

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
 Data File : VU059385.D
 Acq On : 20 Jun 2024 17:31
 Operator : MD/SY
 Sample : P2960-13ME
 Misc : 5.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHB50ME

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\SFAMULM052924WMA.M
 Title : VOC Analysis

Signal : TIC: VU059385.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.592	87	94	117	rVB	27163	47149	7.40%	1.017%
2	1.827	138	167	168	rBV4	38949	142318	22.32%	3.071%
3	2.535	376	387	402	rVB	74606	120803	18.95%	2.607%
4	2.673	428	430	436	rVB3	514	416	0.07%	0.009%
5	2.711	436	442	445	rBV3	435	528	0.08%	0.011%
6	2.756	452	456	465	rBV2	777	1146	0.18%	0.025%
7	2.824	474	477	480	rVB3	291	212	0.03%	0.005%
8	2.853	483	486	487	rBV	322	198	0.03%	0.004%
9	2.949	514	516	522	rVB3	229	218	0.03%	0.005%
10	3.026	529	540	557	rVV3	4477	9554	1.50%	0.206%
11	3.168	578	584	587	rBV4	844	1034	0.16%	0.022%
12	3.226	599	602	605	rBV2	284	199	0.03%	0.004%
13	3.589	709	715	717	rBV2	222	222	0.03%	0.005%
14	3.718	750	755	759	rBV2	291	357	0.06%	0.008%
15	3.811	779	784	788	rVV2	197	223	0.03%	0.005%
16	4.158	890	892	897	rVB	275	224	0.04%	0.005%
17	4.342	944	949	958	rBV2	324	544	0.09%	0.012%
18	4.631	1027	1039	1076	rBV2	47468	167606	26.29%	3.617%
19	5.052	1154	1170	1192	rBV	84335	189651	29.75%	4.092%
20	5.296	1244	1246	1253	rVV2	388	320	0.05%	0.007%
21	5.377	1269	1271	1277	rVB2	276	265	0.04%	0.006%
22	5.409	1277	1281	1285	rBV2	261	270	0.04%	0.006%
23	5.711	1357	1375	1398	rVV3	176437	469877	73.70%	10.139%
24	5.853	1414	1419	1423	rBV2	223	232	0.04%	0.005%
25	5.891	1429	1431	1436	rVB2	386	242	0.04%	0.005%
26	5.968	1450	1455	1457	rBV3	631	565	0.09%	0.012%
27	6.033	1472	1475	1482	rVB3	269	280	0.04%	0.006%
28	6.242	1527	1540	1572	rBV	248412	489627	76.80%	10.565%
29	6.351	1572	1574	1577	rVB	360	200	0.03%	0.004%
30	6.496	1614	1619	1620	rBV	312	248	0.04%	0.005%
31	6.528	1620	1629	1642	rVB8	5110	11179	1.75%	0.241%
32	6.595	1642	1650	1652	rBV2	1214	1357	0.21%	0.029%
33	6.682	1664	1677	1703	rVB	107474	217811	34.17%	4.700%
34	6.772	1703	1705	1710	rVV2	280	206	0.03%	0.004%
35	6.946	1754	1759	1763	rBV	420	480	0.08%	0.010%
36	7.149	1819	1822	1825	rBV2	236	217	0.03%	0.005%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
 Title : VOC Analysis

37	7.194	1829	1836	1839	rBV5	1352	1574	0.25%	0.034%
38	7.332	1875	1879	1887	rBV2	265	414	0.06%	0.009%
39	7.480	1921	1925	1926	rBV2	277	201	0.03%	0.004%
40	7.560	1940	1950	1970	rBV2	51272	95539	14.99%	2.062%
41	7.698	1989	1993	1994	rBV2	500	348	0.05%	0.008%
42	7.894	2041	2054	2072	rVV	184864	325923	51.12%	7.033%
43	8.020	2091	2093	2097	rVB2	518	360	0.06%	0.008%
44	8.177	2132	2142	2161	rBV2	34959	64696	10.15%	1.396%
45	8.464	2226	2231	2233	rBV2	260	276	0.04%	0.006%
46	8.547	2246	2257	2272	rBV2	55955	95628	15.00%	2.063%
47	8.640	2274	2286	2317	rBV	129201	289958	45.48%	6.257%
48	8.849	2347	2351	2358	rBV3	372	340	0.05%	0.007%
49	8.901	2364	2367	2372	rBV2	207	245	0.04%	0.005%
50	9.296	2485	2490	2496	rBV2	226	340	0.05%	0.007%
51	9.415	2511	2527	2552	rBV	360371	637524	100.00%	13.756%
52	9.579	2575	2578	2583	rVB4	864	709	0.11%	0.015%
53	9.698	2608	2615	2619	rBV3	872	1289	0.20%	0.028%
54	9.740	2626	2628	2633	rVB2	265	193	0.03%	0.004%
55	9.824	2651	2654	2658	rVB2	247	202	0.03%	0.004%
56	9.920	2680	2684	2688	rBV2	265	285	0.04%	0.006%
57	10.110	2738	2743	2746	rBV2	437	381	0.06%	0.008%
58	10.364	2818	2822	2824	rBV2	301	256	0.04%	0.006%
59	10.438	2840	2845	2849	rBV2	270	308	0.05%	0.007%
60	10.463	2849	2853	2859	rVV2	267	350	0.05%	0.008%
61	10.570	2882	2886	2888	rBV2	201	204	0.03%	0.004%
62	10.756	2931	2944	2964	rBV	189531	312642	49.04%	6.746%
63	11.029	3026	3029	3035	rVB2	194	203	0.03%	0.004%
64	11.094	3047	3049	3055	rVB2	278	219	0.03%	0.005%
65	11.129	3056	3060	3064	rVV2	234	193	0.03%	0.004%
66	11.180	3070	3076	3080	rBV	277	344	0.05%	0.007%
67	11.412	3142	3148	3154	rVB5	731	763	0.12%	0.016%
68	11.480	3162	3169	3177	rBV2	710	1071	0.17%	0.023%
69	11.615	3208	3211	3215	rVB	445	347	0.05%	0.007%
70	11.637	3215	3218	3220	rBV	271	213	0.03%	0.005%
71	11.753	3248	3254	3260	rBV4	914	1254	0.20%	0.027%
72	11.811	3260	3272	3294	rBV	359933	579057	90.83%	12.495%
73	12.004	3329	3332	3336	rVB2	305	300	0.05%	0.006%
74	12.029	3336	3340	3349	rVB2	404	492	0.08%	0.011%
75	12.190	3378	3390	3414	rBV	198126	333281	52.28%	7.192%
76	12.473	3475	3478	3483	rBV2	254	285	0.04%	0.006%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
 Title : VOC Analysis

77	13.206	3703	3706	3710	rBV	280	193	0.03%	0.004%
78	13.287	3727	3731	3735	rBV2	419	460	0.07%	0.010%
79	13.367	3750	3756	3758	rBV2	238	259	0.04%	0.006%
80	13.438	3773	3778	3780	rBV2	330	278	0.04%	0.006%
81	13.679	3850	3853	3857	rVB2	274	200	0.03%	0.004%
82	13.820	3891	3897	3903	rBV2	377	478	0.07%	0.010%
83	13.859	3903	3909	3910	rBV	734	705	0.11%	0.015%
84	14.010	3953	3956	3961	rVB	314	219	0.03%	0.005%
85	14.110	3978	3987	3990	rBV4	1326	1745	0.27%	0.038%
86	14.206	4014	4017	4021	rBV3	380	292	0.05%	0.006%
87	14.245	4025	4029	4031	rBV	542	357	0.06%	0.008%
88	14.331	4052	4056	4057	rBV3	447	309	0.05%	0.007%
89	14.389	4071	4074	4078	rBV2	233	201	0.03%	0.004%
90	14.457	4092	4095	4097	rBV3	394	291	0.05%	0.006%
91	14.508	4108	4111	4114	rBV3	305	252	0.04%	0.005%
92	14.631	4146	4149	4151	rBV2	262	195	0.03%	0.004%
93	14.647	4152	4154	4159	rVV2	310	240	0.04%	0.005%
94	14.717	4171	4176	4179	rBV3	497	525	0.08%	0.011%
95	14.769	4188	4192	4197	rVB3	472	474	0.07%	0.010%
96	14.939	4239	4245	4250	rBV3	375	548	0.09%	0.012%
97	15.023	4267	4271	4275	rBV	650	692	0.11%	0.015%
98	15.402	4385	4389	4392	rBV2	874	752	0.12%	0.016%
99	15.470	4408	4410	4412	rBV	457	276	0.04%	0.006%
100	15.656	4467	4468	4470	rBV2	446	244	0.04%	0.005%

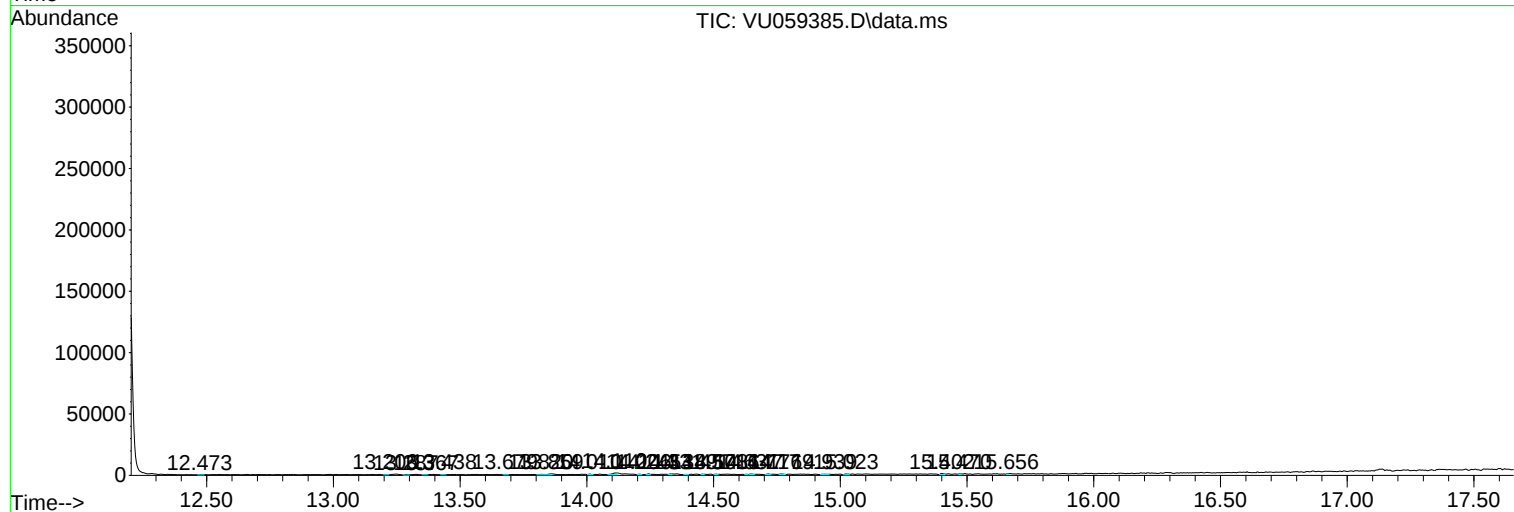
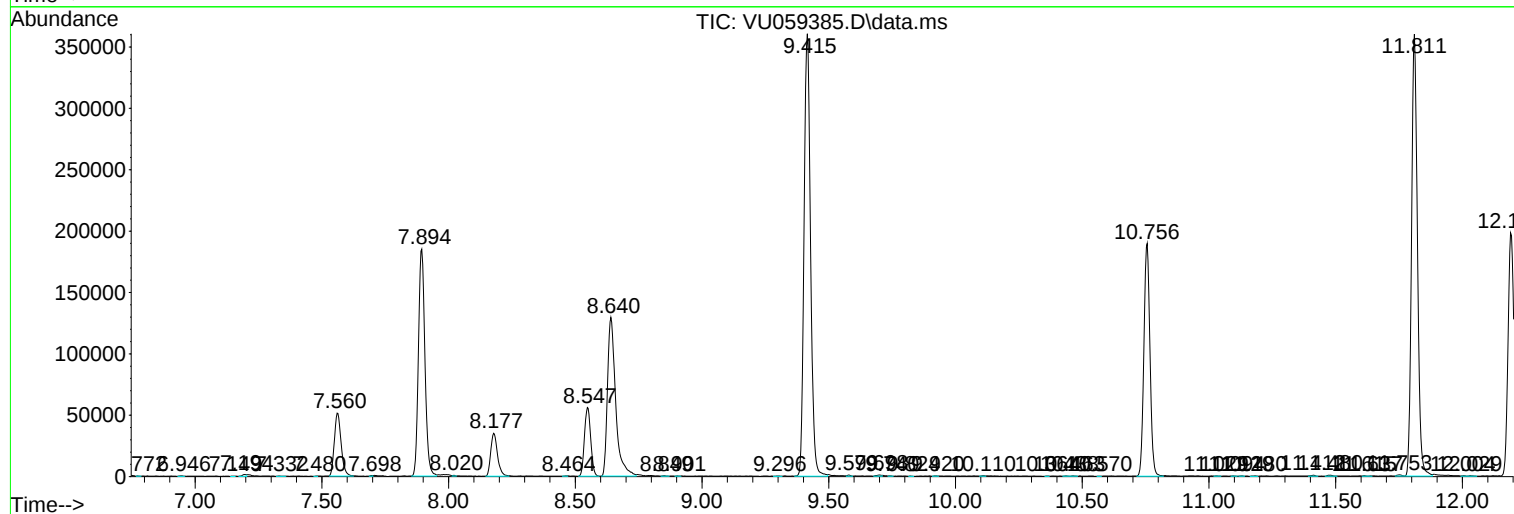
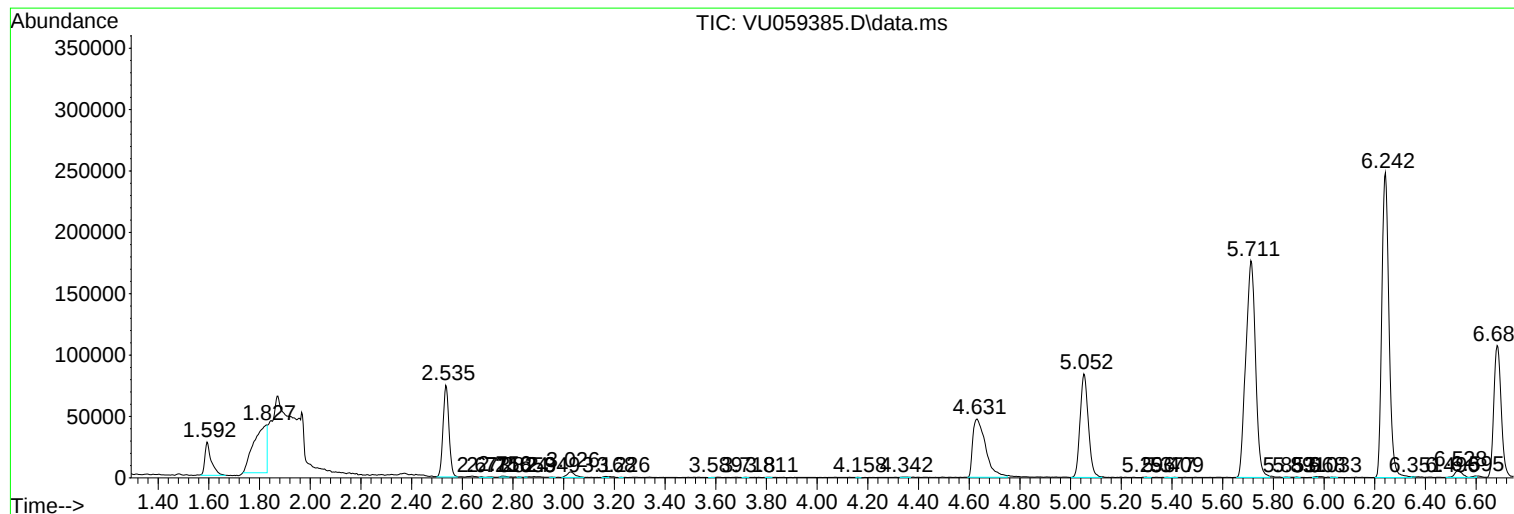
Sum of corrected areas: 4634370

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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.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_U\Method\SFAMULM052924WMA.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