Supporting Information
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Visible-Light Photoredox Catalyzed Cascade Reaction for the Synthesis of Pyrrolo[2,1-\textit{a}]isoquinoline-Substituted Phosphonates

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1. Preparation and Spectral Data of Substrates 1a-f

1.1 General procedure for preparation of [(3,4-dihydroisoquinolin-2(1H)-yl)methyl]phosphonates 1a-f

\[
\text{NH} \quad \overset{\text{(HCHO)n \quad + \quad O}}{\text{toluene, 120°C}} \quad \overset{\text{TsOH}}{\text{N}} \quad \overset{\text{O}}{\text{P(OEt)₂}} \quad \overset{\text{1a}}{\text{1,2,3,4-tetrahydroisoquinoline \quad diethyl phosphite \quad paraformaldehyde \quad toluene-4-sulfonic acid}}
\]

To a stirred solution of 1,2,3,4-tetrahydroisoquinoline (1.33 g, 10 mmol), diethyl phosphite (1.73 g, 12.5 mmol) in toluene (15 mL), paraformaldehyde (0.40 g, 12.5 mmol) and toluene-4-sulfonic acid (45 mg) were added in a 100 mL three-necked flask. The mixture was stirred at 120 °C until the reaction was completed (monitored by TLC). After the solvent was removed under reduced pressure, the residue was purified by flash column chromatography to give compound 1a as a yellow oil (1.92 g, 68% yield). Other dihydroisoquinoline phosphonates 1b-f were prepared according to the above procedure.[1-2]


1.2 Spectral data of the substrates 1a-f
Substrate 1a
1a. yellow oil; 1.92 g (68% yield); ^1H NMR (400 MHz, CDCl3): \( \delta \) 7.08-7.15 (m, 3H), 7.00-7.04 (m, 1H), 4.13-4.23 (m, 4H), 3.85 (s, 2H), 2.87-3.02 (m, 6H), 1.34 (t, \( J = 7.0 \) Hz, 6H); ^13C NMR (100 MHz, CDCl3): \( \delta \) 134.4, 133.8, 128.6, 126.5, 126.1, 125.6, 62.2 (d, \( J = 7.0 \) Hz), 57.3 (d, \( J = 11.0 \) Hz), 54.4, 52.8, 52.4 (d, \( J = 10 \) Hz), 28.8, 16.5 (d, \( J = 6 \) Hz); ^31P NMR (162 MHz, CDCl3): \( \delta \) 24.31; HRMS (ESI): \( m/z \) [M + H]^+ calcd for C14H22NO3P: 284.1410; found: 284.1405

Substrate 1b
1b. yellow oil: 1.56 g (61% yield); ^1H NMR (400 MHz, CDCl3): \( \delta \) 7.08-7.15 (m, 3H), 7.00-7.04 (m, 1H), 3.84 (s, 2H), 3.82 (s, 3H), 3.80 (s, 3H), \( \delta \) 3.00 (d, \( J = 11.6 \) Hz, 2H), 2.96 (d, \( J = 5.2 \) Hz, 2H), 2.92 (d, \( J = 5.4 \) Hz, 2H); ^13C NMR (100 MHz, CDCl3): \( \delta \) 134.2, 133.7, 128.6, 126.5, 125.6, 57.3 (d, \( J = 11.0 \) Hz), 53.7, 52.9 (d, \( J = 6.9 \) Hz), 52.6, 51.9, 28.8; ^31P NMR (162 MHz, CDCl3): \( \delta \) 26.65; HRMS (ESI): \( m/z \) [M + Na]^+ calcd for C12H18NO3P: 278.0917; found: 278.0909.

Substrate 1c
1c. yellow oil: 2.27 g (73% yield); ^1H NMR (400 MHz, CDCl3): \( \delta \) 6.98-7.15 (m, 4H), 4.70-4.82 (m, 2H), 3.85 (s, 2H), 2.86-2.99 (m, 6H), \( \delta \) 3.00 (d, \( J = 6.7 \) Hz), 2.96 (d, \( J = 5.2 \) Hz, 2H), 2.92 (d, \( J = 5.4 \) Hz, 2H); ^13C NMR (100 MHz, CDCl3): \( \delta \) 134.6, 133.9, 128.5, 126.4, 126.0, 125.6, 70.5 (d, \( J = 6.7 \) Hz), 57.3 (d, \( J = 10.8 \) Hz), 55.3, 53.6, 52.4 (d, \( J = 10.2 \) Hz), 28.9, 24.0; ^31P NMR (162 MHz, CDCl3): \( \delta \) 22.45; HRMS (ESI): \( m/z \) [M + H]^+ calcd for C16H26NO3P: 312.1723; found: 312.1714.

Substrate 1d
1d. yellow oil: 2.00 g (59% yield); ^1H NMR (400 MHz, CDCl3): \( \delta \) 7.09-7.11 (m, 3H), 6.95–7.04 (m, 1H), 3.99–4.18 (m, 4H), 3.84 (s, 2H), 2.70-3.08 (m, 6H), 1.55-1.75 (m, 4H), 1.37-1.43 (m, 4H), 0.92 (t, \( J = 7.4 \) Hz, 6H); ^13C NMR (100 MHz, CDCl3): \( \delta \) 134.3, 133.7, 128.5, 126.3, 126.0, 125.5, 65.8 (d, \( J = 7.0 \) Hz), 57.2 (d, \( J = 10.7 \) Hz), 54.2, 53.9, 50.6, 32.5 (d, \( J = 5.8 \) Hz), 28.8, 18.6, 13.5; ^31P NMR (162 MHz, CDCl3): \( \delta \) 24.35; HRMS (ESI): \( m/z \) [M + H]^+ calcd for C18H30NO3P: 340.2036; found: 340.2037.

Substrate 1e
1e. yellow oil: 2.82 g (78% yield); ^1H NMR (400 MHz, CDCl3): \( \delta \) 7.24 (d,
$J = 8.7$ Hz, 1H), 7.16 (s, 1H), 6.96 (d, $J = 8.1$ Hz, 1H), 4.07-4.26 (m, 4H), 3.81 (s, 2H), 2.92-2.99 (m, 4H), 2.84 (t, $J = 6.0$ Hz, 2H), 1.34 (t, $J = 7.0$ Hz, 6H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 136.6, 132.8, 130.3, 129.2, 129.2, 119.1, 62.2 (d, $J = 6.7$ Hz), 56.6 (d, $J = 10.6$ Hz), 54.1, 53.2, 50.9, 28.2, 16.5 (d, $J = 5.8$ Hz); $^{31}$P NMR (162 MHz, CDCl$_3$): $\delta$ 24.05; HRMS (ESI): $m/z$ [M + H]$^+$ calcd for C$_{14}$H$_{21}$NO$_3$PBr: 362.0515; found: 362.0507.

**Substrate 1f**

1f, yellow oil; 2.64 g (77% yield); $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 6.51 (s, 1H), 6.44 (s, 1H), 4.10 (t, $J = 7.1$ Hz, 4H), 3.76 (s, 3H), 3.75 (s, 3H), 3.71 (s, 2H), 2.82-2.99 (m, 4H), 2.74 (t, $J = 6.0$ Hz, 2H), 1.26 (t, $J = 7.1$ Hz, 6H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 147.4, 147.1, 126.1, 125.6, 111.2, 109.3, 62.0 (d, $J = 7.0$ Hz), 56.8 (d, $J = 10.7$ Hz), 55.8, 54.2, 53.3, 49.7, 28.2, 16.4 (d, $J = 5.4$ Hz); $^{31}$P NMR (162 MHz, CDCl$_3$): $\delta$ 24.29; HRMS (ESI): $m/z$ [M + H]$^+$ calcd for C$_{16}$H$_{26}$NO$_5$P: 344.1621; found: 344.1611.

2. Details for Condition Optimization

Table S1. Optimization the condition for the photocatalytic oxidation/[3+2] cycloaddition/oxidative aromatization cascade reaction$^a$. 

S4
| entry | photocatalyst | Base  | Solvent | Yield/%
|-------|--------------|-------|---------|--------
| 1     | Ru(bpy)₃Cl₂·6H₂O | none  | CH₃CN   | Trace  
| 2     | Ru(bpy)₃Cl₂·6H₂O | NaOH  | CH₃CN   | 8%     
| 3     | Ru(bpy)₃Cl₂·6H₂O | NaOAc | CH₃CN   | 44%    
| 4     | Ru(bpy)₃Cl₂·6H₂O | K₂CO₃ | CH₃CN   | 40%    
| 5     | Ru(bpy)₃Cl₂·6H₂O | K₂HPO₄| CH₃CN   | 28%    
| 6     | Ru(bpy)₃Cl₂·6H₂O | DABCO | CH₃CN   | Trace  
| 7     | Ru(bpy)₃Cl₂·6H₂O | DBU   | CH₃CN   | Trace  
| 8     | Ru(bpy)₃Cl₂·6H₂O | Et₃N  | CH₃CN   | Trace  
| 9     | Ru(bpy)₃Cl₂·6H₂O | NaOAc | DCM     | 65%    
| 10    | Ru(bpy)₃Cl₂·6H₂O | NaOAc | THF     | 34     
| 11    | Ru(bpy)₃Cl₂·6H₂O | NaOAc | DMF     | 28     
| 12    | Ru(bpy)₃Cl₂·6H₂O | NaOAc | DMSO    | 20     
| 13    | Ru(bpy)₃Cl₂·6H₂O | NaOAc | CH₃OH   | 47     
| 14    | RB            | NaOAc | DCM     | 24     
| 15    | Eosin Y      | NaOAc | DCM     | 23     
| 16    | fac-Ir(ppy)₃ | NaOAc | DCM     | 21     
| 17    | Ru(bpy)₃Cl₂·6H₂O | NaOAc | DCM     | 71%    
| 18    | Ru(bpy)₃Cl₂·6H₂O | NaOAc | DCM     | Trace  

1) Ru(bpy)₃Cl₂·6H₂O (5 mol%) NaOAc (1.6 equiv), DCM (3 ml), 1 atm O₂, rt, 36 W CFL, 24 h
2) NBS (1.1 equiv), rt, 1-1.5 h
According to the general procedure from 1\(\text{a} \) (0.6 mmol), 2\(\text{a} \) (0.5 mmol), sodium acetate (0.8 mmol), Ru(bpy)\(_3\)Cl\(_2\).6H\(_2\)O (0.025 mmol) and DCM (3.0 mL) under an oxygen atmosphere, the mixture was stirred for 10 h under ambient sunlight irradiation, then followed by the oxidative aromatization with NBS (5.5 mmol equiv.), 3\(\text{a} \) was obtained as a yellow solid in 80% yield (155 mg).
4. Gram-scale reaction.
1a (2.0 g, 7.2 mmol), dimethyl but-2-ynedioate (0.60 g, 4 mmol), sodium acetate (0.5 g, 6.4 mmol), Ru(bpy)₃Cl₂·6H₂O (150 mg, 0.2 mmol) and DCM (24 mL) were added to a 100 ml flask linking with an oxygen balloon, the mixture was stirred for 36 h under ambient temperature while cooling with an electric fan. After the reaction completed (monitored by TLC), the mixture was concentrated in vacuo, and the residue was purified by flash chromatography on silica gel (eluent: petroleum ether / ethyl acetate 5:1 to 3:1) to obtain 3e as a yellow oil (1.15 g, 68.5% yield).
5. X-Ray Structures of 3a

Figure. ORTEP diagram of the X-ray crystal structure of 3a and ethyl acetate complex. Platon plot of 3a (298 k) with thermal ellipsoids at the 50% probability level.

Single crystal of compound 3a and ethyl acetate complex was obtained from the mixed petroleum ether and ethyl acetate (V/V, 4:1). CCDC 1818810 contains the supplementary crystallographic data which can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Crystal data. C$_{23}$H$_{29}$N$_2$O$_7$P, $M = 476.45$, monoclinic, $a = 14.503(3)$ Å, $b = 13.807(2)$ Å, $c = 12.156(2)$ Å, $V = 2371.1(7)$Å$^3$. 
6. Copies of NMR Spectra of the Substrates 1a-f and Products 3a–3p
Figure 1. $^1$H NMR (400 MHz, CDCl$_3$) spectra of substrate 1a

Figure 2. $^{13}$C NMR (100 MHz, CDCl$_3$) spectra of substrate 1a
Figure 3. $^{31}$P NMR (162 MHz, CDCl$_3$) spectra of substrate 1a
Figure 4. $^1$H NMR (400 MHz, CDCl$_3$) spectra of substrate 1b
Figure 5. $^{13}$C NMR (100 MHz, CDCl$_3$) spectra of substrate 1b
Figure 6. $^{31}$P NMR (162 MHz, CDCl$_3$) spectra of substrate 1b
Figure 7. $^1$H NMR (400 MHz, CDCl$_3$) spectra of substrate substrate 1c
Figure 8. $^{13}$C NMR (100 MHz, CDCl$_3$) spectra of substrate 1c
Figure 9. $^{31}$P NMR (162 MHz, CDCl$_3$) spectra of substrate 1c

Figure 10. $^1$H NMR (400 MHz, CDCl$_3$) spectra of substrate 1d
Figure 11. $^{13}$C NMR (100 MHz, CDCl$_3$) spectra of substrate 1d
Figure 12. $^{31}$P NMR (162 MHz, CDCl$_3$) spectra of substrate 1d
Figure 13. $^1$H NMR (400 MHz, CDCl$_3$) spectra of substrate 1e

Figure 14. $^{13}$C NMR (100 MHz, CDCl$_3$) spectra of substrate 1e
Figure 15. $^{31}$P NMR (162 MHz, CDCl$_3$) spectra of substrate 1e
Figure 16. $^1$H NMR (400 MHz, CDCl$_3$) spectra of substrate 1f
Figure 17. $^{13}$C NMR (100 MHz, CDCl$_3$) spectra of substrate 1f
Figure 18. $^{31}$P NMR (162 MHz, CDCl$_3$) spectra of substrate 1f
NMR Spectra of the Product 3

Figure 19. $^1$H NMR (600 MHz, CDCl$_3$) spectra of product 3a
Figure 20. $^{13}$C NMR (100 MHz, CDCl$_3$) spectra of product 3a
Figure 21. $^{31}$P NMR (162 MHz, CDCl$_3$) spectra of product 3a

Figure 22. $^1$H NMR (400 MHz, CDCl$_3$) spectra of product 3b
Figure 23. $^{13}$C NMR (100 MHz, CDCl$_3$) spectra of product 3b
Figure 24. $^{31}$P NMR (162 MHz, CDCl$_3$) spectra of product 3b
Figure 25. $^1$H NMR (400 MHz, CDCl$_3$) spectra of product 3c

Figure 26. $^{13}$C NMR (100 MHz, CDCl$_3$) spectra of product 3c
Figure 27. $^{31}$P NMR (162 MHz, CDCl$_3$) spectra of product 3c
Figure 28. $^1$H NMR (400 MHz, CDCl$_3$) spectra of product 3d
Figure 29. $^{13}$C NMR (100 MHz, CDCl$_3$) spectra of product 3d

Figure 30. $^{31}$P NMR (162 MHz, CDCl$_3$) spectra of product 3d
Figure 31. $^1$H NMR (400MHz, CDCl$_3$) spectra of product 3e
Figure 32. $^{13}$C NMR (100MHz, CDCl$_3$) spectra of product 3e
Figure 33. $^{31}$P NMR (162MHz, CDCl$_3$) spectra of product 3e

Figure 34. $^1$H NMR (400 MHz, CDCl$_3$) spectra of product 3f
Figure 35. $^{13}$C NMR (100 MHz, CDCl$_3$) spectra of product 3f
Figure 36. $^{31}$P NMR (162 MHz, CDCl$_3$) spectra of product 3f
Figure 37. $^1$H NMR (400 MHz, CDCl$_3$) spectra of product 3g
Figure 38. $^{13}$C NMR (100 MHz, CDCl$_3$) spectra of product 3g

Figure 39. $^{31}$P NMR (162 MHz, CDCl$_3$) spectra of product 3g
Figure 40. $^1$H NMR (400 MHz, CDCl$_3$) spectra of product $3h$
Figure 41. $^{13}$C NMR (100 MHz, CDCl$_3$) spectra of product 3h
Figure 42. $^{31}$P NMR (162 MHz, CDCl$_3$) spectra of product 3h
Figure 43. $^1$H NMR (400 MHz, CDCl$_3$) spectrum of product 3i
Figure 44. $^{13}$C NMR (100 MHz, CDCl$_3$) spectrum of product 3i
Figure 45. $^{31}$P NMR (162 MHz, CDCl$_3$) spectrum of product 3i

Figure 46. $^1$H NMR (400 MHz, CDCl$_3$) spectra of product 3j
Figure 47. $^{13}$C NMR (100 MHz, CDCl$_3$) spectra of product 3j
Figure 48. $^{31}$P NMR (162 MHz, CDCl$_3$) spectra of product 3j
Figure 49. $^1$H NMR (400 MHz, CDCl$_3$) spectrum of product 3k.
Figure 50. $^{13}$C NMR (100 MHz, CDCl$_3$) spectrum of product 3k

Figure 51. $^{31}$P NMR (162 MHz, CDCl$_3$) spectrum of product 3k
Figure 52. $^1$H NMR (400 MHz, CDCl$_3$) spectra of product 3l
Figure 53. $^{13}$C NMR (100 MHz, CDCl$_3$) spectra of product 3l
Figure 54. $^{31}$P NMR (162 MHz, CDCl$_3$) spectra of product 3l

![Figure 54. $^{31}$P NMR (162 MHz, CDCl$_3$) spectra of product 3l](image)

Figure 55. $^1$H NMR (400 MHz, CDCl$_3$) spectrum of product 3m

![Figure 55. $^1$H NMR (400 MHz, CDCl$_3$) spectrum of product 3m](image)
Figure 56. $^{13}$C NMR (100 MHz, CDCl$_3$) spectrum of product 3m
Figure 57. $^{31}$ P NMR (162 MHz, CDCl$_3$) spectrum of product 3m
Figure 58. $^1$H NMR (400 MHz, CDCl$_3$) spectra of product 3n
Figure 59. $^{13}$C NMR (100 MHz, CDCl3) spectra of product 3n

Figure 60. $^{31}$P NMR (162 MHz, CDCl3) spectra of product 3n
Figure 61. $^1$H NMR (400 MHz, CDCl$_3$) spectrum of product 3o
Figure 62. $^{13}$C NMR (100 MHz, CDCl$_3$) spectrum of product 3o

Figure 63. $^{31}$P NMR (162 MHz, CDCl$_3$) spectrum of product 3o
Figure 64. $^1$H NMR (400 MHz, CDCl$_3$) spectra of product 3p
Figure 65. $^{13}$C NMR (150 MHz, CDCl$_3$) spectra of product 3p
Figure 66. $^{31}$P NMR (162 MHz, CDCl$_3$) spectra of product 3p
7. Copies of HRMS Spectra of the Substrates 1a-f, and Products 3a-3p
Figure 67. HRMS spectra of substrate 1a
Figure 68. HRMS spectra of substrate 1b
Figure 69. HRMS spectra of substrate 1c
Figure 70. HRMS spectra of substrate 1d
Figure 71. HRMS spectra of substrate 1e
Figure 72. HRMS spectra of substrate 1f
Figure 73. HRMS spectra of substrate 3a
Figure 74. HRMS spectra of substrate 3b
Figure 75. HRMS spectra of substrate 3c
Figure 76. HRMS spectra of substrate 3d
Figure 77. HRMS spectra of substrate 3e
Figure 78. HRMS spectra of substrate 3f
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![Chemical Structure] P(OEt)_2

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Figure 79. HRMS spectra of substrate 3g
Figure 80. HRMS spectra of substrate 3h
Figure 81. HRMS spectra of substrate 3i
Figure 82. HRMS spectra of substrate 3j
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Measured region for 417.1564 m/z

C21 H25 N2 O5 P [M+H]+ - Predicted region for 417.1574 m/z
Figure 83. HRMS spectra of substrate 3k
Figure 84. HRMS spectra of substrate 3l
Figure 85. HRMS spectra of substrate 3m
Figure 86. HRMS spectra of substrate 3n
Figure 87. HRMS spectra of substrate 3o
Figure 88. HRMS spectra of substrate 3p