

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042923\
 Data File : VU053973.D
 Acq On : 28 Apr 2023 16:46
 Operator : JC/MD
 Sample : 02525-07ME
 Misc : 5.88g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DCCK4ME

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_U\Method\SFAMULM033123WMA.M
 Title : VOC Analysis

Signal : TIC: VU053973.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	73	80	101	rBV	72250	109379	14.84%	1.859%
2	2.549	364	376	394	rBV	156469	255948	34.73%	4.349%
3	2.645	394	406	429	rBV	26177	63011	8.55%	1.071%
4	2.915	488	490	494	rBV	292	188	0.03%	0.003%
5	3.041	517	529	541	rBV7	3204	7009	0.95%	0.119%
6	3.089	541	544	547	rVB2	629	359	0.05%	0.006%
7	3.163	566	567	571	rVB	362	205	0.03%	0.003%
8	3.186	571	574	580	rBV2	521	503	0.07%	0.009%
9	3.407	638	643	647	rBB	212	272	0.04%	0.005%
10	3.436	648	652	656	rBB	293	289	0.04%	0.005%
11	3.459	657	659	662	rBV	264	145	0.02%	0.002%
12	3.578	691	696	701	rVV4	550	643	0.09%	0.011%
13	3.629	708	712	713	rBV	191	162	0.02%	0.003%
14	3.639	713	715	718	rVB2	359	228	0.03%	0.004%
15	3.687	727	730	731	rBV2	369	183	0.02%	0.003%
16	3.735	743	745	748	rBV	264	171	0.02%	0.003%
17	3.977	817	820	821	rBV	271	157	0.02%	0.003%
18	4.227	892	898	900	rBV	338	296	0.04%	0.005%
19	4.272	910	912	916	rBB	297	231	0.03%	0.004%
20	4.446	962	966	970	rBV	192	256	0.03%	0.004%
21	4.517	985	988	989	rBV	200	130	0.02%	0.002%
22	4.562	1000	1002	1006	rBV	146	151	0.02%	0.003%
23	4.636	1012	1025	1045	rBV2	29221	92755	12.58%	1.576%
24	4.980	1129	1132	1137	rBV	259	171	0.02%	0.003%
25	5.057	1141	1156	1181	rBV	131588	303862	41.23%	5.164%
26	5.211	1195	1204	1211	rBV5	906	1626	0.22%	0.028%
27	5.298	1227	1231	1235	rBV2	305	314	0.04%	0.005%
28	5.330	1239	1241	1243	rBV2	257	128	0.02%	0.002%
29	5.375	1253	1255	1258	rBV	159	129	0.02%	0.002%
30	5.465	1280	1283	1286	rBV	206	188	0.03%	0.003%
31	5.716	1341	1361	1386	rBV2	277746	737032	100.00%	12.525%
32	5.964	1434	1438	1439	rBV2	905	651	0.09%	0.011%
33	6.111	1479	1484	1486	rBV	288	213	0.03%	0.004%
34	6.179	1502	1505	1507	rBV	437	286	0.04%	0.005%
35	6.240	1511	1524	1551	rBV	273812	535113	72.60%	9.093%
36	6.388	1568	1570	1571	rBV	387	149	0.02%	0.003%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
 Title : VOC Analysis

37	6.423	1579	1581	1585	rVB	341	178	0.02%	0.003%
38	6.462	1589	1593	1594	rBV	176	144	0.02%	0.002%
39	6.526	1602	1613	1622	rBV7	3143	5310	0.72%	0.090%
40	6.600	1627	1636	1646	rBV3	1887	3463	0.47%	0.059%
41	6.684	1649	1662	1684	rVV	163803	319179	43.31%	5.424%
42	6.790	1693	1695	1699	rVV2	297	256	0.03%	0.004%
43	6.864	1715	1718	1721	rBV	191	187	0.03%	0.003%
44	6.877	1721	1722	1726	rVB	268	167	0.02%	0.003%
45	6.899	1727	1729	1731	rBB	272	126	0.02%	0.002%
46	6.912	1731	1733	1738	rBV	261	249	0.03%	0.004%
47	7.083	1783	1786	1790	rVB	319	237	0.03%	0.004%
48	7.195	1815	1821	1822	rBV4	1258	1217	0.17%	0.021%
49	7.269	1840	1844	1847	rBV3	325	227	0.03%	0.004%
50	7.304	1851	1855	1860	rBB2	375	320	0.04%	0.005%
51	7.330	1861	1863	1864	rBV2	238	133	0.02%	0.002%
52	7.375	1875	1877	1880	rBV	170	137	0.02%	0.002%
53	7.562	1922	1935	1960	rBV2	86270	164085	22.26%	2.788%
54	7.706	1977	1980	1983	rBV	208	146	0.02%	0.002%
55	7.732	1985	1988	1992	rVB	370	209	0.03%	0.004%
56	7.783	2001	2004	2007	rBV	205	129	0.02%	0.002%
57	7.893	2025	2038	2064	rBV	338355	615721	83.54%	10.463%
58	8.076	2092	2095	2098	rBV2	279	277	0.04%	0.005%
59	8.092	2098	2100	2103	rVB	403	198	0.03%	0.003%
60	8.111	2104	2106	2108	rBV	260	146	0.02%	0.002%
61	8.131	2109	2112	2113	rVV	252	138	0.02%	0.002%
62	8.179	2115	2127	2150	rVV2	51667	111370	15.11%	1.893%
63	8.549	2232	2242	2255	rVB3	8467	13913	1.89%	0.236%
64	8.600	2256	2258	2260	rBV3	234	144	0.02%	0.002%
65	8.658	2260	2276	2298	rBV2	124649	258819	35.12%	4.398%
66	8.777	2310	2313	2316	rVB3	428	247	0.03%	0.004%
67	8.812	2321	2324	2330	rVB2	258	282	0.04%	0.005%
68	8.873	2341	2343	2347	rVB	253	163	0.02%	0.003%
69	8.931	2356	2361	2363	rBV	199	211	0.03%	0.004%
70	9.053	2397	2399	2403	rBV2	240	157	0.02%	0.003%
71	9.150	2426	2429	2434	rBV	251	291	0.04%	0.005%
72	9.208	2445	2447	2450	rBV2	310	172	0.02%	0.003%
73	9.298	2472	2475	2477	rBV	276	198	0.03%	0.003%
74	9.417	2497	2512	2538	rBV	339020	656999	89.14%	11.165%
75	9.719	2602	2606	2607	rBV	203	162	0.02%	0.003%
76	9.732	2608	2610	2615	rVB	205	149	0.02%	0.003%

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77	9.844	2641	2645	2648	rBV	179	203	0.03%	0.003%
78	10.545	2857	2863	2866	rBV	379	369	0.05%	0.006%
79	10.706	2911	2913	2916	rVB2	272	148	0.02%	0.003%
80	10.758	2916	2929	2948	rBV	237923	386682	52.46%	6.571%
81	10.886	2967	2969	2970	rBV	279	137	0.02%	0.002%
82	11.111	3034	3039	3044	rBV2	1142	1218	0.17%	0.021%
83	11.372	3117	3120	3123	rBV2	328	220	0.03%	0.004%
84	11.481	3151	3154	3155	rBV2	390	191	0.03%	0.003%
85	11.751	3236	3238	3241	rBV	339	178	0.02%	0.003%
86	11.812	3244	3257	3279	rBV	418806	645304	87.55%	10.966%
87	12.073	3335	3338	3342	rVB	356	293	0.04%	0.005%
88	12.192	3362	3375	3397	rBV	357567	577969	78.42%	9.822%
89	12.336	3417	3420	3424	rBV	252	213	0.03%	0.004%
90	12.497	3467	3470	3476	rBV	310	286	0.04%	0.005%
91	12.696	3530	3532	3537	rBV	226	128	0.02%	0.002%
92	12.928	3600	3604	3608	rBV2	283	219	0.03%	0.004%
93	13.217	3692	3694	3699	rVB	399	228	0.03%	0.004%
94	13.365	3736	3740	3745	rVB	309	266	0.04%	0.005%
95	13.719	3847	3850	3854	rVB	289	180	0.02%	0.003%
96	13.741	3854	3857	3860	rBV2	351	238	0.03%	0.004%
97	13.761	3860	3863	3870	rVB2	410	418	0.06%	0.007%
98	13.854	3884	3892	3896	rBV2	565	722	0.10%	0.012%
99	14.838	4195	4198	4201	rBV	427	244	0.03%	0.004%
100	15.545	4416	4418	4420	rBV	578	257	0.03%	0.004%

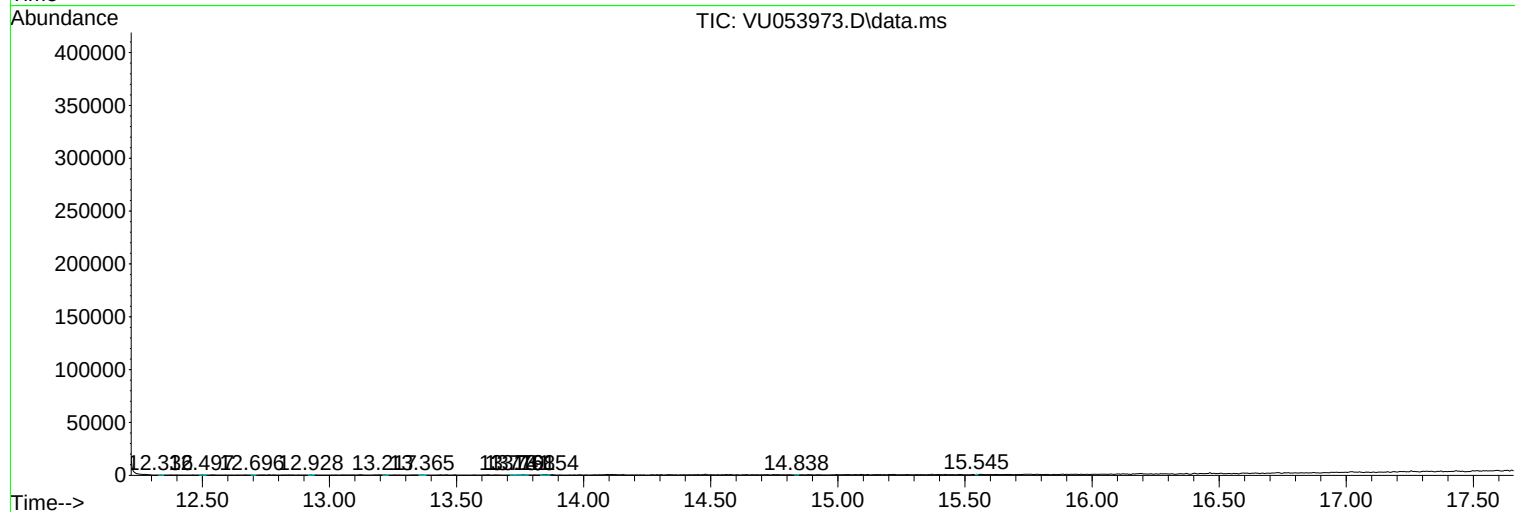
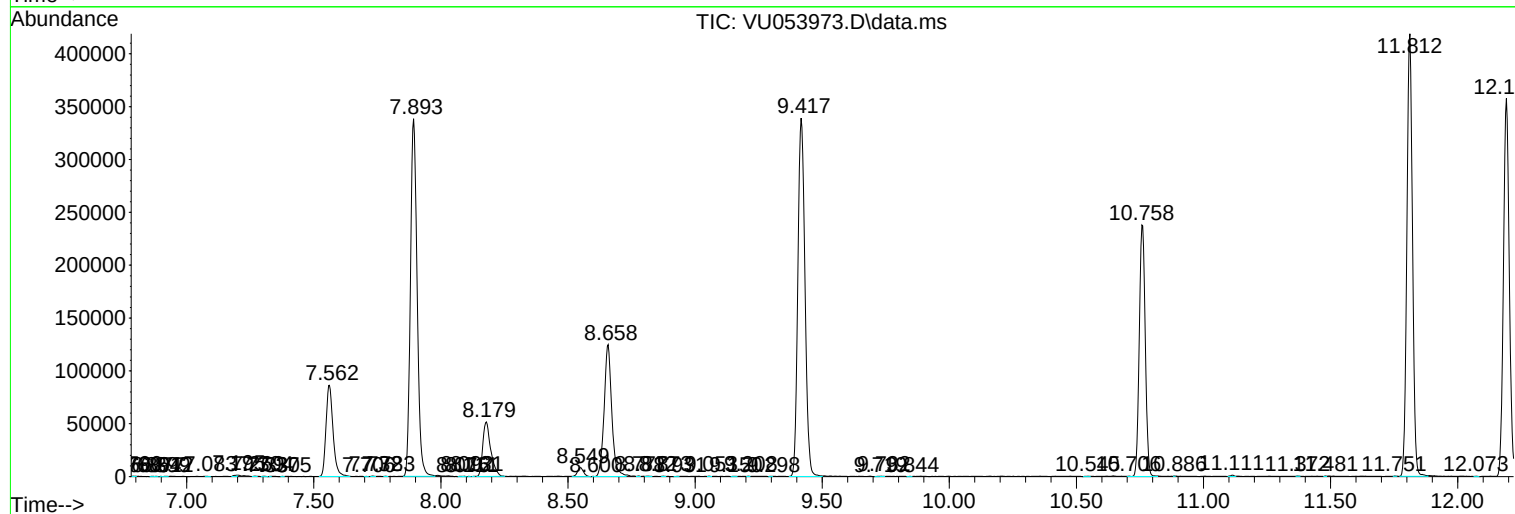
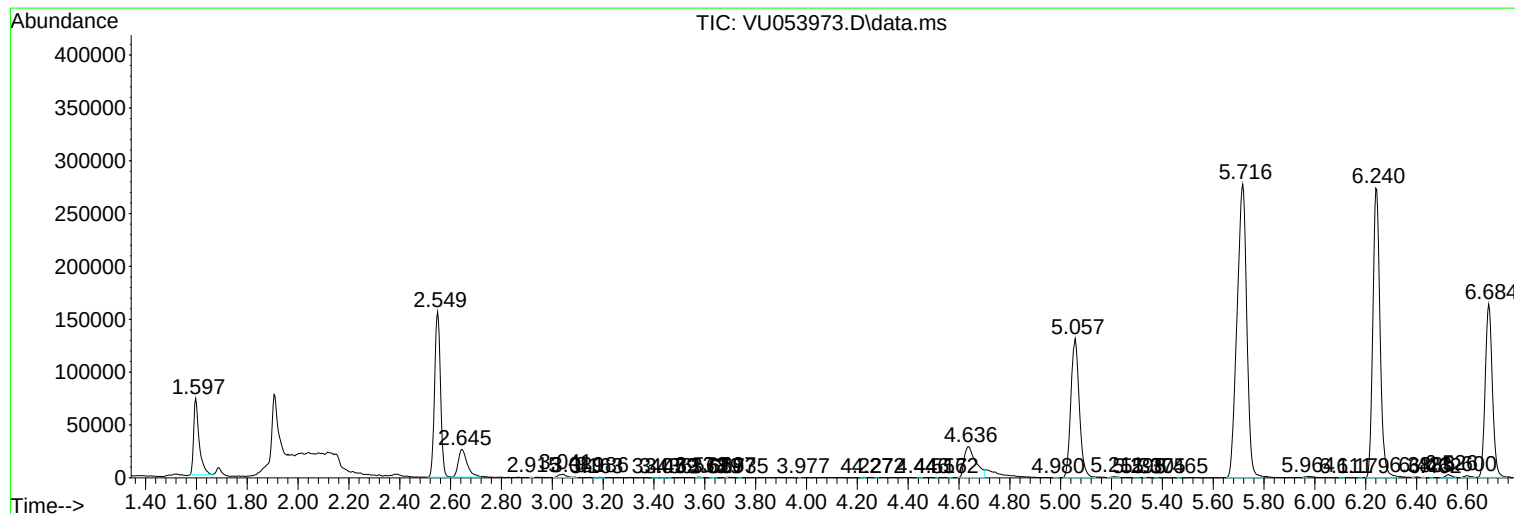
Sum of corrected areas: 5884700

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.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	#	RT	Resp	Conc
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