Laccase-catalysed a-Arylation of Cyclic B-Dicarbonyl Compounds

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Supporting Information

¹H- and ¹³C-NMR spectra:

| 3a | |
|----|----|
| 3b | |
| 3d | |
| 3e | |
| 3f | |
| 3g | |
| 3h | |
| 3i | |
| 3j | |
| 3k | |
| 31 | |
| 3m | |
| 3n | |
| 30 | |
| 3p | |
| 3q | |
| 5 | 38 |
| | |

HPLC-traces:

| 3q |
|-----------|
|-----------|



Figure S1. ¹H NMR (600 MHz, CDCl₃) spectrum of **3a**.



Figure S2. ¹³C NMR spectrum (CDCl₃, 151 MHz) of **3a**



Figure S3. ¹H NMR (600 MHz, CDCl₃) spectrum of **3b**



Figure S4. ¹³C NMR (151 MHz, CDCl₃) spectrum of **3b**

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Figure S5. ¹H NMR spectrum (600 MHz, CDCl₃) of 3d and 4d

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Figure S6. ¹³C NMR spectrum (151 MHz, CDCl₃) of **3d** and **4d**



Figure S7. ¹H NMR spectrum (600 MHz, CDCl₃) of (**3e**).



I



Figure S9. ¹H NMR spectrum (600 MHz, CDCl₃) of (**3f**).



Figure S10. ¹³C NMR spectrum (151 MHz, CDCl₃) of **3f**





*Figure S*11. ¹H NMR spectrum (600 MHz, CDCl₃) of **3g**.



Figure S12. ¹³C NMR spectrum (151 MHz, CDCl₃) of **3g**



Figure S13. ¹H NMR spectrum (600 MHz, CDCl₃) of **3h**.



Figure S14. ¹³C NMR spectrum (151 MHz, CDCl₃) of **3h**.



Figure S15. ¹H NMR spectrum (600 MHz, CDCl₃) of **3i**.



Figure S16. ¹³C NMR spectrum (151 MHz, CDCl₃) of **3i**.



Figure S17. ¹H NMR spectrum (600 MHz, CDCl₃) of **3j**.



Figure S18. ¹³C NMR spectrum (151 MHz, CDCl₃) of **3**j.



Figure S19. ¹H NMR spectrum (600 MHz, CDCl₃) of **3k**.



Figure S20. ¹³C NMR spectrum (151 MHz, CDCl₃)of **3k**.



Figure S21. ¹H NMR spectrum (600 MHz, CDCl₃) of 3l.



Figure S22. ¹³C NMR spectrum (151 MHz, CDCl₃) of 3l.



Figure S23. ¹H NMR spectrum (600 MHz, CDCl₃) of **3m**.



Figure S24. ¹³C NMR spectrum (151 MHz, CDCl₃) of **3m**.



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Figure S26. ¹³C NMR spectrum (151 MHz, CDCl₃) of **3n**.



Figure S27. ¹H NMR spectrum (600 MHz, CDCl₃) of **30**.



Figure S28. ¹³C NMR spectrum (151 MHz, CDCl₃) of **30**.



Figure S29. ¹H NMR spectrum (600 MHz, CDCl₃) of **3p**.



Figure S30. ¹³C NMR spectrum (151 MHz, CDCl₃) of **3p**.



Figure S31. ¹H NMR spectrum (600 MHz, CDCl₃) of 3q.



Figure S32. ¹³C NMR spectrum (151 MHz, CDCl₃) of **3q**.



Figure S33. H_COSY spectrum (600 MHz, CDCl₃) of **3q**.



Figure S34. DEPT spectrum (151 MHz, CDCl₃) of 3q.



Figure S35. HSQC spectrum (600 MHz, CDCl₃) of **3q**.

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Figure S37. ¹H NMR spectrum (600 MHz, CDCl₃) of 5.



Figure S38. ¹³C NMR spectrum (151 MHz, CDCl₃) of **5**.

| Operator:henssen | Timebase:SYS_1 | Sequence:Standards | |
|------------------|----------------|--------------------|--|
|------------------|----------------|--------------------|--|

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| 274 Chuan CW 115A Chiralpak IC Sample Name: Chuan CW 115A Injection Volume: 2,0 | | | | |
|---|-------------------------|-------------------|----------|--|
| Chiralpak IC | | | | |
| Sample Name: | Chuan CW 115A | Injection Volume: | 2,0 | |
| Vial Number: | BA6 | Channel: | UV_VIS_1 | |
| Sample Type: | unknown | Wavelength: | 205.0 | |
| Control Program: | Heptan-2-Propanol 80-20 | Bandwidth: | 2 | |
| Quantif. Method: | default | Dilution Factor: | 1,0000 | |
| Recording Time: | 2.4.2012 17:19 | Sample Weight: | 1,0000 | |
| Run Time (min): | 240,00 | Sample Amount: | 1,0000 | |



| | No. | Ret.Time | Peak Name | Height | Area | Rel.Area | Amount | Туре |
|---|-------|----------|-----------|--------|---------|----------|--------|------|
| | | min | | mAU | mAU*min | % | | |
| Г | 1 | 6,78 | n.a. | 7,029 | 2,083 | 0,58 | n.a. | BMB |
| | 2 | 89,72 | n.a. | 32,759 | 112,634 | 31,24 | n.a. | BMB* |
| | 3 | 147,76 | n.a. | 46,310 | 245,863 | 68,19 | n.a. | BMB* |
| Т | otal: | | | 86,098 | 360,580 | 100,00 | 0,000 | |

Operator:henssen Timebase:SYS_1 Sequence:Standards

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| 283 Chuan CW 115 B Chiralpak IC | | | | |
|------------------------------------|-------------------------|------------------|--------|--|
| | | | | |
| Sample Type: | unknown | Wavelength: | 205.0 | |
| Control Program: | Heptan-2-Propanol 80-20 | Bandwidth: | 2 | |
| Quantif. Method: | default | Dilution Factor: | 1,0000 | |
| Recording Time: | 3.4.2012 21:28 | Sample Weight: | 1,0000 | |
| Run Time (min): | 240,00 | Sample Amount: | 1,0000 | |



Figure S39. HPLC of 3q; racemic (left), non-racemic (right).