

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040423\
 Data File : VU053564.D
 Acq On : 04 Apr 2023 16:20
 Operator : JC/MD
 Sample : 02130-14ME
 Misc : 5.31g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C11A3ME

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: VU053564.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.594	72	79	96	rBV	61235	89544	10.48%	1.332%
2	2.540	361	373	392	rVB	142723	233158	27.30%	3.468%
3	2.623	394	399	400	rBV4	1012	830	0.10%	0.012%
4	2.880	475	479	480	rBV2	323	194	0.02%	0.003%
5	2.941	494	498	499	rBV	1044	738	0.09%	0.011%
6	3.035	517	527	543	rVB9	4292	11263	1.32%	0.168%
7	3.176	561	571	573	rBV4	910	1412	0.17%	0.021%
8	3.543	683	685	687	rBV4	394	189	0.02%	0.003%
9	3.675	714	726	736	rVB6	2664	5599	0.66%	0.083%
10	3.774	754	757	761	rVB	241	193	0.02%	0.003%
11	3.900	791	796	801	rVB	285	211	0.02%	0.003%
12	4.057	841	845	851	rVB	335	287	0.03%	0.004%
13	4.179	881	883	887	rVV2	335	222	0.03%	0.003%
14	4.514	985	987	990	rBV	320	191	0.02%	0.003%
15	4.623	1008	1021	1066	rBV2	54881	167764	19.64%	2.495%
16	4.880	1098	1101	1109	rVB2	280	319	0.04%	0.005%
17	5.054	1138	1155	1181	rBV	135354	315894	36.98%	4.699%
18	5.176	1187	1193	1195	rBV2	513	410	0.05%	0.006%
19	5.369	1250	1253	1256	rBV2	430	354	0.04%	0.005%
20	5.449	1276	1278	1285	rVB3	504	459	0.05%	0.007%
21	5.488	1285	1290	1293	rBV	245	196	0.02%	0.003%
22	5.568	1313	1315	1319	rBV2	299	271	0.03%	0.004%
23	5.636	1331	1336	1340	rBV	285	233	0.03%	0.003%
24	5.713	1340	1360	1388	rVV2	287933	759054	88.87%	11.291%
25	5.864	1404	1407	1412	rVB2	577	493	0.06%	0.007%
26	5.925	1418	1426	1427	rBV	176	219	0.03%	0.003%
27	5.970	1434	1440	1447	rBV5	1430	2328	0.27%	0.035%
28	6.067	1469	1470	1475	rVB2	278	191	0.02%	0.003%
29	6.112	1480	1484	1485	rVV	729	411	0.05%	0.006%
30	6.125	1487	1488	1496	rVV3	899	682	0.08%	0.010%
31	6.240	1509	1524	1547	rBV	315347	615839	72.10%	9.161%
32	6.420	1578	1580	1583	rVB	378	213	0.02%	0.003%
33	6.520	1602	1611	1622	rVB6	5093	9626	1.13%	0.143%
34	6.594	1625	1634	1635	rBV5	1860	2127	0.25%	0.032%
35	6.681	1648	1661	1679	rBV	171085	344077	40.28%	5.118%
36	6.797	1695	1697	1704	rBV3	663	552	0.06%	0.008%

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

37	7.192	1811	1820	1822	rBV4	1407	1555	0.18%	0.023%
38	7.308	1851	1856	1860	rVV2	325	282	0.03%	0.004%
39	7.346	1860	1868	1875	rVB3	498	783	0.09%	0.012%
40	7.485	1908	1911	1914	rVB2	256	192	0.02%	0.003%
41	7.562	1921	1935	1953	rBV	91081	168956	19.78%	2.513%
42	7.694	1974	1976	1980	rBV3	449	360	0.04%	0.005%
43	7.816	2011	2014	2017	rBV2	279	189	0.02%	0.003%
44	7.893	2023	2038	2054	rBV	344858	615113	72.02%	9.150%
45	8.176	2114	2126	2148	rVB2	59600	118028	13.82%	1.756%
46	8.343	2176	2178	2183	rBV2	310	251	0.03%	0.004%
47	8.549	2235	2242	2249	rVB5	1947	2918	0.34%	0.043%
48	8.642	2257	2271	2295	rBV	196626	384209	44.98%	5.715%
49	8.780	2310	2314	2315	rBV2	509	277	0.03%	0.004%
50	8.858	2335	2338	2343	rVB2	220	189	0.02%	0.003%
51	9.121	2416	2420	2426	rVB2	373	341	0.04%	0.005%
52	9.414	2499	2511	2537	rBV	420840	761965	89.21%	11.334%
53	9.575	2551	2561	2562	rBV3	907	1417	0.17%	0.021%
54	9.694	2588	2598	2608	rVV3	2134	4074	0.48%	0.061%
55	9.742	2608	2613	2617	rVB3	571	427	0.05%	0.006%
56	9.838	2640	2643	2646	rBV	369	245	0.03%	0.004%
57	9.925	2668	2670	2677	rVB	291	225	0.03%	0.003%
58	9.970	2678	2684	2686	rBV2	210	220	0.03%	0.003%
59	10.009	2690	2696	2703	rVV2	260	275	0.03%	0.004%
60	10.102	2713	2725	2728	rBV2	1130	1509	0.18%	0.022%
61	10.266	2772	2776	2782	rVB2	351	411	0.05%	0.006%
62	10.481	2839	2843	2845	rBV2	369	283	0.03%	0.004%
63	10.523	2853	2856	2864	rVB2	253	290	0.03%	0.004%
64	10.594	2874	2878	2882	rVB	384	277	0.03%	0.004%
65	10.642	2891	2893	2899	rVB2	277	220	0.03%	0.003%
66	10.684	2903	2906	2912	rVB	276	202	0.02%	0.003%
67	10.758	2913	2929	2945	rBV	303533	484188	56.69%	7.202%
68	10.883	2964	2968	2970	rBV2	429	341	0.04%	0.005%
69	10.999	2998	3004	3009	rBV2	495	677	0.08%	0.010%
70	11.192	3060	3064	3069	rVV	229	277	0.03%	0.004%
71	11.407	3126	3131	3136	rVB4	589	829	0.10%	0.012%
72	11.475	3143	3152	3160	rVB4	1374	2394	0.28%	0.036%
73	11.597	3186	3190	3192	rBV2	268	194	0.02%	0.003%
74	11.613	3192	3195	3200	rBV	373	296	0.03%	0.004%
75	11.748	3230	3237	3243	rVB4	2321	2990	0.35%	0.044%
76	11.809	3243	3256	3277	rBV	529932	854144	100.00%	12.705%

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

77	12.057	3330	3333	3337	rBV	241	225	0.03%	0.003%
78	12.192	3362	3375	3393	rBV	435837	703042	82.31%	10.458%
79	12.324	3413	3416	3422	rVB3	1956	1887	0.22%	0.028%
80	12.414	3443	3444	3447	rBV	323	201	0.02%	0.003%
81	12.459	3453	3458	3461	rBV2	454	376	0.04%	0.006%
82	12.710	3533	3536	3541	rVB3	413	326	0.04%	0.005%
83	12.809	3565	3567	3571	rVB2	376	223	0.03%	0.003%
84	12.835	3571	3575	3577	rBV2	528	394	0.05%	0.006%
85	12.996	3622	3625	3629	rBV	354	278	0.03%	0.004%
86	13.015	3629	3631	3633	rBV2	634	327	0.04%	0.005%
87	13.031	3633	3636	3639	rVB3	599	378	0.04%	0.006%
88	13.076	3647	3650	3653	rBV	608	344	0.04%	0.005%
89	13.121	3657	3664	3665	rBV	496	450	0.05%	0.007%
90	13.140	3668	3670	3673	rVB2	401	203	0.02%	0.003%
91	13.282	3712	3714	3716	rBV2	376	214	0.03%	0.003%
92	13.365	3736	3740	3742	rBV2	467	369	0.04%	0.005%
93	13.423	3753	3758	3767	rBV6	2182	3306	0.39%	0.049%
94	13.841	3879	3888	3901	rBV4	9482	15200	1.78%	0.226%
95	13.912	3908	3910	3914	rVB2	915	452	0.05%	0.007%
96	13.941	3916	3919	3921	rVV2	626	295	0.03%	0.004%
97	13.996	3930	3936	3942	rBV6	959	1454	0.17%	0.022%
98	14.089	3959	3965	3980	rVB2	5596	10295	1.21%	0.153%
99	14.169	3987	3990	3991	rBV2	884	461	0.05%	0.007%
100	14.336	4032	4042	4047	rBV9	2505	4270	0.50%	0.064%

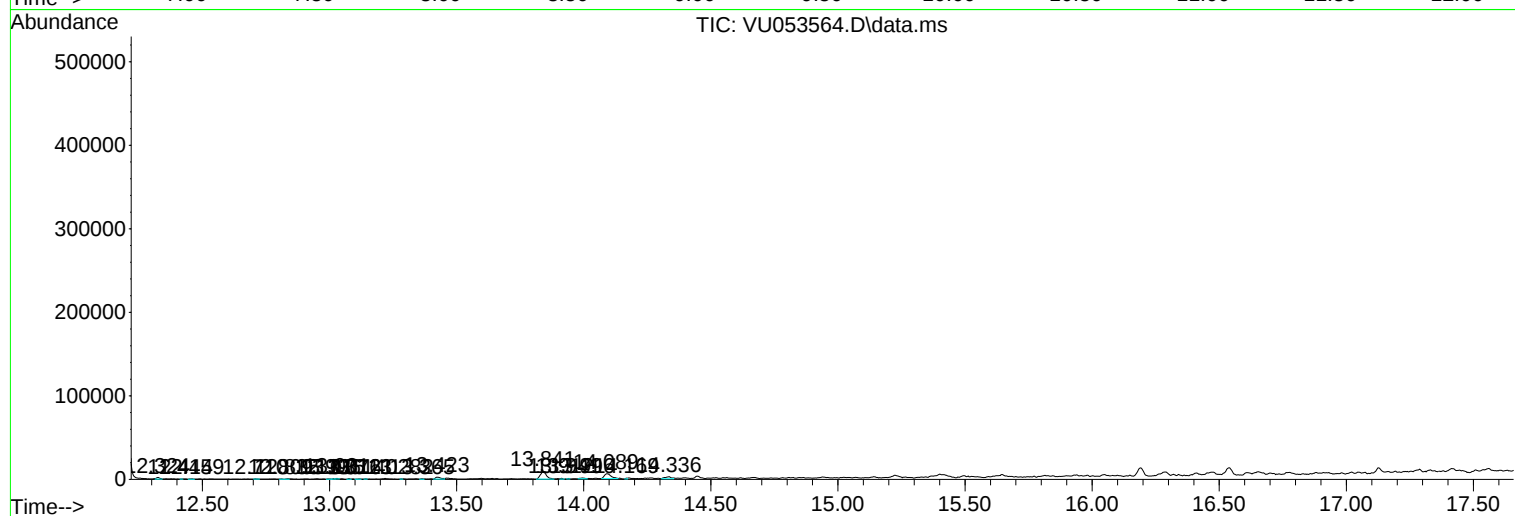
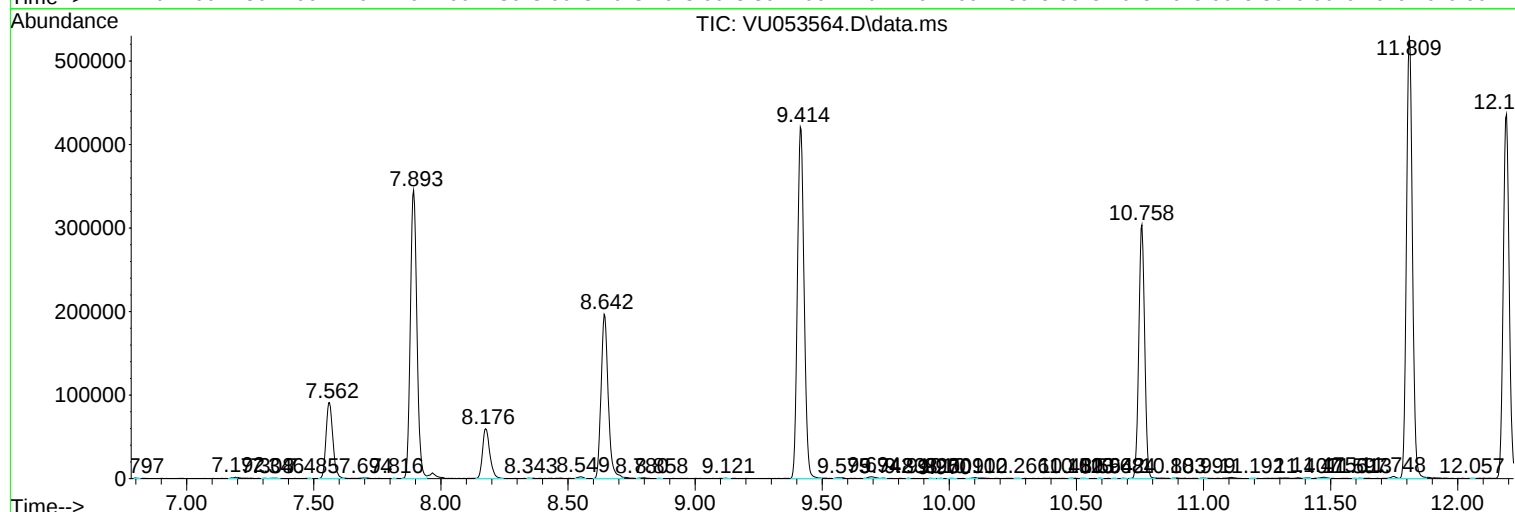
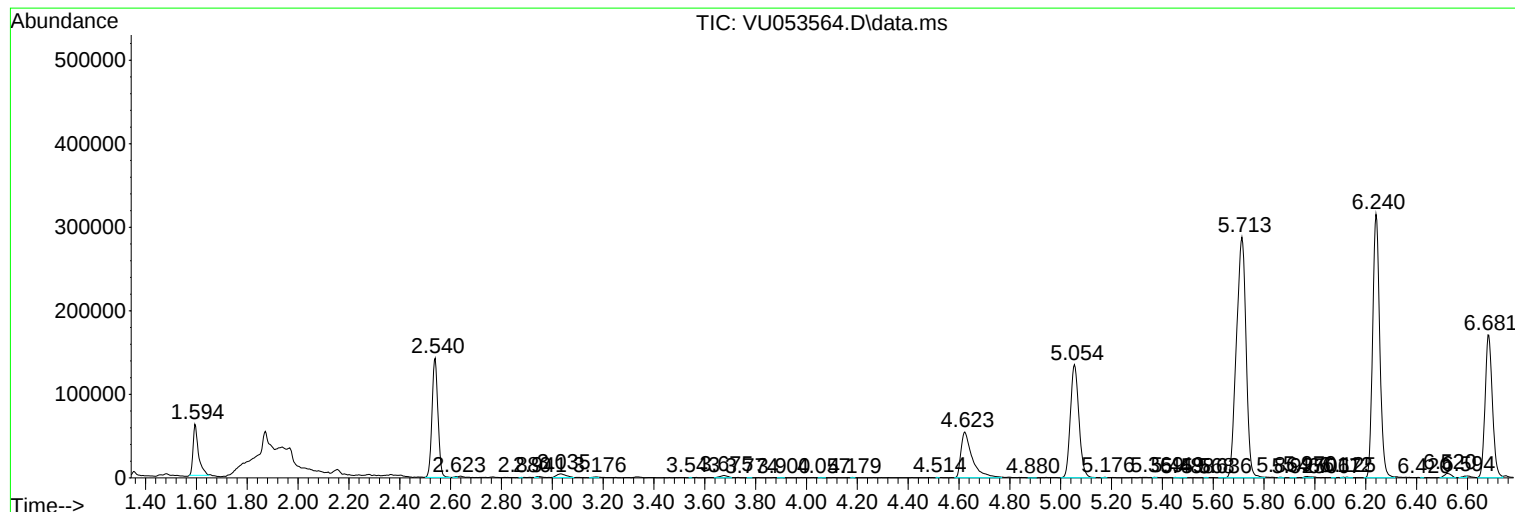
Sum of corrected areas: 6722726

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Instrument :
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C11A3ME

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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