

Discovery of Flavone Derivatives Containing Carboxamide Fragments as Novel Antiviral Agents

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† These authors contributed equally to this work.

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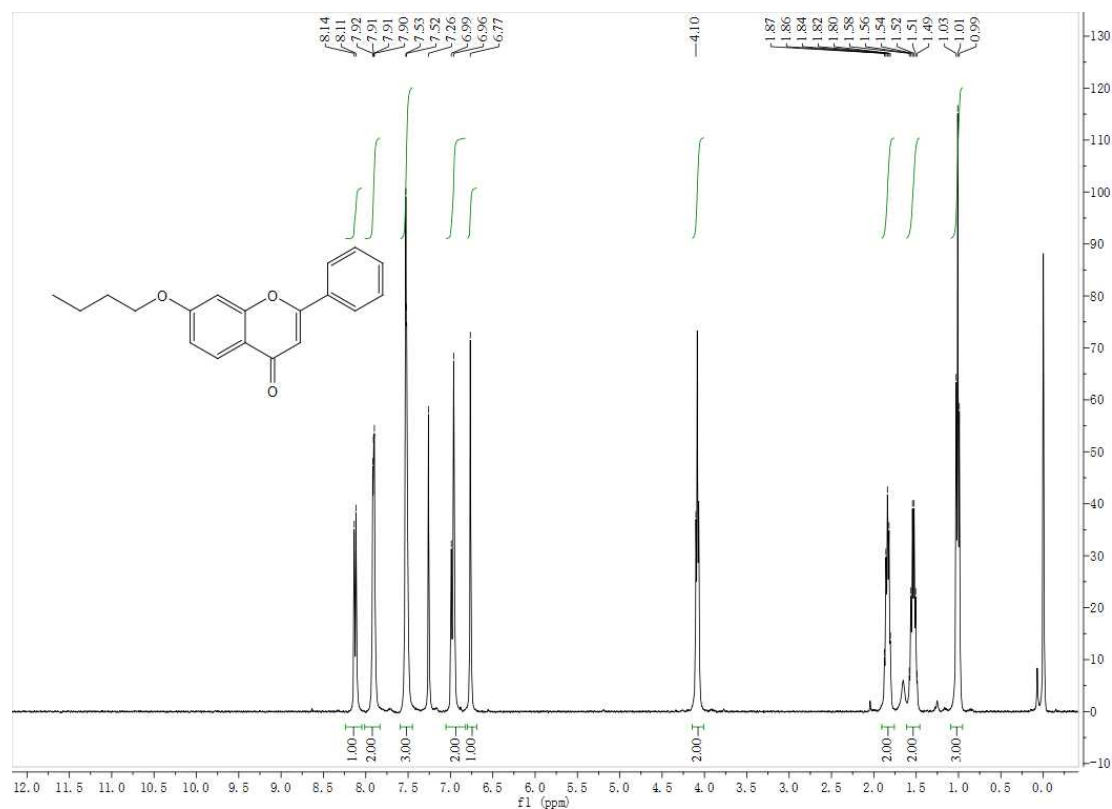
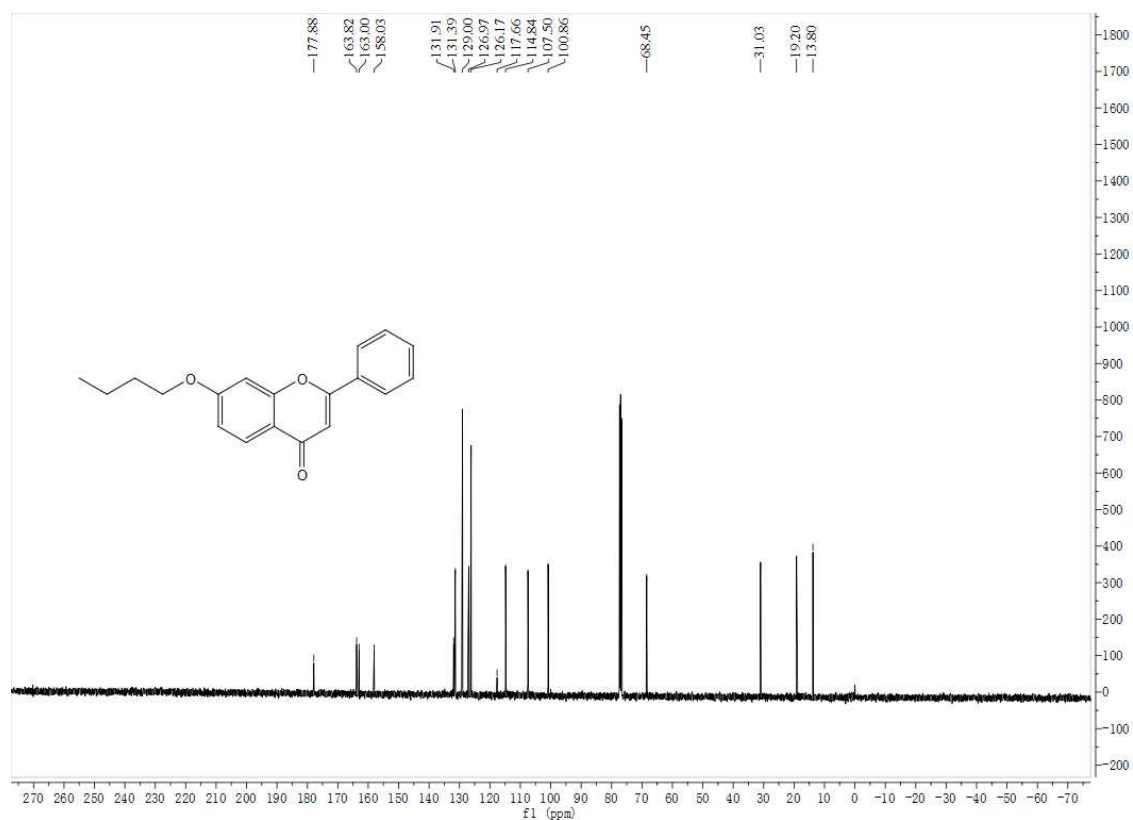
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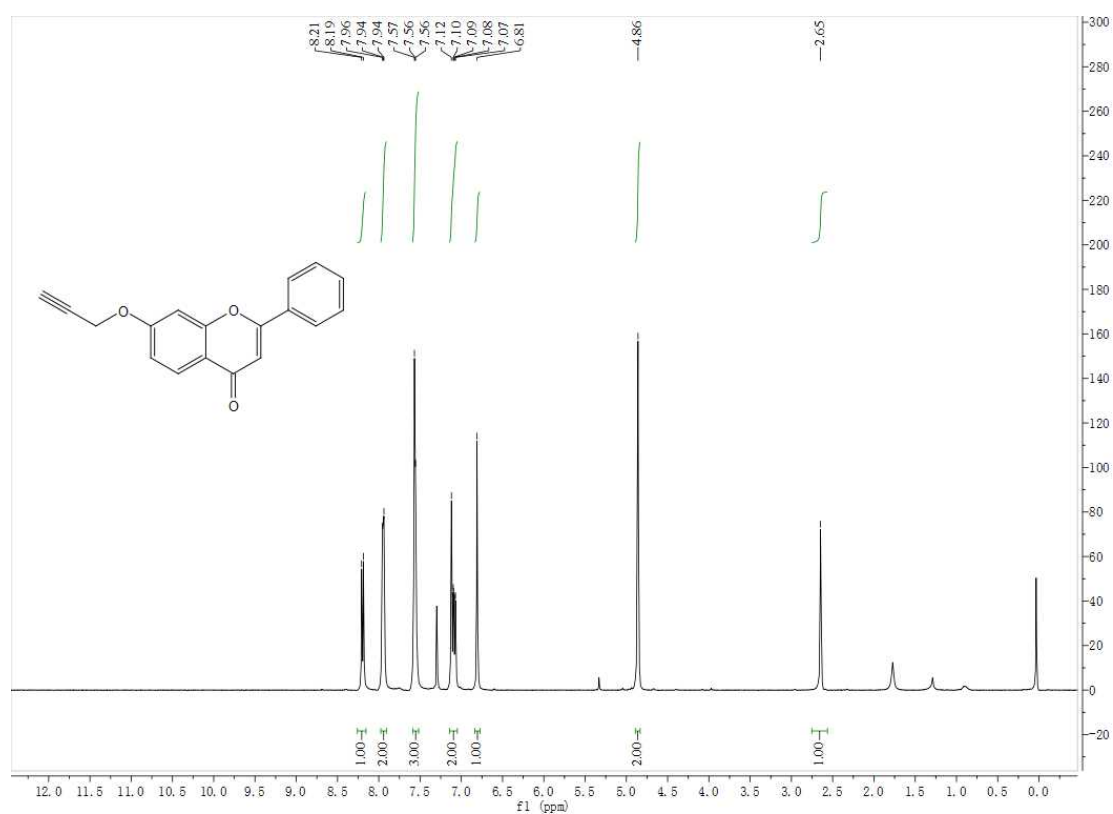
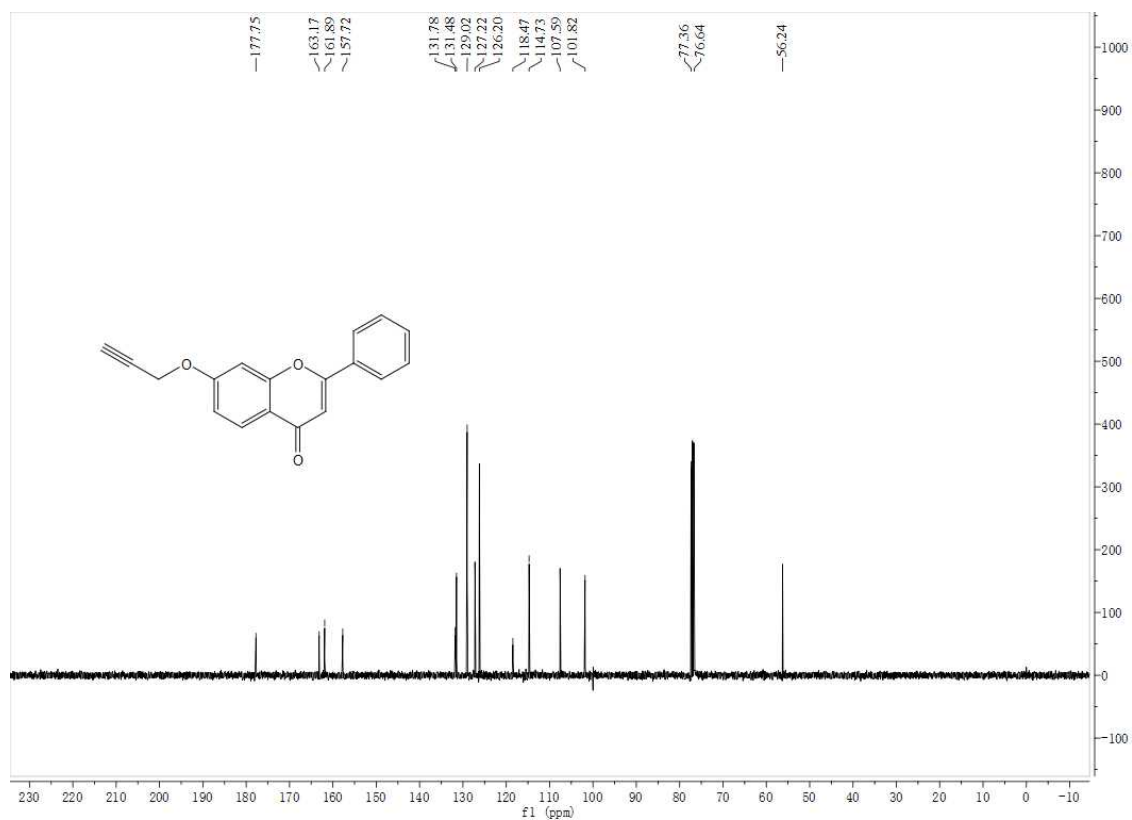
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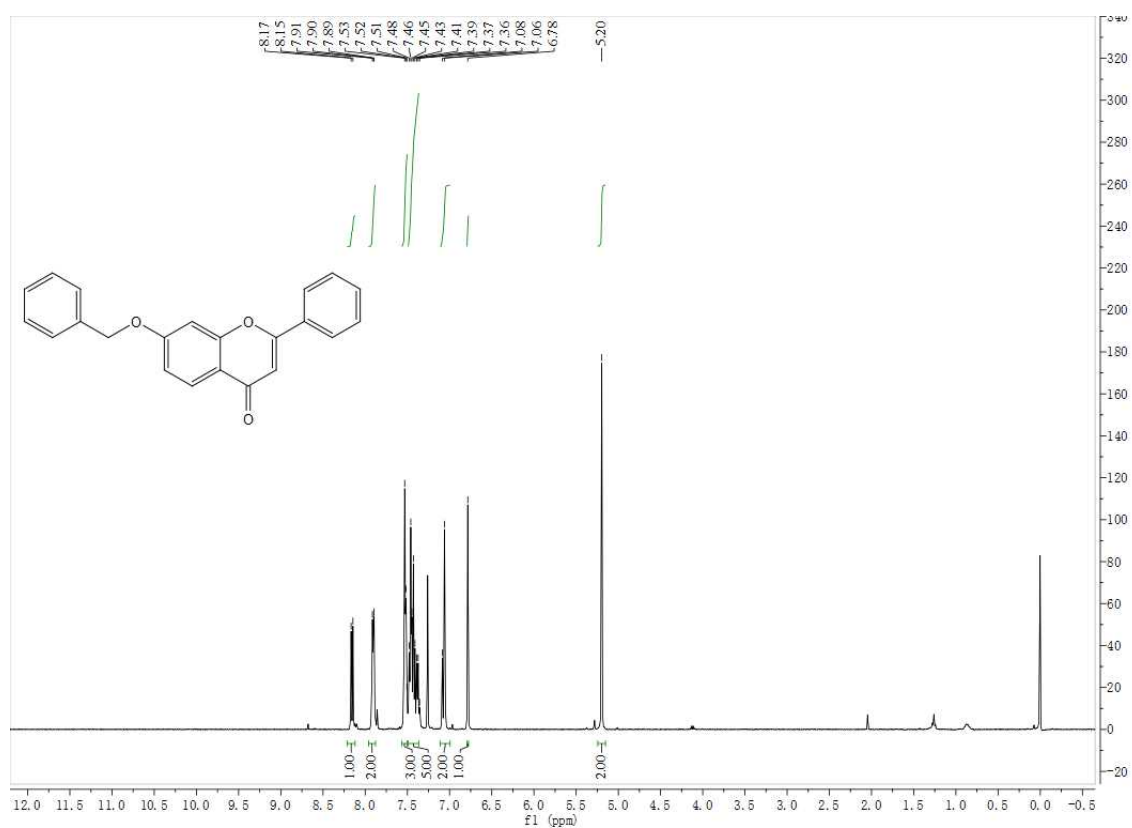
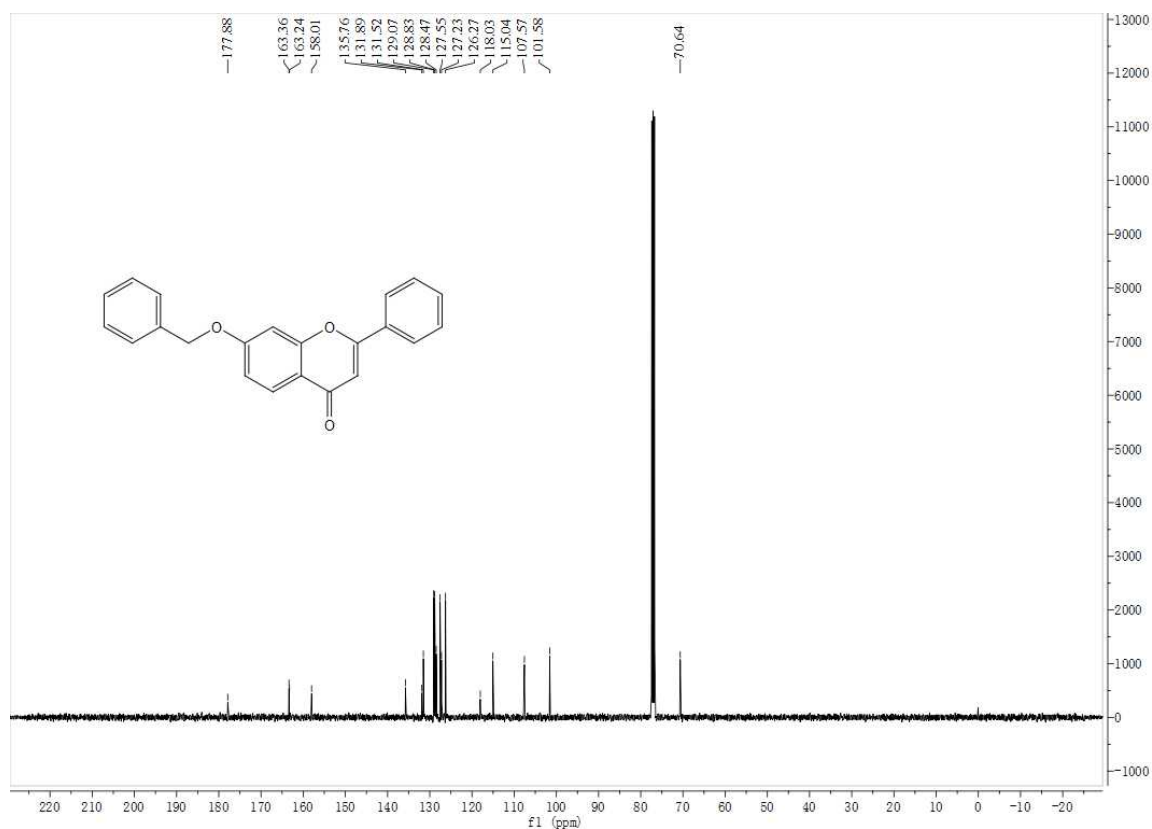
Section S1. Phytotoxic Activity

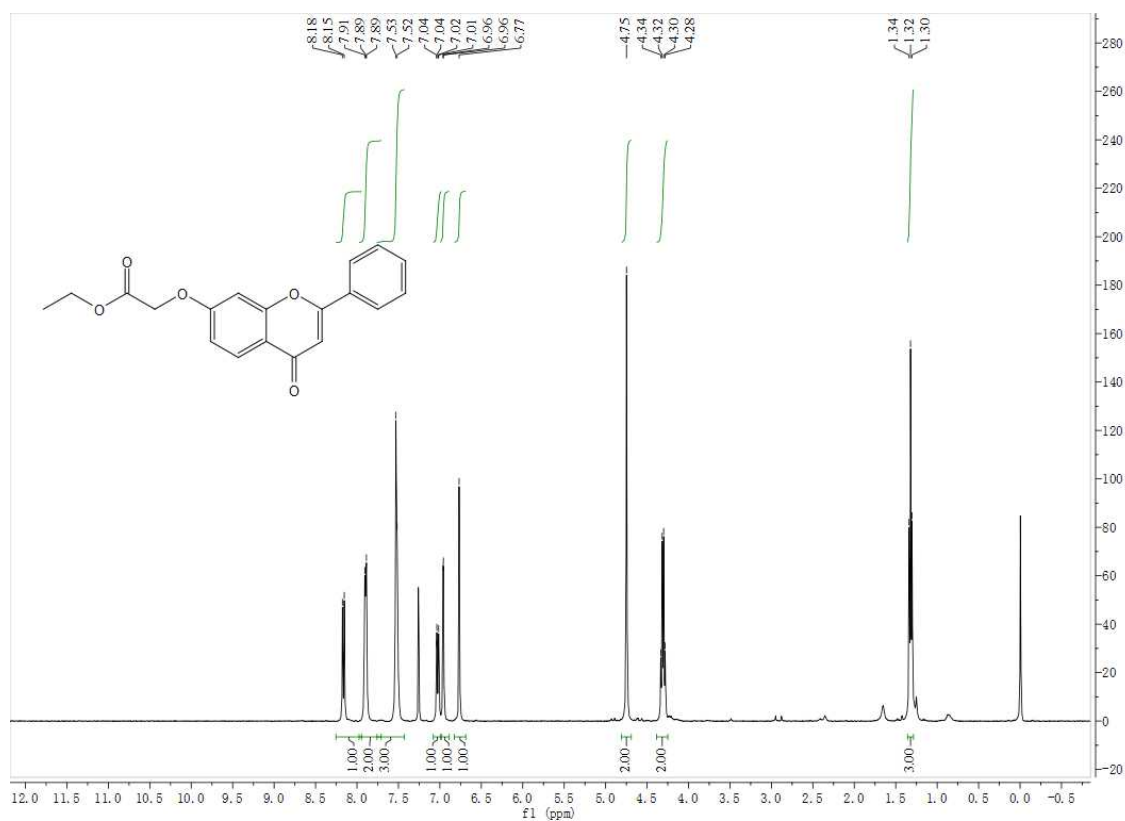
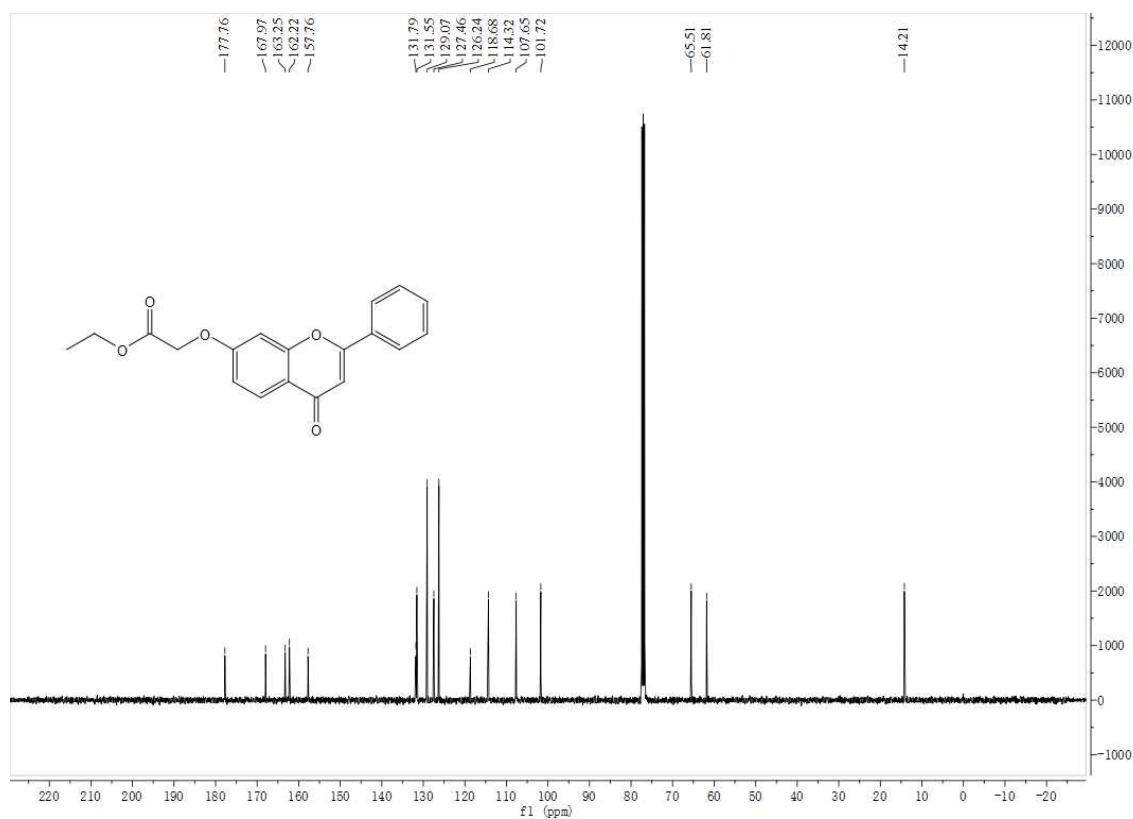
The growing 5–6 leaf stage tobaccos (*Nicotiana tabacum* var *Xanthi nc*) were selected. The compound solution (500 µg/mL) was smeared on the leaves and calculated the number of lesions after 0, 3, 7 and 10 days respectively. [7,51] There are three replicates for each compound.

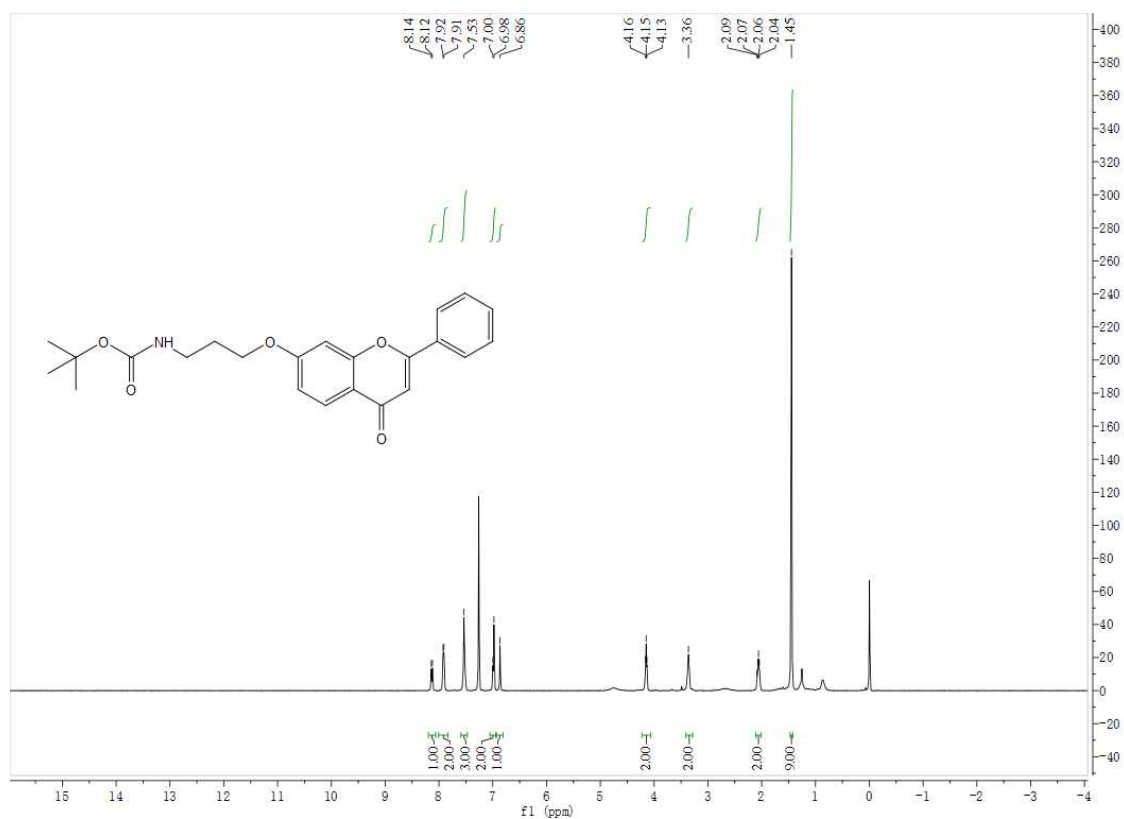
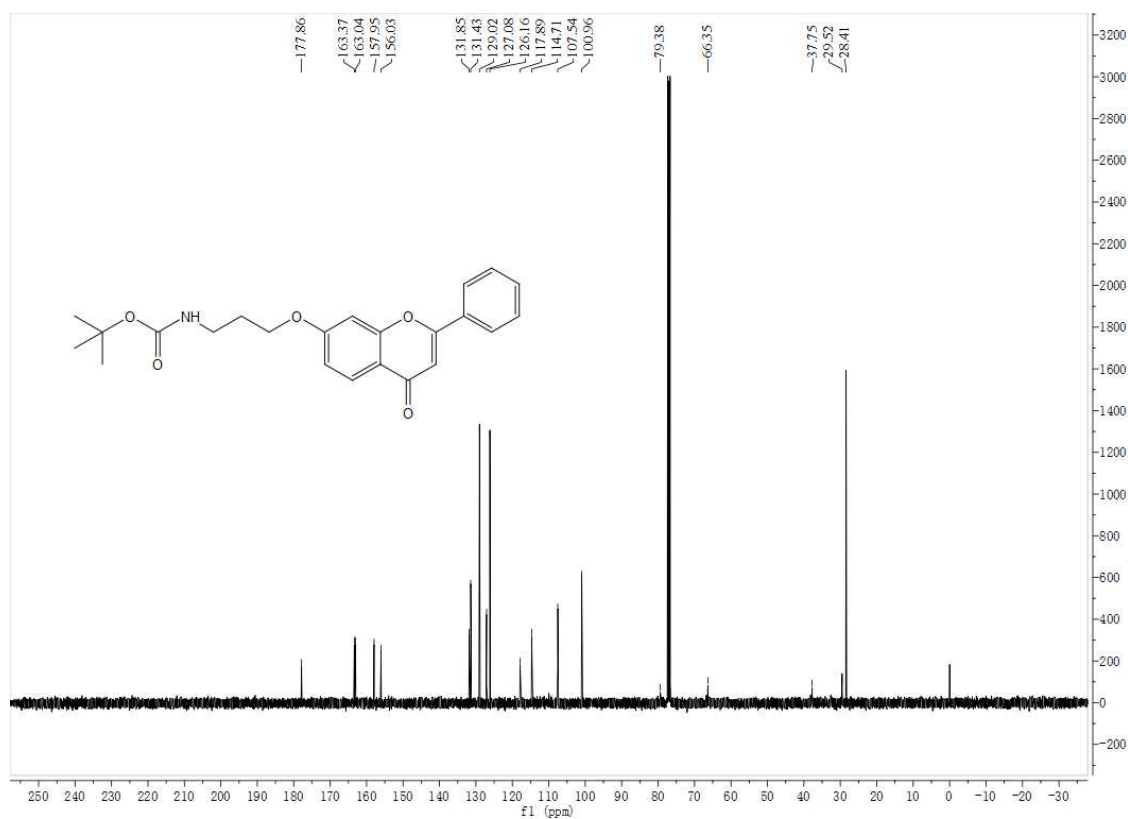
Section S3. Copies of NMR spectra (Figures S1–S60)

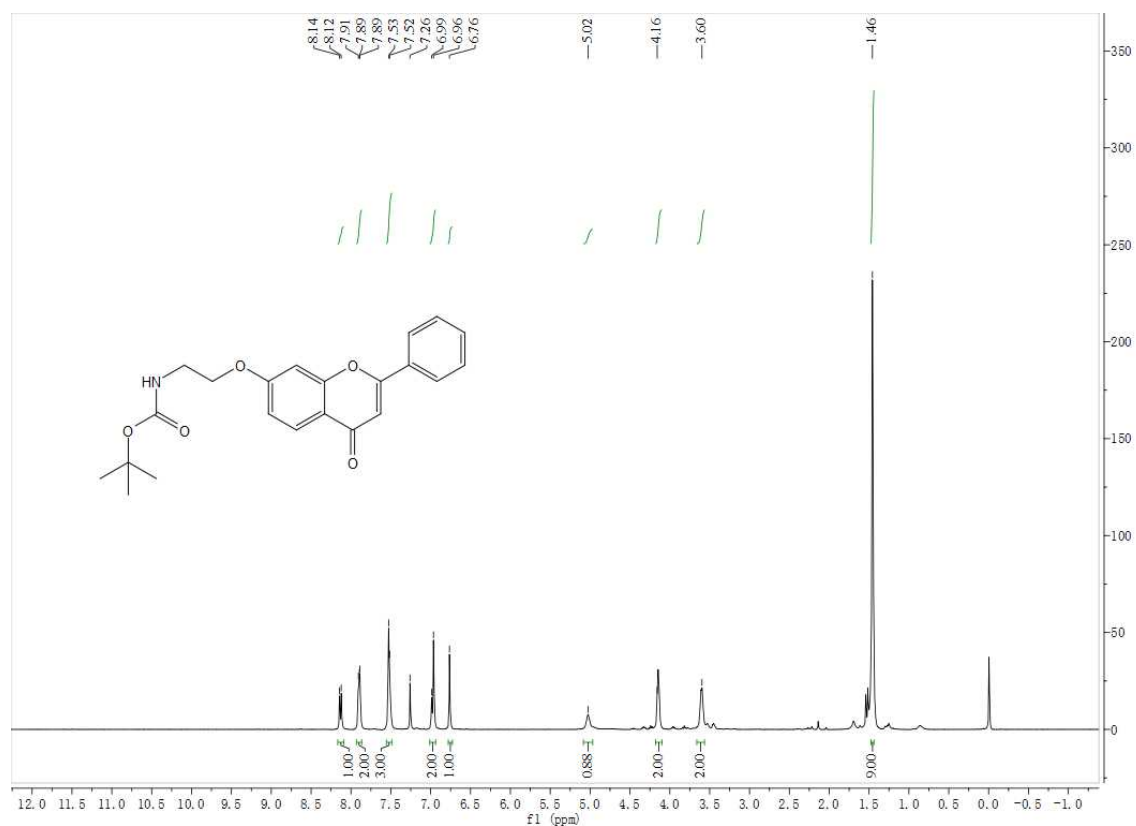
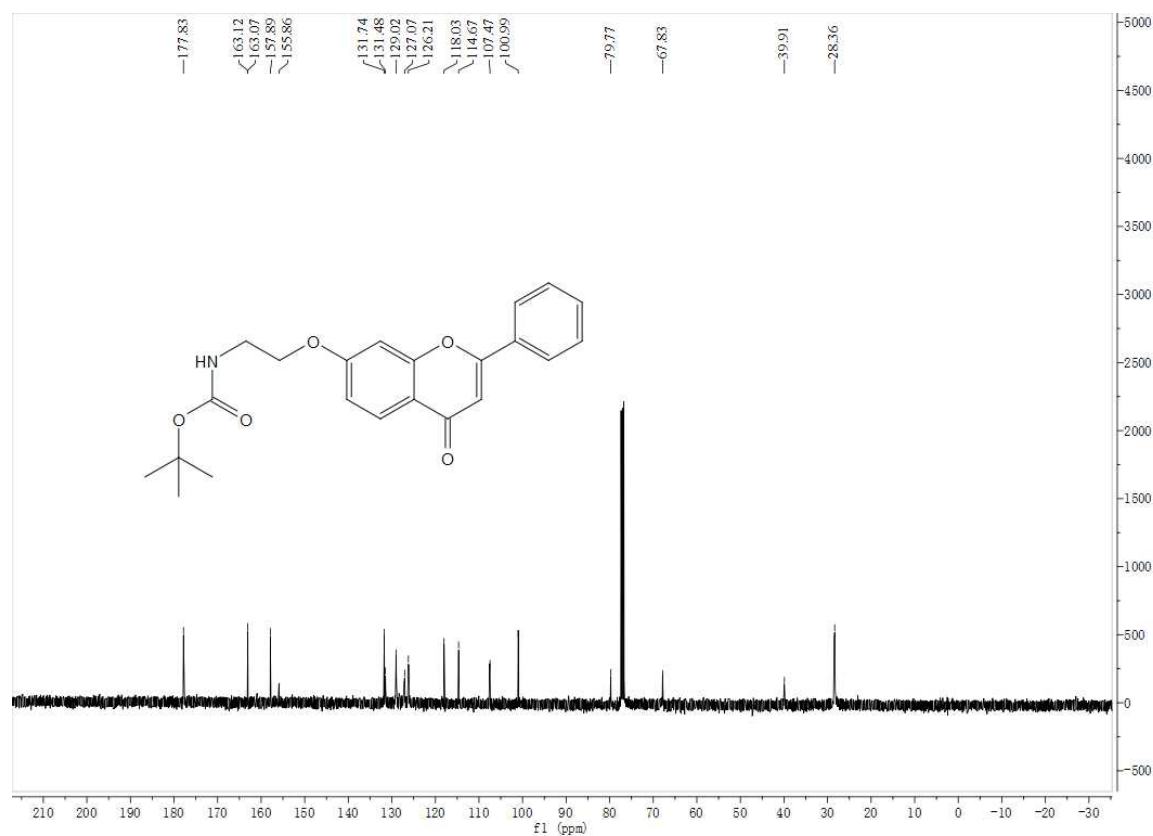
Figure S1. ¹H NMR spectrum of 2aFigure S2. ¹³C NMR spectrum of 2a

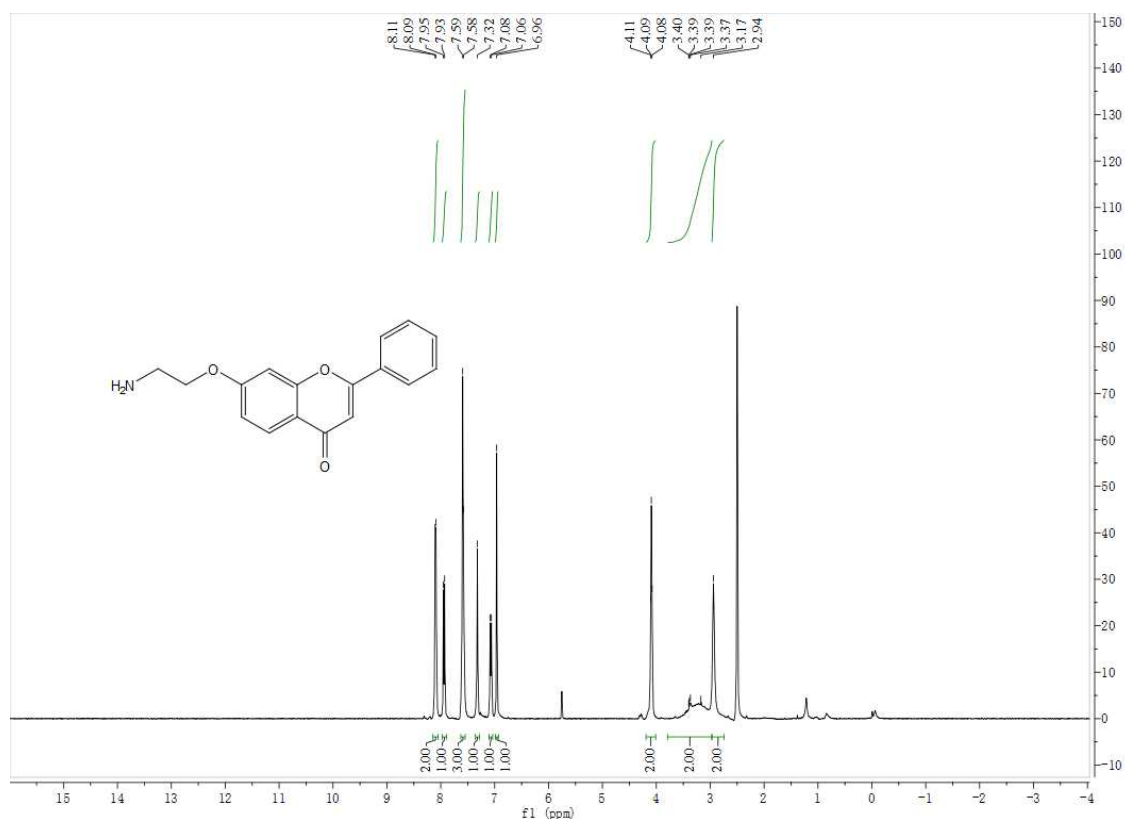
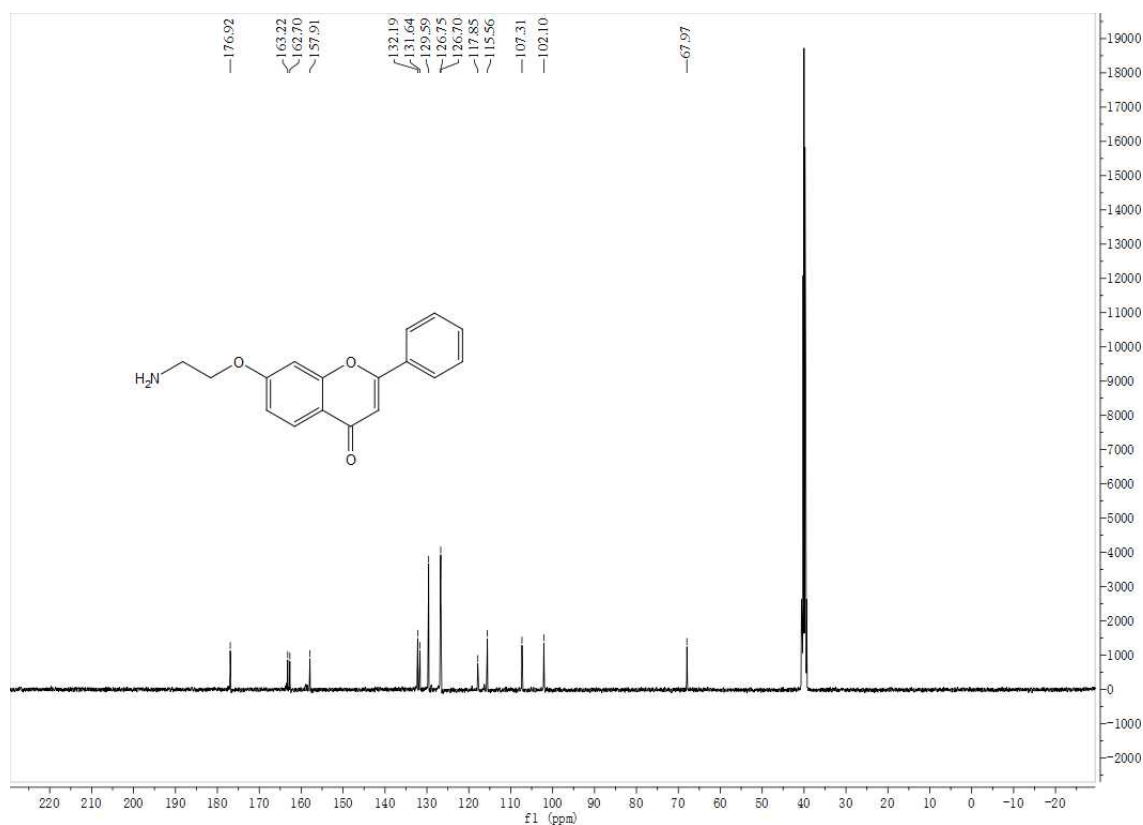
Figure S3. ¹H NMR spectrum of 2bFigure S4. ¹³C NMR spectrum of 2b

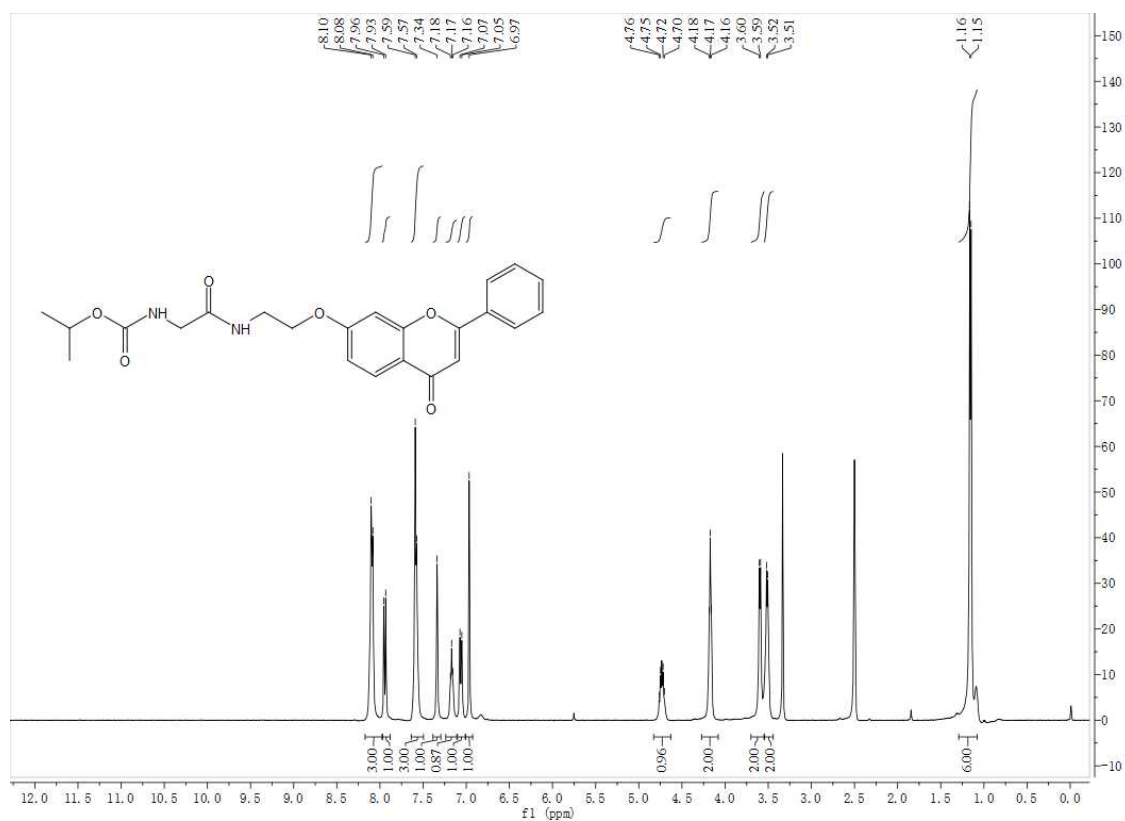
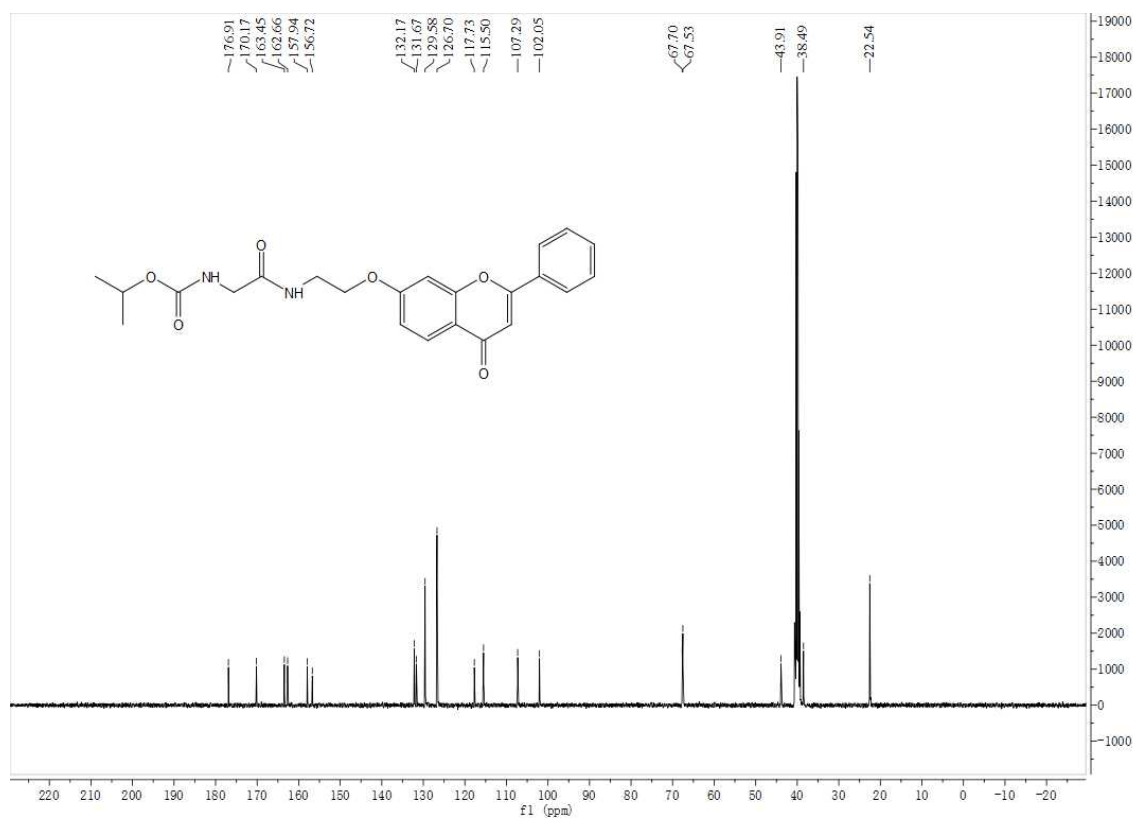
Figure S5. ¹H NMR spectrum of 2cFigure S6. ¹³C NMR spectrum of 2c

Figure S7. ¹H NMR spectrum of 2dFigure S8. ¹³C NMR spectrum of 2d

Figure S9. ¹H NMR spectrum of 2eFigure S10. ¹³C NMR spectrum of 2e

Figure S11. ¹H NMR spectrum of **2f**NMR spectrum of **2f**Figure S12. ¹³C

Figure S13. ¹H NMR spectrum of 3Figure S14. ¹³C NMR spectrum of 3

Figure S15. ¹H NMR spectrum of 4aFigure S16. ¹³C NMR spectrum of 4a

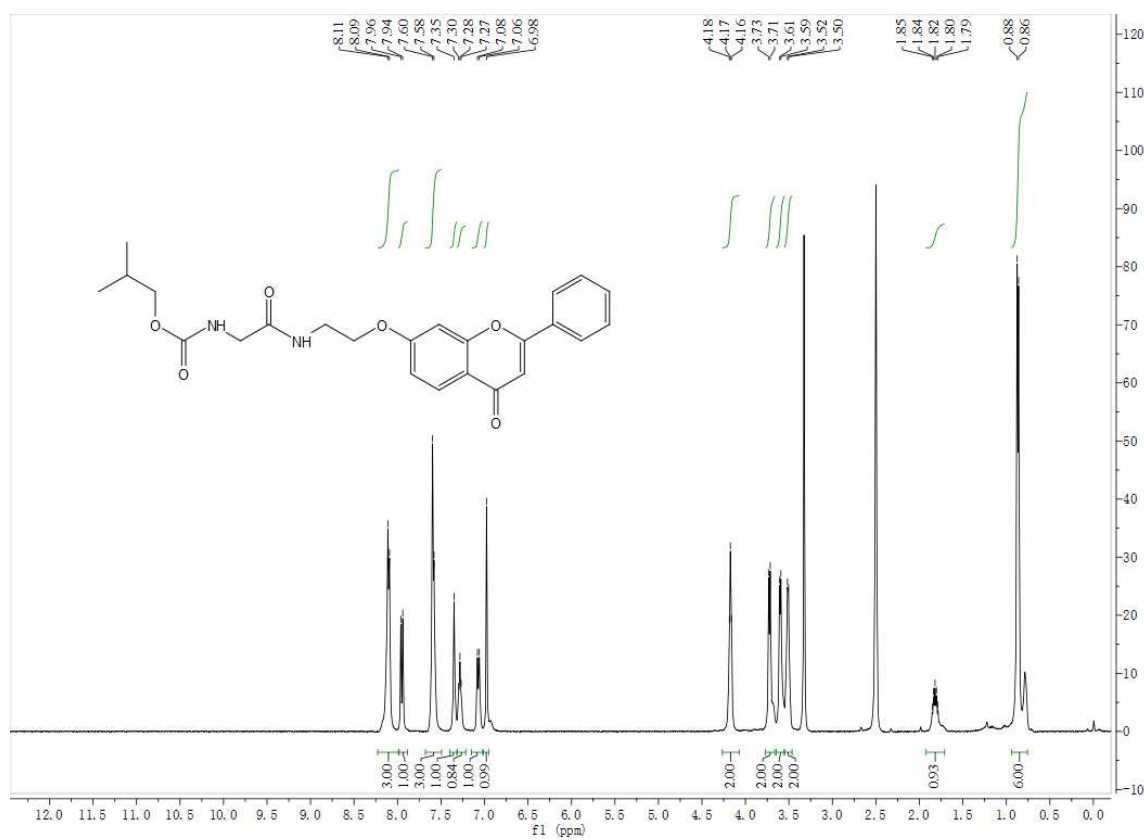
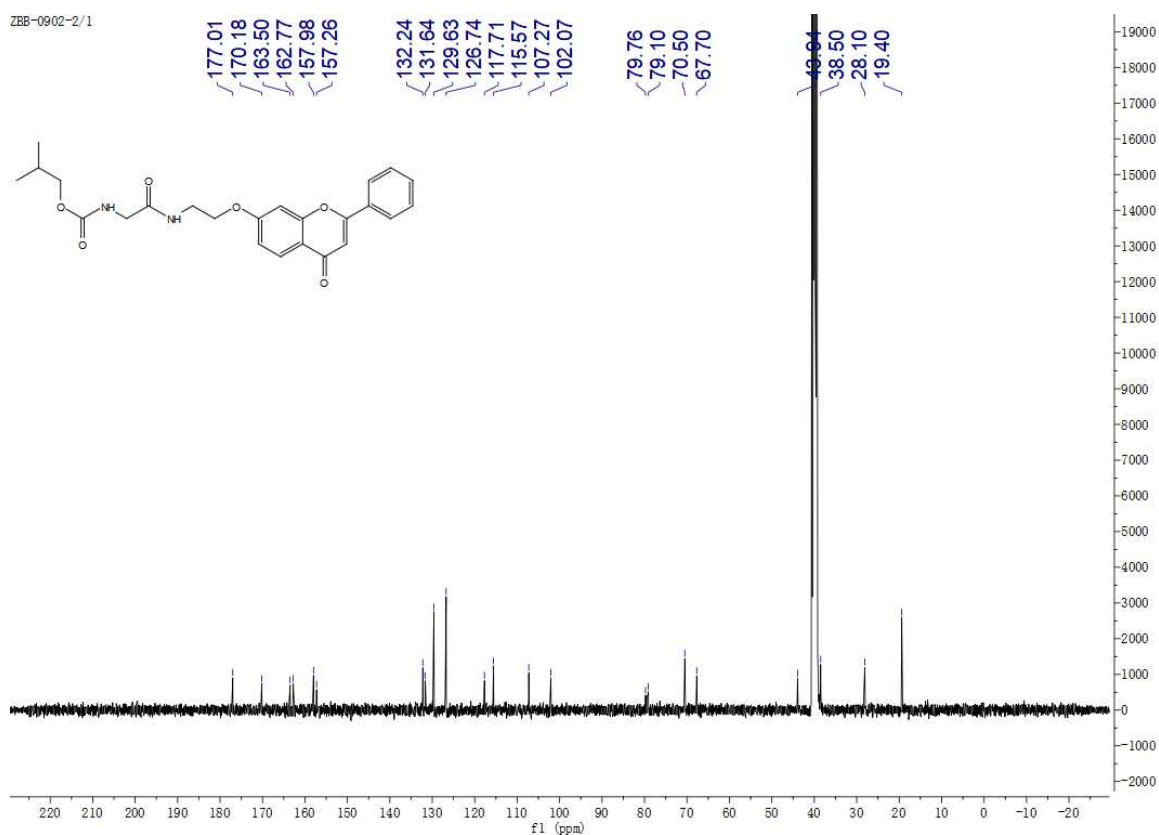
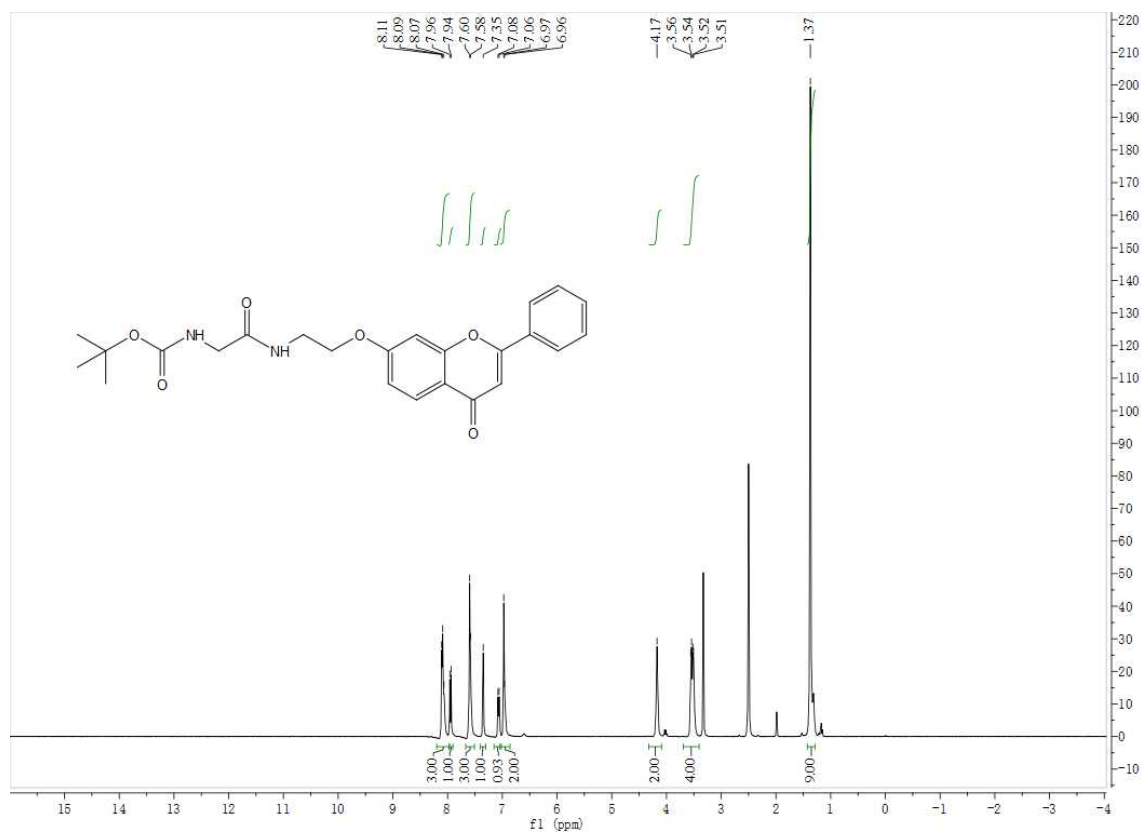


Figure S17. ^1H NMR spectrum of **4b**

Figure S18. ¹³C NMR spectrum of 4bFigure S19. ¹H NMR spectrum of 4c

Chemical structure of compound 10: CC(C)OC(=O)N[C@@H](C(=O)NCCOC1=CC=C2C(=C1)O[C@H](C2=O)C3=CC=CC=C3)C

¹H NMR spectrum (CDCl₃) of compound 10. The x-axis represents the chemical shift in ppm (f1), ranging from -0.5 to 12.0. The y-axis represents the intensity. The spectrum shows several peaks with corresponding integrations and chemical shifts labeled at the top.

Chemical shifts (ppm) labeled at the top: 8.09, 8.08, 7.95, 7.93, 7.59, 7.57, 7.32, 7.14, 7.13, 7.06, 7.04, 6.96, 4.72, 4.71, 4.69, 4.16, 4.03, 4.02, 4.00, 3.51, 3.50, 3.49, 1.19, 1.17, 1.14, 1.13.

Integrations labeled below the spectrum: 3.00, 1.00, 3.00, 1.00, 0.88, 1.00, 1.00, 1.00, 1.00, 1.00, 2.00, 2.00, 2.00, 3.00, 6.00.

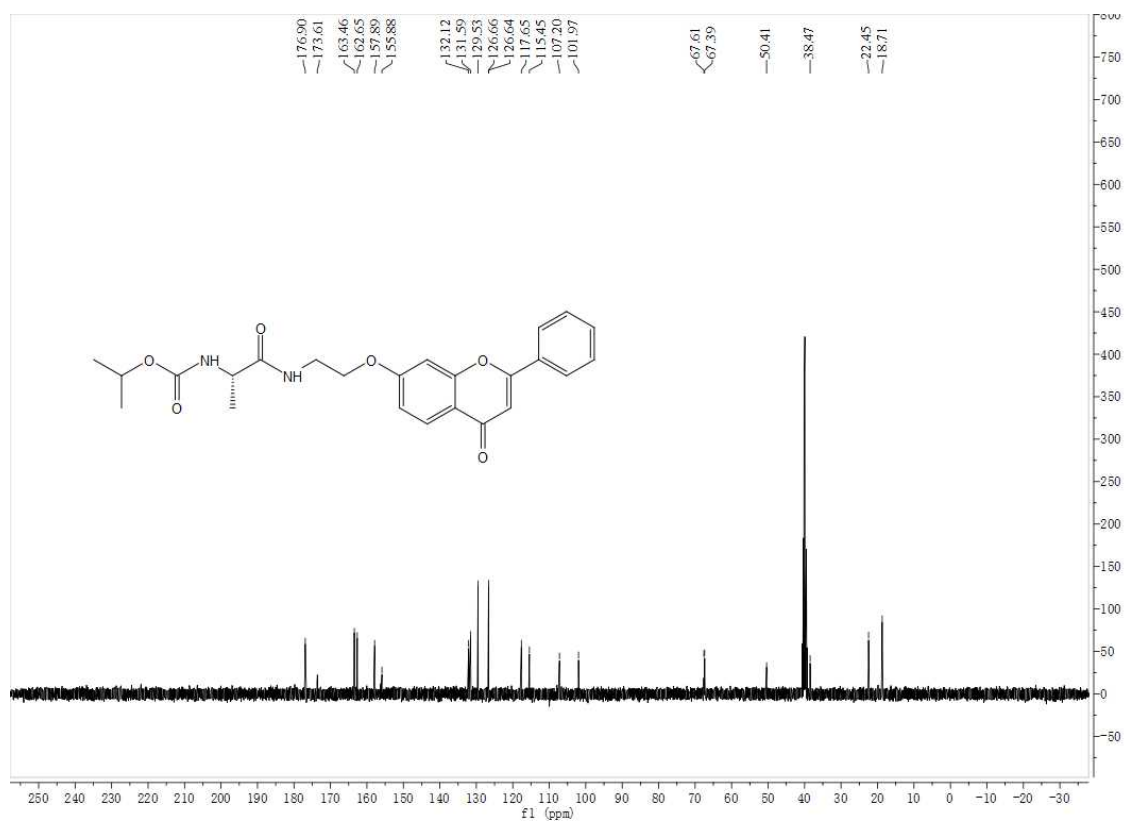
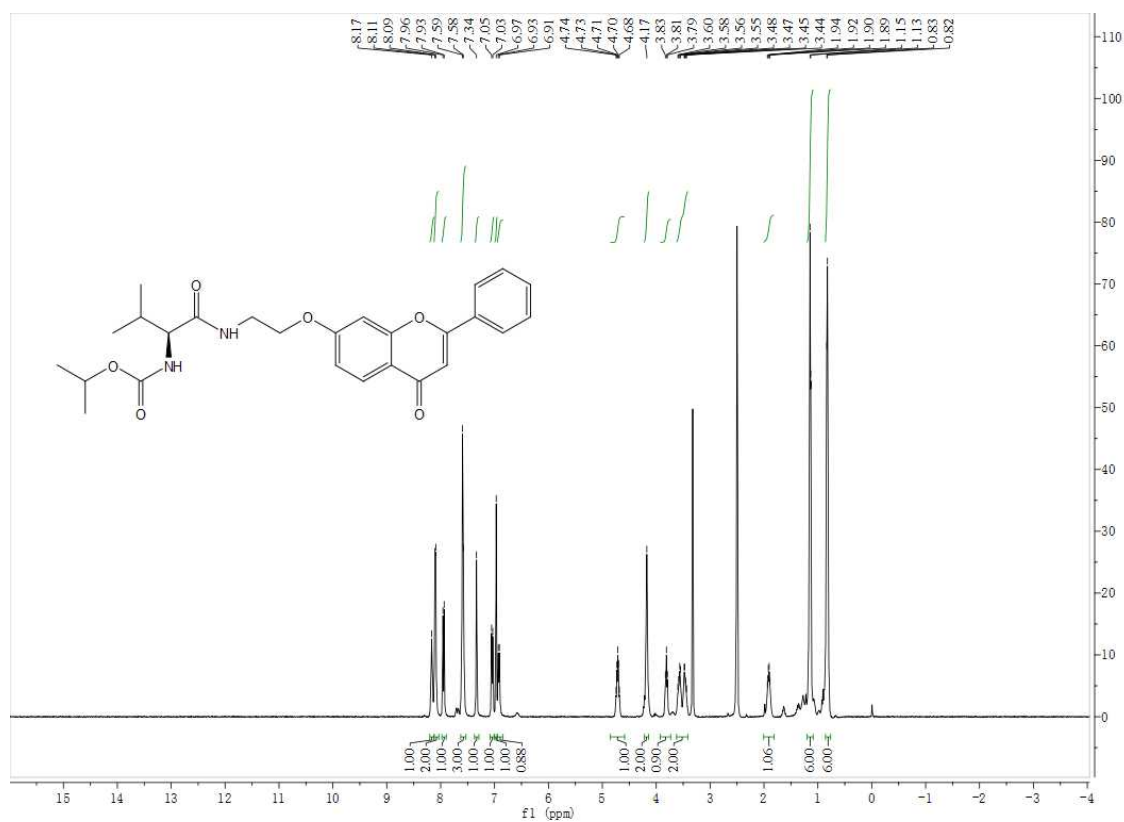
Figure S21. ^1H NMR spectrum of 4dFigure S22. ^{13}C NMR spectrum of 4d

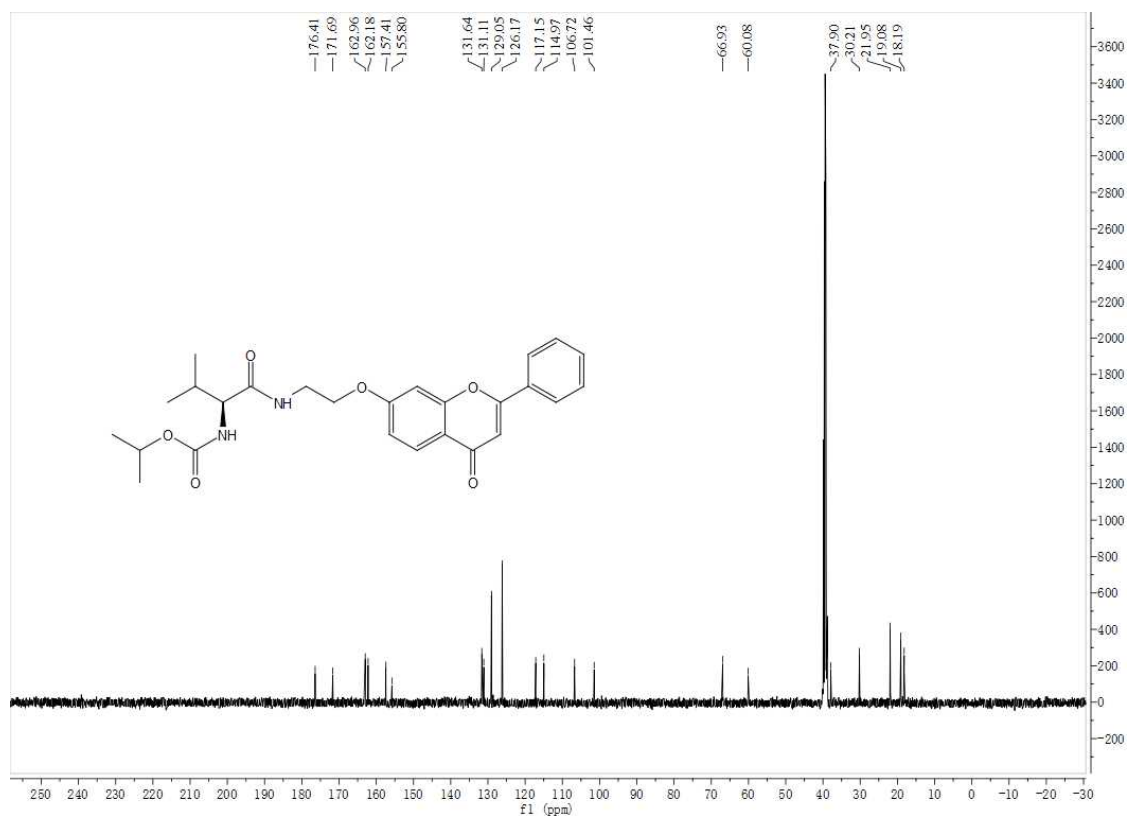
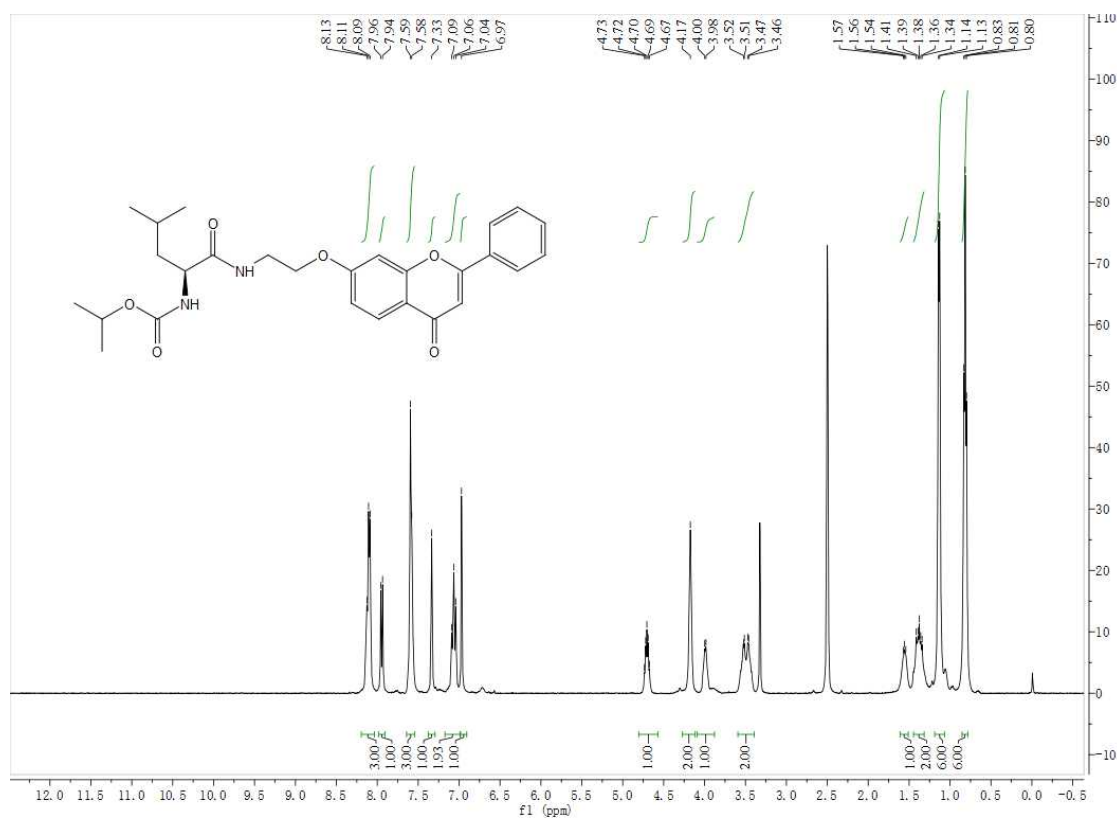
Figure S23. ^1H NMR spectrum of 4eFigure S24. ^{13}C NMR spectrum of 4e

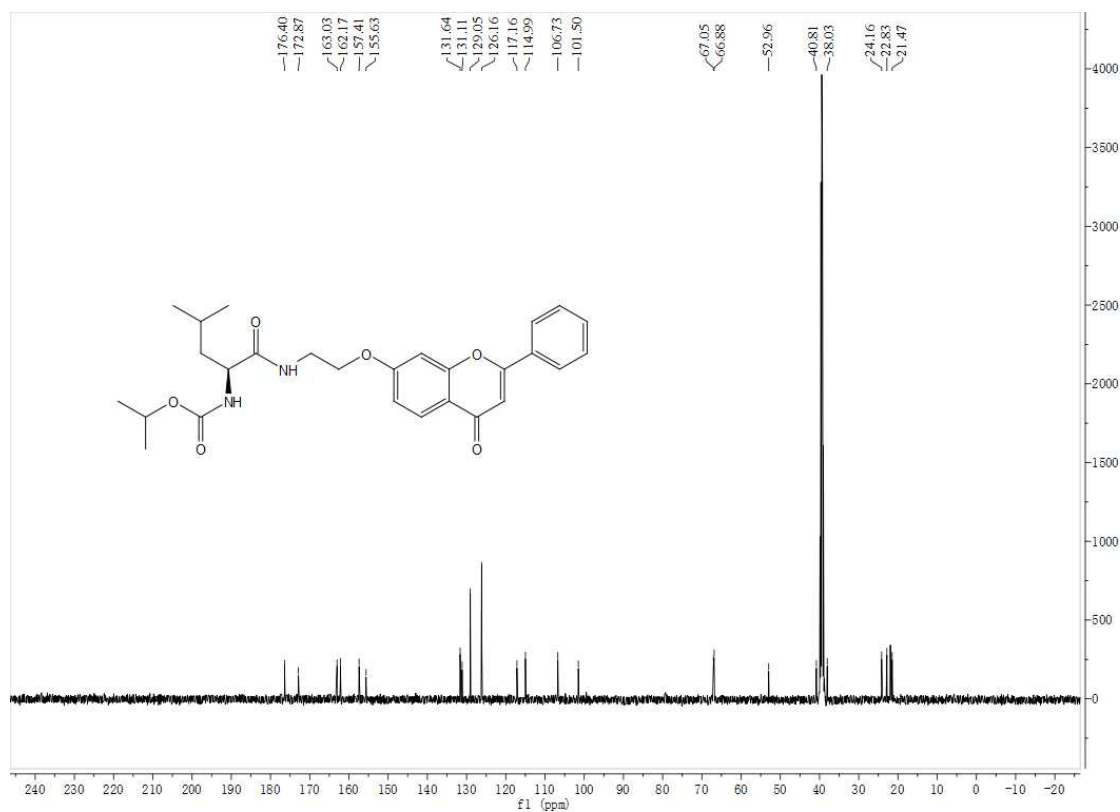
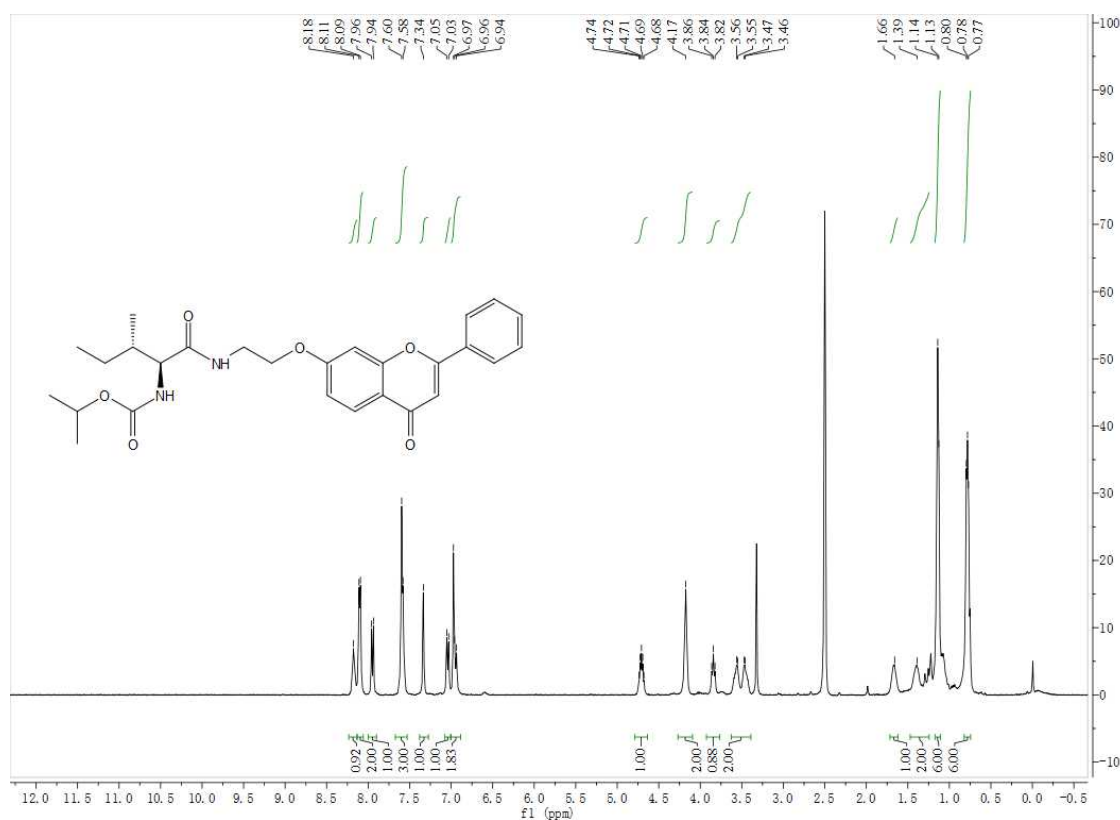
Figure S25. ^1H NMR spectrum of 4fFigure S26. ^{13}C NMR spectrum of 4f

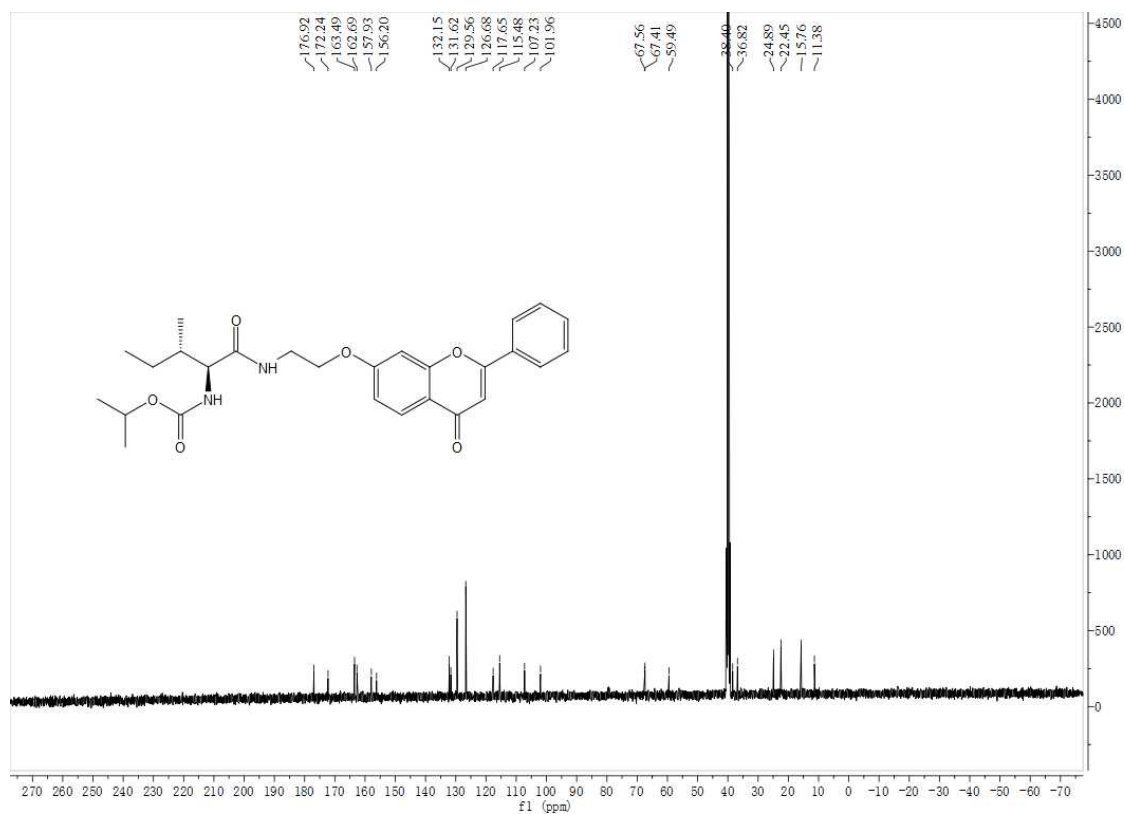
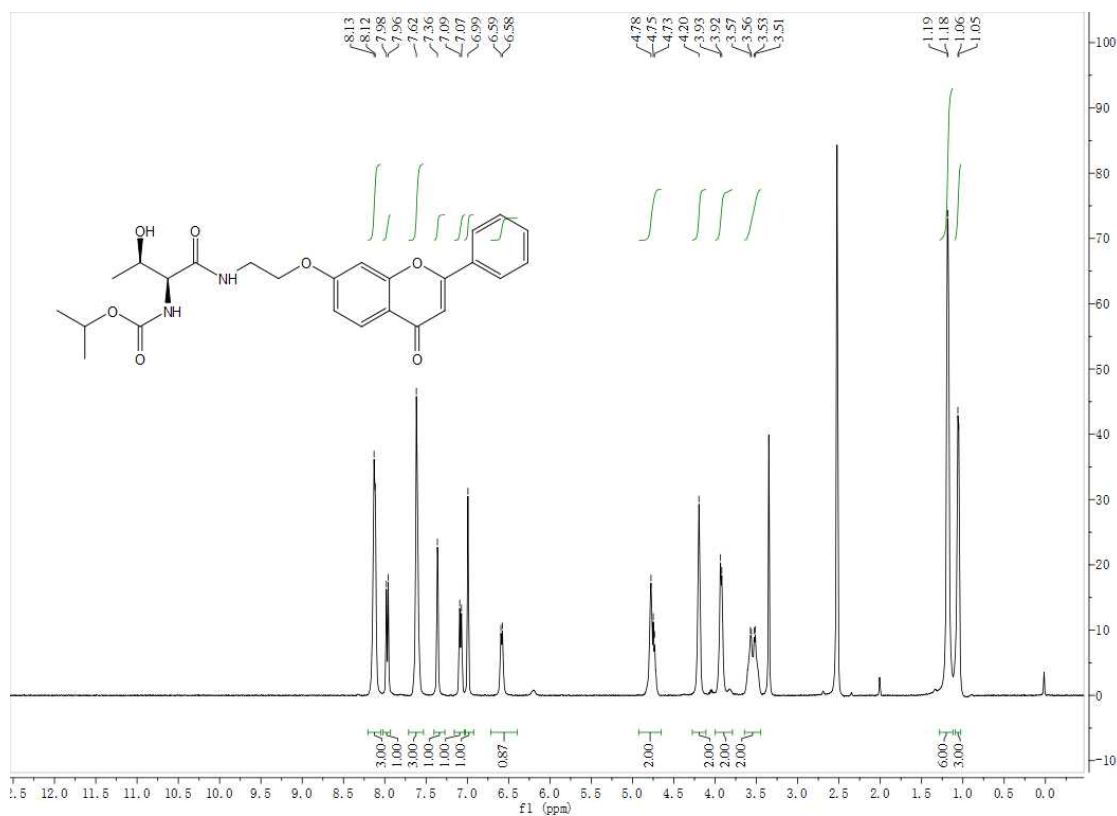
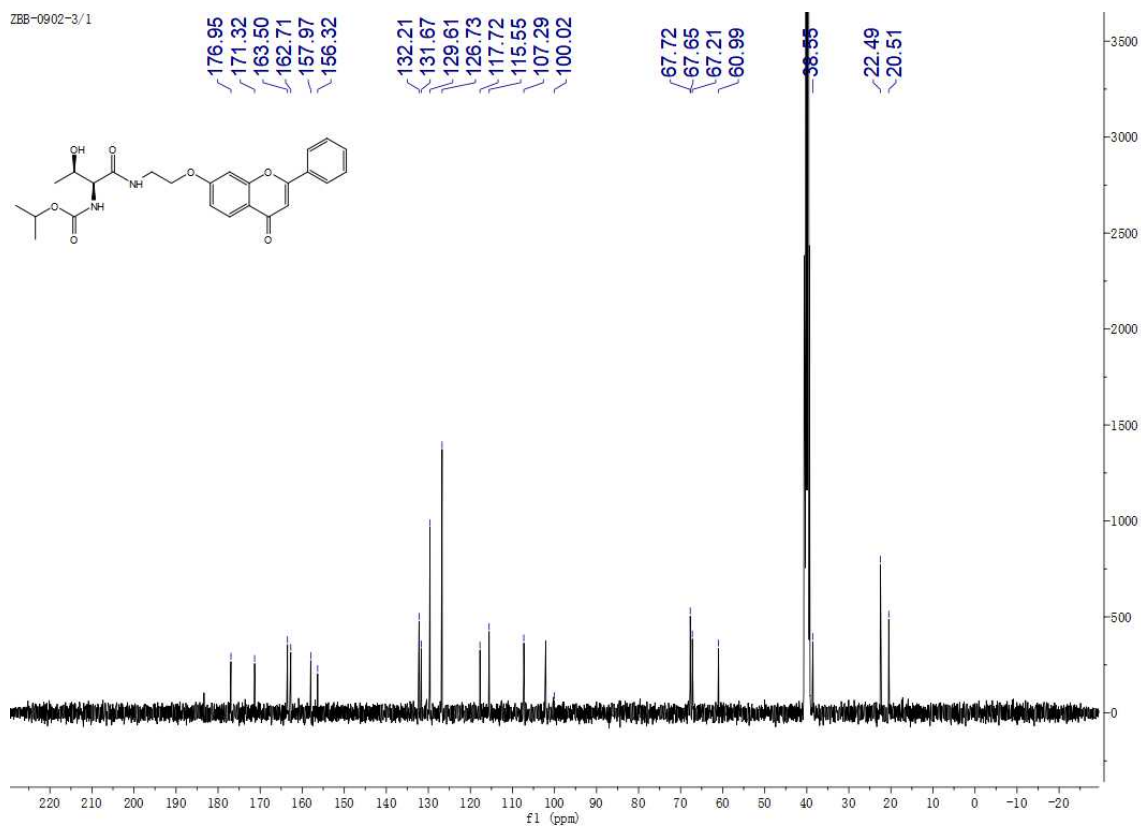
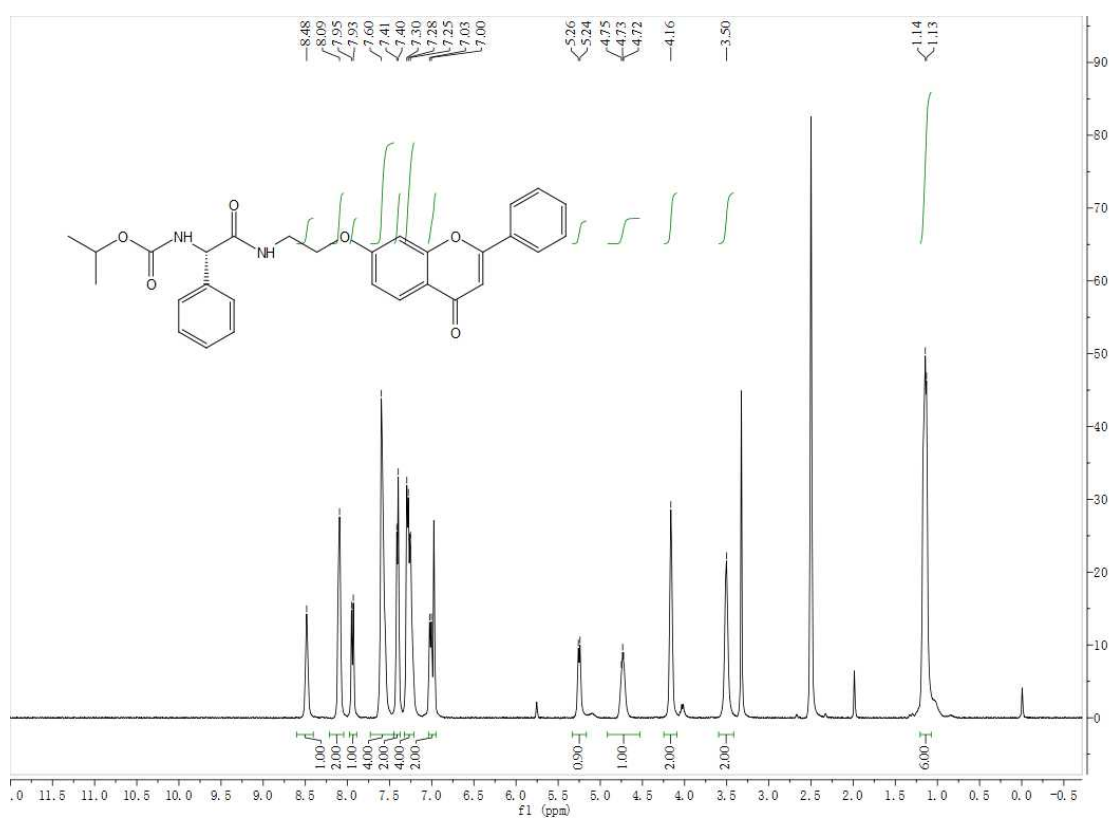
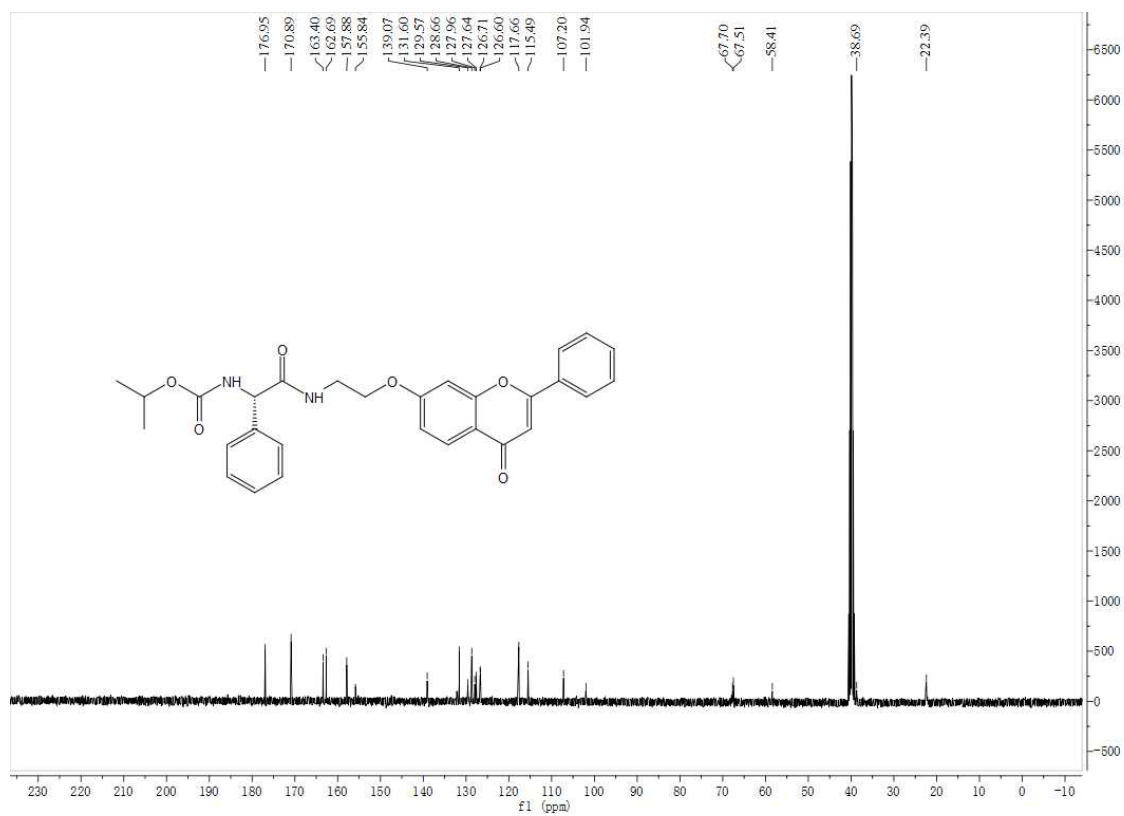
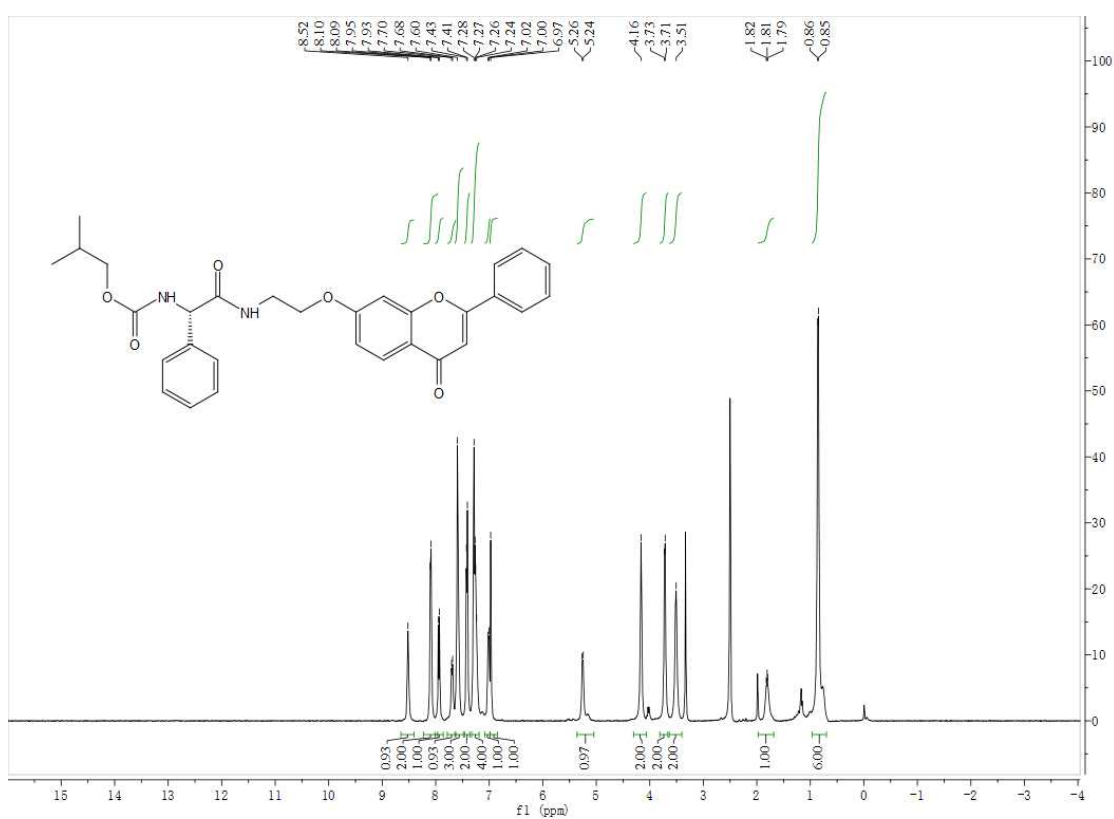
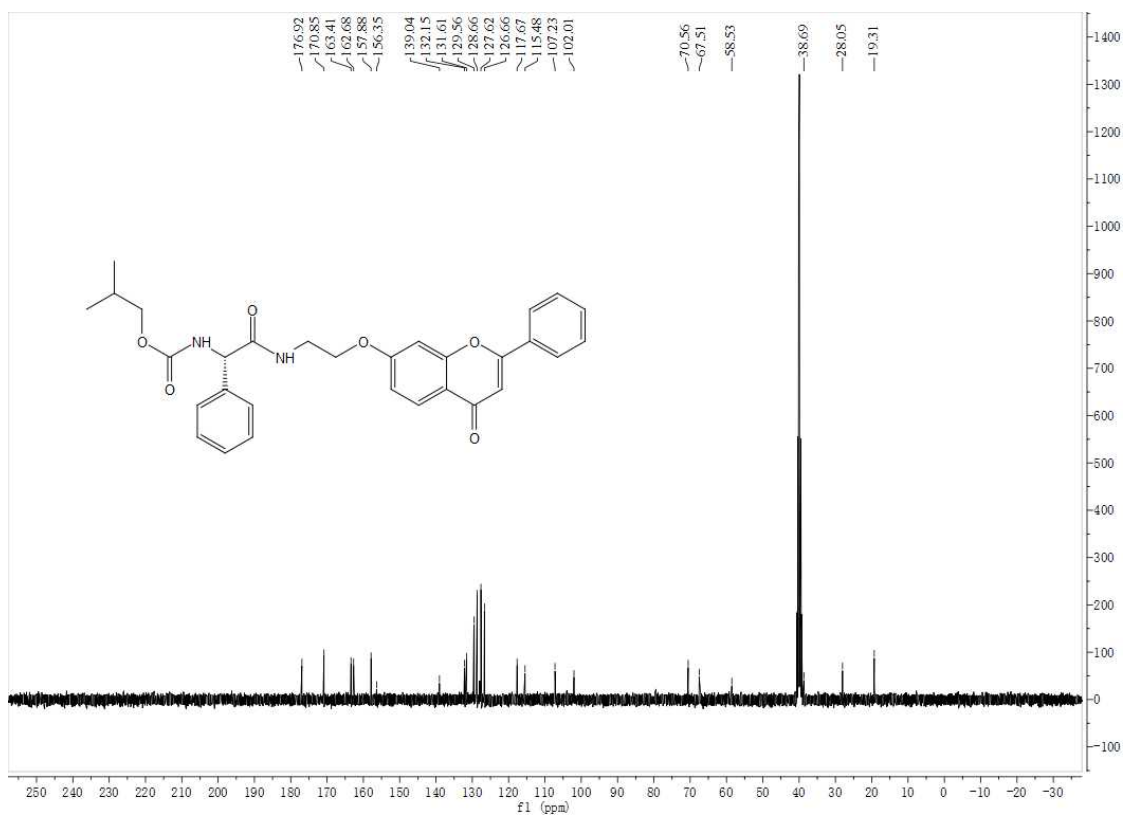
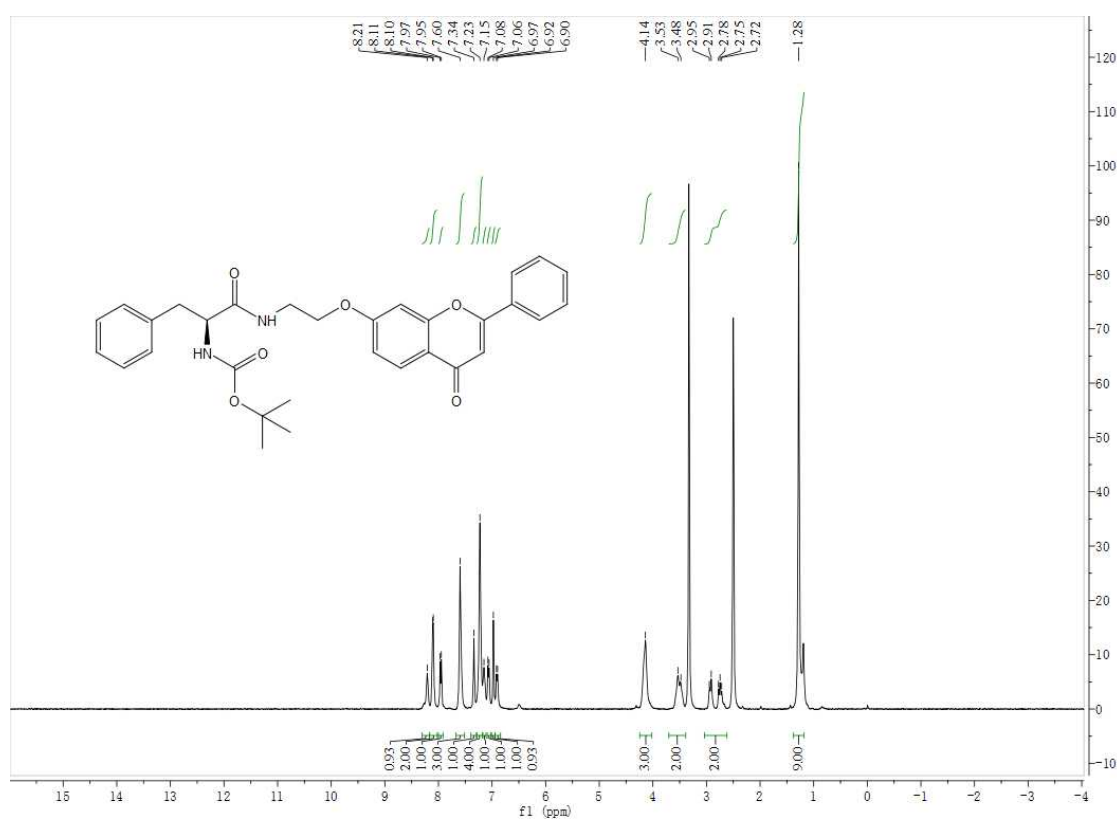
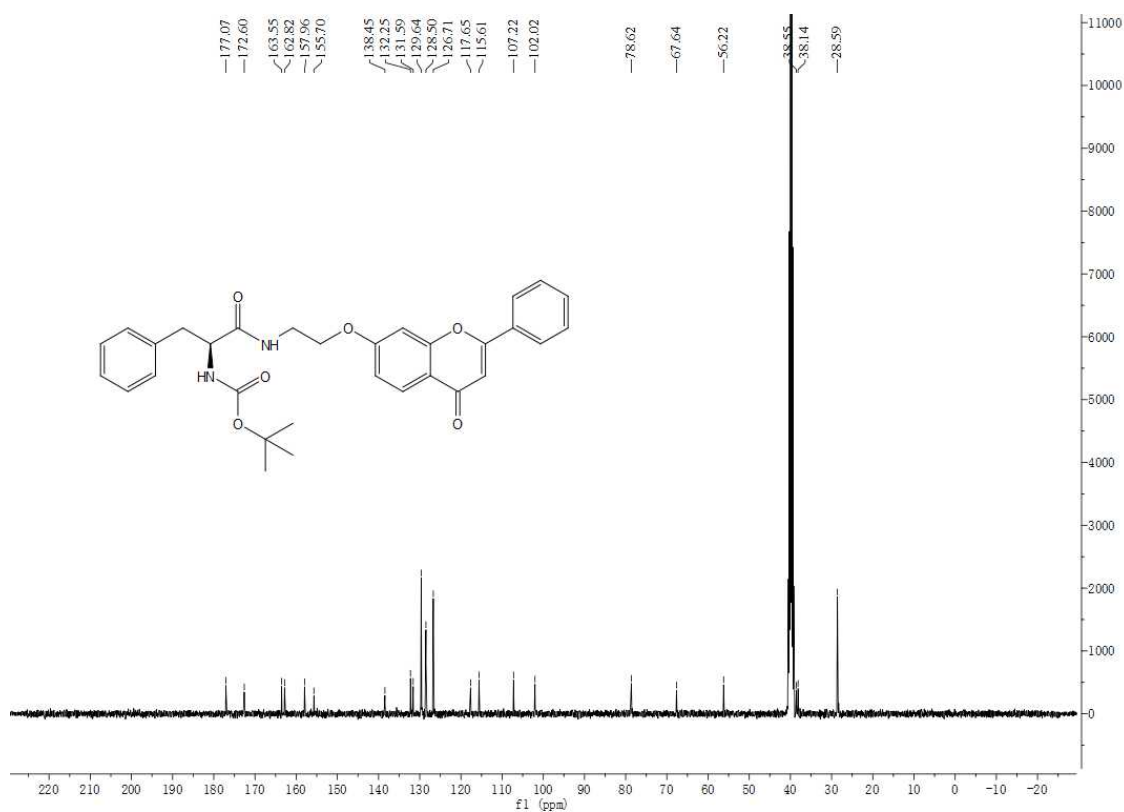
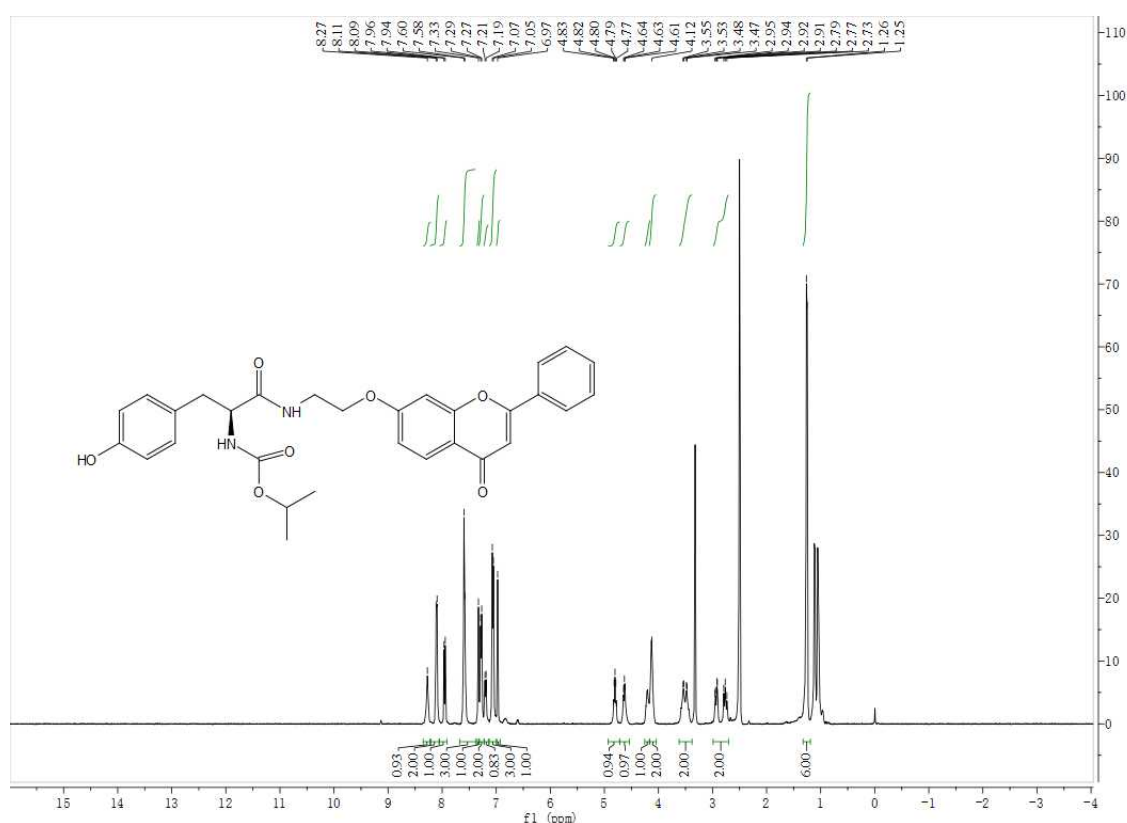
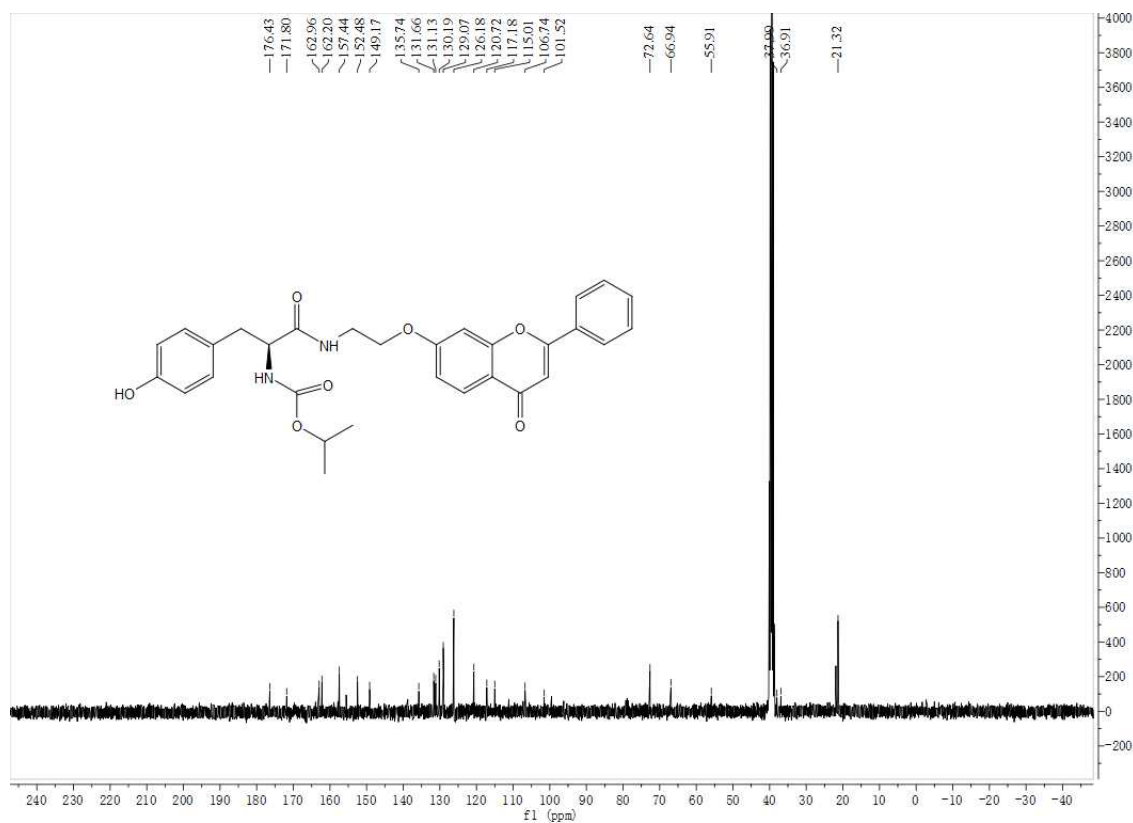
Figure S27. ^1H NMR spectrum of 4gFigure S28. ^{13}C NMR spectrum of 4g

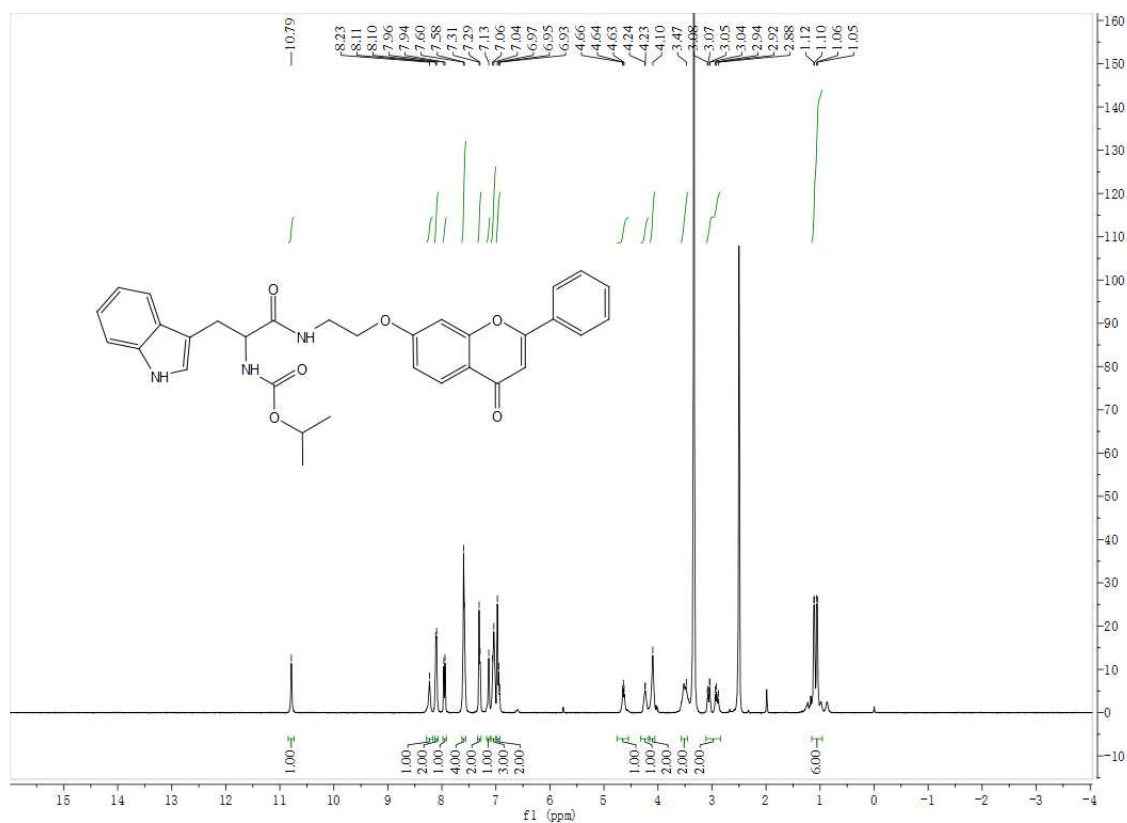
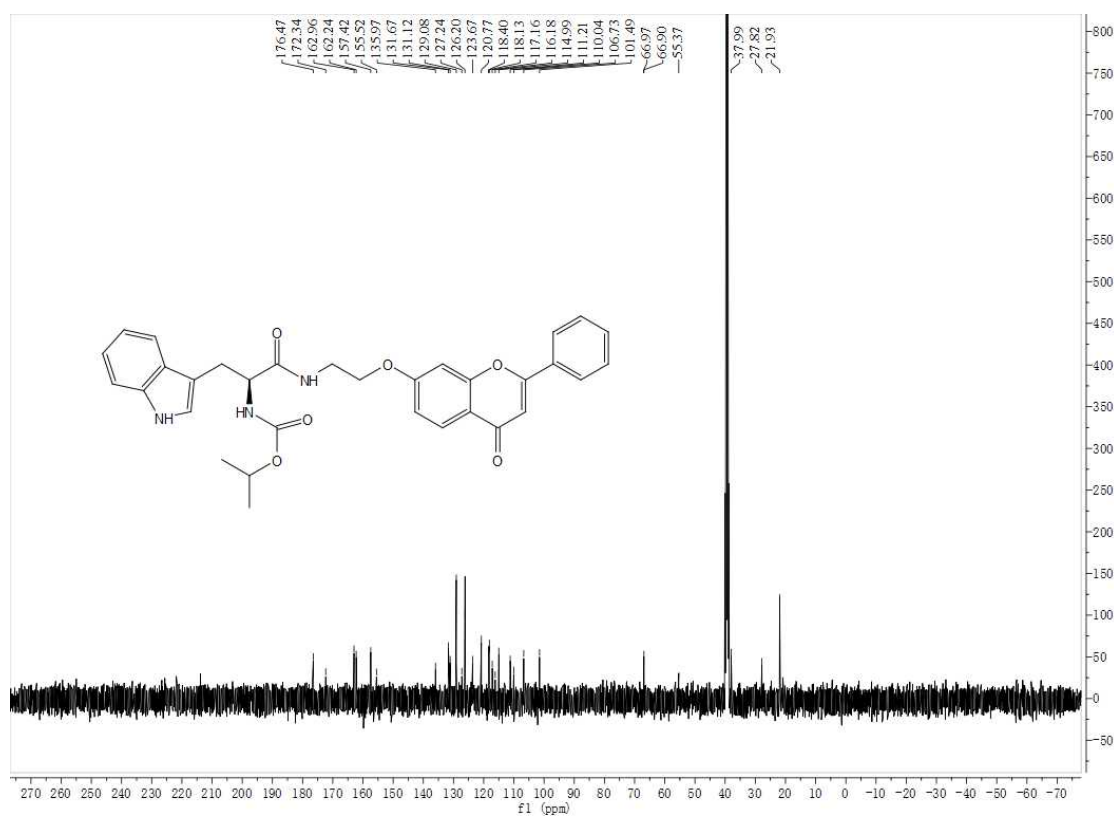
Figure S29. ^1H NMR spectrum of 4hFigure S30. ^{13}C NMR spectrum of 4h

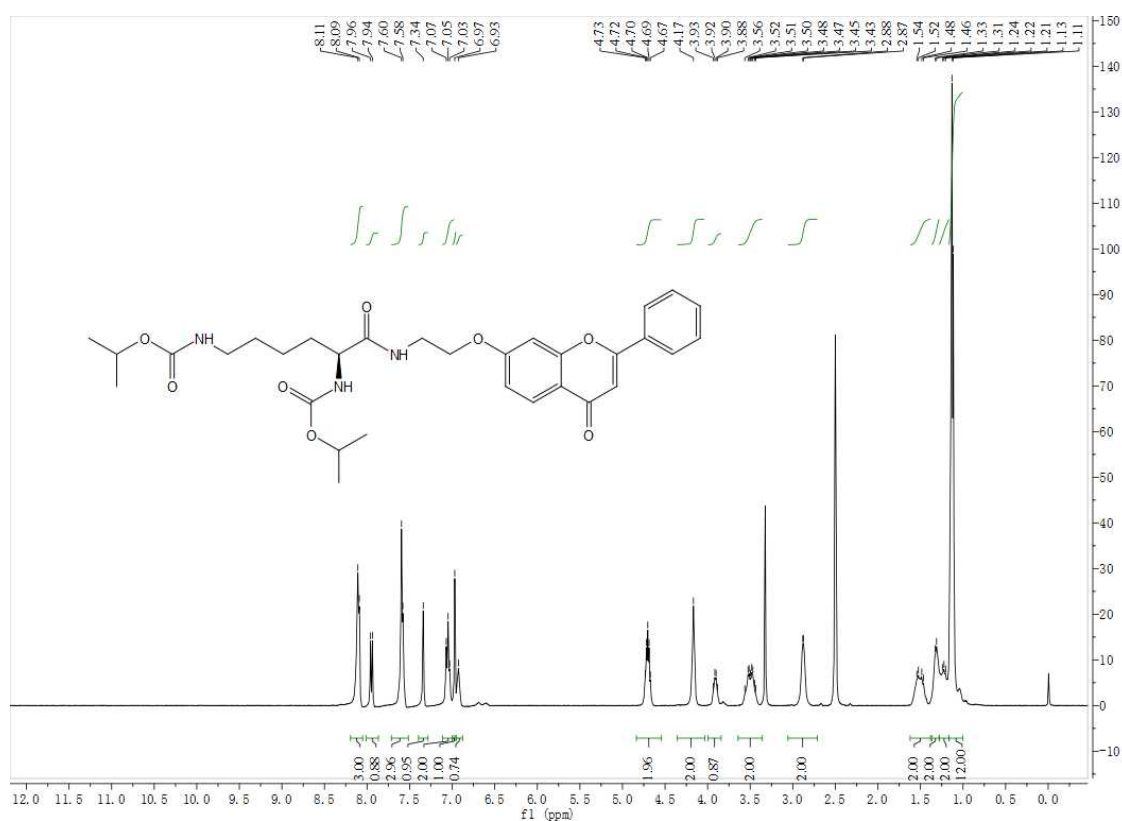
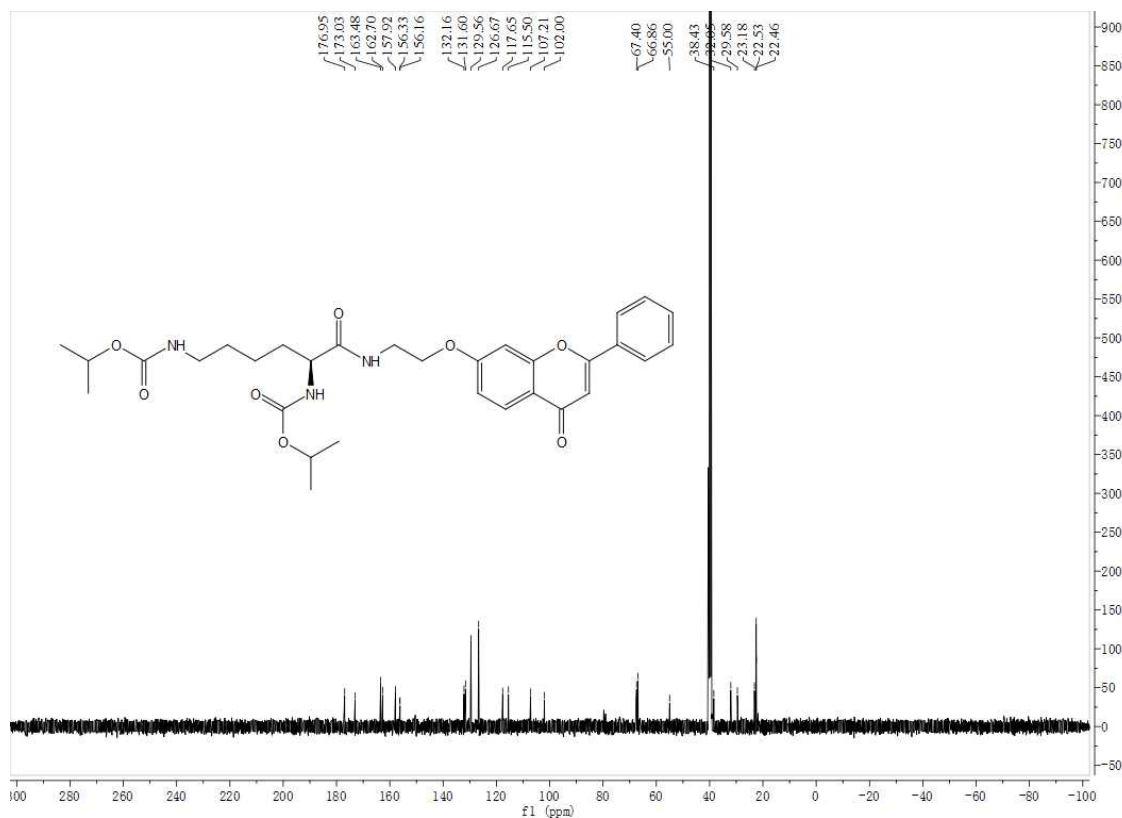
Figure S31. ¹H NMR spectrum of **4i**Figure S32. ¹³C NMR spectrum of **4i**

Figure S33. ¹H NMR spectrum of 4jFigure S34. ¹³C NMR spectrum of 4j

Figure S35. ¹H NMR spectrum of 4kFigure S36. ¹³C NMR spectrum of 4k

Figure S37. ¹H NMR spectrum of 41Figure S38. ¹³C NMR spectrum of 41

Figure S39. ¹H NMR spectrum of **4m**Figure S40. ¹³C NMR spectrum of **4m**

Figure S41. ¹H NMR spectrum of 4nFigure S42. ¹³C NMR spectrum of 4n

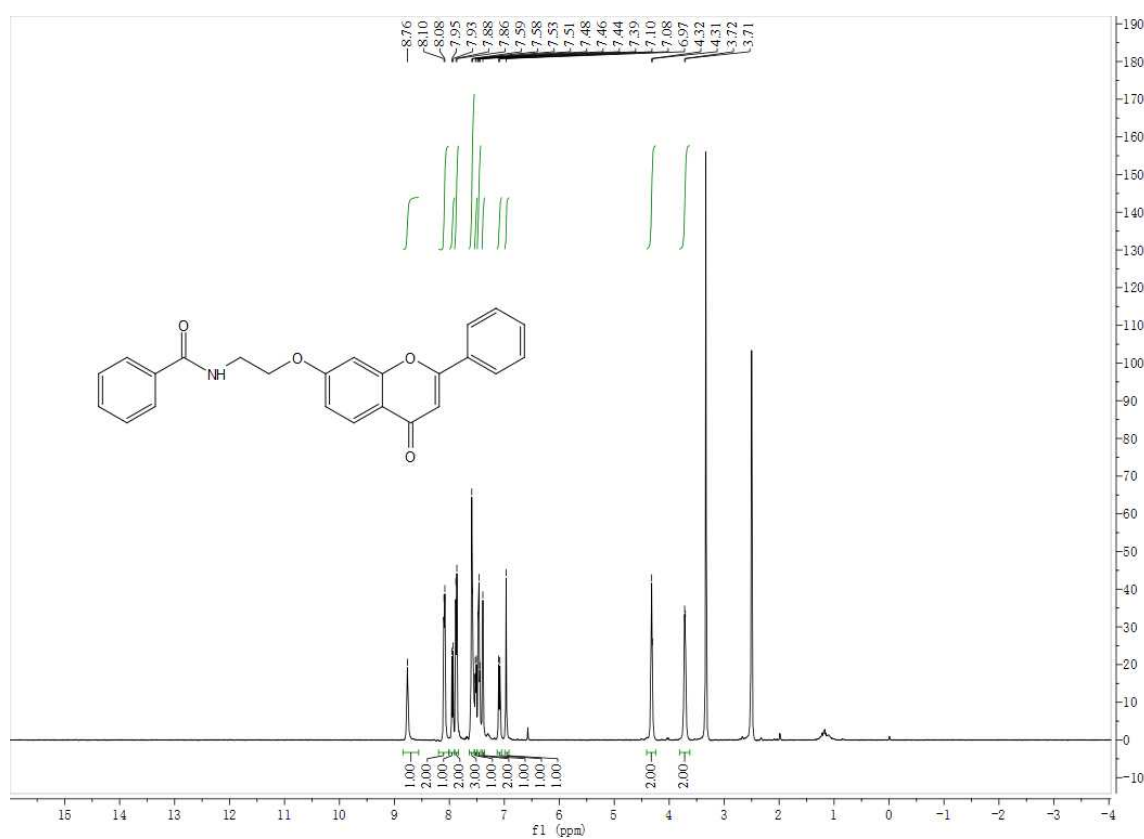
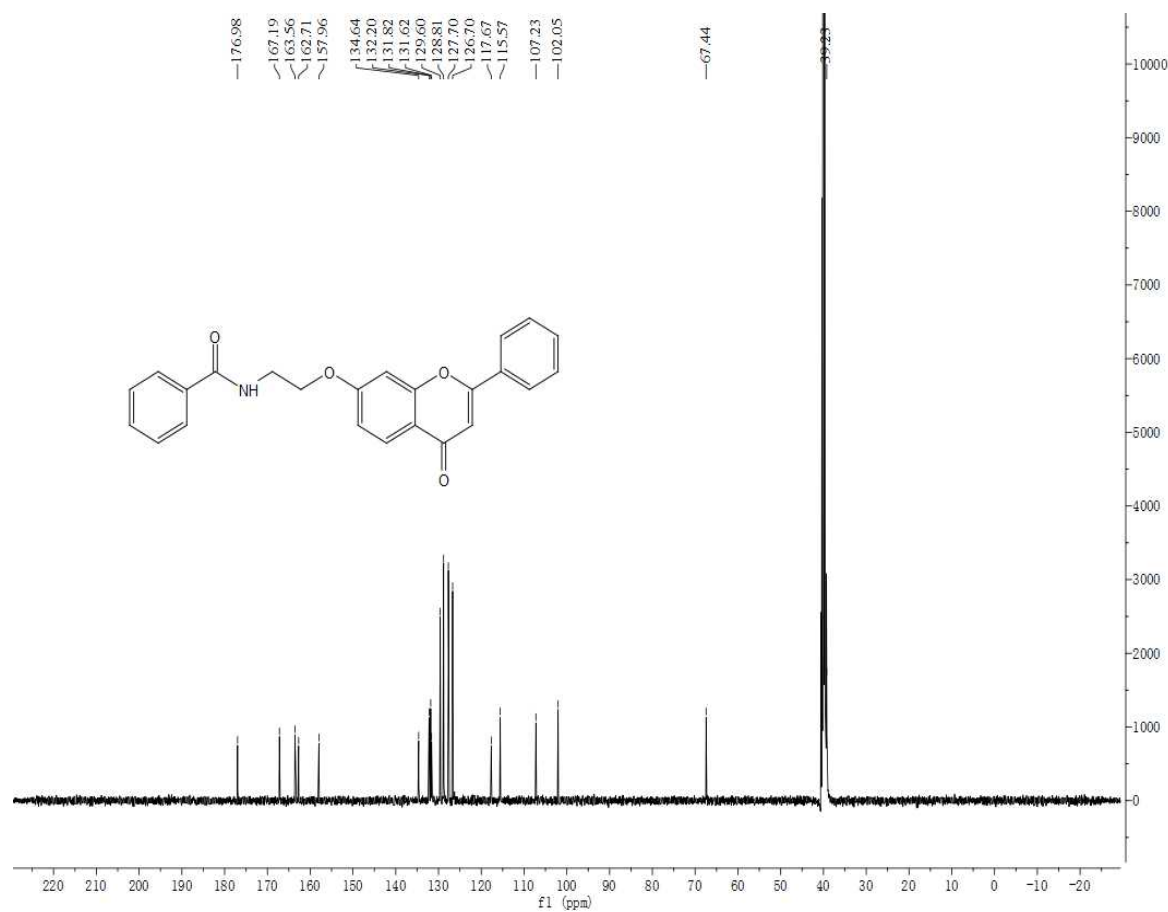
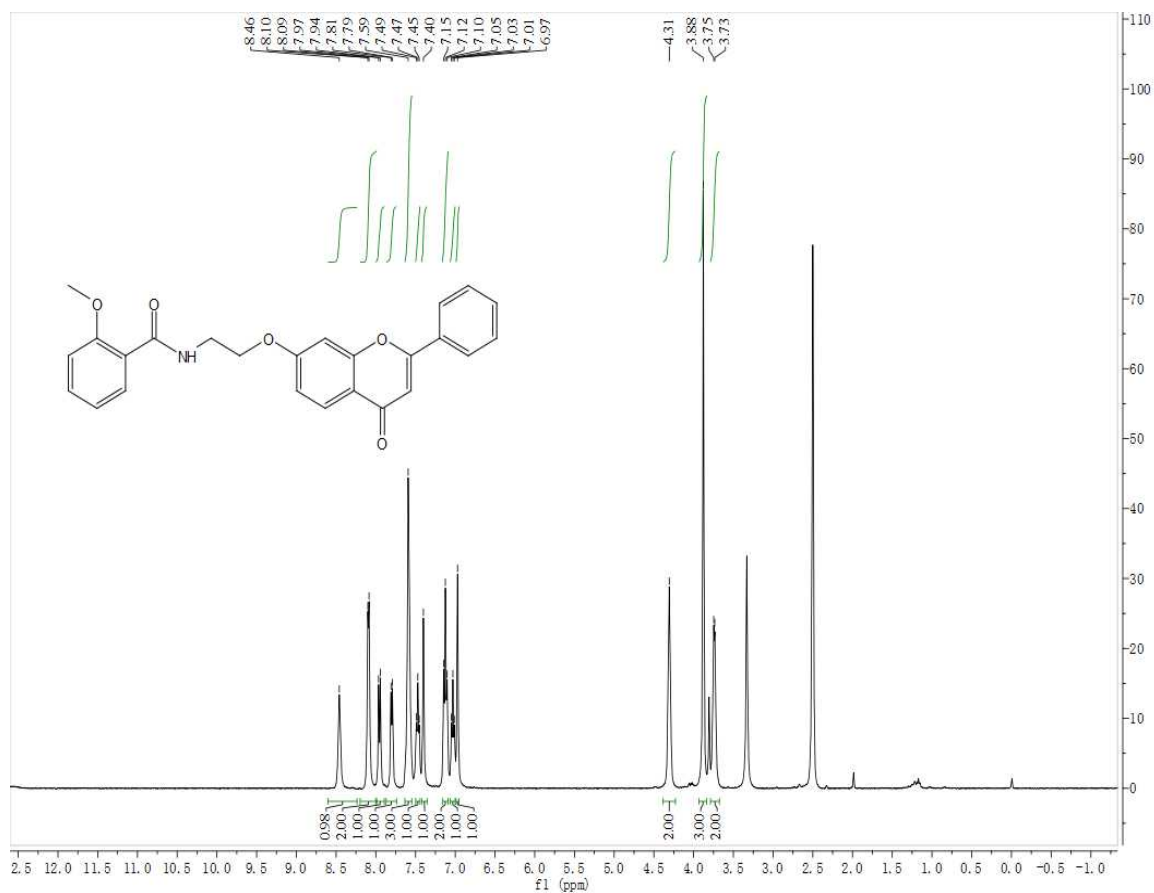
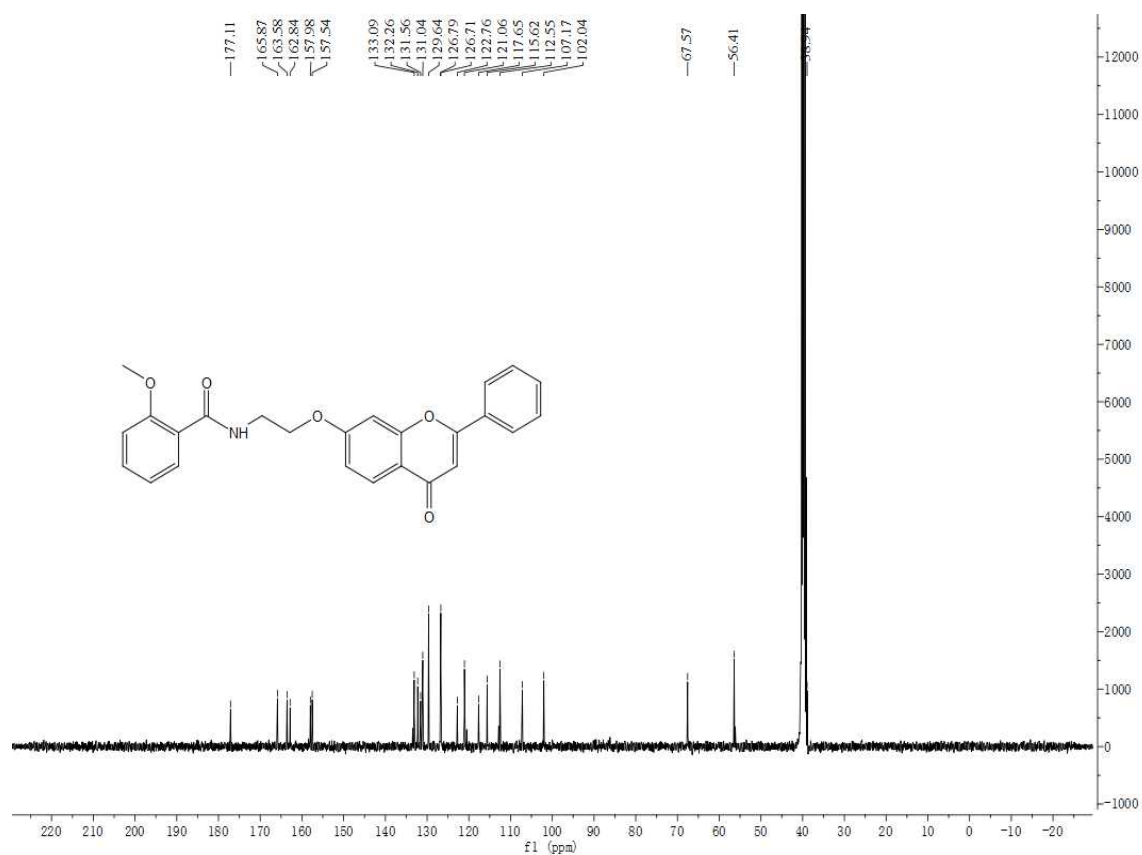
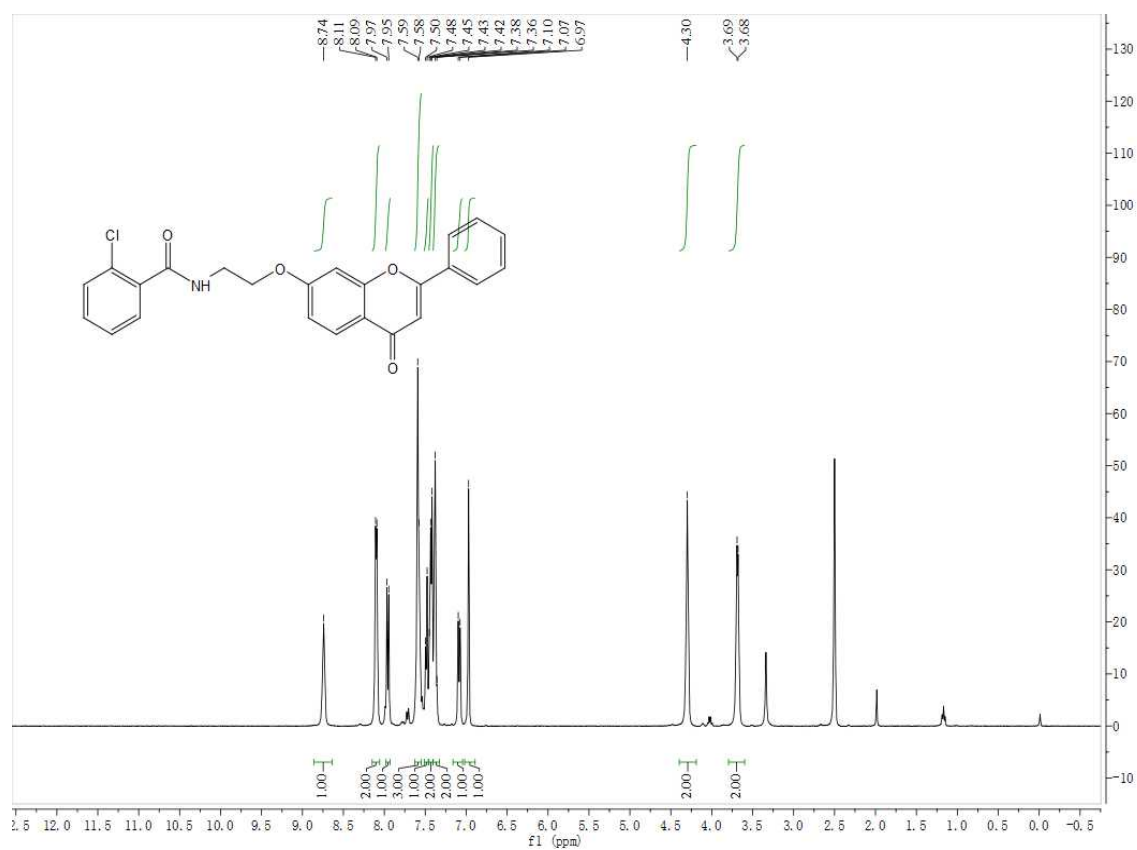
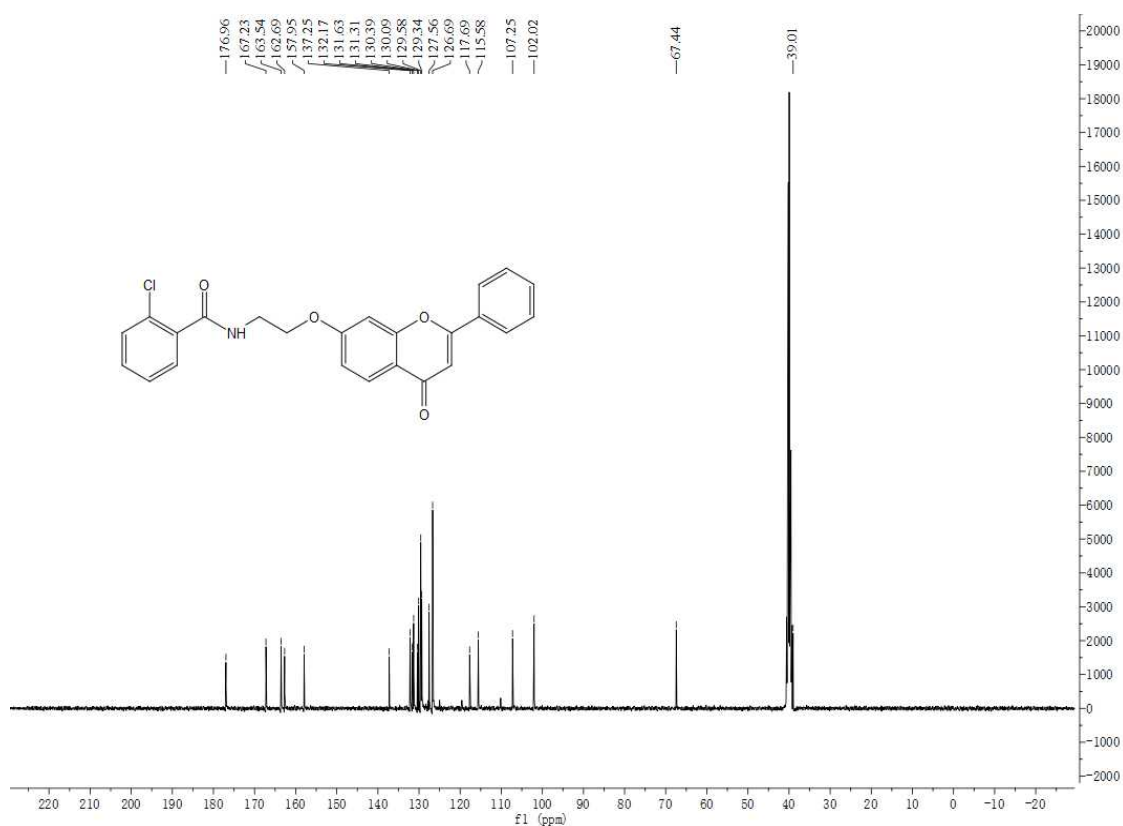
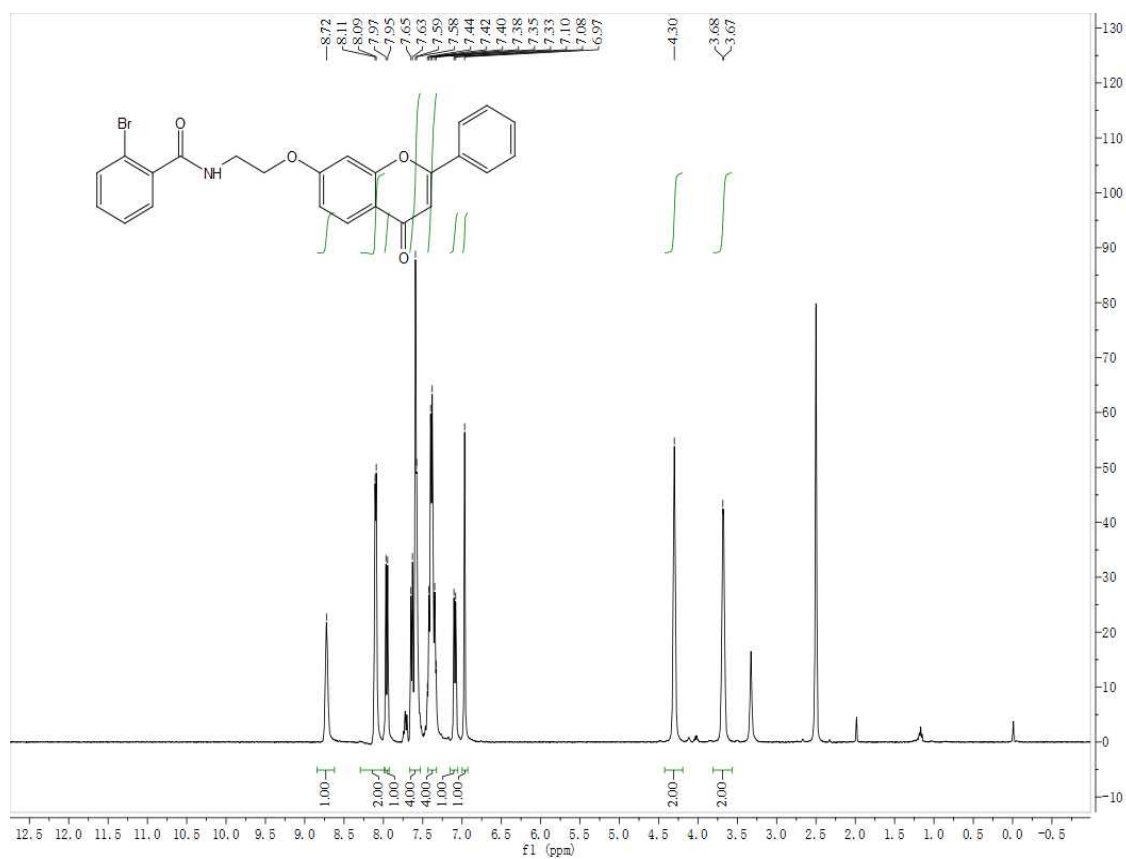
Figure S43. ¹H NMR spectrum of 5a

Figure S44. ^{13}C NMR spectrum of **5a****Figure S45.** ^1H NMR spectrum of **5b**

Figure S46. ¹³C NMR spectrum of **5b**Figure S47. ¹H NMR spectrum of **5c**

Figure S48. ¹³C NMR spectrum of 5cFigure S49. ¹H NMR spectrum of 5d

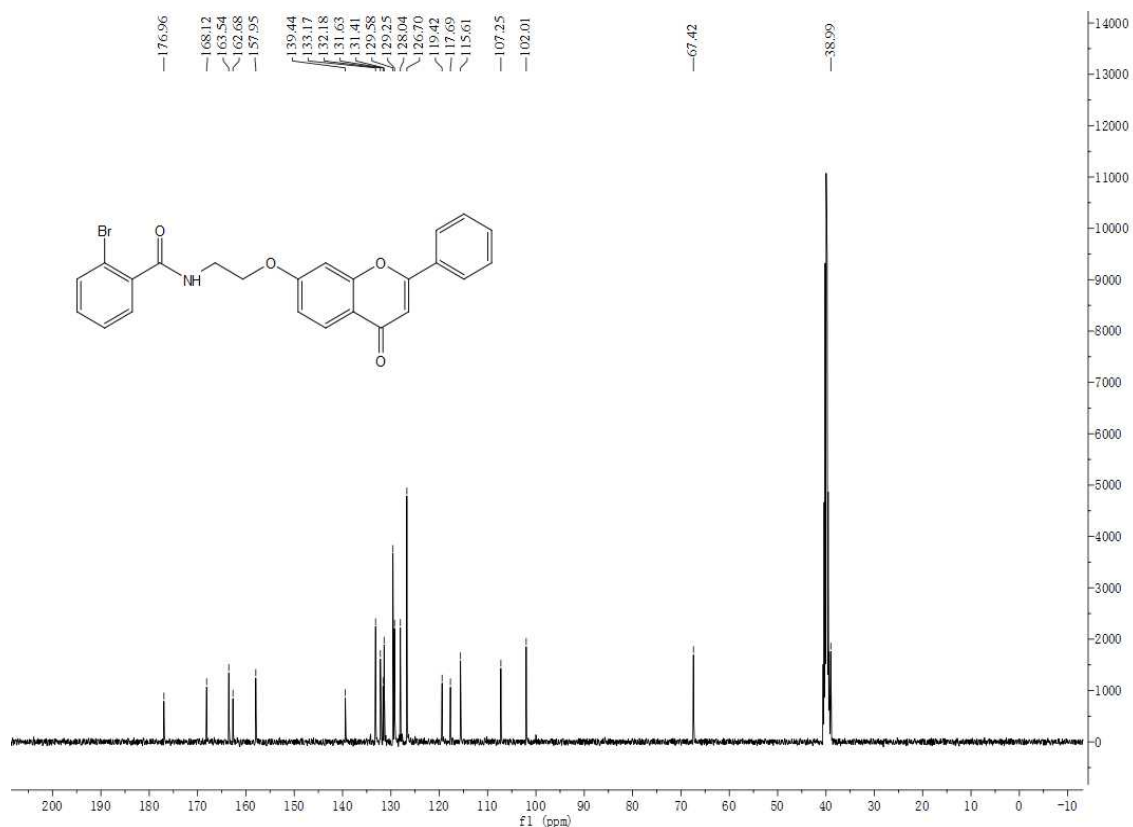


Figure S50. ^{13}C NMR spectrum of **5d**

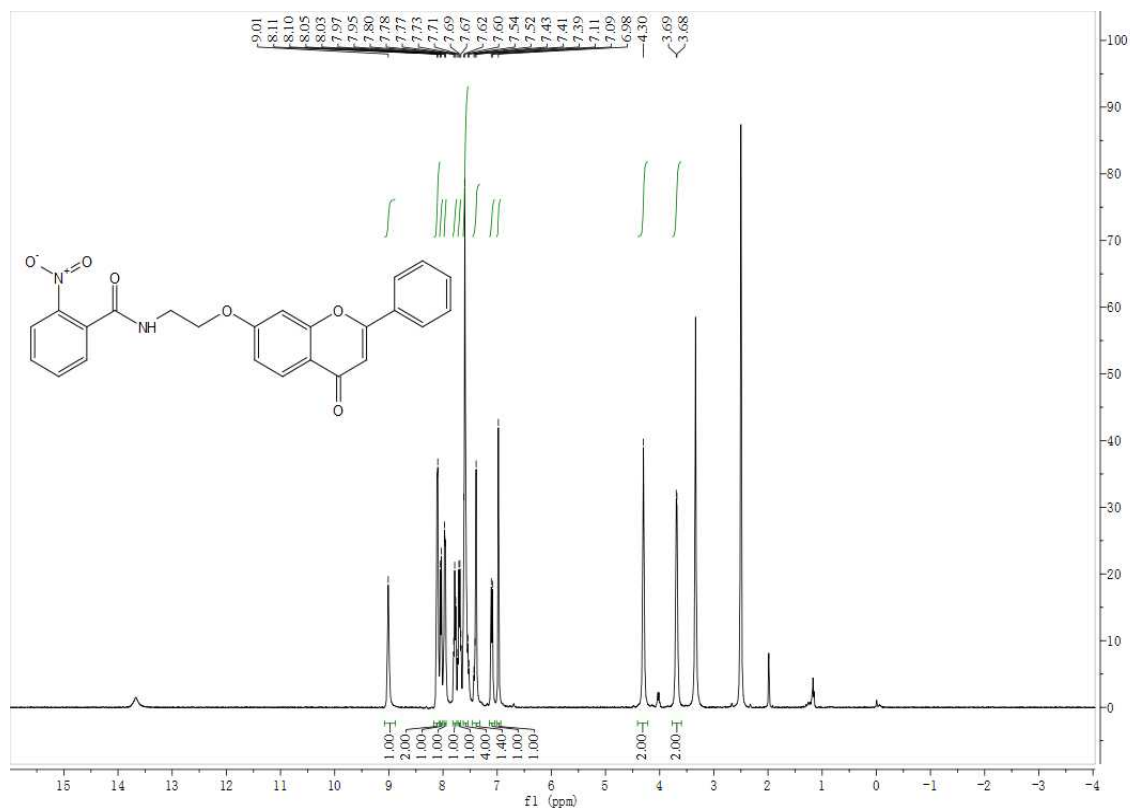
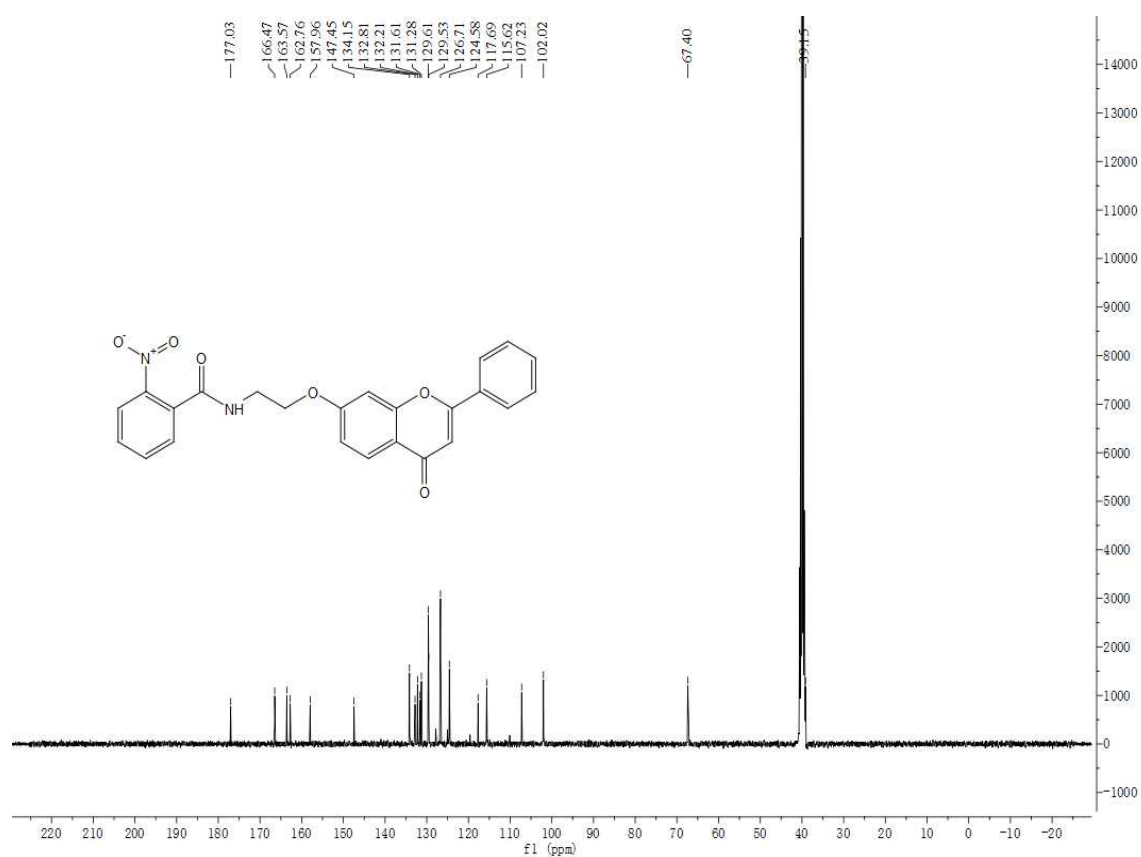
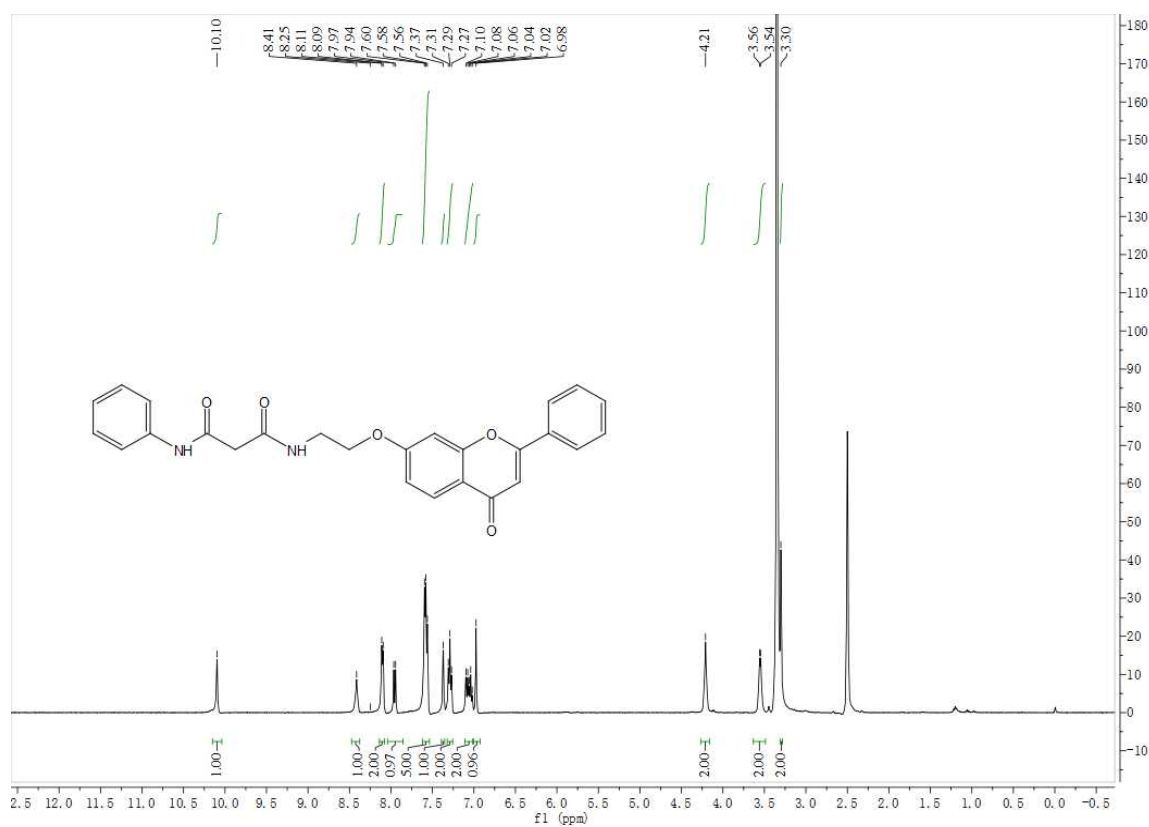
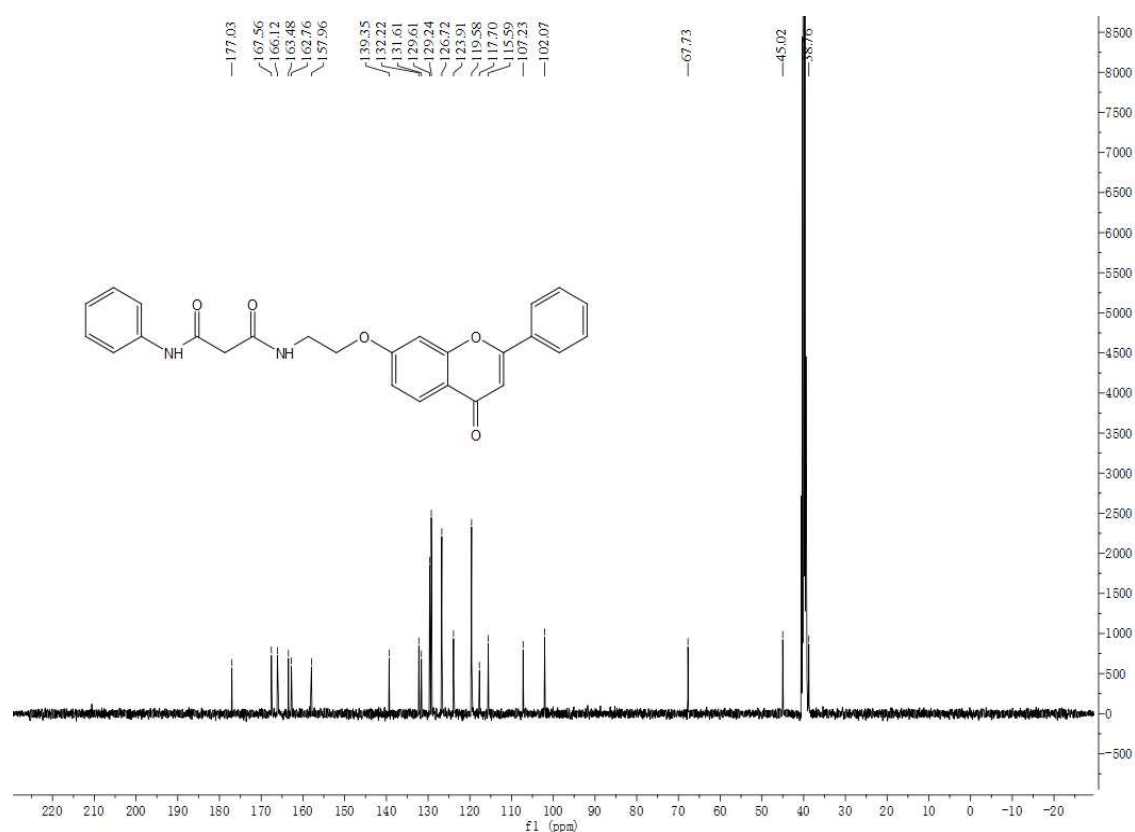
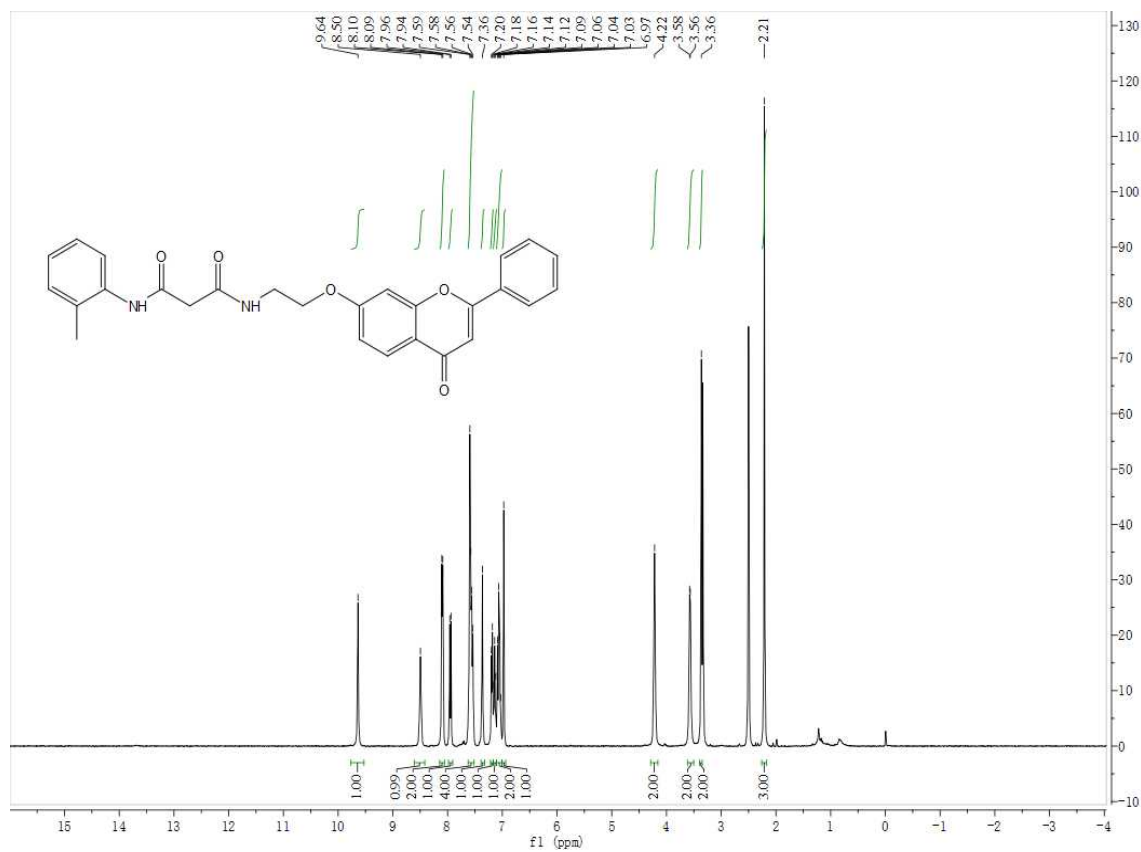
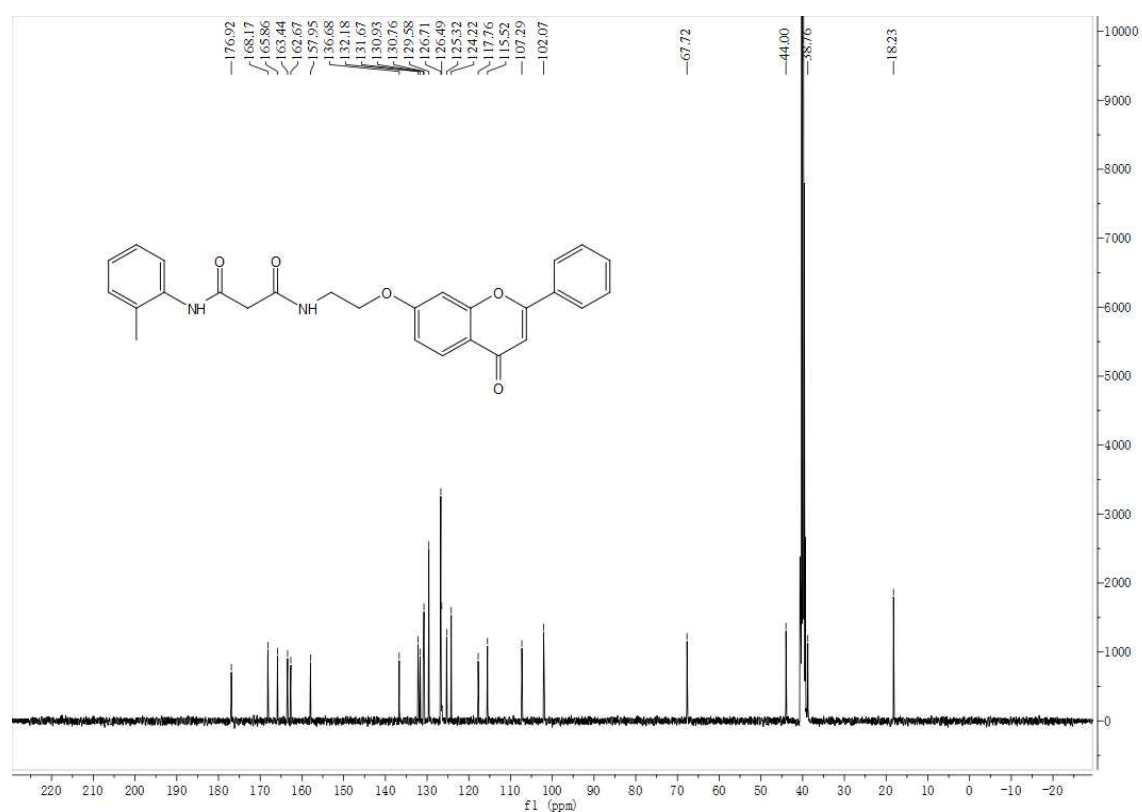
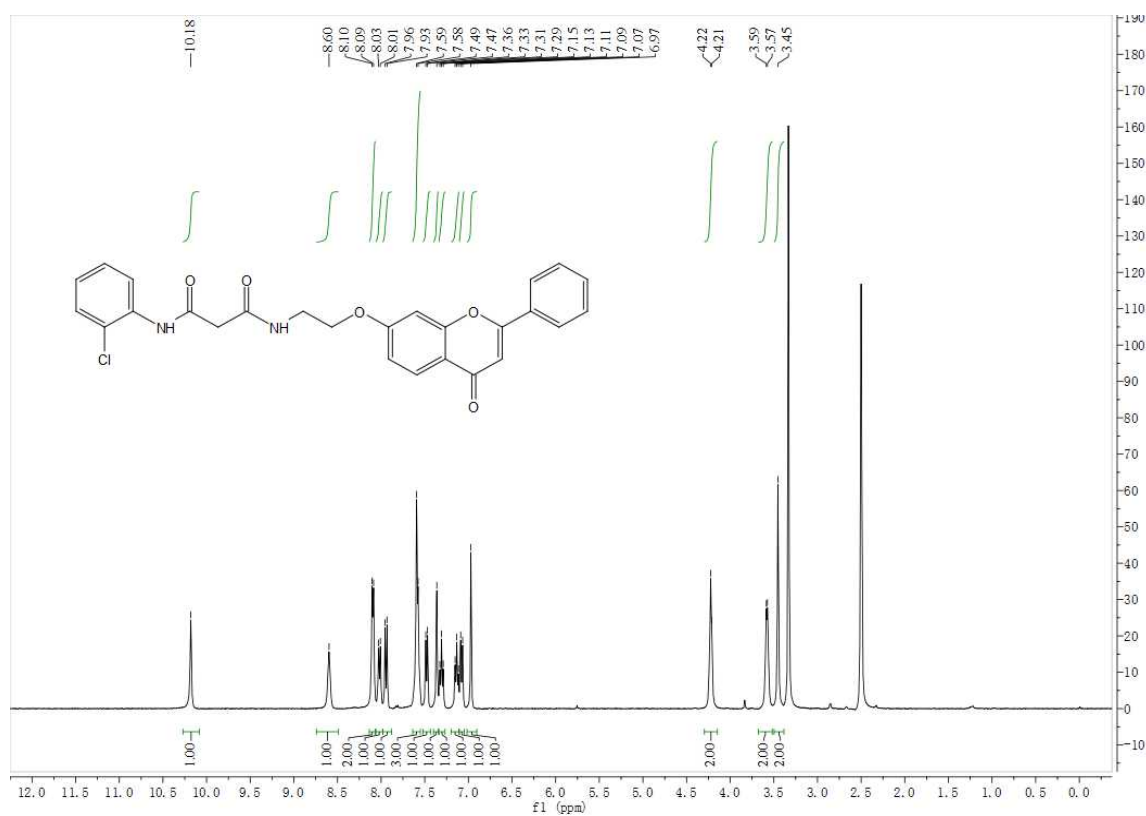


Figure S51. ^1H NMR spectrum of **5e**

Figure S52. ¹³C NMR spectrum of 5eFigure S53. ¹H NMR spectrum of 6a

Figure S54. ¹³C NMR spectrum of 6aFigure S55. ¹H NMR spectrum of 6b

Figure S56. ¹³C NMR spectrum of **6b**Figure S57. ¹H NMR spectrum of **6c**

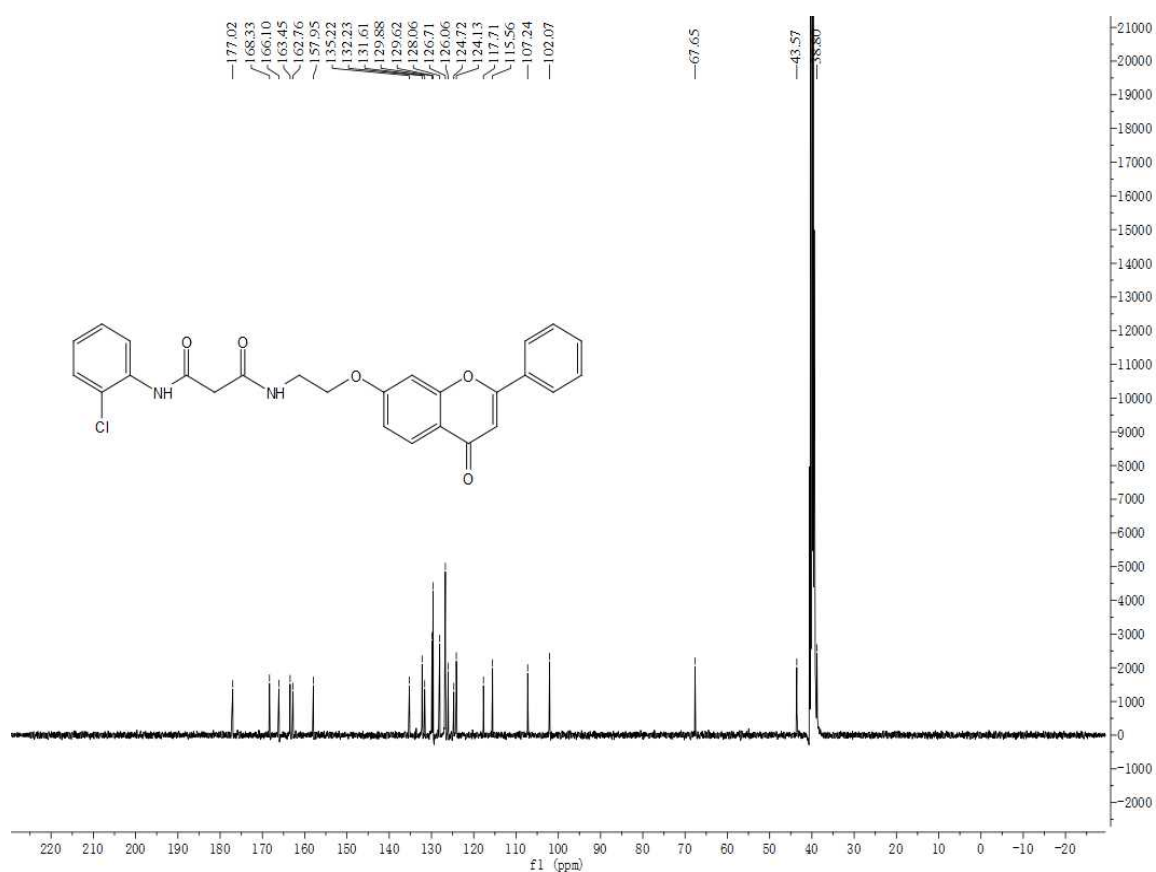
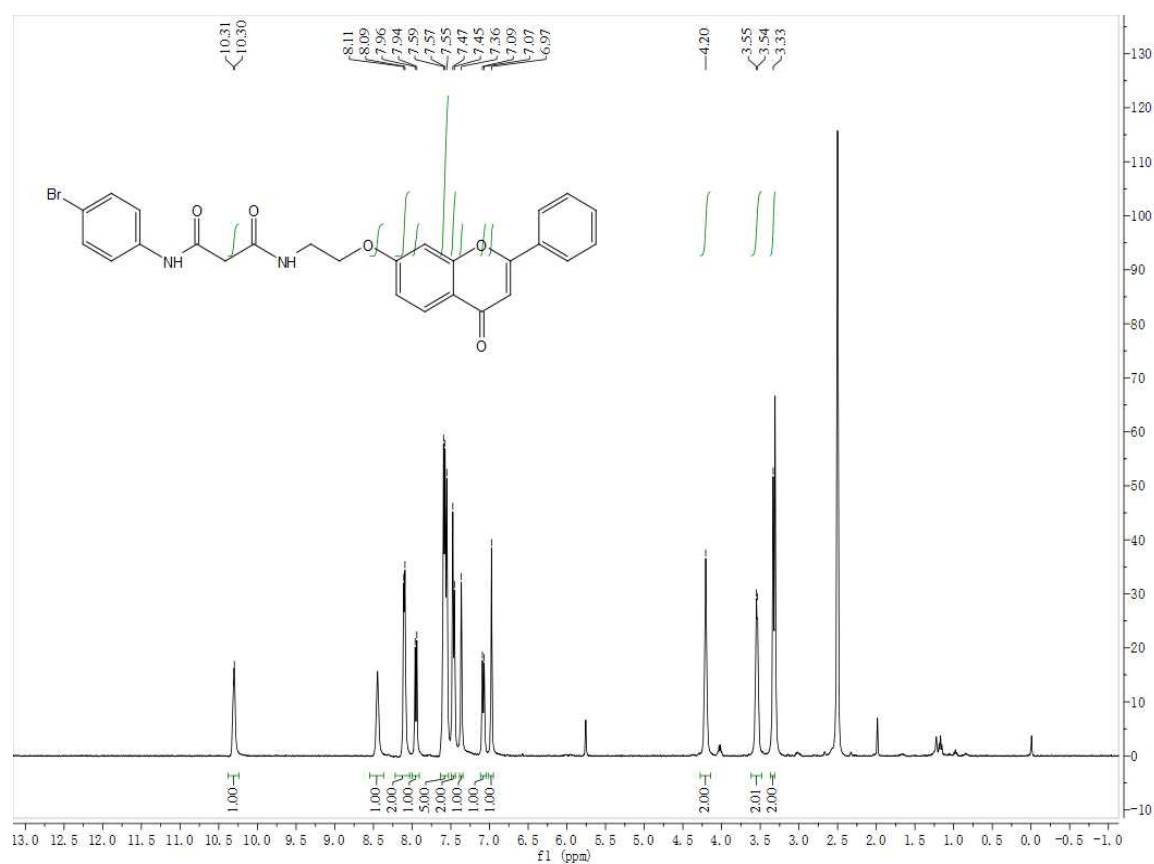
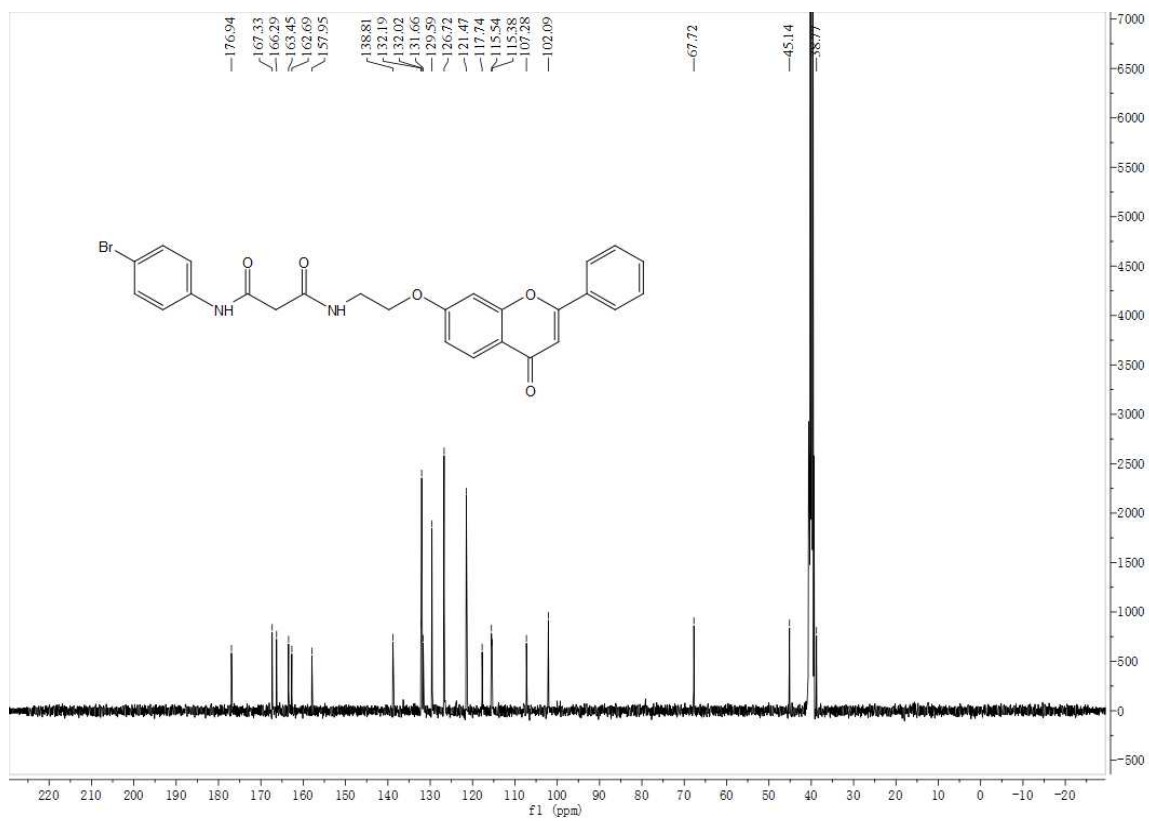
Figure S58. ¹³C NMR spectrum of 6c

Figure S59. ^1H NMR spectrum of **6d****Figure S60.** ^{13}C NMR spectrum of **6d**

Section S3: Molecule docking results of **1** and **2a** with TMV CP.

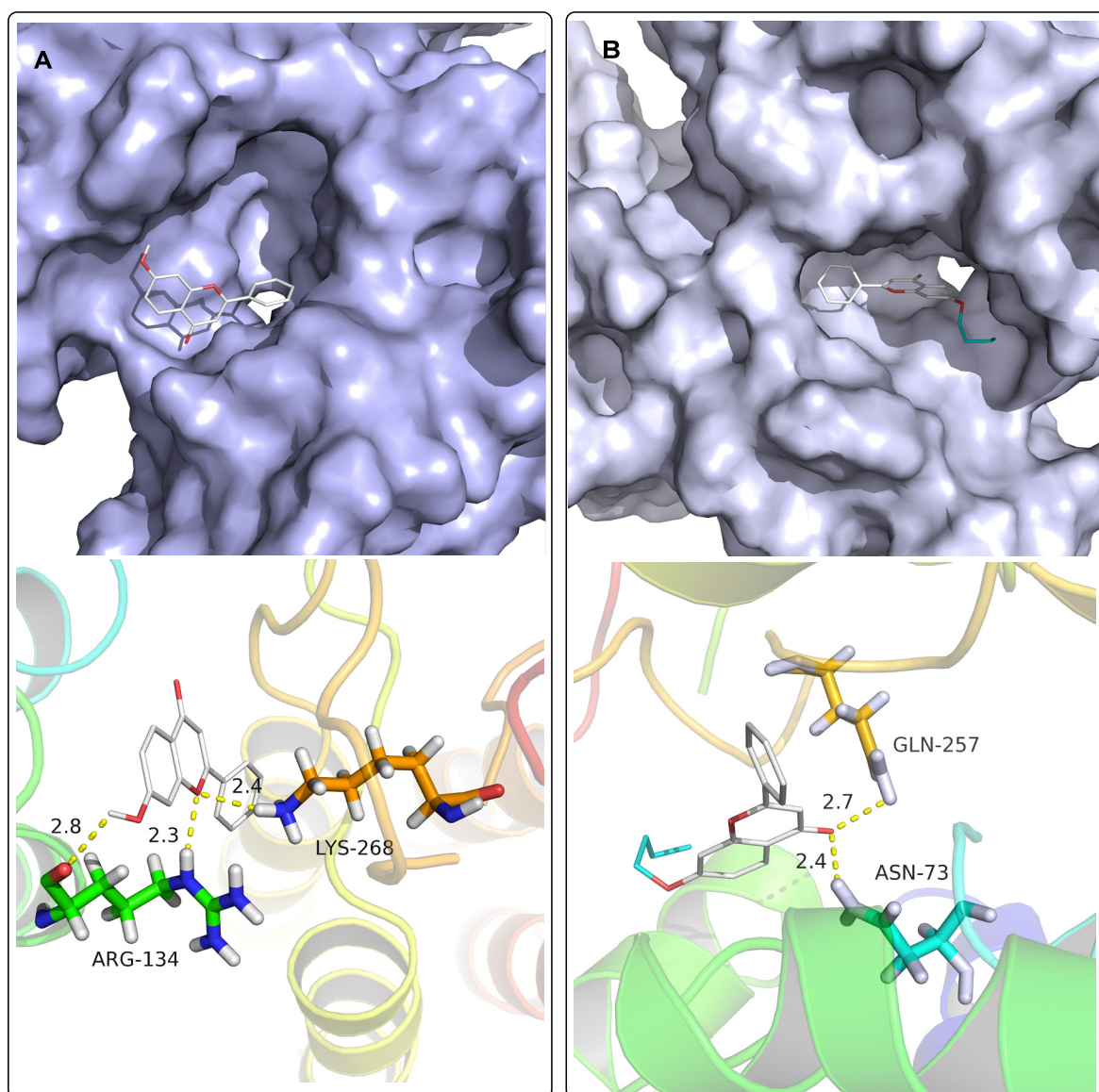


Figure S61. Molecule docking results of **1** (A) and **2a** (B) with TMV CP