**Supplemental Data**

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

*Sean Ekins\*1, Joe Olechno2 and Antony J. Williams3*

1 Collaborations in Chemistry, 5616 Hilltop Needmore Road, Fuquay-Varina, NC 27526, U.S.A.

2 Labcyte Inc., 1190 Borregas Avenue, Sunnyvale, CA 94089, U.S.A.

3 Royal Society of Chemistry, 904 Tamaras Circle, Wake Forest, NC 27587, U.S.A.

**Table S2.** Test set data for searching with ‘acoustic dispensing’ pharmacophore – data ranked by predicted value. ND = no experimental data.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | | **Name** | **Acoustic IC50 Prediction (µM)** | | **Tip-based IC50 Actual(µM)** | **Acoustic IC50 Actual (µM)** | | | W085.1 | 0.0196 | ND | | 0.00231 | | W084.1 | 0.025542 | 0.297 | | ND | | W085.2 | 0.026467 | ND | | 0.00325 | | W082.2 | 0.033615 | 0.808 | | ND | | W084.4 | 0.060011 | 0.374 | | ND | | W084.2 | 0.0761 | 0.456 | | ND | | W084.3 | 3.38573 | 0.473 | | ND | | W083 | 3.84933 | 0.198 | | ND | | W081 | 5.47847 | 38.3 | | ND | | W082.3 | 7.49263 | 1.78 | | ND | | W082.1 | 7.82218 | 1.12 | | ND | | W082.4 | 12,622.20 | 6.27 | | ND | | | | |  |  |  |
|  | | | |  |  |  |
|  |  |  |
|  |  |  |