

## Supplementary Materials

# Design, Synthesis, and Biological Evaluation of Pyridinesulfonamide Derivatives as Novel PI3K/mTOR Dual Inhibitors

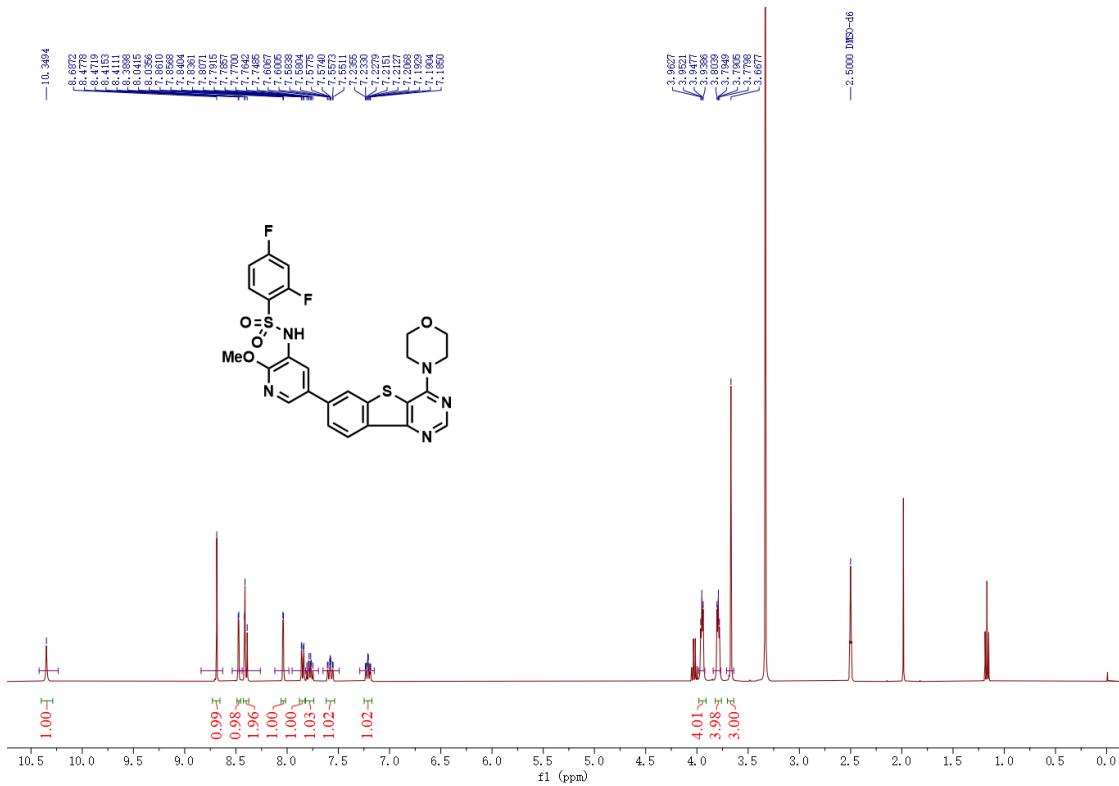
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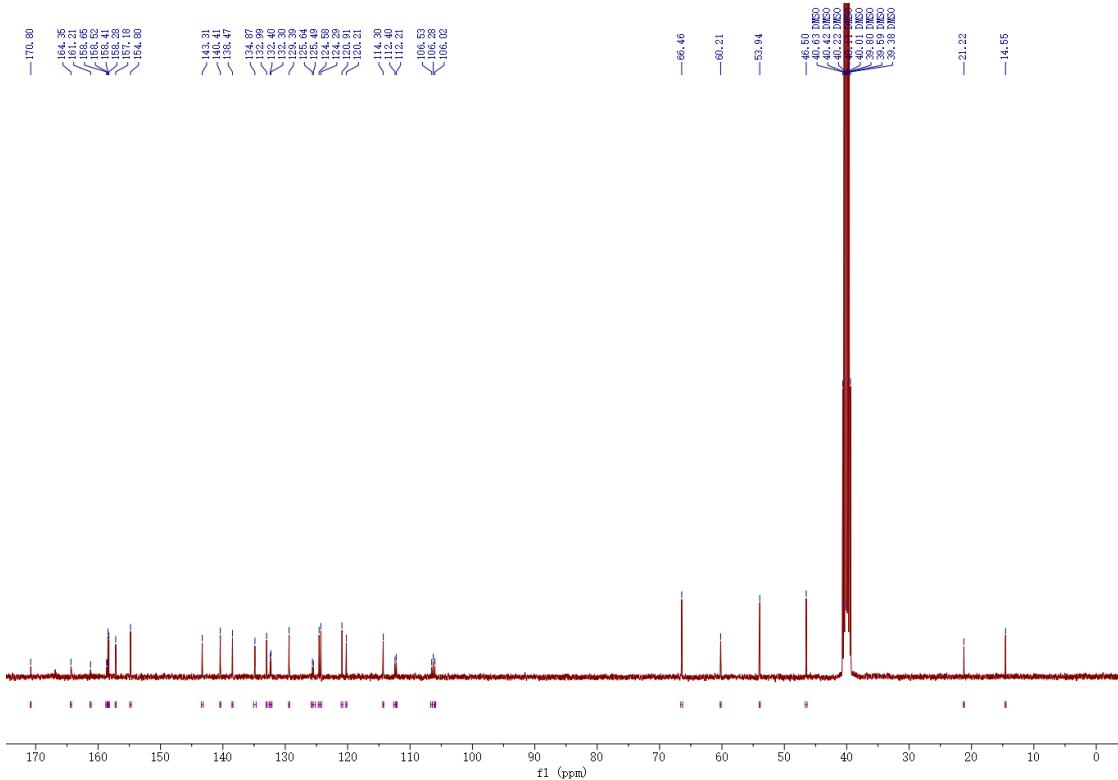
1 Key Laboratory of Structure-Based Drug Design and Discovery (Ministry of Education), School of Pharmaceutical Engineering, Shenyang Pharmaceutical University, Shenyang, 110016, China

2 Faculty of functional food and wine, Shenyang Pharmaceutical University, Shenyang 110016, China

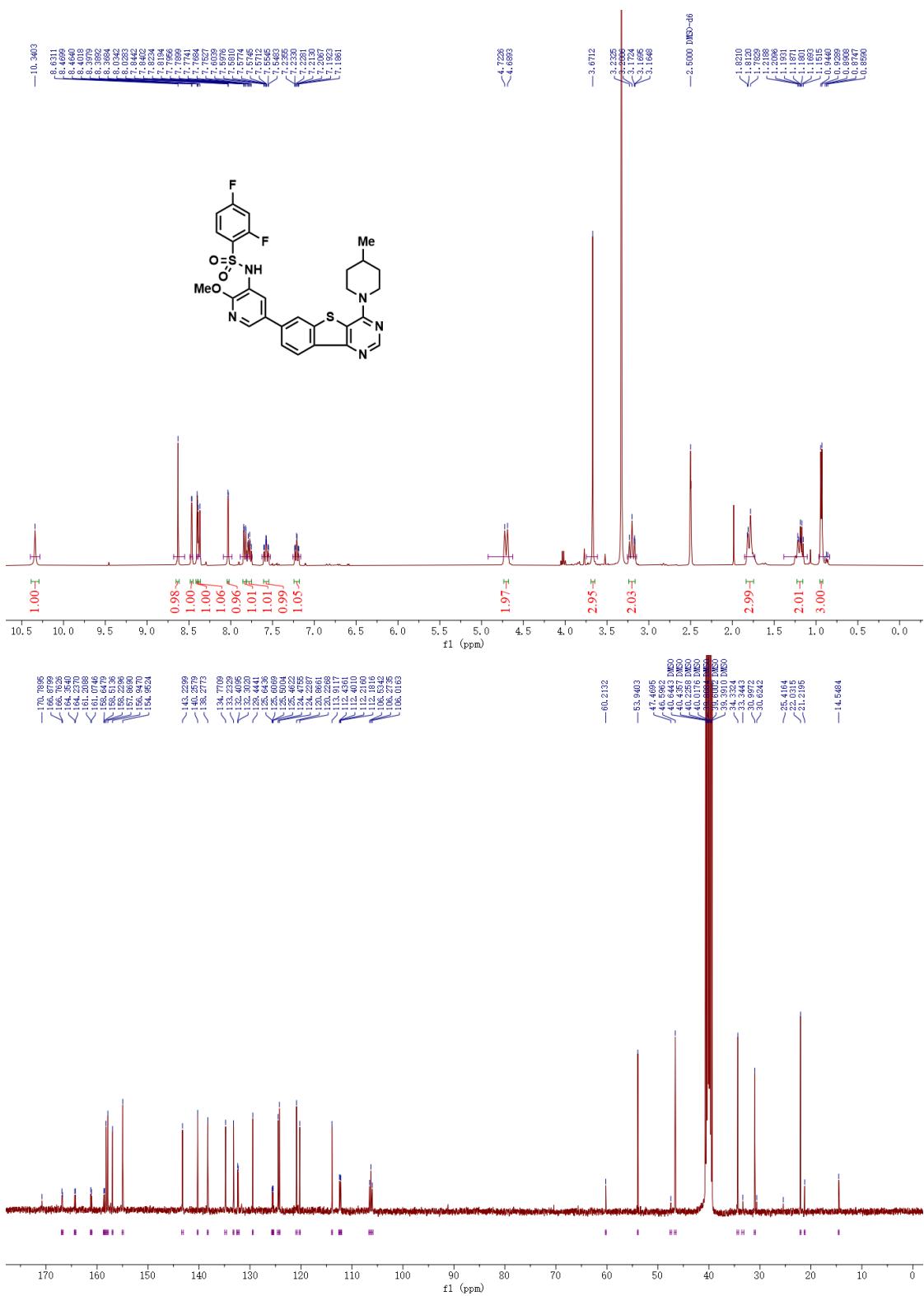
\* Correspondence: e-mail@e-mail.com: ([xuyoujun@sypmu.edu.cn](mailto:xuyoujun@sypmu.edu.cn) (Y. Xu); [Wangf@sypmu.edu.cn](mailto:Wangf@sypmu.edu.cn) (F. Wang))

### NMR spectra for final compounds

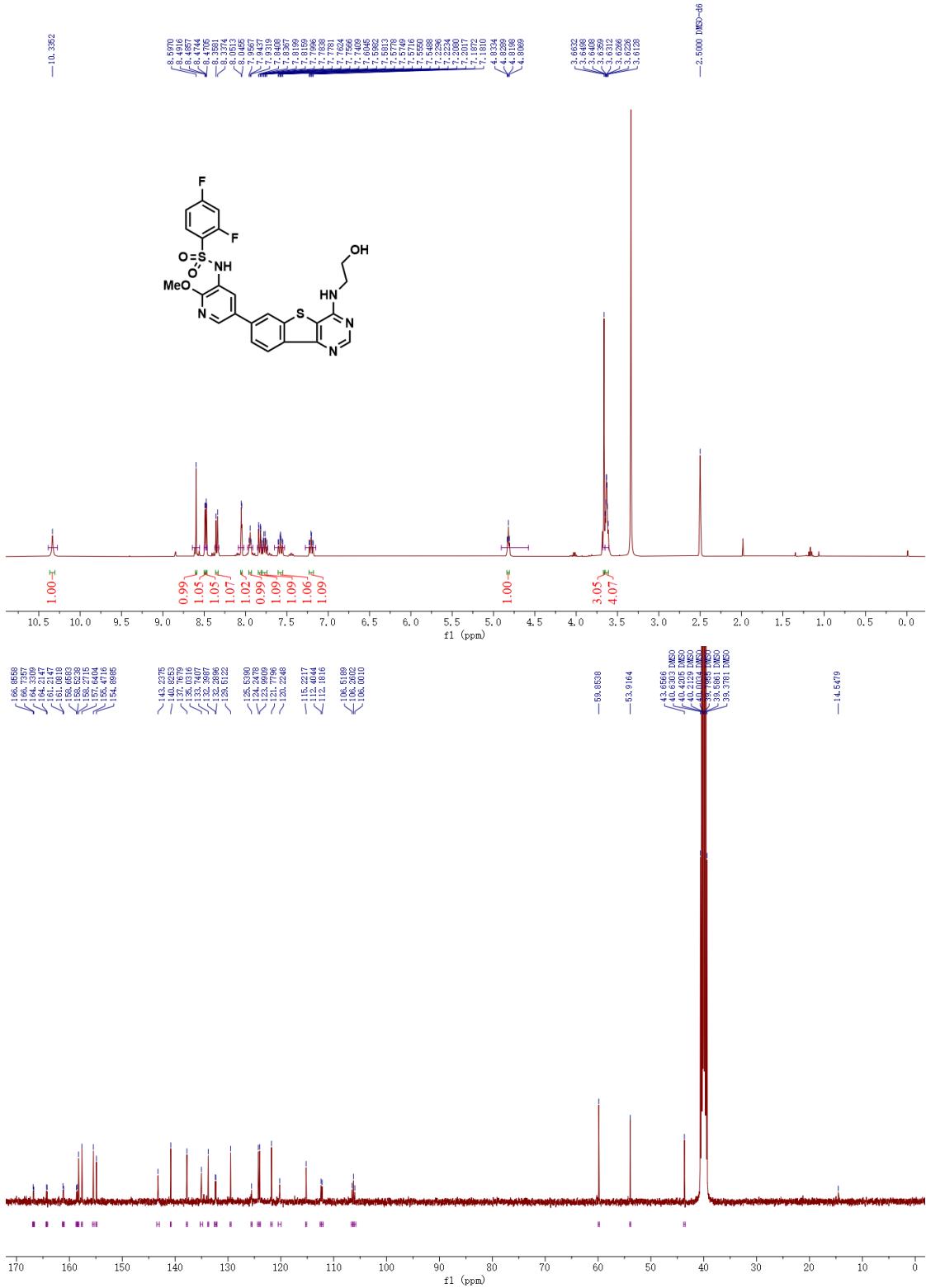




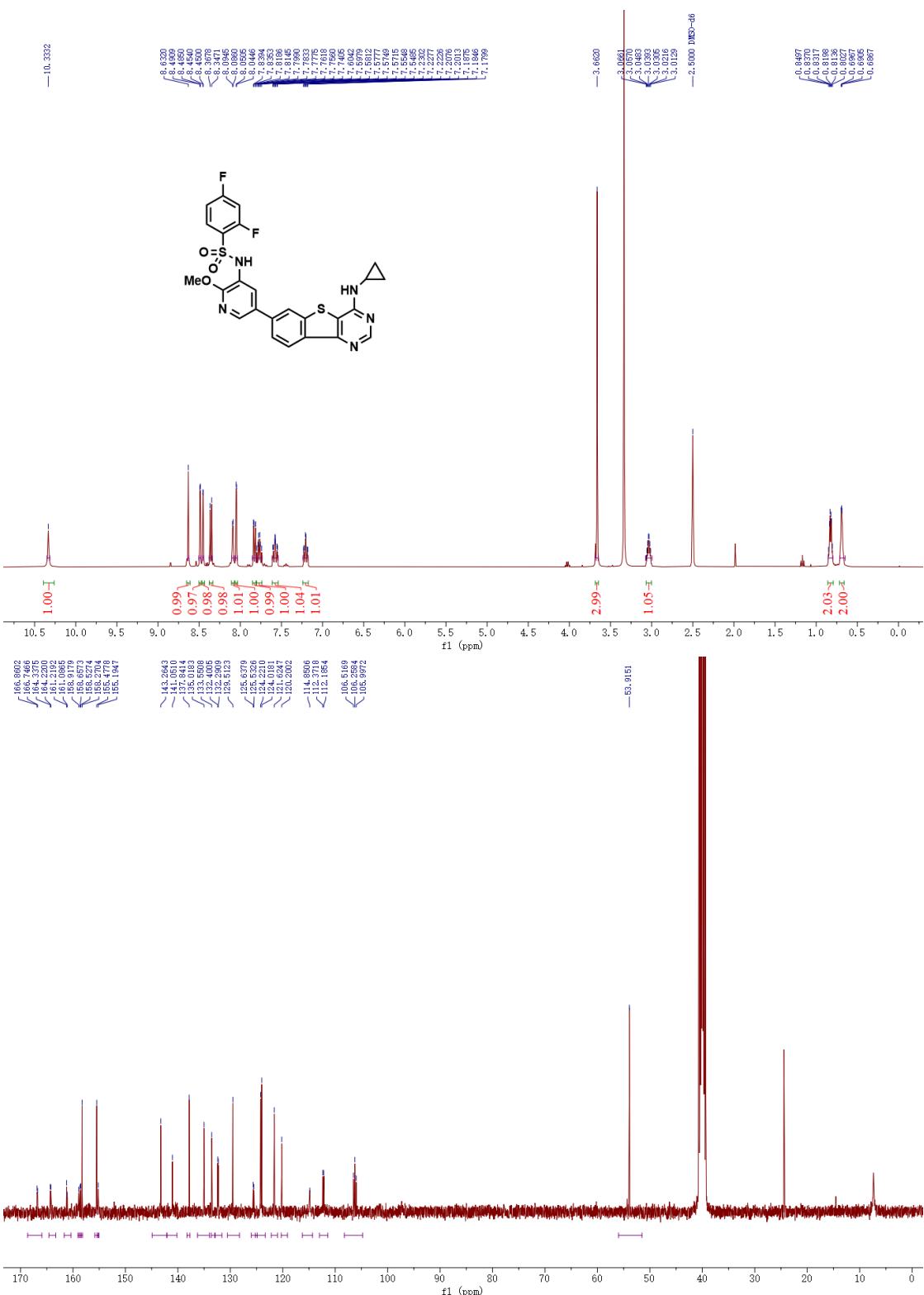
**Figure S1.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **11a** (DMSO-d6).



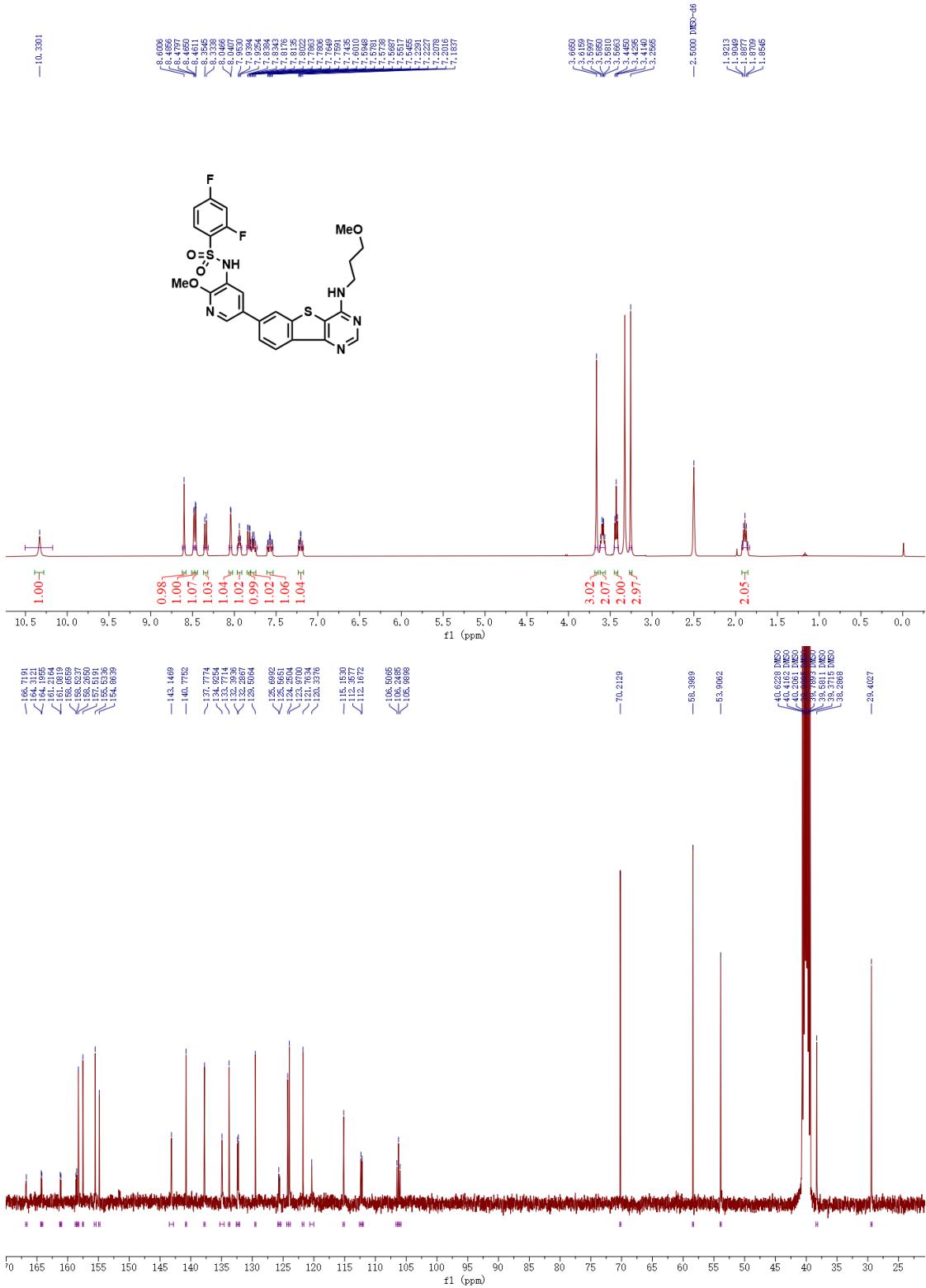
**Figure S2.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **11b** (DMSO-d6).



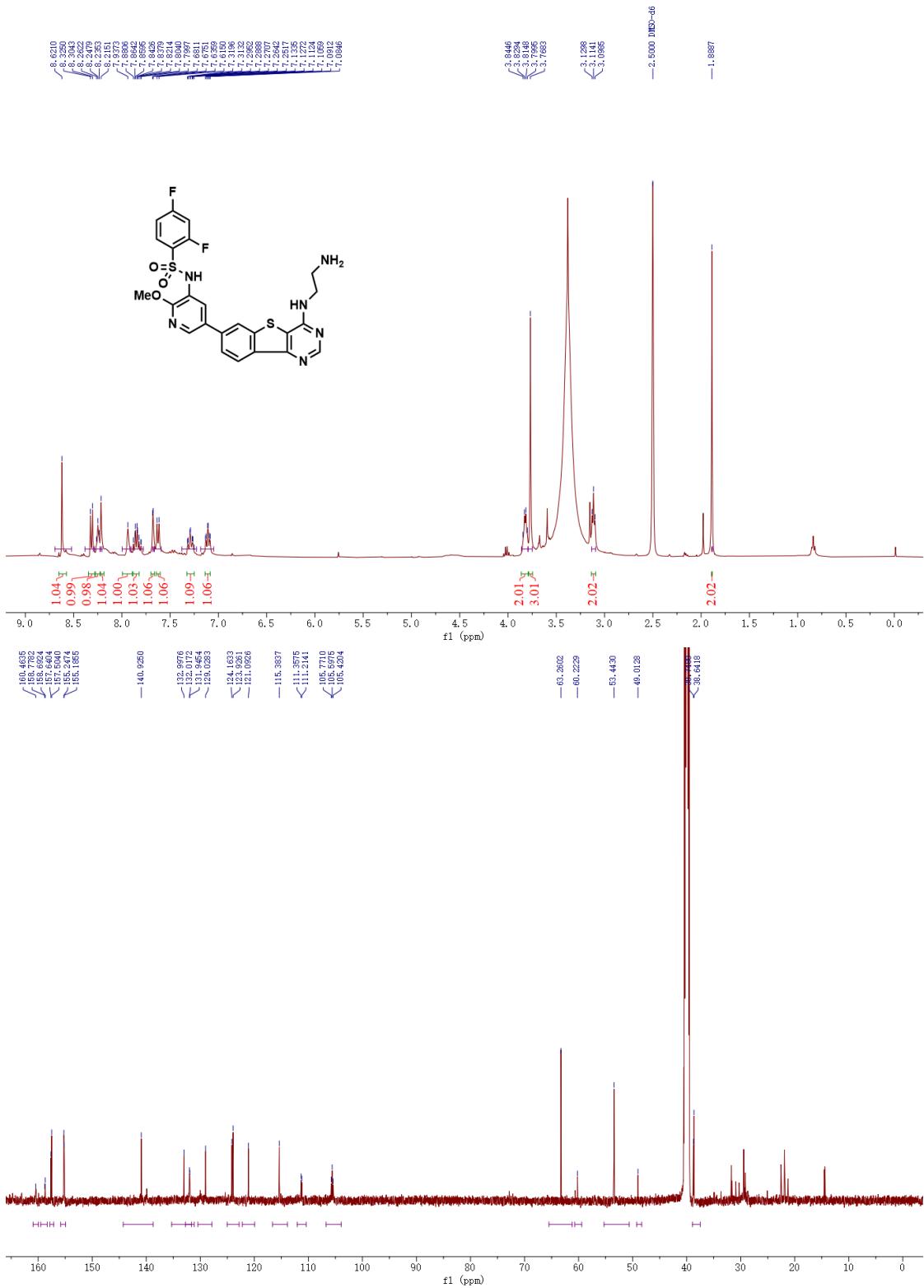
**Figure S3.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **11c** (DMSO-d6).



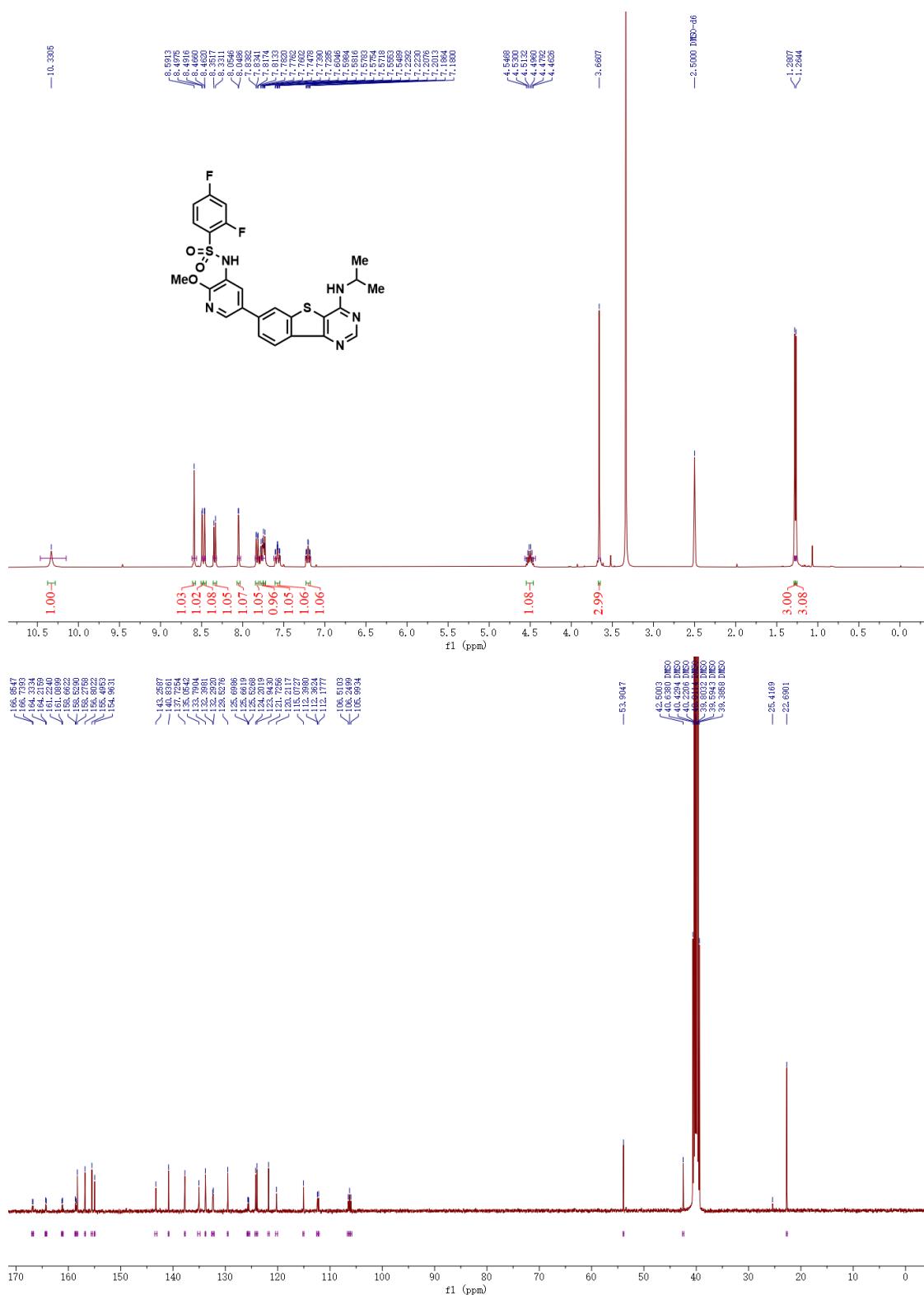
**Figure S4.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **11d** (DMSO-d6).



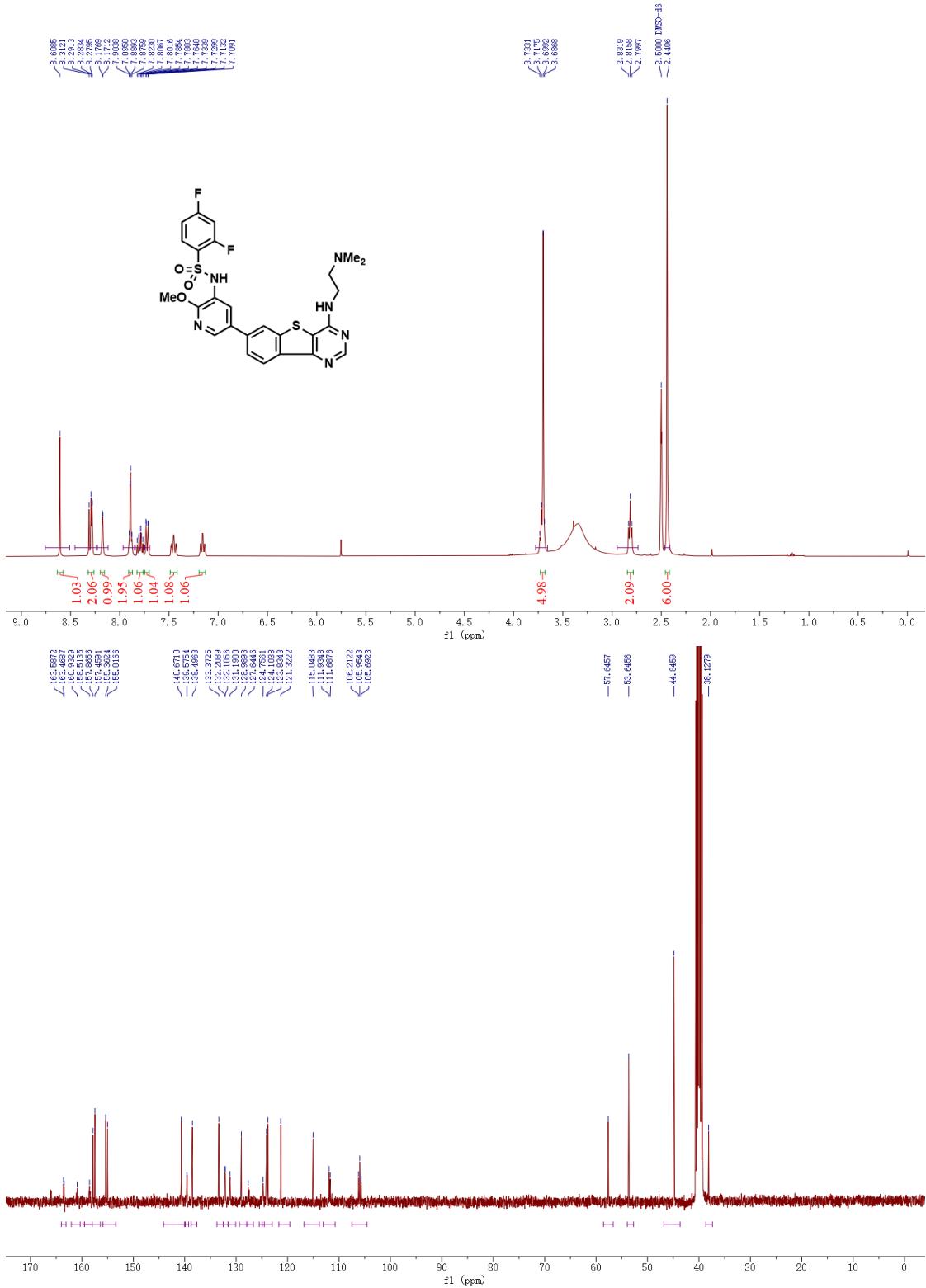
**Figure S5.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **11e** (DMSO-d6).



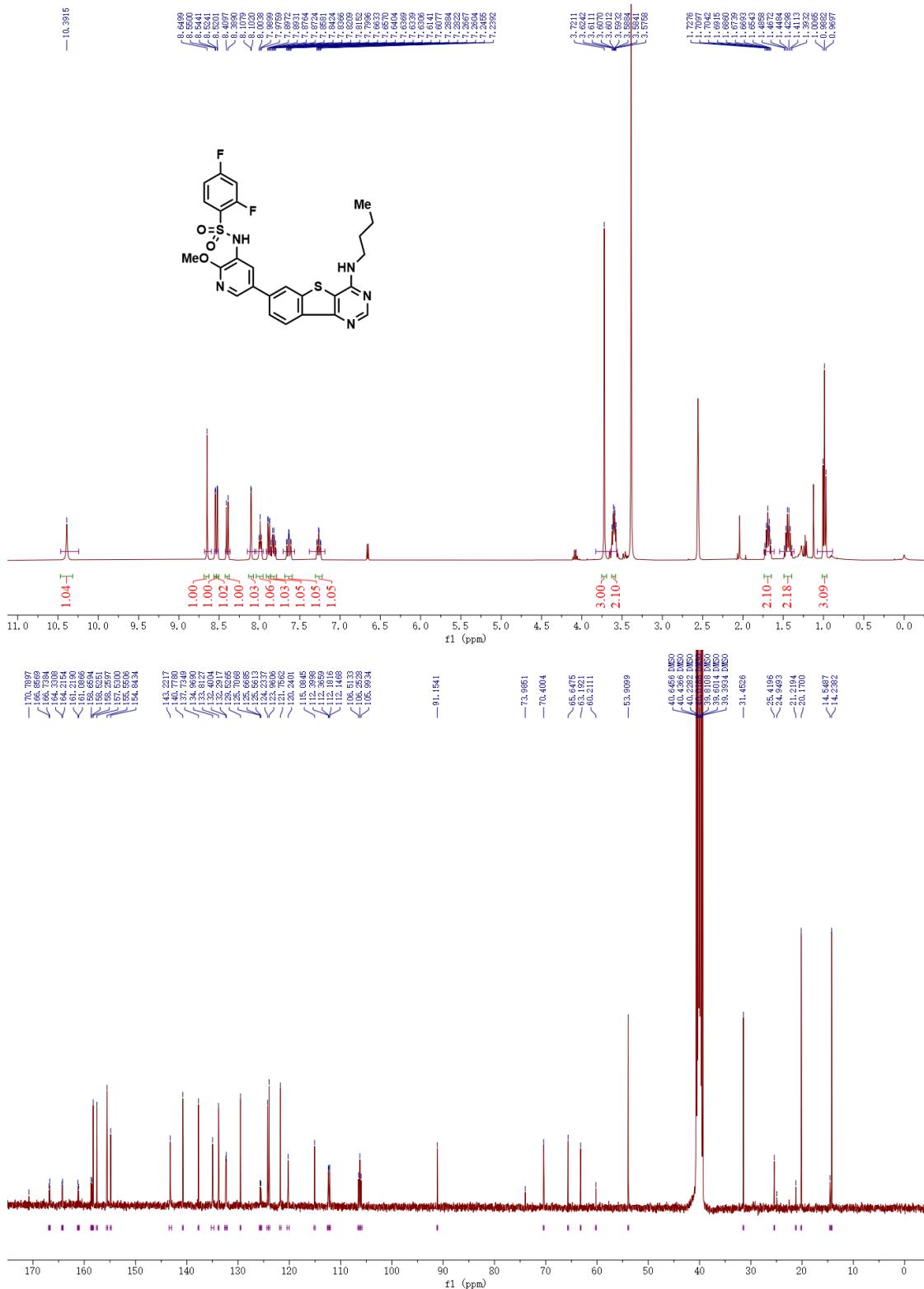
**Figure S6.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **11f** (DMSO-d6).



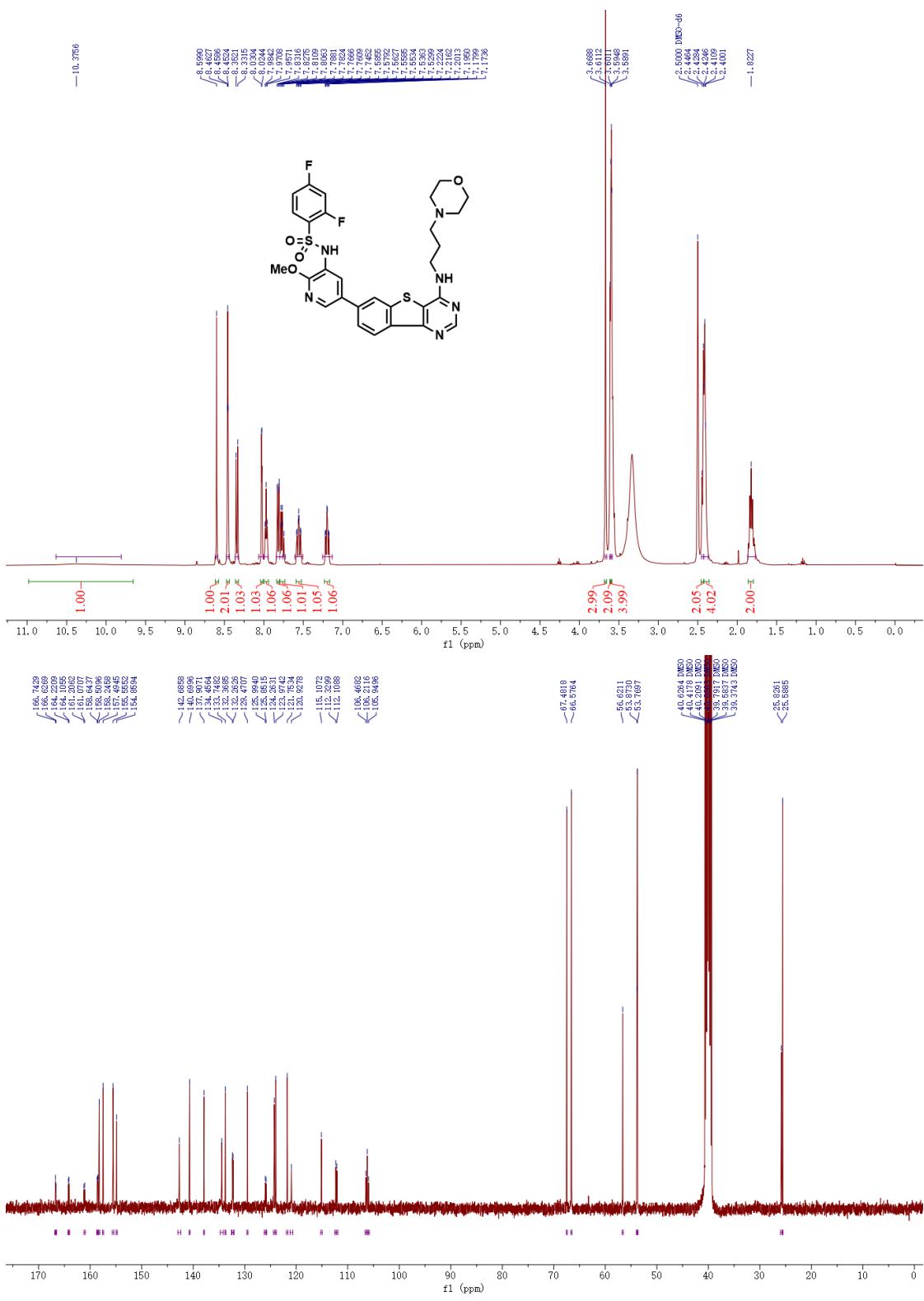
**Figure S7.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **11g** (DMSO-d6).



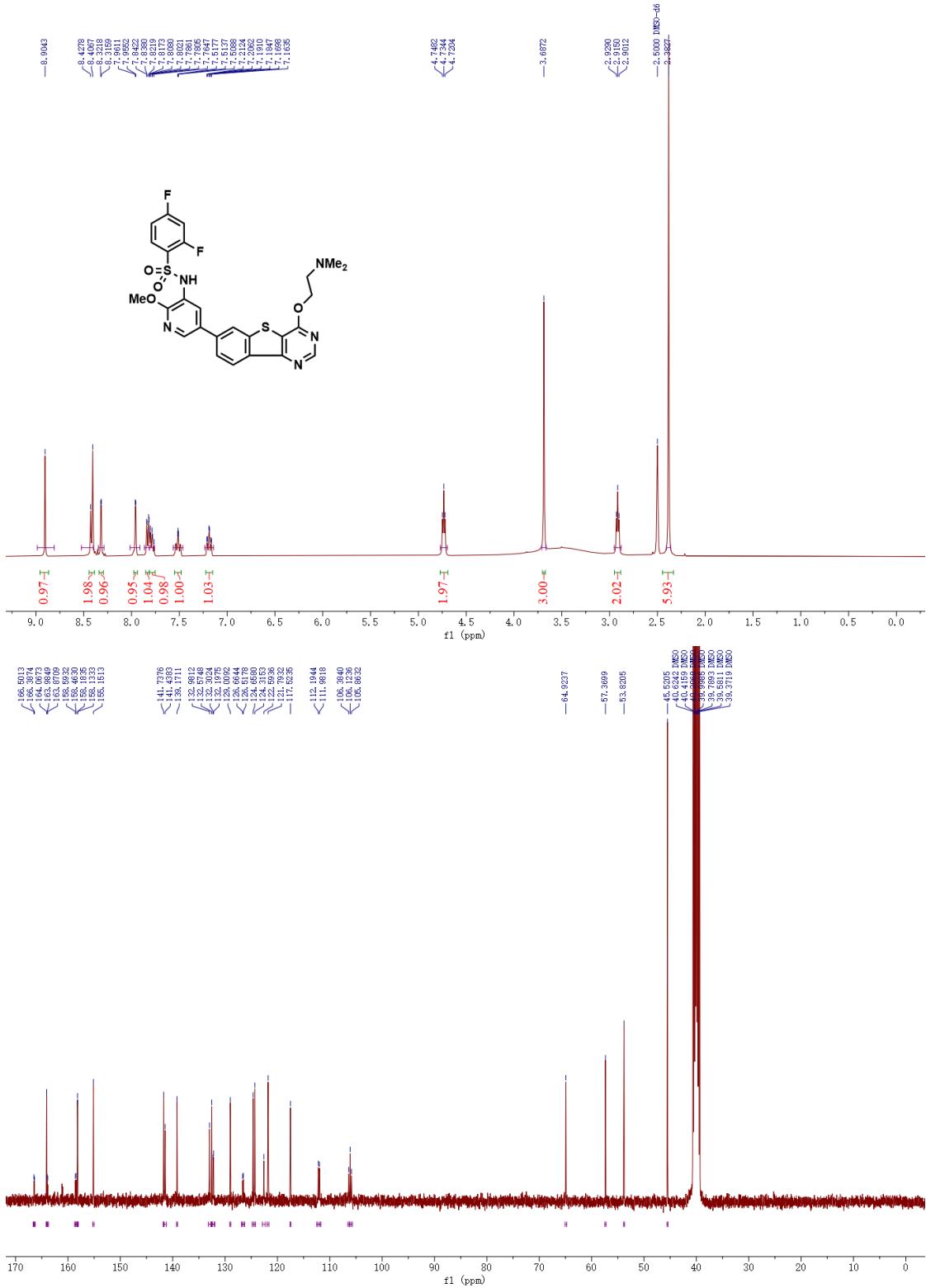
**Figure S8**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **11h** (DMSO-d6).



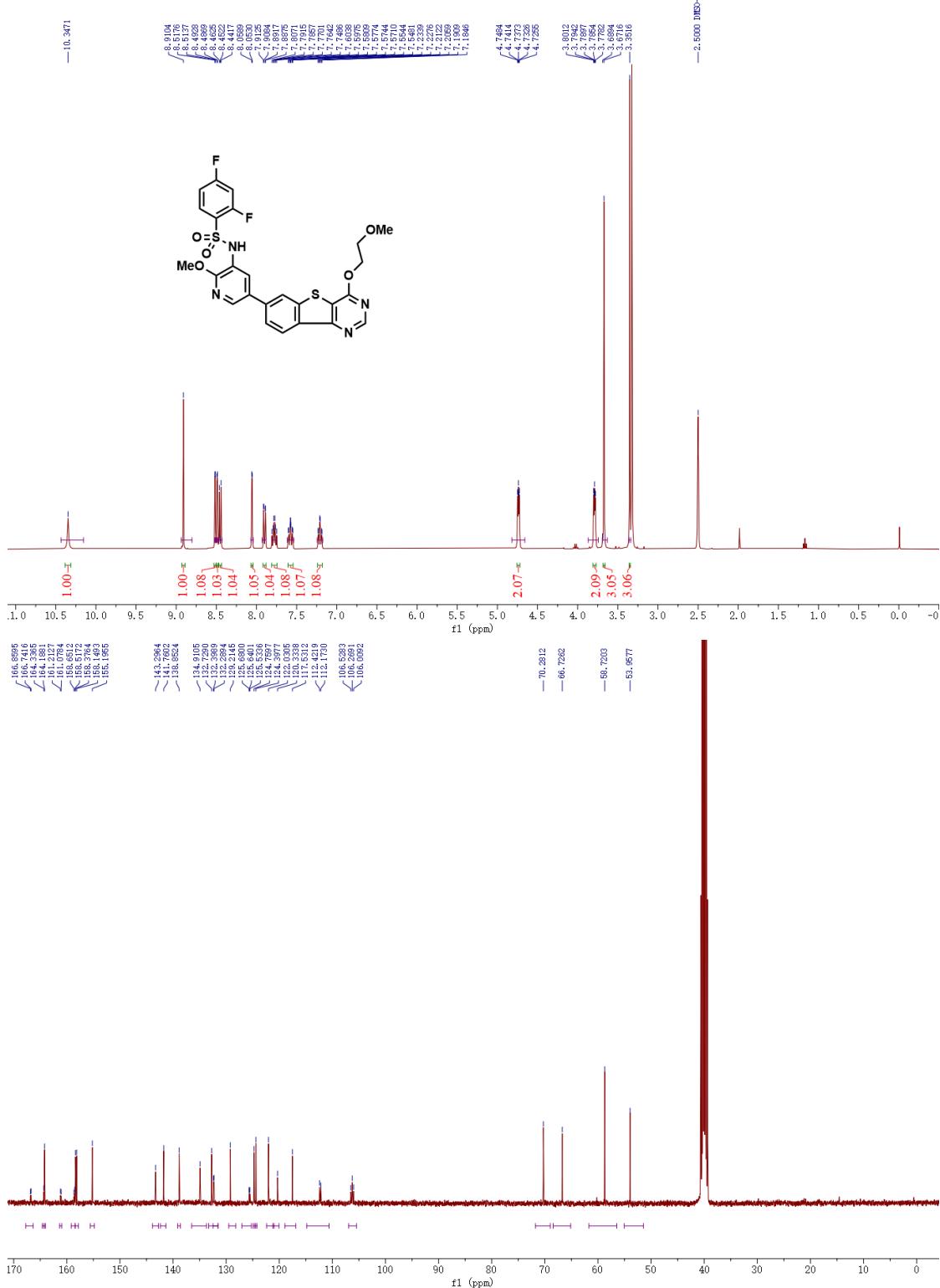
**Figure S9.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **11i** (DMSO-d<sub>6</sub>).



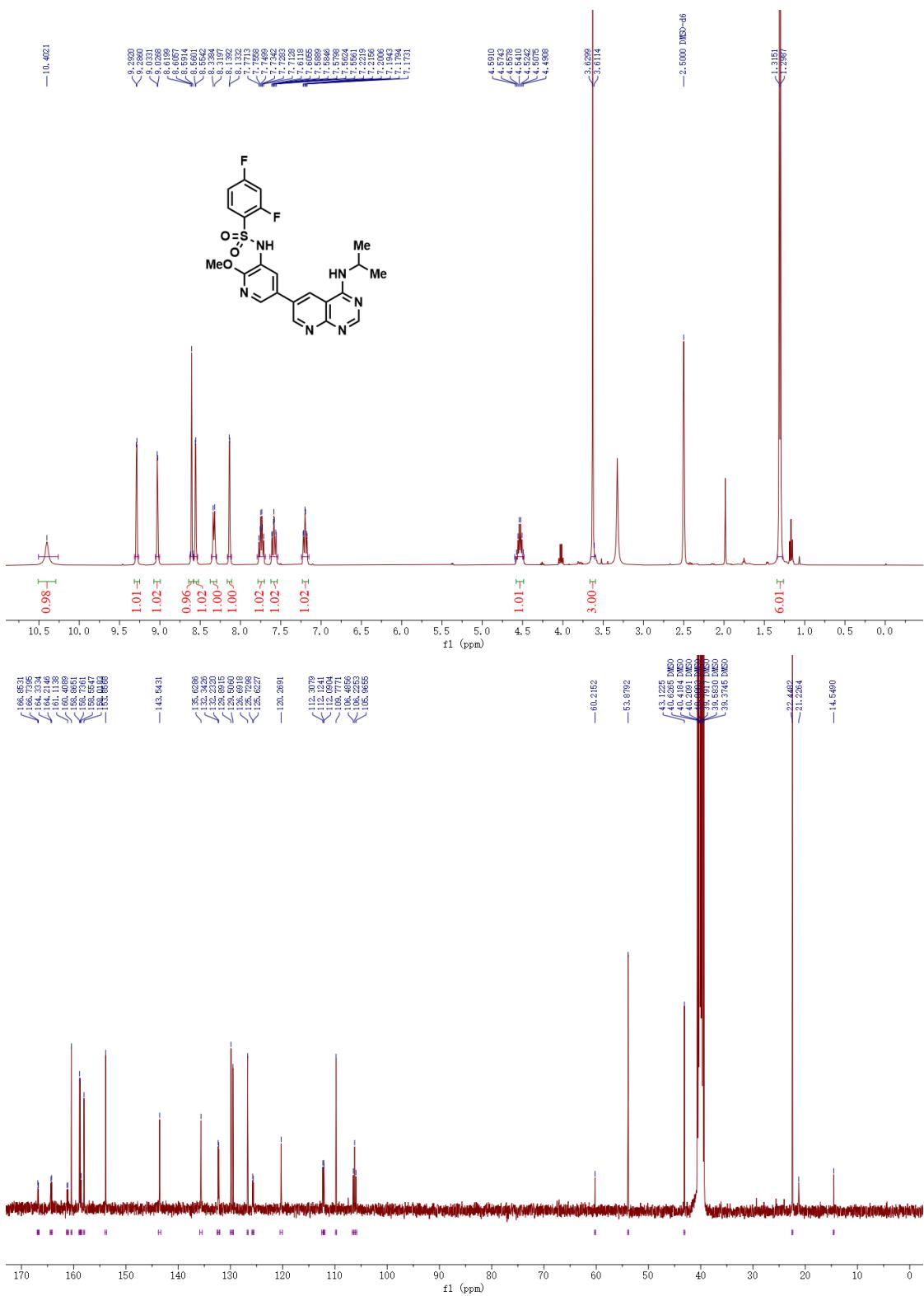
**Figure S10.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **11j** (DMSO-d6).



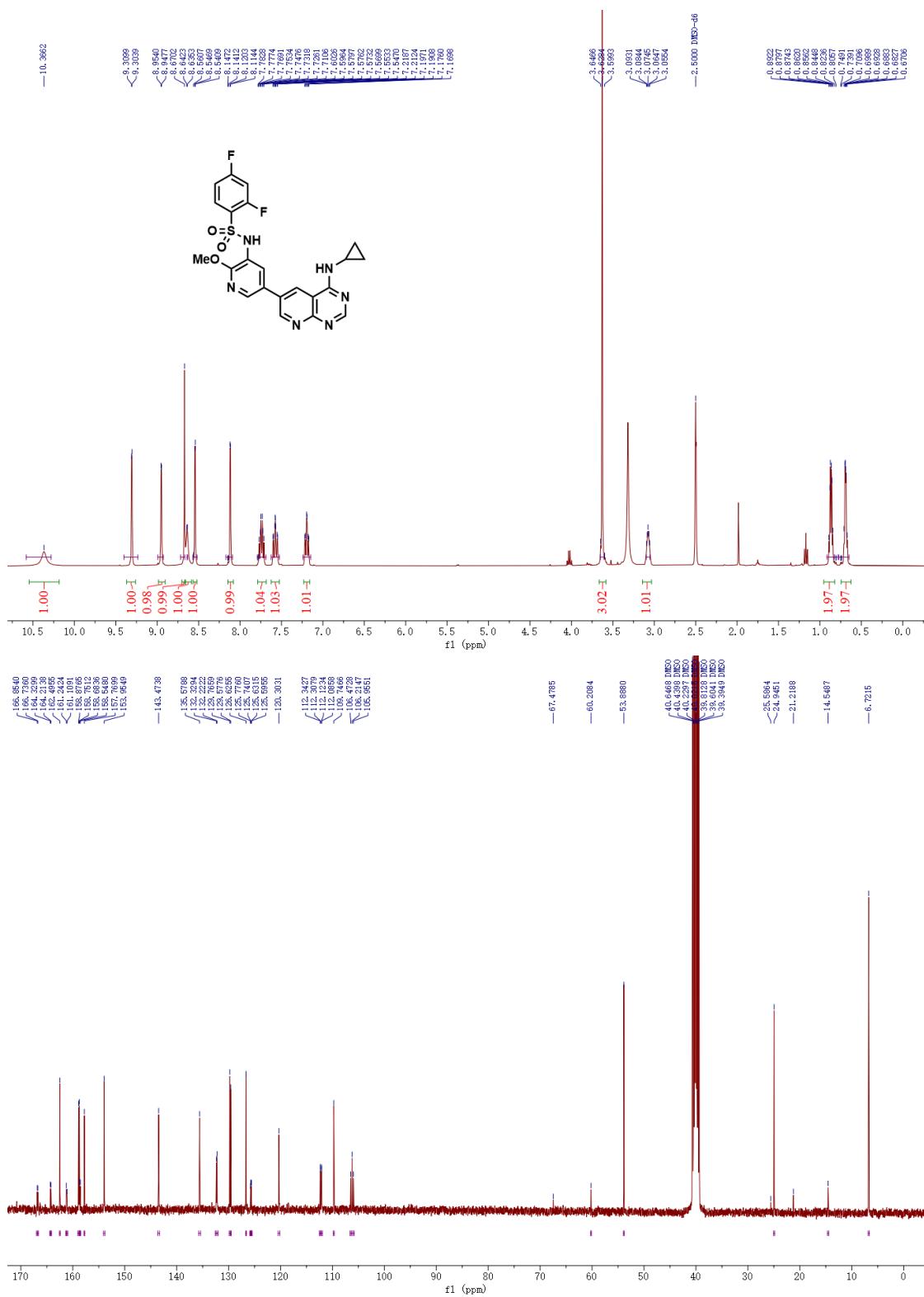
**Figure S11.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **11k** (DMSO-d6).



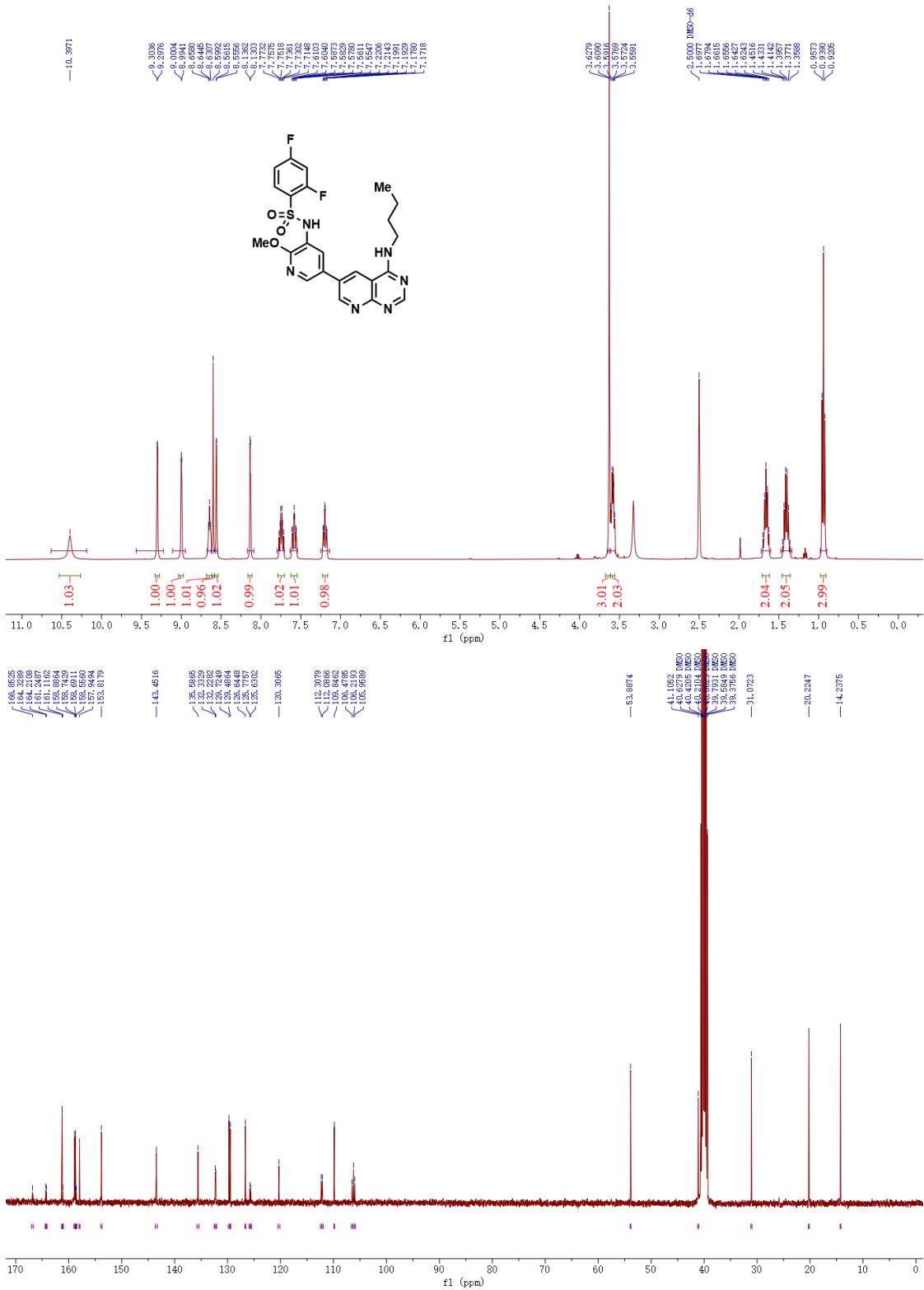
**Figure S12.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **11l** (DMSO-d6).



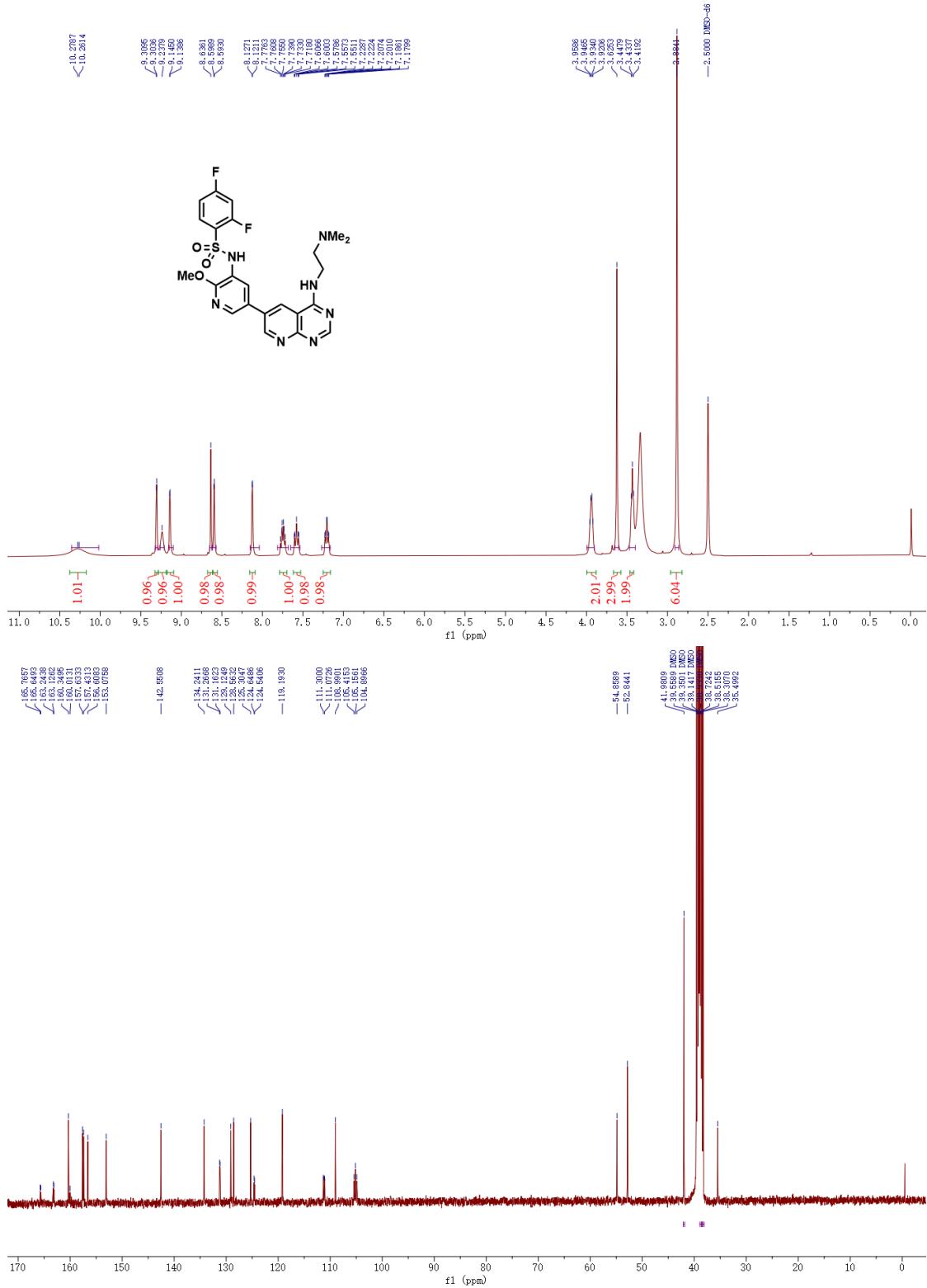
**Figure S13.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **17a** (DMSO-d6).



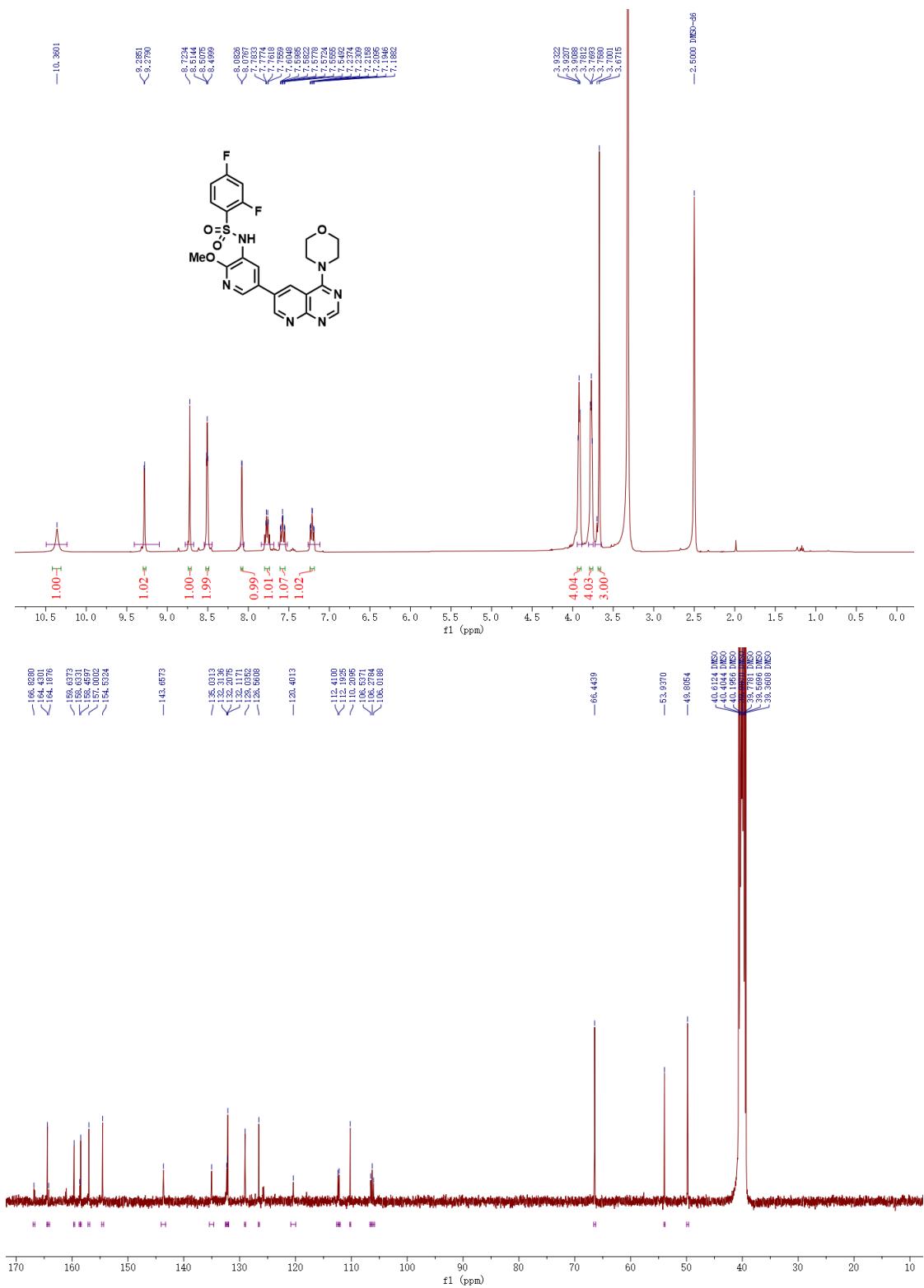
**Figure S14.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **17b** (DMSO-d6).



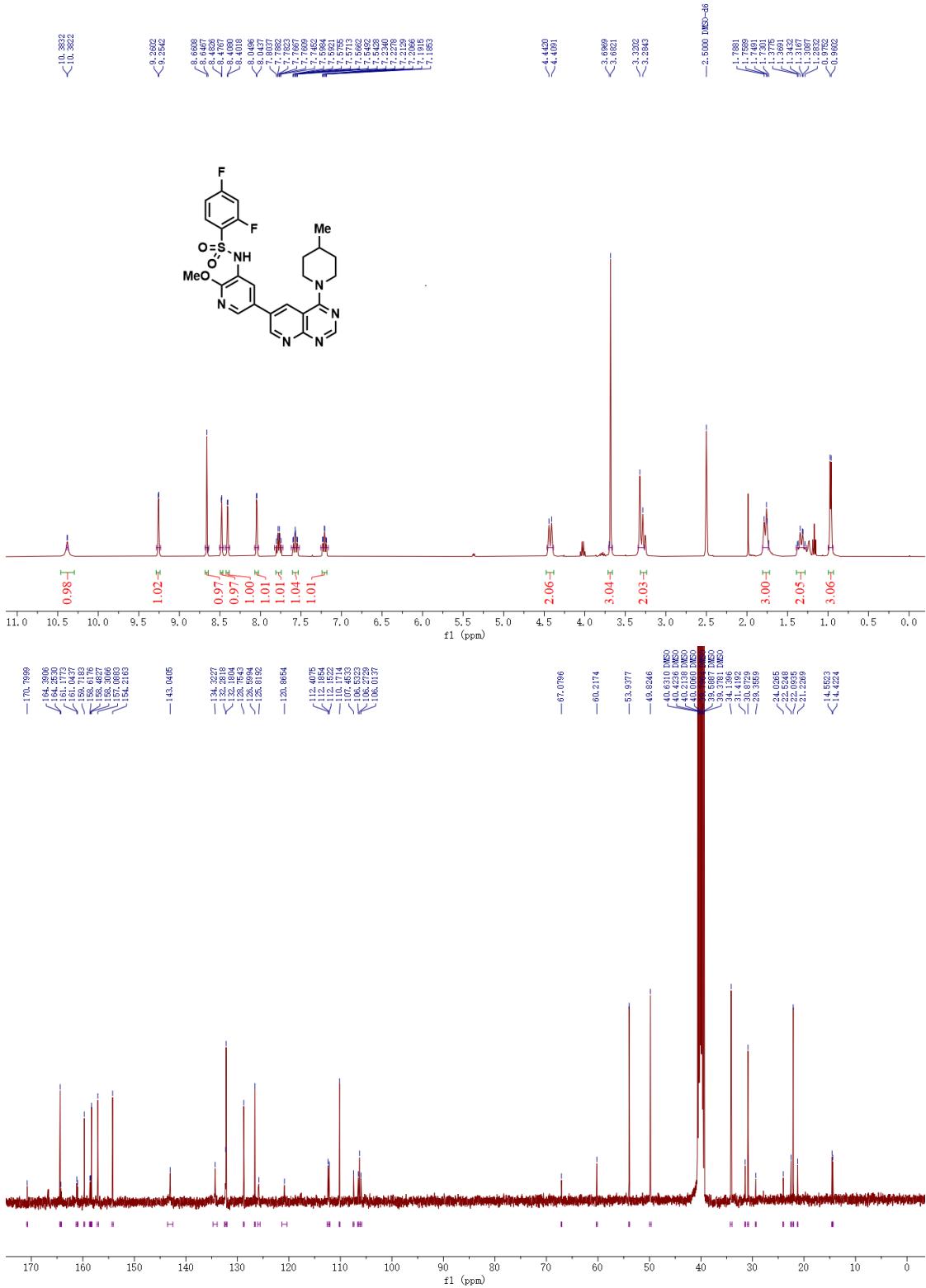
**Figure S15**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **17c** (DMSO-d6).



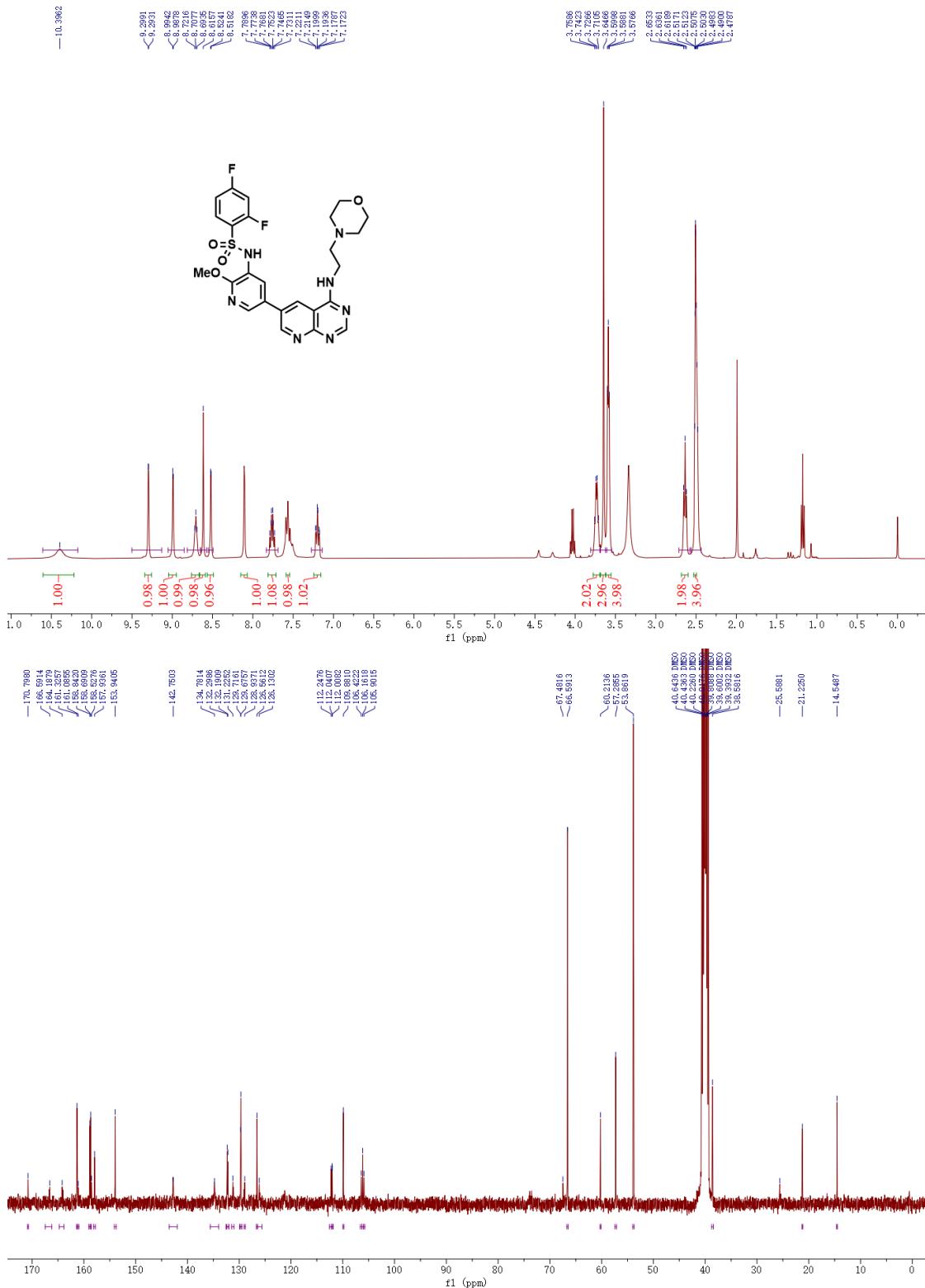
**Figure S16.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **17d** (DMSO-d6).



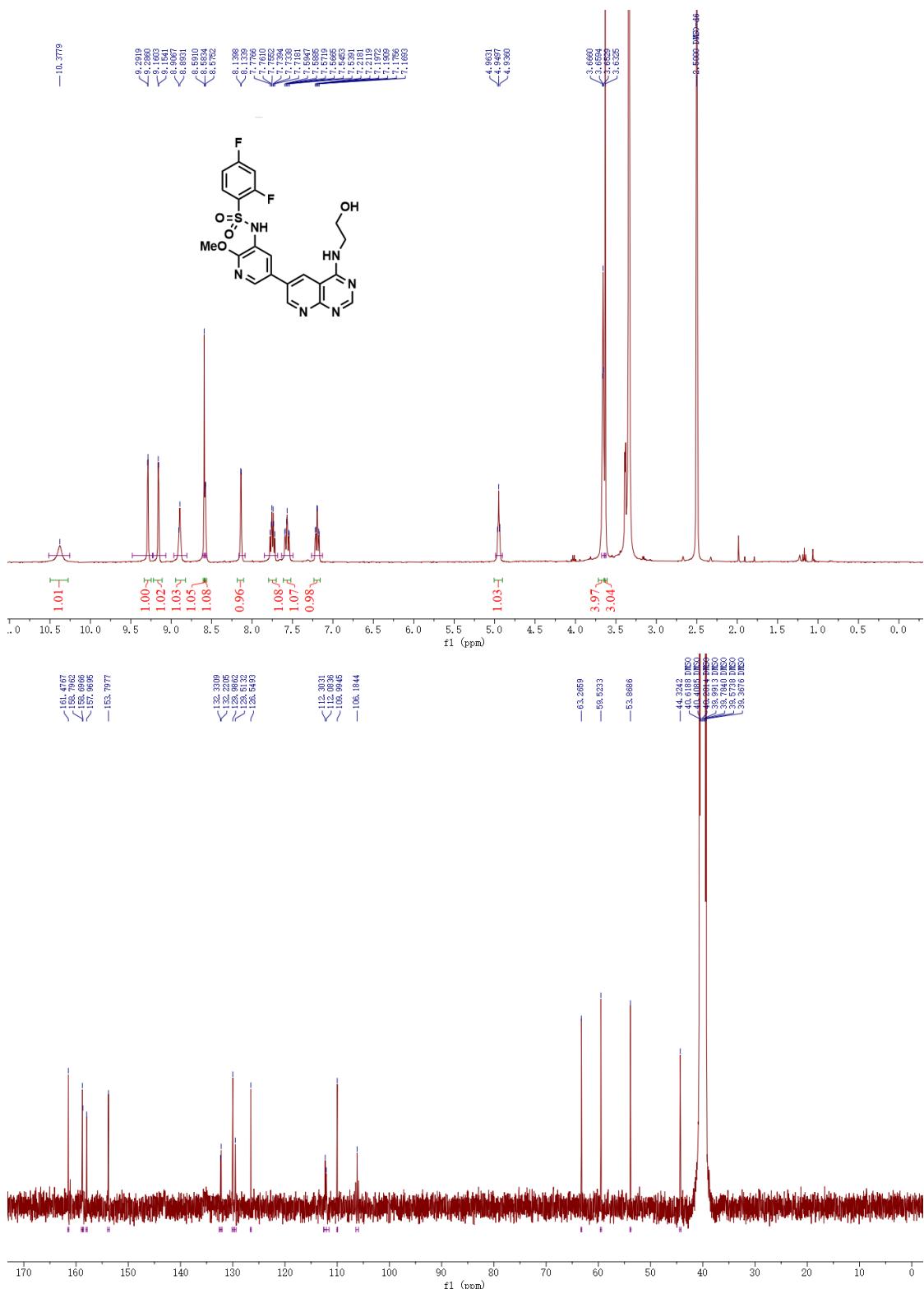
**Figure S17.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **17e** (DMSO-d6).



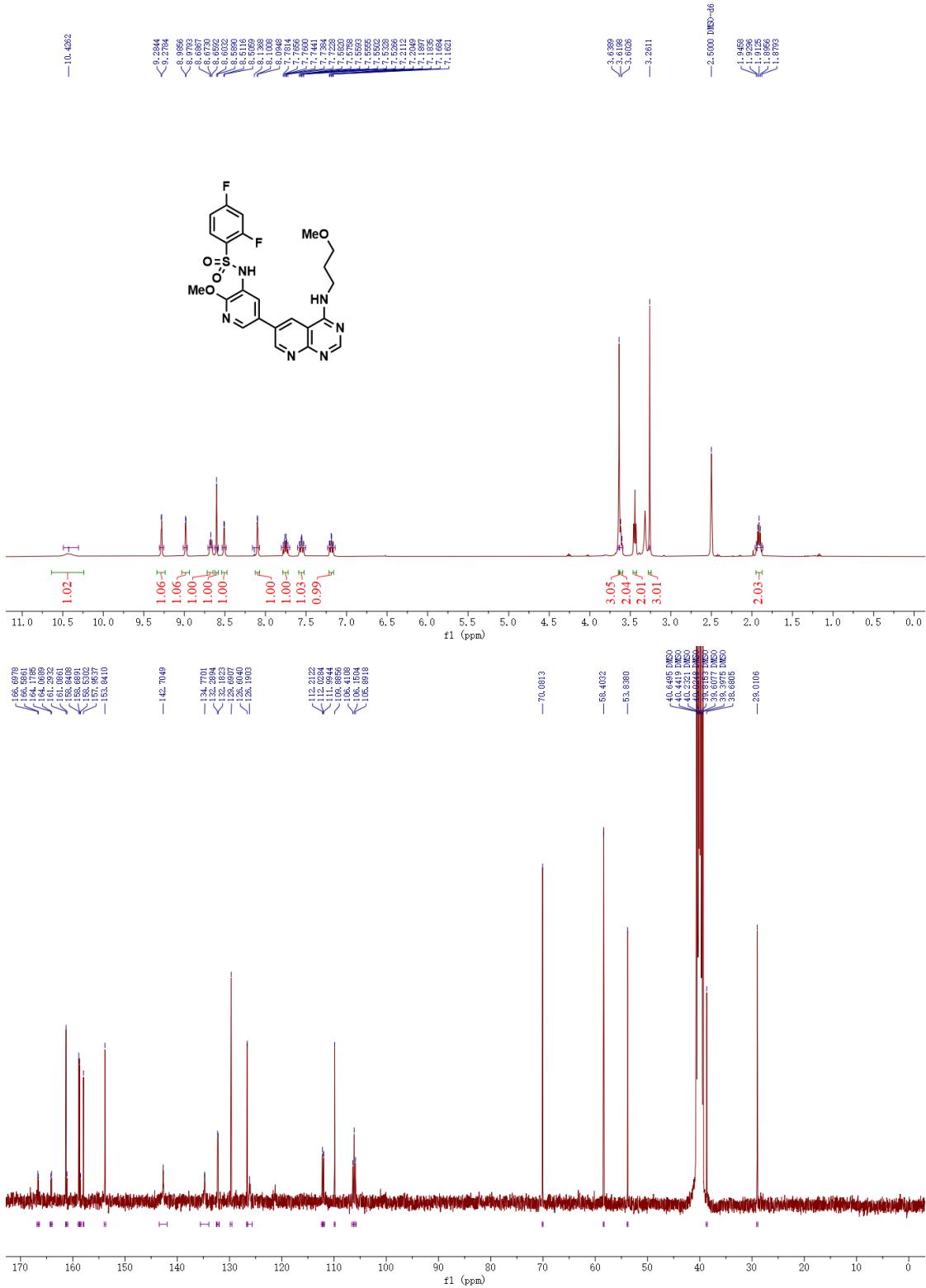
**Figure S18.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **17f** (DMSO-d6).



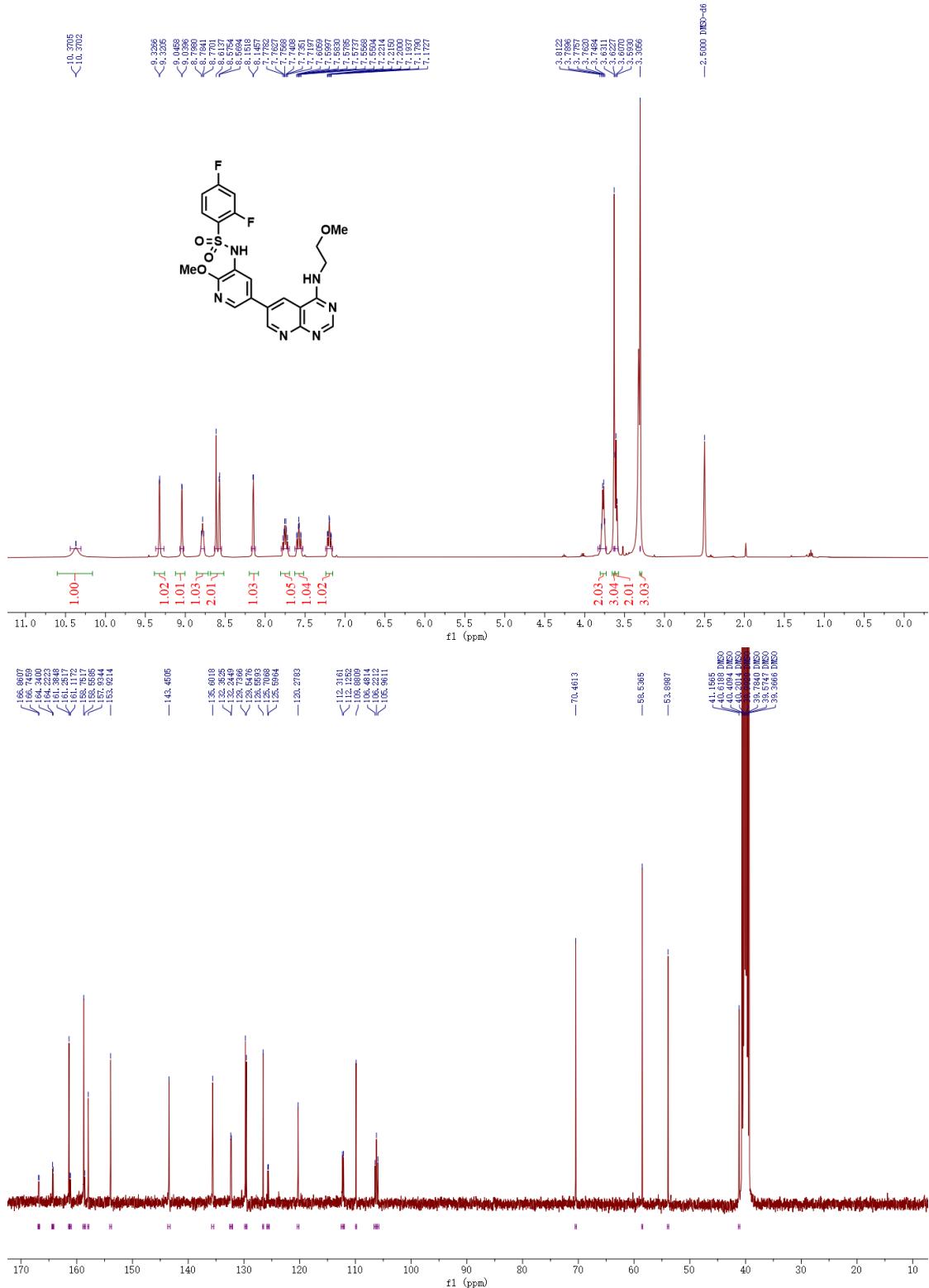
**Figure S19.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **17g** (DMSO-d<sub>6</sub>).



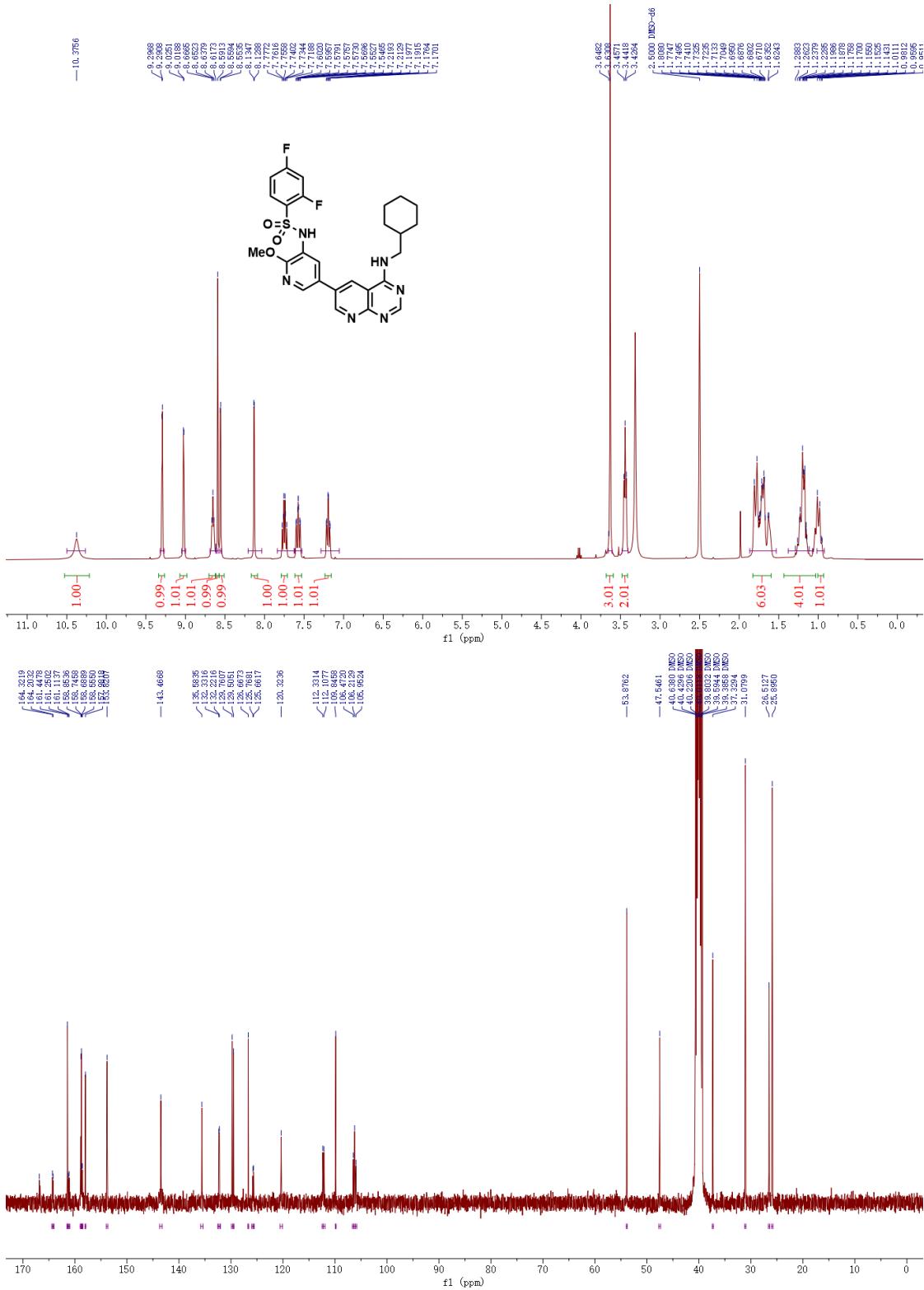
**Figure S20.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **17h** (DMSO-d<sub>6</sub>).



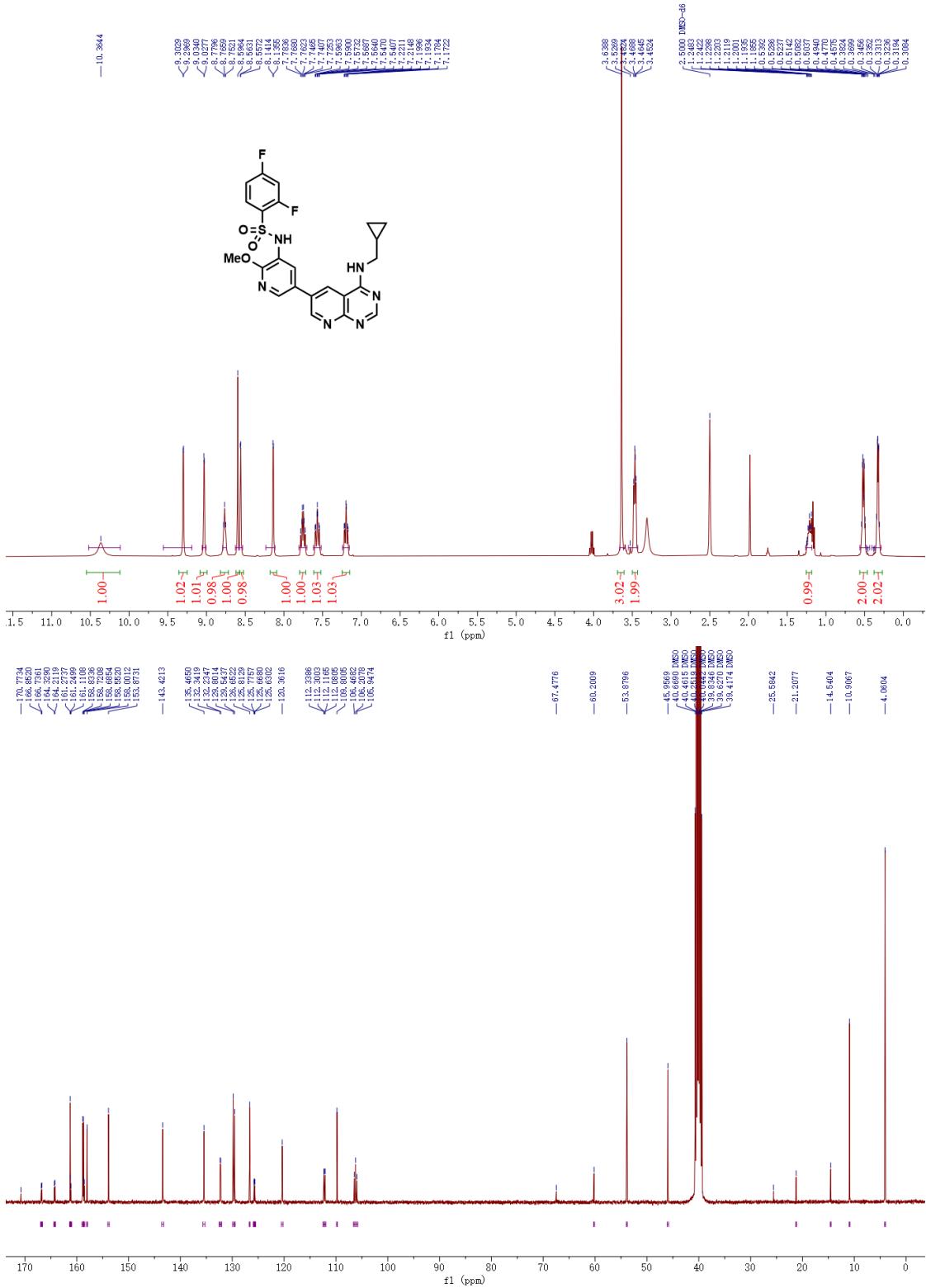
**Figure S21.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **17i** (DMSO-d6).



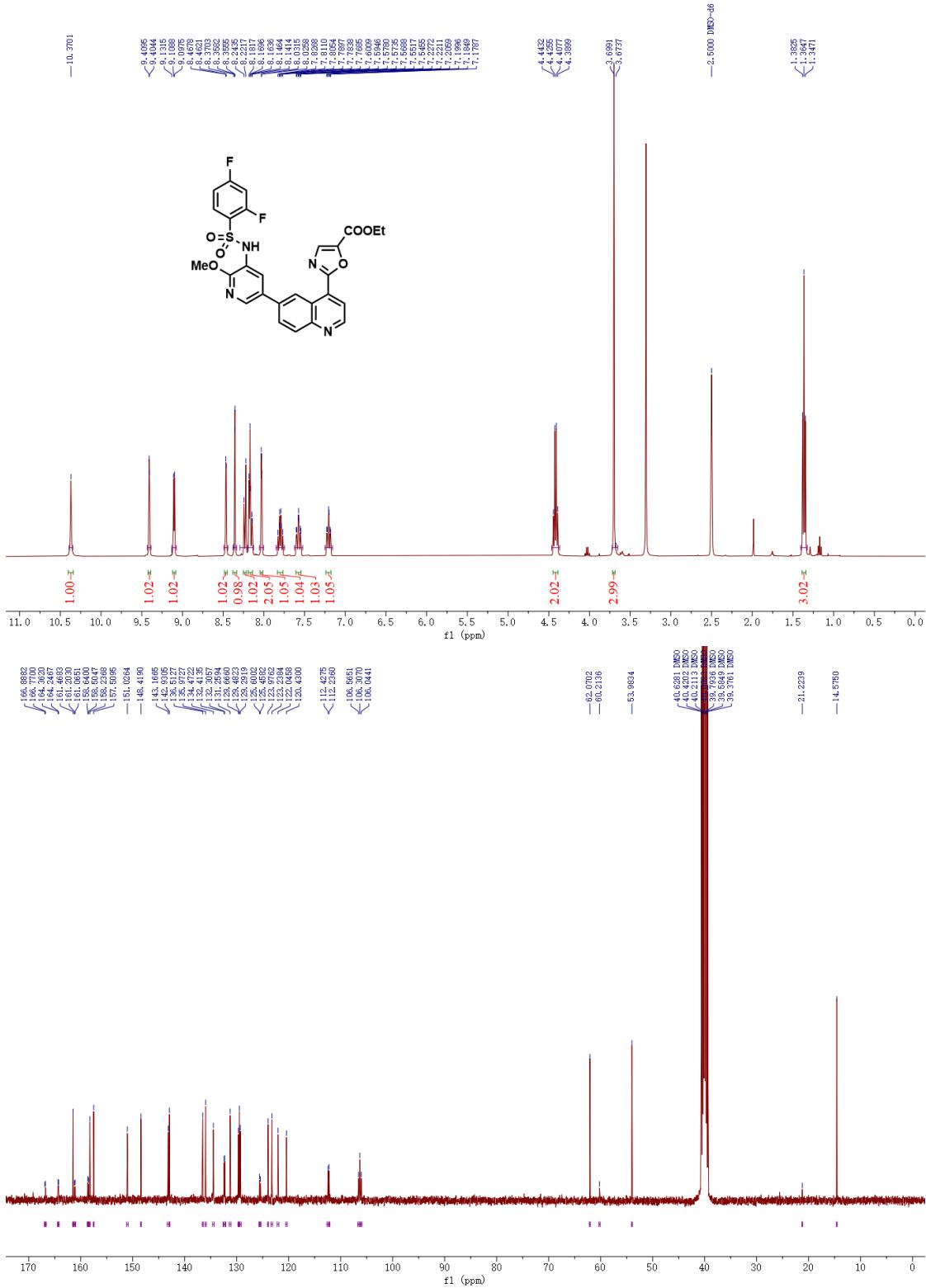
**Figure S22.** <sup>1</sup>H and <sup>13</sup>C NMR spectra of **17j** (DMSO-d<sub>6</sub>).



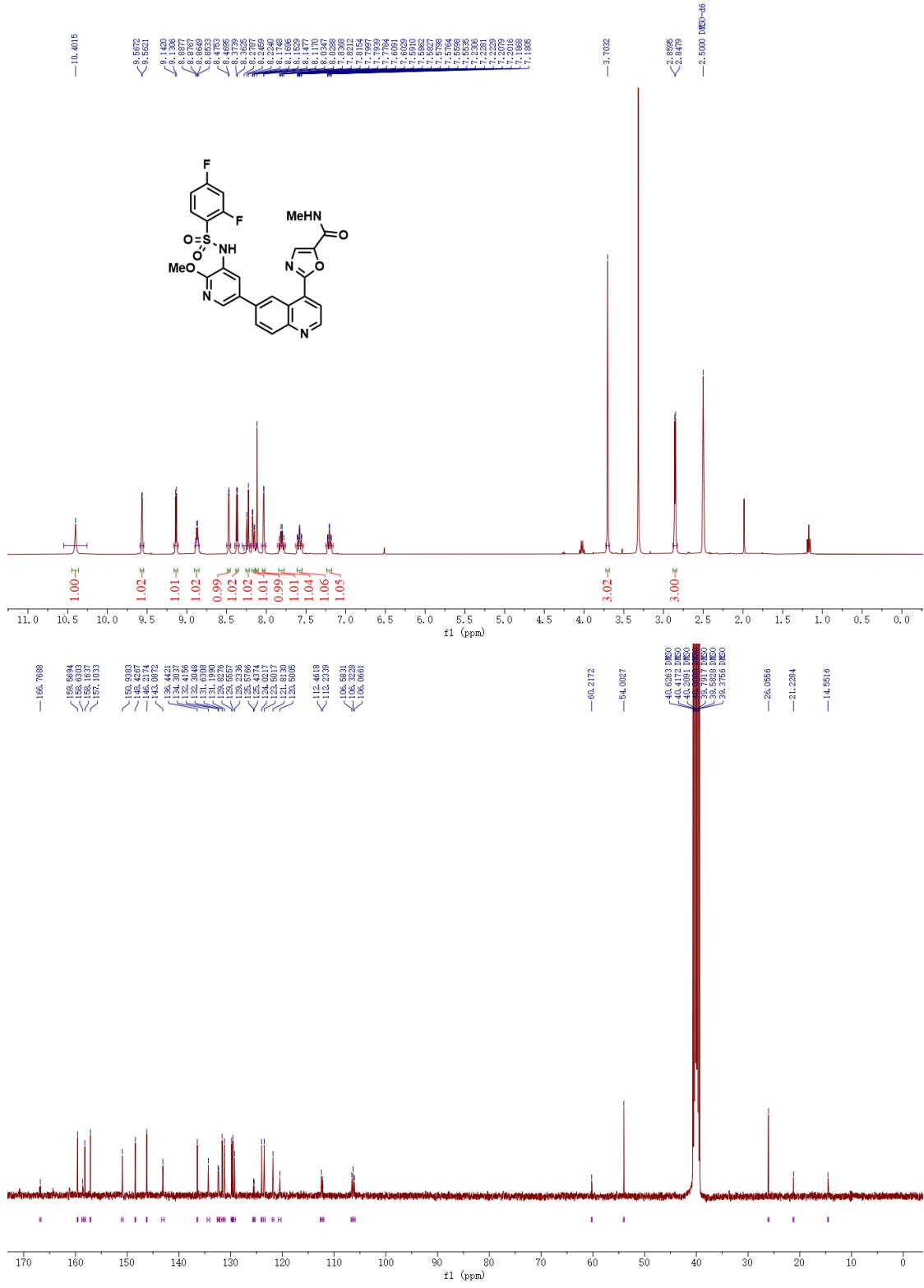
**Figure S23.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **17k** (DMSO-d<sub>6</sub>).



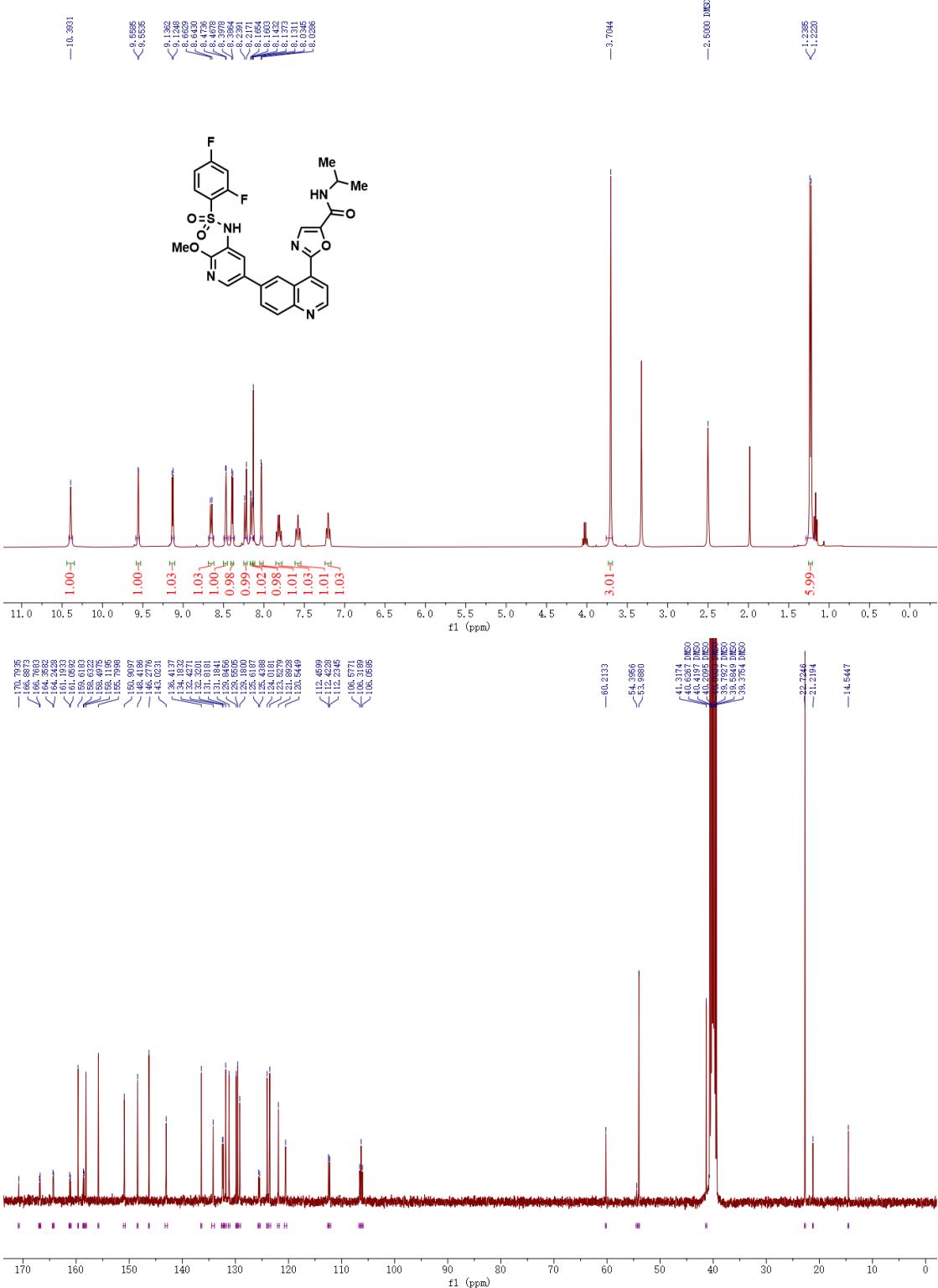
**Figure S24.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **17l** (DMSO-d6).



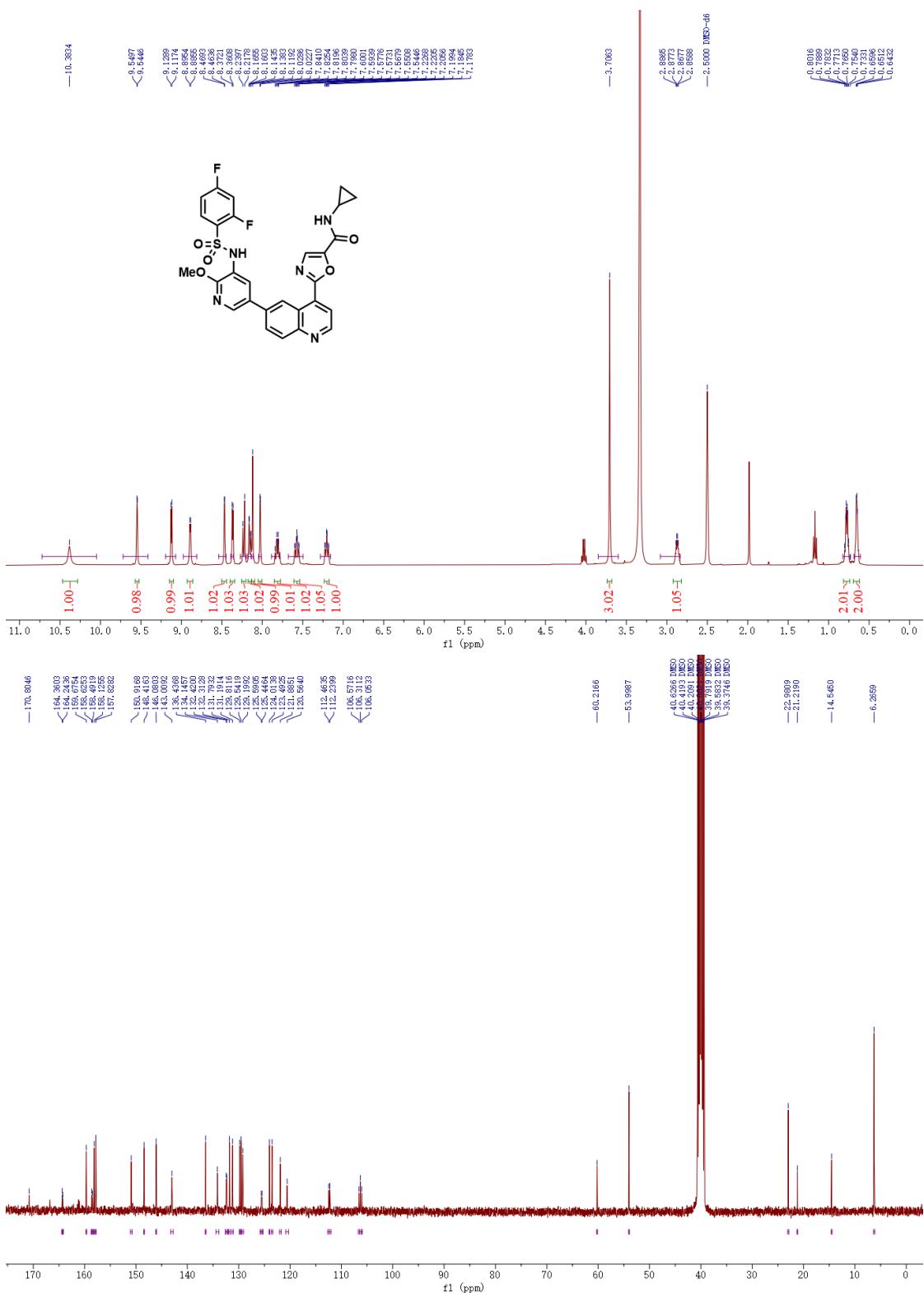
**Figure S25.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **22a** (DMSO-d6).



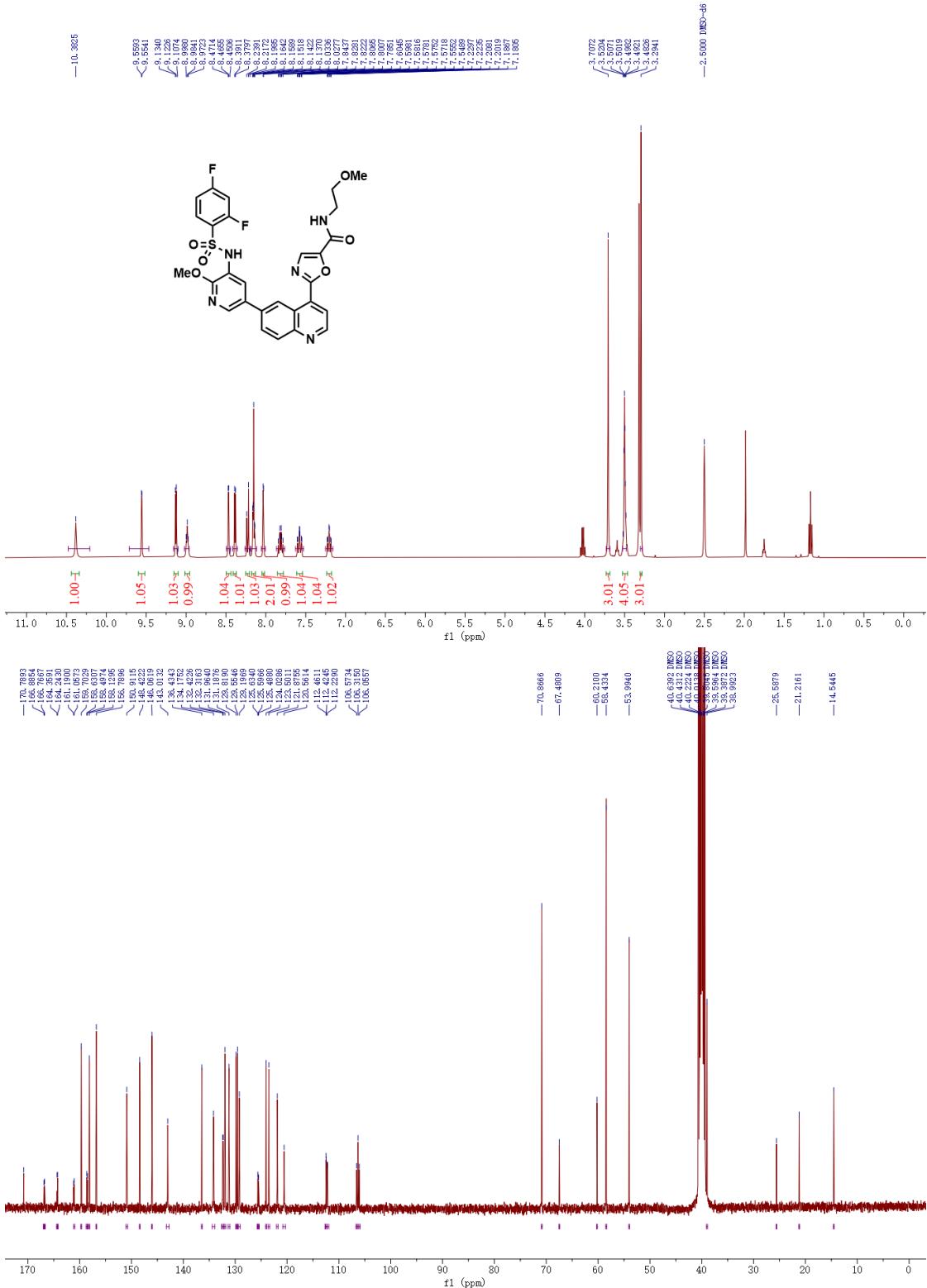
**Figure S26.** <sup>1</sup>H and <sup>13</sup>C NMR spectra of **22b** (DMSO-d<sub>6</sub>).



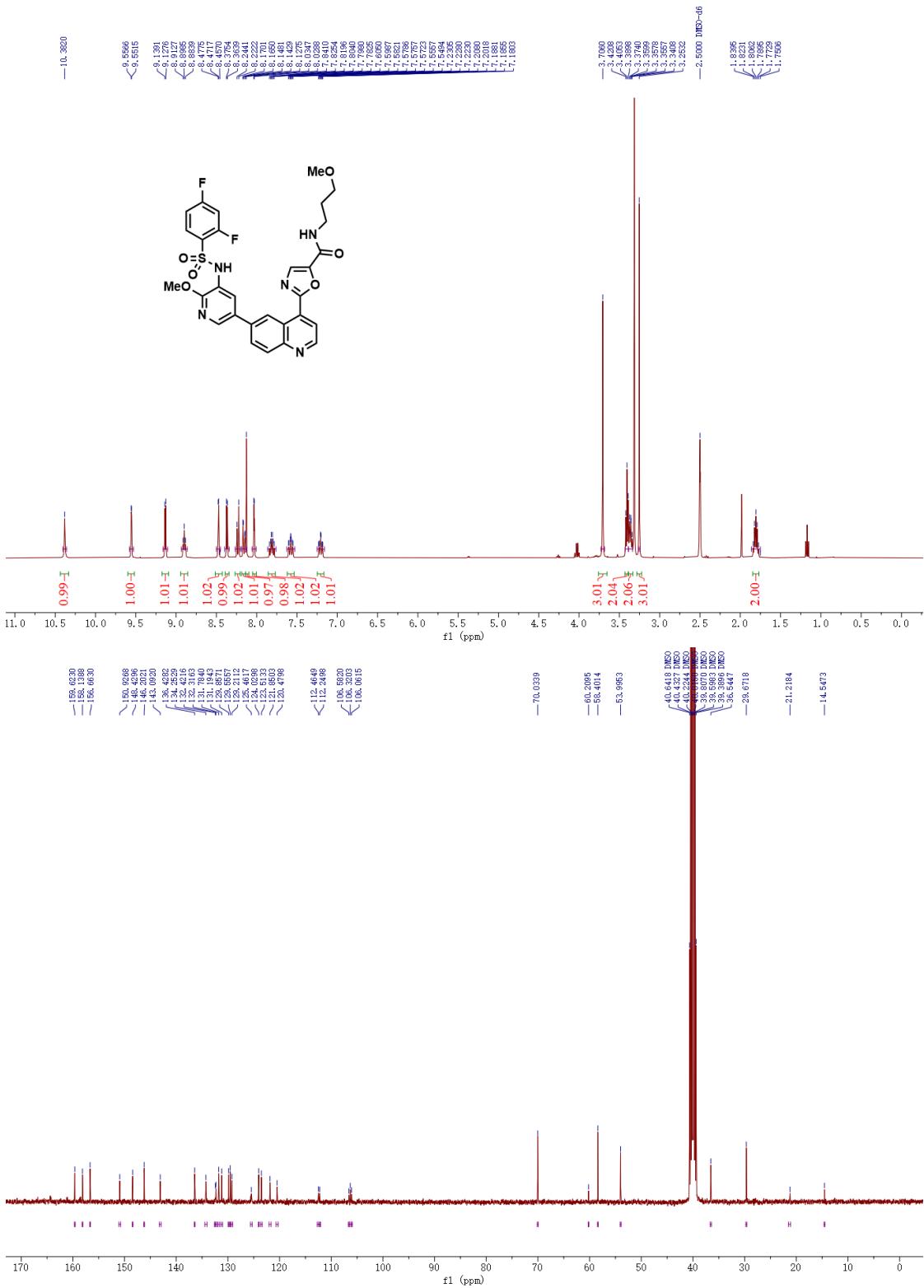
**Figure S27.** <sup>1</sup>H and <sup>13</sup>C NMR spectra of **22c** (DMSO-d<sub>6</sub>).



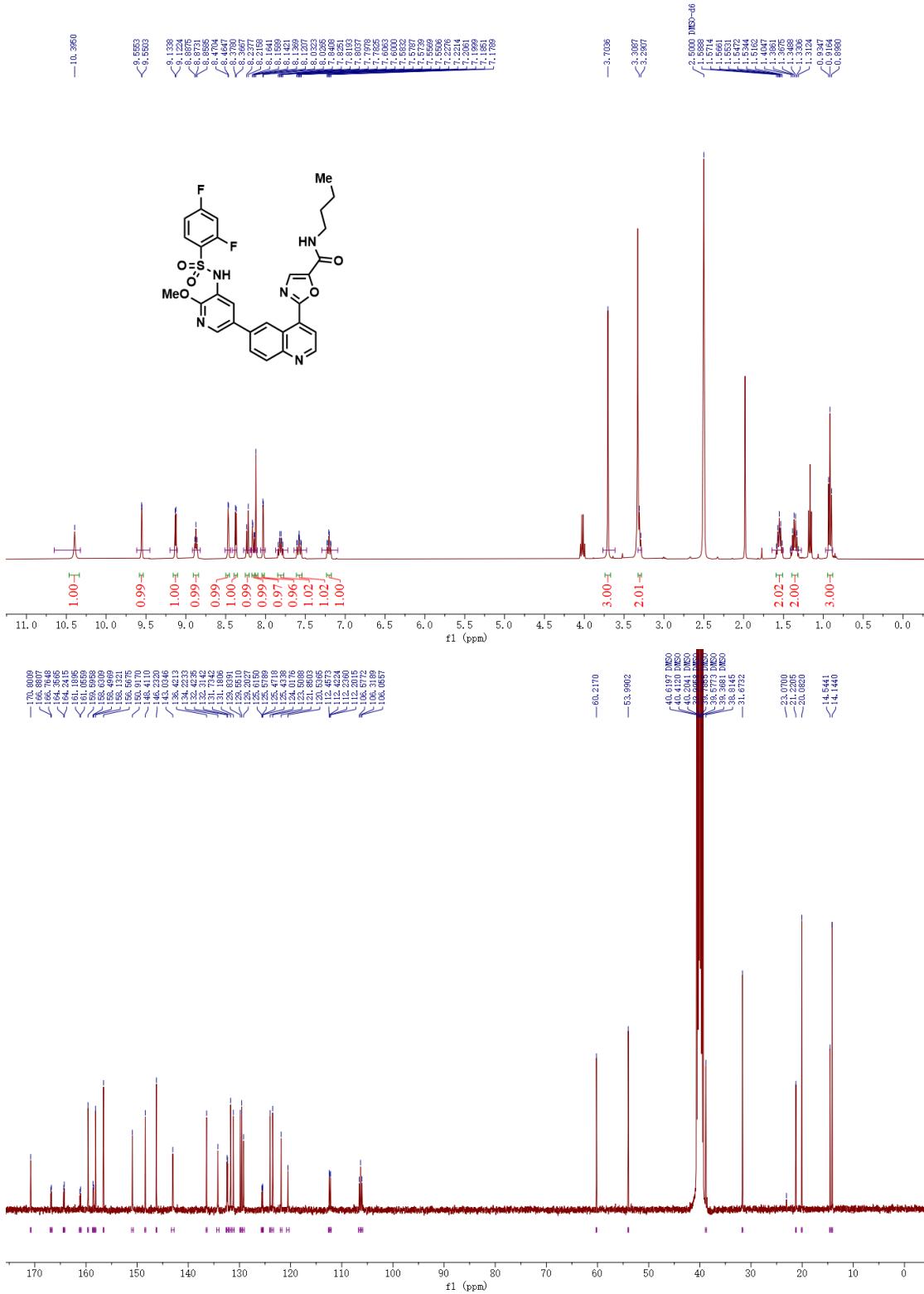
**Figure S28.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **22d** (DMSO-d<sub>6</sub>).



**Figure S29.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **22e** (DMSO-d6).



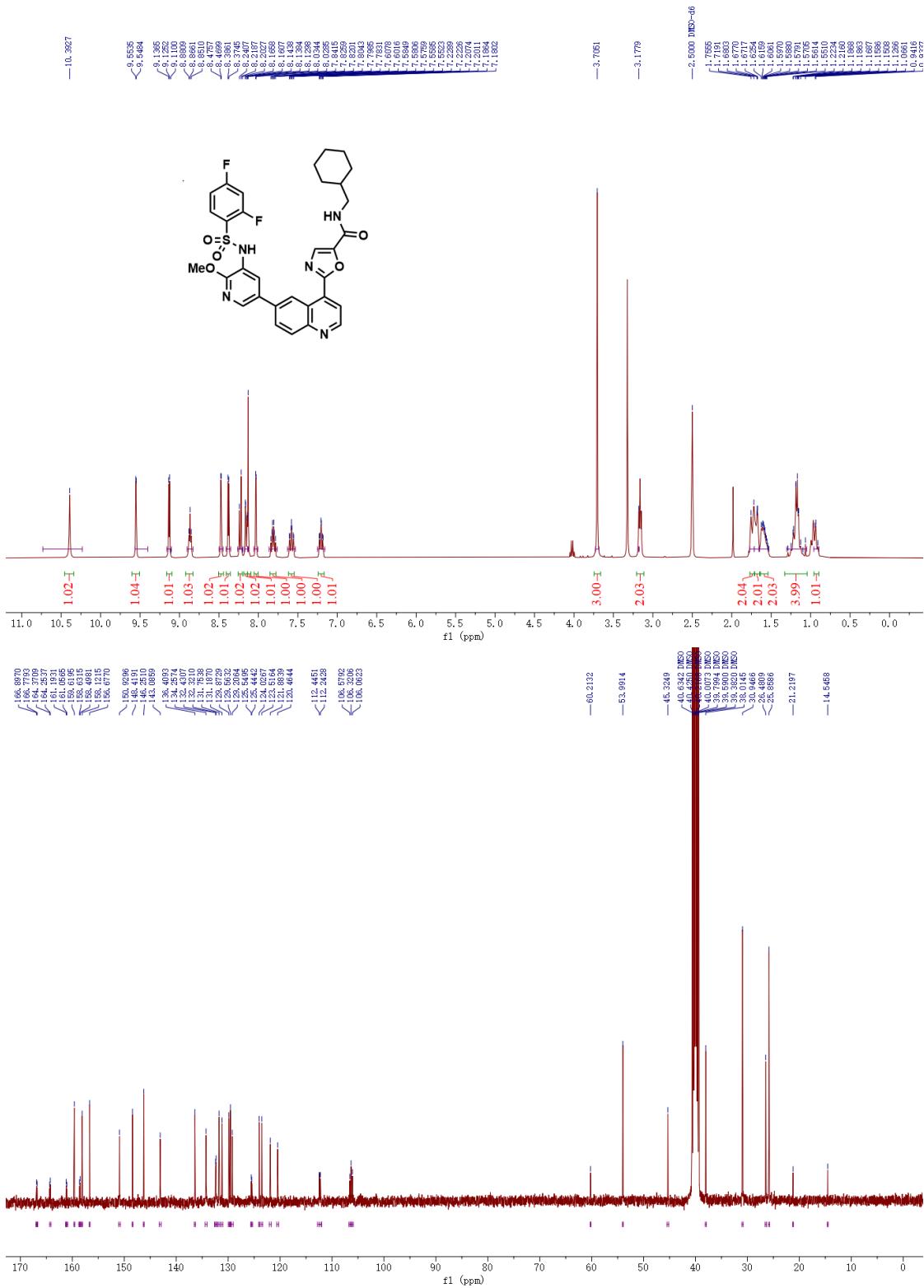
**Figure S30.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **22f** (DMSO-d6).



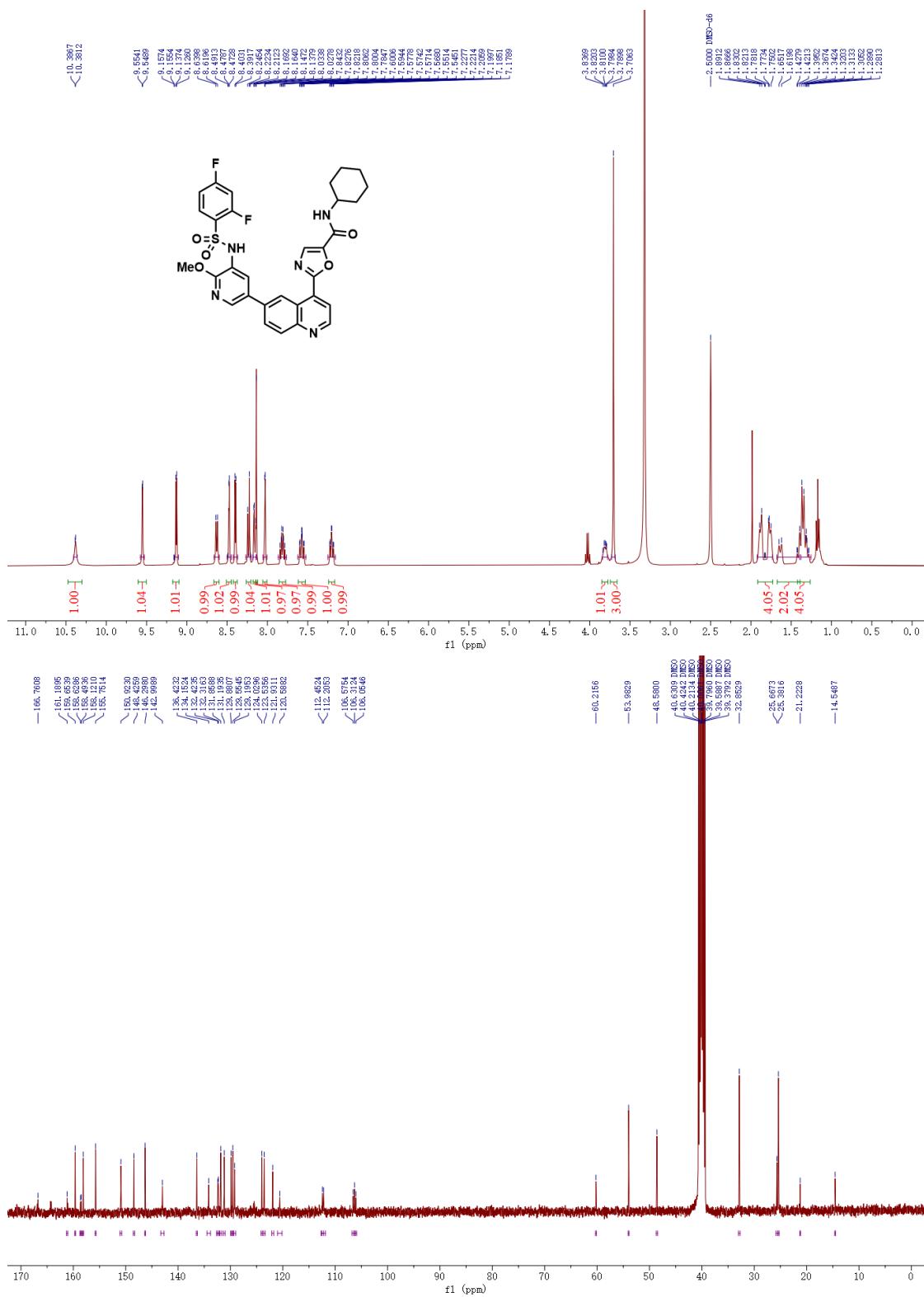
**Figure S31.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **22g** (DMSO-d<sub>6</sub>).



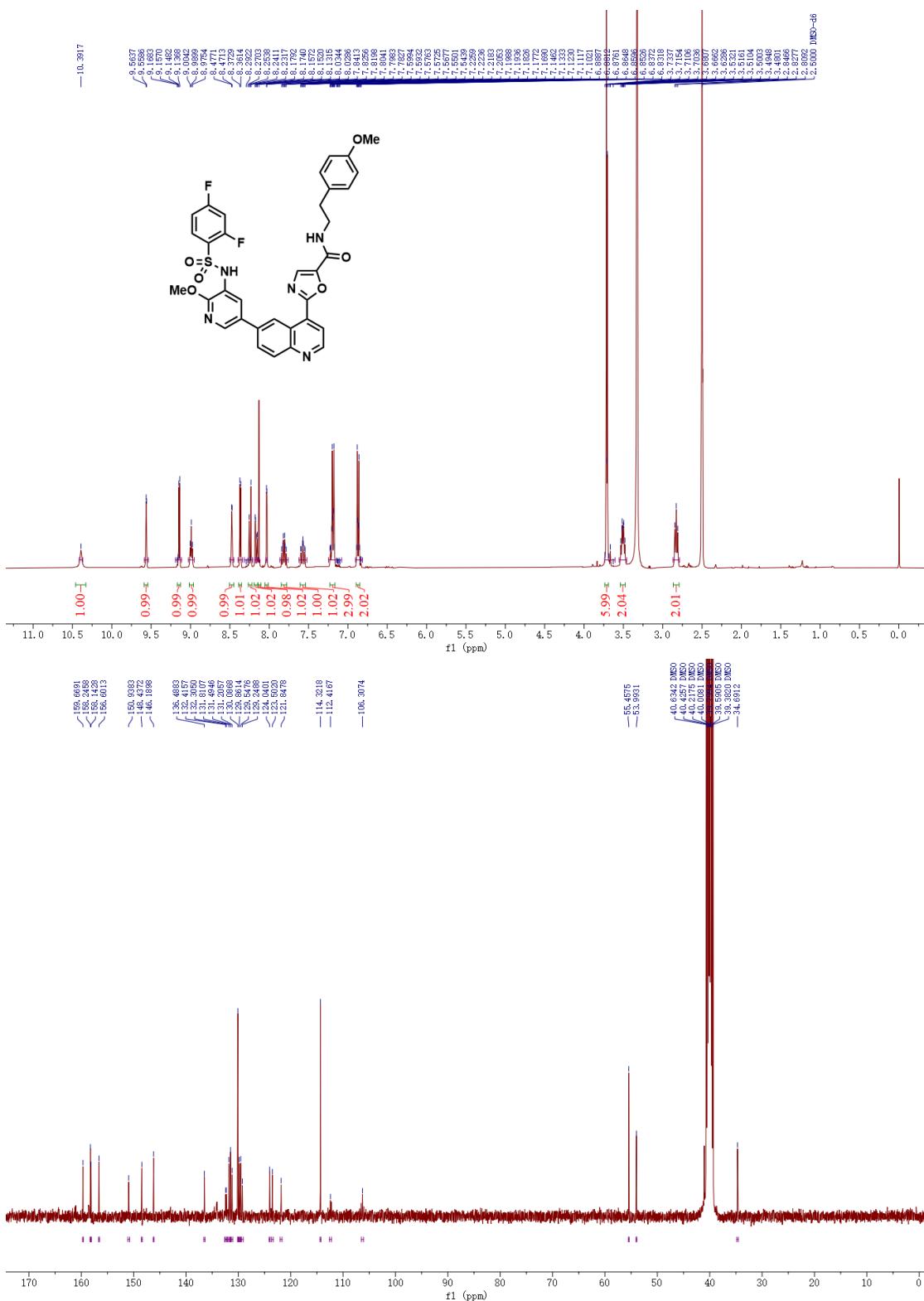
**Figure S32.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **22h** (DMSO-d6).



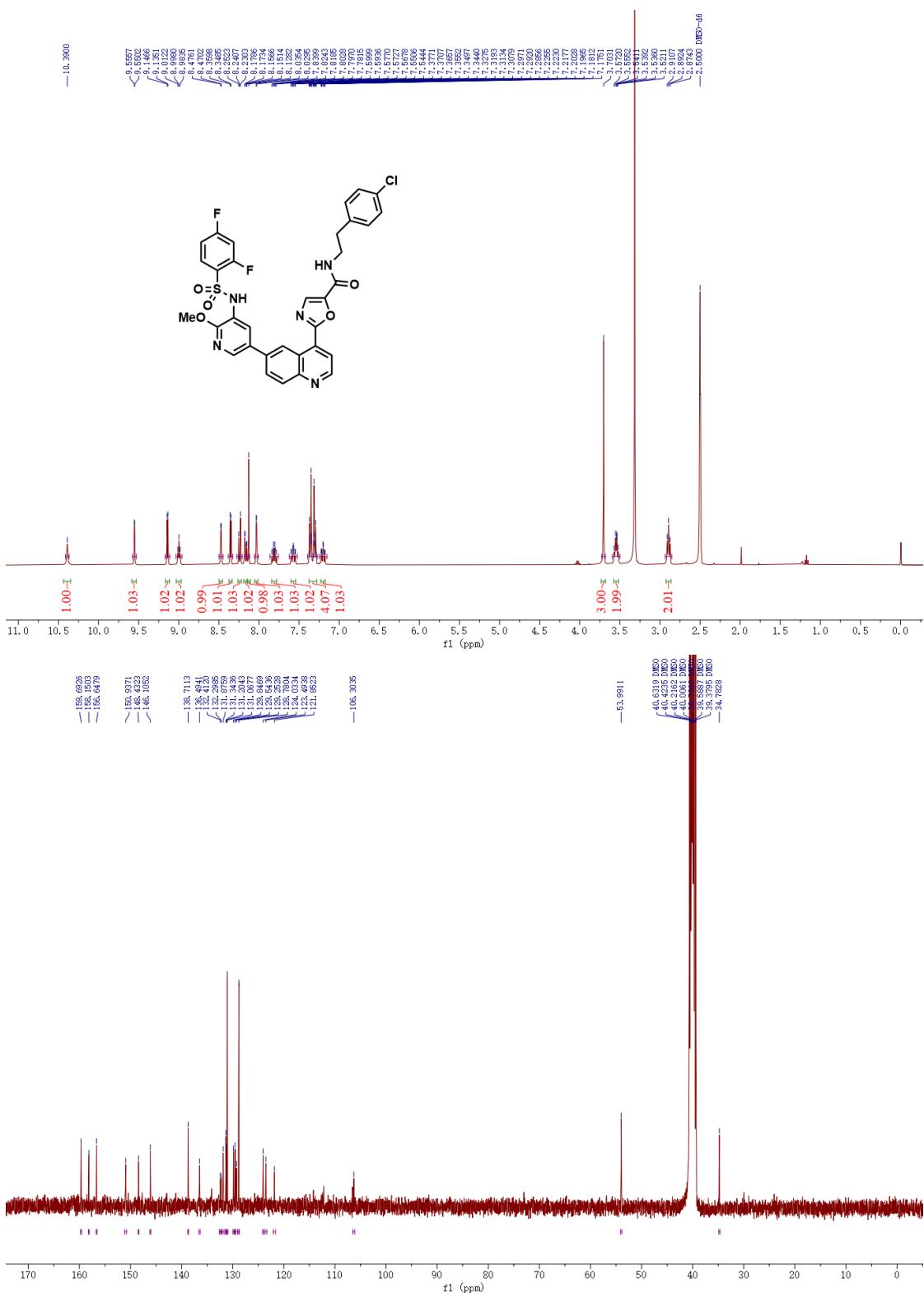
**Figure S33.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **22i** (DMSO-d<sub>6</sub>).



**Figure S34.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **22j** (DMSO-d<sub>6</sub>).



**Figure S35.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **22k** (DMSO-d<sub>6</sub>).



**Figure S36.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **22l** (DMSO-d6).