

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072824\
 Data File : VX042620.D
 Acq On : 26 Jul 2024 23:54
 Operator : JC/MD
 Sample : P3335-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E20K1

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_X\Method\SFAMXML072624WMA.M
 Title : VOC Analysis

Signal : TIC: VX042620.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.368	43	46	56	rVB	49677	59210	10.35%	1.463%
2	1.648	89	92	100	rVB	31079	39406	6.89%	0.973%
3	1.935	135	139	144	rVV2	1425	2020	0.35%	0.050%
4	1.996	147	149	152	rVB	431	361	0.06%	0.009%
5	2.197	178	182	184	rBV2	308	452	0.08%	0.011%
6	2.294	192	198	208	rBV	108163	171992	30.08%	4.249%
7	2.502	230	232	237	rBV3	449	482	0.08%	0.012%
8	2.569	237	243	248	rVV	3664	6585	1.15%	0.163%
9	2.672	258	260	262	rBV	191	203	0.04%	0.005%
10	2.941	297	304	313	rBV	5542	12434	2.17%	0.307%
11	3.014	314	316	318	rVB	494	322	0.06%	0.008%
12	3.038	318	320	322	rBB	199	179	0.03%	0.004%
13	3.056	322	323	324	rBV	267	162	0.03%	0.004%
14	3.075	324	326	330	rBV2	375	451	0.08%	0.011%
15	3.197	344	346	348	rBV	174	200	0.03%	0.005%
16	3.331	365	368	370	rBV3	400	614	0.11%	0.015%
17	3.410	379	381	383	rBV3	175	147	0.03%	0.004%
18	3.630	415	417	419	rVB	254	190	0.03%	0.005%
19	3.873	453	457	461	rBB2	182	313	0.05%	0.008%
20	3.928	462	466	470	rBV2	219	323	0.06%	0.008%
21	4.014	478	480	482	rVB	225	208	0.04%	0.005%
22	4.081	488	491	493	rBB	219	262	0.05%	0.006%
23	4.105	493	495	496	rBV	235	201	0.04%	0.005%
24	4.465	546	554	571	rBV2	38514	118212	20.67%	2.920%
25	5.050	639	650	664	rBV	76063	231911	40.56%	5.729%
26	5.337	695	697	699	rBV	194	217	0.04%	0.005%
27	5.397	705	707	708	rBV	197	140	0.02%	0.003%
28	5.458	713	717	718	rBV4	477	552	0.10%	0.014%
29	5.562	731	734	735	rBV	285	263	0.05%	0.006%
30	5.715	756	759	761	rBV	175	168	0.03%	0.004%
31	5.812	773	775	779	rBV2	213	316	0.06%	0.008%
32	5.879	785	786	789	rBB2	185	147	0.03%	0.004%
33	5.971	789	801	816	rBV2	192036	571809	100.00%	14.125%
34	6.263	848	849	852	rBV	149	170	0.03%	0.004%
35	6.312	852	857	860	rVV2	322	589	0.10%	0.015%
36	6.367	864	866	869	rVB2	422	458	0.08%	0.011%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072824\
 Data File : VX042620.D
 Acq On : 26 Jul 2024 23:54
 Operator : JC/MD
 Sample : P3335-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E20K1

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_X\Method\SFAMXML072624WMA.M
 Title : VOC Analysis

37	6.397	869	871	872	rBV	217	165	0.03%	0.004%
38	6.556	894	897	898	rBV	179	167	0.03%	0.004%
39	6.659	911	914	915	rBV	233	180	0.03%	0.004%
40	6.763	921	931	945	rBV	139934	342516	59.90%	8.461%
41	7.025	973	974	976	rBV	202	171	0.03%	0.004%
42	7.123	983	990	1000	rBV	44523	99650	17.43%	2.462%
43	7.306	1012	1020	1040	rBV	116032	257818	45.09%	6.369%
44	7.476	1046	1048	1050	rBV2	270	320	0.06%	0.008%
45	7.611	1068	1070	1073	rBV	241	244	0.04%	0.006%
46	7.659	1075	1078	1079	rVB2	182	147	0.03%	0.004%
47	7.946	1124	1125	1126	rBV2	269	154	0.03%	0.004%
48	8.037	1138	1140	1143	rBV2	152	153	0.03%	0.004%
49	8.062	1143	1144	1146	rBV	227	140	0.02%	0.003%
50	8.110	1151	1152	1154	rBV	157	167	0.03%	0.004%
51	8.324	1181	1187	1196	rBV	64157	109924	19.22%	2.715%
52	8.647	1234	1240	1249	rBV	276499	428903	75.01%	10.595%
53	8.830	1269	1270	1273	rVB2	440	344	0.06%	0.008%
54	8.952	1285	1290	1302	rBV	45735	70855	12.39%	1.750%
55	9.220	1330	1334	1337	rBV2	229	383	0.07%	0.009%
56	9.275	1339	1343	1348	rBV2	3922	5588	0.98%	0.138%
57	9.348	1352	1355	1356	rBV	219	201	0.04%	0.005%
58	9.385	1356	1361	1374	rBV	166301	251434	43.97%	6.211%
59	9.738	1417	1419	1421	rBV	224	226	0.04%	0.006%
60	10.055	1465	1471	1487	rBV	274757	379232	66.32%	9.368%
61	10.244	1501	1502	1505	rVB	312	193	0.03%	0.005%
62	10.305	1508	1512	1517	rBV2	1495	2173	0.38%	0.054%
63	10.378	1522	1524	1525	rBV	153	153	0.03%	0.004%
64	10.427	1531	1532	1535	rVB	180	155	0.03%	0.004%
65	10.470	1535	1539	1541	rBB	258	320	0.06%	0.008%
66	10.525	1544	1548	1549	rBV	236	323	0.06%	0.008%
67	10.732	1581	1582	1585	rBV	200	175	0.03%	0.004%
68	10.994	1624	1625	1627	rBV	203	144	0.03%	0.004%
69	11.098	1639	1642	1645	rBB2	233	278	0.05%	0.007%
70	11.189	1652	1657	1666	rBV	210218	281798	49.28%	6.961%
71	11.610	1720	1726	1729	rBV	285	587	0.10%	0.015%
72	11.762	1746	1751	1754	rVB	1041	1245	0.22%	0.031%
73	11.890	1767	1772	1774	rBV	280	350	0.06%	0.009%
74	11.915	1774	1776	1780	rVB	264	197	0.03%	0.005%
75	12.024	1789	1794	1803	rVV	210487	273482	47.83%	6.756%
76	12.140	1810	1813	1815	rBV	358	326	0.06%	0.008%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072824\
 Data File : VX042620.D
 Acq On : 26 Jul 2024 23:54
 Operator : JC/MD
 Sample : P3335-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E20K1

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_X\Method\SFAMXML072624WMA.M
 Title : VOC Analysis

77	12.219	1822	1826	1829	rBV3	1895	2612	0.46%	0.065%
78	12.274	1834	1835	1837	rBV3	199	163	0.03%	0.004%
79	12.317	1837	1842	1851	rBV	235299	305983	53.51%	7.558%
80	12.482	1867	1869	1871	rBV	307	259	0.05%	0.006%
81	12.756	1911	1914	1916	rBV	226	243	0.04%	0.006%
82	12.774	1916	1917	1921	rBV	177	270	0.05%	0.007%
83	12.866	1929	1932	1934	rBV3	798	724	0.13%	0.018%
84	12.927	1941	1942	1943	rBV3	301	153	0.03%	0.004%
85	13.134	1973	1976	1978	rBV3	1091	1058	0.19%	0.026%
86	13.219	1988	1990	1993	rVB4	672	726	0.13%	0.018%
87	13.518	2037	2039	2041	rVB	272	148	0.03%	0.004%
88	13.902	2100	2102	2105	rBV	212	263	0.05%	0.006%
89	14.000	2116	2118	2120	rBV	173	236	0.04%	0.006%
90	14.048	2124	2126	2129	rBV	186	214	0.04%	0.005%
91	14.189	2147	2149	2150	rBV	245	148	0.03%	0.004%
92	14.219	2153	2154	2158	rVB	272	238	0.04%	0.006%
93	14.262	2160	2161	2164	rVB	236	168	0.03%	0.004%
94	14.298	2164	2167	2170	rBV	272	368	0.06%	0.009%
95	14.432	2187	2189	2191	rVB	275	237	0.04%	0.006%
96	14.475	2194	2196	2197	rBV	259	157	0.03%	0.004%
97	14.640	2221	2223	2224	rBV	267	177	0.03%	0.004%
98	14.743	2239	2240	2243	rBV	263	279	0.05%	0.007%
99	15.152	2304	2307	2309	rVB2	462	443	0.08%	0.011%
100	15.682	2391	2394	2396	rVB	318	341	0.06%	0.008%

Sum of corrected areas: 4048258

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072824\
Data File : VX042620.D
Acq On : 26 Jul 2024 23:54
Operator : JC/MD
Sample : P3335-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20K1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.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_X\Data\VX072824\
Data File : VX042620.D
Acq On : 26 Jul 2024 23:54
Operator : JC/MD
Sample : P3335-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20K1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.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
------------------	----	---------	-------	----------	---	----	------	------