

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052824\
 Data File : VU059035.D
 Acq On : 28 May 2024 17:19
 Operator : MD/SY
 Sample : P2570-22ME
 Misc : 5.13g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH654ME

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: VU059035.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.476	53	58	66	rBV	8308	9270	1.14%	0.154%
2	1.592	86	94	120	rVB	63475	118061	14.51%	1.963%
3	1.814	136	163	164	rBV6	59845	192088	23.60%	3.194%
4	2.525	374	384	400	rVB	157193	249983	30.71%	4.156%
5	3.020	532	538	553	rVB6	4405	9457	1.16%	0.157%
6	3.168	570	584	603	rBV2	9339	24884	3.06%	0.414%
7	3.460	670	675	677	rBV	219	195	0.02%	0.003%
8	3.537	694	699	702	rBV2	197	208	0.03%	0.003%
9	3.663	735	738	740	rVV2	404	230	0.03%	0.004%
10	3.869	801	802	808	rVV2	243	189	0.02%	0.003%
11	4.187	898	901	906	rVB	304	260	0.03%	0.004%
12	4.222	908	912	916	rBV2	228	211	0.03%	0.004%
13	4.627	1026	1038	1082	rBV	60578	214320	26.33%	3.564%
14	4.869	1109	1113	1116	rVB3	337	230	0.03%	0.004%
15	4.955	1137	1140	1148	rVB3	457	533	0.07%	0.009%
16	4.991	1148	1151	1153	rBV3	436	249	0.03%	0.004%
17	5.049	1153	1169	1197	rVV2	134828	313479	38.51%	5.212%
18	5.168	1202	1206	1212	rVB3	217	302	0.04%	0.005%
19	5.203	1212	1217	1220	rBV2	311	248	0.03%	0.004%
20	5.341	1257	1260	1268	rVB	293	330	0.04%	0.005%
21	5.389	1268	1275	1279	rBV2	368	364	0.04%	0.006%
22	5.708	1355	1374	1398	rVV2	313814	813932	100.00%	13.533%
23	5.897	1429	1433	1437	rBV3	376	356	0.04%	0.006%
24	5.942	1442	1447	1449	rBV2	368	347	0.04%	0.006%
25	5.981	1449	1459	1465	rBV6	2557	5335	0.66%	0.089%
26	6.065	1481	1485	1487	rBV3	256	192	0.02%	0.003%
27	6.158	1511	1514	1519	rVB2	254	216	0.03%	0.004%
28	6.187	1519	1523	1525	rBV	274	219	0.03%	0.004%
29	6.238	1526	1539	1560	rBV	237492	480401	59.02%	7.988%
30	6.463	1606	1609	1612	rVV	377	311	0.04%	0.005%
31	6.524	1615	1628	1637	rVV4	4636	8400	1.03%	0.140%
32	6.595	1637	1650	1664	rVV5	3775	9454	1.16%	0.157%
33	6.682	1664	1677	1703	rVV	185921	375090	46.08%	6.237%
34	6.775	1703	1706	1708	rVV2	528	387	0.05%	0.006%
35	6.801	1712	1714	1718	rVV2	367	271	0.03%	0.005%
36	6.891	1735	1742	1747	rVB2	325	356	0.04%	0.006%

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

37	6.920	1747	1751	1760	rBV	314	472	0.06%	0.008%
38	7.068	1794	1797	1803	rBV2	213	198	0.02%	0.003%
39	7.110	1803	1810	1813	rVB2	214	249	0.03%	0.004%
40	7.193	1834	1836	1838	rVV2	303	190	0.02%	0.003%
41	7.222	1839	1845	1852	rVB6	1133	1611	0.20%	0.027%
42	7.309	1868	1872	1878	rVV4	635	685	0.08%	0.011%
43	7.370	1885	1891	1895	rVV3	189	190	0.02%	0.003%
44	7.470	1915	1922	1924	rBV2	200	211	0.03%	0.004%
45	7.486	1924	1927	1928	rBV	349	209	0.03%	0.003%
46	7.560	1938	1950	1971	rBV	91530	172577	21.20%	2.869%
47	7.778	2011	2018	2019	rBV2	698	486	0.06%	0.008%
48	7.817	2027	2030	2033	rBV2	309	203	0.02%	0.003%
49	7.891	2038	2053	2074	rBV	330459	582820	71.61%	9.691%
50	8.174	2130	2141	2169	rVB2	61032	115752	14.22%	1.925%
51	8.466	2226	2232	2238	rVB3	335	548	0.07%	0.009%
52	8.640	2273	2286	2322	rBV	155792	413216	50.77%	6.871%
53	8.817	2339	2341	2345	rVB3	469	310	0.04%	0.005%
54	8.975	2384	2390	2392	rVV3	347	338	0.04%	0.006%
55	9.219	2461	2466	2471	rVV2	391	436	0.05%	0.007%
56	9.277	2480	2484	2488	rBV2	298	260	0.03%	0.004%
57	9.415	2514	2527	2550	rBV	339234	595311	73.14%	9.898%
58	9.579	2572	2578	2587	rVB3	669	965	0.12%	0.016%
59	9.695	2607	2614	2616	rBV3	1541	1586	0.19%	0.026%
60	9.762	2631	2635	2639	rVB	373	298	0.04%	0.005%
61	9.791	2639	2644	2646	rBV	213	209	0.03%	0.003%
62	9.991	2703	2706	2711	rVV2	241	223	0.03%	0.004%
63	10.055	2723	2726	2730	rBV2	319	289	0.04%	0.005%
64	10.151	2752	2756	2759	rBV2	290	232	0.03%	0.004%
65	10.232	2778	2781	2784	rVB2	292	191	0.02%	0.003%
66	10.283	2794	2797	2802	rVB	323	290	0.04%	0.005%
67	10.470	2852	2855	2859	rBV2	351	282	0.03%	0.005%
68	10.499	2859	2864	2869	rVB2	268	222	0.03%	0.004%
69	10.566	2880	2885	2888	rBV2	286	259	0.03%	0.004%
70	10.756	2931	2944	2959	rBV	242848	401932	49.38%	6.683%
71	10.897	2986	2988	2994	rBV	260	193	0.02%	0.003%
72	11.000	3012	3020	3023	rBV2	289	376	0.05%	0.006%
73	11.167	3066	3072	3075	rBV	226	212	0.03%	0.004%
74	11.273	3100	3105	3107	rBV2	213	185	0.02%	0.003%
75	11.299	3107	3113	3116	rVV2	281	325	0.04%	0.005%
76	11.669	3224	3228	3230	rBV2	276	215	0.03%	0.004%

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Title : VOC Analysis

77	11.810	3260	3272	3294	rBV	282819	449513	55.23%	7.474%
78	12.013	3332	3335	3338	rBV2	431	295	0.04%	0.005%
79	12.135	3370	3373	3378	rVB2	421	257	0.03%	0.004%
80	12.190	3378	3390	3410	rBV	266408	433683	53.28%	7.211%
81	12.286	3418	3420	3422	rVB2	503	199	0.02%	0.003%
82	12.502	3483	3487	3493	rVB3	340	321	0.04%	0.005%
83	12.801	3577	3580	3584	rBV	242	189	0.02%	0.003%
84	12.868	3597	3601	3603	rBV	267	200	0.02%	0.003%
85	12.884	3604	3606	3612	rVB2	394	278	0.03%	0.005%
86	13.003	3641	3643	3647	rVB2	291	187	0.02%	0.003%
87	13.048	3654	3657	3663	rVB2	305	241	0.03%	0.004%
88	13.106	3672	3675	3678	rBV2	356	261	0.03%	0.004%
89	13.206	3703	3706	3709	rVB2	325	186	0.02%	0.003%
90	13.370	3754	3757	3763	rVB2	400	412	0.05%	0.007%
91	13.408	3763	3769	3772	rBV2	392	472	0.06%	0.008%
92	13.492	3792	3795	3802	rVB	294	258	0.03%	0.004%
93	13.913	3923	3926	3928	rBV2	468	274	0.03%	0.005%
94	14.106	3983	3986	3990	rVB2	330	231	0.03%	0.004%
95	14.129	3990	3993	3998	rBV2	435	317	0.04%	0.005%
96	14.624	4145	4147	4153	rVB	560	342	0.04%	0.006%
97	14.669	4157	4161	4164	rBV2	416	361	0.04%	0.006%
98	14.987	4258	4260	4263	rVB	508	230	0.03%	0.004%
99	15.006	4263	4266	4269	rBV2	346	229	0.03%	0.004%
100	15.630	4456	4460	4461	rBV	317	245	0.03%	0.004%

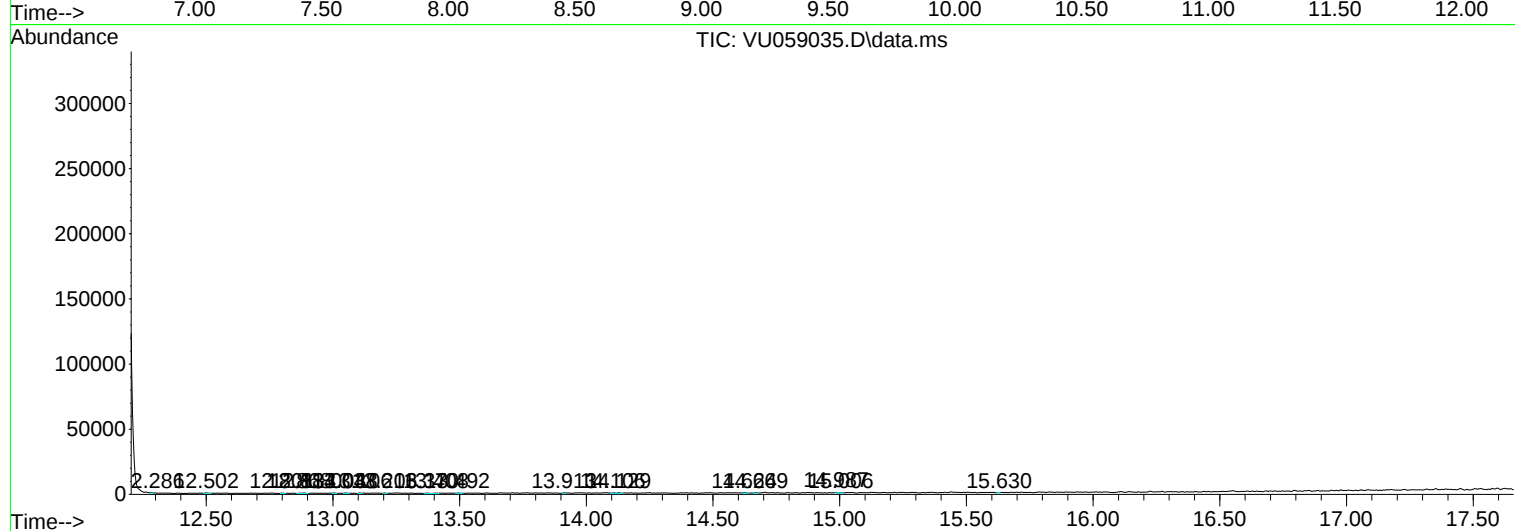
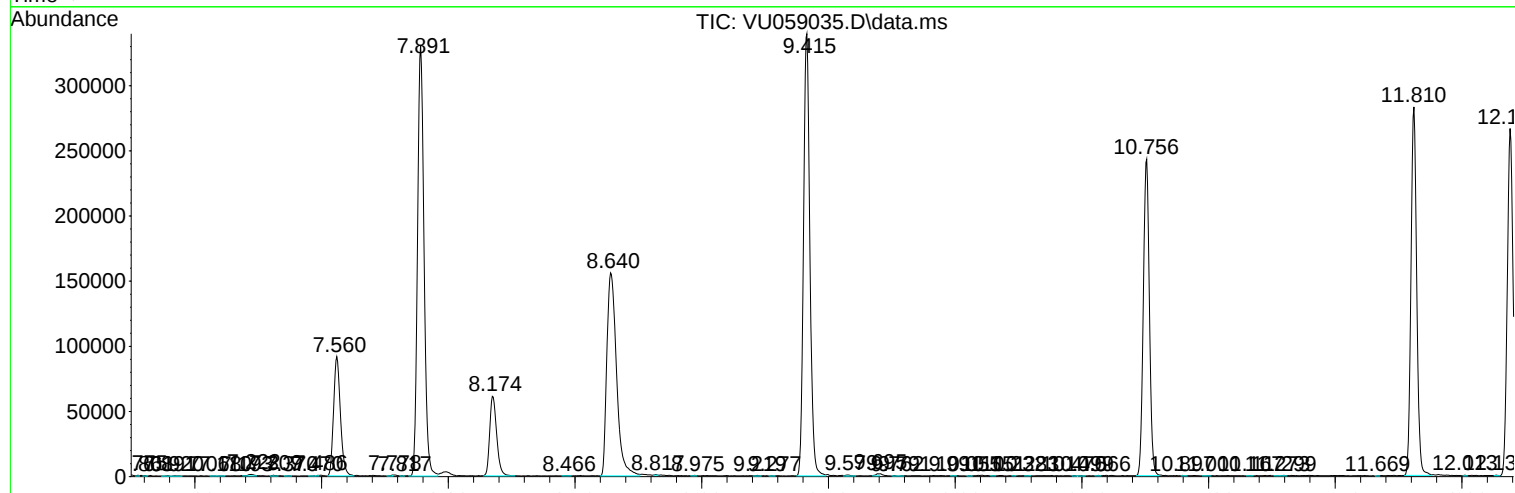
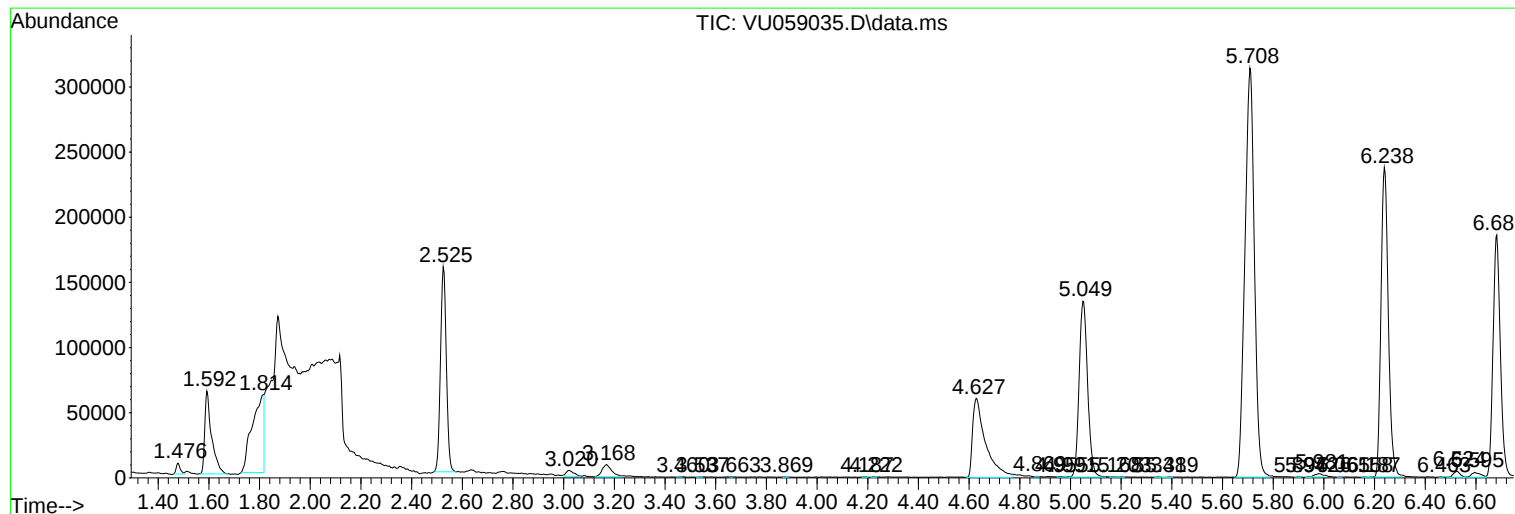
Sum of corrected areas: 6014295

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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	#	RT	Resp	Conc
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