shinyLipidModelFit

# What it does

1. Reads data in generic format (Samples, Features, matrix)
2. Uses `Features` to generate linear models
3. Plots data points onto grid
4. Exports features that agree best with model

# Models

1. Model0 = Rt ~ nCarbon + nDouble
2. Model1 = Rt ~ nCarbon + as.factor(nDouble)
3. Model2 = Rt ~ nCarbon + as.factor(nDouble):position

`Position` means sn1, sn2 etc FA postion.

Models0-2 are increasingly more sophisticated. To choose the best one use BIC as guideline (the more negative, the better).

The model calculates **deltaRt = Rt - predictedRt** (residuals)

# Outliers

`Outlier` are automatically removed if deltaRt>3.5\*MAD (can be changed by user; MAD = median absolute difference to median). MAD=3.5 is a standard value from the literature.

# Export

The linear model can be used to

1. Remove features with deltaRt > cutoff (user defined)
2. For the same lipid ion, retain only the best one in terms of deltaRt
3. Predict Rt of unassigned species (not implemented)

Problems

1. Each lipid class needs to be fit individually and perhaps with different model equation and/or parameters. At the moment cannot export all lipid classes at the same time