Supplementary Information (SI) for New Journal of Chemistry.
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Supporting Information for

Structure-base design to explore the anticancer efficacy of Pt(II)- and Au(III)-N-heterocyclic carbene (NHC) complexes

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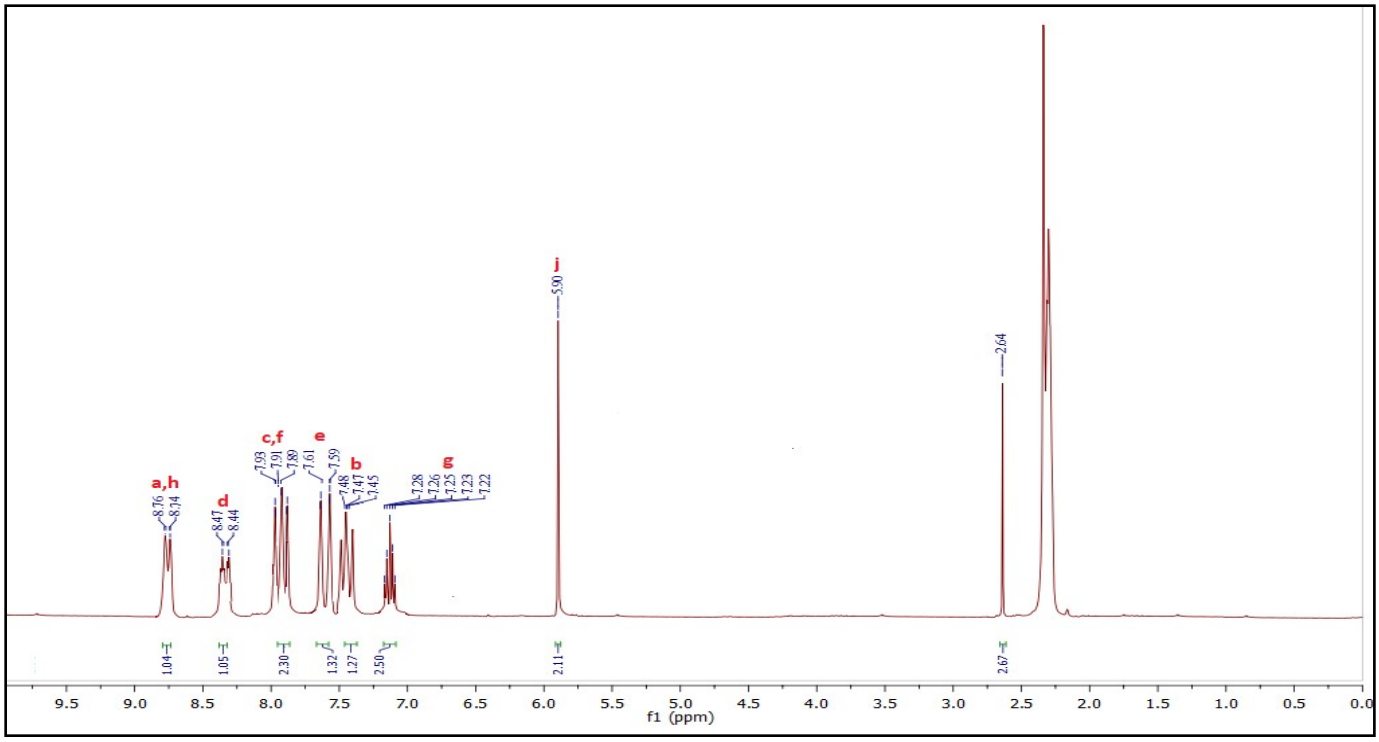

Figure S1: ^{1}H NMR of complex **2**.

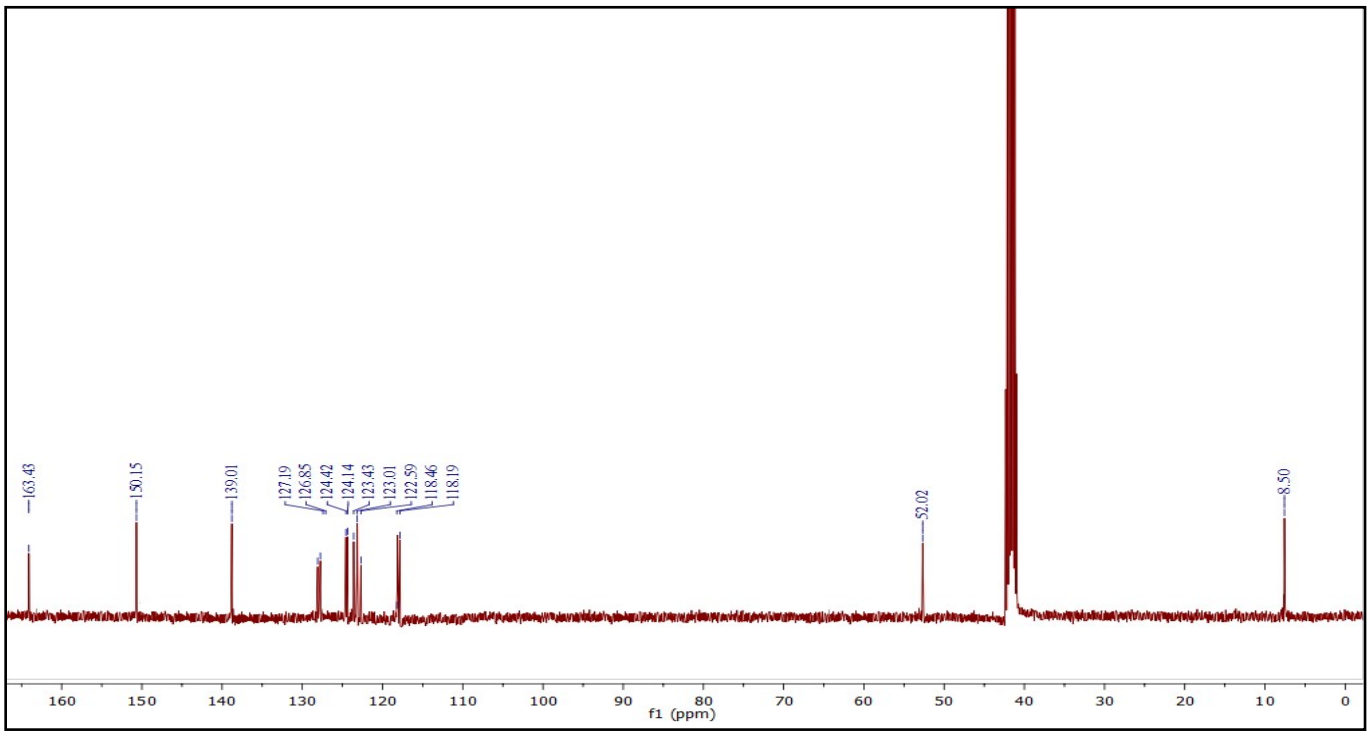

Figure S2: ^{13}C NMR of complex **2**.

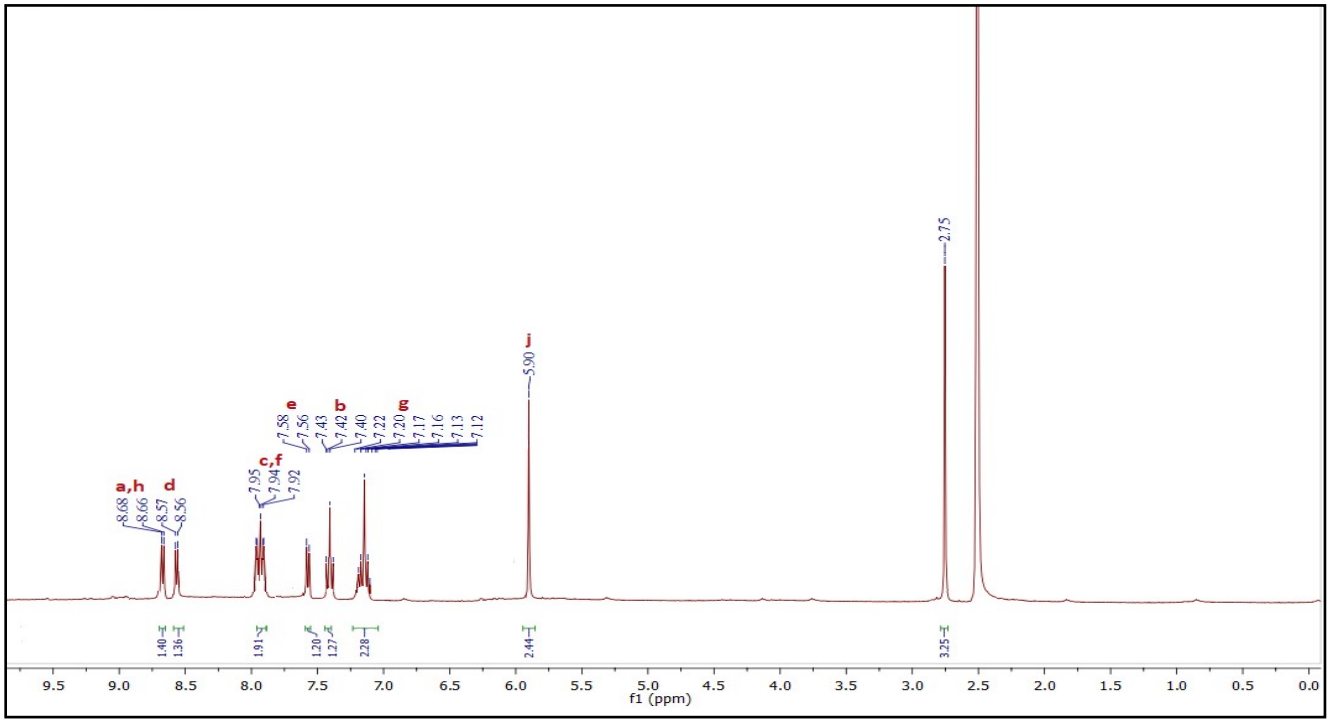

Figure S3: ^{1}H NMR of complex **3**.

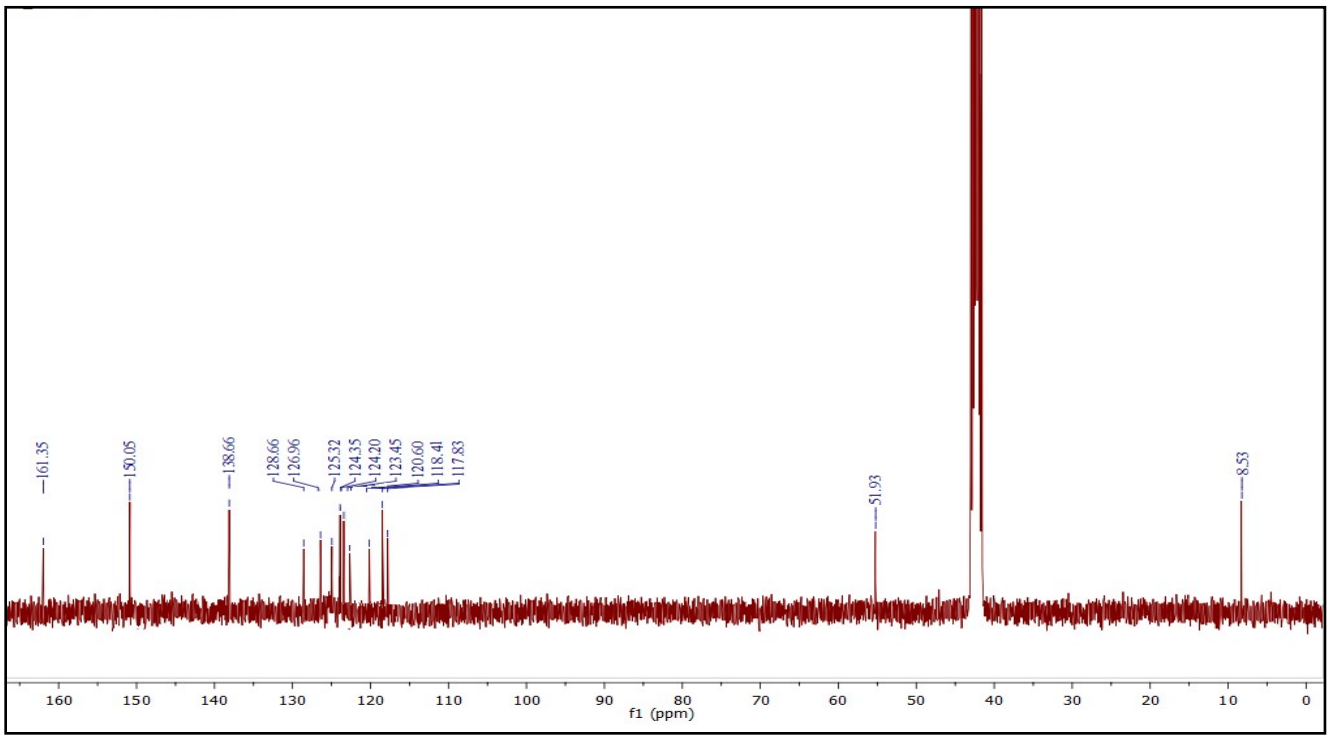

Figure S4: ^{13}C NMR of complex **3**.

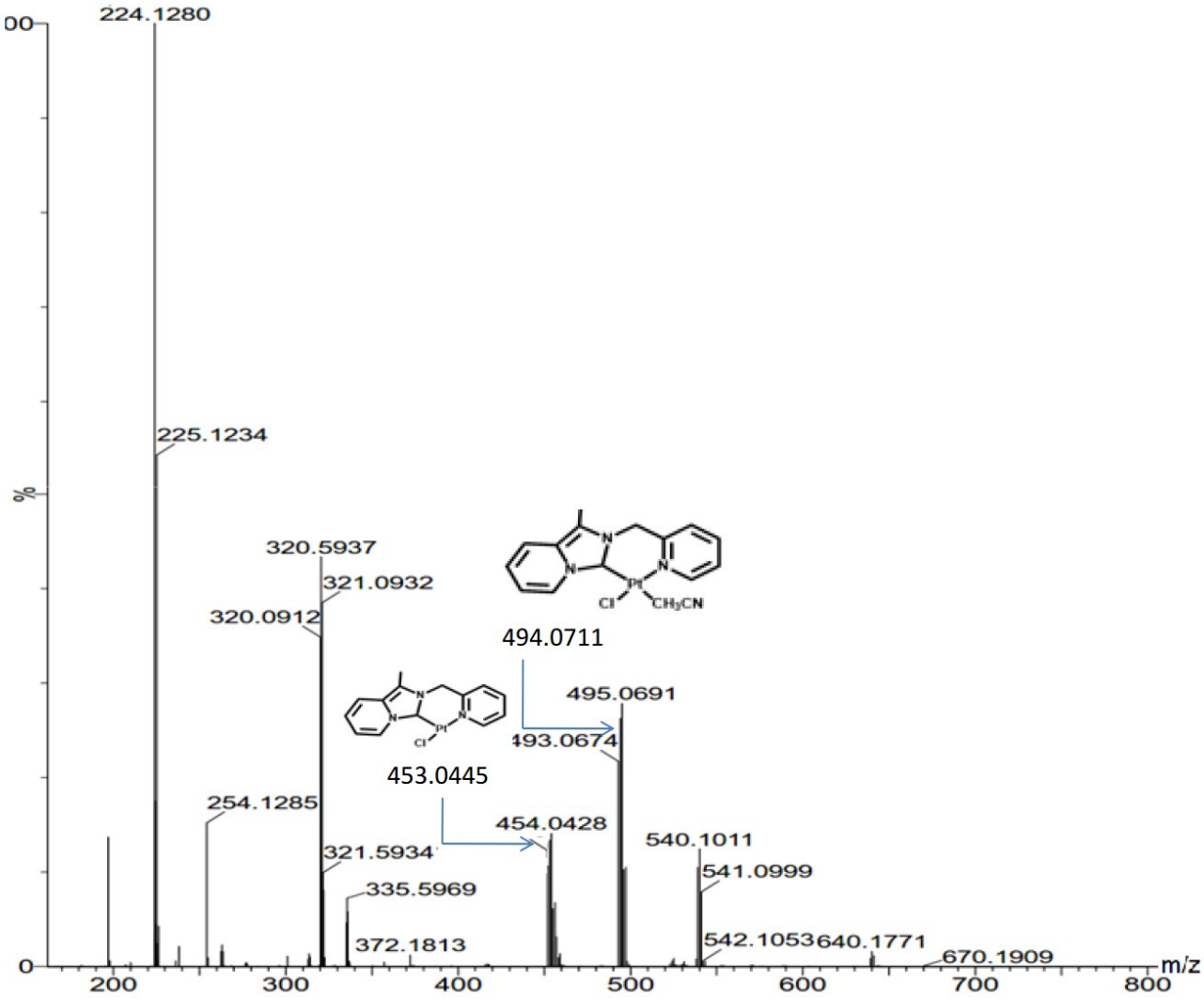

Figure S5: Mass spectra of complex **2**.

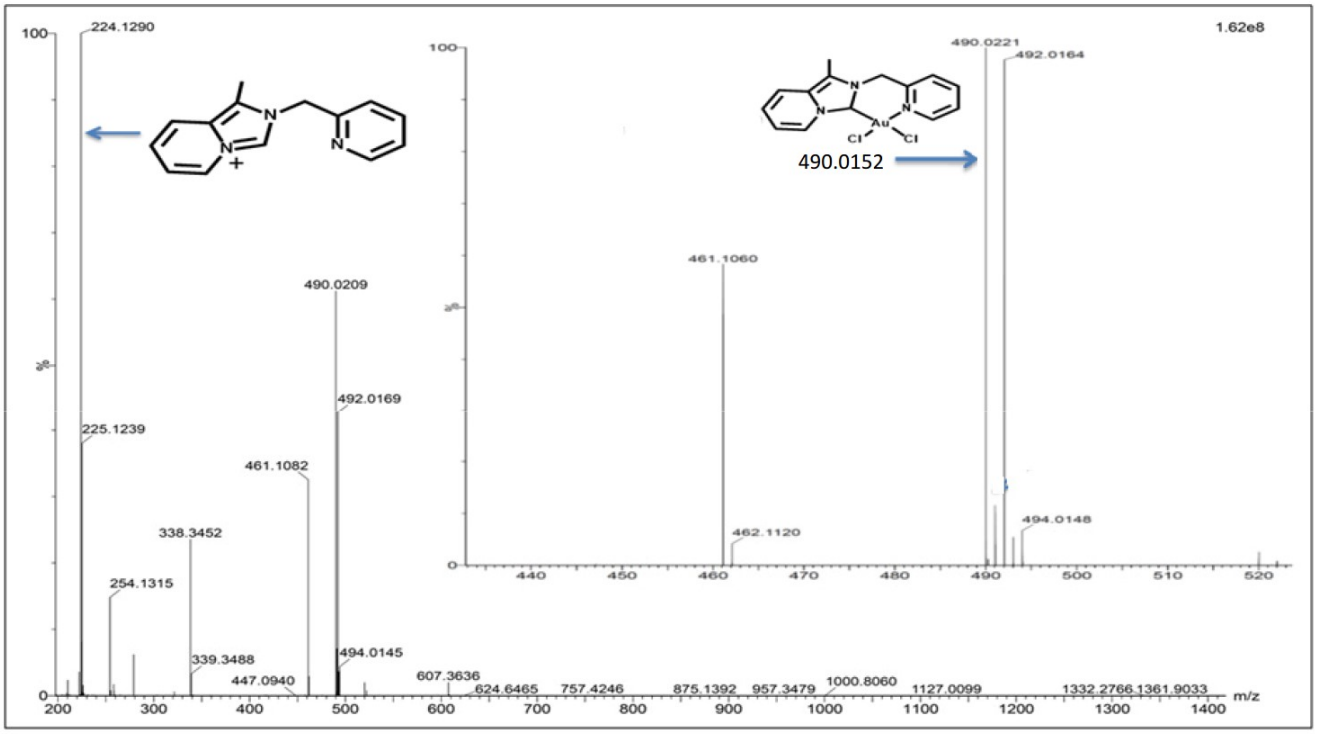

Figure S6: Mass spectra of complex **3**.

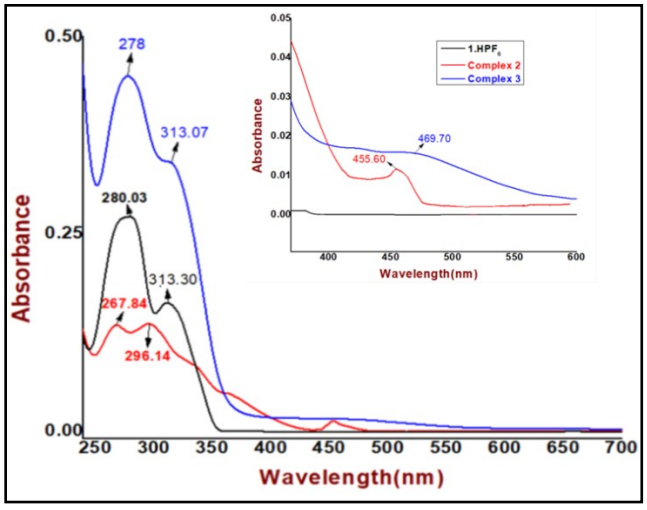

Figure S7: UV-Vis spectra of **1.**HPF_6, complex **2** and complex **3**.

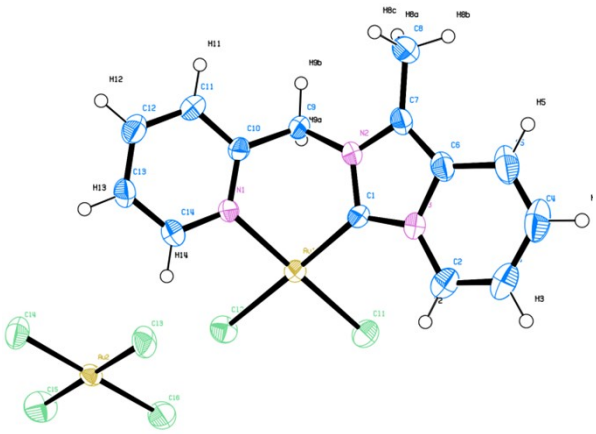

Figure S8: ORTEP view of complex **3**.

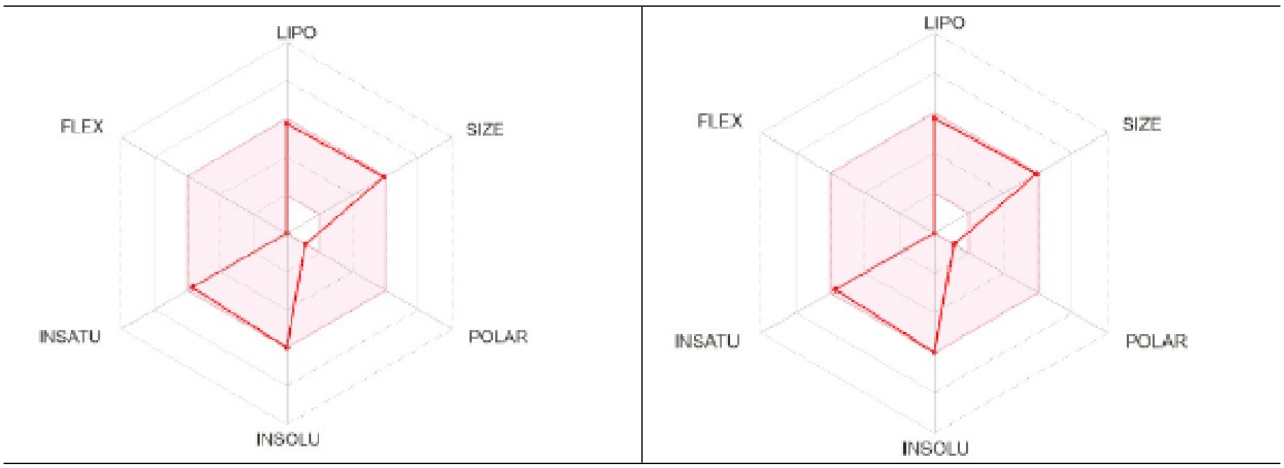

Figure S9. Pharmacokinetic studies of complex **2** (left) and complex **3** (right) shows the similar potency of the complexes to be used as drug.

*(Drug designing and development depends on the assessment of absorption, distribution, metabolism, and excretion (ADME); Swiss ADME is a web tool that offers robust predictive models for physicochemical properties, pharmacokinetics, drug-likeness and medicinal chemistry friendliness. Pioneer work of Lipinski that consider a compound to be used as a drug define some physicochemical parameters, so-called 'Rule-of-five' established the relationship between pharmacokinetics and physicochemical parameters. In this context, six physicochemical properties are taken into consideration: size, solubility, lipophilicity, polarity, flexibility, and saturation. Considering physicochemical range a pink area is obtained in which the radar plot of the molecule has to fall entirely to be considered drug-like. Out of six properties, all the properties remain within the pink area in the case of our present complex **2** and **3** as shown in Figure S9 that supports the similar potency.)*

Table T1:Summary of spectral data of **1.**HPF_6 and complex **2** and **3**.

Complex	λ_{max} (nm) (ε, M^{-1} cm^{-1})
1.HPF_6	280.03 (5485), 311.28 (3222)
2	267.84 (2724), 296.14 (2744), 455.60 (228)
3	(9034), 313.07 (6855), 469.70 (313)

Table T2: Crystallographic parameters of complex **3**.

Empirical formula	$C_{14}H_{13}Au_2Cl_6N_3$
Formula weight	829.91
Temperature/K	293(2)
Crystal system	monoclinic
Space group	P 1 21/c 1
a/Å	17.5971(5)
b/Å	7.7989(2)
c/Å	15.1023(4)
α/°	90
β/°	100.6220(10)
γ/°	90
Volume/$Å^3$	2037.09(10)
Z	4
$\rho_{calc}g/cm^3$	2.706
μ/mm^{-1}	15.178
F(000)	1512.0
Crystal size/mm^3	0.13 × 0.12 × 0.11
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.87 to 27.46
Index ranges	$-22 \leq h \leq 22$, $-10 \leq k \leq 10$, $-19 \leq l \leq 19$
Reflections collected	24453
Independent reflections	4641 [R_{int} = 0.0453, R_{sigma} = 0.0321]
Data/restraints/parameters	4641/0/227
Goodness-of-fit on F^2	1.043
Final R indexes [I>=2σ (I)]	R_1 = 0.0300, wR_2 = 0.0630
Final R indexes [all data]	R_1 = 0.0392, wR_2 = 0.0667
Largest diff. peak/hole / e $Å^{-3}$	1.85/-1.54

***Table T3**:* Summary of binding energy, types of interaction, amino acids involved and the receptive bond lengths involved in the interaction of complex **2** and **3** with BCL2 with human DNA topoisomerase II.

Protein-Ligand	**Docking score**	**Type of interaction**	**Interacting AA chain(or nucleotide chain) name; AA(or nucleotide) name; AA(nucleotide) no.**	**Bond length (Å)**
BCL-2-Complex **2**	-6.24	Pi-Alkyl	A: Leu134	5.48
			A: Phe150	5.37
			A: Met112	4.22
		Alkyl	A: Met112	3.94
			A: Leu134	3.79
			A: Ala146	3.44
		Pi-Pi T-shaped	A: Phe101	5.62
		Pi-Anion	A: Glu133	4.05
		Carbon	A: Asp108	3.17
Human DNA Topoisomerase II-Complex **2**	-7.45	Pi-Alkyl	D: DG9	5.29
			A: Ile856	5.07
		Alkyl	A: Lys868	3.57
			A: Leu995	4.45
			A: Leu995	4.29
		Pi-donor	C: DA8	2.85
		Carbon	A: Glu854	2.95
			C: DC9	2.89
BCL-2-Complex **3**	-6.48	Pi-Alkyl	A: Met112	5.04
			A: Ala146	5.00
			A: Val130	4.82
			A: Leu134	4.50
			A: Phe101	4.32
			A: Phe150	4.18
		Alkyl	A: Leu134	5.23
			A: Val130	4.19
			A: Leu134	3.49
		Pi-Pi T-shaped	A: Phe101	4.84
		Carbon	A: Ala146	2.94
Human DNA Topoisomerase II-Complex **3**	-7.27	Pi-Alkyl	A: Met847	5.46
		Alkyl	A: Pro716	4.82
			A: Lys723	4.53
			A: Leu771	4.19
		Amide-Pi-stacked	A: Leu722	4.79
		Pi-sigma	A: Asn851	3.79
		Carbon	A: Gly852	2.92