**Supporting Information**

**Table S1.** Criteria used to calculate prediction quality of models based on error based metrics.

|  |  |
| --- | --- |
| **Model Prediction Quality** | **Criteria** |
| Good | MAE(95%) ≤ 0.265a and (MAE(95%) + 3 × SD(95%)) ≤ 0.531c |
| Bad | MAE(95%) ≤ 0.398b or (MAE(95%) + 3 × SD(95%)) ≤ 0.664d |
| Moderate | Does not fall in either of criteria |

a0.1×2.659 (Training set range), b0.15×2.659, c0.2×2.659, d0.25×2.659

MAE = Mean absolute error, SD = Standard deviation

**Table S2.** Descriptors used in the development of final models.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Sr. No** | **ShapeRMS-2.66** | **CHI-3\_C-1.67** | **S\_dsCH-1.79** | **LogP** | **COSV** | **S\_dO-34.7** | **CHI-V-3\_C** | **Wiener** |
| 1 | 0.00 | 0.00 | 0.14 | 3.76 | 132.00 | 0.00 | 0.66 | 848 |
| 2 | 0.00 | 0.00 | 0.04 | 3.59 | 133.00 | 0.00 | 0.74 | 965 |
| 3 | 0.00 | 0.00 | 0.17 | 4.41 | 141.00 | 0.00 | 0.76 | 950 |
| 4 | 0.00 | 0.00 | 0.20 | 6.13 | 184.00 | 0.00 | 0.85 | 1900 |
| 5 | 0.00 | 0.18 | 0.19 | 6.20 | 207.00 | 0.00 | 0.91 | 2380 |
| 6 | 0.00 | 0.00 | 0.19 | 4.76 | 175.00 | 0.00 | 0.85 | 1900 |
| 7 | 0.00 | 0.00 | 0.02 | 1.66 | 141.00 | 0.00 | 0.74 | 1520 |
| 8 | 0.00 | 0.00 | 0.19 | 5.60 | 146.00 | 0.00 | 0.78 | 1670 |
| 9 | 0.00 | 0.00 | 0.10 | 2.41 | 155.00 | 0.00 | 0.65 | 848 |
| 10 | 0.00 | 0.00 | 0.16 | 4.78 | 169.00 | 0.00 | 0.83 | 1900 |
| 11 | 0.00 | 0.18 | 0.15 | 4.85 | 183.00 | 0.00 | 0.90 | 2380 |
| 12 | 0.00 | 0.00 | 3.96 | 4.22 | 113.00 | 0.00 | 0.36 | 772 |
| 13 | 0.00 | 0.00 | 3.90 | 4.32 | 112.00 | 0.00 | 0.43 | 1060 |
| 14 | 0.00 | 0.00 | 3.99 | 4.44 | 122.00 | 0.00 | 0.66 | 1210 |
| 15 | 0.00 | 0.00 | 3.77 | 4.27 | 123.00 | 0.00 | 0.74 | 1360 |
| 16 | 0.00 | 0.00 | 4.09 | 6.61 | 140.00 | 0.00 | 0.55 | 1770 |
| 17 | 0.00 | 0.00 | 4.03 | 6.69 | 136.00 | 0.00 | 0.62 | 2250 |
| 18 | 0.00 | 0.00 | 4.06 | 5.09 | 129.00 | 0.00 | 0.76 | 1340 |
| 19 | 0.00 | 0.00 | 4.12 | 6.81 | 140.00 | 0.00 | 0.85 | 2500 |
| 20 | 0.16 | 0.18 | 4.09 | 6.88 | 165.00 | 0.00 | 0.91 | 3050 |
| 21 | 0.00 | 0.48 | 3.92 | 6.53 | 133.00 | 0.30 | 0.96 | 3350 |
| 22 | 0.08 | 0.00 | 4.09 | 5.44 | 118.00 | 0.00 | 0.85 | 2500 |
| 23 | 0.00 | 0.00 | 3.70 | 2.34 | 119.00 | 0.00 | 0.74 | 2040 |
| 24 | 0.00 | 0.00 | 4.08 | 5.70 | 136.00 | 0.00 | 0.94 | 2760 |
| 25 | 0.00 | 0.00 | 4.09 | 6.28 | 122.00 | 0.00 | 0.78 | 2220 |
| 26 | 0.00 | 0.00 | 3.86 | 3.14 | 142.59 | 0.00 | 0.46 | 905 |
| 27 | 0.00 | 0.00 | 3.90 | 3.09 | 106.00 | 0.00 | 0.65 | 1210 |
| 28 | 0.00 | 0.00 | 4.03 | 5.46 | 170.00 | 0.00 | 0.83 | 2500 |
| 29 | 0.00 | 0.18 | 4.01 | 5.53 | 191.00 | 0.00 | 0.90 | 3050 |
| 30 | 0.00 | 0.00 | 0.00 | 3.29 | 143.00 | 0.00 | 0.48 | 848 |
| 31 | 0.00 | 0.00 | 0.00 | 3.29 | 128.00 | 0.00 | 0.48 | 848 |
| 32 | 0.00 | 0.00 | 0.00 | 5.66 | 145.00 | 0.00 | 0.66 | 1900 |
| 33 | 0.00 | 0.00 | 0.00 | 5.66 | 128.00 | 0.00 | 0.66 | 1900 |
| 34 | 0.00 | 0.00 | 3.51 | 3.97 | 124.00 | 0.00 | 0.48 | 1210 |
| 35 | 0.00 | 0.00 | 3.51 | 3.97 | 102.00 | 0.00 | 0.48 | 1210 |
| 36 | 0.00 | 0.00 | 3.64 | 6.34 | 154.00 | 0.00 | 0.66 | 2500 |
| 37 | 0.23 | 0.00 | 3.64 | 6.34 | 130.00 | 0.00 | 0.66 | 2500 |
| 38 | 0.00 | 0.18 | 3.61 | 6.41 | 231.00 | 0.00 | 0.73 | 3050 |
| 39 | 0.25 | 0.18 | 3.61 | 6.41 | 173.00 | 0.00 | 0.73 | 3050 |
| 40 | 0.00 | 0.18 | 3.60 | 6.41 | 196.00 | 0.10 | 0.73 | 3010 |
| 41 | 0.00 | 0.18 | 3.60 | 6.41 | 140.00 | 0.10 | 0.73 | 3010 |
| 42 | 0.00 | 0.31 | 3.58 | 6.56 | 167.00 | 0.20 | 0.78 | 3580 |
| 43 | 0.23 | 0.31 | 3.58 | 6.56 | 161.00 | 0.20 | 0.78 | 3580 |
| 44 | 0.00 | 0.18 | 3.54 | 6.31 | 351.00 | 0.10 | 0.73 | 3730 |
| 45 | 0.19 | 0.18 | 3.54 | 6.31 | 180.00 | 0.10 | 0.73 | 3730 |
| 46 | 0.00 | 0.00 | 2.08 | 1.48 | 108.11 | 0.00 | 0.68 | 1135 |
| 47 | 0.00 | 0.00 | 0.00 | 0.00 | 112.71 | 0.00 | 0.61 | 500 |
| 48 | 0.00 | 0.00 | 0.00 | -0.09 | 119.32 | 0.00 | 0.68 | 968 |