

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100622\
 Data File : VU051170.D
 Acq On : 06 Oct 2022 14:34
 Operator : JC/MD
 Sample : N4893-04
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5J41

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\SFAMULM092922WMA.M
 Title : VOC Analysis

Signal : TIC: VU051170.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.472	35	41	52	rBV	133733	138370	6.11%	0.979%
2	1.597	75	80	115	rVB	200113	274808	12.14%	1.944%
3	1.900	167	174	193	rVB	163434	225046	9.94%	1.592%
4	2.562	369	380	395	rVB	280640	452920	20.00%	3.204%
5	3.183	564	573	587	rVB	11444	23605	1.04%	0.167%
6	3.363	618	629	648	rVB	12332	26741	1.18%	0.189%
7	3.430	648	650	651	rBV	248	86	0.00%	0.001%
8	3.465	657	661	665	rBV2	458	466	0.02%	0.003%
9	3.594	698	701	704	rBV2	338	270	0.01%	0.002%
10	3.716	736	739	741	rBV	266	179	0.01%	0.001%
11	3.829	772	774	777	rBV	263	128	0.01%	0.001%
12	3.928	802	805	807	rBV	350	246	0.01%	0.002%
13	4.022	831	834	836	rBV	334	196	0.01%	0.001%
14	4.038	837	839	843	rVB2	394	211	0.01%	0.001%
15	4.063	844	847	848	rBV2	584	356	0.02%	0.003%
16	4.134	866	869	871	rBV	228	155	0.01%	0.001%
17	4.234	897	900	902	rBV2	271	163	0.01%	0.001%
18	4.247	902	904	908	rVB	369	221	0.01%	0.002%
19	4.356	934	938	941	rBV	284	250	0.01%	0.002%
20	4.385	945	947	952	rVB2	366	271	0.01%	0.002%
21	4.411	952	955	958	rBV	351	214	0.01%	0.002%
22	4.436	959	963	967	rBV2	345	318	0.01%	0.002%
23	4.475	971	975	978	rBV	353	332	0.01%	0.002%
24	4.562	999	1002	1003	rBV2	187	119	0.01%	0.001%
25	4.620	1008	1020	1053	rBV	166949	424490	18.75%	3.003%
26	4.961	1123	1126	1129	rBV2	539	363	0.02%	0.003%
27	5.060	1140	1157	1185	rBV	306869	671653	29.66%	4.751%
28	5.427	1269	1271	1272	rBV2	199	63	0.00%	0.000%
29	5.465	1280	1283	1286	rVB	193	123	0.01%	0.001%
30	5.494	1286	1292	1294	rBV2	311	357	0.02%	0.003%
31	5.510	1294	1297	1298	rBV	520	297	0.01%	0.002%
32	5.568	1312	1315	1317	rBV2	239	161	0.01%	0.001%
33	5.600	1321	1325	1326	rBV	149	106	0.00%	0.001%
34	5.626	1330	1333	1335	rBV	263	146	0.01%	0.001%
35	5.723	1341	1363	1390	rBV2	608209	1654890	73.09%	11.707%
36	6.051	1462	1465	1470	rVB2	467	304	0.01%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100622\
 Data File : VU051170.D
 Acq On : 06 Oct 2022 14:34
 Operator : JC/MD
 Sample : N4893-04
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5J41

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\SFAMULM092922WMA.M
 Title : VOC Analysis

37	6.134	1489	1491	1493	rVB	318	127	0.01%	0.001%
38	6.179	1502	1505	1511	rVB3	317	243	0.01%	0.002%
39	6.247	1511	1526	1545	rBV	426680	816213	36.05%	5.774%
40	6.536	1605	1616	1627	rBV8	7206	14939	0.66%	0.106%
41	6.594	1632	1634	1638	rBV	515	441	0.02%	0.003%
42	6.687	1646	1663	1683	rBV	406642	786514	34.74%	5.564%
43	6.906	1728	1731	1734	rVB2	356	235	0.01%	0.002%
44	6.925	1734	1737	1740	rBV	368	216	0.01%	0.002%
45	6.977	1751	1753	1755	rBV	307	174	0.01%	0.001%
46	6.993	1755	1758	1769	rVB2	424	653	0.03%	0.005%
47	7.102	1787	1792	1793	rBV	651	465	0.02%	0.003%
48	7.160	1808	1810	1811	rBV	246	126	0.01%	0.001%
49	7.256	1838	1840	1842	rVB	290	119	0.01%	0.001%
50	7.298	1851	1853	1855	rBV	71	39	0.00%	0.000%
51	7.324	1855	1861	1863	rBV2	339	372	0.02%	0.003%
52	7.378	1876	1878	1879	rBV	188	88	0.00%	0.001%
53	7.459	1900	1903	1911	rVB2	270	294	0.01%	0.002%
54	7.507	1911	1918	1919	rBV2	426	365	0.02%	0.003%
55	7.565	1923	1936	1953	rBV	177599	314539	13.89%	2.225%
56	7.658	1963	1965	1969	rBV2	488	305	0.01%	0.002%
57	7.793	2005	2007	2010	rBV2	665	412	0.02%	0.003%
58	7.835	2018	2020	2023	rVB	260	114	0.01%	0.001%
59	7.896	2024	2039	2053	rBV	669155	1138414	50.28%	8.053%
60	8.179	2115	2127	2150	rBV	123885	214803	9.49%	1.520%
61	8.552	2229	2243	2257	rBV	1336054	2264272	100.00%	16.018%
62	8.632	2258	2268	2312	rVB3	421834	938391	41.44%	6.638%
63	9.221	2449	2451	2457	rBV3	437	327	0.01%	0.002%
64	9.414	2498	2511	2533	rBV	633751	1050882	46.41%	7.434%
65	9.642	2579	2582	2585	rBV3	468	325	0.01%	0.002%
66	9.697	2590	2599	2609	rVB5	5577	8891	0.39%	0.063%
67	9.909	2661	2665	2667	rBV2	384	351	0.02%	0.002%
68	9.970	2681	2684	2688	rBV2	436	320	0.01%	0.002%
69	10.038	2701	2705	2710	rBV2	364	382	0.02%	0.003%
70	10.092	2719	2722	2723	rBV	893	503	0.02%	0.004%
71	10.275	2776	2779	2782	rBV	327	223	0.01%	0.002%
72	10.391	2812	2815	2817	rBV2	192	118	0.01%	0.001%
73	10.513	2851	2853	2857	rBV	253	128	0.01%	0.001%
74	10.597	2876	2879	2884	rBV2	538	391	0.02%	0.003%
75	10.623	2885	2887	2890	rBV2	292	242	0.01%	0.002%
76	10.755	2914	2928	2951	rBV	587629	967102	42.71%	6.841%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100622\
 Data File : VU051170.D
 Acq On : 06 Oct 2022 14:34
 Operator : JC/MD
 Sample : N4893-04
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5J41

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\SFAMULM092922WMA.M

Title : VOC Analysis

77	10.890	2965	2970	2974	rBV3	1785	1999	0.09%	0.014%
78	11.118	3039	3041	3043	rBV	491	245	0.01%	0.002%
79	11.603	3188	3192	3196	rBV2	335	303	0.01%	0.002%
80	11.629	3196	3200	3202	rBV	521	258	0.01%	0.002%
81	11.809	3244	3256	3278	rBV	467021	751943	33.21%	5.319%
82	12.192	3362	3375	3397	rBV	587850	958197	42.32%	6.778%
83	12.716	3536	3538	3539	rBV	406	138	0.01%	0.001%
84	12.767	3549	3554	3559	rBV4	954	1226	0.05%	0.009%

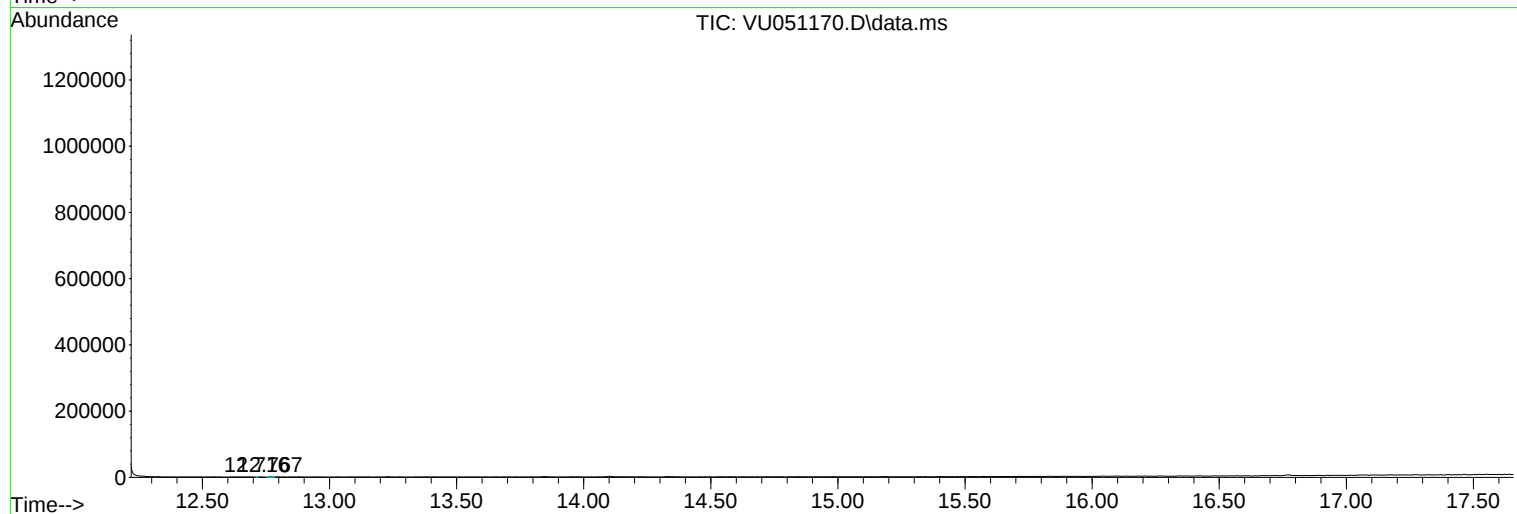
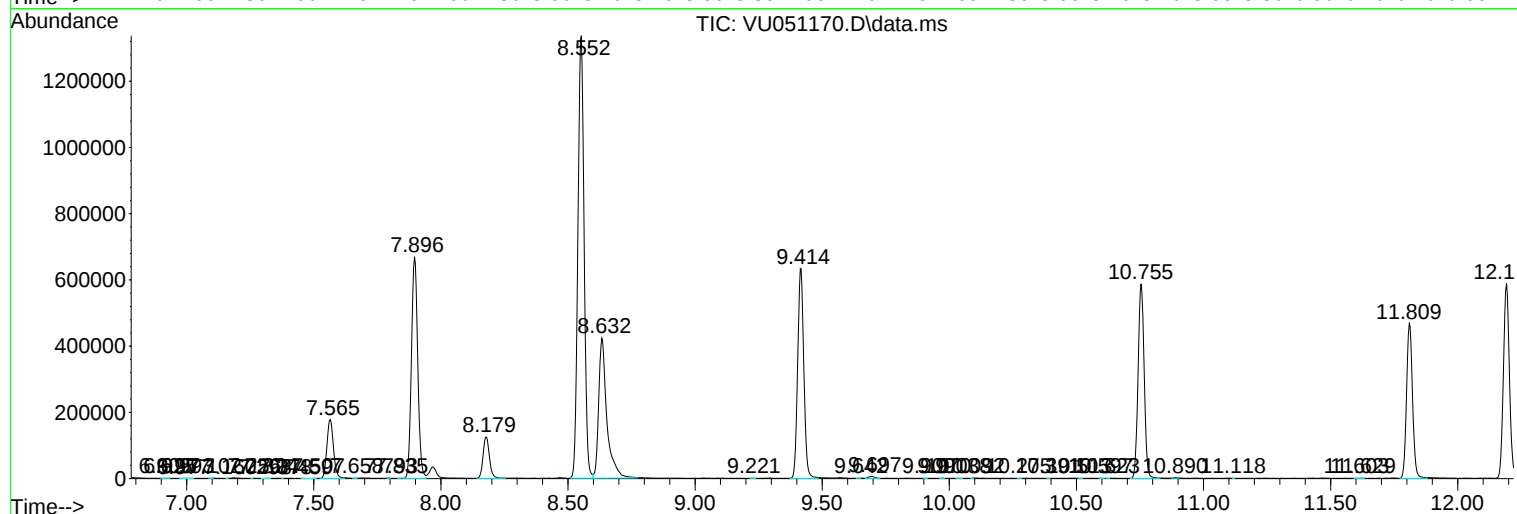
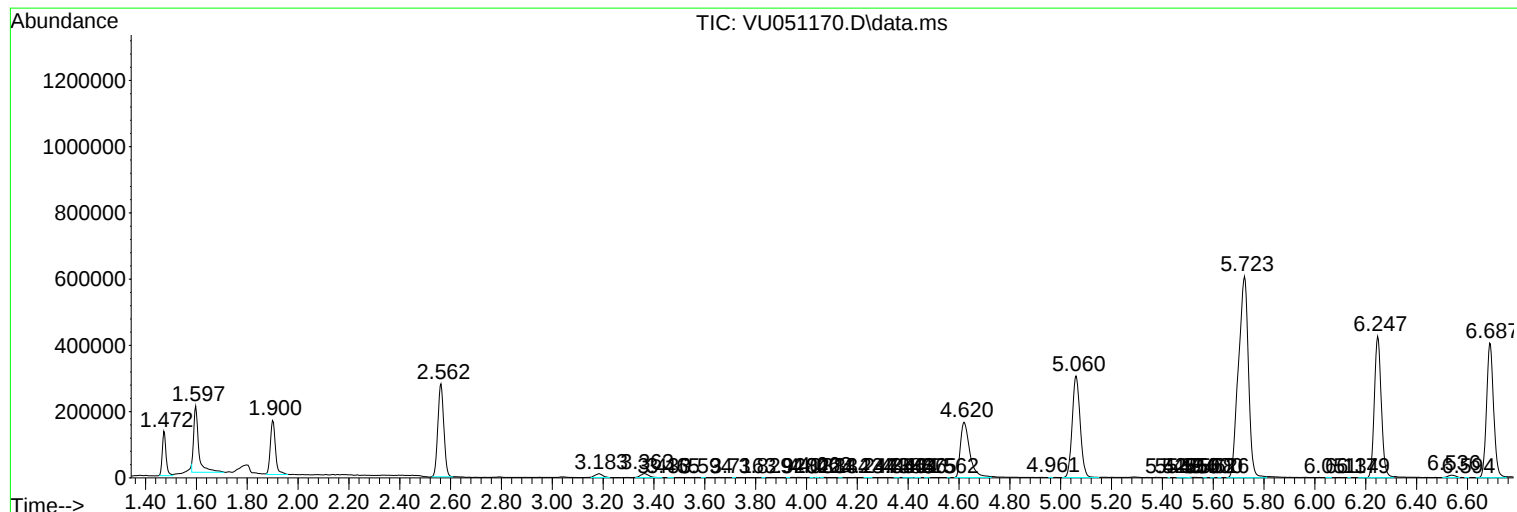
Sum of corrected areas: 14135991

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100622\
Data File : VU051170.D
Acq On : 06 Oct 2022 14:34
Operator : JC/MD
Sample : N4893-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5J41

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092922WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100622\
Data File : VU051170.D
Acq On : 06 Oct 2022 14:34
Operator : JC/MD
Sample : N4893-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5J41

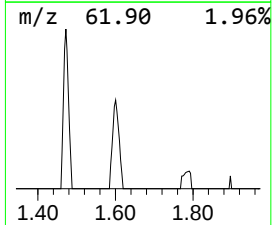
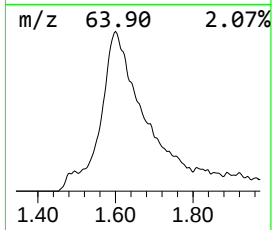
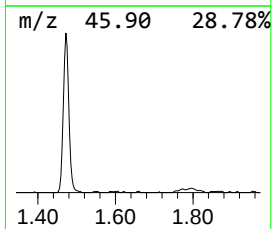
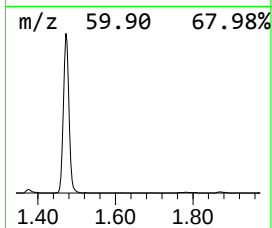
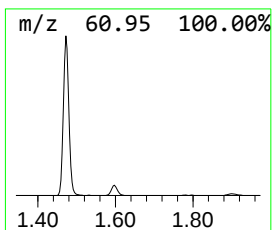
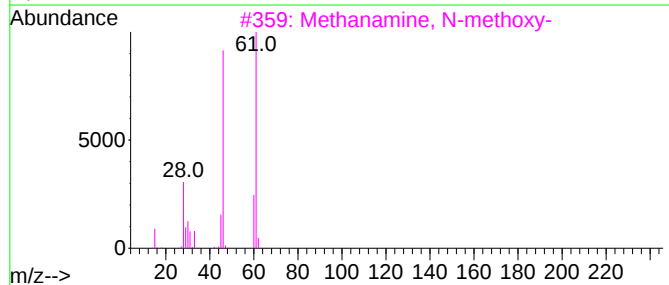
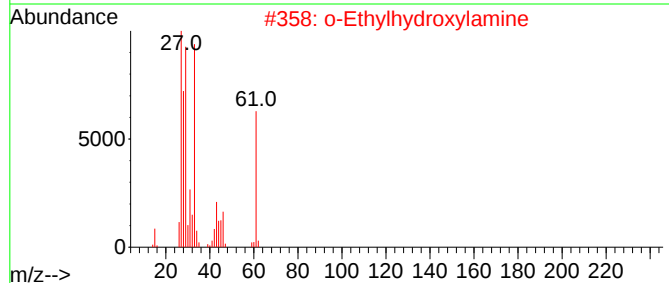
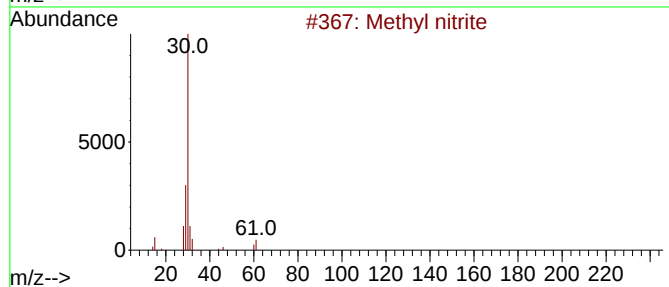
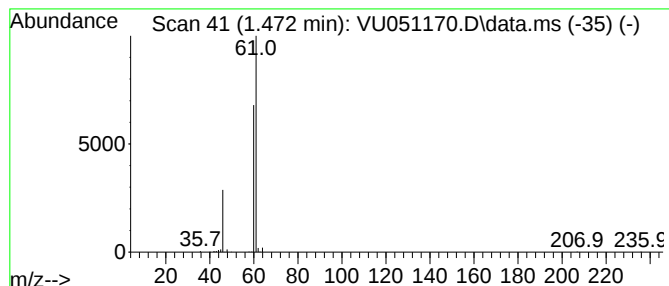
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092922WMA.M
Quant Title : VOC Analysis

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.
1.472	8.48 ug/L	138370	1,4-Difluorobenzene	6.247

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			Trifluoroguanidine	113	CH2F3N3	037950-72-4	4
5			Cyanogen chloride	61	CClN	000506-77-4	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100622\
Data File : VU051170.D
Acq On : 06 Oct 2022 14:34
Operator : JC/MD
Sample : N4893-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5J41

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092922WMA.M
Quant Title : VOC Analysis

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	1.472	8.5	ug/L	138370	1	6.247	816213	50.0