

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU090122\
 Data File : VU050589.D
 Acq On : 01 Sep 2022 18:31
 Operator : SY/MD
 Sample : N4344-23ME 100X
 Misc : 5.58g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBVS0ME

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\SFAMULM083022WMA.M

Title : VOC Analysis

Signal : TIC: VU050589.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.485	40	45	50	rBV3	4998	5294	0.26%	0.037%
2	1.597	72	80	106	rBV	260775	344372	16.94%	2.429%
3	1.899	166	174	197	rVB	217538	301530	14.83%	2.127%
4	2.562	367	380	396	rBV	434805	702910	34.57%	4.957%
5	2.777	439	447	448	rBV2	1030	1071	0.05%	0.008%
6	3.038	520	528	542	rBV4	6141	11263	0.55%	0.079%
7	3.186	560	574	590	rBV	18355	43198	2.12%	0.305%
8	3.372	628	632	634	rBV2	326	217	0.01%	0.002%
9	3.465	657	661	666	rVB3	283	262	0.01%	0.002%
10	3.497	666	671	674	rBV3	286	267	0.01%	0.002%
11	3.726	738	742	749	rVB2	304	278	0.01%	0.002%
12	3.761	750	753	759	rVB2	307	240	0.01%	0.002%
13	3.861	780	784	787	rBV2	224	239	0.01%	0.002%
14	4.047	839	842	846	rVB2	401	263	0.01%	0.002%
15	4.112	856	862	867	rBV2	417	556	0.03%	0.004%
16	4.185	881	885	887	rBV2	341	226	0.01%	0.002%
17	4.221	893	896	900	rVB3	393	334	0.02%	0.002%
18	4.356	935	938	942	rBV2	291	200	0.01%	0.001%
19	4.382	944	946	950	rVB2	514	282	0.01%	0.002%
20	4.401	950	952	958	rBV2	355	395	0.02%	0.003%
21	4.629	1010	1023	1069	rBV	194899	563081	27.69%	3.971%
22	5.063	1141	1158	1180	rBV	360746	796798	39.19%	5.619%
23	5.214	1203	1205	1210	rVB4	850	532	0.03%	0.004%
24	5.365	1248	1252	1255	rBV3	780	716	0.04%	0.005%
25	5.468	1280	1284	1286	rBV2	286	224	0.01%	0.002%
26	5.504	1293	1295	1300	rVB2	460	311	0.02%	0.002%
27	5.722	1342	1363	1397	rBV2	763847	2033310	100.00%	14.340%
28	5.925	1424	1426	1432	rVB4	450	305	0.02%	0.002%
29	5.973	1438	1441	1443	rVV2	521	342	0.02%	0.002%
30	6.095	1475	1479	1480	rBV2	314	237	0.01%	0.002%
31	6.115	1482	1485	1489	rVV2	357	369	0.02%	0.003%
32	6.198	1508	1511	1512	rBV2	381	229	0.01%	0.002%
33	6.247	1512	1526	1555	rVV	588931	1137534	55.94%	8.022%
34	6.391	1568	1571	1574	rBV4	485	347	0.02%	0.002%
35	6.446	1585	1588	1591	rBV2	392	228	0.01%	0.002%
36	6.462	1591	1593	1602	rVV2	436	490	0.02%	0.003%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM083022WMA.M
 Title : VOC Analysis

37	6.533	1606	1615	1622	rVB6	2325	4294	0.21%	0.030%
38	6.587	1628	1632	1633	rBV2	557	394	0.02%	0.003%
39	6.690	1647	1664	1684	rBV	477683	928598	45.67%	6.549%
40	6.800	1693	1698	1708	rVV7	1617	2855	0.14%	0.020%
41	6.838	1708	1710	1717	rVB4	507	422	0.02%	0.003%
42	6.912	1728	1733	1739	rVB4	567	721	0.04%	0.005%
43	6.980	1751	1754	1758	rBV2	306	316	0.02%	0.002%
44	7.137	1799	1803	1806	rVB	377	272	0.01%	0.002%
45	7.185	1812	1818	1824	rBV4	1211	1827	0.09%	0.013%
46	7.240	1832	1835	1840	rVB2	453	420	0.02%	0.003%
47	7.356	1868	1871	1875	rBV2	346	316	0.02%	0.002%
48	7.443	1895	1898	1901	rVV	293	188	0.01%	0.001%
49	7.565	1923	1936	1952	rBV	200567	362624	17.83%	2.557%
50	7.722	1983	1985	1987	rBV2	340	192	0.01%	0.001%
51	7.738	1987	1990	1993	rVV3	362	243	0.01%	0.002%
52	7.832	2017	2019	2023	rBV2	370	232	0.01%	0.002%
53	7.899	2026	2040	2059	rBV	616893	1082632	53.24%	7.635%
54	8.179	2114	2127	2147	rVV	110774	187838	9.24%	1.325%
55	8.423	2201	2203	2206	rVB	480	291	0.01%	0.002%
56	8.475	2216	2219	2223	rVB2	618	444	0.02%	0.003%
57	8.552	2230	2243	2257	rBV2	189311	318018	15.64%	2.243%
58	8.639	2257	2270	2312	rBV5	384979	960150	47.22%	6.771%
59	8.851	2334	2336	2340	rVB3	539	309	0.02%	0.002%
60	8.867	2340	2341	2344	rVB	433	203	0.01%	0.001%
61	8.996	2378	2381	2386	rBV4	438	299	0.01%	0.002%
62	9.050	2395	2398	2403	rVB2	339	297	0.01%	0.002%
63	9.086	2403	2409	2411	rBV2	220	242	0.01%	0.002%
64	9.127	2419	2422	2426	rVB2	412	284	0.01%	0.002%
65	9.153	2426	2430	2434	rBV2	602	518	0.03%	0.004%
66	9.230	2450	2454	2457	rBV2	429	301	0.01%	0.002%
67	9.246	2457	2459	2463	rVB3	369	261	0.01%	0.002%
68	9.269	2463	2466	2468	rBV	381	211	0.01%	0.001%
69	9.285	2468	2471	2473	rVV	394	231	0.01%	0.002%
70	9.346	2486	2490	2494	rVB3	385	262	0.01%	0.002%
71	9.417	2494	2512	2535	rBV	785965	1306385	64.25%	9.213%
72	9.716	2603	2605	2610	rBV2	490	439	0.02%	0.003%
73	9.770	2619	2622	2627	rBV3	239	295	0.01%	0.002%
74	9.893	2656	2660	2666	rVB2	487	523	0.03%	0.004%
75	9.992	2688	2691	2699	rBV	330	441	0.02%	0.003%
76	10.179	2745	2749	2752	rVV2	201	205	0.01%	0.001%

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 Title : VOC Analysis

77	10.291	2780	2784	2790	rBV2	743	839	0.04%	0.006%
78	10.478	2838	2842	2844	rBV2	344	286	0.01%	0.002%
79	10.626	2883	2888	2891	rBV	496	389	0.02%	0.003%
80	10.661	2895	2899	2901	rBV2	478	311	0.02%	0.002%
81	10.758	2915	2929	2949	rBV	560769	920303	45.26%	6.490%
82	10.915	2975	2978	2984	rVB2	572	610	0.03%	0.004%
83	10.973	2994	2996	3002	rBV3	565	632	0.03%	0.004%
84	11.153	3050	3052	3055	rVB2	401	189	0.01%	0.001%
85	11.205	3066	3068	3072	rBV2	455	280	0.01%	0.002%
86	11.301	3094	3098	3100	rBV3	265	261	0.01%	0.002%
87	11.414	3130	3133	3137	rVB2	469	289	0.01%	0.002%
88	11.446	3139	3143	3147	rBV2	359	340	0.02%	0.002%
89	11.465	3147	3149	3152	rBV3	481	348	0.02%	0.002%
90	11.536	3169	3171	3175	rBV	379	300	0.01%	0.002%
91	11.561	3175	3179	3183	rVV	366	369	0.02%	0.003%
92	11.812	3244	3257	3286	rBV	614796	1012633	49.80%	7.142%
93	12.192	3362	3375	3404	rVV	665015	1115328	54.85%	7.866%
94	12.815	3567	3569	3571	rBV2	328	221	0.01%	0.002%
95	12.921	3600	3602	3605	rBV2	352	224	0.01%	0.002%
96	13.082	3649	3652	3653	rBV	494	297	0.01%	0.002%
97	13.262	3706	3708	3712	rVB2	363	188	0.01%	0.001%
98	13.439	3760	3763	3767	rBV2	552	457	0.02%	0.003%
99	13.844	3882	3889	3901	rBV5	5906	10669	0.52%	0.075%
100	14.542	4103	4106	4107	rBV2	450	274	0.01%	0.002%

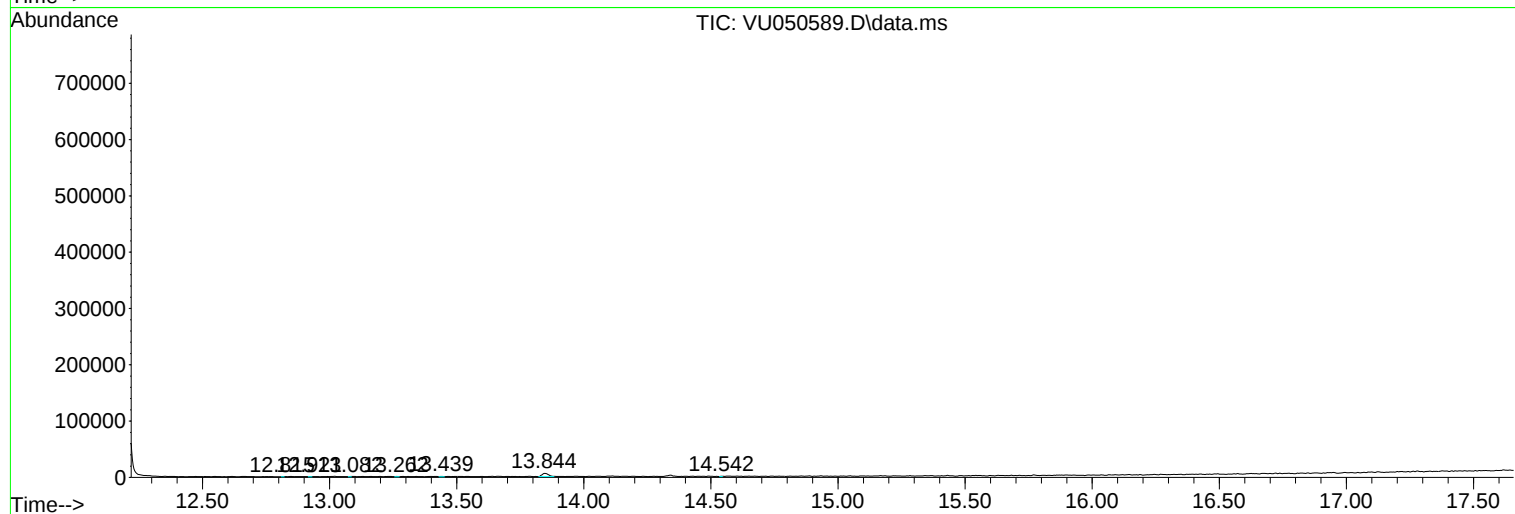
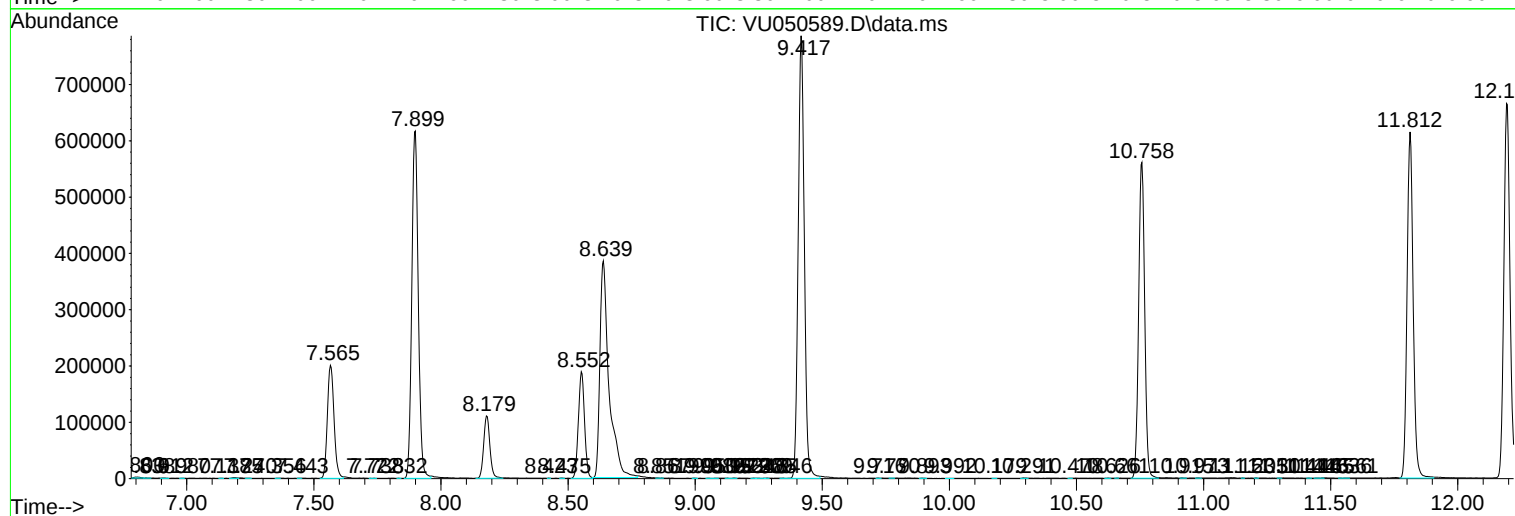
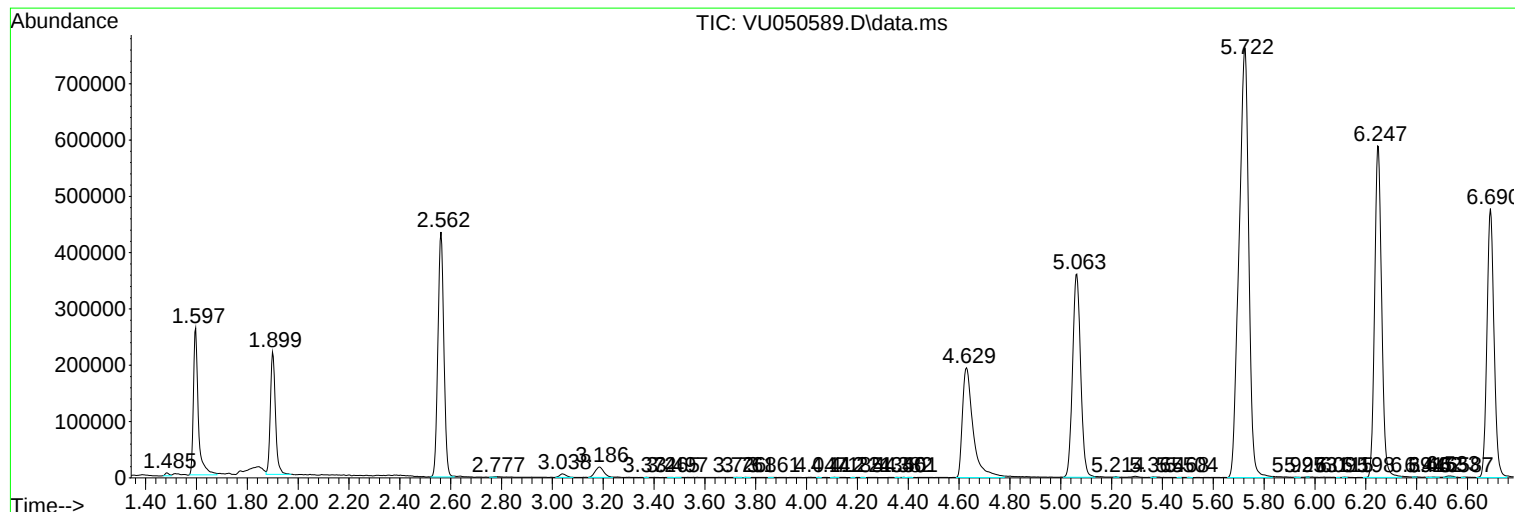
Sum of corrected areas: 14179480

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM083022WMA.M
Quant Title : VOC Analysis

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



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MSVOA_U
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DBVS0ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM083022WMA.M
Quant Title : VOC Analysis

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

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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
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