

**Figure S5.** TOP: Best alignment of structures of luteolin (green) and SKi II (gray) calculated by the program Forge. BOTTOM: Shape and molecular fields comparison of luteolin (A, C, E) vs. SKI II (B, D, F). A and B: Shapes of both molecules represented as atom colored solvent accessible surfaces. C and D: Positive (red) and negative (cyan) molecular electrostatic potential fields contoured at -2.0 kcal/mol. E and F: Hydrophobic (golden) and van der Waals (yellow) molecular interaction fields contoured at -2.0 kcal/mol..