Synthesis, Docking and Biological Evaluation of a Novel Class of Imidazothiazoles as IDO1 Inhibitors

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Table S1. Structure and biological profile of compounds evaluated by molecular docking. Structures of docking poses are depicted as gold sticks, while heme is depicted as cyan sticks. Aminoacids of pocket A, B and C are depicted as red, green and blue shape, respectively.

| Cpd | FRED Chemgauss4 score | Docking pose |
|-----|------------------------|--------------|
| 11a | -15.45                 | ![Docking pose](image) |
| 11b | -13.56                 | ![Docking pose](image) |
| 11c | -13.99                 | ![Docking pose](image) |
| 11d | -13.97                 | ![Docking pose](image) |
| 11e | -14.89                 | ![Docking pose](image) |
| Cpd | FRED Chemgauss4 score | Docking pose |
|-----|-----------------------|--------------|
| 11f | -14.36                | ![Docking pose](image1) |
| 11g | -14.86                | ![Docking pose](image2) |
| 11h | -14.40                | ![Docking pose](image3) |
| 11i | -14.67                | ![Docking pose](image4) |
| 11j | -14.18                | ![Docking pose](image5) |
| Cpd | FRED Chemgauss4 score | Docking pose |
|-----|-----------------------|--------------|
| 11k | -14.35                |              |
| 12a | -11.98                |              |
| 12b | -11.70                |              |
| 12c | -12.38                |              |
| 12d | -12.39                |              |
| Cpd | FRED Chemgauss4 score | Docking pose |
|-----|-----------------------|--------------|
| 12e | -12.74                | ![Docking pose](image1) |
| 12f | -14.46                | ![Docking pose](image2) |
| 12g | -14.87                | ![Docking pose](image3) |
| 12h | -15.99                | ![Docking pose](image4) |
| 12i | -15.16                | ![Docking pose](image5) |
| Cpd | FRED Chemgauss4 score | Docking pose |
|-----|----------------------|--------------|
| 12j | -15.31               | ![Docking pose](image) |
| 12k | -15.37               | ![Docking pose](image) |