Electronic Supplementary Information

Reactivity of alkynylindole-2-carboxamides in [Pd]-catalysed C-H activation and phase transfer catalysis: Formation of pyrrolo-diindolones vs β-carbolinones

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1 Crystal data for the compounds 9a and 10h

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(1) Crystal data for the compounds 9a and 10h

**X-ray Data.** X-ray data for compounds 9a and 10h, were collected using MoK$_\alpha$ ($\lambda = 0.71073$ Å) radiation. The structures were solved and refined by standard methods as mentioned in the main text. The CCDC numbers are 1453189-1453190.

**Compound 9a**

Red color needle, C$_{31}$H$_{20}$N$_2$O$_2$, $M = 454.51$, Triclinic, Space group $P$-$1$, $a = 9.4276(5)$, $b = 11.2761(9)$, $c = 11.6981(10)$ Å, $V = 1137.32(14)$ Å$^3$, $\alpha = 112.674(8)$, $\beta = 90.151(5)$, $\gamma = 96.976(5)$, $Z = 2$, $\mu = 0.660$ mm$^{-1}$, data/restraints/parameters: 4333/0/317, R indices ($I$> $2\sigma(I)$): R1 = 0.0449, wR2 (all data) = 0.1166, CCDC No. 1453189.

**Compound 10h**

Colorless block, C$_{26}$H$_{22}$N$_2$O$_2$, $M = 394.46$, Triclinic, Space group $P$-$1$, $a = 11.5059(4)$, $b = 12.8459(6)$, $c = 15.6020(8)$ Å, $\alpha = 106.081(4)$, $\beta = 93.226(4)$, $\gamma = 109.728(4)$, $V = 2056.95(16)$ Å$^3$, $Z = 4$, $\mu = 0.643$ mm$^{-1}$, data/restraints/parameters: 7879/0/547, R indices ($I$> $2\sigma(I)$): R1 = 0.0488, wR2 (all data) = 0.1277, CCDC No. 1453190.
(2) Copies of $^1$H/$^{13}$C NMR spectra for starting precursors

Figure S1. $^1$H NMR spectrum of compound 5d

Figure S2. $^{13}$C NMR spectrum of compound 5d
Figure S3. $^1$H NMR spectrum of compound 6b

Figure S4. $^{13}$C NMR spectrum of compound 6b
Figure S5. $^1$H NMR spectrum of compound 6d

Figure S6. $^{13}$C NMR spectrum of compound 6d
Figure S7. $^1$H NMR spectrum of compound 7a

Figure S8. $^{13}$C NMR spectrum of compound 7a
**Figure S9.** $^1$H NMR spectrum of compound 7b

**Figure S10.** $^{13}$C NMR spectrum of compound 7b
Figure S11. $^1$H NMR spectrum of compound 7c

Figure S12. $^{13}$C NMR spectrum of compound 7c
Figure S13. $^1$H NMR spectrum of compound 7d

Figure S14. $^{13}$C NMR spectrum of compound 7d
Figure S15. $^1$H NMR spectrum of compound 7e

Figure S16. $^{13}$C NMR spectrum of compound 7e
Figure S17. $^1$H NMR spectrum of compound 7f

Figure S18. $^{13}$C NMR spectrum of compound 7f
Figure S19. $^1$H NMR spectrum of compound 7g

Figure S20. $^{13}$C NMR spectrum of compound 7g
Figure S21. $^1$H NMR spectrum of compound 7h

Figure S22. $^{13}$C NMR spectrum of compound 7h
**Figure S23.** $^1$H NMR spectrum of compound 7i

**Figure S24.** $^{13}$C NMR spectrum of compound 7i
Figure S25. $^1$H NMR spectrum of compound 7j

Figure S26. $^{13}$C NMR spectrum of compound 7j
Figure S27. $^1$H NMR spectrum of compound 7k

Figure S28. $^{13}$C NMR spectrum of compound 7k
Figure S29. $^1$H NMR spectrum of compound 8a

Figure S30. $^{13}$C NMR spectrum of compound 8a
Figure S31. $^{1}$H NMR spectrum of compound 8b

Figure S32. $^{13}$C NMR spectrum of compound 8b
Figure S33. $^1$H NMR spectrum of compound 8c

Figure S34. $^{13}$C NMR spectrum of compound 8c
Figure S35. $^1$H NMR spectrum of compound 8d

Figure S36. $^{13}$C NMR spectrum of compound 8d
Figure S37. $^1$H NMR spectrum of compound 8e

Figure S38. $^{13}$C NMR spectrum of compound 8e
Figure S39. $^1$H NMR spectrum of compound 8f

Figure S40. $^{13}$C NMR spectrum of compound 8f
Figure S41. $^1$H NMR spectrum of compound 8g

Figure S42. $^{13}$C NMR spectrum of compound 8g
Figure S43. $^1$H NMR spectrum of compound 8h

Figure S44. $^{13}$C NMR spectrum of compound 8h
Figure S45. $^1$H NMR spectrum of compound 8i

Figure S46. $^{13}$C NMR spectrum of compound 8i
Figure S47. $^1$H NMR spectrum of compound 8j

Figure S48. $^{13}$C NMR spectrum of compound 8j
Figure S49. $^1$H NMR spectrum of compound 8k

Figure S50. $^{13}$C NMR spectrum of compound 8k
Figure S51. $^1$H NMR spectrum of compound 8l

Figure S52. $^{13}$C NMR spectrum of compound 8l
Figure S53. $^1$H NMR spectrum of compound 8m

Figure S54. $^{13}$C NMR spectrum of compound 8m
Figure S55. $^1$H NMR spectrum of compound 8n

Figure S56. $^{13}$C NMR spectrum of compound 8n
Figure S57. $^1$H NMR spectrum of compound 8o

Figure S58. $^{13}$C NMR spectrum of compound 8o
(2) Copies of $^1\text{H}/^{13}\text{C}$ NMR spectra for pyrrolo diindolones 9a-j and β-Carbolinones 10a-o.

Figure S59. $^1\text{H}$ NMR spectrum of compound 9a

Figure S60. $^{13}\text{C}$ NMR spectrum of compound 9a
Figure S61. $^1$H NMR spectrum of compound 9b

Figure S62. $^{13}$C NMR spectrum of compound 9b
Figure S63. $^1$H NMR spectrum of compound 9c

Figure S64. $^{13}$C NMR spectrum of compound 9c
Figure S65. $^1$H NMR spectrum of compound 9d

Figure S66. $^{13}$C NMR spectrum of compound 9d
Figure S67. $^1$H NMR spectrum of compound 9e

Figure S68. $^{13}$C NMR spectrum of compound 9e
Figure S69. $^1$H NMR spectrum of compound 9f

Figure S70. $^{13}$C NMR spectrum of compound 9f
Figure S71. $^1$H NMR spectrum of compound 9g

Figure S72. $^{13}$C NMR spectrum of compound 9g
**Figure S73.** $^1$H NMR spectrum of compound 9h

**Figure S74.** $^{13}$C NMR spectrum of compound 9h
Figure S75. $^1$H NMR spectrum of compound 9i

Figure S76. $^{13}$C NMR spectrum of compound 9i
Figure S77. $^1$H NMR spectrum of compound 9j

Figure S78. $^{13}$C NMR spectrum of compound 9j
Figure S79. $^1$H NMR spectrum of compound 10a

Figure S80. $^{13}$C NMR spectrum of compound 10a
Figure S81. $^1$H NMR spectrum of compound 10b

Figure S82. $^{13}$C NMR spectrum of compound 10b
Figure S83. $^1$H NMR spectrum of compound 10c

Figure S84. $^{13}$C NMR spectrum of compound 10c
Figure S85. $^1$H NMR spectrum of compound 10d

Figure S86. $^{13}$C NMR spectrum of compound 10d
Figure S87. $^1$H NMR spectrum of compound 10e

Figure S88. $^{13}$C NMR spectrum of compound 10e
Figure S89. $^1$H NMR spectrum of compound 10f

Figure S90. $^{13}$C NMR spectrum of compound 10f
Figure S91. $^1$H NMR spectrum of compound 10g

Figure S92. $^{13}$C NMR spectrum of compound 10g
Figure S93. $^1$H NMR spectrum of compound 10h

Figure S94. $^{13}$C NMR spectrum of compound 10h
**Figure S95.** $^1$H NMR spectrum of compound 10i

**Figure S96.** $^{13}$C NMR spectrum of compound 10i
Figure S97. $^1$H NMR spectrum of compound 10j

Figure S98. $^{13}$C NMR spectrum of compound 10j
Figure S99. $^1$H NMR spectrum of compound 10k

Figure S100. $^{13}$C NMR spectrum of compound 10k
Figure S101. $^1$H NMR spectrum of compound 10l

Figure S102. $^{13}$C NMR spectrum of compound 10l
Figure S103. $^1$H NMR spectrum of compound 10m

Figure S104. $^{13}$C NMR spectrum of compound 10m
Figure S105. $^1$H NMR spectrum of compound 10n

Figure S106. $^{13}$C NMR spectrum of compound 10n
Figure S107. $^1$H NMR spectrum of compound 10o

Figure S108. $^{13}$C NMR spectrum of compound 10o