**Table S4.** Physical and Pharmacokinetic data predicted by QikProp[a] extensions for compounds **5e**, **5f**, and **6a-c,e.**

| **Compound** | % **HOA**[b] | QP**PCaco**[c] | QP**logBB**[d] | QP**logHERG**[e] | QP**logKhsa**[f] | QP**logS**[g] | **PSA**[h] | Number of violations (<3) |
|---|---|---|---|---|---|---|---|---|
| **5e** | 90.757 | 1.454.968 | -1.168 | **-6.064** | 0.665 | **-6.773** | 113.326 | 2 |
| **5f** | 84.271 | 661.610 | -1.628 | **-6.101** | 0.766 | **-7.281** | 115.871 | 2 |
| **6a** | 100.000 | 592.613 | -1.272 | **-6.749** | 0.416 | -5.746 | 78.898 | 1 |
| **6b** | 100.000 | 639.622 | -1.303 | **-6.515** | 0.378 | -5.749 | 87.049 | 1 |
| **6c** | 100.000 | 602.342 | -1.283 | **-6.565** | 0.584 | **-6.260** | 78.848 | 2 |
| **6e** | 100.000 | 559.964 | -1.444 | **-5.799** | 0.274 | -5.312 | 101.681 | 1 |

a: QikProp (QP) version 6.5; [b] HOA, Human oral absorption (>80% - high and <25% - poor) ; [c] QPPCaco: Predicted apparent Caco-2 cell permeability (<25 nm/sec - poor and >500 nm/sec great); [d] QPlogBB: Predicted log brain/blood partition coefficient (appropriate values between -3.0 and 1.2); [e] QPlogHERG: Predicted $IC_{50}$ value for blockage of HERG K+ channels (above −5); [f] QPlogKhsa: Prediction of binding to human serum albumin (appropriate values between -1.5 and 1.5); [g] QPlogS: Predicted log aqueous solubility (appropriate values above -6.5); [h] PSA: polar surface area (appropriate values between 70–200 $Å^2$). The intervals of appropriate values are defined by QP. Bold numbers correspond to violations of the Jorgensen Rule-of-Three.