

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081622\
 Data File : VX030649.D
 Acq On : 16 Aug 2022 12:58
 Operator : JC/MD
 Sample : N4220-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A43K4

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_X\Method\SFAMXML080422WMA.M
 Title : VOC Analysis

Signal : TIC: VX030649.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	7	9	15	rVB3	9178	9787	0.77%	0.106%
2	1.246	23	26	42	rVV	315855	305662	24.08%	3.303%
3	1.368	42	46	57	rVB	150651	157310	12.39%	1.700%
4	1.666	90	95	103	rVB	107135	136154	10.73%	1.471%
5	2.306	194	200	208	rBV	256510	390926	30.80%	4.225%
6	2.380	209	212	217	rVB2	5637	8736	0.69%	0.094%
7	2.508	230	233	235	rBV2	565	737	0.06%	0.008%
8	2.642	252	255	262	rVB5	1440	2503	0.20%	0.027%
9	2.745	270	272	275	rBV2	412	442	0.03%	0.005%
10	2.782	276	278	285	rVB6	1193	1989	0.16%	0.021%
11	2.953	299	306	307	rBV3	2234	4035	0.32%	0.044%
12	3.062	322	324	325	rBV2	516	476	0.04%	0.005%
13	3.117	329	333	337	rVB2	541	804	0.06%	0.009%
14	3.215	345	349	350	rBV	359	420	0.03%	0.005%
15	3.294	359	362	363	rBV	622	534	0.04%	0.006%
16	3.440	385	386	393	rVV4	736	996	0.08%	0.011%
17	3.703	426	429	431	rBV2	556	565	0.04%	0.006%
18	3.965	470	472	475	rBV	424	430	0.03%	0.005%
19	4.020	478	481	484	rBV2	481	361	0.03%	0.004%
20	4.056	484	487	489	rBV	295	344	0.03%	0.004%
21	4.129	495	499	501	rBV2	384	586	0.05%	0.006%
22	4.300	523	527	529	rVB2	629	702	0.06%	0.008%
23	4.324	529	531	535	rVB2	370	485	0.04%	0.005%
24	4.458	545	553	570	rBV	103504	297702	23.46%	3.217%
25	4.739	597	599	603	rBV2	547	768	0.06%	0.008%
26	4.922	627	629	631	rBV	642	394	0.03%	0.004%
27	5.062	639	652	670	rBV	166271	518080	40.82%	5.599%
28	5.202	673	675	676	rBV2	525	451	0.04%	0.005%
29	5.379	699	704	705	rBV2	775	1085	0.09%	0.012%
30	5.556	727	733	741	rBV6	1894	5286	0.42%	0.057%
31	5.739	761	763	768	rBV3	476	638	0.05%	0.007%
32	5.873	783	785	786	rBV	497	366	0.03%	0.004%
33	5.976	789	802	817	rBV2	427516	1269200	100.00%	13.716%
34	6.251	843	847	849	rBV	478	547	0.04%	0.006%
35	6.342	860	862	866	rBV3	565	880	0.07%	0.010%
36	6.763	922	931	947	rBV	276807	669402	52.74%	7.234%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXMLM080422WMA.M
 Title : VOC Analysis

37	6.982	965	967	968	rBV	462	342	0.03%	0.004%
38	7.110	981	988	995	rVV4	7009	16104	1.27%	0.174%
39	7.208	999	1004	1009	rVB2	501	800	0.06%	0.009%
40	7.245	1009	1010	1013	rBV	549	527	0.04%	0.006%
41	7.312	1013	1021	1034	rBV	244458	523623	41.26%	5.659%
42	7.488	1044	1050	1055	rBV4	1309	2125	0.17%	0.023%
43	7.586	1061	1066	1072	rBV5	1066	2417	0.19%	0.026%
44	7.781	1097	1098	1101	rVV2	393	360	0.03%	0.004%
45	7.933	1119	1123	1125	rBV3	995	1454	0.11%	0.016%
46	8.104	1148	1151	1152	rBV	650	510	0.04%	0.006%
47	8.122	1152	1154	1158	rVB2	444	456	0.04%	0.005%
48	8.269	1174	1178	1179	rBV2	454	516	0.04%	0.006%
49	8.330	1181	1188	1198	rBV	157611	259037	20.41%	2.799%
50	8.446	1206	1207	1209	rVB	713	404	0.03%	0.004%
51	8.482	1210	1213	1217	rBV3	802	1295	0.10%	0.014%
52	8.574	1226	1228	1234	rBV5	1324	2000	0.16%	0.022%
53	8.653	1234	1241	1250	rBV	571519	902792	71.13%	9.756%
54	8.952	1285	1290	1298	rBV	116088	171692	13.53%	1.855%
55	9.275	1340	1343	1348	rVB3	3513	5555	0.44%	0.060%
56	9.384	1356	1361	1372	rBV	481798	682053	53.74%	7.371%
57	9.769	1423	1424	1427	rBV2	447	409	0.03%	0.004%
58	9.811	1429	1431	1434	rBV2	323	424	0.03%	0.005%
59	10.055	1465	1471	1482	rBV	579378	786310	61.95%	8.497%
60	10.201	1492	1495	1499	rBV4	1224	1622	0.13%	0.018%
61	10.433	1532	1533	1535	rVB2	653	424	0.03%	0.005%
62	10.531	1547	1549	1551	rVV2	611	476	0.04%	0.005%
63	10.573	1554	1556	1558	rVB2	507	426	0.03%	0.005%
64	10.652	1565	1569	1570	rBV2	655	780	0.06%	0.008%
65	10.774	1587	1589	1597	rVB3	1433	2494	0.20%	0.027%
66	10.829	1597	1598	1600	rBV2	535	426	0.03%	0.005%
67	10.860	1600	1603	1608	rBV5	1205	1922	0.15%	0.021%
68	11.140	1647	1649	1652	rBV2	572	792	0.06%	0.009%
69	11.195	1652	1658	1671	rVV	446945	557161	43.90%	6.021%
70	11.317	1674	1678	1684	rVV3	3261	4873	0.38%	0.053%
71	11.366	1684	1686	1688	rVV	870	492	0.04%	0.005%
72	11.457	1699	1701	1702	rBV	416	372	0.03%	0.004%
73	11.482	1703	1705	1707	rVB	980	694	0.05%	0.007%
74	11.634	1728	1730	1732	rBV2	677	522	0.04%	0.006%
75	11.744	1746	1748	1751	rBV2	802	883	0.07%	0.010%
76	11.921	1775	1777	1778	rBV	642	625	0.05%	0.007%

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
 Title : VOC Analysis

77	11.969	1782	1785	1788	rVV3	1222	1353	0.11%	0.015%
78	12.024	1789	1794	1803	rVV	592564	724871	57.11%	7.833%
79	12.110	1806	1808	1811	rVV3	1001	965	0.08%	0.010%
80	12.152	1814	1815	1817	rBV2	396	347	0.03%	0.004%
81	12.225	1822	1827	1834	rVB5	3931	6916	0.54%	0.075%
82	12.323	1837	1843	1855	rVV	615068	768718	60.57%	8.307%
83	12.427	1858	1860	1861	rVB	1017	453	0.04%	0.005%
84	12.500	1871	1872	1875	rBV	558	360	0.03%	0.004%
85	12.585	1883	1886	1887	rBV2	1007	967	0.08%	0.010%
86	12.768	1912	1916	1924	rVB2	3419	5832	0.46%	0.063%
87	12.908	1936	1939	1941	rBV3	527	539	0.04%	0.006%
88	13.414	2019	2022	2024	rBV2	691	999	0.08%	0.011%
89	13.567	2046	2047	2049	rBV2	572	445	0.04%	0.005%
90	13.859	2093	2095	2099	rVB	546	469	0.04%	0.005%
91	14.127	2136	2139	2144	rVB	2244	3474	0.27%	0.038%
92	14.188	2146	2149	2153	rBV4	1820	2453	0.19%	0.027%
93	14.426	2186	2188	2191	rBV3	509	692	0.05%	0.007%
94	14.536	2202	2206	2207	rBV2	706	766	0.06%	0.008%
95	14.579	2211	2213	2214	rBV	584	396	0.03%	0.004%
96	14.621	2218	2220	2224	rVV4	1177	1500	0.12%	0.016%
97	14.993	2276	2281	2285	rBV6	1582	2750	0.22%	0.030%
98	15.585	2377	2378	2380	rVB2	1179	559	0.04%	0.006%
99	15.609	2380	2382	2387	rBV4	878	1111	0.09%	0.012%
100	16.176	2474	2475	2478	rVB2	824	743	0.06%	0.008%

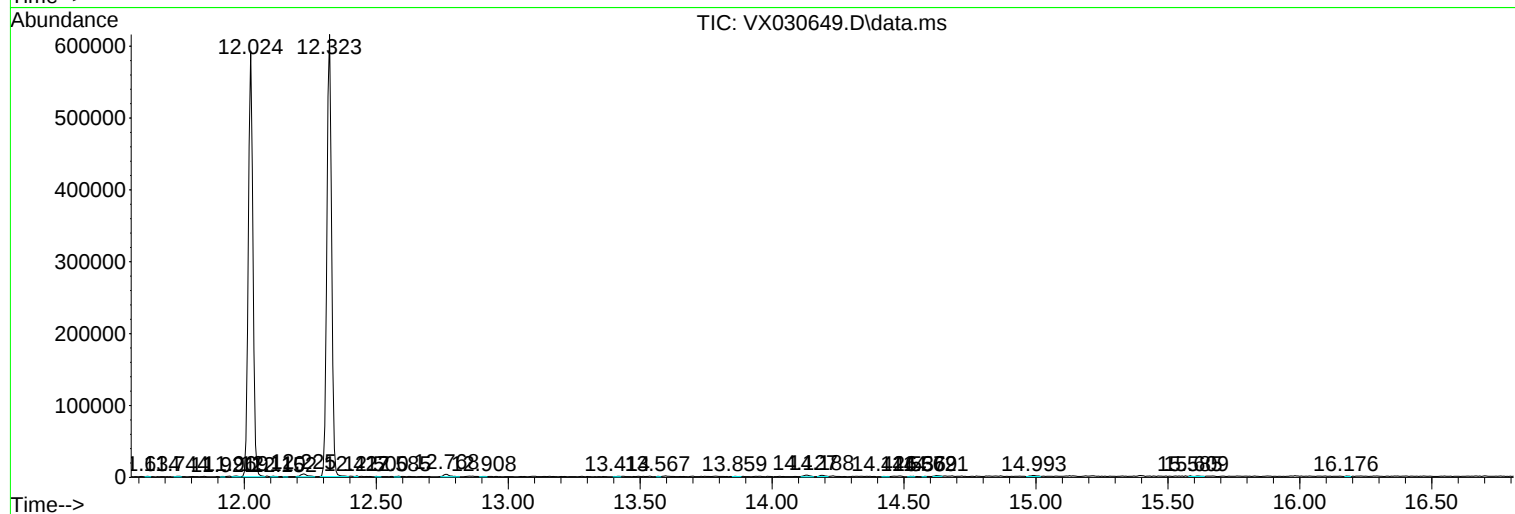
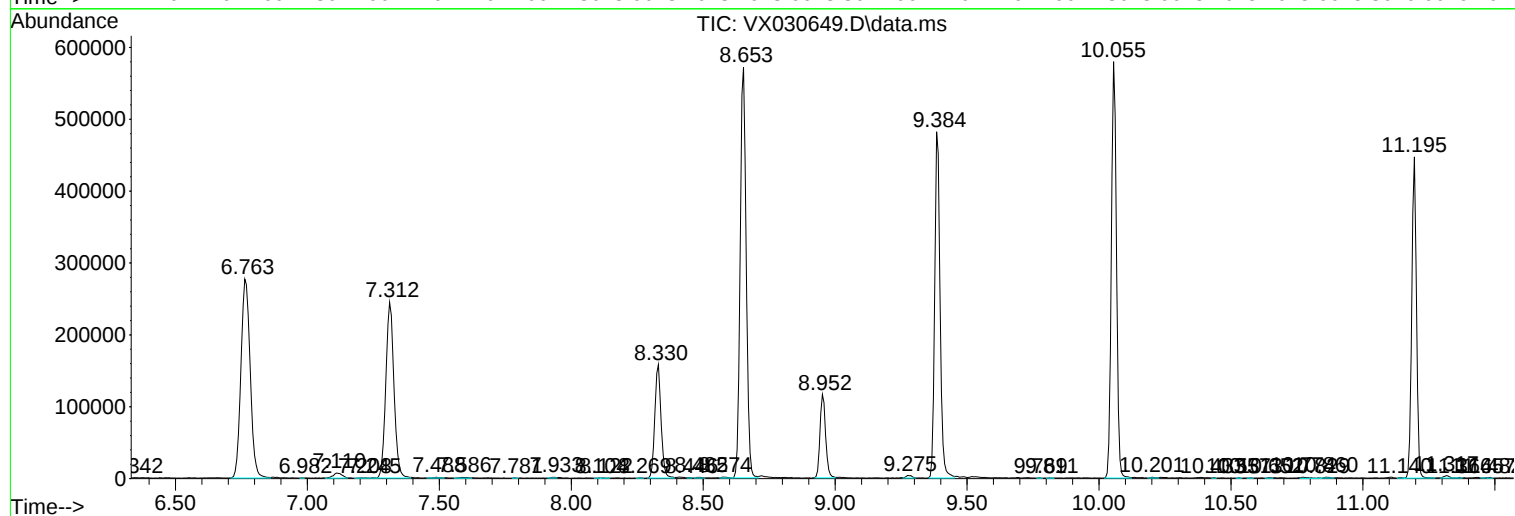
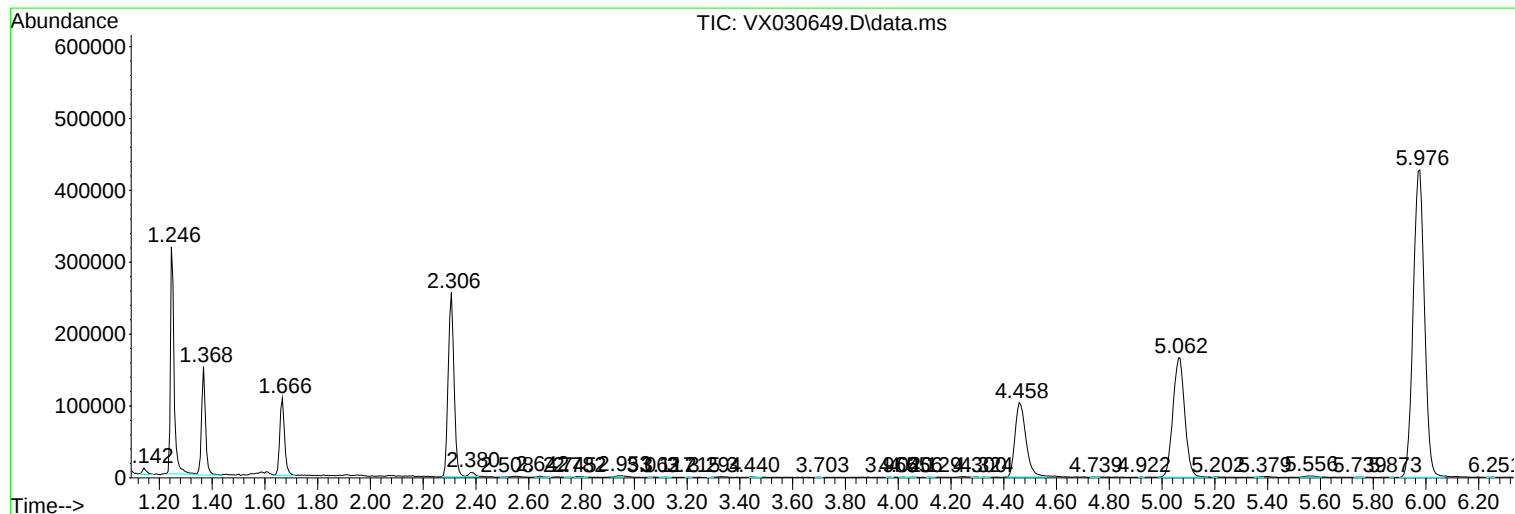
Sum of corrected areas: 9253650

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Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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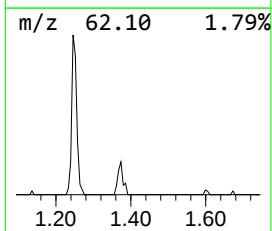
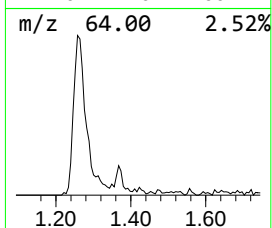
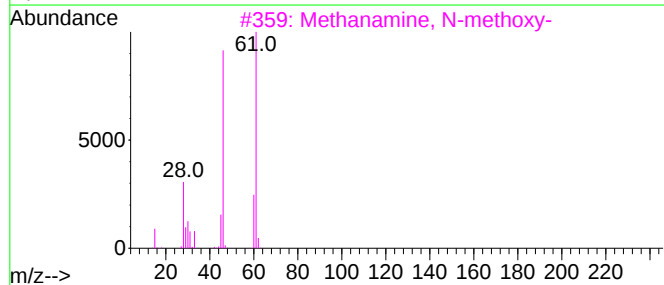
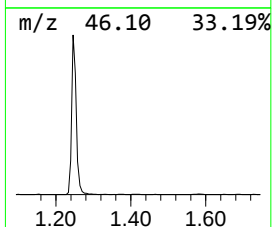
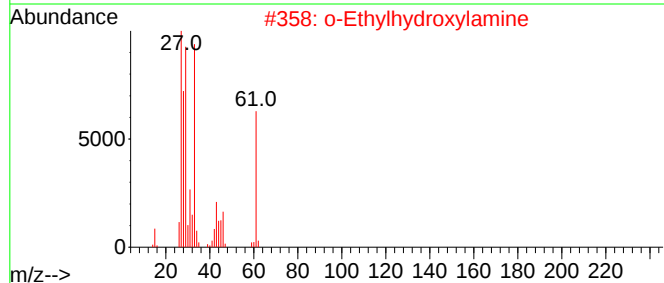
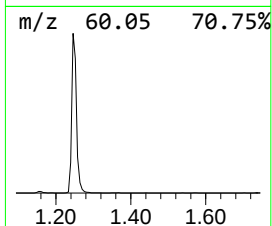
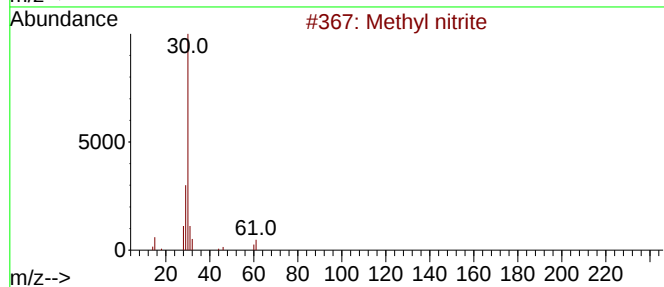
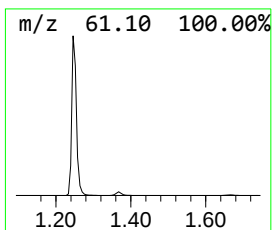
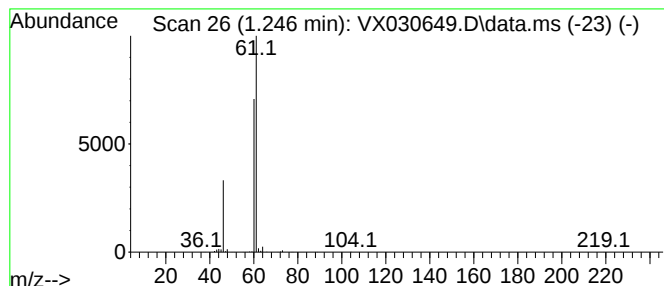
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	22.83 ug/L	305662	1,4-Difluorobenzene	6.763

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			Cyanogen chloride	61	CClN	000506-77-4	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	1.246	22.8	ug/L	305662	1	6.763	669402	50.0