Predicting aberrant Fc-fusion protein pharmacokinetics from in silico structural properties and physiologically based pharmacokinetic (PBPK) modeling

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Supplementary File S1

Table S1. In silico properties considered as potential covariates of the scaling factors F1 and F2 in the modified PBPK model. Properties highlighted in yellow were selected through hierarchical clustering and were considered in the symbolic regression procedures. Properties highlighted in cyan were not only chosen for the symbolic regression, but they also appear in the formulas included in the model.

PROPERTY LABEL	PROPERTY DESCRIPTION
patch_pos	Total area of protein positive patch(es)
patch_pos_[K] ([K]=1,2,3,4,5)	Area of largest K protein positive patch(es)
patch_pos_%	Percentage of total surface area in protein positive patches
patch_pos_n	Number of protein positive patches
patch_neg	Total area of protein negative patch(es)
patch_neg_[K] ([K]=1,2,3,4,5)	Area of largest K protein negative patch(es)
patch_neg_%	Percentage of total surface area in protein negative patches
patch_neg_n	Number of protein negative patches
patch_hyd	Total area of protein hydrophobic patch(es)
patch_hyd_[K] ([K]=1,2,3,4,5)	Area of largest K protein hydrophobic patch(es
patch_hyd_%	Percentage of total surface area in protein hydrophobic patches
patch_hyd_n	Number of protein hydrophobic patches
patch_ion	Total area of protein ionic patch(es)
patch_ion_[K] ([K]=1,2,3,4,5)	Area of largest K protein ionic patch(es)
patch_ion_%	Percentage of total surface area in protein ionic patches
patch_ion_n	Number of protein ionic patches
Mass	Protein mass

debye	Debye screening length
pI_3D	Coordinate-based pI of the fused protein
pI_Fc	sequence-based calculated pI of the whole molecule
pI_seq	Sequence based pI of the fused protein
zquadrupole	Zeta quadrupole moment
Ens_dipole	Ensemble dipole moment
Dipole_moment	Dipole moment based on charge distribution on protein atoms
Asa_hyd	Water accessible surface area of hydrophobic atoms of a protein
Asa_vdw	Water accessible surface area of a protein
R_solv	Hydrodynamic radius
volume	Protein volume
Asa_hph	Water accessible surface area of hydrophilic atoms of a protein
mobility	Velocity of migration in an electric potential
zeta	Zeta potential
Ens_charge	Ensemble net charge
app_charge	Apparent charge of the protein at one Debye length at a given pH
Net_charge	Net charge of the protein at a given pH
eccen	Eccentricity based on two principal directions
helicity	Helicity, percentage of residuals with helical secondary structure
R_gyr	Radius of gyration
henry	Henry function
Hyd_moment	Kyte-Doolittle hydrophobicity moment