1_2 contains the zipped file 1_2.cdf which is the GC × GC-TOFMS chromatogram of 100% conventional diesel. The tutorial uses this chromatogram for the training set.

2_1 contains the zipped file 2_1.cdf which is the GC × GC-TOFMS chromatogram of 100% conventional diesel. The tutorial uses this chromatogram for the training set.

3_1 contains the zipped file 3_1.cdf which is the GC × GC-TOFMS chromatogram of a blend of 5% biodiesel with 95% conventional diesel (by volume). The tutorial uses this chromatogram for the training set.

4_1 contains the zipped file 4_1.cdf which is the GC × GC-TOFMS chromatogram of a blend of 5% biodiesel with 95% conventional diesel (by volume). The tutorial uses this chromatogram for the training set.

5_1 contains the zipped file 5_1.cdf which is the GC × GC-TOFMS chromatogram of a blend of 8.75% biodiesel with 91.25% conventional diesel (by volume). The tutorial uses this chromatogram for the training set.

6_1 contains the zipped file 6_1.cdf which is the GC × GC-TOFMS chromatogram of a blend of 8.75% biodiesel with 91.25% conventional diesel (by volume). The tutorial uses this chromatogram for the training set.

7_1 contains the zipped file 7_1.cdf which is the GC × GC-TOFMS chromatogram of a blend of 12.5% biodiesel with 87.5% conventional diesel (by volume). The tutorial uses this chromatogram for the training set.

8_1 contains the zipped file 8_1.cdf which is the GC × GC-TOFMS chromatogram of a blend of 12.5% biodiesel with 87.5% conventional diesel (by volume). The tutorial uses this chromatogram for the training set.

9_1 contains the zipped file 9_1.cdf which is the GC × GC-TOFMS chromatogram of a blend of 12.5% biodiesel with 87.5% conventional diesel (by volume). The tutorial uses this chromatogram for the training set.

11_1 contains the zipped file 11_1.cdf which is the GC × GC-TOFMS chromatogram of a blend of 16.25% biodiesel with 83.75% conventional diesel (by volume). The tutorial uses this chromatogram for the training set.

12_1 contains the zipped file 12_1.cdf which is the GC × GC-TOFMS chromatogram of a blend of 16.25% biodiesel with 83.75% conventional diesel (by volume). The tutorial uses this chromatogram for the training set.

13_1 contains the zipped file 13_1.cdf which is the GC × GC-TOFMS chromatogram of a blend of 20% biodiesel with 80% conventional diesel (by volume). The tutorial uses this chromatogram for the training set. Electronic Supplementary Material (ESI) for Analytical Methods

14_1 contains the zipped file 14_1.cdf which is the GC × GC-TOFMS chromatogram of a blend of 20% biodiesel with 80% conventional diesel (by volume). The tutorial uses this chromatogram for the training set.

A_1 contains the zipped file A_1.cdf which is the GC × GC-TOFMS chromatogram of a blend of 5% biodiesel with 95% conventional diesel (by volume). The tutorial uses this chromatogram for the test set.

B_1 contains the zipped file B_1.cdf which is the GC × GC-TOFMS chromatogram of a blend of 5% biodiesel with 95% conventional diesel (by volume). The tutorial uses this chromatogram for the test set.

C_1 contains the zipped file C_1.cdf which is the GC × GC-TOFMS chromatogram of a blend of 8.75% biodiesel with 91.25% conventional diesel (by volume). The tutorial uses this chromatogram for the test set.

D_1 contains the zipped file D_1.cdf which is the GC × GC-TOFMS chromatogram of a blend of 8.75% biodiesel with 91.25% conventional diesel (by volume). The tutorial uses this chromatogram for the test set.

E_1 contains the zipped file E_1.cdf which is the GC × GC-TOFMS chromatogram of a blend of 12.5% biodiesel with 87.5% conventional diesel (by volume). The tutorial uses this chromatogram for the test set.

F_1 contains the zipped file F_1.cdf which is the GC × GC-TOFMS chromatogram of a blend of 12.5% biodiesel with 87.5% conventional diesel (by volume). The tutorial uses this chromatogram for the test set.

H_1 contains the zipped file H_1.cdf which is the GC × GC-TOFMS chromatogram of a blend of 16.25% biodiesel with 83.75% conventional diesel (by volume). The tutorial uses this chromatogram for the test set.

I_1 contains the zipped file I_1.cdf which is the GC × GC-TOFMS chromatogram of a blend of 20% biodiesel with 80% conventional diesel (by volume). The tutorial uses this chromatogram for the test set.

J_1 contains the zipped file J_1.cdf which is the GC × GC-TOFMS chromatogram of a blend of 20% biodiesel with 80% conventional diesel (by volume). The tutorial uses this chromatogram for the test set.