

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101322\
 Data File : VV028540.D
 Acq On : 13 Oct 2022 16:29
 Operator : SY/MD
 Sample : N5049-14ME
 Misc : 5.22g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 COBSOME

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_V\Method\SFAMVLM100722WMA.M

Title : VOC Analysis

Signal : TIC: VV028540.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.304	76	82	97	rBV	34989	46198	5.43%	0.697%
2	2.089	320	326	340	rVB	134681	193426	22.73%	2.920%
3	2.886	572	574	577	rBV2	174	111	0.01%	0.002%
4	3.005	608	611	613	rBV3	424	260	0.03%	0.004%
5	3.243	682	685	686	rBV	260	156	0.02%	0.002%
6	3.265	689	692	695	rVB2	303	207	0.02%	0.003%
7	3.500	762	765	766	rBV	151	78	0.01%	0.001%
8	3.590	791	793	797	rBV2	175	131	0.02%	0.002%
9	3.683	819	822	827	rBV2	417	219	0.03%	0.003%
10	3.860	874	877	879	rBV2	329	165	0.02%	0.002%
11	3.915	882	894	925	rBV2	31567	166474	19.56%	2.513%
12	4.339	1014	1026	1053	rVB2	122400	313820	36.87%	4.738%
13	4.613	1107	1111	1114	rBV2	228	194	0.02%	0.003%
14	4.645	1114	1121	1122	rBV4	1089	929	0.11%	0.014%
15	4.744	1151	1152	1155	rBV3	299	157	0.02%	0.002%
16	4.786	1161	1165	1168	rBV	193	158	0.02%	0.002%
17	4.886	1193	1196	1200	rBV3	491	458	0.05%	0.007%
18	5.037	1227	1243	1275	rBV3	266023	678785	79.76%	10.248%
19	5.256	1309	1311	1314	rVB2	825	390	0.05%	0.006%
20	5.278	1314	1318	1319	rBV2	314	195	0.02%	0.003%
21	5.314	1326	1329	1330	rBV2	999	571	0.07%	0.009%
22	5.535	1395	1398	1401	rBV3	440	349	0.04%	0.005%
23	5.609	1409	1421	1454	rBV	298287	611365	71.84%	9.230%
24	5.905	1506	1513	1515	rBV3	3140	3473	0.41%	0.052%
25	6.063	1550	1562	1593	rVB2	165039	353796	41.57%	5.341%
26	6.259	1620	1623	1628	rBV2	438	271	0.03%	0.004%
27	6.368	1655	1657	1664	rBV4	568	601	0.07%	0.009%
28	6.410	1667	1670	1671	rBV	250	153	0.02%	0.002%
29	6.474	1688	1690	1694	rBV2	498	271	0.03%	0.004%
30	6.558	1714	1716	1720	rBV2	207	126	0.01%	0.002%
31	6.638	1733	1741	1743	rBV4	2038	2483	0.29%	0.037%
32	6.818	1794	1797	1800	rBV	402	320	0.04%	0.005%
33	6.860	1808	1810	1812	rBV	173	98	0.01%	0.001%
34	6.883	1815	1817	1821	rVB2	470	299	0.04%	0.005%
35	6.915	1821	1827	1831	rBV3	911	1231	0.14%	0.019%
36	6.982	1837	1848	1873	rBV2	97672	193985	22.79%	2.929%

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100722WMA.M
 Title : VOC Analysis

37	7.233	1920	1926	1928	rBV5	1363	1368	0.16%	0.021%
38	7.310	1939	1950	1978	rBV	270174	487481	57.28%	7.360%
39	7.619	2036	2046	2072	rBV	67707	139810	16.43%	2.111%
40	7.783	2095	2097	2099	rBV2	557	400	0.05%	0.006%
41	7.892	2130	2131	2134	rVB2	410	105	0.01%	0.002%
42	7.915	2134	2138	2139	rBV	510	316	0.04%	0.005%
43	7.963	2151	2153	2155	rBV	269	115	0.01%	0.002%
44	8.014	2164	2169	2173	rBV	338	254	0.03%	0.004%
45	8.034	2173	2175	2177	rBV	399	221	0.03%	0.003%
46	8.108	2184	2198	2228	rBV3	163867	521172	61.24%	7.868%
47	8.429	2291	2298	2311	rBV5	2809	5943	0.70%	0.090%
48	8.516	2322	2325	2332	rVB2	356	308	0.04%	0.005%
49	8.548	2332	2335	2336	rBV2	311	187	0.02%	0.003%
50	8.847	2416	2428	2458	rBV	430787	763668	89.73%	11.529%
51	9.066	2494	2496	2502	rVB3	349	265	0.03%	0.004%
52	9.092	2502	2504	2505	rBV	324	128	0.02%	0.002%
53	9.117	2510	2512	2513	rBV2	299	95	0.01%	0.001%
54	9.146	2515	2521	2525	rVV5	1261	1224	0.14%	0.018%
55	9.317	2572	2574	2578	rVB	175	93	0.01%	0.001%
56	9.548	2639	2646	2657	rVB6	2206	3376	0.40%	0.051%
57	9.593	2657	2660	2663	rBV2	325	209	0.02%	0.003%
58	9.612	2663	2666	2668	rBV2	279	145	0.02%	0.002%
59	9.661	2680	2681	2683	rBV	303	106	0.01%	0.002%
60	9.693	2689	2691	2692	rBV	617	312	0.04%	0.005%
61	9.789	2718	2721	2729	rVB5	865	1033	0.12%	0.016%
62	9.844	2732	2738	2744	rVV4	737	875	0.10%	0.013%
63	9.905	2756	2757	2759	rVB	269	96	0.01%	0.001%
64	10.053	2799	2803	2805	rBV	511	305	0.04%	0.005%
65	10.108	2816	2820	2823	rBV3	571	529	0.06%	0.008%
66	10.214	2838	2853	2876	rBV	292530	497574	58.47%	7.512%
67	10.336	2889	2891	2892	rBV	224	99	0.01%	0.001%
68	10.442	2921	2924	2925	rBV2	470	274	0.03%	0.004%
69	10.532	2948	2952	2954	rBV	457	377	0.04%	0.006%
70	10.571	2958	2964	2975	rVB5	5547	8152	0.96%	0.123%
71	10.674	2995	2996	3000	rVB	205	89	0.01%	0.001%
72	10.722	3007	3011	3012	rBV2	230	161	0.02%	0.002%
73	10.870	3055	3057	3064	rVB3	817	600	0.07%	0.009%
74	11.243	3162	3173	3197	rBV	536188	851048	100.00%	12.849%
75	11.461	3238	3241	3242	rBV	261	116	0.01%	0.002%
76	11.619	3278	3290	3316	rBV	467231	734317	86.28%	11.086%

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 Title : VOC Analysis

77	11.850	3359	3362	3367	rBV2	429	398	0.05%	0.006%
78	12.063	3426	3428	3432	rBV2	347	188	0.02%	0.003%
79	12.146	3445	3454	3456	rBV2	569	740	0.09%	0.011%
80	12.233	3477	3481	3482	rBV3	342	260	0.03%	0.004%
81	12.355	3517	3519	3521	rBV2	408	264	0.03%	0.004%
82	12.374	3524	3525	3526	rBV	423	106	0.01%	0.002%
83	12.419	3538	3539	3541	rBV	176	89	0.01%	0.001%
84	12.464	3550	3553	3556	rBV2	446	254	0.03%	0.004%
85	12.497	3561	3563	3565	rBV	474	266	0.03%	0.004%
86	12.648	3606	3610	3611	rBV	483	266	0.03%	0.004%
87	12.786	3652	3653	3655	rBV2	200	93	0.01%	0.001%
88	12.879	3677	3682	3691	rVB7	1810	2105	0.25%	0.032%
89	13.082	3743	3745	3748	rVB2	348	154	0.02%	0.002%
90	13.133	3758	3761	3763	rVB4	476	269	0.03%	0.004%
91	13.191	3777	3779	3785	rVB2	518	366	0.04%	0.006%
92	13.262	3796	3801	3807	rBV6	958	1192	0.14%	0.018%
93	13.342	3824	3826	3829	rVB	642	278	0.03%	0.004%
94	13.358	3829	3831	3833	rBV	318	171	0.02%	0.003%
95	13.500	3867	3875	3888	rVB2	10163	16682	1.96%	0.252%
96	13.628	3909	3915	3920	rBV5	967	1068	0.13%	0.016%
97	13.963	4013	4019	4020	rBV3	590	581	0.07%	0.009%
98	14.281	4115	4118	4122	rBV2	959	980	0.12%	0.015%
99	14.439	4160	4167	4172	rBV4	1429	1737	0.20%	0.026%
100	14.519	4190	4192	4194	rBV2	556	268	0.03%	0.004%

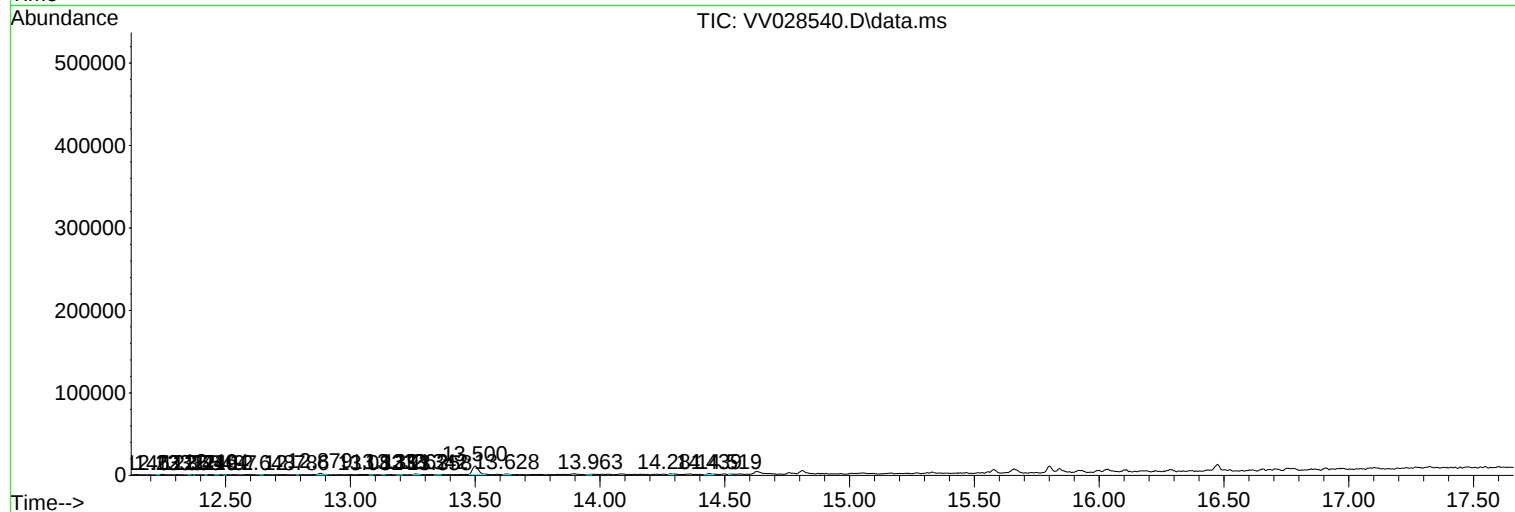
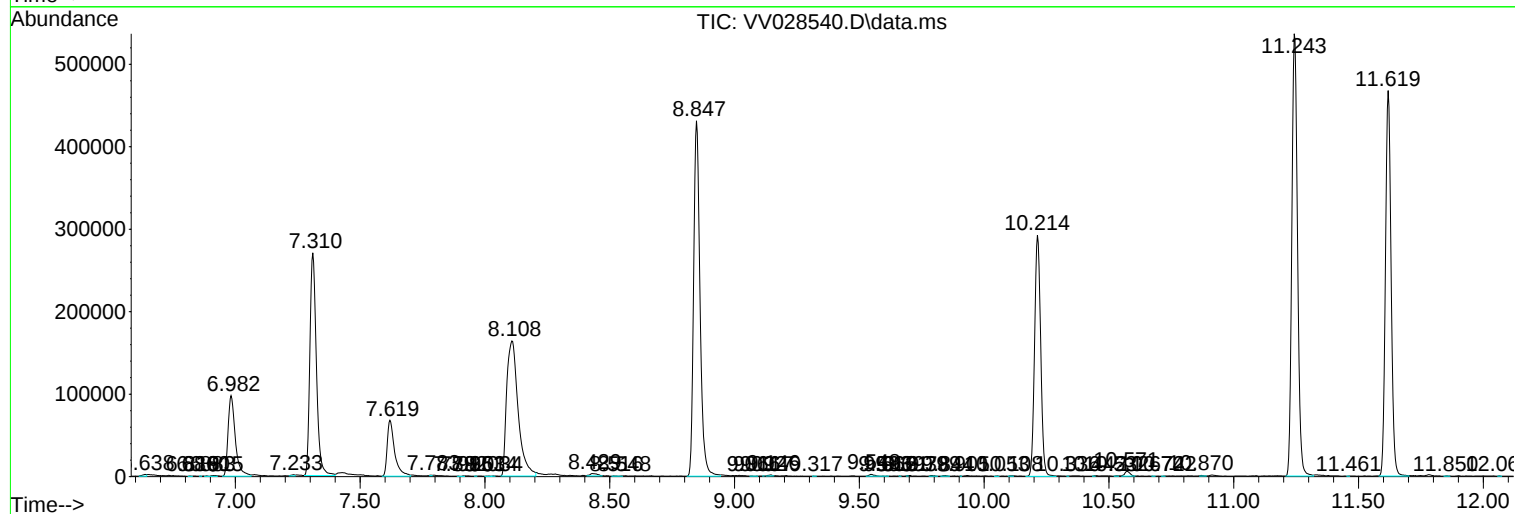
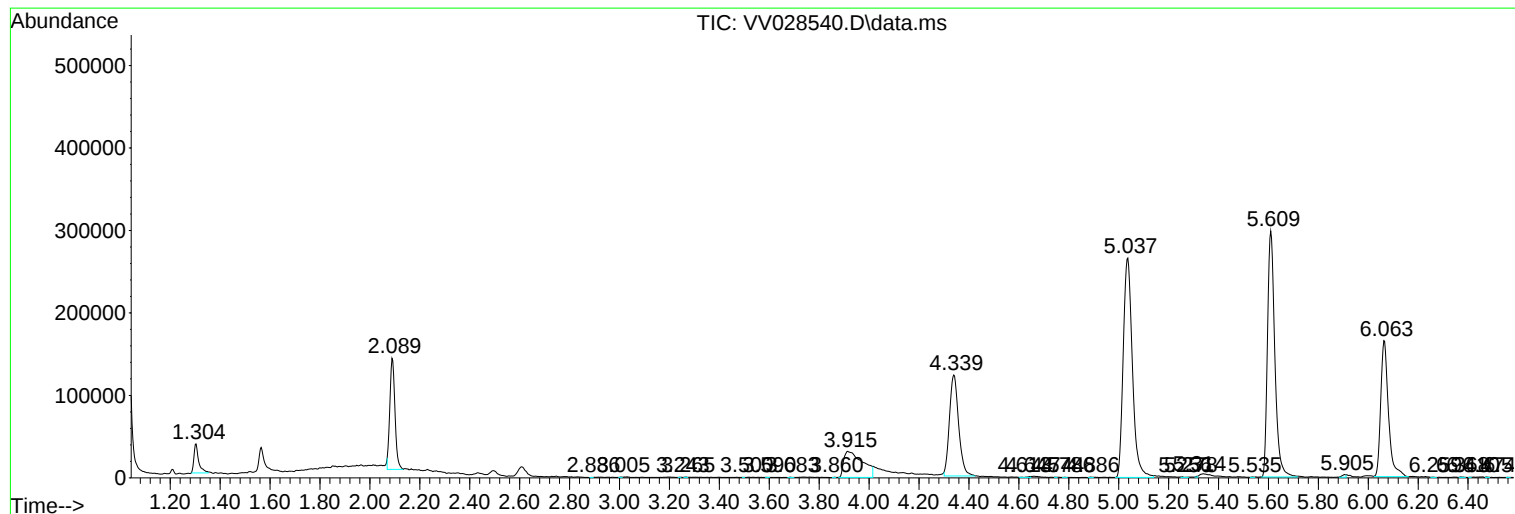
Sum of corrected areas: 6623624

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100722WMA.M
Quant Title : VOC Analysis

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



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Instrument :
MSVOA_V
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C0BS0ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100722WMA.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 Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc