

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
 Data File : VU047992.D
 Acq On : 13 Apr 2022 10:52
 Operator : SY/MD
 Sample : VU0413WBL01
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK089

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\SFAMULM032422WMA.M
 Title : VOC Analysis

Signal : TIC: VU047992.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.600	73	81	99	rVB	162787	189824	14.83%	1.841%
2	1.915	170	179	198	rBV	129874	181411	14.17%	1.759%
3	2.568	370	382	402	rBV	271591	446642	34.88%	4.331%
4	2.796	445	453	461	rVB3	939	1796	0.14%	0.017%
5	2.906	484	487	490	rVB3	448	320	0.02%	0.003%
6	2.925	490	493	496	rVB	365	254	0.02%	0.002%
7	2.948	496	500	501	rBV2	366	250	0.02%	0.002%
8	2.977	507	509	512	rVB3	500	306	0.02%	0.003%
9	3.050	525	532	540	rVB3	1551	2678	0.21%	0.026%
10	3.083	540	542	545	rBV2	303	236	0.02%	0.002%
11	3.118	551	553	558	rBV4	403	318	0.02%	0.003%
12	3.186	571	574	578	rVB2	421	291	0.02%	0.003%
13	3.362	624	629	634	rBV4	812	837	0.07%	0.008%
14	3.491	666	669	673	rVB3	440	404	0.03%	0.004%
15	3.514	673	676	680	rBV	386	361	0.03%	0.004%
16	3.604	700	704	707	rBV	334	249	0.02%	0.002%
17	3.668	717	724	726	rBV3	322	321	0.03%	0.003%
18	3.742	741	747	751	rBV3	317	392	0.03%	0.004%
19	3.796	760	764	767	rBV	294	285	0.02%	0.003%
20	3.880	787	790	795	rVB2	422	352	0.03%	0.003%
21	3.909	795	799	802	rBV3	267	237	0.02%	0.002%
22	4.259	903	908	911	rVB2	405	371	0.03%	0.004%
23	4.417	952	957	961	rVB	411	323	0.03%	0.003%
24	4.475	969	975	978	rBV2	248	258	0.02%	0.003%
25	4.562	995	1002	1006	rBV2	256	343	0.03%	0.003%
26	4.620	1006	1020	1043	rBV	136191	327071	25.54%	3.171%
27	5.063	1142	1158	1184	rBV	231608	507601	39.64%	4.922%
28	5.205	1198	1202	1205	rVB2	310	274	0.02%	0.003%
29	5.259	1215	1219	1223	rBV2	364	322	0.03%	0.003%
30	5.282	1223	1226	1227	rBV2	451	322	0.03%	0.003%
31	5.571	1310	1316	1320	rBV2	242	274	0.02%	0.003%
32	5.726	1341	1364	1392	rBV2	471906	1280426	100.00%	12.415%
33	6.047	1458	1464	1466	rVB4	607	546	0.04%	0.005%
34	6.092	1474	1478	1480	rBV3	396	360	0.03%	0.003%
35	6.111	1480	1484	1485	rBV2	405	290	0.02%	0.003%
36	6.250	1509	1527	1555	rBV	380770	731252	57.11%	7.090%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
 Data File : VU047992.D
 Acq On : 13 Apr 2022 10:52
 Operator : SY/MD
 Sample : VU0413WBL01
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK089

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\SFAMULM032422WMA.M
 Title : VOC Analysis

37	6.529	1605	1614	1615	rBV5	1531	1586	0.12%	0.015%
38	6.690	1650	1664	1687	rBV	294775	576435	45.02%	5.589%
39	6.803	1698	1699	1702	rVB3	487	252	0.02%	0.002%
40	6.854	1712	1715	1723	rVB2	414	468	0.04%	0.005%
41	6.899	1725	1729	1732	rBV2	367	268	0.02%	0.003%
42	7.005	1759	1762	1767	rVV2	341	297	0.02%	0.003%
43	7.041	1767	1773	1779	rVV2	584	760	0.06%	0.007%
44	7.066	1779	1781	1785	rVB2	436	252	0.02%	0.002%
45	7.095	1785	1790	1793	rBV	281	279	0.02%	0.003%
46	7.185	1806	1818	1827	rBV4	3332	6470	0.51%	0.063%
47	7.353	1867	1870	1875	rBV2	318	387	0.03%	0.004%
48	7.494	1907	1914	1918	rBV	273	361	0.03%	0.004%
49	7.565	1924	1936	1960	rVV	151954	268995	21.01%	2.608%
50	7.648	1960	1962	1965	rVV2	571	335	0.03%	0.003%
51	7.690	1967	1975	1985	rVB4	2331	3972	0.31%	0.039%
52	7.748	1990	1993	1997	rVB2	391	345	0.03%	0.003%
53	7.793	1998	2007	2015	rBV4	2768	4600	0.36%	0.045%
54	7.899	2026	2040	2055	rBV	579593	1004975	78.49%	9.744%
55	8.179	2115	2127	2150	rVV	107711	185564	14.49%	1.799%
56	8.356	2178	2182	2185	rBV4	422	289	0.02%	0.003%
57	8.398	2192	2195	2199	rVB4	616	495	0.04%	0.005%
58	8.552	2240	2243	2246	rBV3	368	240	0.02%	0.002%
59	8.632	2252	2268	2301	rBV	415107	761591	59.48%	7.384%
60	8.867	2338	2341	2344	rBV3	408	273	0.02%	0.003%
61	9.025	2384	2390	2393	rVV4	575	646	0.05%	0.006%
62	9.044	2393	2396	2402	rVV2	492	417	0.03%	0.004%
63	9.127	2416	2422	2423	rBV2	383	242	0.02%	0.002%
64	9.160	2429	2432	2433	rBV2	353	233	0.02%	0.002%
65	9.285	2463	2471	2477	rVB3	265	424	0.03%	0.004%
66	9.417	2496	2512	2535	rBV	572562	998699	78.00%	9.683%
67	9.555	2552	2555	2557	rBV	484	336	0.03%	0.003%
68	9.690	2592	2597	2605	rVB3	1432	1842	0.14%	0.018%
69	9.809	2629	2634	2639	rVB2	411	429	0.03%	0.004%
70	9.851	2641	2647	2648	rBV2	344	333	0.03%	0.003%
71	9.893	2657	2660	2663	rVB2	388	242	0.02%	0.002%
72	10.060	2708	2712	2718	rVB2	247	272	0.02%	0.003%
73	10.111	2718	2728	2737	rVB8	1771	3599	0.28%	0.035%
74	10.160	2737	2743	2745	rBV2	317	357	0.03%	0.003%
75	10.288	2780	2783	2786	rBV	303	237	0.02%	0.002%
76	10.481	2837	2843	2853	rBV4	1077	1730	0.14%	0.017%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
 Data File : VU047992.D
 Acq On : 13 Apr 2022 10:52
 Operator : SY/MD
 Sample : VU0413WBL01
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK089

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\SFAMULM032422WMA.M
 Title : VOC Analysis

77	10.674	2894	2903	2910	rVB3	2857	3714	0.29%	0.036%
78	10.758	2916	2929	2946	rBV	442714	722279	56.41%	7.003%
79	10.822	2947	2949	2959	rVB5	1802	1725	0.13%	0.017%
80	10.873	2959	2965	2967	rBV	636	679	0.05%	0.007%
81	11.089	3027	3032	3038	rBV4	861	993	0.08%	0.010%
82	11.275	3087	3090	3093	rBV	347	271	0.02%	0.003%
83	11.352	3110	3114	3117	rBV3	397	297	0.02%	0.003%
84	11.468	3139	3150	3157	rBV6	2669	4809	0.38%	0.047%
85	11.571	3179	3182	3185	rVV2	358	321	0.03%	0.003%
86	11.696	3215	3221	3226	rVB2	906	934	0.07%	0.009%
87	11.748	3229	3237	3245	rBV4	2432	3461	0.27%	0.034%
88	11.812	3245	3257	3276	rBV	635729	1026232	80.15%	9.950%
89	12.192	3361	3375	3396	rVV	595314	985598	76.97%	9.556%
90	12.381	3430	3434	3437	rBV2	464	372	0.03%	0.004%
91	12.539	3481	3483	3489	rVB3	294	265	0.02%	0.003%
92	12.979	3610	3620	3621	rBV4	984	1295	0.10%	0.013%
93	13.224	3688	3696	3706	rVB5	2983	4187	0.33%	0.041%
94	13.844	3880	3889	3897	rBV3	6330	9407	0.73%	0.091%
95	14.089	3955	3965	3982	rBV	15177	26954	2.11%	0.261%
96	14.243	4010	4013	4015	rBV2	391	311	0.02%	0.003%
97	14.330	4033	4040	4051	rVB5	6492	10305	0.80%	0.100%
98	14.378	4051	4055	4058	rBV2	489	421	0.03%	0.004%
99	15.217	4312	4316	4319	rBV2	1042	784	0.06%	0.008%
100	15.484	4396	4399	4403	rBV4	665	566	0.04%	0.005%

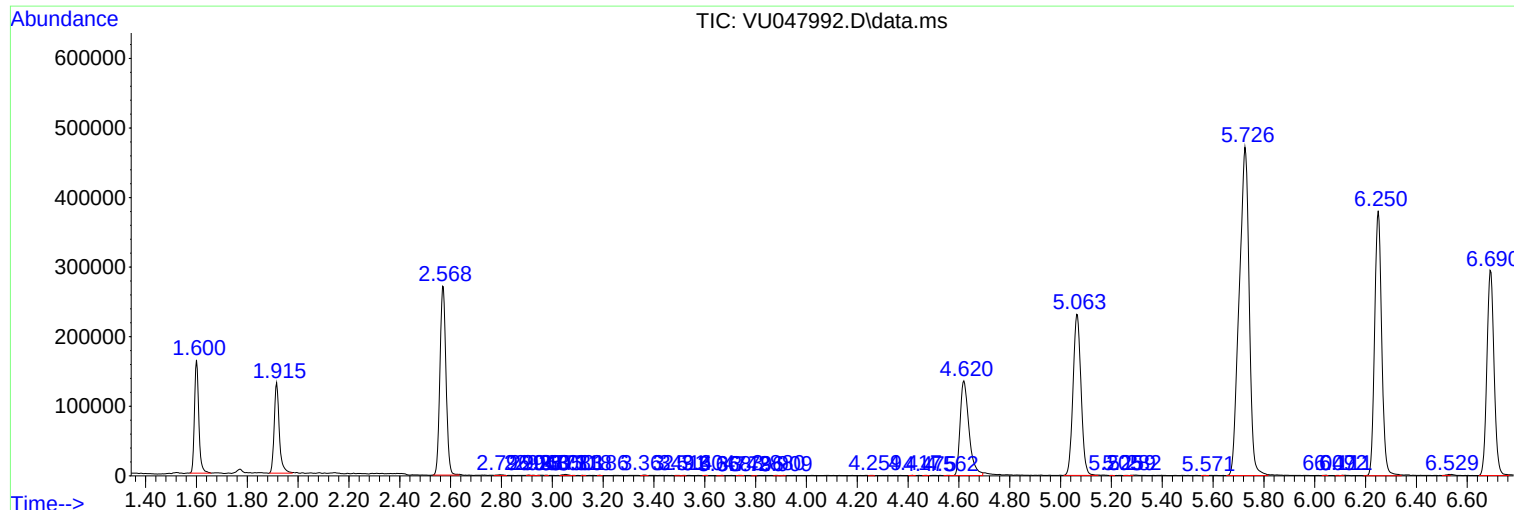
Sum of corrected areas: 10313504

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
Data File : VU047992.D
Acq On : 13 Apr 2022 10:52
Operator : SY/MD
Sample : VU0413WBL01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK089

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
Data File : VU047992.D
Acq On : 13 Apr 2022 10:52
Operator : SY/MD
Sample : VU0413WBL01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK089

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.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\VU041322\
Data File : VU047992.D
Acq On : 13 Apr 2022 10:52
Operator : SY/MD
Sample : VU0413WBL01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK089

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.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
------------------	----	---------	-------	----------	---	----	------	------