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.

ζ Department of Chemistry, University of Utah, Salt Lake City, Utah 84112-0850, U.S.A.

*E-mail: kwchi@ulsan.ac.kr, sckang@semyung.ac.kr, stang@chem.utah.edu
# 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...............................S10
8. HR-ESI-MS spectra of the metalla-rectangles 5 and 6...............................S11
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).
Figure 8. Calculated and experimental ESI-MS spectra of the metalla-rectangles 3 (a) and 4 (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).