DAFTAR GAMBAR JURNAL SGLT-2

|  |
| --- |
| Tabel 1: Roìoìt-Meìan-Squareì Deìviatioìn dari Proìteìin Data Bank Koìdeì 7VSI |
| *Scoring Function**Algorithm* | MolDock *Optimizer* (Å) | MolDock SE (Å) | *Iterated Simplex* (Å) |
| MolDock *Score* | 1.10886 | 1.06717 | 1.20246 |
| MolDock Score (GRID) | 1.24845 | 0.9767 | 1.12646 |
| PLANTS *Score* | 0.446412 | 0.923043 | 0.825914 |
| PLANTS *Score* (GRID) | 0.663754 | 0.762987 | 0.780602 |

|  |
| --- |
| Tabel 2. Reìsidu asam aminoì koìmpleìks-ligan |
| No. | Senyawa | Rerank score | Residu asam amino |
| 1. | Eìmpaglifloìzin | -139.194 | SEìR 287 (3,04 Å), PHEì 98 (2,53 Å), GLN 457 (2,10 Å), TRP 291 (2,25 Å), ASN 75 (2,33 Å) |
| 2. | 4,5-Dicaffeìoìylquinic acid | -147.778 | SEìR 287 (2,52 Å), PHEì 98 (2,74 Å), GLN 457 (2,06 Å), ASN 75 (1,99 Å), GLY 79 (2,17 Å), ASP 158 (1,90 Å) |
| 3. | 1,3-Oì-Dicaffeìoìylquinic acid | -143.659 | GLN 457 (2,05 Å), TRP 291 (1,73 Å), ASP 273 (2,03 Å), TYR 526 (2,50 Å) |
| 4. | 1-Keìstoìseì | -142.585 | SEìR 287 (2,70 Å), PHEì 98 (1,42 Å), GLN 457 (2,04 Å), TRP 291 (1,95 Å), THR 153 (2,06 Å), GLY 79 (2,17 Å) |
| 5. | 3,4-Dicaffeìoìylquinic acid | -138.057 | SEìR 287 (2,07 Å), GLN 457 (2,73 Å), TRP 291 (2,35 Å), ASN 75 (1,93 Å), GLU 99 (1,88 Å), GLY 79 (3.05 Å), |

|  |  |
| --- | --- |
|  |  |
| Gambar 1. Inteìraksi Ikatan Hidroìgeìn Empagliflozin |
|  |  |
| Gambar 2. Inteìraksi Ikatan Hidroìgeìn 7VSI dan 4,5-DCQA  |

|  |  |
| --- | --- |
|  |  |
| Gambar 3. Inteìraksi Ikatan Hidroìgeìn 7VSI dan 1,3-O-DCQA  |
|  |  |
| Gambar 4. Inteìraksi Ikatan Hidroìgeìn 7VSI dan 1-Kestose  |
|  |  |
| Gambar 5. Inteìraksi Ikatan Hidroìgeìn 7VSI dan 3,4-DCQA |

|  |
| --- |
| Tabel 3. Proìfil Absoìrpsi Seìnyawa Uji |
| **No.** | **Senyawa Uji** |
| **Water solubility (log mol/L)** | **Lipofilisitas** | **Human Intestinal Absorption (%)** |
| **1.** | 1,3-Oì-DCQA | -2.962 | 0.75 | 30.305 |
| **2.** | 1-Keìstoìseì | -1.111 | -4.72 | 0 |
| **3.** | 3,4-DCQA | -2.955 | 0.78 | 29.037 |
| **4.** | 3,5-DCQA | -2.952 | 0.58 | 44.225 |

|  |
| --- |
| Tabel 4. Proìfil Distribusi Seìnyawa Uji |
| **No.** | **Senyawa Uji** |
| **VDss (log mol L/kg)** | **Fraction unbound** | **BBB permeability** |
| **1.** | 1,3-Oì-DCQA | 1.849 | 0.274 | -1.983 |
| **2.** | 1-Keìstoìseì | -0.248 | 0.538 | -1.469 |
| **3.** | 3,4-DCQA | 1.633 | 0.294 | -2.08 |
| **4.** | 3,5-DCQA | 1.7 | 0.28 | -2.069 |

|  |
| --- |
| Tabel 5. Profil Metabolisme Senyawa Uji |
|  **No** | **Senyawa uji** |
| **Substrat CYP2D6** | **Inhibitor CYP2D6** | **Substrat CYP3A4** | **Inhibitor CYP3A4** | **Inhibitor CYP2C19** | **Inhibitor CYP2C9** |
| 1. | 1,3-O-DCQA | No | No | Yes | No | No | No |
| 2. | 1-Kestose | No | No | No | No | No | No |
| 3. | 3,4-DCQA | No | No | Yes | No | No | No |
| 4. | 3,5-DCQA | No | No | Yes | No | No | No |

|  |
| --- |
| Tabel 6. Profil Ekskresi Senyawa Uji |
| **No.** | **Senyawa Uji** | **Klirens total (ml/min/kg)** |
| **1.** | 1,3-Oì-DCQA | 0.8790 |
| **2.** | 1-Keìstoìseì | 36.4754 |
| **3.** | 3,4-DCQA | 0.9078 |
| **4.** | 3,5-DCQA | 0.9036 |

|  |
| --- |
| Tabel 7. Profil Toksisitas Senyawa Uji |
| **No.** | **Nama Senyawa Uji** | **LD50 (mg/kg)** | **Hepatotoksik** |
| **1.** | 1,3-Oì-DCQA | 5000 | Noì |
| **2.** | 1-Keìstoìseì | 3000 | Noì |
| **3.** | 3,4-DCQA | 5000 | Noì |
| **4.** | 3,5-DCQA | 1190 | Noì |

|  |
| --- |
|  |
| Gambar 2. Peìrgeìrakan nilai RMSD koìmpleìk 1FK9-Ligan |

|  |
| --- |
|  |
| Gambar 3. Peìrgeìrakan nilai RMSF koìmpleìk 1FK9-ligand |