Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Materials

In vitro biological and *in silico* screening of the novel iron(III) complexes for DNA-targeted antitumor drug component

Serap Nigdelioglu Dolanbay[1], Zehra Kübra Yilmaz[1], Büşra Kaya[2*], Belma Aslim[1], Bahri Ülküseven[2]

[1]*Gazi University, Faculty of Science, Department of Biology, 06500 Ankara, Turkey*

[2]*Department of Chemistry, Engineering Faculty, Istanbul University-Cerrahpasa, 34320, Avcilar, Istanbul, Turkey*

Table S1. SMILES notations of complexes from Cheminfo software.

Complexes	SMILES notations*
Fe1	c1ccc2c(c1)O[Fe]13(OC(=C(C(c4ccccc4)OC)C(=[N]1N=C(SC)[N]3=C2)C)C)Cl
Fe2	c1(ccc2c(c1)O[Fe]13(OC(=C(C(c4ccccc4)OC)C(=[N]1N=C(SC)[N]3=C2)C)C)Cl)OC

* SMILES notations used in Molinspiration and PASS online software.

Table S2. Selected supercoiled pBR322 DNA cleavage data in the presence of varying concentrations of complex **Fe1** in Fig. 7.

Lane no.	Reaction conditions	Form I (%)	Form II (%)
0	DNA	87.5	12.5
1	DNA+ Fe1 (500 µM)	83.3	16.7
2	DNA+ Fe1 (750 µM)	71.1	28.9
3	DNA+ Fe1 (1000 µM)	80.7	19.3
4	DNA+ Fe1 (1500 µM)	66.9	33.1
5	DNA+ Fe1 (2500 µM)	22.5	77.5

Table S3. Selected supercoiled pBR322 DNA cleavage data in the presence of varying concentrations of complex **Fe2** in Fig. 7.

Lane no.	Reaction conditions	Form I (%)	Form II (%)
0	DNA	90.2	9.8
1	DNA+ Fe2 (500 µM)	86.4	13.6
2	DNA+ Fe2 (750 µM)	84.3	15.7
3	DNA+ Fe2 (1000 µM)	81.5	18.5
4	DNA+ Fe2 (1500 µM)	83.9	16.1
5	DNA+ Fe2 (2500 µM)	75.4	24.6

Table S4. The optimized geometrical parameters of Fe(III) complexes 1 and 2 in the ground state at the B3LYP/LANL2DZ level, together with the published crystal data[1].

Bond length (Å)	**Calculated**		**Experimental**
Complexes	**Fe1**	**Fe2**	**Similar structure[1]**
Fe1-O1	1.872	1.872	1.897(2)
Fe1-O3	1.877	1.876	1.907(2)
Fe1-N1	1.893	1.894	2.067(3)
Fe1-N3	1.941	1.942	2.076(3)
Fe1-Cl1	2.290	2.293	2.2146(11)
Bond angle (deg)			
O1-Fe1-O3	91.6	91.6	92.51(10)
O1-Fe1-N1	89.3	89.4	87.07(10)
O3-Fe1-N1	167.0	167.0	144.71(11)
O1-Fe1-N3	158.4	158.3	147.74(11)
O3-Fe1-N3	91.2	91.1	87.47(11)
N1-Fe1-N3	83.2	83.2	74.99(11)
O1-Fe1-Cl1	102.4	102.4	108.50(8)
O3-Fe1-Cl1	100.3	100.5	108.66(9)
N1-Fe1-Cl1	92.2	92.0	104.86(8)
N3-Fe1-Cl1	98.7	98.8	102.00(9)

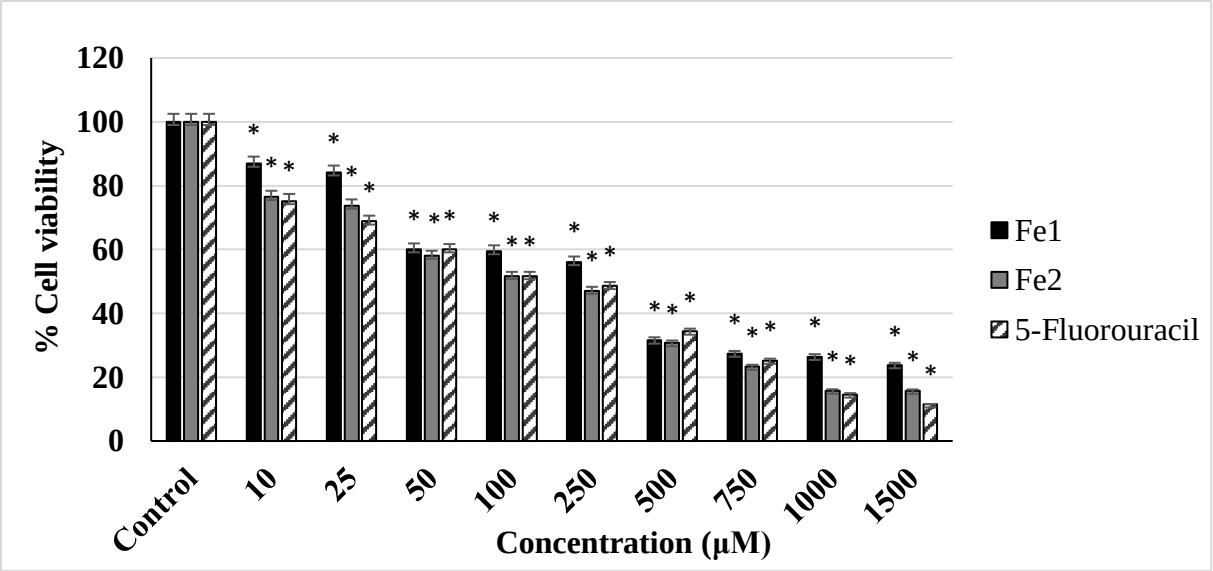


Figure S1a. The effects of complexes **Fe1**, **Fe2** and 5-Fluorouracil on viability of HT-29 cell line for 24 h. Results are represented as mean of three replicates ± standard deviation. *$p < 0.05$ compared to control.

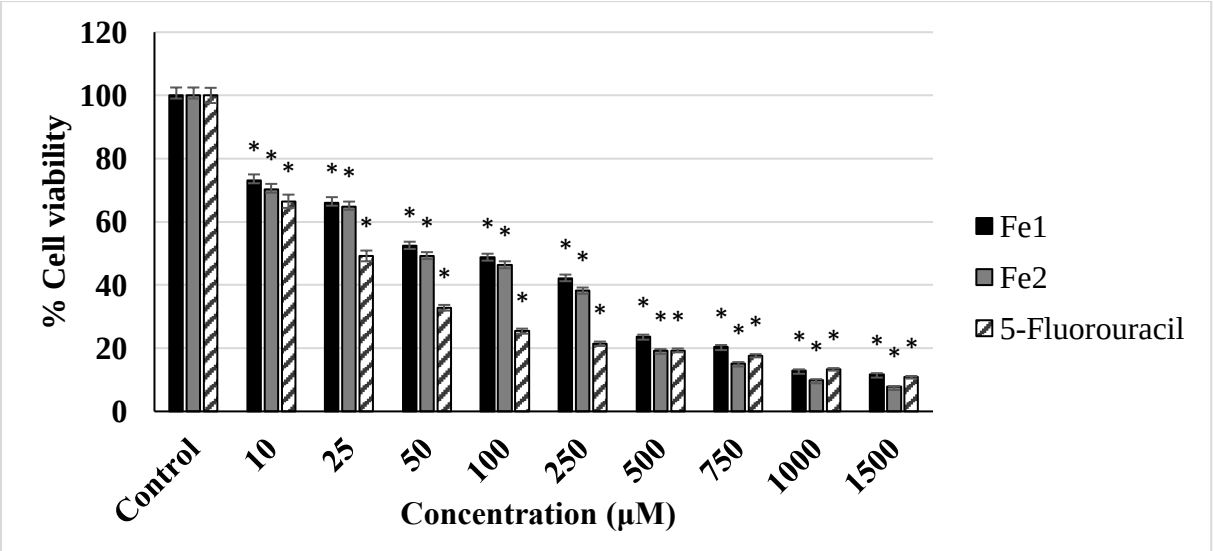


Figure S1b. The effects of complexes **Fe1**, **Fe2** and 5-Fluorouracil on viability of HT-29 cell line for 48 h. Results are represented as mean of three replicates ± standard deviation. *$p < 0.05$ compared to control.

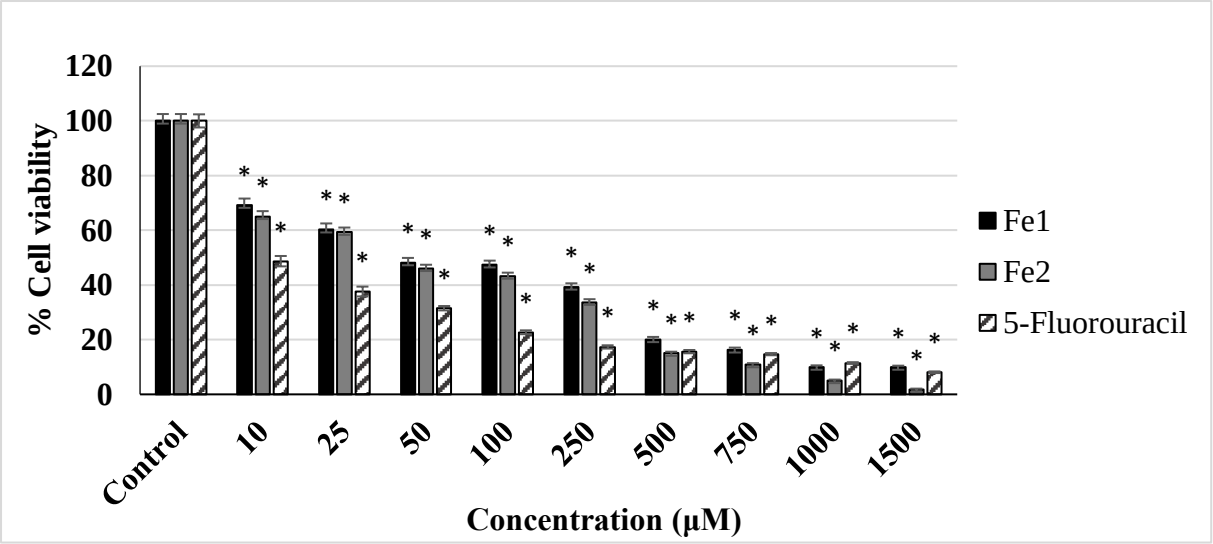


Figure S1c. The effects of complexes **Fe1**, **Fe2** and 5-Fluorouracil on viability of (a) HT-29 cell line for 72 h. Results are represented as mean of three replicates ± standard deviation. *$p < 0.05$ compared to control.

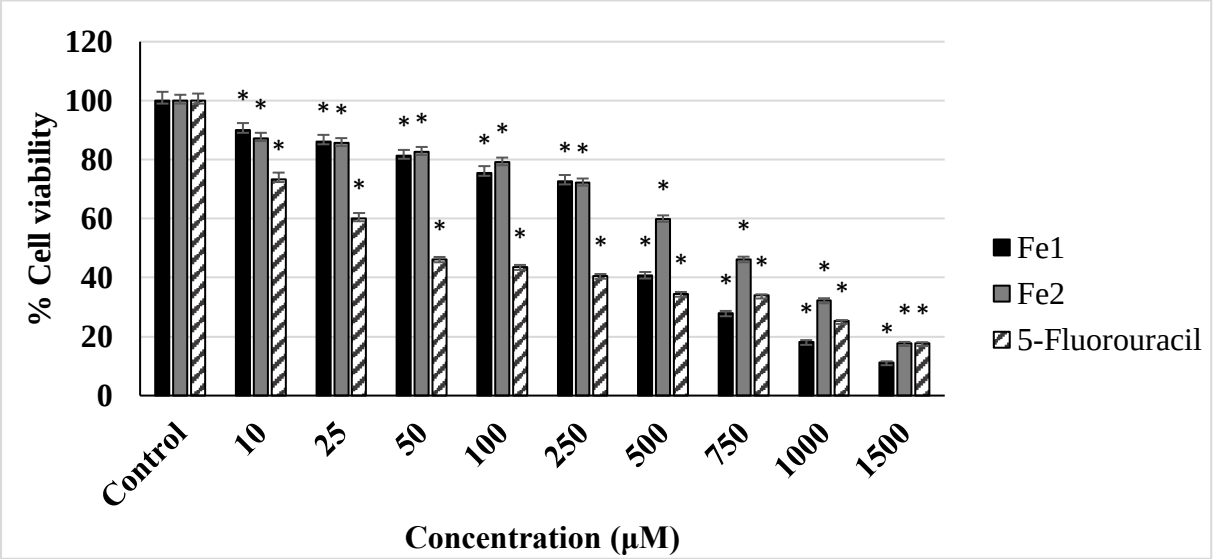


Figure S2a. The effects of complexes **Fe1, Fe2** and 5-Fluorouracil on viability of HeLa cell line for 24 h. Results are represented as mean of three replicates ± standard deviation. *$p < 0.05$ compared to control.

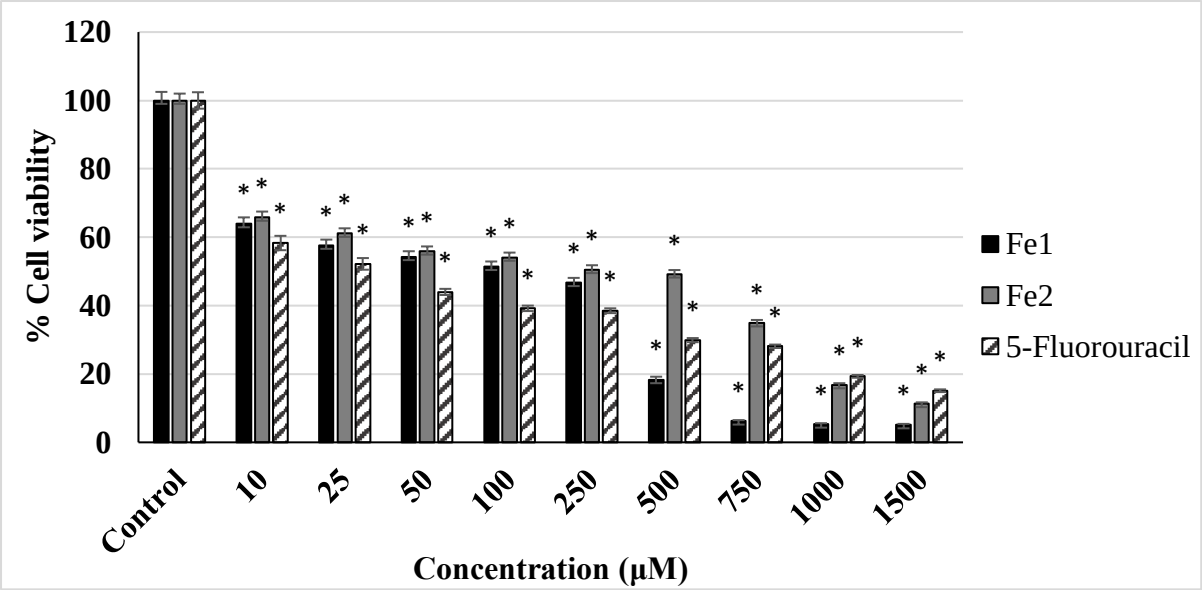


Figure S2b. The effects of complexes **Fe1**, **Fe2** and 5-Fluorouracil on viability of HeLa cell line for 48 h. Results are represented as mean of three replicates ± standard deviation. *$p < 0.05$ compared to control.

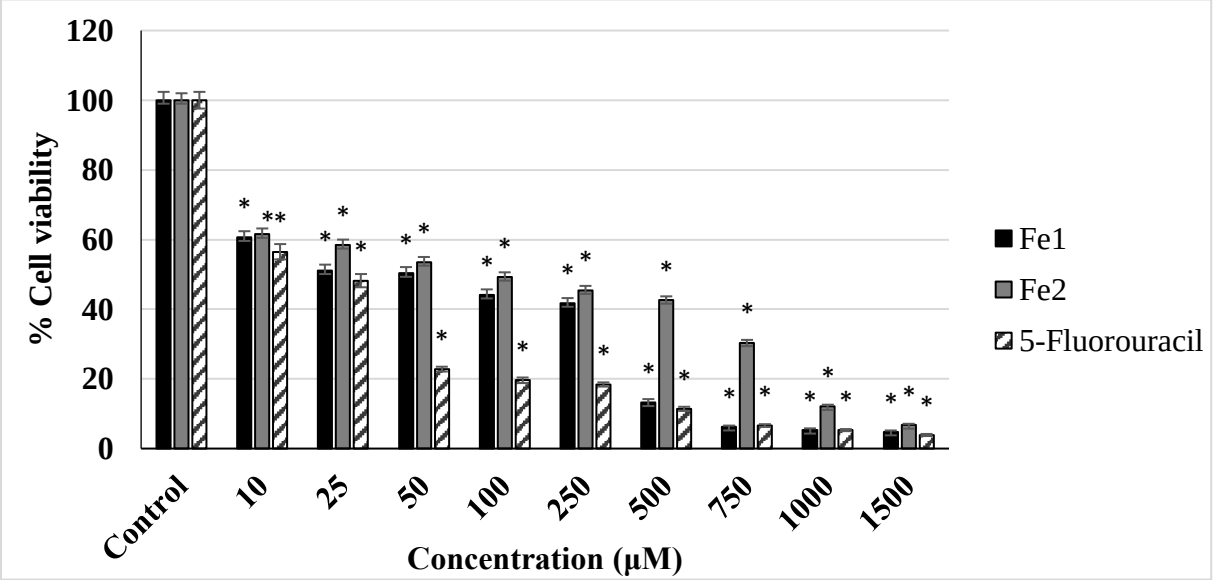


Figure S2c. The effects of complexes **Fe1**, **Fe2** and 5-Fluorouracil on viability of HeLa cell line for 72 h. Results are represented as mean of three replicates ± standard deviation. *$p < 0.05$ compared to control.

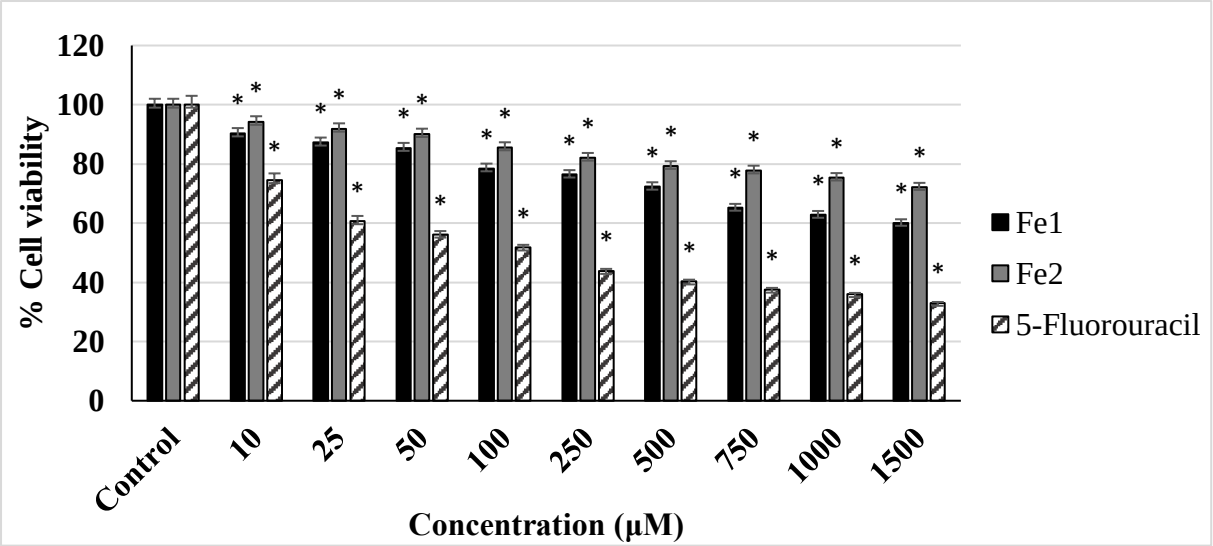


Figure S3a. The effects of complexes **Fe1, Fe2** and 5-Fluorouracil on viability of L929 cell line for 24 h. Results are represented as mean of three replicates ± standard deviation. *$p < 0.05$ compared to control.

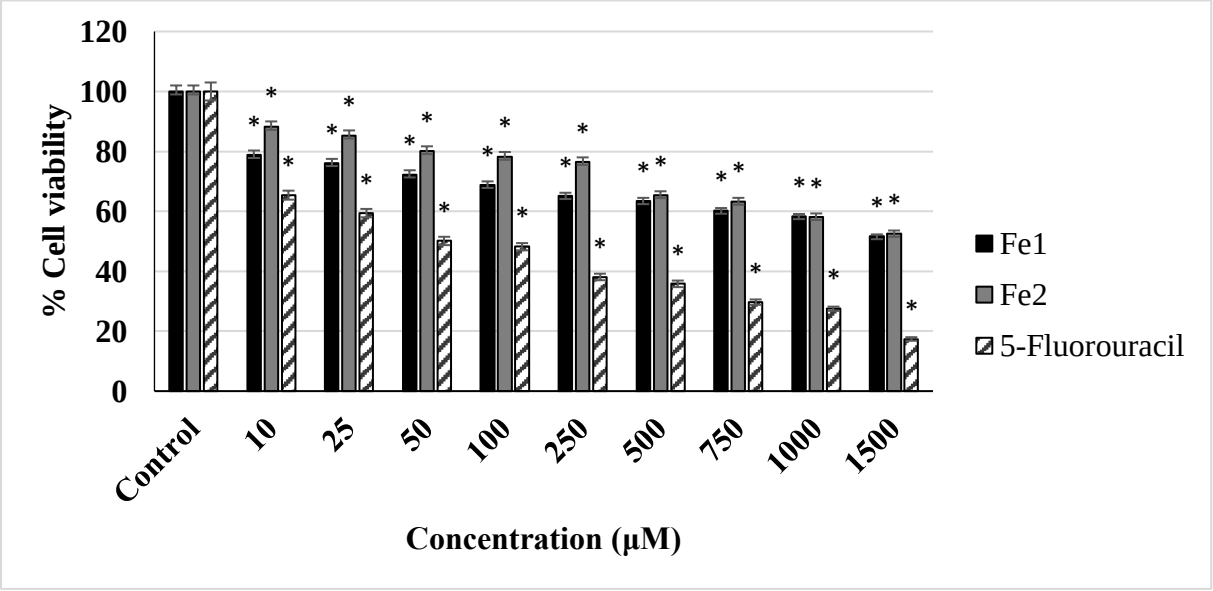


Figure S3b. The effects of complexes **Fe1**, **Fe2** and 5-Fluorouracil on viability of L929 cell line for 48 h. Results are represented as mean of three replicates ± standard deviation. *$p < 0.05$ compared to control.

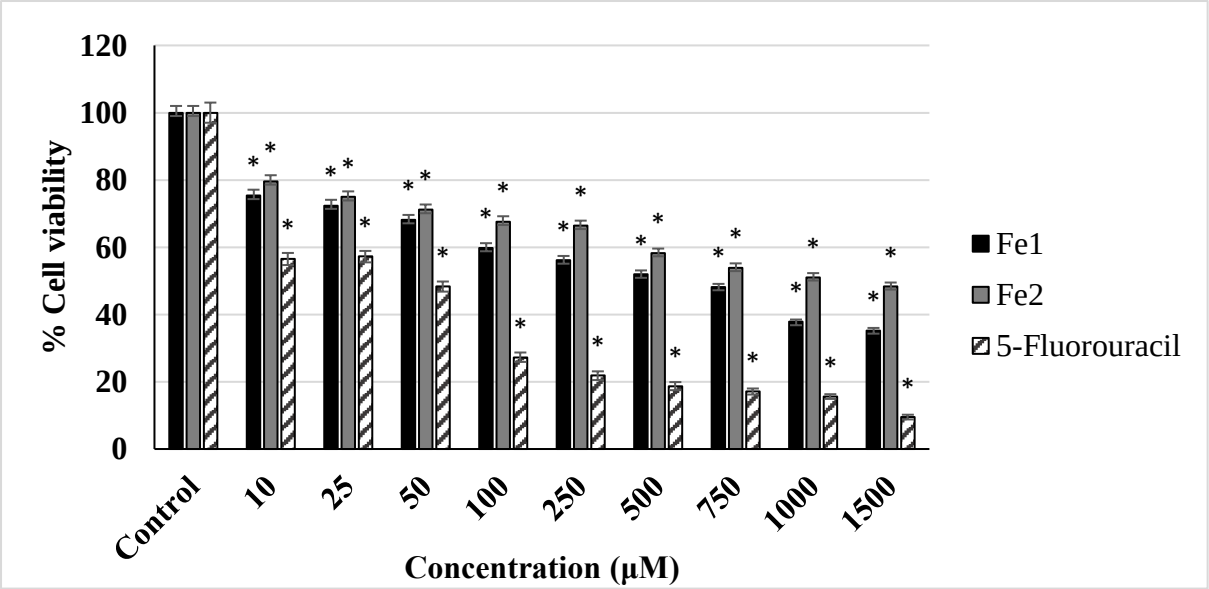


Figure S3c. The effects of complexes **Fe1**, **Fe2** and 5-Fluorouracil on viability of L929 cell line for 72 h. Results are represented as mean of three replicates ± standard deviation. *$p < 0.05$ compared to control.

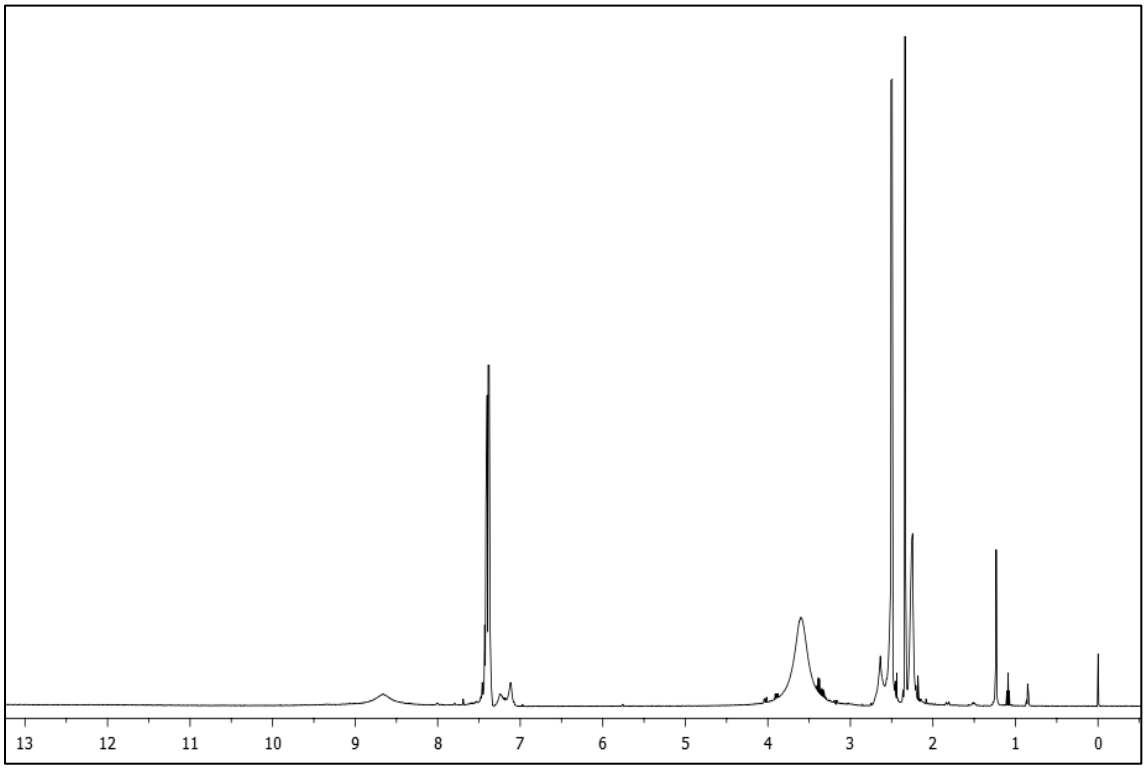


Figure S4. ^{1}H NMR spectrum of 3-benzylidene-2,4-pentanedione-S-methylthiosemicarbazone hydrogen iodide in DMSO-d_6.

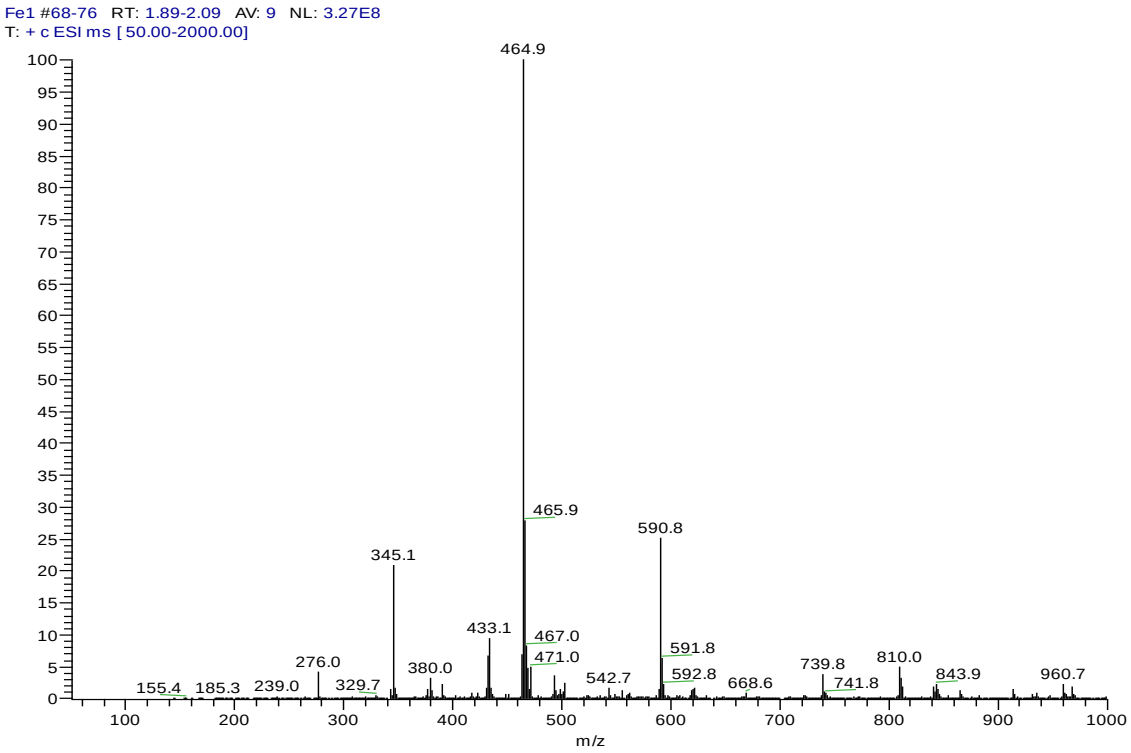


Figure S5. ESI-MS of **Fe1** in $CHCl_3$.

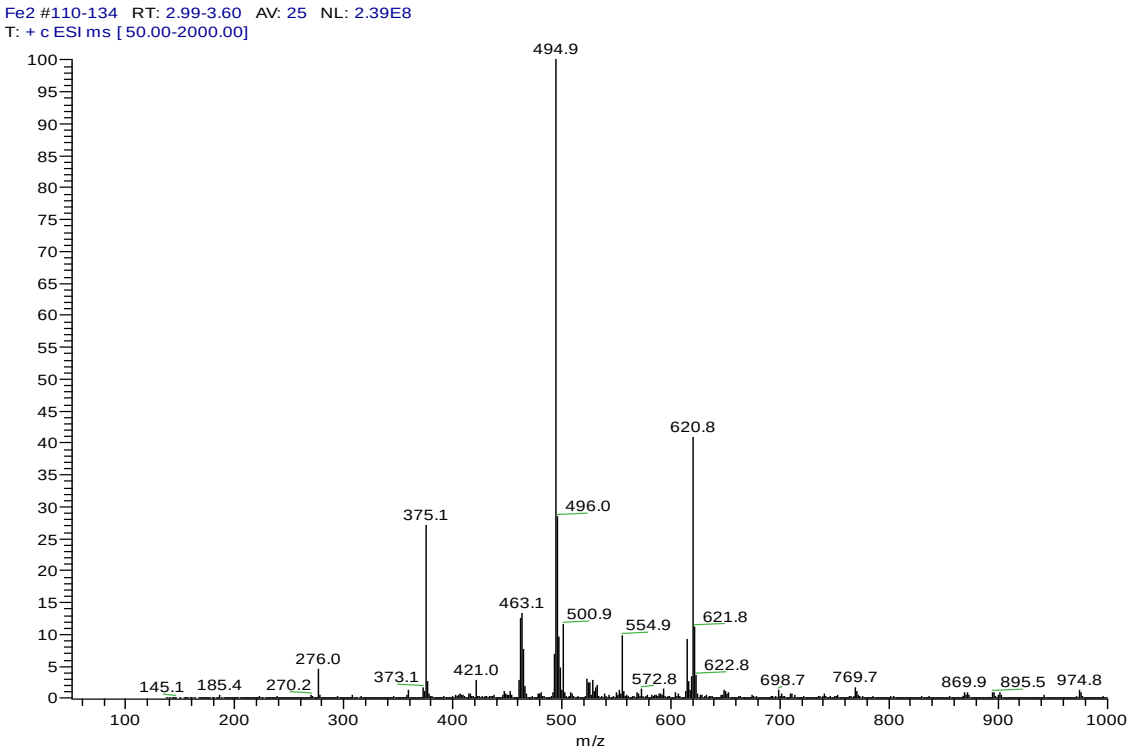


Figure S6. ESI-MS of **Fe2** in $CHCl_3$.

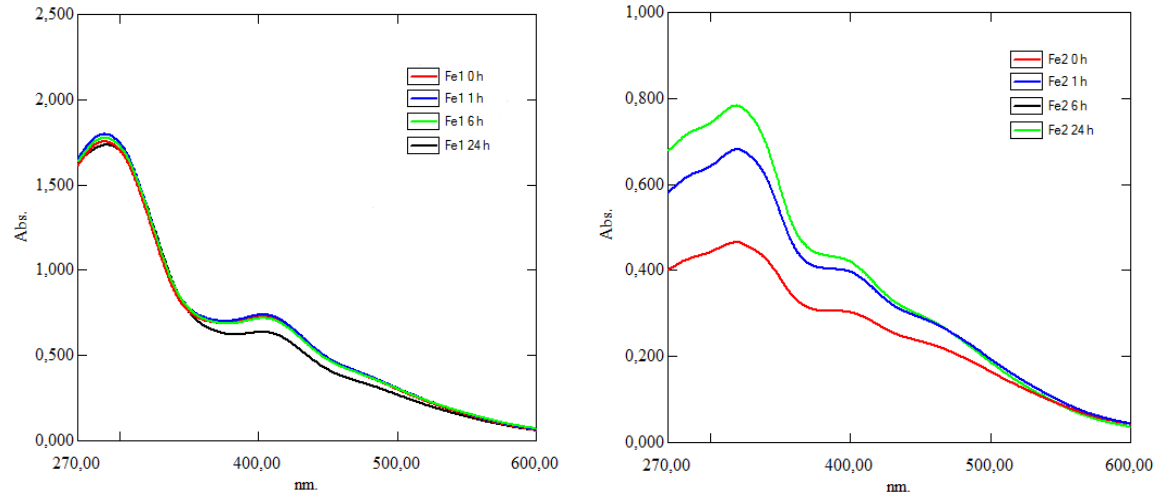
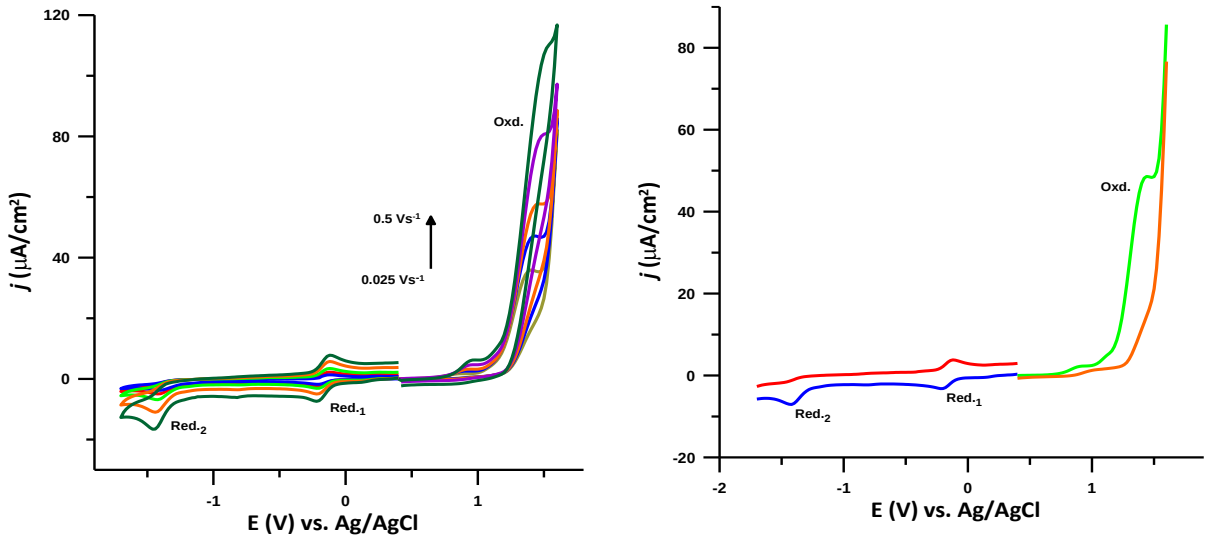
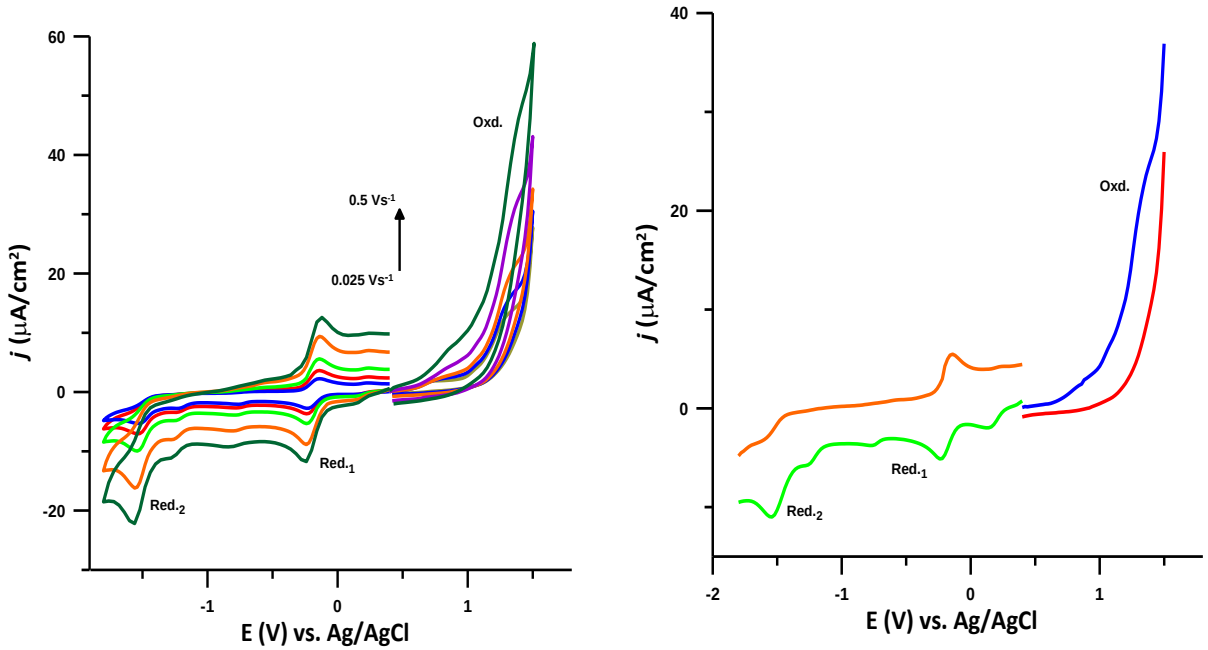


Figure S7. UV-Visible spectra of **Fe1** and **Fe2** in 1% DMSO-water mixture.



(a) **(b)**

Figure S8. CVs of **Fe1** (1.0 x 10^{-3}M) at different scan rates (0.025, 0.05, 0.1, 0.25, 0.5 Vs^{-1}) **(a)** and LSVs at a scan rate of 0.1 Vs^{-1} in 0.1 M TBAP/DMSO solution on GC working electrode **(b)**.



(a) **(b)**

Figure S9. CVs of **Fe2** (1.0 x 10^{-3}M) at different scan rates (0.025, 0.05, 0.1, 0.25, 0.5 Vs^{-1}) **(a)** and LSVs at a scan rate of 0.1 Vs^{-1} in 0.1 M TBAP/DMSO solution on GC working electrode **(b)**.

References

1. B. A. Arslan, B. Kaya, O. Şahin, S. Baday, C. C. Saylan and B. Ülküseven, *J. Mol. Struct.*, 2021, **1246**, 131166.