Electronic Supplementary Material (ESI) for Dalton Transactions.

Lipophilicity-dependent ruthenium N-heterocyclic carbene complexes as potential anticancer agents†

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Table S1. Crystallographic data for complex **1**.

Complex **1**			
Empirical formula	$C_{27}H_{30}N_2Cl_2Ru$	V (Å^3)	2452.8(10)
Formula weight	554.50	Z	4
Crystal system	Monoclinic	Dc (g·cm^{-3})	1.502
Space group	$P2_1/c$	μ (mm^{-1})	0.875
a (Å)	12.180(3)	F(000)	1136
b (Å)	16.920(4)	R_{int}	0.0857
c (Å)	12.171(3)	Goodness-of-fit	1.080
α (º)	90.00	R_1 [I>2σ (I)]	0.0792
β (º)	102.072(3)	wR_2 [I>2σ (I)]	0.2029
γ (º)	90.00	R_1 (all data)[a]	0.1105
T (K)	296	wR_2 (all data)[b]	0.2462

[a] $R_1=\Sigma||F_o|-|F_c||/\Sigma|F_o|$. [b] $wR_2= |\Sigma w(|F_o|^2 -|F_c|^2)|/\Sigma|w(F_o)^2|^{1/2}$, where $w = 1/[\sigma^2(F_o^2) +(aP)^2+bP]$. P = $(F_o^2 + 2F_c^2)/3$.

Table S2 Selected bond lengths (Å) and angles (°) for **1**.

Complex **1**			
Ru(1)-Cl(1)	2.4270(18)	Ru(1)-C(1)	2.096
Ru(1)-Cl(2)	2.4257(17)	N(2)-C(1)	1.361(7)
N(1)-C(1)	1.351(7)		
Cl(1)-Ru(1)-Cl(2)	83.61(5)	Cl(1)-Ru(1)-C(1)	89.08(14)
Cl(2)-Ru(1)-C(1)	90.75(14)	Ru(1)-C(1)-N(1)	128.6(4)
Ru(1)-C(1)-N(2)	127.7(4)	N(1)-C(1)-N(2)	103.6(4)

Table S3 Hydrogen bond lengths (Å) and Angles (°) of **1**.

D–H···A	d(D–H)	d(H···A)	d(D···A)	∠DHA
C4-H4B ···Cl1	0.9700	2.5500	3.303(6)	135.00
C10-H10 ··· Cl1	0.9300	2.7900	3.563(7)	142.00
C11-H11B ··· Cl2	0.9700	2.5600	3.374(7)	141.00
C20-H20 ··· Cl1 [i]	0.9300	2.5900	3.437(5)	151.00
C23-H23 ··· Cl2 [ii]	0.9300	2.5900	3.498(6)	165.00
C26-H26 ··· Cl2	0.9600	2.8000	3.513(7)	132.00

Symmetry codes: i: 2-x, -y, 1-z; ii: x, 1/2-y, 1/2+z.

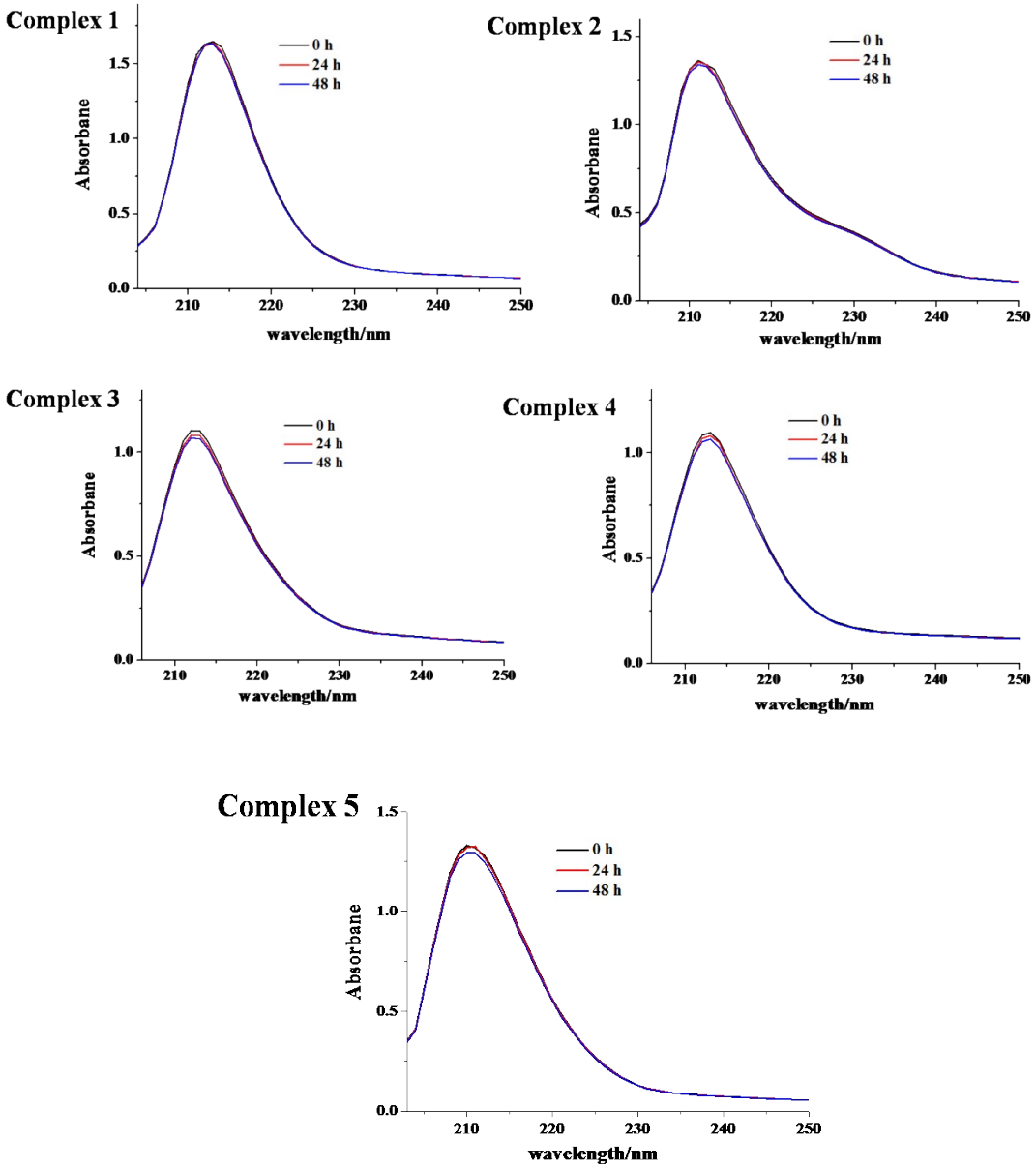


Fig. S1 The stability of complexes **1-5** in PBS indicated by UV-Vis spectra.

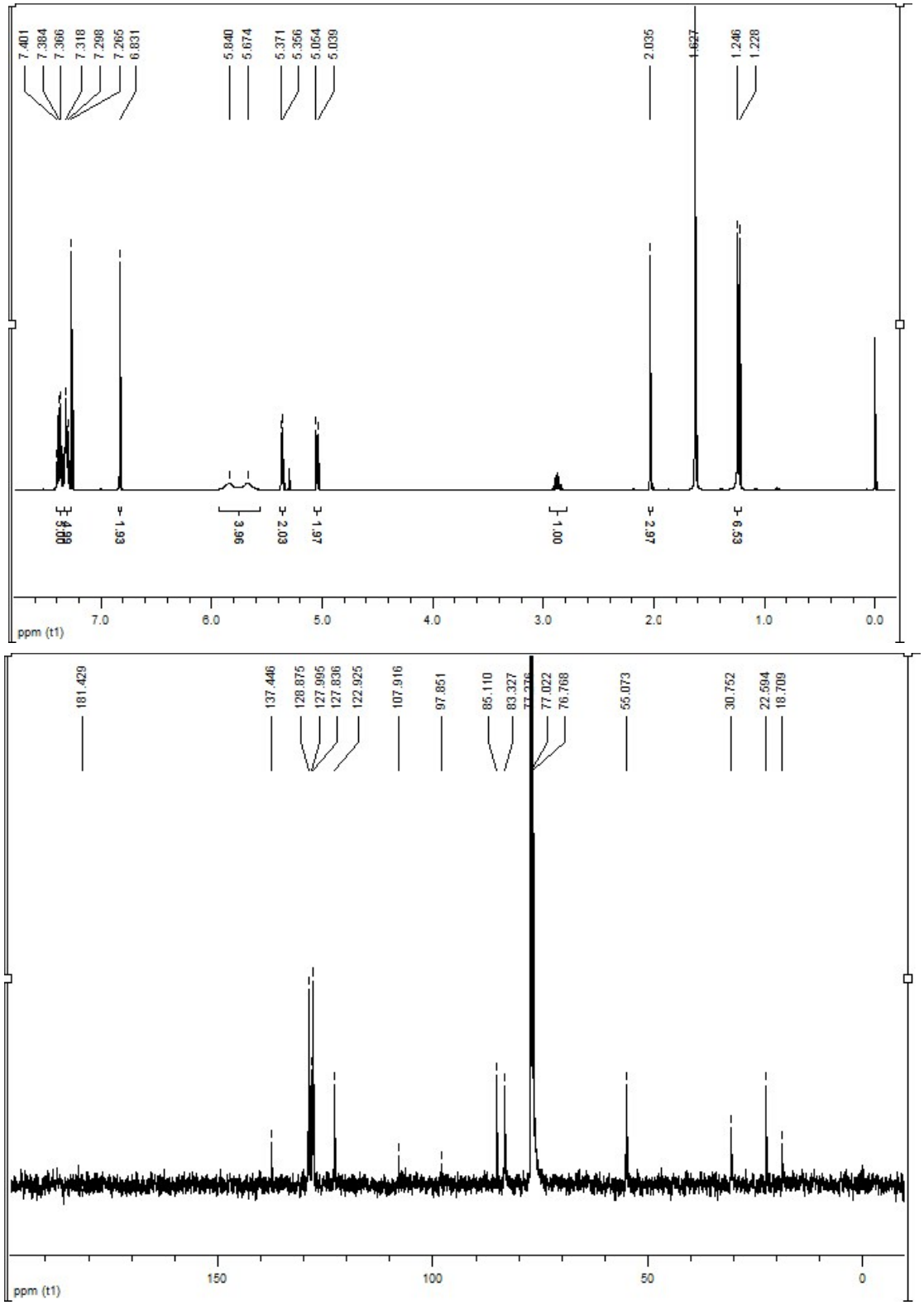


Fig.S2-1 ^{1}H/NMR (up) and ^{13}C/NMR (down) of complex **1**.

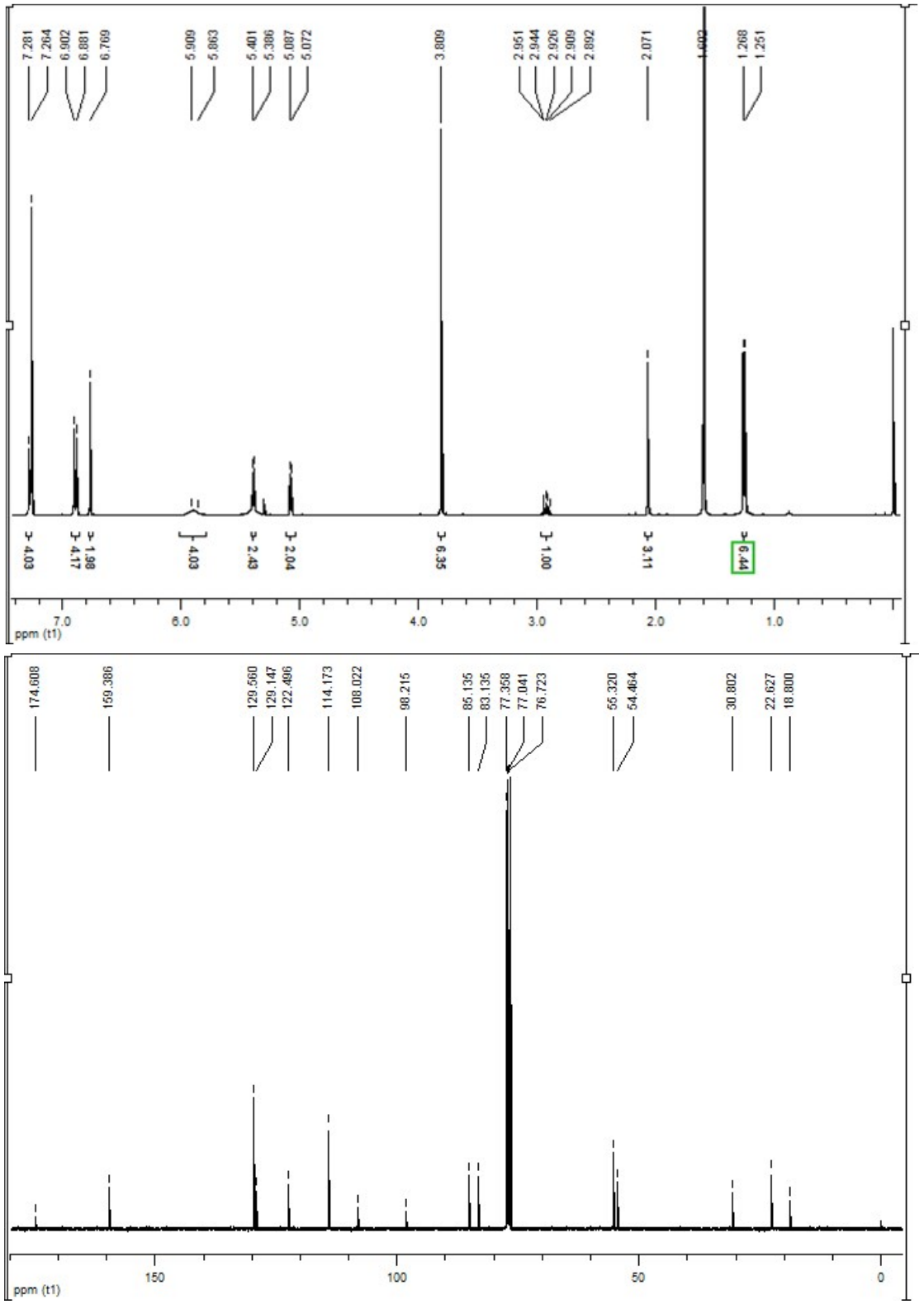


Fig.S2-2 ^{1}H/NMR (up) and ^{13}C/NMR (down) of complex **2**.

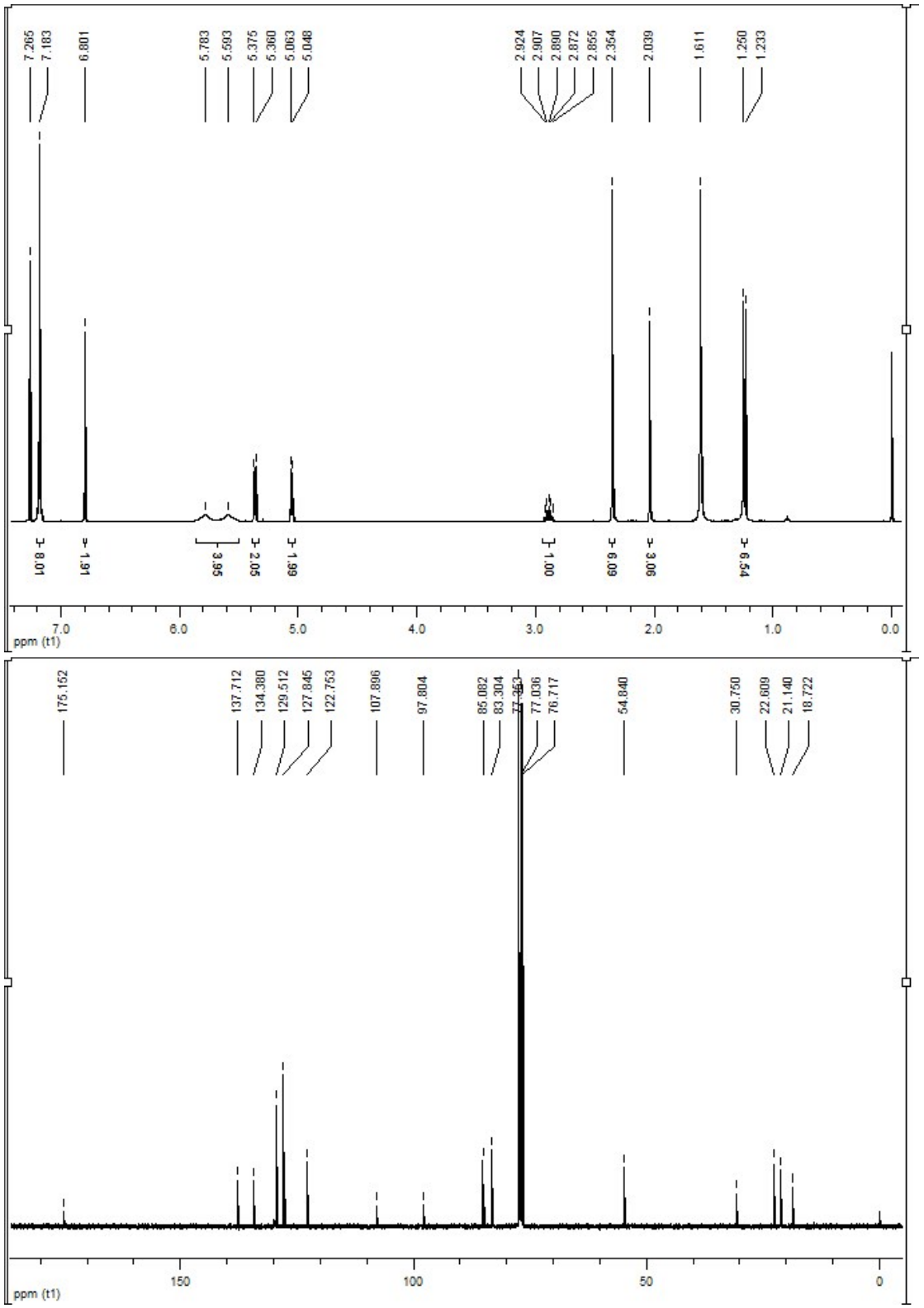


Fig.S2-3 ^{1}H/NMR (up) and ^{13}C/NMR (down) of complex **3**.

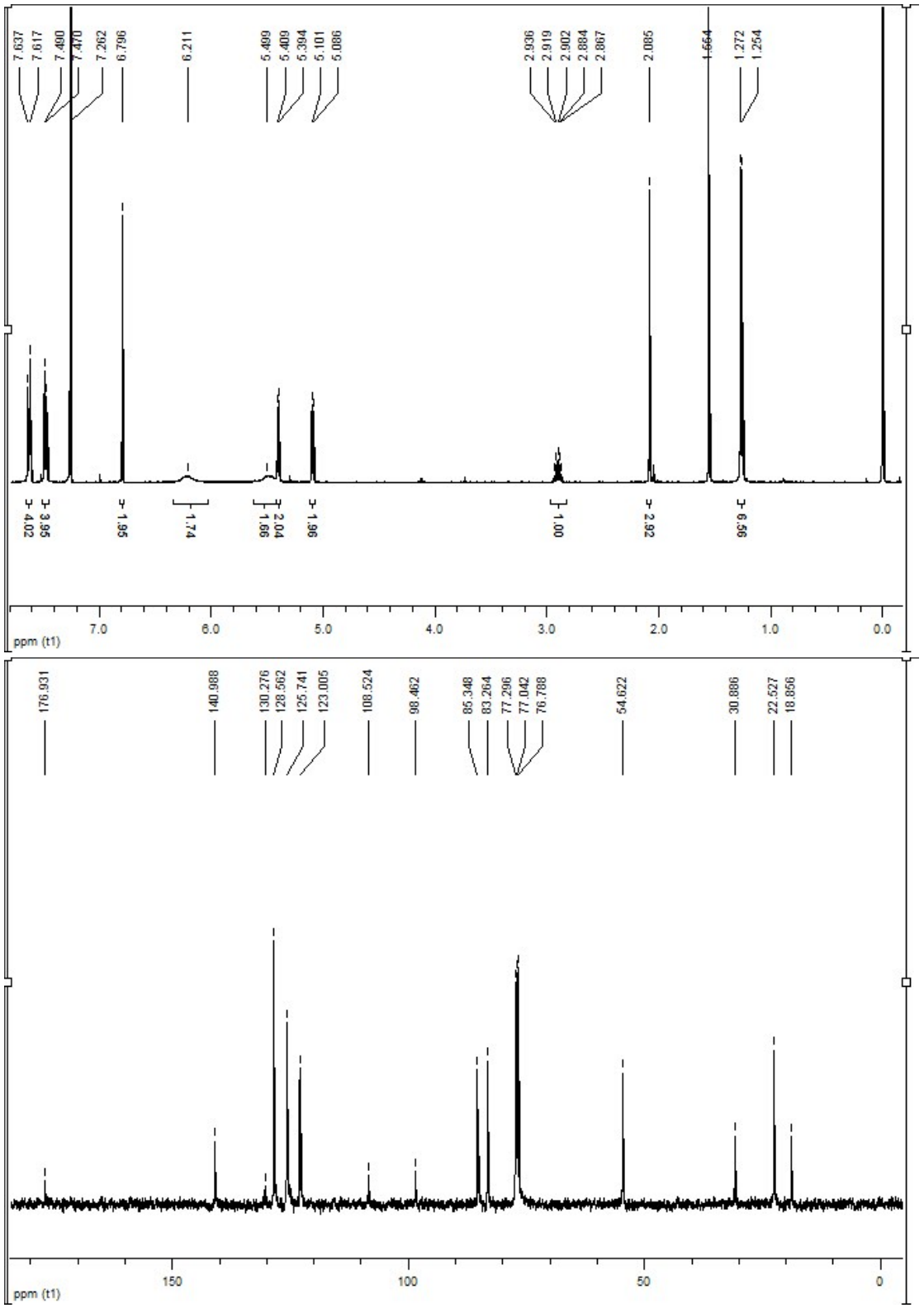


Fig.S2-4 ^{1}H/NMR (up) and ^{13}C/NMR (down) of complex **4**.

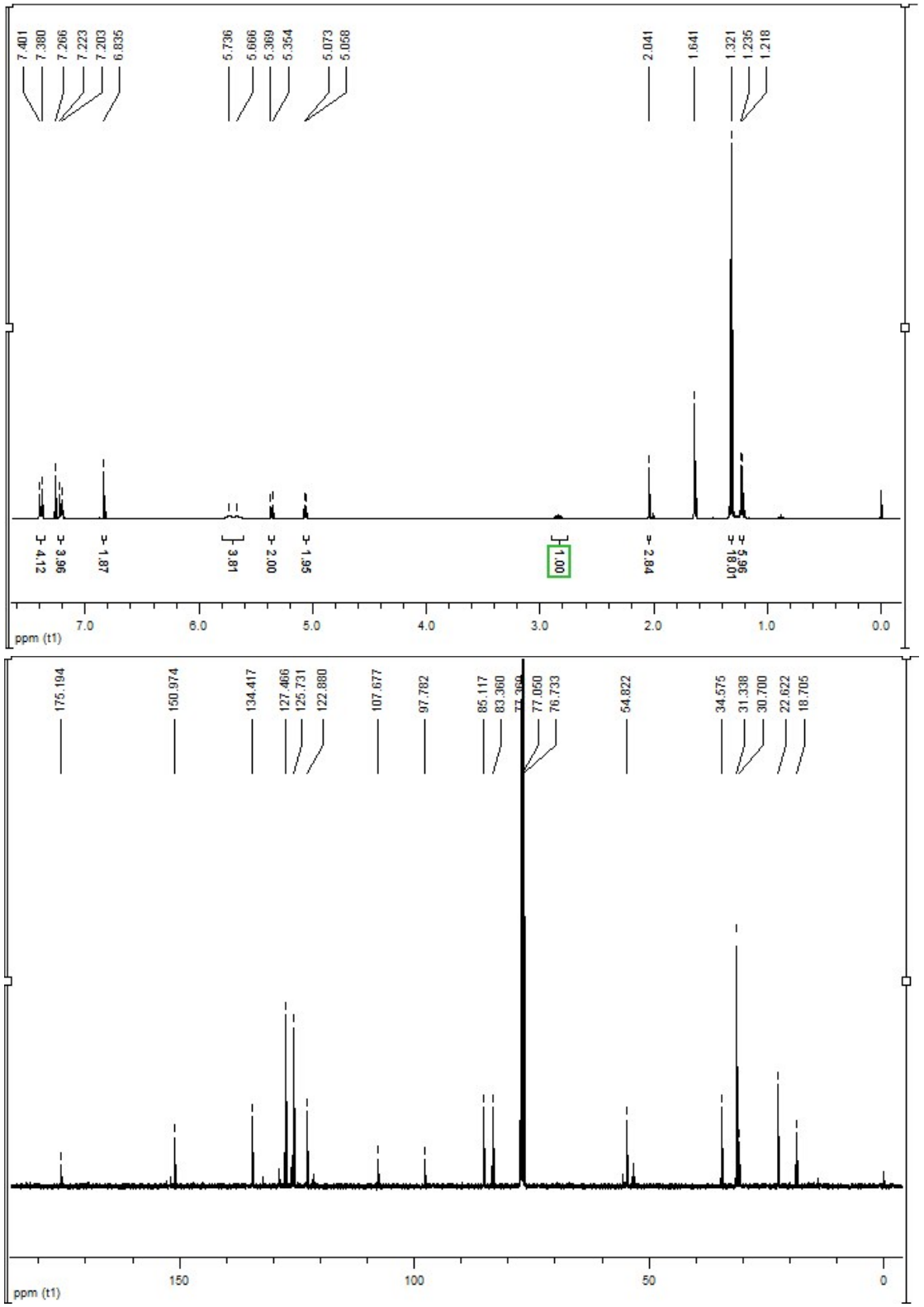


Fig.S2-5 ^{1}H/NMR (up) and ^{13}C/NMR (down) complex **5**.

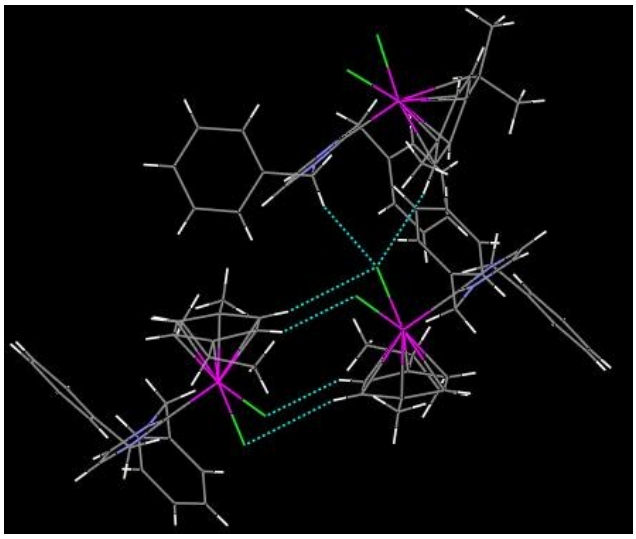
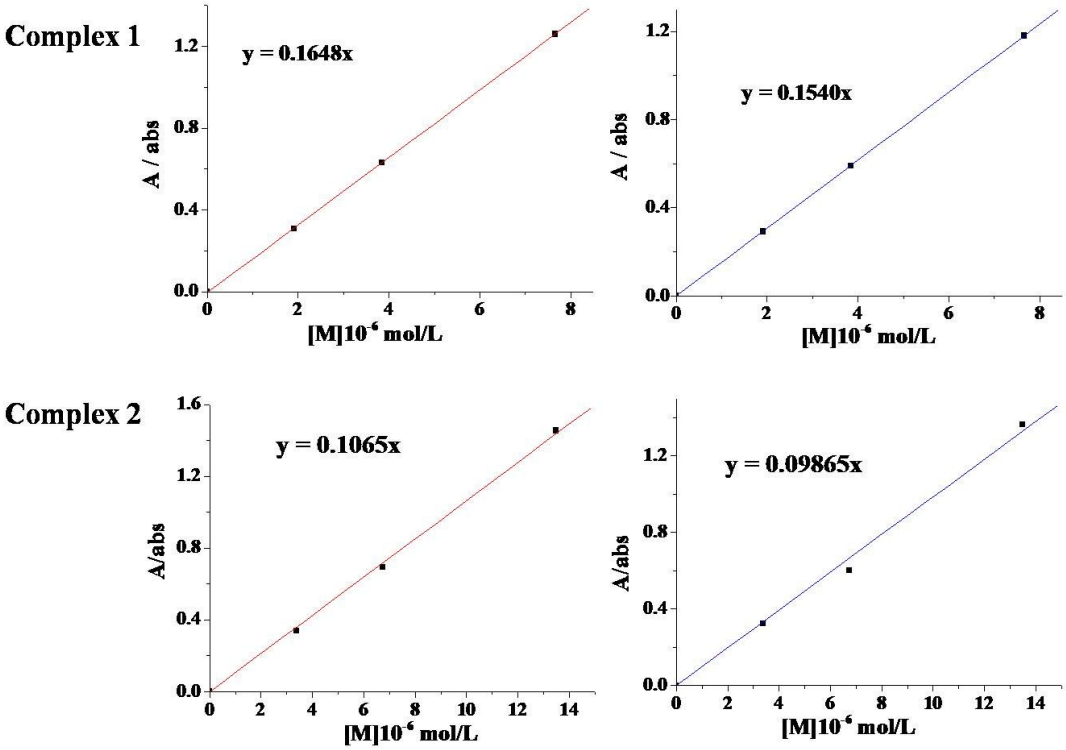


Fig. S3 The hydrogen bonds (dotted line) between adjacent molecules of complex **1**.



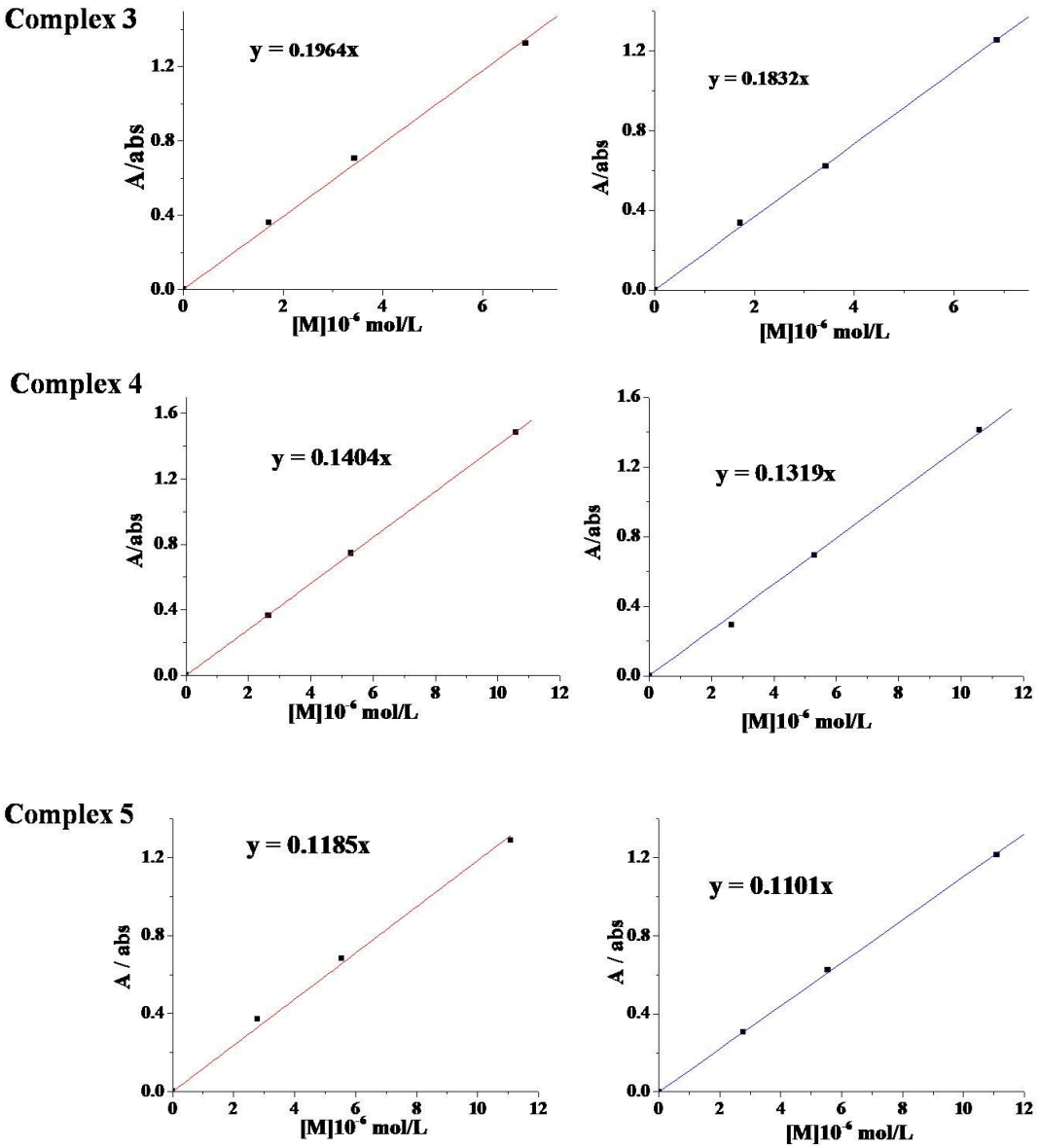


Fig. S4 The standard curves of complexes **1-5** in water (left, red line) and octanol (right, blue line).

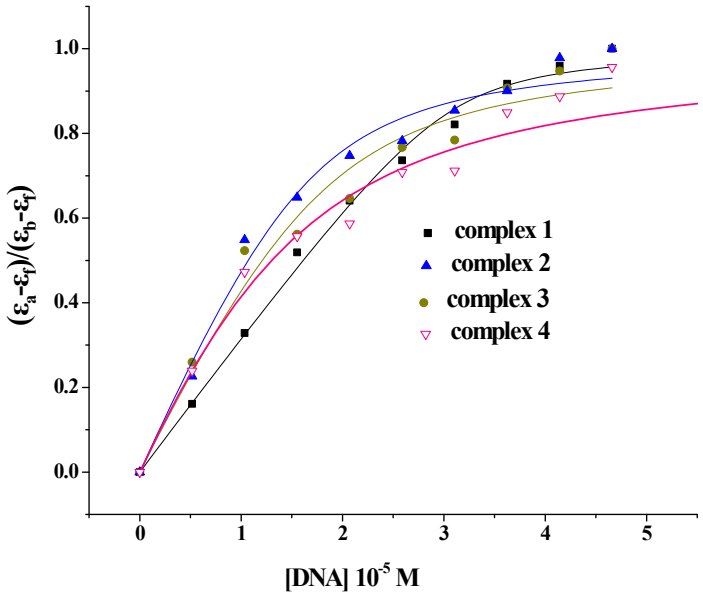


Fig. S5 The least-squares fit of $\Delta\varepsilon_{af}/\Delta\varepsilon_{bf}$ vs [DNA] for complexes **1-4**.