Pharmacokinetics properties of predicted compounds.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Ligands | GI absorption | BBB permeability | Pgp substrate | CYP1A2 inhibitor | CYP2C19 inhibitor | CYP2C9 inhibitor | CYP2D6 inhibitor | CYP3A4 inhibitor | log Kp (cm/s) |
| 4,5-di-p-trans-coumaroylquinic acid | Low | No | Yes | No | No | No | No | No | -7.67 |
| (+)-pipoxide | High | No | No | Yes | No | Yes | No | Yes | -6.75 |
| Thymelol | High | No | No | Yes | No | Yes | No | No | -6.14 |
| Zinc000095485961 | Low | No | Yes | No | No | No | No | No | -8.1 |
| Rutamontine | High | No | No | Yes | No | Yes | No | No | -6.14 |
| (-)-tingtanoxide | High | No | No | No | Yes | Yes | No | Yes | -6.6 |
| Tricoccin s13 acetate | High | No | Yes | No | No | Yes | No | No | -5.73 |
| Lactupicrin | High | No | Yes | No | No | No | No | No | -8.02 |
| Naamidine A | High | No | Yes | No | Yes | Yes | No | Yes | -6.91 |
| Zinc000000134782 | High | Yes | No | Yes | Yes | Yes | No | Yes | -5.2 |
| Sigmoidin b 4'-methylether diacetate | High | No | No | Yes | Yes | Yes | No | Yes | -5.88 |
| (-)-pipoxide | High | No | No | Yes | No | Yes | Yes | Yes | -6.75 |
| Abyssinone ii | High | Yes | No | Yes | Yes | Yes | Yes | Yes | -5.28 |
| (+)-strigol | High | No | No | No | No | No | No | No | -7.52 |
| Norisojamicin | High | No | No | Yes | Yes | Yes | No | Yes | -5.99 |
| Calopogonium isoflavone b | High | Yes | No | Yes | Yes | Yes | No | Yes | -5.64 |
| Isosamarcandin | High | No | Yes | No | No | No | Yes | Yes | -5.79 |
| (+)-pipoxide-2-methyl ether | High | Yes | No | Yes | Yes | Yes | Yes | Yes | -6.45 |
| Zinc000095485890 | High | No | No | No | No | No | No | No | -7.58 |
| 1,6-di-o-p-hydroxybenzoyl-beta-d-glucopyranoside | Low | No | Yes | No | No | No | No | No | -8.43 |

*Blood brain barrier permeability (BBB), P-glycoprotein (P-gp) substrates, and gastrointestinal (GI) absorption*

**Druglikeness and Toxicity Profiling of the Top 20 Compound**

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Ligands | MW | #HA | #HD | Log P | Log S | Solubility | LV | GI absorption | Hepatotoxicity | Acute Oral    Toxicity | Nephrotoxicity | Carcinogenicity | mutagenesis |
| 4,5-di-p-trans-coumaroylquinic acid | 484.45 | 10 | 5 | 1.98 | -3.91 | Soluble | 0 | Low | Yes | 0.79 | 0.75 | 0.89 | 0.86 |
| **(+)-pipoxide** | 366.36 | 6 | 1 | 2.76 | -3.56 | Soluble | 0 | High | 0.54 | 0.50 | 0.64 | 0.90 | 0.68 |
| Thymelol | 352.29 | 7 | 1 | 2.87 | -4.44 | Moderately soluble | 0 | High | 0.81 | 0.67 | 0.52 | 0.99 | 0.64 |
| **Zinc000095485961** | 446.45 | 9 | 5 | 2.08 | -3.11 | Soluble | 0 | Low | 0.83 | 0.68 | 0.88 | 0.96 | 0.81 |
| Rutamontine | 352.29 | 7 | 1 | 2.87 | -4.44 | Moderately soluble | 0 | High | 0.79 | 0.67 | 0.54 | 0.99 | 0.64 |
| (-)-tingtanoxide | 408.4 | 7 | 0 | 3.95 | -4.02 | Moderately soluble | 0 | High | 0.51 | 0.50 | 0.47 | 0.85 | 0.68 |
| Tricoccin s13 acetate | 470.6 | 6 | 0 | 3.34 | -5.62 | Moderately soluble | 0 | High | 0.56 | 0.63 | 0.61 | 0.93 | 0.70 |
| Lactupicrin | 410.42 | 7 | 2 | 1.99 | -2.9 | Soluble | 0 | High | Yes | 0.48 | 0.74 | 0.92 | 0.55 |
| **Naamidine a** | 433.46 | 6 | 2 | 2.44 | -4.27 | Moderately soluble | 0 | High | 0.60 | 0.67 | 0.63 | 0.71 | 0.56 |
| Zinc000000134782 | 344.36 | 4 | 0 | 3.53 | -5.29 | Moderately soluble | 0 | High | 0.58 | 0.63 | 0.49 | 0.99 | 0.52 |
| **Sigmoidin\_b\_4'-methylether\_diacetate** | 454.47 | 8 | 1 | 3.97 | -5.23 | Moderately soluble | 0 | High | Yes | 0.49 | 0.57 | 1.00 | 0.52 |
| **(-)-pipoxide** | 366.36 | 6 | 1 | 3.25 | -3.56 | Soluble | 0 | High | 0.54 | 0.50 | 0.64 | 0.90 | 0.68 |
| Abyssinone\_ii | 324.37 | 4 | 2 | 2.83 | -4.68 | Moderately soluble | 0 | High | Yes | 0.60 | 0.54 | 0.96 | 0.55 |
| **(+)-strigol** | 346.37 | 6 | 1 | 2.89 | -2.65 | Soluble | 0 | High | Yes | 0.37 | 0.60 | 0.93 | 0.66 |
| Norisojamicin | 364.35 | 6 | 1 | 3.51 | -4.71 | Moderately soluble | 0 | High | Yes | 0.43 | 0.56 | 1.00 | 0.53 |
| Calopogonium\_isoflavone\_b | 348.35 | 5 | 0 | 3.64 | -4.86 | Moderately soluble | 0 | High | Yes | 0.60 | 0.65 | 1.00 | 0.61 |
| **Isosamarcandin** | 400.51 | 5 | 2 | 3.47 | -5 | Moderately soluble | 0 | High | 0.68 | 0.43 | 0.92 | 0.95 | 0.63 |
| (+)-pipoxide-2-methyl\_ether | 380.39 | 6 | 0 | 3.08 | -3.91 | Soluble | 0 | High | Yes | 0.50 | 0.64 | 0.86 | 0.68 |
| Zinc000095485890 | 438.47 | 7 | 0 | 3.01 | -3.64 | Soluble | 0 | High | Yes | 0.72 | 0.63 | 0.93 | 0.64 |
| **1,6-di-o-p-hydroxybenzoyl-beta-d-glucopyranoside** | 420.37 | 10 | 5 | 1.25 | -2.66 | Soluble | 0 | Low | 0.81 | 0.74 | 0.82 | 0.95 | 0.76 |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |

For toxicity compounds highlighted in Red is Toxic and Green is Non-toxic

*LV=Lipinski’s rule violation GI= Gastrointestinal*