Table 1: Docking results of 1-(substituted phenyl)-3-(naphthalene-1,2-d-thiazol-2-yl)urea/thiourea derivatives with AA/2AR. Data of % reduction in catalepsy were taken from reference [10]. Compound number is same as given in the literature. a) Binding free energy (kcal/mol); b) Inhibition constant estimated by docking (in nM); c) Root mean square deviation (in Å); d) Amino acid; e) Bond distance (in Å); f) No H-bond or pi-interaction.

| Comp. | R | X | % Reduction in catalepsy | ΔG\text{b} | K\text{i} | RMSD | Hydrogen bonds | π-Interactions |
|-------|---|---|---------------------------|-----------|----------|------|----------------|---------------|
| 3     | H | O | 44.44                     | -8.27     | 863.78   | 4.29 | f              | -             |
| 4     | 4-OCH\text{3} | O | 58.51                     | -8.81     | 346.16   | 3.99 | Glu-169        | 2.16          |
|       |    |   |                           |           |          |      | Tyr-271        | 1.95          |
| 5     | 2-OCH\text{3} | O | 76.9                      | -9.00     | 250.84   | 4.21 | Phe-168        | 1.97          |
|       |    |   |                           |           |          |      | Tyr-271        | 1.94          |
| 6     | 2,4-OCH\text{3} | O | 75                         | -9.25     | 164.57   | 4.03 | Phe-168        | 2.15          |
|       |    |   |                           |           |          |      | Glu-169        | 2.38          |
|       |    |   |                           |           |          |      | Tyr-271        | 1.96          |
| 7     | 3,4,5-OCH\text{3} | O | 70.29                     | -9.07     | 224.23   | 3.93 | His-278        | 1.87          |
| 8     | 4-Phenoxy | O | 55.56                     | -9.53     | 102.63   | 2.52 | f              | -             |
| 9     | 2-F | O | 29.12                     | -8.16     | 1040     | 4.85 | Phe-168        | 2.02          |
|       |    |   |                           |           |          |      | Tyr-271        | 2.08          |
| 10    | 4-F | O | 30.3                      | -8.14     | 1080     | 4.83 | Phe-168        | 2.07          |
|       |    |   |                           |           |          |      | Tyr-271        | 2.05          |
| 11    | 2-Br | O | 38.74                     | -8.72     | 405.86   | 4.15 | Phe-168        | 4.55          |
|       |    |   |                           |           |          |      | Tyr-271        | 4.52          |
| 12    | 4-Br | O | 37.76                     | -8.55     | 542.28   | 4.36 | Phe-168        | 4.61          |
|       |    |   |                           |           |          |      | Tyr-271        | 4.59          |
| 13    | 2-Cl | O | 37.37                     | -8.54     | 546.60   | 4.09 | Phe-168        | 4.54          |
|       |    |   |                           |           |          |      | Phe-168        | 5.28          |
| 14    | 4-Cl | O | 38.61                     | -8.38     | 721.26   | 4.34 | Phe-168        | 4.60          |
|       |    |   |                           |           |          |      | Phe-168        | 5.19          |
| 15    | 2-Cl, 5-CF\text{3} | O | 51.37                     | -8.94     | 281.80   | 4.1  | Phe-168        | 4.55          |
|       |    |   |                           |           |          |      | Tyr-271        | 4.52          |
| 16    | 2-NO\text{2} | O | 72.05                     | -9.87     | 58.72    | 4.69 | Phe-168        | 4.61          |
|       |    |   |                           |           |          |      | Phe-168        | 5.19          |
| 17    | 4-NO\text{2} | O | 31.28                     | -8.61     | 484.40   | 3.93 | Val-84         | 2.04          |
| 18    | 2-CH\text{2} | O | 47.64                     | -8.46     | 626.58   | 4.01 | Phe-168        | 1.74          |
|       |    |   |                           |           |          |      | Phe-168        | 4.13          |
|       |    |   |                           |           |          |      | Phe-168        | 4.57          |
| 19    | 4-CH\text{3} | O | 48.56                     | -8.65     | 455.03   | 4.03 | Phe-168        | 6.03          |
|       |    |   |                           |           |          |      | Phe-168        | 4.38          |
| 20    | H | S | 44.63                     | -8.45     | 636.96   | 3.95 | Ala-81         | 2.17          |
|       |    |   |                           |           |          |      | Glu-169        | 2.09          |
|       |    |   |                           |           |          |      | Tyr-271        | 1.88          |
| 21    | 4-OCH\text{3} | S | 58.05                     | -9.26     | 162.54   | 5.02 | Glu-169        | 1.95          |
|       |    |   |                           |           |          |      | Asn-253        | 2.39          |
|       |    |   |                           |           |          |      | Glu-169        | 1.98          |
|       |    |   |                           |           |          |      | Asn-253        | 3.19          |
| 22    | 2-OCH\text{3} | S | 75.46                     | -9.06     | 229.22   | 2.72 | Glu-169        | 1.95          |
|       |    |   |                           |           |          |      | Asn-253        | 2.39          |
|       |    |   |                           |           |          |      | Glu-169        | 1.98          |
|       |    |   |                           |           |          |      | Glu-169        | 3.19          |
| 23    | 2-F | S | 38.35                     | -8.18     | 1010     | 1.39 | f              | -             |
| 24    | 4-F | S | 34.95                     | -8.11     | 1130     | 4.24 | f              | -             |
| 25    | 2-Br | S | 30.96                     | -8.53     | 562.85   | 4.05 | f              | -             |
| 26    | 4-Br | S | 35.27                     | -8.75     | 388.83   | 4.22 | f              | -             |
| 27    | 2-Cl | S | 39.14                     | -8.55     | 544.16   | 3.1  | f              | -             |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 28 | 4-Cl | S | 27.88 | 3.88 | Phe-168 | 3.88 |
| 29 | 2-NO₂ | S | 72.97 | -9.61 | 90.07 | 2.63 | Phe-168 | 2.15 |
| 30 | 4-NO₂ | S | 32.13 | -8.72 | 405.62 | 4.45 | His-278 | 2.05 |
| 31 | 2-CH₃ | S | 49.87 | -8.66 | 448.49 | 4.77 | Phe-168 | 4.12 |
| 32 | 4-CH₃ | S | 47.97 | -8.56 | 529.05 | 4.30 | Phe-168 | 4.18 |