

Electronic Supplementary Information (ESI) for

**Photoswitchable Alkoxy-Bridged Binuclear Rhenium(I) Complexes – A
Potential Probe for Biomolecules and Optical Cell Imaging**

Veerasamy Sathish,^a Eththilu Babu,^a Arumugam Ramdass,^a Zong-Zhan Lu,^b Tzu-Ting Chang,^b
Murugesan Velayudham,^b Pounraj Thanasekaran,^b Kuang-Lieh Lu,^{*b} Wen-Shan Li,^{*b} and
Seenivasan Rajagopal^{*a}

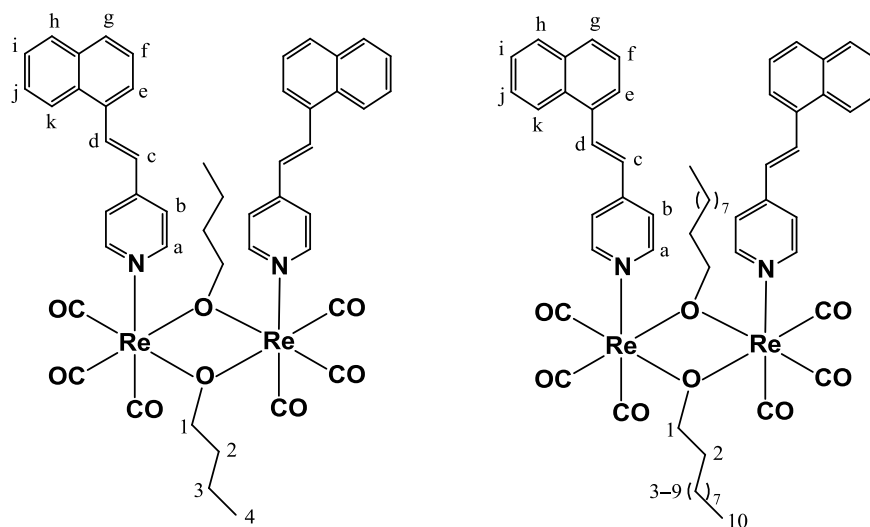
^a*Department of Physical Chemistry, School of Chemistry, Madurai Kamaraj University,
Madurai, Tamilnadu, India*

^b*Institute of Chemistry, Academia Sinica, Taipei 115, Taiwan*

Table S1. Crystallographic data of **1**.

1	
empirical formula	C ₄₈ H ₄₄ N ₂ O ₈ Re ₂
<i>M_w</i>	1149.27
crystal system	orthorhombic
space group	<i>P</i> 2 ₁ 2 ₁ 2 ₁
<i>a</i> (Å)	14.0169(3)
<i>b</i> (Å)	16.7072(3)
<i>c</i> (Å)	19.0984(4)
<i>V</i> (Å ³)	4472.52(16)
<i>Z</i>	4
<i>T</i> (K)	296
λ (Å)	0.71073
<i>D_{calc}</i> (g cm ⁻³)	1.707
μ (mm ⁻¹)	5.463
Flack parameter	[0.005(16)]
<i>F</i> ₀₀₀	2240
GOF	1.073
<i>R</i> ₁ ^{<i>a</i>} (<i>I</i> > 2σ(<i>I</i>))	0.0483
<i>wR</i> ₂ ^{<i>b</i>} (<i>I</i> > 2σ(<i>I</i>))	0.1223
<i>R</i> ₁ ^{<i>a</i>} (all data)	0.0595
<i>wR</i> ₂ ^{<i>b</i>} (all data)	0.1154
$\Delta\rho_{\max}/\Delta\rho_{\min}$ (e Å ⁻³)	2.069/-1.351

$${}^a R_1 = \sum ||F_0| - |F_c|| / \sum |F_0|. \quad {}^b wR_2 = \{ \sum [w(F_0^2 - F_c^2)^2] / \sum [w(F_0^2)^2] \}^{1/2}.$$



Scheme S1. ^1H NMR numbering for complexes **1** and **2**.

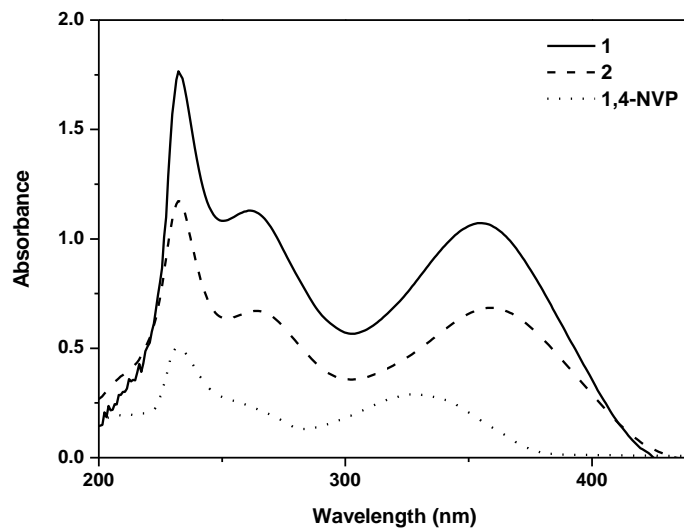


Figure S1. UV-vis spectra of complexes **1** (solid line) and **2** (dash line) and free ligand 1,4-NVP (dot line) in CH_2Cl_2 .

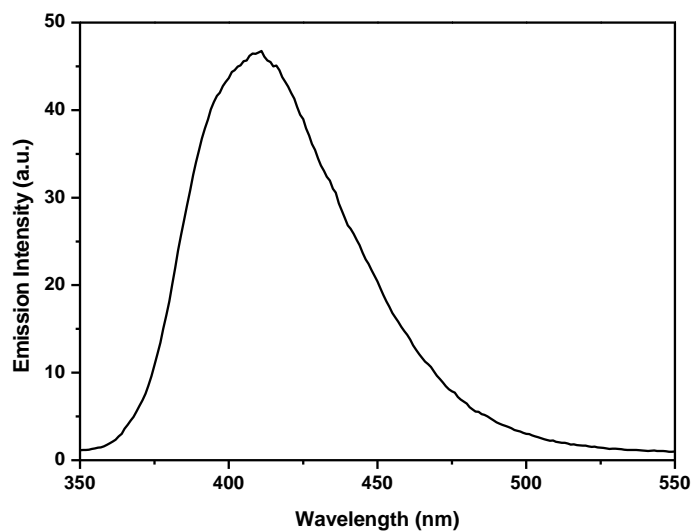


Figure S2. Emission spectrum of 4-(1-naphthylvinyl)pyridine ligand in CH_2Cl_2 .

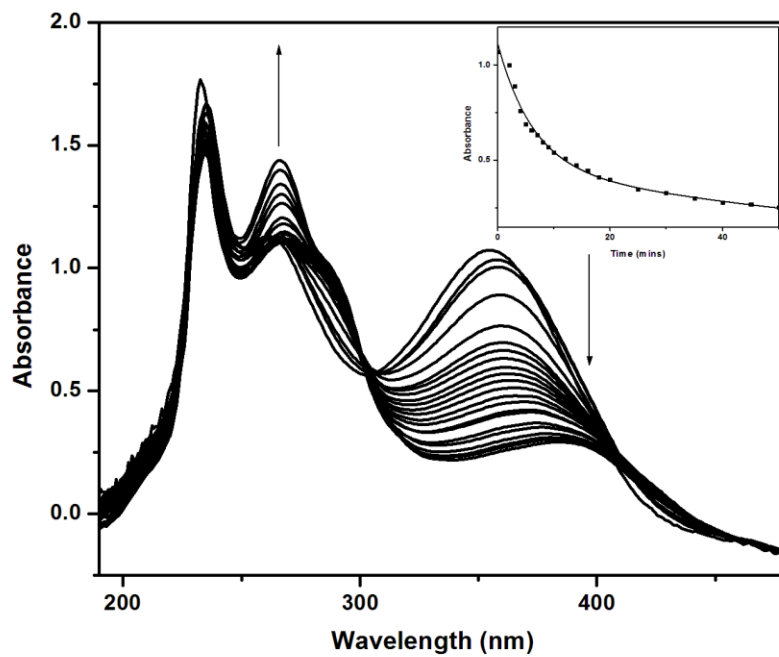


Figure S3. UV-vis spectral changes of complex **1** (3×10^{-5} M) in CH₂Cl₂ upon irradiation at 365 nm.

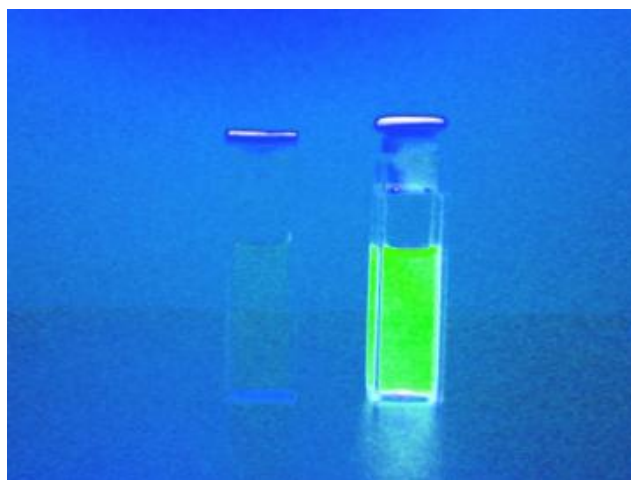


Figure S4. Photograph taken before and after the irradiation of **2** under illumination from a UV lamp at 365 nm in CH₂Cl₂.

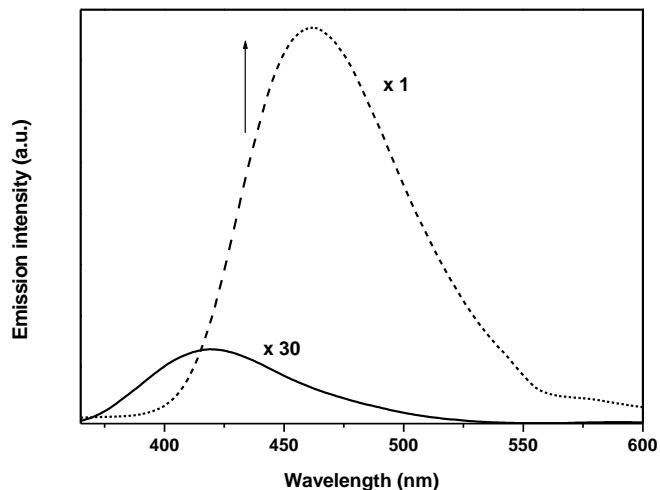


Figure S5. Emission spectra of **2** (3×10^{-5} M) before (—) and after (-----) photolysis in CH₂Cl₂.

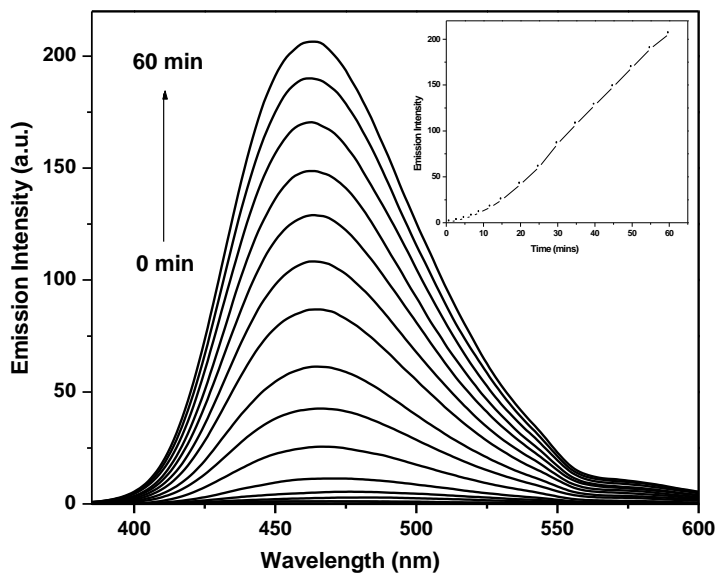


Figure S6. Enhancement in emission intensity upon 365 nm irradiation of complex **1** (3×10^{-5} M) in CH₂Cl₂.

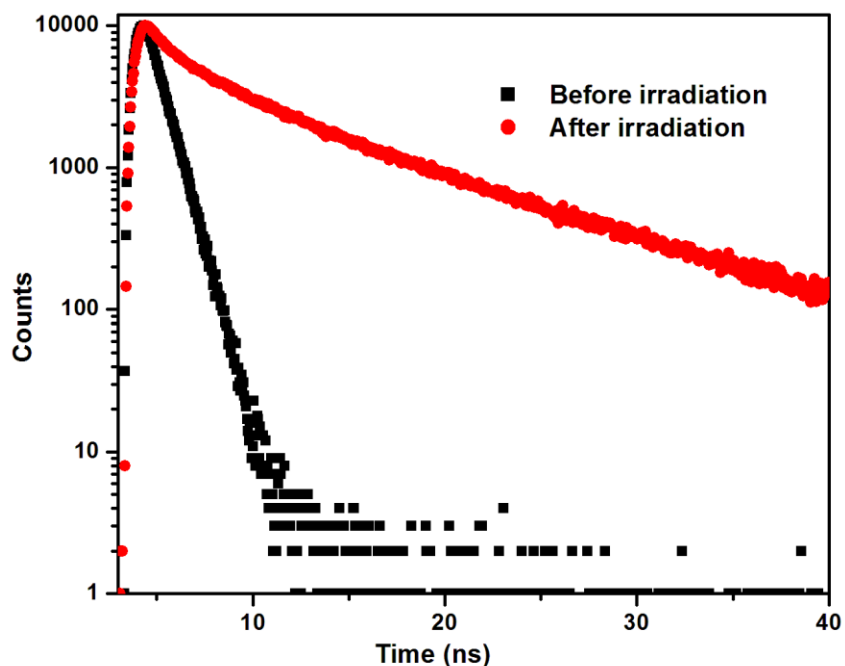


Figure S7. Lifetime decay profiles of **2** in CH₂Cl₂ before (black line) and after (red line) irradiation.

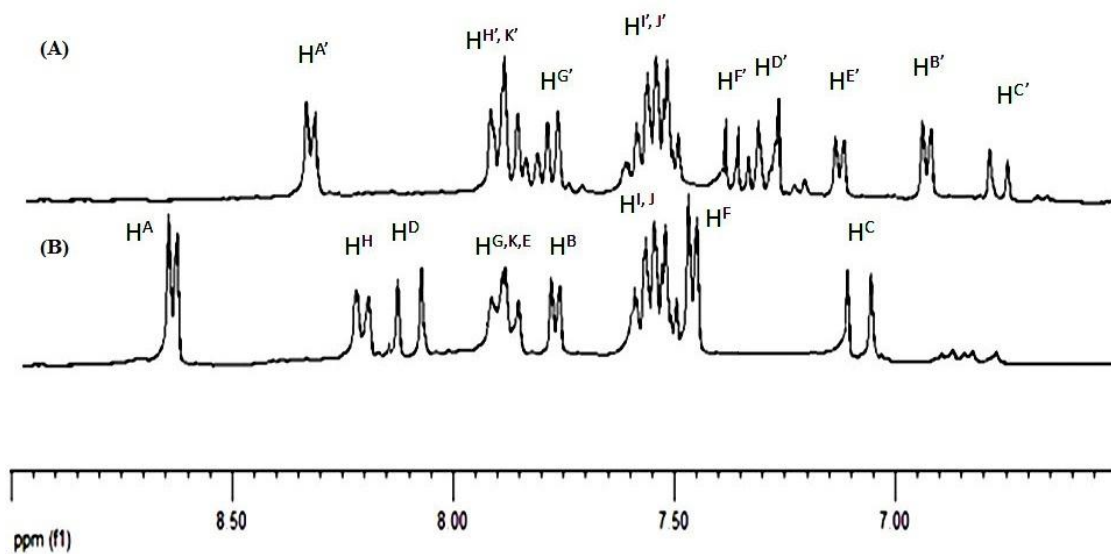


Figure S8. ¹H NMR spectra of complex **2** after (A) and before (B) irradiation at 365 nm in CDCl₃.

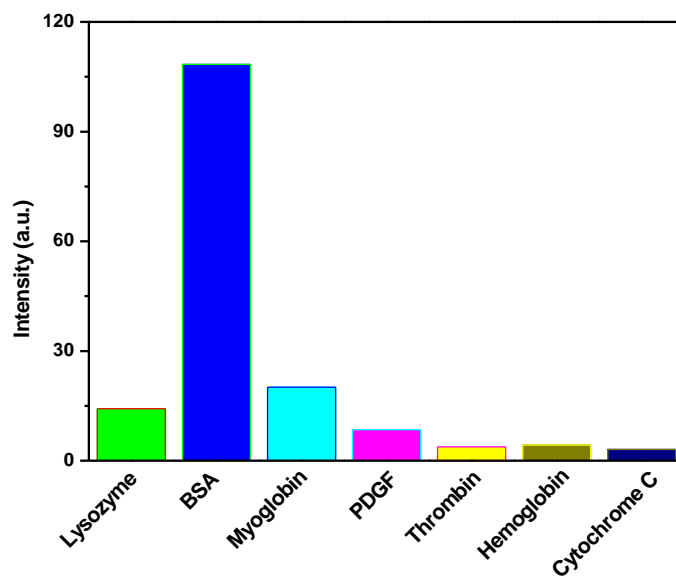


Figure S9. Comparison of the fluorescence intensity of **2** (20 μM) in the presence of various proteins.

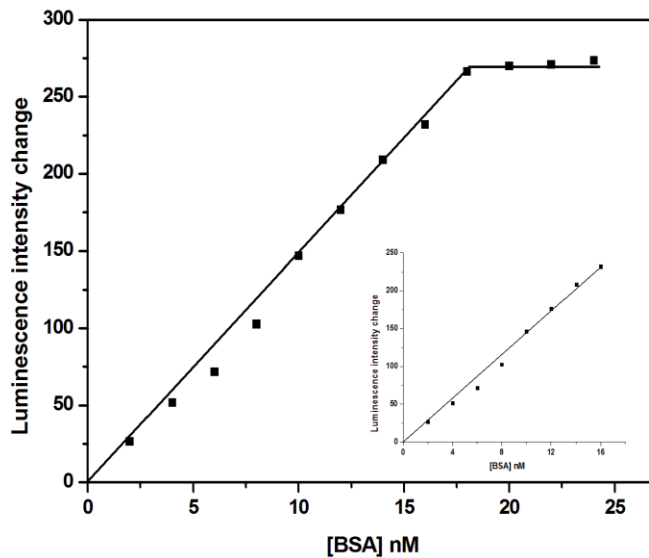


Figure S10. Luminescence intensity change of complex **2** versus [BSA] in PBS buffer. The concentration of BSA is 0–24 $\times 10^{-9}$ M. Inset: calibration plot of BSA sensor ($R = 0.993$).

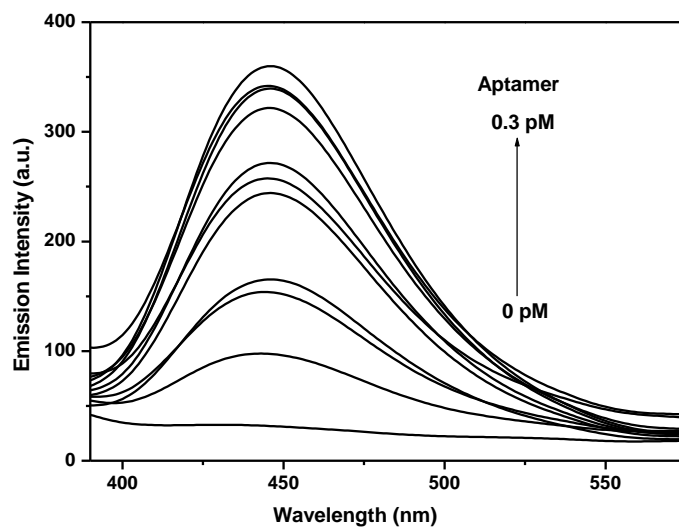


Figure S11. Emission spectral changes of complex **1** (10 μM) with the addition of PDGF aptamer (0 pM to 0.3 pM) in PBS buffer.

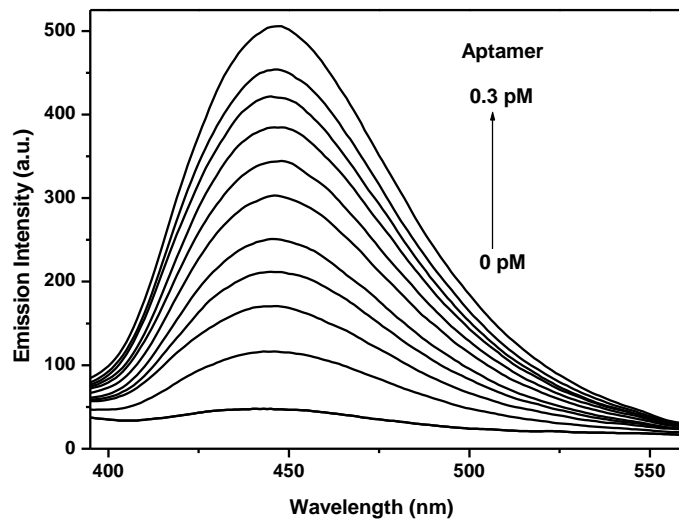


Figure S12. Emission spectral changes of **2** (10 μM) with the addition of PDGF binding aptamer (0 pM to 0.3 pM) in PBS buffer (pH = 7.4).

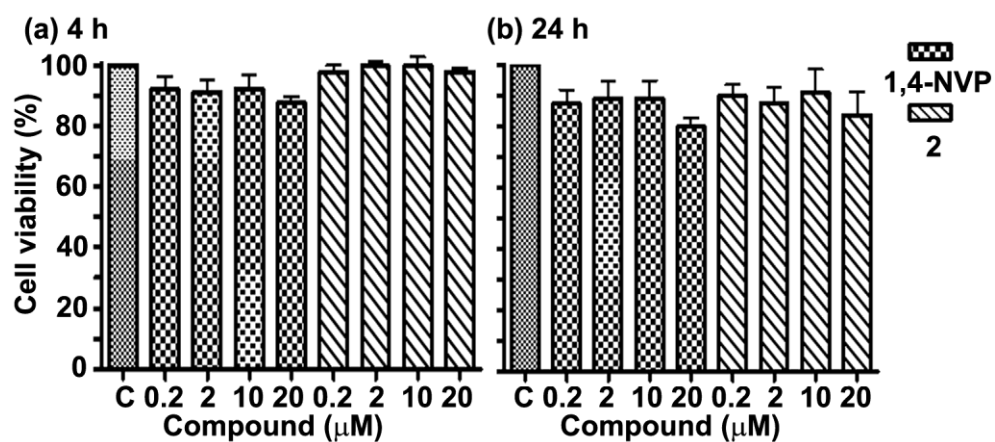


Figure S13. *In vitro* cell viability effects of 1,4-NVP and rhenium(I) complex **2** in inhibiting the growth of breast epithelium cells, M10, at 4 and 24 h..