

VirtualToxLab Results – Praktikum HS 2016/2017

Groppe 2 (23.11. - 5.12.)

Compound	Toxic Potential
FM-BT.pdb	0.479
RT_MS_JB.pdb	0.471 ^A
Tyr-Val-Pro.pdb	0.450
IS_AZ_RR.pdb	0.367
JK_LH.pdb	0.428
MA-KZ.pdb	0.429
PD-BS.pdb	0.367
HU_AG_JH.pdb	0.469
JG-MB-NC.pdb	0.299
NC_EV.pdb	Wurde nicht gesendet!!!

ToxPot < 0.50 → **Low**
0.50 < ToxPot < 0.65 → **Medium**
0.65 < ToxPot → **High**

A Original: 0.521 → downscaled due to unsatisfied salt bridges in hERG (3), AR (3), AR (4), GR (3), MR (4)