**Supplemental Data**

**Dispensing Processes Impact Apparent Biological Activity as Determined by Computational and Statistical Analyses**

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**Table S3**. Test set data for searching with ‘tip-based dispensing’ pharmacophore– data ranked by predicted value. Note W081 and W082.3 were not retrieved by the pharmacophore indicating they do not fit to the Tip-based pharmacophore. These correspond to IC50 values of 38.3 M and 1.78 M, respectively. ND = no experimental data.

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| **Name** | **Tip-based IC50 Prediction (µM)** | **Tip-based IC50 Actual (µM)** | **Acoustic IC50 Actual (µM)** |
| W084.1 | 0.348797 | 0.297 | ND |
| W084.2 | 0.380588 | 0.456 | ND |
| W084.4 | 0.699411 | 0.374 | ND |
| W082.2 | 0.839169 | 0.808 | ND |
| W085.2 | 1.32573 | ND | 0.00325 |
| W082.4 | 1.49893 | 6.27 | ND |
| W083 | 2.82285 | 0.198 | ND |
| W084.3 | 2.91191 | 0.473 | ND |
| W082.1 | 3.38289 | 1.12 | ND |
| W085.1 | 3.54739 | ND | 0.00231 |