	3.536	680	683	686	rBB	168	133	0.03%	0.003%
21	3.877	773	789	807	rBV	51273	120715	24.69%	2.608%
22	3.938	807	808	816	rVB	252	146	0.03%	0.003%
23	4.671	1013	1036	1066	rBV2	124865	376789	77.06%	8.141%
24	4.803	1074	1077	1083	rVB	198	139	0.03%	0.003%
25	4.871	1094	1098	1101	rBV2	141	122	0.02%	0.003%
26	4.909	1108	1110	1114	rVB2	214	148	0.03%	0.003%
27	5.067	1144	1159	1177	rBV	93257	203590	41.64%	4.399%
28	5.150	1184	1185	1189	rVB2	283	148	0.03%	0.003%
29	5.199	1198	1200	1202	rVB2	378	155	0.03%	0.003%
30	5.224	1206	1208	1211	rVB2	191	129	0.03%	0.003%
31	5.321	1223	1238	1255	rVB2	29235	65787	13.45%	1.421%
32	5.729	1344	1365	1396	rBV2	179452	488984	100.00%	10.565%
33	6.253	1514	1528	1546	rBV	184524	344012	70.35%	7.432%
34	6.546	1610	1619	1630	rBB2	8223	14085	2.88%	0.304%
35	6.694	1651	1665	1685	rBB	117397	224654	45.94%	4.854%
36	7.186	1814	1818	1822	rBB	271	274	0.06%	0.006%

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

37	7.449	1898	1900	1902	rBV2	265	151	0.03%	0.003%
38	7.459	1902	1903	1908	rVB	247	141	0.03%	0.003%
39	7.568	1925	1937	1954	rBV	61272	106764	21.83%	2.307%
40	7.629	1954	1956	1959	rVB2	322	179	0.04%	0.004%
41	7.694	1973	1976	1978	rBB	251	136	0.03%	0.003%
42	7.903	2027	2041	2057	rBV	212210	362437	74.12%	7.831%
43	7.973	2058	2063	2072	rVB2	2372	3638	0.74%	0.079%
44	8.182	2115	2128	2144	rBV	44339	73694	15.07%	1.592%
45	8.237	2144	2145	2151	rVB	325	199	0.04%	0.004%
46	8.459	2210	2214	2215	rBV	397	271	0.06%	0.006%
47	8.481	2215	2221	2227	rVV4	1508	2441	0.50%	0.053%
48	8.555	2237	2244	2254	rVB5	5768	10018	2.05%	0.216%
49	8.636	2258	2269	2294	rBV	166294	279895	57.24%	6.047%
50	8.806	2318	2322	2325	rBB	130	136	0.03%	0.003%
51	9.022	2386	2389	2393	rBB	175	166	0.03%	0.004%
52	9.047	2394	2397	2399	rBV	148	122	0.02%	0.003%
53	9.166	2431	2434	2437	rBB	158	128	0.03%	0.003%
54	9.237	2451	2456	2459	rBV	135	189	0.04%	0.004%
55	9.298	2472	2475	2478	rBB	145	121	0.02%	0.003%
56	9.356	2489	2493	2497	rBB	132	162	0.03%	0.004%
57	9.420	2500	2513	2532	rBV	276685	450724	92.18%	9.738%
58	9.536	2546	2549	2553	rBB	148	154	0.03%	0.003%
59	9.600	2566	2569	2571	rBV	140	122	0.02%	0.003%
60	9.694	2594	2598	2603	rBB	337	345	0.07%	0.007%
61	9.755	2614	2617	2620	rBV	152	155	0.03%	0.003%
62	9.803	2629	2632	2635	rBB	166	136	0.03%	0.003%
63	10.025	2699	2701	2704	rBV	149	128	0.03%	0.003%
64	10.118	2727	2730	2732	rVV	173	130	0.03%	0.003%
65	10.266	2773	2776	2779	rBV	154	159	0.03%	0.003%
66	10.382	2809	2812	2815	rBV	144	156	0.03%	0.003%
67	10.504	2846	2850	2856	rBB	167	244	0.05%	0.005%
68	10.542	2858	2862	2866	rBB	131	159	0.03%	0.003%
69	10.652	2893	2896	2899	rBB	149	128	0.03%	0.003%
70	10.674	2899	2903	2909	rBV	424	551	0.11%	0.012%
71	10.758	2915	2929	2947	rBV	183056	290693	59.45%	6.280%
72	10.867	2957	2963	2965	rBV	188	234	0.05%	0.005%
73	10.896	2965	2972	2984	rVB2	1208	2314	0.47%	0.050%
74	11.031	3011	3014	3017	rBV	160	160	0.03%	0.003%
75	11.083	3027	3030	3034	rBB	195	174	0.04%	0.004%
76	11.253	3080	3083	3086	rBV	168	160	0.03%	0.003%

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 Title : VOC Analysis

77	11.349	3108	3113	3115	rBV	181	210	0.04%	0.005%
78	11.568	3177	3181	3189	rVB	204	323	0.07%	0.007%
79	11.668	3209	3212	3215	rBV	144	149	0.03%	0.003%
80	11.700	3218	3222	3225	rBV	254	184	0.04%	0.004%
81	11.812	3245	3257	3274	rBV	297356	458315	93.73%	9.902%
82	11.980	3305	3309	3311	rBV	186	155	0.03%	0.003%
83	12.195	3364	3376	3392	rBV	233845	371535	75.98%	8.027%
84	12.465	3457	3460	3462	rBV	172	146	0.03%	0.003%
85	12.517	3472	3476	3478	rBV	155	137	0.03%	0.003%
86	12.777	3550	3557	3564	rVB2	554	730	0.15%	0.016%
87	12.890	3587	3592	3594	rBV	204	234	0.05%	0.005%
88	13.854	3888	3892	3895	rBV2	298	221	0.05%	0.005%
89	14.340	4042	4043	4047	rVB	294	127	0.03%	0.003%
90	14.394	4058	4060	4071	rVB	145	153	0.03%	0.003%
91	14.578	4109	4117	4124	rBV2	224	335	0.07%	0.007%
92	14.902	4215	4218	4220	rBV	170	122	0.02%	0.003%
93	15.455	4387	4390	4397	rBV2	235	235	0.05%	0.005%
94	15.610	4436	4438	4441	rBV	145	122	0.02%	0.003%
95	15.648	4447	4450	4453	rBV	218	143	0.03%	0.003%
96	15.777	4485	4490	4492	rBV2	227	246	0.05%	0.005%
97	15.848	4506	4512	4515	rBV2	199	261	0.05%	0.006%
98	15.941	4537	4541	4543	rBV	140	136	0.03%	0.003%
99	16.828	4815	4817	4822	rBV3	391	263	0.05%	0.006%
100	16.902	4838	4840	4845	rBV	327	289	0.06%	0.006%

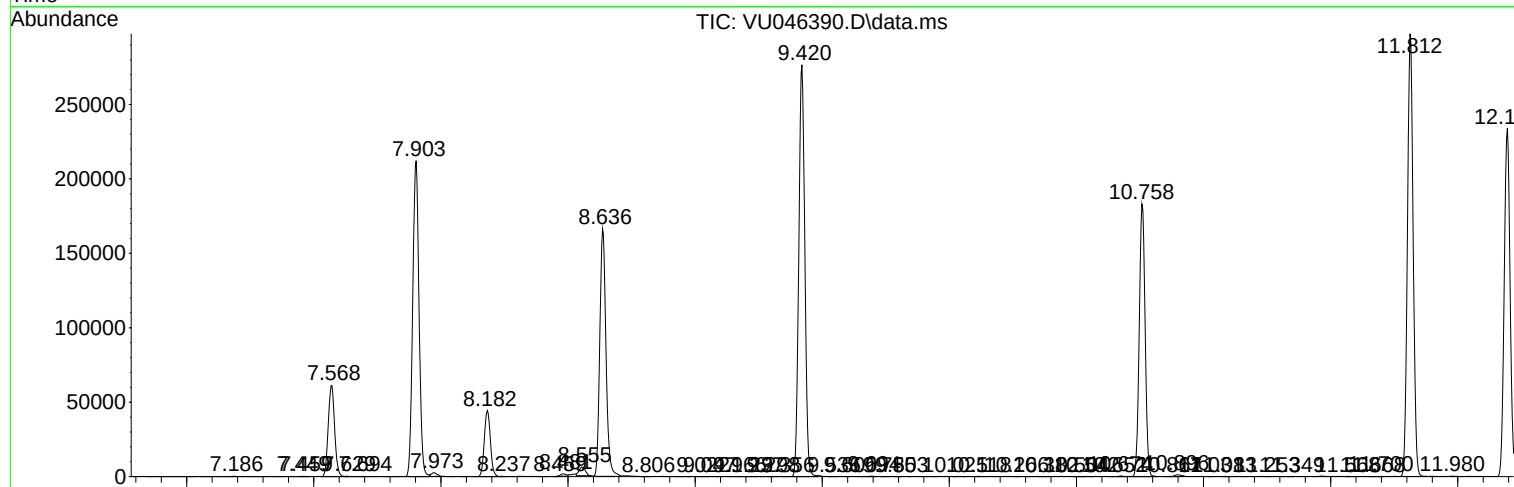
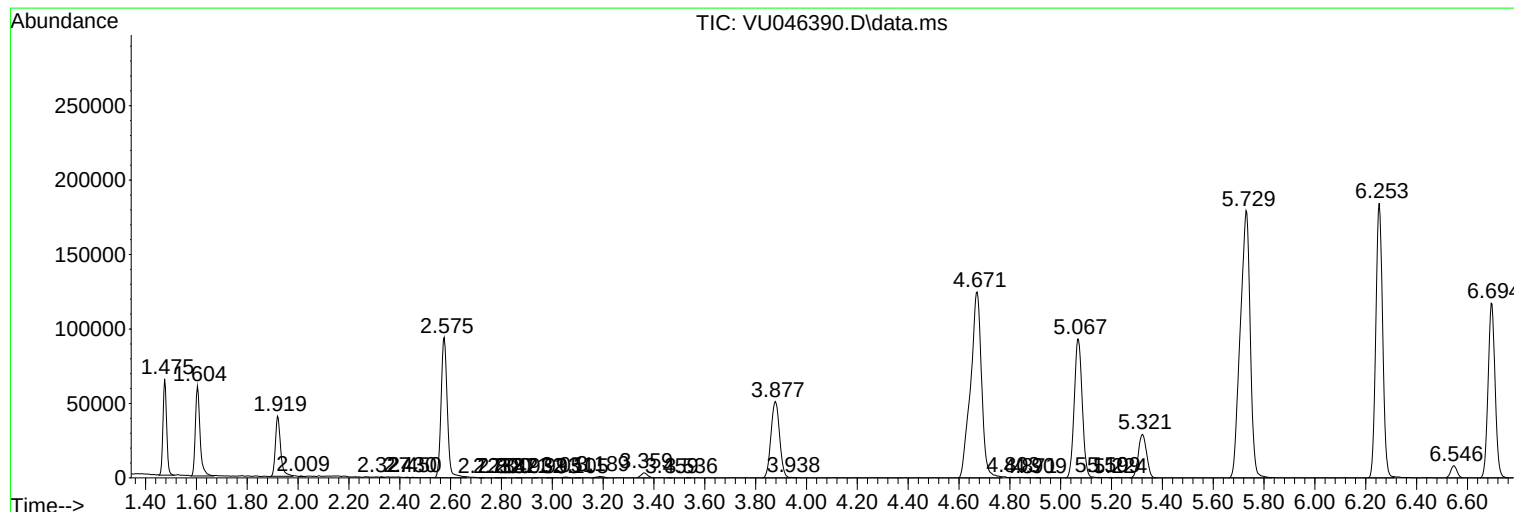
Sum of corrected areas: 4628522

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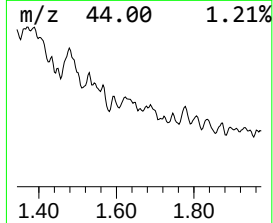
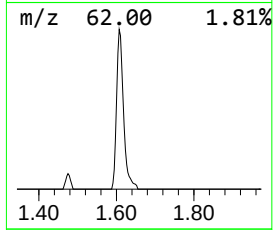
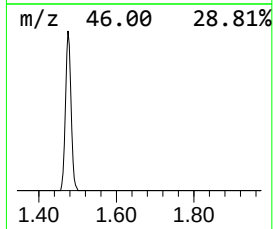
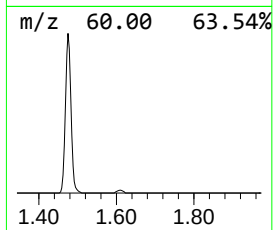
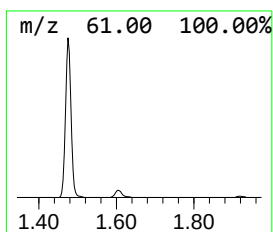
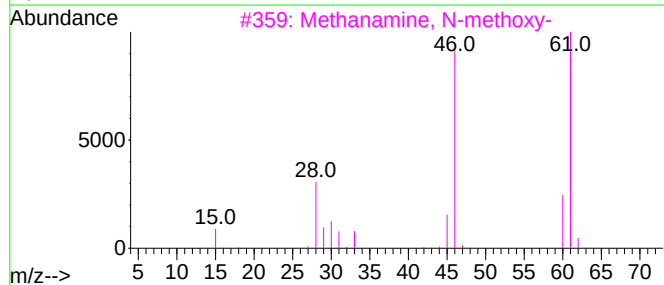
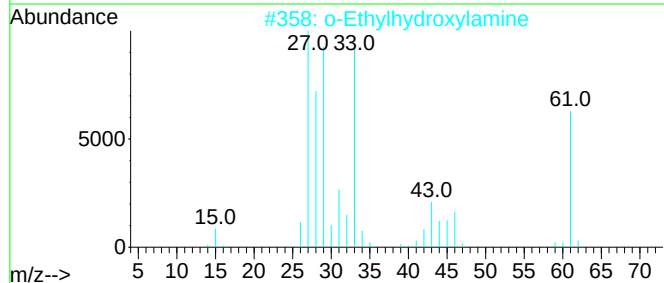
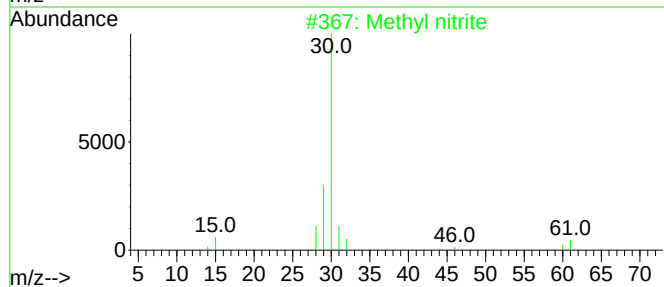
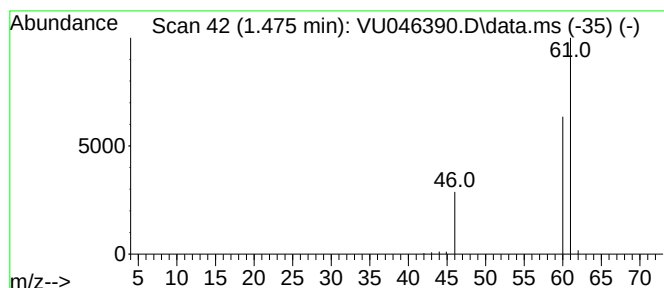
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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	9.31 ug/L	64061	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			Methanamine, N-methoxy-	61	C2H7NO	001117-97-1	4
4			Methyl formate	60	C2H4O2	000107-31-3	3
5			Urea	60	CH4N2O	000057-13-6	3



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.475	9.3	ug/L	64061	1	6.253	344012	50.0