**Supplementary Information**

# Characterizations of cationic γ-carbolines binding with double-stranded DNA by spectroscopic methods and AFM imaging

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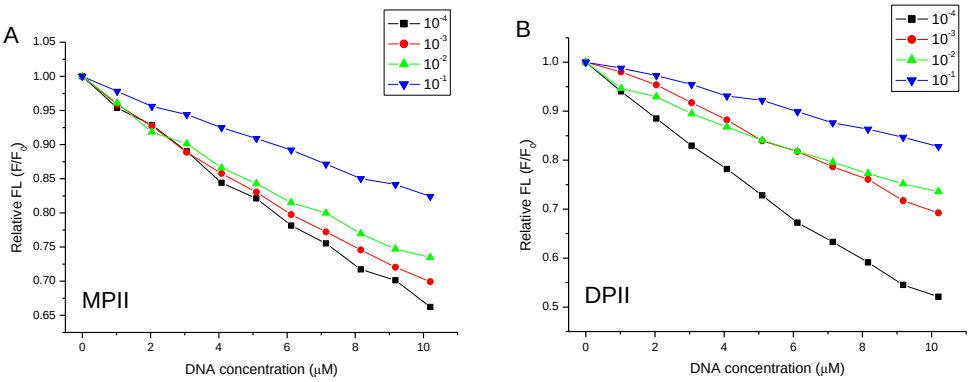



Fig. S1. Relative fluorescence intensity decreases with the titration of **MPII** and **DPII** (0.1 μM) by CT-DNA (0–10.2 μM). Black line and squares: an ionic strength of $10^{-4}$ M; red line and diamonds: an ionic strength of $10^{-3}$ M; green line and triangles: an ionic strength of $10^{-2}$ M; blue line and inverted triangles: an ionic strength of $10^{-1}$ M.

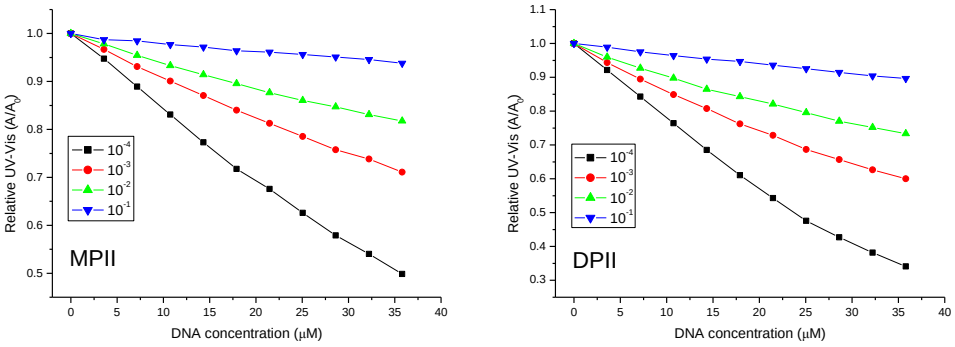
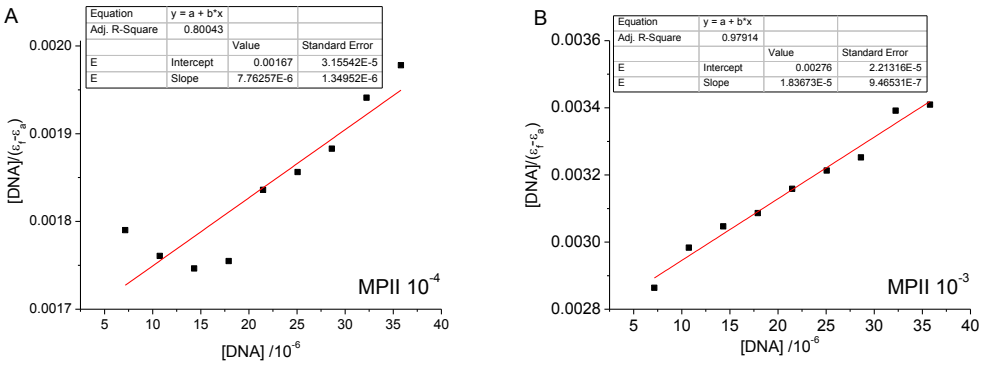



Fig. S2. Relative UV-Vis absorbance decreases with the titration of **MPII** ($\lambda_{max}$=260 nm) and **DPII** ($\lambda_{max}$=262 nm) (10 μM) by CT-DNA (0–35.8 μM). Black line and squares: an ionic strength of $10^{-4}$ M; red line and diamonds: an ionic strength of $10^{-3}$ M; green line and triangles: an ionic strength of $10^{-2}$ M; blue line and inverted triangles: an ionic strength of $10^{-1}$ M.



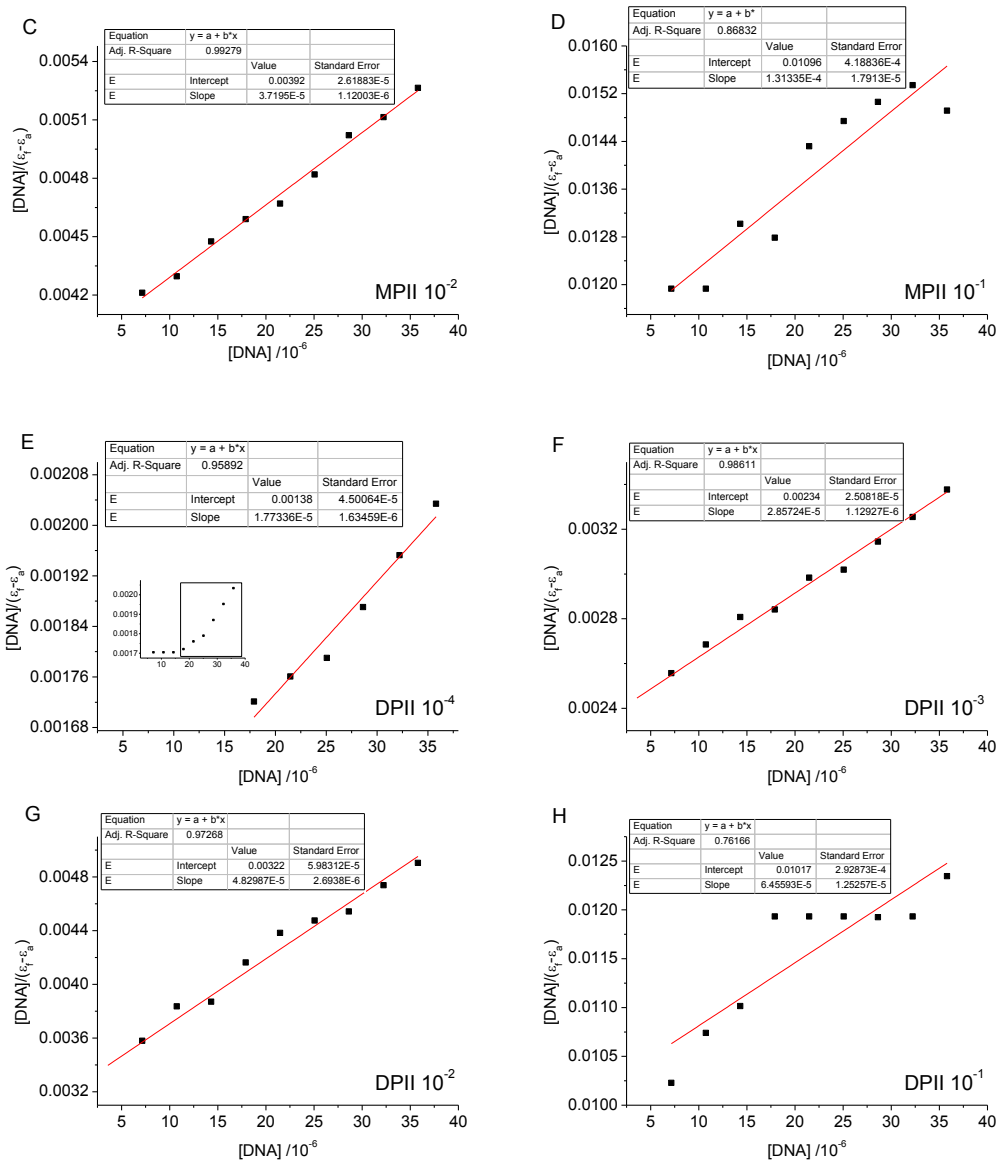



Fig. S3. The plots of $[DNA]/(e_f–e_a)$ versus [DNA] for the titrations of DNA with **MPII** (A-D)and **DPII** (E-H) in various ionic strengths.

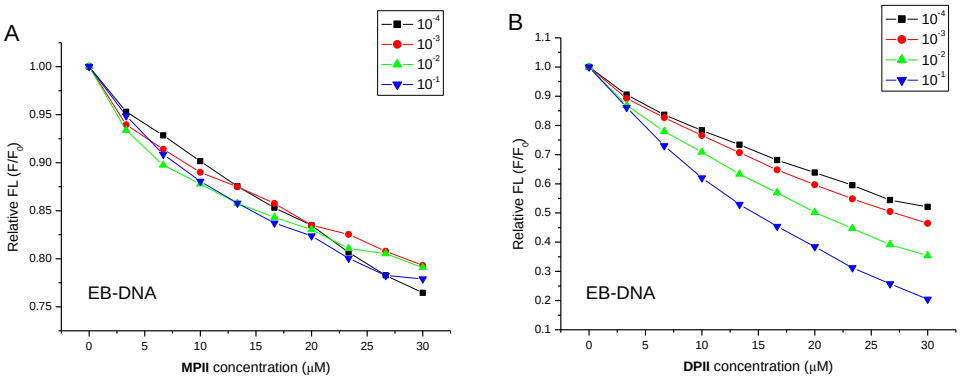



Fig. S4. Relative fluorescence intensity decreases with the titration of **EB**-DNA (2 μM : 5 μM) by **MPII** (A) and **DPII** (B) (0–30 μM). Black line and squares: an ionic strength of $10^{-4}$ M; red line and diamonds: an ionic strength

of $10^{-3}$ M; green line and triangles: an ionic strength of $10^{-2}$ M; blue line and inverted triangles: an ionic strength of $10^{-1}$ M.

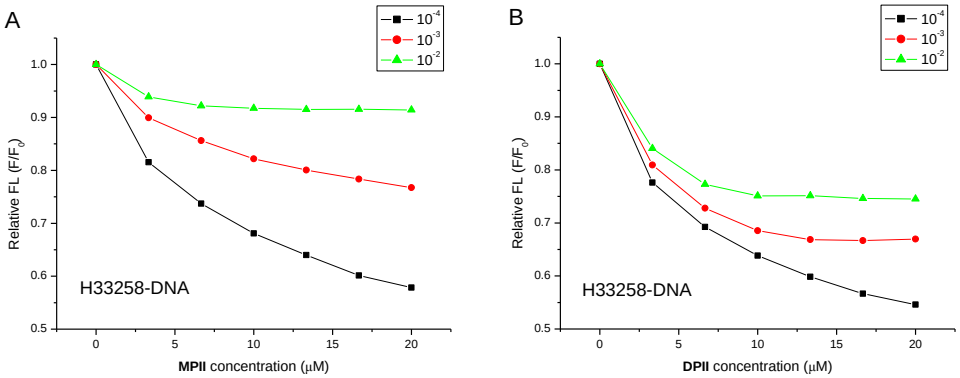



Fig. S5. Relative fluorescence intensity decreases with the titration of H33258-DNA (2 μM : 5 μM) by **MPII** (A) and **DPII** (B) (0–20 μM). Black line and squares: an ionic strength of $10^{-4}$ M; red line and diamonds: an ionic strength of $10^{-3}$ M; green line and triangles: an ionic strength of $10^{-2}$ M.

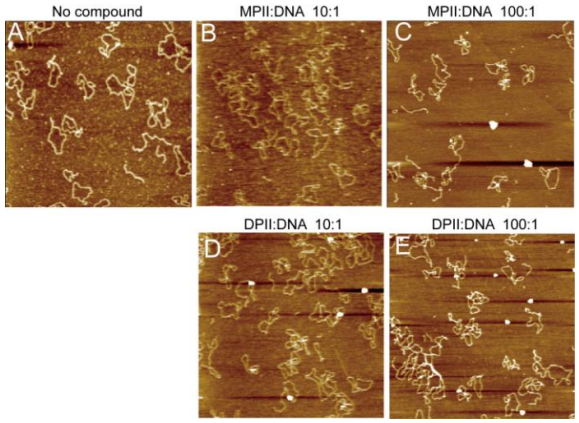



Fig. S6. AFM images for pBR322 with the increase of **MPII** and **DPII** at the mole ratio of compound:DNA=0:1 (A), 10:1((B) and (D)), 100:1 ((C) and (E)). Scan area: 3000 nm×3000 nm. Z range is 2 nm.

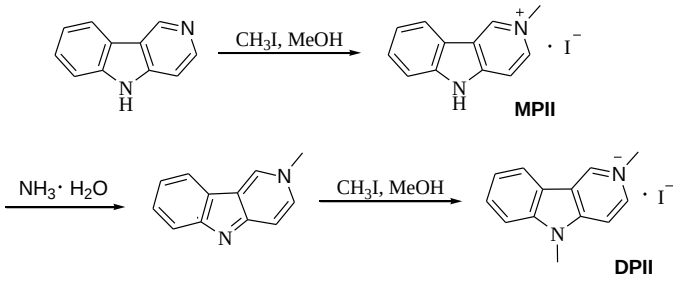



Fig.S7. Synthesis of the two cationic γ-carbolines

## Spectroscopic data about three synthetic compounds

**1. 2-Methyl-5*H*-pyrido[4,3-*b*]indolium iodide (MPII) (Fig. S2-4)**

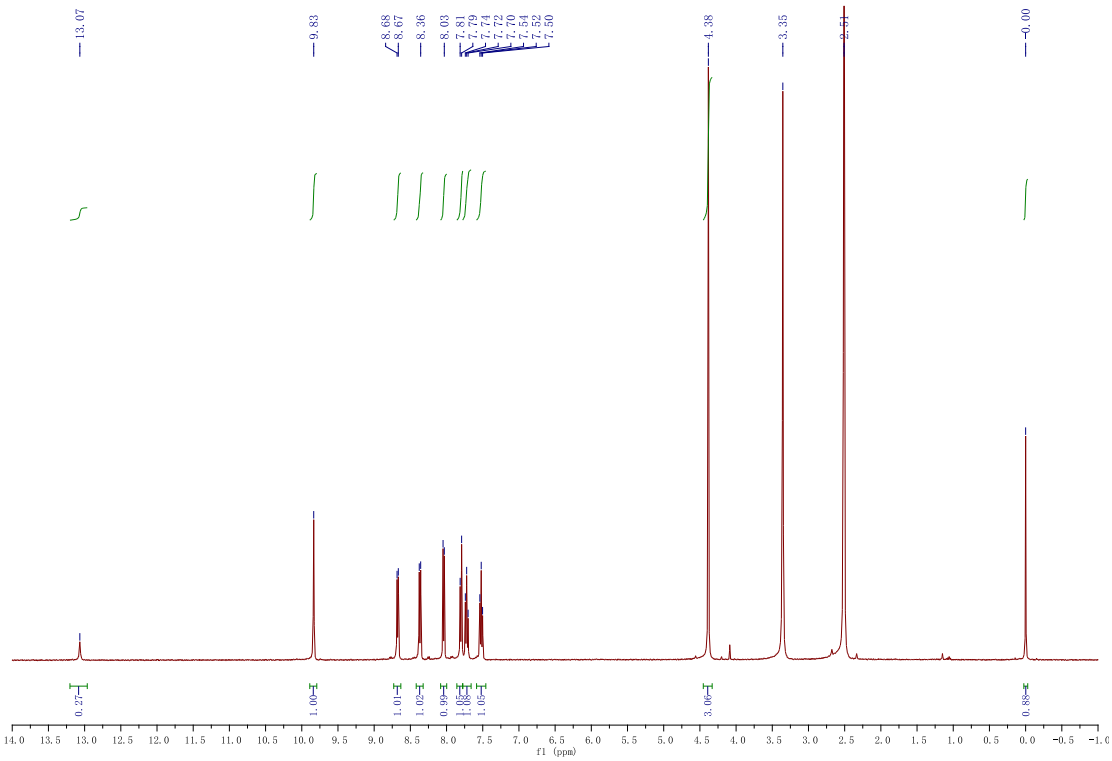



Fig. S8. $^{1}$H NMR of 2-methyl-5*H*-pyrido[4,3-*b*]indolium iodide (MPII)

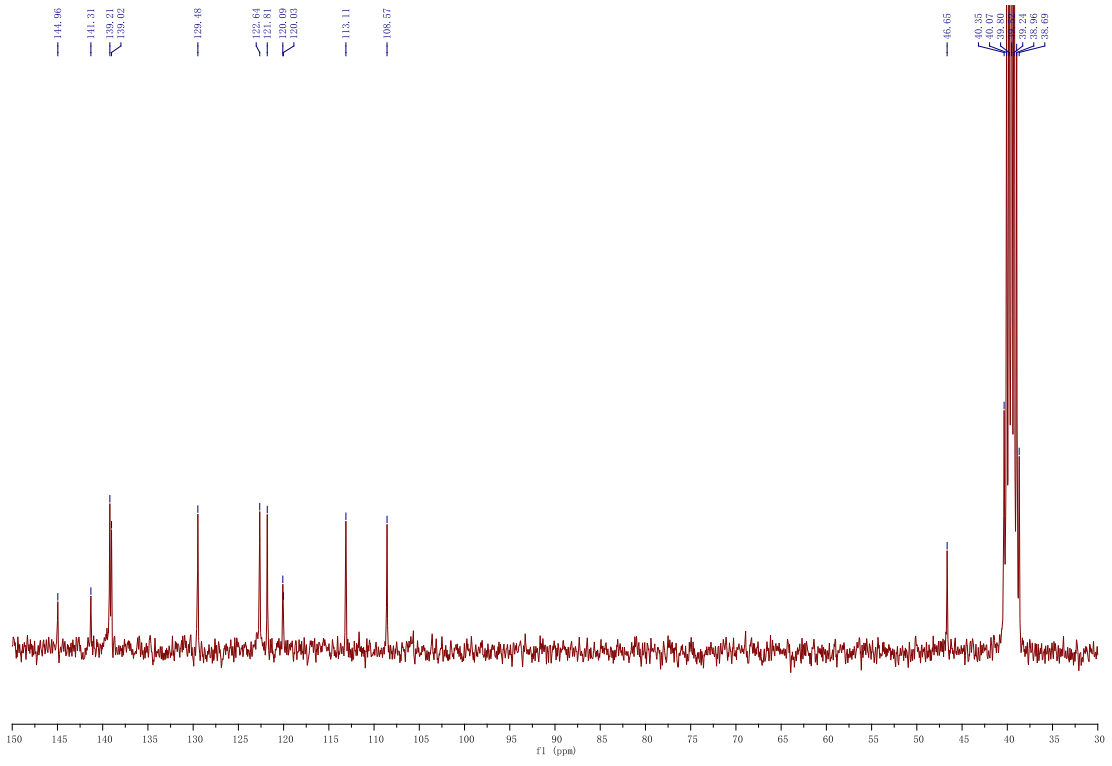
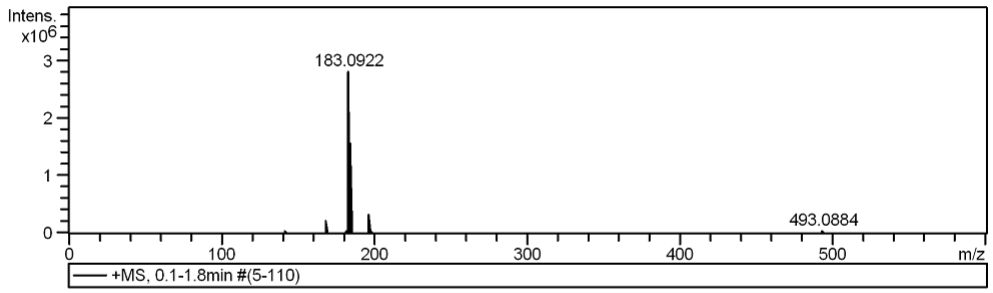



Fig. S9. $^{13}$C NMR of 2-methyl-5*H*-pyrido[4,3-*b*]indolium iodide (MPII)

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.3 Bar |
| Focus | Not active | | | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set Capillary | 4500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 3000 m/z | Set End Plate Offset | -500 V | Set Divert Valve | Waste |




| # | m/z | Res. | S/N | I | FWHM |
|---|---|---|---|---|---|
| 1 | 168.0683 | 4485 | 6604.5 | 239251 | 0.0375 |
| 2 | 183.0922 | 2561 | 83228.4 | 2825307 | 0.0715 |
| 3 | 197.1076 | 4803 | 10415.4 | 331688 | 0.0410 |
| 4 | 493.0884 | 6173 | 7681.4 | 57840 | 0.0799 |

Fig. S10. HRMS of 2-methyl-5*H*-pyrido[4,3-*b*]indolium iodide (MPII)

2. 2-Methyl-2H-pyrido[4,3-b]indole (Fig. S5-7)

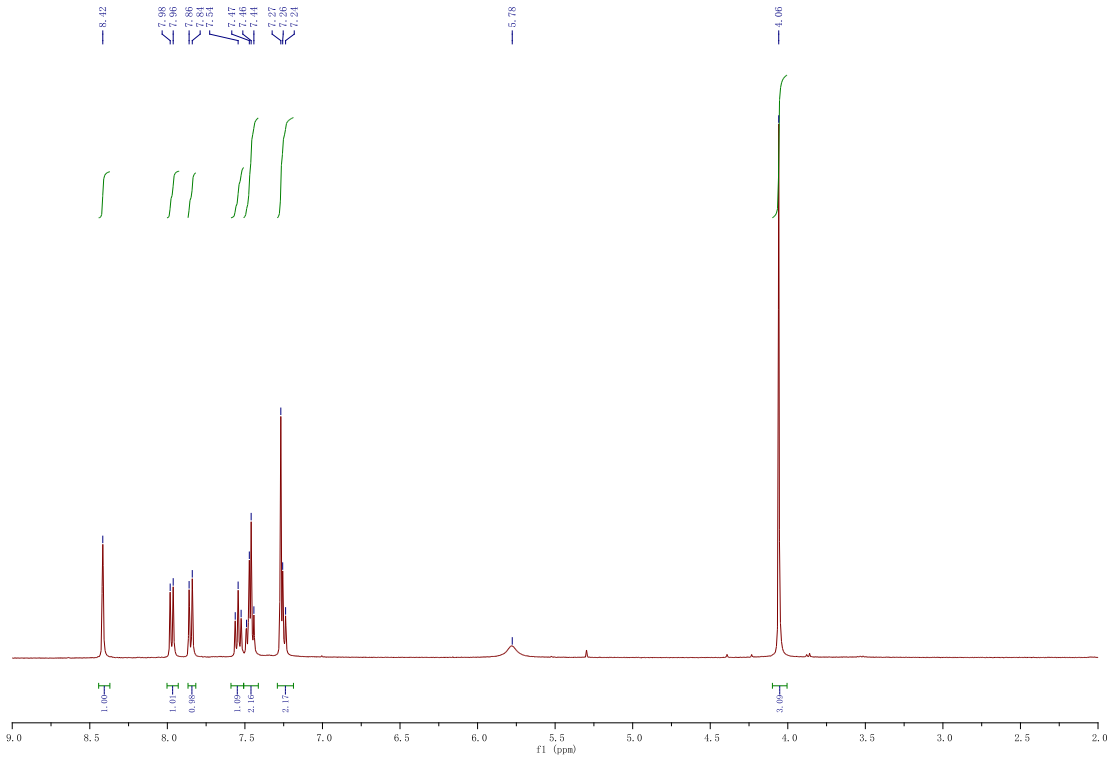



Fig. S11. $^{1}$H NMR of 2-methyl-2H-pyrido[4,3-b]indole

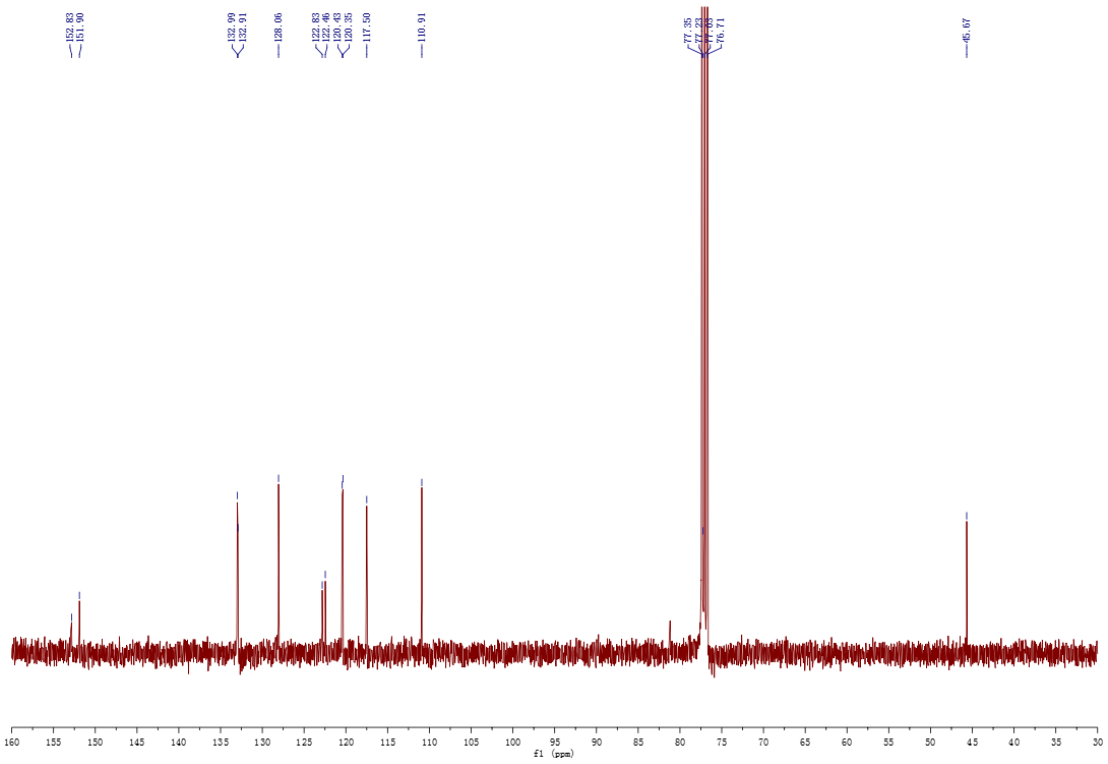
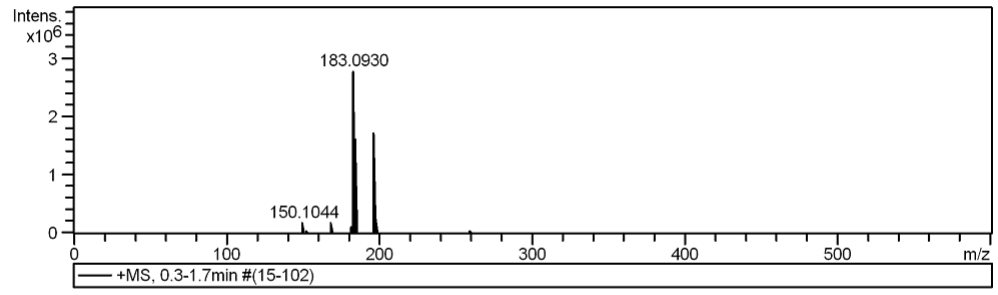



Fig. S12. $^{13}$C NMR of 2-methyl-2H-pyrido[4,3-b]indole

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.3 Bar |
| Focus | Not active | | | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set Capillary | 4500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 3000 m/z | Set End Plate Offset | -500 V | Set Divert Valve | Waste |




| # | m/z | Res. | S/N | I | FWHM |
|---|---|---|---|---|---|
| 1 | 150.1044 | 4455 | 3249.5 | 193296 | 0.0337 |
| 2 | 168.0682 | 4441 | 3365.8 | 186418 | 0.0378 |
| 3 | 183.0930 | 2454 | 53635.1 | 2789761 | 0.0746 |
| 4 | 197.1085 | 4228 | 35203.3 | 1720289 | 0.0466 |

Fig. S13. HRMS of 2-methyl-2H-pyrido[4,3-b]indole

3. 2,5-Dimethyl-5*H*-pyrido[4,3-*b*]indolium iodide (DPII) (Fig. S8-10)

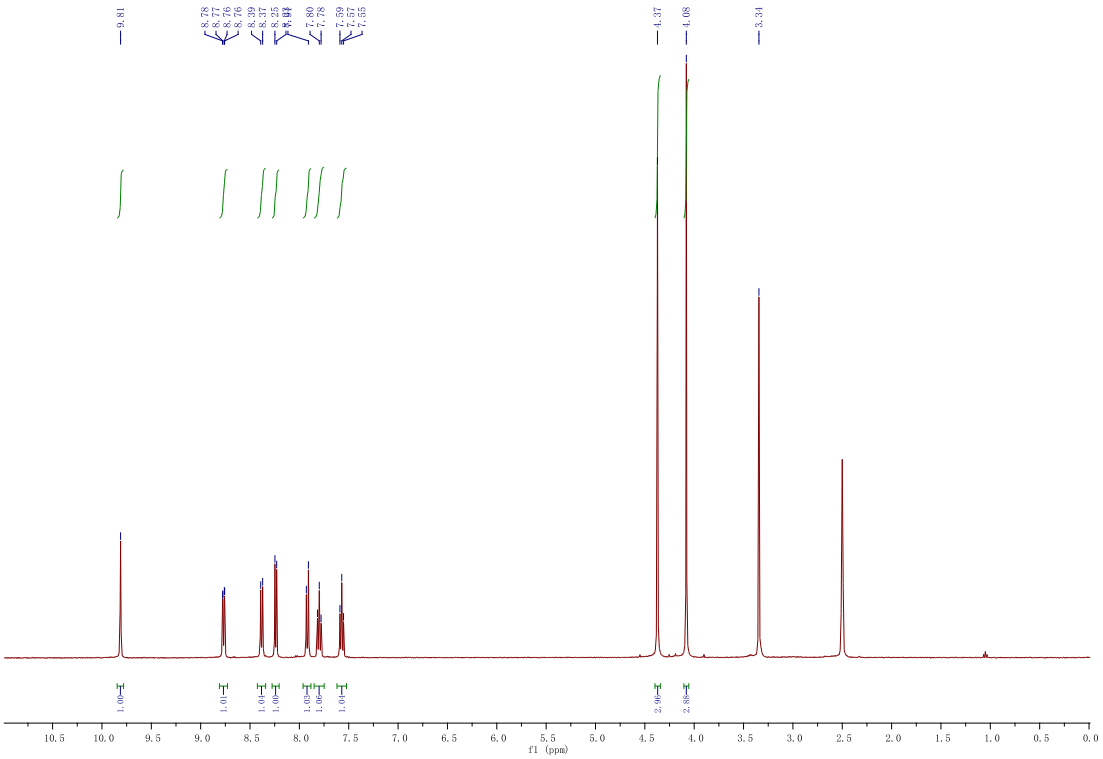



Fig. S14. $^{1}$H NMR of 2,5-dimethyl-5*H*-pyrido[4,3-*b*]indolium iodide (DPII)

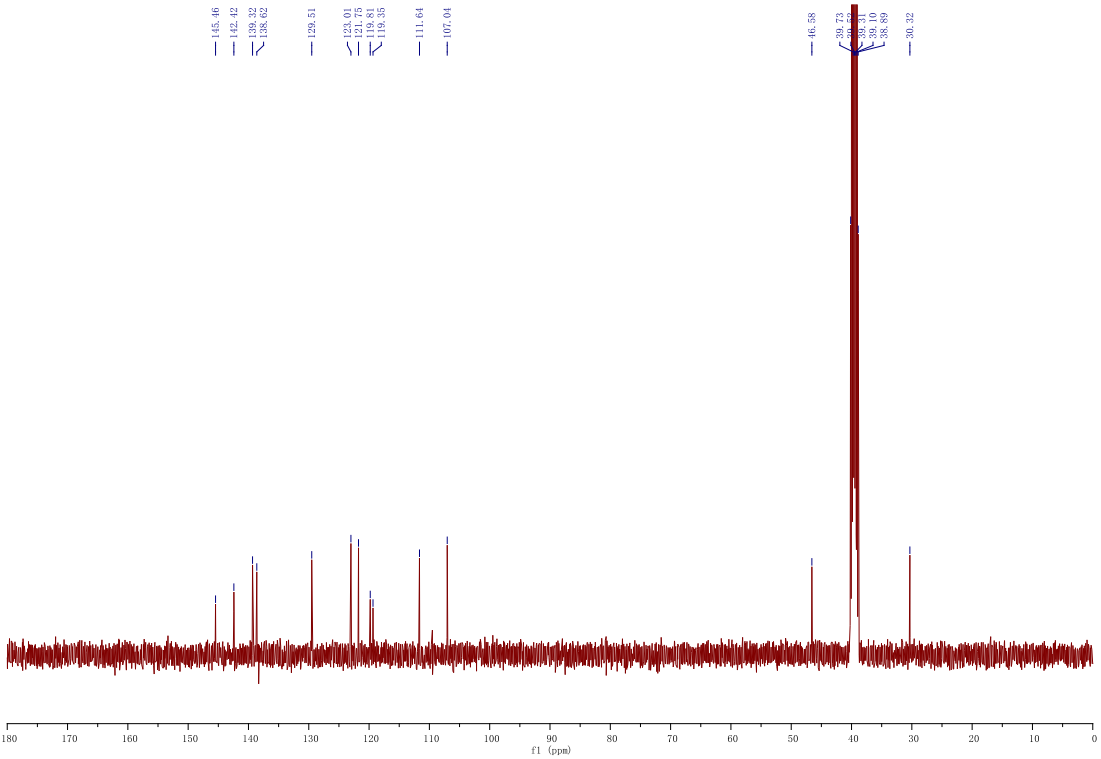
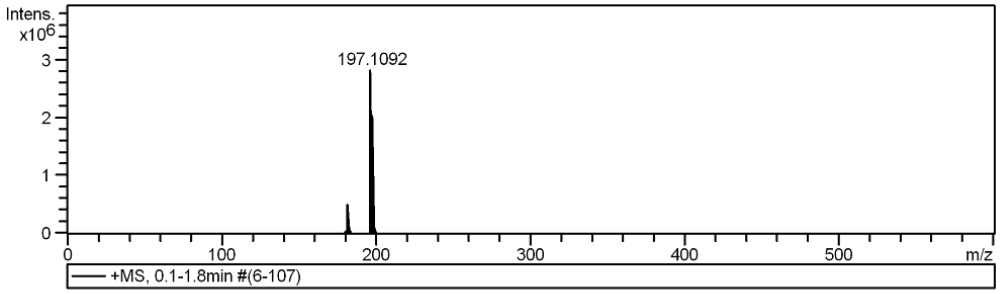



Fig. S15. $^{13}$C NMR of 2,5-dimethyl-5*H*-pyrido[4,3-*b*]indolium iodide (DPII)

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.3 Bar |
| Focus | Not active | | | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set Capillary | 4500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 3000 m/z | Set End Plate Offset | -500 V | Set Divert Valve | Waste |




| # | m/z | Res. | S/N | I | FWHM |
|---|---|---|---|---|---|
| 1 | 182.0842 | 4554 | 14027.2 | 505927 | 0.0400 |
| 2 | 197.1092 | 2360 | 82799.8 | 2833069 | 0.0835 |
| 3 | 198.1118 | 4410 | 59670.8 | 2034387 | 0.0449 |
| 4 | 199.1126 | 5539 | 3577.4 | 121529 | 0.0359 |

Fig. S16. HRMS of 2,5-dimethyl-5*H*-pyrido[4,3-*b*]indolium iodide (DPII)