

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122023\
 Data File : VX039395.D
 Acq On : 20 Dec 2023 12:48
 Operator : JC/MD
 Sample : 05807-13 10X
 Misc : 1.26g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AZ5

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: VX039395.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	23	25	26	rBV	1943	1577	0.14%	0.026%
2	1.368	43	46	56	rVB	63080	69544	5.98%	1.125%
3	1.660	90	94	100	rBV	48729	62194	5.34%	1.006%
4	2.306	194	200	211	rBV	105665	166571	14.31%	2.696%
5	2.459	223	225	226	rBV2	284	250	0.02%	0.004%
6	2.599	246	248	250	rBV	181	170	0.01%	0.003%
7	2.703	262	265	271	rVB2	694	1245	0.11%	0.020%
8	2.788	274	279	286	rBV3	2855	5473	0.47%	0.089%
9	2.941	296	304	316	rVB2	13166	32200	2.77%	0.521%
10	3.093	327	329	332	rBV	267	294	0.03%	0.005%
11	3.117	332	333	338	rVB2	407	439	0.04%	0.007%
12	3.154	338	339	341	rBV	273	210	0.02%	0.003%
13	3.312	364	365	367	rBV2	210	163	0.01%	0.003%
14	3.416	380	382	384	rVB2	236	187	0.02%	0.003%
15	3.483	387	393	394	rVB2	216	245	0.02%	0.004%
16	3.599	410	412	416	rBV2	329	397	0.03%	0.006%
17	3.855	451	454	455	rVB2	348	330	0.03%	0.005%
18	3.879	455	458	459	rBV	224	160	0.01%	0.003%
19	3.916	463	464	467	rVV2	216	194	0.02%	0.003%
20	4.202	509	511	513	rVB2	307	204	0.02%	0.003%
21	4.251	515	519	521	rBV2	168	202	0.02%	0.003%
22	4.446	544	551	564	rBV	64857	183381	15.76%	2.968%
23	5.056	639	651	669	rBV	82015	257394	22.12%	4.165%
24	5.550	728	732	735	rBV4	445	810	0.07%	0.013%
25	5.690	752	755	757	rBV2	214	293	0.03%	0.005%
26	5.714	757	759	761	rBV	175	192	0.02%	0.003%
27	5.867	780	784	786	rBV2	133	204	0.02%	0.003%
28	5.964	789	800	820	rBV2	208749	641276	55.10%	10.378%
29	6.501	887	888	891	rVB2	227	197	0.02%	0.003%
30	6.550	894	896	898	rBV	224	199	0.02%	0.003%
31	6.757	922	930	946	rVV	169046	410415	35.26%	6.642%
32	7.031	973	975	978	rVB	219	219	0.02%	0.004%
33	7.123	982	990	997	rVV5	1240	2815	0.24%	0.046%
34	7.306	1012	1020	1034	rBV	137174	302749	26.01%	4.899%
35	7.482	1048	1049	1052	rVB2	547	445	0.04%	0.007%
36	7.507	1052	1053	1058	rBV2	234	305	0.03%	0.005%

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 Title : VOC Analysis

37	7.586	1064	1066	1070	rVB2	169	169	0.01%	0.003%
38	7.787	1097	1099	1102	rBV	389	252	0.02%	0.004%
39	7.842	1107	1108	1112	rVB	342	285	0.02%	0.005%
40	7.873	1112	1113	1115	rBV2	286	205	0.02%	0.003%
41	7.964	1126	1128	1131	rVB3	253	269	0.02%	0.004%
42	8.086	1145	1148	1149	rBV	206	167	0.01%	0.003%
43	8.257	1173	1176	1177	rBV	211	177	0.02%	0.003%
44	8.324	1181	1187	1206	rBV	86803	143547	12.33%	2.323%
45	8.476	1210	1212	1214	rVV2	277	179	0.02%	0.003%
46	8.574	1225	1228	1229	rBV2	194	160	0.01%	0.003%
47	8.647	1233	1240	1253	rBV	263389	416581	35.79%	6.741%
48	8.903	1280	1282	1285	rBV2	215	246	0.02%	0.004%
49	8.952	1285	1290	1306	rVV	62195	96323	8.28%	1.559%
50	9.080	1308	1311	1312	rBV2	228	221	0.02%	0.004%
51	9.177	1326	1327	1329	rBV	293	224	0.02%	0.004%
52	9.256	1338	1340	1342	rBV2	168	225	0.02%	0.004%
53	9.275	1342	1343	1348	rVB2	322	324	0.03%	0.005%
54	9.384	1355	1361	1378	rBV	304488	448839	38.57%	7.263%
55	9.701	1409	1413	1418	rBV4	1030	1466	0.13%	0.024%
56	9.805	1428	1430	1432	rBV2	200	161	0.01%	0.003%
57	9.927	1447	1450	1454	rVB2	195	224	0.02%	0.004%
58	10.055	1465	1471	1472	rBV	375414	478550	41.12%	7.744%
59	10.262	1503	1505	1509	rVB	195	153	0.01%	0.002%
60	10.299	1509	1511	1512	rBV	530	356	0.03%	0.006%
61	10.842	1597	1600	1601	rBV2	231	176	0.02%	0.003%
62	10.963	1617	1620	1624	rVB3	375	520	0.04%	0.008%
63	11.091	1635	1641	1643	rBV2	431	439	0.04%	0.007%
64	11.189	1652	1657	1666	rBV	274169	350143	30.09%	5.666%
65	11.305	1674	1676	1680	rVB3	332	361	0.03%	0.006%
66	11.591	1721	1723	1727	rVB	266	215	0.02%	0.003%
67	11.628	1727	1729	1730	rBV	207	169	0.01%	0.003%
68	11.750	1745	1749	1751	rBV3	269	380	0.03%	0.006%
69	11.969	1780	1785	1789	rBV	52837	66657	5.73%	1.079%
70	12.036	1789	1796	1808	rVB2	575848	1163828	100.00%	18.834%
71	12.329	1837	1844	1853	rBV2	410039	774995	66.59%	12.542%
72	12.475	1867	1868	1870	rBV	241	188	0.02%	0.003%
73	12.701	1903	1905	1909	rVB2	341	322	0.03%	0.005%
74	12.762	1909	1915	1922	rVB2	2216	2849	0.24%	0.046%
75	12.927	1936	1942	1946	rBV4	1863	2637	0.23%	0.043%
76	12.987	1950	1952	1956	rVB	201	176	0.02%	0.003%

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 Title : VOC Analysis

77	13.109	1971	1972	1977	rVB2	248	258	0.02%	0.004%
78	13.207	1985	1988	1992	rVB2	713	960	0.08%	0.016%
79	13.457	2028	2029	2031	rBV	311	205	0.02%	0.003%
80	13.536	2041	2042	2045	rBV2	179	188	0.02%	0.003%
81	13.585	2045	2050	2057	rBV	50387	62207	5.35%	1.007%
82	13.786	2079	2083	2088	rVB3	620	1171	0.10%	0.019%
83	13.835	2088	2091	2092	rBV	364	279	0.02%	0.005%
84	13.932	2105	2107	2108	rBV	221	168	0.01%	0.003%
85	13.963	2108	2112	2118	rVV3	6948	9369	0.81%	0.152%
86	14.128	2135	2139	2145	rVB2	2828	4099	0.35%	0.066%
87	14.182	2145	2148	2149	rBV	250	237	0.02%	0.004%
88	14.304	2164	2168	2170	rVV2	180	265	0.02%	0.004%
89	14.506	2197	2201	2203	rVV2	220	303	0.03%	0.005%
90	14.579	2211	2213	2214	rBV	250	180	0.02%	0.003%
91	14.652	2222	2225	2232	rVB3	377	805	0.07%	0.013%
92	14.701	2232	2233	2234	rBV	367	216	0.02%	0.003%
93	14.865	2258	2260	2263	rVB2	368	337	0.03%	0.005%
94	15.048	2288	2290	2292	rBV	237	163	0.01%	0.003%
95	15.554	2371	2373	2375	rBV3	333	347	0.03%	0.006%
96	16.072	2456	2458	2459	rBV	366	257	0.02%	0.004%
97	16.133	2466	2468	2472	rVB	346	307	0.03%	0.005%
98	16.292	2492	2494	2495	rBV	384	199	0.02%	0.003%
99	16.316	2497	2498	2499	rBV	256	162	0.01%	0.003%
100	16.597	2542	2544	2545	rBV	317	215	0.02%	0.003%

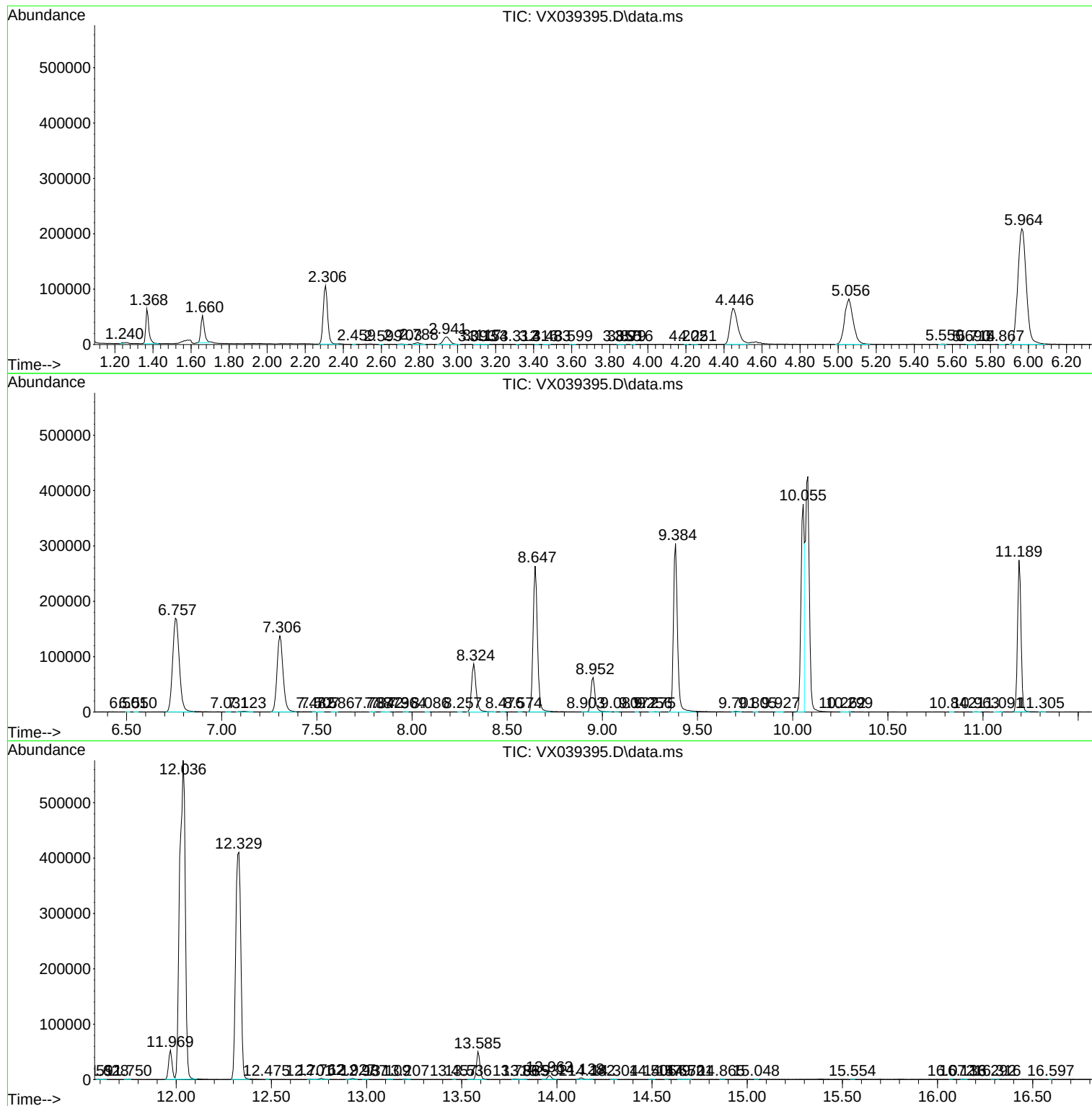
Sum of corrected areas: 6179398

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.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
TIC Integration Parameters: LSCINT.P

No Library Search Compounds Detected

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