

# Structural Optimization of Isoquinoline Derivatives from Lycobetaine and Their Inhibitory Activity against Neuroendocrine Prostate Cancer Cells

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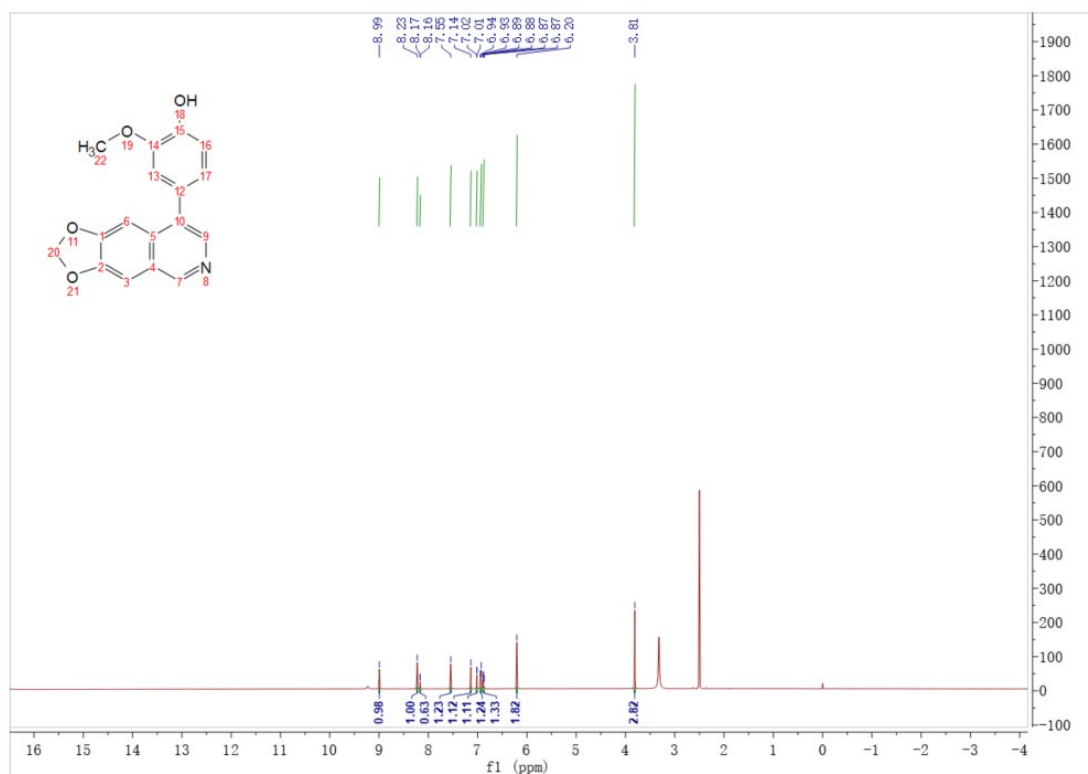
## **Supporting Information**

### **Content**

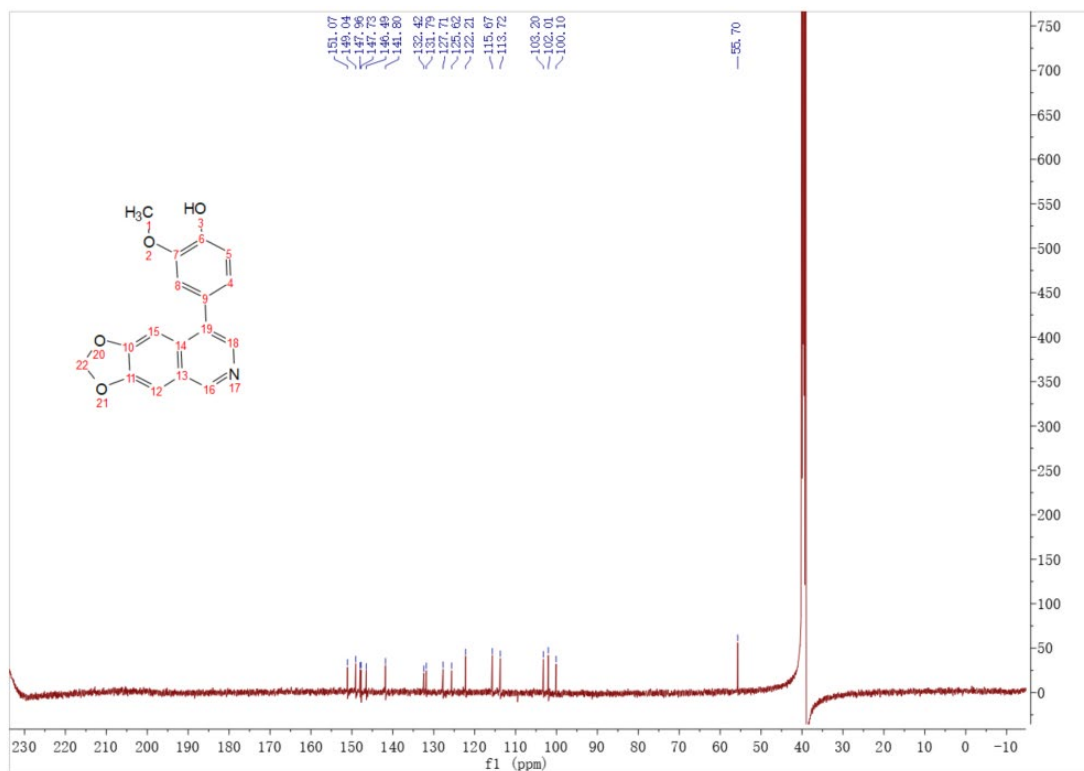
1. NMR Spectrums of representative compounds.....S3–S13
2. HPLC Spectrums of representative compounds..... ·S14–S15

## 1. NMR Spectrums

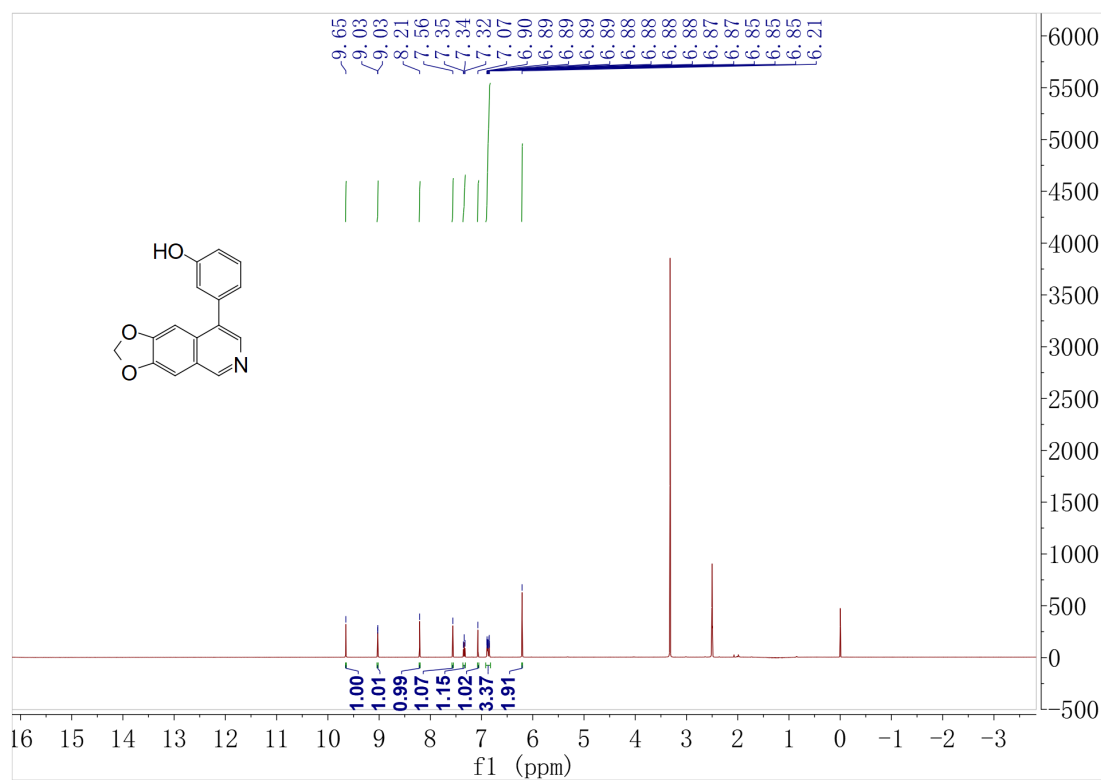
### $^1\text{H}$ NMR Spectrum of compound 1



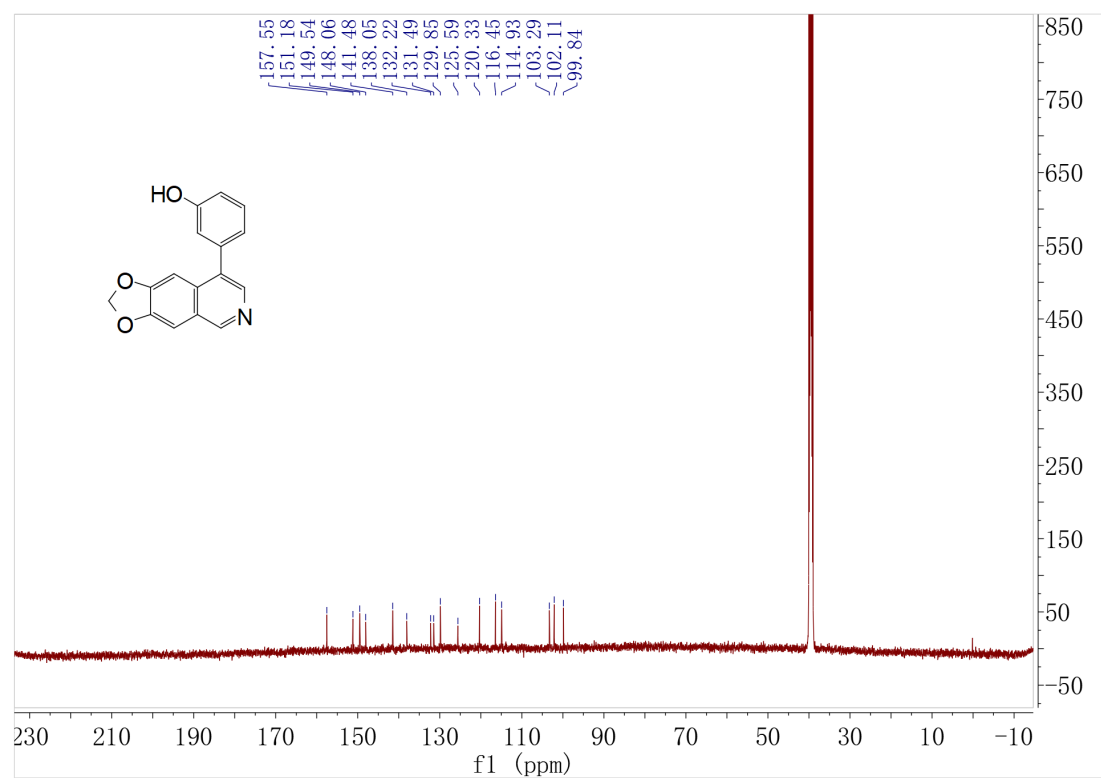
### $^{13}\text{C}$ NMR Spectrum of compound 1



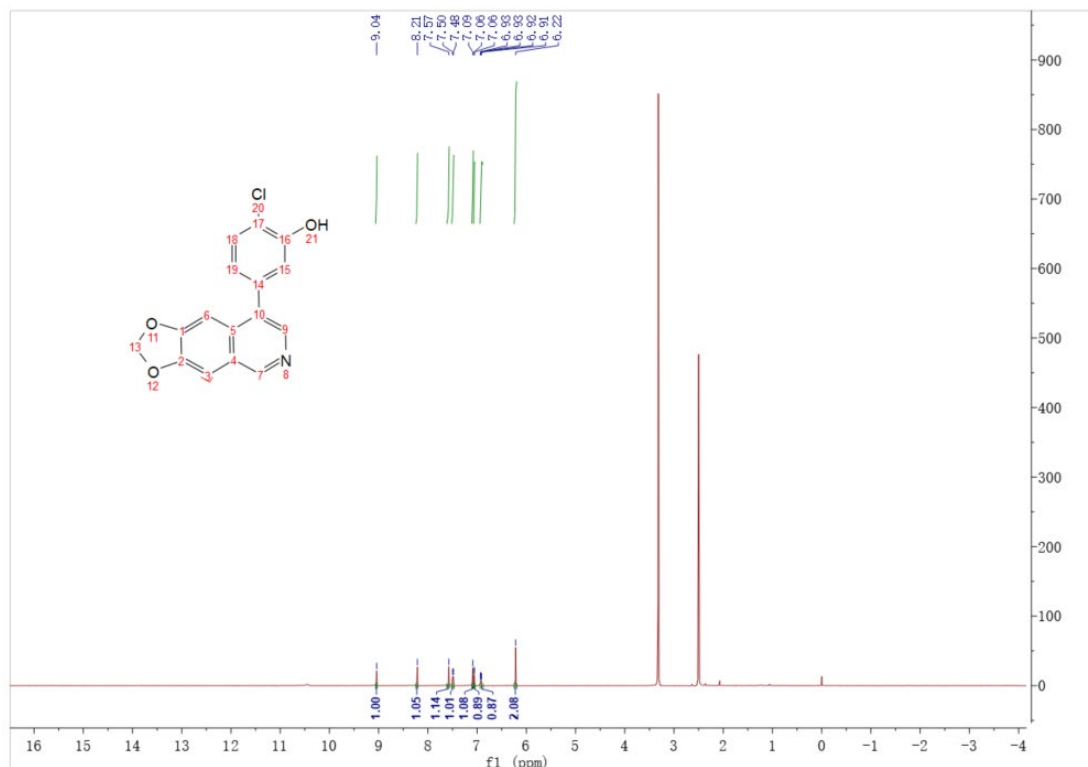
# <sup>1</sup>H NMR Spectrum of compound **19**



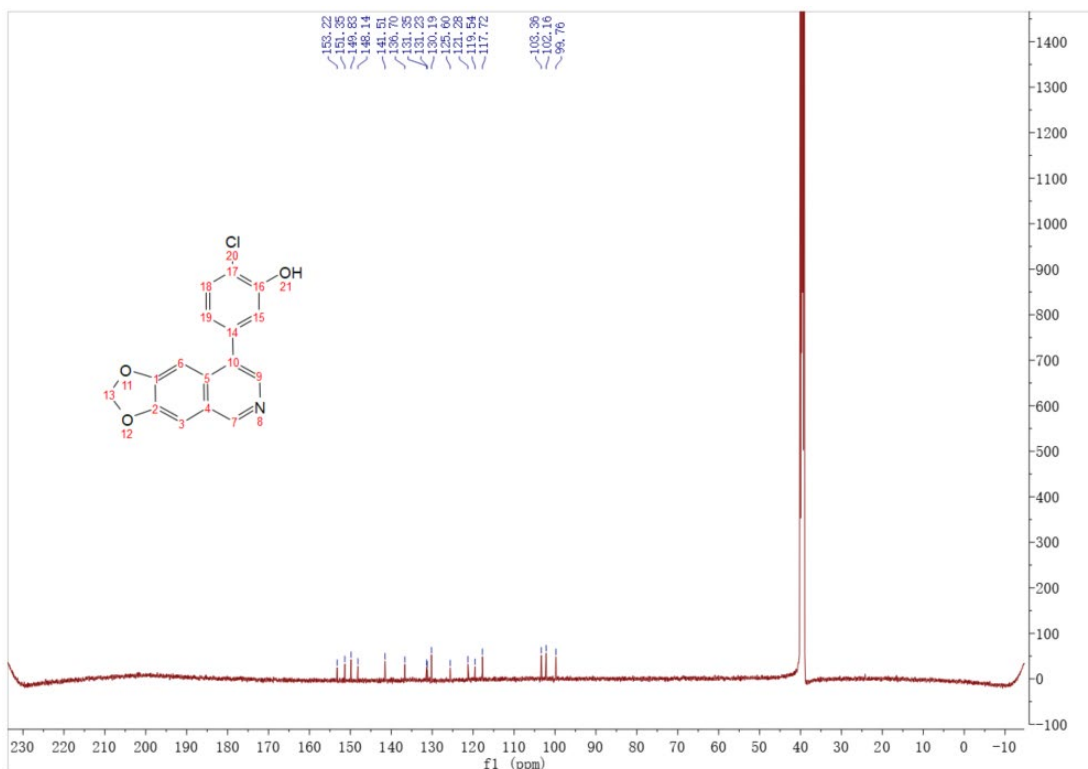
# <sup>13</sup>C NMR Spectrum of compound **19**



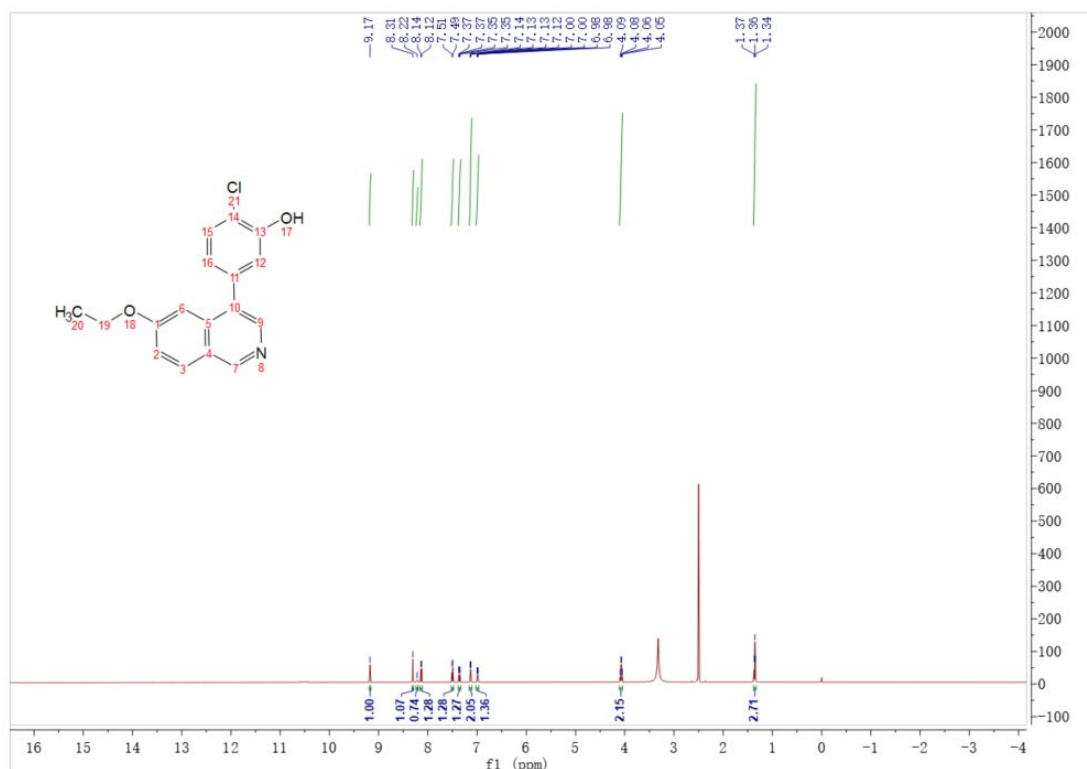
# <sup>1</sup>H NMR Spectrum of compound 20



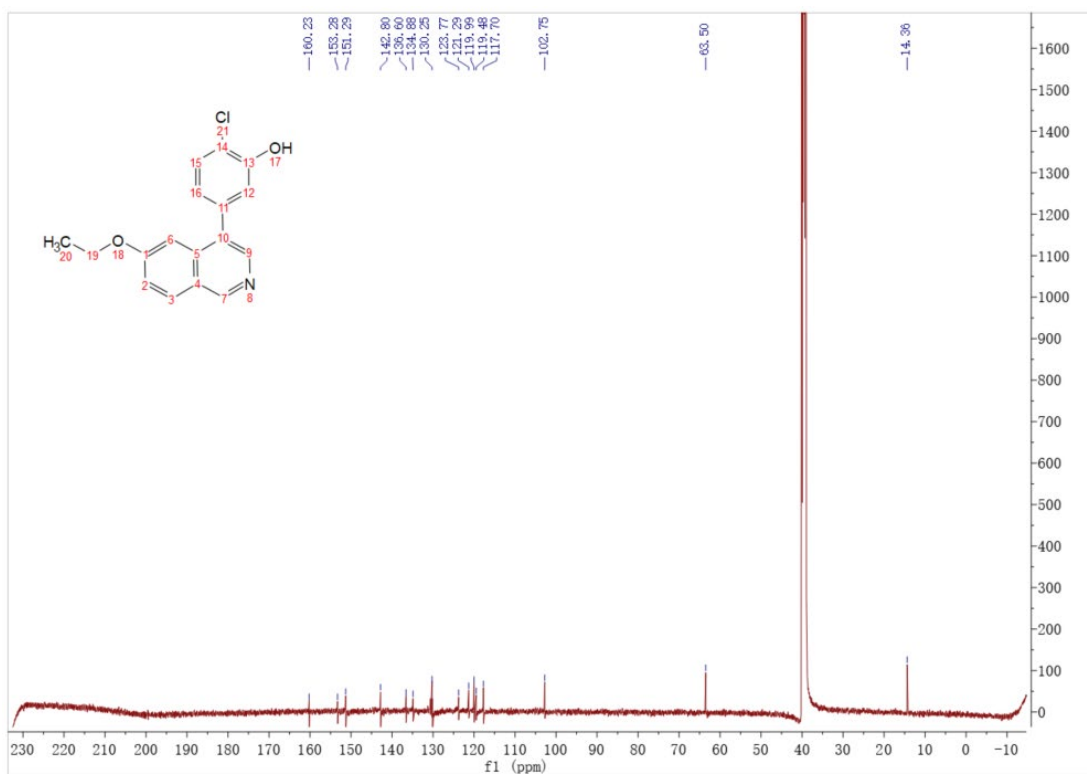
# <sup>13</sup>C NMR Spectrum of compound 20



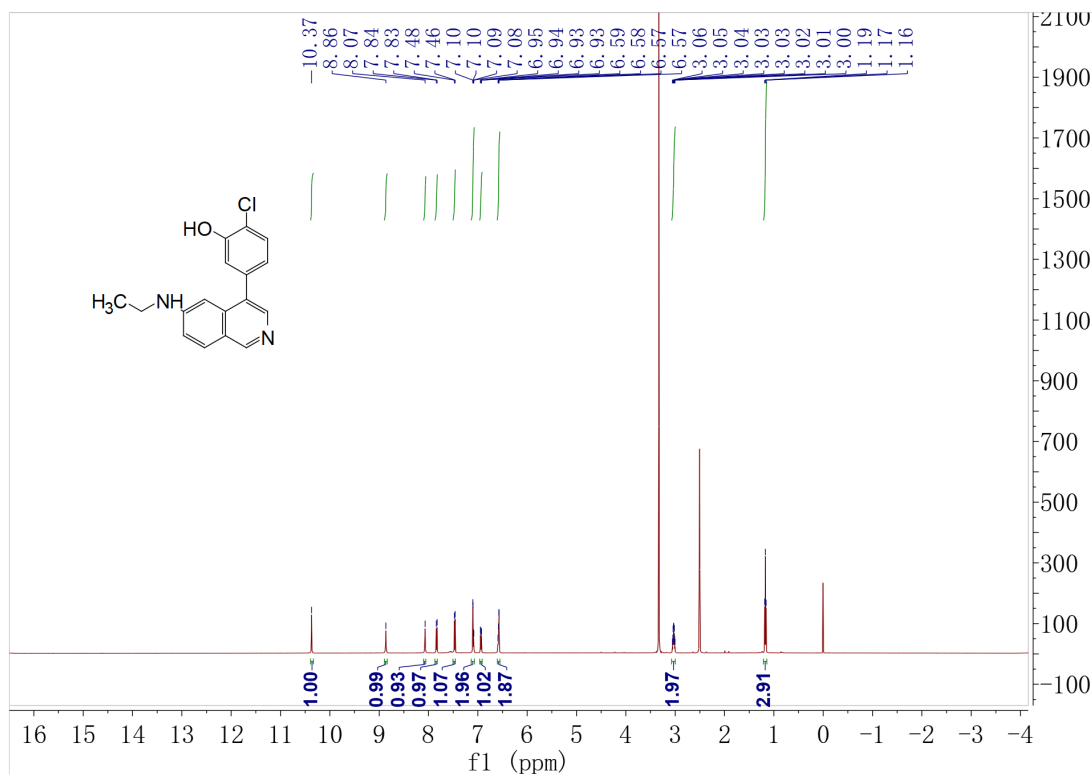
### <sup>1</sup>H NMR Spectrum of compound 23



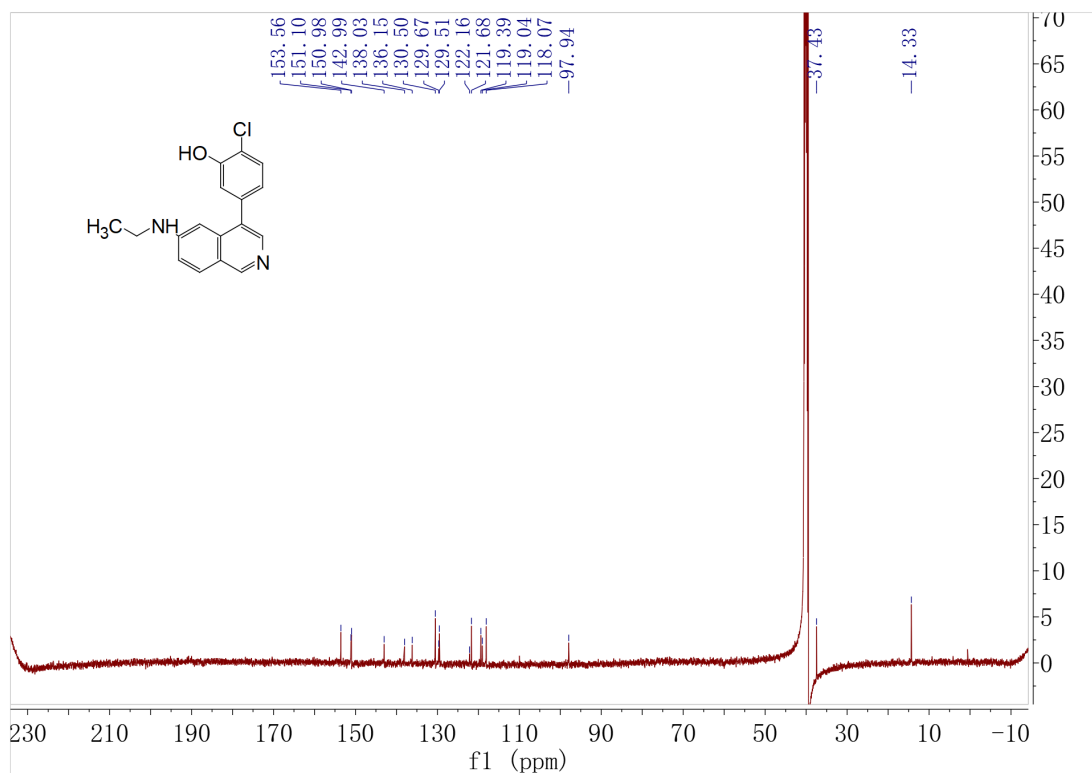
<sup>13</sup>C NMR Spectrum of compound **23**



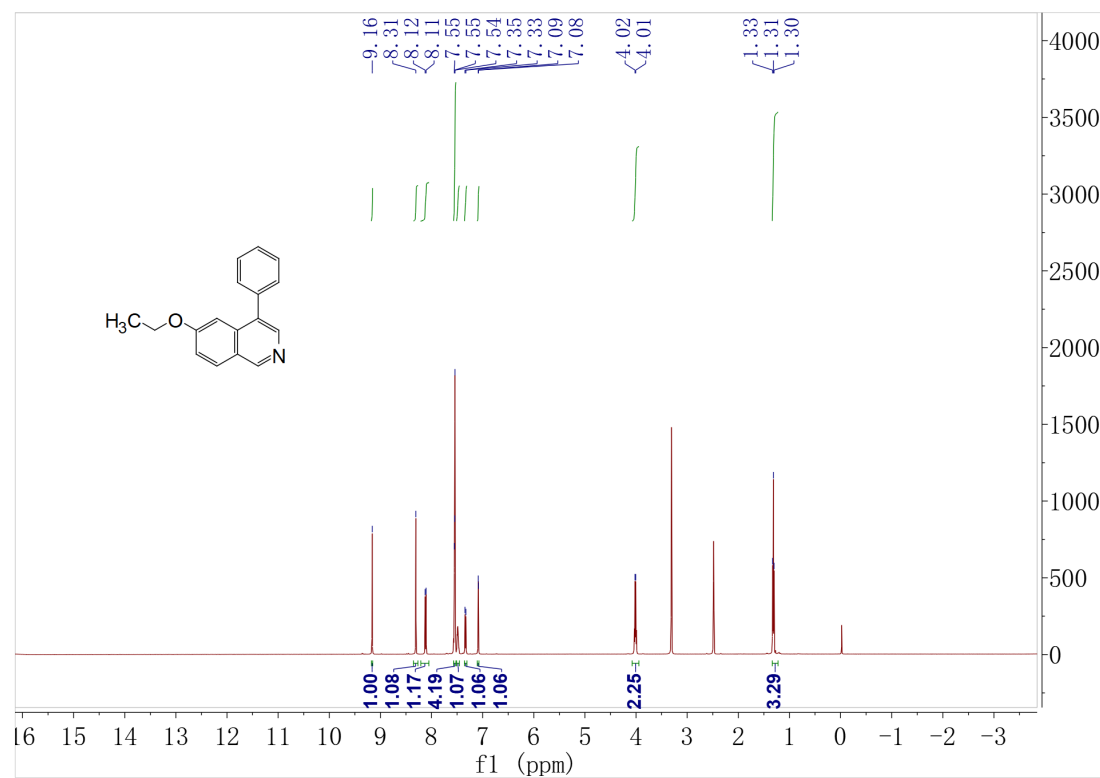
# <sup>1</sup>H NMR Spectrum of compound **34**



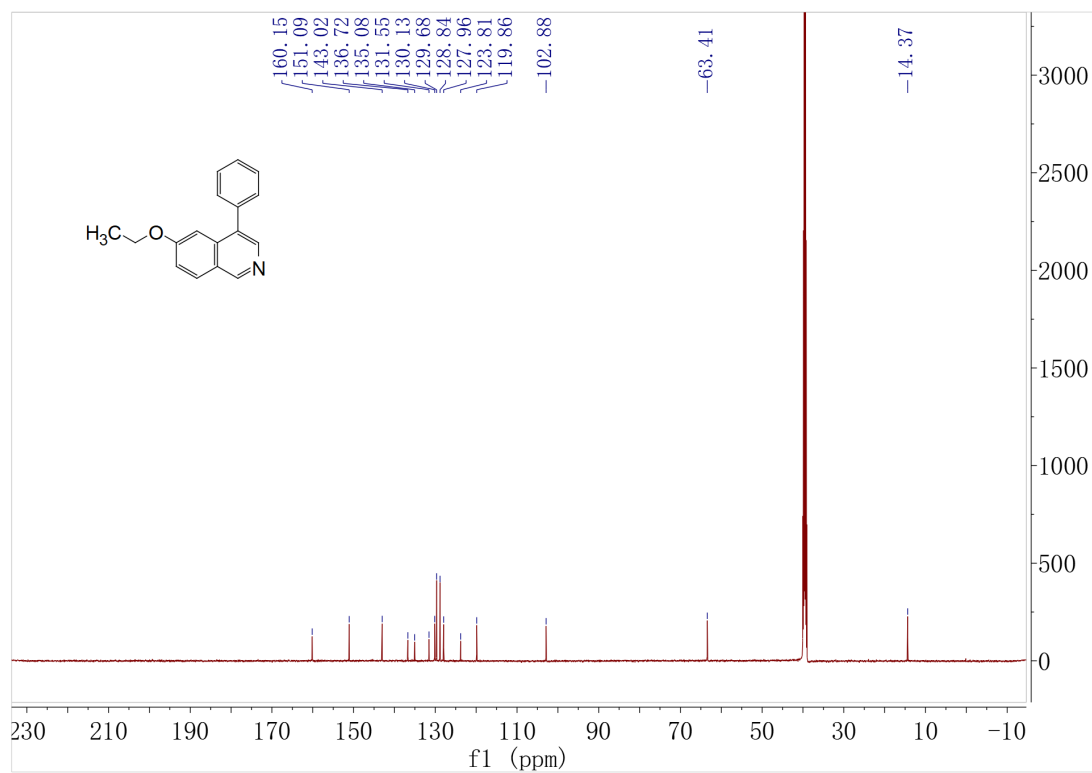
# <sup>13</sup>C NMR Spectrum of compound **34**



### $^1\text{H}$ NMR Spectrum of compound **37**

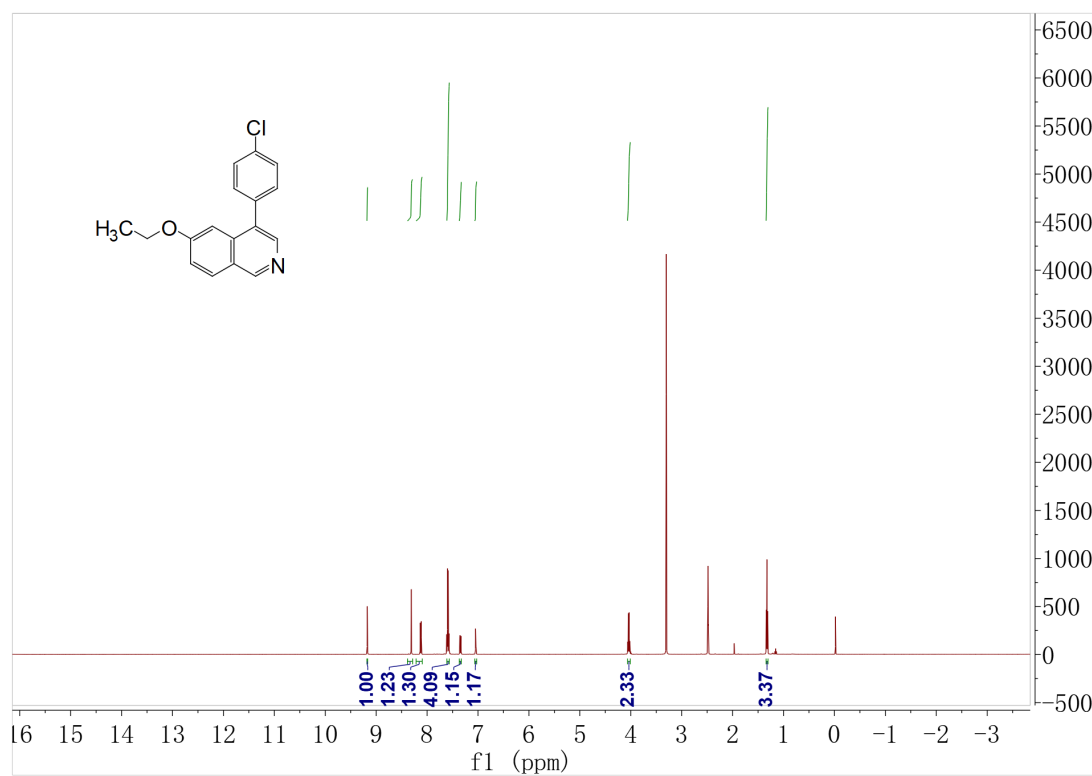


### $^{13}\text{C}$ NMR Spectrum of compound **37**

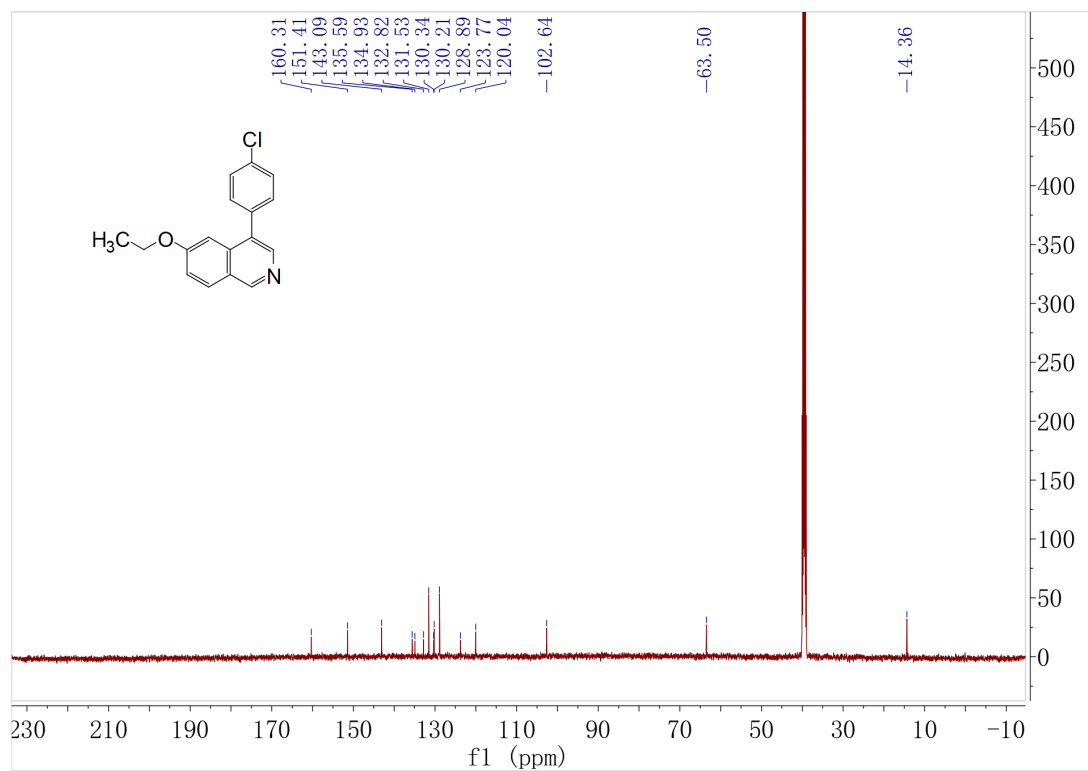




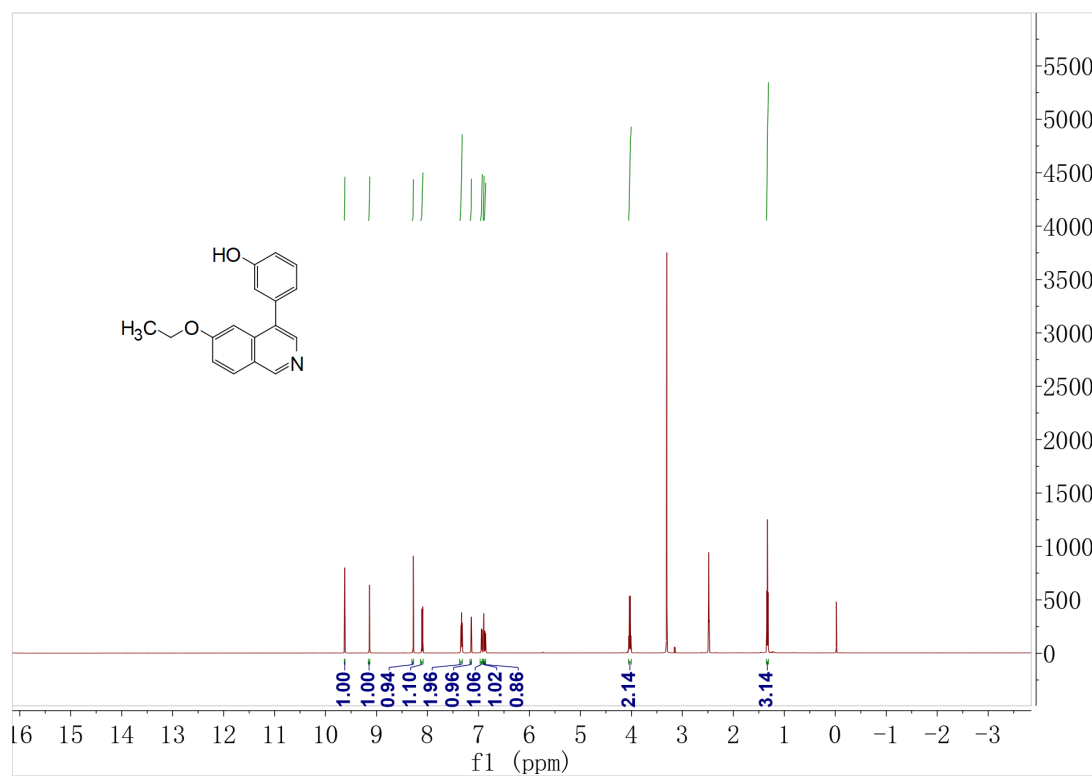
### <sup>1</sup>H NMR Spectrum of compound **38**



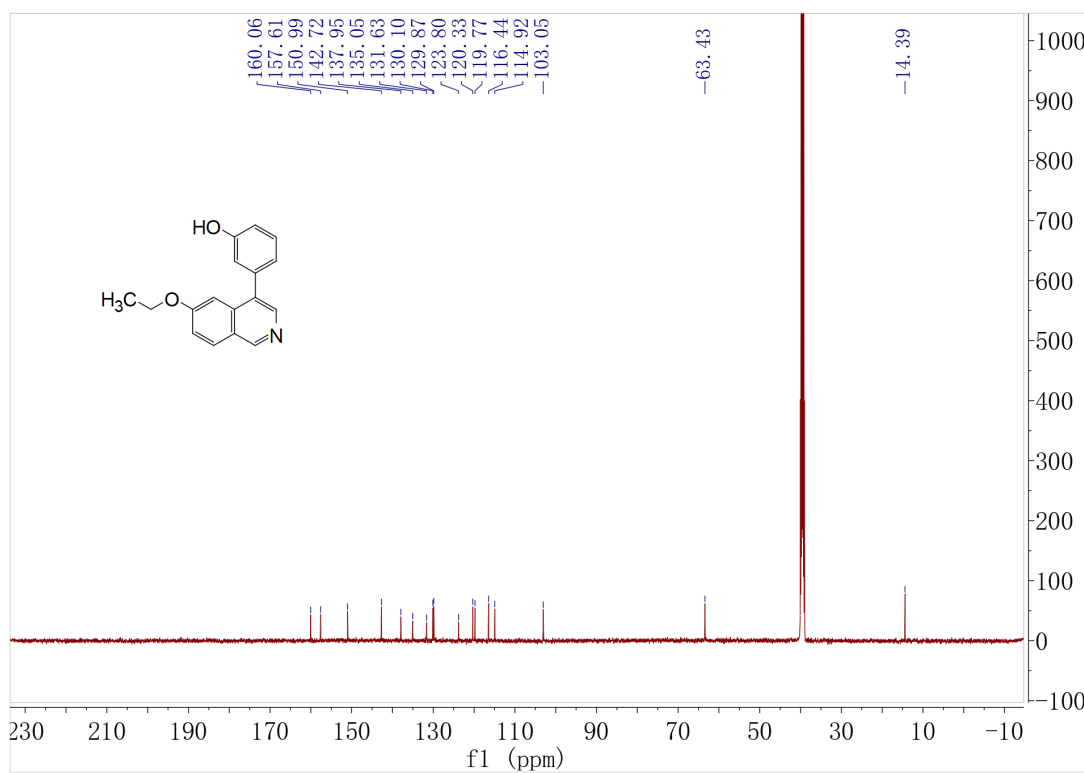
### <sup>13</sup>C NMR Spectrum of compound **38**



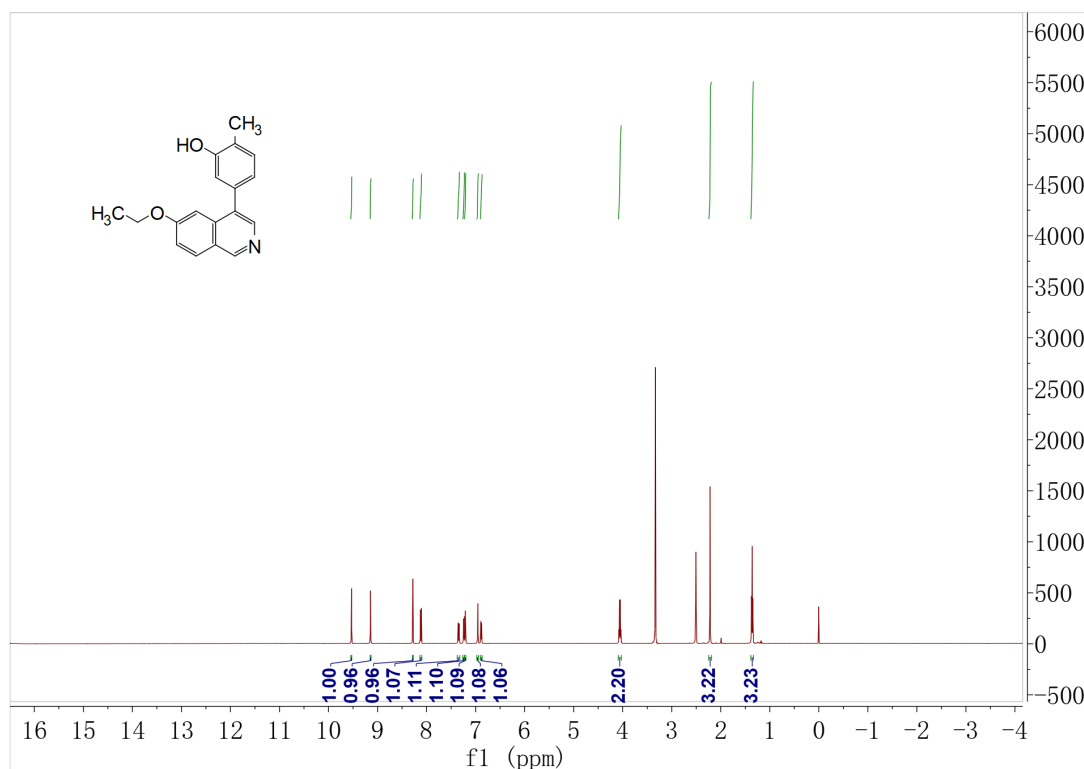
### $^1\text{H}$ NMR Spectrum of compound **39**



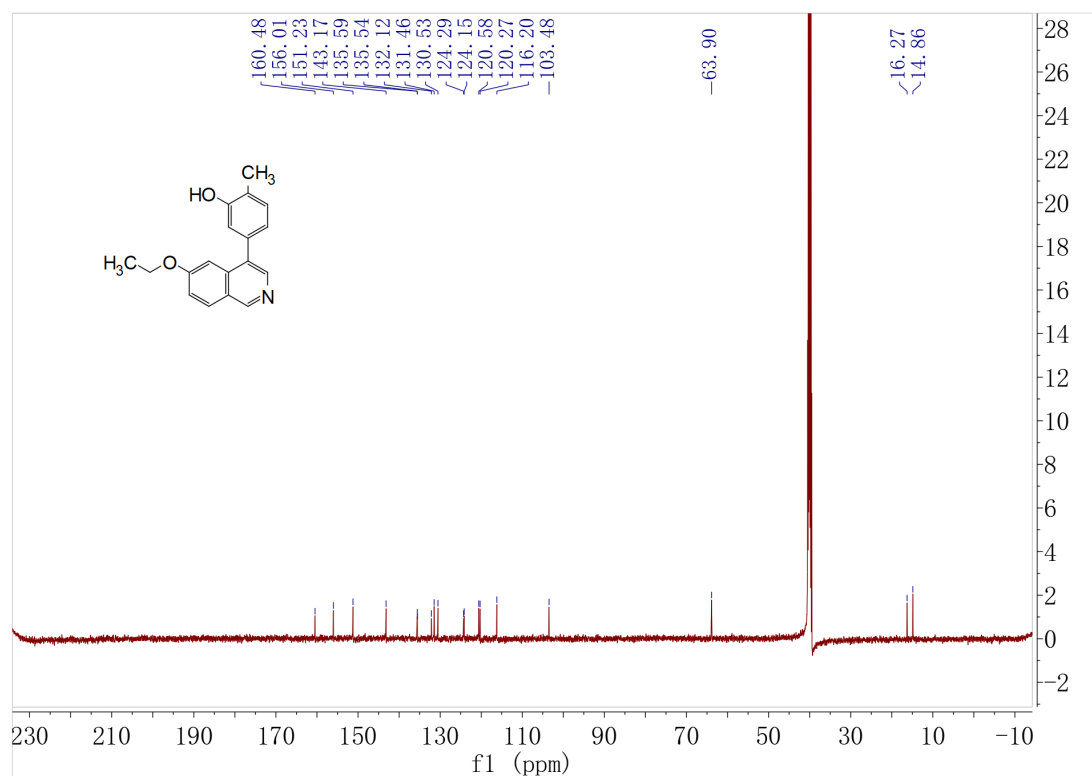
### $^{13}\text{C}$ NMR Spectrum of compound **39**



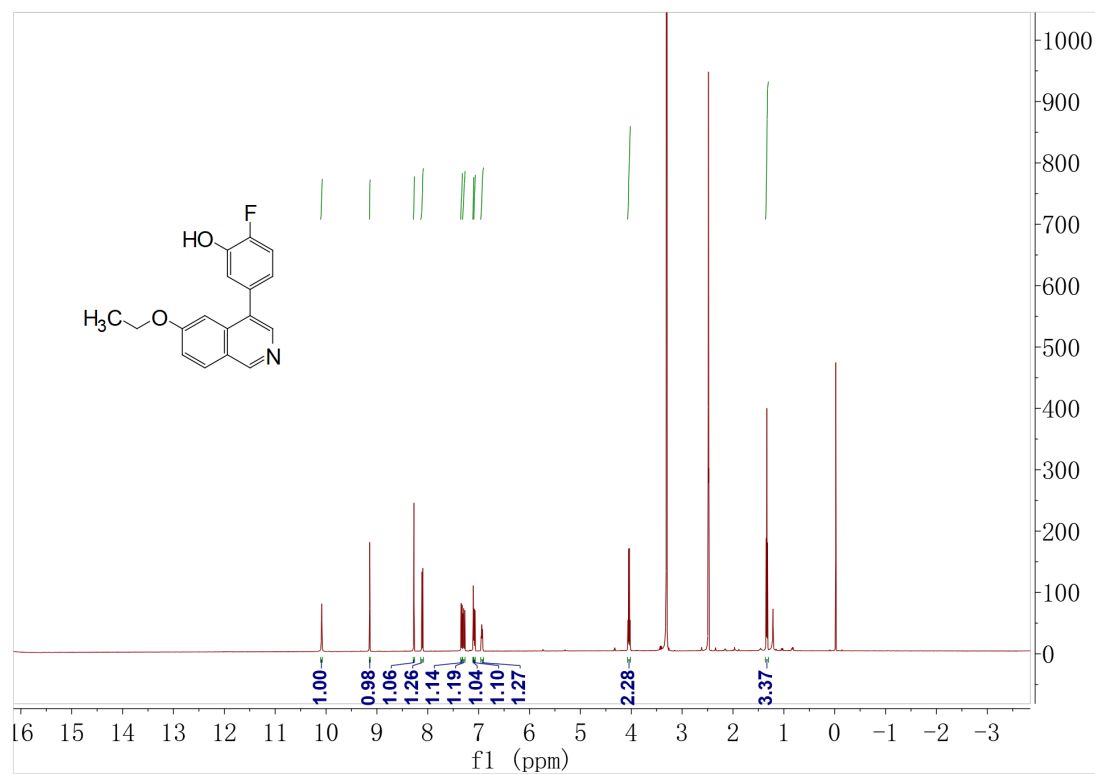
# <sup>1</sup>H NMR Spectrum of compound 40



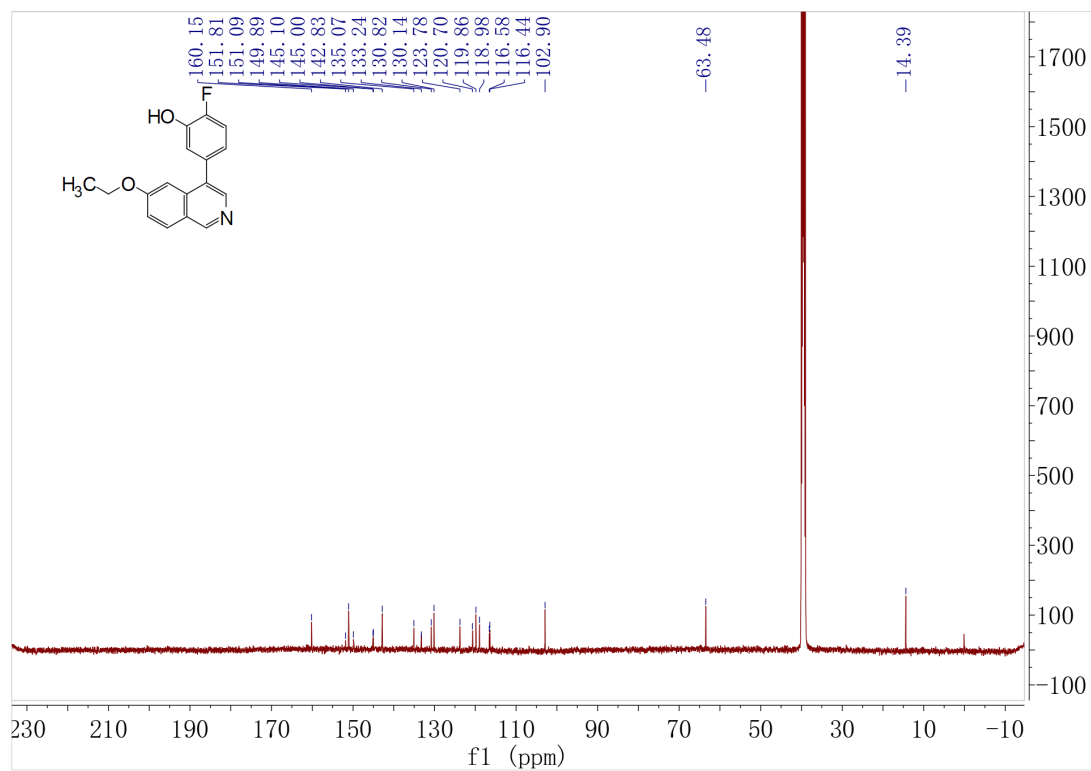
# <sup>13</sup>C NMR Spectrum of compound 40



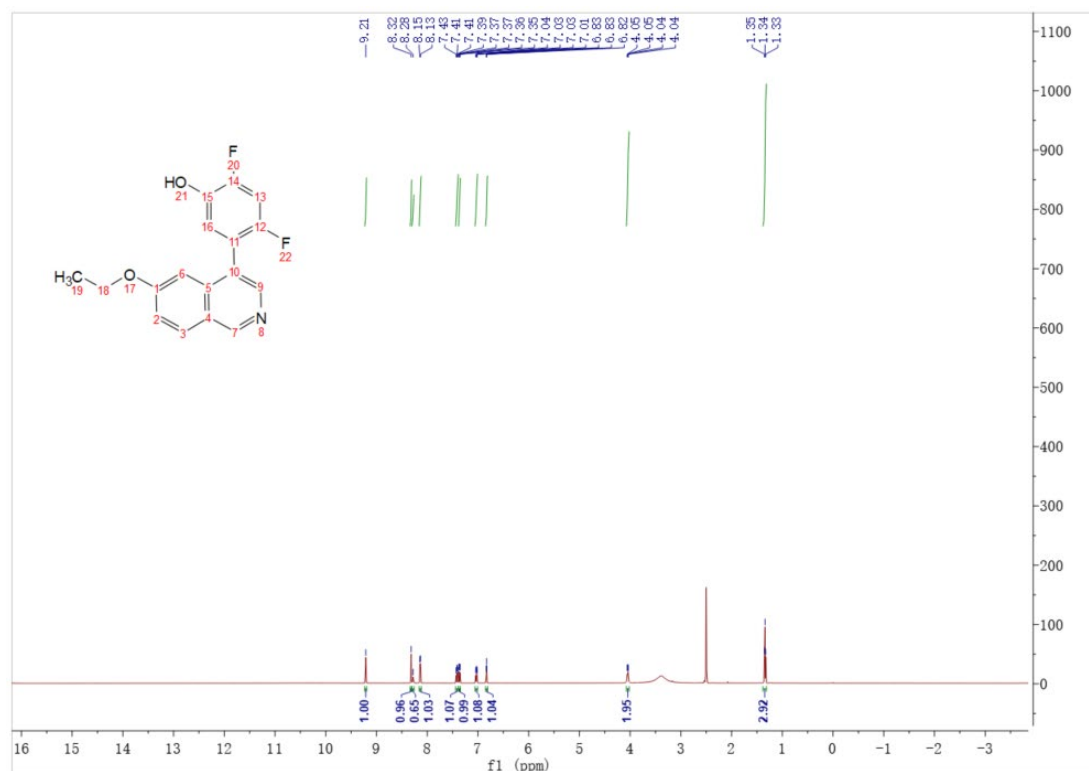
### <sup>1</sup>H NMR Spectrum of compound **45**



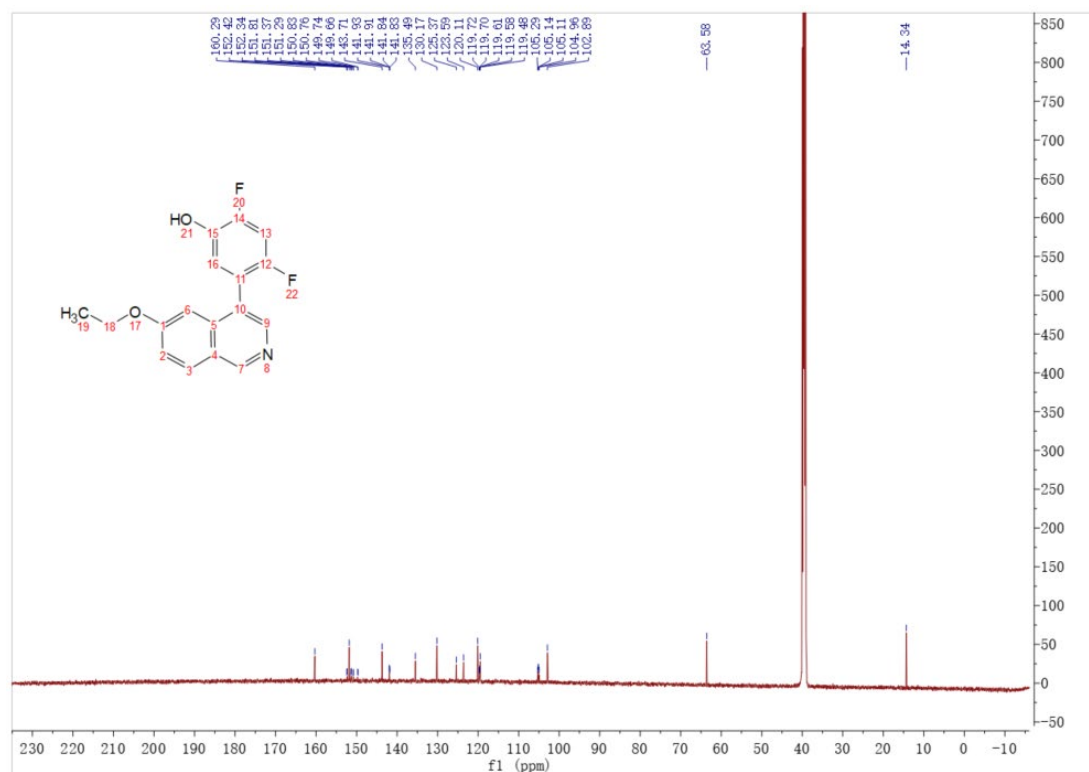
### <sup>13</sup>C NMR Spectrum of compound **45**



# <sup>1</sup>H NMR Spectrum of compound 46

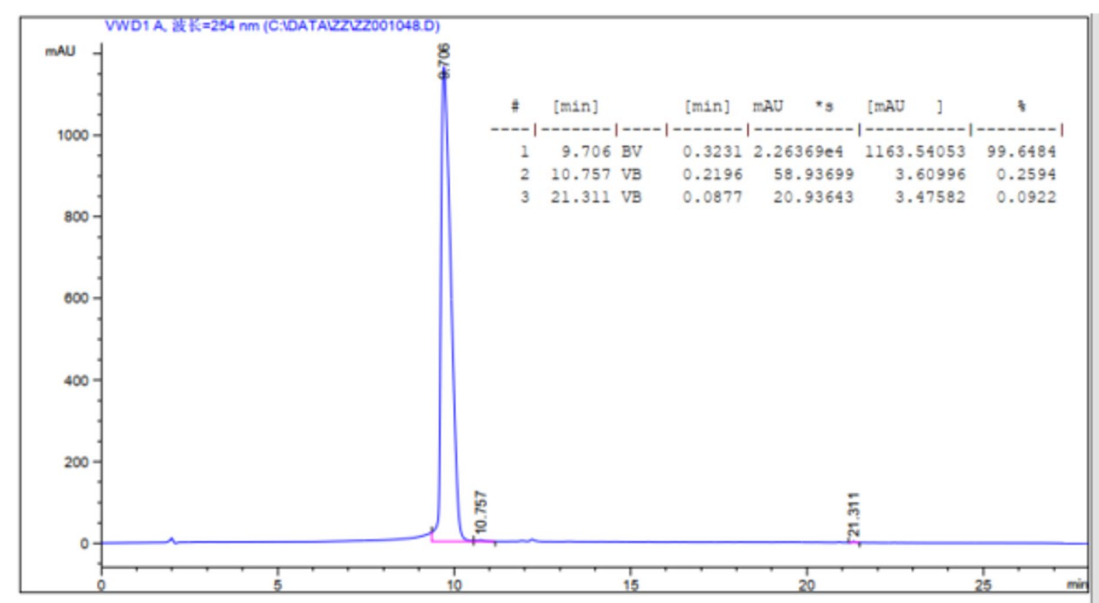


# <sup>13</sup>C NMR Spectrum of compound 46

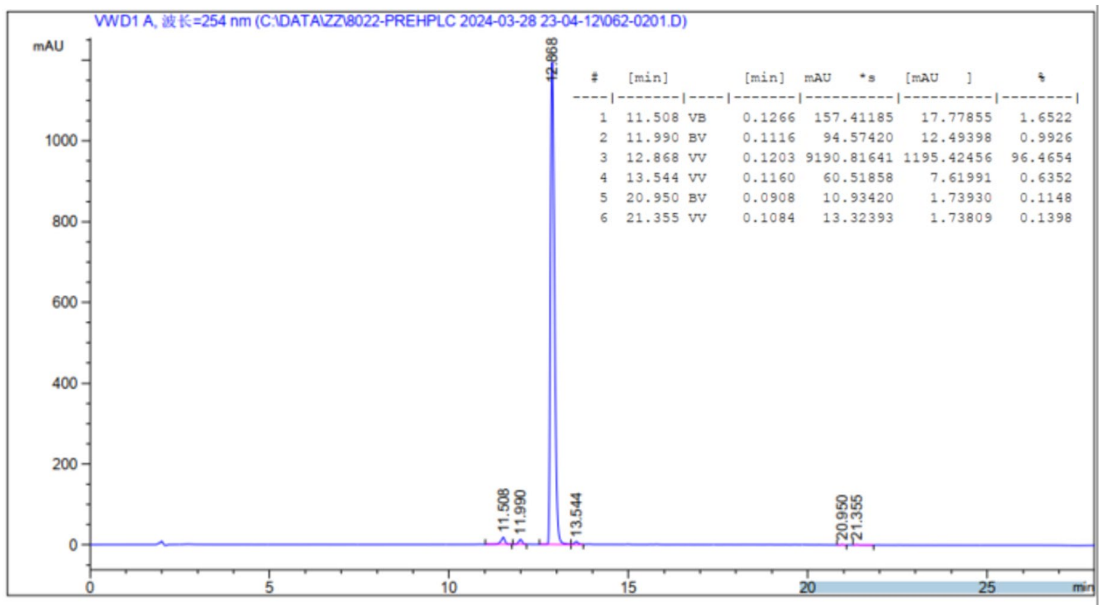


2. HPLC Spectrums

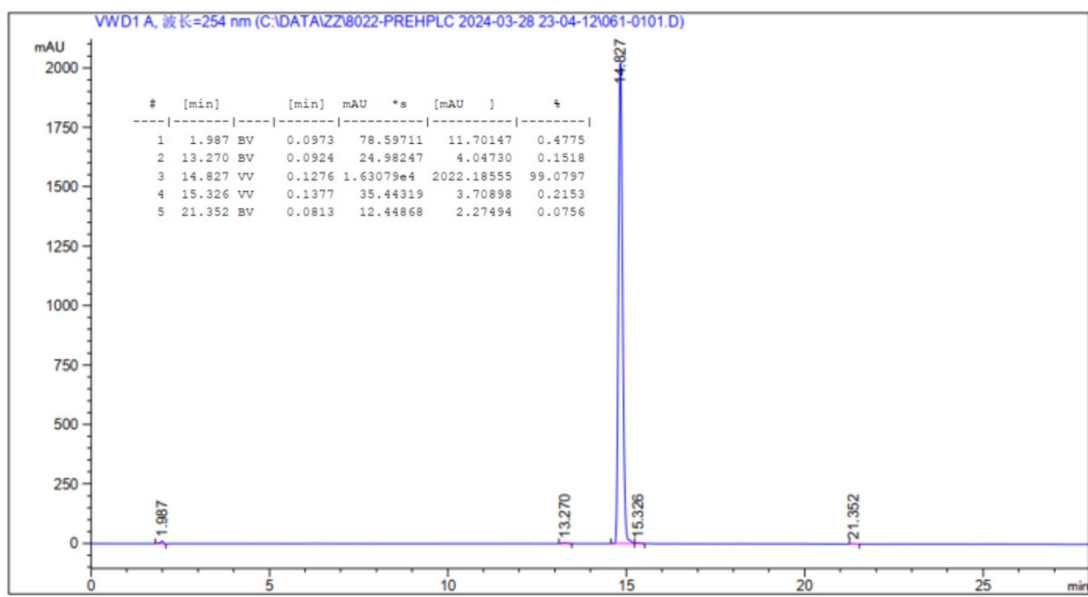
HPLC Spectrum of compound **1** (99.6% purity)



HPLC Spectrum of compound **20** (96.5% purity)



## HPLC Spectrum of compound **23** (99.1% purity)



## HPLC Spectrum of compound **46** (99.5% purity)

