**Supplementary Table S2.** In silico drug-likeness and early ADME profiling for lignin-derived oligomers (mol10–mol14) and reference inhibitors (Rapamycin, Everolimus) computed with SwissADME. Reported are compliance/violations for Lipinski, Veber, Ghose, Egan, and Muegge filters; PAINS and Brenk structural alerts; molecular weight (MW), topological polar surface area (TPSA), and consensus log Po/w. Input structures derive from the SMILES in Table 1.

| | Mol10 | Mol11 | Mol12 | Mol13 | Mol14 | Rapamycin | Everolimus |
|---|---|---|---|---|---|---|---|
| Lipinski | No; 3 violations: MW>500, NorO>10, NHorOH>5 | No; 3 violations: MW>500, NorO>10, NHorOH>5 | No; 3 violations: MW>500, NorO>10, NHorOH>5 | No; 3 violations: MW>500, NorO>10, NHorOH>5 | No; 3 violations: MW>500, NorO>10, NHorOH>5 | No; 2 violations: MW>500, NorO>10 | No; 2 violations: MW>500, NorO>10 |
| Ghose | No; 3 violations: MW>480, MR>130, #atoms>70 | No; 3 violations: MW>480, MR>130, #atoms>70 | No; 4 violations: MW>480, WLOGP<-0.4, MR>130, #atoms>70 | No; 3 violations: MW>480, MR>130, #atoms>70 | No; 3 violations: MW>480, MR>130, #atoms>70 | No; 4 violations: MW>480, WLOGP>5.6, MR>130, #atoms>70 | No; 4 violations: MW>480, WLOGP>5.6, MR>130, #atoms>70 |
| Veber | No; 2 violations: Rotors>10, TPSA>140 | No; 2 violations: Rotors>10, TPSA>140 | No; 2 violations: Rotors>10, TPSA>140 | No; 2 violations: Rotors>10, TPSA>140 | No; 2 violations: Rotors>10, TPSA>140 | No; 1 violation: TPSA>140 | No; 1 violation: TPSA>140 |
| Egan | No; 1 violation: TPSA>131.6 | No; 1 violation: TPSA>131.6 | No; 1 violation: TPSA>131.6 | No; 1 violation: TPSA>131.6 | No; 1 violation: TPSA>131.6 | No; 1 violation: TPSA>131.6 | No; 1 violation: TPSA>131.6 |
| Muegge | No; 5 violations: MW>600, TPSA>150, Rotors>15, H-acc>10, H-don>5 | No; 5 violations: MW>600, TPSA>150, Rotors>15, H-acc>10, H-don>5 | No; 4 violations: MW>600, TPSA>150, H-acc>10, H-don>5 | No; 4 violations: MW>600, TPSA>150, H-acc>10, H-don>5 | No; 5 violations: MW>600, TPSA>150, Rotors>15, H-acc>10, H-don>5 | No; 4 violations: MW>600, XLOGP3>5, TPSA>150, H-acc>10 | No; 4 violations: MW>600, XLOGP3>5, TPSA>150, H-acc>10 |
| PAINS | 0 alert | 0 alert | 3 alerts: imine_one_A, quinone_A, quinone_D | 2 alerts: catechol_A, quinone_A | 1 alert: quinone_A | 0 alert | 0 alert |
| Brenk | 0 alert | 1 alert: hydroquinone | 3 alerts: chinone_1, chinone_2, diketo_group | 2 alerts: catechol, chinone_1 | 1 alert: chinone_1 | 2 alerts: diketo_group, isolated_alkene | 2 alerts: diketo_group, isolated_alkene |
| Molecular Weight | 692.75 g/mol | 724.75 g/mol | 690.65 g/mol | 692.66 g/mol | 722.73 g/mol | 914.17 g/mol | 958.22 g/mol |
| TPSA | 198.76 Å² | 239.22 Å² | 242.26 Å² | 248.58 Å² | 226.58 Å² | 195.43 Å² | 204.66 Å² |
| Consensus Log $P_{o/w}$ | 2.84 | 2.20 | -0.40 | 0.45 | 0.41 | 4.19 | 4.62 |