

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121823\
 Data File : VX039310.D
 Acq On : 18 Dec 2023 14:41
 Operator : JC/MD
 Sample : 05799-14ME
 Misc : 4.40g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BGR35ME

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\SFAMXML120523WMA.M
 Title : VOC Analysis

Signal : TIC: VX039310.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	26	28	33	rBV3	1816	1939	0.21%	0.025%
2	1.368	43	46	64	rVB	66945	113057	12.08%	1.469%
3	1.581	71	81	83	rBV4	6908	19778	2.11%	0.257%
4	1.648	89	92	97	rBV	24572	36590	3.91%	0.475%
5	2.276	189	195	209	rBV	170633	285601	30.52%	3.711%
6	2.684	258	262	265	rBV2	387	579	0.06%	0.008%
7	2.733	265	270	272	rBV2	709	1206	0.13%	0.016%
8	2.782	274	278	287	rVB3	2877	5594	0.60%	0.073%
9	2.940	298	304	312	rBV2	3297	8292	0.89%	0.108%
10	3.416	379	382	384	rBV2	414	504	0.05%	0.007%
11	3.593	409	411	413	rVB	403	327	0.03%	0.004%
12	3.696	426	428	431	rVB2	240	203	0.02%	0.003%
13	3.745	433	436	439	rVB	324	279	0.03%	0.004%
14	4.135	497	500	502	rBV2	252	217	0.02%	0.003%
15	4.282	523	524	527	rVV	259	237	0.03%	0.003%
16	4.367	537	538	543	rVB2	308	360	0.04%	0.005%
17	4.416	543	546	547	rBV2	209	212	0.02%	0.003%
18	4.489	549	558	583	rBV	57020	255613	27.32%	3.322%
19	5.062	640	652	669	rVB	115719	360894	38.57%	4.690%
20	5.257	682	684	685	rVB2	412	258	0.03%	0.003%
21	5.538	728	730	731	rBV	256	225	0.02%	0.003%
22	5.550	731	732	736	rVB2	321	300	0.03%	0.004%
23	5.800	769	773	774	rBV2	165	216	0.02%	0.003%
24	5.964	789	800	817	rBV2	329656	935652	100.00%	12.159%
25	6.159	830	832	836	rVB2	411	391	0.04%	0.005%
26	6.293	851	854	857	rBV2	316	510	0.05%	0.007%
27	6.367	860	866	869	rBV3	1304	2744	0.29%	0.036%
28	6.519	889	891	892	rBV2	283	218	0.02%	0.003%
29	6.763	921	931	949	rBV	228653	574010	61.35%	7.459%
30	7.068	980	981	983	rBV	268	226	0.02%	0.003%
31	7.129	983	991	998	rBV9	1933	5948	0.64%	0.077%
32	7.208	1000	1004	1011	rVV5	2578	5938	0.63%	0.077%
33	7.306	1012	1020	1035	rVB	184323	419616	44.85%	5.453%
34	7.482	1044	1049	1054	rBV4	668	1262	0.13%	0.016%
35	7.623	1070	1072	1077	rVV2	249	288	0.03%	0.004%
36	7.708	1084	1086	1089	rVB	413	256	0.03%	0.003%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
 Title : VOC Analysis

37	7.976	1124	1130	1132	rBV3	989	1589	0.17%	0.021%
38	8.141	1156	1157	1160	rVB	335	223	0.02%	0.003%
39	8.238	1172	1173	1177	rBV2	315	333	0.04%	0.004%
40	8.324	1181	1187	1206	rVV	120281	211110	22.56%	2.743%
41	8.647	1234	1240	1257	rBV	446050	731150	78.14%	9.501%
42	8.952	1285	1290	1308	rBV	87195	139662	14.93%	1.815%
43	9.110	1314	1316	1318	rBV3	507	650	0.07%	0.008%
44	9.269	1336	1342	1357	rBV	299776	455304	48.66%	5.917%
45	9.397	1357	1363	1379	rBV	322086	582855	62.29%	7.574%
46	9.720	1410	1416	1420	rBV4	881	1748	0.19%	0.023%
47	9.994	1458	1461	1465	rBV2	280	386	0.04%	0.005%
48	10.055	1465	1471	1489	rBV	491877	695682	74.35%	9.040%
49	10.311	1508	1513	1517	rBV2	840	1115	0.12%	0.014%
50	10.384	1522	1525	1526	rVB	197	199	0.02%	0.003%
51	10.451	1534	1536	1540	rBV2	150	199	0.02%	0.003%
52	10.646	1566	1568	1572	rBV2	282	469	0.05%	0.006%
53	10.963	1618	1620	1621	rVV2	574	571	0.06%	0.007%
54	11.037	1628	1632	1633	rBV	237	321	0.03%	0.004%
55	11.091	1636	1641	1648	rBV4	837	1548	0.17%	0.020%
56	11.195	1652	1658	1673	rVV	349453	451068	48.21%	5.862%
57	11.305	1674	1676	1680	rVB3	364	519	0.06%	0.007%
58	11.457	1698	1701	1704	rBV3	540	726	0.08%	0.009%
59	11.591	1721	1723	1726	rBV2	246	313	0.03%	0.004%
60	11.634	1727	1730	1733	rVB2	555	627	0.07%	0.008%
61	11.677	1736	1737	1741	rVV3	621	671	0.07%	0.009%
62	11.713	1741	1743	1746	rVV3	400	370	0.04%	0.005%
63	11.756	1748	1750	1758	rVB3	501	1024	0.11%	0.013%
64	11.841	1760	1764	1767	rBV	359	469	0.05%	0.006%
65	11.939	1777	1780	1783	rBV2	237	260	0.03%	0.003%
66	11.975	1783	1786	1788	rBV3	616	792	0.08%	0.010%
67	12.024	1789	1794	1807	rVV	563970	711455	76.04%	9.245%
68	12.323	1837	1843	1860	rBV	499813	649047	69.37%	8.434%
69	12.719	1906	1908	1909	rBV	323	240	0.03%	0.003%
70	12.756	1912	1914	1919	rVB3	656	907	0.10%	0.012%
71	13.091	1967	1969	1971	rVB	256	245	0.03%	0.003%
72	13.122	1971	1974	1976	rBV2	624	563	0.06%	0.007%
73	13.183	1982	1984	1987	rVB2	275	283	0.03%	0.004%
74	13.274	1997	1999	2002	rBV	400	316	0.03%	0.004%
75	13.378	2014	2016	2020	rVB2	270	214	0.02%	0.003%
76	13.439	2023	2026	2028	rBV2	299	279	0.03%	0.004%

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77	13.713	2068	2071	2073	rVB2	193	204	0.02%	0.003%
78	13.774	2079	2081	2083	rBV2	274	245	0.03%	0.003%
79	13.969	2110	2113	2116	rVB2	551	451	0.05%	0.006%
80	14.048	2121	2126	2131	rVB2	375	687	0.07%	0.009%
81	14.134	2134	2140	2146	rVB	1746	2368	0.25%	0.031%
82	14.304	2164	2168	2170	rBV3	169	218	0.02%	0.003%
83	14.323	2170	2171	2173	rVB	341	211	0.02%	0.003%
84	14.505	2199	2201	2203	rBV	271	206	0.02%	0.003%
85	14.603	2216	2217	2219	rBV2	312	263	0.03%	0.003%
86	14.633	2219	2222	2223	rVV2	238	259	0.03%	0.003%
87	14.676	2227	2229	2231	rBV2	181	221	0.02%	0.003%
88	14.755	2240	2242	2244	rVB2	561	435	0.05%	0.006%
89	14.810	2249	2251	2252	rBV2	270	227	0.02%	0.003%
90	14.859	2257	2259	2263	rVB2	313	343	0.04%	0.004%
91	15.085	2293	2296	2299	rVB2	457	513	0.05%	0.007%
92	15.115	2299	2301	2303	rBV2	323	331	0.04%	0.004%
93	15.139	2303	2305	2307	rBV	349	297	0.03%	0.004%
94	15.158	2307	2308	2311	rVV2	381	299	0.03%	0.004%
95	15.213	2315	2317	2321	rVB2	527	480	0.05%	0.006%
96	15.493	2361	2363	2365	rVB2	623	451	0.05%	0.006%
97	15.554	2371	2373	2374	rBV	526	420	0.04%	0.005%
98	15.731	2400	2402	2404	rVB2	374	263	0.03%	0.003%
99	16.158	2470	2472	2474	rBV2	572	544	0.06%	0.007%
100	16.682	2556	2558	2560	rBV2	289	224	0.02%	0.003%

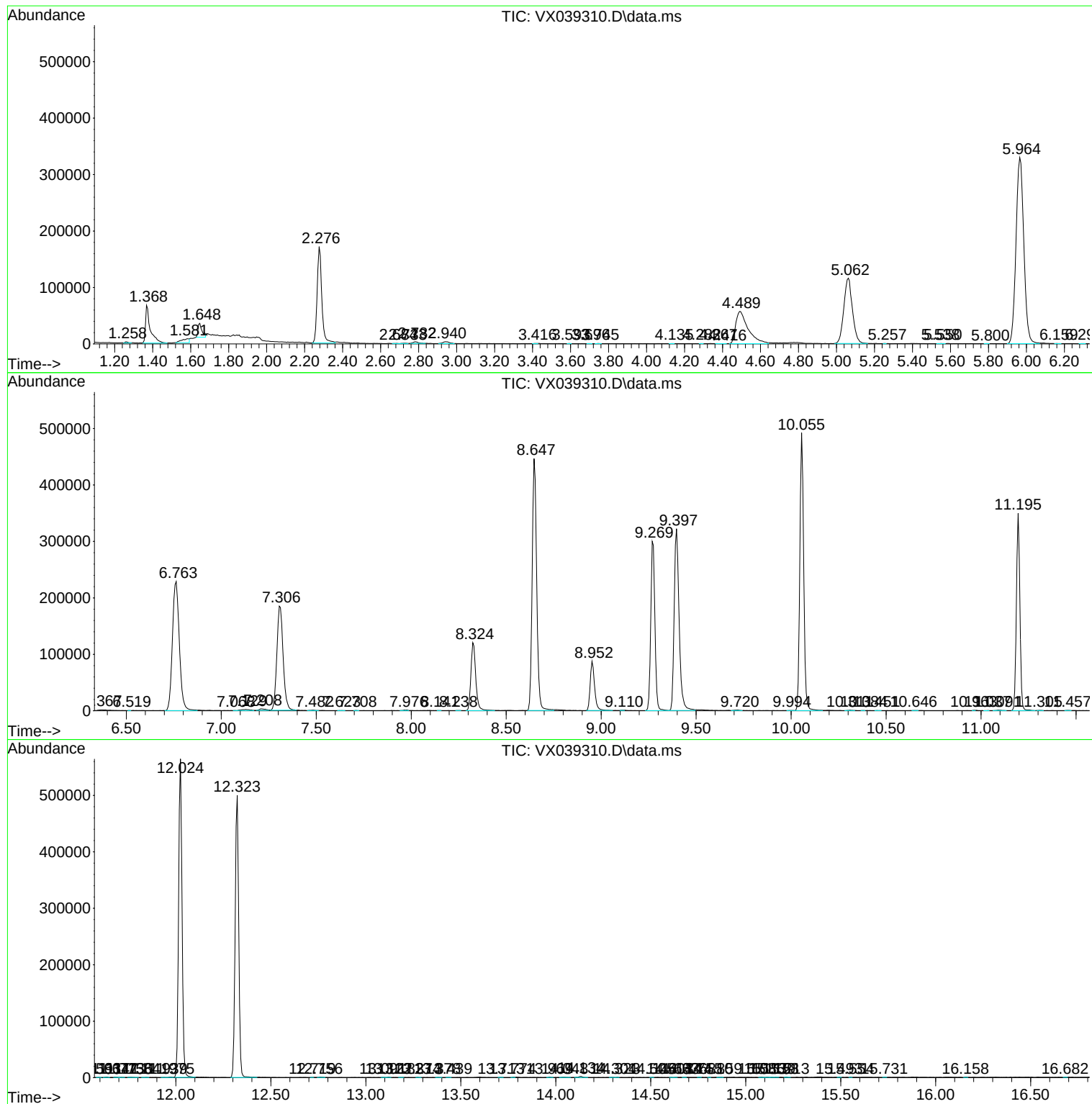
Sum of corrected areas: 7695202

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120523WMA.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\SFAMXML120523WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
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No Library Search Compounds Detected

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