Supplementary Materials

Table of Contents

- 1. NMR spectra
- 2. Diagram of Calculation Targets

1. NMR Spectra





Compound **6a** ¹³C-NMR (100 MHz, CDCl₃).



For the NMR Spectra of compound **18a**, see the Supporting Information of the following paper:

1. Wu, Y.C.; Liron, M.; Zhu, J.P. Asymmetric total synthesis of (-)-quinocarcin. J. Am. Chem. Soc. **2008**, 130, 7148–7152.

For the NMR Spectra of compound 22a, see the Supporting Information of the following paper:

Wu, Y.C.; Bernadat, G.; Masson, G.; Couturier, C.; Schlama, T.; Zhu, J.P. Synthetic studies on (-)-lemonomycin: An efficient asymmetric synthesis of lemonomycinone amide. *J. Org. Chem.* 2009, 74, 2046–2052.

For the NMR Spectra of compound **28a** and compound **28b**, see the Supporting Information of the following paper:

3. Wu Y.C.; Zhu, J.P. Asymmetric total syntheses of (–)-renieramycin M and G and (–)-jorumycin using aziridine as a lynchpin. *Org. Lett.* **2009**, *11*, 5558–5561.

2. Diagram of Calculation Targets



Figure S1. Charge distribution of the arenium ion.

Figure S2. Total of electronic energy (Hartree) of the transition-state of the *ortho*-isomer product in the electrophilic aromatic bromination of anisole.



Figure S3. Total of electronic energy (Hartree) of the transition-state of the *meta*-isomer product in the electrophilic aromatic bromination of anisole.



Figure S4. Total of electronic energy (Hartree) of the transition-state of the *para*-isomer product in the electrophilic aromatic bromination of anisole.



Figure S5. Total of electronic energy (Hartree) of the *ortho*-isomer product in the electrophilic aromatic bromination of anisole.



Figure S6. Total of electronic energy (Hartree) of the *meta*-isomer product in the electrophilic aromatic bromination of anisole.



Figure S7. Total of electronic energy (Hartree) of the *para*-isomer product in the electrophilic aromatic bromination of anisole.

