

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122121\
 Data File : VX025957.D
 Acq On : 21 Dec 2021 15:22
 Operator : JC/MD
 Sample : M5150-17DL 20X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 GBBX5DL

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\SFAMXLM122021WMA.M
 Title : VOC Analysis

Signal : TIC: VX025957.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	23	27	41	rBV2	25945	32473	5.34%	0.602%
2	1.368	43	46	54	rVB	71072	72601	11.94%	1.346%
3	1.666	91	95	103	rBV	64550	81424	13.39%	1.509%
4	2.307	194	200	210	rBV	111046	185017	30.43%	3.429%
5	2.489	229	230	233	rBV2	328	350	0.06%	0.006%
6	2.794	274	280	286	rBV2	1376	2597	0.43%	0.048%
7	2.947	300	305	311	rVB4	1276	2921	0.48%	0.054%
8	3.032	318	319	324	rBV3	257	338	0.06%	0.006%
9	3.355	371	372	376	rBV2	216	203	0.03%	0.004%
10	3.593	409	411	414	rBV	206	232	0.04%	0.004%
11	4.172	503	506	510	rBV	229	372	0.06%	0.007%
12	4.209	510	512	515	rVV	238	269	0.04%	0.005%
13	4.239	515	517	520	rVV2	155	183	0.03%	0.003%
14	4.270	520	522	525	rVB2	175	204	0.03%	0.004%
15	4.306	525	528	530	rVB2	172	190	0.03%	0.004%
16	4.459	544	553	567	rBV	49149	140749	23.15%	2.609%
17	4.654	583	585	588	rVB	322	274	0.05%	0.005%
18	4.940	630	632	637	rVB2	256	305	0.05%	0.006%
19	5.062	640	652	668	rBV2	82224	248273	40.84%	4.602%
20	5.397	704	707	709	rBV	228	260	0.04%	0.005%
21	5.489	721	722	725	rBV2	222	253	0.04%	0.005%
22	5.544	728	731	733	rBV	294	298	0.05%	0.006%
23	5.775	767	769	774	rBV2	203	258	0.04%	0.005%
24	5.855	780	782	784	rBV	210	223	0.04%	0.004%
25	5.970	789	801	819	rBV2	201418	607953	100.00%	11.269%
26	6.184	834	836	838	rBV2	157	176	0.03%	0.003%
27	6.312	855	857	860	rBV2	201	258	0.04%	0.005%
28	6.367	862	866	867	rVV2	239	266	0.04%	0.005%
29	6.531	890	893	896	rVB2	291	403	0.07%	0.007%
30	6.623	905	908	912	rVB2	273	287	0.05%	0.005%
31	6.763	922	931	944	rBV	140631	335223	55.14%	6.214%
32	6.982	966	967	970	rBV	252	241	0.04%	0.004%
33	7.129	982	991	1002	rBV	158866	347455	57.15%	6.440%
34	7.312	1012	1021	1033	rBV	125096	277593	45.66%	5.145%
35	7.501	1051	1052	1055	rBV2	252	225	0.04%	0.004%
36	7.641	1073	1075	1078	rBV2	225	218	0.04%	0.004%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML122021WMA.M
 Title : VOC Analysis

37	7.812	1099	1103	1104	rBV3	330	367	0.06%	0.007%
38	7.866	1109	1112	1113	rBV2	348	279	0.05%	0.005%
39	7.921	1119	1121	1122	rBV2	279	290	0.05%	0.005%
40	8.037	1137	1140	1141	rVB	323	272	0.04%	0.005%
41	8.324	1182	1187	1197	rVV	90863	151902	24.99%	2.816%
42	8.476	1210	1212	1218	rVB2	419	575	0.09%	0.011%
43	8.653	1234	1241	1249	rBV	354047	588607	96.82%	10.910%
44	8.952	1285	1290	1302	rVB	59105	87131	14.33%	1.615%
45	9.281	1339	1344	1349	rBV4	959	1154	0.19%	0.021%
46	9.385	1355	1361	1377	rBV	243579	373569	61.45%	6.924%
47	9.616	1397	1399	1402	rBV2	334	289	0.05%	0.005%
48	9.884	1441	1443	1444	rBV	231	214	0.04%	0.004%
49	9.939	1450	1452	1454	rBV2	220	219	0.04%	0.004%
50	10.055	1465	1471	1487	rVB	423082	570045	93.76%	10.566%
51	10.305	1509	1512	1515	rVB3	646	890	0.15%	0.016%
52	10.348	1518	1519	1523	rVB	403	328	0.05%	0.006%
53	10.390	1523	1526	1527	rBV	231	241	0.04%	0.004%
54	10.457	1536	1537	1542	rVB	276	291	0.05%	0.005%
55	10.500	1542	1544	1546	rBV2	236	200	0.03%	0.004%
56	10.646	1566	1568	1570	rVB2	379	299	0.05%	0.006%
57	10.848	1599	1601	1603	rBV	274	271	0.04%	0.005%
58	11.122	1642	1646	1650	rVB2	1499	2017	0.33%	0.037%
59	11.195	1652	1658	1669	rVB	320892	393462	64.72%	7.293%
60	11.281	1669	1672	1680	rBV4	758	1545	0.25%	0.029%
61	11.409	1689	1693	1696	rBV2	218	274	0.05%	0.005%
62	11.457	1698	1701	1702	rBV2	304	374	0.06%	0.007%
63	11.549	1713	1716	1718	rBV	342	310	0.05%	0.006%
64	11.719	1742	1744	1745	rBV2	310	279	0.05%	0.005%
65	11.750	1746	1749	1755	rVB5	1813	2565	0.42%	0.048%
66	11.933	1776	1779	1782	rVB2	899	829	0.14%	0.015%
67	11.982	1785	1787	1789	rBV2	278	260	0.04%	0.005%
68	12.024	1789	1794	1807	rVV	403311	489272	80.48%	9.069%
69	12.116	1807	1809	1810	rVV2	735	568	0.09%	0.011%
70	12.146	1813	1814	1821	rVV4	1252	1202	0.20%	0.022%
71	12.323	1837	1843	1853	rVB	288144	376641	61.95%	6.981%
72	12.427	1858	1860	1863	rVB2	551	451	0.07%	0.008%
73	12.567	1881	1883	1886	rVB2	159	179	0.03%	0.003%
74	12.713	1904	1907	1908	rVB	219	203	0.03%	0.004%
75	12.731	1908	1910	1912	rBV2	225	191	0.03%	0.004%
76	13.048	1959	1962	1964	rVB2	269	276	0.05%	0.005%

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Peak Location: TOP

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 Title : VOC Analysis

77	13.073	1964	1966	1970	rVB	226	193	0.03%	0.004%
78	13.213	1985	1989	1992	rVV2	178	312	0.05%	0.006%
79	13.378	2014	2016	2019	rBV	230	302	0.05%	0.006%
80	13.536	2040	2042	2045	rVV	220	242	0.04%	0.004%
81	13.585	2048	2050	2051	rVV	312	220	0.04%	0.004%
82	13.658	2060	2062	2065	rBV2	266	279	0.05%	0.005%
83	13.945	2106	2109	2113	rBV2	188	329	0.05%	0.006%
84	14.365	2176	2178	2181	rBV2	179	192	0.03%	0.004%
85	14.426	2186	2188	2190	rBV2	332	370	0.06%	0.007%
86	14.749	2239	2241	2246	rBV2	156	217	0.04%	0.004%
87	14.914	2266	2268	2271	rVB2	255	257	0.04%	0.005%
88	15.066	2291	2293	2296	rBV2	207	174	0.03%	0.003%
89	15.188	2312	2313	2315	rBV2	358	265	0.04%	0.005%
90	15.353	2337	2340	2343	rBV3	203	331	0.05%	0.006%
91	15.597	2377	2380	2381	rBV2	158	186	0.03%	0.003%
92	15.627	2383	2385	2388	rVB2	295	226	0.04%	0.004%
93	15.676	2391	2393	2396	rBV3	195	203	0.03%	0.004%
94	15.774	2406	2409	2411	rBV2	253	209	0.03%	0.004%
95	16.109	2463	2464	2466	rBV	353	313	0.05%	0.006%
96	16.249	2485	2487	2490	rVV2	169	211	0.03%	0.004%
97	16.286	2492	2493	2495	rVV2	296	185	0.03%	0.003%
98	16.469	2521	2523	2526	rBV2	403	421	0.07%	0.008%
99	16.511	2529	2530	2533	rVB2	357	246	0.04%	0.005%
100	16.572	2539	2540	2545	rVB2	211	205	0.03%	0.004%

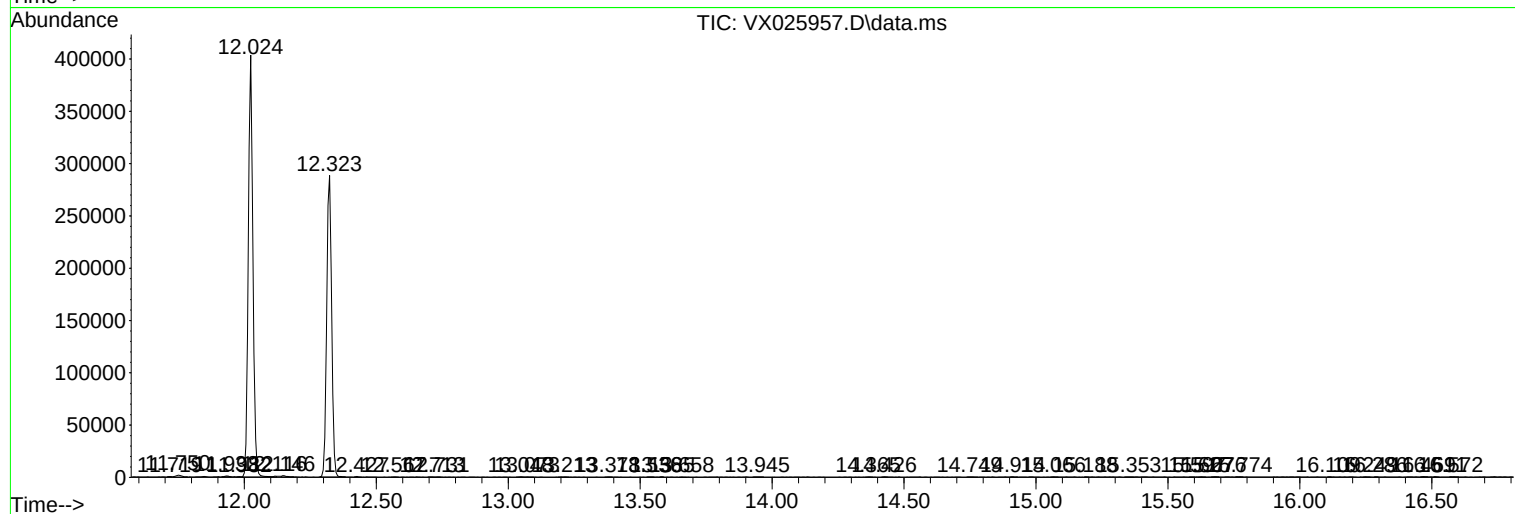
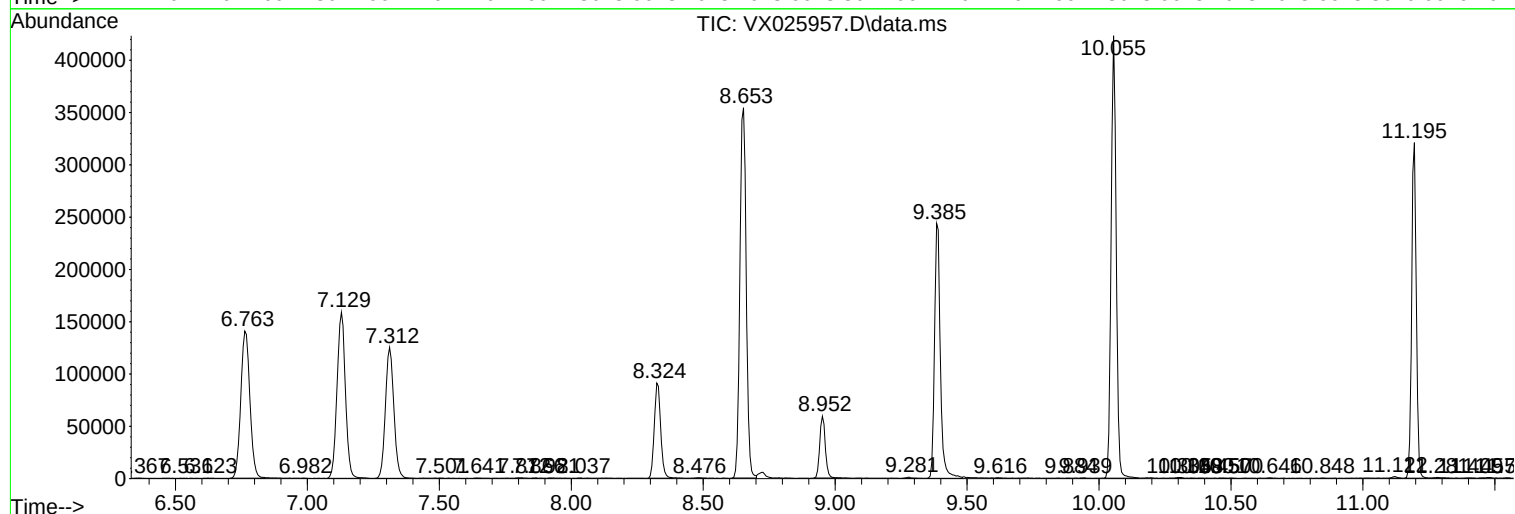
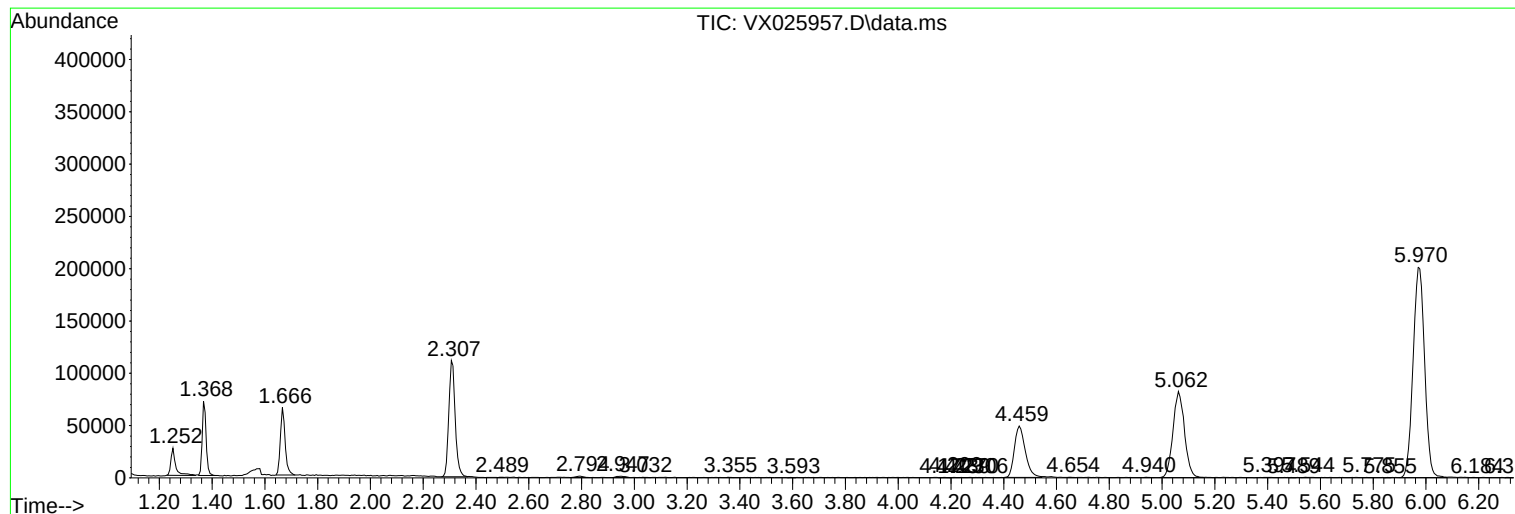
Sum of corrected areas: 5394984

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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GBBX5DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122021WMA.M
Quant Title : VOC Analysis

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



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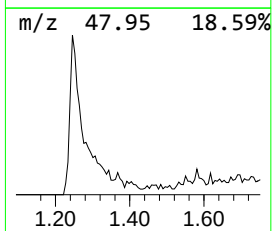
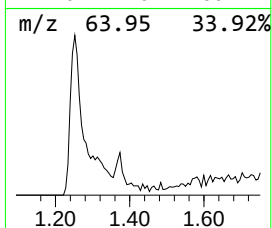
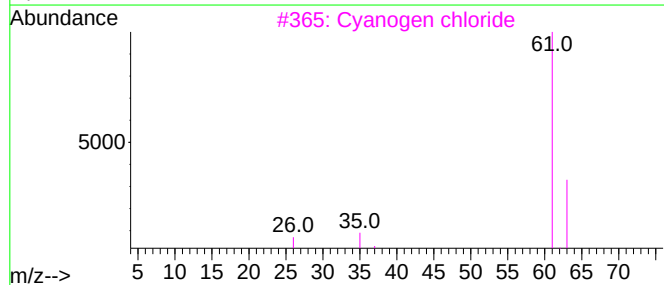
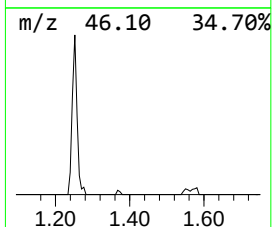
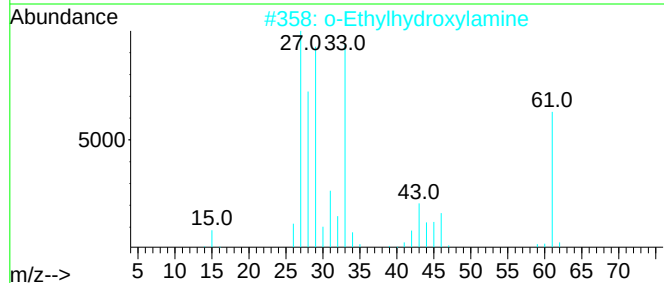
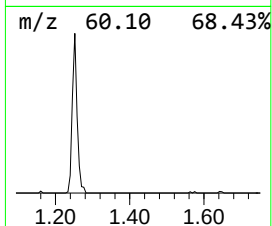
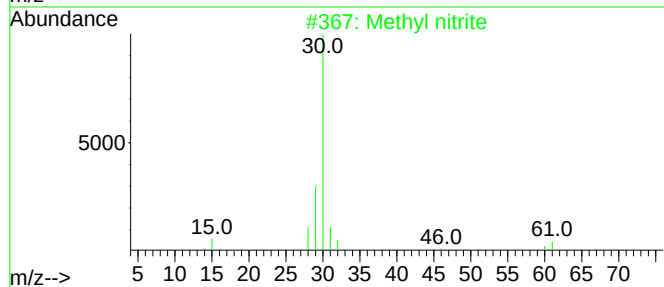
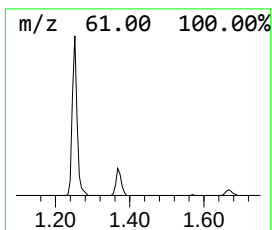
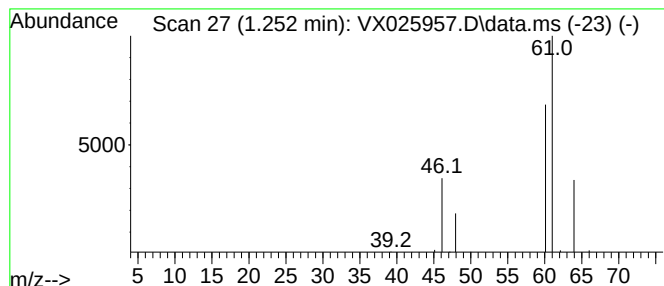
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122021WMA.M
Quant Title : VOC Analysis

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.
1.252	4.84 ug/L	32473	1,4-Difluorobenzene	6.769

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			Cyanogen chloride	61	CClN	000506-77-4	4
5			Methyl formate	60	C2H4O2	000107-31-3	3



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.252	4.8	ug/L	32473	1	6.769	335223	50.0