

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120921\
 Data File : VU046249.D
 Acq On : 10 Dec 2021 02:32
 Operator : SY/MD
 Sample : M4982-14
 Misc : 5.6mL/MSVOA_U/WATER
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0CS5

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\SFAMULM112921WMA.M
 Title : VOC Analysis

Signal : TIC: VU046249.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.604	75	82	104	rVB	91661	102149	15.94%	1.975%
2	1.919	172	180	198	rVB	68248	87748	13.69%	1.697%
3	2.318	301	304	308	rBV2	291	324	0.05%	0.006%
4	2.446	341	344	346	rBV	369	258	0.04%	0.005%
5	2.520	363	367	370	rBV	350	291	0.05%	0.006%
6	2.572	371	383	404	rBV	140070	232423	36.27%	4.495%
7	2.758	439	441	443	rBV	295	170	0.03%	0.003%
8	2.838	463	466	469	rVB	369	201	0.03%	0.004%
9	2.919	485	491	494	rBV	496	504	0.08%	0.010%
10	2.986	509	512	515	rBV2	259	213	0.03%	0.004%
11	3.247	590	593	596	rBV2	274	167	0.03%	0.003%
12	3.305	608	611	613	rBV	376	245	0.04%	0.005%
13	3.353	620	626	630	rBV2	329	387	0.06%	0.007%
14	3.401	638	641	644	rBV	320	210	0.03%	0.004%
15	3.601	699	703	707	rBV	399	349	0.05%	0.007%
16	3.629	709	712	719	rVV	371	415	0.06%	0.008%
17	3.883	788	791	794	rBV	250	192	0.03%	0.004%
18	3.932	803	806	809	rBV2	332	235	0.04%	0.005%
19	4.019	829	833	836	rBV	406	302	0.05%	0.006%
20	4.057	842	845	849	rBV	328	280	0.04%	0.005%
21	4.157	874	876	878	rBV2	224	127	0.02%	0.002%
22	4.308	919	923	925	rBV	376	268	0.04%	0.005%
23	4.437	961	963	966	rVB	306	151	0.02%	0.003%
24	4.465	966	972	975	rBV	447	515	0.08%	0.010%
25	4.485	975	978	981	rVB	331	207	0.03%	0.004%
26	4.507	981	985	991	rBV	418	560	0.09%	0.011%
27	4.549	995	998	1001	rBV	299	195	0.03%	0.004%
28	4.581	1005	1008	1011	rBV	410	299	0.05%	0.006%
29	4.639	1011	1026	1054	rBV	56492	165275	25.79%	3.196%
30	4.919	1108	1113	1115	rBV3	274	261	0.04%	0.005%
31	4.954	1121	1124	1127	rBV2	360	225	0.04%	0.004%
32	4.983	1130	1133	1138	rVB	391	316	0.05%	0.006%
33	5.070	1145	1160	1181	rVB	110040	258427	40.33%	4.998%
34	5.176	1190	1193	1195	rBV3	415	277	0.04%	0.005%
35	5.305	1228	1233	1236	rBV	465	368	0.06%	0.007%
36	5.327	1236	1240	1242	rBV2	544	365	0.06%	0.007%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120921\
 Data File : VU046249.D
 Acq On : 10 Dec 2021 02:32
 Operator : SY/MD
 Sample : M4982-14
 Misc : 5.6mL/MSVOA_U/WATER
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0CS5

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\SFAMULM112921WMA.M
 Title : VOC Analysis

37	5.382	1252	1257	1259	rBV	454	355	0.06%	0.007%
38	5.424	1267	1270	1271	rBV	206	107	0.02%	0.002%
39	5.520	1297	1300	1302	rBV2	242	170	0.03%	0.003%
40	5.549	1306	1309	1314	rBV	246	235	0.04%	0.005%
41	5.613	1326	1329	1331	rBV	186	137	0.02%	0.003%
42	5.729	1343	1365	1383	rBV2	237423	640764	100.00%	12.391%
43	6.170	1498	1502	1504	rBV2	327	262	0.04%	0.005%
44	6.250	1512	1527	1545	rBV	198167	373068	58.22%	7.214%
45	6.498	1601	1604	1606	rBV	315	228	0.04%	0.004%
46	6.546	1606	1619	1632	rVV4	24862	48735	7.61%	0.942%
47	6.694	1652	1665	1685	rBV	146316	284061	44.33%	5.493%
48	6.851	1710	1714	1717	rBV	436	356	0.06%	0.007%
49	6.970	1743	1751	1754	rBV	503	697	0.11%	0.013%
50	7.337	1862	1865	1870	rBV	371	337	0.05%	0.007%
51	7.501	1913	1916	1919	rBV2	219	202	0.03%	0.004%
52	7.568	1922	1937	1957	rBV	83033	143497	22.39%	2.775%
53	7.729	1985	1987	1992	rBV	146	122	0.02%	0.002%
54	7.751	1992	1994	1998	rVB	287	168	0.03%	0.003%
55	7.777	1998	2002	2004	rBV2	261	208	0.03%	0.004%
56	7.899	2027	2040	2057	rBV	294274	511021	79.75%	9.882%
57	8.134	2111	2113	2116	rBV2	204	147	0.02%	0.003%
58	8.179	2116	2127	2143	rVV	56637	94596	14.76%	1.829%
59	8.462	2209	2215	2220	rBV3	717	1010	0.16%	0.020%
60	8.636	2257	2269	2295	rBV	189065	335238	52.32%	6.483%
61	8.948	2362	2366	2370	rBV2	377	378	0.06%	0.007%
62	8.989	2374	2379	2387	rVB	488	713	0.11%	0.014%
63	9.028	2387	2391	2394	rBV2	400	258	0.04%	0.005%
64	9.047	2394	2397	2399	rBV	292	209	0.03%	0.004%
65	9.192	2439	2442	2448	rVB	438	381	0.06%	0.007%
66	9.221	2448	2451	2455	rBV2	396	372	0.06%	0.007%
67	9.259	2460	2463	2464	rBV2	297	181	0.03%	0.004%
68	9.295	2471	2474	2477	rBV2	372	234	0.04%	0.005%
69	9.311	2477	2479	2487	rVV2	211	214	0.03%	0.004%
70	9.420	2500	2513	2537	rBV	299698	501909	78.33%	9.706%
71	9.636	2578	2580	2584	rBV	315	214	0.03%	0.004%
72	9.751	2612	2616	2619	rBV	255	274	0.04%	0.005%
73	9.954	2673	2679	2682	rBV	404	449	0.07%	0.009%
74	10.050	2705	2709	2714	rBV2	386	422	0.07%	0.008%
75	10.137	2732	2736	2739	rBV	411	358	0.06%	0.007%
76	10.202	2753	2756	2759	rBV	473	352	0.05%	0.007%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120921\
 Data File : VU046249.D
 Acq On : 10 Dec 2021 02:32
 Operator : SY/MD
 Sample : M4982-14
 Misc : 5.6mL/MSVOA_U/WATER
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0CS5

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\SFAMULM112921WMA.M
 Title : VOC Analysis

77	10.362	2803	2806	2810	rVB	345	232	0.04%	0.004%
78	10.443	2829	2831	2835	rBV2	269	181	0.03%	0.004%
79	10.462	2835	2837	2840	rVV2	210	112	0.02%	0.002%
80	10.510	2849	2852	2856	rVB	550	382	0.06%	0.007%
81	10.539	2856	2861	2863	rBV	237	242	0.04%	0.005%
82	10.758	2917	2929	2951	rVB	220524	353500	55.17%	6.836%
83	10.857	2957	2960	2963	rBV2	351	226	0.04%	0.004%
84	10.877	2963	2966	2969	rBV	352	319	0.05%	0.006%
85	11.259	3082	3085	3090	rBV2	360	450	0.07%	0.009%
86	11.452	3141	3145	3146	rBV2	471	337	0.05%	0.007%
87	11.513	3161	3164	3167	rBV2	266	174	0.03%	0.003%
88	11.549	3171	3175	3177	rBV2	303	240	0.04%	0.005%
89	11.636	3200	3202	3205	rBV	288	161	0.03%	0.003%
90	11.812	3245	3257	3276	rVB	335405	521611	81.40%	10.087%
91	12.124	3350	3354	3357	rBV	614	445	0.07%	0.009%
92	12.195	3363	3376	3391	rBV	301923	491251	76.67%	9.500%
93	12.295	3401	3407	3411	rBV2	552	670	0.10%	0.013%
94	12.337	3417	3420	3421	rBV	281	178	0.03%	0.003%
95	12.484	3462	3466	3469	rBV	427	346	0.05%	0.007%
96	12.504	3469	3472	3475	rBV	381	263	0.04%	0.005%
97	12.552	3483	3487	3494	rBV	614	667	0.10%	0.013%
98	13.645	3824	3827	3830	rBV2	361	306	0.05%	0.006%
99	15.626	4439	4443	4446	rBV2	629	645	0.10%	0.012%
100	15.719	4468	4472	4475	rBV	716	626	0.10%	0.012%

Sum of corrected areas: 5171102

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120921\
Data File : VU046249.D
Acq On : 10 Dec 2021 02:32
Operator : SY/MD
Sample : M4982-14
Misc : 5.6mL/MSVOA_U/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0CS5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.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\VU120921\
Data File : VU046249.D
Acq On : 10 Dec 2021 02:32
Operator : SY/MD
Sample : M4982-14
Misc : 5.6mL/MSVOA_U/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0CS5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.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
------------------	----	---------	-------	----------	---	----	------	------