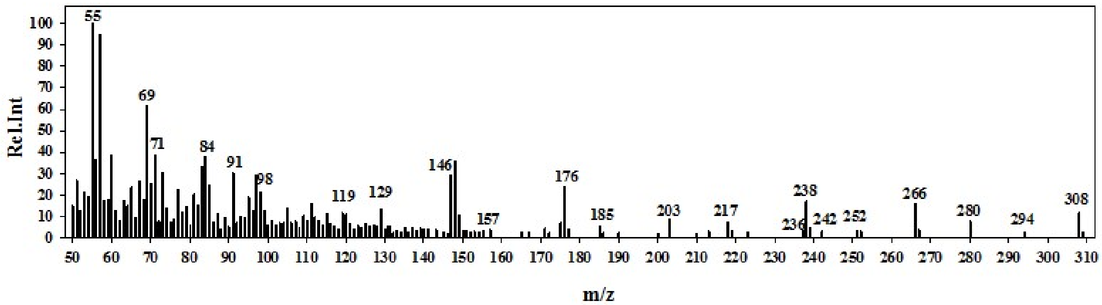

Fig. S1 Mass spectrum of Sbat

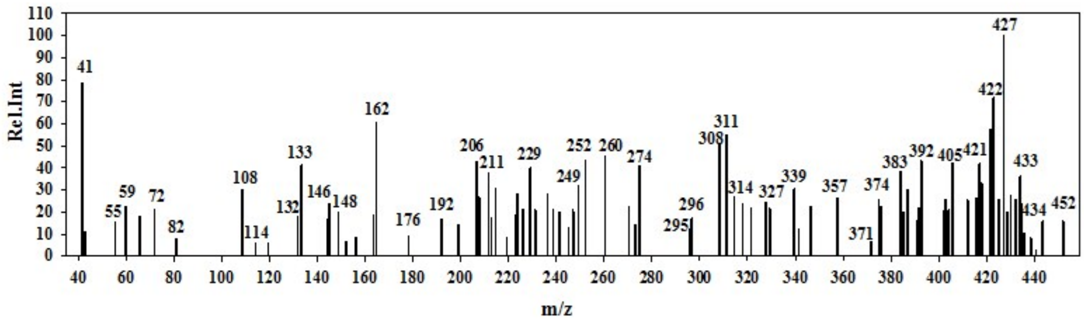

Fig. S2 Mass spectrum of Ag-Sbat

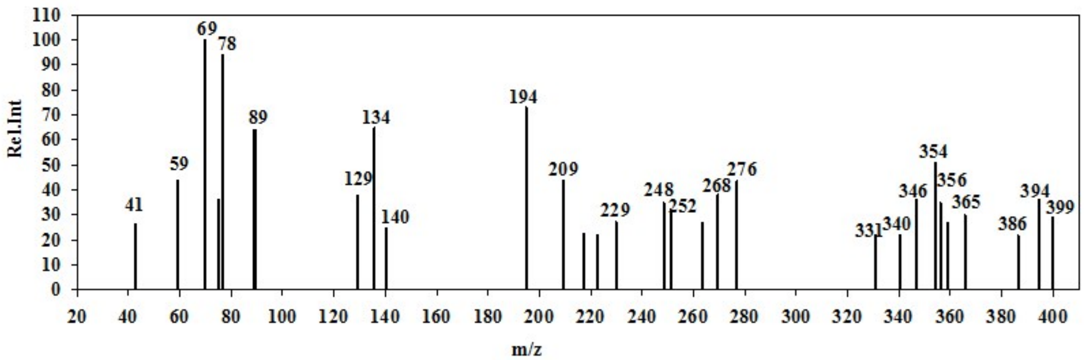

Fig. S3 Mass spectrum of Cu-Sbat

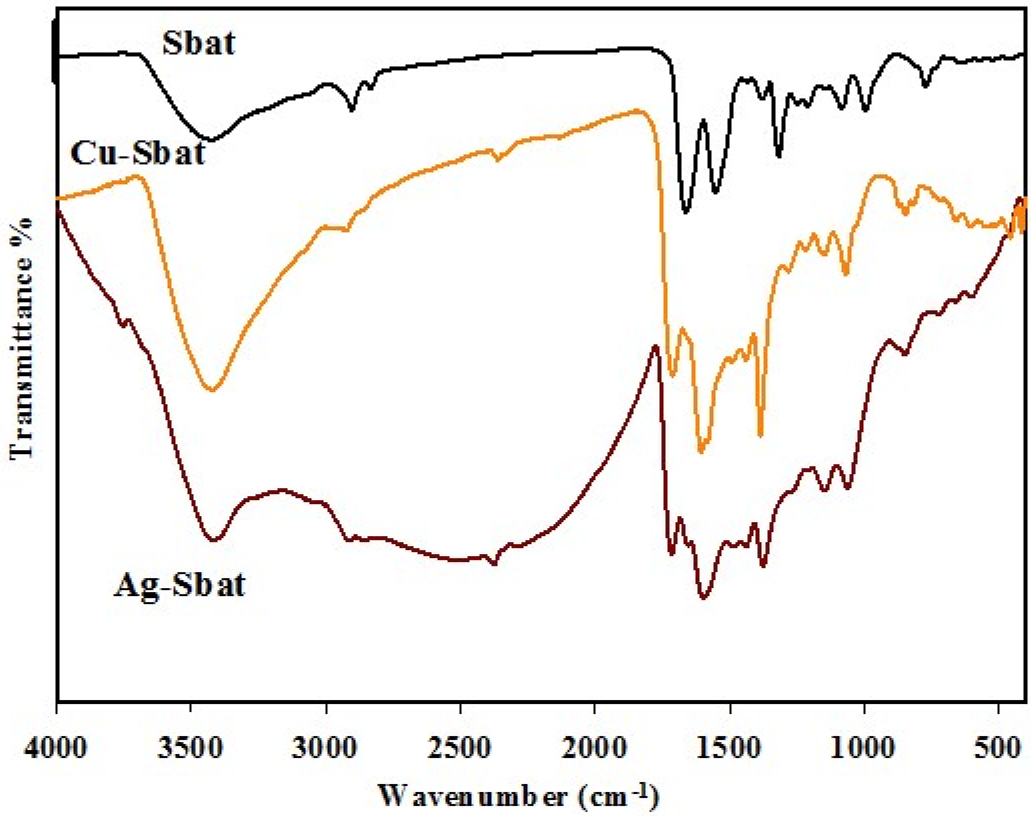

Fig. S4 IR spectra of the Schiff base and its complexes

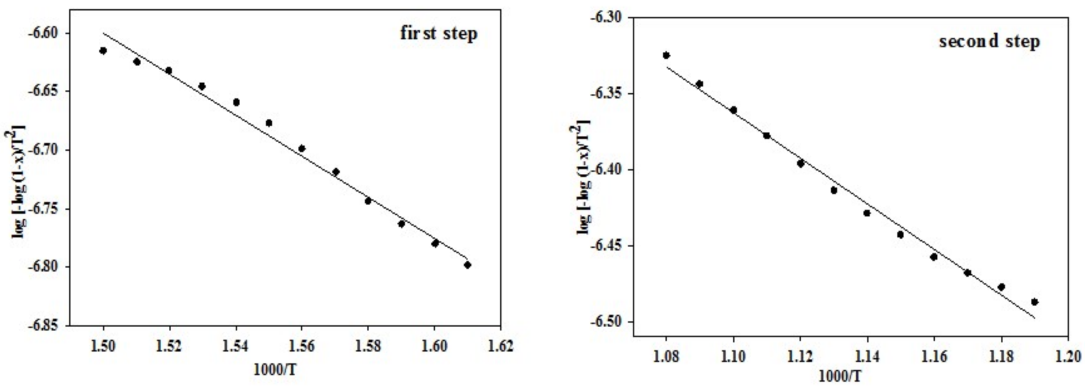

Fig. S5 A plot of log (–log (1 – x)/T^2) vs. 1000/T of silver complex based on Coats-Redfern equation

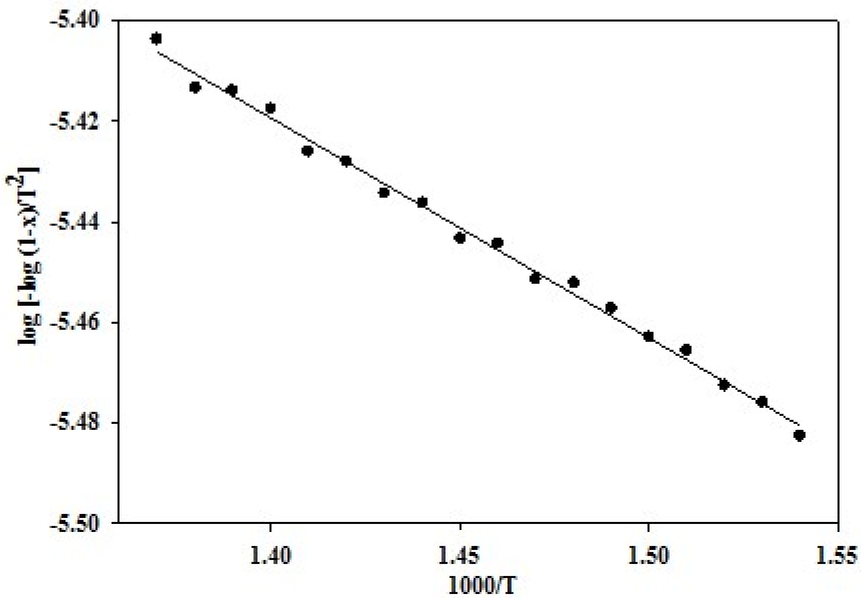

Fig. S6 A plot of log (–log (1 – x)/T^2) vs. 1000/T of copper complex based on Coats-Redfern equation

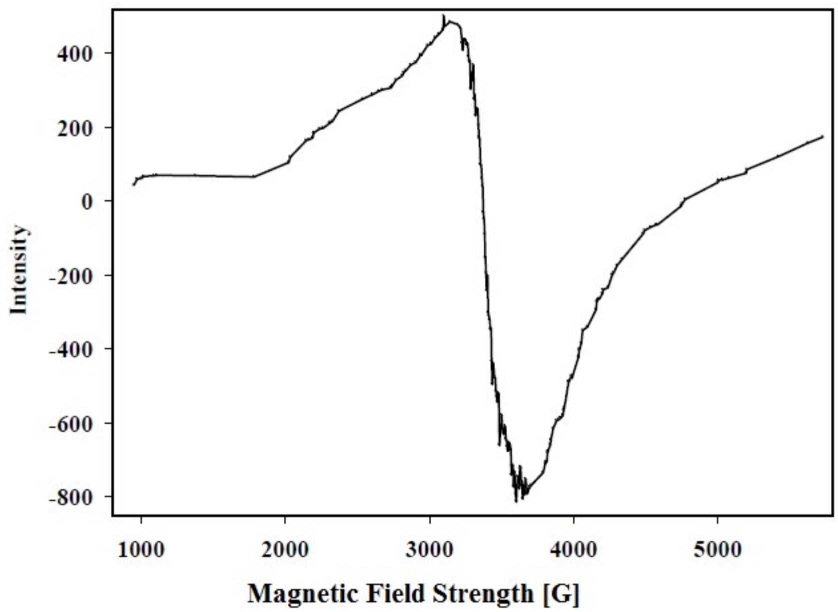

Fig. S7 The ESR spectrum of Cu-Sbat complex

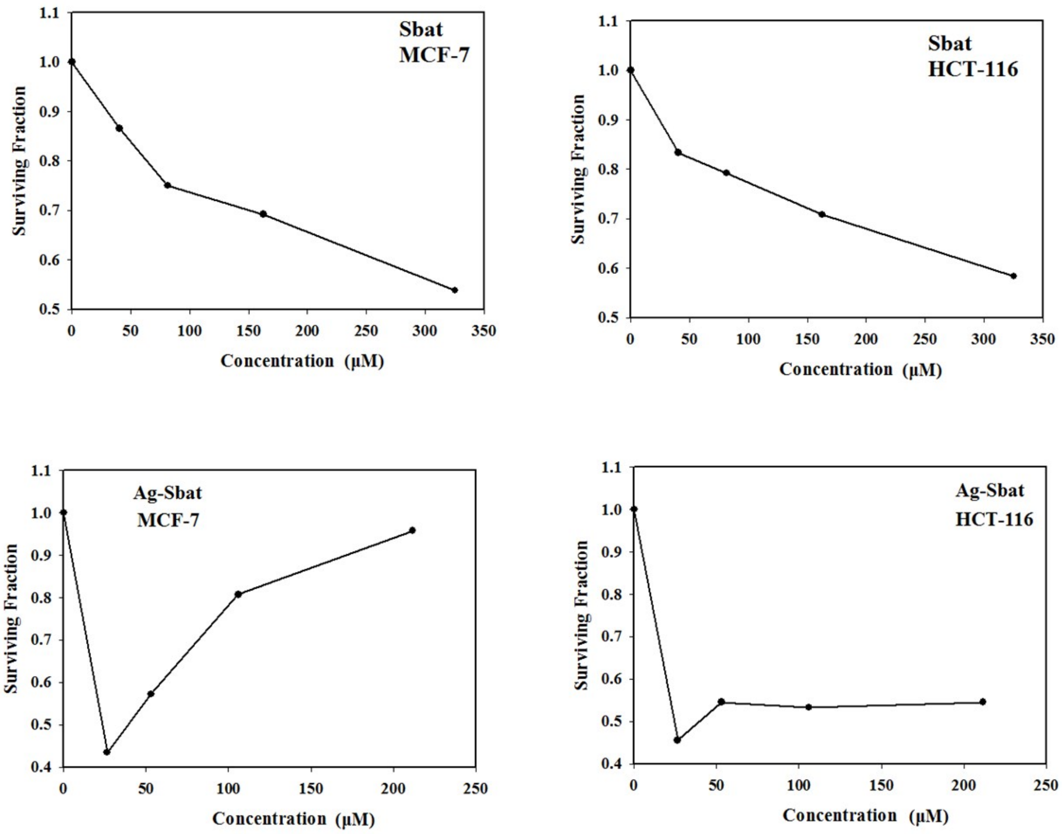

Fig. S8 The IC_{50} values of the studied Sbat Schiff base and its complex Ag-Sbat against MCF-7 and HCT-116 cell lines

Table S1 Natural population of the total electrons in the complexes on the sub-shells using B3LYP/LANL2DZ

	Ag-Sbat	Cu-Sbat
Effective Core	28.00000	10.00000
Core	57.97789 (99.9619% of 58)	55.97833 (99.9613% of 56)
Valence	139.50109 (99.6436% of 140)	138.53080 (99.6624% of 139)
Natural Minimal Basis	225.47899 (99.7695% of 226)	204.50912 (99.7605% of 205)
Natural Rydberg Basis	0.52101 (0.2305% of 226)	0.49088 (0.2395% of 205)

Table S2 Total static dipole moment (μ), the mean polarizibility $<\alpha>$, the anisotropy of the polarizibility Δα and the first order hyperpolarizibility $<\beta >$ for the complexes using B3LYP/LANL2DZ

Property	Urea	Sbat	Ag-Sbat	Cu-Sbat
$_x\mu$		-1.8302	0.8845	2.8811
$_y\mu$		2.0683	6.5057	0.0263
$_z\mu$		0.5491	1.0940	0.6637
μ(,D)	1.3197	2.8159	6.6551	2.9567
α_{xx}, au		-66.5128	-144.2016	-116.7465
α_{yy}		-140.6692	-163.4716	-149.2615
α_{zz}		-123.2214	-161.2235	-155.8040
α_{xy}		21.4380	-64.1960	41.3467
α_{xz}		-0.0708	2.9646	3.7723
α_{yz}		-1.8738	-0.6322	5.1133
$<\alpha>$, esu		-1.632×10^{-23}	-2.316×10^{-23}	-2.084×10^{-23}
Δα, esu		9.952×10^{-24}	2.705×10^{-24}	5.370×10^{-24}
β_{xxx}, au.		-236.4058	-159.5028	157.1280
β_{yyy}		47.9714	159.2092	-72.7442
β_{zzz}		0.2297	-34.0541	-28.8688
β_{xyy}		-20.1473	-92.0317	146.0700
β_{xxy}		-6.0145	44.0277	32.9440
β_{xxz}		-6.4757	-6.9564	33.2657
β_{xzz}		-4.9762	-46.5174	28.2583
β_{yzz}		-7.1374	-5.1148	-11.3472
β_{yyz}		1.7659	7.2477	-10.9779
β_{xyz}		-0.0682	43.9141	26.2119
$<\beta>$, esu	$0.1947x10^{-30}$	$2.280x10^{-30}$	$3.106x10^{-30}$	$2.898\ x10^{-30}$

Table S3 Orbital involved in vertical transition, coefficient, oscillator strength, transition energy, observed and calculated wavelength for Ag-Sbat and Cu-Sbat

State	Orbital	Coefficient	f	ΔE, eV	λ_{max}	
					Exp.	Calc.
			Ag-Sbat			
S1	96-100	0.1405	0.046	3.9	320	326
	97-100	0.1551				
	98-100	0.6192				
	98-101	0.1485				
	98-102	0.1139				
	94-101	0.1007				
S2	97-100	0.2507	0.483	4.90	290	289
	98-102	0.1152				
	99-100	0.2025				
	98-101	0.6001				
			Cu-Sbat			
S1	91A-99A	0.1062	0.015	3.9	327	335
	93A-99A	0.1384				
	96A-99A	0.1948				
	97A-99A	0.4883				
	98A-100A	0.3602				
	89B-98B	0.1219				
	96B-99B	0.4668				
	96B-100B	0.1876				
	97B-100B	0.3762				
S2	93A-100A	0.662	0.433	4.13	298	300
	94A-99A	0.1141				
	96A-99A	0.2710				
	97A-100A	0.1167				
	98A-102A	0.1942				
	87B-98B	0.1592				
	88B-98B	0.2910				
	92B-100B	0.1021				
	93B-100B	0.1391				
	94B-99B	0.4617				
	95B-99B	0.5221				
	96B-100B	0.1752				
	97B-102B	0.1582				