

Table S1. Shape, field and global similarity scores (SSim, FSim and Sim, respectively) for the best alignments of compounds quercetin, (+)-taxifolin and SKI II to luteolin, as calculated by Forge. Numer of conformations (Confs) and alignments (Alns) generated are also shown.

	Sim	FSim	SSim	Confs	Alns
quercetin	0.869	0.775	0.964	20	10
(+)-taxifolin	0.915	0.868	0.961	93	10
SKI II	0.719	0.616	0.822	13	10