

Supporting Information

Table SI 1. Docking data of selected tetracyclic compounds **17**, **21** and for tricyclic compounds **32**, **34**, **36**, **38**, **41** and **42**, compounds mentioned in the discussion, with comparable binding of the inhibitors to the enzyme with GoldScore and per-atom-score for the *R*-enantiomeric form.

cpd	IC ₅₀ (<i>Ee</i> AChE) [μ M]	# heavy atoms	position of tert. amine	GoldScore	per-atom-score
17	0.23	33	CAS	106.63	3.23
21	0.25	31	CAS	103.87	3.35
32	0.07	24	CAS	96.51	4.02
34	0.39	27	CAS	101.39	3.76
36	0.51	23	CAS	100.78	4.38
38	0.41	26	CAS	112.53	4.33
41	0.07	23	CAS	94.50	4.11
42	0.09	26	CAS	105.29	4.05