

## VirtualToxLab Results – Praktikum HS 2016/2017

Group 2 (22.2. - 3.3.)

Compound	Toxic Potential
SS_MS.pdb	0.402
SG_MB.pdb	0.469
AI_PJR.pdb	0.466 <sup>A</sup>
KR_JS_ES.pdb	0.463
AE_JT.pdb	0.466 <sup>B</sup>
MM_LK_AS.pdb	0.309
ED_AB.pdb	0.430
MK_DM.pdb	0.547 <sup>C</sup>
SM_MK_CV.pdb	0.487 <sup>D</sup>
SG_AS_JS.pdb	0.351

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

- A Original: 0.516 → downscaled due to unsatisfied salt bridges in hERG (3), PPAR $\gamma$  (5)  
B Original: 0.516 → downscaled due to unsatisfied salt bridges in hERG (3), PPAR $\gamma$  (5)  
C Original: 0.597 → downscaled due to unsatisfied salt bridges in ER $\alpha$  (3), ER $\beta$  (3)  
D Original: 0.537 → downscaled due to unsatisfied salt bridges in ER $\alpha$  (3), CYP2C9 (4), AR (1)