

ToxComp 1.2 – an Open Source *iv vitro in vivo* extrapolation (IVIVE) system for cardiotoxicity prediction with Marvin plugins embedded

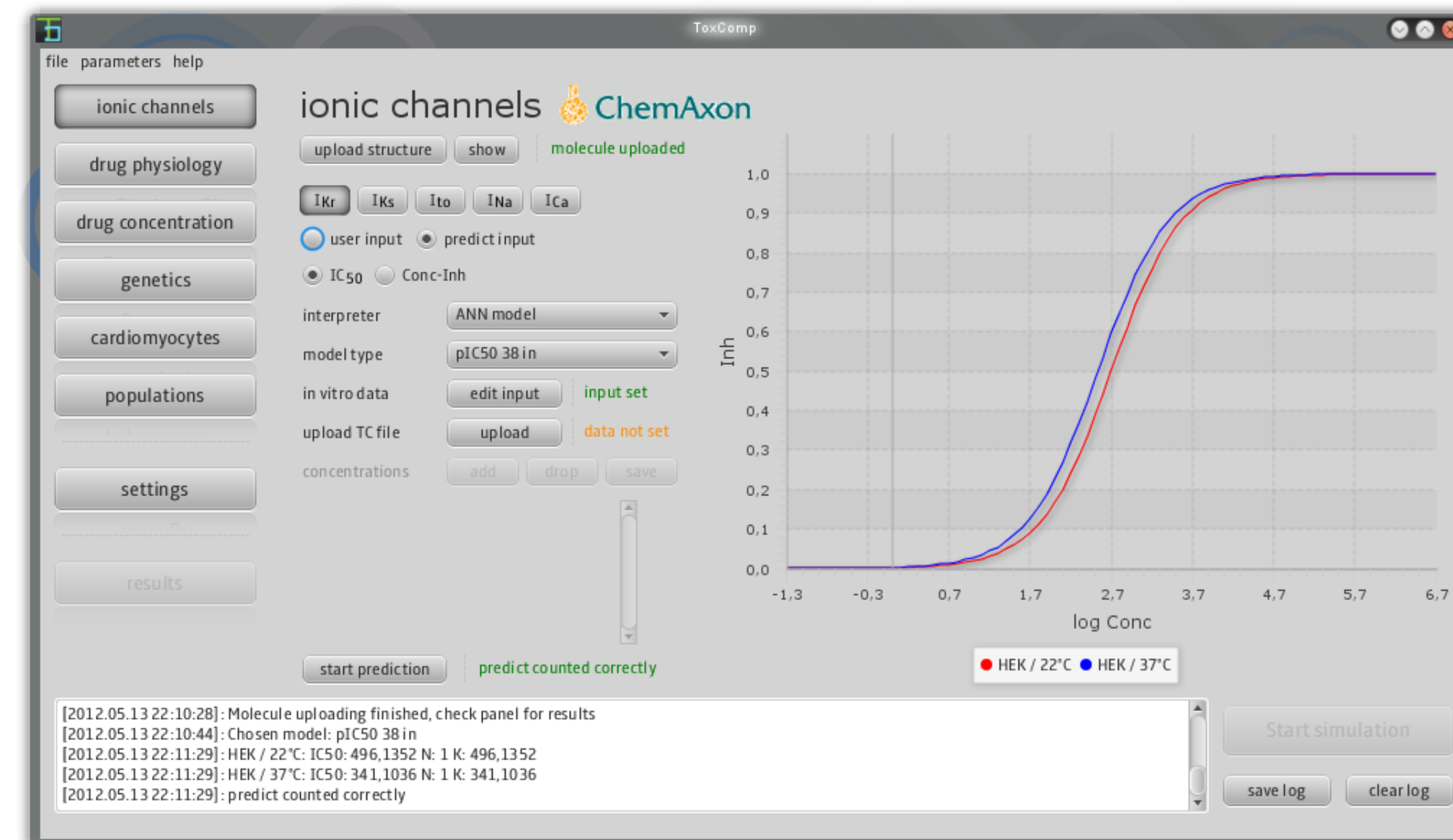
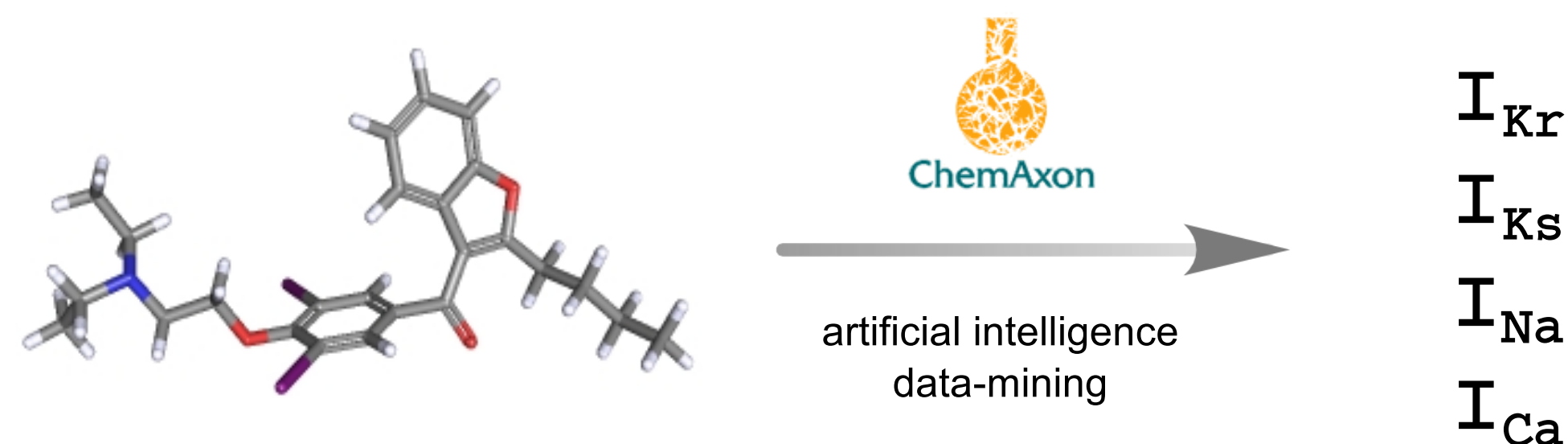


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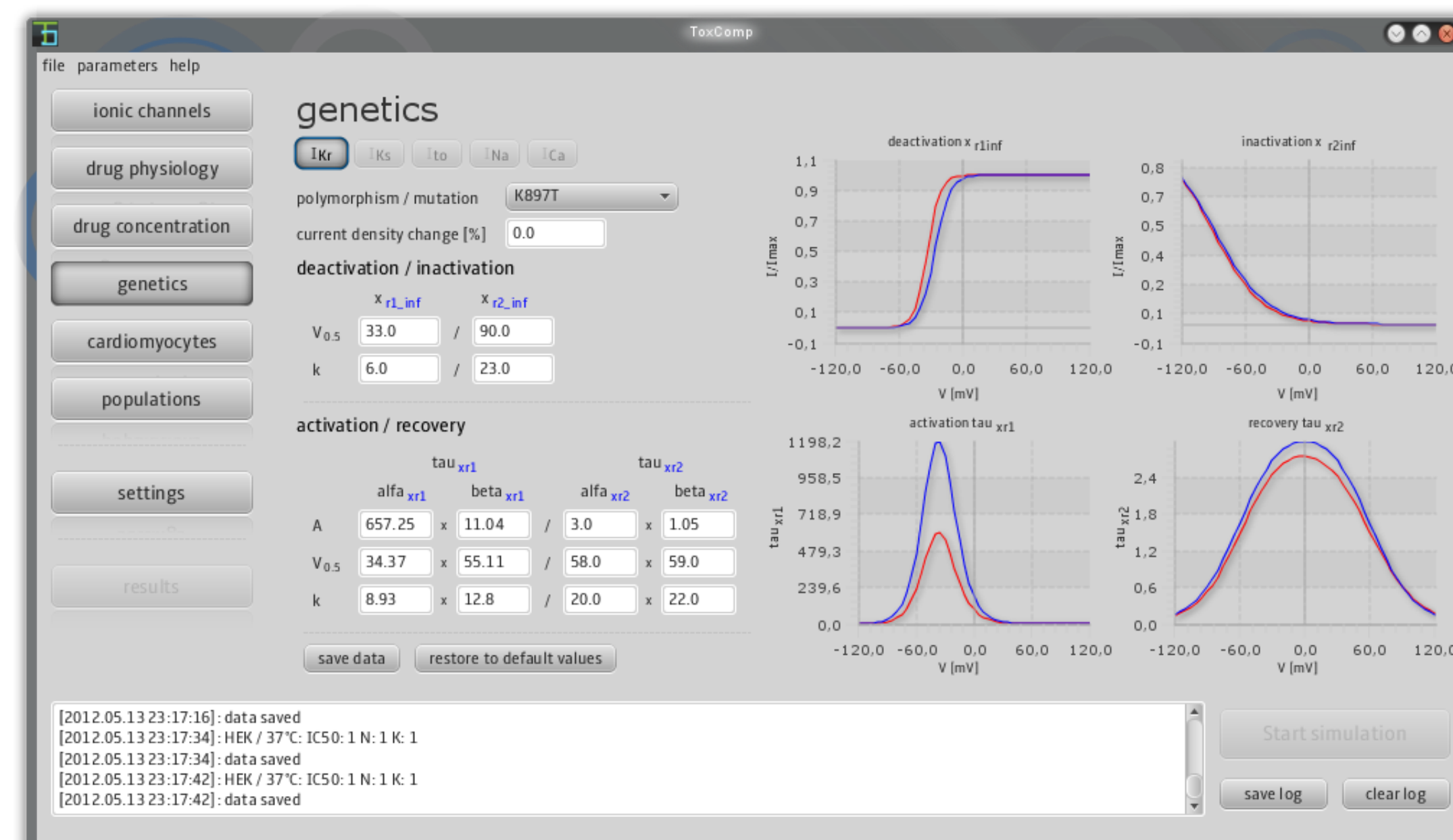
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ionic channels



genetics

- HERG channel (I_{Kr})
- genetic polymorphism
 - channel gating activity
 - pre-defined mutations (WT, K897T)
 - user-defined mutations

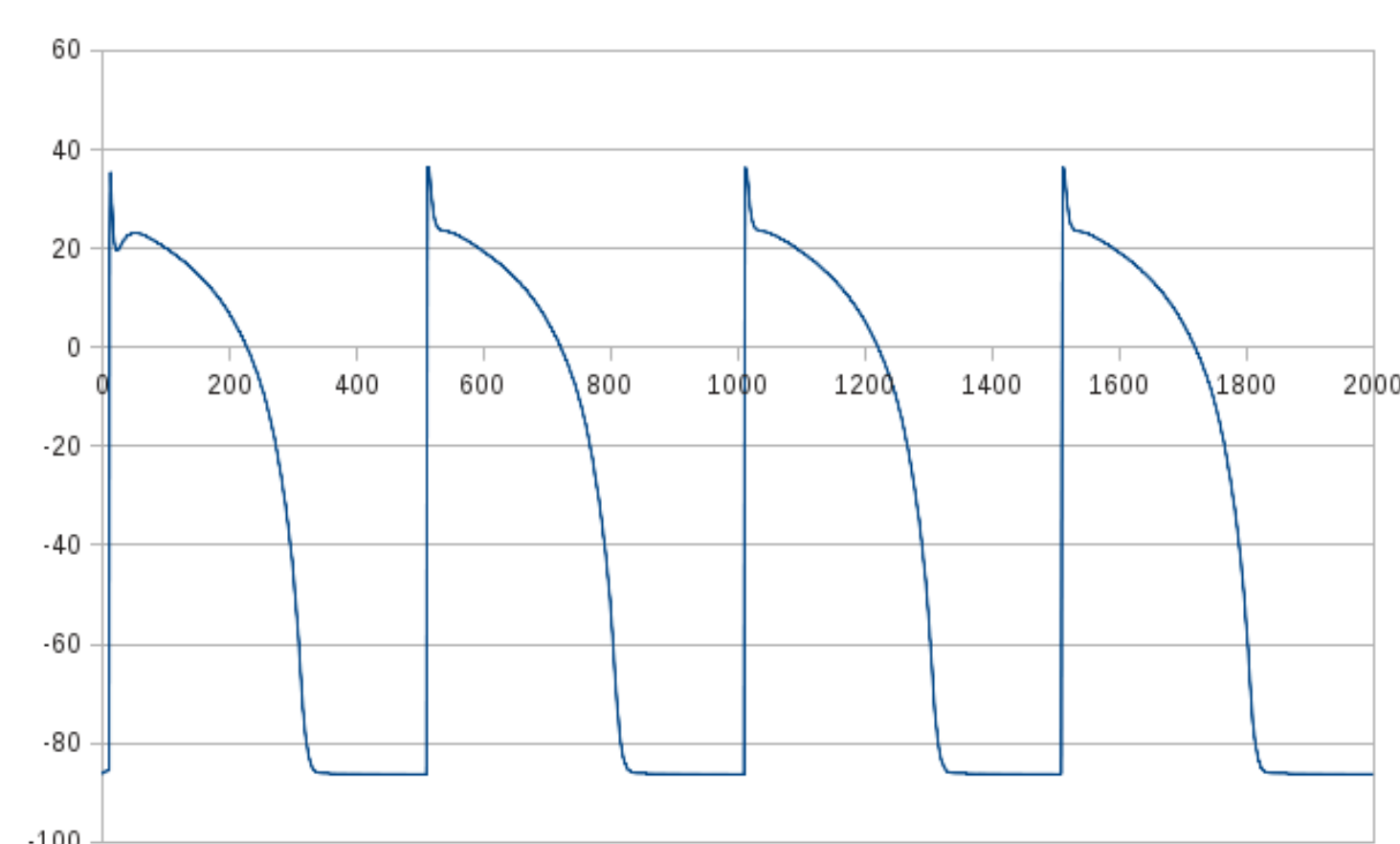


population

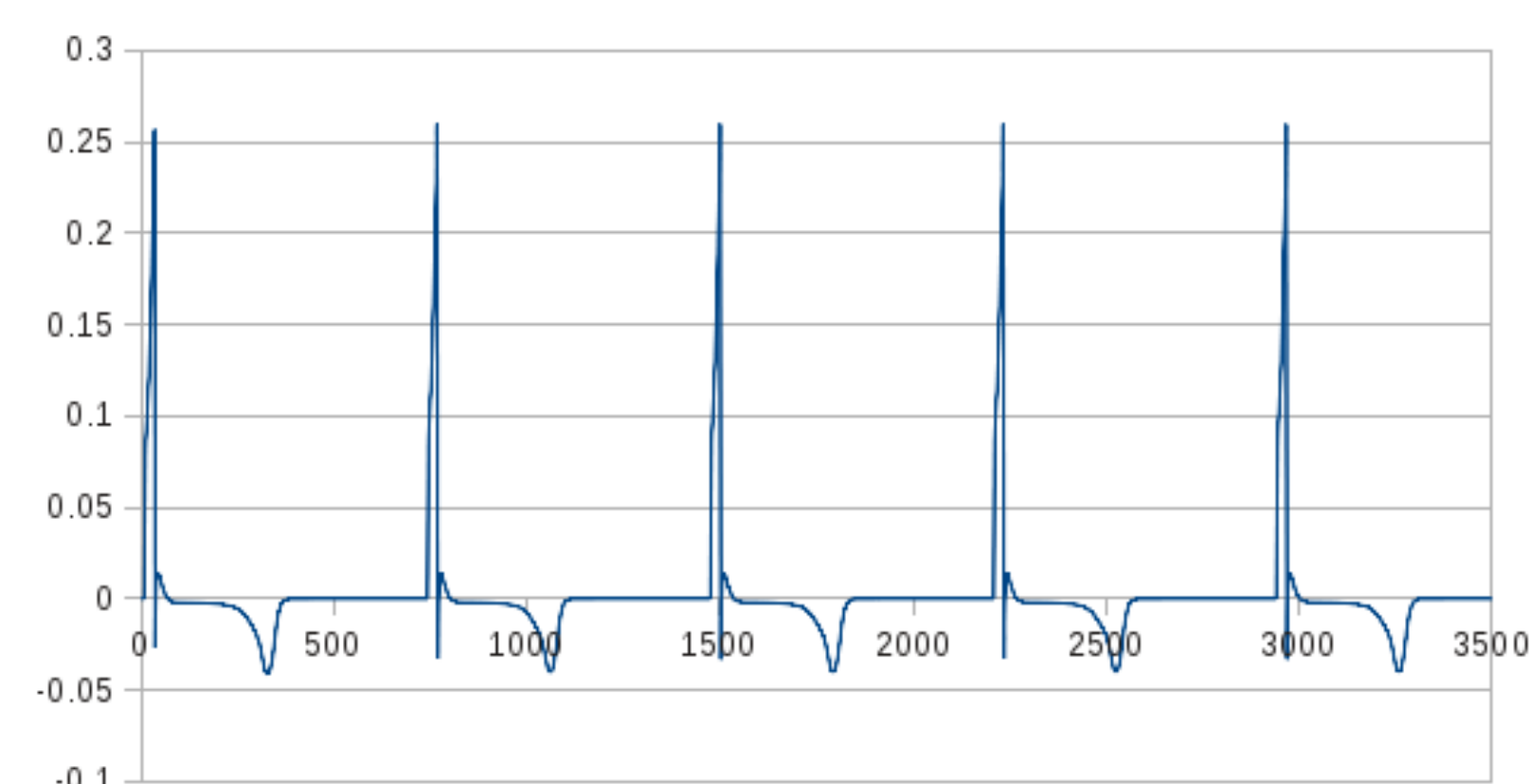
- statistical modeling
- pre-set distributions
 - cardiomyocyte volume & area
 - sarcoplasmic reticulum volume
 - ionic concentrations: K^+ , Na^+ , Ca^{++}



output



Action Potential



Pseudo-ECG

technology

- Java, JavaFX, OS-independent

