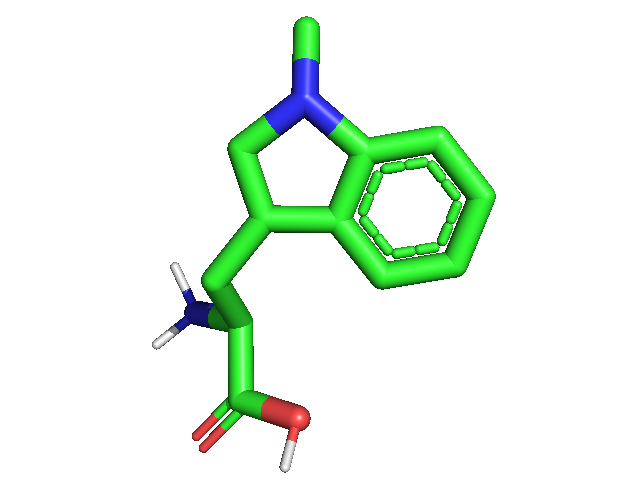
**SUPPORTING INFORMATION**

**Molecular docking of Acetylacetone-Based Oxindole against indoleamine 2,3-dioxygenase: Study of Energy Minimization**

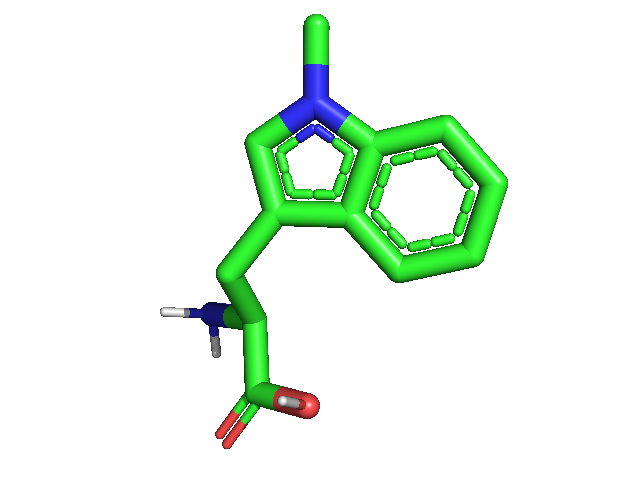


Figure 1. The structure of ligand **1** and **L-1MT**



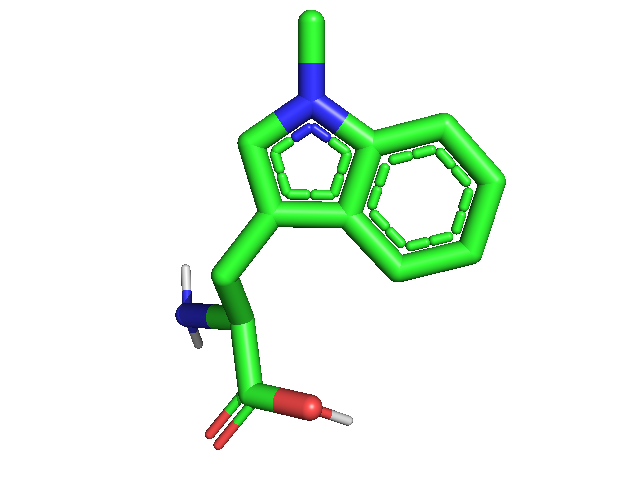
**L-1MTa**

**E = 73.90 Kkal/mol**



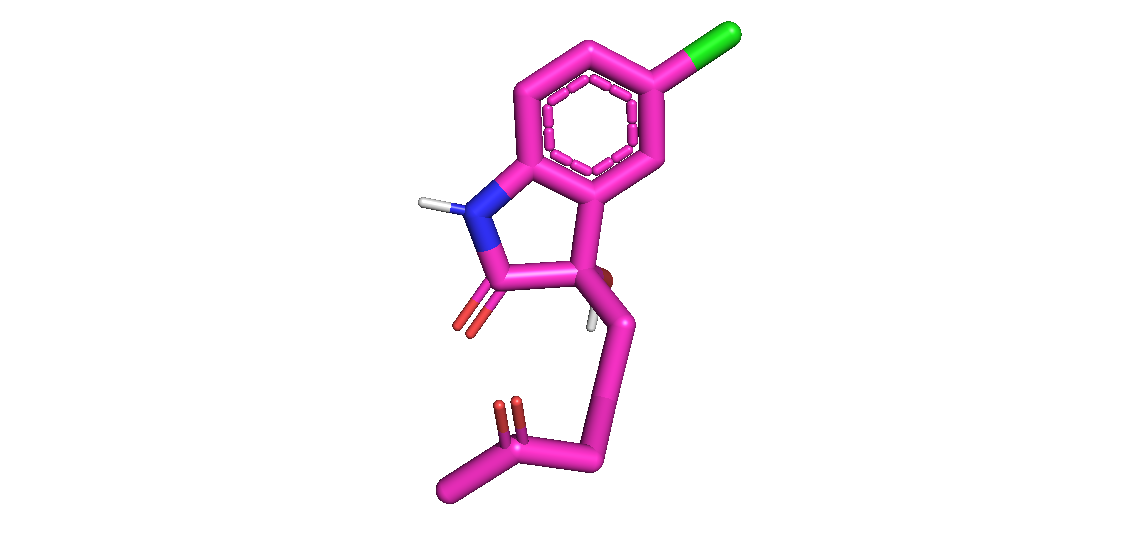
**L-1MTb**

**E = 53.88 Kkal/mol**

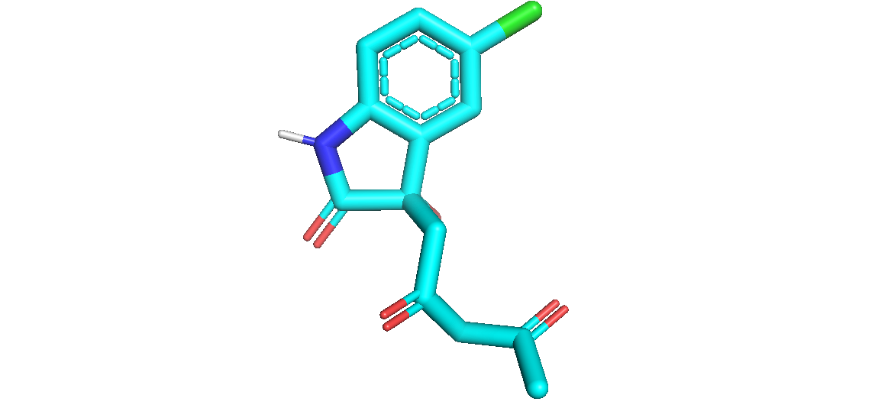


**E = 54.94 Kkal/mol**

**1a**

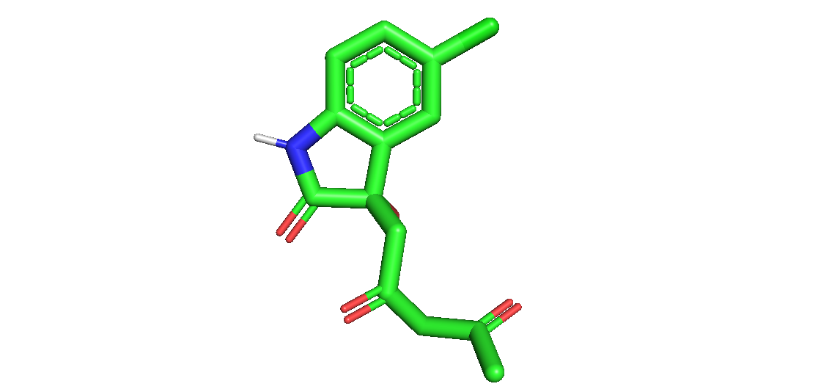


**E = 16.64 Kkal/mol**



**1b**

**E = 21.86 Kkal/mol**

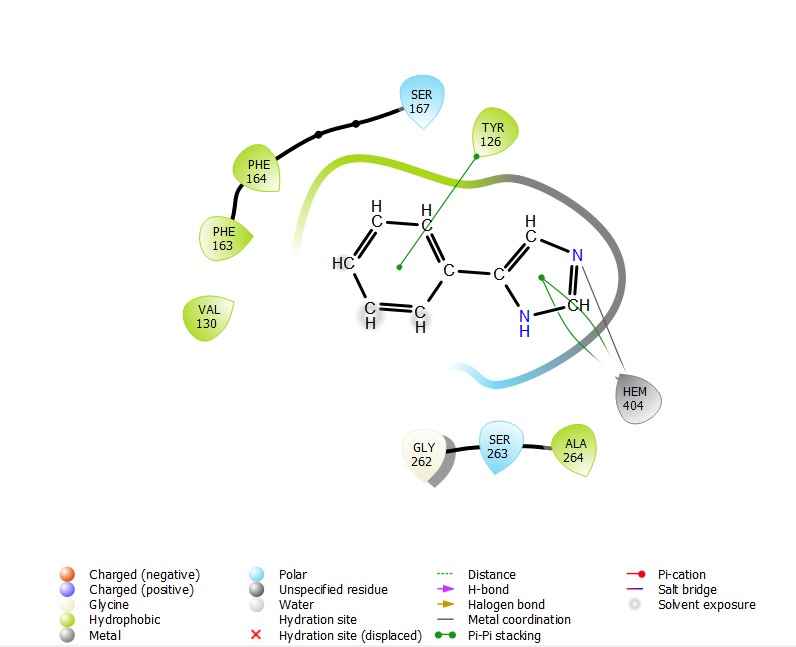


**1c**

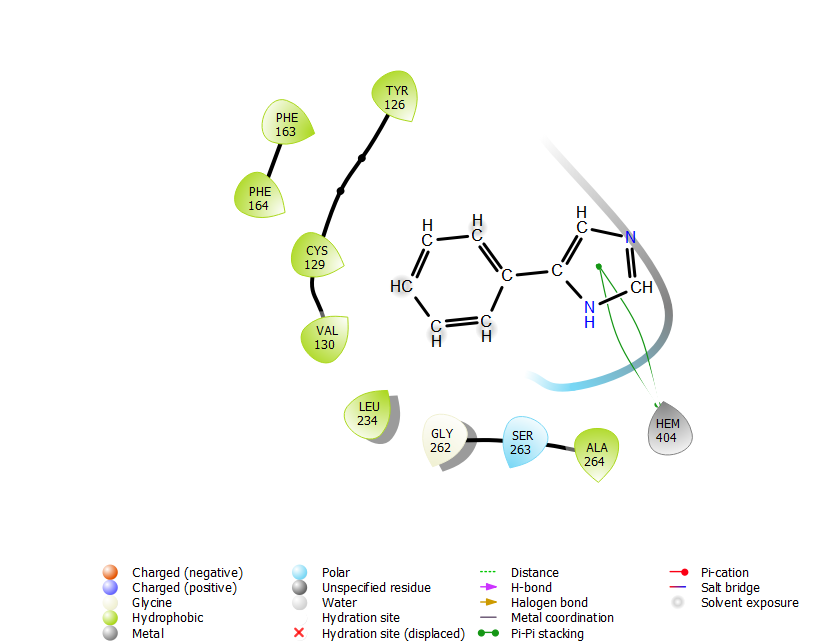
**E = 23.52 Kkal/mol**

**L-1MTc**

Figure 2. The structure conformation of ligand 1 and L-1MT resulting from minimization using (a) *MarvinSketch,* (b) *Open Babel*, and (c) without minimization



**(A)**

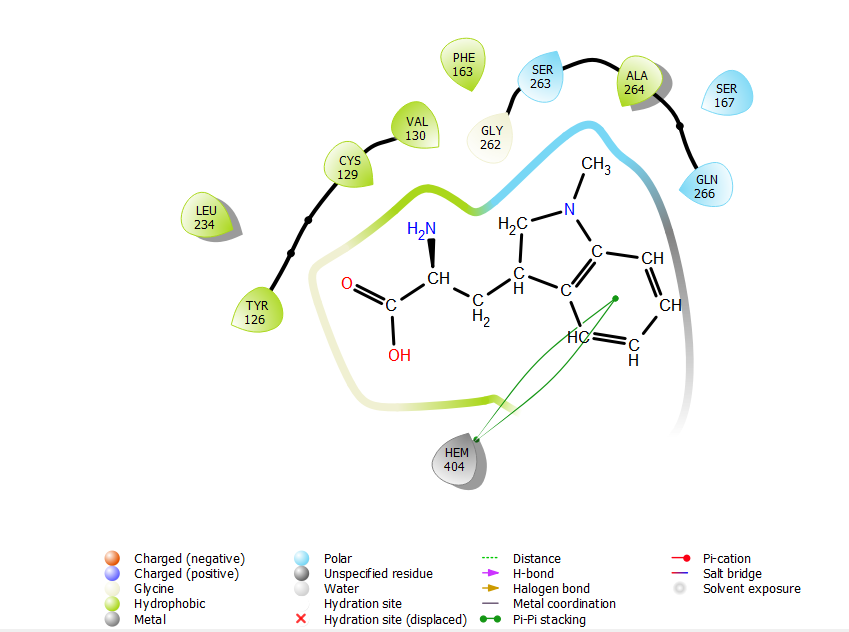


**(B)**

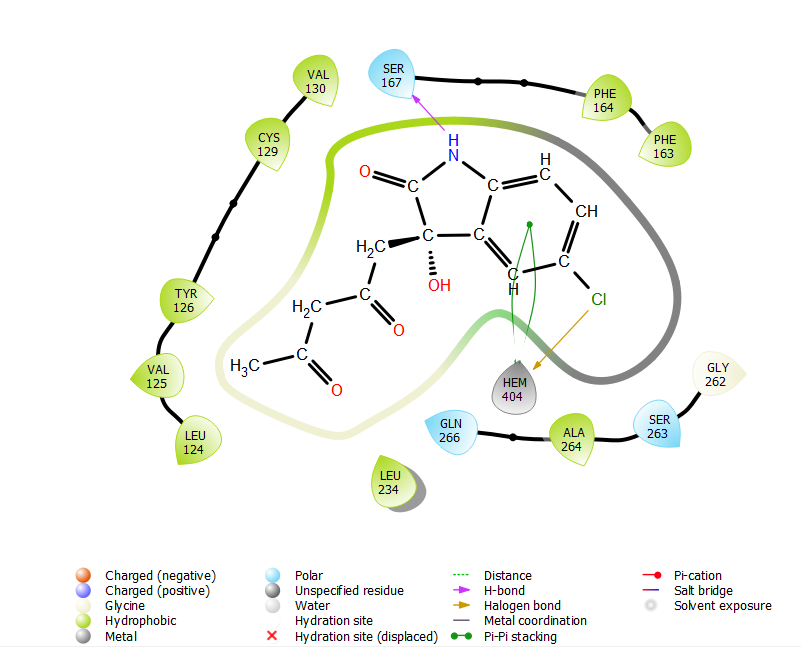
Figure 3. Representation of co-crystallized (**A**) and redocked PIM (**B**) to 2D0T

Table 1. Binding energy of ligand **1** and **L-1MT**

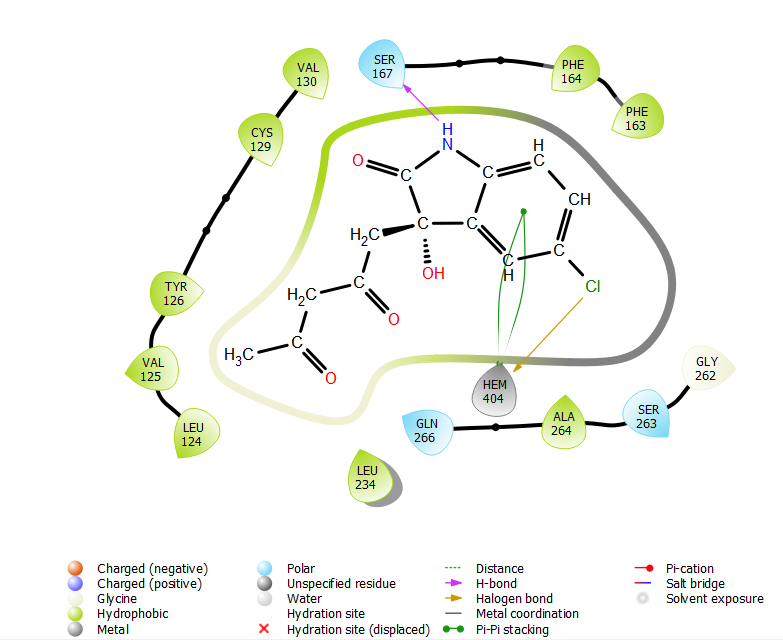
|  |  |
| --- | --- |
| **Ligand** | **(Pose) Binding Affinity (Kcal/mol)** |
| **1a** | (1) -0.4; (2) 2.4; (3) 2.4 |
| **1b** | (1) 0.2; (2) 2.4 |
| **1c** | (1) 0.3; (2) 2.3; (3) 2.7; (4) 2.9 |
| **L-1MTa** | (1) -2.8; (2) -2.1; (3) -1.3; (4) -0.9; (5) -0.7; (6) -0.1 |
| **L-1MTb** | (1) -1.0; (2) -0.9; (3) -0.7; (4) -0.6; (5) -0.2; (6) -0.2; (7) 0.6 |
| **L-1MTc** | (1) -1.1; (2) -1.1; (3) -0.8; (4) -0.8; (5) -0.2; (6) 1.2; (7) 1.5; (8) 1.8 |



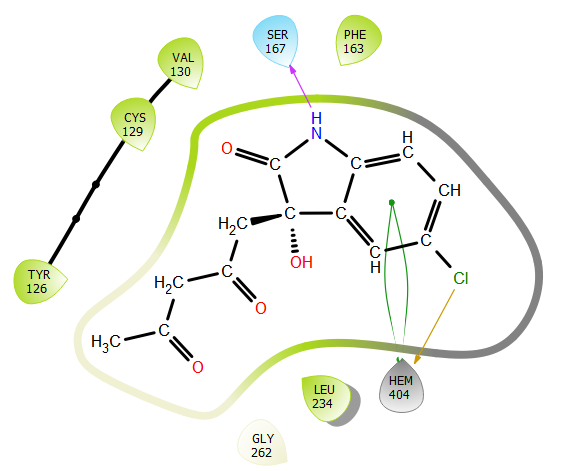
**L-1MTa**



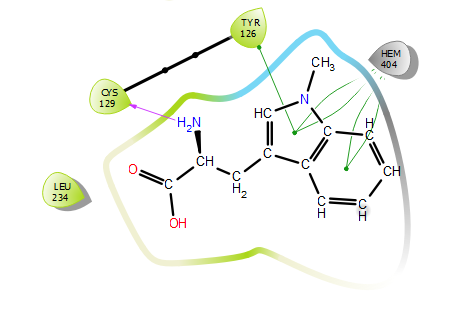
**1a**



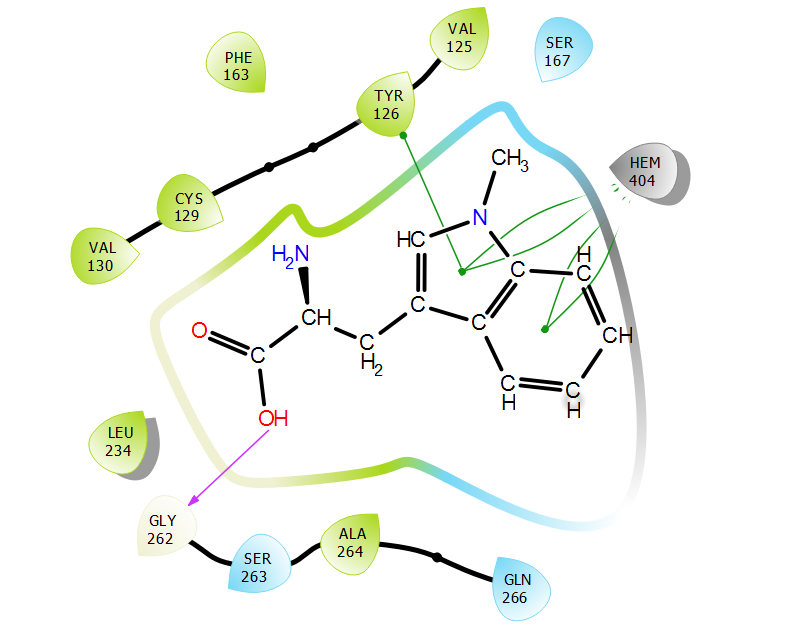
**1b**



**1c**



**L-1MTb**



**L-1MTc**

Figure 4. Interactions of ligand **1** and **L-1MT** with 2D0T