

Supporting Information

Discovery of Antibacterial Agents Targeting Biofilm Formation: Total Synthesis and *in vitro* Investigation of Amycolasporins

Wenxi Wu,^a Yu Mu,^a Junfeng Tan,^a Zixuan Wang,^a Chen Zhang,^a Guiding Li,^a Ying Jin,^a Xueshi Huang^{a*} and Li Han^{a*}

*^aInstitute of Microbial Pharmaceuticals, College of Life and Health Sciences,
Northeastern University, Shenyang 110819, China.*

**Corresponding authors*

Tel: 86-24-8365-6106. Fax: 86-24-8365-6106. E-mail: huangxs@mail.neu.edu.cn (X. Huang);

Tel: 86-24-8365-6122. Fax: 86-24-8365-6122. E-mail: hanli@mail.neu.edu.cn (L. Han).

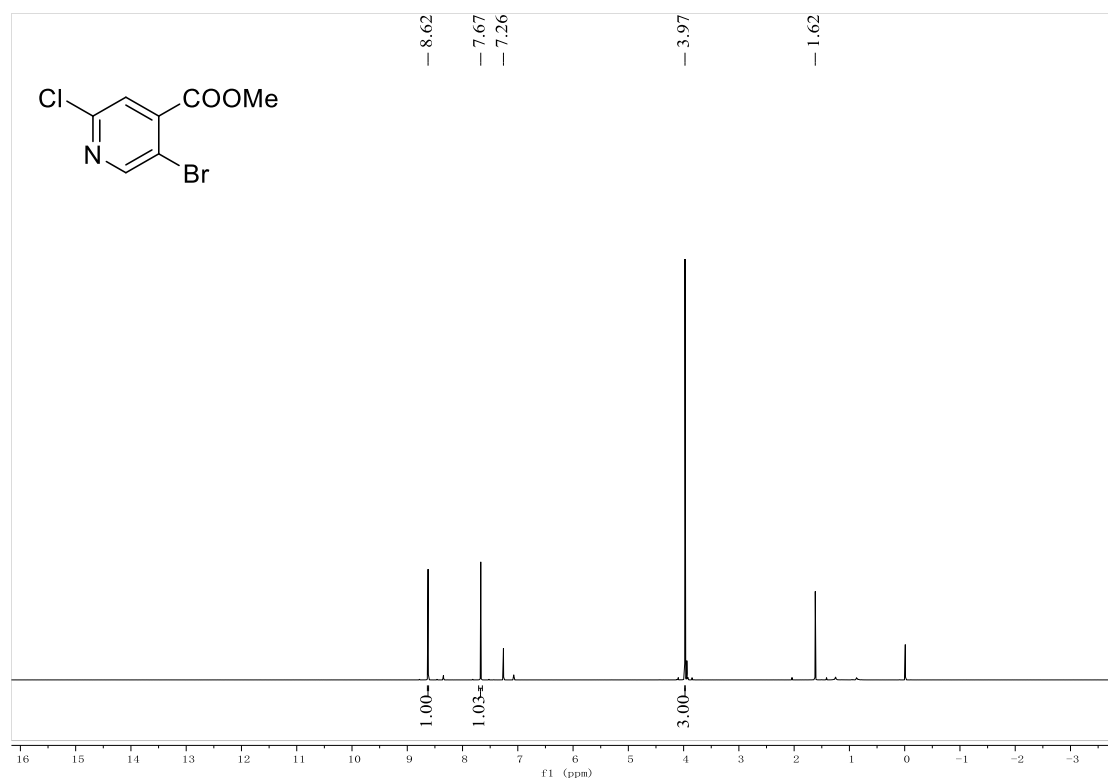


Figure S1 ^1H NMR Spectra of compound **9** (600 MHz, CDCl_3)

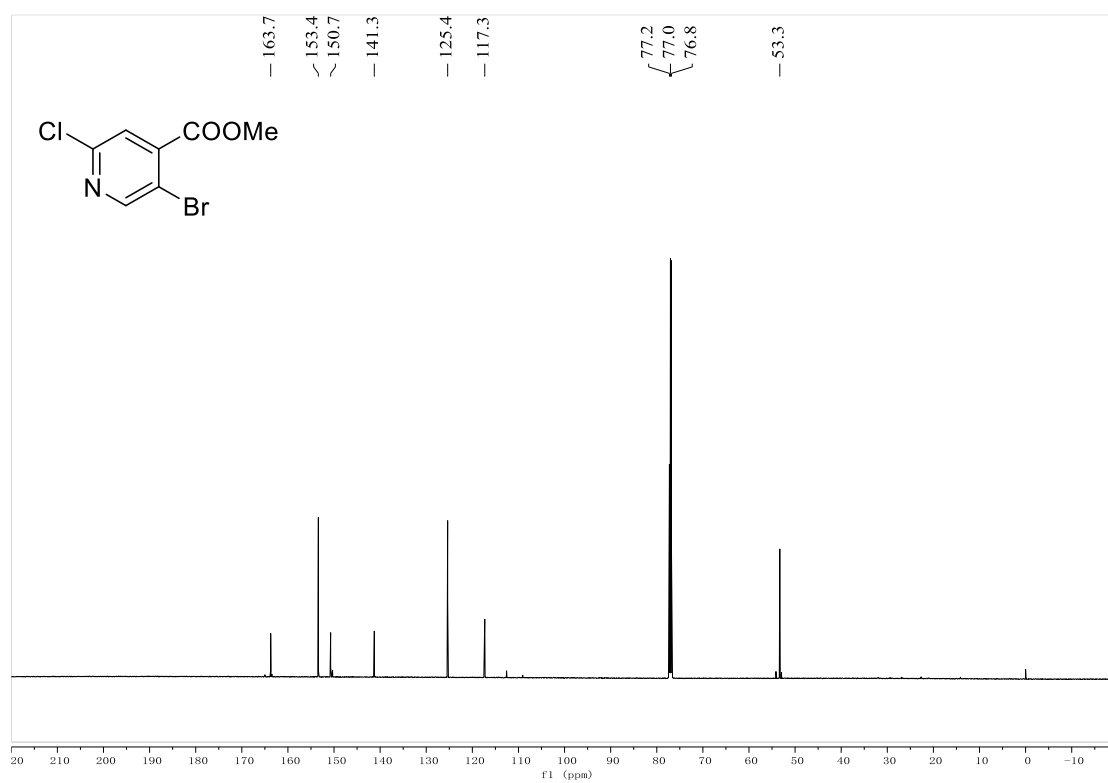


Figure S2 ^{13}C NMR Spectra of compound **9** (150 MHz, CDCl_3)

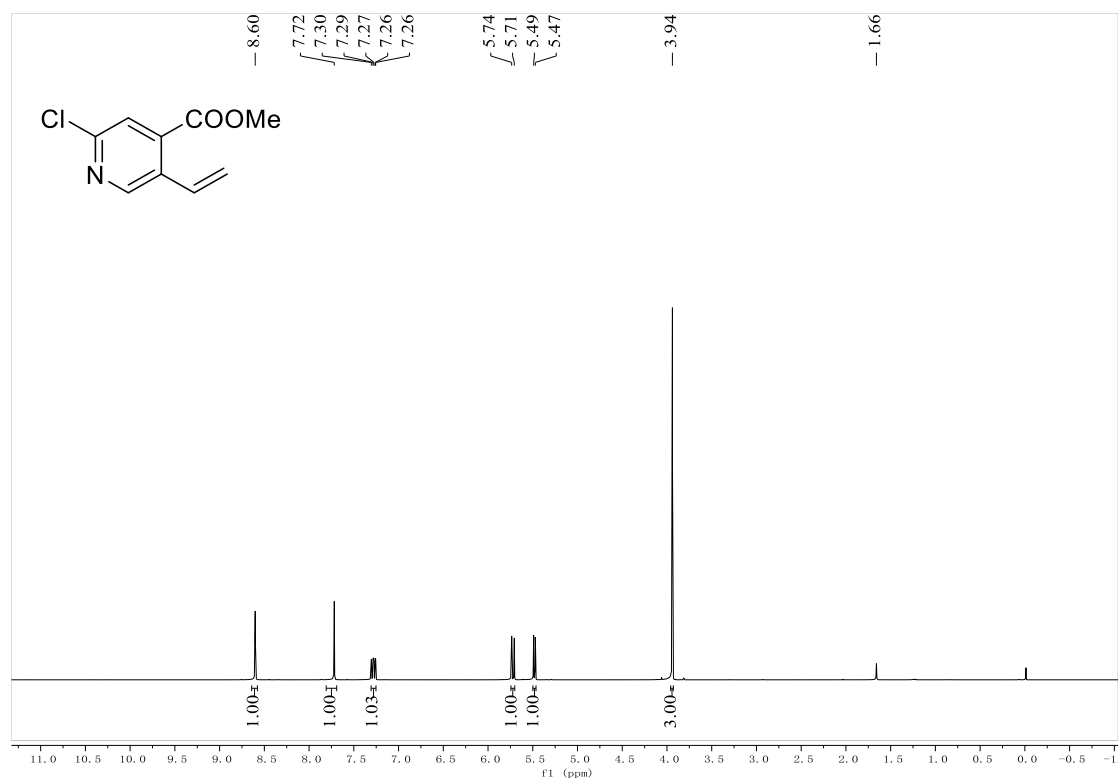


Figure S3 ¹H NMR Spectra of compound **10** (600 MHz, CDCl₃)

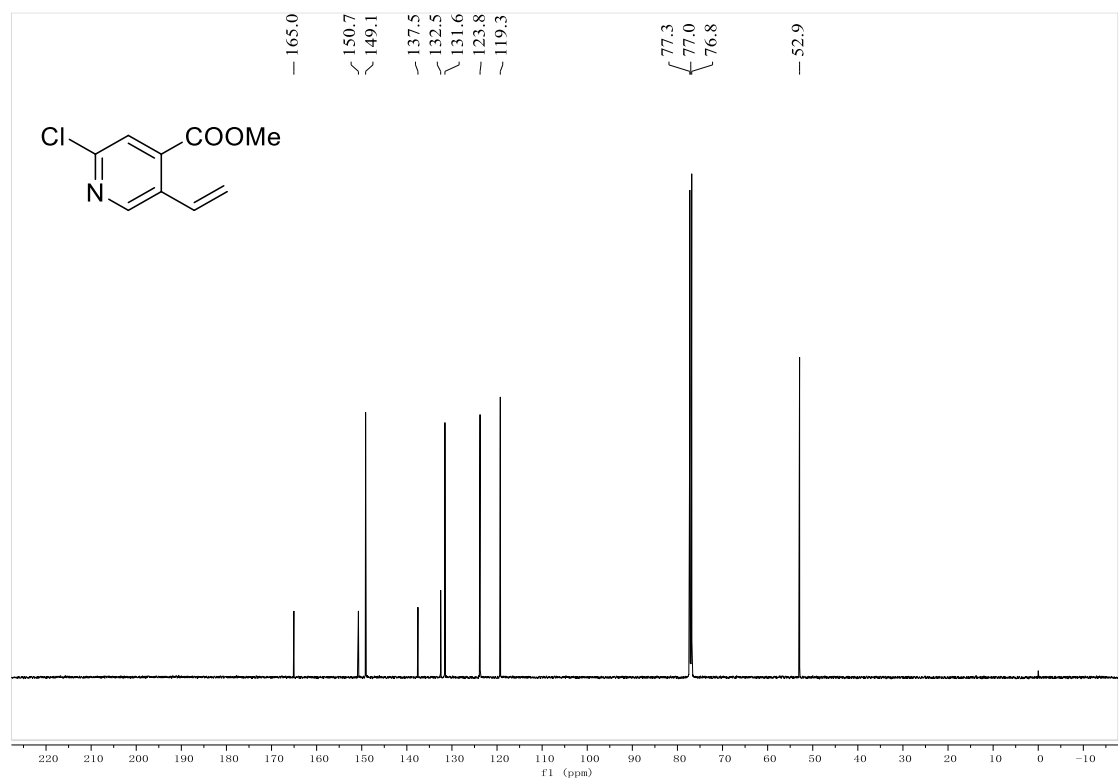


Figure S4 ¹³C NMR Spectra of compound **10** (150 MHz, CDCl₃)

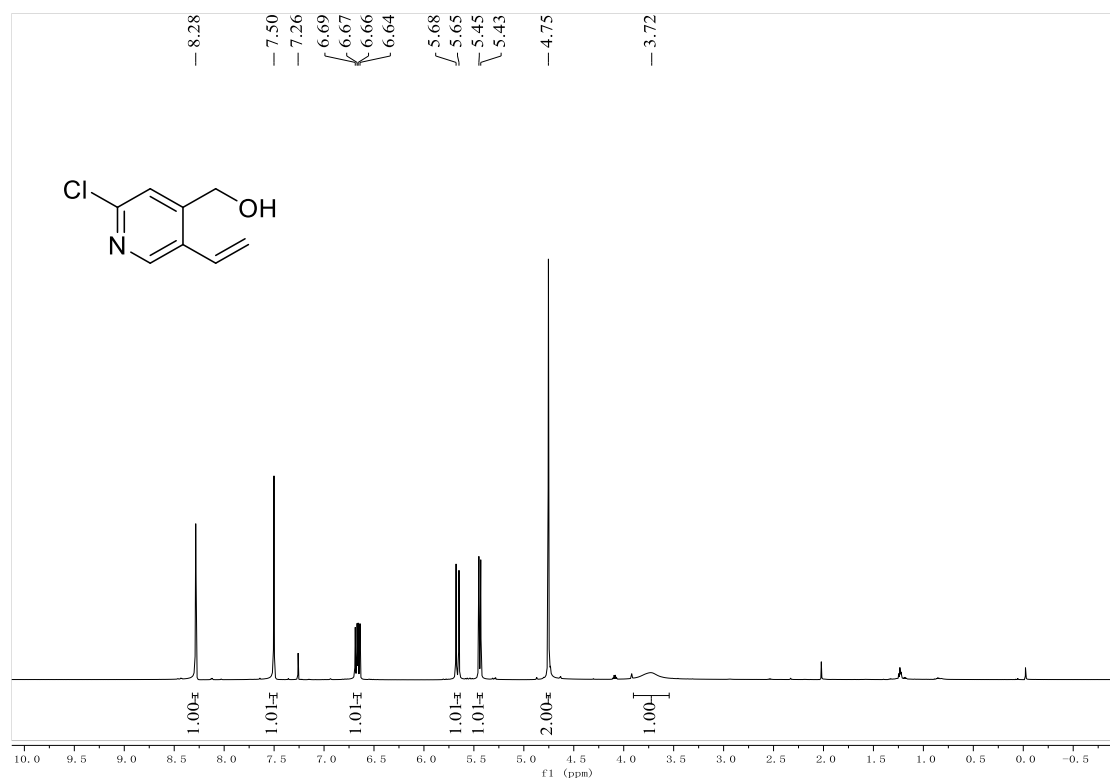


Figure S5 ¹H NMR Spectra of compound **11** (600 MHz, CDCl₃)

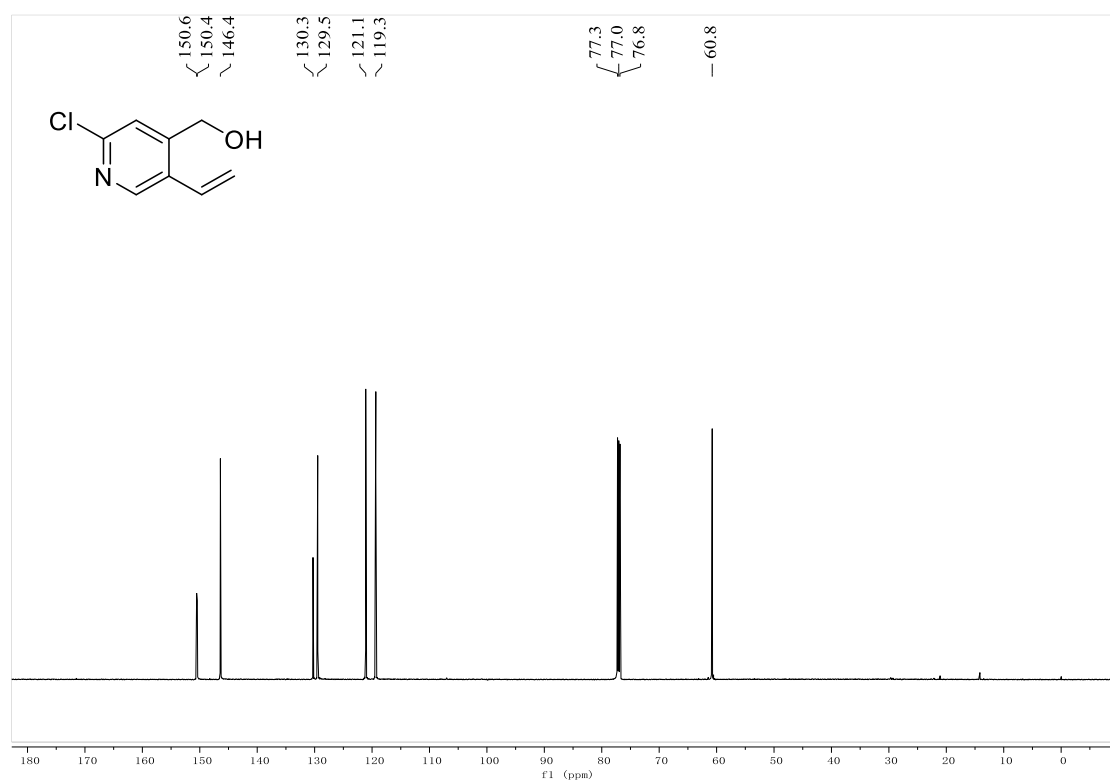


Figure S6 ¹³C NMR Spectra of compound **11** (150 MHz, CDCl₃)

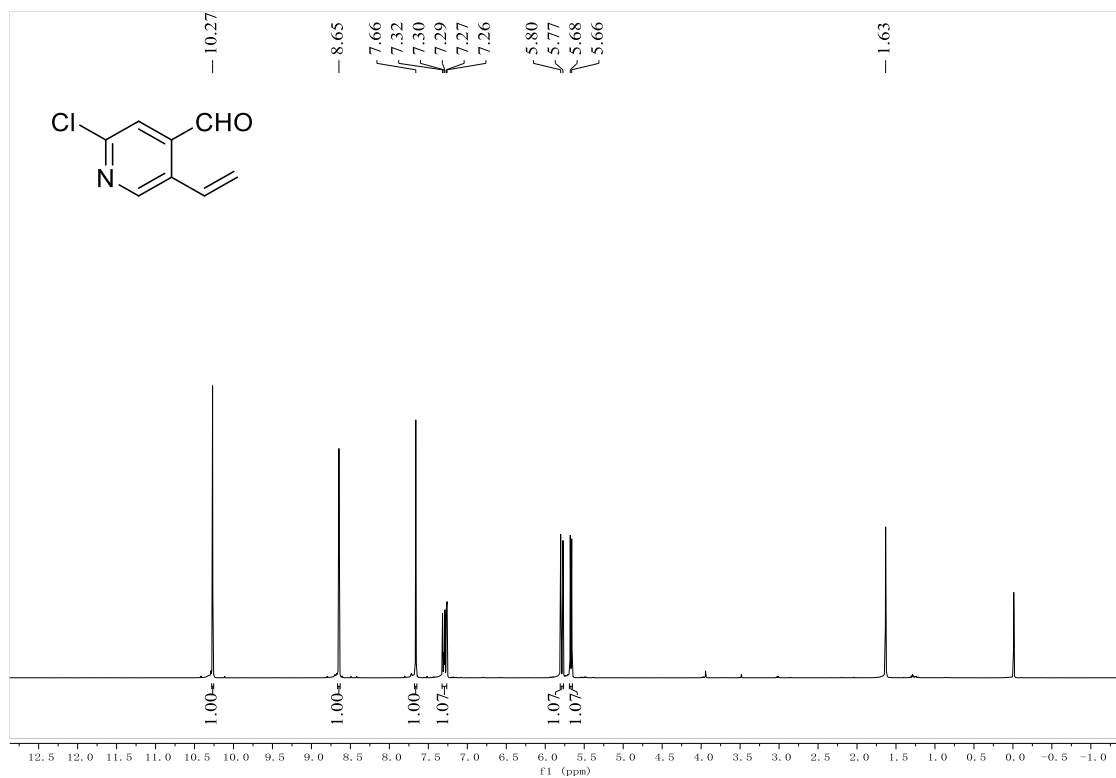


Figure S7 ¹H NMR Spectra of compound **7** (600 MHz, CDCl₃)

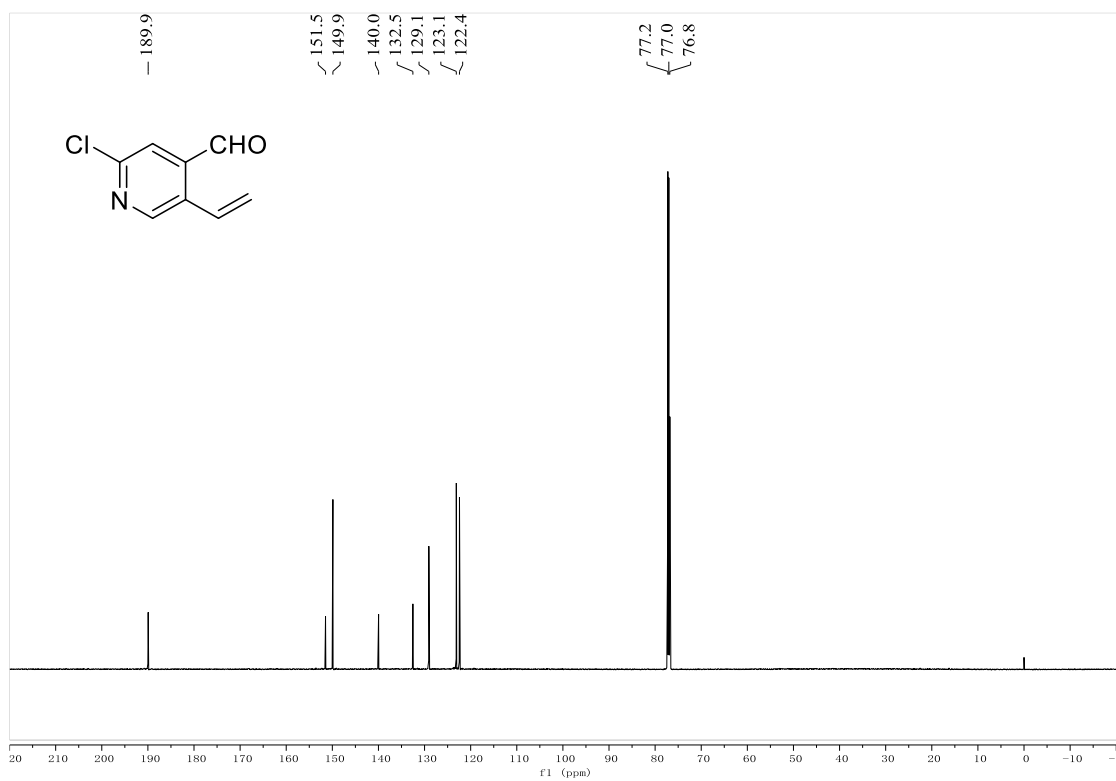


Figure S8 ¹³C NMR Spectra of compound **7** (150 MHz, CDCl₃)

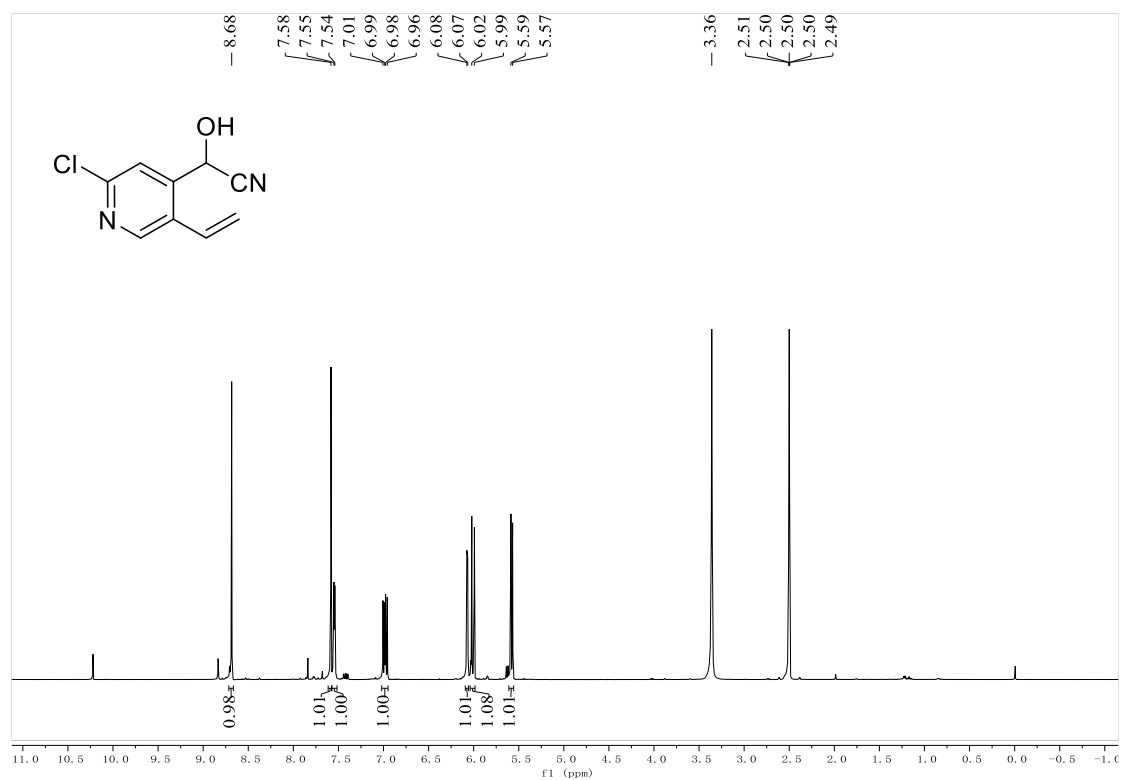


Figure S9 $^1\text{H NMR}$ Spectra of compound **6** (600 MHz, $\text{DMSO-}d_6$)

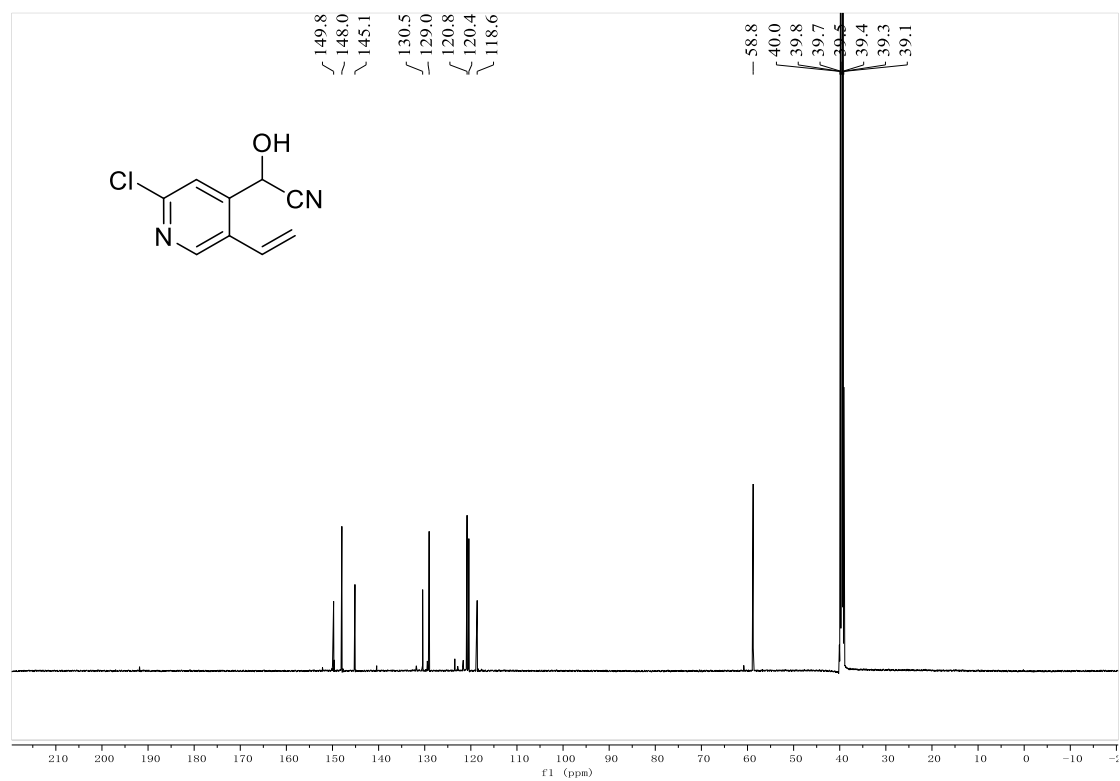


Figure S10 $^{13}\text{C NMR}$ Spectra of compound **6** (150 MHz, $\text{DMSO-}d_6$)

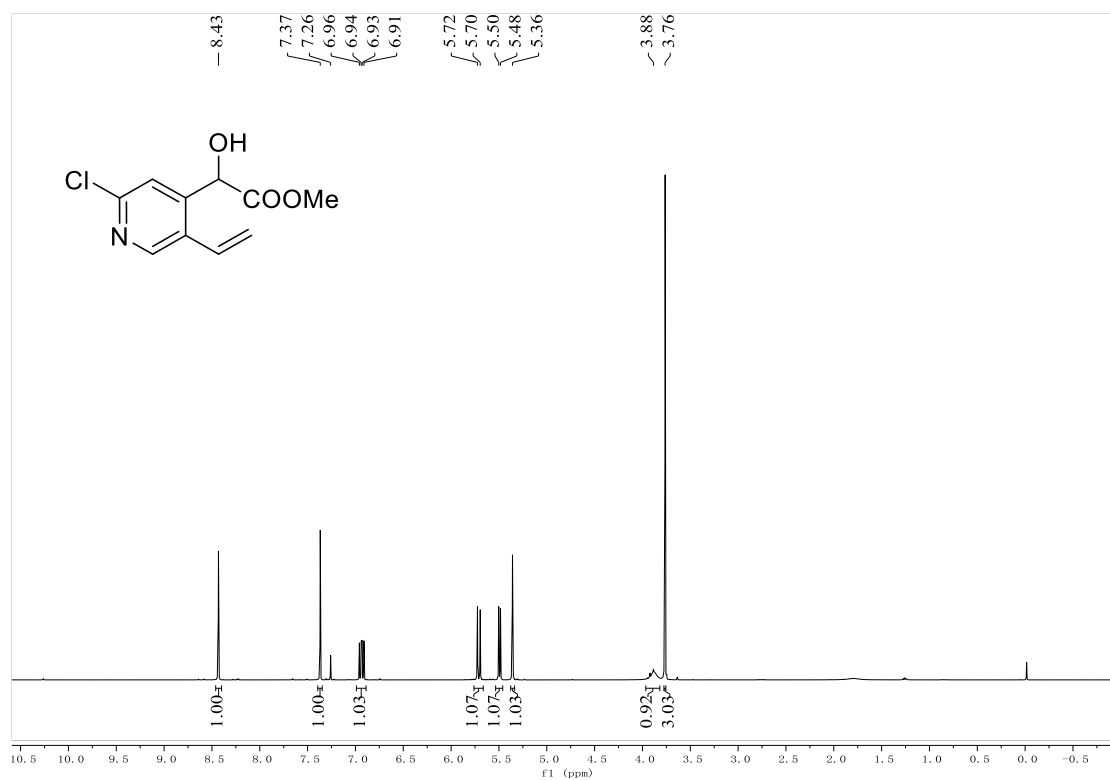


Figure S11 ^1H NMR Spectra of compound **13** (600 MHz, CDCl_3)

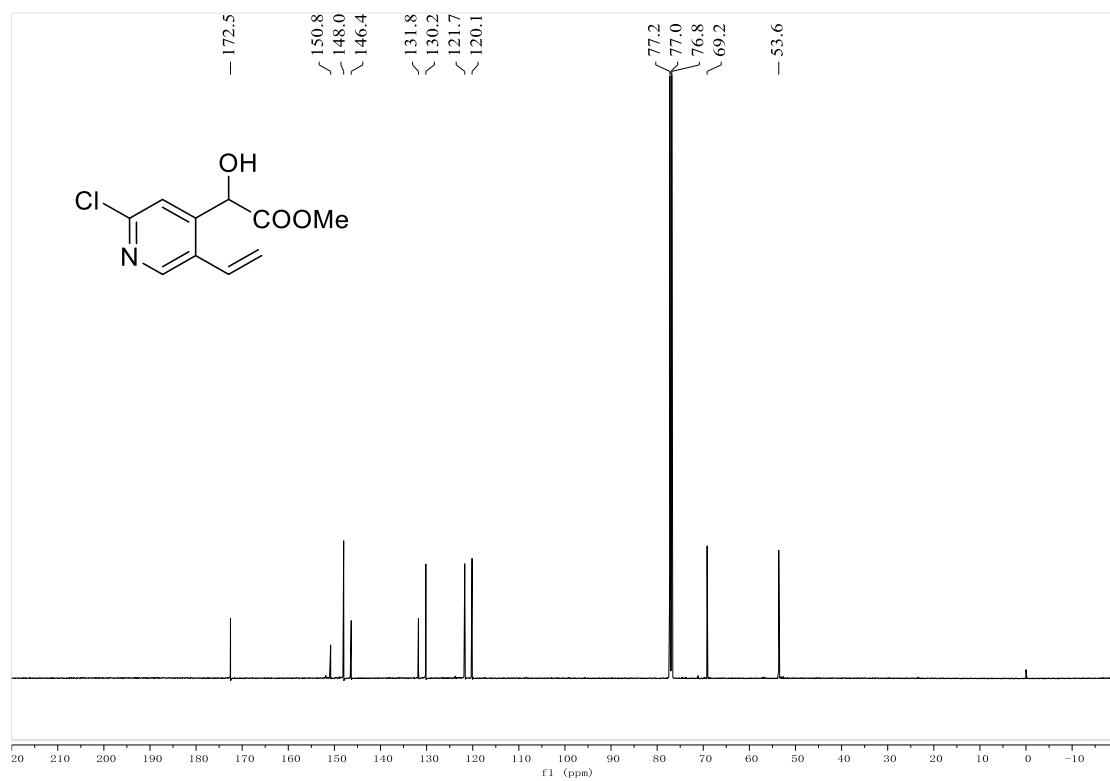


Figure S12 ^{13}C NMR Spectra of compound **13** (150 MHz, CDCl_3)

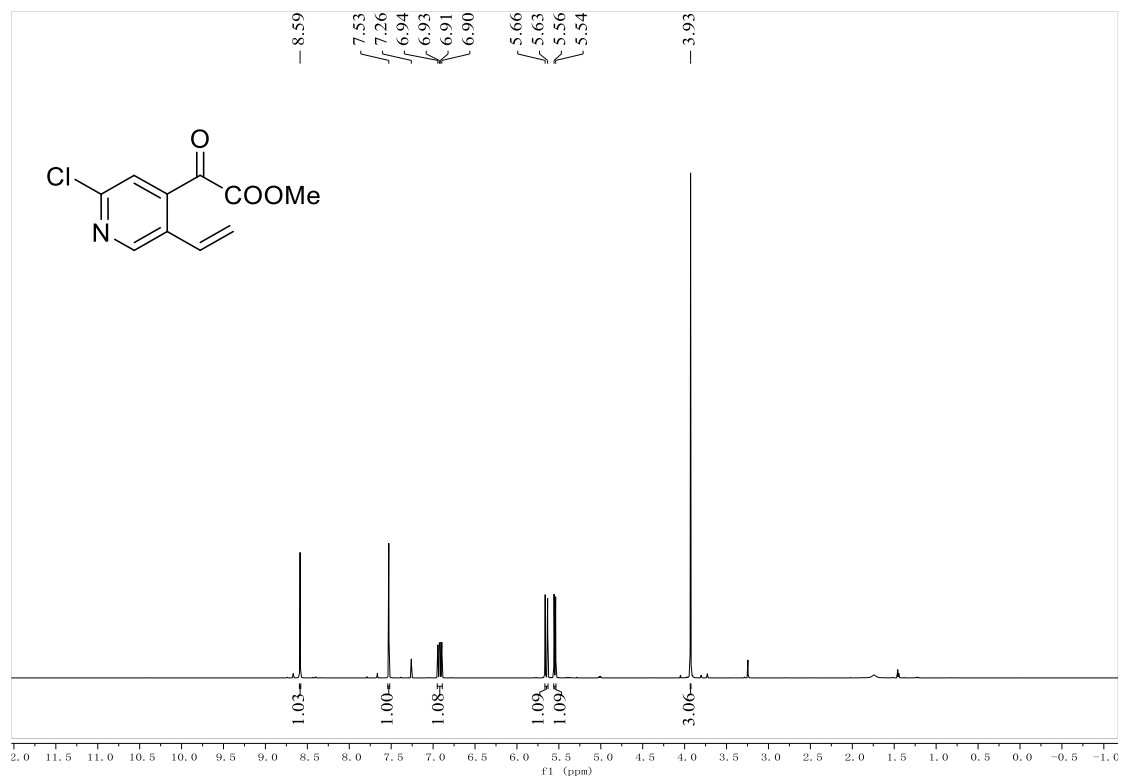


Figure S13 ¹H NMR Spectra of compound **5** (600 MHz, CDCl₃)



Figure S14 ¹³C NMR Spectra of compound **5** (150 MHz, CDCl₃)

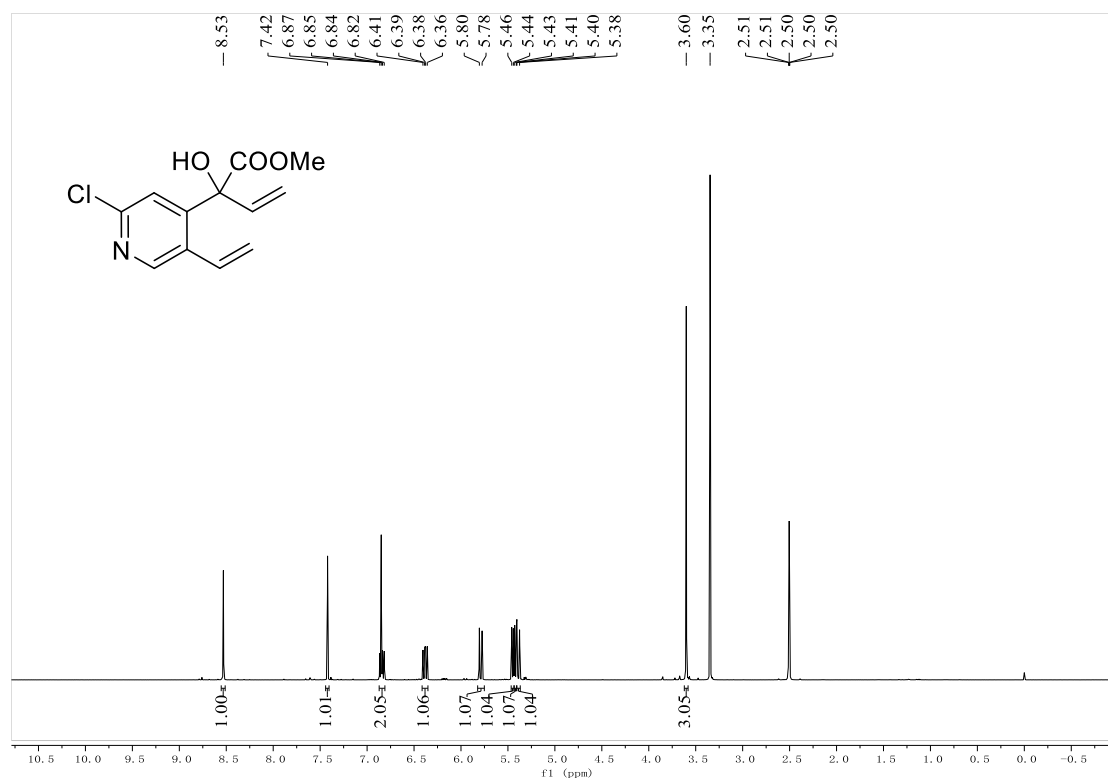


Figure S15 ¹H NMR Spectra of compound **5b** (600 MHz, DMSO-*d*₆)

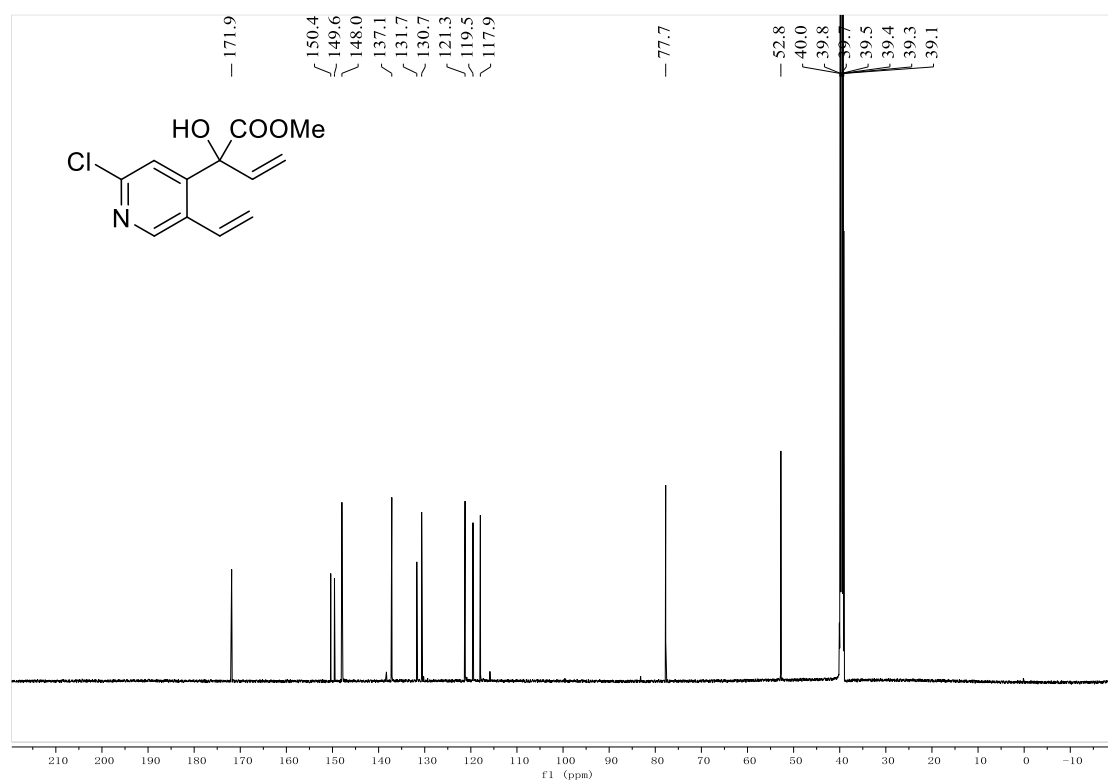


Figure S16 ¹³C NMR Spectra of compound **5b** (150 MHz, DMSO-*d*₆)

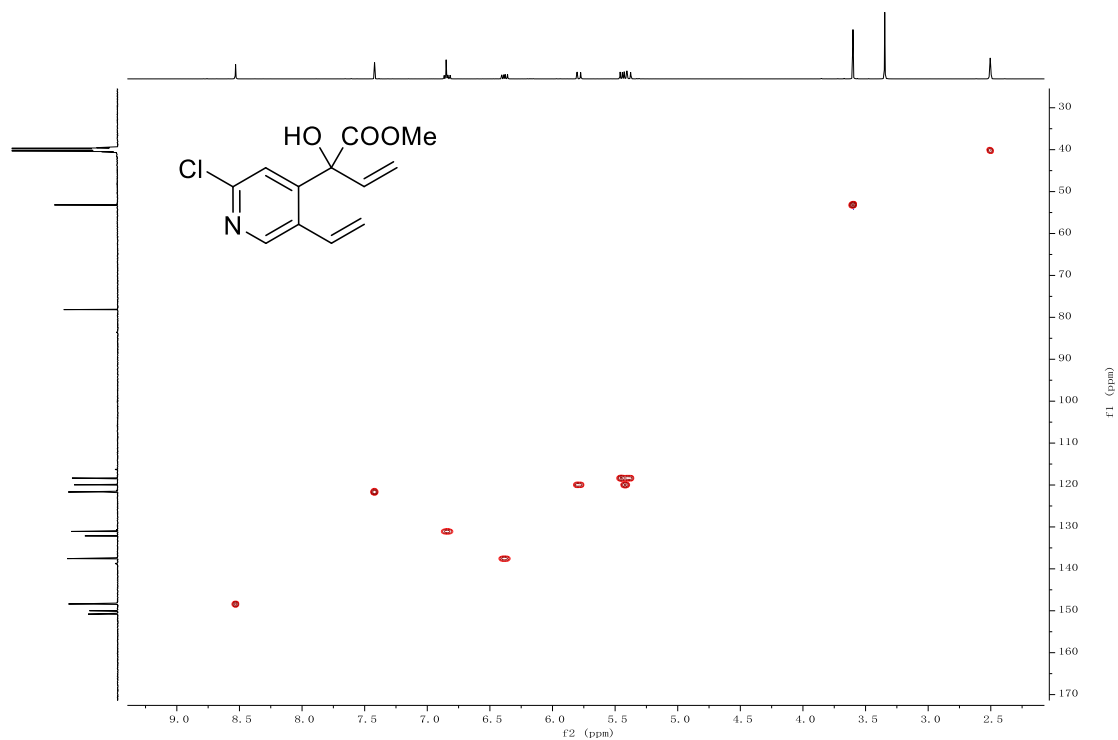


Figure S17 HSQC Spectra of compound **4** (150 MHz, DMSO-*d*₆)

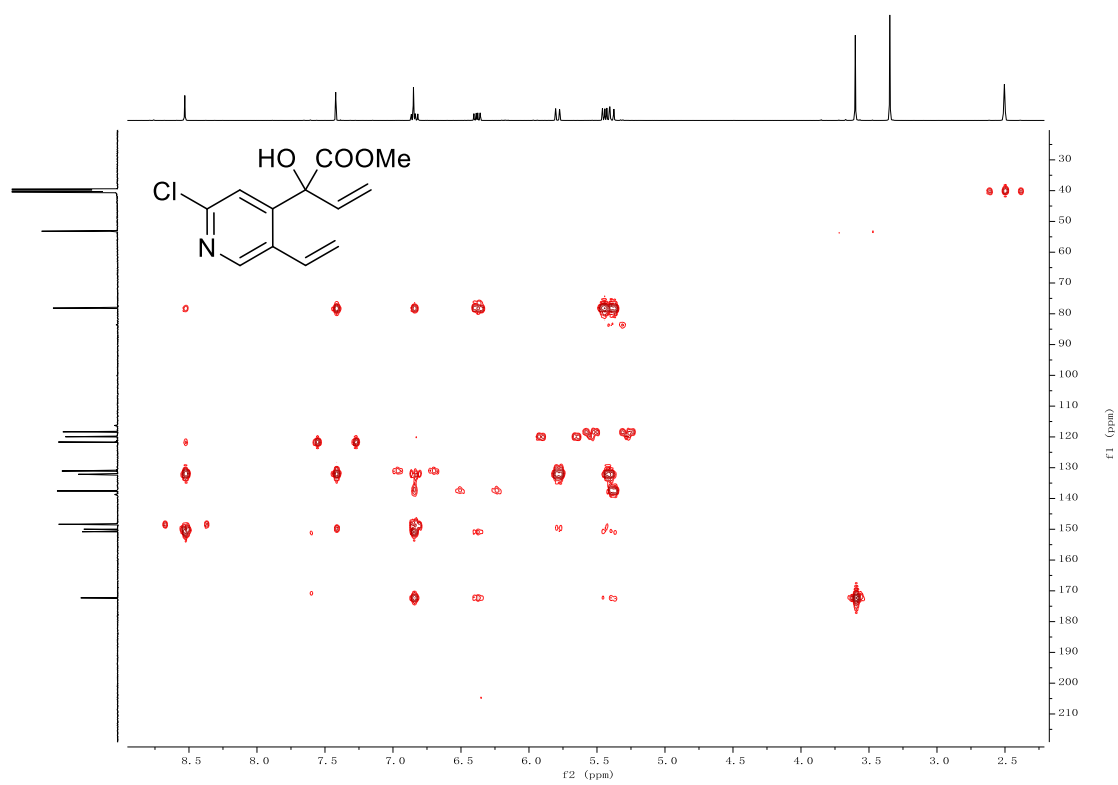


Figure S18 HMBC Spectra of compound **4** (150 MHz, DMSO-*d*₆)

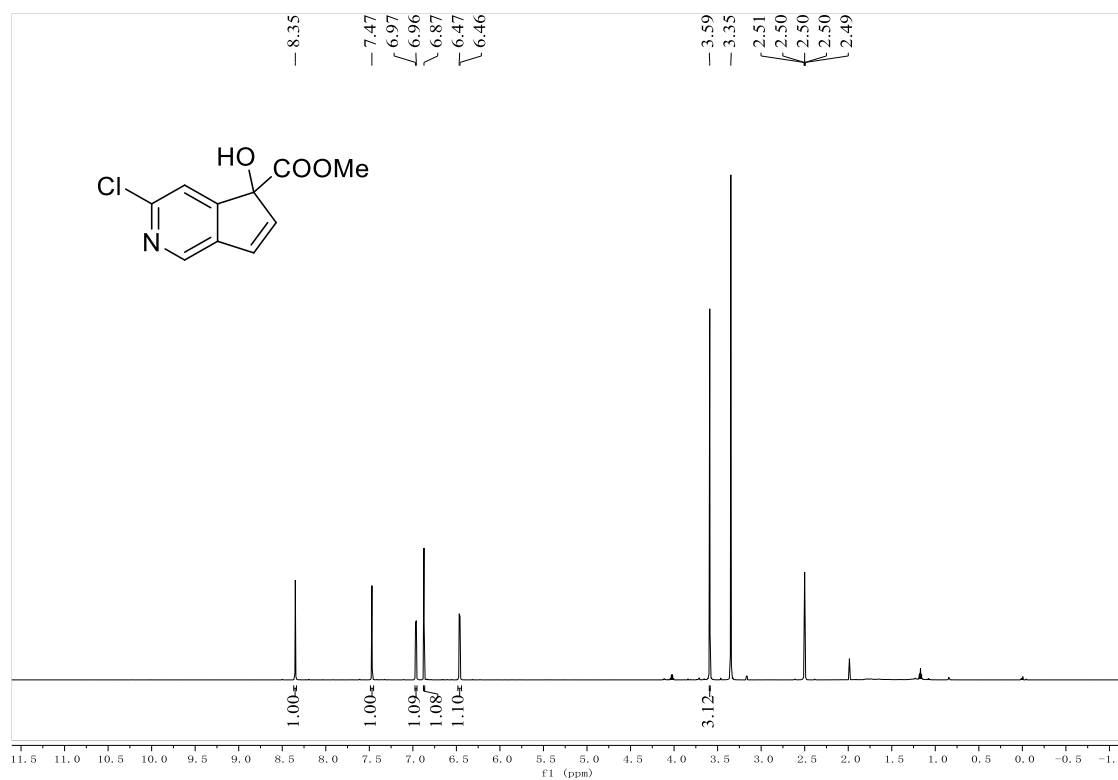


Figure S19 ¹H NMR Spectra of compound **18** (600 MHz, DMSO-*d*₆)

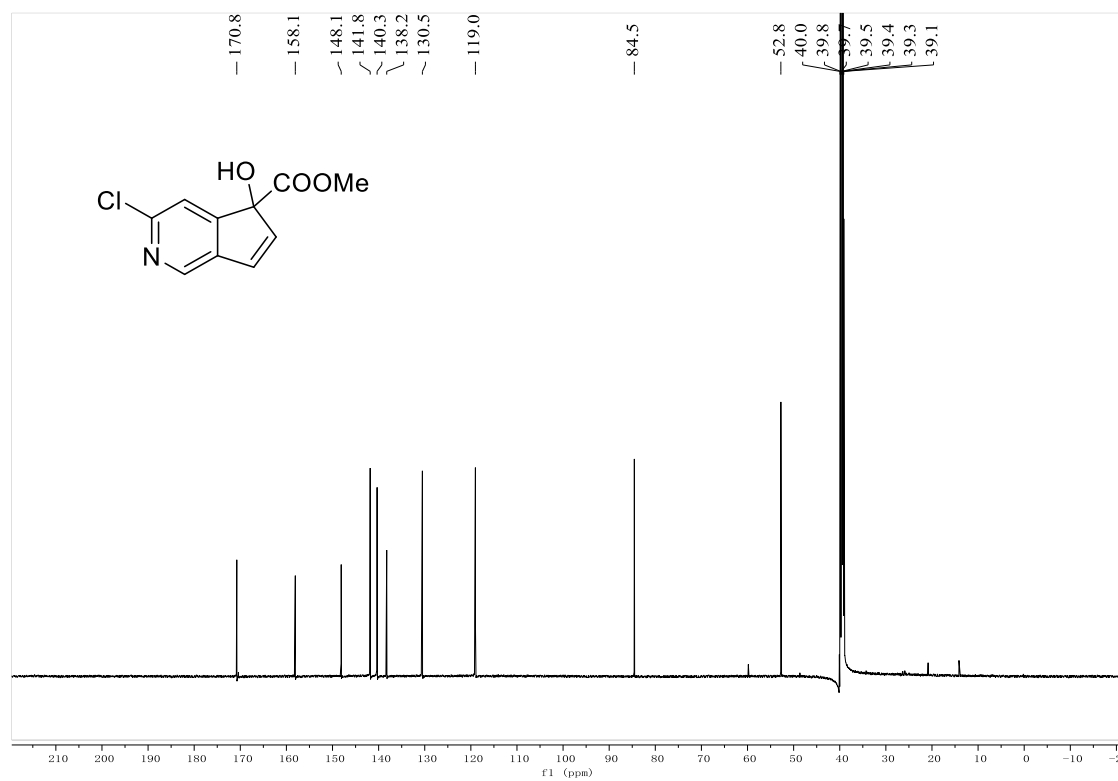


Figure S20 ¹³C NMR Spectra of compound **18** (150 MHz, DMSO-*d*₆)

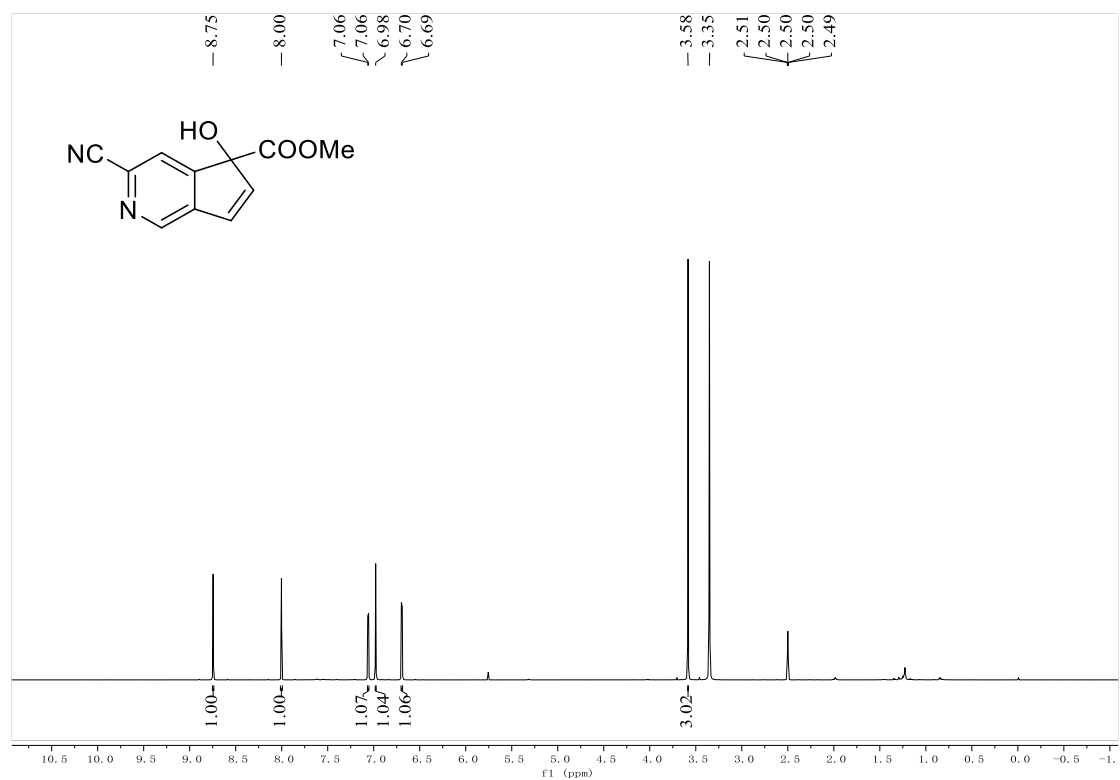


Figure S21 ¹H NMR Spectra of compound **19** (600 MHz, DMSO-*d*₆)

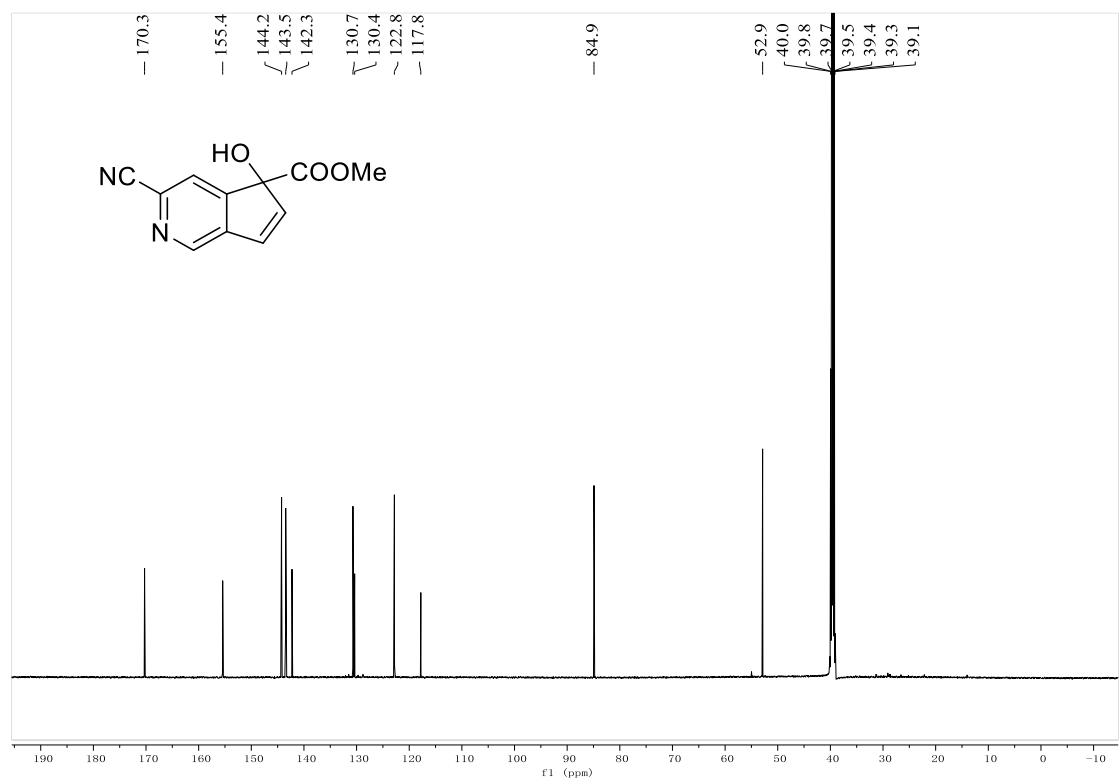


Figure S22 ¹³C NMR Spectra of compound **19** (150 MHz, DMSO-*d*₆)

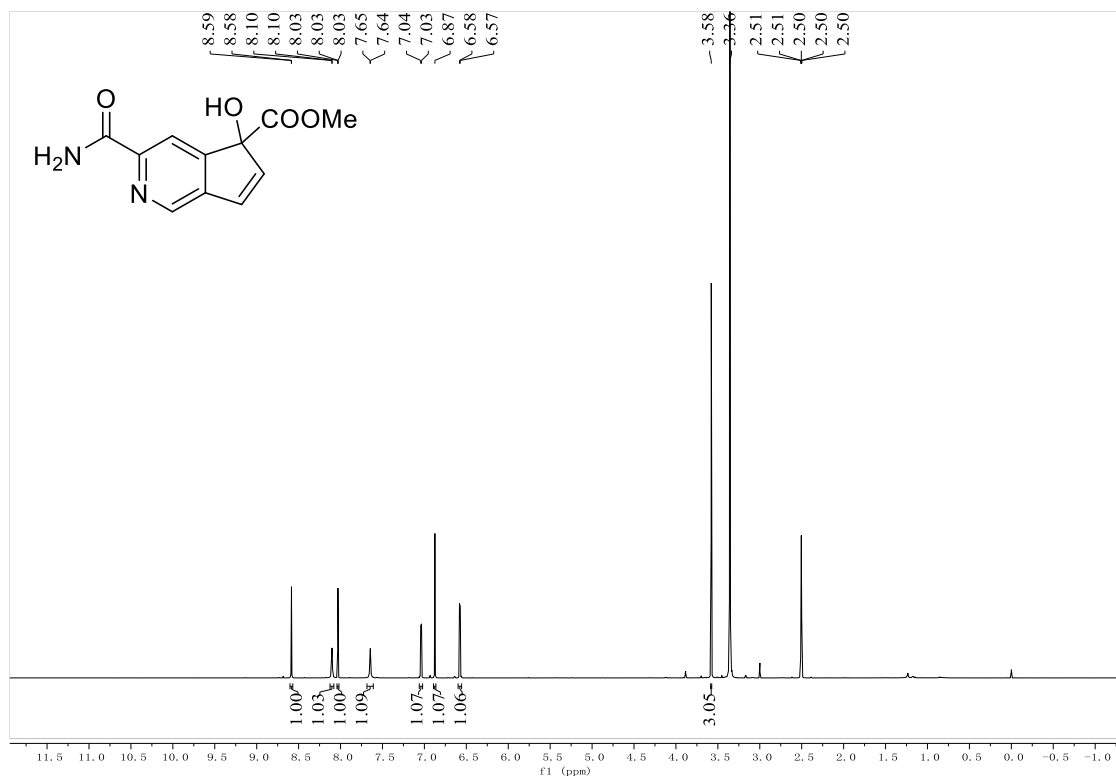


Figure S23 ¹H NMR Spectra of amycolasporin C (3) (600 MHz, DMSO-*d*₆)

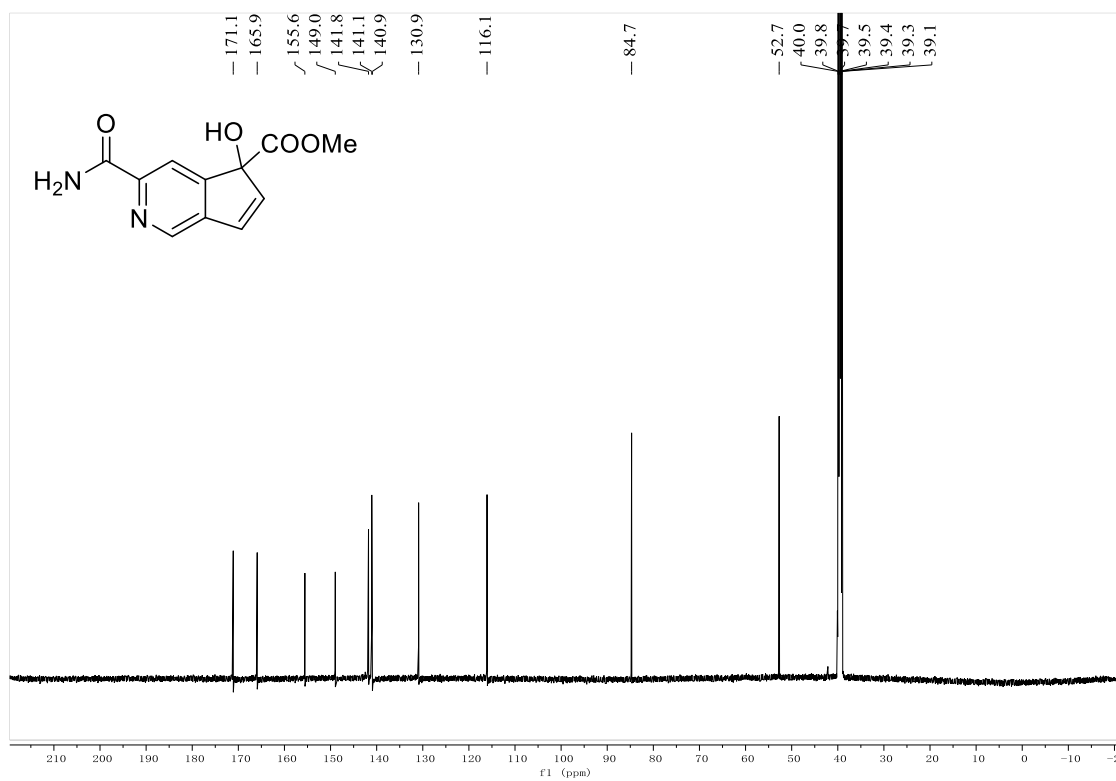


Figure S24 ¹³C NMR Spectra of amycolasporin C (3) (150 MHz, DMSO-*d*₆)

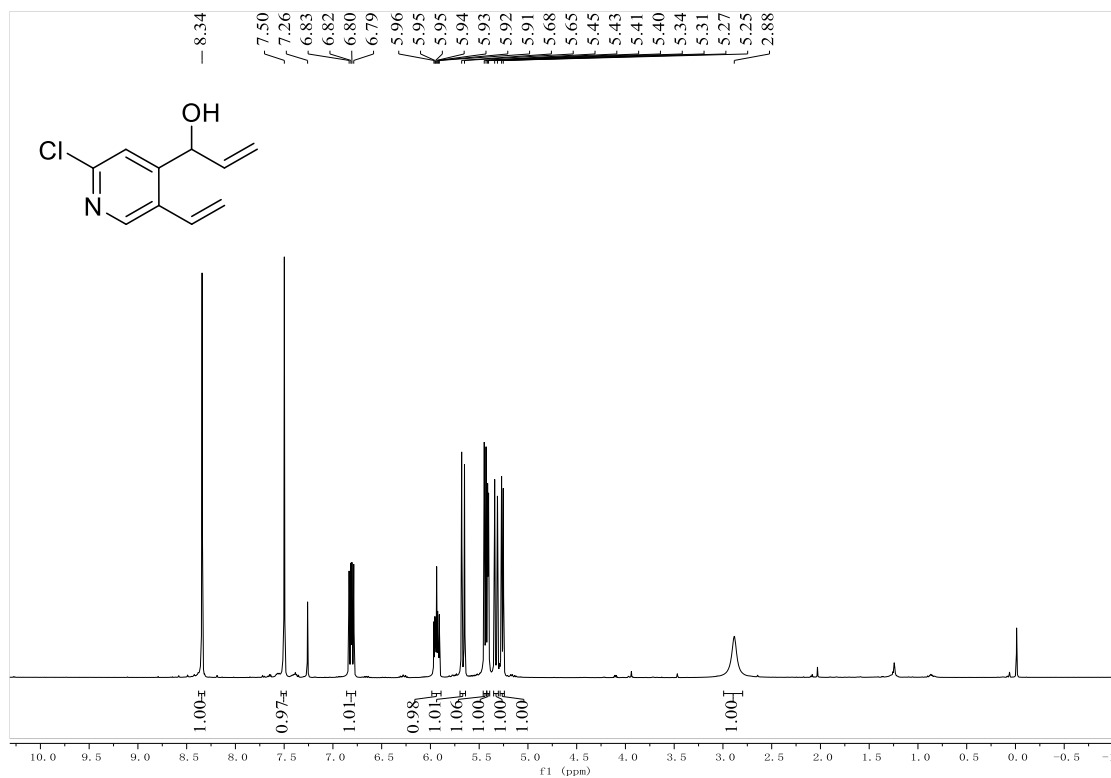


Figure S25 ¹H NMR Spectra of compound **20** (600 MHz, CDCl₃)

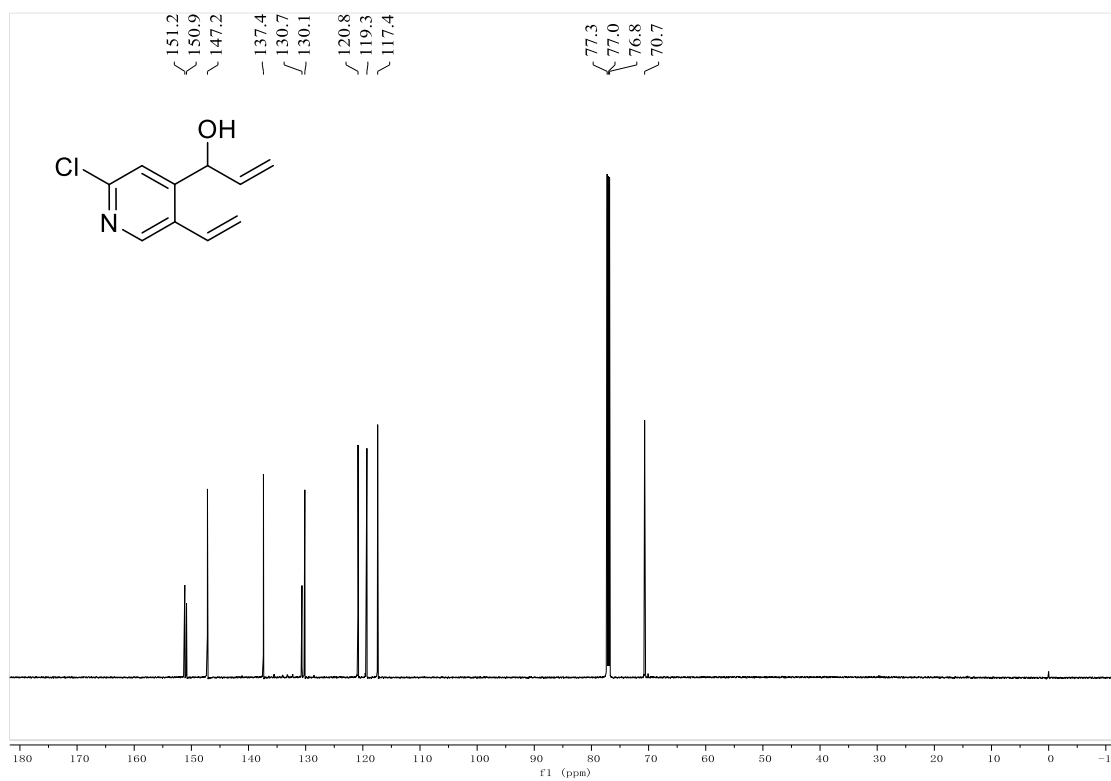


Figure S26 ¹³C NMR Spectra of compound **20** (150 MHz, CDCl₃)

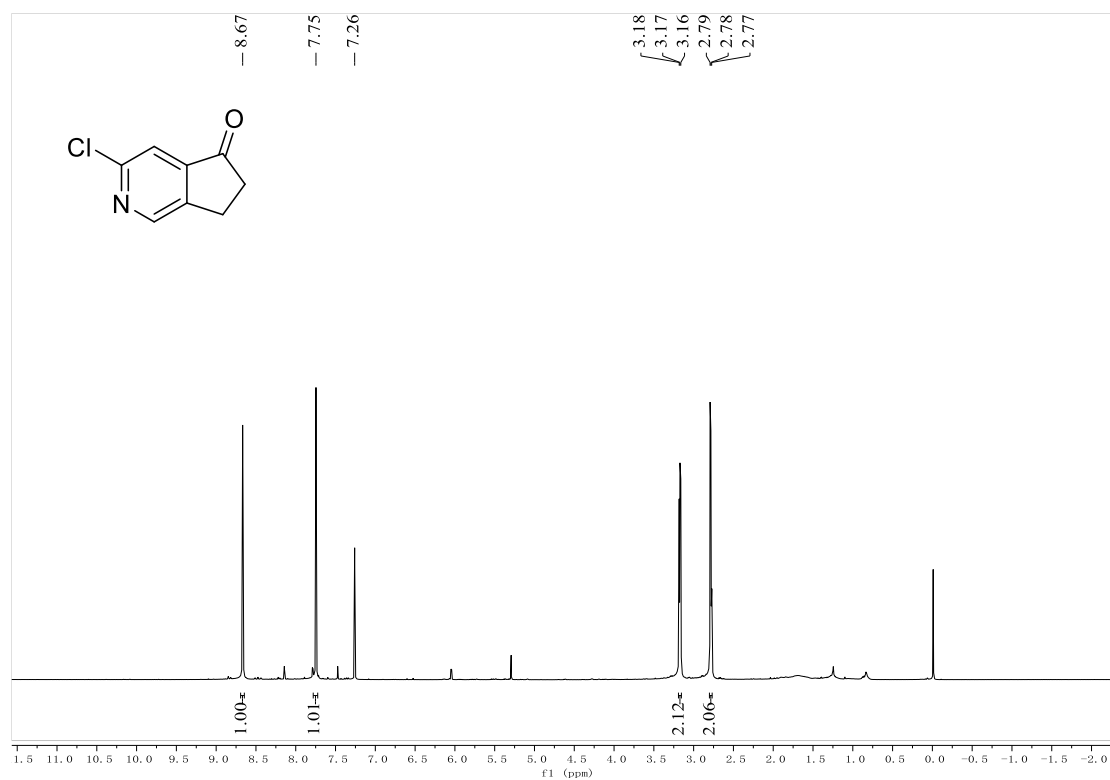


Figure S27 ¹H NMR Spectra of compound **21** (600 MHz, CDCl₃)

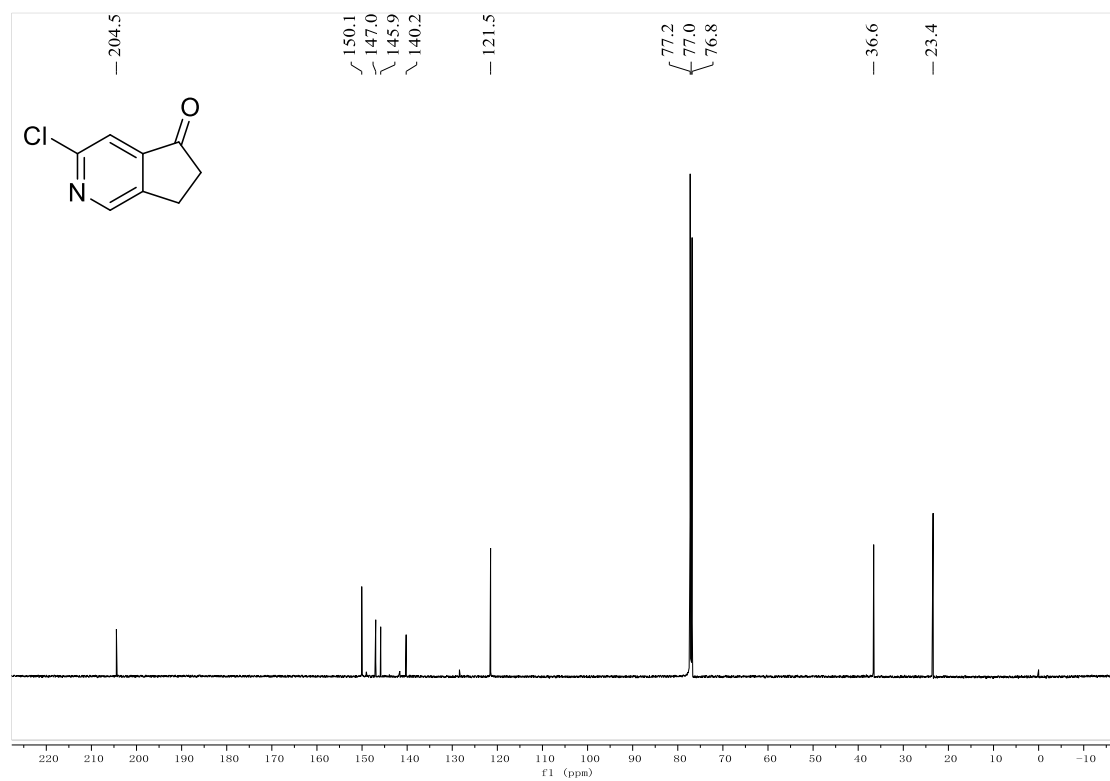


Figure S28 ¹³C NMR Spectra of compound **21** (150 MHz, CDCl₃)

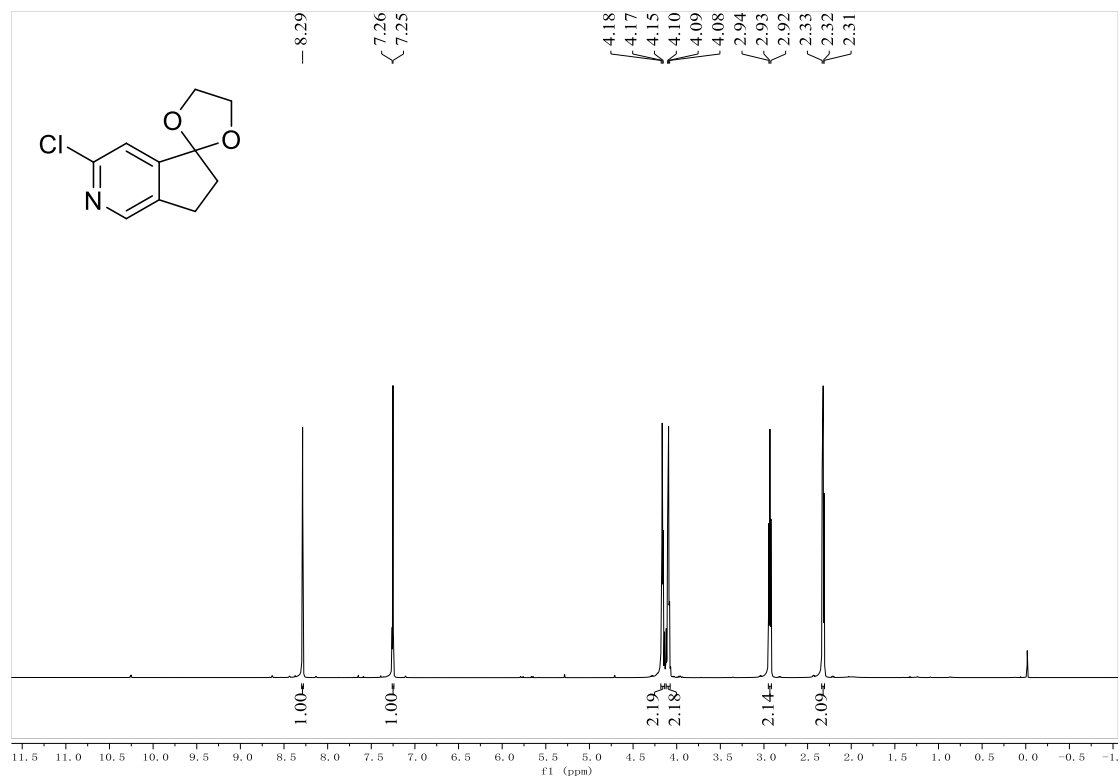


Figure S29 ¹H NMR Spectra of compound **22** (600 MHz, CDCl₃)

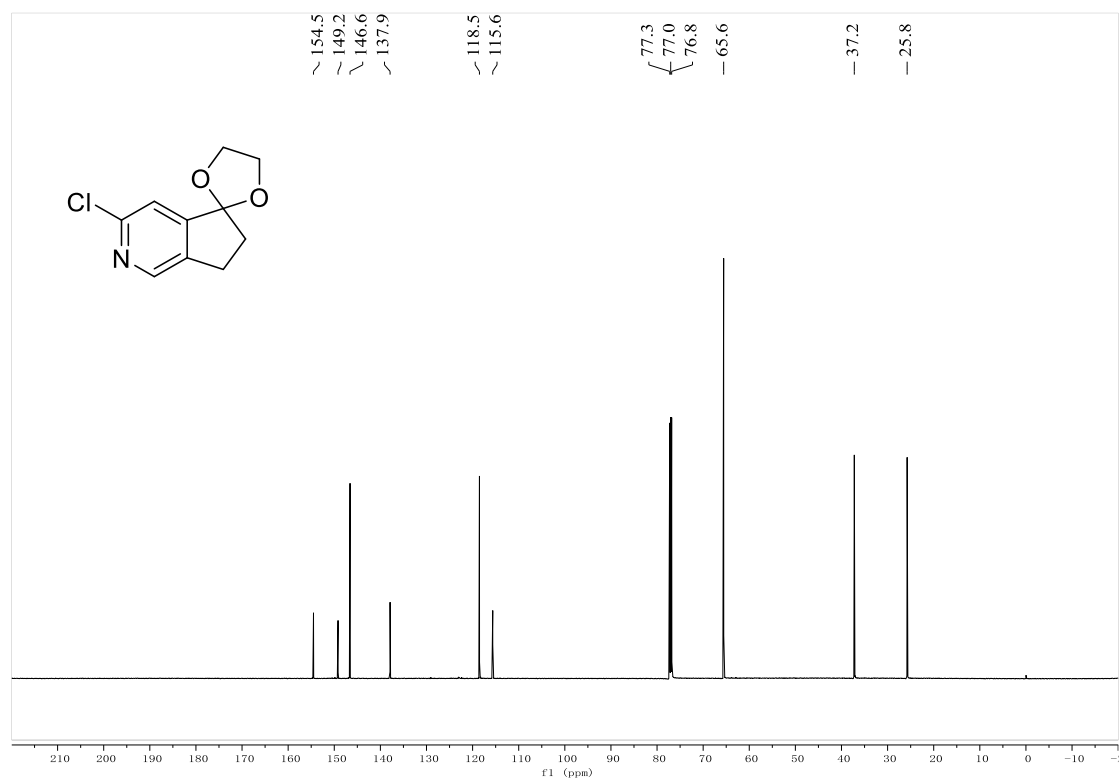


Figure S30 ¹³C NMR Spectra of compound **22** (150 MHz, CDCl₃)

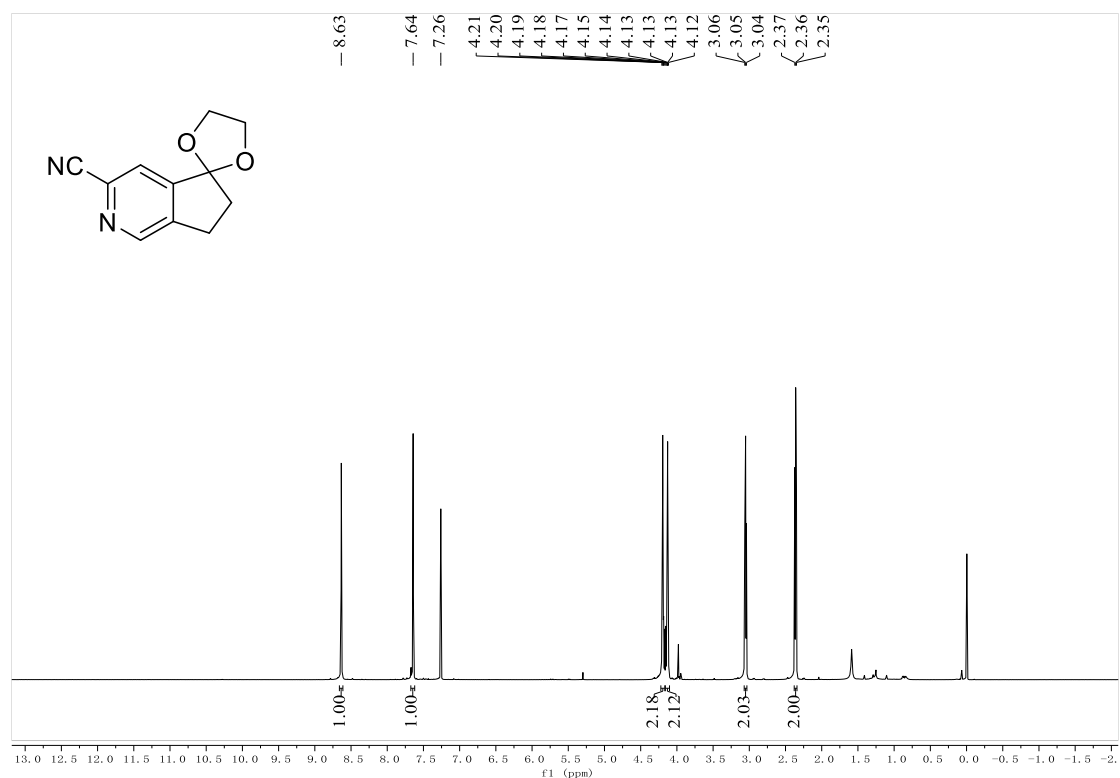


Figure S31 ¹H NMR Spectra of compound **23** (600 MHz, CDCl₃)

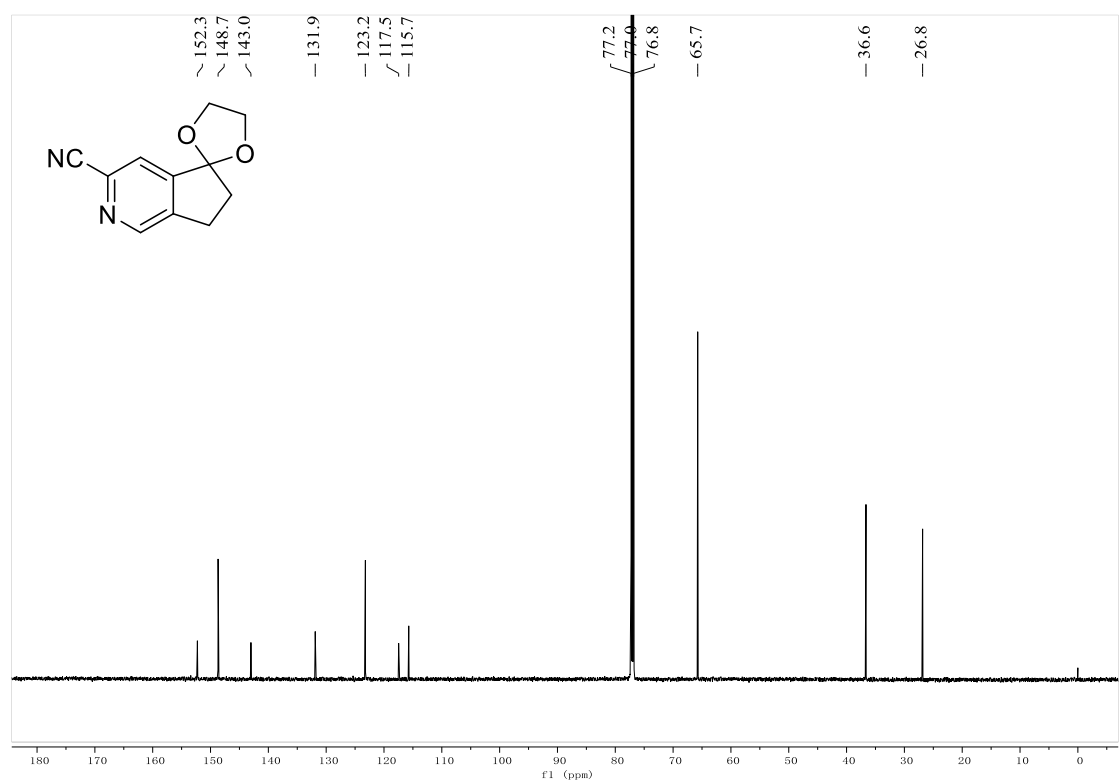


Figure S32 ¹³C NMR Spectra of compound **23** (150 MHz, CDCl₃)

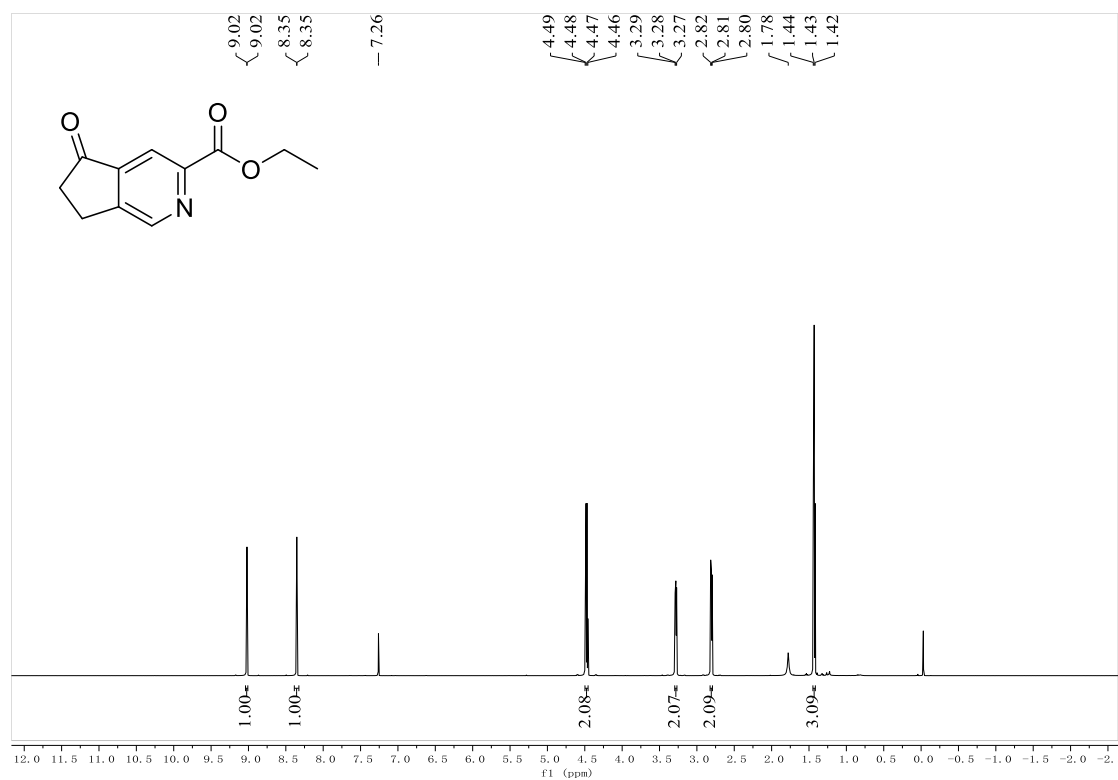


Figure S33 ¹H NMR Spectra of compound **24** (600 MHz, CDCl₃)

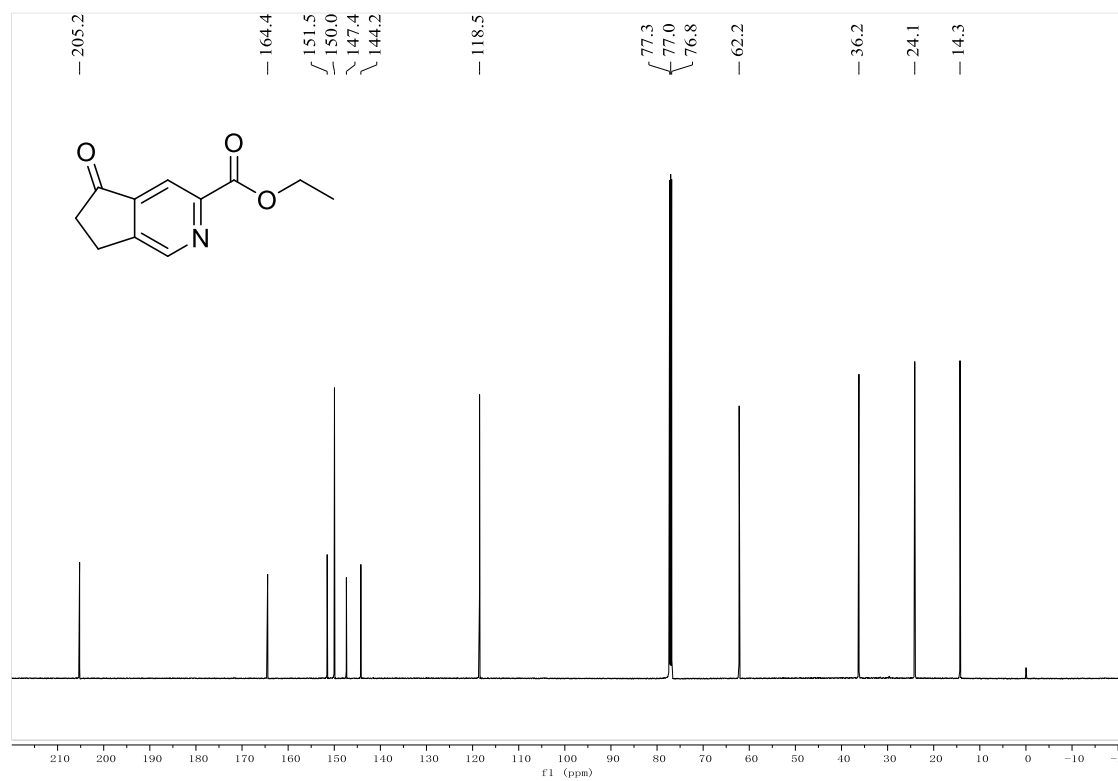


Figure S34 ¹³C NMR Spectra of compound **24** (150 MHz, CDCl₃)

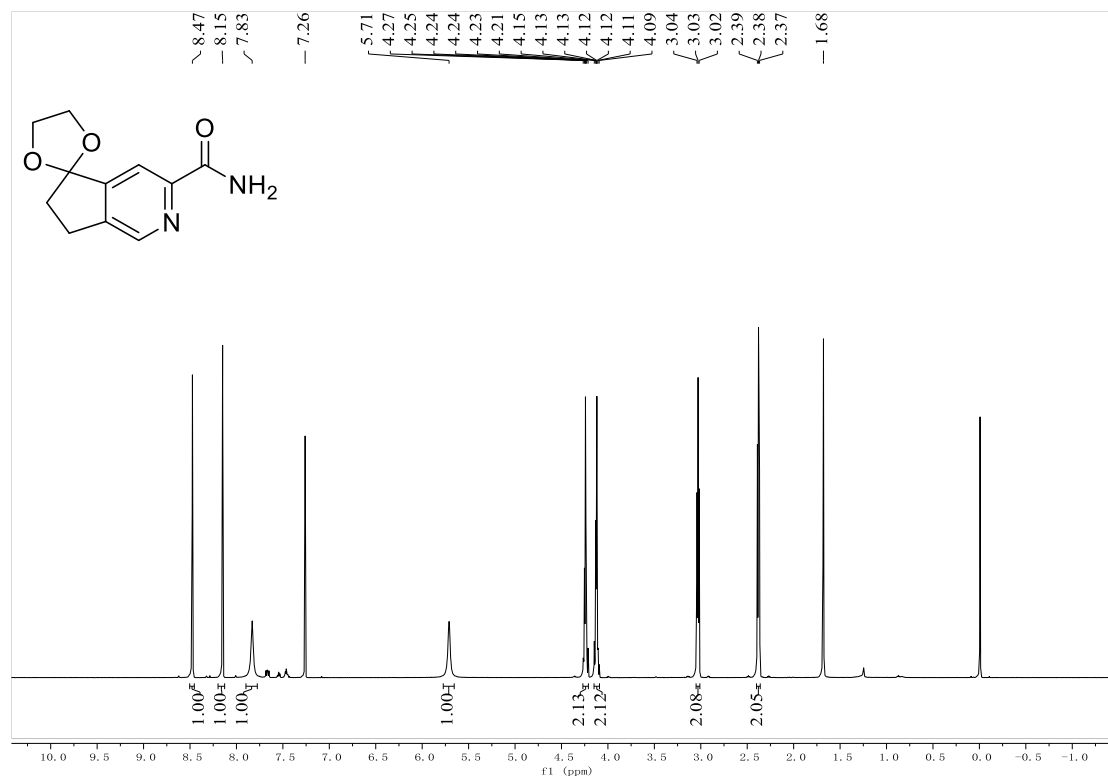


Figure S35 ¹H NMR Spectra of compound **25** (600 MHz, CDCl₃)

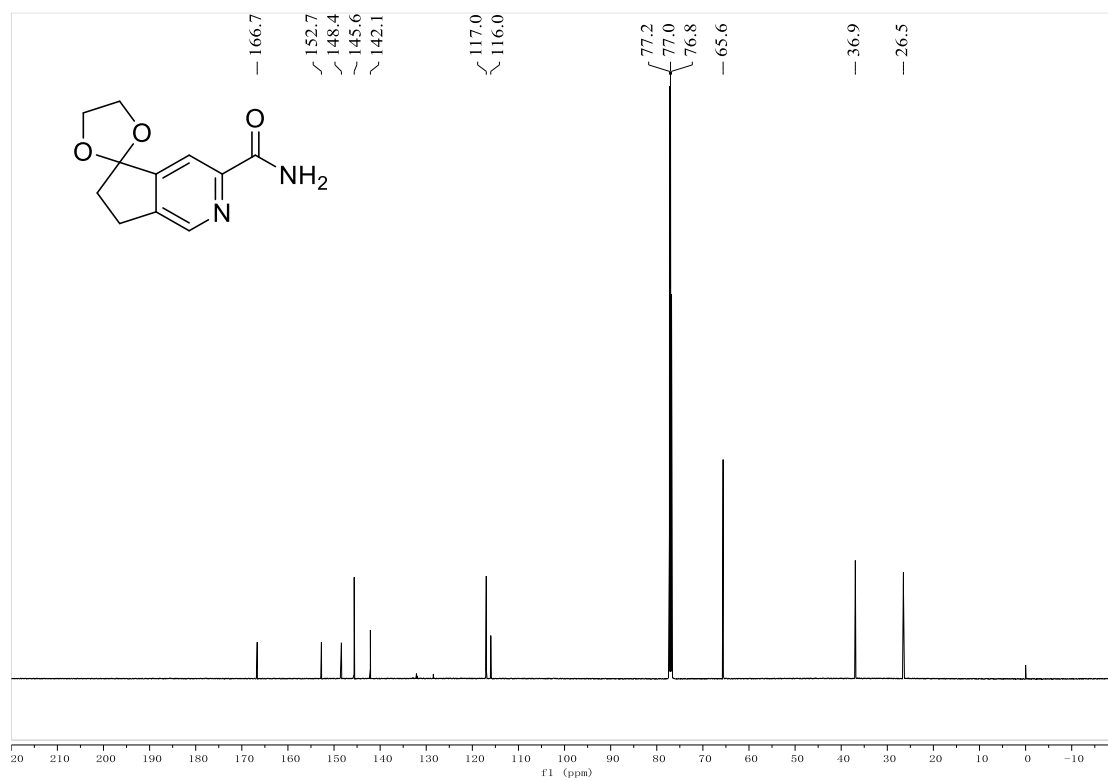


Figure S36 ¹³C NMR Spectra of compound **25** (150 MHz, CDCl₃)

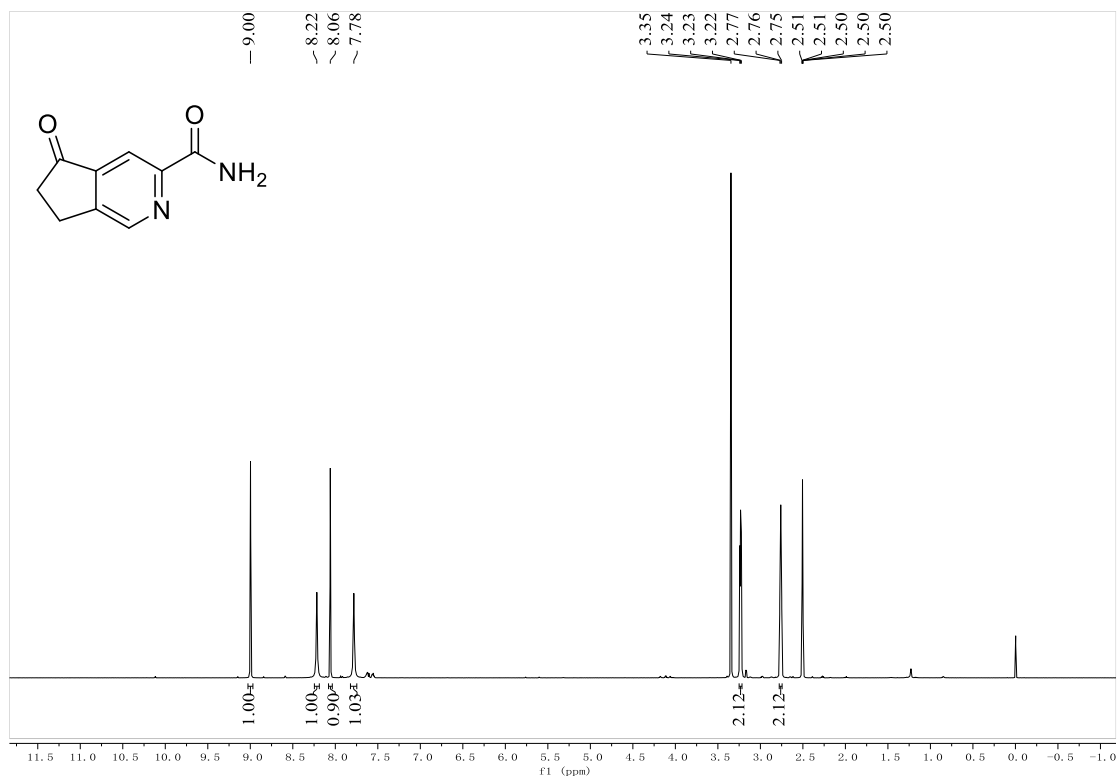


Figure S37 ^1H NMR Spectra of amycolasporin A (**1**) (600 MHz, $\text{DMSO-}d_6$)

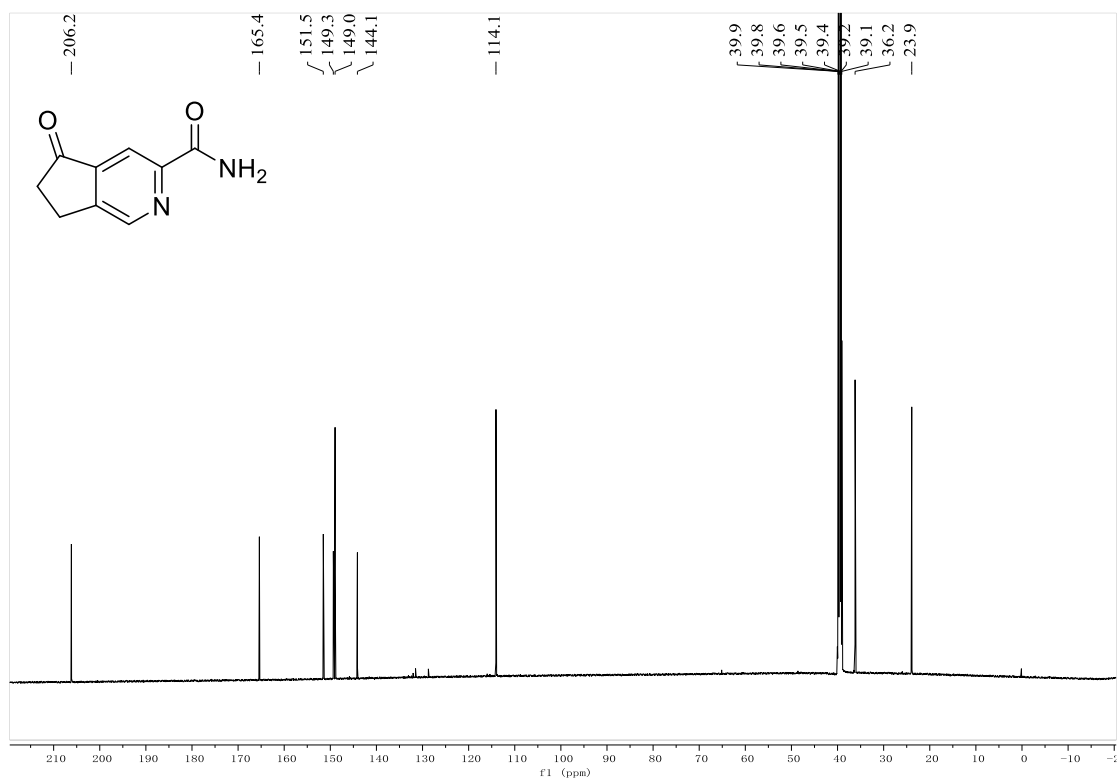


Figure S38 ^{13}C NMR Spectra of amycolasporin A (**1**) (150 MHz, $\text{DMSO-}d_6$)

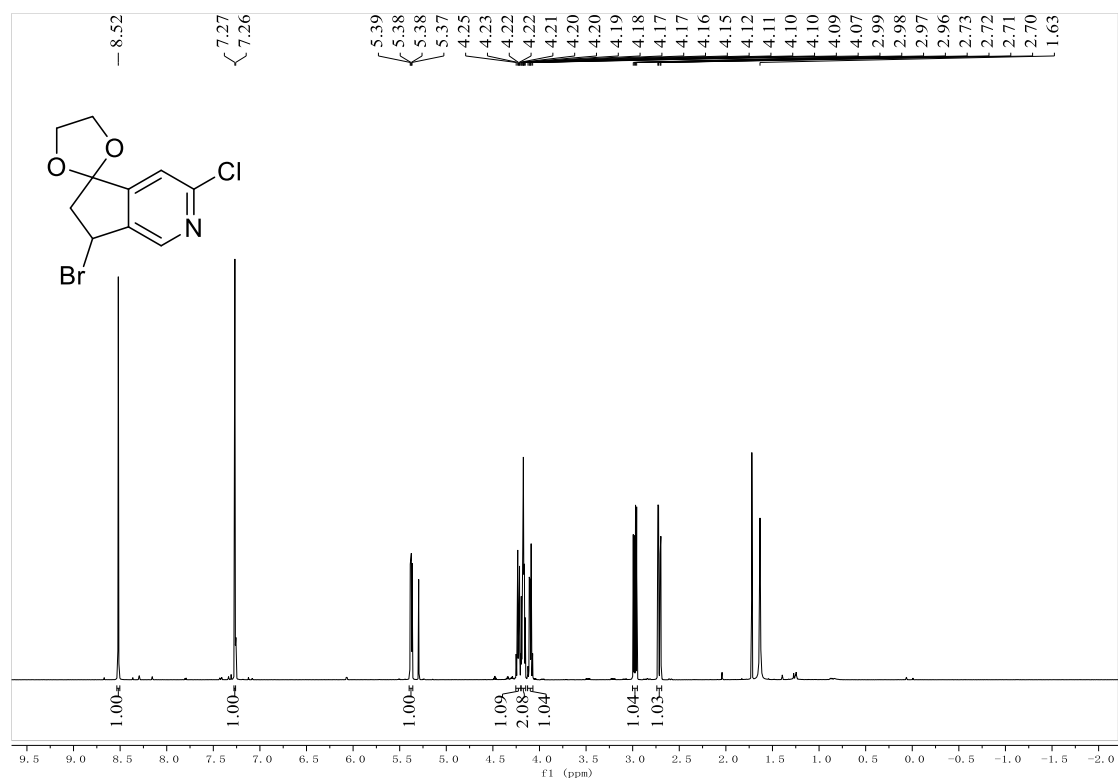


Figure S39 ^1H NMR Spectra of compound **26** (600 MHz, CDCl_3)

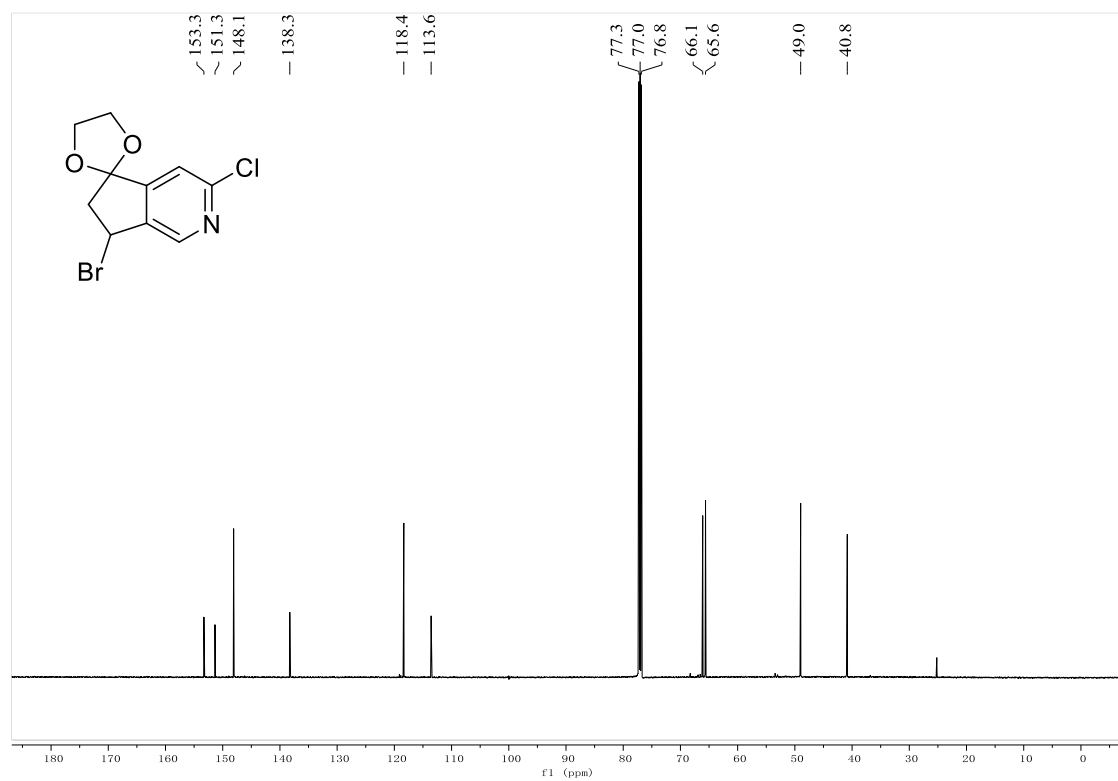


Figure S40 ^{13}C NMR Spectra of compound **26** (150 MHz, CDCl_3)

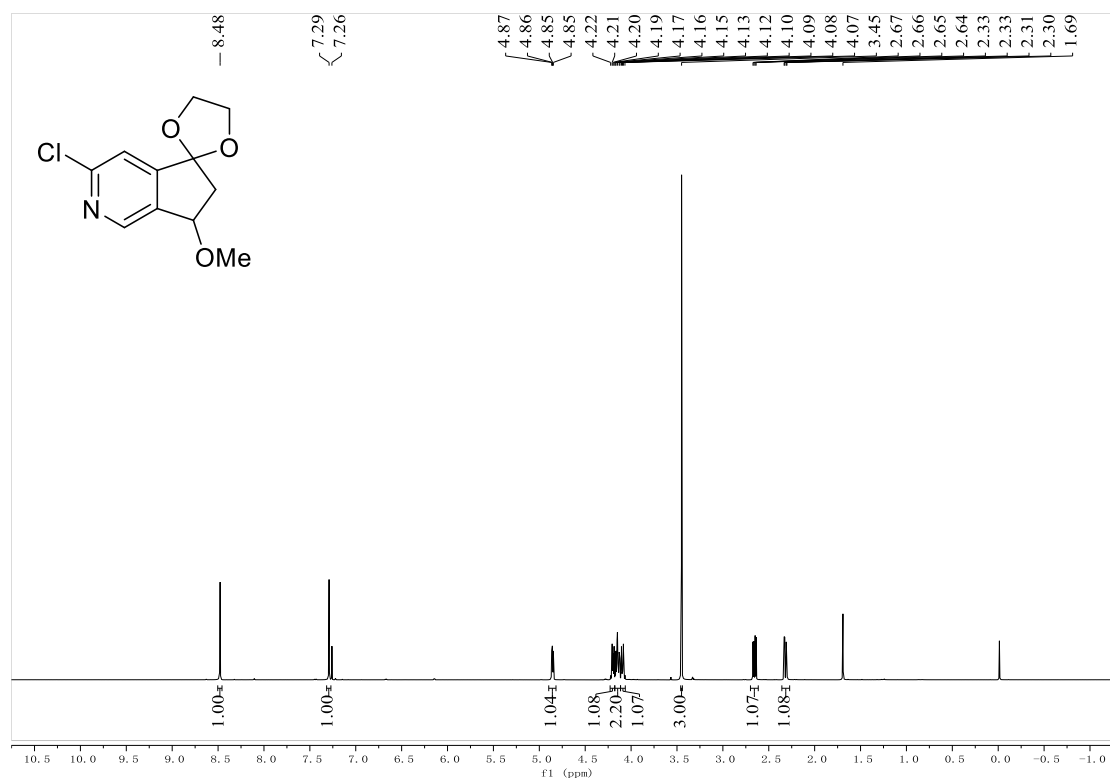


Figure S41 ¹H NMR Spectra of compound **27** (600 MHz, CDCl₃)

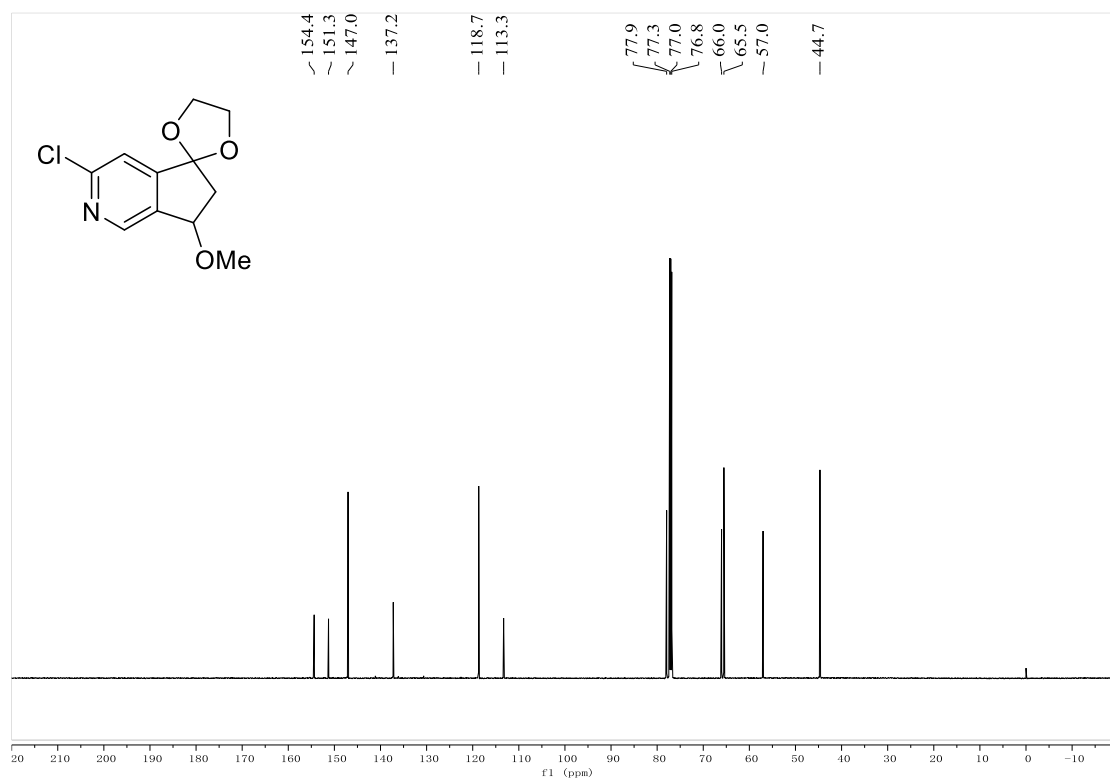


Figure S42 ¹³C NMR Spectra of compound **27** (150 MHz, CDCl₃)

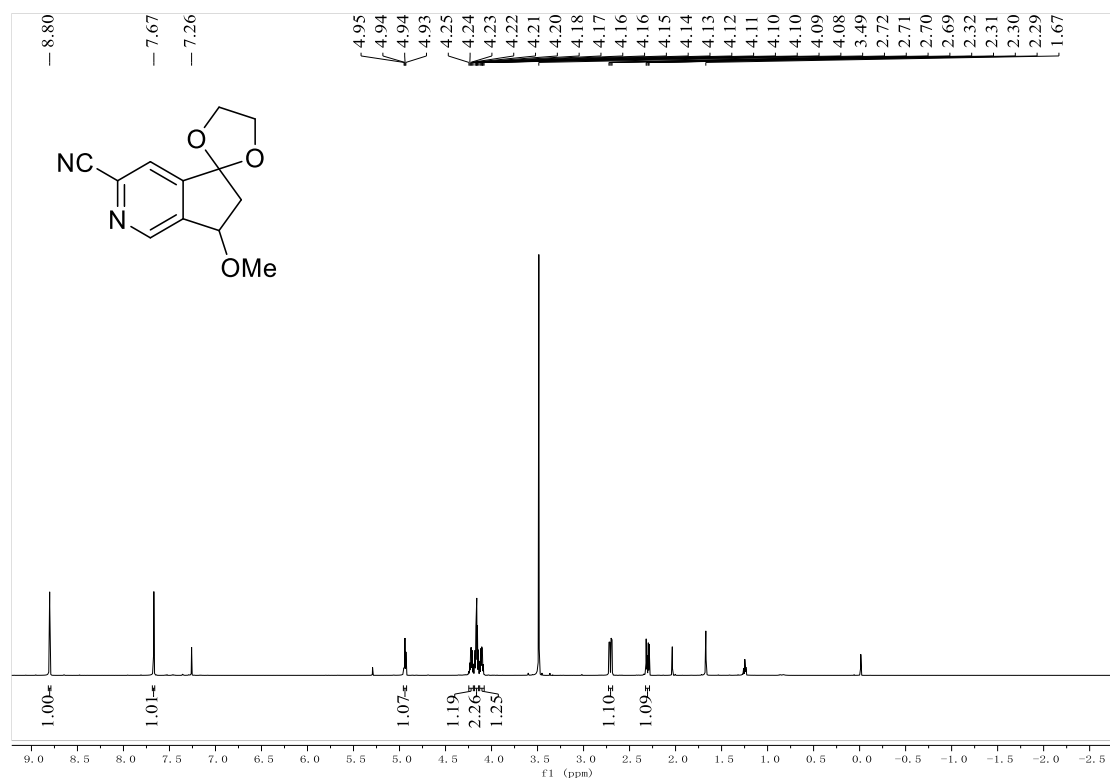


Figure S43 ^1H NMR Spectra of compound **28** (600 MHz, CDCl_3)

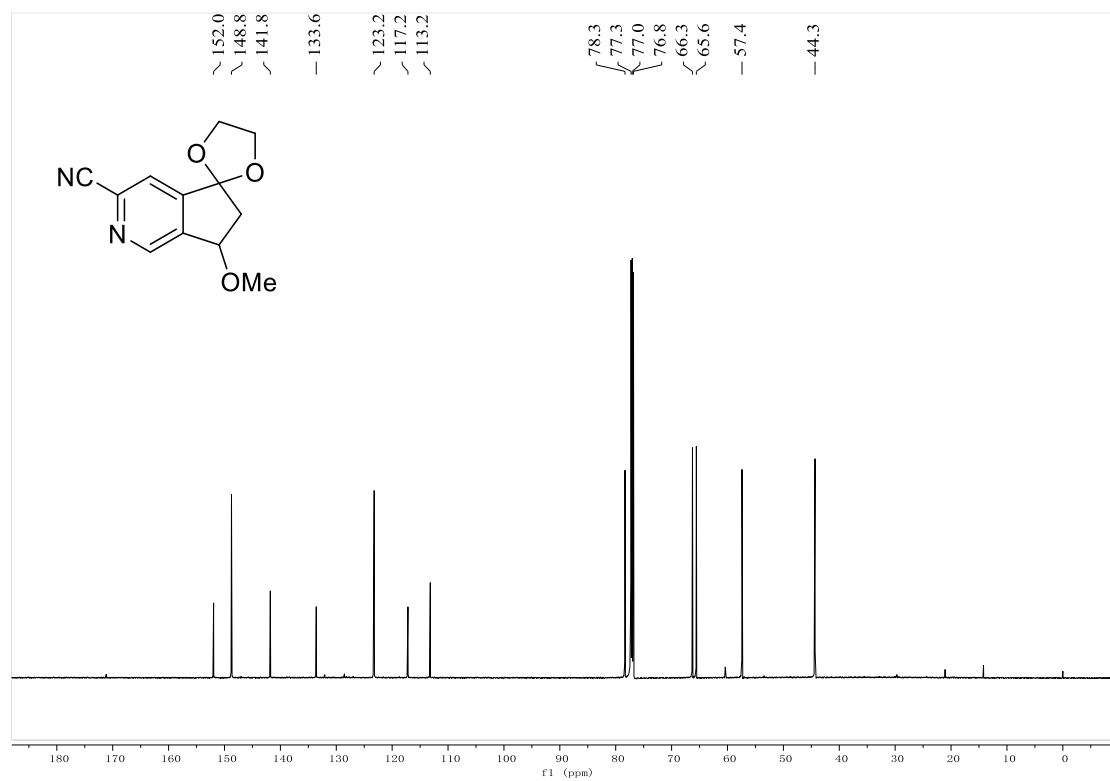


Figure S44 ^{13}C NMR Spectra of compound **28** (150 MHz, CDCl_3)

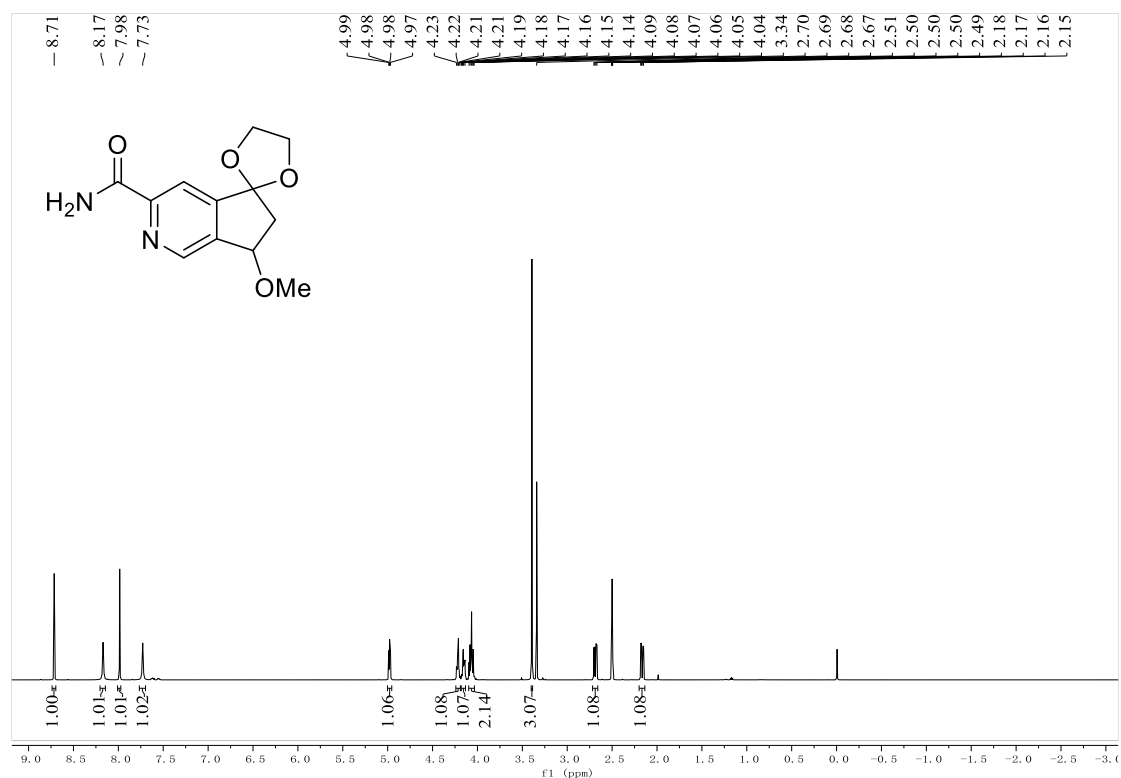


Figure S45 ¹H NMR Spectra of compound **29** (600 MHz, DMSO-*d*₆)

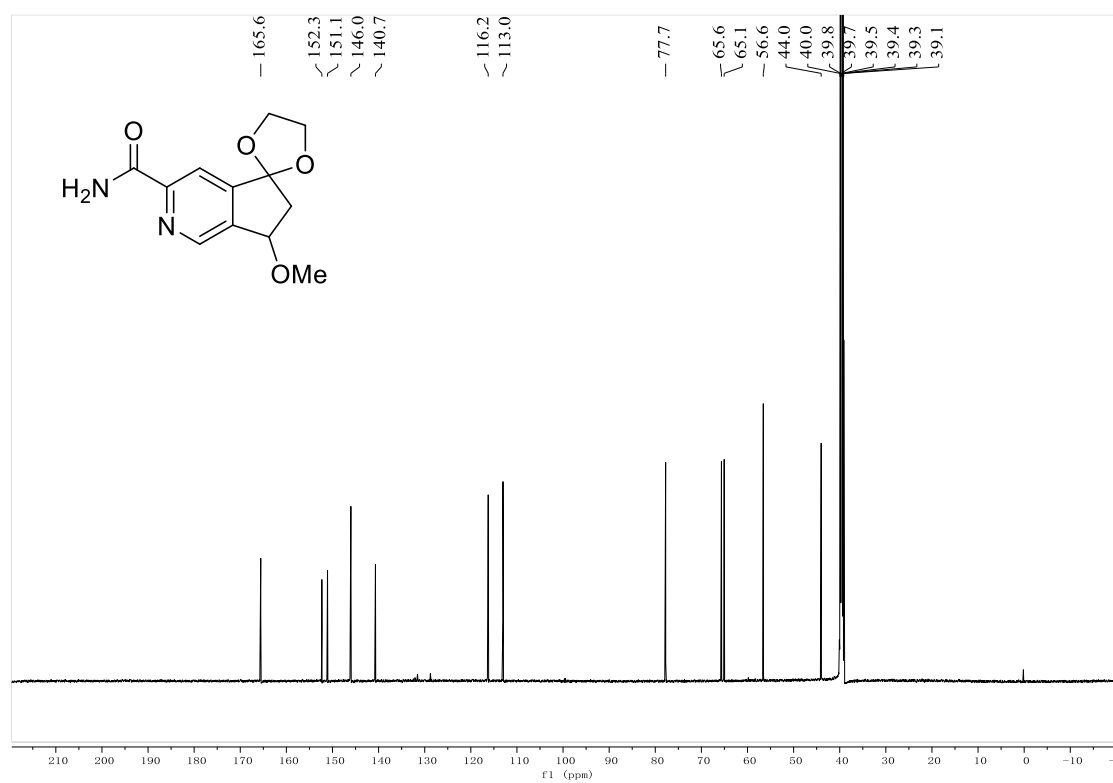


Figure S46 ¹³C NMR Spectra of compound **29** (150 MHz, DMSO-*d*₆)

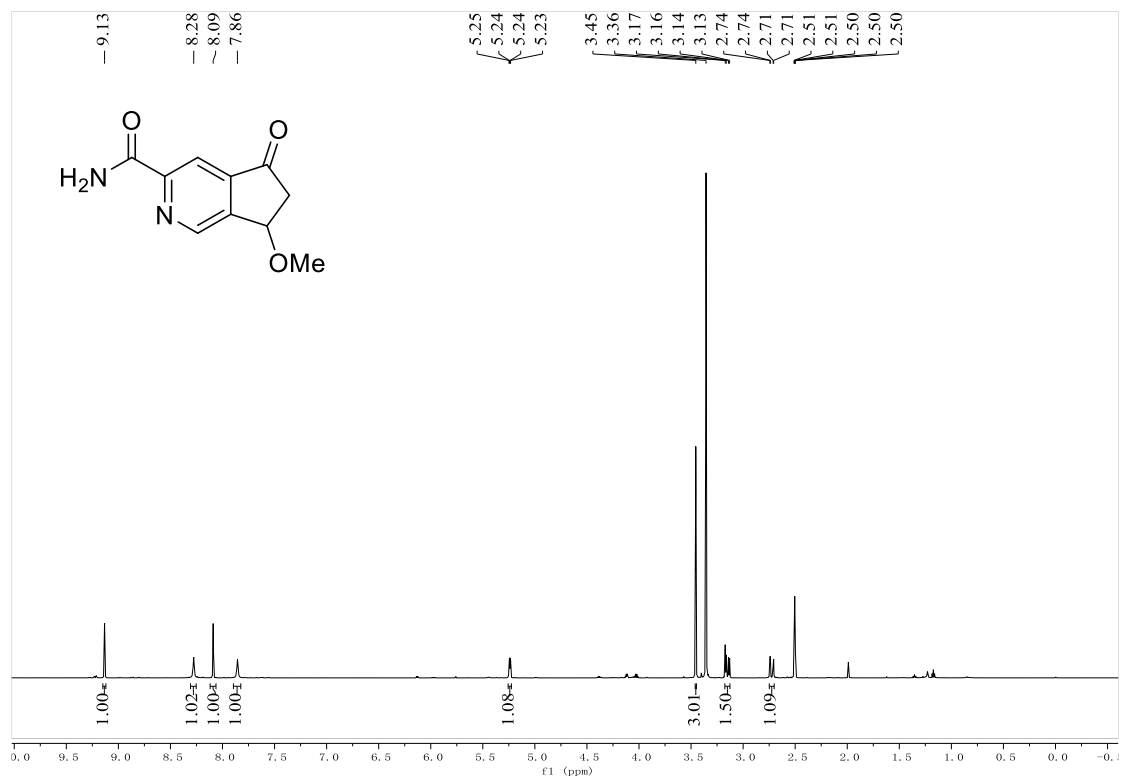


Figure S47 ^1H NMR Spectra of amycolasporin B (**2**) (600 MHz, $\text{DMSO-}d_6$)

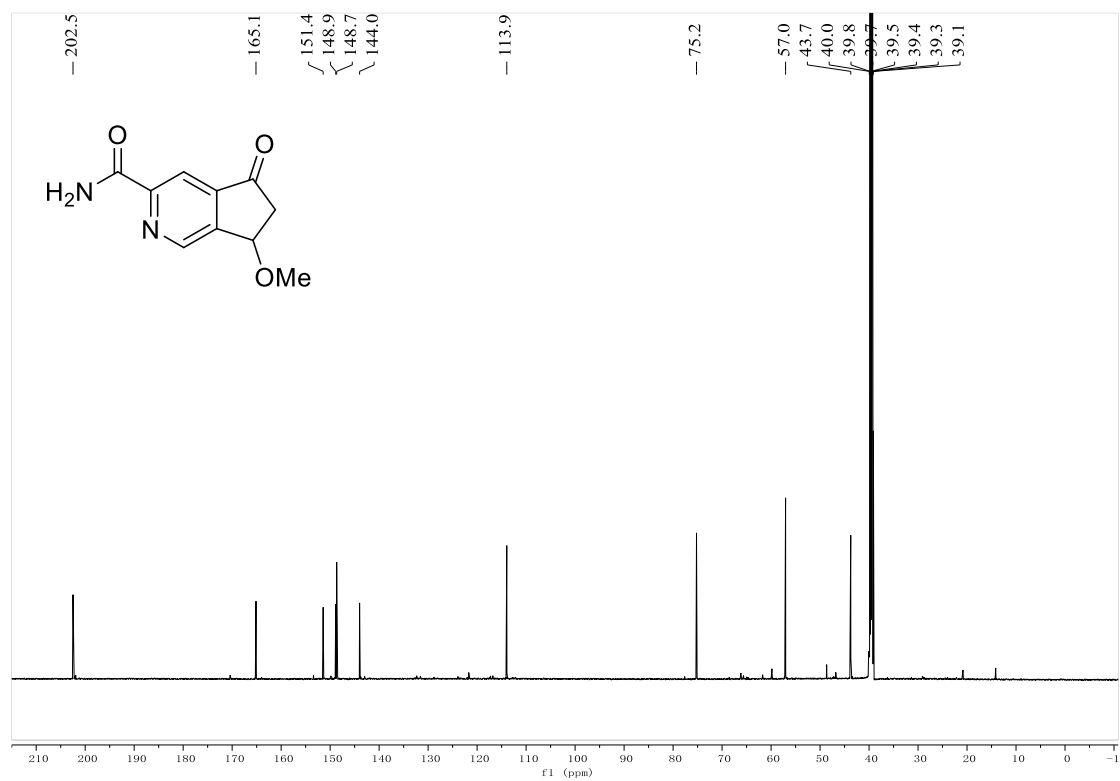


Figure S48 ^{13}C NMR Spectra of amycolasporin B (**2**) (150 MHz, $\text{DMSO-}d_6$)

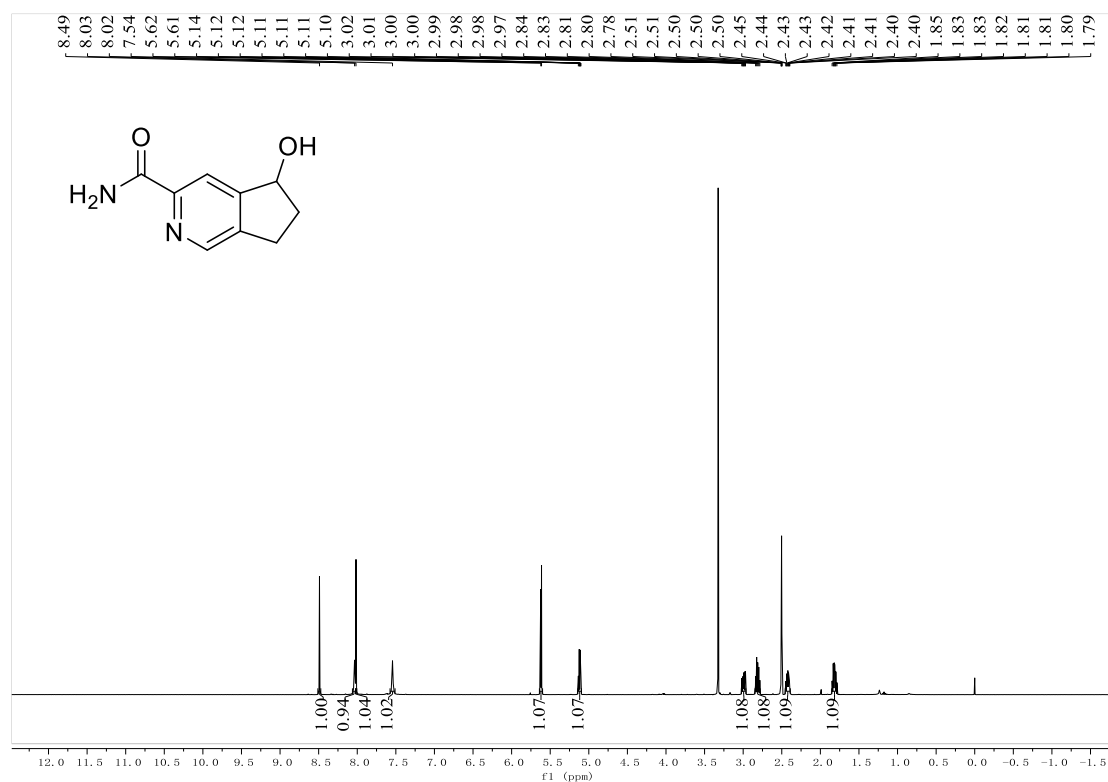


Figure S49 ¹H NMR Spectra of compound **30a** (600 MHz, DMSO-*d*₆)

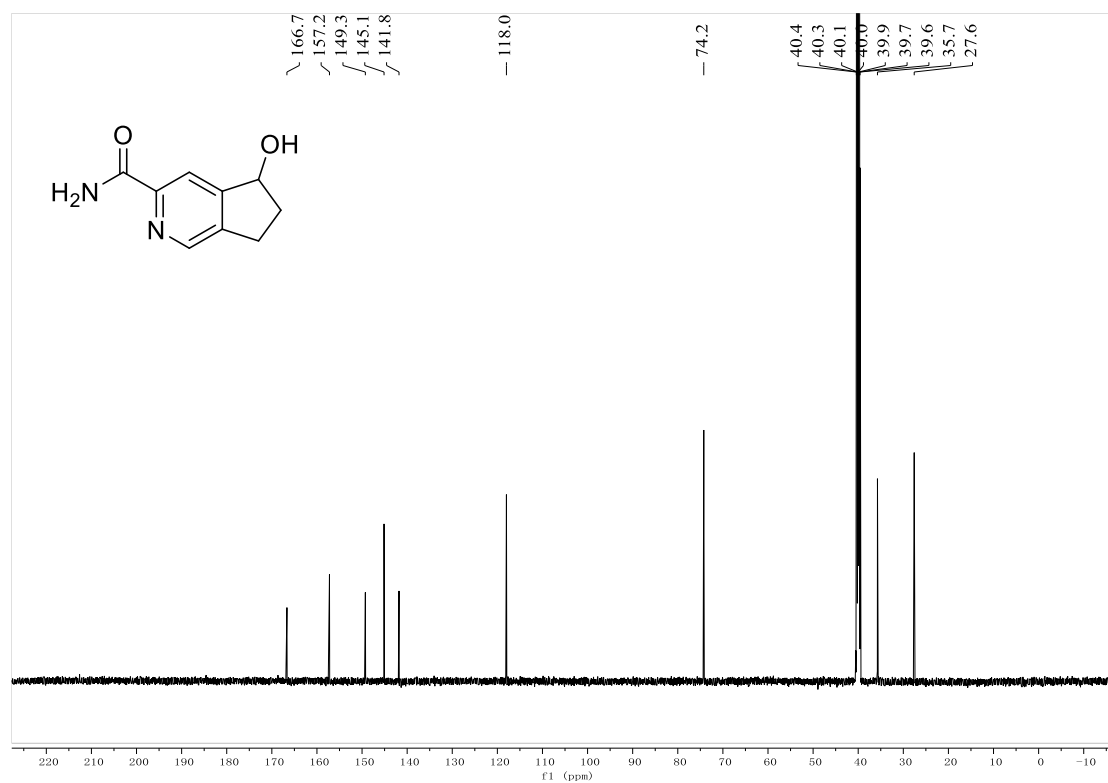


Figure S50 ¹³C NMR Spectra of compound **30a** (150 MHz, DMSO-*d*₆)

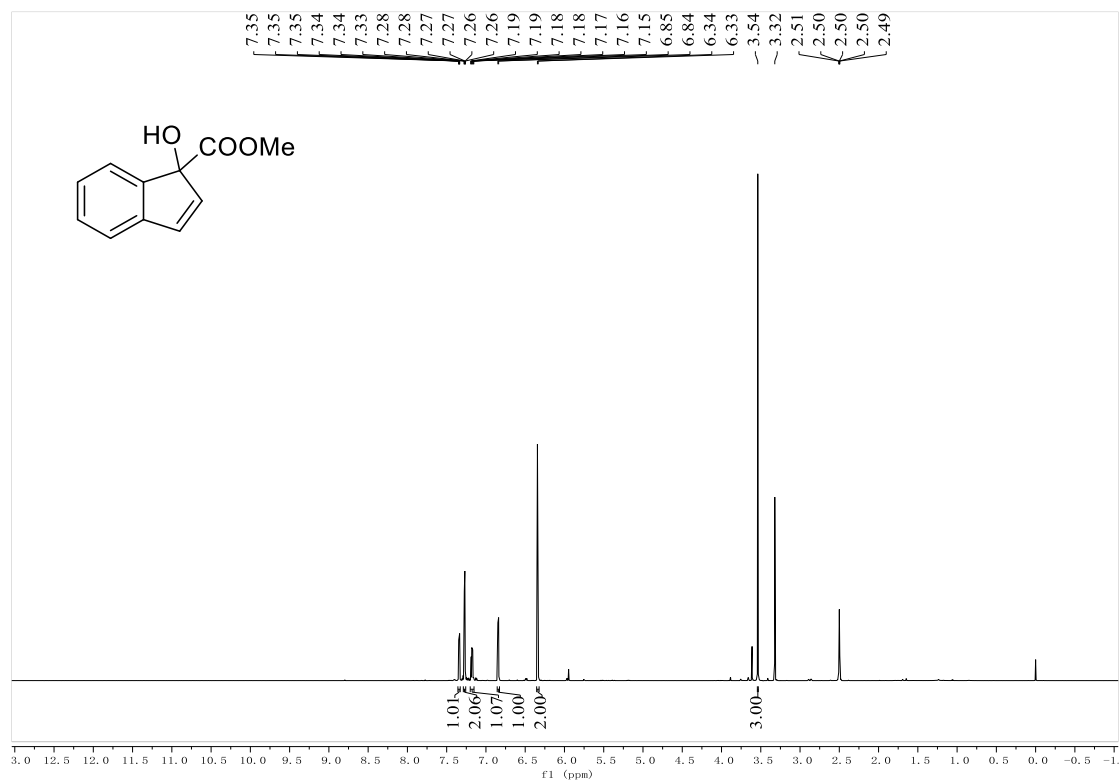


Figure S51 ¹H NMR Spectra of compound **30b** (600 MHz, DMSO-*d*₆)

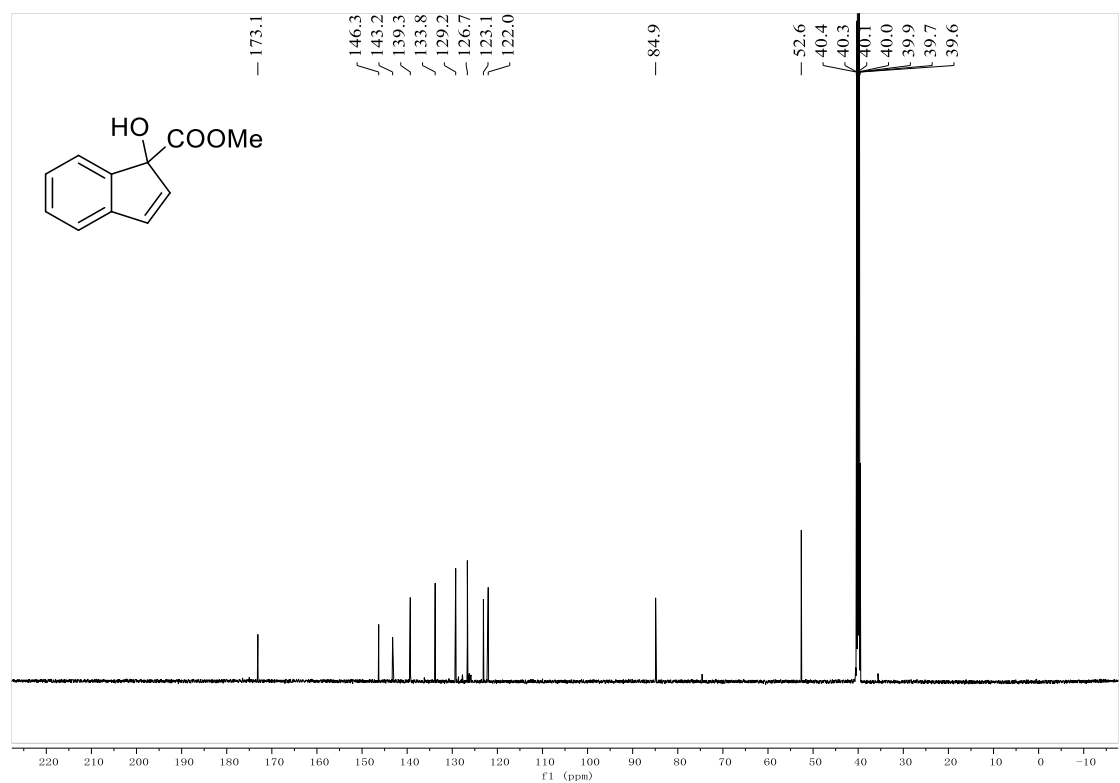


Figure S52 ¹³C NMR Spectra of compound **30b** (150 MHz, DMSO-*d*₆)

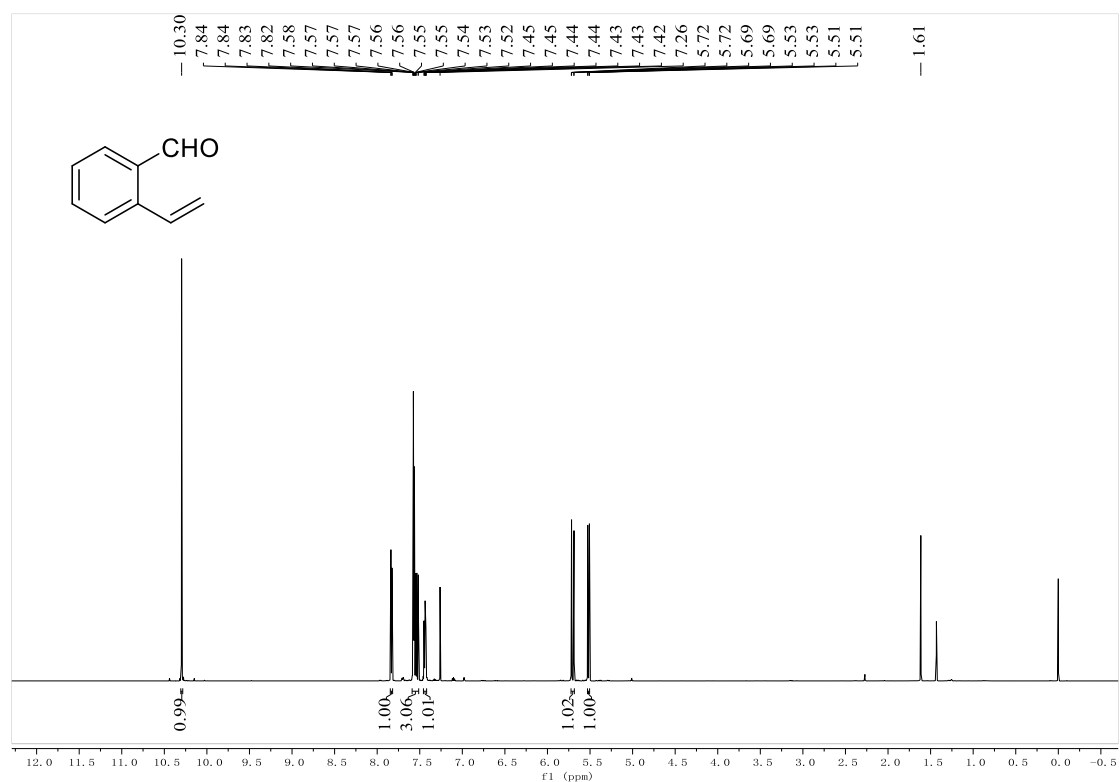


Figure S53 ^1H NMR Spectra of 2-ethenyl- α -hydroxy-benzeneacetonitrile (600 MHz, CDCl_3)

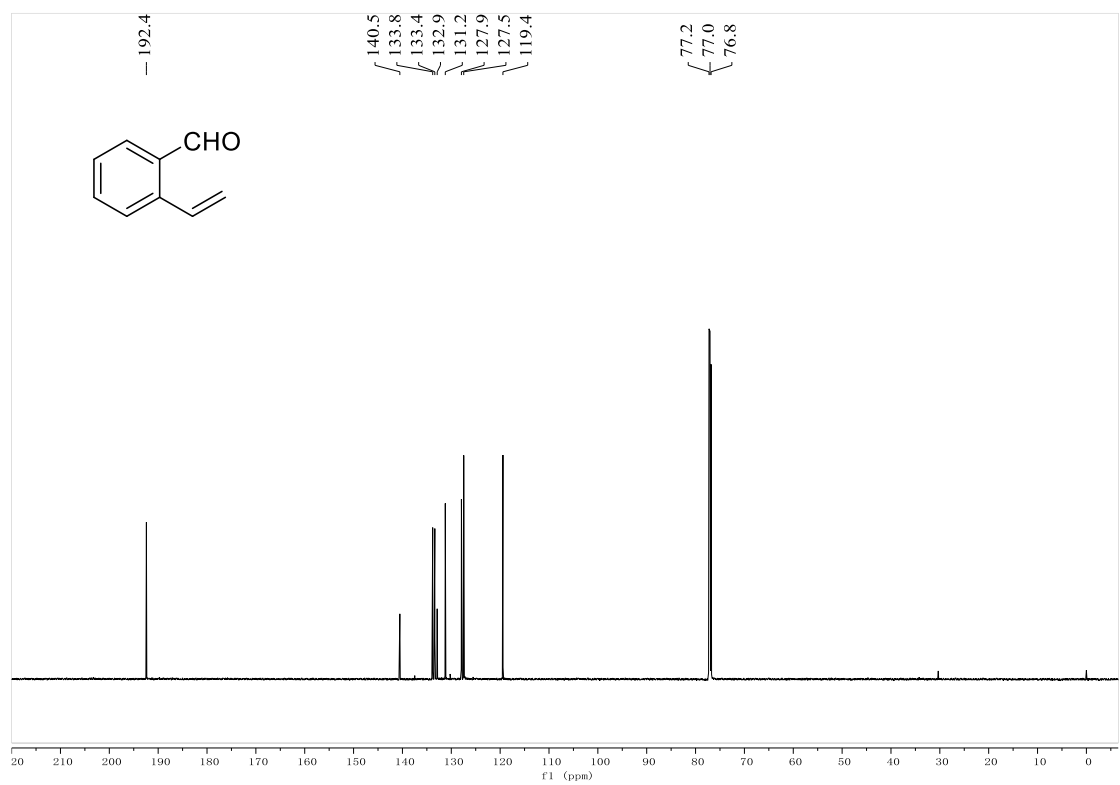


Figure S54 ^{13}C NMR Spectra of 2-ethenyl- α -hydroxy-benzeneacetonitrile (150 MHz, CDCl_3)

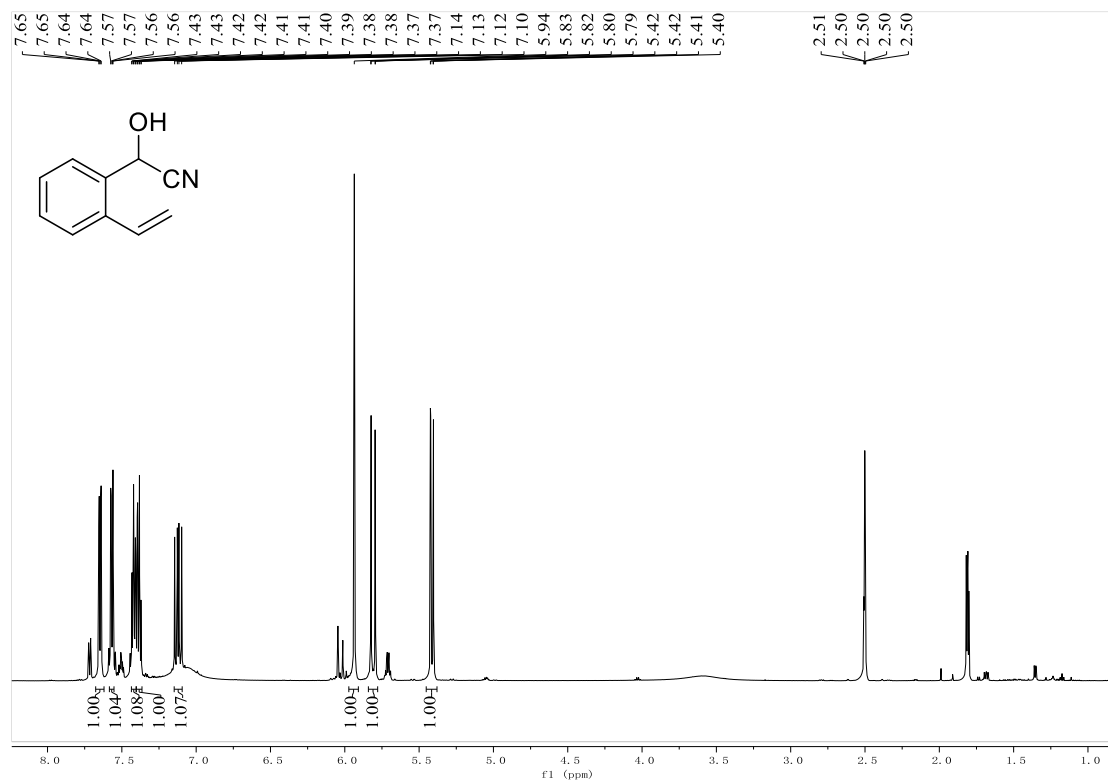


Figure S55 ^1H NMR Spectra of methyl 2-ethenyl- α -hydroxy-benzeneacetate (600 MHz, CDCl_3)

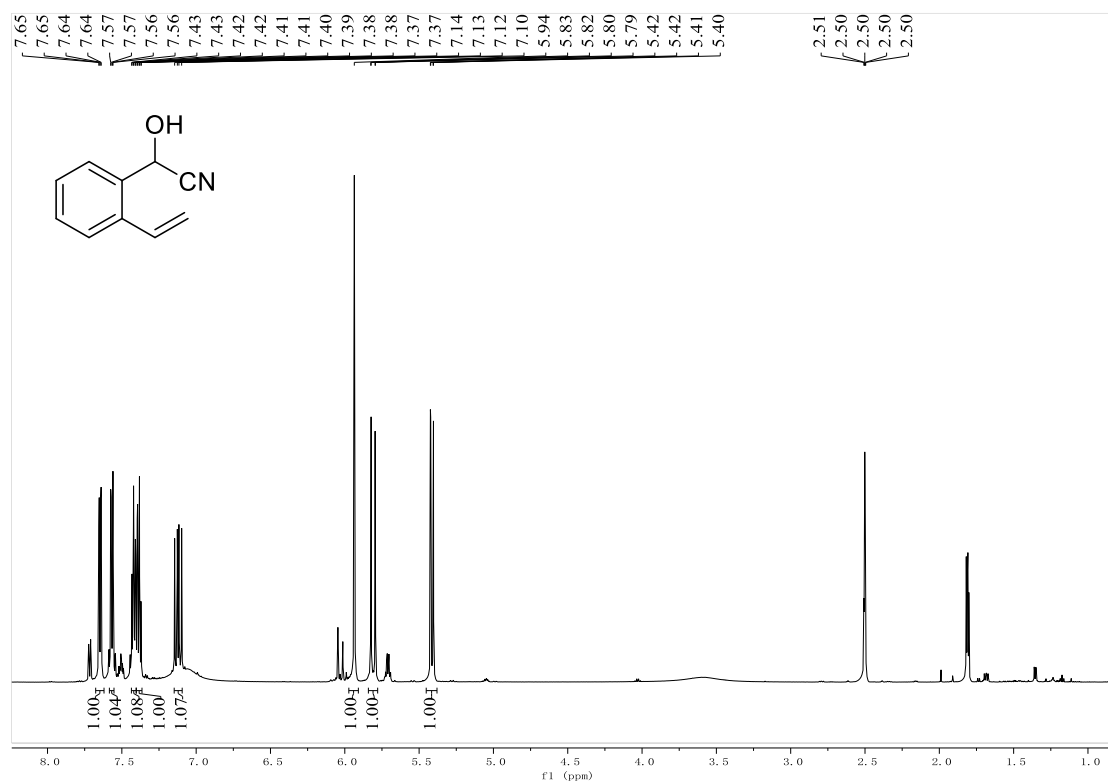


Figure S56 ^{13}C NMR Spectra of methyl 2-ethenyl- α -hydroxy-benzeneacetate (150 MHz, $\text{DMSO}-d_6$)

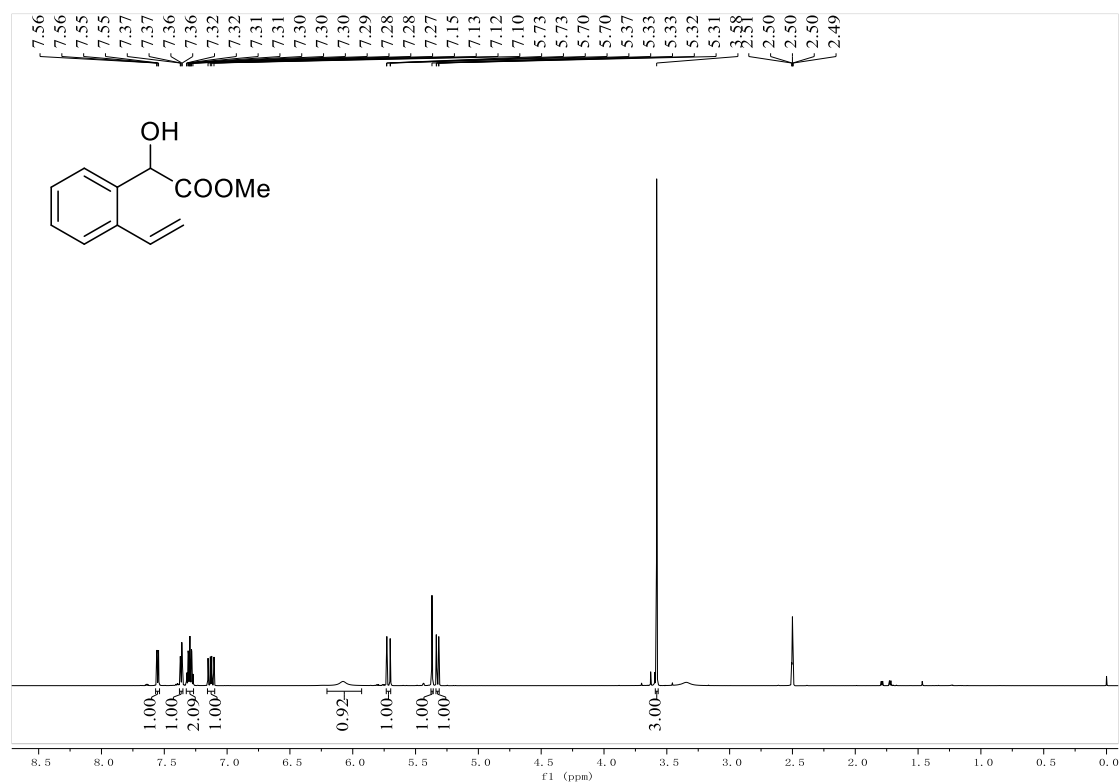


Figure S57 ^1H NMR Spectra of 2-ethenyl- α -oxo-benzeneacetate
(600 MHz, $\text{DMSO-}d_6$)

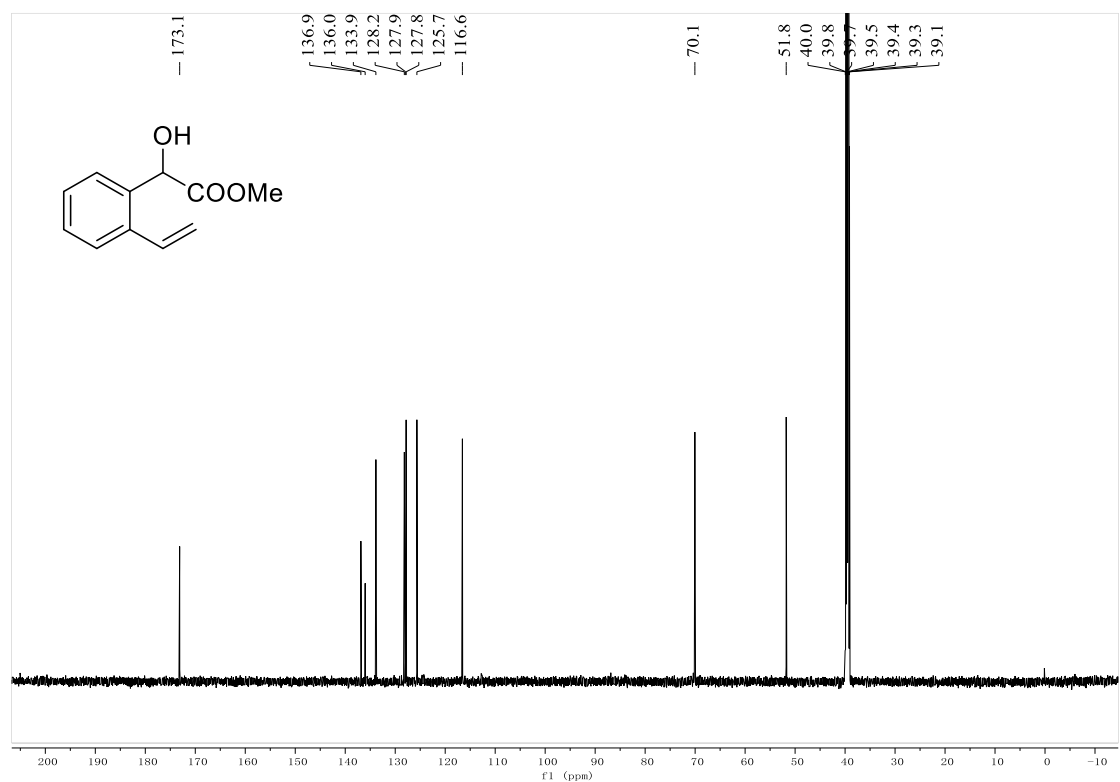


Figure S58 ^{13}C NMR Spectra of 2-ethenyl- α -oxo-benzeneacetate
(150 MHz, $\text{DMSO-}d_6$)

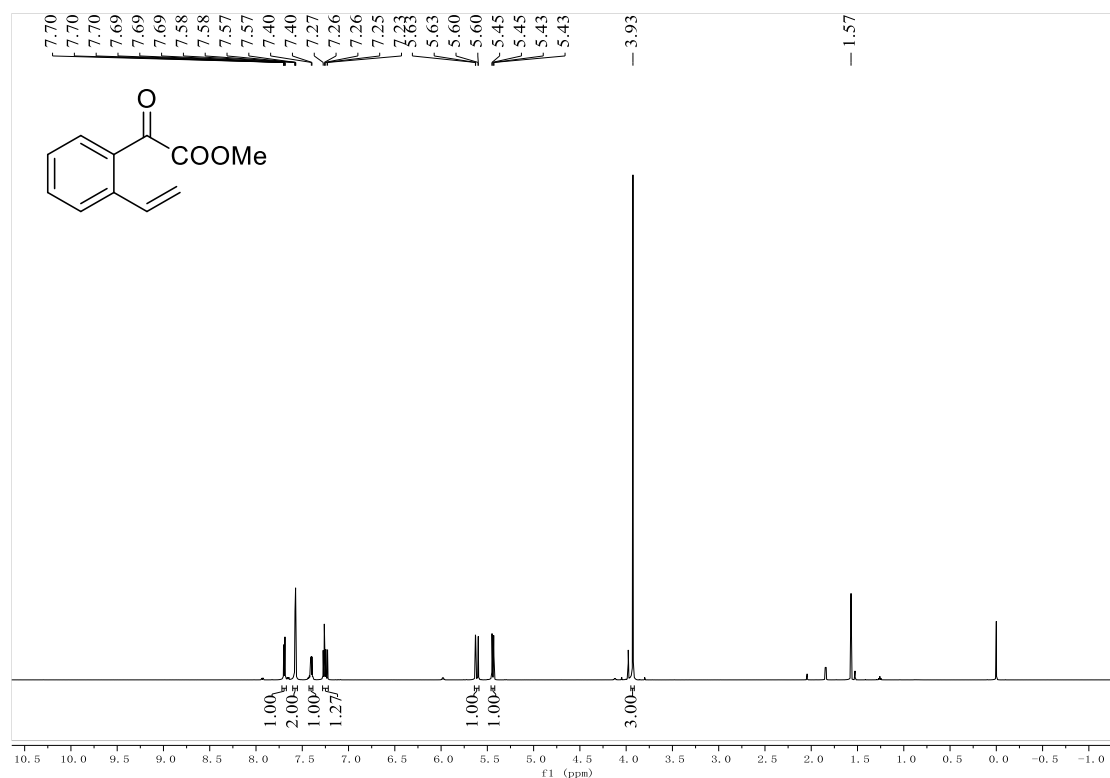


Figure S59 ¹H NMR Spectra of 2-ethenyl- α -oxo-benzeneacetate (600 MHz, CDCl₃)

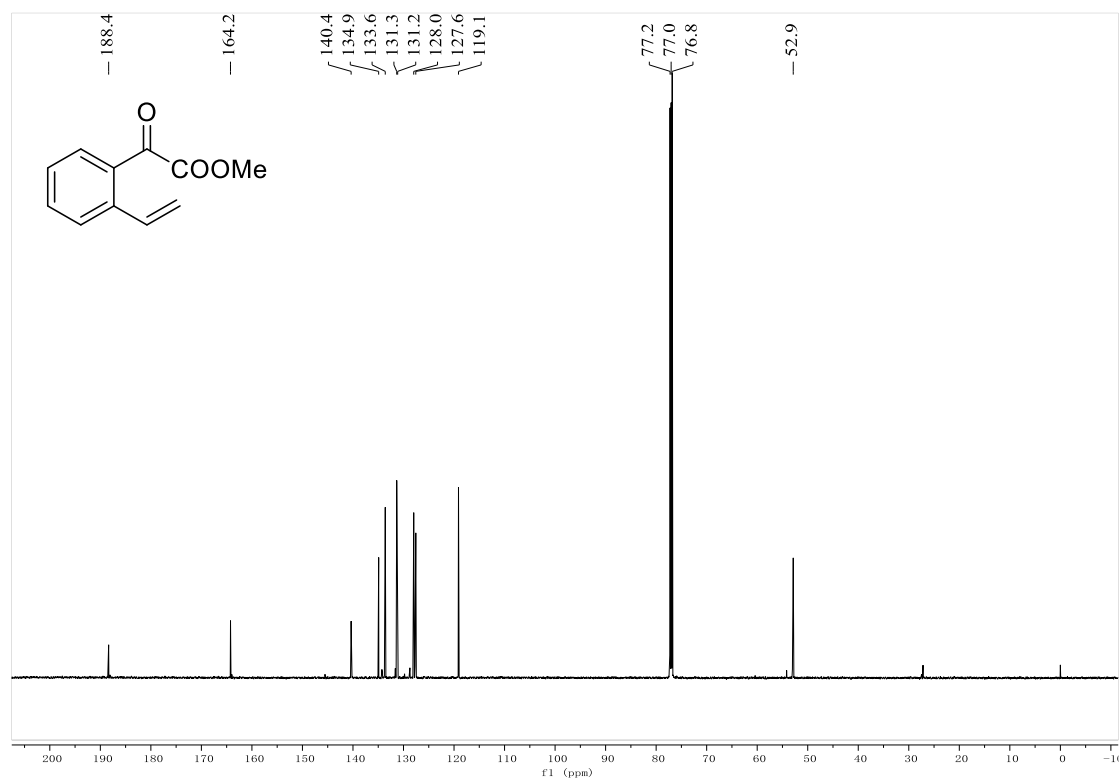


Figure S60 ¹³C NMR Spectra of 2-ethenyl- α -oxo-benzeneacetate (150 MHz, CDCl₃)

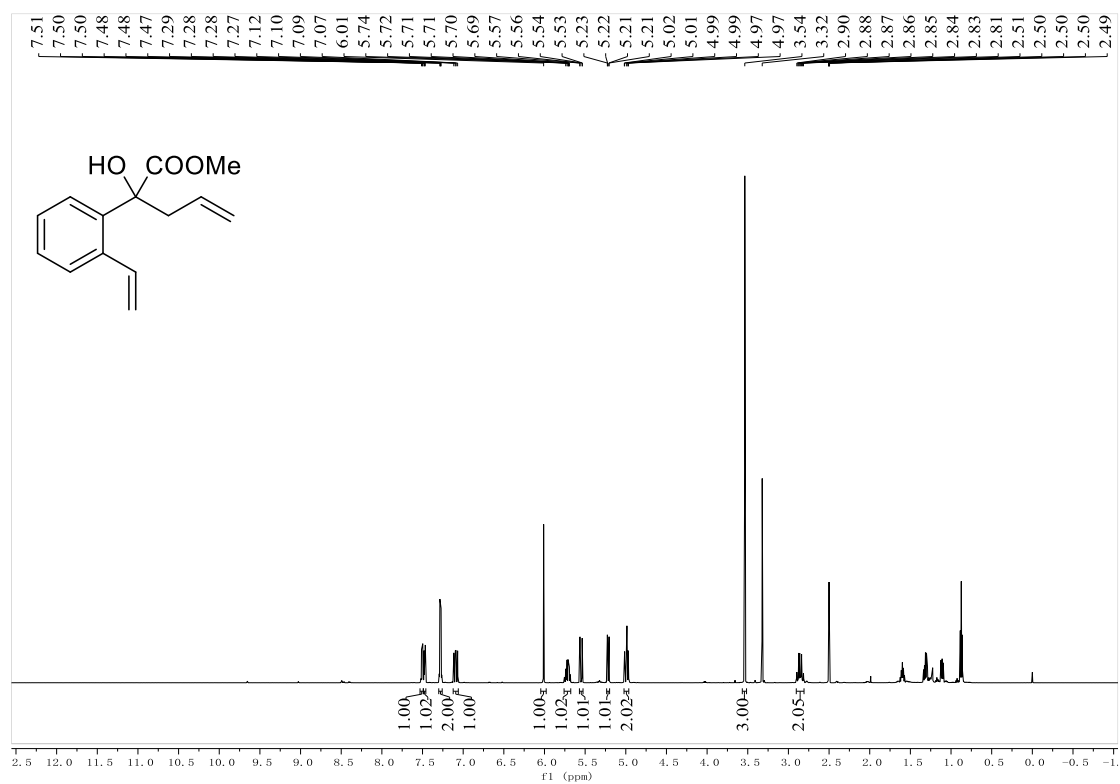


Figure S61 ¹H NMR Spectra of compound **33a** (600 MHz, DMSO-*d*₆)

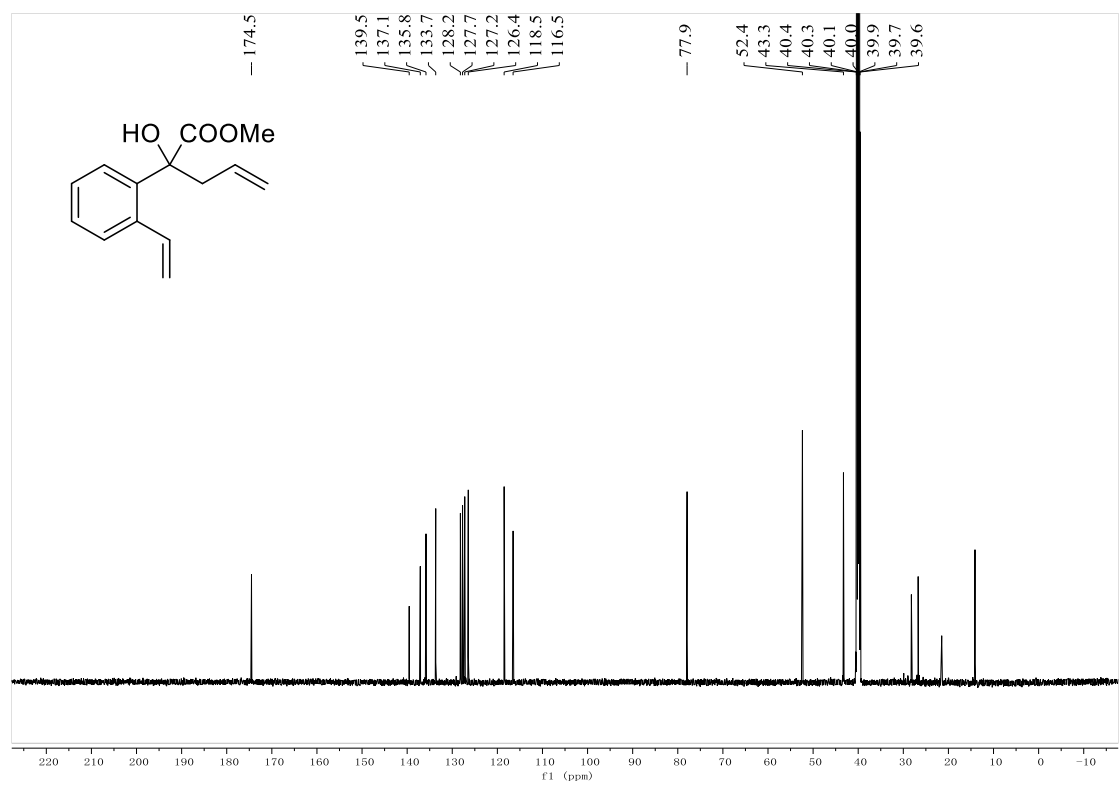


Figure S62 ¹³C NMR Spectra of compound **33a** (150 MHz, DMSO-*d*₆)

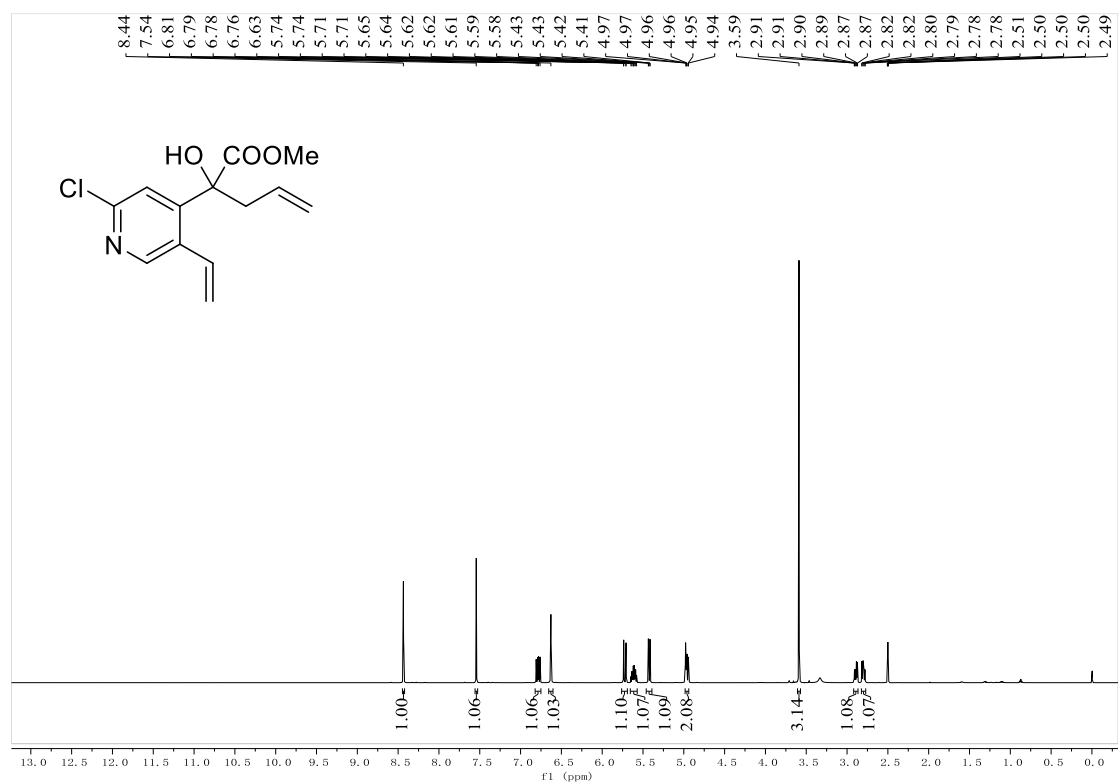


Figure S63 ^1H NMR Spectra of compound **33b** (600 MHz, $\text{DMSO-}d_6$)

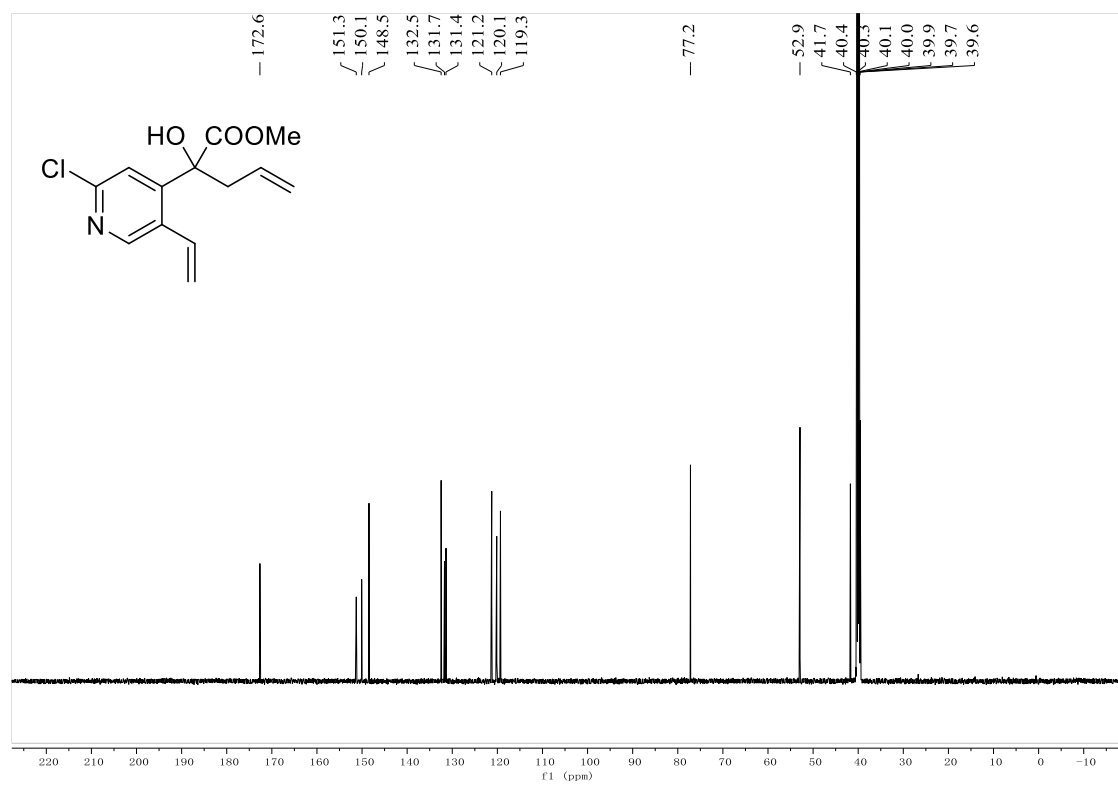


Figure S64 ^{13}C NMR Spectra of compound **33b** (150 MHz, $\text{DMSO-}d_6$)

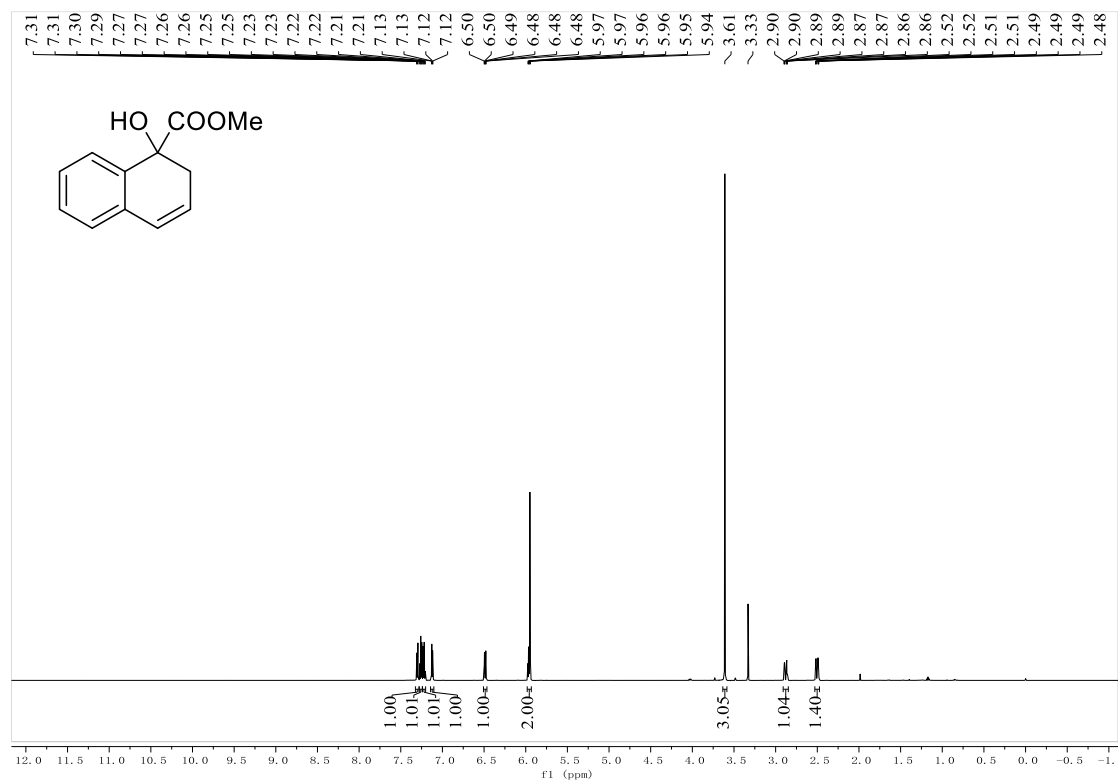


Figure S65 ¹H NMR Spectra of compound **30c** (600 MHz, DMSO-*d*₆)

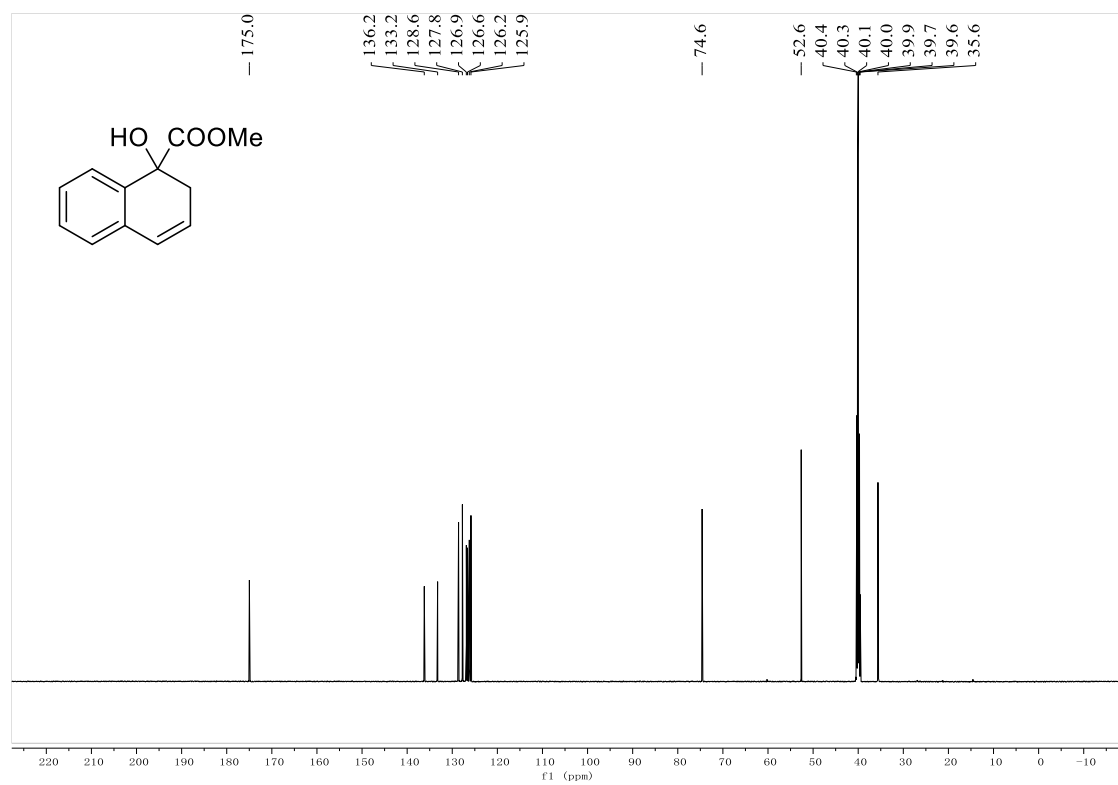


Figure S66 ¹³C NMR Spectra of compound **30c** (150 MHz, DMSO-*d*₆)

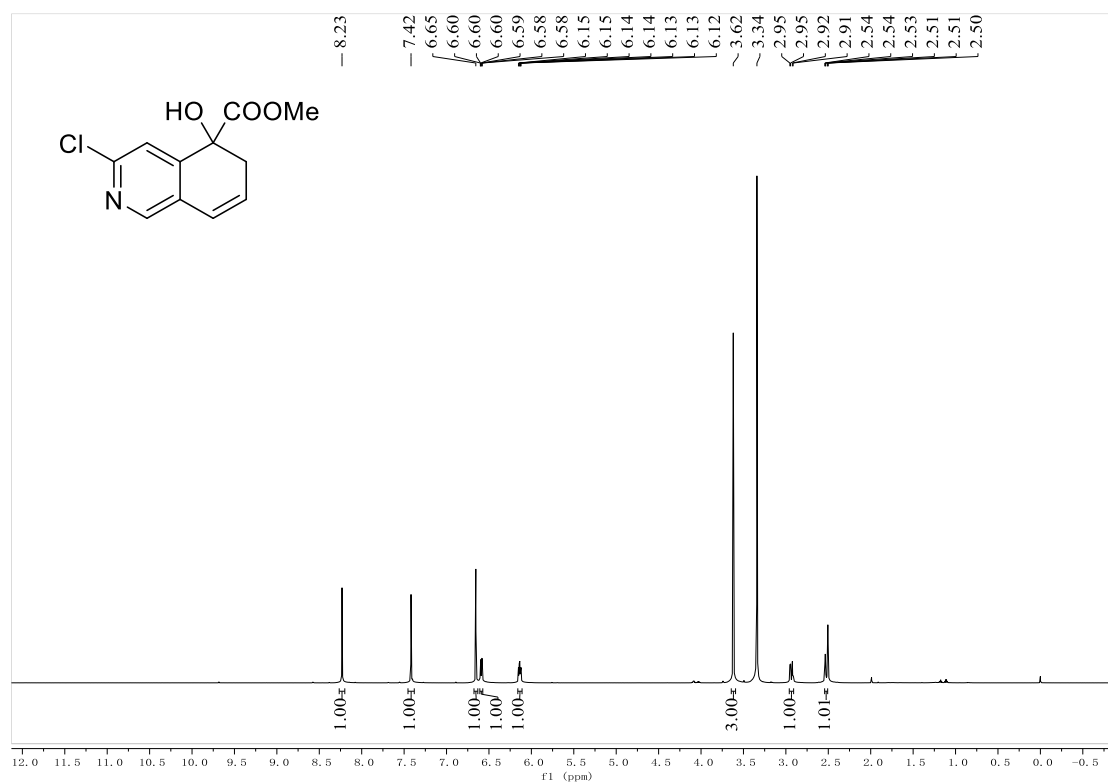


Figure S67 ¹H NMR Spectra of compound **30d** (600 MHz, DMSO-*d*₆)

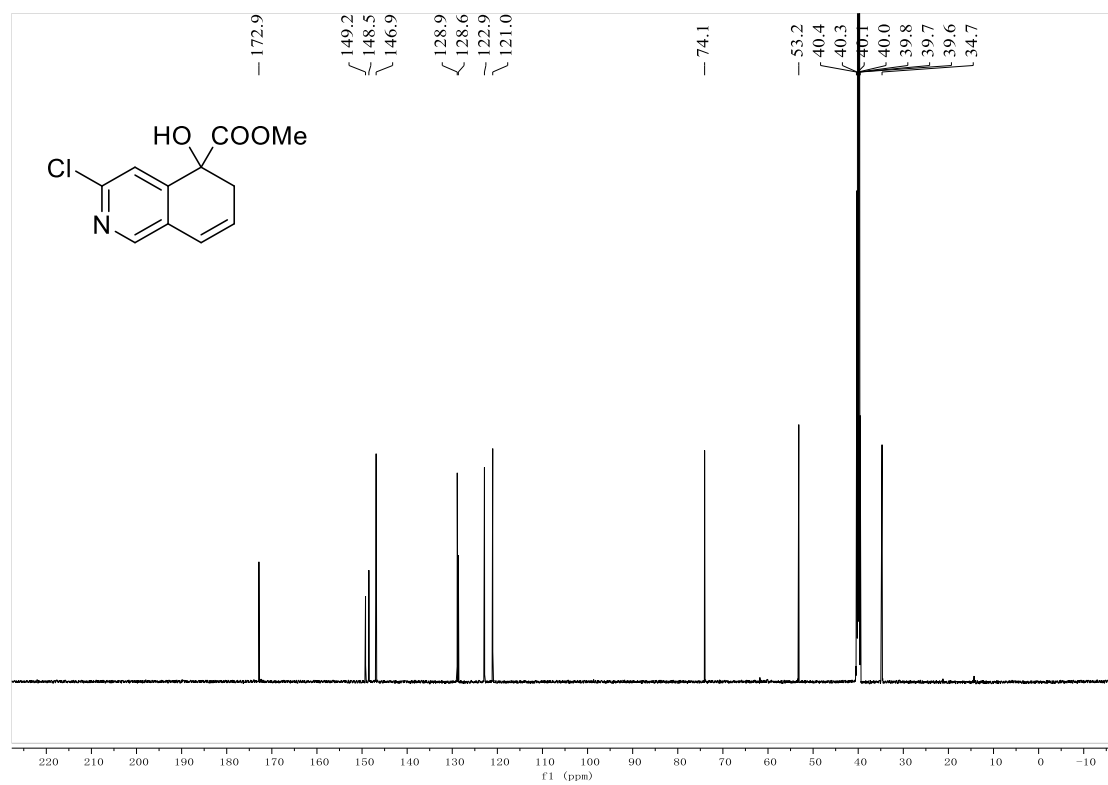


Figure S68 ¹³C NMR Spectra of compound **30d** (150 MHz, DMSO-*d*₆)

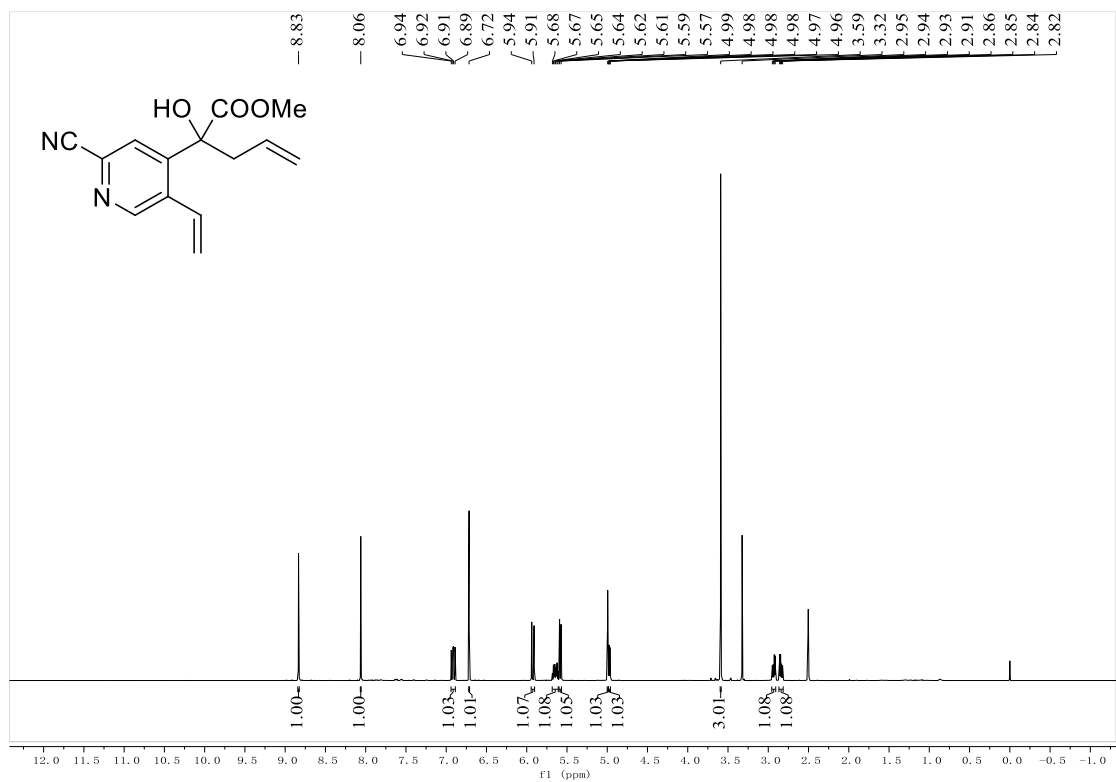


Figure S69 ¹H NMR Spectra of compound **34** (600 MHz, DMSO-*d*₆)

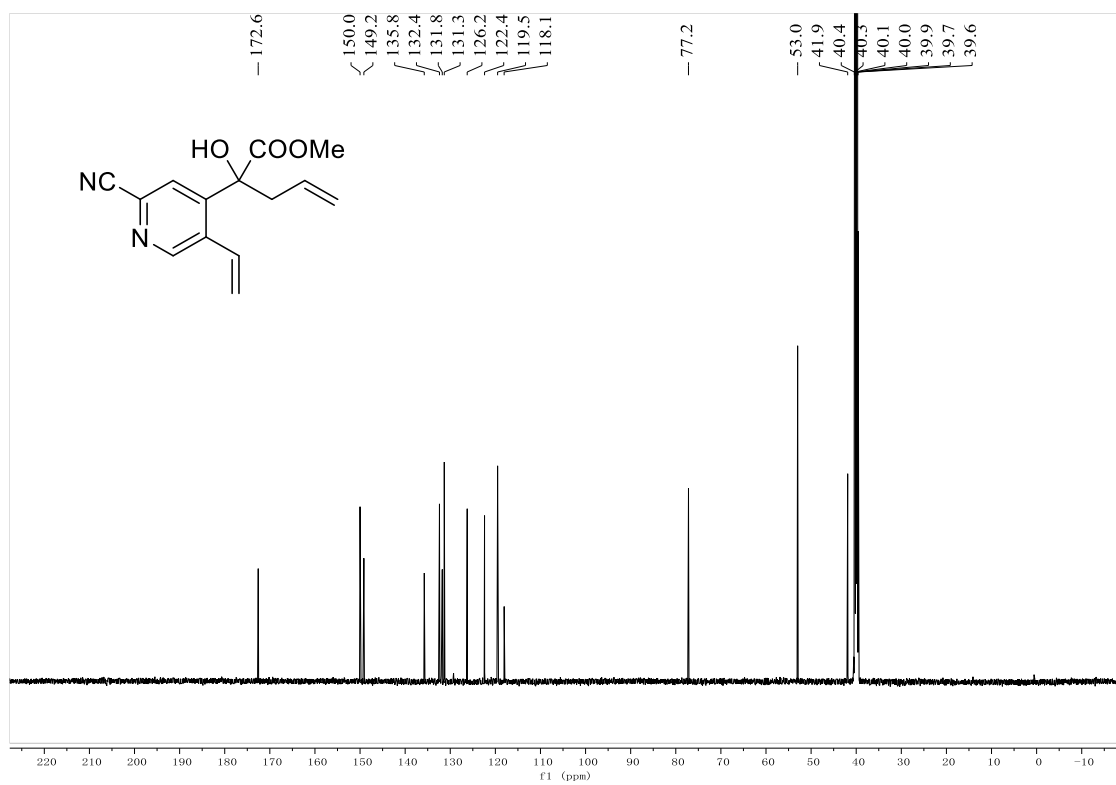


Figure S70 ¹³C NMR Spectra of compound **34** (150 MHz, DMSO-*d*₆)

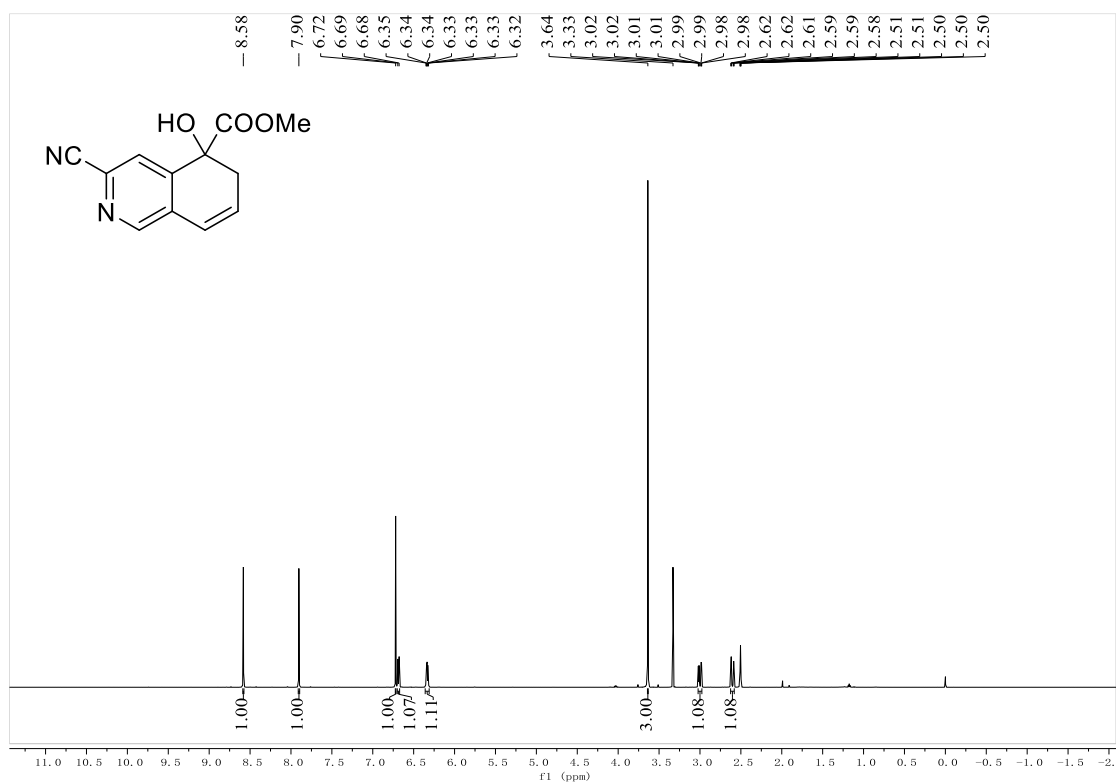


Figure S71 ^1H NMR Spectra of compound **30e** (600 MHz, $\text{DMSO-}d_6$)

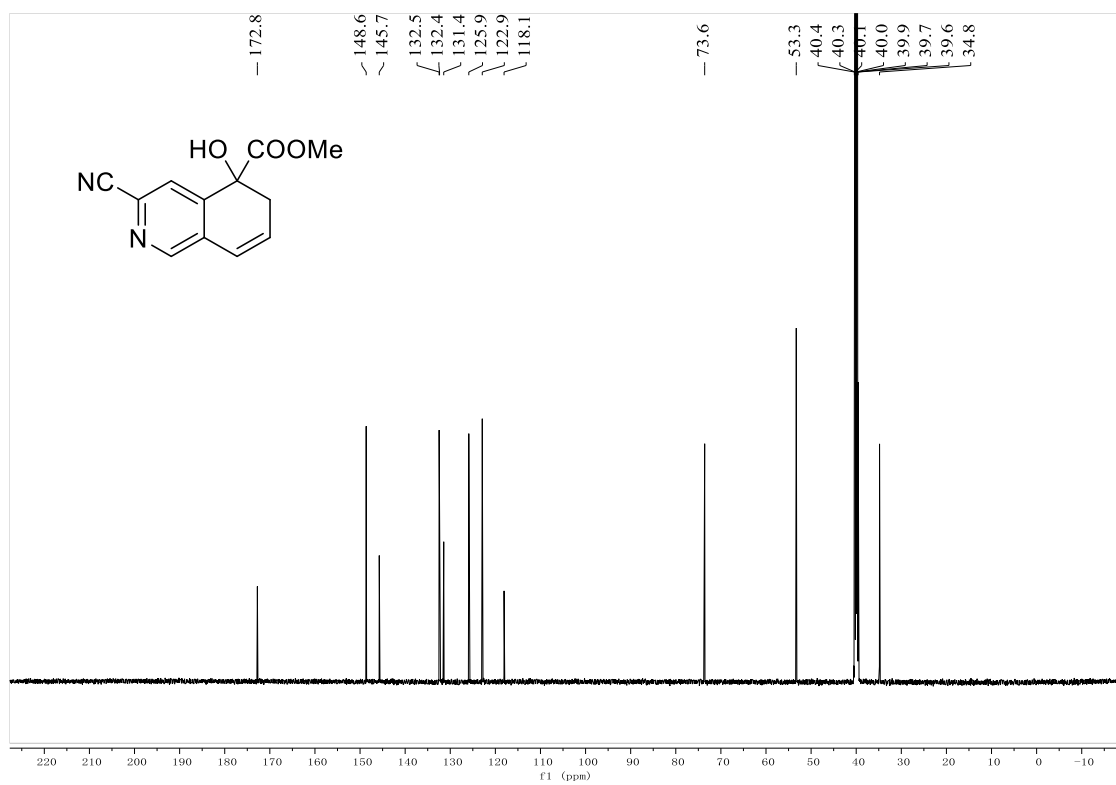


Figure S72 ^{13}C NMR Spectra of compound **30e** (150 MHz, $\text{DMSO-}d_6$)

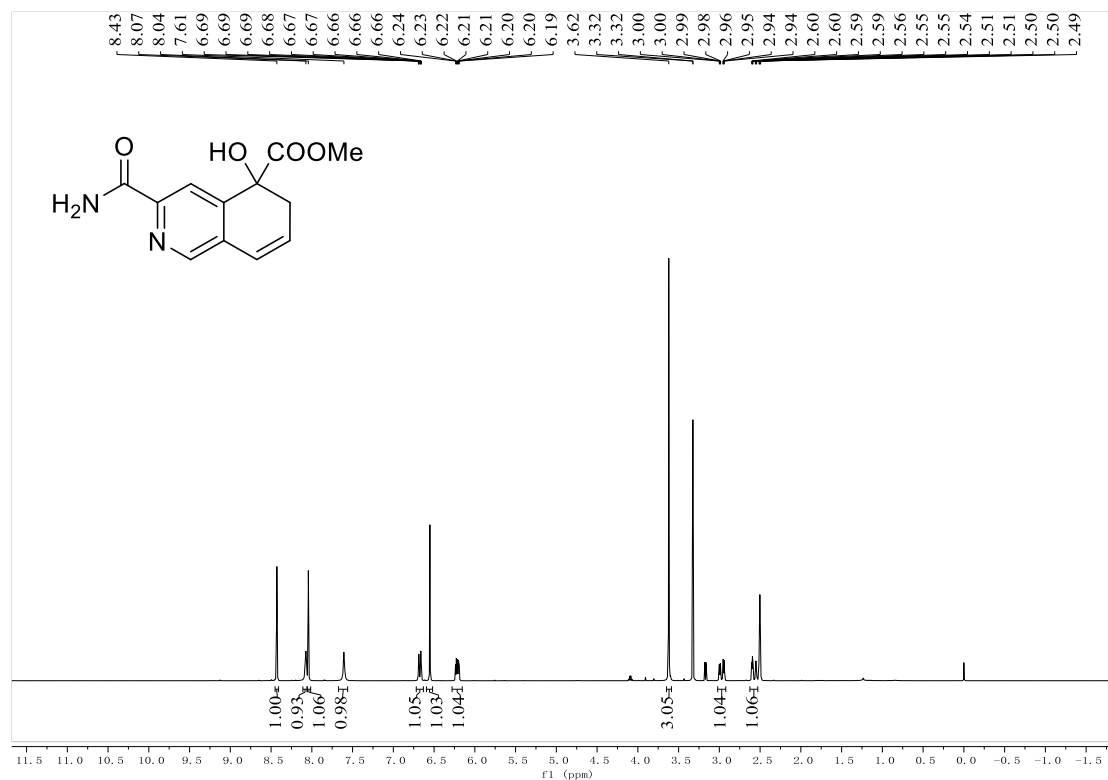


Figure S73 ¹H NMR Spectra of compound **30f** (600 MHz, DMSO-*d*₆)

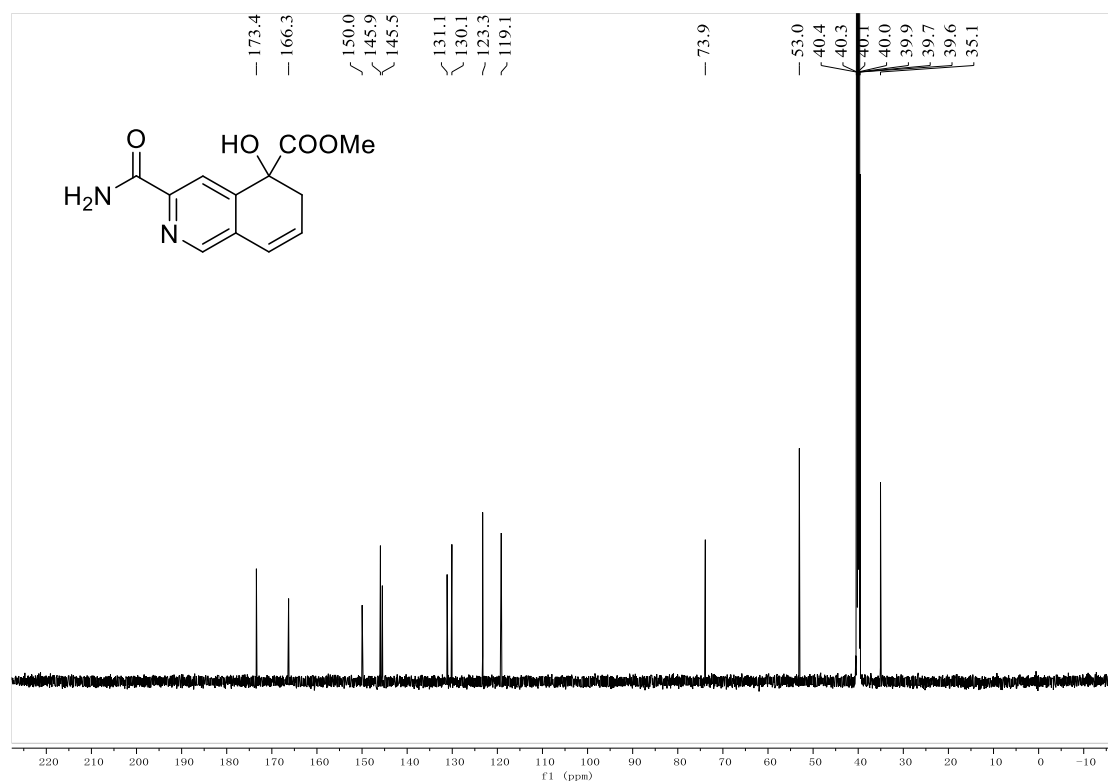


Figure S74 ¹³C NMR Spectra of compound **30f** (150 MHz, DMSO-*d*₆)