

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052424\
 Data File : VU058973.D
 Acq On : 24 May 2024 16:06
 Operator : MD/SY
 Sample : P2547-12ME
 Misc : 6.20g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH5W9ME

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: VU058973.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.595	88	95	123	rVB	77339	137973	14.65%	2.212%
2	2.534	376	387	404	rBV	175461	287498	30.52%	4.609%
3	2.820	474	476	479	rVB	351	143	0.02%	0.002%
4	2.930	504	510	513	rBV2	324	377	0.04%	0.006%
5	3.026	530	540	560	rVB4	6705	14702	1.56%	0.236%
6	3.103	560	564	565	rBV	320	237	0.03%	0.004%
7	3.171	573	585	596	rBV2	5142	11683	1.24%	0.187%
8	3.473	676	679	683	rBV	144	113	0.01%	0.002%
9	3.492	683	685	688	rVB2	181	99	0.01%	0.002%
10	3.582	707	713	715	rBV	294	271	0.03%	0.004%
11	3.640	728	731	734	rBV	422	286	0.03%	0.005%
12	3.724	755	757	759	rBV2	66	30	0.00%	0.000%
13	3.869	796	802	806	rBV2	293	327	0.03%	0.005%
14	3.917	812	817	820	rBV2	161	178	0.02%	0.003%
15	4.152	887	890	899	rVB	250	246	0.03%	0.004%
16	4.216	905	910	919	rBV2	273	387	0.04%	0.006%
17	4.319	935	942	945	rBV2	271	306	0.03%	0.005%
18	4.345	945	950	953	rVV2	187	168	0.02%	0.003%
19	4.396	958	966	969	rBV2	258	339	0.04%	0.005%
20	4.447	979	982	983	rBV2	142	84	0.01%	0.001%
21	4.518	997	1004	1008	rBV2	283	359	0.04%	0.006%
22	4.576	1018	1022	1023	rBV2	208	148	0.02%	0.002%
23	4.637	1030	1041	1086	rBV2	57338	226625	24.06%	3.633%
24	5.052	1155	1170	1195	rBV	158964	365505	38.80%	5.859%
25	5.213	1217	1220	1224	rBV3	290	197	0.02%	0.003%
26	5.245	1227	1230	1232	rBV	285	184	0.02%	0.003%
27	5.335	1255	1258	1261	rBV2	187	162	0.02%	0.003%
28	5.492	1305	1307	1309	rBV	154	88	0.01%	0.001%
29	5.595	1336	1339	1341	rBV	149	121	0.01%	0.002%
30	5.711	1356	1375	1409	rBV2	358403	942016	100.00%	15.101%
31	5.981	1445	1459	1471	rBV6	2443	6074	0.64%	0.097%
32	6.061	1481	1484	1486	rBV2	243	171	0.02%	0.003%
33	6.090	1490	1493	1495	rBV	123	82	0.01%	0.001%
34	6.177	1516	1520	1526	rBV	310	300	0.03%	0.005%
35	6.242	1526	1540	1563	rBV	242963	492158	52.25%	7.890%
36	6.483	1612	1615	1616	rBV	146	73	0.01%	0.001%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052424\
 Data File : VU058973.D
 Acq On : 24 May 2024 16:06
 Operator : MD/SY
 Sample : P2547-12ME
 Misc : 6.20g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH5W9ME

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	6.531	1620	1630	1642	rVV10	8393	17072	1.81%	0.274%
38	6.598	1643	1651	1664	rVV3	3104	6867	0.73%	0.110%
39	6.682	1664	1677	1704	rVB2	209715	428810	45.52%	6.874%
40	6.804	1713	1715	1719	rVB4	477	240	0.03%	0.004%
41	6.875	1734	1737	1740	rBV	169	144	0.02%	0.002%
42	6.917	1748	1750	1751	rVB	135	39	0.00%	0.001%
43	6.930	1751	1754	1756	rBV2	211	140	0.01%	0.002%
44	7.016	1779	1781	1784	rBV2	113	68	0.01%	0.001%
45	7.071	1794	1798	1802	rBV	225	190	0.02%	0.003%
46	7.110	1805	1810	1813	rBV2	291	252	0.03%	0.004%
47	7.171	1826	1829	1831	rBV	143	80	0.01%	0.001%
48	7.193	1831	1836	1839	rBV4	460	426	0.05%	0.007%
49	7.209	1839	1841	1842	rBV2	413	170	0.02%	0.003%
50	7.261	1855	1857	1861	rBV	186	93	0.01%	0.001%
51	7.315	1872	1874	1875	rBV2	307	156	0.02%	0.003%
52	7.360	1885	1888	1889	rBV	139	65	0.01%	0.001%
53	7.451	1913	1916	1919	rBV2	201	183	0.02%	0.003%
54	7.560	1938	1950	1969	rBV2	99567	194983	20.70%	3.126%
55	7.682	1985	1988	1991	rBV2	242	216	0.02%	0.003%
56	7.711	1994	1997	2001	rBV3	325	290	0.03%	0.005%
57	7.746	2006	2008	2013	rVB	192	102	0.01%	0.002%
58	7.782	2015	2019	2026	rVB3	432	475	0.05%	0.008%
59	7.891	2040	2053	2073	rBV	387516	692728	73.54%	11.105%
60	8.116	2121	2123	2124	rVB	212	64	0.01%	0.001%
61	8.129	2124	2127	2129	rBV2	126	87	0.01%	0.001%
62	8.177	2130	2142	2167	rVV	65657	129674	13.77%	2.079%
63	8.335	2189	2191	2193	rVB2	165	58	0.01%	0.001%
64	8.354	2193	2197	2199	rBV	414	284	0.03%	0.005%
65	8.531	2246	2252	2256	rBV2	211	222	0.02%	0.004%
66	8.637	2274	2285	2289	rBV	103821	172074	18.27%	2.758%
67	8.894	2361	2365	2371	rVB3	398	373	0.04%	0.006%
68	8.987	2391	2394	2396	rBV	173	119	0.01%	0.002%
69	9.135	2438	2440	2443	rBV	267	168	0.02%	0.003%
70	9.415	2514	2527	2554	rBV	330619	621498	65.98%	9.963%
71	9.695	2608	2614	2625	rVB4	2161	3375	0.36%	0.054%
72	9.769	2634	2637	2639	rBV	184	103	0.01%	0.002%
73	9.849	2660	2662	2664	rBV2	154	104	0.01%	0.002%
74	9.907	2676	2680	2682	rBV	240	169	0.02%	0.003%
75	10.048	2721	2724	2725	rBV	176	89	0.01%	0.001%
76	10.225	2772	2779	2782	rBV2	316	398	0.04%	0.006%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052424\
 Data File : VU058973.D
 Acq On : 24 May 2024 16:06
 Operator : MD/SY
 Sample : P2547-12ME
 Misc : 6.20g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH5W9ME

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	10.682	2919	2921	2924	rBV2	206	102	0.01%	0.002%
78	10.759	2932	2945	2964	rBV	248092	461786	49.02%	7.403%
79	10.881	2980	2983	2987	rBV	420	394	0.04%	0.006%
80	11.029	3026	3029	3030	rBV	201	118	0.01%	0.002%
81	11.814	3261	3273	3292	rBV	300271	491890	52.22%	7.885%
82	12.016	3332	3336	3345	rBV	459	493	0.05%	0.008%
83	12.193	3377	3391	3414	rBV	310558	519363	55.13%	8.326%
84	12.765	3563	3569	3571	rBV2	728	775	0.08%	0.012%
85	14.974	4254	4256	4264	rBV2	579	778	0.08%	0.012%

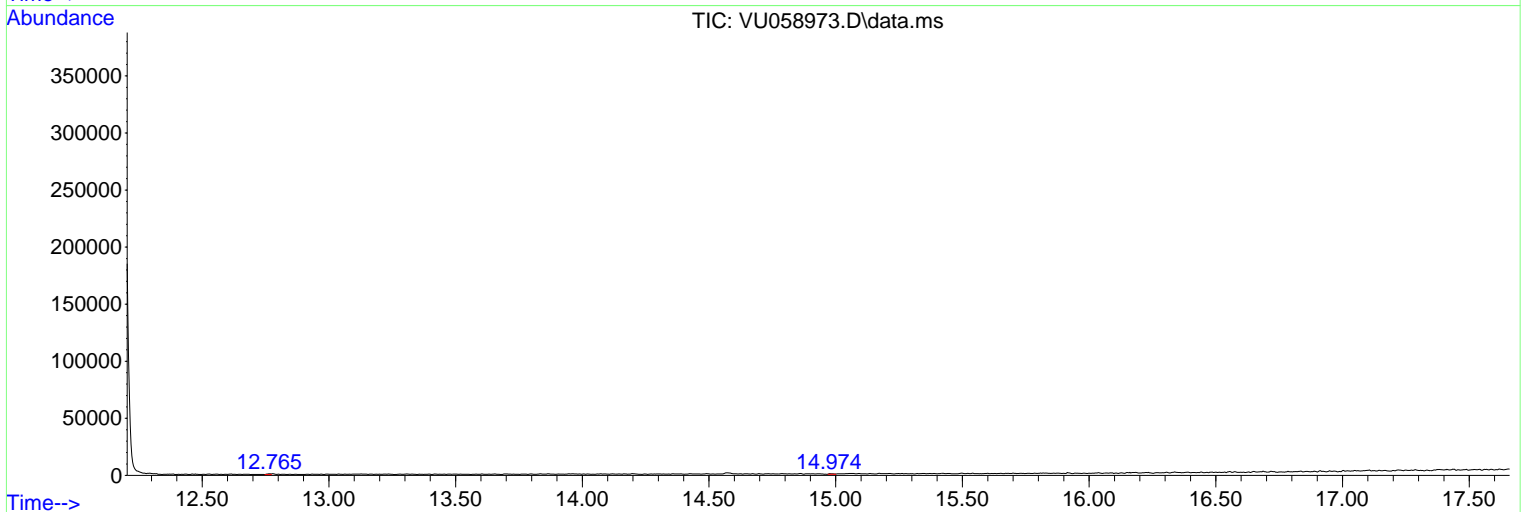
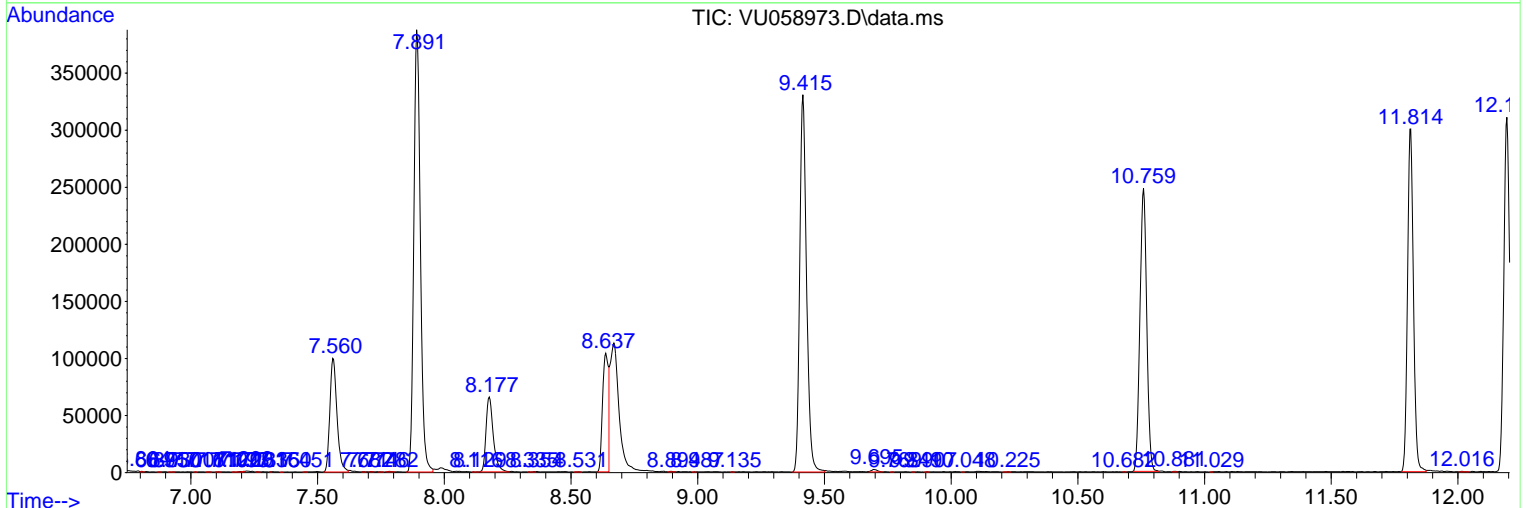
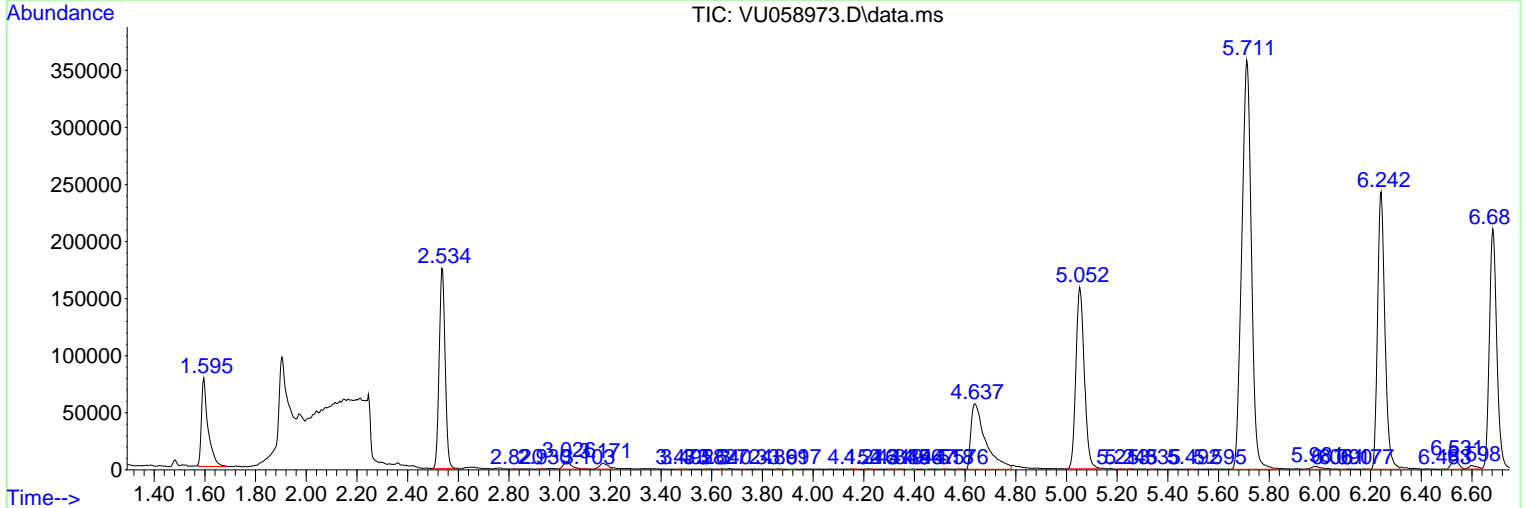
Sum of corrected areas: 6238057

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052424\
 Data File : VU058973.D
 Acq On : 24 May 2024 16:06
 Operator : MD/SY
 Sample : P2547-12ME
 Misc : 6.20g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH5W9ME

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\VU052424\
Data File : VU058973.D
Acq On : 24 May 2024 16:06
Operator : MD/SY
Sample : P2547-12ME
Misc : 6.20g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH5W9ME

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\VU052424\
Data File : VU058973.D
Acq On : 24 May 2024 16:06
Operator : MD/SY
Sample : P2547-12ME
Misc : 6.20g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH5W9ME

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

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