

Development of Classification Models for Identifying “True” P-glycoprotein (P-gp) Inhibitors Through Inhibition, ATPase Activation and Monolayer Efflux Assays

Supplementary Information

Figure S1. Graphical representation of the best performing decision trees for the inhibition experiment. Two classes were used: inhibitors (Y) and non-inhibitors compounds (N). Molecular descriptors and their corresponding decision criteria are reported in rectangles. The number of classified compounds for Y/N are reported between brackets. The arrows at the bottom right show the direction of the branches. See the text for an explanation of the descriptors.

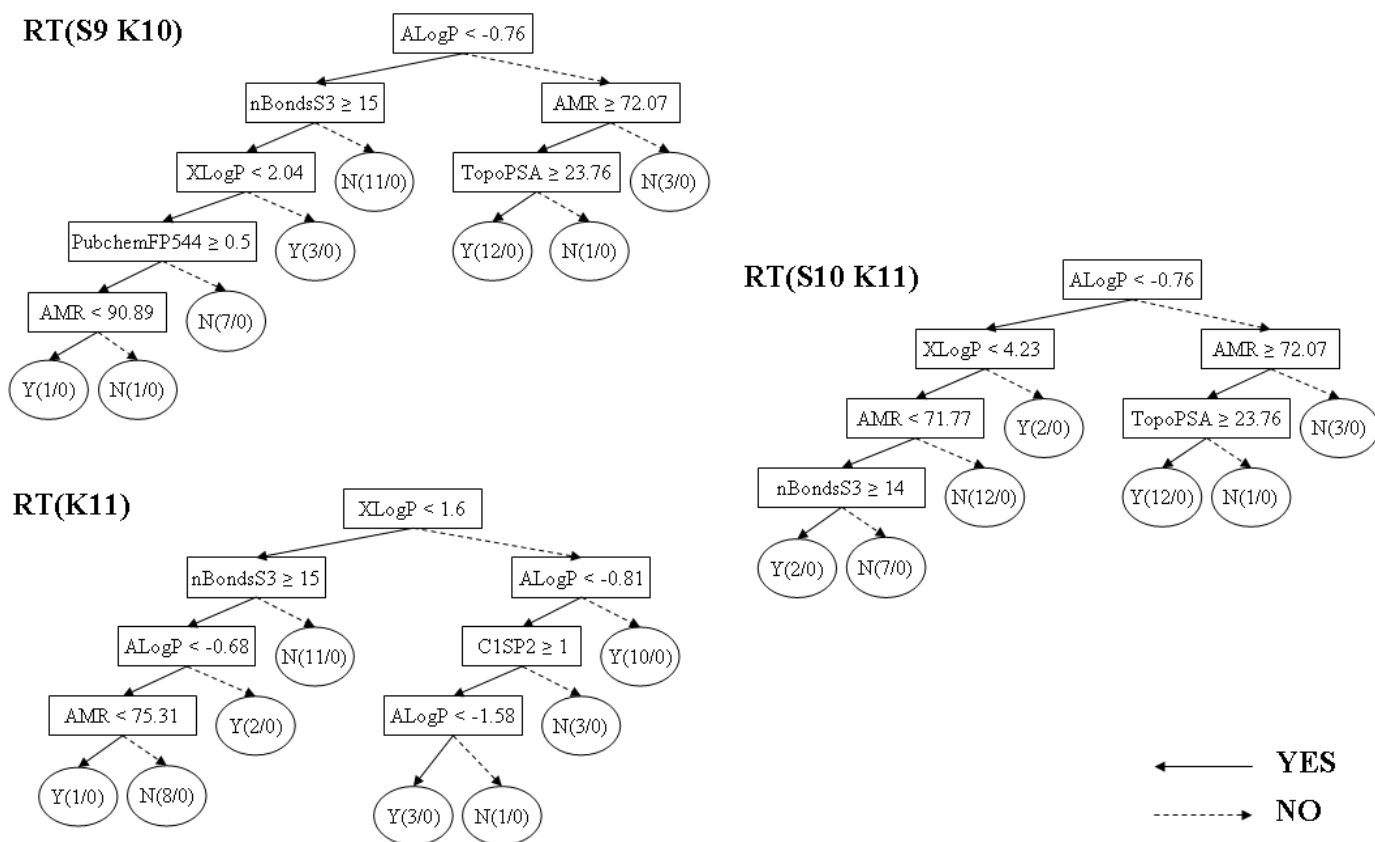


Figure S2. Graphical representation of the best performing decision trees for the ATP-ase experiment. Two classes were used: ATP-ase activators (Y) and non-activators (N). Molecular descriptors and their corresponding decision criteria are reported in rectangles. The number of classified compounds for Y/N are reported between brackets. The arrows at the bottom right show the direction of the branches. See the text for an explanation of the descriptors.

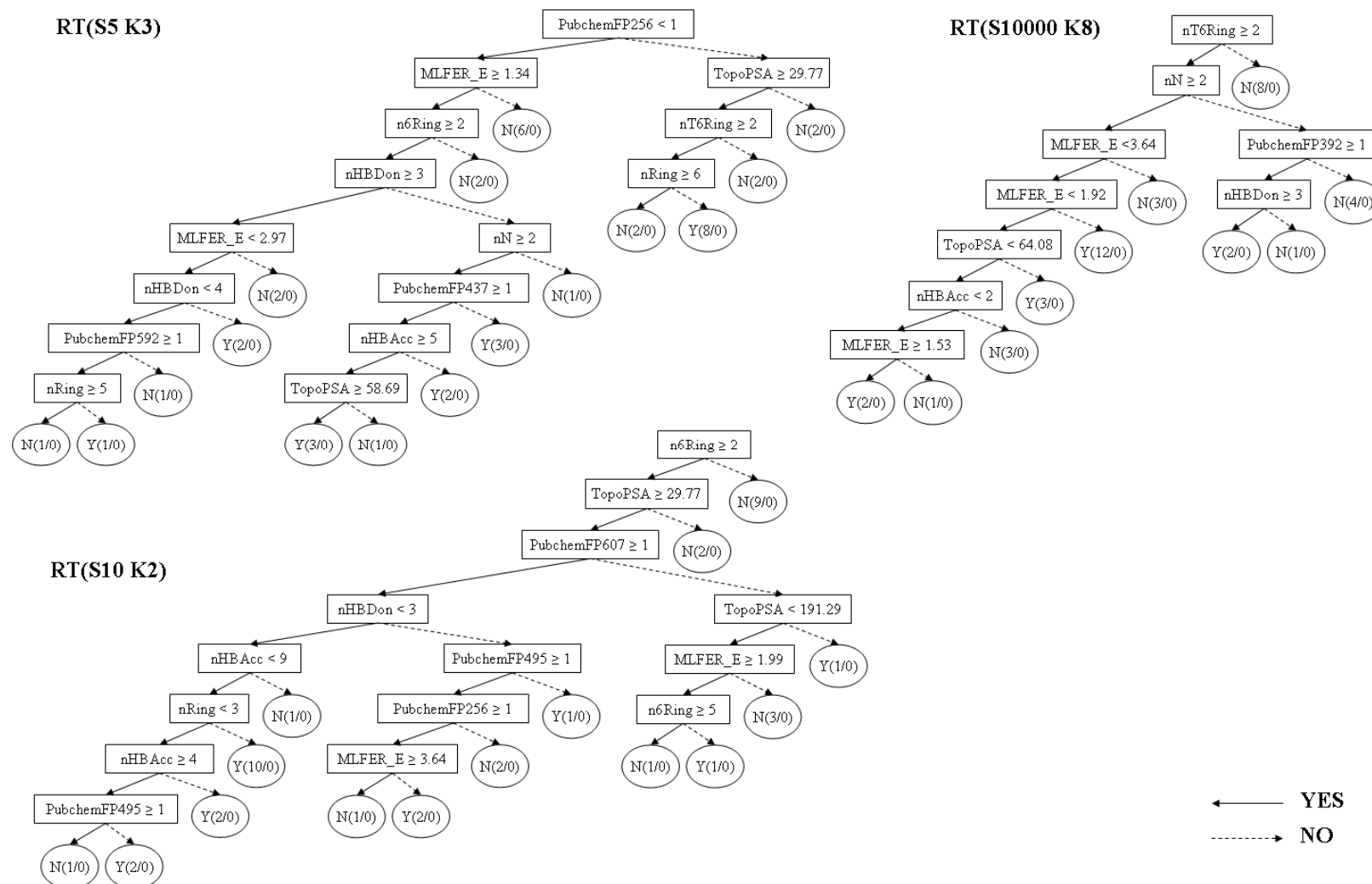


Figure S3. Graphical representation of the best performing decision trees for the monolayer efflux experiment. Two classes were used: effluxed (Y) and non-effluxed compounds (N). Molecular descriptors and their corresponding decision criteria are reported in rectangles. The number of classified compounds for Y/N are reported between brackets. The arrows at the bottom right show the direction of the branches. See the text for an explanation of the descriptors.

