Electronic Supplementary Information

Tetrahydroacridine derivative and its conjugate with gold nanoparticles: Promising agents for the treatment of Alzheimer's disease

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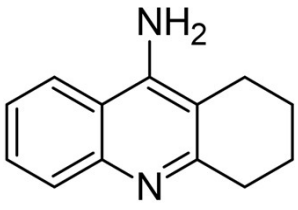

Scheme S1. Chemical structure of tacrine.

Table S1. Crystal data and structure refinement for CHDA

Empirical formula	C_{15} H_{21} Cl_2 N_3 O_2
Formula weight	346.25
Temperature	293(2) K
Wavelength	1.54178 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 7.0963(5) Å, α= 111.519(6)°
	b = 9.7638(7) Å, β= 96.992(5)°
	c = 12.7882(7) Å, γ = 92.865(6)°
Volume	813.85(9) $Å^3$
Z	2
Density (calculated)	1.413 Mg/m^3
Absorption coefficient	3.679 mm^{-1}
F(000)	364
Crystal size	0.1914 x 0.0456 x 0.0246 mm^3
Theta range for data collection	3.76 to 69.92°
Index ranges	-8≤h≤7, -11≤k≤11, -15≤l≤15
Reflections collected	14996
Independent reflections	3030 [R(int) = 0.0764]
Completeness to theta = 69.92°	98.2 %
Absorption correction	Analytical
Max. and min. transmission	0.924 and 0.691
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3030 / 0 / 221
Goodness-of-fit on F^2	0.762
Final R indices [I>2sigma(I)]	R1 = 0.0364, wR2 = 0.0702
R indices (all data)	R1 = 0.0880, wR2 = 0.0791
Extinction coefficient	0.0016(2)
Largest diff. peak and hole	0.245 and -0.204 $e·Å^{-3}$

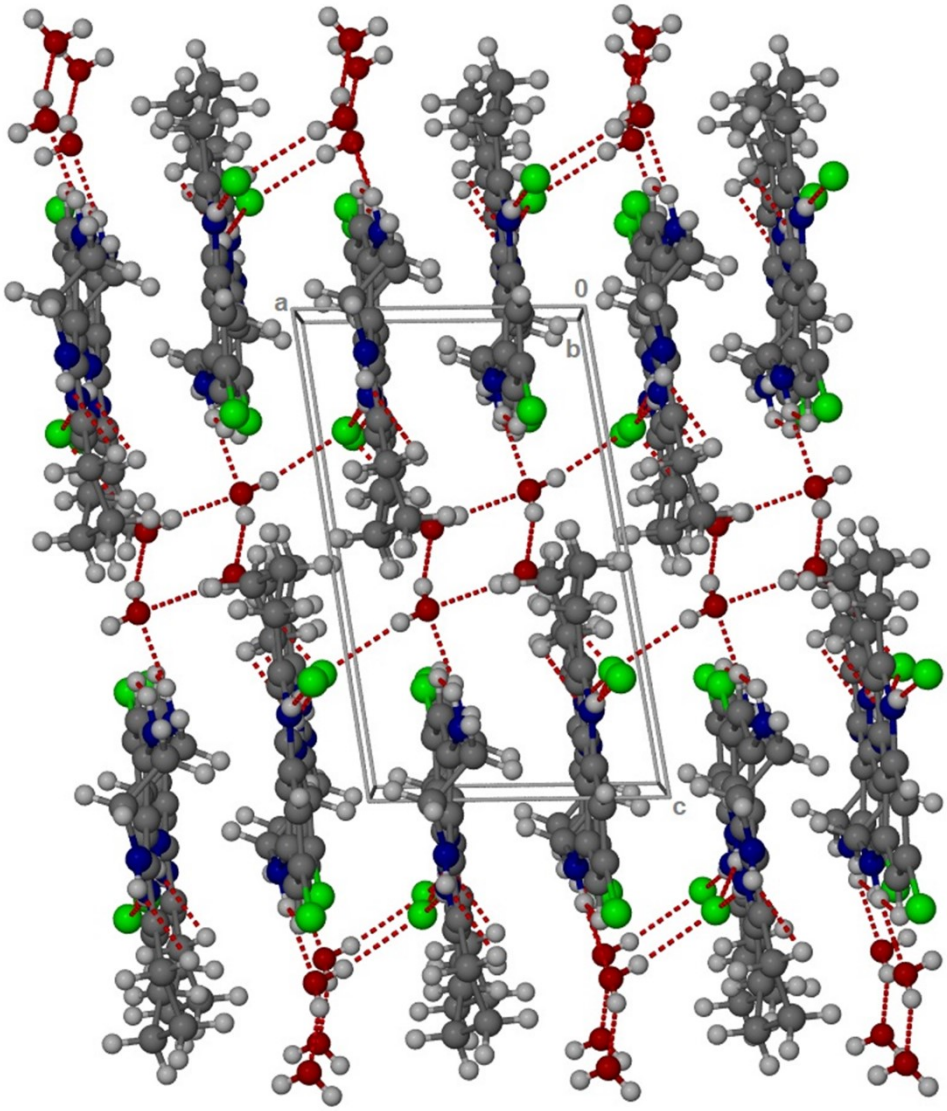

Fig. S1. The view of crystal packing in the b direction. The molecules are shown in a ball-and-sticks representation. The N-H···O, O-H···O and N-H···Cl hydrogen bonds are shown as the dashed lines.

Table S2. Hydrogen bonds for CHDA [Å and °].

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
N(1)-H(1)···Cl(2)	0.87(2)	2.33(3)	3.198(2)	170(2)
N(15)-H(15)···Cl(2)#1	0.84(2)	2.57(3)	3.330(2)	151(2)
N(18)-H(18)···O(1)	0.87(3)	2.06(3)	2.883(3)	158(3)
O(1)-H(1A)···O(2)	0.81(4)	1.97(4)	2.758(4)	165(4)
O(1)-H(1B)···Cl(2)#2	0.81(4)	2.44(4)	3.243(3)	172(4)
O(2)-H(2A)···Cl(2)#3	0.78(4)	2.45(4)	3.232(3)	177(5)
O(2)-H(2B)···O(1)#4	0.80(5)	2.04(5)	2.835(4)	175(5)

Symmetry transformations used to generate equivalent atoms:
#1 x,y+1,z #2 -x,-y+2,-z+2 #3 x,y+1,z+1 #4 -x+1,-y+3,-z+3

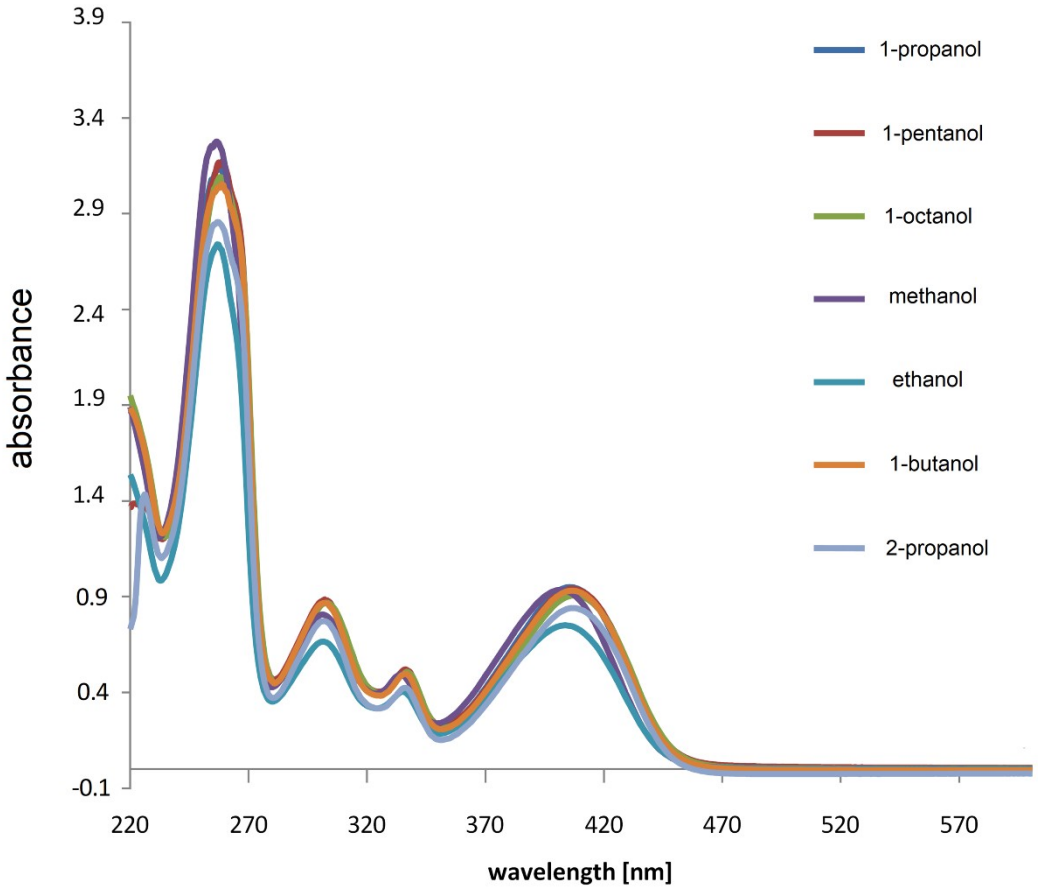

Fig. S2. UV VIS absorption spectra of CHDA recorded in various solvents.

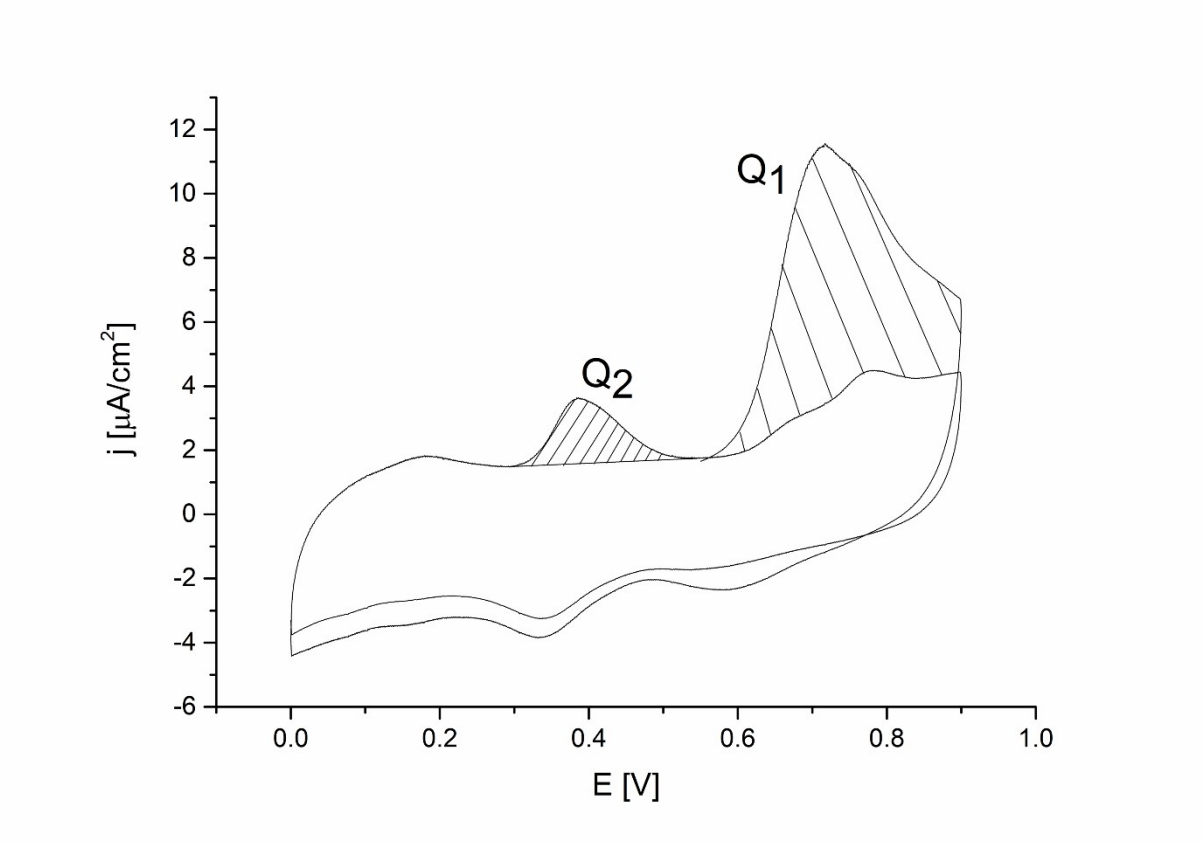

Fig. S3. Schematic diagram of the determination of the charge associated with one-electron oxidation of CHDA adsorbed on the gold electrode surface (the charge is equal to the difference of Q_1 and Q_2).

c

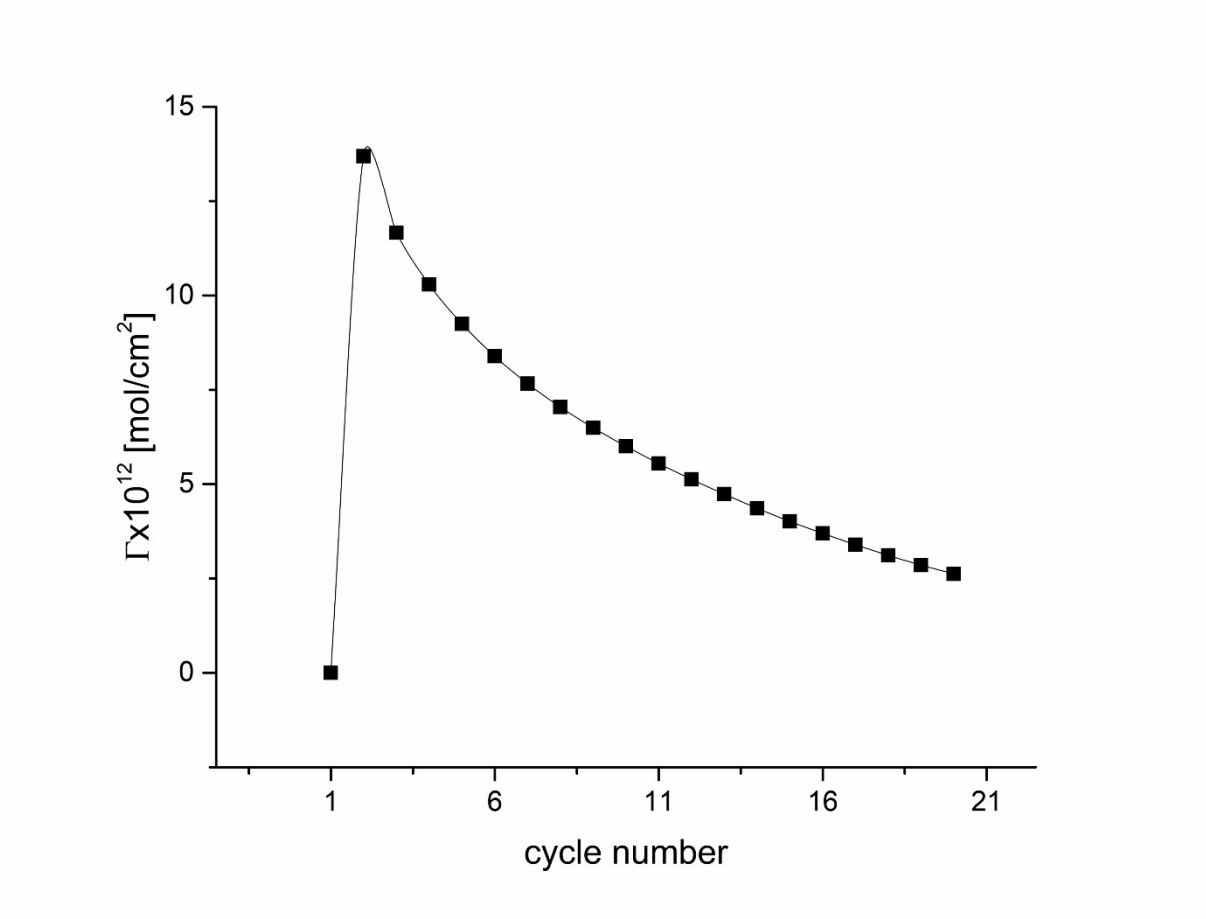

Fig. S4. Dependence of surface concentration of redox species giving oxidation peaks at 0.35 V (both isomeric forms) as a function of voltammetric cycle number.

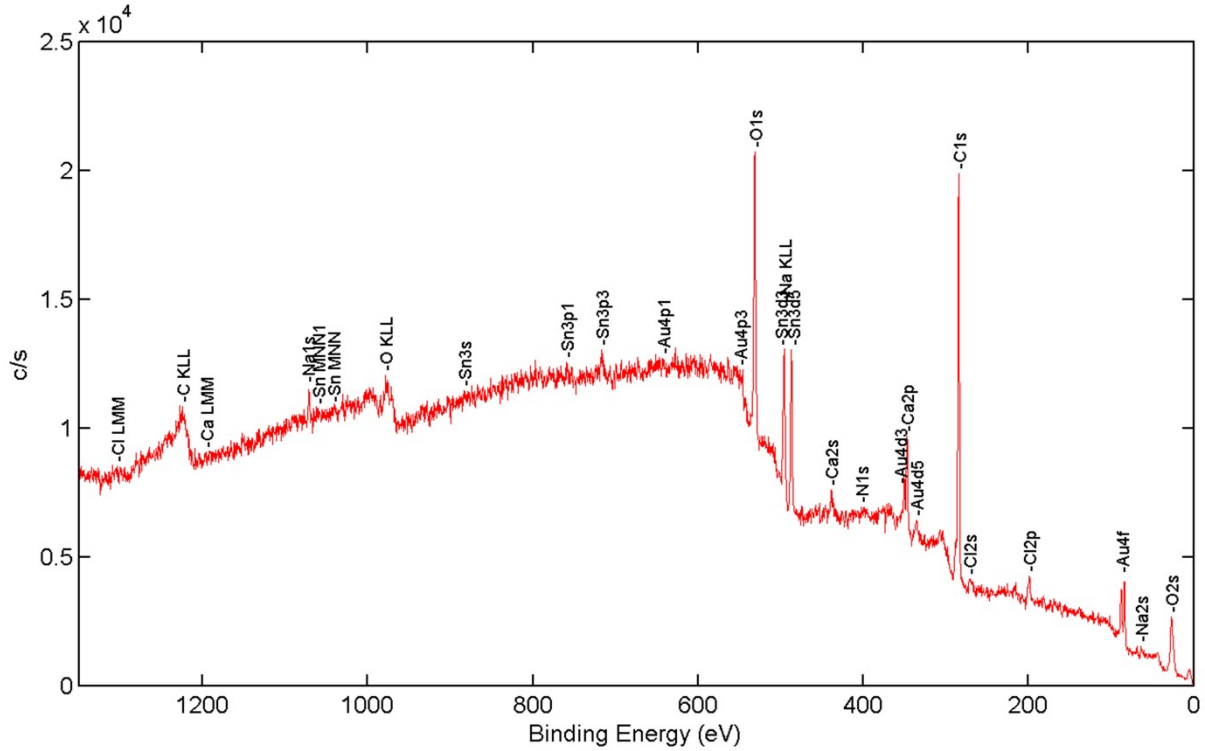

Fig. S5. XPS survey spectrum of CHDA/AuNps conjugate.

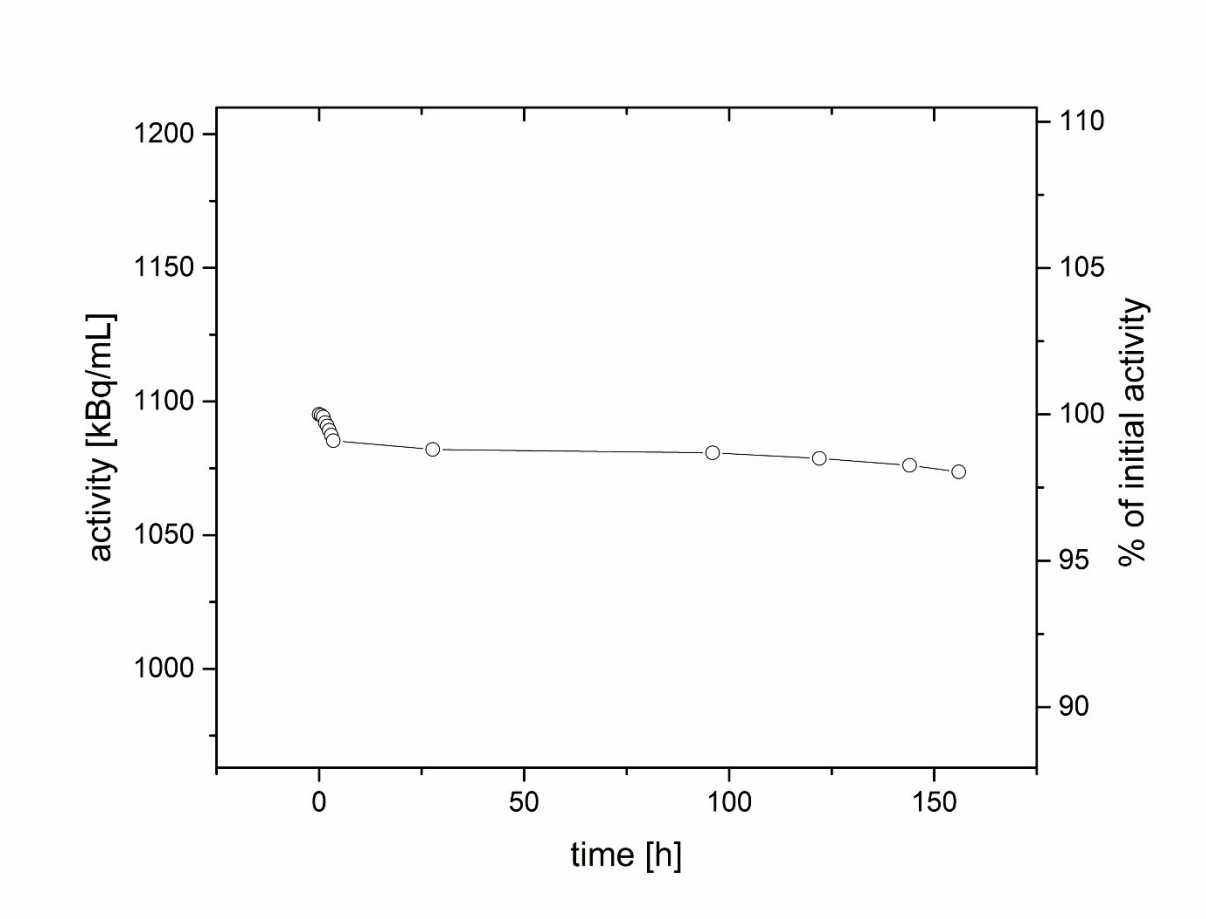

Fig. S6. Purification of CHDA/^{198}AuNps conjugates by dialysis. Activity (left axis) and % of initial activity (right axis) of conjugate solution versus dialysis time.