

Conjugation of Aminoadamantane and γ -Carboline Pharmacophores Gives Rise to Unexpected Properties of Multifunctional Ligands

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Supplementary

Table S1. Docking scores of aminoadamantane- γ -carboline conjugates.

No	R	Estimated docked binding energies (kcal/mol)	
		AChE	BChE
4a	H	-9.80	-11.25
4b	Me	-10.47	-10.21
4c	F	-10.10	-11.01
8a	H	-9.72	-10.66
8b	Me	-9.53	-10.36
8c	F	-9.49	-10.22
4d	H	-10.38	-10.75
4e	Me	-10.46	-10.64
4f	F	-10.68	-10.70
8d	H	-8.94	-10.60
8e	Me	-9.33	-10.09
8f	F	-9.72	-10.60
dimebon		-9.98	-10.35
donepezil		-11.66	-10.42

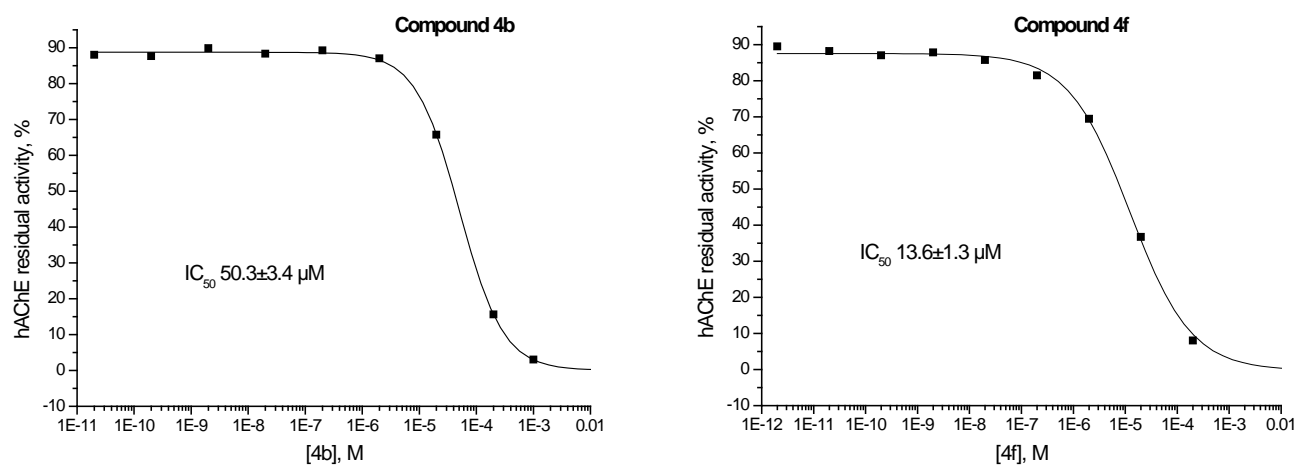


Figure S1. IC_{50} values for hAChE inhibition by compounds **4** (MEAN \pm SEM, $n = 3$).

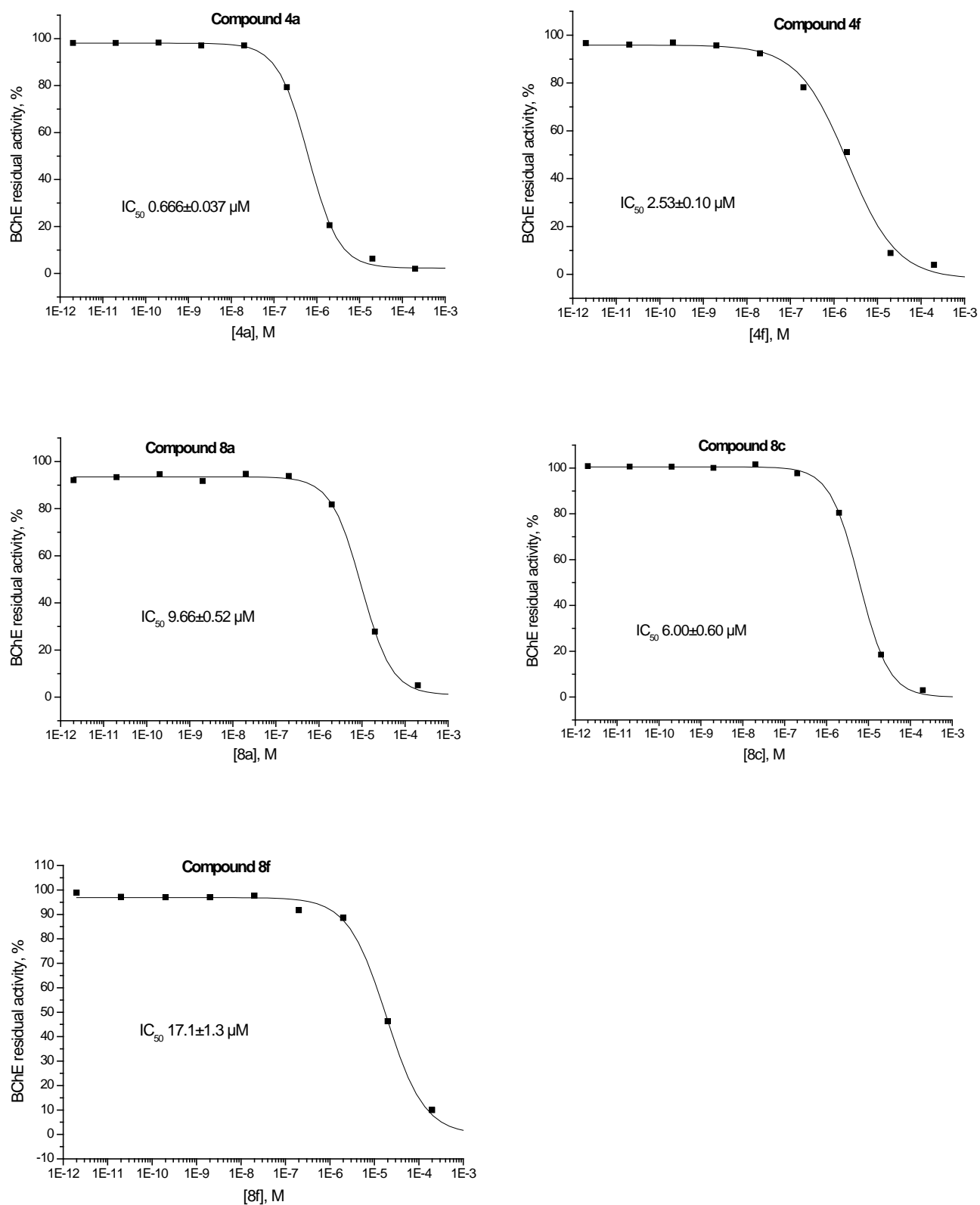


Figure S2. IC₅₀ values for eqBChE inhibition by compounds **4**, **8** (MEAN ± SEM, n = 3).

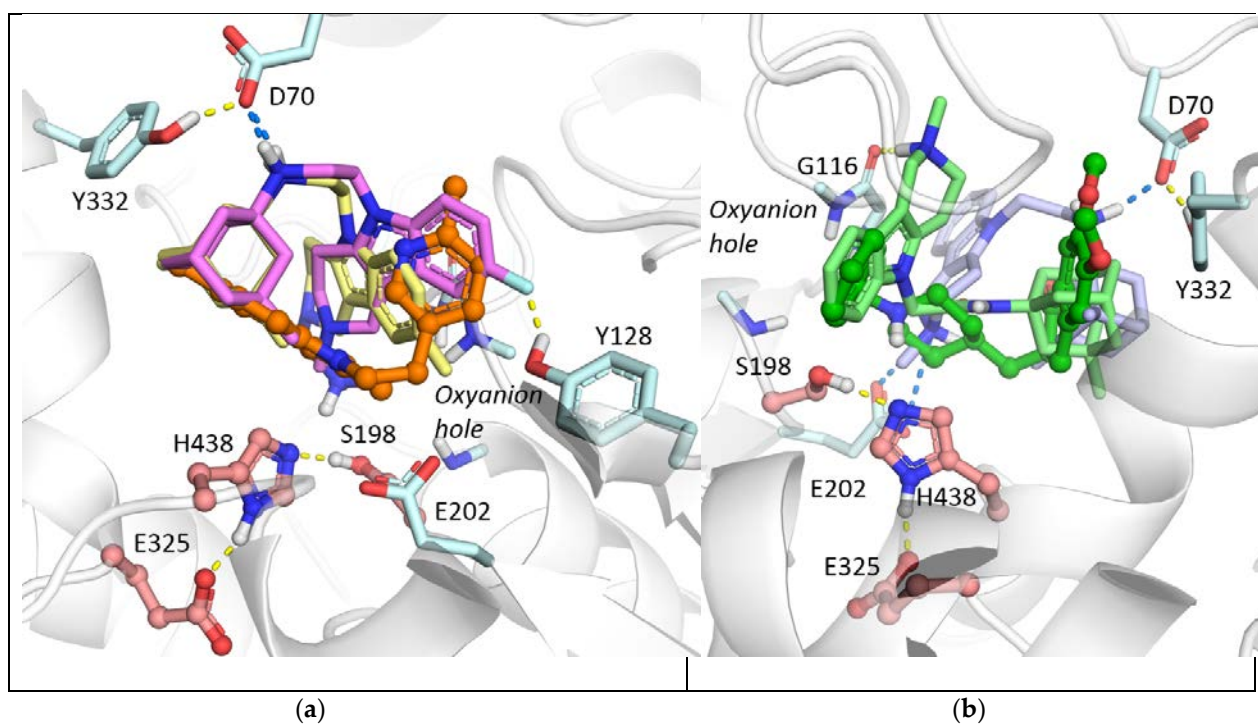


Figure S3. Docking of conjugates linked *via* ethylene and 1-oxoethylene spacers to BChE (a) Fig. 4 overlapped with binding pose of dimebon (carbon atoms are shown in orange) (b) Fig 3a overlapped with binding pose of donepezil (carbon atoms are shown in bright green), viewpoint differs from the original figures in the text.

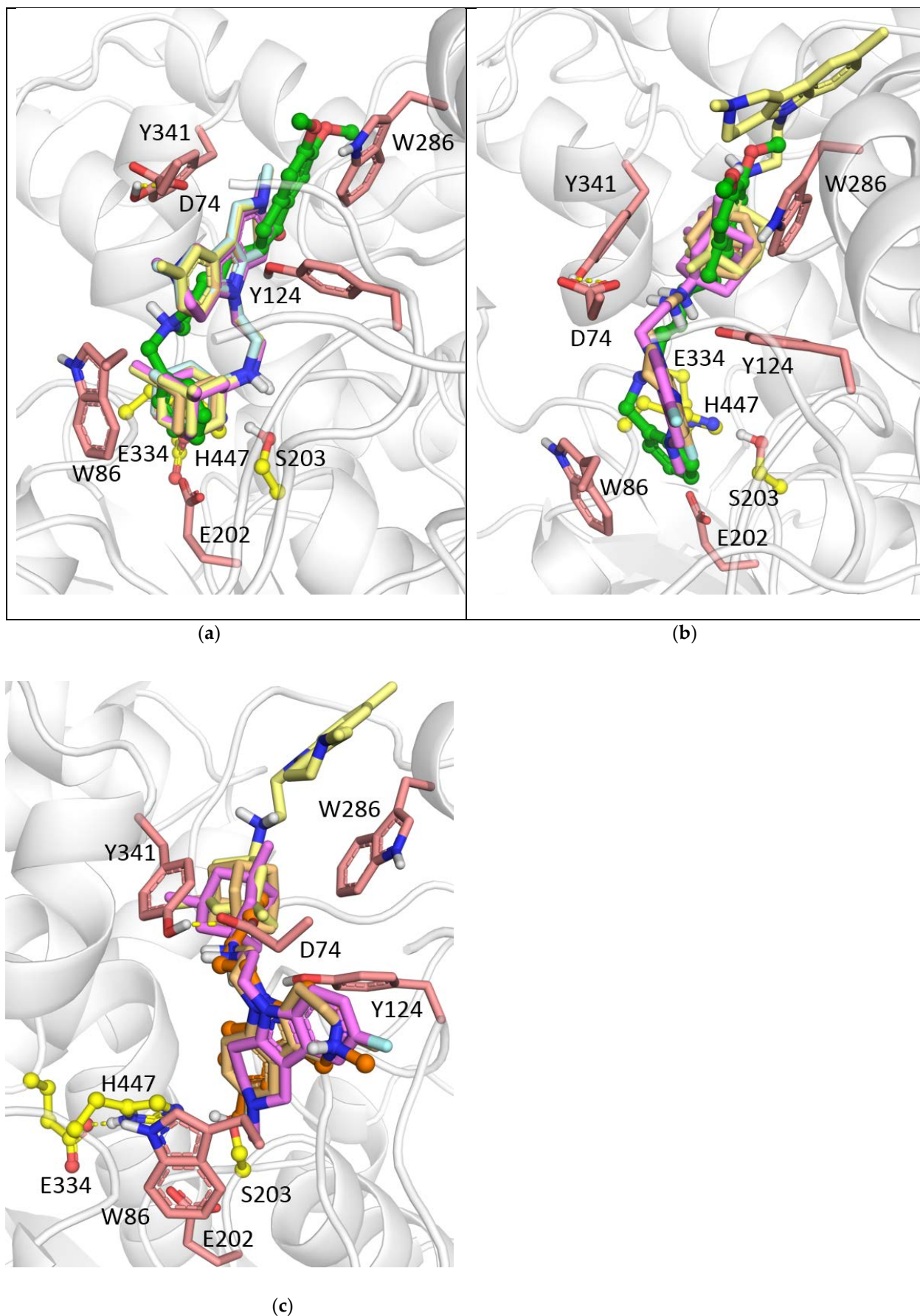


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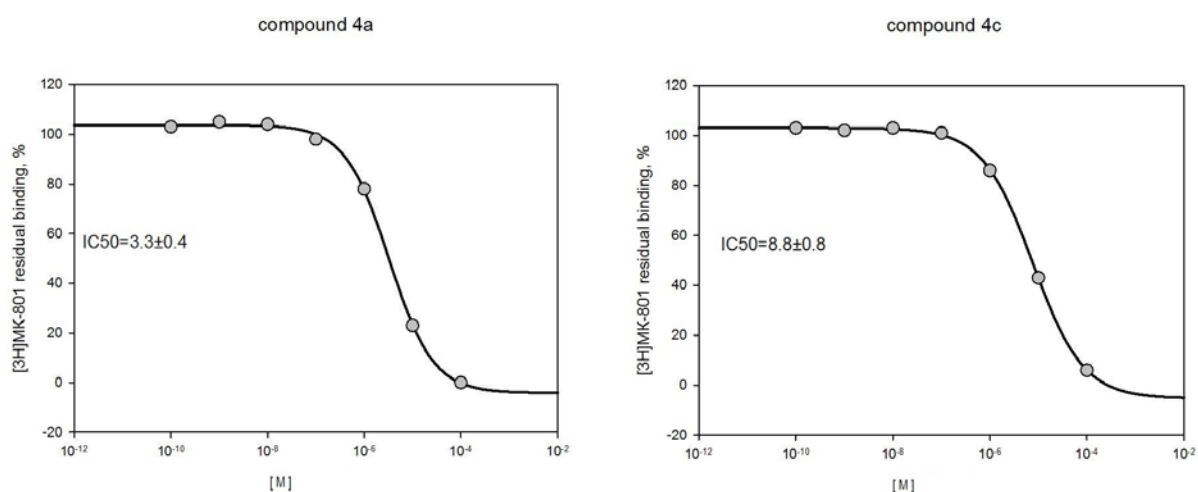


Figure S5. Representative curves for calculation of IC_{50} values for compounds binding with MK-801 specific site of NMDA receptor in semilogarithmic plots (MEAN \pm SEM, $n = 3$).

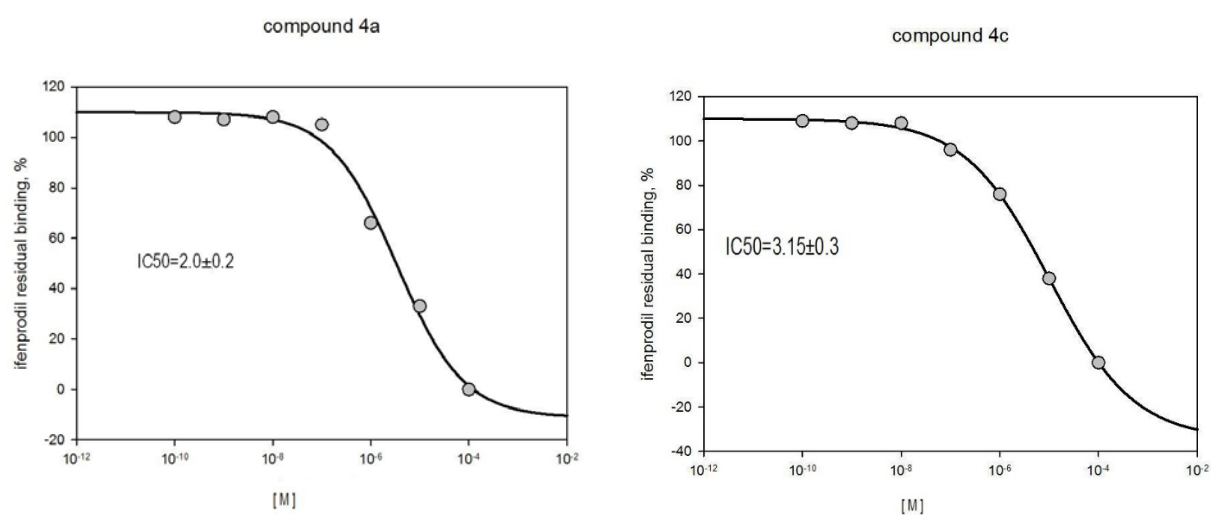


Figure S6. Representative curves for calculation of IC_{50} values for compounds binding with ifenprodil specific site of NMDA receptor in semilogarithmic plots (MEAN \pm SEM, $n = 3$).