(±)-2-Cyclohexyl-5-methoxy-2H-chromene, a synthetic 5-methoxyflavone derivative, is a selective DNA polymerase-β inhibitor with neuroprotective activity against β-amyloid toxicity

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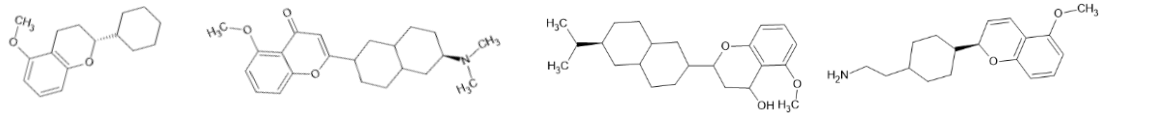
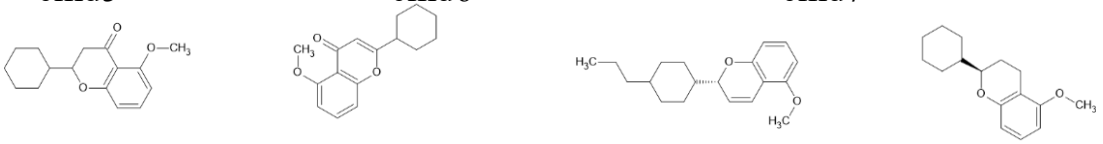
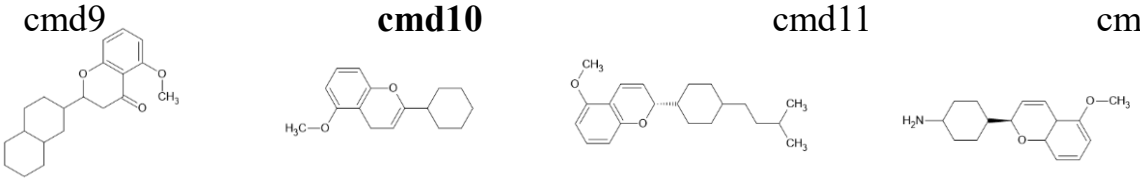
cmd1 cmd2 cmd3 cmd4



cmd5 cmd6 cmd7 cmd8



cmd9 **cmd10** cmd11 cmd12



cmd13 cmd14 cmd15 cmd16

Compound	Complementarity	Complementarity r	Complementarity rho
cmd1	0,471	0,571	0,597
cmd2	0,418	0,354	0,433
cmd3	0,435	0,351	0,441
cmd4	0,412	0,299	0,448
cmd5	0,424	0,389	0,51
cmd6	0,416	0,329	0,541
cmd7	0,44	0,044	0,514
cmd8	0,431	0,526	0,496
cmd9	0,441	0,378	0,502
cmd10	0,473	0,569	0,597
cmd11	0,42	0,035	0,433
cmd12	0,414	0,472	0,576
cmd13	0,39	0,387	0,539
cmd14	0,41	0,205	0,544
cmd15	0,454	0,456	0,54
cmd16	0,427	0,423	0,369

Supplementary Figure 1. Scaffold hopping from 5-methoxyflavone. Computational design yielded derivatives with evaluated complementarity, complementarity *r* and complementarity *rho* scores. Bold highlights the top-performing derivatives. Structural formulas and scores are displayed.