## 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.



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