

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052824\
 Data File : VU059028.D
 Acq On : 28 May 2024 14:27
 Operator : MD/SY
 Sample : P2577-06ME
 Misc : 5.97g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHBN4ME

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\SFAMULM052324WMA.M
 Title : VOC Analysis

Signal : TIC: VU059028.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	120	rVB	72099	118010	14.63%	2.035%
2	2.534	375	387	403	rBV	155140	249210	30.89%	4.298%
3	2.917	504	506	508	rBV	380	108	0.01%	0.002%
4	3.026	529	540	551	rBV4	3957	7993	0.99%	0.138%
5	3.168	573	584	601	rBV4	4100	10578	1.31%	0.182%
6	3.300	622	625	629	rBV2	259	157	0.02%	0.003%
7	3.357	639	643	646	rBV2	418	362	0.04%	0.006%
8	3.393	651	654	657	rBV	143	96	0.01%	0.002%
9	3.438	665	668	674	rVB2	286	269	0.03%	0.005%
10	3.573	707	710	714	rVB	314	205	0.03%	0.004%
11	3.599	715	718	719	rBV	99	61	0.01%	0.001%
12	3.669	737	740	744	rBV3	618	440	0.05%	0.008%
13	3.792	775	778	779	rBV	79	45	0.01%	0.001%
14	3.840	790	793	796	rBV2	265	161	0.02%	0.003%
15	3.875	799	804	807	rBV	174	163	0.02%	0.003%
16	3.907	809	814	817	rBV2	159	125	0.02%	0.002%
17	3.962	829	831	834	rBV2	97	51	0.01%	0.001%
18	4.065	860	863	866	rBV2	174	116	0.01%	0.002%
19	4.161	889	893	895	rBV	296	192	0.02%	0.003%
20	4.177	895	898	901	rVB2	111	79	0.01%	0.001%
21	4.264	917	925	930	rBV2	120	250	0.03%	0.004%
22	4.319	939	942	946	rVV	294	188	0.02%	0.003%
23	4.415	968	972	974	rBV	114	97	0.01%	0.002%
24	4.451	979	983	986	rVB2	105	85	0.01%	0.001%
25	4.473	986	990	993	rBV	304	242	0.03%	0.004%
26	4.509	998	1001	1003	rBV2	183	119	0.01%	0.002%
27	4.563	1016	1018	1020	rBV2	77	43	0.01%	0.001%
28	4.624	1026	1037	1064	rBV	63095	192940	23.91%	3.327%
29	4.939	1133	1135	1136	rBV	176	71	0.01%	0.001%
30	5.052	1154	1170	1199	rVB2	135177	309550	38.37%	5.338%
31	5.187	1210	1212	1216	rBV2	121	58	0.01%	0.001%
32	5.219	1221	1222	1226	rBV2	263	94	0.01%	0.002%
33	5.242	1226	1229	1235	rVB2	147	126	0.02%	0.002%
34	5.280	1239	1241	1247	rVB2	254	151	0.02%	0.003%
35	5.309	1247	1250	1253	rBV2	212	188	0.02%	0.003%
36	5.354	1261	1264	1269	rVB	217	135	0.02%	0.002%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052324WMA.M
 Title : VOC Analysis

37	5.409	1275	1281	1284	rBV	274	278	0.03%	0.005%
38	5.428	1284	1287	1292	rVV2	197	204	0.03%	0.004%
39	5.537	1318	1321	1323	rBV2	214	148	0.02%	0.003%
40	5.631	1346	1350	1352	rVB2	111	66	0.01%	0.001%
41	5.711	1352	1375	1403	rBV2	302621	806795	100.00%	13.914%
42	5.888	1426	1430	1432	rBV2	193	180	0.02%	0.003%
43	5.914	1436	1438	1441	rBV	228	126	0.02%	0.002%
44	5.972	1448	1456	1466	rBV6	2061	4188	0.52%	0.072%
45	6.119	1499	1502	1506	rVB2	289	238	0.03%	0.004%
46	6.171	1512	1518	1521	rVB2	206	168	0.02%	0.003%
47	6.187	1521	1523	1525	rBV	144	96	0.01%	0.002%
48	6.238	1527	1539	1566	rBV	242141	477737	59.21%	8.239%
49	6.396	1586	1588	1589	rBV	287	82	0.01%	0.001%
50	6.431	1597	1599	1601	rBV2	166	91	0.01%	0.002%
51	6.492	1615	1618	1619	rVV	134	68	0.01%	0.001%
52	6.521	1619	1627	1638	rVB6	3683	6970	0.86%	0.120%
53	6.599	1638	1651	1663	rBV6	2889	6603	0.82%	0.114%
54	6.682	1663	1677	1703	rVV	180423	366455	45.42%	6.320%
55	6.904	1742	1746	1752	rBV2	187	192	0.02%	0.003%
56	6.926	1752	1753	1756	rBV	132	67	0.01%	0.001%
57	7.033	1784	1786	1789	rBV2	172	110	0.01%	0.002%
58	7.071	1792	1798	1800	rBV2	173	143	0.02%	0.002%
59	7.090	1800	1804	1806	rVB	168	101	0.01%	0.002%
60	7.110	1807	1810	1816	rVB2	252	244	0.03%	0.004%
61	7.148	1816	1822	1824	rBV	211	148	0.02%	0.003%
62	7.168	1824	1828	1830	rBV2	148	120	0.01%	0.002%
63	7.216	1840	1843	1845	rBV3	942	725	0.09%	0.013%
64	7.341	1880	1882	1884	rBV2	106	60	0.01%	0.001%
65	7.389	1894	1897	1900	rVB	172	107	0.01%	0.002%
66	7.415	1900	1905	1907	rBV2	284	209	0.03%	0.004%
67	7.499	1926	1931	1935	rBV3	389	386	0.05%	0.007%
68	7.560	1938	1950	1972	rBV	89167	169055	20.95%	2.916%
69	7.814	2027	2029	2032	rBV2	153	87	0.01%	0.002%
70	7.891	2040	2053	2075	rBV	329155	578703	71.73%	9.980%
71	8.090	2113	2115	2123	rVB2	361	272	0.03%	0.005%
72	8.126	2123	2126	2128	rBV	140	93	0.01%	0.002%
73	8.174	2130	2141	2161	rBV2	59733	112863	13.99%	1.946%
74	8.319	2183	2186	2189	rBV2	334	208	0.03%	0.004%
75	8.341	2189	2193	2195	rBV	281	200	0.02%	0.003%
76	8.457	2225	2229	2232	rBV	381	437	0.05%	0.008%

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052324WMA.M
 Title : VOC Analysis

77	8.508	2241	2245	2249	rVB2	346	248	0.03%	0.004%
78	8.531	2249	2252	2254	rBV2	254	180	0.02%	0.003%
79	8.647	2273	2288	2321	rBV	157064	425966	52.80%	7.346%
80	9.078	2420	2422	2428	rBV	252	213	0.03%	0.004%
81	9.119	2432	2435	2437	rBV	226	152	0.02%	0.003%
82	9.151	2441	2445	2447	rBV2	297	177	0.02%	0.003%
83	9.299	2488	2491	2495	rBV2	167	131	0.02%	0.002%
84	9.322	2495	2498	2505	rBV2	268	239	0.03%	0.004%
85	9.415	2514	2527	2546	rBV	320124	589392	73.05%	10.165%
86	9.791	2641	2644	2648	rBV2	230	223	0.03%	0.004%
87	9.840	2656	2659	2662	rBV	241	209	0.03%	0.004%
88	9.894	2674	2676	2678	rBV2	154	69	0.01%	0.001%
89	9.933	2686	2688	2690	rBV	130	72	0.01%	0.001%
90	9.955	2691	2695	2697	rVV	311	222	0.03%	0.004%
91	10.010	2706	2712	2714	rBV2	352	377	0.05%	0.007%
92	10.193	2766	2769	2771	rBV	217	118	0.01%	0.002%
93	10.357	2817	2820	2824	rBV2	362	278	0.03%	0.005%
94	10.460	2849	2852	2855	rBV2	243	199	0.02%	0.003%
95	10.563	2880	2884	2885	rBV2	270	196	0.02%	0.003%
96	10.756	2931	2944	2965	rBV	247621	419453	51.99%	7.234%
97	11.190	3076	3079	3082	rBV	266	200	0.02%	0.003%
98	11.486	3168	3171	3173	rBV	262	158	0.02%	0.003%
99	11.811	3260	3272	3293	rBV	293650	475640	58.95%	8.203%
100	12.190	3378	3390	3415	rBV	275430	456562	56.59%	7.874%

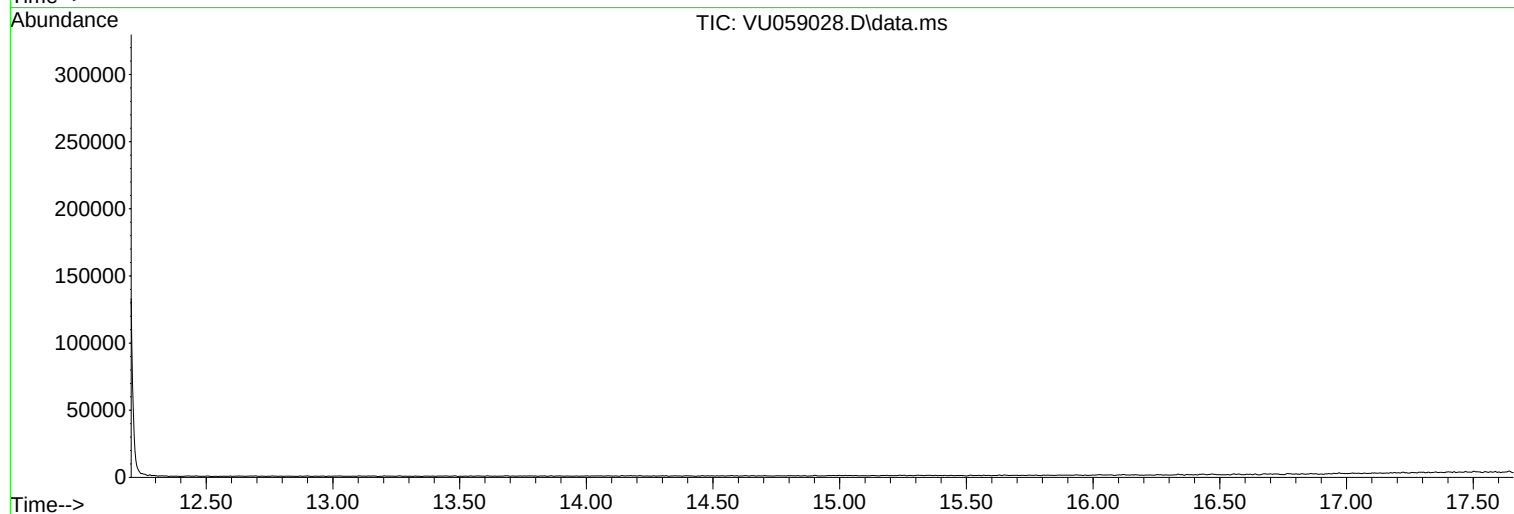
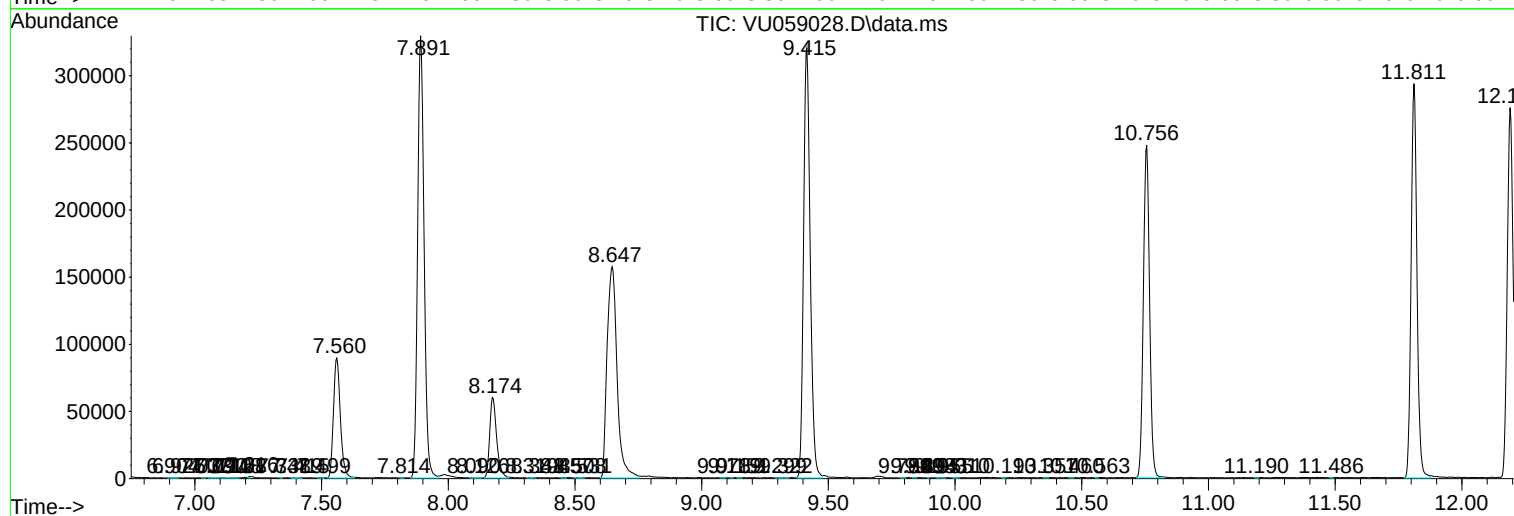
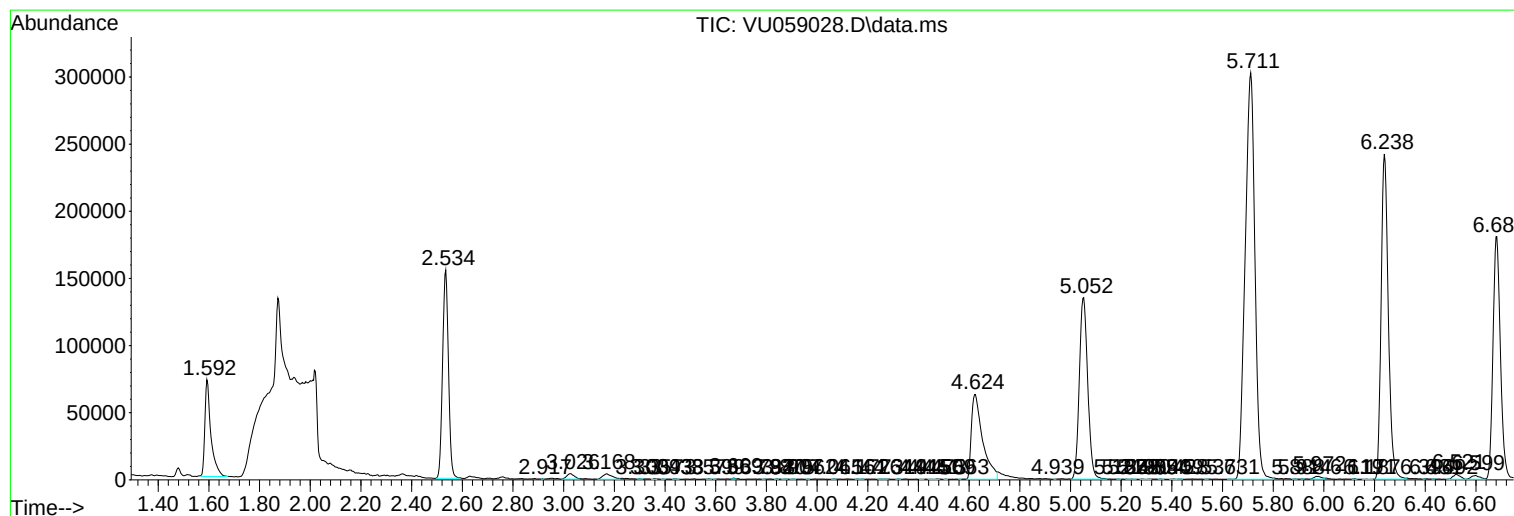
Sum of corrected areas: 5798455

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ClientSampleId :
BHBN4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052324WMA.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\SFAMULM052324WMA.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