Potent Acetylcholinesterase Selective and Reversible Homodimeric Agent based on Tacrine for Theranostics

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Fig S1. ^{1}H NMR spectrum of 9-Chloro-1,2,3,4-tetrahydroacridine (**1**).

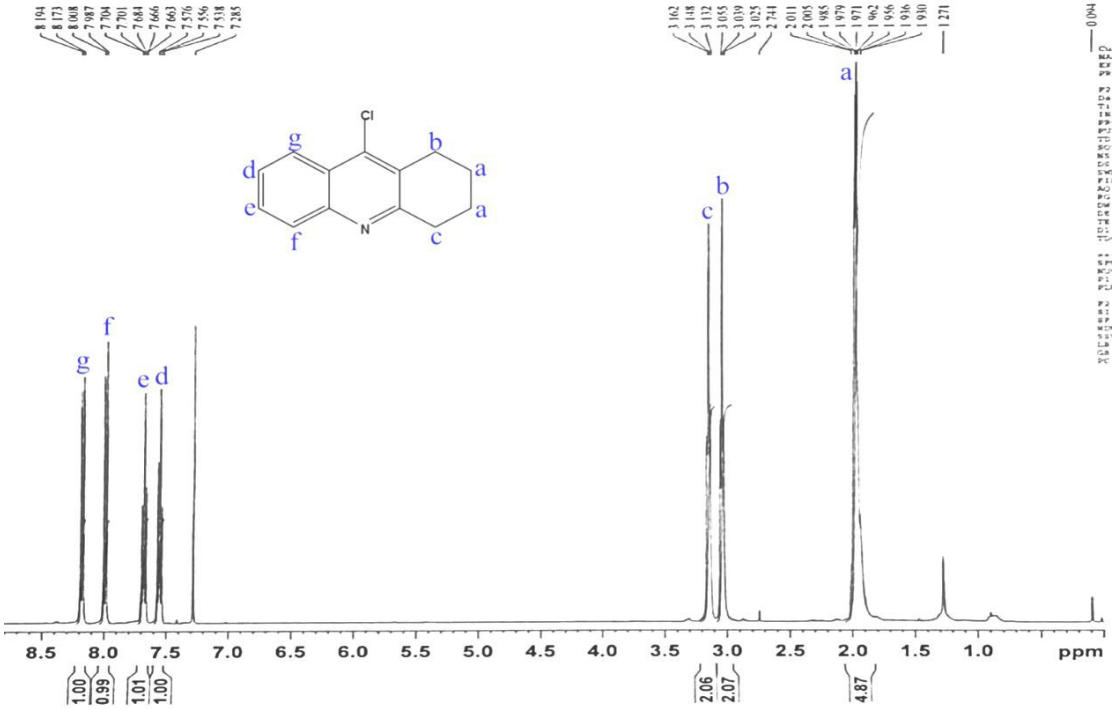


Fig S2. ^{13}C NMR spectrum of 9-Chloro-1,2,3,4-tetrahydroacridine (**1**).

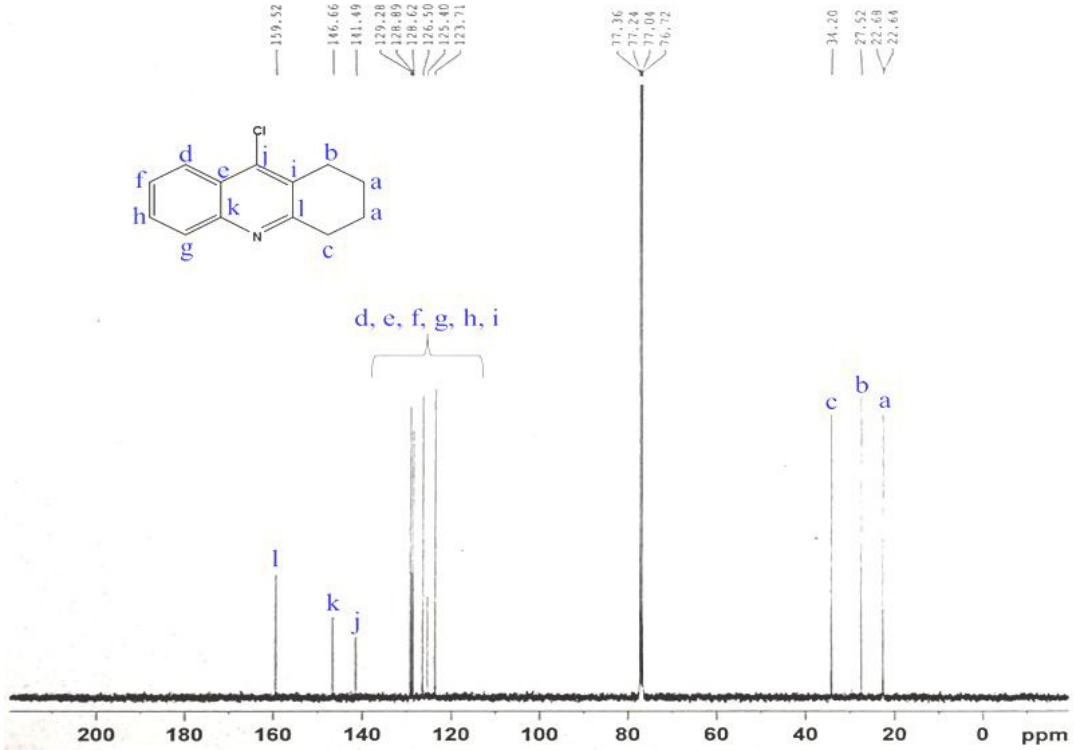


Fig S3. LC-MS mass spectrum of 9-Chloro-1,2,3,4-tetrahydroacridine (**1**).

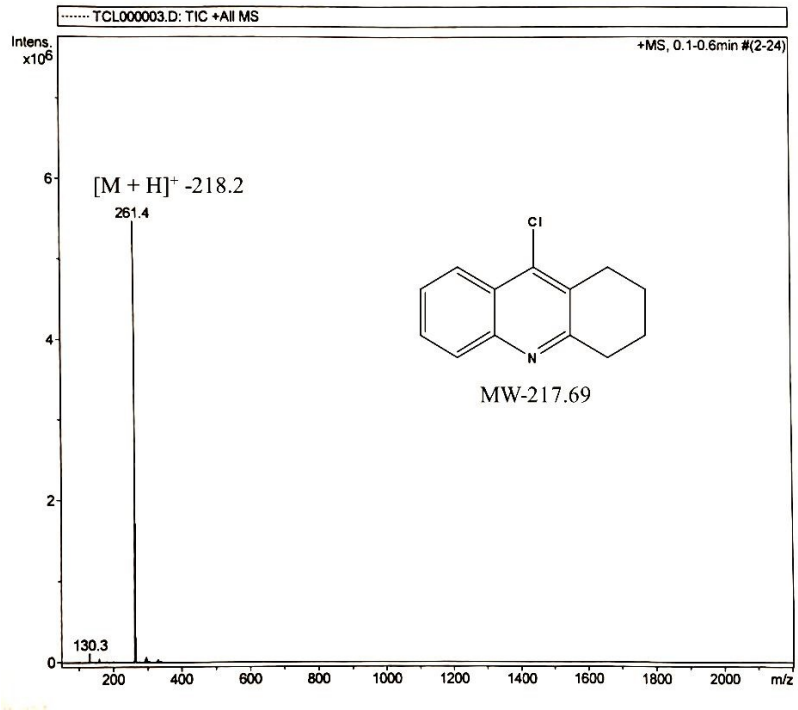


Fig S4. ^{1}H NMR spectrum of N^{1}-(1,2,3,4-tetrahydroacridin-9-yl)ethane-1,2-diamine (**2**).

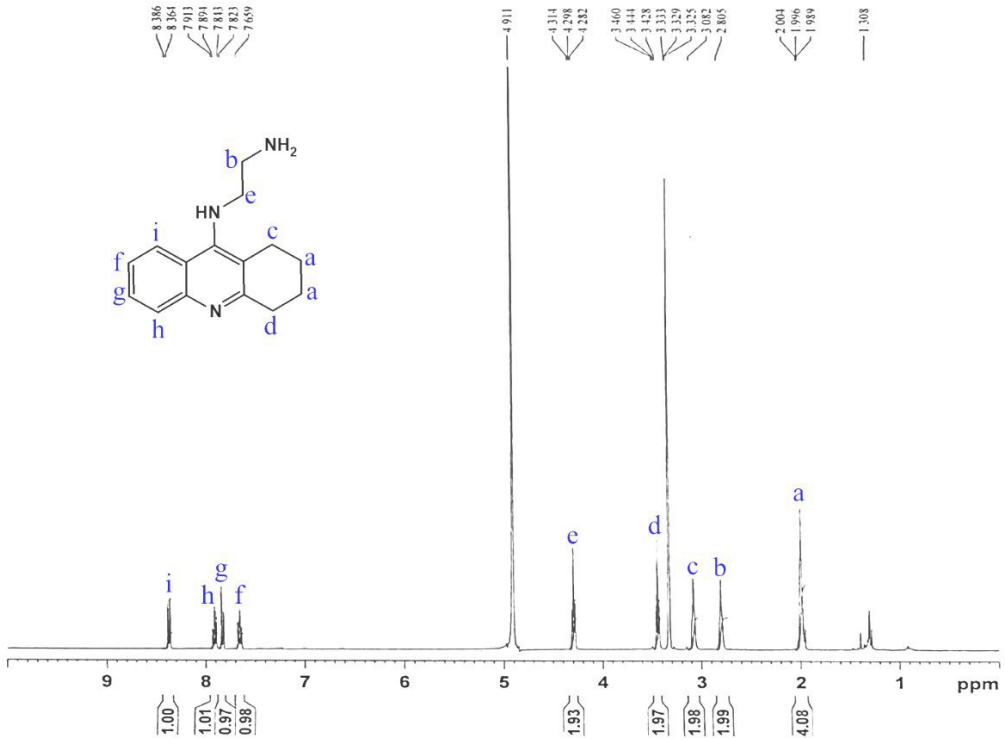


Fig S5. ^{13}C NMR spectrum of N^1-(1,2,3,4-tetrahydroacridin-9-yl)ethane-1,2-diamine (**2**).

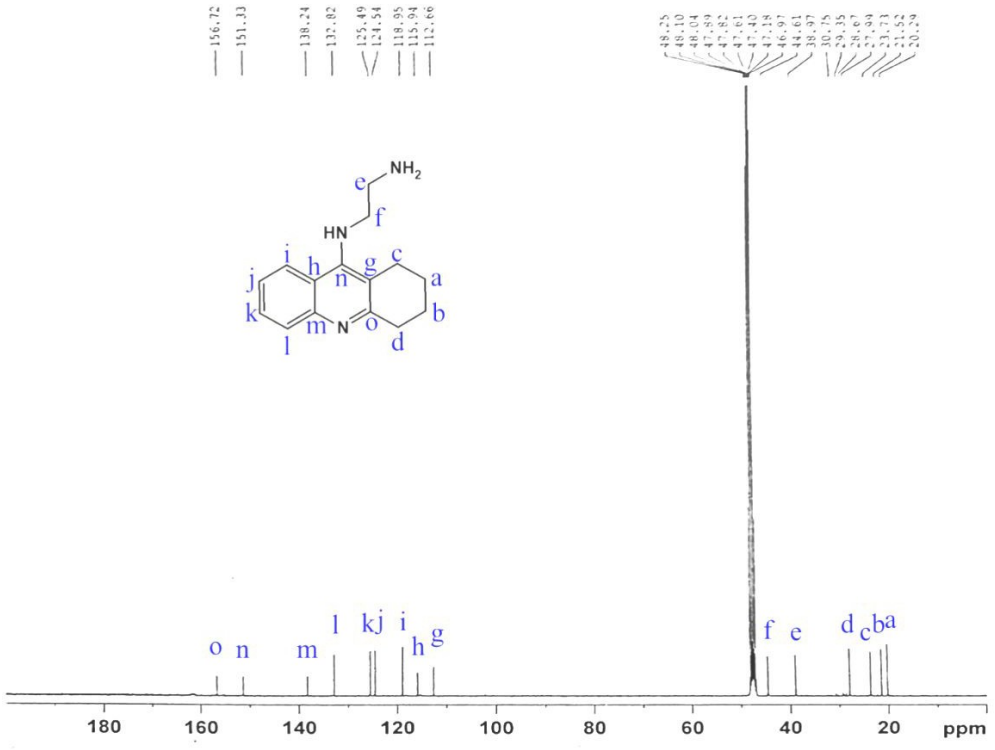


Fig S6. LC-MS spectrum of N^1-(1,2,3,4-tetrahydroacridin-9-yl)ethane-1,2-diamine (**2**).

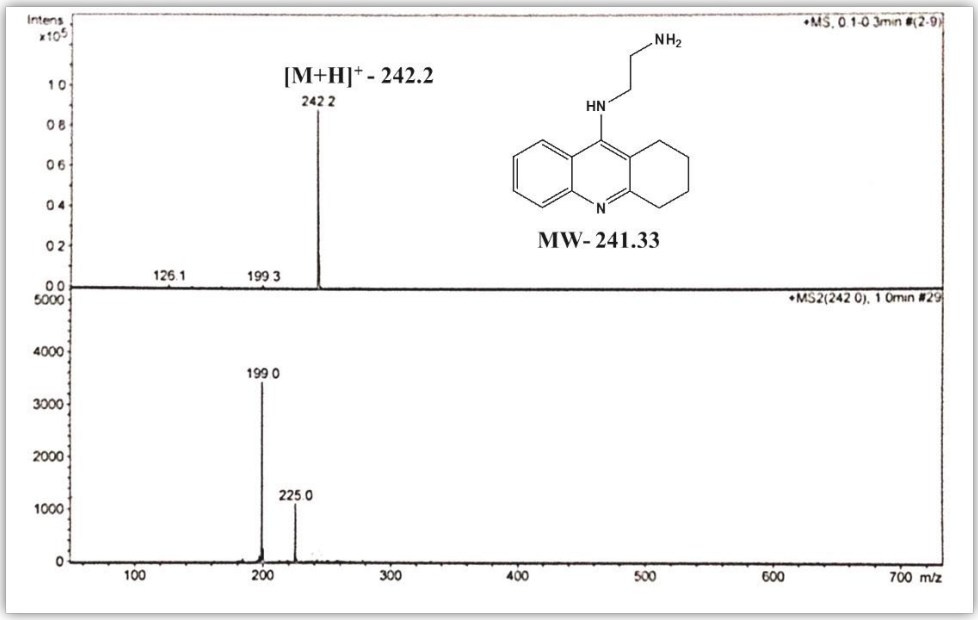


Fig S7. ^{1}H NMR spectrum of 5-amino-N^{1},N^{3}-bis(2-(1,2,3,4-tetrahydroacridin-9-ylamino)ethyl)isophthalamide**(4) .**

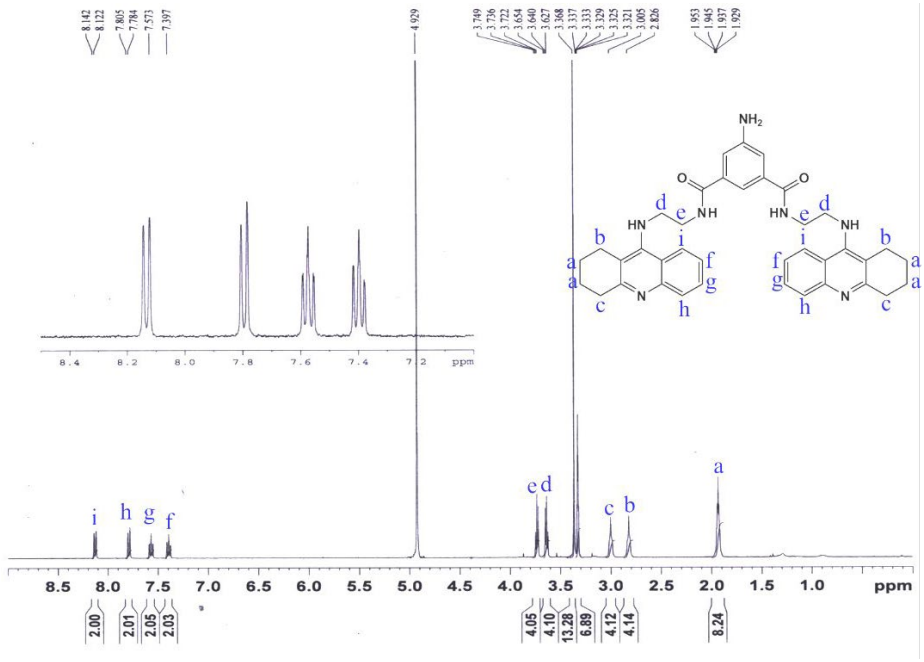


Fig S8. ^{13}C NMR Spectrum of 5-amino-N^{1},N^{3}-bis(2-(1,2,3,4-tetrahydroacridin-9-ylamino)ethyl)isophthalamide **(4) .**

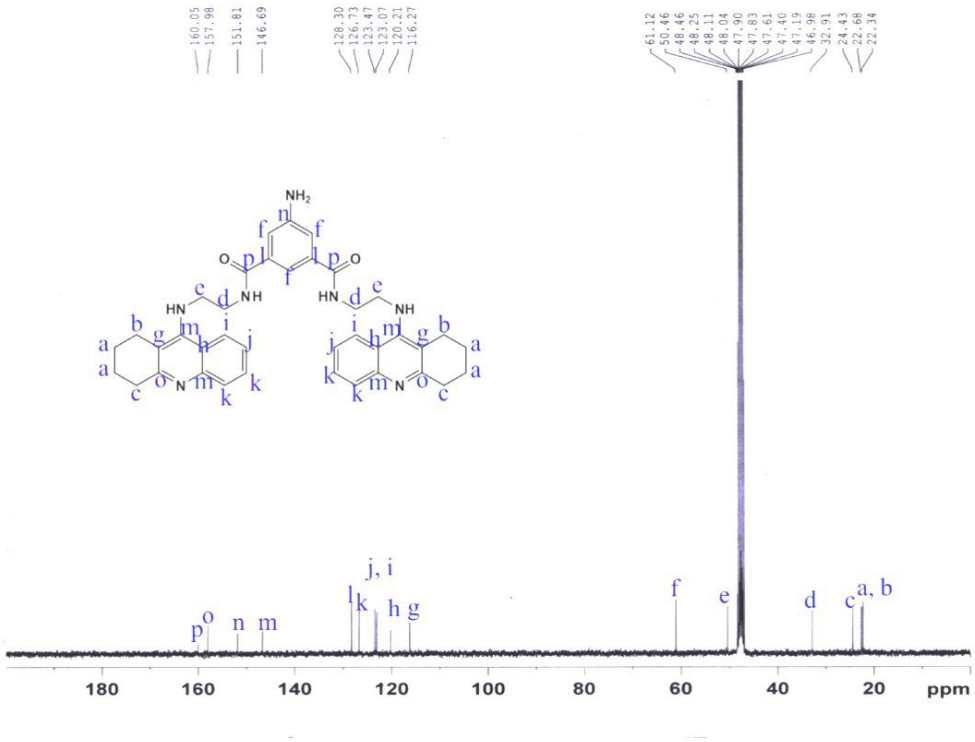


Fig S9.LC-MS spectrum of 5-amino-N^1,N^3-bis(2-(1,2,3,4-tetrahydroacridin-9-ylamino)ethyl)isophthalamide **(4)**

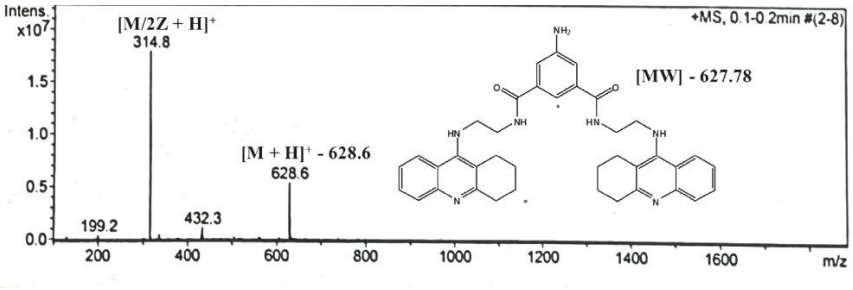


Fig S10.HR-MS spectrum of 5-amino-N^1,N^3-bis(2-(1,2,3,4-tetrahydroacridin-9-ylamino)ethyl)isophthalamide **(4)**

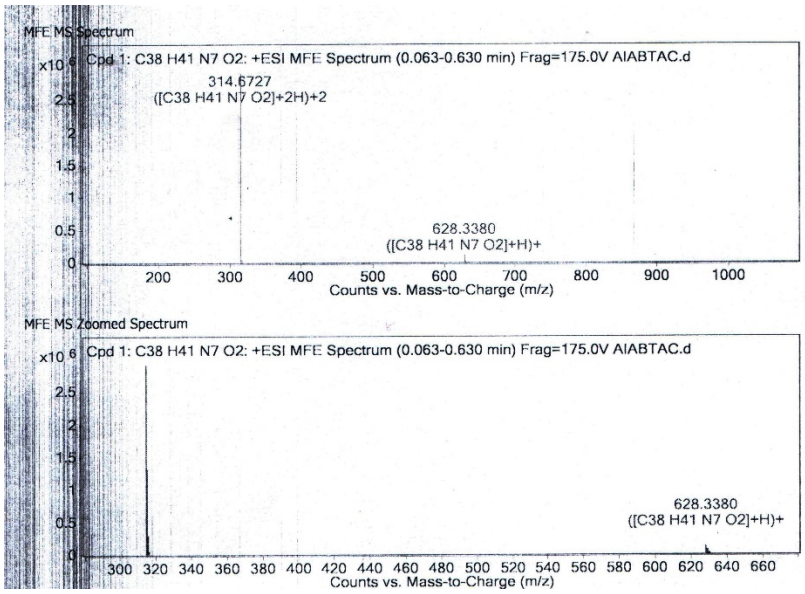


Fig S11. Enzyme kinetic curves (Michaelis-Menton curve) of compound **(4)** on AChE (a) and BuChE (b).

(a) (b)

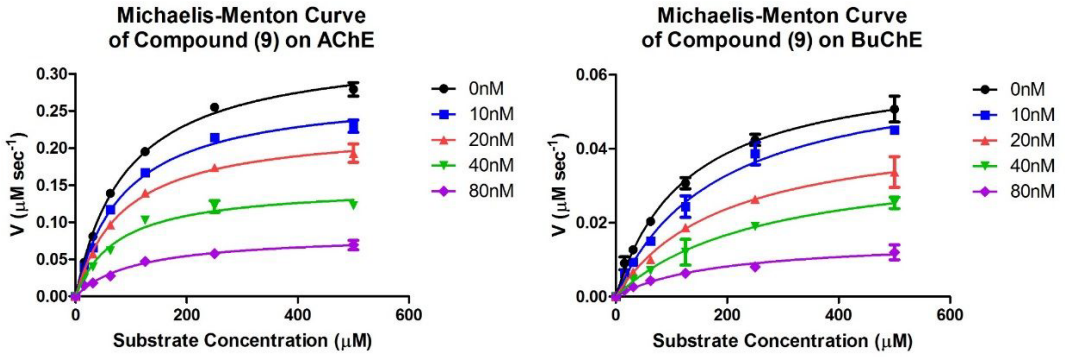
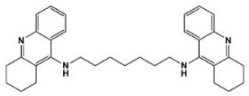
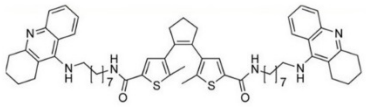
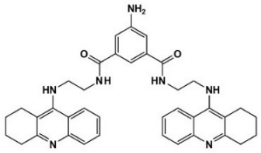


Fig S12. Molecular docking analysis of various reference THA derivatives with compound **4**.

Compound	Structure	Docking Score	Glide Score
Bis(7)-tacrine		19.897	19.897
11b		17.488	17.489
Compound **(4)**		20.746	20.747

In molecular docking analysis, docking and glide score were calculated in percentage with respect to bis(7)-tacrine by using the below formula:

% docking score/Glide score W.R.T. bis(7)-tacrine =

[Docking/Glide Score of Inhibitor – Docking/Glide Score of bis(7)-tacrine] / [Docking/Glide Score of bis(7)-tacrine] X 100