

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112824\
 Data File : VU062061.D
 Acq On : 27 Nov 2024 19:06
 Operator : MD/SY
 Sample : VU1128MBL01
 Misc : 5.00g/5mL/100ul/5mL/MSVOA_U/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK109

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112724WMA.M
 Title : VOC Analysis

Signal : TIC: VU062061.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	107	rVB	80478	90294	13.36%	1.758%
2	1.904	184	191	211	rVB	56980	78200	11.57%	1.523%
3	2.229	289	292	294	rBV2	455	323	0.05%	0.006%
4	2.560	383	395	413	rBV	136669	225283	33.34%	4.386%
5	2.833	477	480	483	rBV2	191	143	0.02%	0.003%
6	2.924	504	508	510	rBV2	196	139	0.02%	0.003%
7	3.036	539	543	547	rBV2	511	527	0.08%	0.010%
8	3.107	562	565	568	rBV	265	204	0.03%	0.004%
9	3.351	634	641	652	rVB4	1043	1814	0.27%	0.035%
10	3.396	653	655	658	rBV2	254	169	0.03%	0.003%
11	3.612	719	722	724	rBV	278	171	0.03%	0.003%
12	3.692	740	747	758	rBV5	711	1171	0.17%	0.023%
13	3.776	771	773	776	rBB	260	142	0.02%	0.003%
14	3.795	776	779	781	rBV	255	182	0.03%	0.004%
15	3.859	795	799	802	rBV2	285	252	0.04%	0.005%
16	3.882	802	806	810	rVV	311	281	0.04%	0.005%
17	3.914	813	816	819	rBB2	246	161	0.02%	0.003%
18	3.965	829	832	834	rBV	266	188	0.03%	0.004%
19	4.110	874	877	879	rBV2	174	142	0.02%	0.003%
20	4.203	903	906	909	rBV2	284	253	0.04%	0.005%
21	4.251	918	921	924	rVB	191	151	0.02%	0.003%
22	4.296	932	935	937	rVB	295	179	0.03%	0.003%
23	4.319	938	942	947	rBB2	287	288	0.04%	0.006%
24	4.409	967	970	974	rBB2	244	202	0.03%	0.004%
25	4.438	975	979	982	rBB2	242	219	0.03%	0.004%
26	4.470	982	989	994	rBV2	260	444	0.07%	0.009%
27	4.563	1015	1018	1023	rBV2	265	280	0.04%	0.005%
28	4.618	1025	1035	1074	rBV2	55432	155573	23.02%	3.029%
29	5.052	1154	1170	1200	rVV	120208	270300	40.00%	5.263%
30	5.264	1232	1236	1238	rBV	212	150	0.02%	0.003%
31	5.367	1263	1268	1273	rBV3	402	492	0.07%	0.010%
32	5.470	1295	1300	1303	rBV2	165	165	0.02%	0.003%
33	5.486	1303	1305	1308	rVB2	261	168	0.02%	0.003%
34	5.557	1323	1327	1329	rBV	235	157	0.02%	0.003%
35	5.612	1341	1344	1346	rVB	250	140	0.02%	0.003%
36	5.637	1349	1352	1357	rBV	141	191	0.03%	0.004%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112824\
 Data File : VU062061.D
 Acq On : 27 Nov 2024 19:06
 Operator : MD/SY
 Sample : VU1128MBL01
 Misc : 5.00g/5mL/100ul/5mL/MSVOA_U/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK109

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112724WMA.M
 Title : VOC Analysis

37	5.714	1357	1376	1414	rBV2	242902	675670	100.00%	13.156%
38	6.004	1459	1466	1468	rBV3	361	426	0.06%	0.008%
39	6.062	1482	1484	1487	rBB2	246	135	0.02%	0.003%
40	6.081	1487	1490	1493	rBV	171	163	0.02%	0.003%
41	6.126	1501	1504	1506	rBV	236	155	0.02%	0.003%
42	6.200	1523	1527	1528	rBV	265	186	0.03%	0.004%
43	6.239	1528	1539	1567	rBV	211377	409453	60.60%	7.972%
44	6.428	1597	1598	1602	rVB2	364	167	0.02%	0.003%
45	6.518	1622	1626	1627	rBV2	400	294	0.04%	0.006%
46	6.534	1627	1631	1639	rVB4	1589	2327	0.34%	0.045%
47	6.589	1643	1648	1651	rBV2	286	300	0.04%	0.006%
48	6.637	1659	1663	1664	rBV	282	203	0.03%	0.004%
49	6.679	1664	1676	1704	rVV	149227	296532	43.89%	5.774%
50	6.894	1741	1743	1747	rVB	285	223	0.03%	0.004%
51	7.033	1784	1786	1788	rBV	292	184	0.03%	0.004%
52	7.126	1810	1815	1817	rVV2	202	194	0.03%	0.004%
53	7.139	1817	1819	1821	rVB	252	137	0.02%	0.003%
54	7.155	1822	1824	1828	rBB2	262	193	0.03%	0.004%
55	7.200	1836	1838	1840	rBV	241	160	0.02%	0.003%
56	7.377	1890	1893	1899	rVB2	308	350	0.05%	0.007%
57	7.412	1900	1904	1906	rBV2	244	174	0.03%	0.003%
58	7.428	1907	1909	1913	rVB	284	191	0.03%	0.004%
59	7.454	1914	1917	1918	rBV	255	144	0.02%	0.003%
60	7.557	1937	1949	1971	rBV	83103	154393	22.85%	3.006%
61	7.692	1988	1991	1995	rBV	304	184	0.03%	0.004%
62	7.730	2000	2003	2005	rBV2	269	167	0.02%	0.003%
63	7.804	2021	2026	2031	rBV3	376	448	0.07%	0.009%
64	7.888	2040	2052	2081	rBV	303393	543076	80.38%	10.574%
65	8.171	2130	2140	2163	rBV	56796	101223	14.98%	1.971%
66	8.341	2190	2193	2195	rBV	272	175	0.03%	0.003%
67	8.412	2212	2215	2217	rBV2	308	257	0.04%	0.005%
68	8.550	2252	2258	2262	rBV2	1265	1333	0.20%	0.026%
69	8.586	2266	2269	2272	rBV	176	166	0.02%	0.003%
70	8.627	2272	2282	2319	rBV2	165854	335585	49.67%	6.534%
71	8.923	2369	2374	2376	rVB2	349	321	0.05%	0.006%
72	8.959	2382	2385	2389	rVB2	260	175	0.03%	0.003%
73	9.020	2400	2404	2406	rBV	211	144	0.02%	0.003%
74	9.187	2452	2456	2458	rBV2	241	184	0.03%	0.004%
75	9.245	2471	2474	2479	rBV2	273	308	0.05%	0.006%
76	9.290	2486	2488	2492	rVB	229	148	0.02%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112824\
 Data File : VU062061.D
 Acq On : 27 Nov 2024 19:06
 Operator : MD/SY
 Sample : VU1128MBL01
 Misc : 5.00g/5mL/100ul/5mL/MSVOA_U/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK109

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\SFAMULM112724WMA.M
 Title : VOC Analysis

77	9.316	2492	2496	2499	rBV2	189	163	0.02%	0.003%
78	9.409	2513	2525	2550	rBV	288951	500121	74.02%	9.738%
79	9.637	2590	2596	2599	rBV	342	348	0.05%	0.007%
80	9.695	2607	2614	2617	rBV3	768	998	0.15%	0.019%
81	9.769	2634	2637	2639	rBV	207	138	0.02%	0.003%
82	10.016	2711	2714	2720	rBV2	198	204	0.03%	0.004%
83	10.232	2779	2781	2786	rVB2	223	142	0.02%	0.003%
84	10.428	2838	2842	2846	rBV	240	200	0.03%	0.004%
85	10.457	2848	2851	2854	rBV	177	145	0.02%	0.003%
86	10.586	2888	2891	2894	rBV	354	249	0.04%	0.005%
87	10.746	2929	2941	2960	rBV	210491	349821	51.77%	6.811%
88	10.869	2977	2979	2982	rVB	306	141	0.02%	0.003%
89	11.087	3041	3047	3060	rVB3	627	1238	0.18%	0.024%
90	11.473	3159	3167	3173	rVB	831	1174	0.17%	0.023%
91	11.640	3216	3219	3221	rBV2	221	157	0.02%	0.003%
92	11.746	3245	3252	3258	rBV3	1750	2621	0.39%	0.051%
93	11.804	3258	3270	3300	rBV	264759	443603	65.65%	8.637%
94	12.184	3376	3388	3415	rBV	275245	466485	69.04%	9.083%
95	12.534	3494	3497	3499	rBV2	193	137	0.02%	0.003%
96	12.994	3634	3640	3643	rBV2	302	335	0.05%	0.007%
97	13.232	3707	3714	3724	rVB6	1705	2848	0.42%	0.055%
98	14.103	3977	3985	3987	rBV4	2401	3261	0.48%	0.063%
99	14.328	4049	4055	4069	rVB7	3150	5694	0.84%	0.111%
100	14.901	4230	4233	4236	rBV3	345	252	0.04%	0.005%

Sum of corrected areas: 5135861

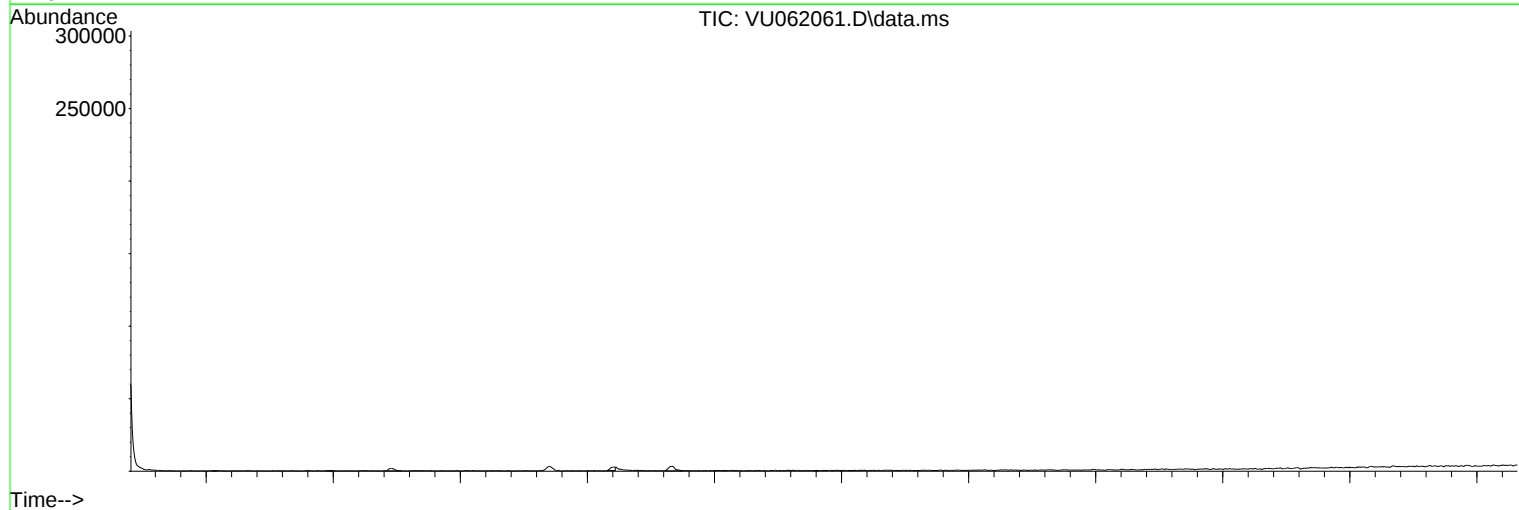
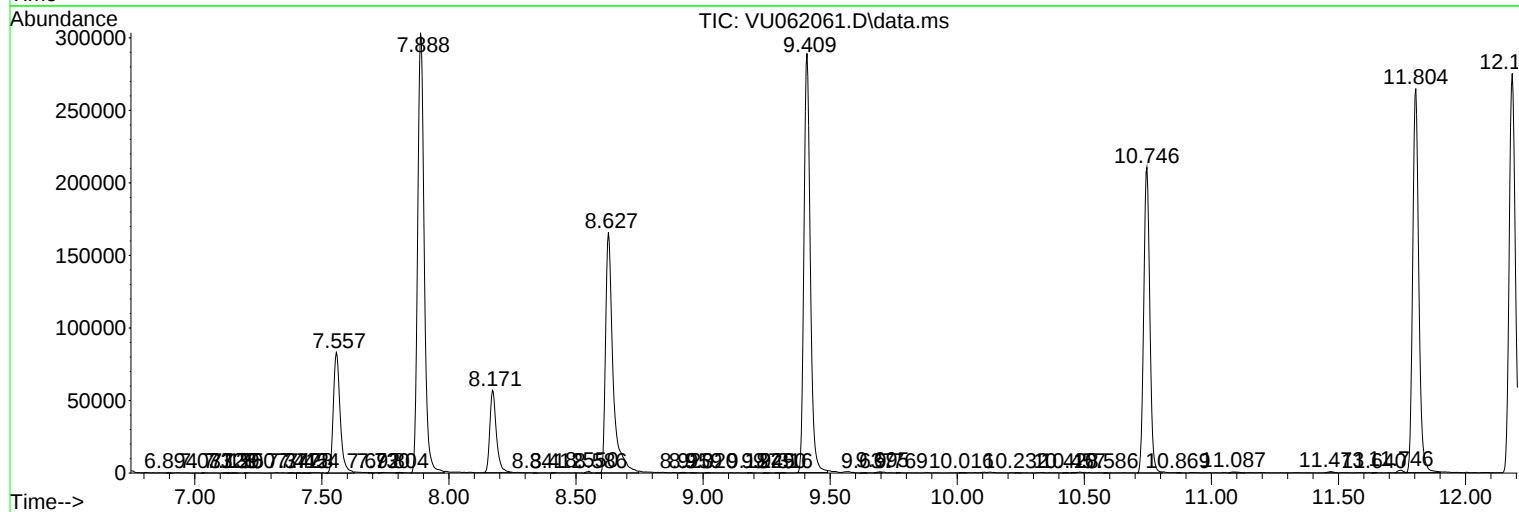
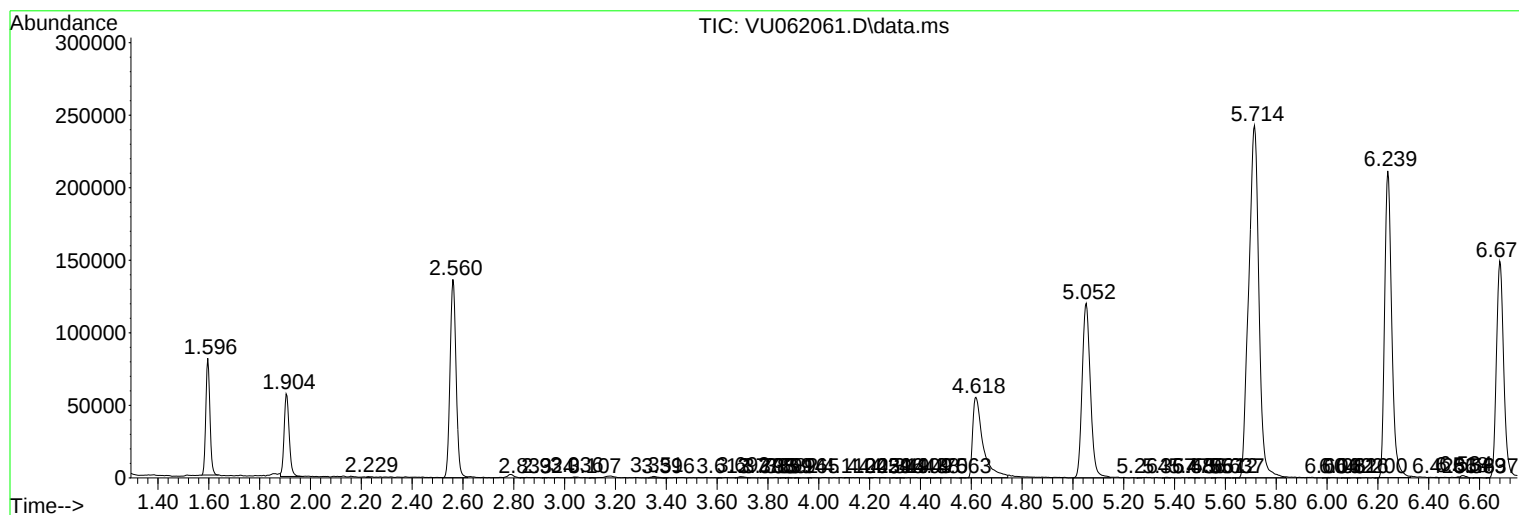
Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112824\
Data File : VU062061.D
Acq On : 27 Nov 2024 19:06
Operator : MD/SY
Sample : VU1128MBL01
Misc : 5.00g/5mL/100ul/5mL/MSVOA_U/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK109

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112724WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112824\
Data File : VU062061.D
Acq On : 27 Nov 2024 19:06
Operator : MD/SY
Sample : VU1128MBL01
Misc : 5.00g/5mL/100ul/5ml/MSVOA_U/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK109

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112724WMA.M
Quant Title : VOC Analysis

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

No Library Search Compounds Detected

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112824\
Data File : VU062061.D
Acq On : 27 Nov 2024 19:06
Operator : MD/SY
Sample : VU1128MBL01
Misc : 5.00g/5mL/100ul/5mL/MSVOA_U/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK109

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112724WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--
				#	RT Resp Conc
