Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Material

Synthesis, characterization, *in vitro* cytotoxicity, *in silico* ADMET analysis and interaction studies of 5-dithiocarbamato-1,3,4-thiadiazole-2-thiol and its Zinc(II) Complex with Human Serum Albumin: Combined spectroscopy and molecular docking investigations

Fereshteh.Shiri[a],*, Somaye Shahraki[a], Sadegh Baneshi[a], Massoud Nejati-Yazdinejad[a], Mostafa Heidari Majd[b]

[a]Department of Chemistry, University of Zabol, P.O. Box 98615-538, Zabol, Iran.
[b]Faculty of Pharmacy, Zabol University of Medical Sciences, Zabol, Iran

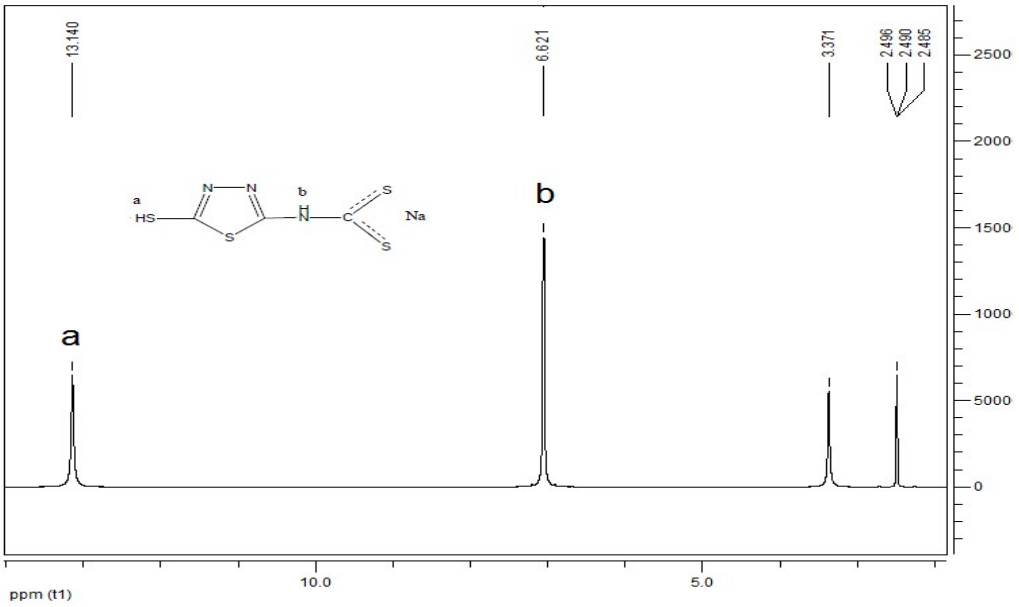
13.140
6.621
3.371
2.496
2.490
2.485
a
b
HS
N
N
S
H
N
C
S
S
Na
2500
2000
1500
1000
5000
0
10.0
5.0
ppm (t1)

Figure 1S

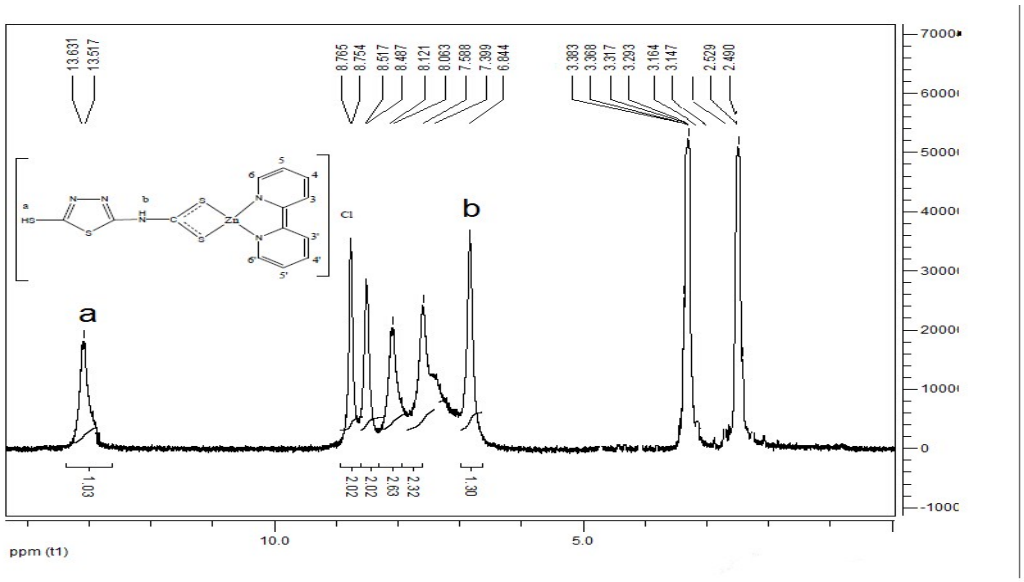

Figure 2S

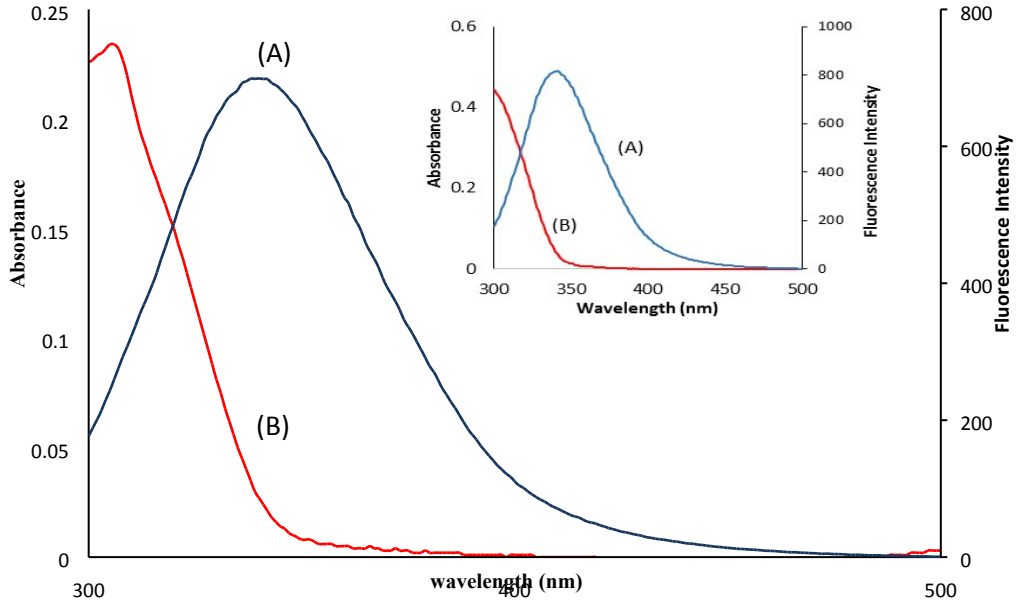

Figure 3S

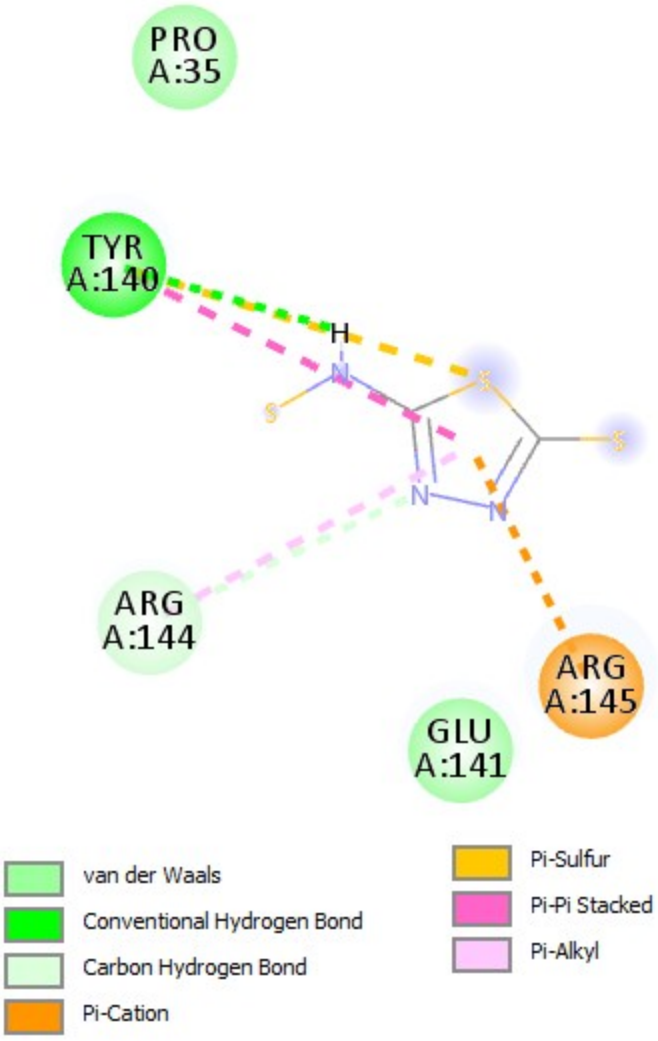
PRO
A:35
TYR
A:140
H
N
S
S
S
N
N
ARG
A:144
ARG
A:145
GLU
A:141
van der Waals
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Pi-Cation
Pi-Sulfur
Pi-Pi Stacked
Pi-Alkyl

Figure 4S(A)

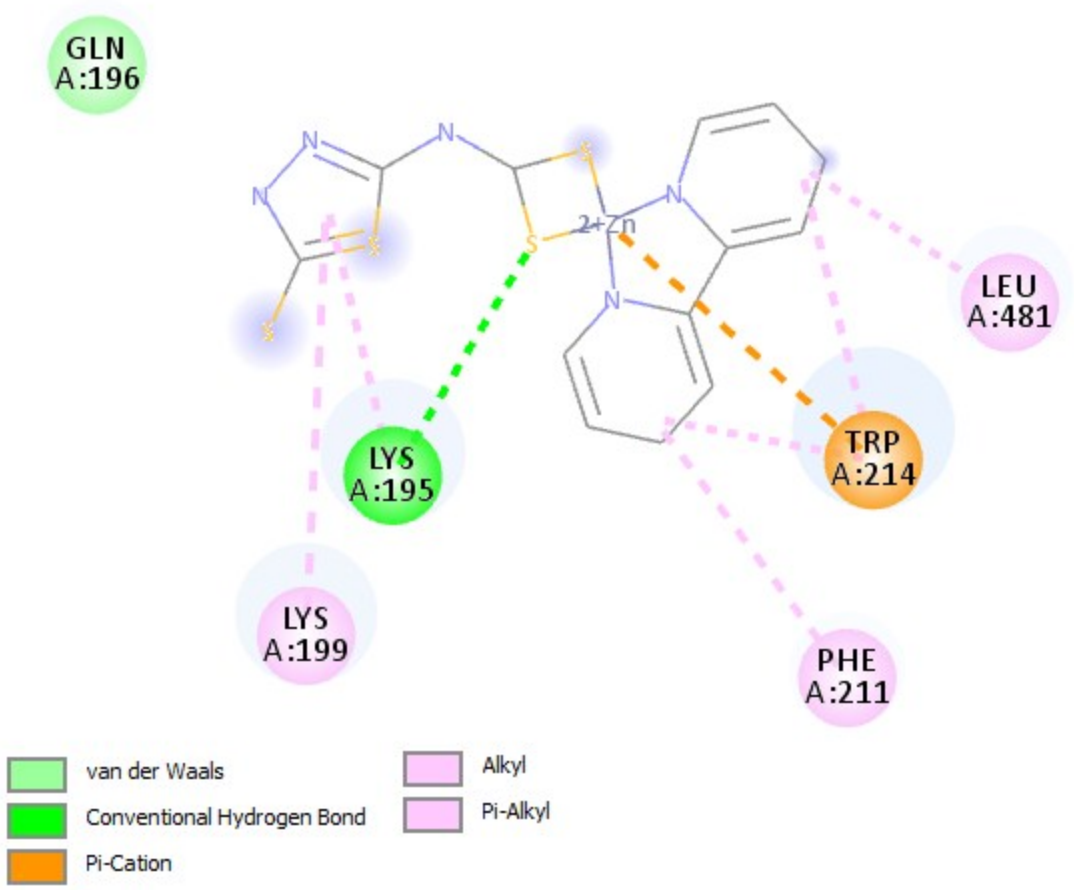

Figure 4S(B)

Figure 1S. 1H NMR spectrum (DMSO-d6, 500 MHz) of dithiocarbamate ligand.

Figure 2S. 1H NMR spectrum (DMSO-d6, 500 MHz) Zn(II) complex.

Figure 3S. Spectral overlap between the fluorescence emission spectrum of HSA (10 µM) (A) and absorption spectrum of Zn complex (10 µM), Insert for dithiocarbamate ligand (10 µM), at 310 K.

Figure 4S. Two-dimensional scheme of interactions between the Ligand (A), Complex (B) and HSA. Only the more important residues for binding are shown.

Table 1S. Prediction of ADMET properties

Parameter	ligand	complex
Molweight	165.265	430.919
LogP	0.5163	2.8386
LogS	-3.752	-4.458
H-Acceptors	3	5
H-Donors	1	1
Polar Surface Area	119.65	137.93
Mutagenic	none	none
Tumorigenic	none	none
Reproductive Effective	none	none
Irritant	none	none

Table 2S. Smina score of HSA with different conformers of ligand and complex

Ligand		Complex	
Pose	Affinity (kcal/mol)	Pose	Affinity (kcal/mol)
1	-4.3	1	-8.1
2	-4.0	2	-7.6
3	-4.0	3	-7.3
4	-4.0	4	-7.2
5	-3.9	5	-7.2
6	-3.9	6	-7.0
7	-3.8	7	-6.9
8	-3.8	8	-6.8
9	-3.7	9	-6.7