

Electronic Supplementary Information

Cycloplatinated(II) complexes bearing 1,1'-bis(diphenylphosphino)ferrocene ligand: Biological evaluation and molecular docking studies

*Masood Fereidoonzehad,^a Hamid R. Shamsavari,^{*b} Sedigheh Abedanzadeh,^c Behnoosh Behchenari,^{la} Mojdeh Hossein-Abadi,^{lb} Zahra Faghih,^d and M. Hassan Beyzavi^{*e}*

^aDepartment of Medicinal Chemistry, School of Pharmacy; Cancer, Environmental and Petroleum Pollutants Research Center, Ahvaz Jundishapur University of Medical Sciences, Ahvaz, Iran.

^bDepartment of Chemistry, Institute for Advanced Studies in Basic Sciences (IASBS), Yousef Sobouti Blvd., Zanjan 45137-66731, Iran.

^cDepartment of Chemistry, Isfahan University of Technology, Isfahan 84156, Islamic Republic of Iran.

^dShiraz Institute for Cancer Research, School of Medicine, Shiraz University of Medical Sciences, Shiraz, Iran.

^eDepartment of Chemistry and Biochemistry, University of Arkansas, Fayetteville, Arkansas 72701, United States.

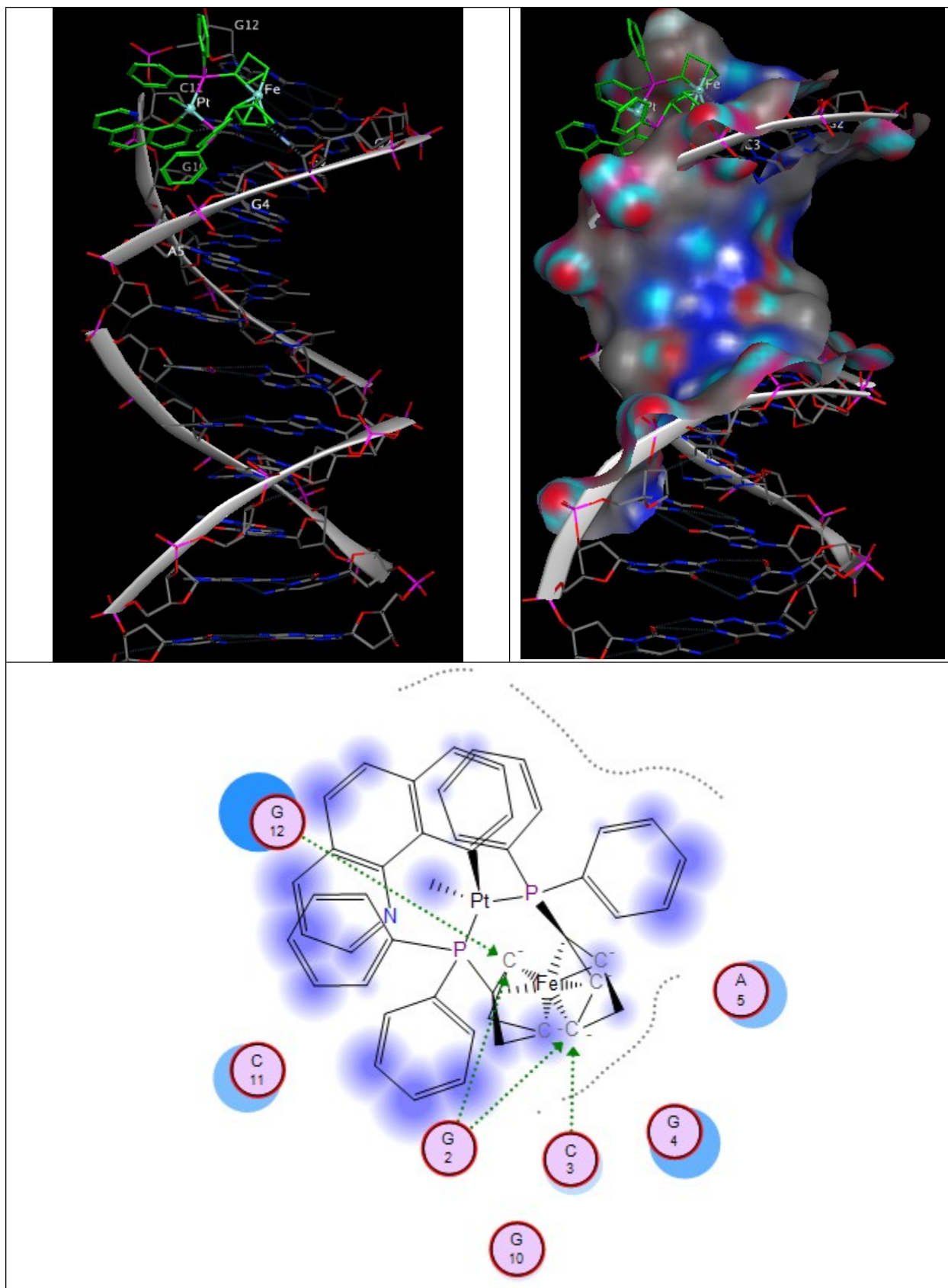
*Email: shamsavari@iasbs.ac.ir. (H.R.S.), beyzavi@uark.edu. (M.H.B.).

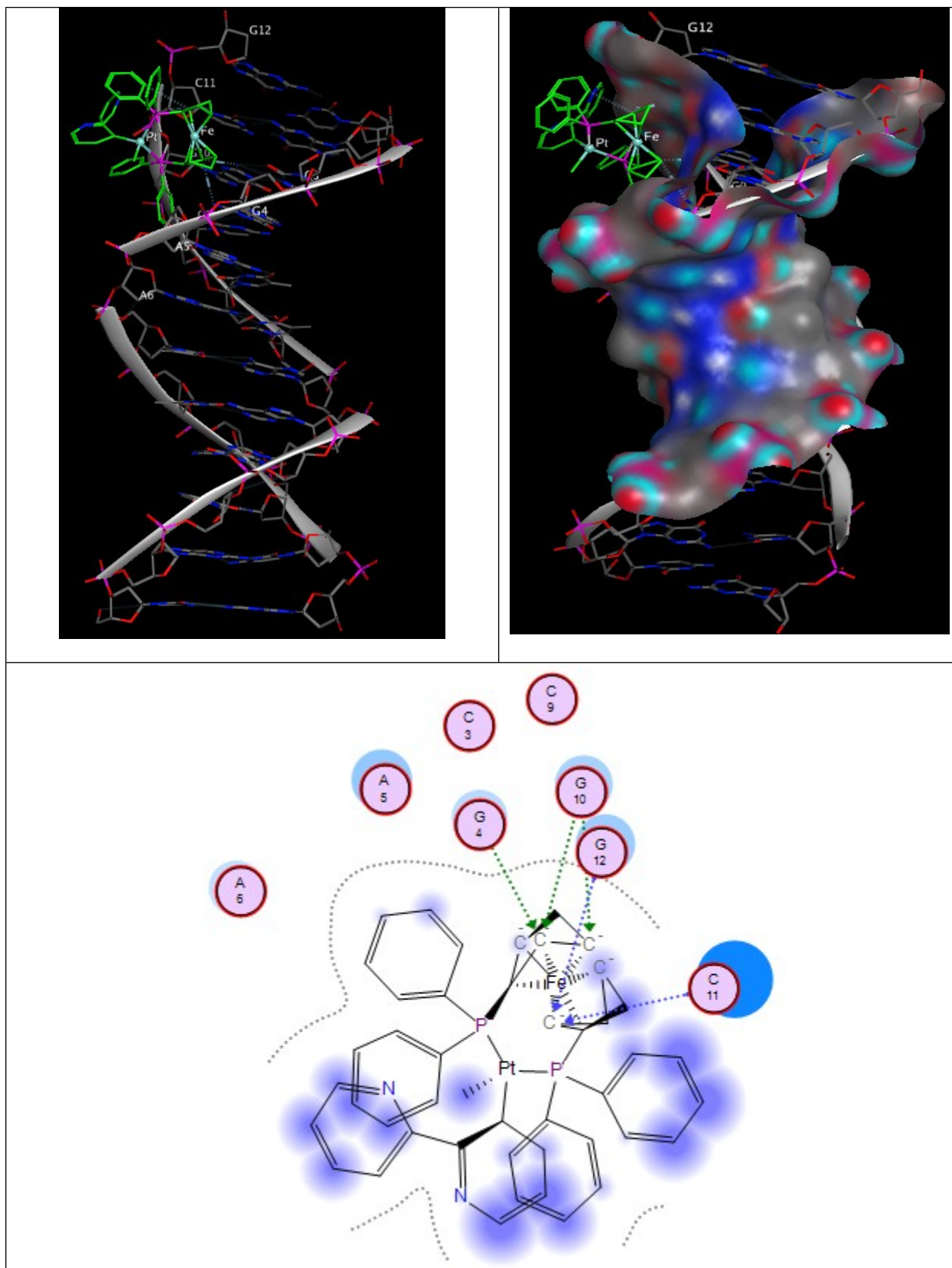
^lThese authors contributed equally to this work.

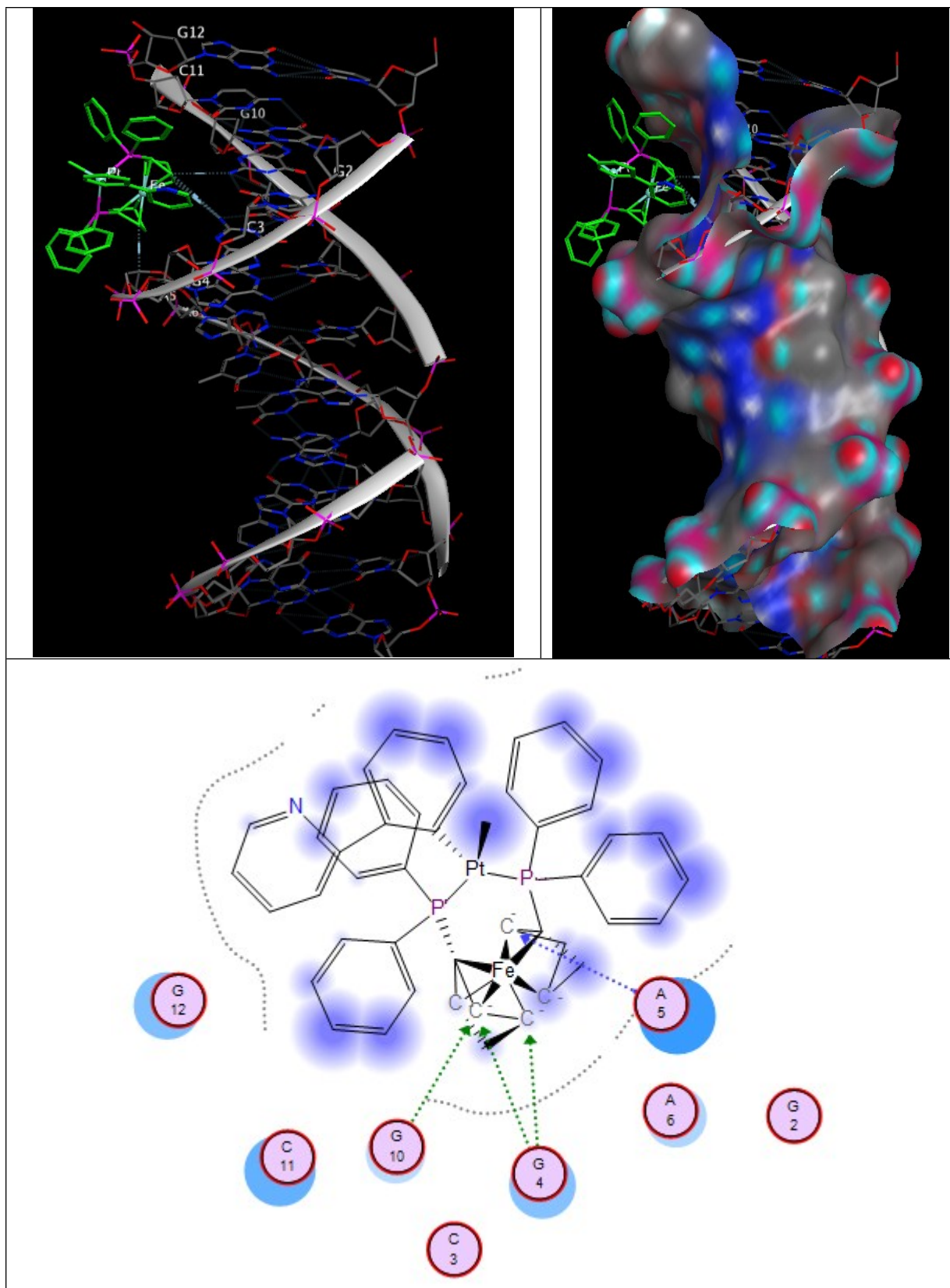
Contents:	Page
Table S1. <i>In vitro</i> cytotoxicity of 2a–2e , 3a , and 3b against cancer cell lines A549 , SKOV3 , and MCF-7 .	3
Figure S1. Molecular docking simulation studies of the interaction between 2b and 1BNA.	4
Figure S2. Molecular docking simulation studies of the interaction between 2c and 1BNA.	5
Figure S3. Molecular docking simulation studies of the interaction between 2e and 1BNA.	6
Figure S4. Molecular docking simulation studies of the interaction between 3b and 1BNA.	7
Figure S5. Molecular docking simulation studies of the interaction between 2b and 1LU5.	8
Figure S6. Molecular docking simulation studies of the interaction between 2c and 1LU5.	9
Figure S7. Molecular docking simulation studies of the interaction between 2e and 1LU5.	10
Figure S8. Molecular docking simulation studies of the interaction between 3b and 1LU5.	11
Figure S9. The best docked conformation of complex 2d , in the best binding sites with 3CO3.	12

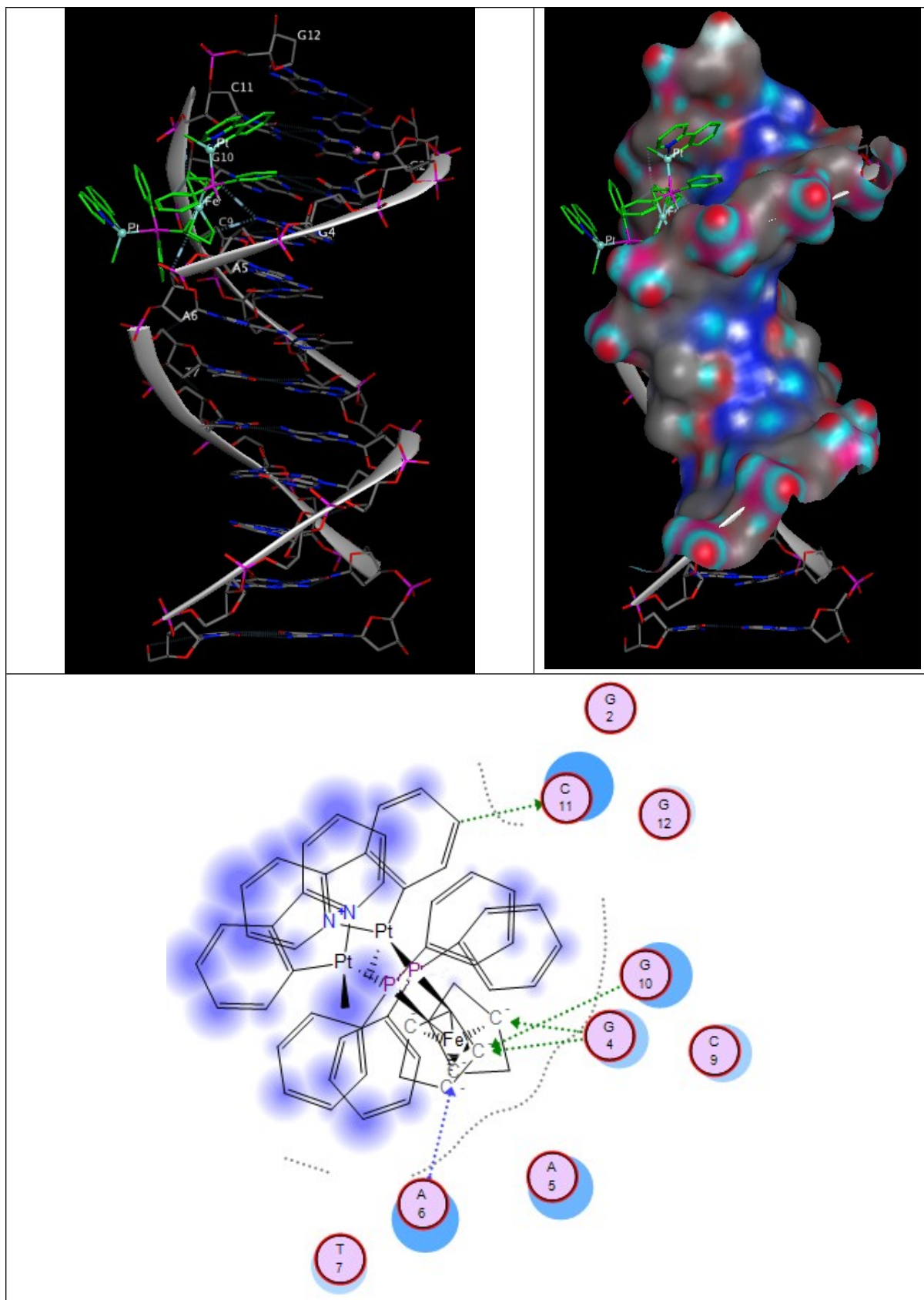
Table S1. *In vitro* cytotoxicity against cancer cell lines.

Complex	IC₅₀ (μM ± SD)		
	A549	SKOV3	MCF-7
2a	6.84 ± 1.37	15.65 ± 0.71	8.48 ± 1.12
2b	28.42 ± 1.66	23.99 ± 3.47	34.55 ± 1.59
2c	7.44 ± 1.51	8.79 ± 1.16	11.58 ± 2.18
2d	3.65 ± 0.68	12.69 ± 1.09	9.29 ± 1.35
2e	18.84 ± 1.37	15.81 ± 2.07	20.39 ± 2.65
3a	27.49 ± 2.21	21.26 ± 1.38	32.85 ± 2.64
3b	24.5 ± 0.73	13.60 ± 0.92	24.35 ± 0.89
<i>cis-platin</i>	9.75 ± 1.52	18.57 ± 1.29	15.29 ± 1.72









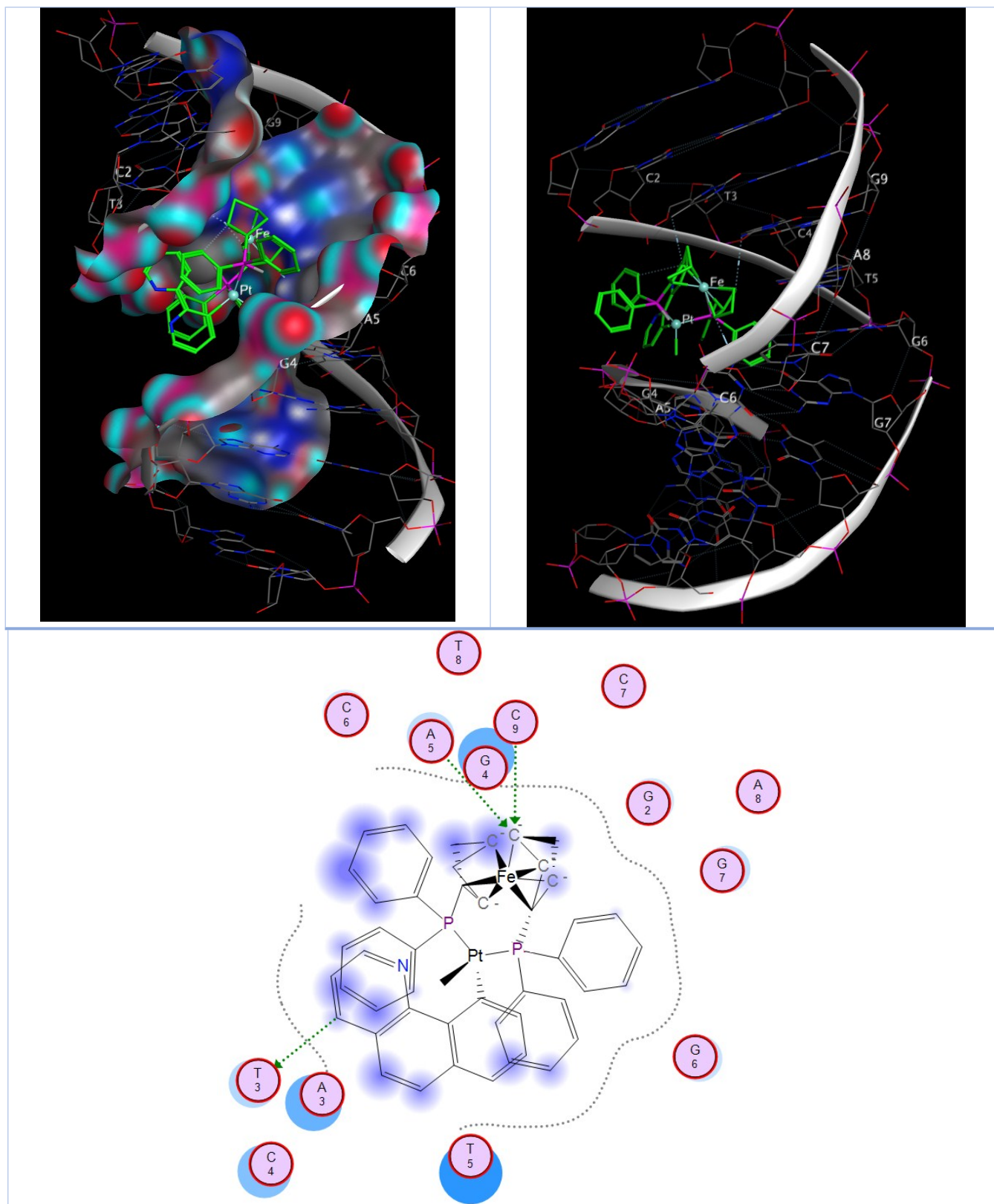




Figure S6. Molecular docking simulation studies of the interaction between **2c** and 1LU5.

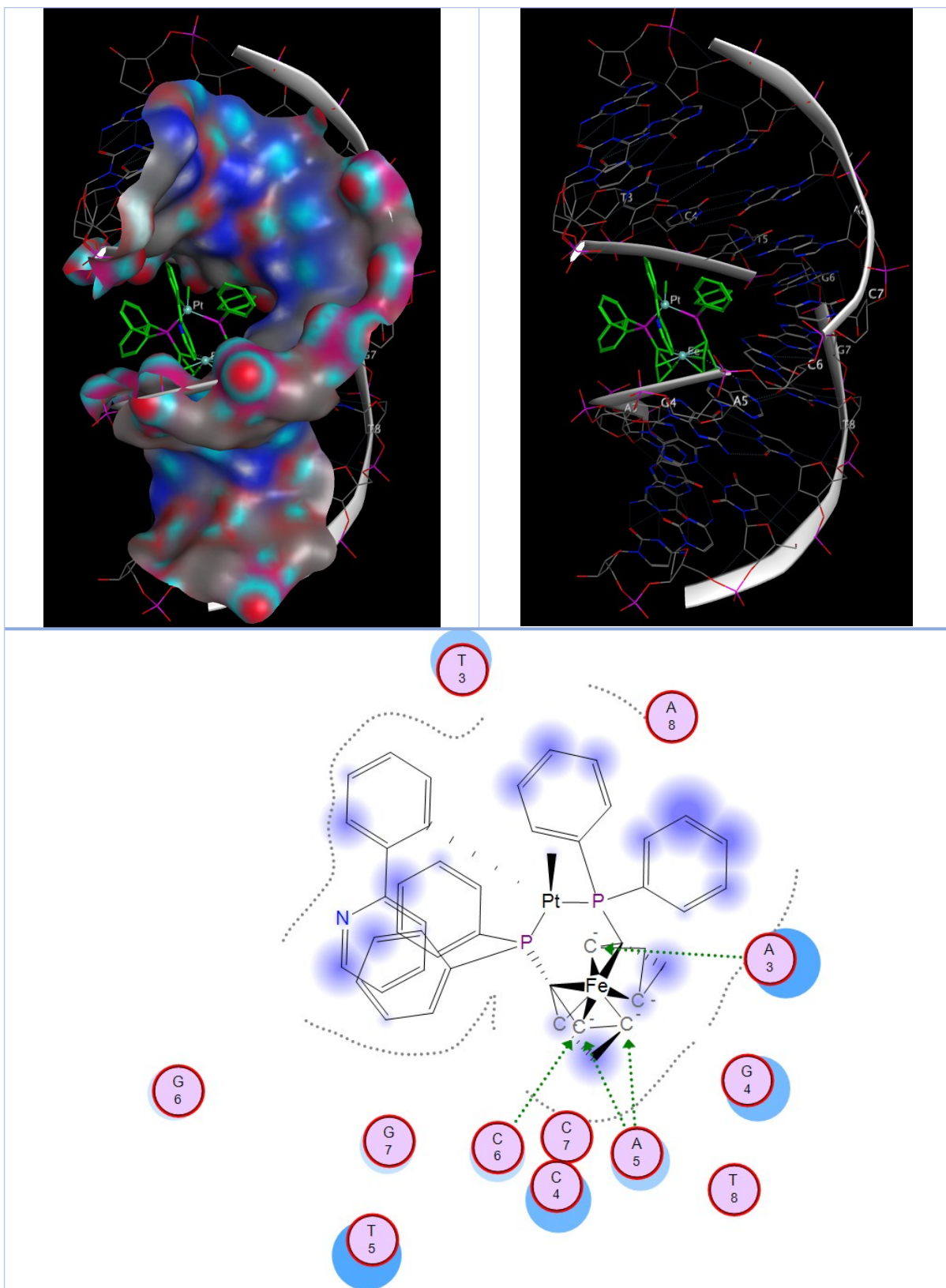


Figure S7. Molecular docking simulation studies of the interaction between **2e** and 1LU5.

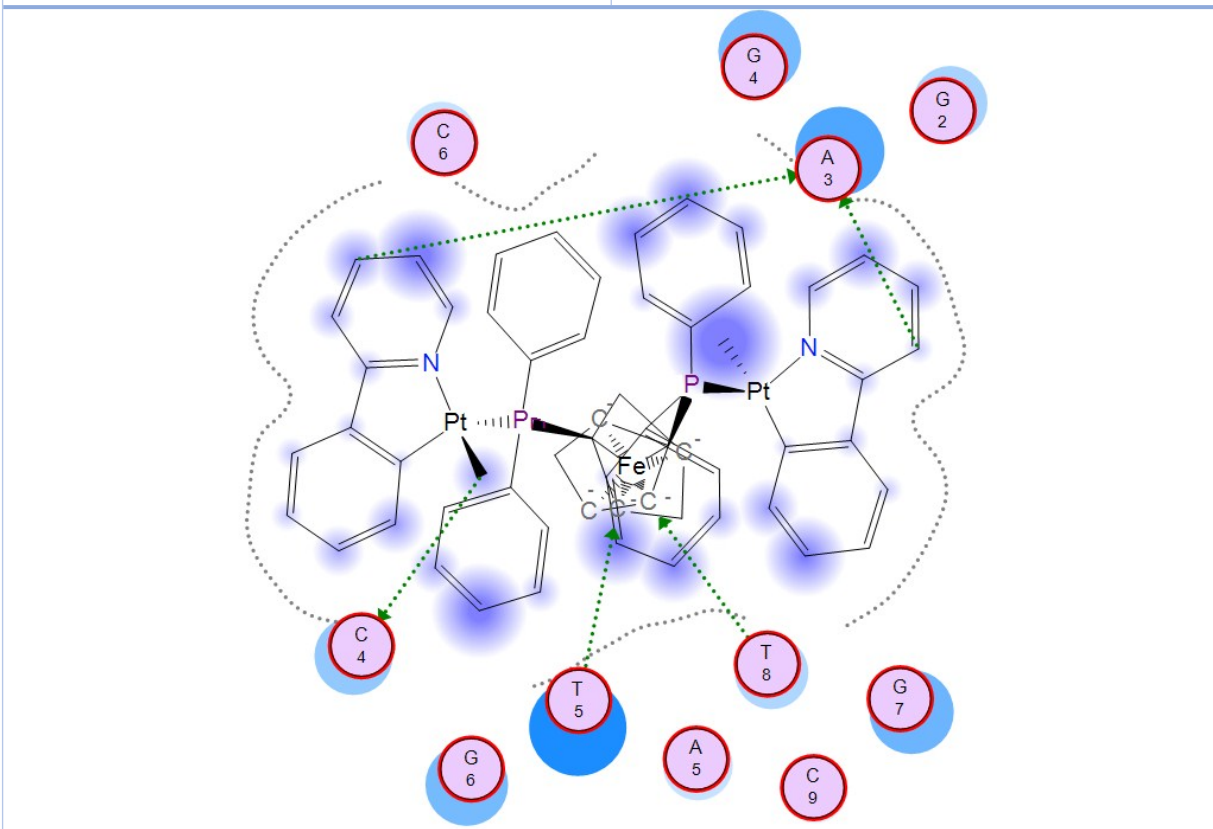
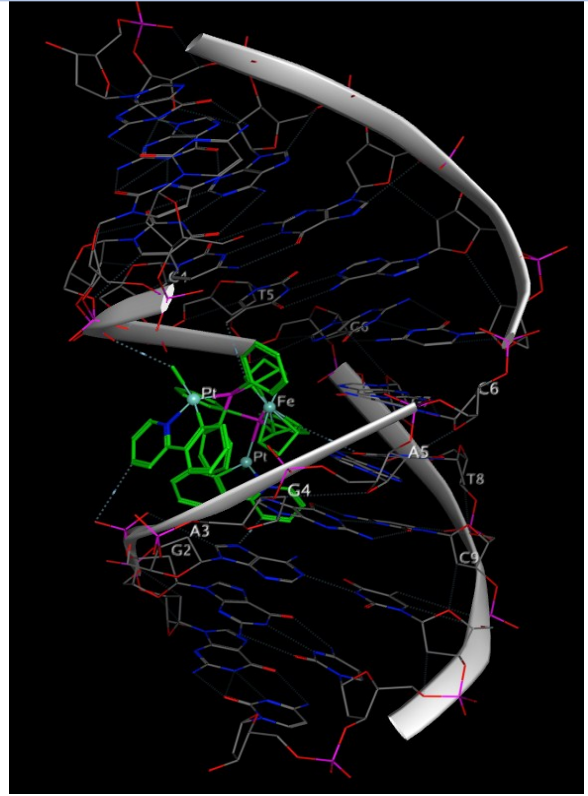
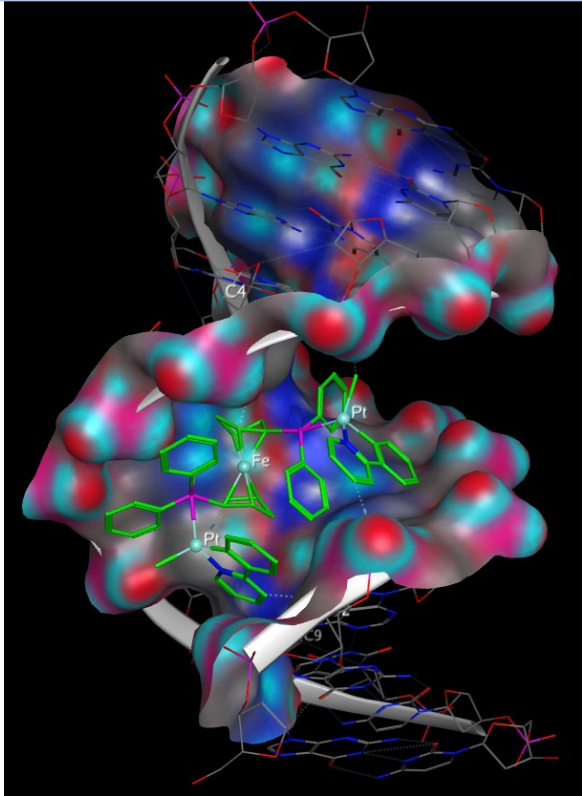


Figure S8. Molecular docking simulation studies of the interaction between **3b** and 1LU5.

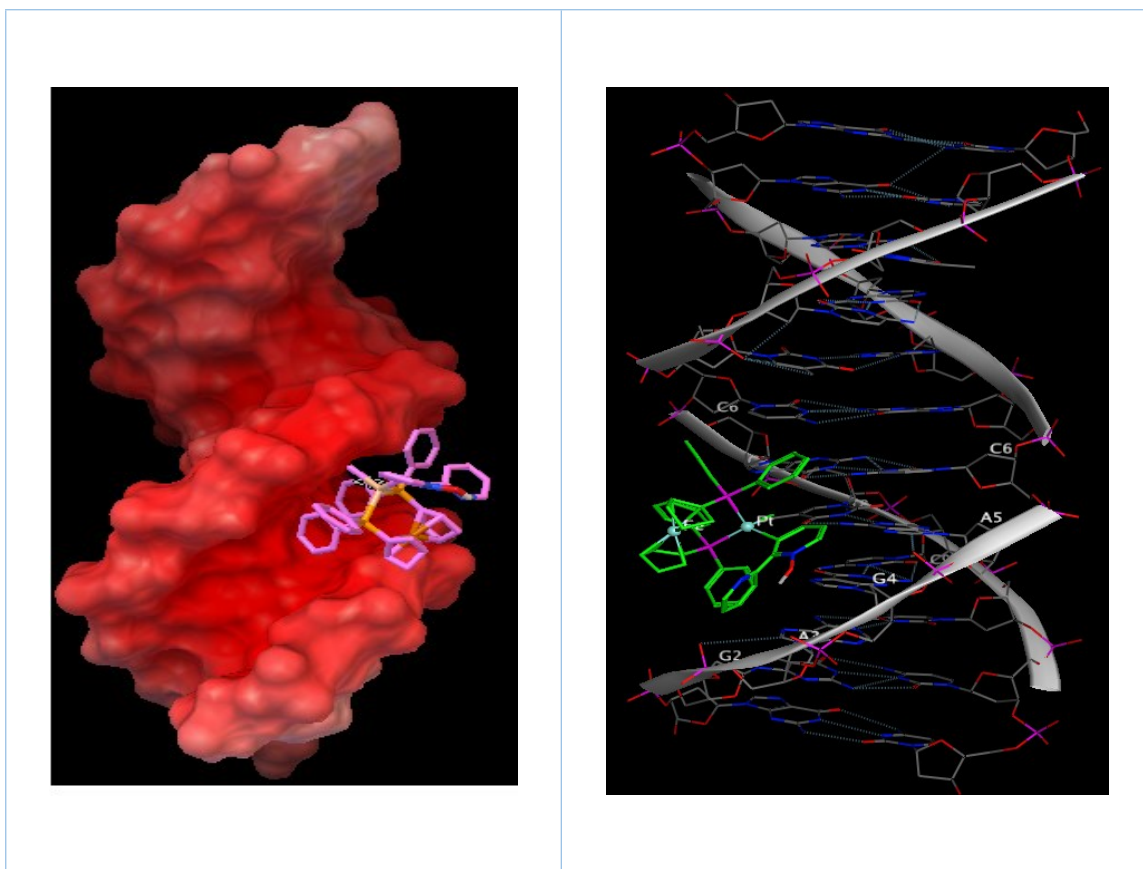


Figure S9. The best docked conformation of complex **2d**, in the best binding sites with 3CO3.