Supplementary Information

Synthesis, structural, spectral and molecular docking of Ni(II) and Pd(II) complexes with isatin moiety and their DNA cleavage activity

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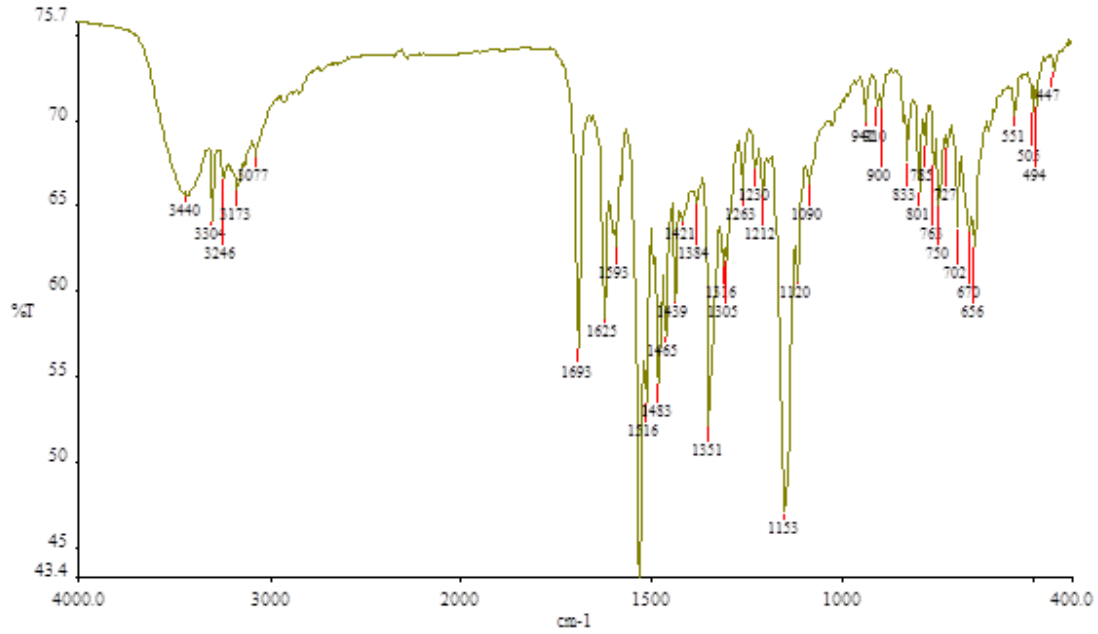

Fig. S1 —FT-IR spectrum of [(*Z*)-2-(5-nitro-2-oxoindolin-3-ylidene)-*N*-phenylhydrazinecarbothioamide] in KBr

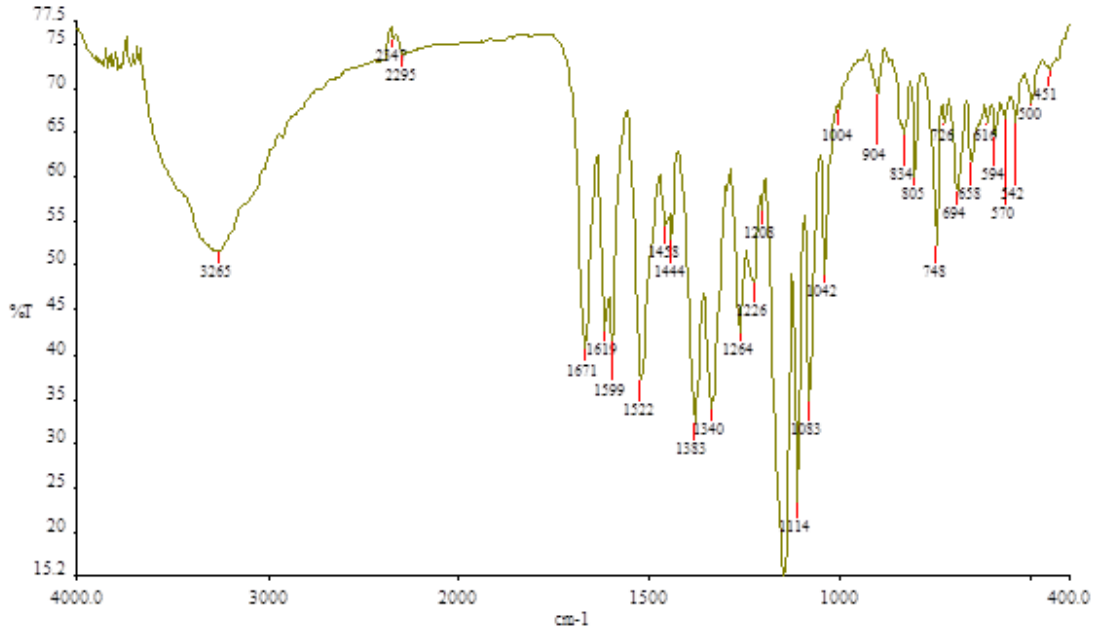

Fig. S2— FT-IR spectrum of Bis[2-(5-nitro-2-oxoindolin-3-ylidene)-*N*-phenylhydrazinecarbothioamidato-κ^3O, N^2, S]nickel(II) dihydrate in KBr

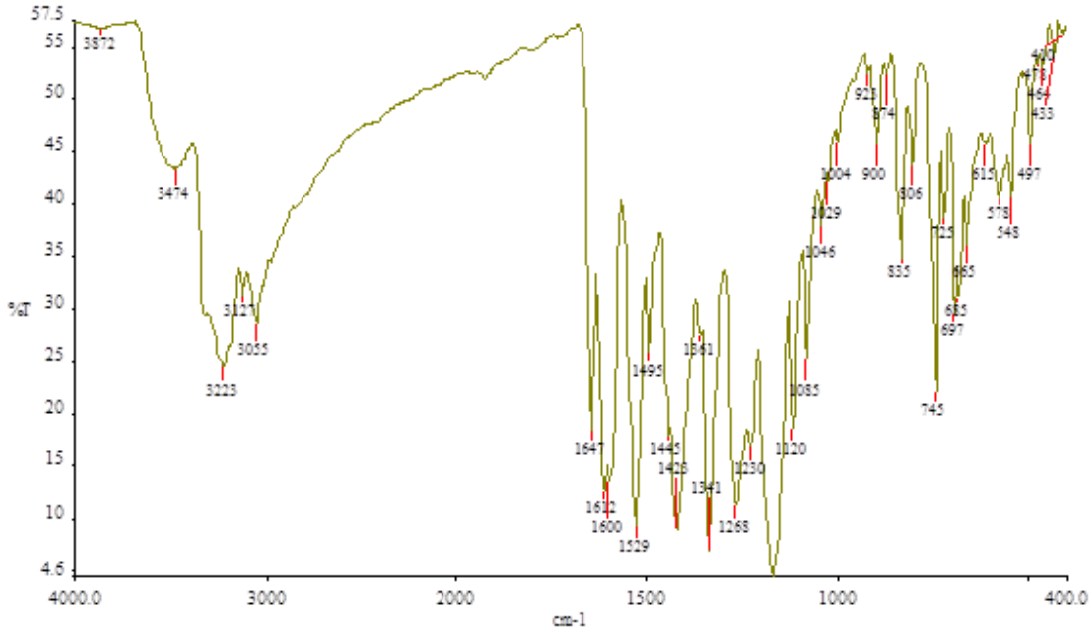

Fig. S3— FT-IR spectrum of chloro{*N*′-[5-chloro-2-(oxo-κ*O*)-1, 2-dihydro-3*H*-indol-3-ylidene]-*N*-phenylcarbamohydrazonothioato- $\kappa^2 N'$, *S*}palladium(II) in KBr

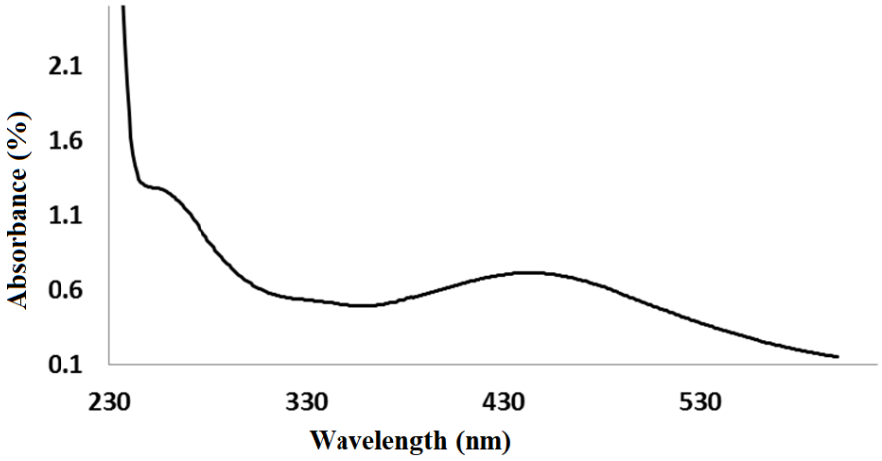

Fig. S4— Electronic spectrum of [(*Z*)-2-(5-nitro-2-oxoindolin-3-ylidene)-*N*-phenylhydrazinecarbothioamide] in DMSO

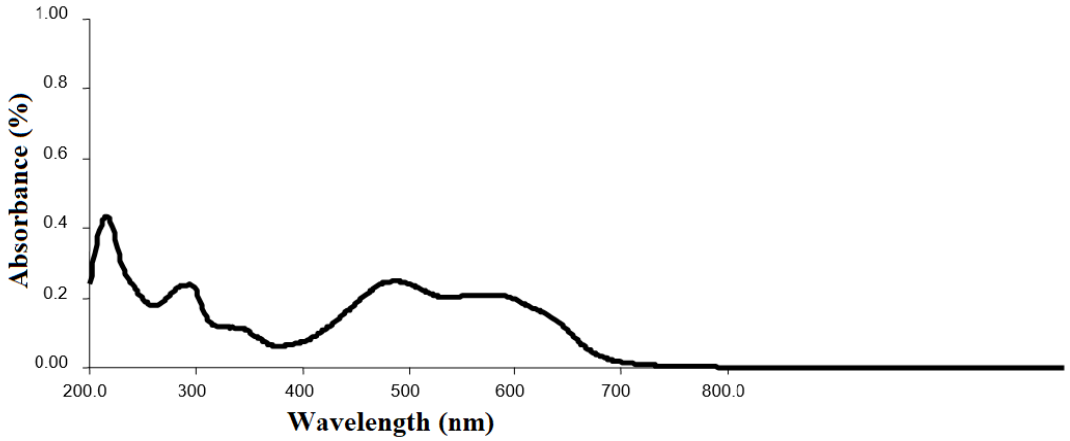

Fig. S5— Electronic spectrum of Bis[2-(5-nitro-2-oxoindolin-3-ylidene)-*N*-phenylhydrazinecarbothioamidato-$\kappa^3 O$, N^2, *S*]nickel(II) di hydrate in DMSO

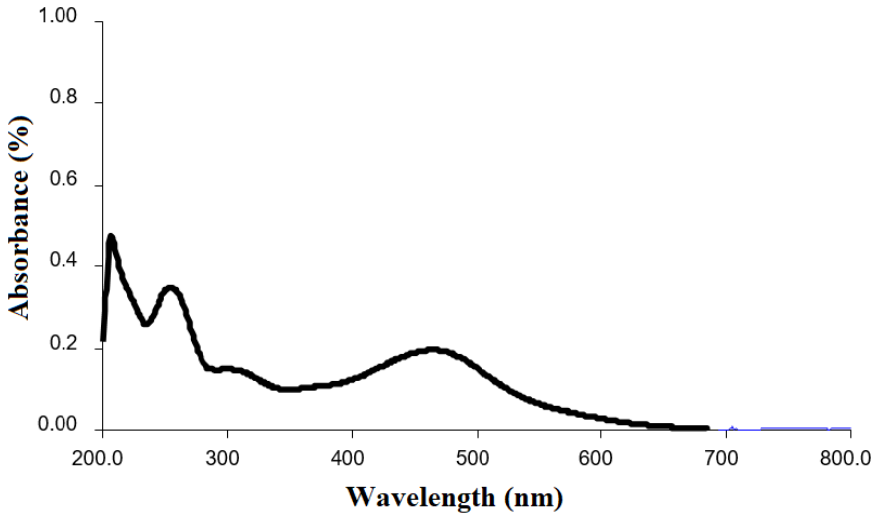

Fig. S6— Electronic spectrum of chloro{*N*′-[5-chloro-2-(oxo- κ*O*)-1, 2-dihydro-3*H*-indol-3-ylidene]-*N*-phenylcarbamohydrazonothioato- $\kappa^2 N'$, *S*} palladium(II) in DMSO

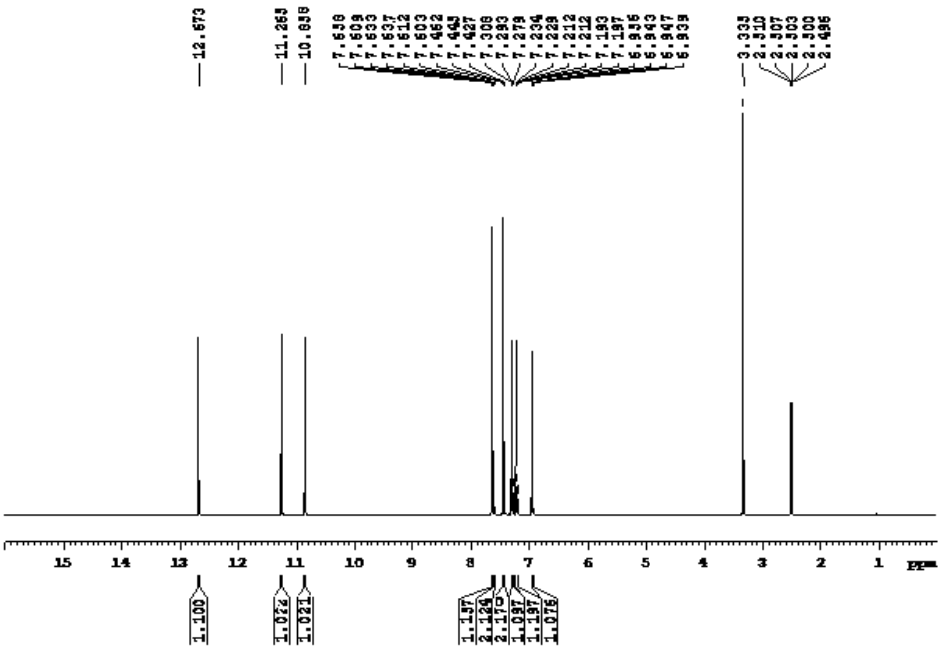

Fig. S7—^{1}H NMR spectrum of [(*Z*)-2-(5-nitro-2-oxoindolin-3-ylidene)-*N*-phenylhydrazinecarbthioamide]

Table S1 — Percentages of the different intermolecular contacts in the studied crystal structure			
	A	**B**	**C**
S…S	0.2	0.5	0.2
S…H	9.8	8.8	9.8
S…O	0	1	0.8
S…N	0.2	0.8	0.6
S…C	1.7	1.9	0.3
O…O	0.4	0.5	0.4
O…N	2.6	1.3	2.8
C…O	1.7	2.2	2.2
O…H	24.7	21.1	25.1
N…N	1.5	1	1.4
C…N	4.1	4.5	2.8
N…H	4	5.4	3.4
C…C	12.3	8.4	9.6
H…C	7.7	13.3	11.7
H…H	29.1	29.4	28.9

Table S2 — The calculated bond distances (R, Å) and angles (A,˚) of [(Z)-2-(5-nitro-2-oxoindolin-3-ylidene)-N-phenylhydrazinecarbothioamide]

Bond(s)	**Calc.**	**Exp.**	**Bond(s)**	**Calc.**	**Exp.**
R(1-21)	1.669	1.662	A(4-9-15)	117.601	118.104
R(2-20)	1.225	1.236	A(10-5-20)	111.727	111.006
R(3-9)	1.231	1.232	A(5-10-11)	129.045	128.235
R(4-9)	1.232	1.232	A(5-10-18)	109.119	109.582
R(5-10)	1.394	1.402	A(5-20-19)	105.375	106.351
R(5-20)	1.389	1.366	A(7-6-19)	119.247	117.579
R(6-7)	1.327	1.342	A(6-7-21)	121.594	120.965
R(6-19)	1.302	1.298	A(6-19-18)	126.468	125.122
R(7-21)	1.403	1.392	A(6-19-20)	126.433	128.366
R(8-21)	1.35	1.337	A(7-21-8)	112.517	114.155
R(8-22)	1.412	1.422	A(21-8-22)	132.968	129.749
R(9-15)	1.467	1.457	A(8-22-23)	115.592	116.333
R(10-11)	1.391	1.382	A(8-22-31)	124.861	125.078
R(10-18)	1.418	1.408	A(9-15-13)	118.715	118.732
R(11-13)	1.395	1.39	A(9-15-16)	118.613	118.334
R(13-15)	1.398	1.392	A(11-10-18)	121.837	122.171
R(15-16)	1.397	1.397	A(10-11-13)	117.895	117.575
R(16-18)	1.387	1.377	A(10-18-16)	120.141	120.591
R(18-19)	1.456	1.453	A(10-18-19)	106.68	106.564
R(19-20)	1.494	1.498	A(11-13-15)	119.967	119.911
R(22-23)	1.406	1.381	A(13-15-16)	122.672	122.931
R(22-31)	1.401	1.374	A(15-16-18)	117.488	116.799
R(23-25)	1.39	1.388	A(16-18-19)	133.179	132.834
R(25-27)	1.397	1.362	A(18-19-20)	107.099	106.477
R(27-29)	1.394	1.361	A(23-22-31)	119.547	118.585
R(29-31)	1.395	1.396	A(22-23-25)	120.487	121.316
A(1-21-7)	116.77	116.351	A(22-31-29)	119.221	118.887
A(1-21-8)	130.713	129.485	A(22-31-32)	119.934	120.571
A(2-20-5)	126.635	126.712	A(23-25-27)	120.174	120.225
A(2-20-19)	127.989	126.929	A(25-27-29)	119.22	118.437
A(3-9-4)	124.589	123.332	A(28-27-29)	120.444	120.777
A(3-9-15)	117.81	118.563	A(27-29-31)	121.35	122.502
			A(30-29-31)	118.684	118.757

Table S3 —Cartesian coordinates of the optimized structure of the studied compound			
S	-3.534372000	-2.579213000	-0.000238000
O	0.929240000	-3.747710000	-0.000025000
O	5.334009000	3.155922000	-0.000155000
O	3.184442000	3.524707000	0.000095000
N	3.013510000	-2.691459000	0.000533000
N	-0.050711000	-0.888864000	-0.000068000
N	-1.041801000	-1.771627000	-0.000197000
N	-2.522108000	-0.025153000	-0.001193000
N	4.162645000	2.775871000	-0.000020000
C	3.483968000	-1.379756000	0.000214000
C	4.796965000	-0.919603000	0.000313000
H	5.637328000	-1.605552000	0.000528000
C	5.005116000	0.459689000	0.000178000
H	6.004262000	0.876053000	0.000183000
C	3.912123000	1.330607000	0.000075000
C	2.589511000	0.880884000	0.000061000
H	1.774261000	1.592603000	-0.000038000
C	2.379492000	-0.490158000	0.000116000
C	1.179519000	-1.313950000	0.000087000
C	1.625567000	-2.739821000	0.000152000
C	-2.385652000	-1.368068000	-0.000473000
C	-3.647683000	0.828158000	-0.000428000
C	-3.365654000	2.205240000	-0.001030000
H	-2.331858000	2.543419000	-0.001960000
C	-4.397628000	3.136440000	-0.000406000
H	-4.159993000	4.195854000	-0.000803000
C	-5.727560000	2.710364000	0.000758000
H	-6.535466000	3.435264000	0.001108000
C	-6.004452000	1.344018000	0.001343000
H	-7.034261000	0.999263000	0.002311000
C	-4.980652000	0.395757000	0.000759000
H	-5.204556000	-0.661157000	0.001279000
H	-0.846350000	-2.776459000	-0.000269000
H	3.584280000	-3.524229000	-0.000494000
H	-1.627835000	0.458817000	-0.001044000