

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052524\
 Data File : VU059012.D
 Acq On : 25 May 2024 20:40
 Operator : MD/SY
 Sample : P2568-21ME
 Misc : 5.64g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH642ME

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: VU059012.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	115	rVB	54745	85779	12.44%	1.757%
2	2.534	375	387	404	rBV	117193	190694	27.65%	3.905%
3	2.634	412	418	422	rBV5	2001	2529	0.37%	0.052%
4	2.933	508	511	512	rBV2	484	324	0.05%	0.007%
5	2.991	526	529	531	rBV	380	203	0.03%	0.004%
6	3.026	533	540	552	rVB3	2579	5110	0.74%	0.105%
7	3.171	571	585	600	rBV2	8543	21220	3.08%	0.435%
8	3.528	693	696	697	rBV2	170	96	0.01%	0.002%
9	3.611	718	722	725	rBV	169	139	0.02%	0.003%
10	3.782	770	775	776	rBV	153	135	0.02%	0.003%
11	3.862	797	800	803	rBV2	273	180	0.03%	0.004%
12	3.936	820	823	826	rVB2	255	169	0.02%	0.003%
13	3.978	833	836	838	rBV	105	76	0.01%	0.002%
14	4.139	883	886	889	rBV	237	129	0.02%	0.003%
15	4.190	899	902	905	rVB2	255	160	0.02%	0.003%
16	4.306	933	938	944	rBV2	296	313	0.05%	0.006%
17	4.367	954	957	960	rBV	130	83	0.01%	0.002%
18	4.406	964	969	971	rBV2	241	223	0.03%	0.005%
19	4.464	983	987	990	rBV2	144	100	0.01%	0.002%
20	4.537	1005	1010	1011	rBV	209	180	0.03%	0.004%
21	4.624	1025	1037	1084	rBV	58514	193315	28.03%	3.959%
22	5.052	1154	1170	1193	rBV	117494	271005	39.29%	5.550%
23	5.190	1208	1213	1214	rBV	152	118	0.02%	0.002%
24	5.254	1230	1233	1235	rBV	137	88	0.01%	0.002%
25	5.312	1249	1251	1253	rBV2	207	123	0.02%	0.003%
26	5.341	1257	1260	1264	rBV2	149	103	0.01%	0.002%
27	5.364	1265	1267	1269	rBV	123	82	0.01%	0.002%
28	5.444	1289	1292	1294	rBV	161	81	0.01%	0.002%
29	5.460	1294	1297	1301	rVB2	145	116	0.02%	0.002%
30	5.515	1311	1314	1318	rVB2	199	150	0.02%	0.003%
31	5.711	1356	1375	1402	rBV2	262934	689674	100.00%	14.124%
32	5.885	1426	1429	1432	rBV	136	100	0.01%	0.002%
33	5.917	1437	1439	1443	rBV	238	197	0.03%	0.004%
34	5.971	1451	1456	1472	rVB6	2619	5301	0.77%	0.109%
35	6.033	1472	1475	1477	rBV2	192	130	0.02%	0.003%
36	6.110	1495	1499	1504	rBV2	282	280	0.04%	0.006%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052524\
 Data File : VU059012.D
 Acq On : 25 May 2024 20:40
 Operator : MD/SY
 Sample : P2568-21ME
 Misc : 5.64g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH642ME

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

37	6.238	1527	1539	1572	rBV	186908	368200	53.39%	7.541%
38	6.399	1586	1589	1591	rBV2	228	176	0.03%	0.004%
39	6.431	1596	1599	1603	rBV3	272	183	0.03%	0.004%
40	6.528	1614	1629	1640	rBV3	3716	7937	1.15%	0.163%
41	6.595	1640	1650	1655	rBV6	2932	4915	0.71%	0.101%
42	6.682	1664	1677	1701	rVB	160612	320150	46.42%	6.557%
43	6.804	1712	1715	1716	rBV2	231	138	0.02%	0.003%
44	6.846	1723	1728	1730	rBV2	109	119	0.02%	0.002%
45	6.949	1758	1760	1765	rBV2	162	154	0.02%	0.003%
46	7.081	1798	1801	1802	rBV	160	91	0.01%	0.002%
47	7.184	1831	1833	1835	rBV2	142	82	0.01%	0.002%
48	7.200	1836	1838	1839	rBV2	336	137	0.02%	0.003%
49	7.312	1869	1873	1877	rVB	439	325	0.05%	0.007%
50	7.338	1877	1881	1882	rBV	119	98	0.01%	0.002%
51	7.370	1888	1891	1895	rBV2	140	124	0.02%	0.003%
52	7.489	1925	1928	1931	rVB2	303	230	0.03%	0.005%
53	7.560	1939	1950	1969	rBV	76976	142679	20.69%	2.922%
54	7.714	1996	1998	2000	rVB2	160	81	0.01%	0.002%
55	7.743	2000	2007	2009	rBV2	230	258	0.04%	0.005%
56	7.772	2015	2016	2019	rBV3	271	181	0.03%	0.004%
57	7.836	2033	2036	2038	rBV	107	77	0.01%	0.002%
58	7.891	2041	2053	2074	rBV	266509	477538	69.24%	9.780%
59	8.100	2113	2118	2122	rVB2	270	283	0.04%	0.006%
60	8.123	2122	2125	2128	rBV	166	123	0.02%	0.003%
61	8.174	2130	2141	2164	rVV2	49051	93608	13.57%	1.917%
62	8.277	2171	2173	2174	rBV2	360	139	0.02%	0.003%
63	8.312	2181	2184	2189	rBV2	212	214	0.03%	0.004%
64	8.341	2192	2193	2198	rVB2	404	199	0.03%	0.004%
65	8.370	2200	2202	2205	rVB2	221	82	0.01%	0.002%
66	8.573	2260	2265	2267	rBV	214	177	0.03%	0.004%
67	8.643	2273	2287	2321	rBV2	142958	385921	55.96%	7.904%
68	8.865	2354	2356	2362	rVB2	500	351	0.05%	0.007%
69	9.010	2398	2401	2405	rBV2	181	171	0.02%	0.004%
70	9.049	2410	2413	2414	rBV	171	108	0.02%	0.002%
71	9.074	2418	2421	2428	rVB2	232	169	0.02%	0.003%
72	9.113	2428	2433	2436	rVB	147	123	0.02%	0.003%
73	9.132	2436	2439	2442	rBV2	160	118	0.02%	0.002%
74	9.293	2485	2489	2493	rVB	229	178	0.03%	0.004%
75	9.328	2496	2500	2503	rBV	253	241	0.03%	0.005%
76	9.415	2515	2527	2553	rBV	253982	459093	66.57%	9.402%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052524\
 Data File : VU059012.D
 Acq On : 25 May 2024 20:40
 Operator : MD/SY
 Sample : P2568-21ME
 Misc : 5.64g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH642ME

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

77	9.695	2607	2614	2616	rBV4	1276	1411	0.20%	0.029%
78	9.868	2666	2668	2671	rVB	255	130	0.02%	0.003%
79	9.888	2671	2674	2678	rBV2	256	186	0.03%	0.004%
80	10.335	2811	2813	2818	rBV2	137	128	0.02%	0.003%
81	10.425	2835	2841	2842	rBV2	142	148	0.02%	0.003%
82	10.531	2871	2874	2877	rBV	161	124	0.02%	0.003%
83	10.605	2892	2897	2901	rBV2	194	201	0.03%	0.004%
84	10.640	2901	2908	2910	rBV	402	389	0.06%	0.008%
85	10.695	2922	2925	2927	rBV	126	84	0.01%	0.002%
86	10.756	2931	2944	2967	rVV	221006	380679	55.20%	7.796%
87	10.971	3009	3011	3015	rBV2	219	155	0.02%	0.003%
88	11.097	3047	3050	3053	rBV	242	183	0.03%	0.004%
89	11.373	3132	3136	3141	rBV2	359	287	0.04%	0.006%
90	11.505	3174	3177	3179	rBV	220	129	0.02%	0.003%
91	11.601	3203	3207	3210	rBV2	244	221	0.03%	0.005%
92	11.666	3224	3227	3231	rBV2	338	311	0.05%	0.006%
93	11.810	3260	3272	3293	rBV	231388	376725	54.62%	7.715%
94	11.933	3307	3310	3311	rBV2	566	302	0.04%	0.006%
95	11.987	3325	3327	3328	rBV	271	100	0.01%	0.002%
96	12.190	3378	3390	3410	rBV2	227459	385728	55.93%	7.900%
97	12.544	3497	3500	3503	rBV2	374	285	0.04%	0.006%
98	14.029	3958	3962	3966	rBV	442	421	0.06%	0.009%
99	14.402	4076	4078	4080	rBV	351	225	0.03%	0.005%
100	14.669	4157	4161	4163	rBV	523	449	0.07%	0.009%

Sum of corrected areas: 4882877

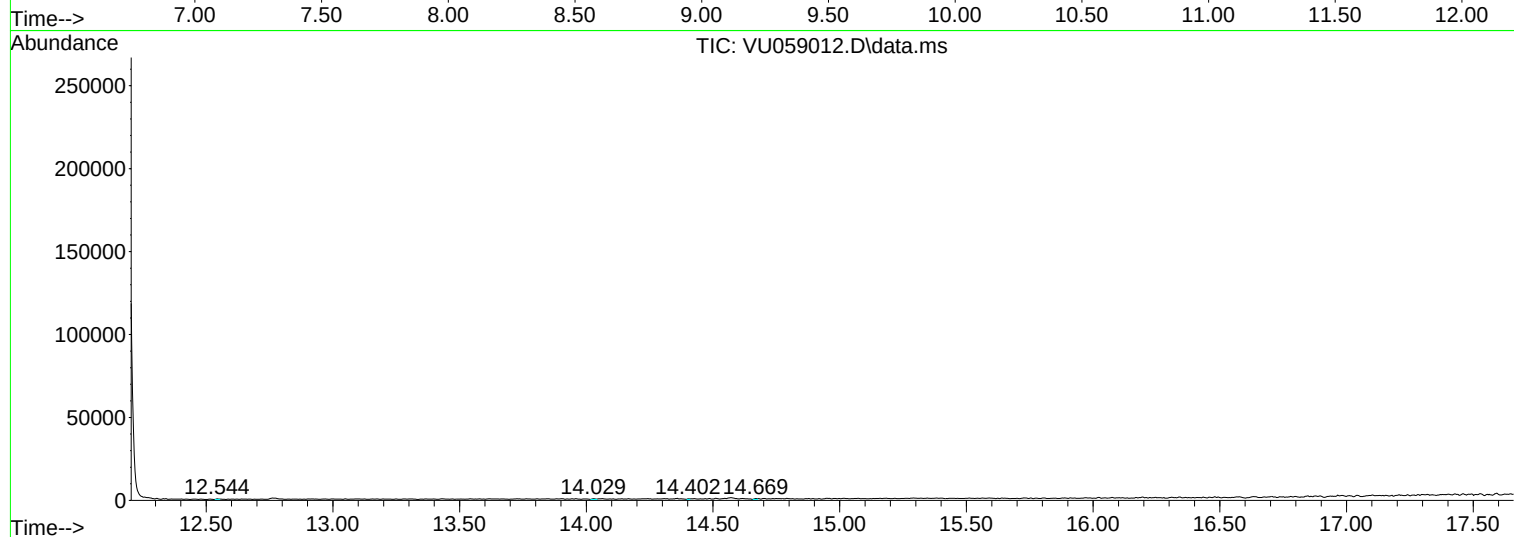
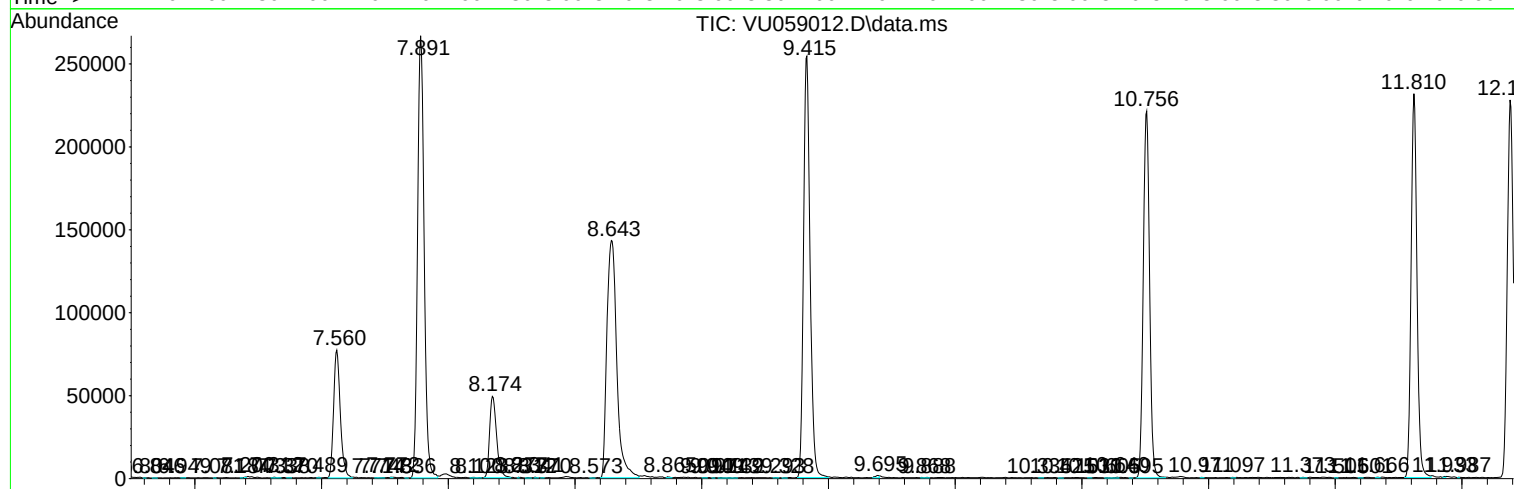
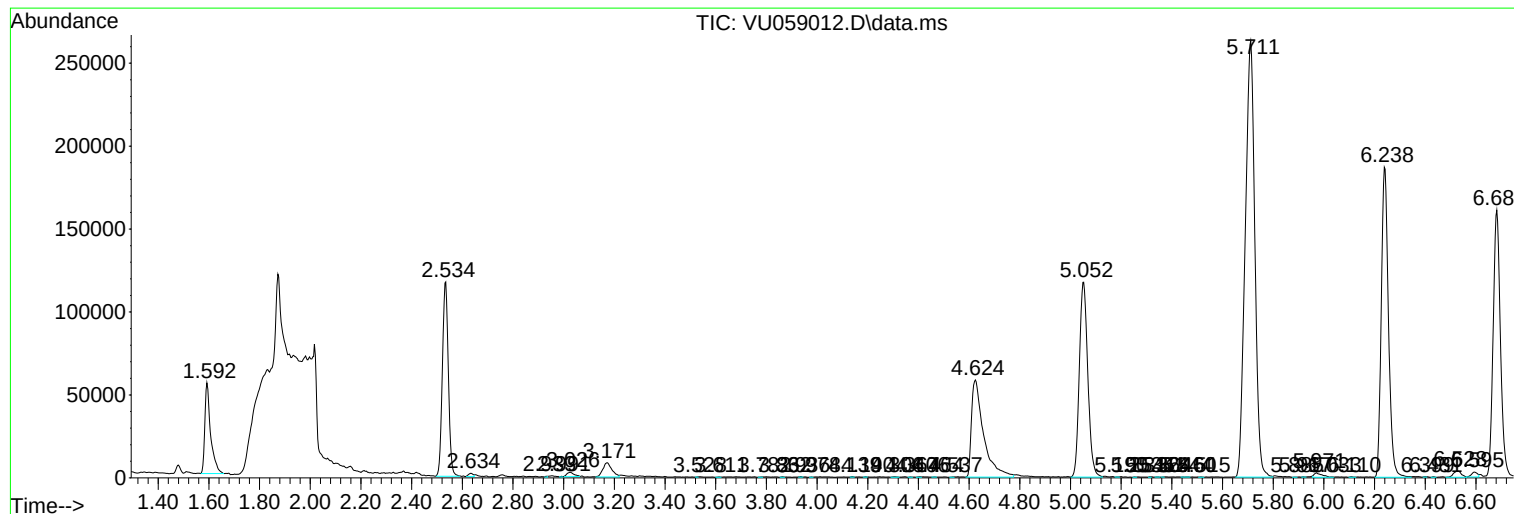
Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052524\
Data File : VU059012.D
Acq On : 25 May 2024 20:40
Operator : MD/SY
Sample : P2568-21ME
Misc : 5.64g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH642ME

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052524\
Data File : VU059012.D
Acq On : 25 May 2024 20:40
Operator : MD/SY
Sample : P2568-21ME
Misc : 5.64g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH642ME

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

No Library Search Compounds Detected

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052524\
Data File : VU059012.D
Acq On : 25 May 2024 20:40
Operator : MD/SY
Sample : P2568-21ME
Misc : 5.64g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH642ME

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

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