

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX121021\  
 Data File : VX025727.D  
 Acq On : 11 Dec 2021 01:24  
 Operator : JC/MD  
 Sample : M4981-19  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 37 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 C0CR8

Integration Parameters: LSCINT.P

Integrator: RTE  
 Smoothing : OFF  
 Sampling : 1  
 Start Thrs: 0.2  
 Stop Thrs : 0

Filtering: 5  
 Min Area: 0 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXLM112221WMA.M  
 Title : VOC Analysis

Signal : TIC: VX025727.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.367	43	46	53	rVB	43653	41764	5.01%	1.247%
2	1.666	91	95	104	rBV	33412	43138	5.18%	1.288%
3	2.312	194	201	214	rBV2	75507	141572	16.99%	4.227%
4	2.587	243	246	247	rBV	374	380	0.05%	0.011%
5	3.251	353	355	358	rBV	376	349	0.04%	0.010%
6	3.733	432	434	437	rBV	261	301	0.04%	0.009%
7	3.842	449	452	454	rBV2	336	370	0.04%	0.011%
8	3.964	470	472	476	rBV2	270	223	0.03%	0.007%
9	4.105	493	495	498	rBV	303	414	0.05%	0.012%
10	4.178	505	507	508	rBV	318	213	0.03%	0.006%
11	4.220	513	514	515	rBV	284	132	0.02%	0.004%
12	4.476	543	556	570	rBV2	28295	122793	14.74%	3.666%
13	4.702	592	593	596	rBV2	313	255	0.03%	0.008%
14	5.062	640	652	665	rBV	40281	127482	15.30%	3.806%
15	5.391	695	706	717	rVB2	12166	36640	4.40%	1.094%
16	5.507	724	725	727	rBV	237	177	0.02%	0.005%
17	5.562	733	734	737	rBV3	317	329	0.04%	0.010%
18	5.659	748	750	751	rBV	312	190	0.02%	0.006%
19	5.848	779	781	784	rBV2	212	245	0.03%	0.007%
20	5.976	790	802	817	rBV2	104419	307095	36.85%	9.169%
21	6.525	890	892	893	rBV	243	156	0.02%	0.005%
22	6.763	923	931	942	rBV	82516	196338	23.56%	5.862%
23	6.976	963	966	967	rBV	259	202	0.02%	0.006%
24	7.128	982	991	1008	rBV	388947	833297	100.00%	24.879%
25	7.311	1013	1021	1033	rVB	64954	139042	16.69%	4.151%
26	7.567	1061	1063	1064	rBV2	272	183	0.02%	0.005%
27	7.738	1089	1091	1094	rVB2	292	251	0.03%	0.007%
28	8.329	1182	1188	1197	rBV	44445	72326	8.68%	2.159%
29	8.652	1234	1241	1248	rBV	162133	253061	30.37%	7.555%
30	8.720	1249	1252	1258	rVB	1894	3061	0.37%	0.091%
31	8.835	1269	1271	1273	rBV2	246	239	0.03%	0.007%
32	8.866	1274	1276	1278	rBV	230	222	0.03%	0.007%
33	8.951	1285	1290	1297	rVB	31796	45782	5.49%	1.367%
34	9.085	1310	1312	1316	rVB	224	278	0.03%	0.008%
35	9.116	1316	1317	1321	rBV	313	311	0.04%	0.009%
36	9.159	1321	1324	1326	rBV2	638	597	0.07%	0.018%

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 MSVOA\_X  
 ClientSampleId :  
 C0CR8

Integration Parameters: LSCINT.P

Integrator: RTE  
 Smoothing : OFF  
 Sampling : 1  
 Start Thrs : 0.2  
 Stop Thrs : 0

Filtering: 5  
 Min Area: 0 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXLM112221WMA.M  
 Title : VOC Analysis

37	9.207	1329	1332	1336	rBV2	319	602	0.07%	0.018%
38	9.244	1336	1338	1341	rBV2	234	213	0.03%	0.006%
39	9.274	1341	1343	1346	rVV2	935	780	0.09%	0.023%
40	9.384	1356	1361	1374	rBV	100032	148771	17.85%	4.442%
41	9.524	1381	1384	1385	rBV2	305	315	0.04%	0.009%
42	9.689	1409	1411	1413	rBV2	252	254	0.03%	0.008%
43	9.982	1457	1459	1460	rBV	312	282	0.03%	0.008%
44	10.055	1465	1471	1480	rBV	183975	244143	29.30%	7.289%
45	10.366	1521	1522	1524	rVB	337	157	0.02%	0.005%
46	10.402	1526	1528	1530	rBV2	363	341	0.04%	0.010%
47	10.500	1542	1544	1545	rBV	148	64	0.01%	0.002%
48	10.616	1560	1563	1564	rBV	308	315	0.04%	0.009%
49	10.731	1580	1582	1583	rBV	290	206	0.02%	0.006%
50	10.750	1583	1585	1586	rVB	265	147	0.02%	0.004%
51	10.853	1601	1602	1603	rBV	223	96	0.01%	0.003%
52	10.939	1613	1616	1618	rBV2	263	360	0.04%	0.011%
53	11.122	1643	1646	1650	rVB3	707	913	0.11%	0.027%
54	11.195	1652	1658	1665	rVV	118850	150709	18.09%	4.500%
55	11.384	1687	1689	1692	rBV2	266	209	0.03%	0.006%
56	11.408	1692	1693	1694	rVV	254	98	0.01%	0.003%
57	11.530	1711	1713	1714	rBV	364	364	0.04%	0.011%
58	11.573	1719	1720	1723	rVV	374	239	0.03%	0.007%
59	11.609	1723	1726	1727	rVV	259	281	0.03%	0.008%
60	11.756	1746	1750	1752	rVV2	390	575	0.07%	0.017%
61	11.780	1752	1754	1756	rVV2	186	123	0.01%	0.004%
62	11.810	1756	1759	1760	rVV2	297	254	0.03%	0.008%
63	11.829	1760	1762	1765	rVB2	310	351	0.04%	0.010%
64	11.981	1785	1787	1789	rBV	232	253	0.03%	0.008%
65	12.024	1789	1794	1802	rVV	167472	210475	25.26%	6.284%
66	12.146	1812	1814	1820	rVB3	488	765	0.09%	0.023%
67	12.268	1832	1834	1837	rBV	287	363	0.04%	0.011%
68	12.323	1838	1843	1850	rVB	168095	210066	25.21%	6.272%
69	12.426	1859	1860	1861	rVB	429	157	0.02%	0.005%
70	12.560	1881	1882	1887	rBV	296	397	0.05%	0.012%
71	12.658	1896	1898	1899	rVB	225	96	0.01%	0.003%
72	12.804	1921	1922	1926	rVB	336	417	0.05%	0.012%
73	12.871	1932	1933	1934	rBV	279	134	0.02%	0.004%
74	12.951	1943	1946	1947	rBV2	222	273	0.03%	0.008%
75	13.127	1973	1975	1976	rBV	228	190	0.02%	0.006%
76	13.182	1980	1984	1986	rBV2	300	382	0.05%	0.011%

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Instrument :  
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 ClientSampleId :  
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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\SFAMXLM112221WMA.M  
 Title : VOC Analysis

77	13.304	2002	2004	2007	rVB	216	162	0.02%	0.005%
78	13.359	2012	2013	2015	rBV	187	140	0.02%	0.004%
79	13.408	2019	2021	2022	rBV	360	208	0.02%	0.006%
80	13.530	2037	2041	2043	rBV	266	338	0.04%	0.010%
81	13.597	2050	2052	2056	rBV	294	257	0.03%	0.008%
82	13.652	2059	2061	2064	rBV	294	330	0.04%	0.010%
83	13.700	2068	2069	2070	rBV	216	116	0.01%	0.003%
84	13.719	2070	2072	2074	rVB	237	144	0.02%	0.004%
85	13.792	2078	2084	2086	rVB	331	517	0.06%	0.015%
86	13.834	2090	2091	2092	rBV	155	73	0.01%	0.002%
87	13.895	2099	2101	2102	rBB	184	86	0.01%	0.003%
88	13.932	2106	2107	2110	rBV	254	278	0.03%	0.008%
89	13.987	2114	2116	2119	rVB	237	197	0.02%	0.006%
90	14.322	2170	2171	2172	rVB	253	92	0.01%	0.003%
91	14.920	2268	2269	2270	rVB	214	78	0.01%	0.002%
92	15.127	2302	2303	2306	rVB	322	293	0.04%	0.009%
93	15.462	2357	2358	2364	rBV2	376	594	0.07%	0.018%
94	15.755	2404	2406	2407	rBV2	307	148	0.02%	0.004%
95	15.846	2419	2421	2423	rBV	260	295	0.04%	0.009%
96	15.987	2442	2444	2446	rVB3	403	281	0.03%	0.008%
97	16.590	2541	2543	2546	rVB	298	216	0.03%	0.006%

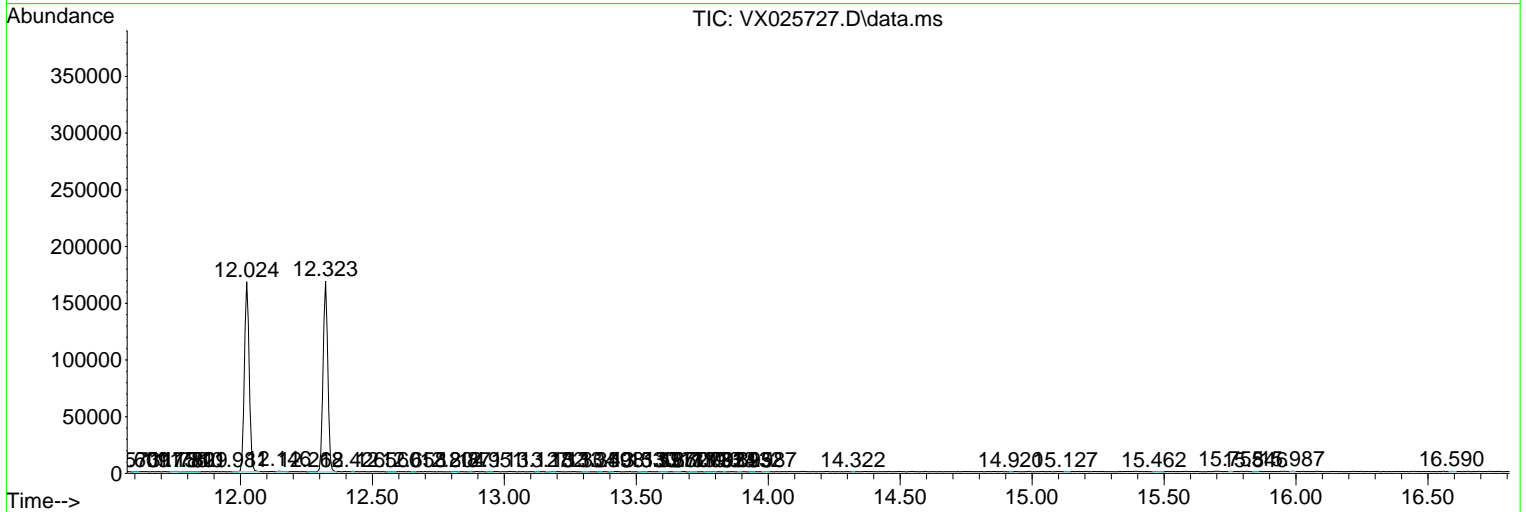
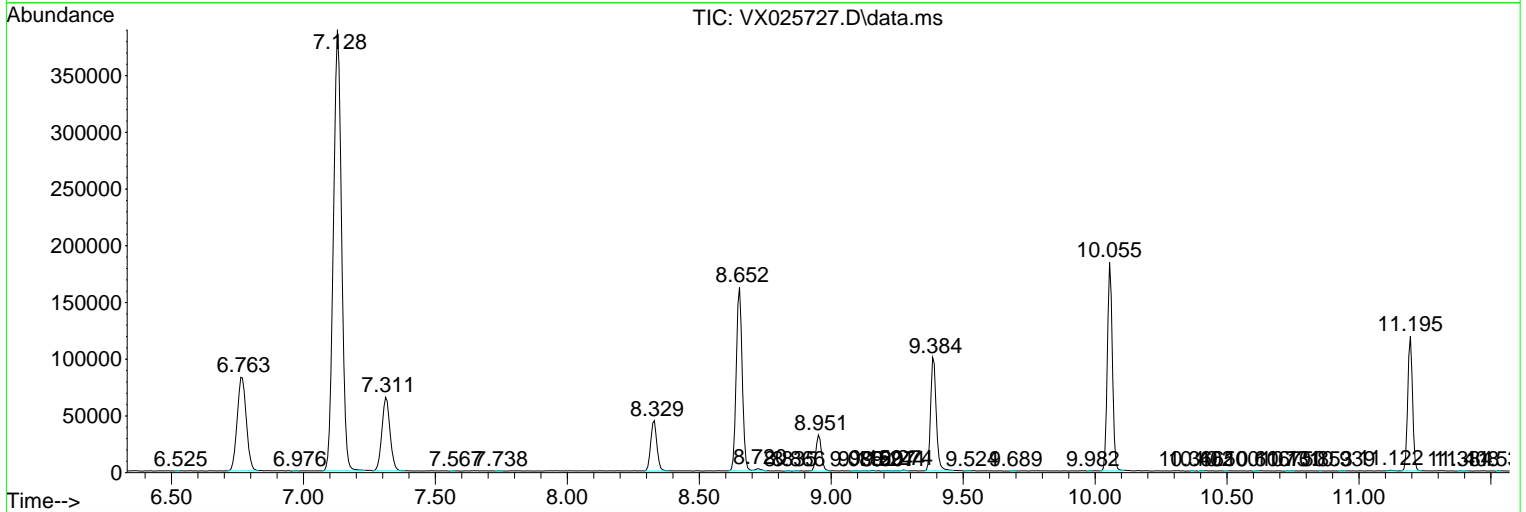
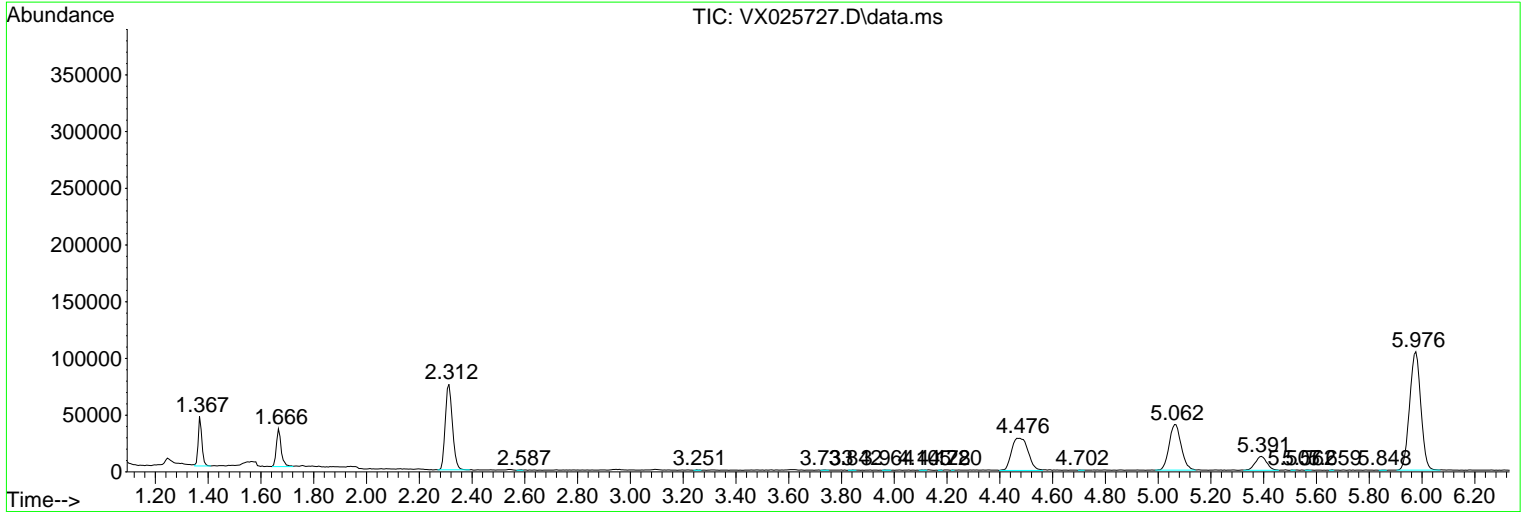
Sum of corrected areas: 3349381

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXLM112221WMA.M  
 Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX121021\  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXLM112221WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

No Library Search Compounds Detected

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXLM112221WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--		
					#	RT	Resp Conc

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