**Table S1. Detailed absorption, distribution, metabolism, toxicity and excretion in silico assessment.**

| Attributes | F9 | CB18 |
|---|---|---|
| **Molecular Property** | | |
| Mass | 230.304 | 258.35 |
| logP | 2.61 | 3.39 |
| H-bond acceptors | 4 | 4 |
| H-bond donors | 1 | 1 |
| Rotatable bonds | 10 | 11 |
| PSA | 96.98 | 109.71 |
| Refractivity | 62.85 | 72.46 |
| **Druglikeness** | | |
| Lipinski | Yes; 0 violation | Yes; 0 violation |
| Ghose filter | Yes | Yes |
| Veber (GSK) filter | Yes | No; 1 violation: Rot > 10 |
| Egan (Pharmacia) filter | Yes | Yes |
| Muegge (Bayer) filter | Yes | Yes |
| Abbott Bioavailability score | 0.56 | 0.56 |
| **Medicinal Chemistry (Friendly)** | | |
| PAINS | 0 alert | 0 alert |
| Brenk structural alert | 0 alert | 0 alert |
| **ADMET** | | |
| **A (Absorption)** | | |
| Water solubility | -1.913 | -2.73 |
| Human Intestinal Absorption (HIA) | 95.87 | 94.5 |
| Human oral bioavailability (HOB) | | |
| Caco-2 permeability | 0.92 | 0.89 |
| P-glycoprotein inhibitior I/II | No | No |
| P-glycoprotein substrate | No | No |
| | | |
| **D (Distribution)** | | |
| BBB Permeability | Yes | Yes |
| **M (Metabolism)** | | |
| *CYP Inhibitors and Substrates* | | |
| CYP1A2 inhibition | No | No |
| CYP2C19 inhibition | No | No |
| CYP2C9 inhibition | No | No |
| CYP2C9 substrate | No | No |
| CYP2D6 inhibition | No | No |
| CYP2D6 substrate | No | No |
| CYP3A4 inhibition | No | No |
| CYP3A4 substrate | No | No |
| **E (Excretion)** | | |
| Renal Organic Cation Transporter | - | - |
| **T (Toxicity)** | | |
| AMES toxicity | No | No |
| hERG I inhibitor | No | No |
| hERG II inhibitor | No | No |
| Hepatotoxicty | No | No |
| Carcinogenicity | No | No |
| Mutagenic | No | No |
| Irritant | No | No |