

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102924\
 Data File : VU061289.D
 Acq On : 29 Oct 2024 16:54
 Operator : MD/SY
 Sample : P4493-13ME
 Misc : 5.69g/5mL/100ul/5mL/MSVOA_U/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A4F20ME

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\SFAMULM102824WMA.M
 Title : VOC Analysis

Signal : TIC: VU061289.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.596	88	95	113	rVB	91974	125332	12.83%	1.636%
2	2.544	379	390	408	rBV	195180	321779	32.95%	4.200%
3	2.946	506	515	534	rBV	11006	22627	2.32%	0.295%
4	3.174	572	586	609	rBV2	14972	40014	4.10%	0.522%
5	3.557	701	705	709	rVB2	265	229	0.02%	0.003%
6	3.586	709	714	717	rBV3	338	315	0.03%	0.004%
7	3.657	733	736	738	rBV2	307	212	0.02%	0.003%
8	3.676	739	742	744	rBV3	711	467	0.05%	0.006%
9	3.721	752	756	761	rBV3	263	271	0.03%	0.004%
10	3.817	784	786	789	rBV2	233	157	0.02%	0.002%
11	3.866	799	801	803	rBV	128	71	0.01%	0.001%
12	3.988	834	839	843	rBV	224	238	0.02%	0.003%
13	4.036	852	854	855	rBV	152	68	0.01%	0.001%
14	4.139	882	886	889	rBV2	169	123	0.01%	0.002%
15	4.161	889	893	897	rBV2	254	270	0.03%	0.004%
16	4.238	915	917	920	rBV	249	157	0.02%	0.002%
17	4.354	948	953	955	rBV	262	237	0.02%	0.003%
18	4.390	961	964	966	rBV2	236	150	0.02%	0.002%
19	4.457	981	985	990	rVB2	205	251	0.03%	0.003%
20	4.489	991	995	998	rBV2	155	133	0.01%	0.002%
21	4.525	998	1006	1009	rBV2	209	333	0.03%	0.004%
22	4.618	1024	1035	1067	rBV	73014	210391	21.54%	2.746%
23	5.049	1154	1169	1194	rBV	168587	376352	38.54%	4.912%
24	5.219	1220	1222	1224	rBV2	132	68	0.01%	0.001%
25	5.283	1238	1242	1247	rVB	258	258	0.03%	0.003%
26	5.309	1247	1250	1251	rBV2	175	116	0.01%	0.002%
27	5.373	1266	1270	1271	rBV	161	80	0.01%	0.001%
28	5.457	1292	1296	1300	rBV2	304	260	0.03%	0.003%
29	5.515	1311	1314	1316	rBV	186	148	0.02%	0.002%
30	5.563	1323	1329	1333	rBV	183	256	0.03%	0.003%
31	5.599	1338	1340	1343	rBV2	190	137	0.01%	0.002%
32	5.711	1355	1375	1405	rBV2	367695	976629	100.00%	12.748%
33	6.126	1500	1504	1505	rBV	193	121	0.01%	0.002%
34	6.181	1514	1521	1524	rBB2	261	283	0.03%	0.004%
35	6.238	1524	1539	1569	rBV	316284	615412	63.01%	8.033%
36	6.528	1623	1629	1632	rBV3	1413	1852	0.19%	0.024%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM102824WMA.M
 Title : VOC Analysis

37	6.679	1663	1676	1705	rBV	215383	425053	43.52%	5.548%
38	6.885	1738	1740	1742	rVB	157	84	0.01%	0.001%
39	6.904	1742	1746	1749	rBV	187	153	0.02%	0.002%
40	7.010	1776	1779	1780	rBV	253	138	0.01%	0.002%
41	7.020	1780	1782	1786	rVB2	262	165	0.02%	0.002%
42	7.042	1786	1789	1791	rBV	224	126	0.01%	0.002%
43	7.078	1798	1800	1802	rBV	189	128	0.01%	0.002%
44	7.132	1814	1817	1820	rBV	162	158	0.02%	0.002%
45	7.164	1825	1827	1828	rBV	177	92	0.01%	0.001%
46	7.248	1851	1853	1856	rBV2	230	132	0.01%	0.002%
47	7.316	1871	1874	1876	rBV	191	139	0.01%	0.002%
48	7.357	1885	1887	1889	rBV	118	81	0.01%	0.001%
49	7.412	1901	1904	1906	rBV	211	120	0.01%	0.002%
50	7.451	1913	1916	1918	rBV	209	138	0.01%	0.002%
51	7.489	1925	1928	1929	rBV	151	107	0.01%	0.001%
52	7.557	1936	1949	1974	rBV	122842	222864	22.82%	2.909%
53	7.689	1988	1990	1992	rBV2	165	105	0.01%	0.001%
54	7.717	1996	1999	2004	rVB3	351	394	0.04%	0.005%
55	7.743	2004	2007	2010	rBV2	222	175	0.02%	0.002%
56	7.888	2040	2052	2076	rBV	455952	810043	82.94%	10.573%
57	8.174	2129	2141	2163	rBV	82147	149019	15.26%	1.945%
58	8.332	2188	2190	2192	rBV2	134	85	0.01%	0.001%
59	8.348	2192	2195	2202	rVB2	322	335	0.03%	0.004%
60	8.380	2202	2205	2209	rBV	256	232	0.02%	0.003%
61	8.406	2209	2213	2218	rVB2	197	235	0.02%	0.003%
62	8.428	2218	2220	2223	rVB	166	100	0.01%	0.001%
63	8.451	2223	2227	2229	rBV2	367	333	0.03%	0.004%
64	8.531	2246	2252	2255	rVB2	295	312	0.03%	0.004%
65	8.547	2255	2257	2259	rBV	181	117	0.01%	0.002%
66	8.589	2268	2270	2273	rBV	133	87	0.01%	0.001%
67	8.634	2273	2284	2326	rBV	240982	548744	56.19%	7.163%
68	8.968	2386	2388	2390	rBV2	331	131	0.01%	0.002%
69	9.049	2408	2413	2414	rBV	214	186	0.02%	0.002%
70	9.100	2424	2429	2431	rBV2	263	242	0.02%	0.003%
71	9.225	2466	2468	2472	rBV	247	186	0.02%	0.002%
72	9.251	2472	2476	2480	rVB2	211	191	0.02%	0.002%
73	9.287	2482	2487	2491	rBV2	217	239	0.02%	0.003%
74	9.332	2499	2501	2504	rBV2	152	85	0.01%	0.001%
75	9.412	2514	2526	2555	rBV	443572	784173	80.29%	10.236%
76	9.608	2585	2587	2589	rBV2	134	77	0.01%	0.001%

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 Title : VOC Analysis

77	9.688	2610	2612	2615	rBV2	295	144	0.01%	0.002%
78	9.778	2636	2640	2642	rBV2	269	195	0.02%	0.003%
79	9.814	2646	2651	2654	rBV2	221	237	0.02%	0.003%
80	9.949	2689	2693	2694	rBV	224	148	0.02%	0.002%
81	9.991	2702	2706	2709	rBV2	283	250	0.03%	0.003%
82	10.161	2754	2759	2764	rVB2	268	311	0.03%	0.004%
83	10.187	2764	2767	2769	rBV	235	134	0.01%	0.002%
84	10.216	2771	2776	2779	rBV2	253	265	0.03%	0.003%
85	10.315	2801	2807	2808	rBV2	220	192	0.02%	0.003%
86	10.524	2870	2872	2875	rBV2	148	103	0.01%	0.001%
87	10.749	2930	2942	2962	rBV	319561	538530	55.14%	7.029%
88	11.029	3024	3029	3032	rBV	297	392	0.04%	0.005%
89	11.158	3064	3069	3070	rBV2	223	215	0.02%	0.003%
90	11.200	3079	3082	3083	rBV2	226	155	0.02%	0.002%
91	11.364	3129	3133	3134	rBV2	183	139	0.01%	0.002%
92	11.415	3147	3149	3150	rBV2	196	69	0.01%	0.001%
93	11.737	3247	3249	3251	rBV	259	138	0.01%	0.002%
94	11.804	3259	3270	3294	rBV	462455	759382	77.76%	9.912%
95	12.187	3376	3389	3419	rBV	415897	711742	72.88%	9.290%
96	12.637	3525	3529	3533	rVB	343	290	0.03%	0.004%
97	12.920	3610	3617	3632	rBV6	2659	6383	0.65%	0.083%
98	13.106	3671	3675	3678	rBV2	251	252	0.03%	0.003%
99	13.804	3890	3892	3894	rBV2	243	141	0.01%	0.002%
100	14.084	3976	3979	3981	rBV	281	176	0.02%	0.002%

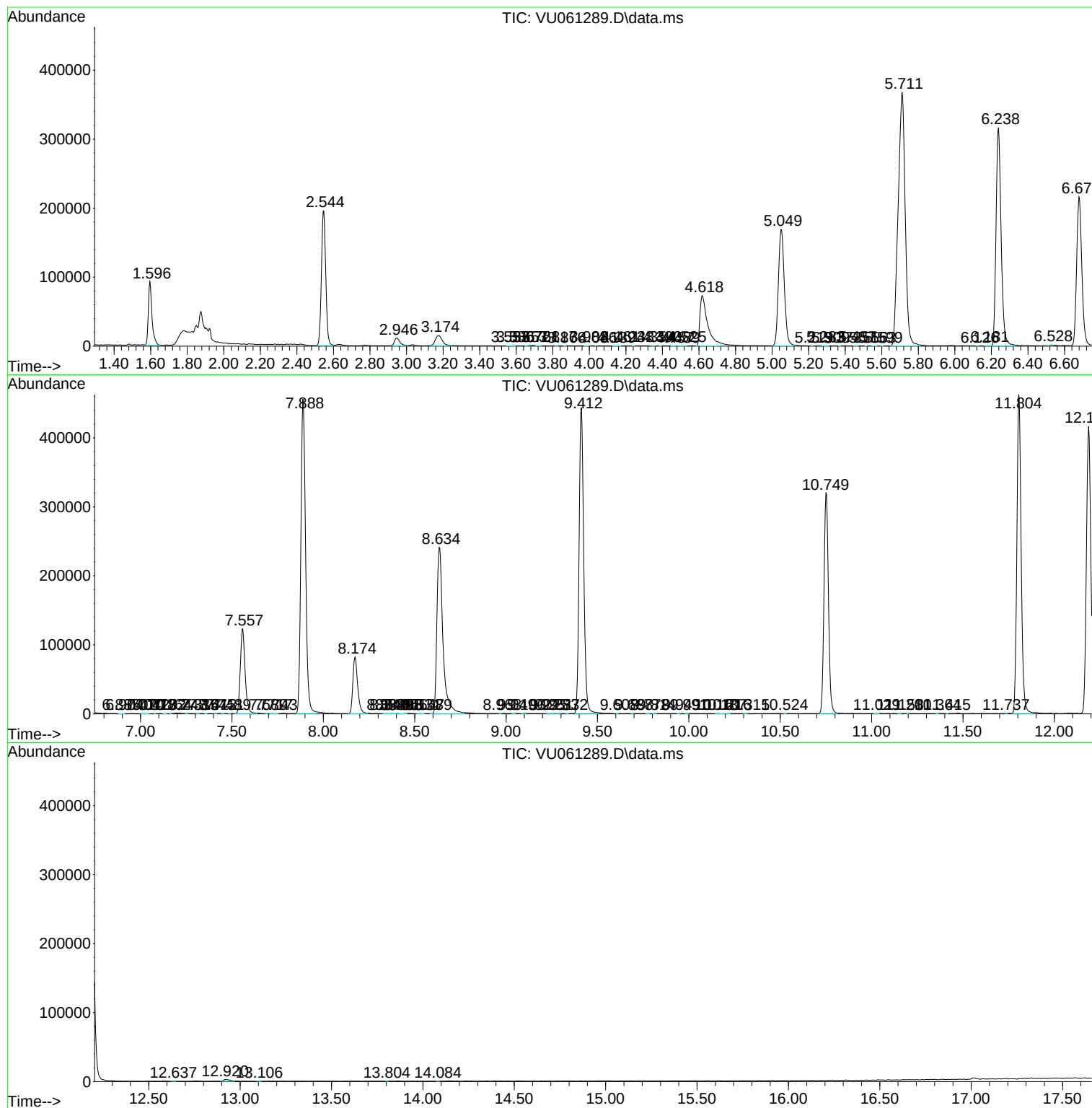
Sum of corrected areas: 7661284

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Instrument :
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A4F20ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM102824WMA.M
Quant Title : VOC Analysis

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



Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102924\
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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A4F20ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM102824WMA.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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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM102824WMA.M
Quant Title : VOC Analysis

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

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