

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121921\
 Data File : VU046498.D
 Acq On : 19 Dec 2021 16:31
 Operator : SY/MD
 Sample : M5103-02DL 40X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AW1DL

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: VU046498.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	36	42	54	rVB	23390	23587	4.41%	0.494%
2	1.604	74	82	101	rBV	59735	72418	13.53%	1.515%
3	1.854	158	160	161	rBV	247	114	0.02%	0.002%
4	1.922	171	181	197	rBV	44932	64274	12.01%	1.345%
5	2.096	233	235	238	rVB	319	153	0.03%	0.003%
6	2.205	266	269	271	rBV	253	174	0.03%	0.004%
7	2.231	274	277	279	rBV	193	157	0.03%	0.003%
8	2.427	336	338	344	rVB	235	133	0.02%	0.003%
9	2.575	372	384	409	rBV	108382	180756	33.78%	3.783%
10	2.748	436	438	443	rBB	152	123	0.02%	0.003%
11	2.777	444	447	448	rBV	131	95	0.02%	0.002%
12	2.803	452	455	459	rVB	162	162	0.03%	0.003%
13	2.867	471	475	478	rBV	149	167	0.03%	0.003%
14	3.054	529	533	539	rBB3	698	743	0.14%	0.016%
15	3.189	566	575	586	rBB	1503	2888	0.54%	0.060%
16	3.362	625	629	630	rBV	265	218	0.04%	0.005%
17	4.350	933	936	939	rBB	134	118	0.02%	0.002%
18	4.658	1013	1032	1065	rBV2	47513	186363	34.83%	3.900%
19	5.067	1143	1159	1179	rBV	101539	218700	40.87%	4.577%
20	5.729	1344	1365	1393	rBV2	195621	535132	100.00%	11.198%
21	6.124	1485	1488	1491	rBB	139	120	0.02%	0.003%
22	6.253	1514	1528	1551	rBV	171219	320392	59.87%	6.705%
23	6.546	1605	1619	1642	rBV	159017	295038	55.13%	6.174%
24	6.693	1652	1665	1683	rBV2	124829	241497	45.13%	5.054%
25	6.767	1685	1688	1691	rBB	243	173	0.03%	0.004%
26	6.803	1696	1699	1701	rBB	213	103	0.02%	0.002%
27	7.185	1813	1818	1824	rBB	259	381	0.07%	0.008%
28	7.568	1925	1937	1958	rBV	68119	116295	21.73%	2.434%
29	7.690	1971	1975	1978	rBV2	285	254	0.05%	0.005%
30	7.899	2026	2040	2055	rBV	239410	411261	76.85%	8.606%
31	7.970	2057	2062	2072	rVV2	3152	5136	0.96%	0.107%
32	8.073	2091	2094	2097	rVB	259	164	0.03%	0.003%
33	8.182	2116	2128	2143	rBV	47780	78940	14.75%	1.652%
34	8.240	2145	2146	2149	rVB2	238	130	0.02%	0.003%
35	8.285	2158	2160	2164	rVB2	235	149	0.03%	0.003%
36	8.475	2210	2219	2228	rBV2	673	1237	0.23%	0.026%

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Integrator: RTE

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

37	8.555	2232	2244	2257	rVV	117563	196181	36.66%	4.105%
38	8.636	2257	2269	2301	rVV	174405	300113	56.08%	6.280%
39	8.877	2341	2344	2346	rBV	162	146	0.03%	0.003%
40	8.938	2360	2363	2365	rBV	128	114	0.02%	0.002%
41	9.095	2408	2412	2415	rBV	141	145	0.03%	0.003%
42	9.150	2424	2429	2434	rBV	141	240	0.04%	0.005%
43	9.176	2435	2437	2441	rVB	175	148	0.03%	0.003%
44	9.211	2445	2448	2451	rBB	136	115	0.02%	0.002%
45	9.259	2460	2463	2465	rBB	151	102	0.02%	0.002%
46	9.291	2470	2473	2477	rBB	185	166	0.03%	0.003%
47	9.417	2500	2512	2529	rBV	253191	416504	77.83%	8.716%
48	9.526	2543	2546	2549	rVB	165	137	0.03%	0.003%
49	9.639	2578	2581	2585	rBB	159	159	0.03%	0.003%
50	9.700	2596	2600	2607	rVB3	324	321	0.06%	0.007%
51	9.764	2617	2620	2623	rBV	129	129	0.02%	0.003%
52	9.822	2635	2638	2642	rBV	129	158	0.03%	0.003%
53	10.012	2693	2697	2699	rBV	152	151	0.03%	0.003%
54	10.095	2718	2723	2726	rBV	167	202	0.04%	0.004%
55	10.127	2731	2733	2736	rVB	167	109	0.02%	0.002%
56	10.208	2753	2758	2763	rBB	154	231	0.04%	0.005%
57	10.246	2767	2770	2772	rBV	149	131	0.02%	0.003%
58	10.288	2779	2783	2787	rBB	150	173	0.03%	0.004%
59	10.404	2816	2819	2822	rVB	178	143	0.03%	0.003%
60	10.436	2825	2829	2834	rBB	190	200	0.04%	0.004%
61	10.465	2835	2838	2840	rBV	149	126	0.02%	0.003%
62	10.500	2847	2849	2851	rBV	141	100	0.02%	0.002%
63	10.558	2862	2867	2869	rBB	129	140	0.03%	0.003%
64	10.587	2874	2876	2880	rBV	120	132	0.02%	0.003%
65	10.626	2884	2888	2889	rBV	149	126	0.02%	0.003%
66	10.671	2896	2902	2909	rBV2	682	608	0.11%	0.013%
67	10.758	2917	2929	2948	rVB	190160	301290	56.30%	6.305%
68	10.902	2969	2974	2981	rVB2	445	673	0.13%	0.014%
69	10.938	2981	2985	2990	rBV	174	247	0.05%	0.005%
70	11.012	3006	3008	3011	rVB	183	122	0.02%	0.003%
71	11.034	3012	3015	3018	rBV	183	160	0.03%	0.003%
72	11.143	3043	3049	3051	rBB	163	150	0.03%	0.003%
73	11.169	3052	3057	3060	rBV	222	240	0.04%	0.005%
74	11.455	3142	3146	3148	rBV	400	302	0.06%	0.006%
75	11.465	3148	3149	3156	rVB	384	305	0.06%	0.006%
76	11.635	3196	3202	3211	rBV	108	176	0.03%	0.004%

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Integration Parameters: LSCINT.P

Integrator: RTE

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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

77	11.812	3244	3257	3276	rVB	263295	409232	76.47%	8.564%
78	11.944	3294	3298	3301	rVB	255	239	0.04%	0.005%
79	11.970	3301	3306	3312	rVV	510	624	0.12%	0.013%
80	12.195	3363	3376	3391	rBV	241464	385449	72.03%	8.066%
81	12.777	3550	3557	3562	rVB3	442	596	0.11%	0.012%
82	13.610	3812	3816	3819	rBV	124	114	0.02%	0.002%
83	13.667	3831	3834	3837	rBV	150	118	0.02%	0.002%
84	14.204	3998	4001	4004	rBV	115	96	0.02%	0.002%
85	14.304	4029	4032	4037	rVB	145	98	0.02%	0.002%
86	14.574	4111	4116	4118	rBV2	682	622	0.12%	0.013%
87	14.883	4207	4212	4218	rBV	168	248	0.05%	0.005%
88	15.147	4292	4294	4297	rVB	198	109	0.02%	0.002%
89	15.474	4393	4396	4400	rBV2	161	141	0.03%	0.003%
90	15.520	4407	4410	4412	rVB	179	110	0.02%	0.002%
91	15.577	4425	4428	4431	rBV2	199	117	0.02%	0.002%
92	15.603	4433	4436	4438	rBV	232	146	0.03%	0.003%
93	15.677	4456	4459	4462	rBV2	206	124	0.02%	0.003%
94	15.709	4466	4469	4475	rVB	248	188	0.04%	0.004%
95	15.738	4475	4478	4480	rBV	224	153	0.03%	0.003%
96	15.793	4492	4495	4501	rBV2	342	317	0.06%	0.007%
97	15.989	4552	4556	4558	rBV2	269	238	0.04%	0.005%
98	16.185	4614	4617	4621	rVB2	330	239	0.04%	0.005%
99	16.481	4703	4709	4713	rBV3	339	397	0.07%	0.008%
100	16.989	4865	4867	4868	rBV	392	132	0.02%	0.003%

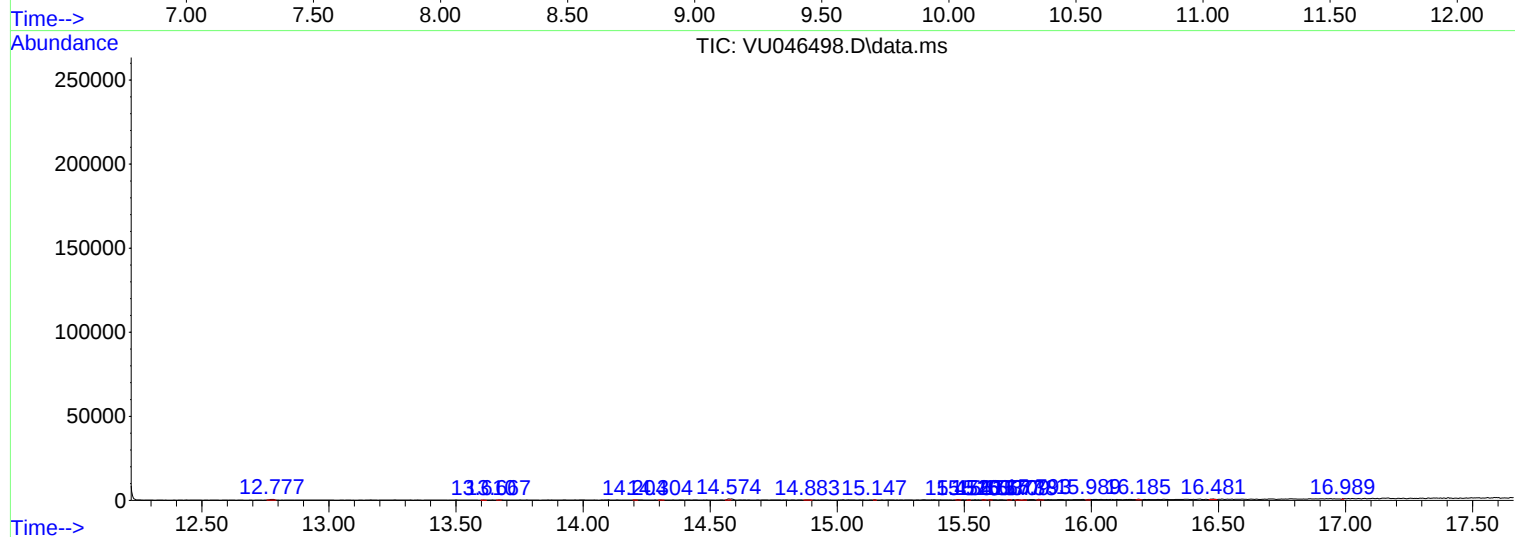
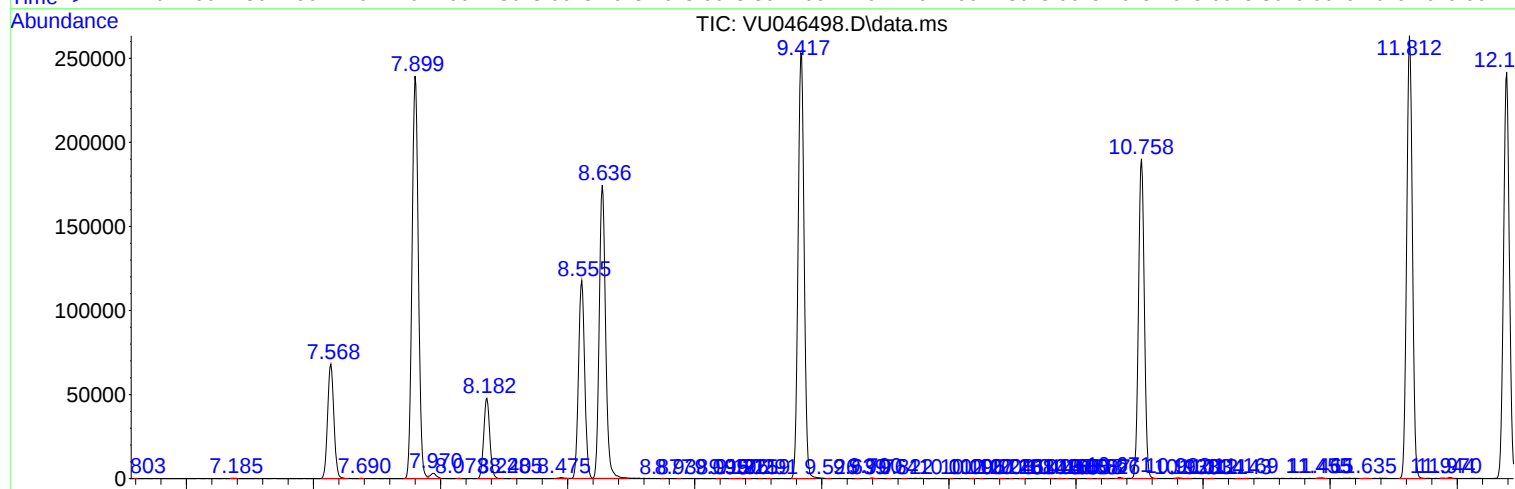
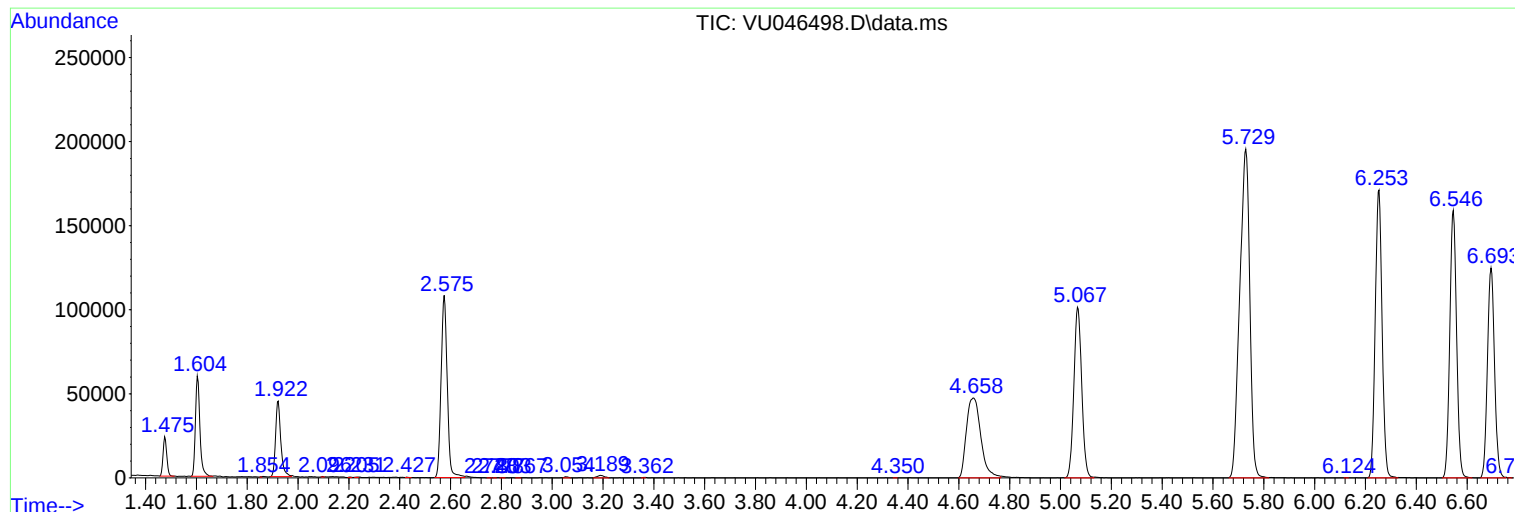
Sum of corrected areas: 4778707

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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AW1DL

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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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

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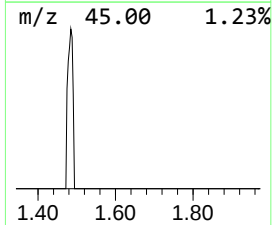
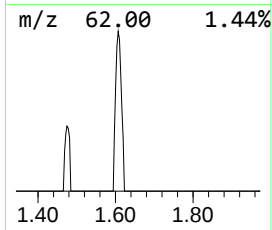
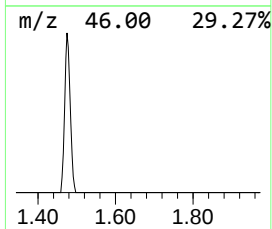
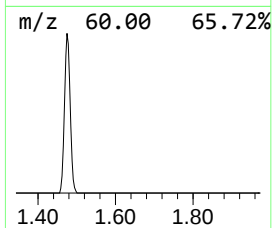
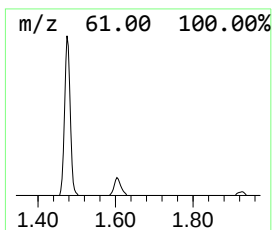
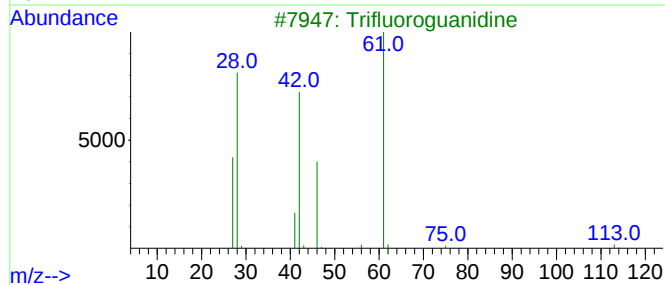
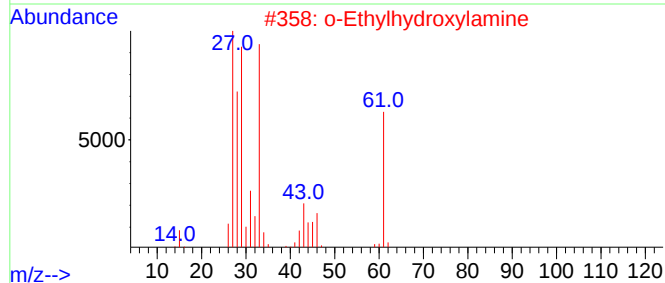
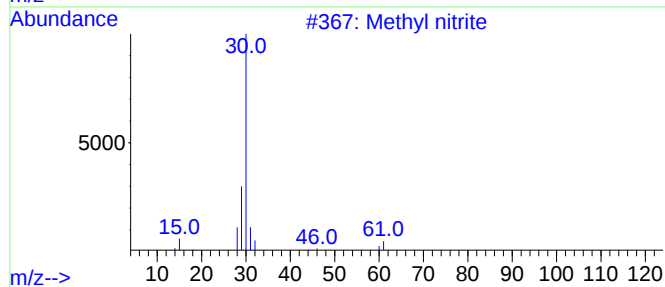
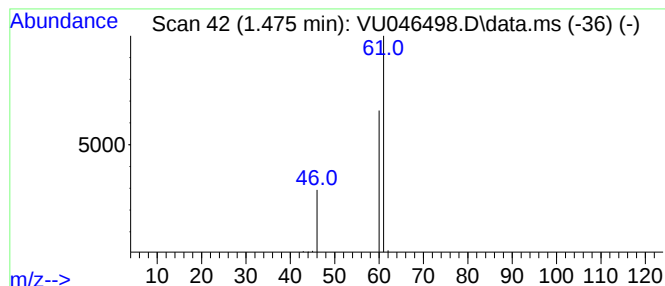
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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	3.68 ug/L	23587	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			Trifluoroguanidine	113	CH2F3N3	037950-72-4	4
4			Methyl formate	60	C2H4O2	000107-31-3	3
5			Urea	60	CH4N2O	000057-13-6	3



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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
unknown-01	1.475	3.7	ug/L	23587	1	6.253	320392	50.0