

DNA / Protein Binding and Apoptotic induced Anti-cancer property of First Time Reported Quercetin – Iron (III) Complex Having Secondary Anionic Residue: A combine Experimental and Theoretical Approach

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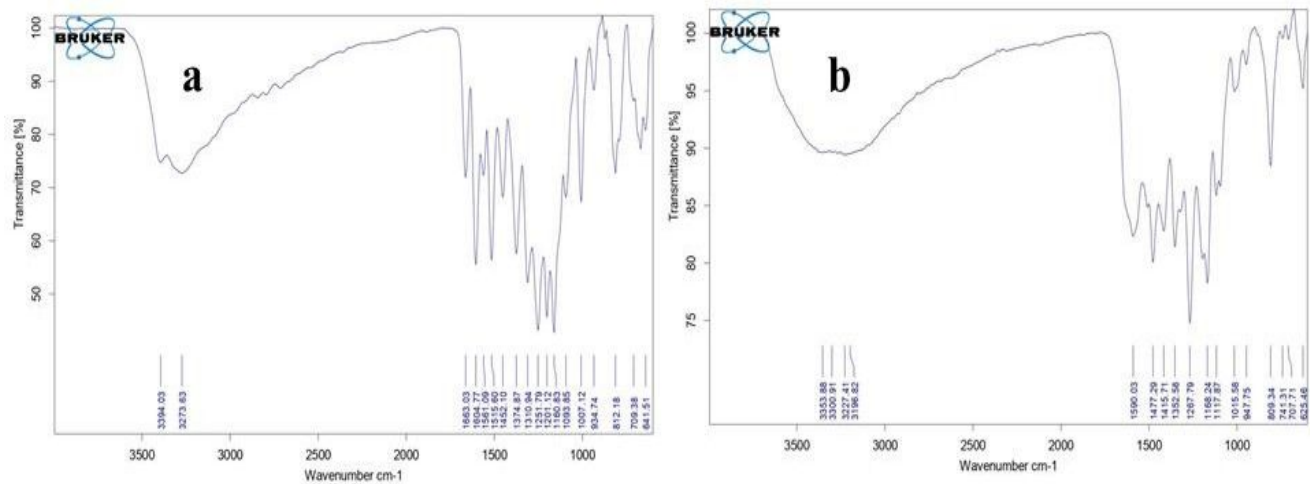


Figure S1: IR spectra of a) Quercetin and b) Complex 1

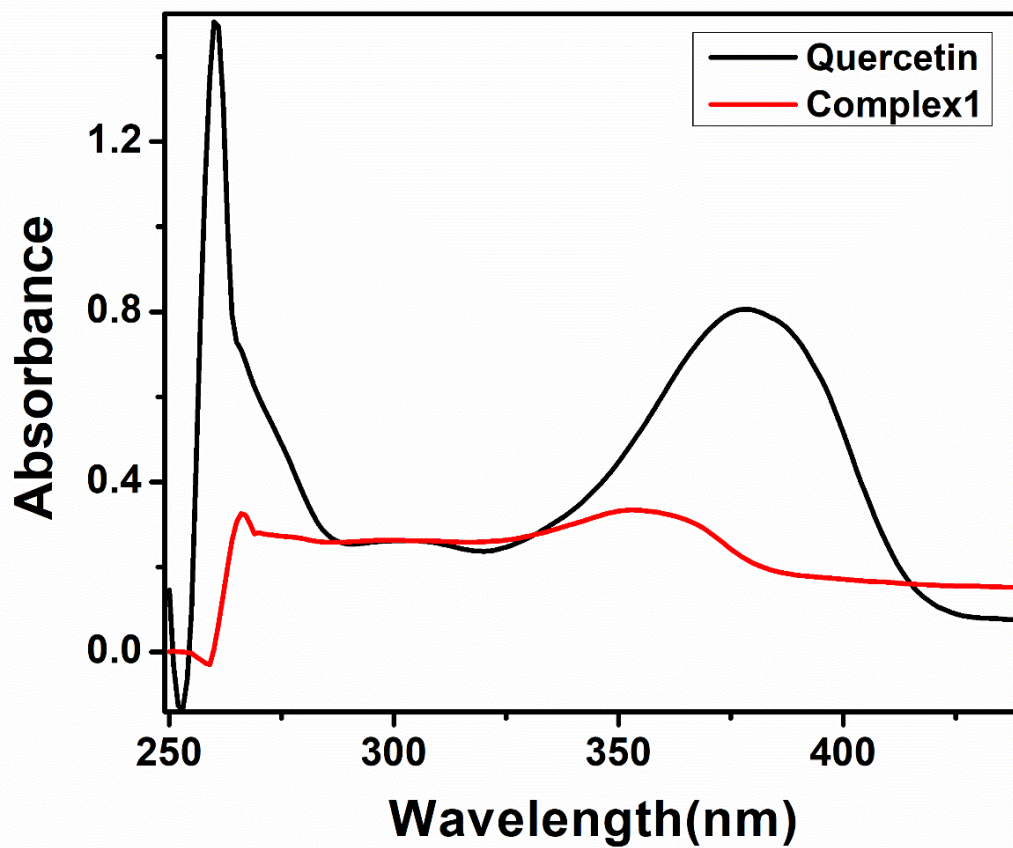


Figure S2: UV spectrum of Quercetin and complex 1

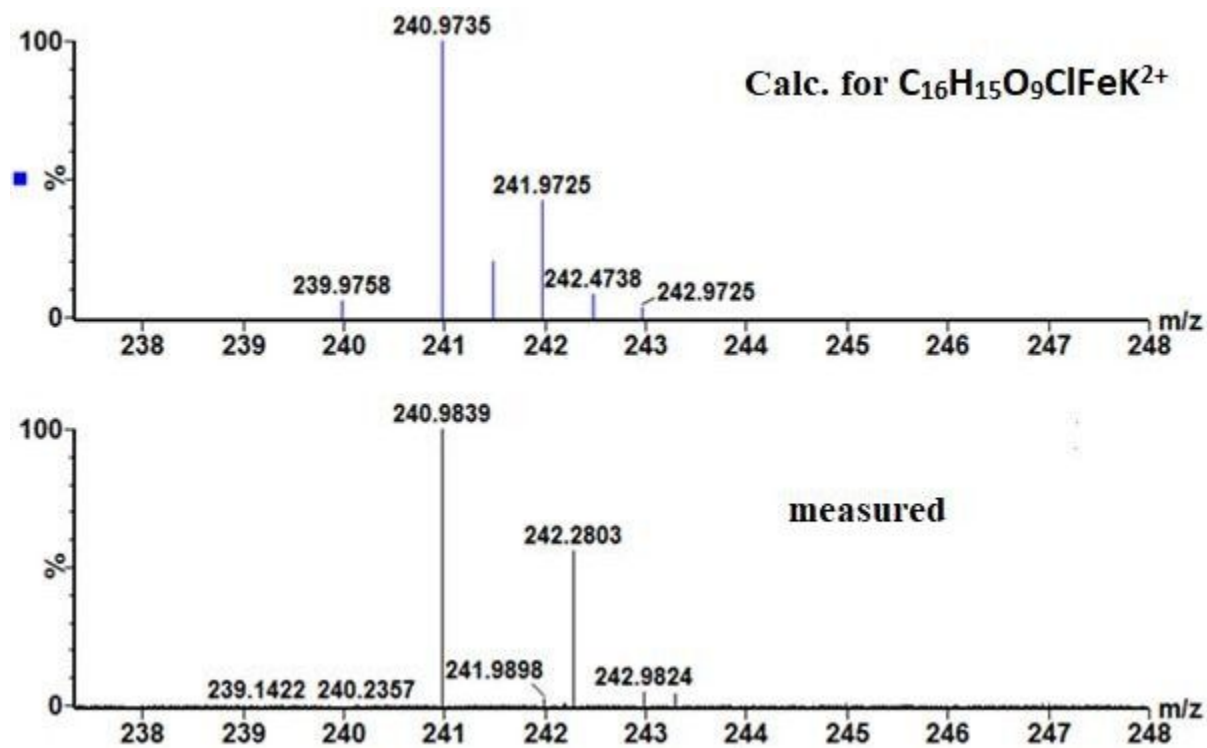


Figure S3: Mass spectra of complex 1

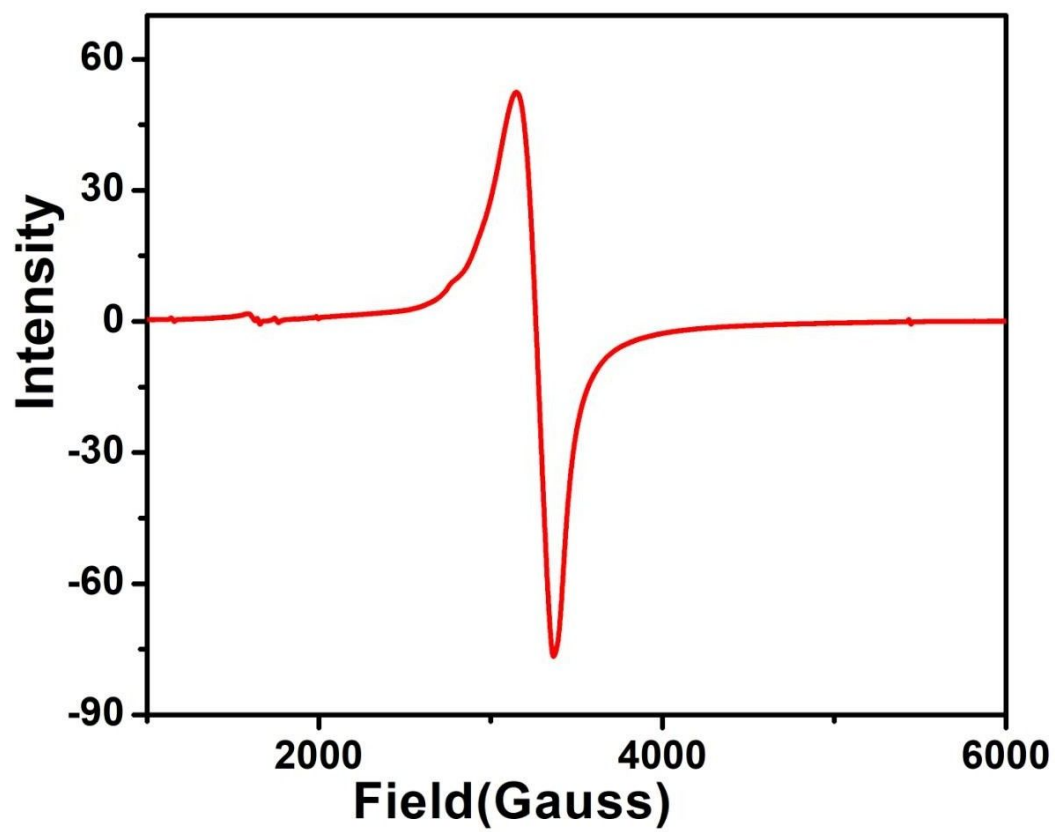


Figure S4: Electron paramagnetic resonance (EPR) spectroscopy of Complex 1

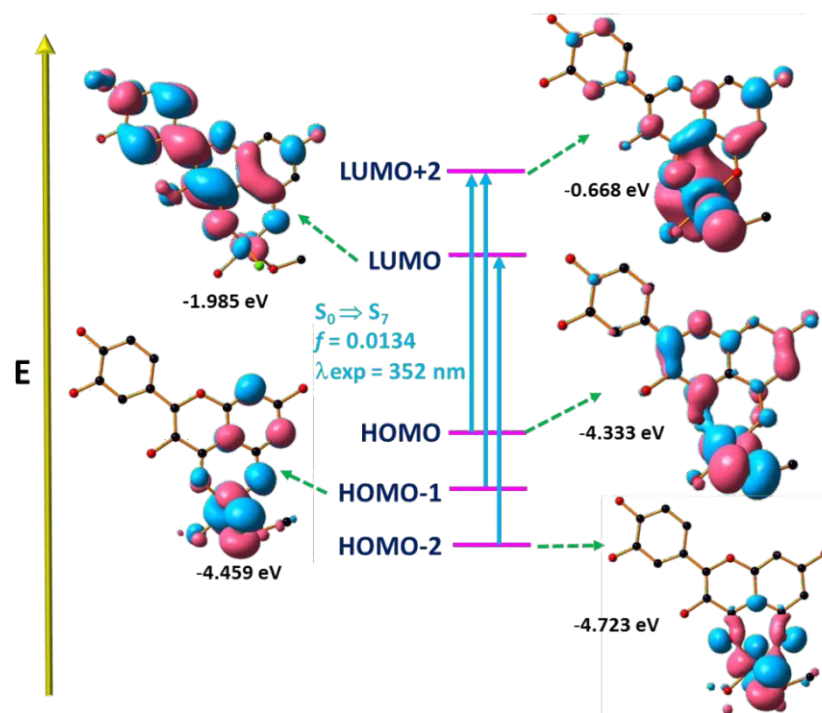


Figure S5: Frontier molecular orbitals involved in the absorbance of complex **1** in DMSO solution

Table S1: Selective bond distances and bond angles of **1**.

Bond distance(Å)		Bond angles (°)	
Fe1-Cl1	2.337	Cl1- Fe1-O1	106.50
Fe1-O1	1.875	Cl1- Fe1-O2	93.80
Fe1-O2	1.902	O1- Fe1-O2	93.59
Fe1-O1W	2.008	O1- Fe1-O1M	161.27
Fe1-O1M	2.020	O1- Fe1-O1W	86.52
		O2- Fe1-O1M	86.31
		O2- Fe1-O1W	179.87
		Cl1- Fe1-O1W	86.21
		Cl1- Fe1-O1M	92.17

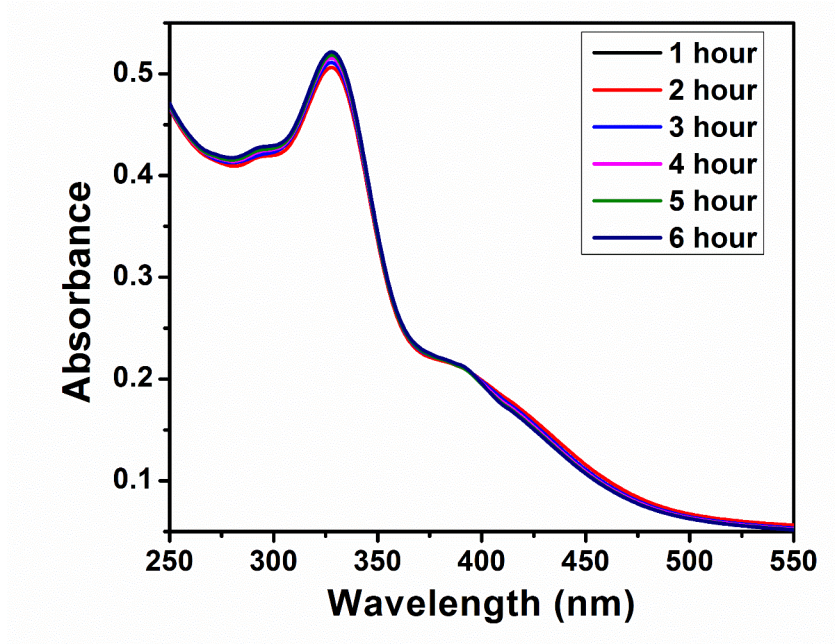


Figure S6: At CP buffer at pH 7.4 the stability curve of complex **1** as a function of time

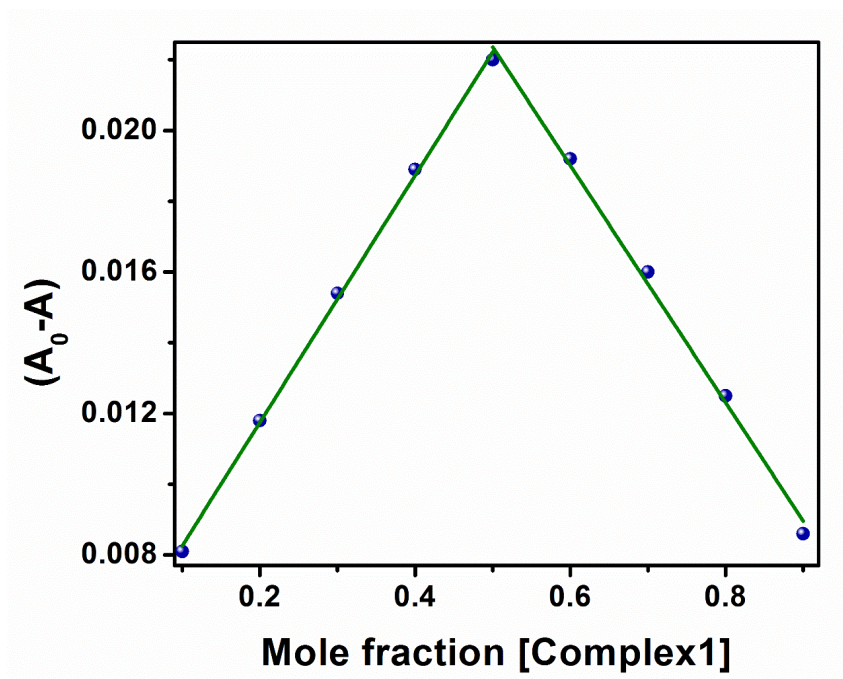


Figure S7: Job's plot by using fluorescence quenching of the HSA by complex **1**

Table S2: Fluorescence Lifetime decay parameters of HSA in the absence and presence of Complex 1

Sample	α_1	τ_1 (ns)	α_2	τ_2 (ns)	τ_{av} (ns)	χ^2
HSA	0.80	0.61	0.20	5.21	3.74	1.60
HSA + Complex1_a	0.85	0.50	0.15	4.76	3.18	1.64
HSA + Complex1_b	0.88	0.43	0.12	4.14	2.54	1.62
HSA + Complex1_c	0.90	0.38	0.10	3.86	2.22	1.65

Table S3: Statistical data analysis in 48 hrs incubation

Dose (μ M)	Survival (%)						AVG	SD	P
	repeat 1		repeat 2		repeat 3				
0	100	100	100	100	100	100	100	0	-
1.25	35.434 08	38.342 85	41.516 05	40.987 18	42.838 22	58.439 79	42.926 36	8.0444 58	0.0003
2.5	18.774 77	13.750 54	18.774 77	15.072 71	14.808 27	19.568 07	16.791 52	2.5183 73	0.0001
5	9.7840 37	10.841 77	11.106 2	12.692 81	12.163 94	15.072 71	11.943 58	1.8428 31	<0.00 01

10	8.7263 03	5.0242 35	6.3464 03	8.1974 37	6.6108 36	12.957 24	7.9770 75	2.7805 36	<0.00 01
20	8.7263 03	6.3464 03	8.9907 37	6.6108 36	5.2886 69	11.899 5	7.9770 75	2.3969 79	<0.00 01

