Supporting Information

Coordination Driven Self-assembly of Ruthenium-Based Molecular-Rectangle: Synthesis, Characterization, Photo-physical and Anticancer Potency Studies

Vaishali Vajpayee,[†] Young Ho Song, [†] Young Jun Jung,[‡] Se Chan Kang, ^{*‡} Hyunuk Kim,[±] In Su Kim, [†] Ming Wang,^ζ Timothy R. Cook,^ζ Peter J. Stang, ^{*ζ} and Ki-Whan Chi ^{*†}

[†] Department of Chemistry, University of Ulsan, Ulsan 680-749, Republic of Korea.

[‡]Department of Natural Medicine Resources, University of Semyung, Jecheon 390-711,

Republic of Korea.

[±] Department of Chemistry, POSTECH, Pohang 690-784, Republic of Korea.

^ζDepartment of Chemistry, University of Utah, Salt Lake City, Utah 84112-0850, U.S.A.

*E-mail: <u>kwchi@ulsan.ac.kr</u>, <u>sckang@semyung.ac.kr</u>, <u>stang@chem.utah.edu</u>

Table of Contents

1.	¹³ C NMR spectra of the metalla-rectangles 1 and 2	S3
2.	¹³ C NMR spectra of the metalla-rectangles 3 and 4	S4
3.	¹ H and ¹³ C NMR spectra of the metalla-rectangles 5	.S5
4.	¹ H and ¹³ C NMR spectra of the metalla-rectangles 6	.S6
5.	¹ H and ¹³ C NMR spectra of the metalla-rectangles 7	.S8
6.	¹ H and ¹³ C NMR spectra of the metalla-rectangles 8	.S9
7.	HR-ESI-MS spectra of the metalla-rectangles 3 and 4	S 10
8.	HR-ESI-MS spectra of the metalla-rectangles 5 and 6	S 11
9.	HR-ESI-MS spectra of the metalla-rectangles 7 and 8	S12



Figure 1. 13 C NMR spectra of the metalla-rectangles 1 (a) and 2 (b).



Figure 2. 13 C NMR spectra of the metalla-rectangles **3** (a) and **4** (b).



Figure 3. 1 H (a) and 13 C NMR (b) spectra of the metalla-rectangle 5.



Figure 4. 1 H (a) and 13 C NMR (b) spectra of the metalla-rectangle **6**.



Figure 5. 1 H (a) and 13 C NMR (b) spectra of the metalla-rectangle 7.



Figure 6. 1 H (a) and 13 C NMR (b) spectra of the metalla-rectangle **8**.



Figure 7. Calculated and experimental ESI-MS spectra of the metalla-rectangles 1 (a) and 2 (b).





(b)



Figure 8. Calculated and experimental ESI-MS spectra of the metalla-rectangles 3 (a) and 4 (b).



(b)



Figure 9. Calculated and experimental ESI-MS spectra of the metalla-rectangles 5 (a) and 6 (b).



Figure 10. Calculated and experimental ESI-MS spectra of the metalla-rectangles 7 (a) and 8 (b).