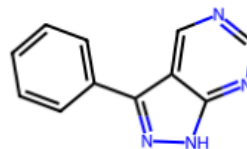
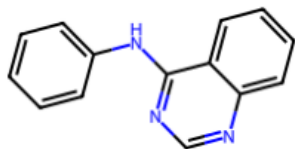


Figure 4 — Six largest Murcko scaffold series (RDKit, fixed bond length)

S1 — 504 molecules share this scaffold (11% of cohort) | mean pIC50 7.29 | 79% active (2% of cohort) | mean pIC50 4.19 | 2% active



S4 — 51 molecules share this scaffold (1% of cohort) | mean pIC50 8.51 | 98% active (1% of cohort) | mean pIC50 8.12 | 96% active

