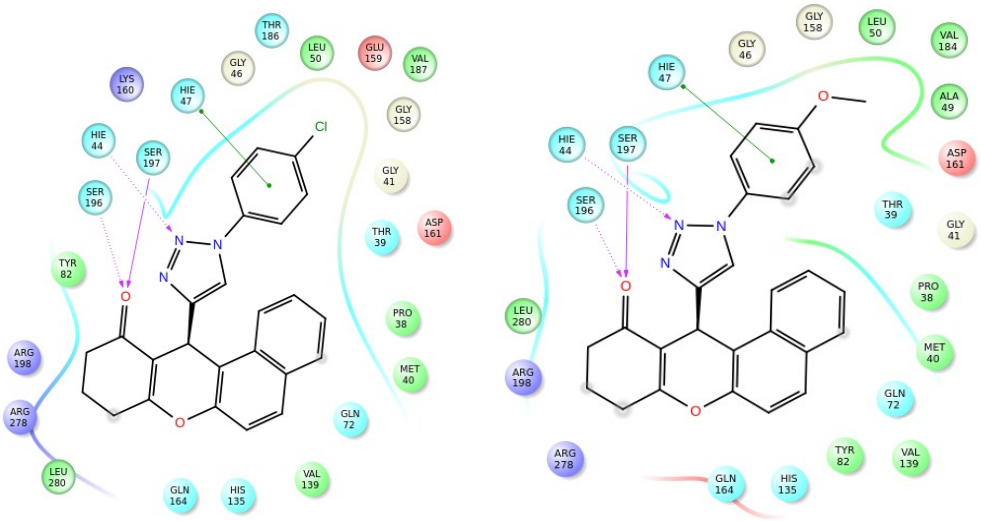

Figure 1: Ligand interaction diagram of *S*-configuration 7k and 7m

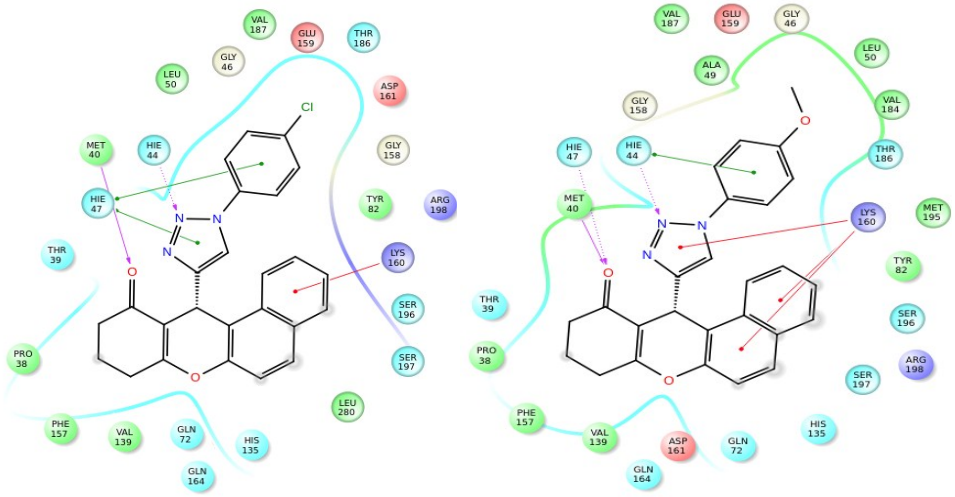

Figure 2: Ligand interaction diagram of *R*-configuration 7k and 7m

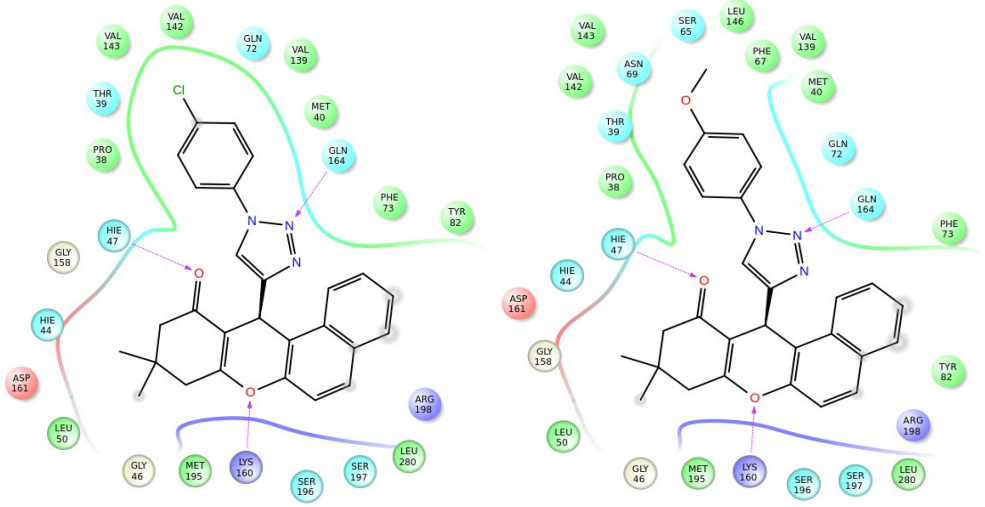

Figure 3: Ligand interaction diagram of *S*-configuration 7c and 7e

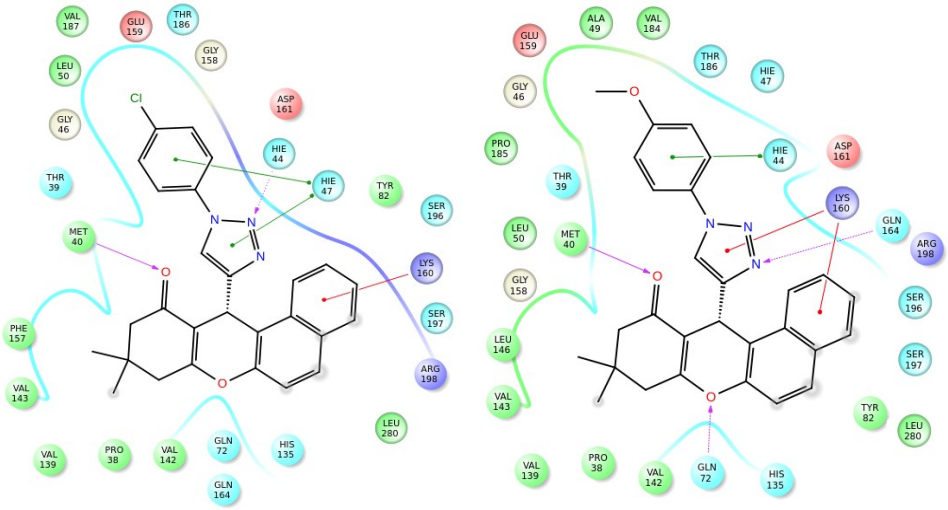

Figure 4: Ligand interaction diagram of *R*-configuration 7c and 7e

**Table 1:** Dock score, Emodel, bond length and bond angles of ***R*** and ***S*-**compounds of **7c, 7e, 7k** and **7m.**

| Compound | Dock score | Emodel | Bond length | Bond angle |
|---|---|---|---|---|
| *R*-7c | -6.63 | -64.66 | 2.24 Aº (MET 40)<br>2.72 Aº (HIE 44) | 105.0º |
| *R*-7e | -6.77 | -60.12 | 2.41 Aº (MET 40)<br>2.40 Aº (GLN 72)<br>2.38 Aº (GLN 164) | 106.8º |
| *R*-7k | -6.03 | -59.56 | 2.37 Aº (MET 40)<br>2.71 Aº (HIE 44) | 92.6º |
| *R*-7m | -6.58 | -59.40 | 2.22 Aº (MET 40)<br>2.56 Aº (HIE 44)<br>2.77 Aº (HIE 47) | 97.7º |
| *S*-7c | -5.91 | -54-70 | 1.93 Aº (HIE 47)<br>2.26 Aº (GLN 164)<br>2.30 Aº (LYS 160) | 69.9º |
| *S*-7e | -5.52 | -51.66 | 1.95 Aº (HIE 47)<br>2.27 Aº (GLN 164)<br>2.24 Aº (LYS 160) | 76.2º |
| *S*-7k | -6.77 | -58.79 | 2.05 Aº (SER 196)<br>2.01 Aº & 2.64 Aº (SER 197)<br>2.03 Aº (HIE 44) | 67.2º |
| *S*-7m | -6.98 | -58.25 | 2.14 Aº (SER 196)<br>1.82 Aº & 2.39 Aº (SER 197)<br>2.09 Aº (HIE 44) | 62.5º |