

Supplementary Information

Discovery of a series of Theophylline derivatives containing 1,2,3-triazole for treatment of non-small cell lung cancer (NSCLC)

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Figure S32-2. ^{13}C NMR spectrum (100 MHz, DMSO- d_6) of compound D32	Error! Bookmark not defined.

Figure S1-1. ^1H NMR spectrum (400MHz, DMSO-d_6) of compound D1

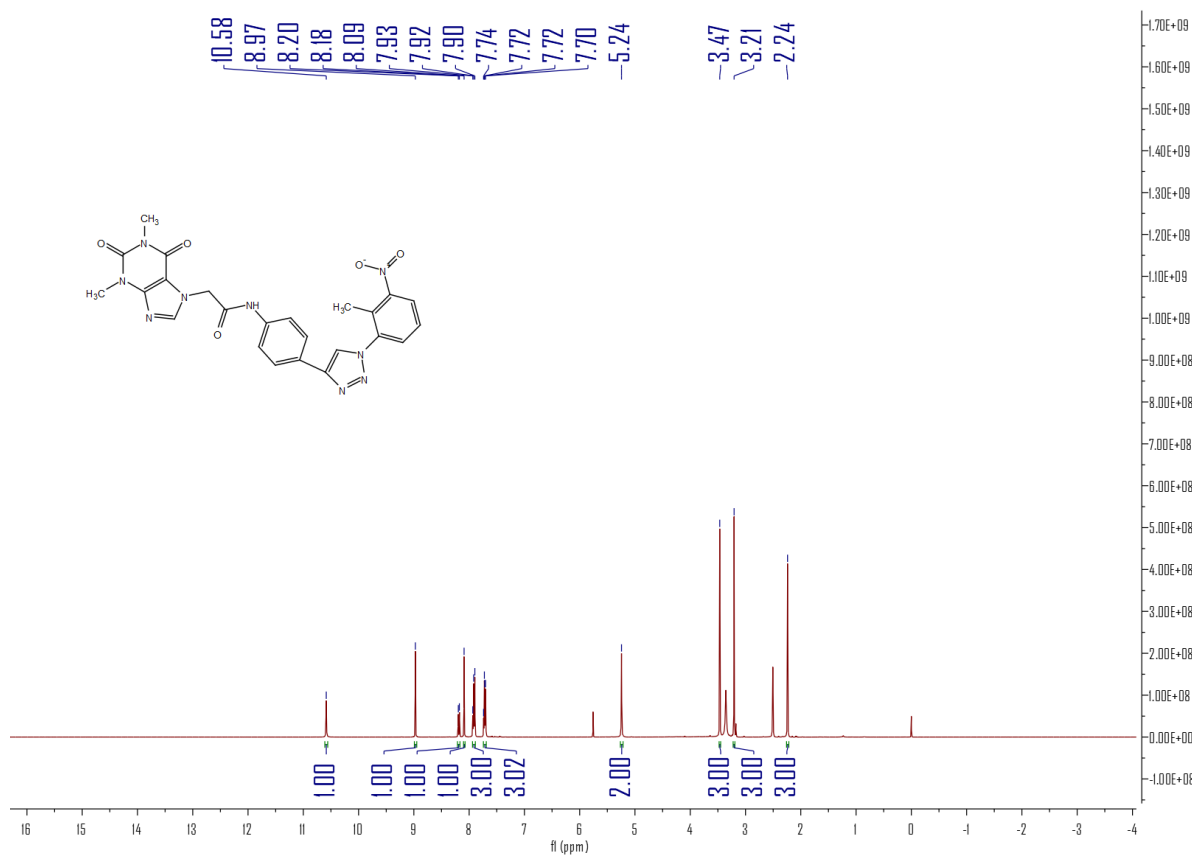


Figure S1-2. ^{13}C NMR spectrum (100MHz, DMSO- d_6) of compound D1

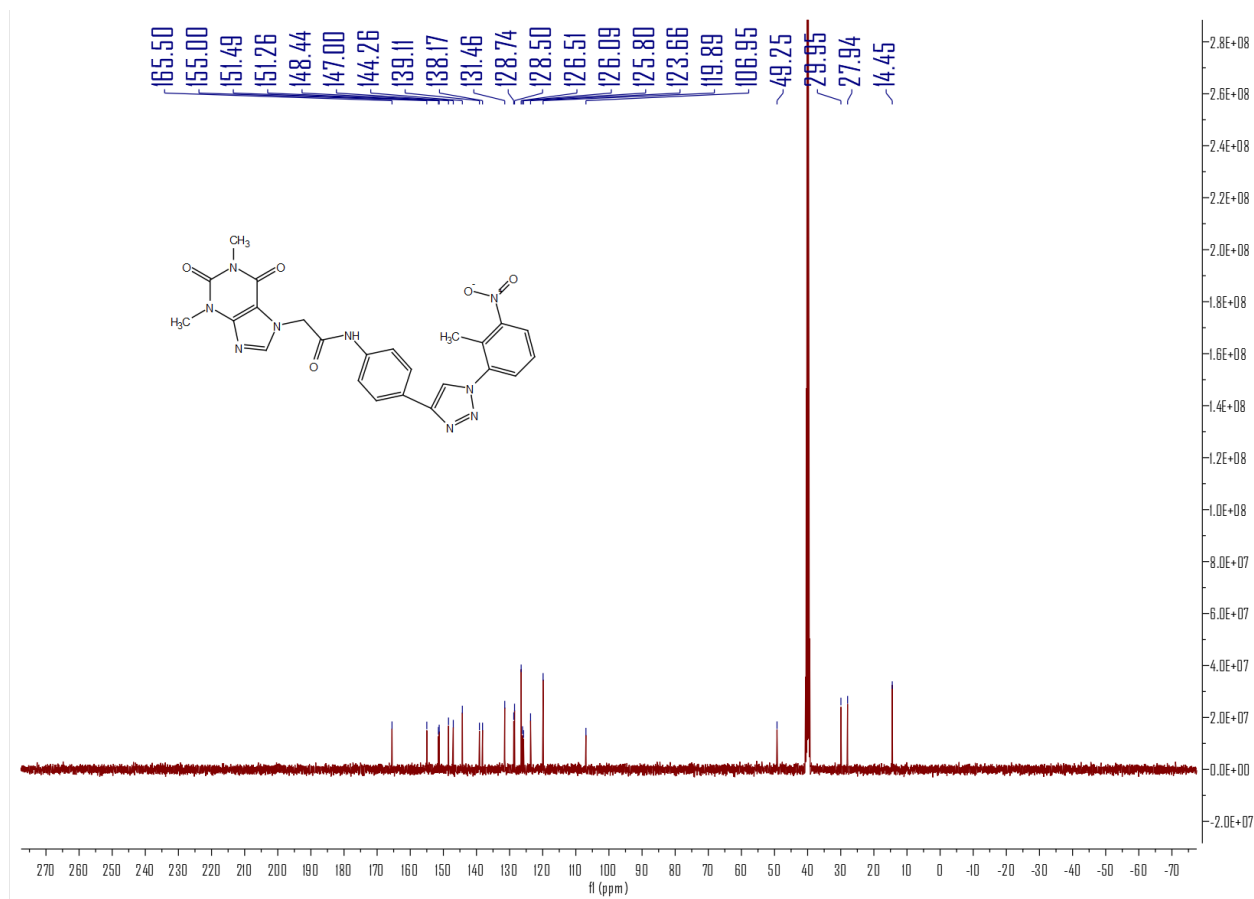


Figure S2-1. ^1H NMR spectrum (400MHz, DMSO-d_6) of compound D2

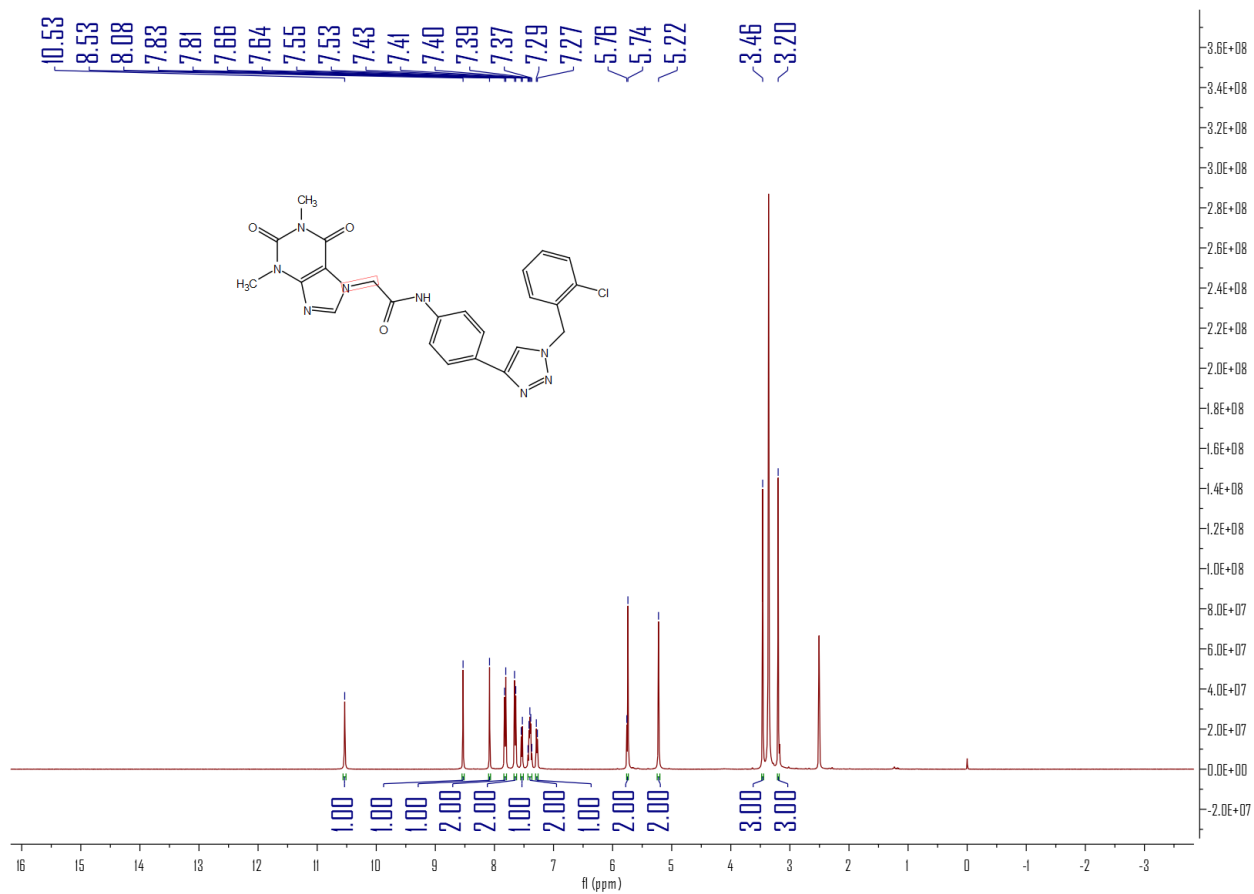


Figure S2-2. ^{13}C NMR spectrum (100MHz, DMSO- d_6) of compound D2

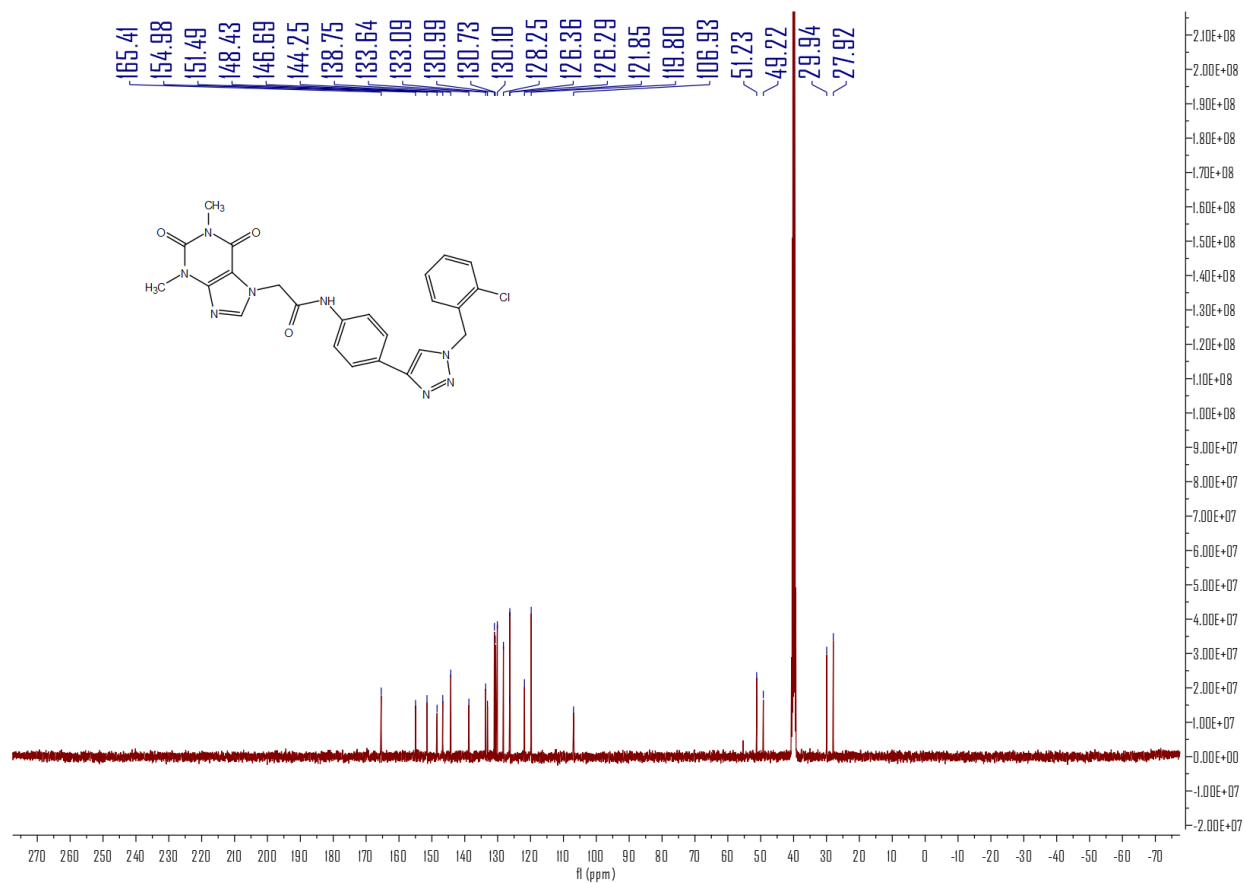


Figure S3-1. ^1H NMR spectrum (400MHz, DMSO-d_6) of compound D3

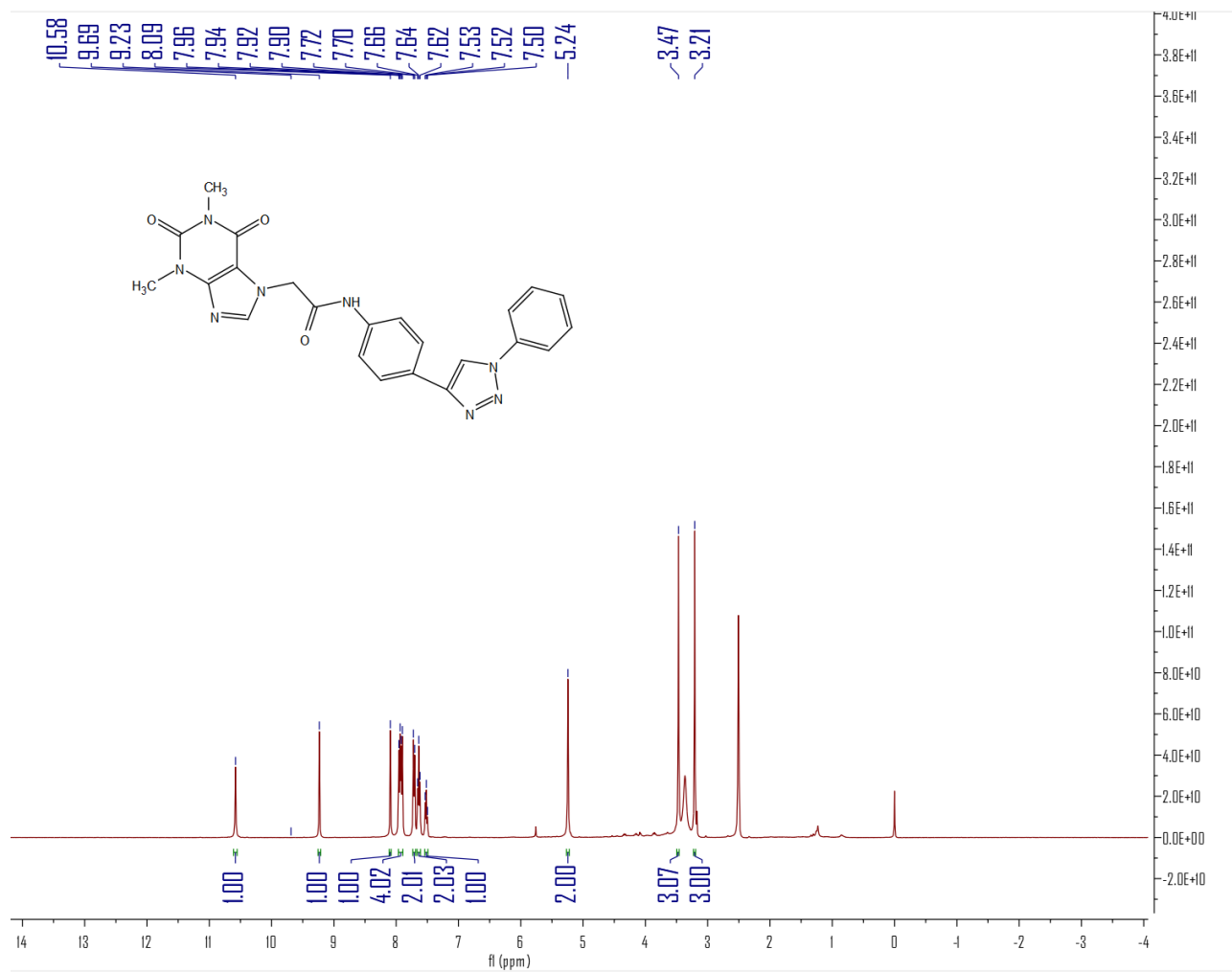


Figure S3-2. ^{13}C NMR spectrum (100MHz, DMSO- d_6) of compound D3

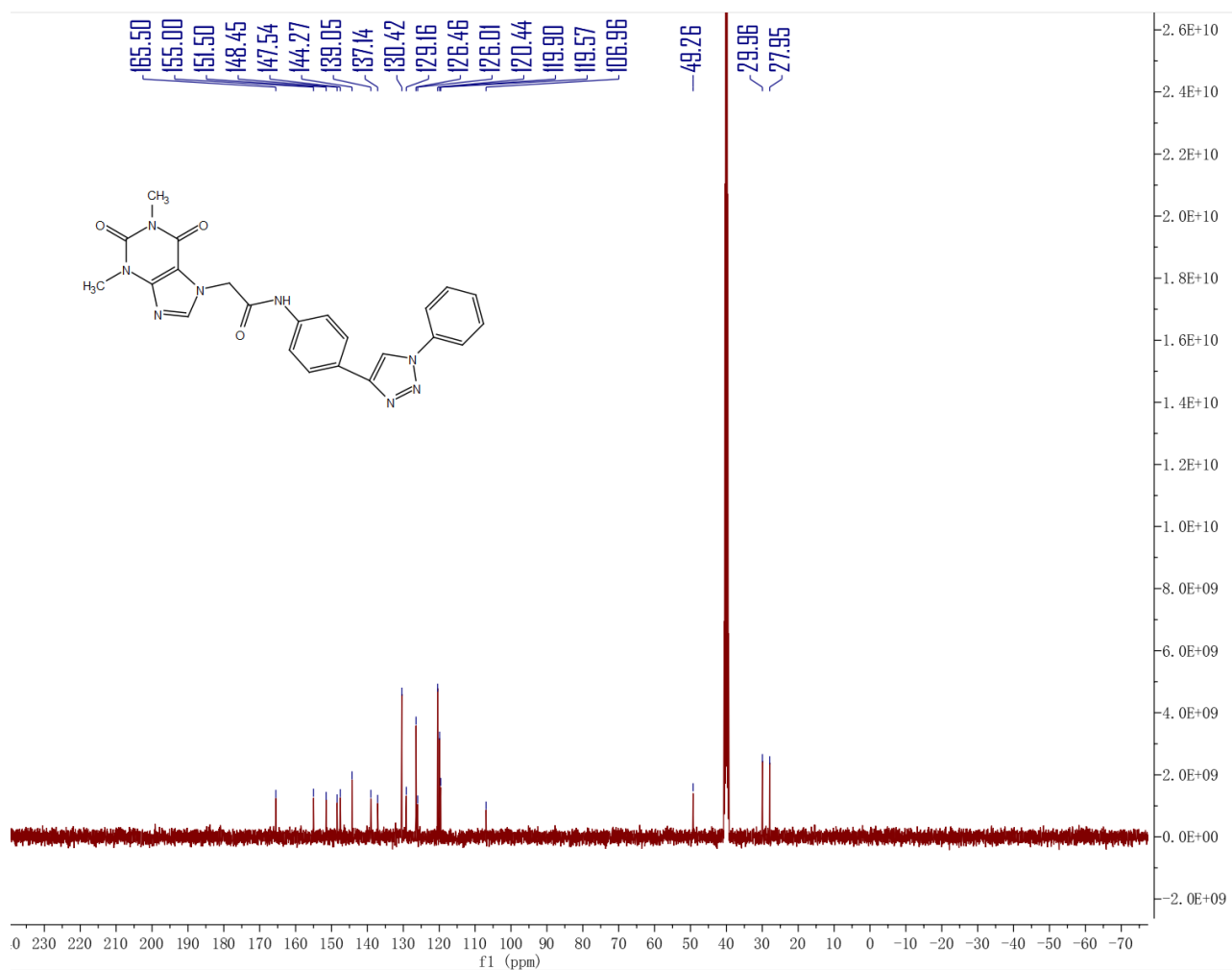


Figure S4-1. ^1H NMR spectrum (400MHz, DMSO- d_6) of compound D4



Figure S4-2. ^{13}C NMR spectrum (100MHz, DMSO- d_6) of compound D4

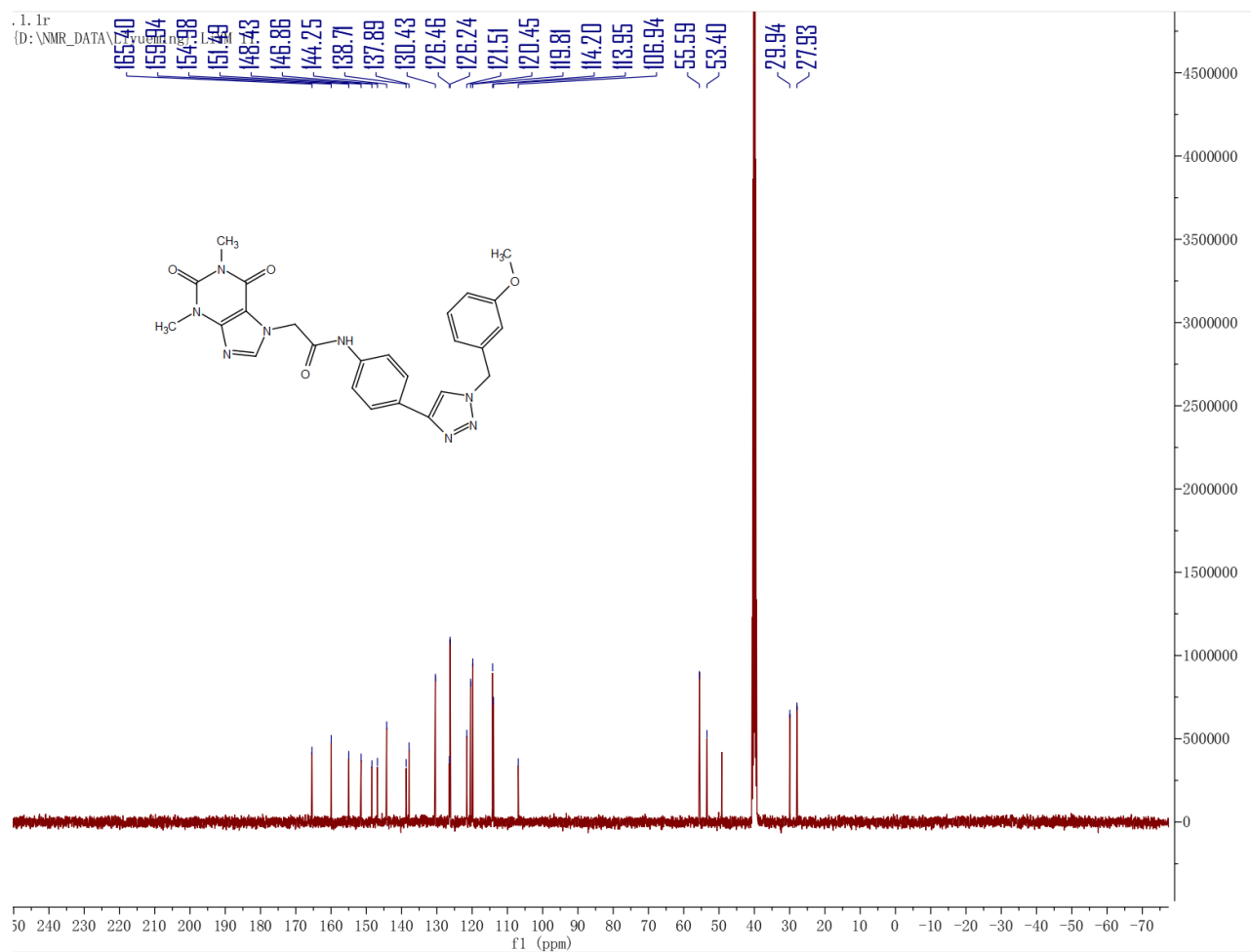


Figure S5-1. ^1H NMR spectrum (400MHz, DMSO- d_6) of compound D5

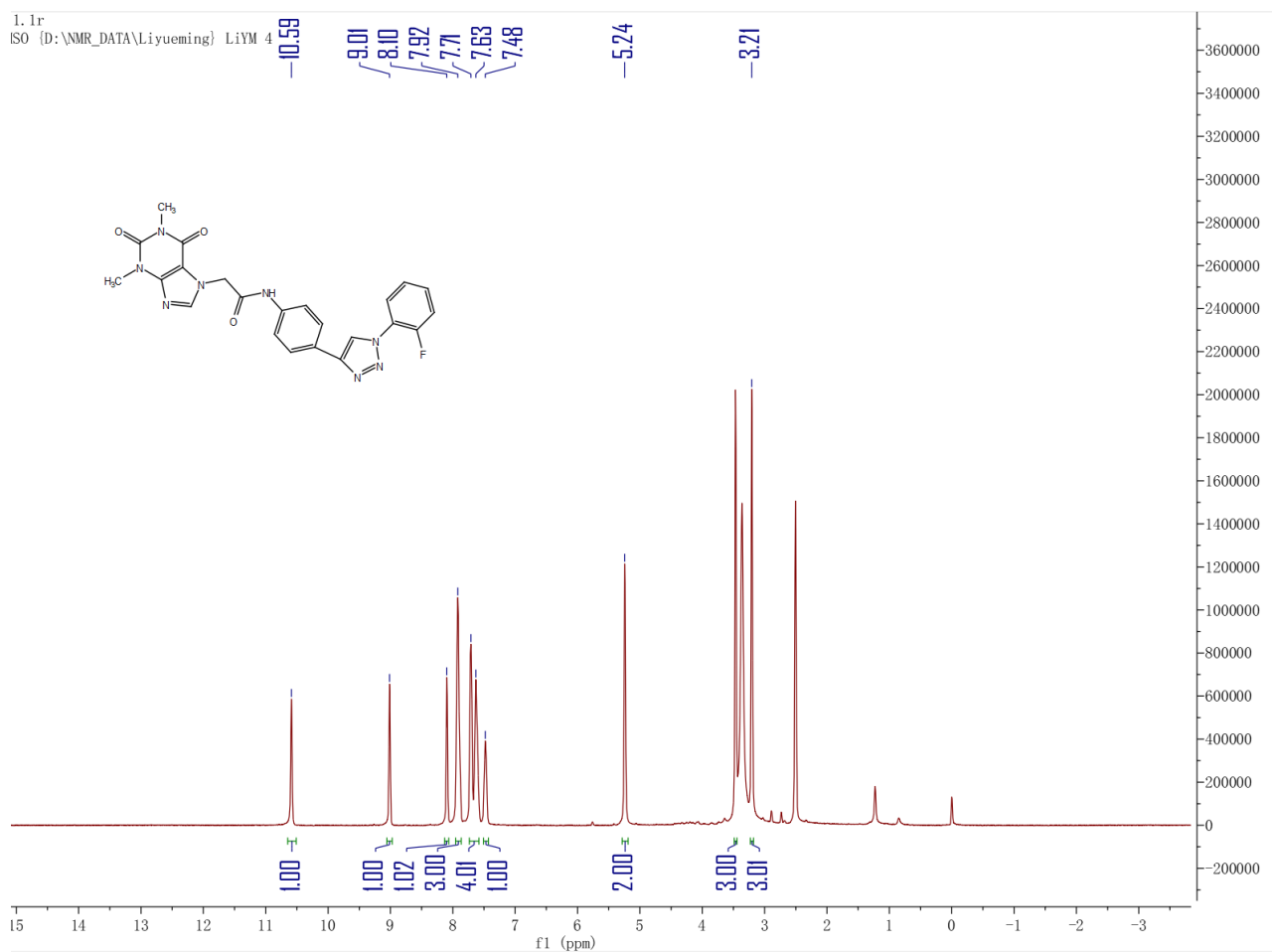


Figure S5-2. ^{13}C NMR spectrum (100MHz, DMSO- d_6) of compound D5

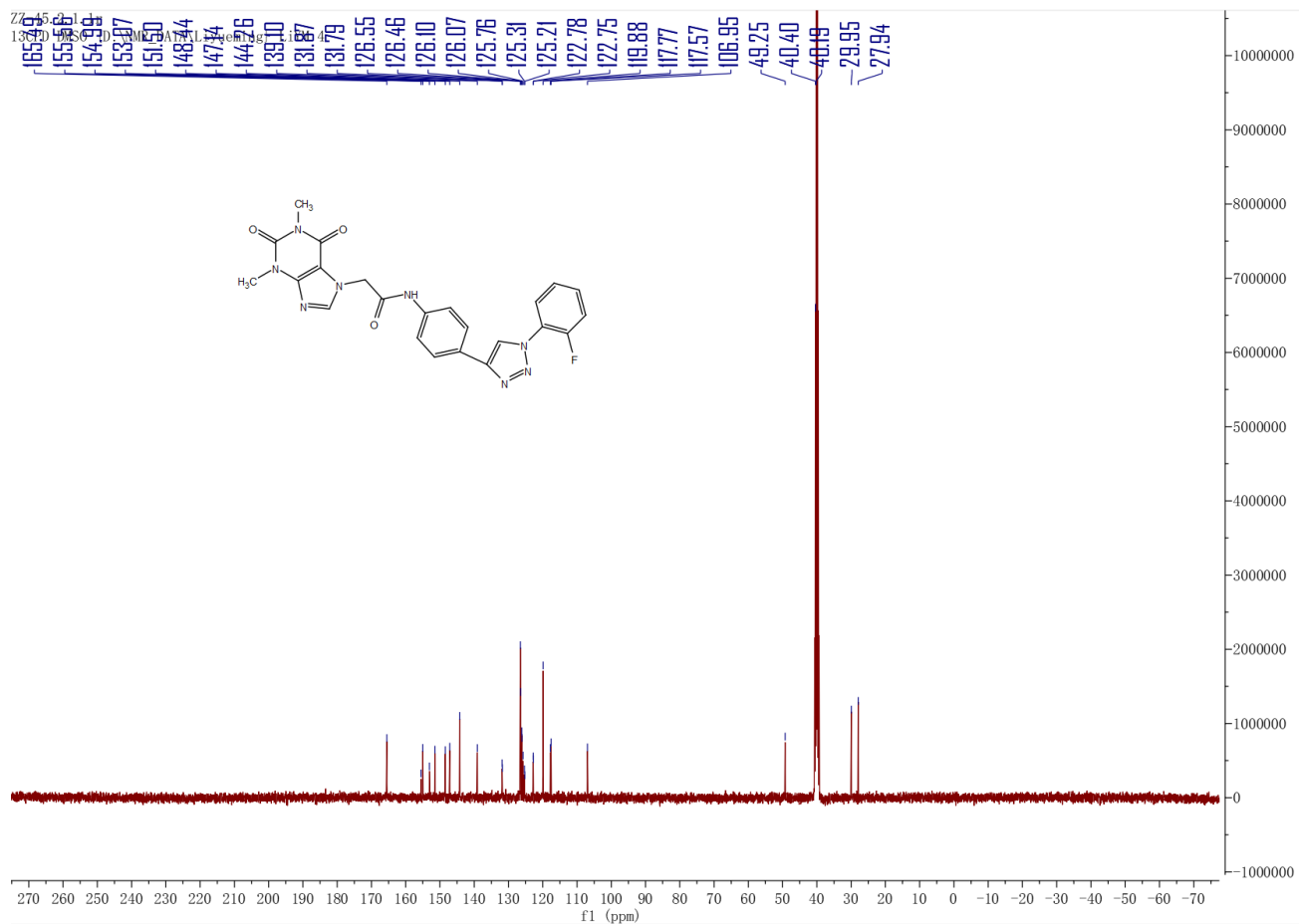


Figure S6-1. ^1H NMR spectrum (400MHz, DMSO-d_6) of compound D6

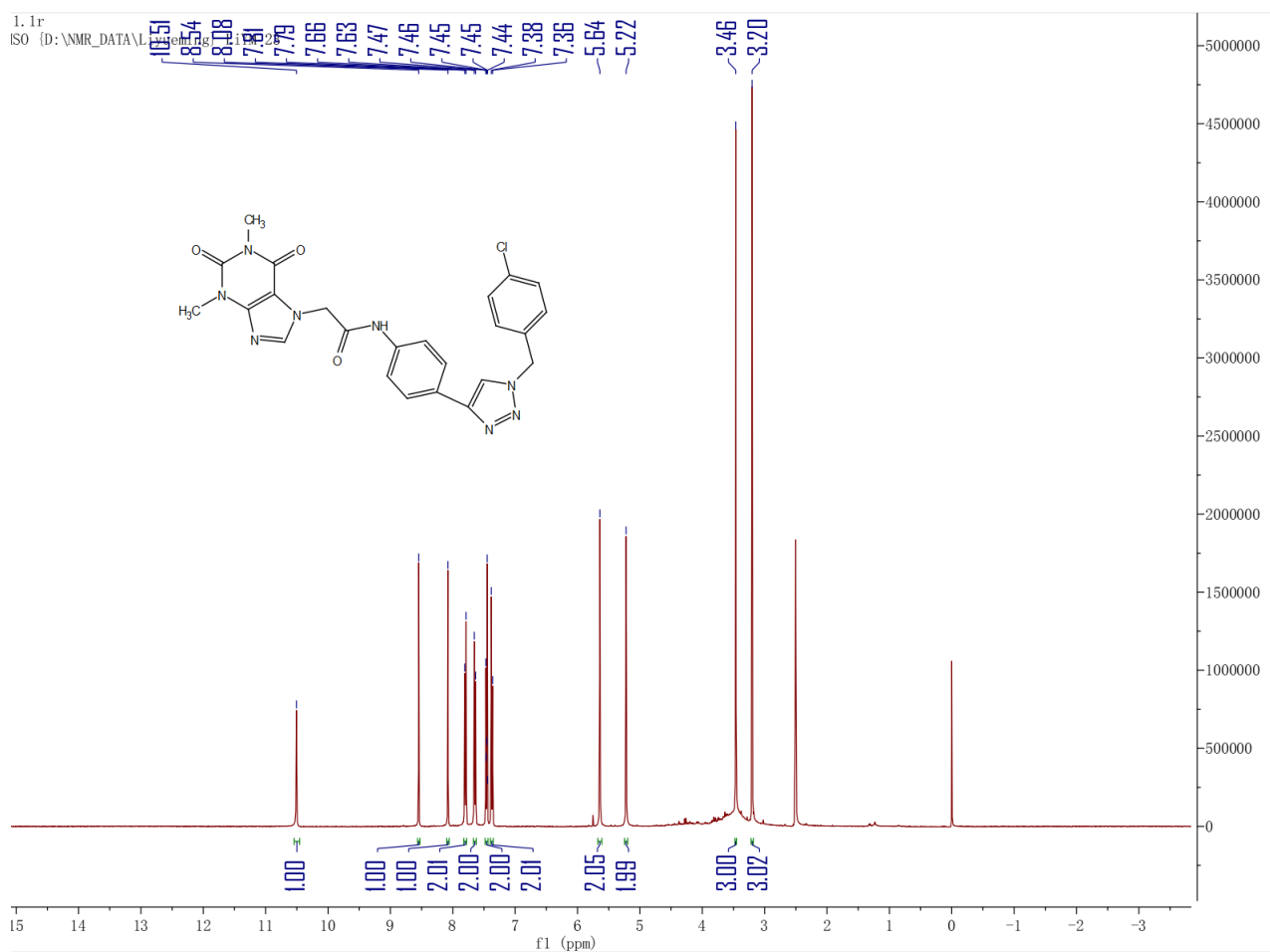


Figure S6-2. ^{13}C NMR spectrum (100MHz, DMSO- d_6) of compound D6

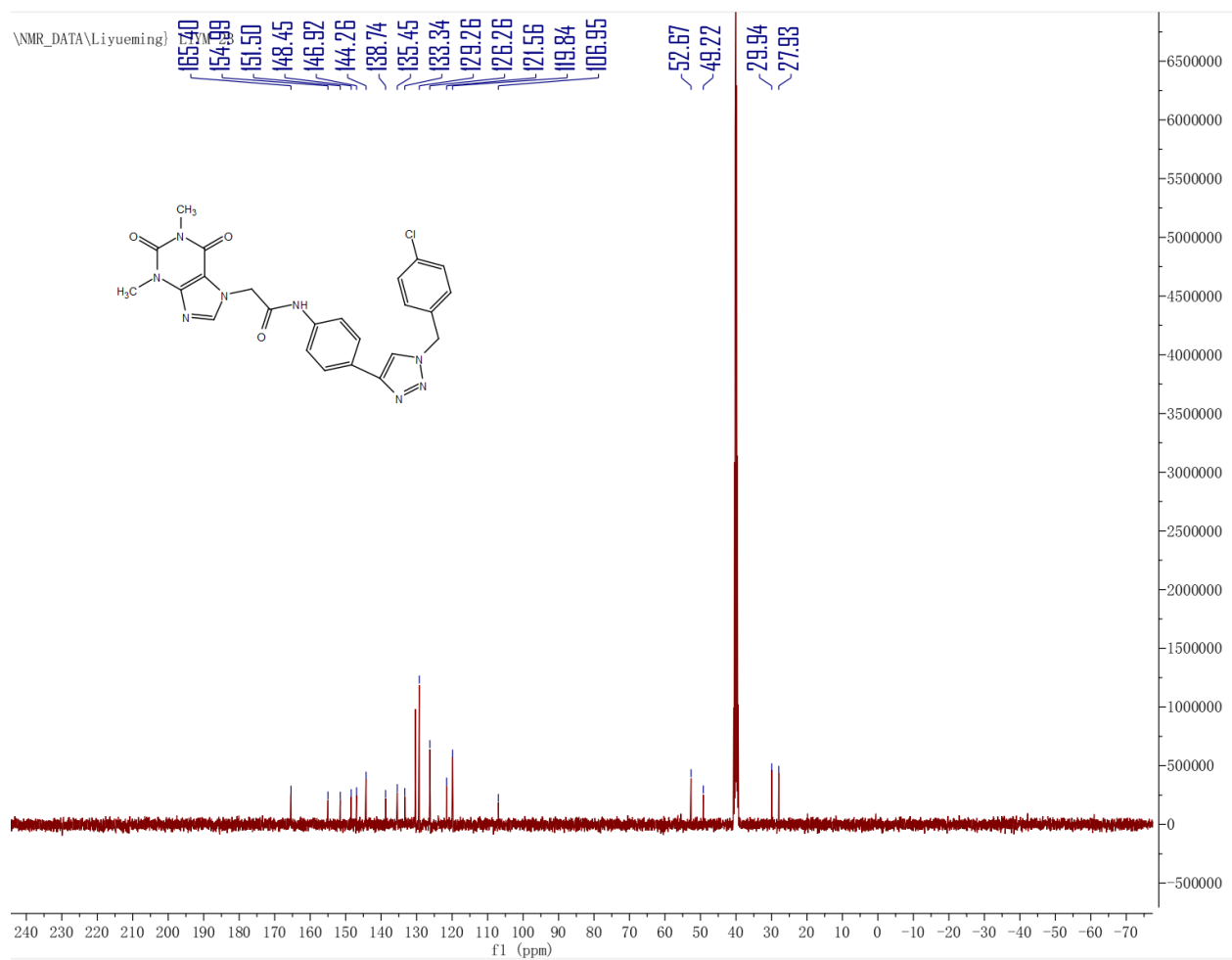


Figure S7-1. ^1H NMR spectrum (400MHz, DMSO-d_6) of compound D7

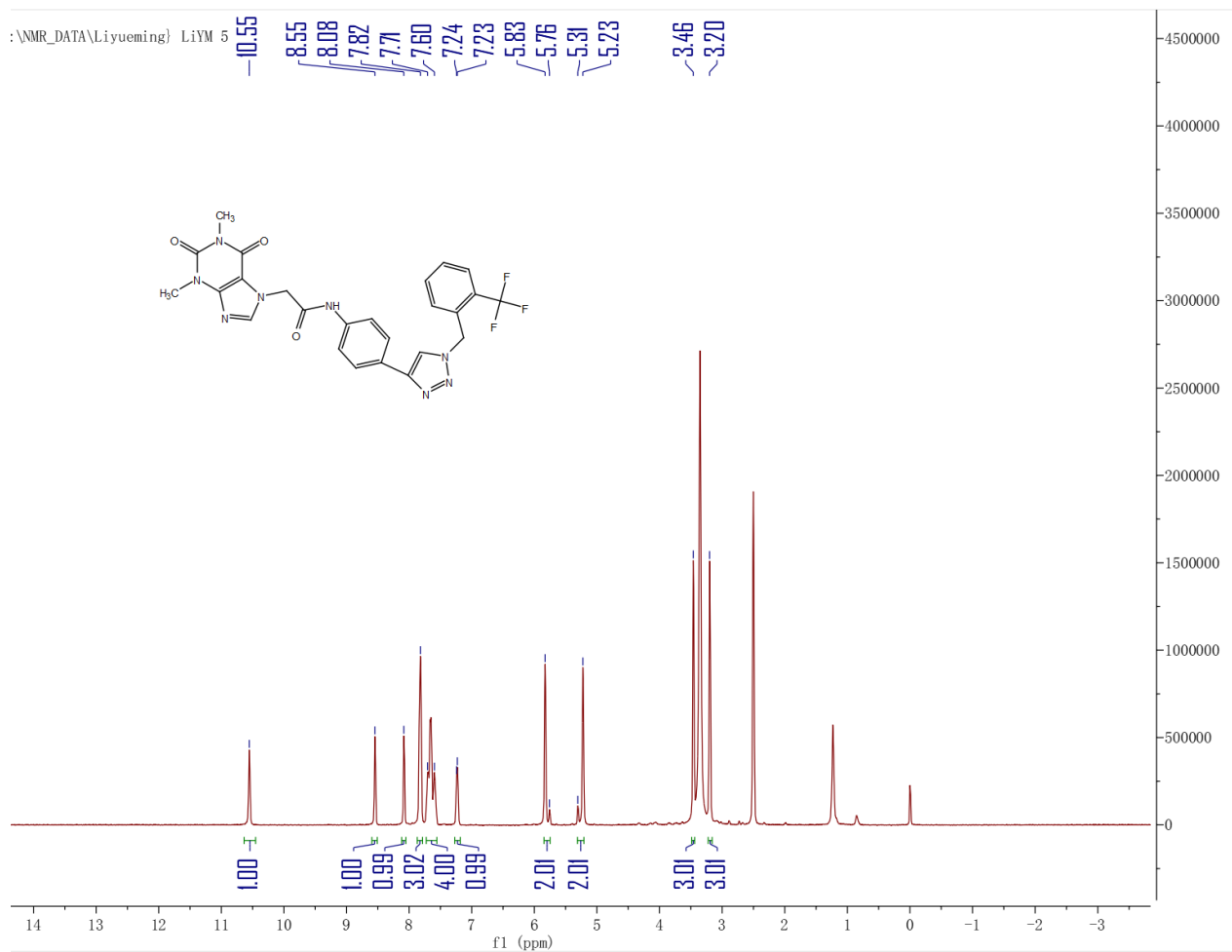


Figure S7-2. ^{13}C NMR spectrum (100MHz, DMSO- d_6) of compound D7

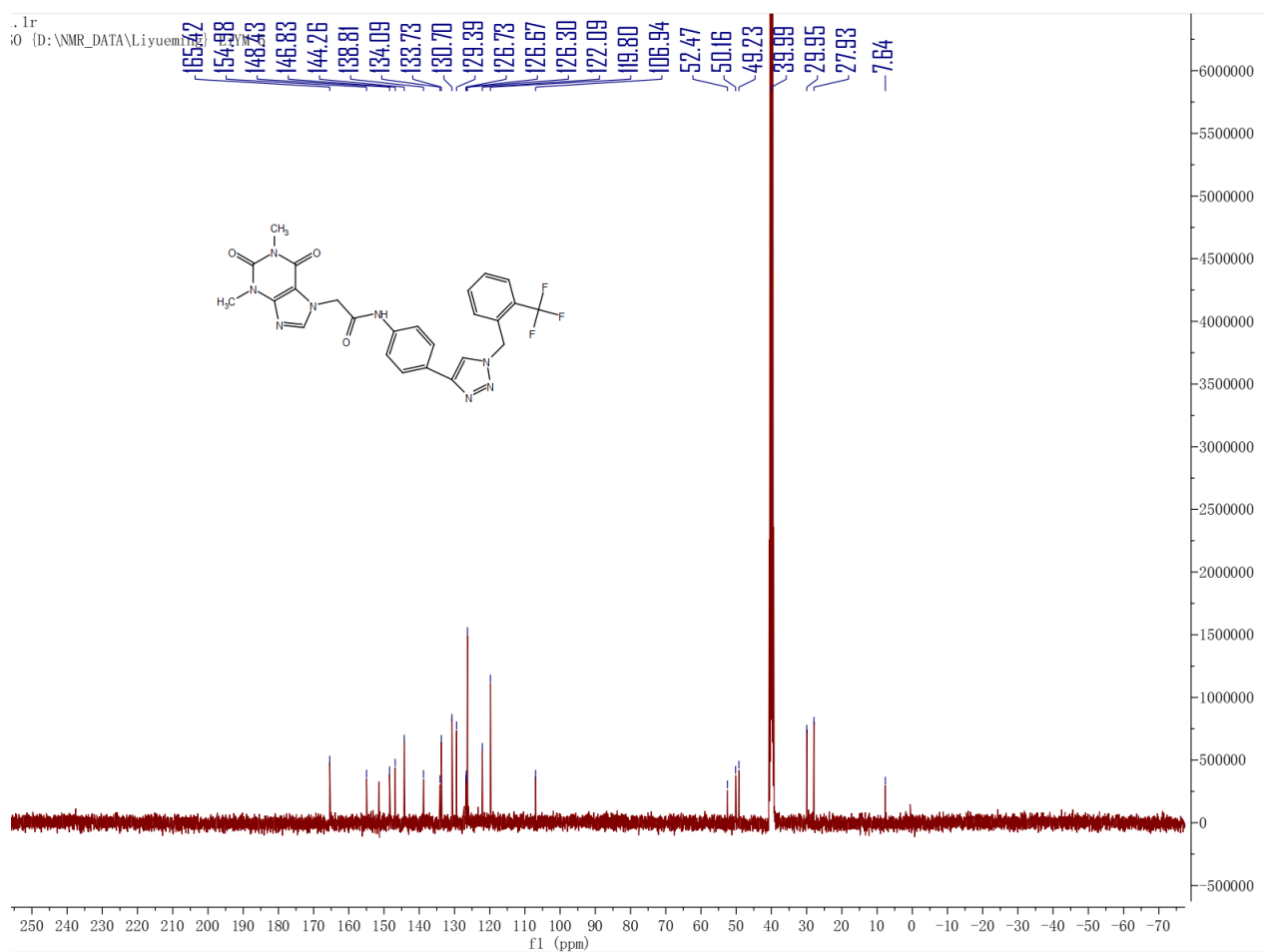


Figure S8-1. ^1H NMR spectrum (400MHz, DMSO-d_6) of compound D8

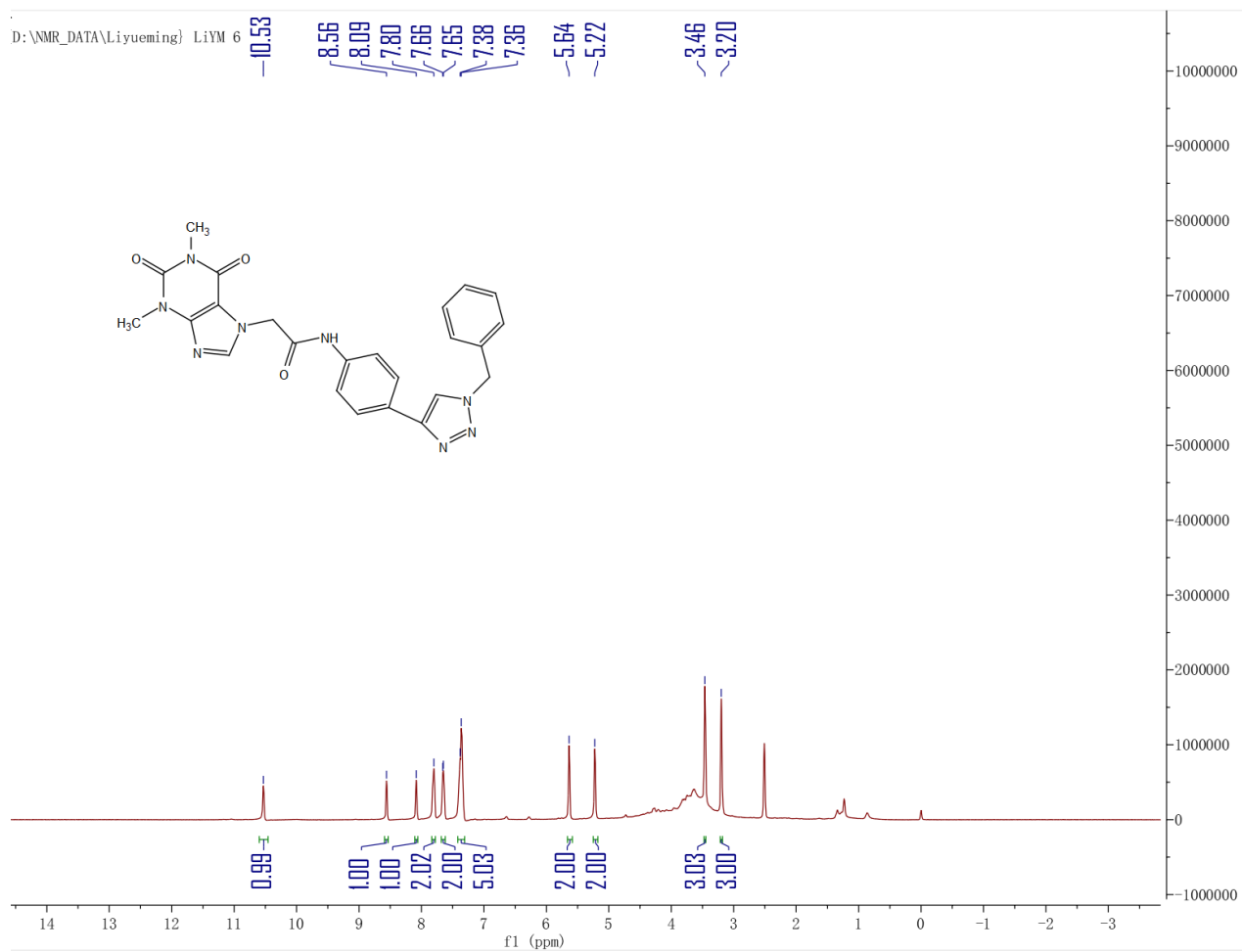


Figure S8-2. ^{13}C NMR spectrum (100MHz, DMSO- d_6) of compound D8

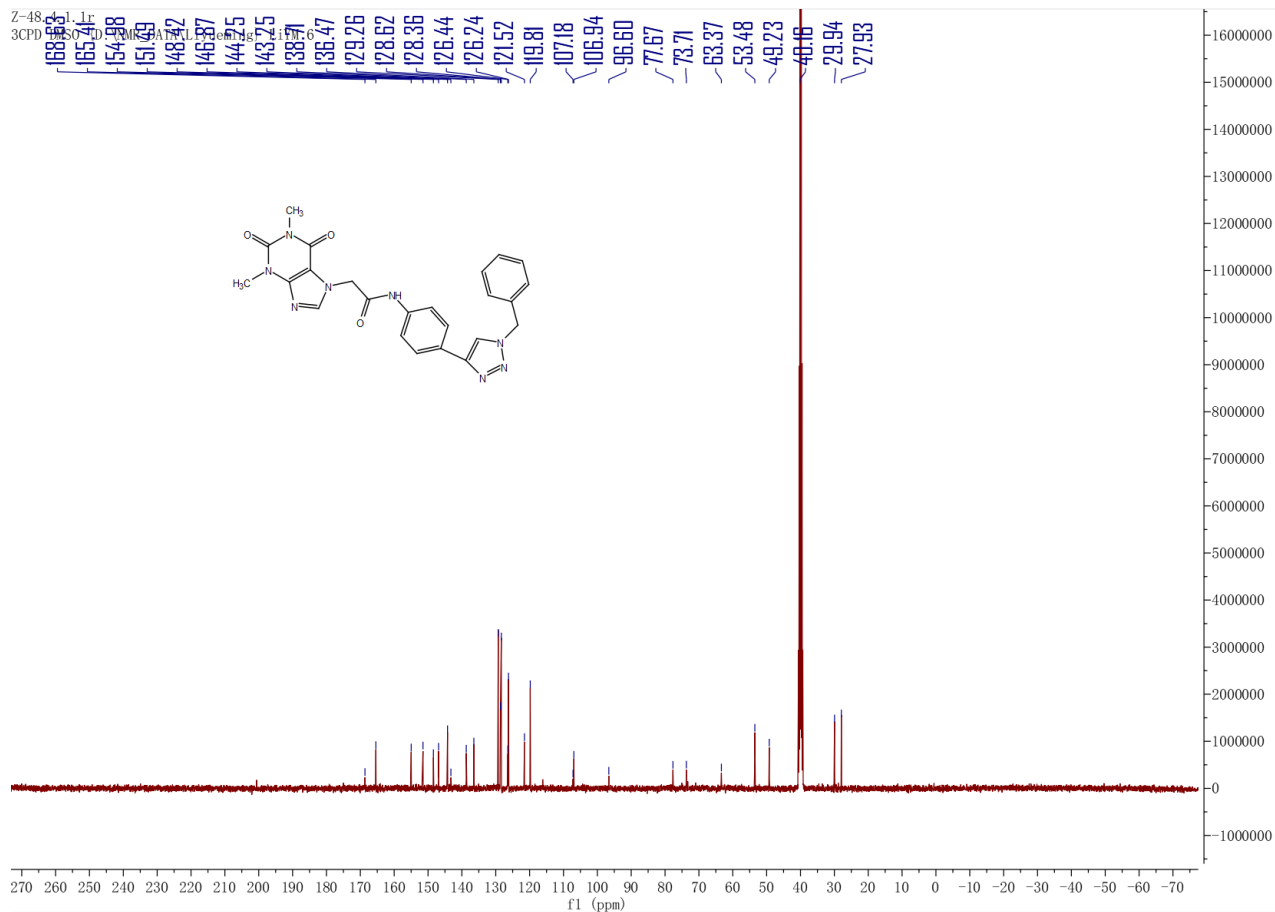


Figure S9-1. ^1H NMR spectrum (400MHz, DMSO-d_6) of compound D9

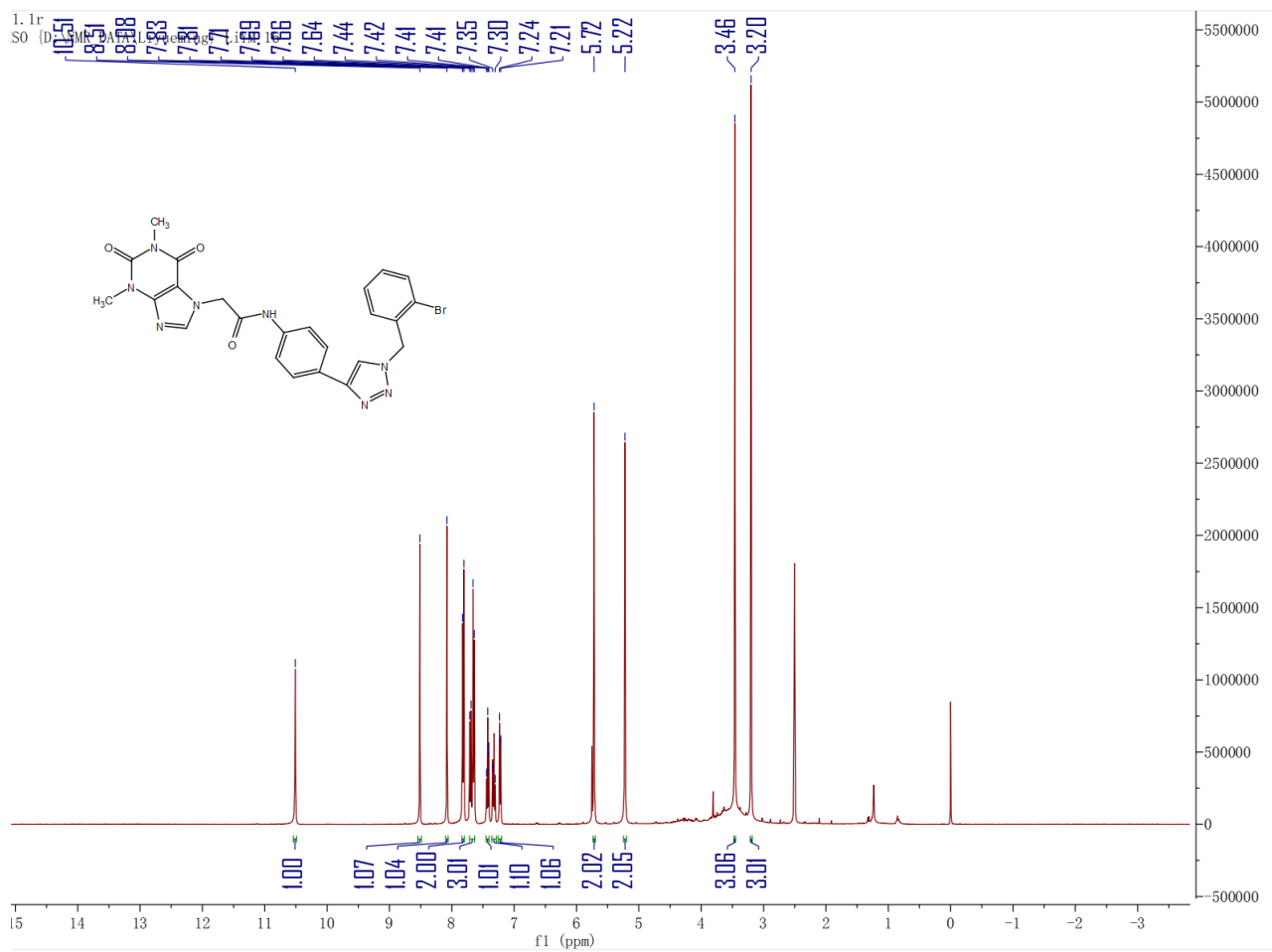


Figure S9-2. ^{13}C NMR spectrum (100MHz, DMSO- d_6) of compound D9

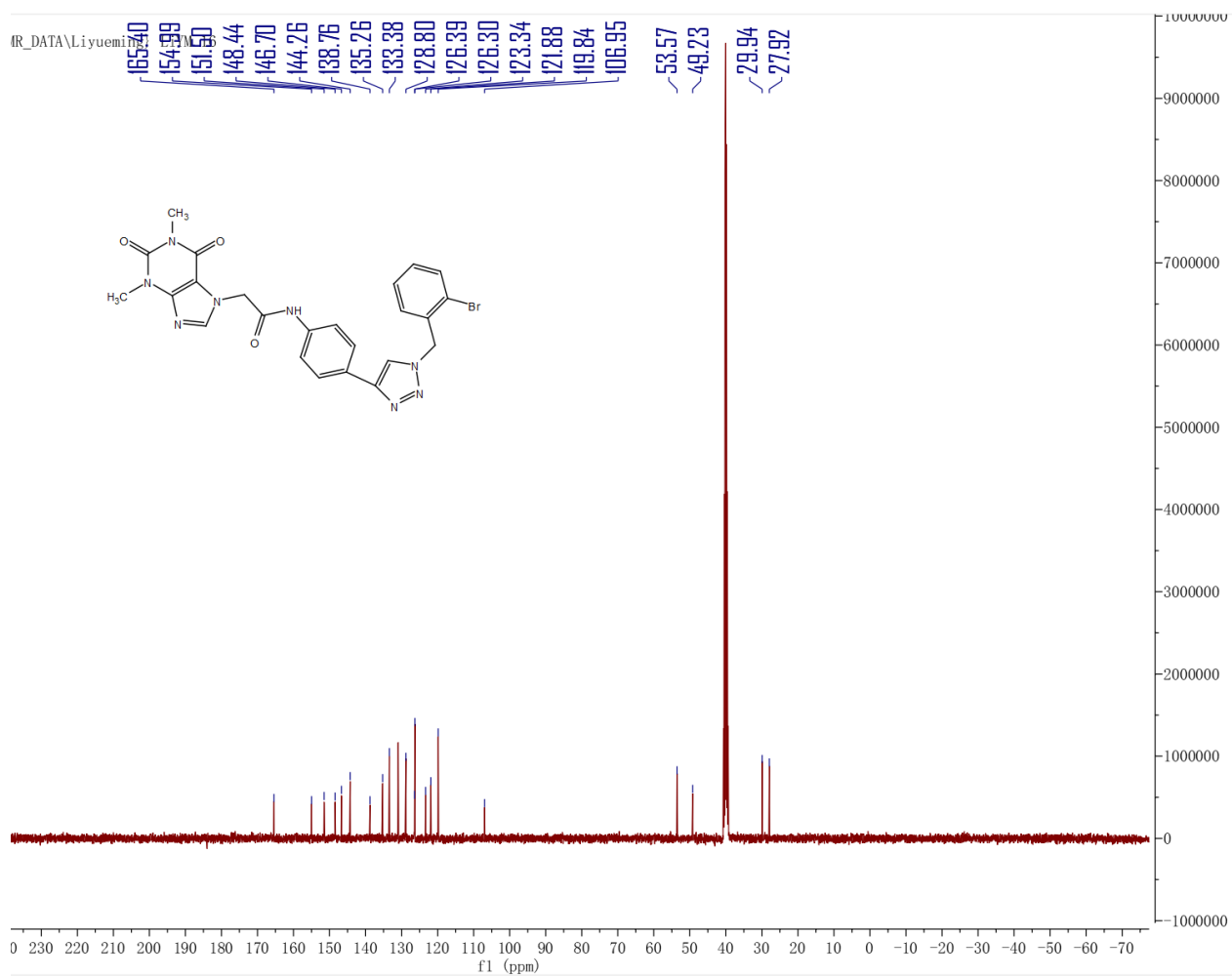


Figure S10-1. ^1H NMR spectrum (400MHz, DMSO-d_6) of compound D10

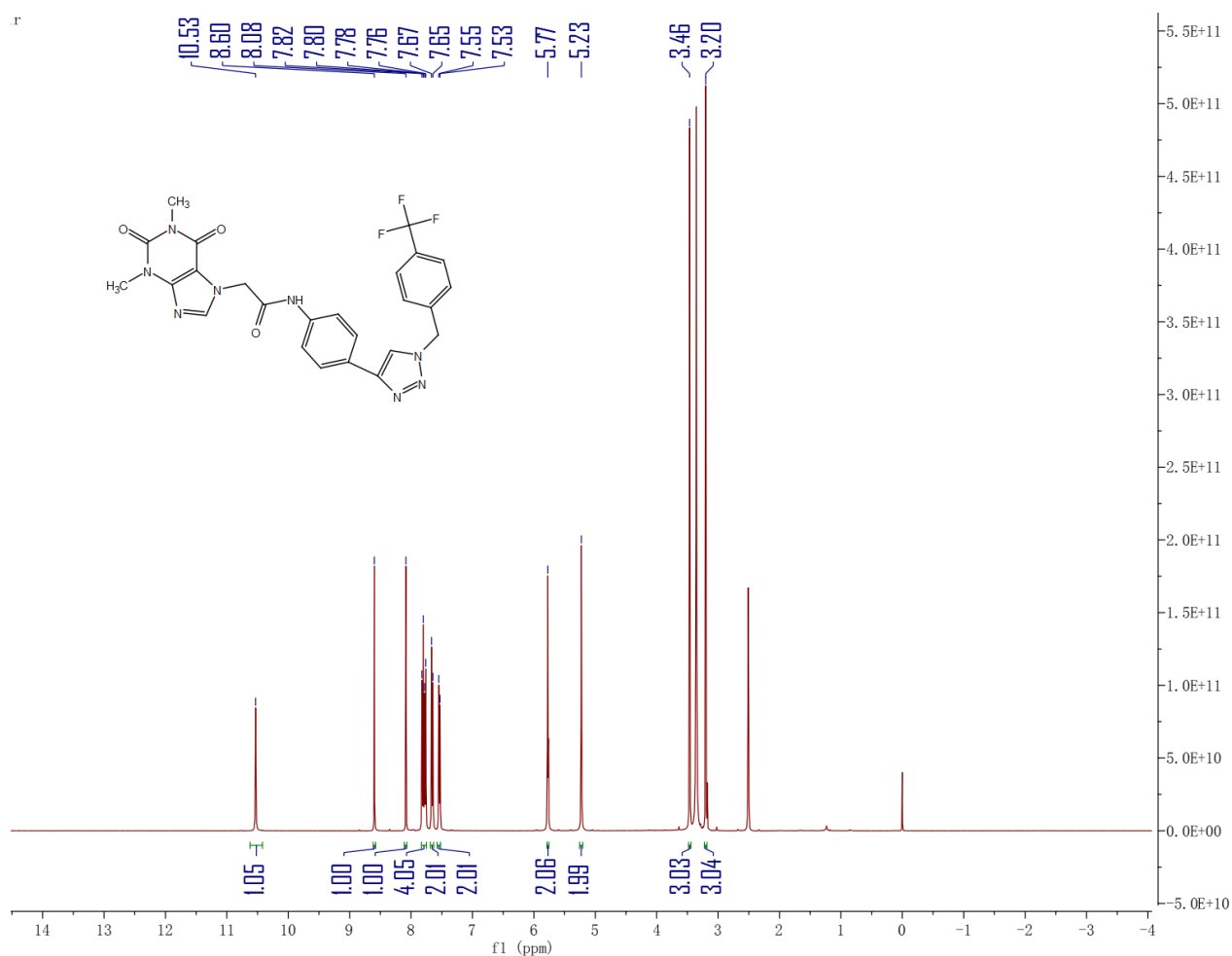


Figure S10-2. ^{13}C NMR spectrum (100MHz, DMSO- d_6) of compound D10

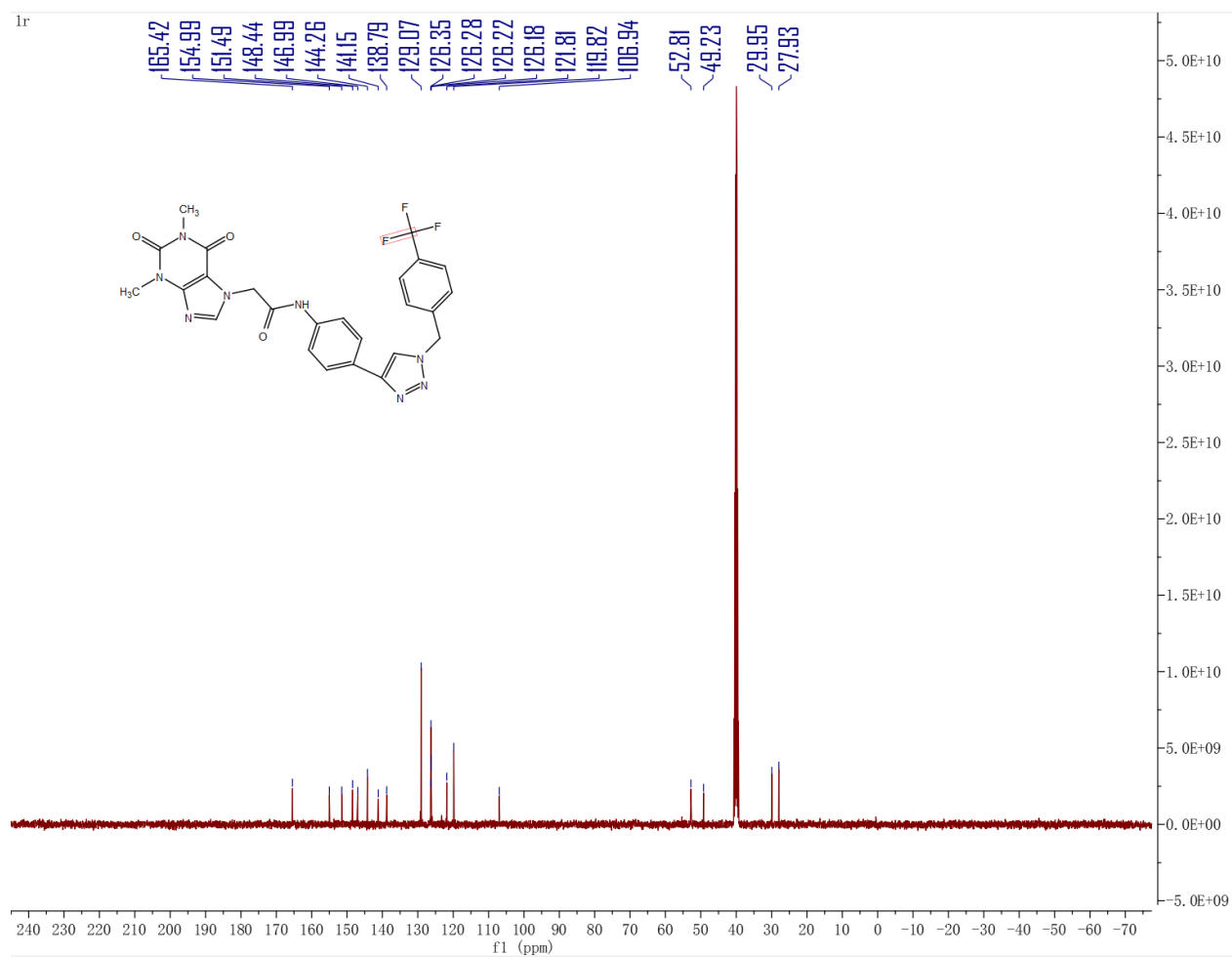


Figure S11-1. ^1H NMR spectrum (400MHz, DMSO- d_6) of compound D11

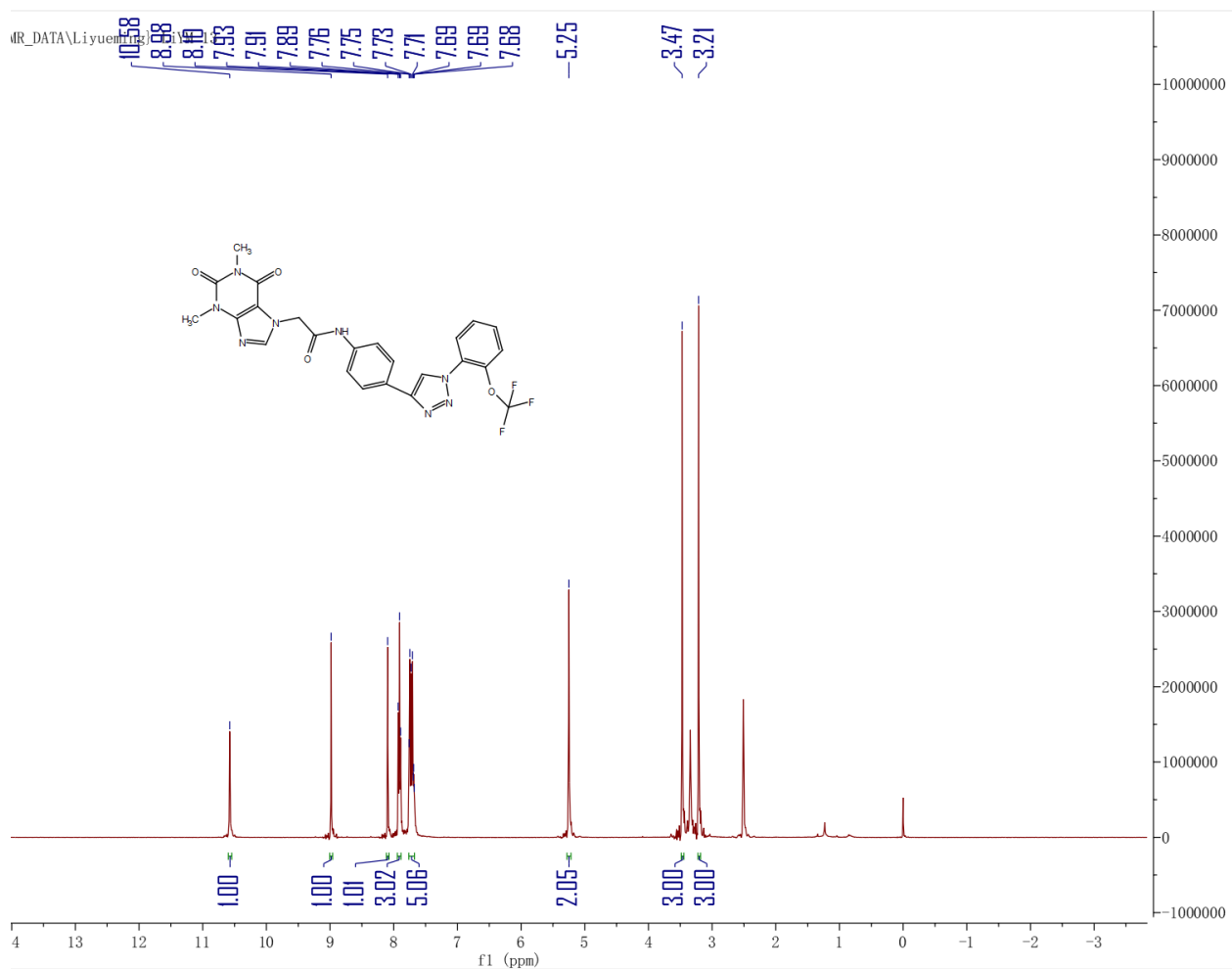


Figure S11-2. ^{13}C NMR spectrum (100MHz, DMSO- d_6) of compound D11

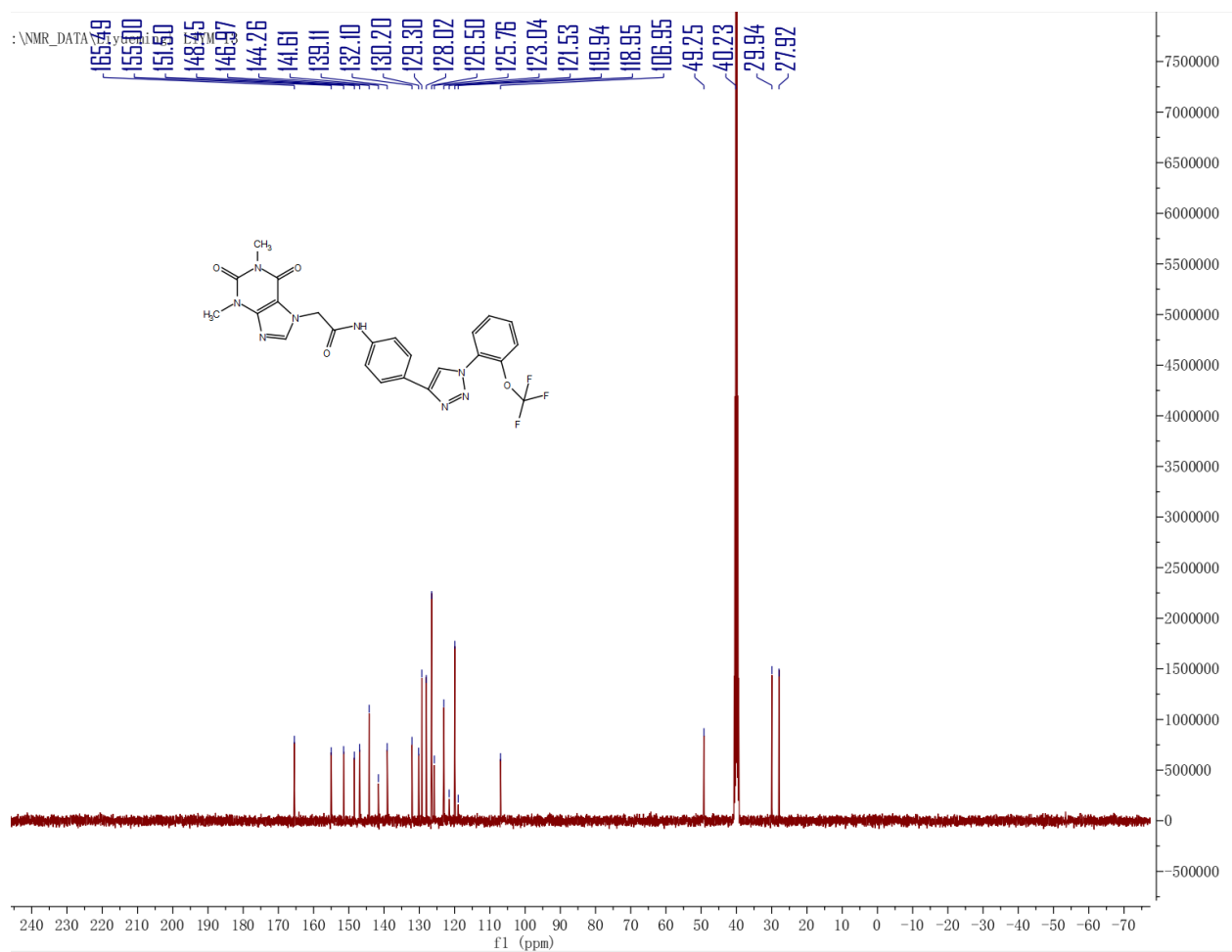


Figure S12-1. ^1H NMR spectrum (400MHz, DMSO- d_6) of compound D12

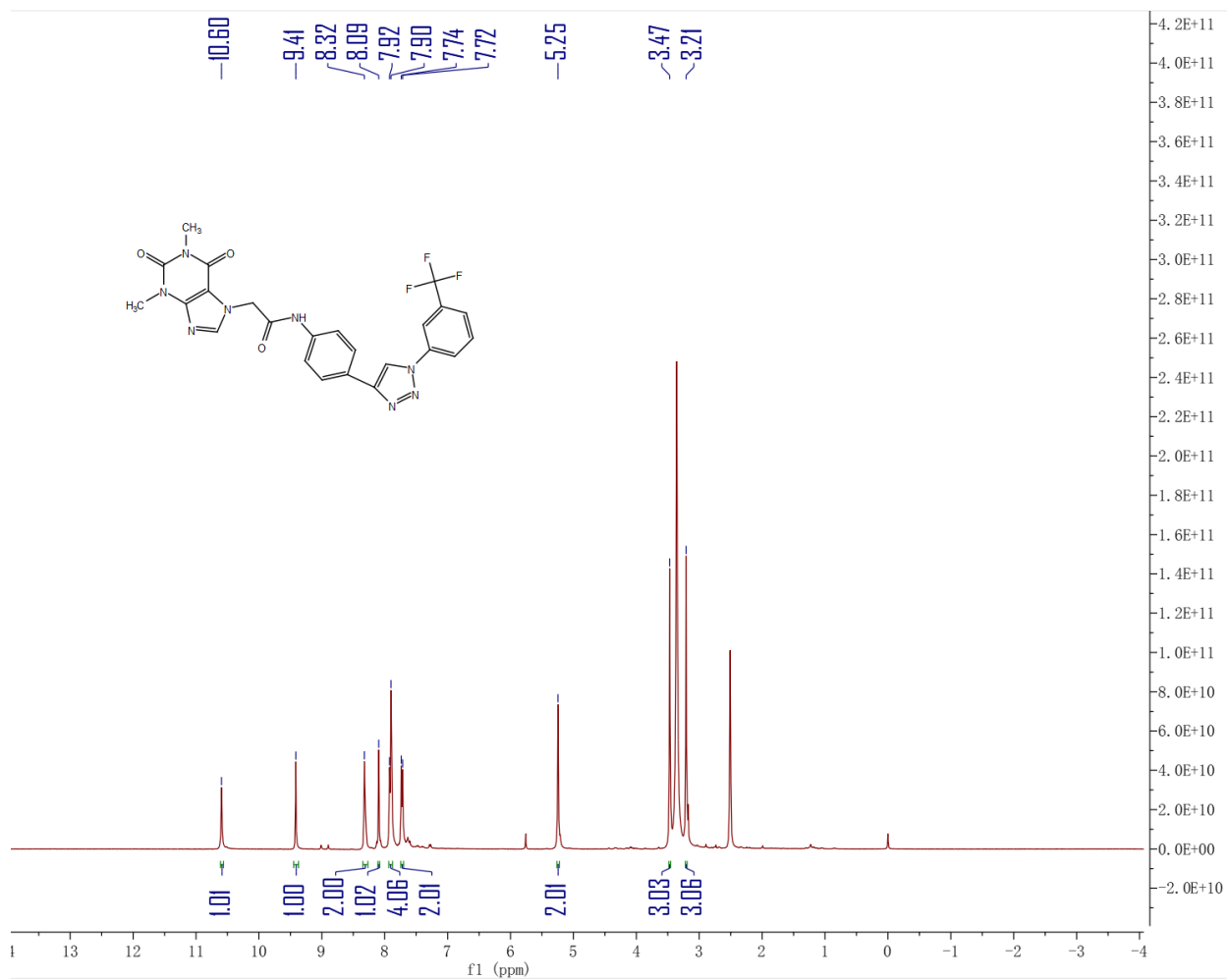


Figure S12-2. ^{12}C NMR spectrum (100MHz, DMSO- d_6) of compound D12

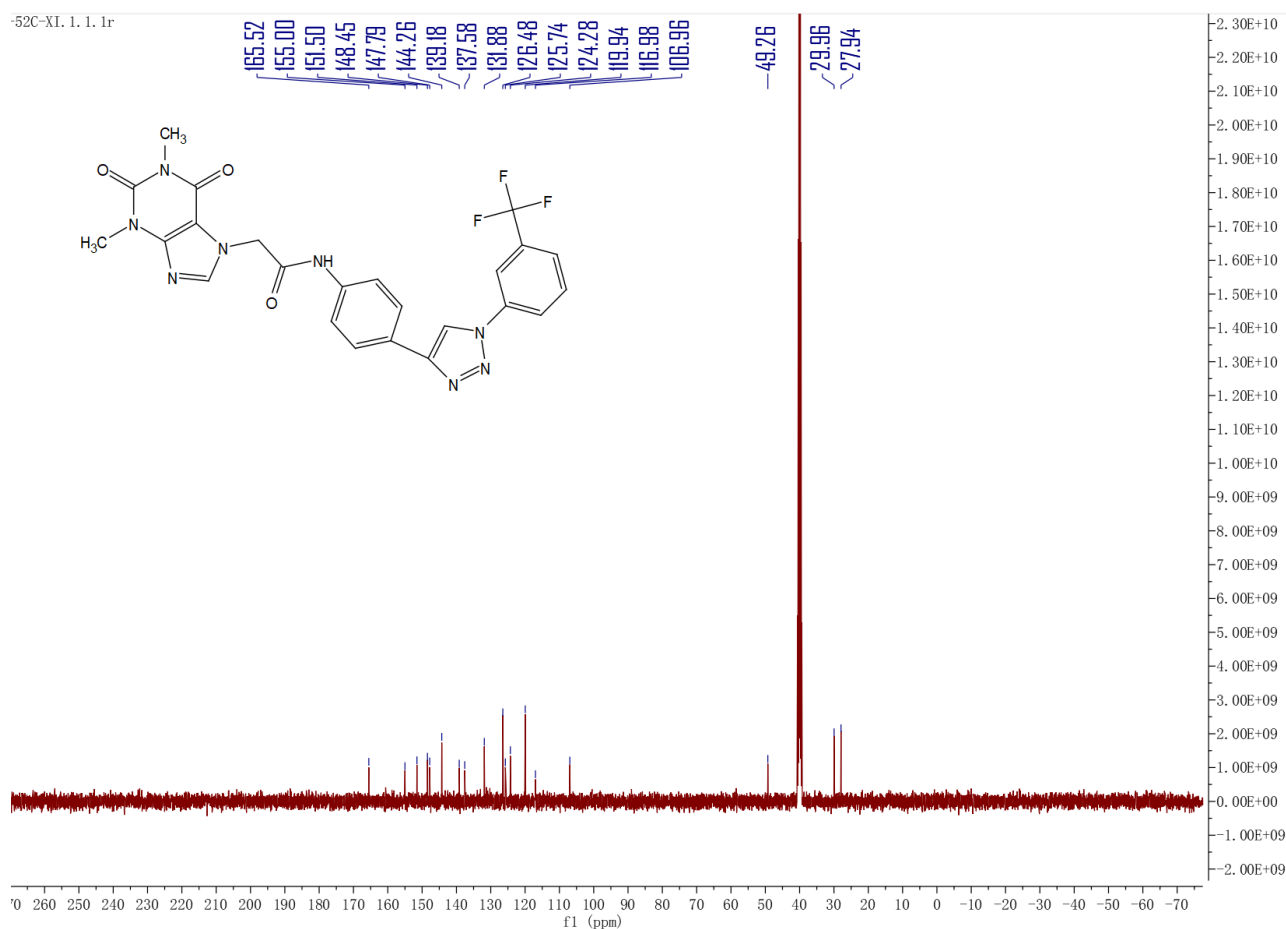


Figure S13-1. ^1H NMR spectrum (400MHz, DMSO- d_6) of compound D13



Figure S13-2. ^{13}C NMR spectrum (100MHz, DMSO- d_6) of compound D13

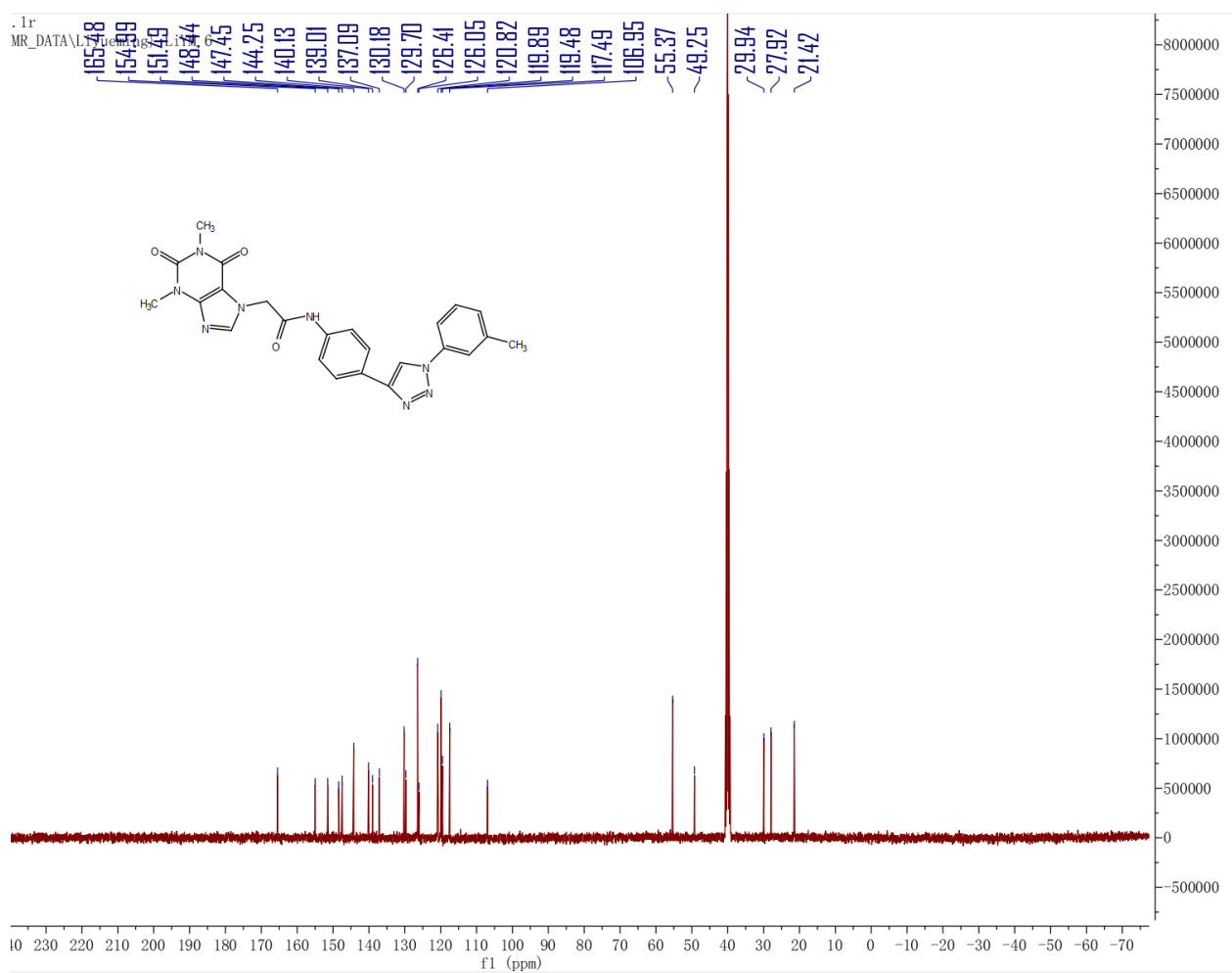


Figure S14-1. ^1H NMR spectrum (400MHz, DMSO- d_6) of compound D14



Figure S14-2. ^{13}C NMR spectrum (100MHz, DMSO- d_6) of compound D14

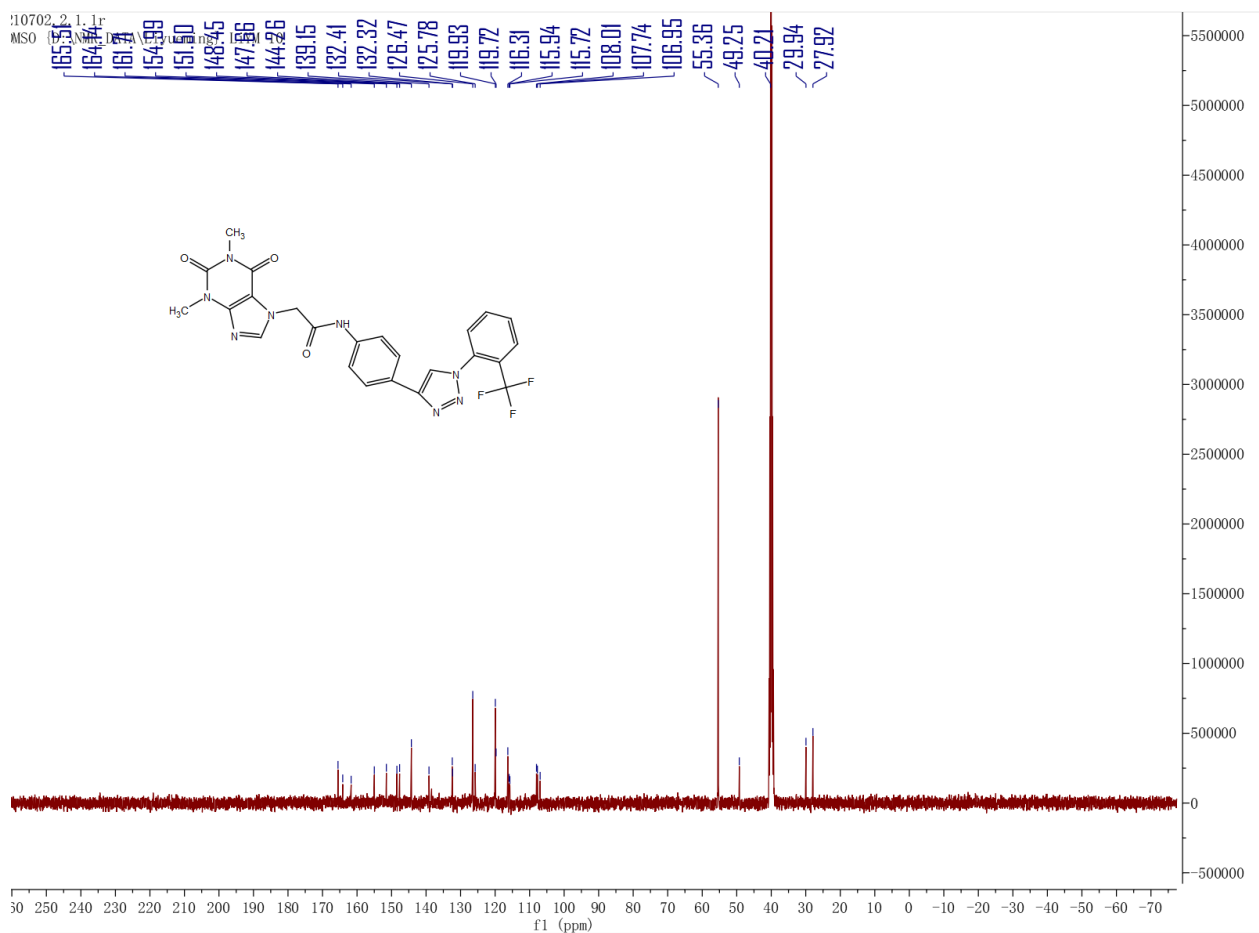


Figure S15-1. ^1H NMR spectrum (400MHz, DMSO-d_6) of compound D15



Figure S15-2. ^{13}C NMR spectrum (100MHz, DMSO- d_6) of compound D15

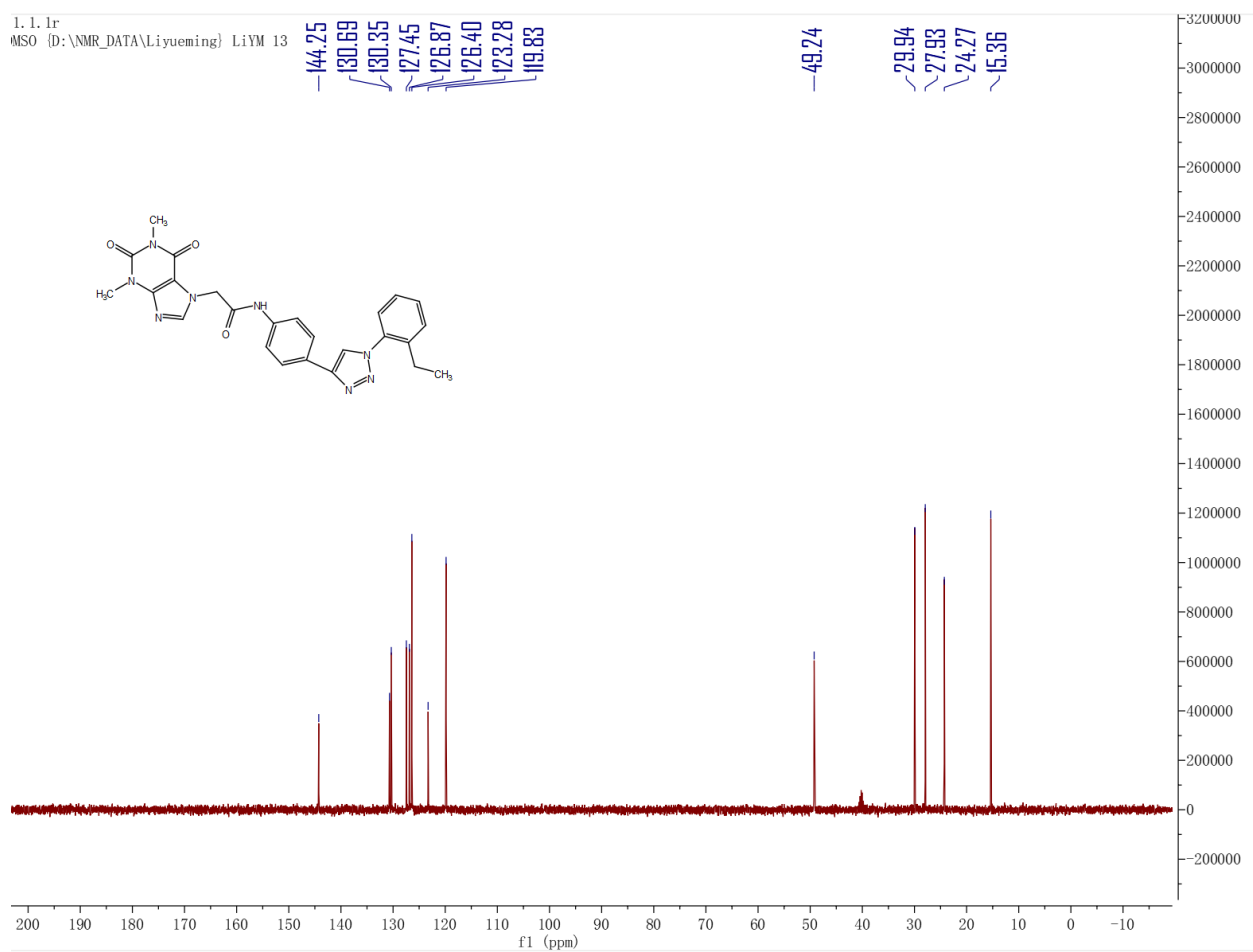


Figure S16-1. ^1H NMR spectrum (400MHz, DMSO-d_6) of compound D16

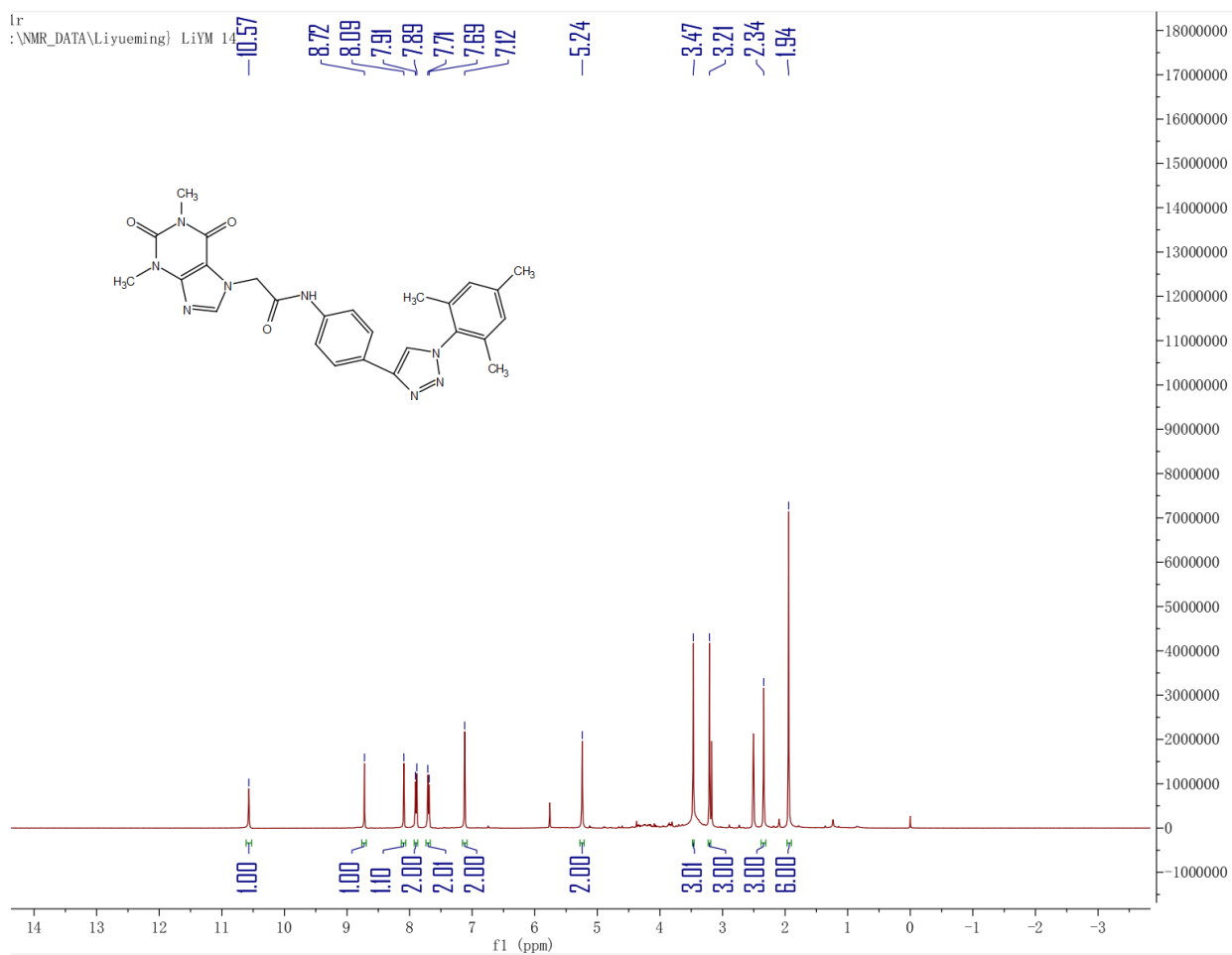


Figure S16-2. ^{13}C NMR spectrum (100MHz, DMSO- d_6) of compound D16

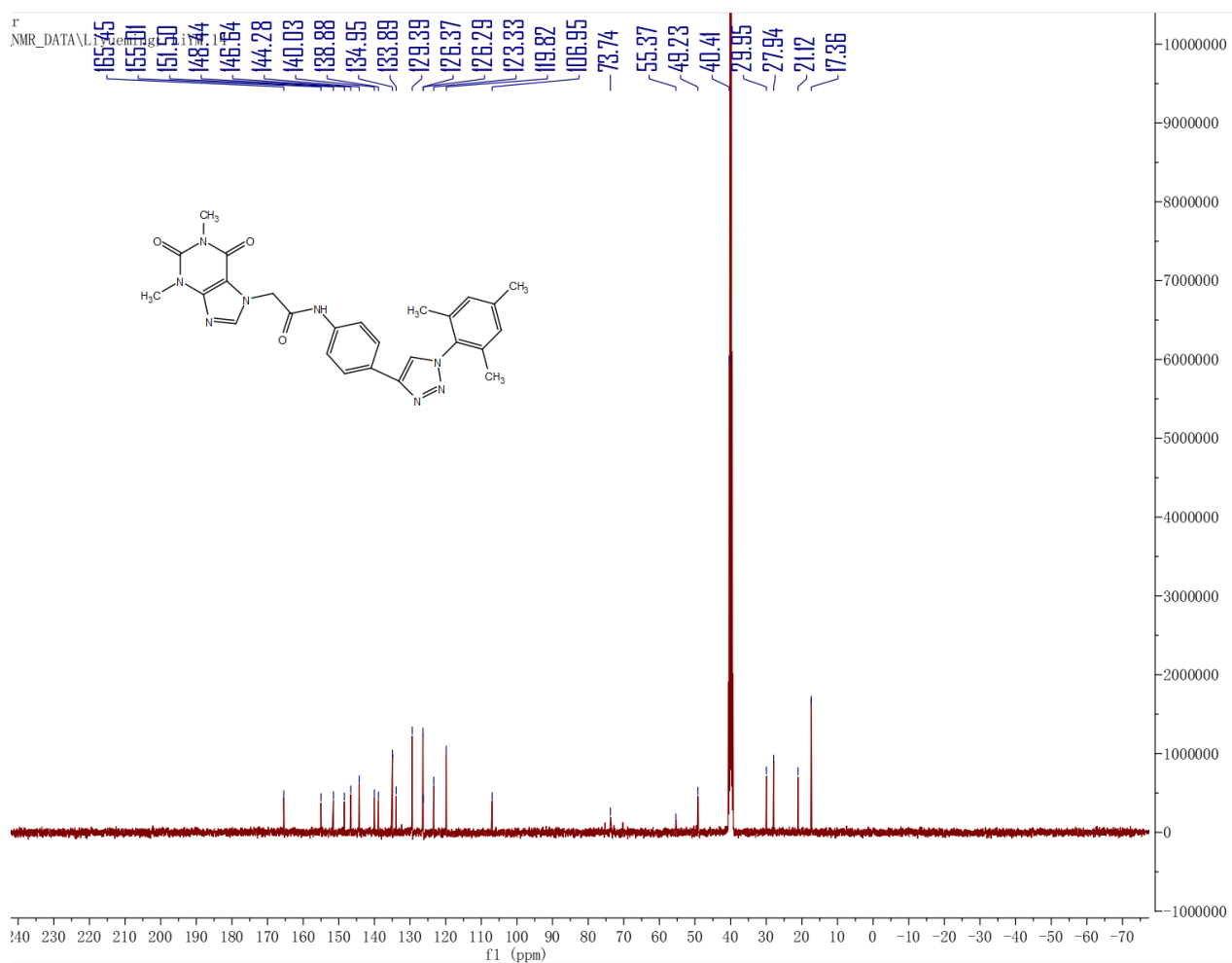


Figure S17-1. ^1H NMR spectrum (400MHz, DMSO- d_6) of compound D17

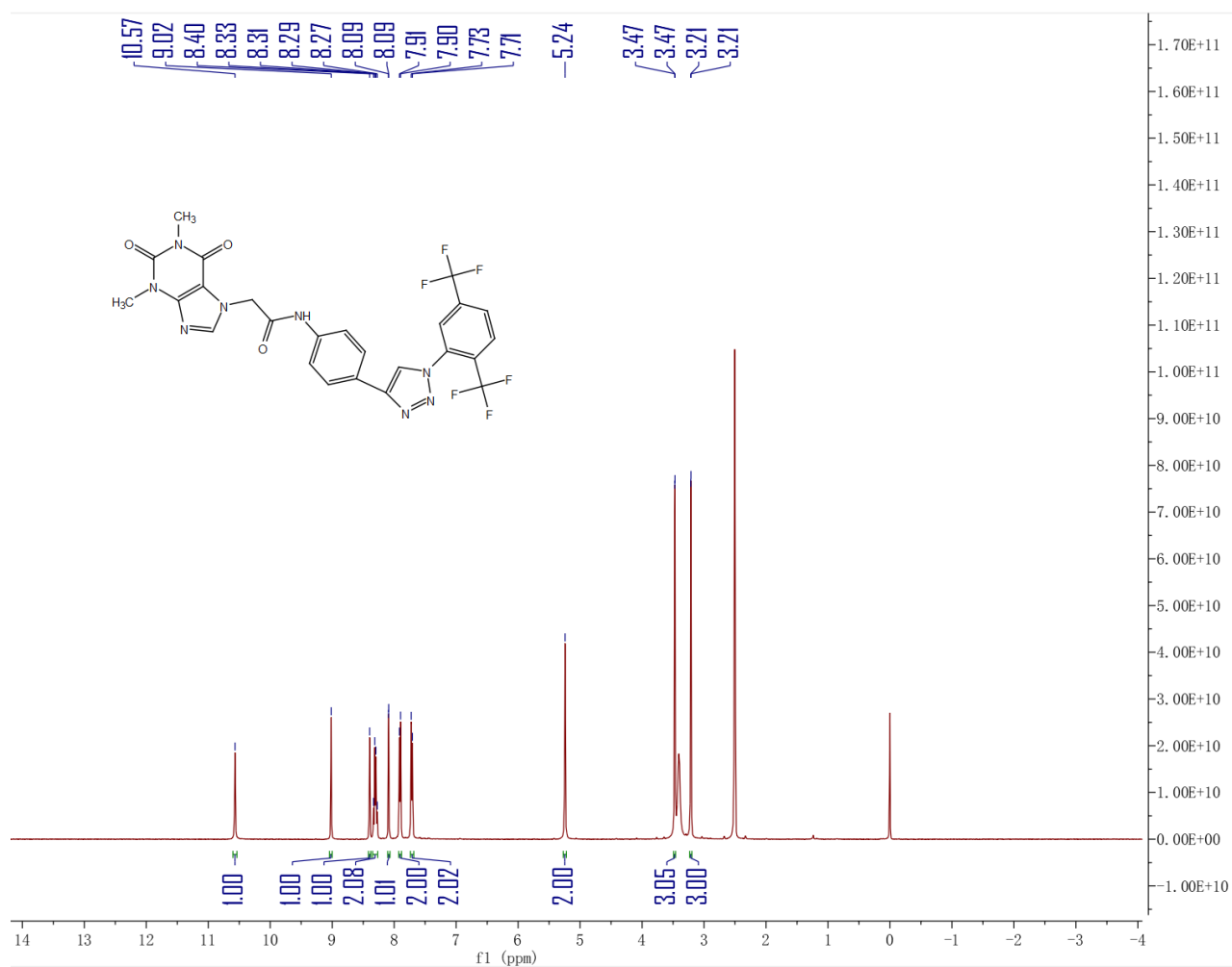


Figure S17-2. ^{13}C NMR spectrum (100MHz, DMSO- d_6) of compound D17

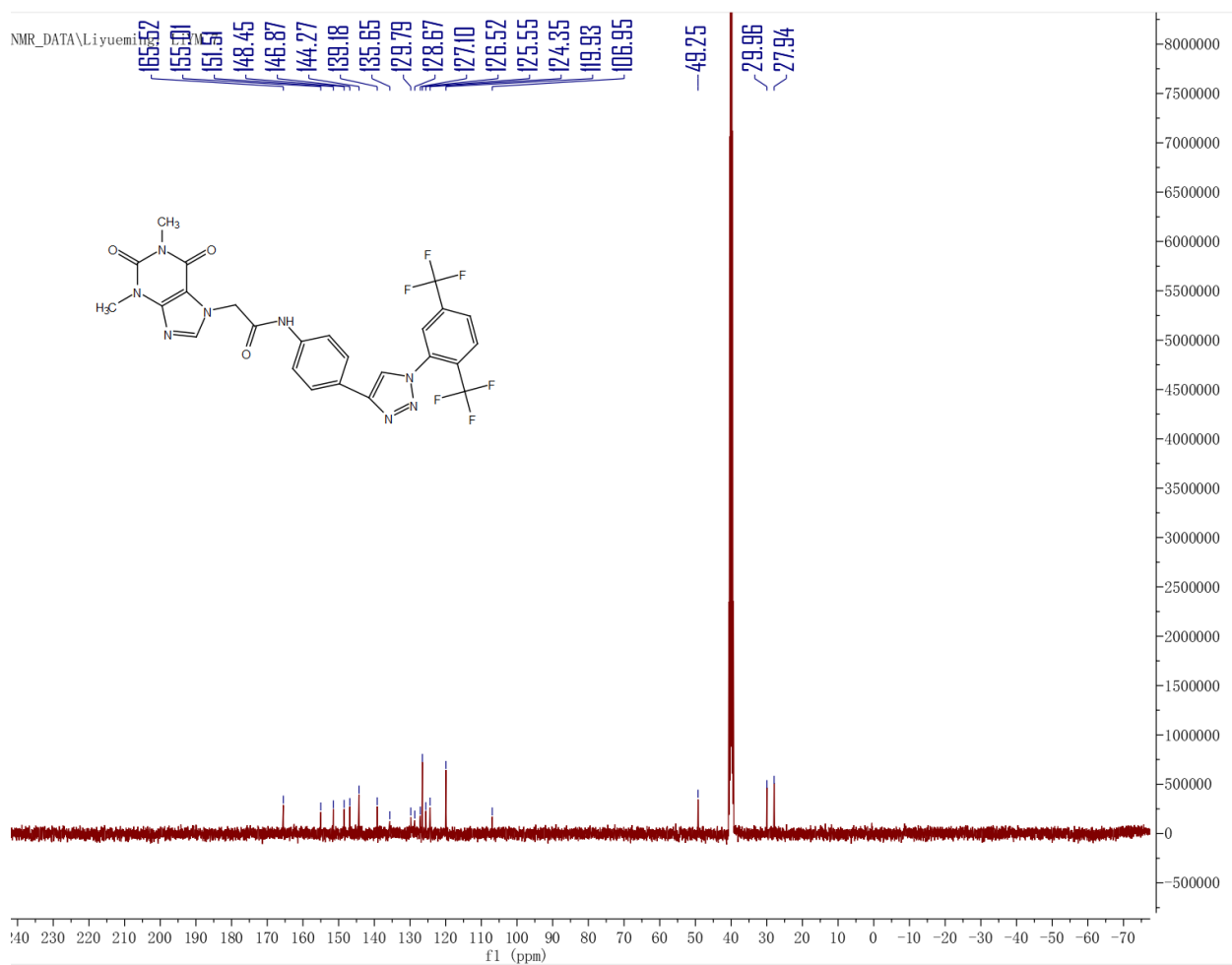


Figure S18-1. ^1H NMR spectrum (400MHz, DMSO- d_6) of compound D18

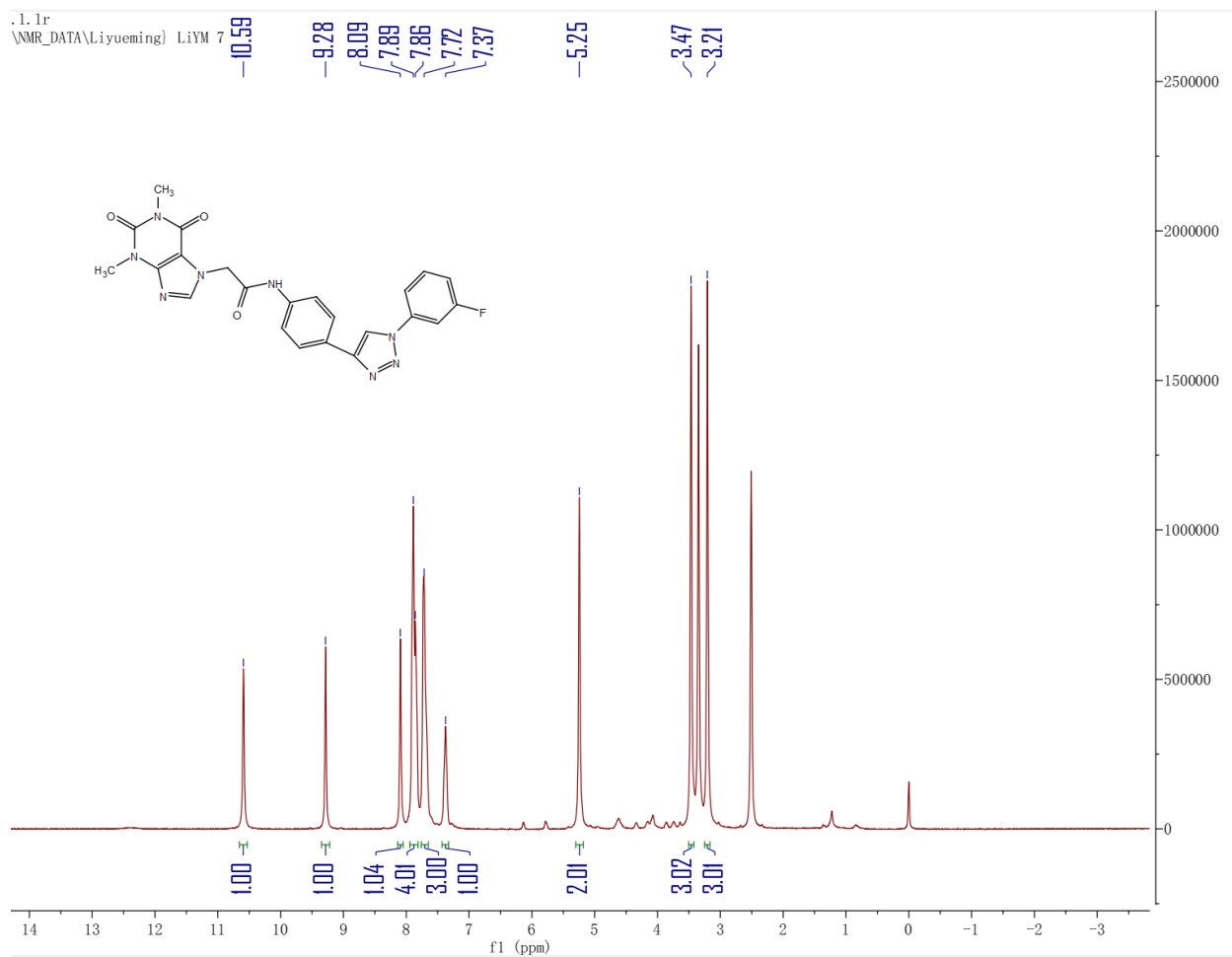


Figure S18-2. ^{13}C NMR spectrum (100MHz, DMSO- d_6) of compound D18

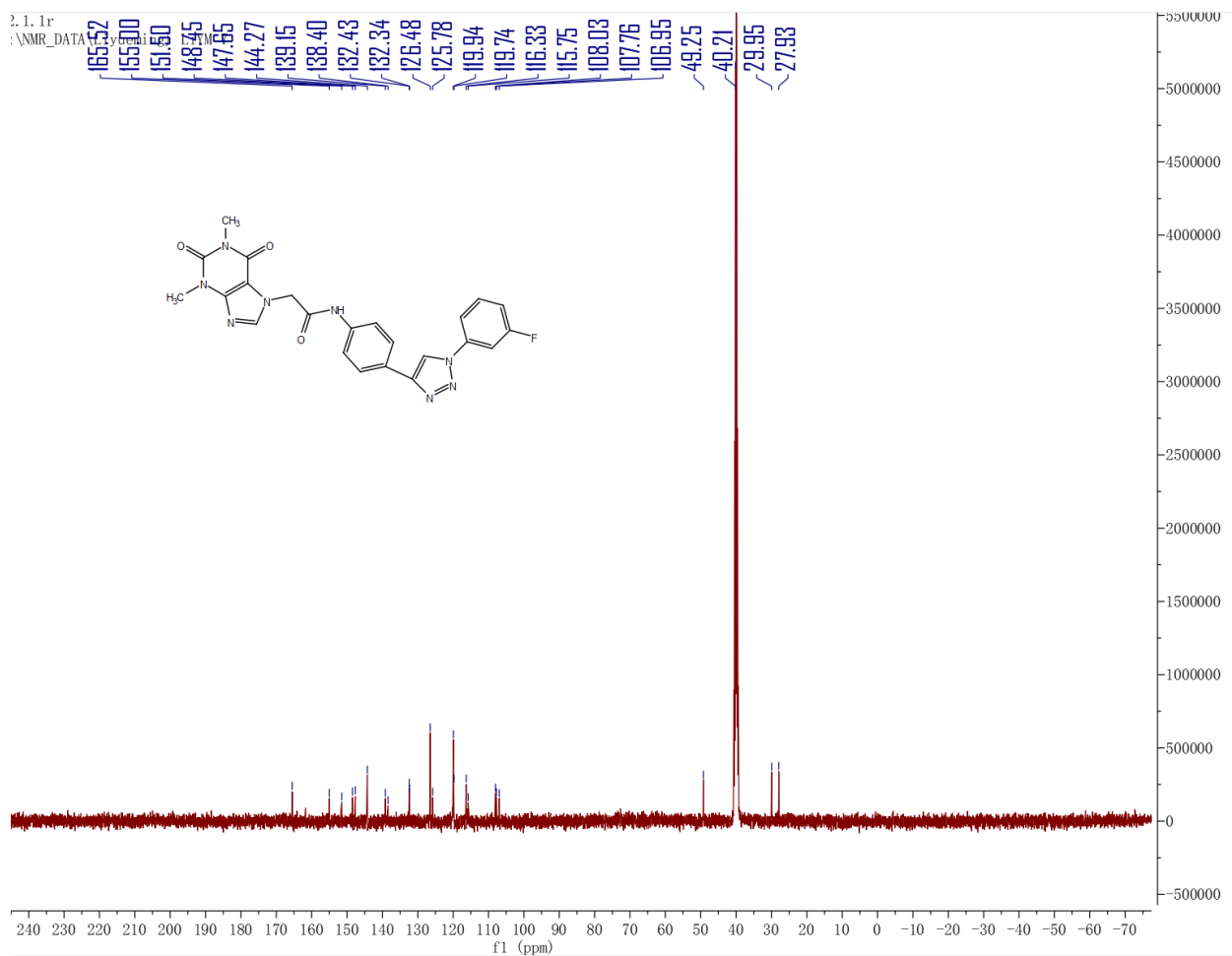


Figure S19-1. ¹H NMR spectrum (400MHz, DMSO-d₆) of compound D19

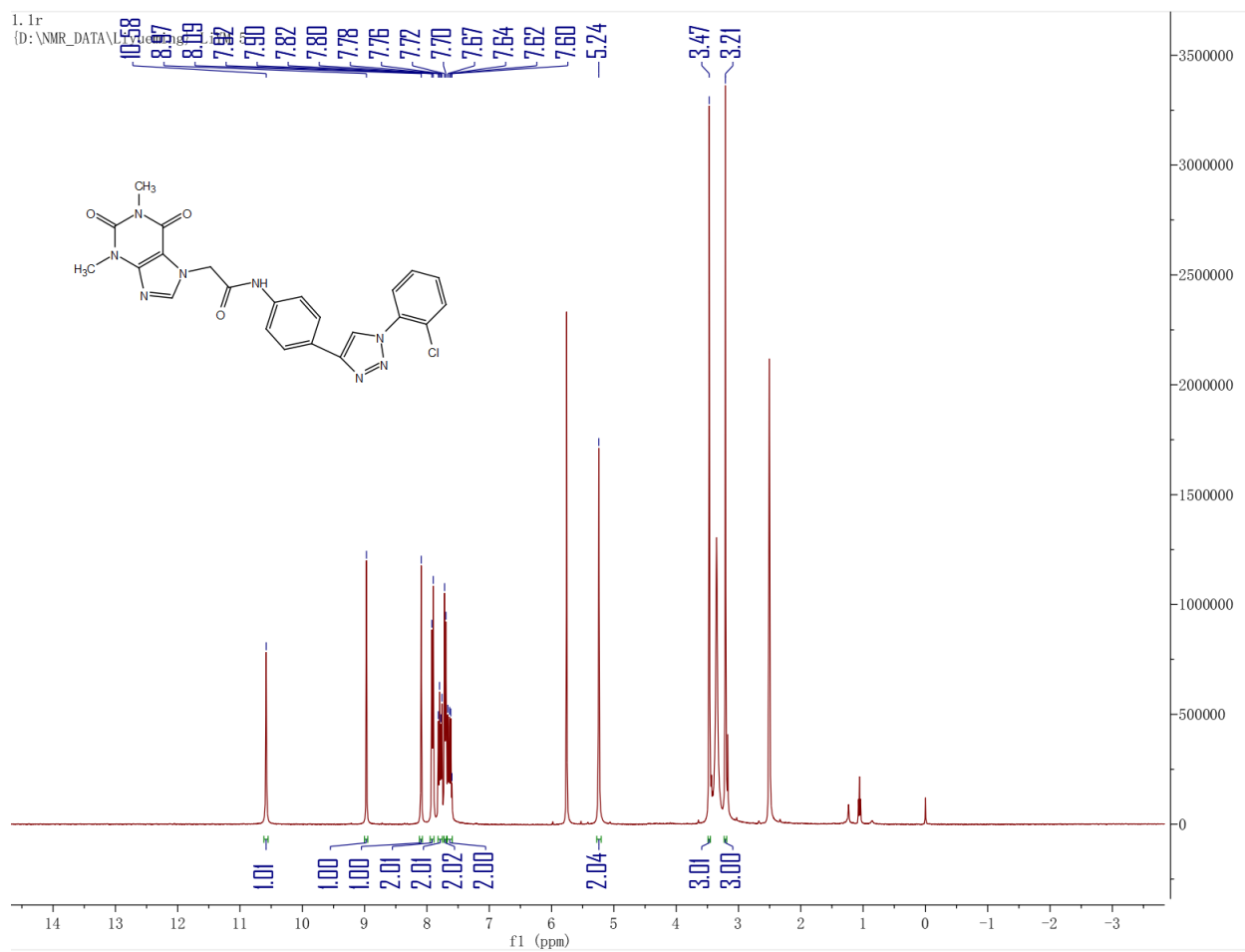


Figure S19-2. ^{13}C NMR spectrum (100MHz, DMSO- d_6) of compound D19

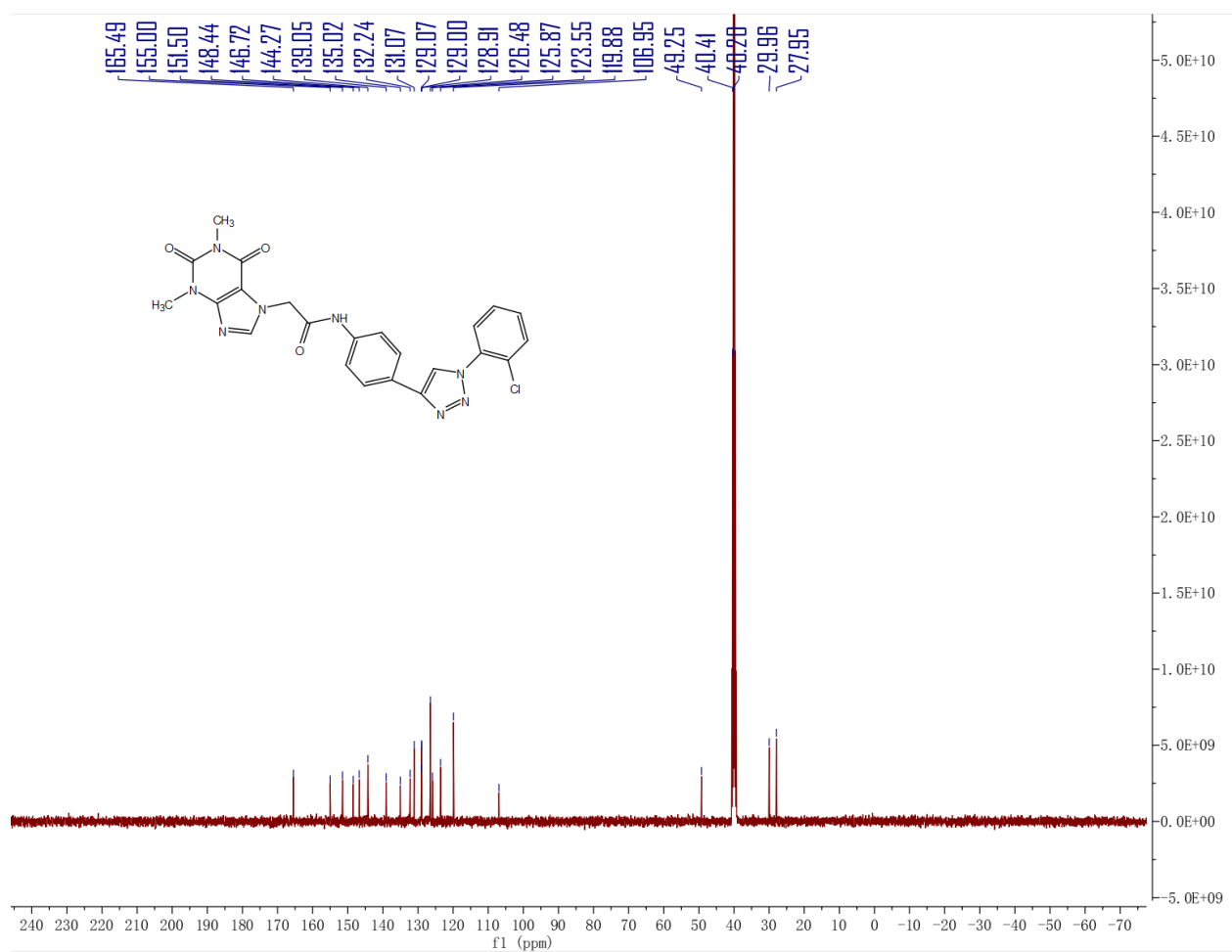


Figure S20-1. ^1H NMR spectrum (400MHz, DMSO- d_6) of compound D20

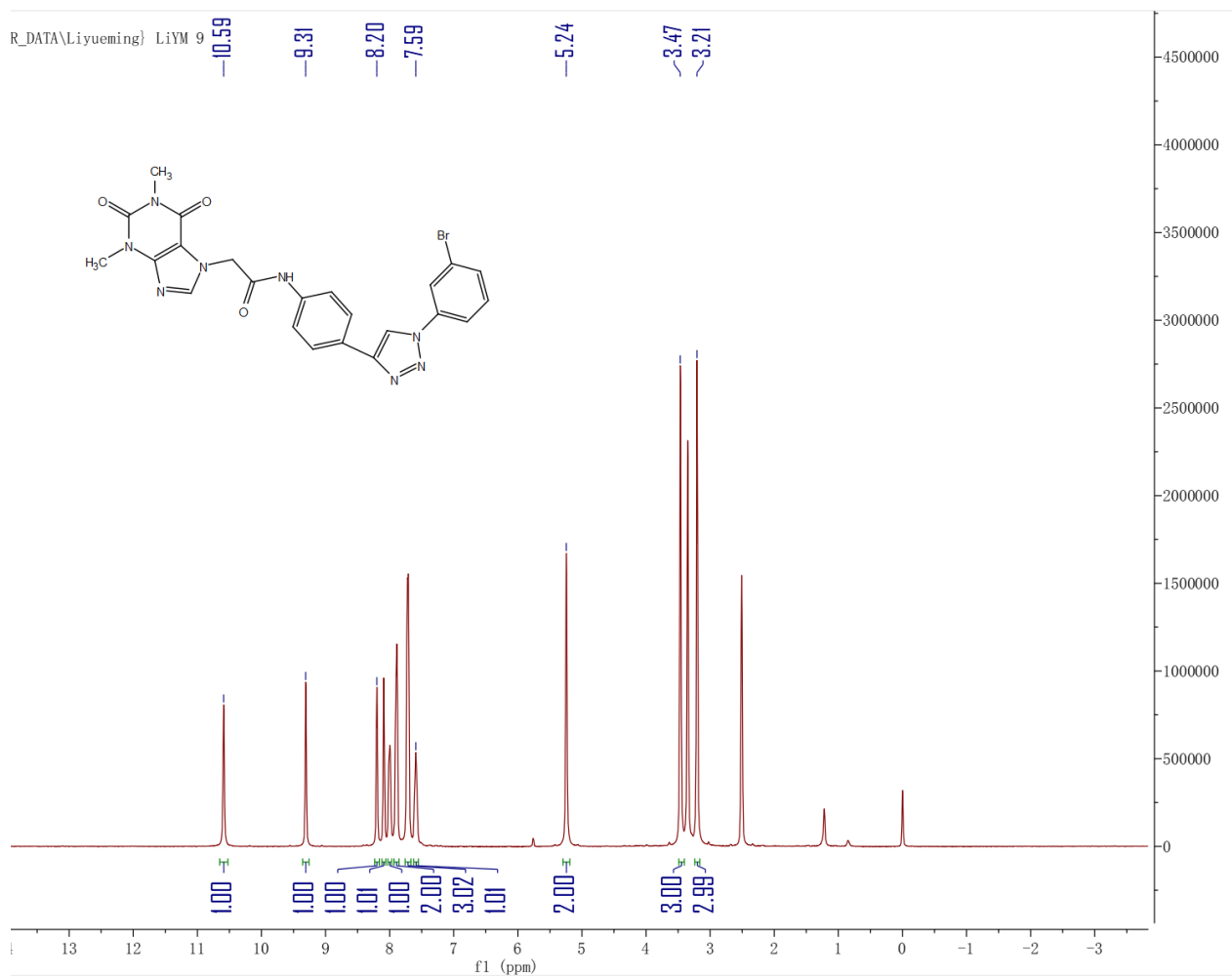


Figure S20-2. ^{13}C NMR spectrum (100MHz, DMSO- d_6) of compound D20

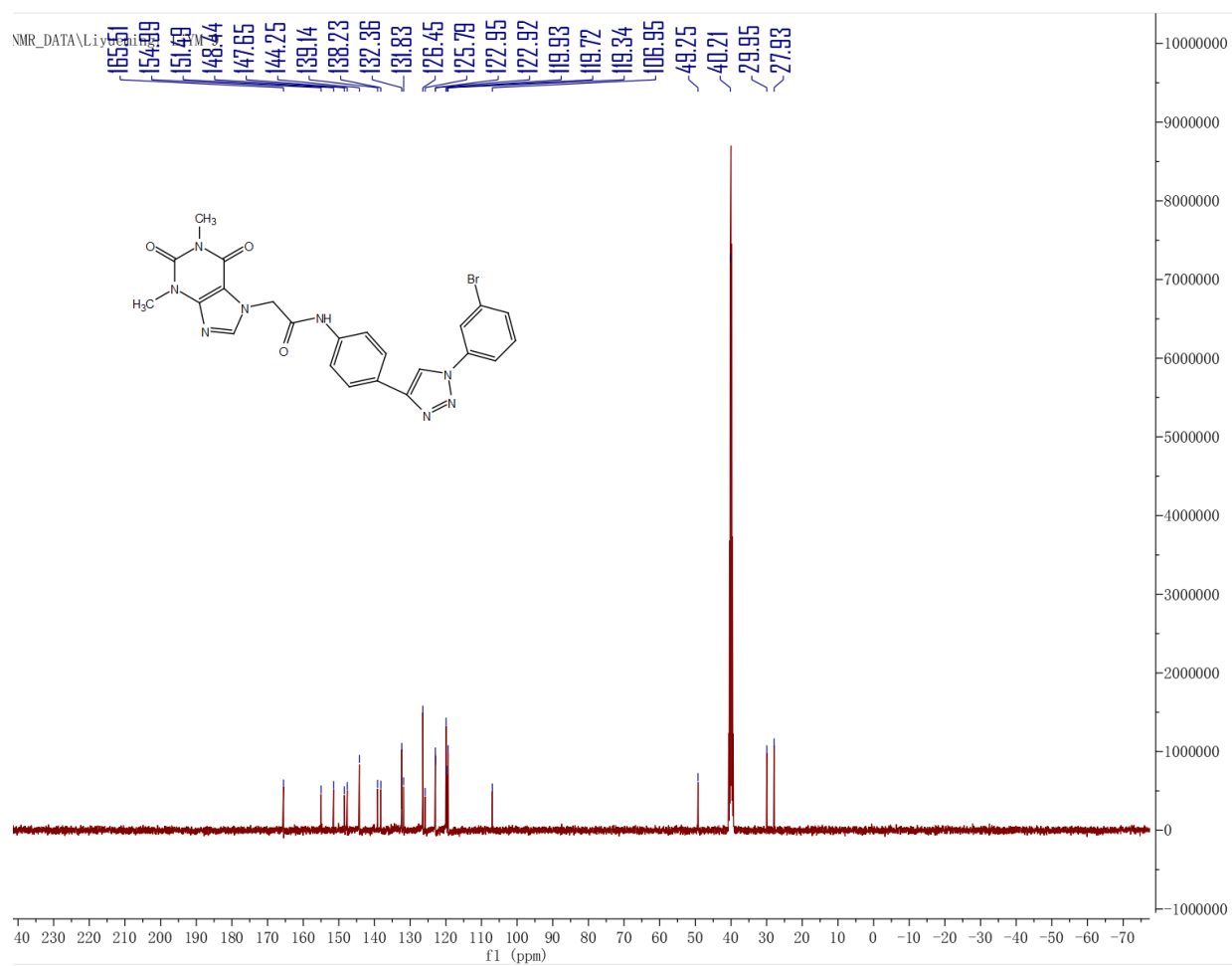


Figure S21-1. ^1H NMR spectrum (400MHz, DMSO- d_6) of compound D21

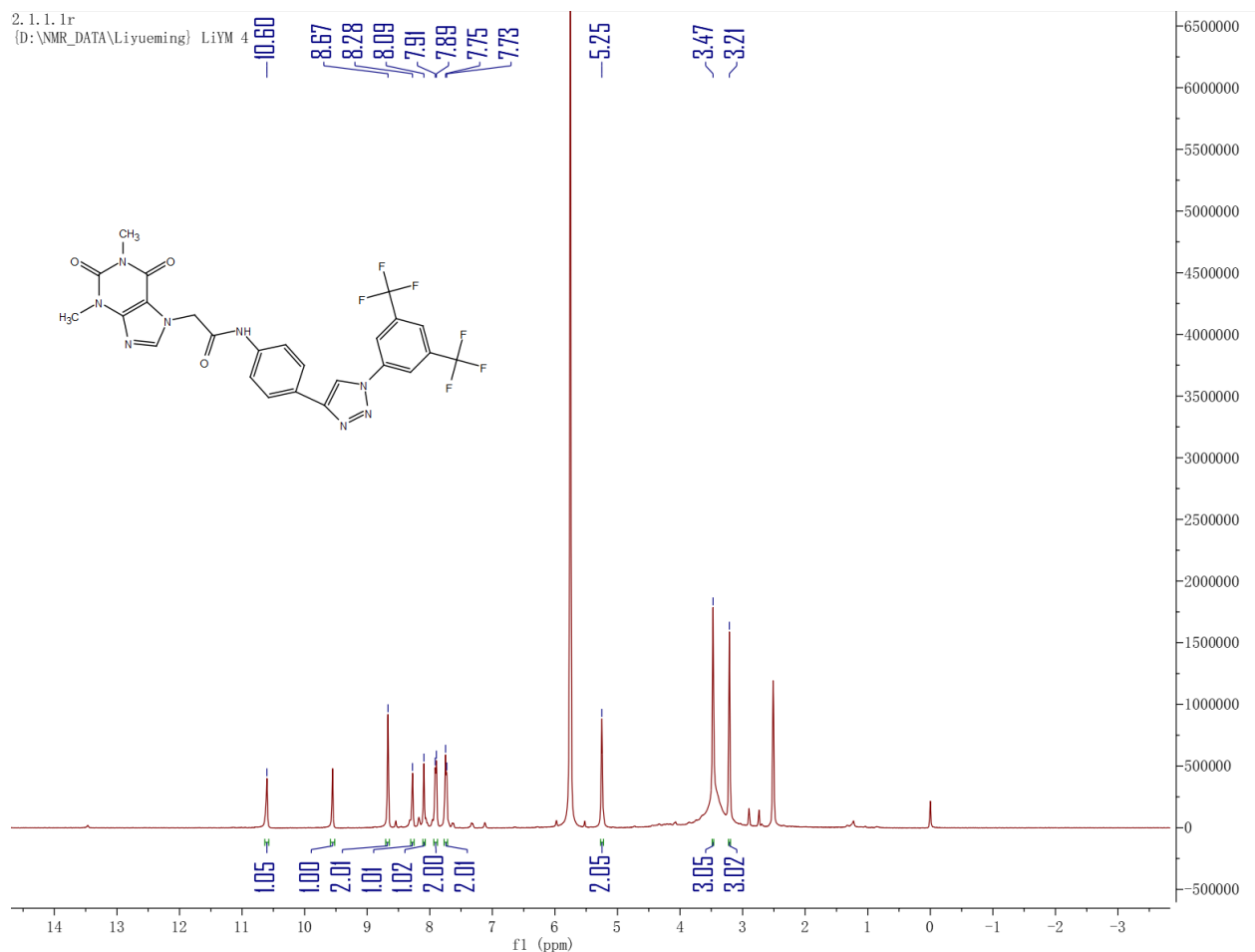


Figure S21-2. ^{13}C NMR spectrum (100MHz, DMSO- d_6) of compound D21

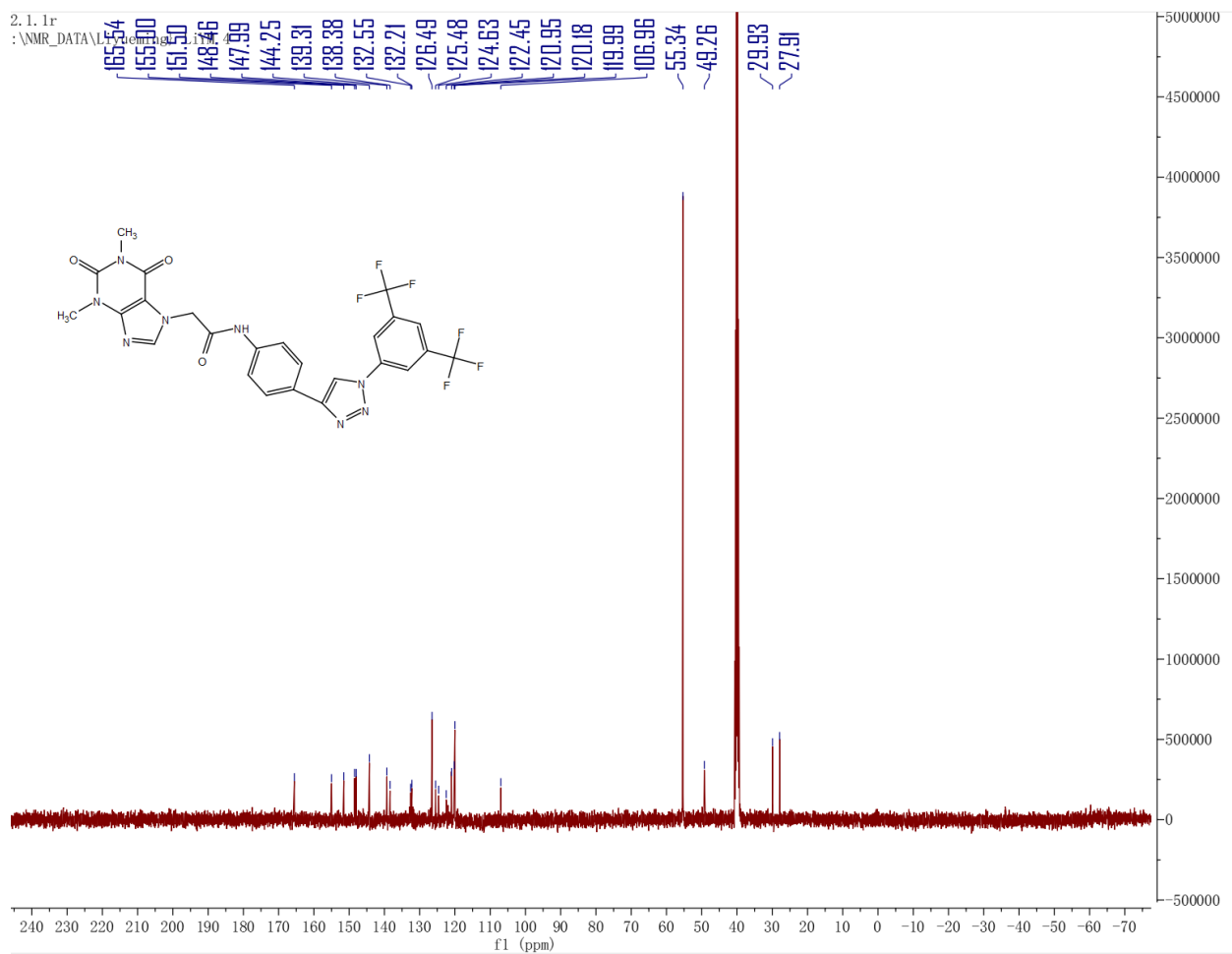


Figure S22-1. ^1H NMR spectrum (400MHz, DMSO- d_6) of compound D22



Figure S22-2. ^{13}C NMR spectrum (100MHz, DMSO- d_6) of compound D22

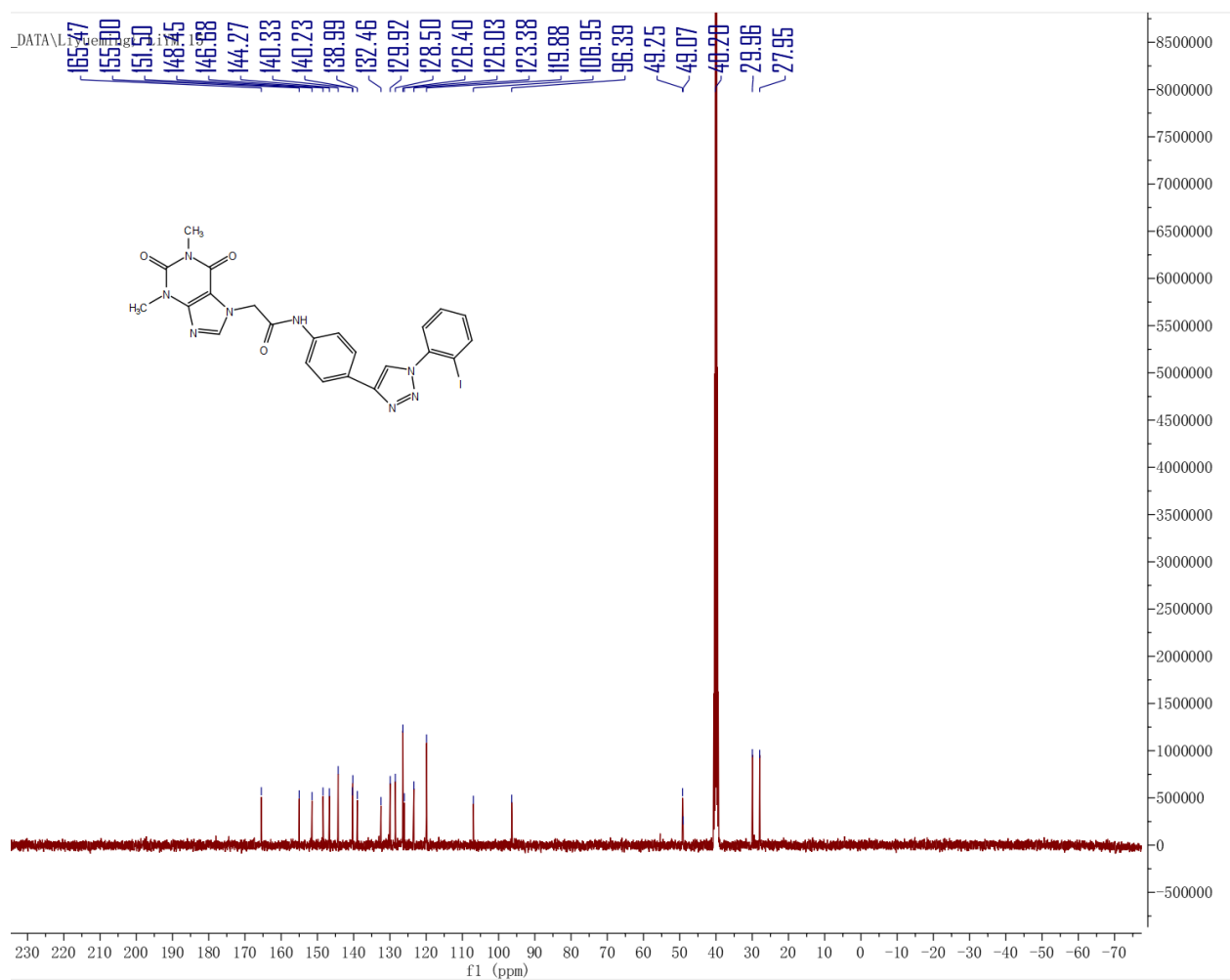


Figure S23-1. ^1H NMR spectrum (400MHz, DMSO- d_6) of compound D23

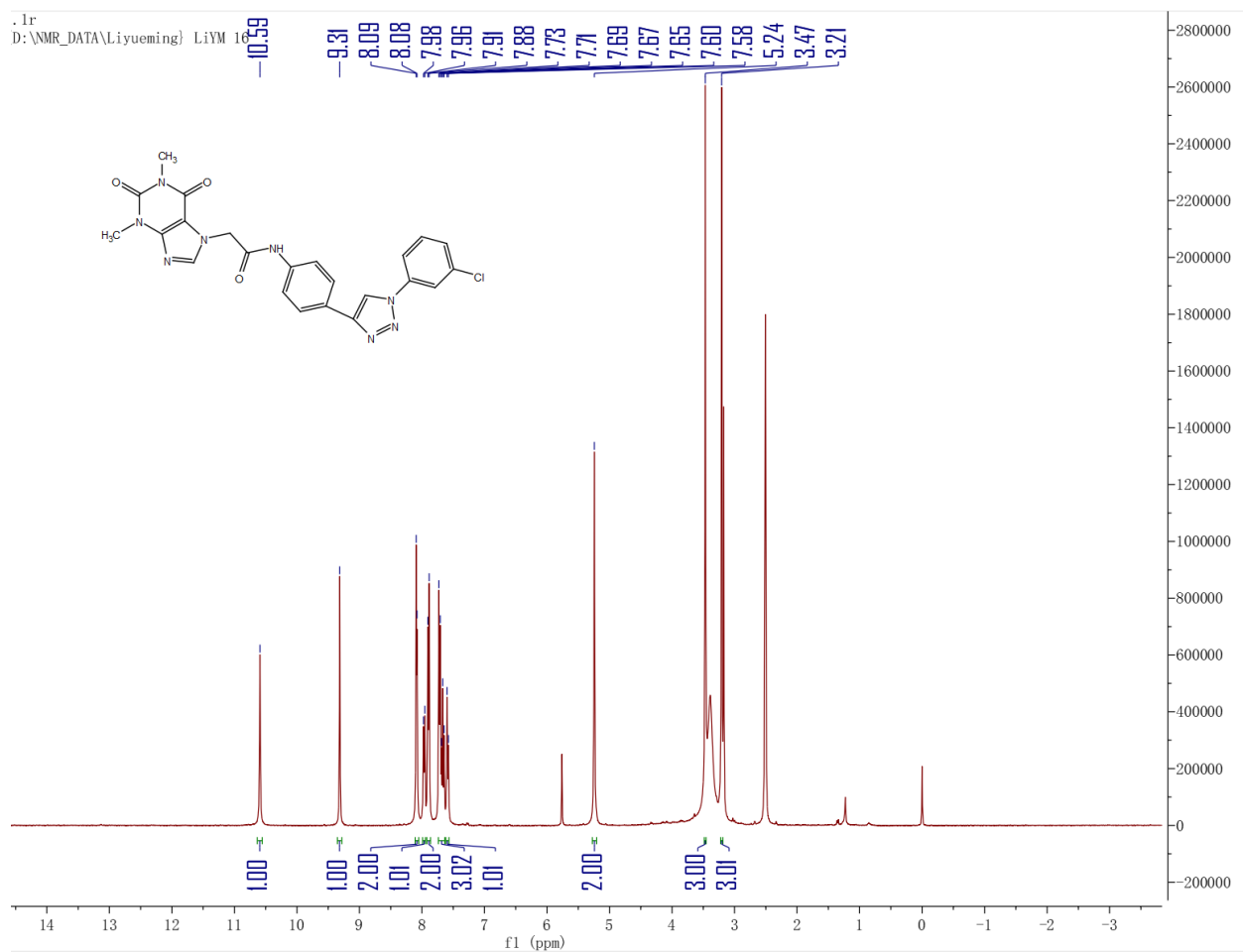


Figure S23-2. ^{13}C NMR spectrum (100MHz, DMSO- d_6) of compound D23

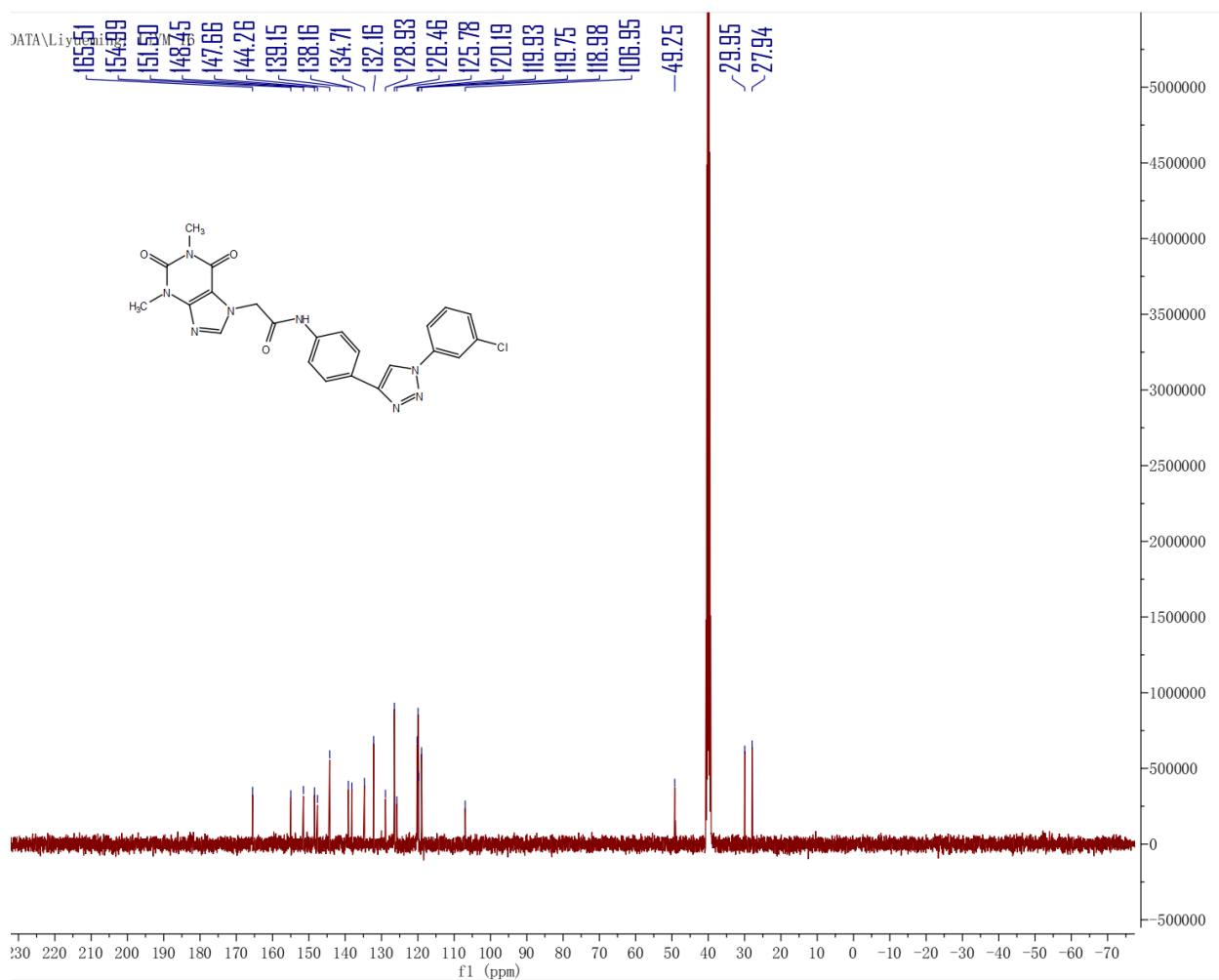


Figure S24-1. ^1H NMR spectrum (400MHz, DMSO- d_6) of compound D24

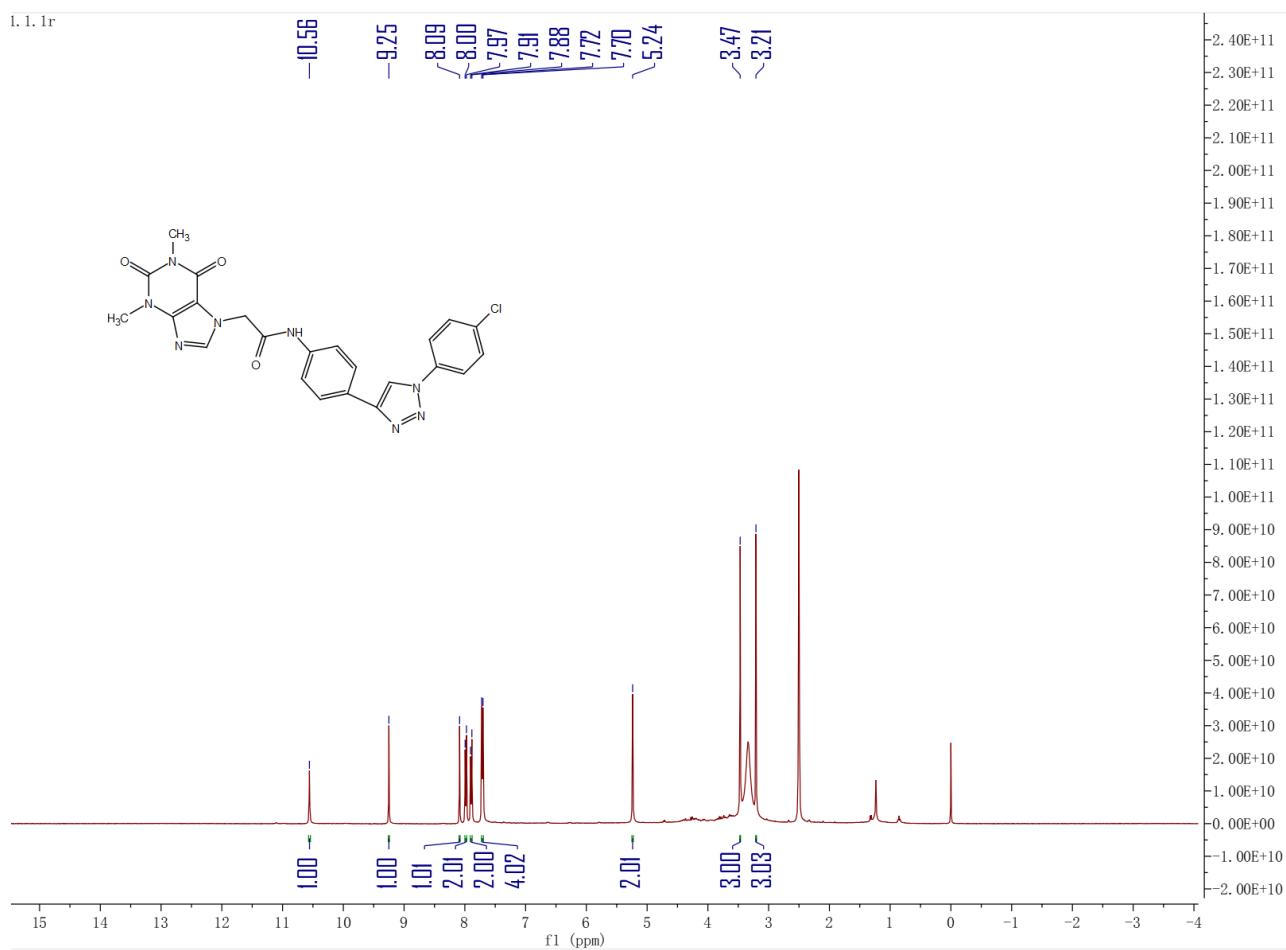
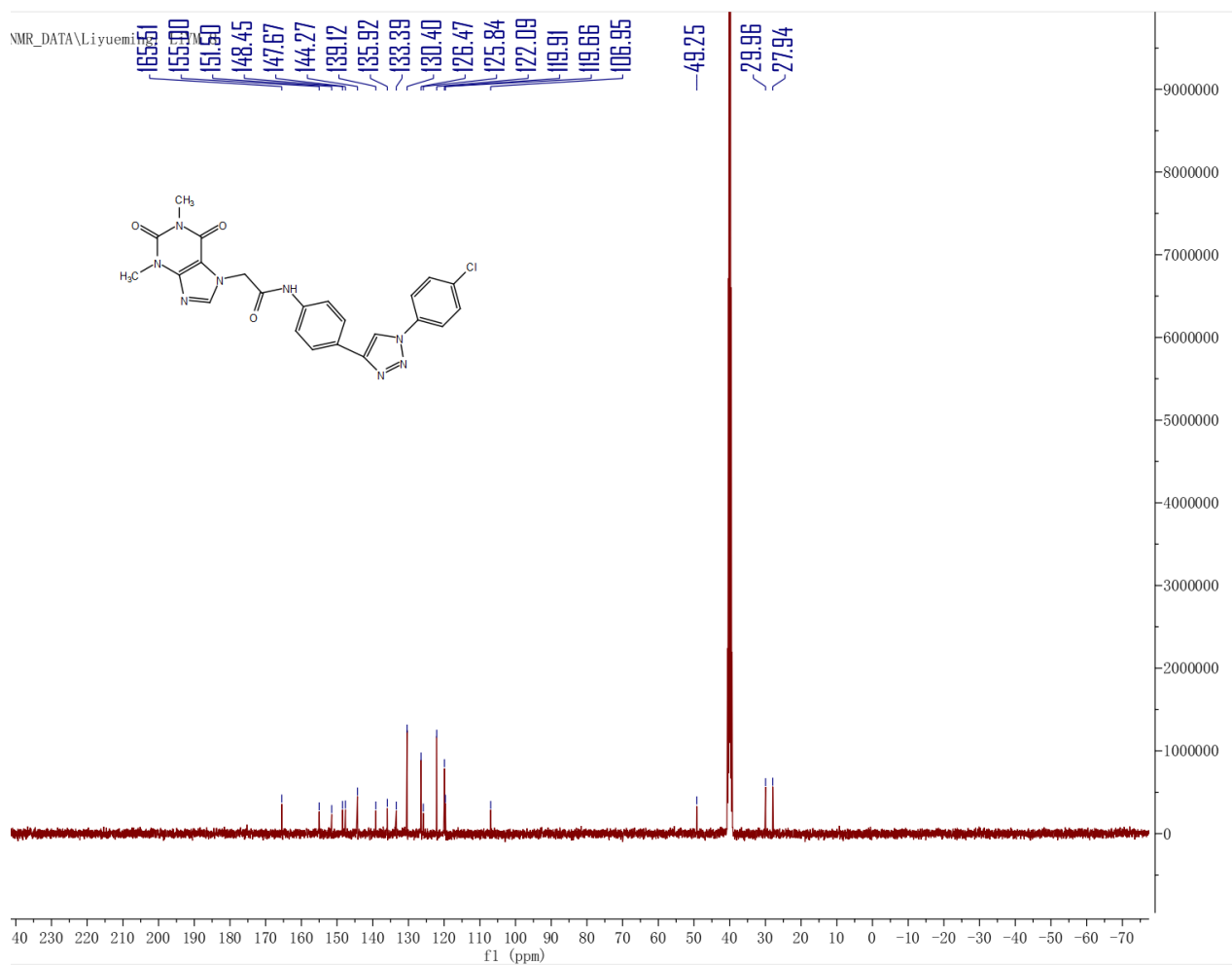


Figure S24-2. ^{13}C NMR spectrum (100MHz, DMSO- d_6) of compound D24



Chemical structure of compound 10 is shown in the top left corner. The ^1H NMR spectrum (DMSO- d_6) is displayed below the structure, showing peaks corresponding to the protons in the molecule. The x-axis represents the chemical shift in ppm (f1), ranging from 14 to -4. The y-axis represents the intensity, ranging from -5.0×10^{10} to 6.0×10^{11} .

Key peaks and their integration values are labeled:

- 10.50 (1.00)
- 8.54 (1.00)
- 8.08 (1.00)
- 7.81 (2.01)
- 7.79 (2.04)
- 7.65 (1.05)
- 7.63 (3.09)
- 7.32 (2.00)
- 7.30 (3.02)
- 7.28 (3.05)
- 6.94 (3.01)
- 6.88
- 5.22
- 3.75
- 3.46
- 3.20

Figure S25-2. ^{13}C NMR spectrum (100MHz, DMSO- d_6) of compound D25

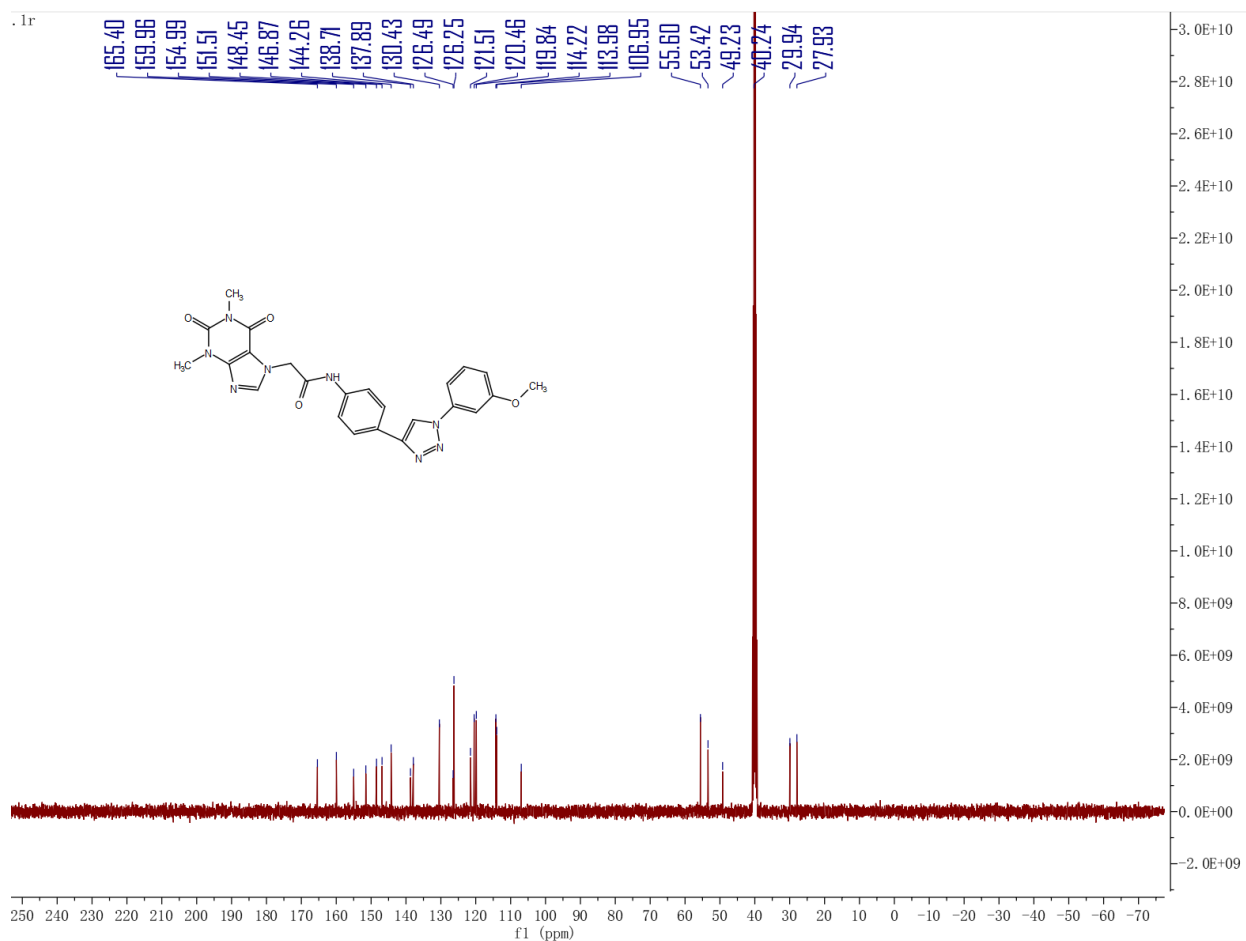


Figure S26-1. ^1H NMR spectrum (400MHz, DMSO- d_6) of compound D26

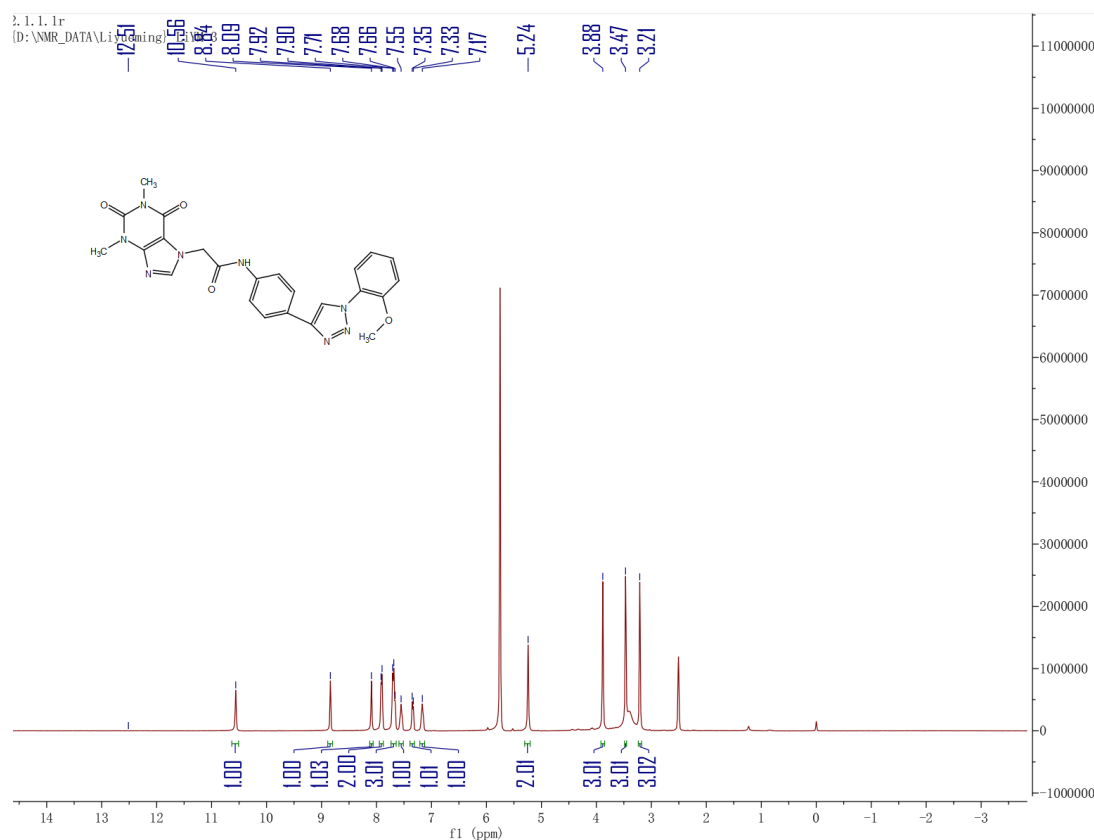


Figure S26-2. ^{13}C NMR spectrum (100MHz, DMSO- d_6) of compound D26

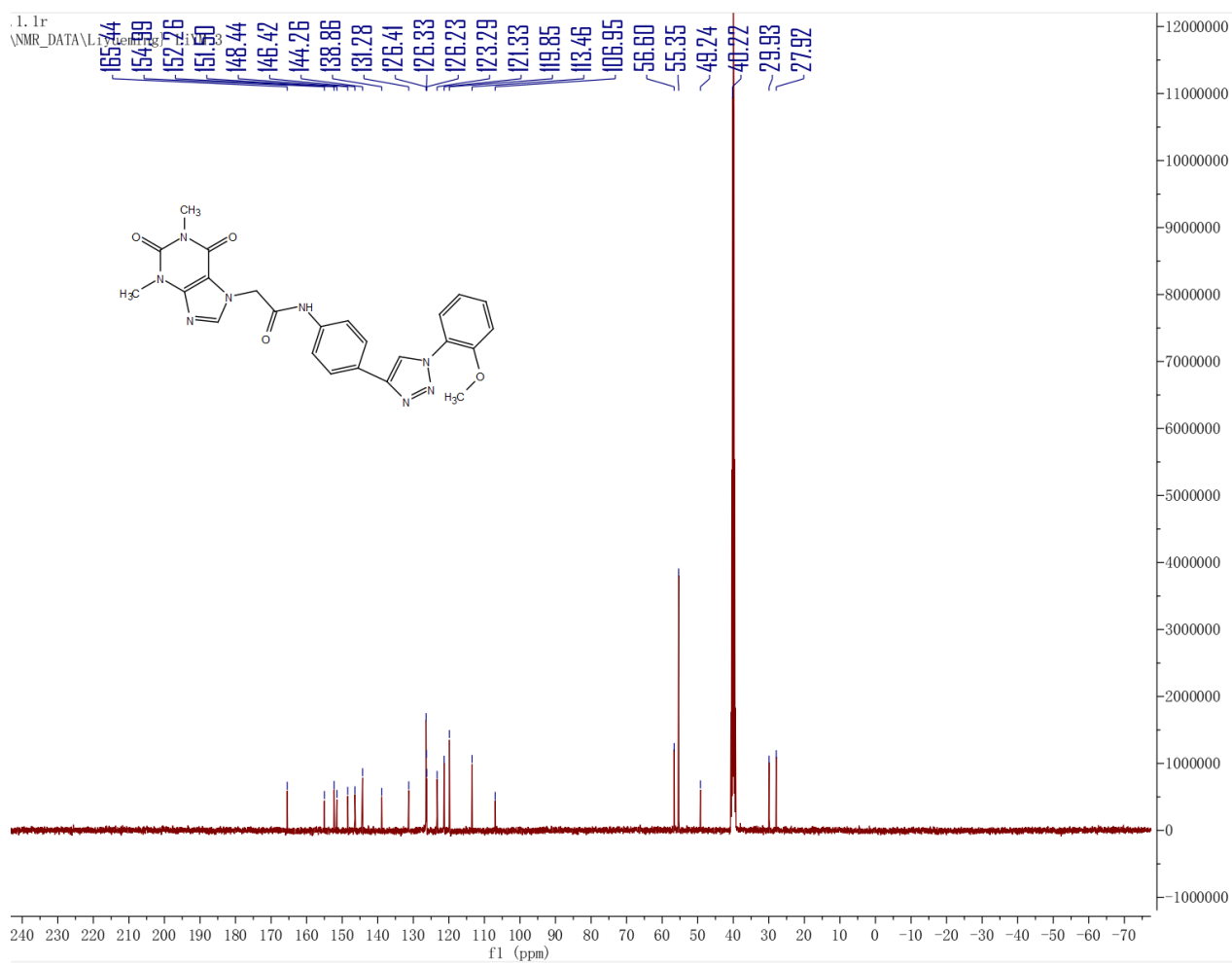


Figure S27-1. ^1H NMR spectrum (400MHz, DMSO- d_6) of compound D27

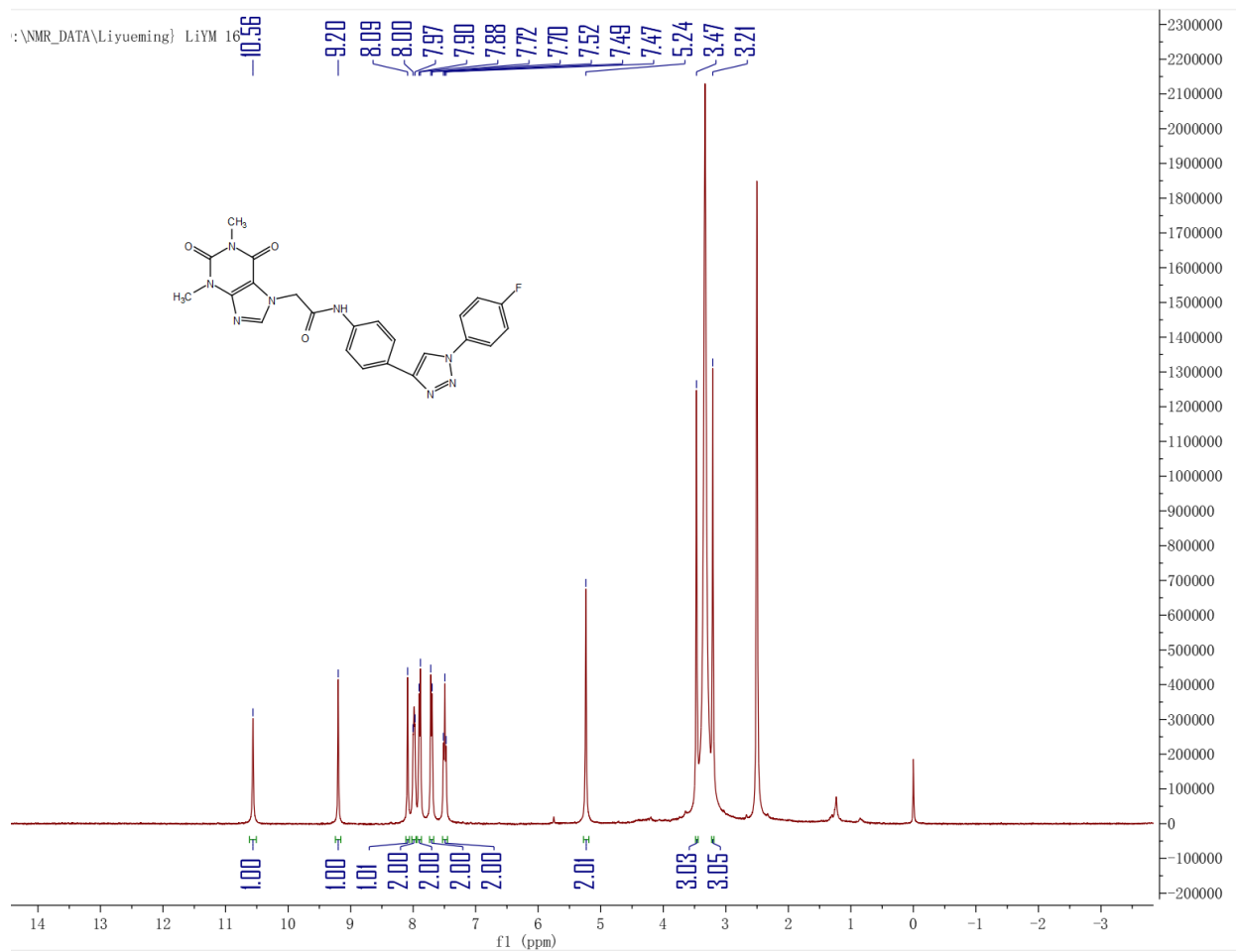


Figure S27-2. ^{13}C NMR spectrum (100MHz, DMSO- d_6) of compound D27

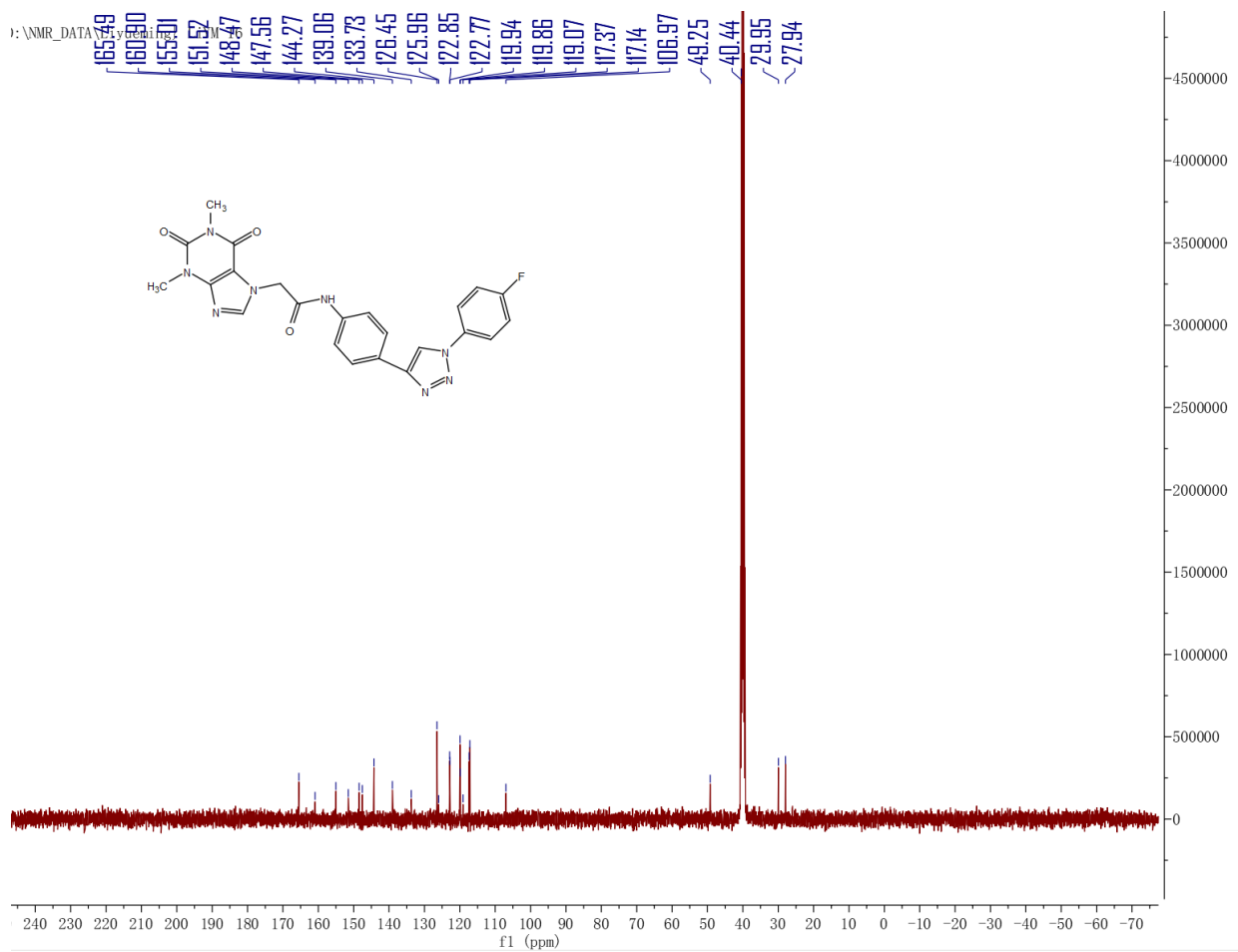


Figure S28-1. ^1H NMR spectrum (400MHz, DMSO- d_6) of compound D28

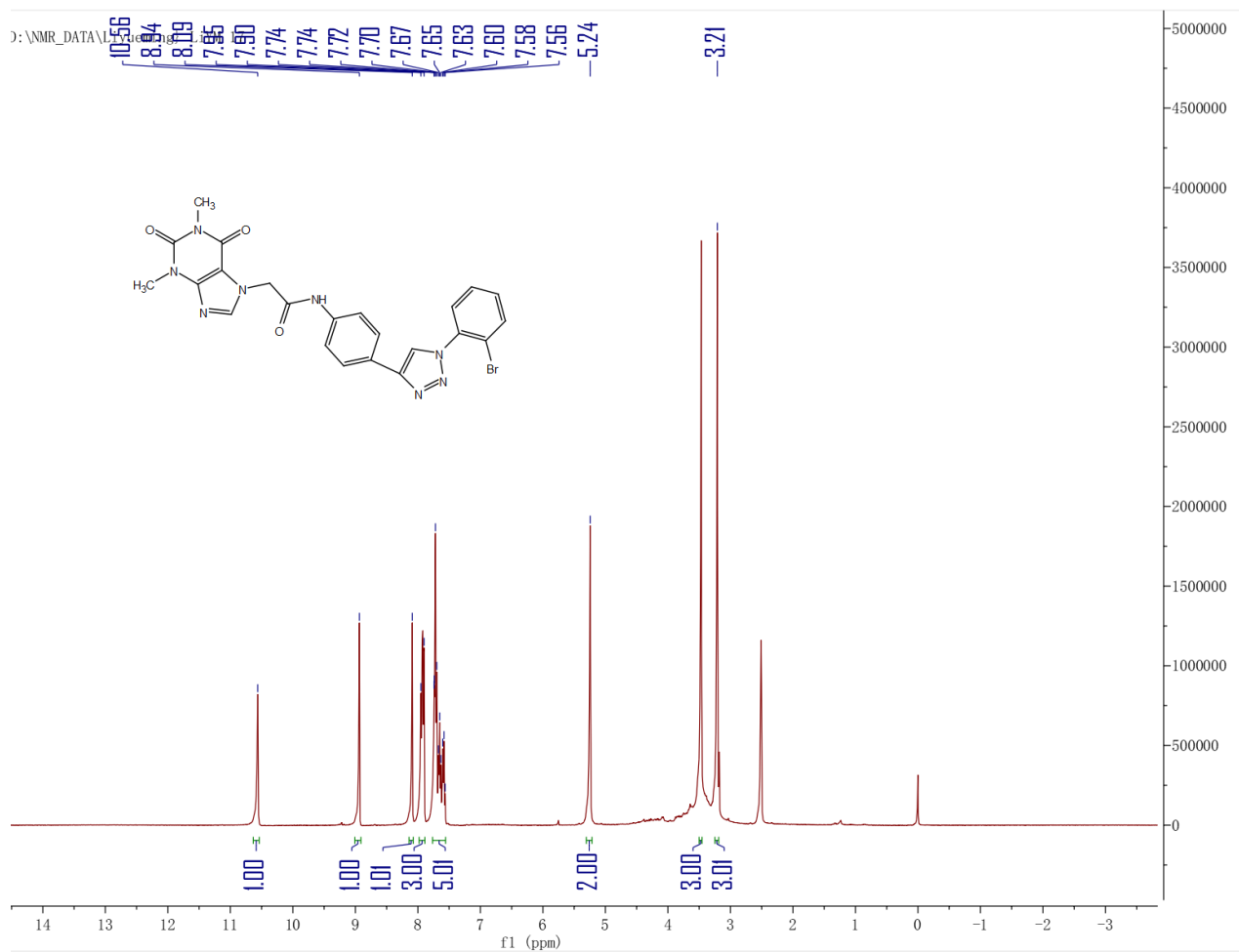


Figure S28-2. ^{13}C NMR spectrum (100MHz, DMSO- d_6) of compound D28

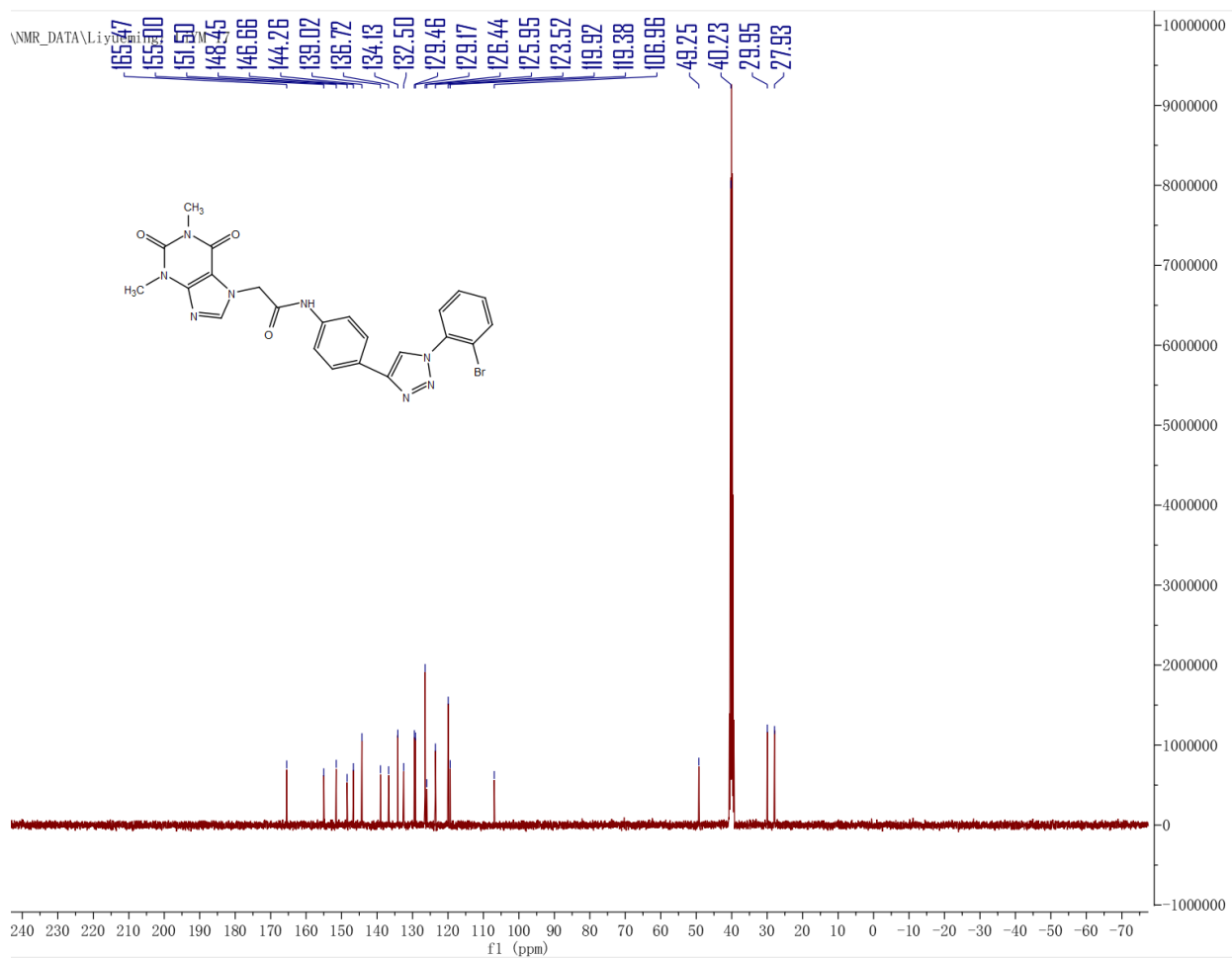


Figure S29-1. ^1H NMR spectrum (400MHz, DMSO- d_6) of compound D29

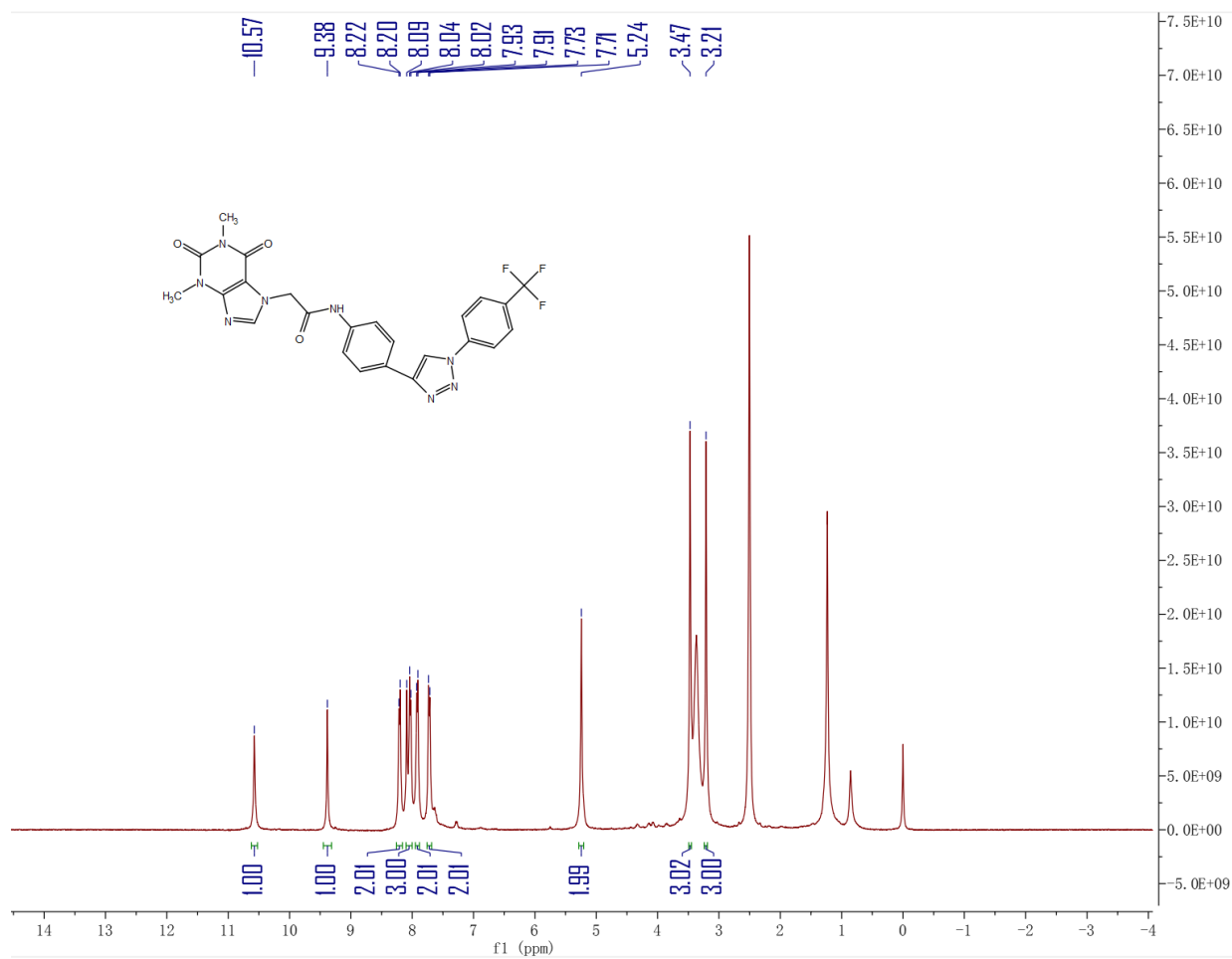


Figure S29-2. ^{13}C NMR spectrum (100MHz, DMSO- d_6) of compound D29

