**Table 3. ADME/T and drug-likeness analyses of the highest-ranked drug molecules.**

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **ADME/T Analysis** | | | | | | | | | | | | | | | | |
| **Compound** | **Absorption** | | **Desorption** | | | | **Metabolism (CYP)** | | | | **Excretion** | **Toxicity** | | | | |
| **Water solubility**  **LogS cm/s** | **HIA** | **BBB** | **VDss** | | **CNS** | **Substrate** | | **Inhibitors** | | **TC** | **carcinogenicity** | **AMES** | **Hepatotoxicity** | | **Cytotoxicity** |
| **2D6** | **3A4** | **2D6** | **3A4** |
| **Pazopanib** | -3.011 | 92.477 | -1.161 | 0.268 | | -2.541 | No | Yes | No | Yes | 0.322 | Yes | No | No | | Yes |
| **Ponatinib** | -2.903 | 84.958 | 0.243 | -0.045 | | -2.06 | No | Yes | No | Yes | 0.389 | Yes | Yes | No | | No |
| **Irinotecan** | -3.57 | 99.879 | -1.303 | 1.128 | | -3.232 | No | Yes | No | Yes | 0.939 | No | No | No | | Yes |
| **Drug-likeness properties** | | | | | | | | | | | | | | | | |
| **Compound** | **Molecular Weight** | | **LogPo/w** | | **nHBA** | | **nHBD** | | **nRotB** | | **Lipinski’s rule** | | | | **Decision** | |
| **Follow** | **Violation** | | |
| **Pazopanib** | 437.529 | | 3.13904 | | 8 | | 2 | | 5 | | 5 | 0 | | | Accepted | |
| **Ponatinib** | 532.57 | | 4.45602 | | 6 | | 1 | | 4 | | 4 | 1 | | | Accepted | |
| **Irinotecan** | 586.689 | | 4.0911 | | 9 | | 1 | | 4 | | 4 | 1 | | | Accepted | |
| LogP (<5)—Measure of Lipophilicity index; nRotB (<5)—Number of rotatable bonds; MW (<500Da)—Molecular weight; nHBA (<10)—H-bond acceptor; nHBD (<5)—H-bond donor. | | | | | | | | | | | | | | | | |