ChemistryOPEN

# Supporting Information



## Enzymatic Strategy for the Resolution of New 1-Hydroxymethyl Tetrahydro-$\beta$-carboline Derivatives in Batch and Continuous-Flow Systems

Rita Megyesi,[a] Enikő Forró,*[a] and Ferenc Fülöp*[a, b]

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HPLC with Chiralpak OD-H column (4.6 mm × 250 mm), eluent: *n*-hexane: *i*PA (93:7), flow rate: 0.5 mL $min^{-1}$, detection at 260 nm, at room temperature. Retention times (min): for (*R*)-**7**: 27.7, (*S*)-**7**: 16.6, (*S*)-**10**: 13.8 and (*R*)-**10**: 18.8.

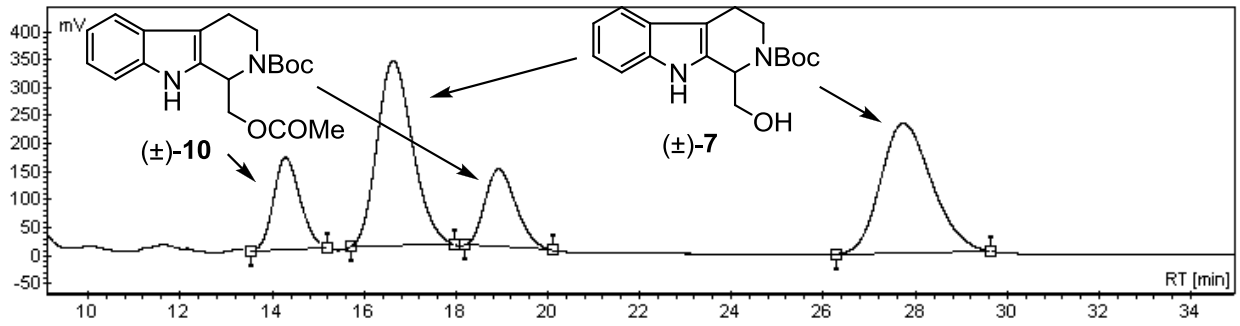


**Figure S1** HPLC chromatogram of (±)-**7** and (±)-**10**

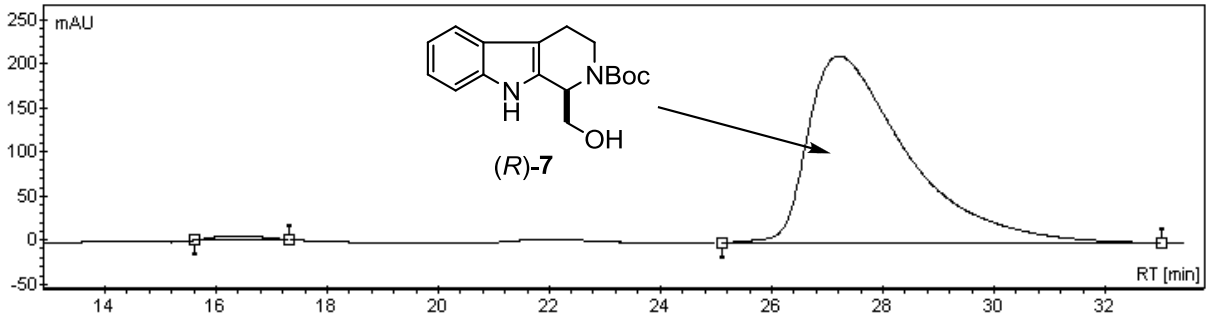


**Figure S2** HPLC chromatogram of the (*R*)-**7** (*ee* = 98%) after a column chromatography separation of the preparative-scale enzymatic resolution of (±)-**7**.

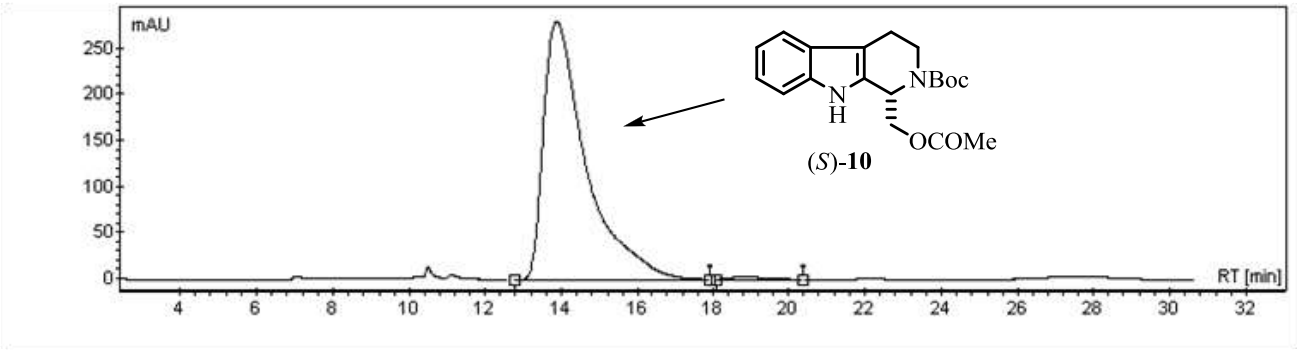


**Figure S3** HPLC chromatogram of the (*S*)-**10** (*ee* = 98%) after a column chromatography separation of the preparative-scale enzymatic resolution of (±)-**7**.

HPLC with Chiralpak OD-H column (4.6 mm × 250 mm), eluent: *n*-hexane: *i*PA (93:7), flow rate: 0.5 mL $min^{-1}$, detection at 260 nm, at room temperature. Retention times (min): for (*S*)-**8**: 21.9, (*R*)-**8**: 38.6, (*S*)-**11**: 17.0 and (*R*)-**11**: 25.3.

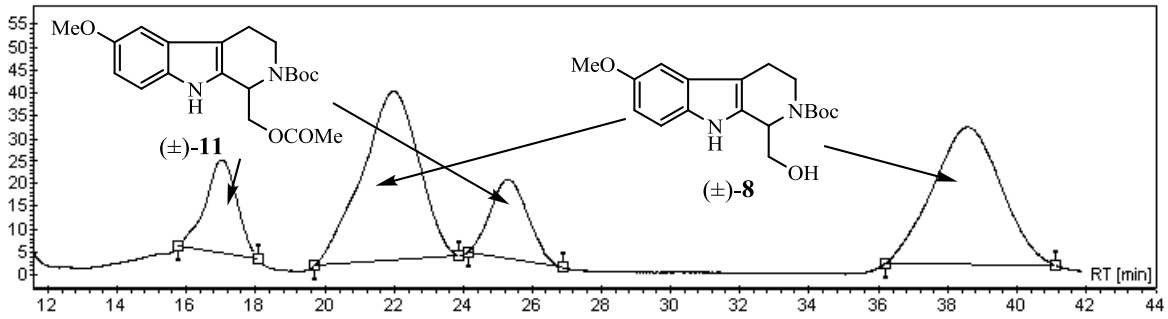


**Figure S4** HPLC chromatogram of (±)-**8** and (±)-**11**.

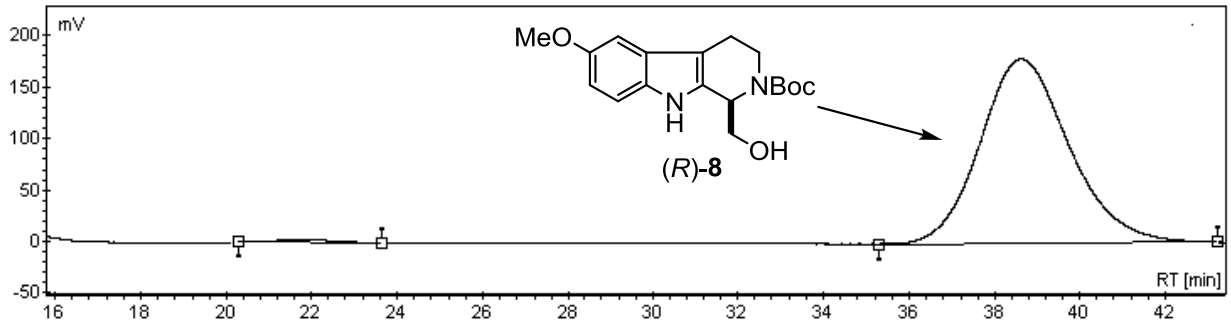


**Figure S5** HPLC chromatogram of the (*R*)-**8** (*ee* = 98%) after a column chromatography separation of the preparative-scale enzymatic resolution of (±)-**8**.

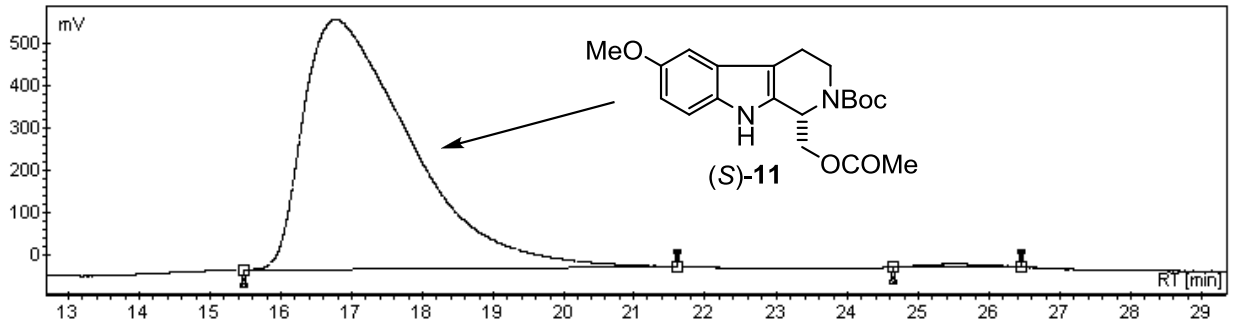


**Figure S6** HPLC chromatogram of the (*S*)-**11** (*ee* = 98%) after a column chromatography separation of the preparative-scale enzymatic resolution of (±)-**8**.

HPLC with Chiralpak OD-H column (4.6 mm × 250 mm), eluent: *n*-hexane: *i*PA (93:7), flow rate: 0.5 mL $min^{-1}$, detection at 260 nm, at room temperature. Retention times (min): for (*S*)-**9**: 15.6, (*R*)-**9**: 28.8, (*S*)-**12**: 12.6 and (*R*)-**12**: 19.9.

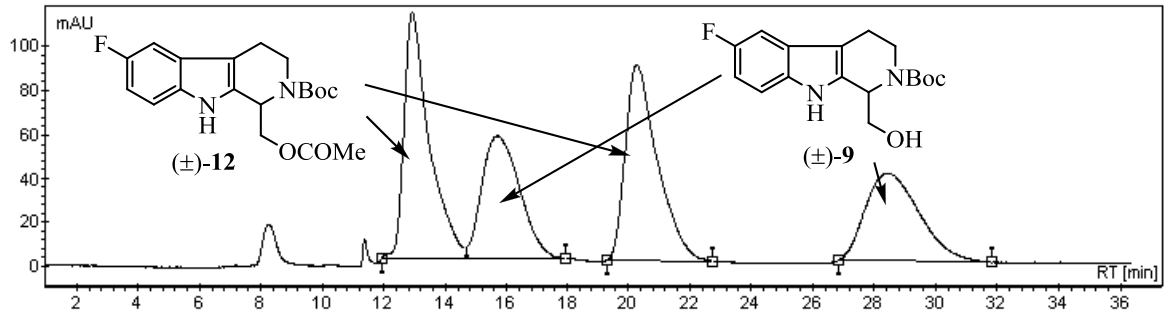


**Figure S7** HPLC chromatogram of (±)-**9** and (±)-**12**.

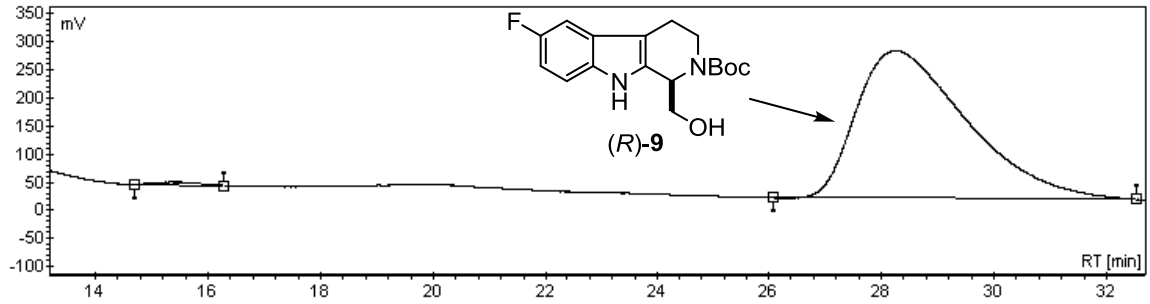


**Figure S8** HPLC chromatogram of the (*R*)-**9** (*ee* = 96%) after a column chromatography separation of the preparative-scale enzymatic resolution of (±)-**9**.

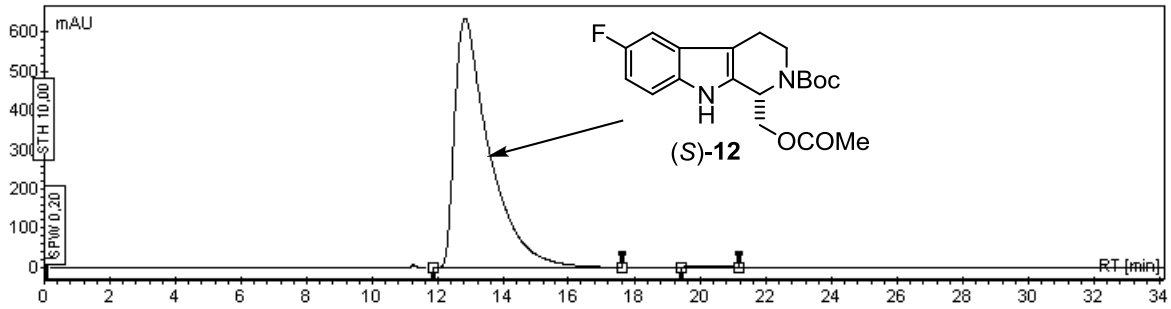


**Figure S9** HPLC chromatogram of the (*S*)-**12** (*ee* = 98%) after a column chromatography separation of the preparative-scale enzymatic resolution of (±)-**9**.

HPLC with Chiralpak IA column (4.6 mm × 250 mm), eluent: *n*-hexane: *i*PA (95:5), flow rate: 0.5 mL $min^{-1}$, detection at 210 nm, at room temperature. Retention times (min): for (*S*)-**13**: 88.2, (*R*)-**13**: 92.8.

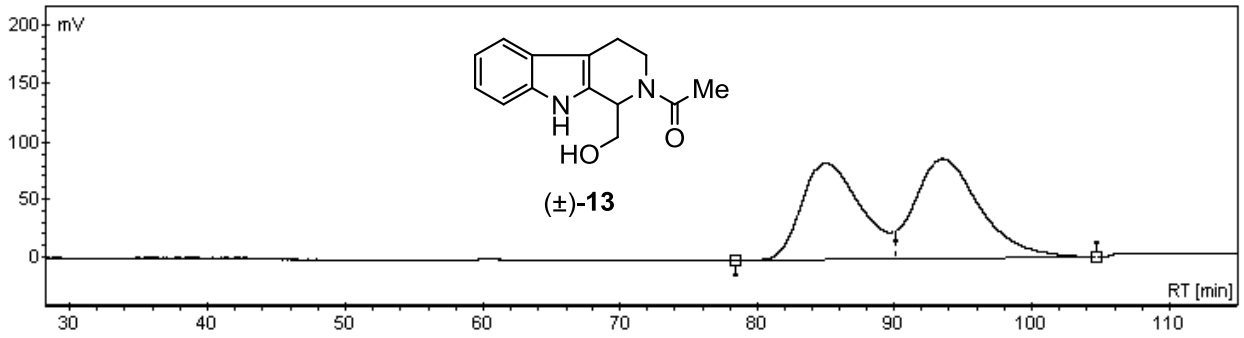


**Figure S10** HPLC chromatogram of (±)-**13**.

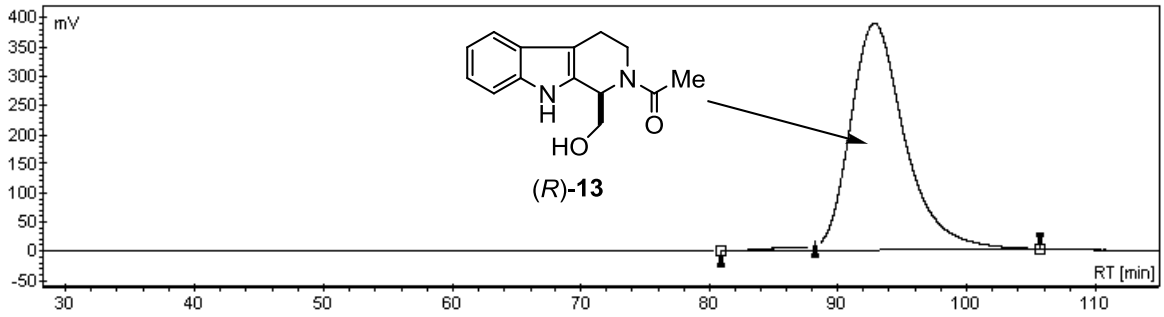


**Figure S11** HPLC chromatogram of (*R*)-**13** (*ee* = 98%).

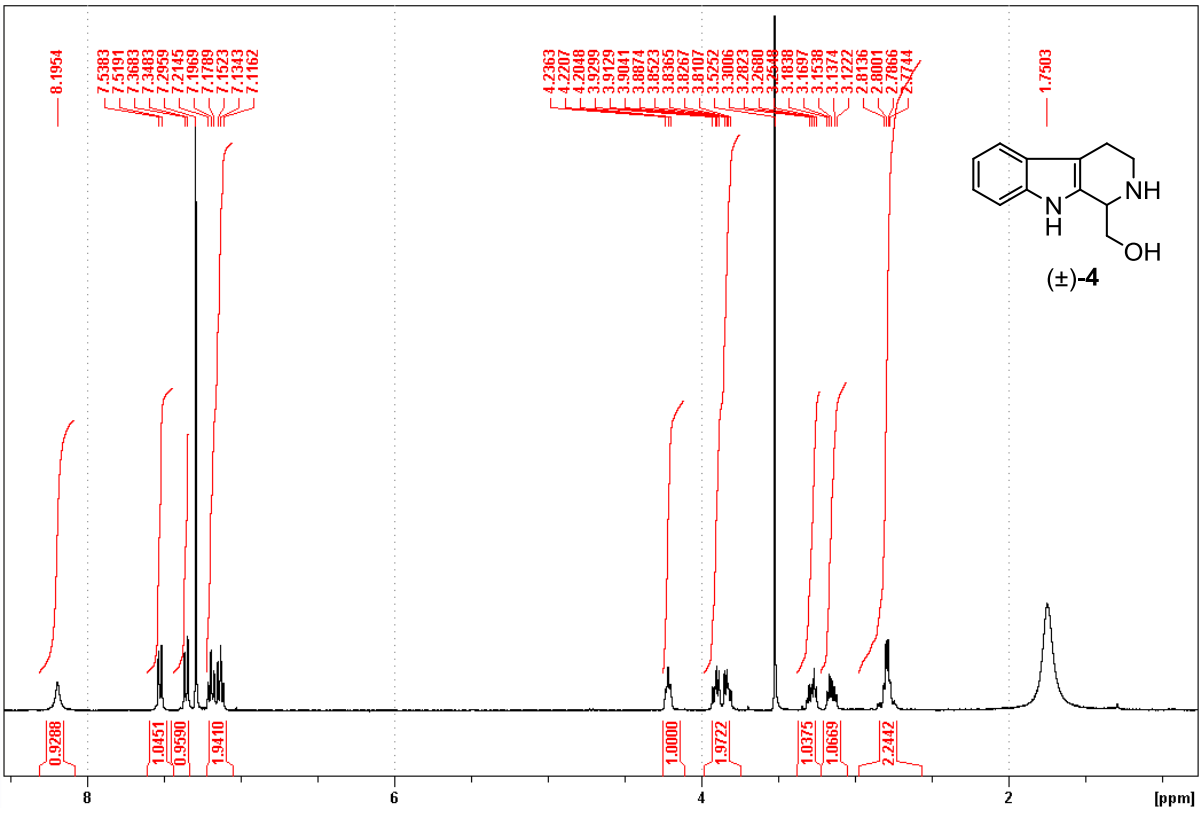


**Figure S12:** $^{1}$H NMR (400 MHz, $CDCl_3$, 25 °C) spectra for (±)-**4**.

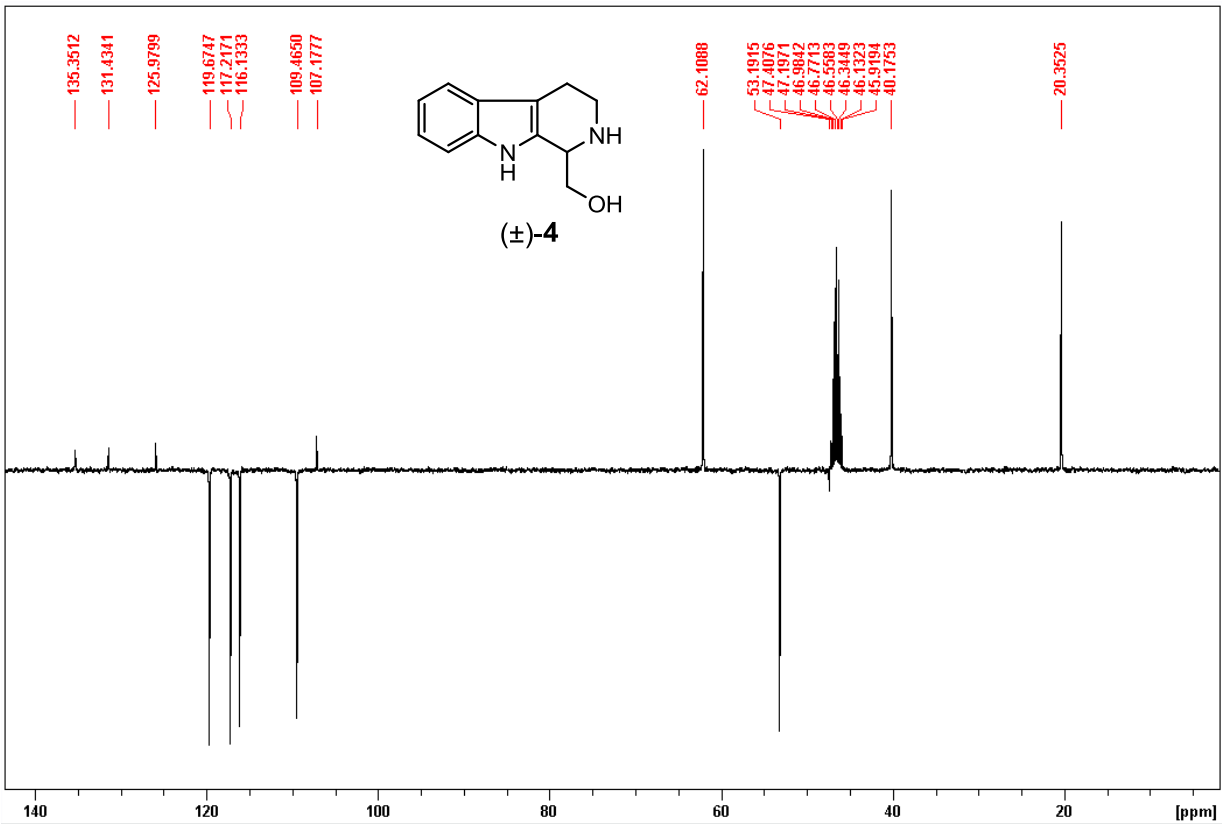


**Figure S13:** $^{13}$C NMR (400 MHz, MeOH-d4, 25 °C) spectra for (±)-**4**.

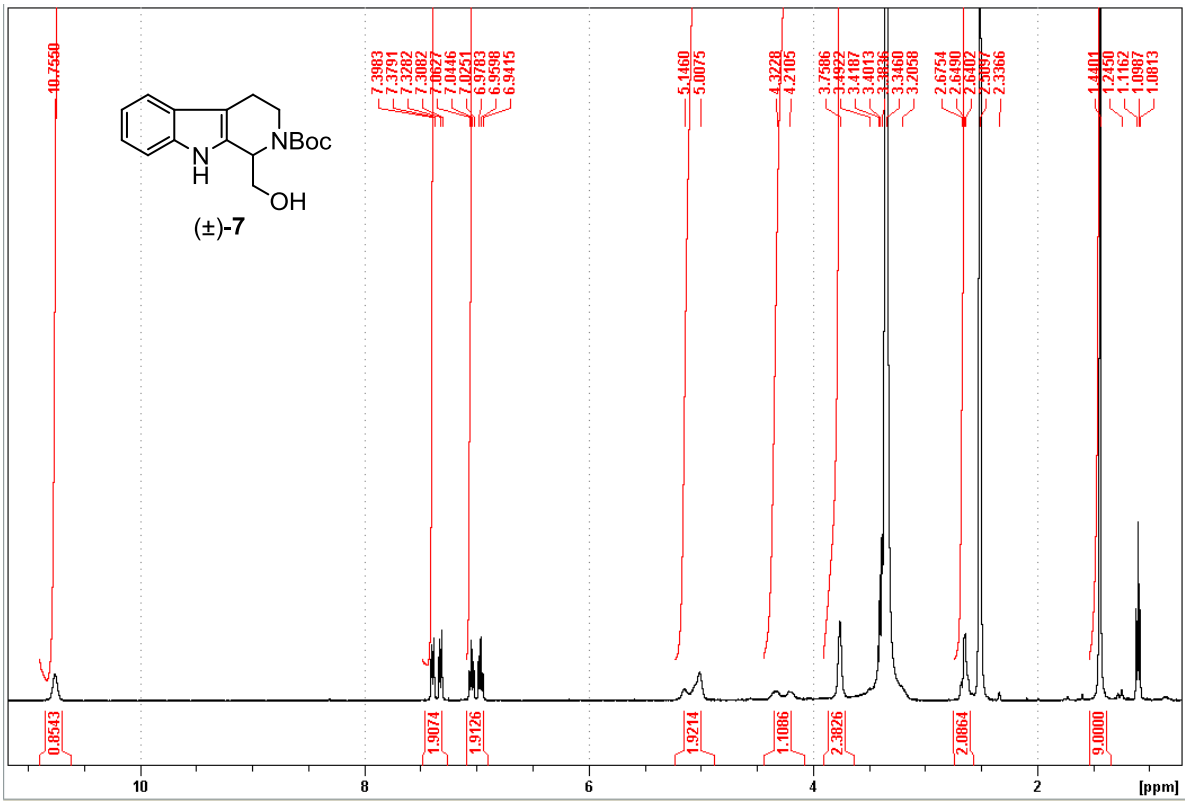


**Figure S14:** $^{1}$H NMR (400 MHz, DMSO, 25 °C) spectra for (±)-**7**.

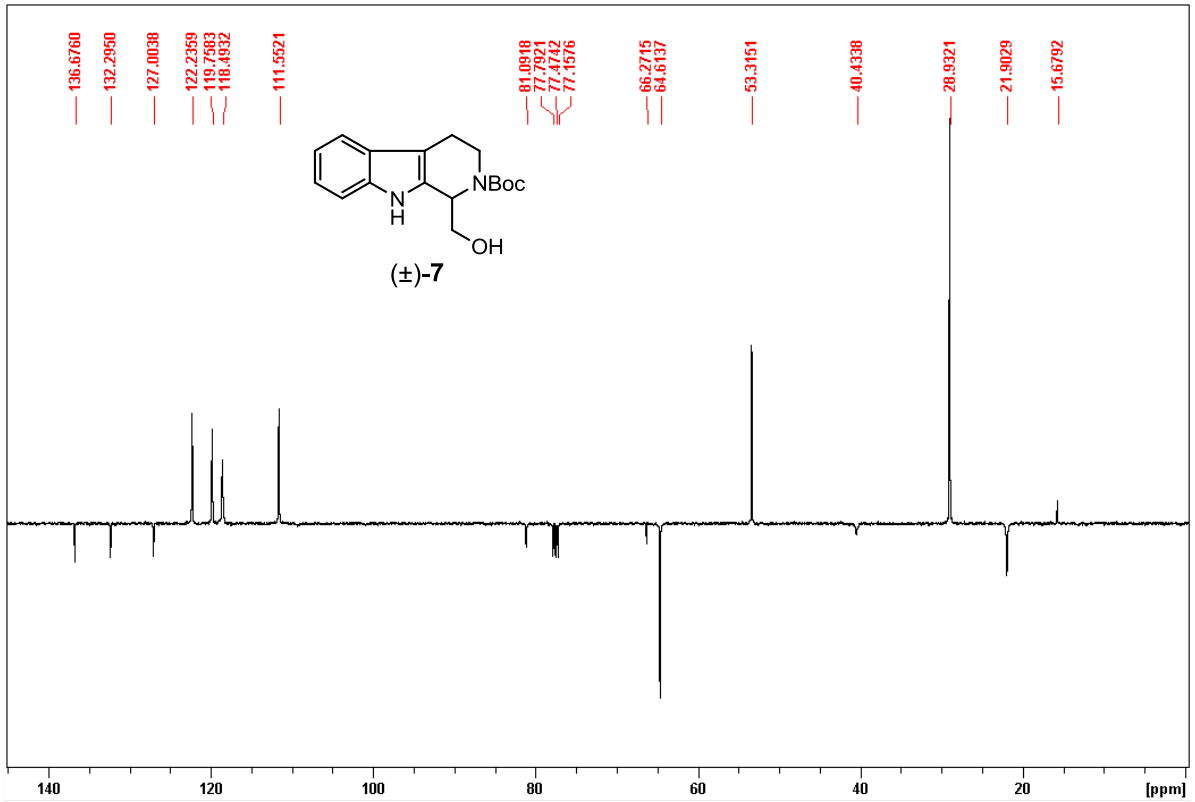


**Figure S15:** $^{13}$C NMR (400 MHz, $CDCl_3$, 25 °C) spectra for (±)-**7**.

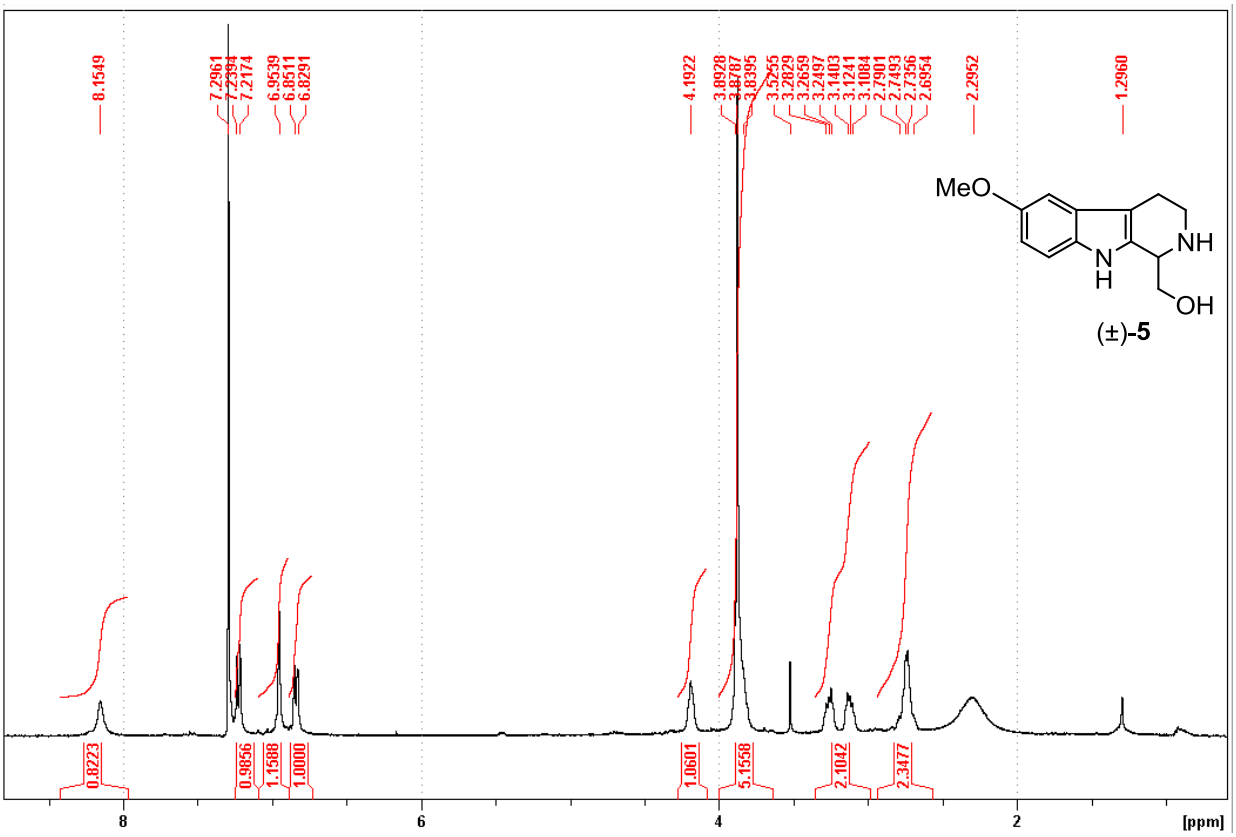


**Figure S16:** $^{1}$H NMR (400 MHz, $CDCl_3$, 25 °C) spectra for (±)-**5**.

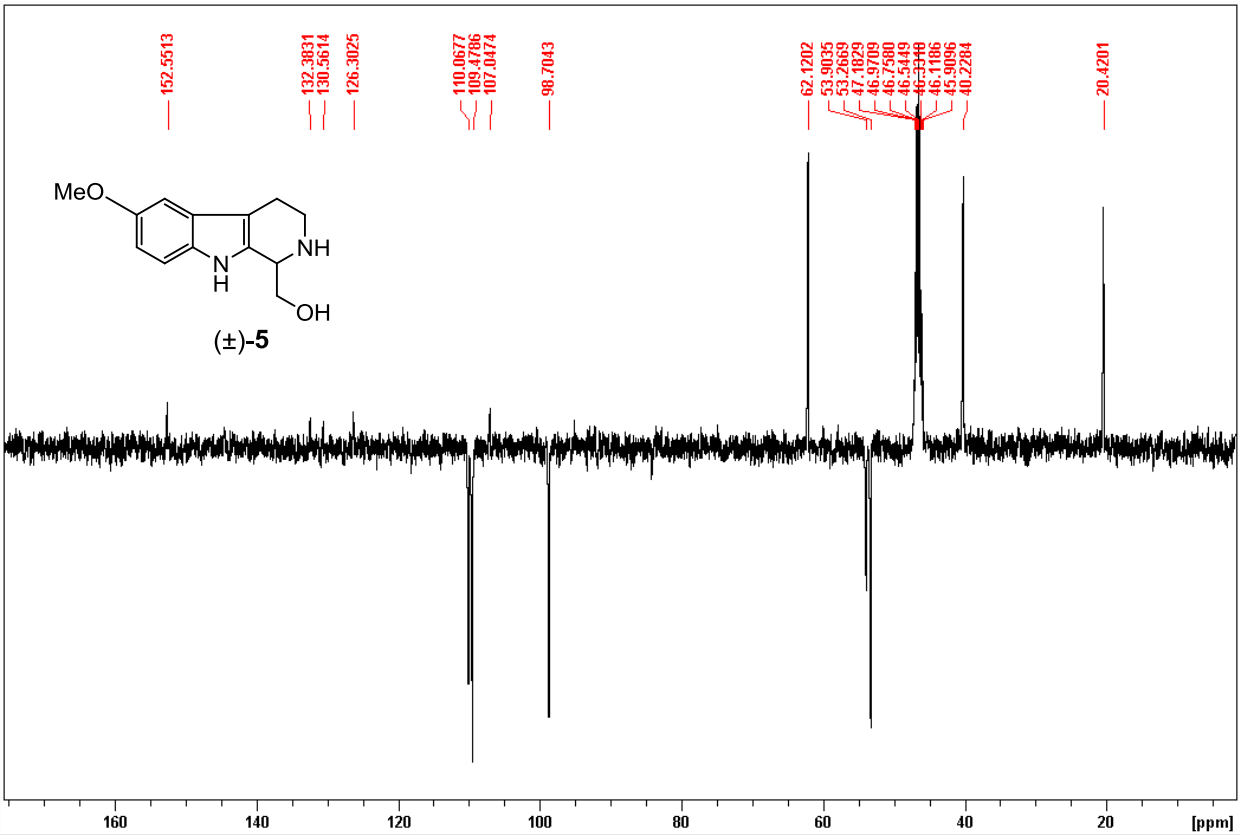


**Figure S17:** $^{13}$C NMR (400 MHz, MeOH-d4, 25 °C) spectra for (±)-**5**.

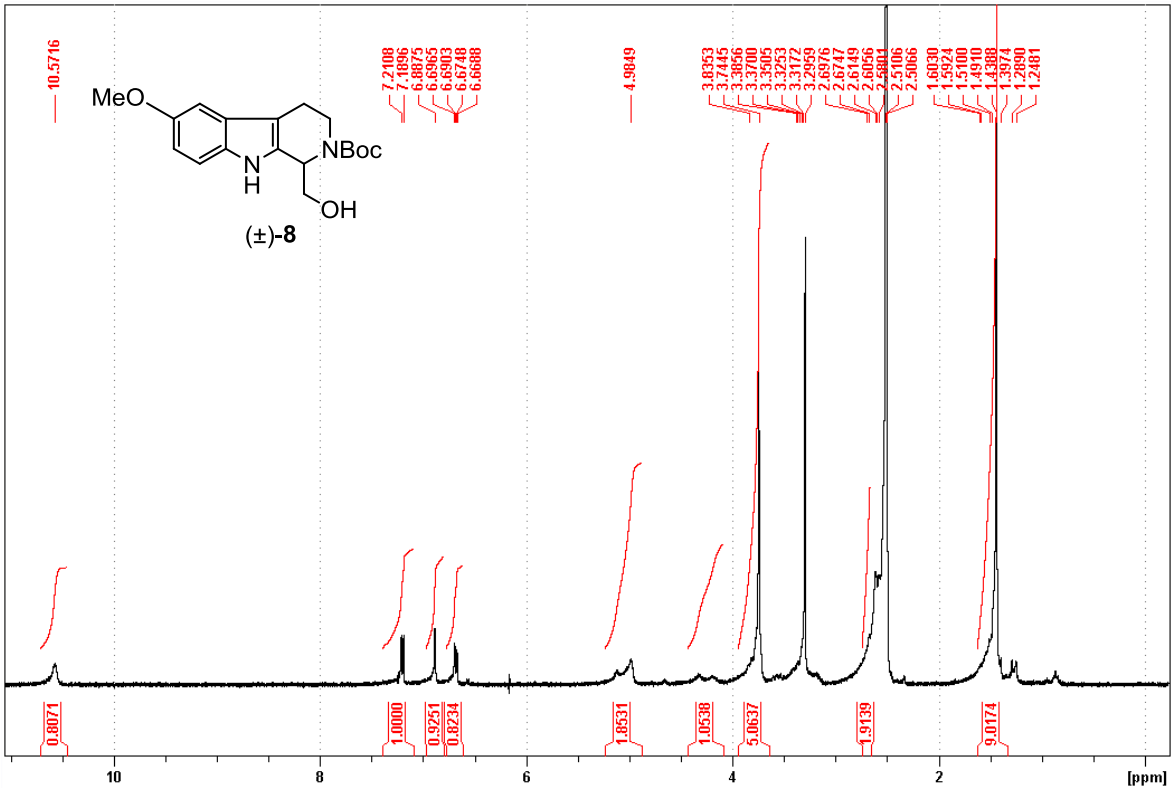


**Figure S18:** $^{1}$H NMR (400 MHz, DMSO, 25 °C) spectra for (±)-**8**.

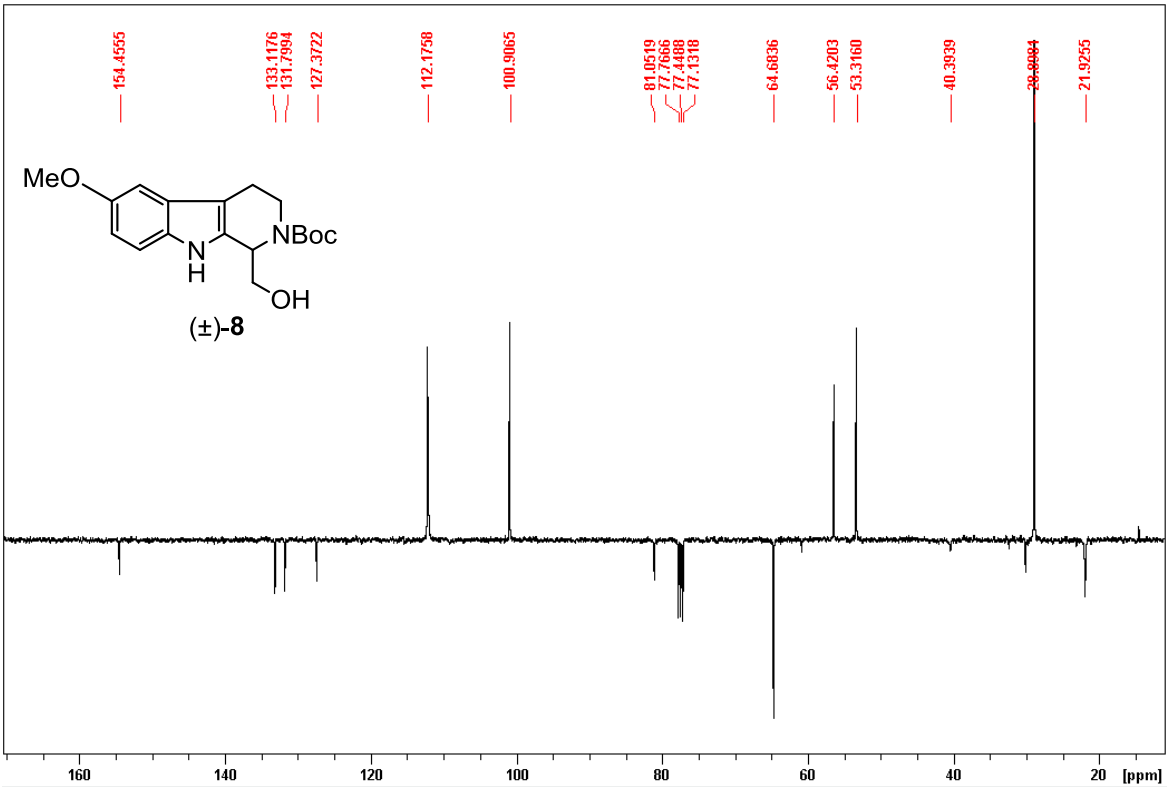


**Figure S19:** $^{13}$C NMR (400 MHz, $CDCl_3$, 25 °C) spectra for (±)-**8**.

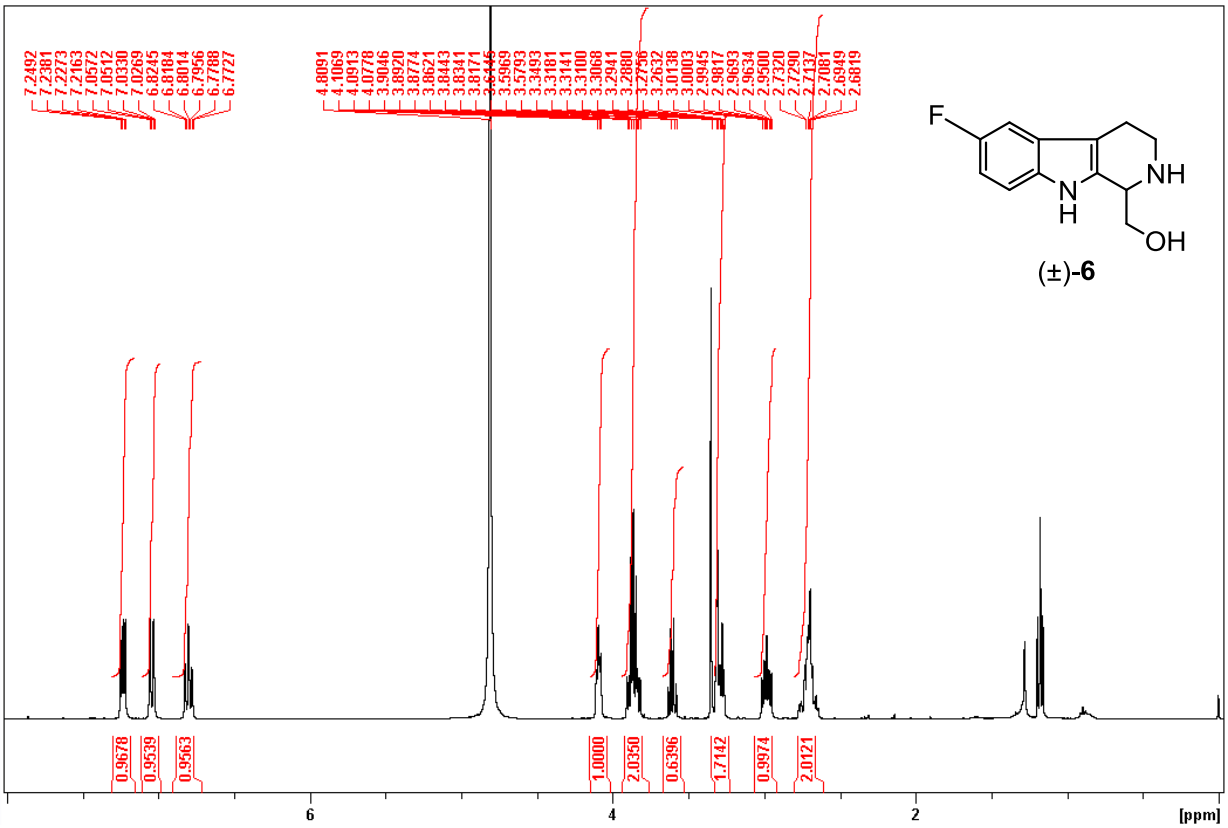


**Figure S20:** $^{1}$H NMR (400 MHz, MeOH-d4, 25 °C) spectra for (±)-**6**.

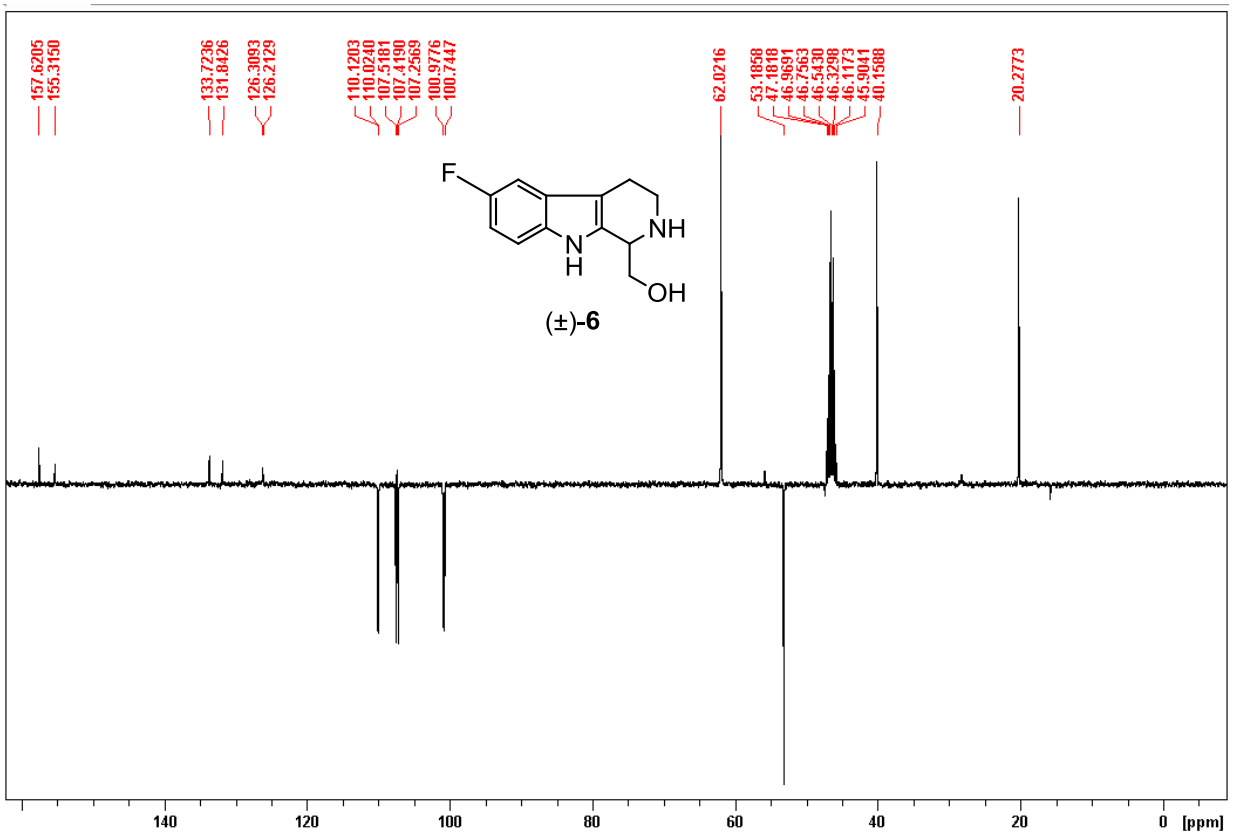


**Figure S21:** $^{13}$C NMR (400 MHz, MeOH-d4, 25 °C) spectra for (±)-**6**.

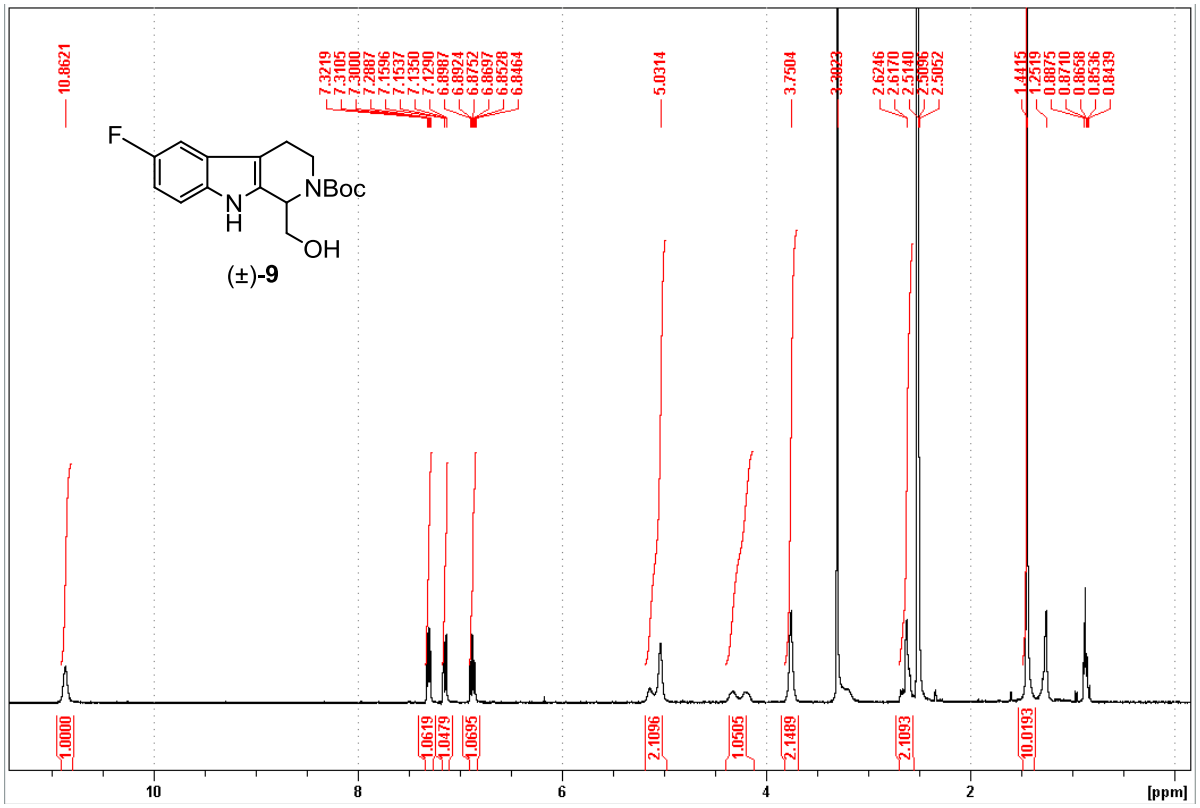


**Figure S22:** $^{1}$H NMR (400 MHz, DMSO, 25 °C) spectra for (±)-**9**.

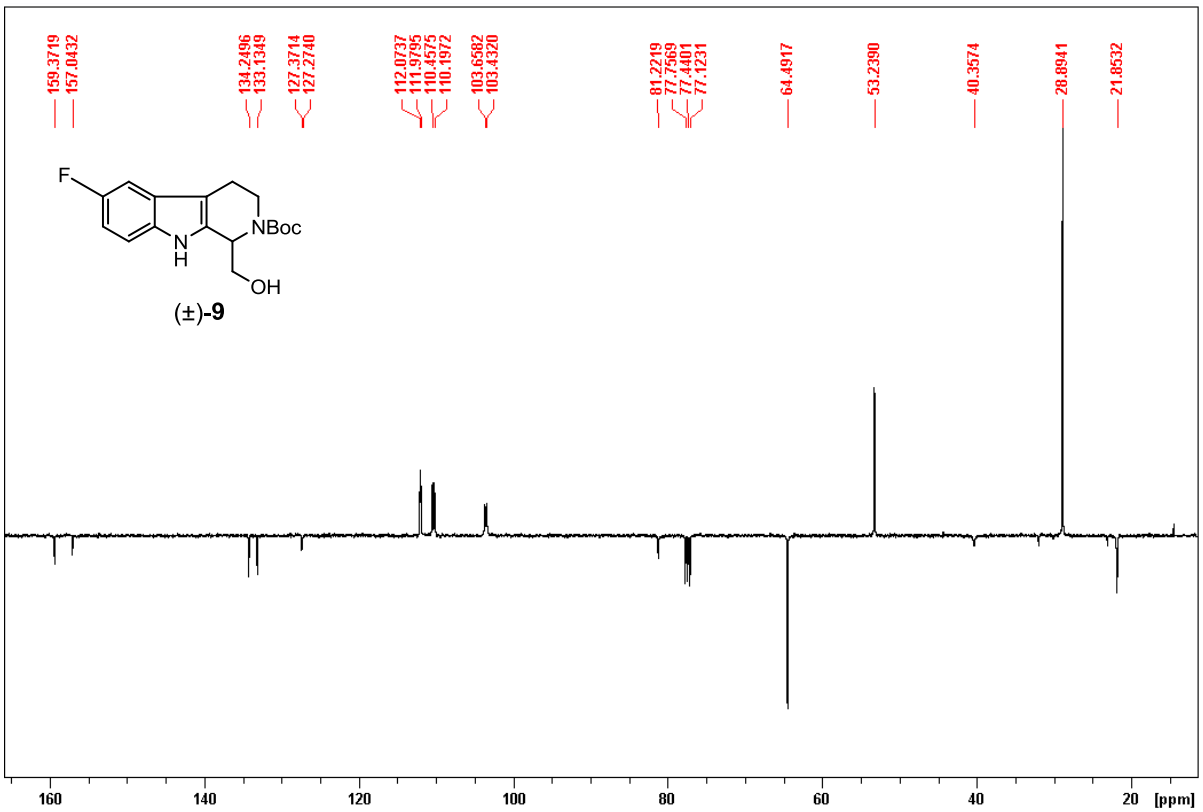


**Figure S23:** $^{13}$C NMR (400 MHz, $CDCl_3$, 25 °C) spectra for (±)-**9**.

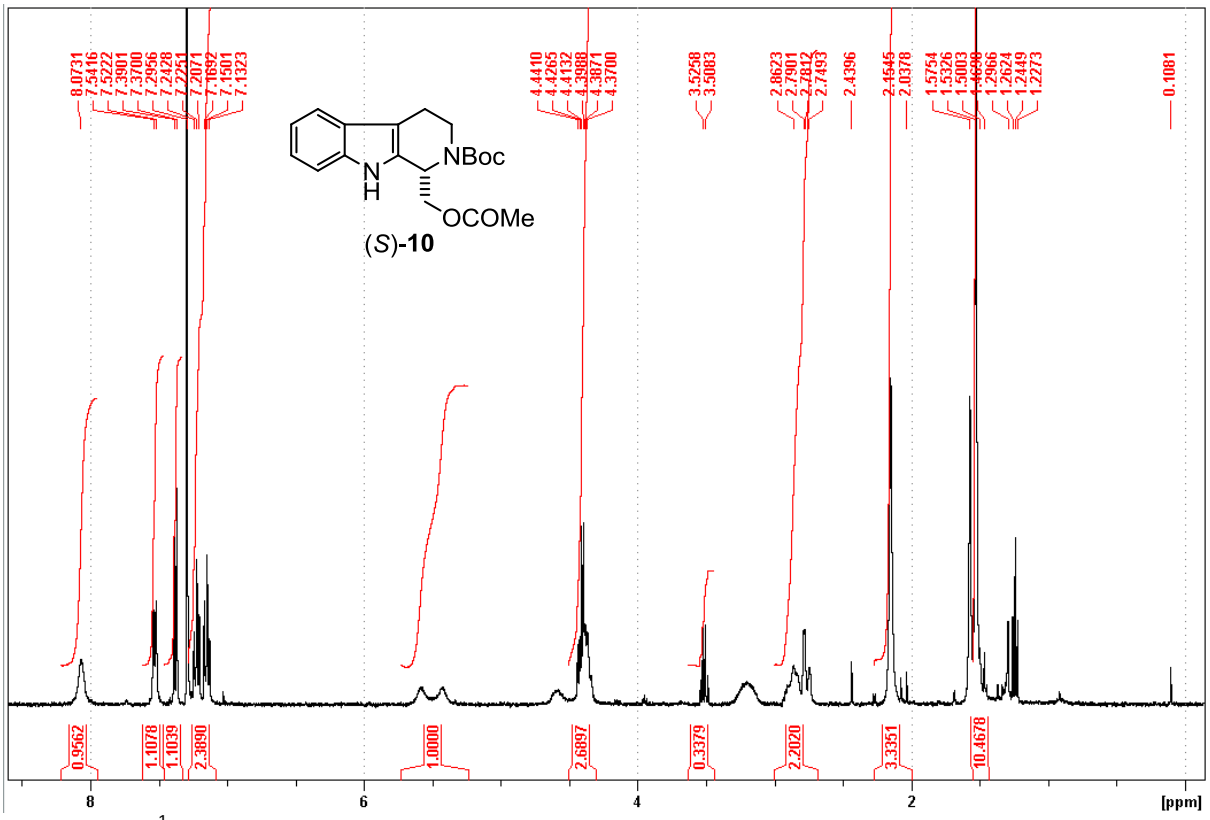


**Figure S24:** $^{1}$H NMR (400 MHz, $CDCl_3$, 25 °C) spectra for (*S*)-**10**.

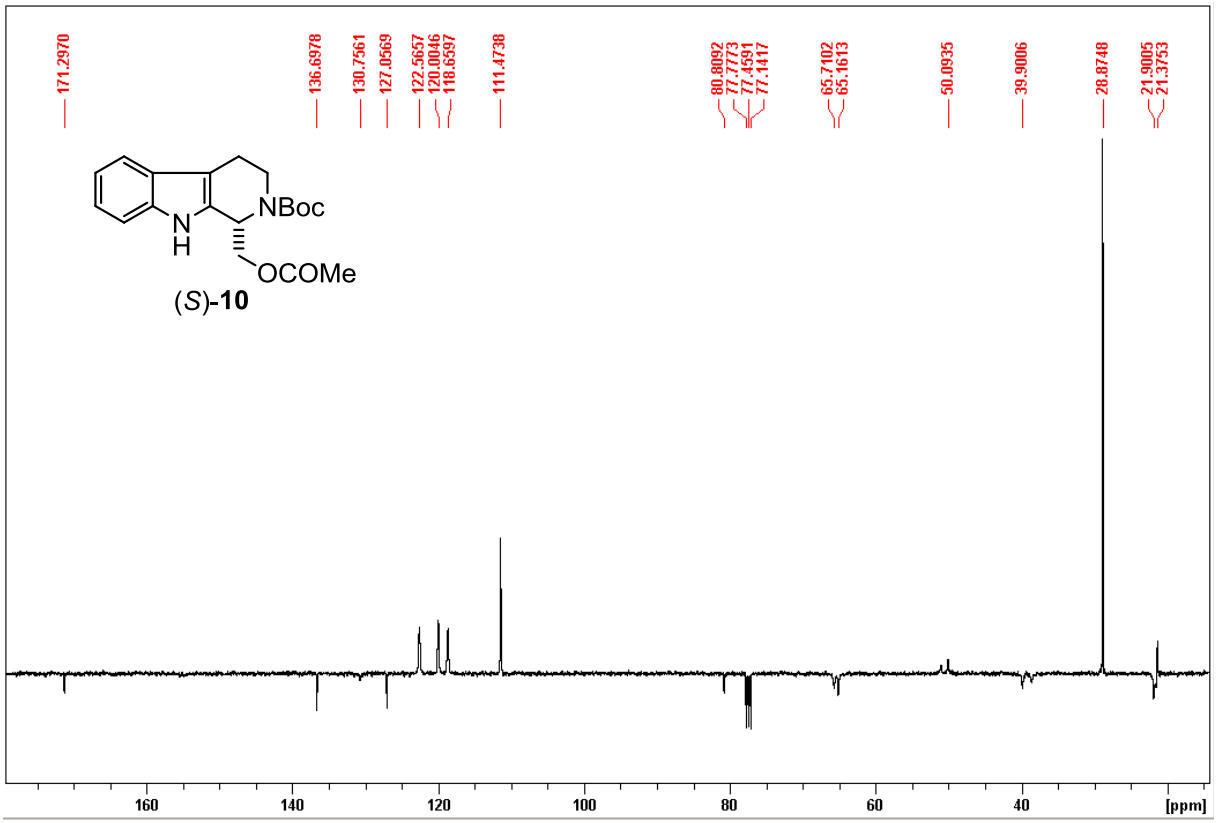


**Figure S25:** $^{13}$C NMR (400 MHz, $CDCl_3$, 25 °C) spectra for (*S*)-**10**.

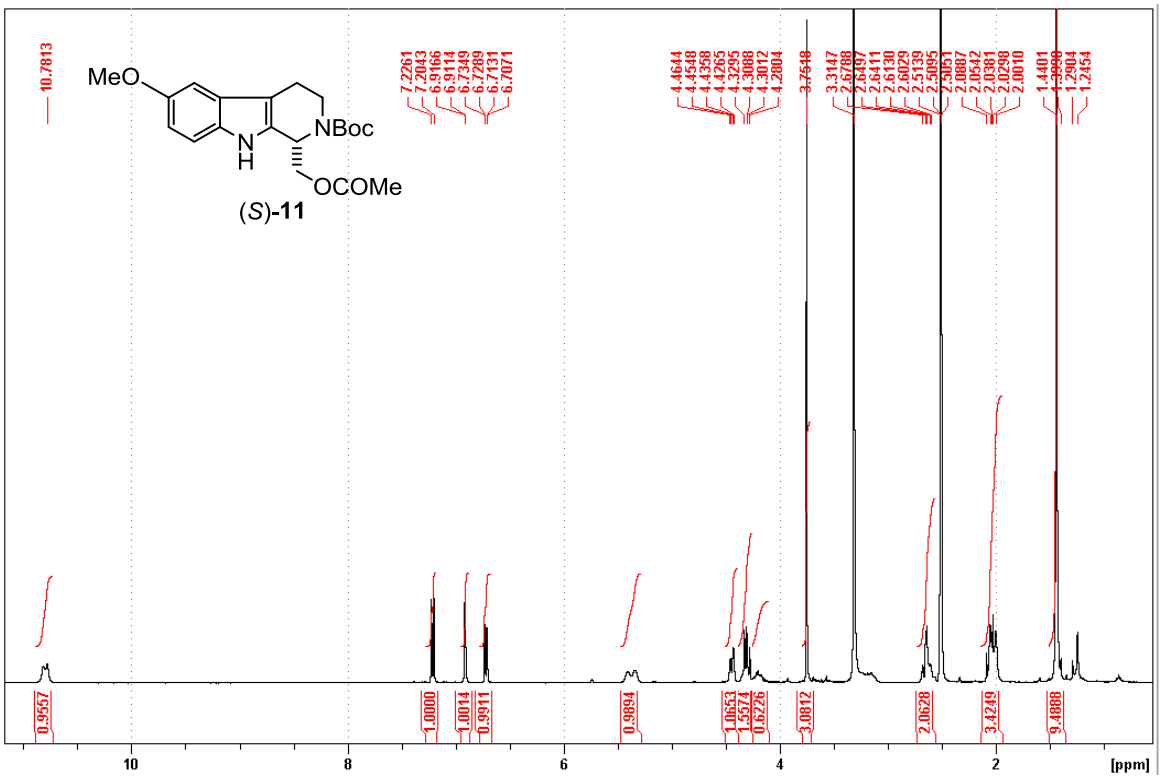


**Figure S26:** $^{1}$H NMR (400 MHz, DMSO, 25 °C) spectra for (*S*)-**11**.

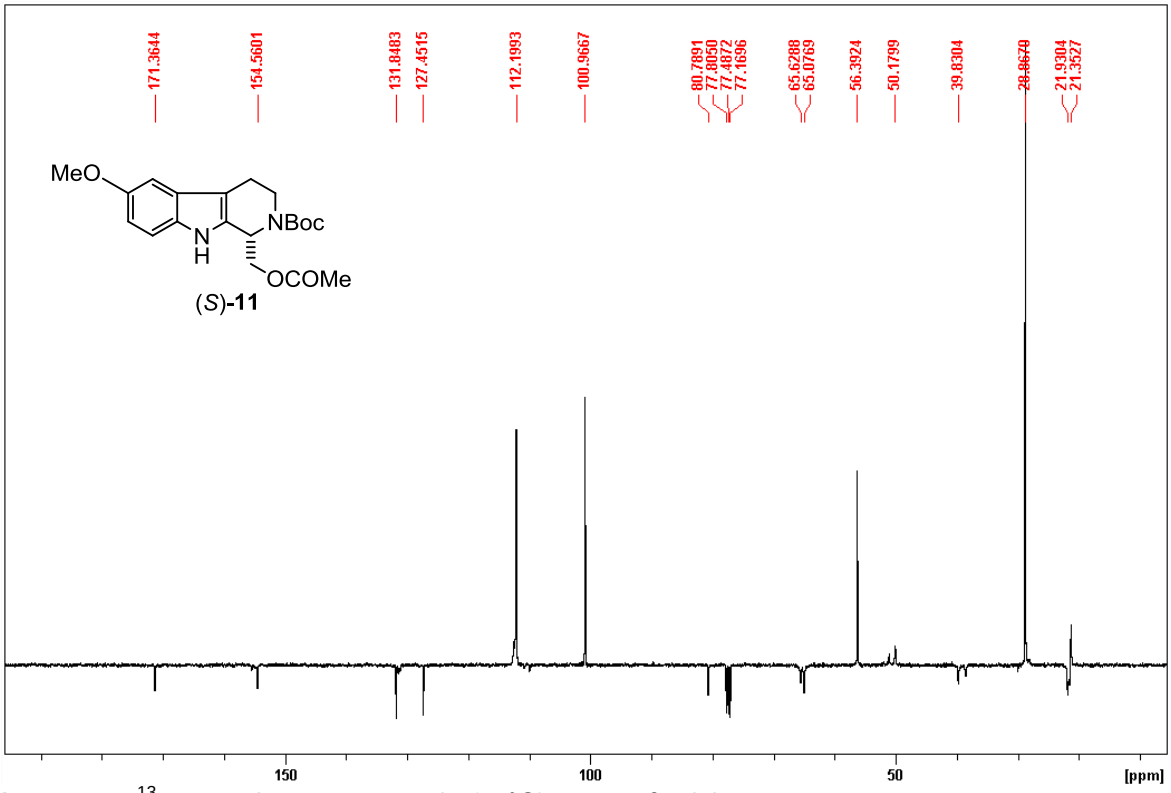


**Figure S27:** $^{13}$C NMR (400 MHz, $CDCl_3$, 25 °C) spectra for (*S*)-**11**.

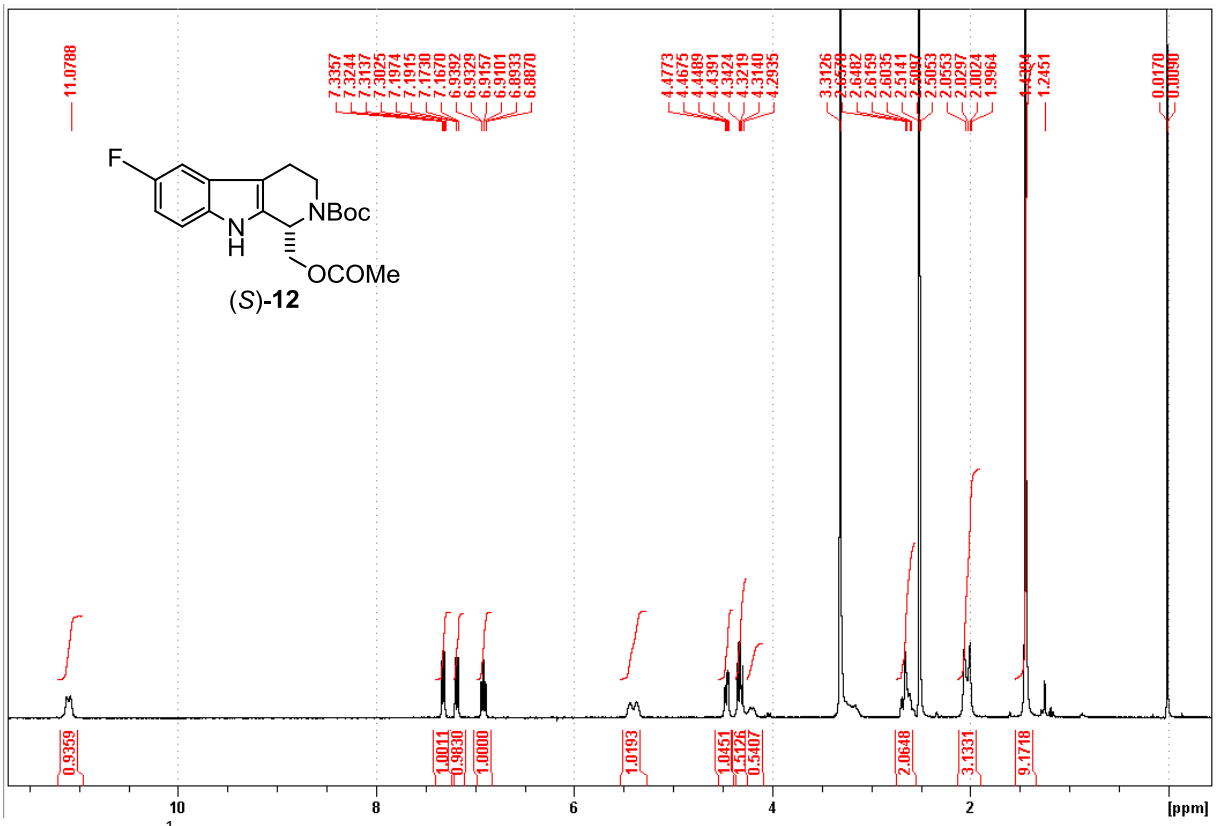


**Figure S28:** $^{1}$H NMR (400 MHz, DMSO, 25 °C) spectra for (*S*)-**12**.

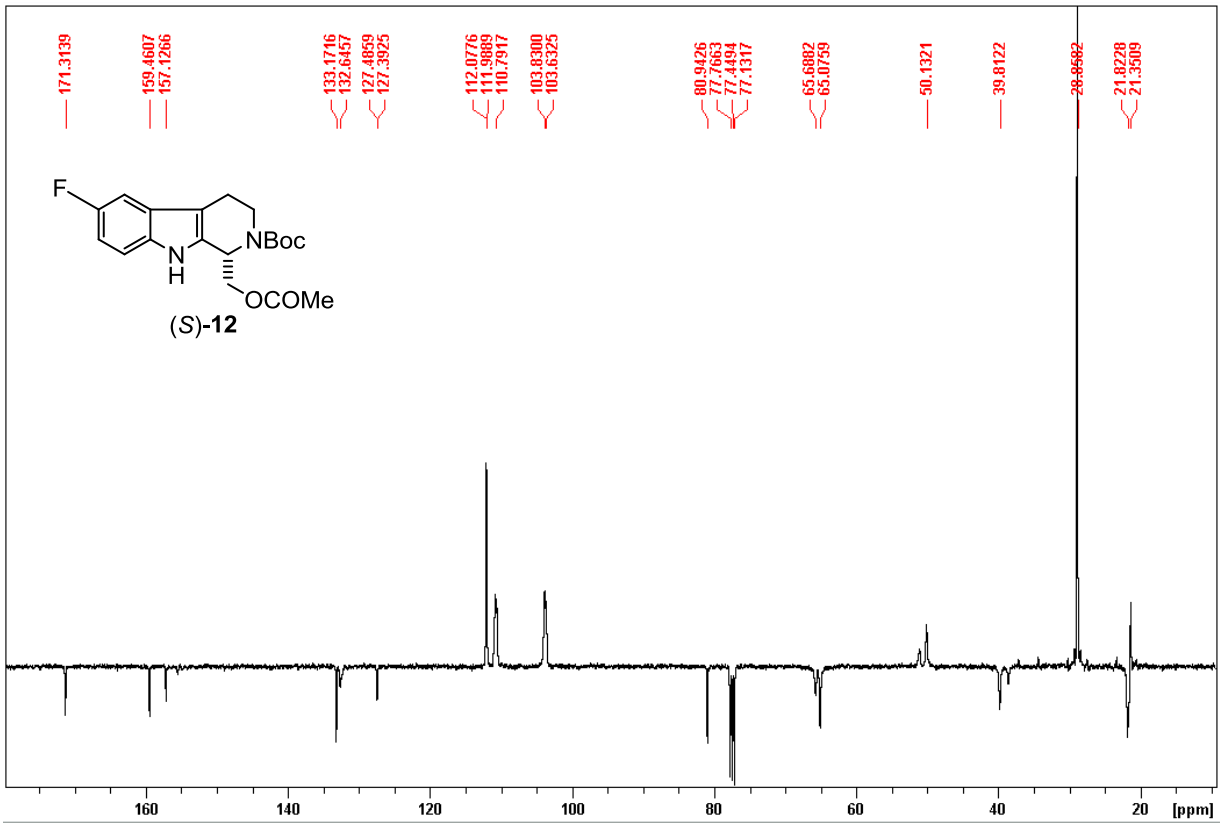


**Figure S29:** $^{13}$C NMR (400 MHz, $CDCl_3$, 25 °C) spectra for (*S*)-**12**.

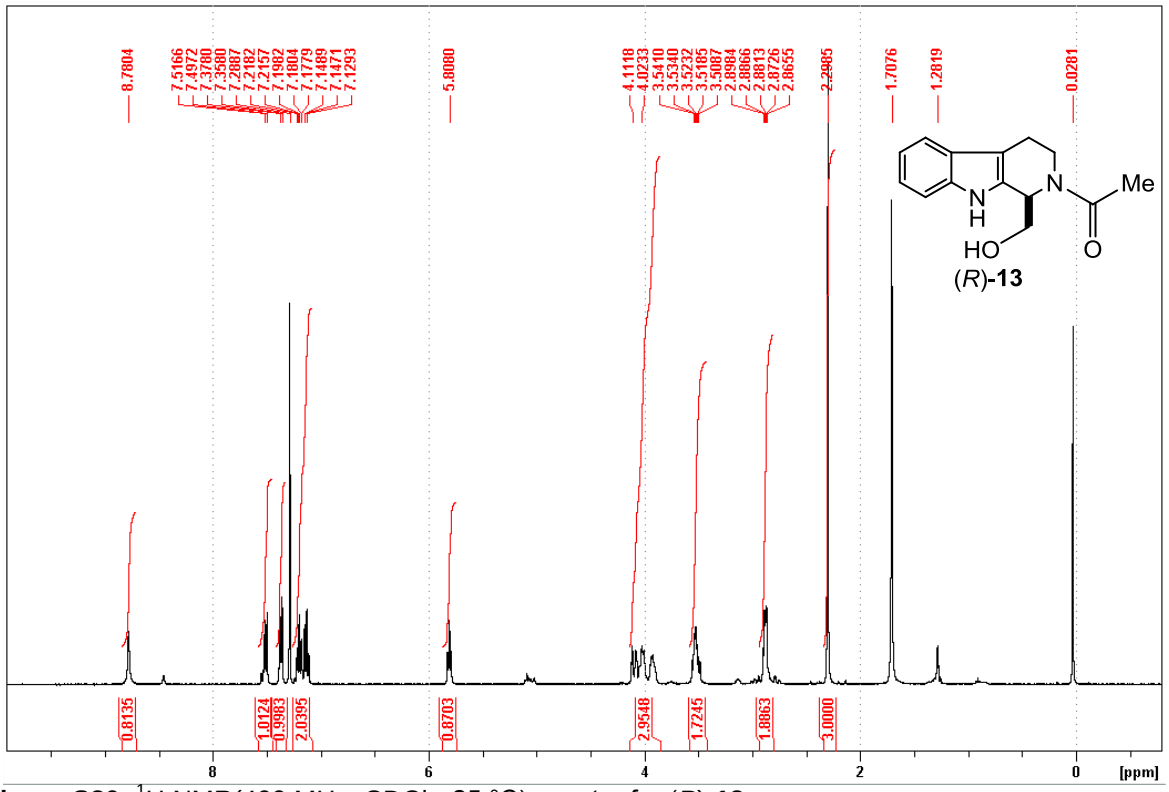


**Figure S30:** $^{1}$H NMR(400 MHz, $CDCl_3$, 25 °C) spectra for (*R*)-**13**.