**Supporting Information for article:**

**Ensemble-based modeling of chemical compounds with antimalarial activity**

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# List of Supplementary files

1. Train.sdf: Training dataset
2. Test.sdf: Test dataset
3. External.sdf: External validation set
4. VSVS.zip: Virtual screening validation dataset
5. Fragments.hdr: 250 most relevant ISIDA fragments employed in the modeling process

# Table TS1. Best ensemble model parameters

|  |  |  |  |
| --- | --- | --- | --- |
| Model | Fragments(\*) | γ | σ2 |
| 1 | 239,244,12,47,33,243,118,187,22,25,149,214,38,139 | 17.57 | 0.00040 |
| 2 | 205,240,196,239,173,33,118,4,152,228,153,242,143,148,120,129,48,220,219,187,85 | 6352.41 | 0.19615 |
| 3 | 163,102,30,61,140,36,201,54,166,205,111,78,95,76,5,14,113,236,44,182,170,129,250,106 | 2.30 | 0.00875 |
| 4 | 111,33,148,47,93,172,22,183,206,107,127,87,218,201,165,210 | 1403.58 | 0.00078 |
| 5 | 24,224,89,64,40,25,67,220,60,83,138,7,119,66,149,164,91,127,179,169,57,244,61,8 | 1098471.28 | 0.00185 |
| 6 | 84,187,198,250,23,116,80,41,225,230,104,111,93,89,33,48,221,5,88,27,118,173,212,72 | 3.42 | 0.00298 |
| 7 | 143,56,138,6,111,226,222,245,165,155,23,20,66,109 | 0.57 | 0.00071 |
| 8 | 32,218,102,13,202,54,55,241,244,194,27,173 | 1.70 | 0.00007 |
| 9 | 46,111,140,95,226,191,98,142,242,85,79,124 | 0.27 | 0.00034 |
| 10 | 220,123,40,26,36,193,166,233,175,62,78,170,137,42,4,217,216,83,242,33,66,24,231,248 | 0.36 | 0.00251 |
| 11 | 97,144,30,82,95,206,250,63,237,18,160,33,241,225,165,107,179,197,109,166,145,174 | 56.13 | 0.00137 |
| 12 | 106,36,234,48,163,41,196,231,141,89,100,38,235,199,149,71,24,101 | 0.43 | 0.00056 |
| 13 | 135,230,228,65,159,137,198,108,84,201,64,76,175,26,156,216 | 1.13 | 0.00332 |
| 14 | 95,139,20,155,4,66,37,105,236,28,78,11,166,112,101,72,248,245,209,223,97,16,147 | 1.28 | 0.00291 |
| 15 | 159,93,233,21,186,68,112,198,69,114,219,97,250,117,62,145,34 | 1.57 | 0.00301 |

(\*) Fragments numbering corresponds to the same numbering provided in the Fragments.hdr file containing ISIDA fragments definitions.