

Table 9. Experimental and HQSAR predicted pIC₅₀ values for UPPS inhibition

| Cpd ID* | UPPS pIC ₅₀ , M | Predicted pIC ₅₀ , M | Cross- validated predicted [†] pIC ₅₀ , M |
|---------------------|-------------------------------|------------------------------------|--|
| BPH-629 | 6.23 | 5.83 | 5.73 |
| BPH-608 | 6.16 | 5.88 | 5.82 |
| BPH-628 | 6.04 | 5.85 | 5.79 |
| BPH-625 | 5.99 | 5.86 | 5.82 |
| BPH-675 | 5.95 | 6.15 | 6.17 |
| BPH-676 | 5.89 | 5.4 | 5.15 |
| BPH-640 | 5.75 | 5.87 | 5.87 |
| BPH-626 | 5.7 | 5.83 | 5.84 |
| BPH-621 | 5.51 | 5.32 | 5.23 |
| BPH-622 | 5.26 | 5.29 | 5.29 |
| BPH-294 | 5.17 | 4.91 | 4.85 |
| BPH-228 | 5.11 | 4.96 | 4.65 |
| BPH-364 | 5.0 | 5.05 | 5.04 |
| BPH-618 | 4.99 | 5.26 | 5.35 |
| BPH-646 | 4.92 | 5.24 | 5.51 |
| BPH-642 | 4.87 | 4.69 | 4.62 |
| BPH-633 | 4.67 | 4.68 | 4.66 |
| BPH-632 | 4.56 | 4.65 | 4.65 |
| BPH-641 | 4.47 | 4.68 | 4.76 |
| BPH-620 | 4.45 | 4.62 | 4.64 |
| BPH-300 | 4.32 | 4.06 | 4.0 |
| BPH-614 | 4.17 | 4.67 | 4.75 |
| BPH-674 | 4.16 | 3.91 | 3.88 |
| BPH-663 | 4.06 | 3.92 | 4.08 |
| BPH-601 | 4.05 | 3.26 | 2.99 |
| BPH-619 | 3.91 | 4.7 | 4.89 |
| BPH-11 | 3.7 | 3.92 | 4.03 |
| BPH-461 | 3.31 | 3.39 | 3.47 |
| Risedronate (BPH-2) | 3.18 | 3.71 | 4.01 |

*Structures are shown in SI Fig. 9.

[†]Cross-validated predictions obtained using a leave-one-out validation scheme as implemented in the HQSAR module of Sybyl 7.3 (Tripos Inc., St. Louis, MO).