

# Supporting Information

## 1,6-Conjugated Addition Mediated [2+1] Annulation: Approach to Spiro[2.5]octa-4,7-dien-6-one

Zhenbo Yuan, Xinxin Fang, Xuanyi Li, Jie Wu, Hequan Yao, \* and Aijun Lin \*

*State Key Laboratory of Natural Medicines and Department of Medicinal Chemistry,*

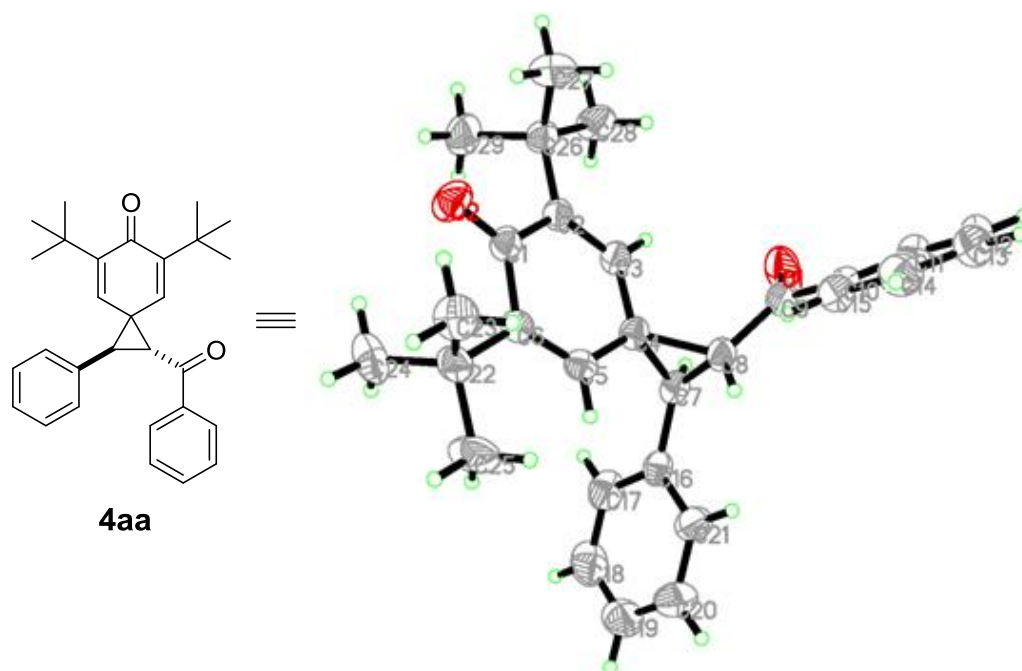
*China Pharmaceutical University, Nanjing 210009, P. R. China.*

E-mail: ajlin@cpu.edu.cn, hyao@cpu.edu.cn

### Contents

|                                                           |           |
|-----------------------------------------------------------|-----------|
| <i>Crystal structure of 4aa</i> .....                     | <i>S1</i> |
| <i>X-ray crystallographic data of 4aa</i> : .....         | <i>S1</i> |
| <i>Crystal structure of 4ma</i> .....                     | <i>S2</i> |
| <i>X-ray crystallographic data of 4ma</i> : .....         | <i>S2</i> |
| <i><sup>1</sup>H and <sup>13</sup>C-NMR Spectra</i> ..... | <i>S3</i> |

### Crystal structure of 4aa

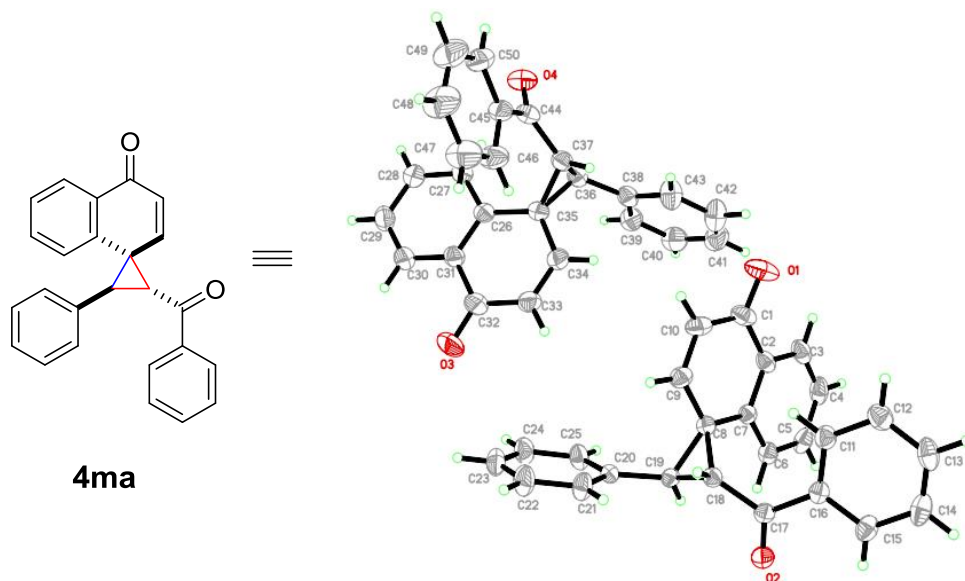


**Figure S1. ORTEP plot of the crystal structure of 4aa (at 30% probability level).**

### X-ray crystallographic data of 4aa

|                                  |                                                     |
|----------------------------------|-----------------------------------------------------|
| CCDC number                      | 1412107                                             |
| Empirical formula                | C <sub>29</sub> H <sub>32</sub> O <sub>2</sub>      |
| Formula weight                   | 412.55                                              |
| Temperature                      | 296 K                                               |
| Wavelength                       | 0.71073 Å                                           |
| Space group                      | P2(1)/c                                             |
| Unit cell dimensions             | a=13.417(2) Å =90°                                  |
|                                  | b=19.553(3) Å =108.595(3)°                          |
|                                  | c=9.7821(16) Å =90°                                 |
| Volume                           | 2432.2(7) Å <sup>3</sup>                            |
| Z                                | 4                                                   |
| Density (calculated)             | 1.127 Mg/m <sup>3</sup>                             |
| F(000)                           | 888.0                                               |
| Completeness to theta = 25.010 ° | 99.8%                                               |
| Absorption correction            | MULTI-SCAN                                          |
| Max. and min. transmission       | 0.985 and 0.981                                     |
| R indices (all data)             | R= 0.0467( 2662)<br>wR2(reflections)= 0.1470( 4280) |

### Crystal structure of 4ma



**Figure S2. ORTEP plot of the crystal structure of 4ma (at 30% probability level).**

### X-ray crystallographic data of 4ma

|                                  |                                                |
|----------------------------------|------------------------------------------------|
| CCDC number                      | 1427612                                        |
| Empirical formula                | C <sub>25</sub> H <sub>18</sub> O <sub>2</sub> |
| Formula weight                   | 350.39                                         |
| Temperature                      | 296 K                                          |
| Wavelength                       | 0.71073 Å                                      |
| Space group                      | C2/c                                           |
| Unit cell dimensions             | a= 43.875(12)Å =90°                            |
|                                  | b= 8.776(2)Å = 98.921(5)°                      |
|                                  | c= 19.789(5)Å =90°                             |
| Volume                           | 7527(3) Å <sup>3</sup>                         |
| Z                                | 16                                             |
| Density (calculated)             | 1.237 Mg/m <sup>3</sup>                        |
| F(000)                           | 2944.0                                         |
| Completeness to theta = 25.010 ° | 99.5%                                          |
| Absorption correction            | MULTI-SCAN                                     |
| Max. and min. transmission       | 0.983 and 0.979                                |
| R indices (all data)             | R= 0.0778( 3730)<br>wR2= 0.1963( 6616)         |

# <sup>1</sup>H and <sup>13</sup>C-NMR Spectra

