

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110821\
 Data File : VX025098.D
 Acq On : 08 Nov 2021 16:21
 Operator : JC/MD
 Sample : M4464-01ME 10X
 Misc : 4.68g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 GB7K1ME

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\SFAMXLM110821WMA.M
 Title : VOC Analysis

Signal : TIC: VX025098.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.368	42	46	53	rVB	163640	163344	3.61%	1.225%
2	1.666	91	95	104	rVB	110167	136760	3.02%	1.025%
3	2.306	192	200	210	rBV	202509	369800	8.16%	2.773%
4	2.709	262	266	272	rVB3	3536	5696	0.13%	0.043%
5	2.794	272	280	284	rBV2	4099	7579	0.17%	0.057%
6	2.940	302	304	312	rVB2	1200	1676	0.04%	0.013%
7	3.087	325	328	330	rBV2	1638	2254	0.05%	0.017%
8	3.221	347	350	352	rBV	273	430	0.01%	0.003%
9	3.349	367	371	373	rBV	339	470	0.01%	0.004%
10	3.440	382	386	387	rBV2	782	787	0.02%	0.006%
11	3.562	402	406	407	rBV2	546	594	0.01%	0.004%
12	3.611	407	414	423	rVB2	19052	46299	1.02%	0.347%
13	3.995	474	477	480	rVB2	536	671	0.01%	0.005%
14	4.135	496	500	501	rVB	647	656	0.01%	0.005%
15	4.300	520	527	530	rBV3	4243	8477	0.19%	0.064%
16	4.489	544	558	576	rBV3	416700	1252735	27.66%	9.393%
17	5.062	639	652	666	rVV2	127787	410177	9.06%	3.076%
18	5.391	694	706	714	rBV4	6618	23251	0.51%	0.174%
19	5.458	714	717	718	rBV3	1070	843	0.02%	0.006%
20	5.562	730	734	739	rVB2	1047	1908	0.04%	0.014%
21	5.684	750	754	755	rBV2	374	527	0.01%	0.004%
22	5.970	788	801	818	rBV2	323573	962774	21.25%	7.219%
23	6.251	841	847	848	rBV2	493	728	0.02%	0.005%
24	6.635	909	910	914	rVB2	822	549	0.01%	0.004%
25	6.763	919	931	943	rBV	234917	539581	11.91%	4.046%
26	7.123	982	990	999	rBV2	244302	497125	10.97%	3.727%
27	7.312	1012	1021	1032	rBV2	175028	378408	8.35%	2.837%
28	7.464	1044	1046	1048	rBV2	862	776	0.02%	0.006%
29	7.659	1076	1078	1082	rBV	349	435	0.01%	0.003%
30	7.714	1084	1087	1088	rBV2	576	537	0.01%	0.004%
31	7.799	1098	1101	1105	rBV2	843	1118	0.02%	0.008%
32	7.836	1105	1107	1112	rVB	509	579	0.01%	0.004%
33	7.921	1119	1121	1123	rBV	438	450	0.01%	0.003%
34	8.104	1148	1151	1153	rVB	526	541	0.01%	0.004%
35	8.220	1165	1170	1173	rVB	377	700	0.02%	0.005%
36	8.257	1173	1176	1181	rBV2	404	721	0.02%	0.005%

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 Title : VOC Analysis

37	8.324	1181	1187	1195	rBV	132944	226509	5.00%	1.698%
38	8.476	1209	1212	1215	rBV3	629	822	0.02%	0.006%
39	8.580	1224	1229	1234	rBV3	2884	4519	0.10%	0.034%
40	8.653	1234	1241	1246	rVV	507328	787473	17.38%	5.905%
41	8.720	1246	1252	1267	rVB	3026700	4529732	100.00%	33.964%
42	8.952	1285	1290	1299	rVV	107875	156430	3.45%	1.173%
43	9.019	1299	1301	1304	rVB2	727	653	0.01%	0.005%
44	9.122	1316	1318	1322	rVB2	792	971	0.02%	0.007%
45	9.214	1330	1333	1335	rBV	671	583	0.01%	0.004%
46	9.275	1338	1343	1351	rVV2	13816	20082	0.44%	0.151%
47	9.391	1356	1362	1376	rBV	318420	461239	10.18%	3.458%
48	9.628	1399	1401	1406	rVB	461	565	0.01%	0.004%
49	10.055	1465	1471	1486	rBV	471446	655130	14.46%	4.912%
50	10.195	1489	1494	1503	rVB2	11543	15420	0.34%	0.116%
51	10.305	1506	1512	1518	rBV	40337	55884	1.23%	0.419%
52	10.640	1563	1567	1573	rBV	12412	17416	0.38%	0.131%
53	10.744	1581	1584	1586	rBV	546	514	0.01%	0.004%
54	10.823	1594	1597	1598	rBV2	662	548	0.01%	0.004%
55	10.854	1598	1602	1608	rVB4	1176	2010	0.04%	0.015%
56	10.902	1608	1610	1613	rBV2	437	585	0.01%	0.004%
57	10.963	1617	1620	1623	rBV	729	823	0.02%	0.006%
58	11.091	1638	1641	1642	rBV	2293	1725	0.04%	0.013%
59	11.195	1653	1658	1665	rBV	338990	385959	8.52%	2.894%
60	11.378	1684	1688	1696	rVB2	2940	4866	0.11%	0.036%
61	11.451	1696	1700	1702	rBV3	1585	1911	0.04%	0.014%
62	11.567	1715	1719	1724	rVB5	2420	3622	0.08%	0.027%
63	11.610	1724	1726	1731	rBV3	1513	2525	0.06%	0.019%
64	11.750	1745	1749	1754	rVB2	9189	11496	0.25%	0.086%
65	11.829	1759	1762	1763	rBV2	755	784	0.02%	0.006%
66	11.939	1774	1780	1783	rBV2	2137	2134	0.05%	0.016%
67	12.024	1789	1794	1800	rBV	457390	551881	12.18%	4.138%
68	12.091	1802	1805	1809	rVB2	3343	3646	0.08%	0.027%
69	12.128	1809	1811	1813	rBV3	1439	1494	0.03%	0.011%
70	12.219	1823	1826	1827	rBV	561	469	0.01%	0.004%
71	12.250	1827	1831	1834	rVV2	13566	16669	0.37%	0.125%
72	12.323	1837	1843	1849	rVB	452054	570103	12.59%	4.275%
73	12.427	1856	1860	1865	rVB4	1943	2584	0.06%	0.019%
74	12.469	1865	1867	1874	rVB2	773	1222	0.03%	0.009%
75	12.591	1884	1887	1890	rBV2	389	464	0.01%	0.003%
76	12.670	1897	1900	1902	rVV2	897	724	0.02%	0.005%

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 Title : VOC Analysis

77	12.878	1930	1934	1936	rVB3	538	631	0.01%	0.005%
78	12.975	1946	1950	1951	rBV2	581	509	0.01%	0.004%
79	13.042	1958	1961	1962	rBV2	874	822	0.02%	0.006%
80	13.158	1976	1980	1981	rBV	770	702	0.02%	0.005%
81	13.280	1998	2000	2002	rBV	531	633	0.01%	0.005%
82	13.420	2019	2023	2025	rBV	390	457	0.01%	0.003%
83	13.859	2091	2095	2096	rBV2	451	527	0.01%	0.004%
84	13.896	2097	2101	2102	rVB2	480	493	0.01%	0.004%
85	13.914	2102	2104	2106	rBV	627	580	0.01%	0.004%
86	13.938	2106	2108	2110	rBV	723	718	0.02%	0.005%
87	14.097	2131	2134	2135	rBV	650	448	0.01%	0.003%
88	14.542	2204	2207	2208	rBV	622	640	0.01%	0.005%
89	14.816	2250	2252	2255	rVB2	448	447	0.01%	0.003%
90	15.207	2314	2316	2319	rVV3	562	603	0.01%	0.005%
91	15.237	2319	2321	2324	rVB2	517	459	0.01%	0.003%
92	15.389	2345	2346	2349	rBV3	653	564	0.01%	0.004%
93	15.560	2372	2374	2377	rBV2	447	504	0.01%	0.004%
94	15.682	2392	2394	2395	rBV	435	459	0.01%	0.003%
95	15.743	2402	2404	2407	rBV	571	607	0.01%	0.005%
96	15.975	2438	2442	2443	rBV2	604	568	0.01%	0.004%
97	16.237	2481	2485	2486	rBV2	494	496	0.01%	0.004%
98	16.401	2508	2512	2515	rBV3	625	1275	0.03%	0.010%
99	16.426	2515	2516	2520	rVB2	835	760	0.02%	0.006%
100	16.731	2563	2566	2569	rBV2	669	755	0.02%	0.006%

Sum of corrected areas: 13336799

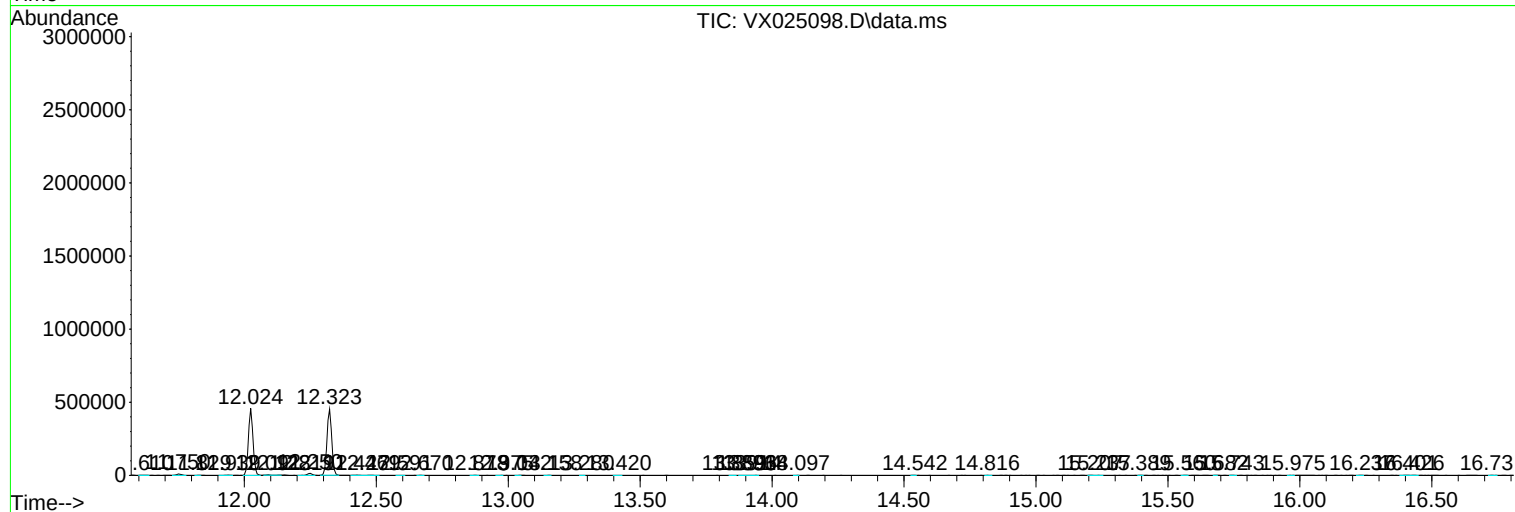
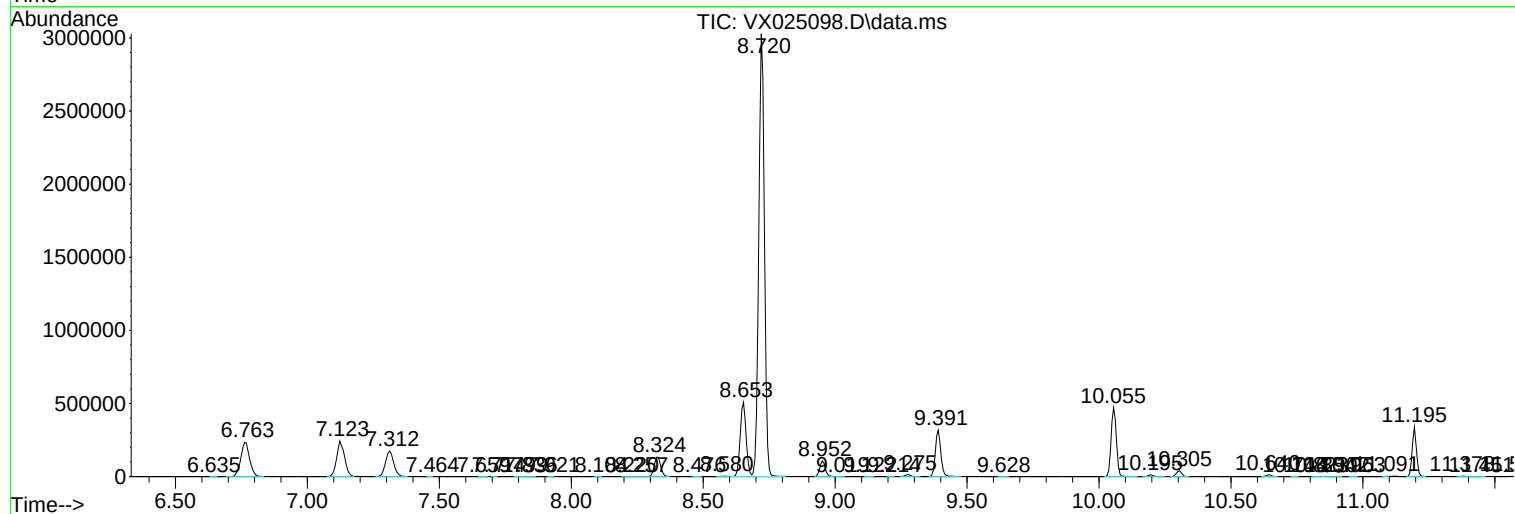
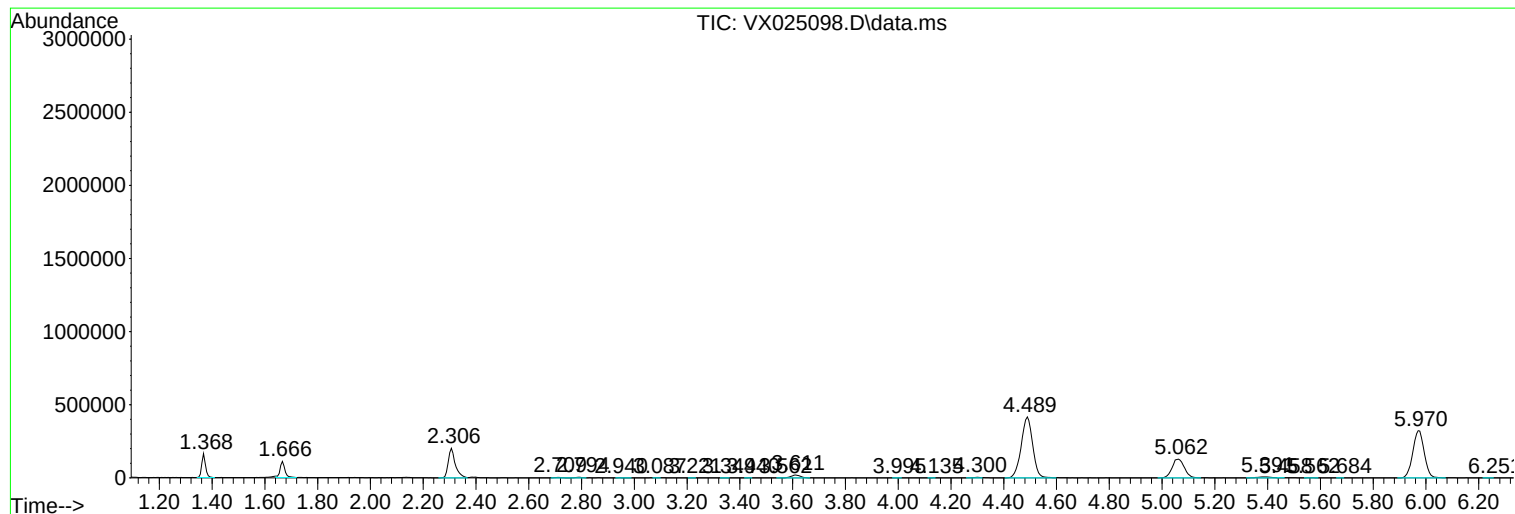
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM110821WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML110821WMA.M
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TIC Library : C:\Database\NIST20.L
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No Library Search Compounds Detected

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