

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101521\
 Data File : VX024822.D
 Acq On : 14 Oct 2021 19:19
 Operator : JC/MD
 Sample : M4103-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AA3

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\SFAMXML100721WMA.M
 Title : VOC Analysis

Signal : TIC: VX024822.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	23	26	32	rBV2	5600	8831	0.95%	0.123%
2	1.367	43	46	55	rVB	108282	98142	10.59%	1.364%
3	1.666	91	95	106	rVB	78528	96688	10.44%	1.344%
4	2.306	194	200	211	rBV	170890	274436	29.62%	3.814%
5	2.550	230	240	249	rBV	20177	37031	4.00%	0.515%
6	2.709	264	266	272	rVB	490	561	0.06%	0.008%
7	2.794	274	280	284	rBV2	838	1387	0.15%	0.019%
8	2.946	299	305	315	rVB2	2478	5618	0.61%	0.078%
9	3.044	319	321	324	rVB2	194	176	0.02%	0.002%
10	3.184	343	344	346	rBV	220	151	0.02%	0.002%
11	3.209	346	348	351	rBV2	204	208	0.02%	0.003%
12	3.721	428	432	433	rVV2	159	197	0.02%	0.003%
13	3.898	459	461	464	rVB2	176	154	0.02%	0.002%
14	4.013	478	480	485	rVB2	155	191	0.02%	0.003%
15	4.135	499	500	504	rBV2	142	199	0.02%	0.003%
16	4.178	504	507	508	rVV2	161	135	0.01%	0.002%
17	4.288	522	525	526	rBV2	148	136	0.01%	0.002%
18	4.464	545	554	572	rBV	80826	241120	26.03%	3.351%
19	5.068	639	653	670	rBV	121307	385253	41.58%	5.354%
20	5.214	675	677	679	rVB	203	163	0.02%	0.002%
21	5.300	689	691	695	rBV2	105	157	0.02%	0.002%
22	5.391	702	706	712	rVB3	411	876	0.09%	0.012%
23	5.678	749	753	755	rBV	242	251	0.03%	0.003%
24	5.763	764	767	768	rBV2	110	132	0.01%	0.002%
25	5.976	789	802	820	rBV2	318958	926476	100.00%	12.876%
26	6.226	840	843	844	rBV2	186	135	0.01%	0.002%
27	6.354	862	864	867	rVV2	210	216	0.02%	0.003%
28	6.409	870	873	874	rBV	204	212	0.02%	0.003%
29	6.464	880	882	884	rBV	307	286	0.03%	0.004%
30	6.525	891	892	895	rVB2	187	132	0.01%	0.002%
31	6.549	895	896	898	rBV	310	157	0.02%	0.002%
32	6.592	901	903	908	rVB2	215	258	0.03%	0.004%
33	6.769	920	932	945	rBV	243674	573660	61.92%	7.972%
34	6.970	963	965	968	rBV2	188	199	0.02%	0.003%
35	7.001	968	970	972	rVB	316	175	0.02%	0.002%
36	7.019	972	973	978	rVB3	212	252	0.03%	0.004%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101521\
 Data File : VX024822.D
 Acq On : 14 Oct 2021 19:19
 Operator : JC/MD
 Sample : M4103-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AA3

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\SFAMXLM100721WMA.M
 Title : VOC Analysis

37	7.116	981	989	996	rBV3	4915	11417	1.23%	0.159%
38	7.226	1003	1007	1012	rBV3	813	1537	0.17%	0.021%
39	7.318	1012	1022	1039	rVB	195021	424566	45.83%	5.900%
40	7.482	1045	1049	1053	rVB3	401	670	0.07%	0.009%
41	7.690	1081	1083	1084	rBV2	238	212	0.02%	0.003%
42	7.811	1099	1103	1107	rVB3	675	836	0.09%	0.012%
43	7.933	1119	1123	1128	rVV3	672	1051	0.11%	0.015%
44	8.061	1142	1144	1147	rBV	292	248	0.03%	0.003%
45	8.330	1181	1188	1200	rBV	128828	210475	22.72%	2.925%
46	8.653	1234	1241	1248	rBV	479249	726374	78.40%	10.095%
47	8.720	1249	1252	1260	rVB	7332	10908	1.18%	0.152%
48	8.951	1285	1290	1302	rVB	100954	144587	15.61%	2.009%
49	9.116	1315	1317	1319	rBV2	230	225	0.02%	0.003%
50	9.226	1331	1335	1337	rBV	144	213	0.02%	0.003%
51	9.281	1341	1344	1348	rBV	508	631	0.07%	0.009%
52	9.390	1356	1362	1381	rBV	340702	514519	55.54%	7.151%
53	9.525	1381	1384	1388	rVB3	1425	1872	0.20%	0.026%
54	9.598	1395	1396	1399	rBV2	165	164	0.02%	0.002%
55	9.646	1402	1404	1406	rBV	168	156	0.02%	0.002%
56	9.903	1443	1446	1447	rBV	185	153	0.02%	0.002%
57	10.055	1465	1471	1487	rBV	511909	690181	74.50%	9.592%
58	10.195	1491	1494	1499	rVB2	639	808	0.09%	0.011%
59	10.281	1506	1508	1509	rBV	156	129	0.01%	0.002%
60	10.305	1509	1512	1517	rVB2	907	1297	0.14%	0.018%
61	10.646	1562	1568	1571	rBV4	579	1094	0.12%	0.015%
62	10.756	1583	1586	1590	rBV2	209	392	0.04%	0.005%
63	10.866	1601	1604	1606	rBV2	394	396	0.04%	0.006%
64	10.963	1618	1620	1624	rVB2	309	331	0.04%	0.005%
65	11.079	1633	1639	1643	rBV4	599	924	0.10%	0.013%
66	11.122	1643	1646	1650	rVV3	1179	1358	0.15%	0.019%
67	11.195	1652	1658	1668	rBV	391381	485781	52.43%	6.751%
68	11.311	1675	1677	1681	rVB3	522	464	0.05%	0.006%
69	11.378	1685	1688	1689	rBV3	353	306	0.03%	0.004%
70	11.457	1699	1701	1706	rVB3	434	595	0.06%	0.008%
71	11.494	1706	1707	1710	rVB2	253	154	0.02%	0.002%
72	11.610	1724	1726	1729	rBV2	233	229	0.02%	0.003%
73	11.756	1746	1750	1754	rBV3	1742	2367	0.26%	0.033%
74	11.847	1763	1765	1766	rVB	292	158	0.02%	0.002%
75	11.896	1770	1773	1775	rBV2	203	234	0.03%	0.003%
76	11.933	1776	1779	1783	rVB2	957	1130	0.12%	0.016%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101521\
 Data File : VX024822.D
 Acq On : 14 Oct 2021 19:19
 Operator : JC/MD
 Sample : M4103-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AA3

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\SFAMXML100721WMA.M
 Title : VOC Analysis

77	11.969	1783	1785	1788	rBV	405	408	0.04%	0.006%
78	12.024	1789	1794	1805	rVB	510098	626949	67.67%	8.713%
79	12.109	1805	1808	1809	rBV2	438	476	0.05%	0.007%
80	12.128	1809	1811	1812	rBV	288	152	0.02%	0.002%
81	12.225	1821	1827	1830	rBV5	1923	2846	0.31%	0.040%
82	12.323	1837	1843	1857	rVB	532207	663830	71.65%	9.226%
83	12.481	1866	1869	1870	rBV2	254	217	0.02%	0.003%
84	12.859	1928	1931	1935	rBV3	2203	2527	0.27%	0.035%
85	12.963	1946	1948	1949	rVB2	221	141	0.02%	0.002%
86	13.097	1968	1970	1971	rBV	254	172	0.02%	0.002%
87	13.115	1971	1973	1977	rVV2	295	300	0.03%	0.004%
88	13.182	1980	1984	1987	rBV2	210	376	0.04%	0.005%
89	13.420	2020	2023	2025	rBV2	224	307	0.03%	0.004%
90	13.524	2038	2040	2042	rVB	138	128	0.01%	0.002%
91	13.591	2049	2051	2054	rBV2	324	444	0.05%	0.006%
92	13.676	2061	2065	2066	rVB2	157	157	0.02%	0.002%
93	13.786	2078	2083	2085	rBV3	297	386	0.04%	0.005%
94	13.963	2110	2112	2116	rVB2	343	303	0.03%	0.004%
95	14.103	2133	2135	2137	rBV	275	270	0.03%	0.004%
96	14.213	2151	2153	2155	rVV	302	193	0.02%	0.003%
97	14.383	2178	2181	2183	rBV3	187	200	0.02%	0.003%
98	15.554	2371	2373	2376	rVB2	329	372	0.04%	0.005%
99	15.597	2376	2380	2381	rBV	384	491	0.05%	0.007%
100	15.804	2412	2414	2416	rBV2	393	401	0.04%	0.006%

Sum of corrected areas: 7195539

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101521\
Data File : VX024822.D
Acq On : 14 Oct 2021 19:19
Operator : JC/MD
Sample : M4103-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0AA3

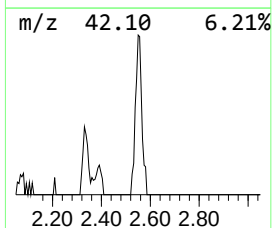
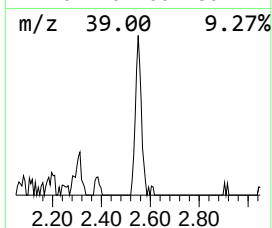
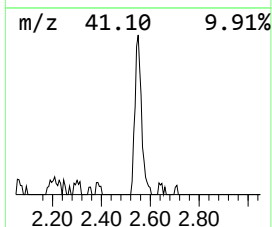
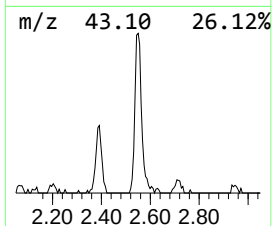
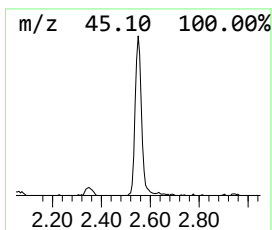
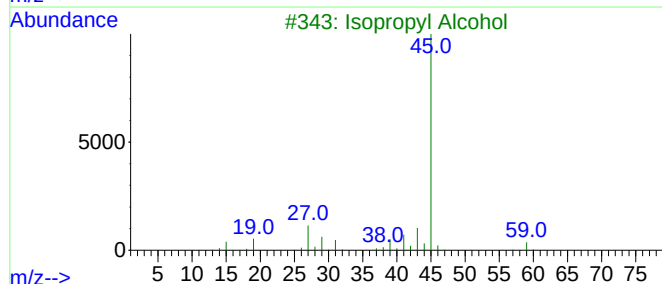
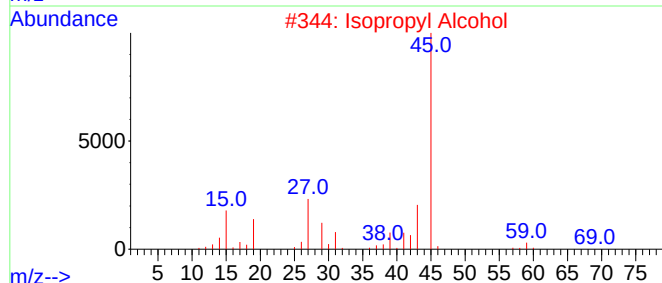
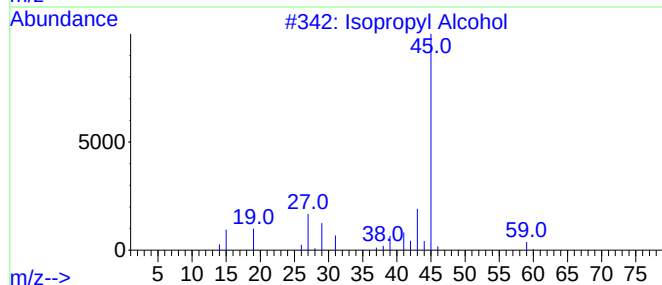
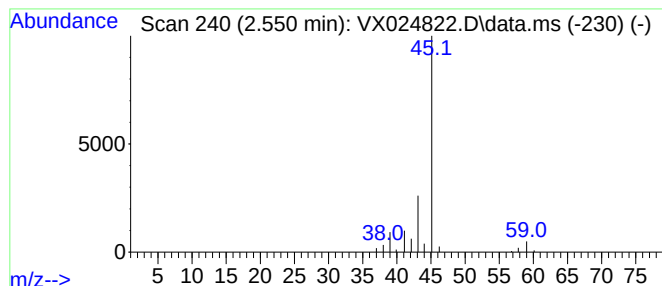
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM100721WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.550	3.23 ug/L	37031	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	83
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
5			Isopropyl Alcohol	60	C3H8O	000067-63-0	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101521\
Data File : VX024822.D
Acq On : 14 Oct 2021 19:19
Operator : JC/MD
Sample : M4103-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0AA3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML100721WMA.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
Isopropyl Alcohol	2.550	3.2	ug/L	37031	1	6.769	573660	50.0