

Supporting Information For:

Synthesis, Characterization and Antifungal Activity of Novel Benzo[4,5]imidazo[1,2-*d*][1,2,4]triazine Derivatives

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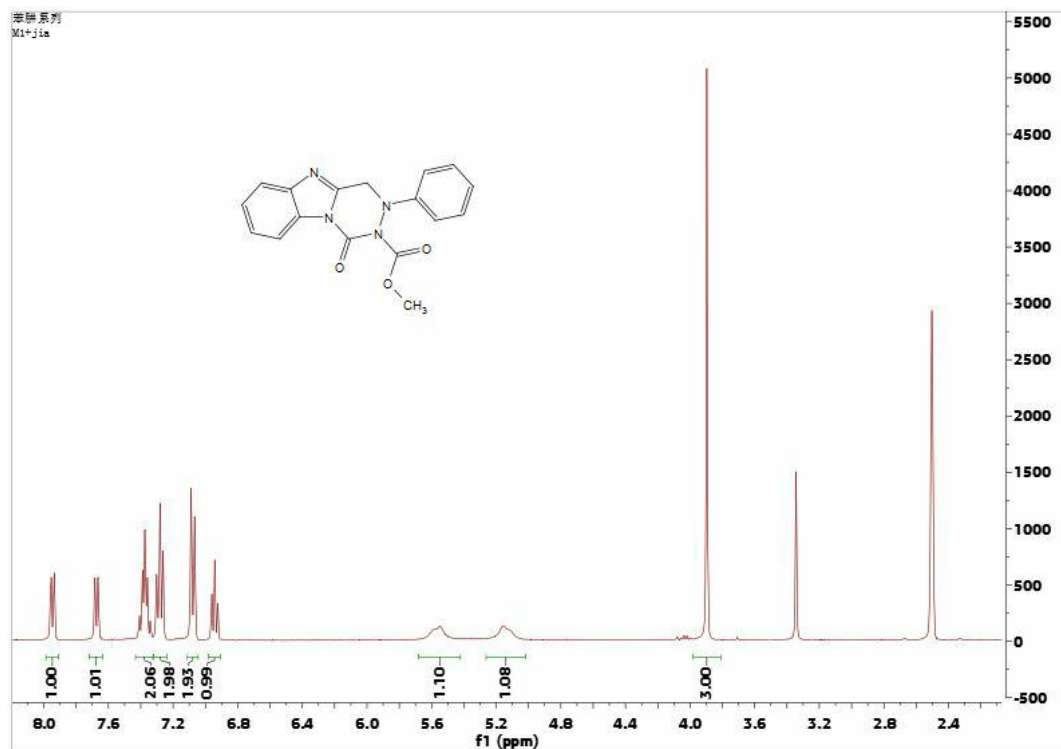
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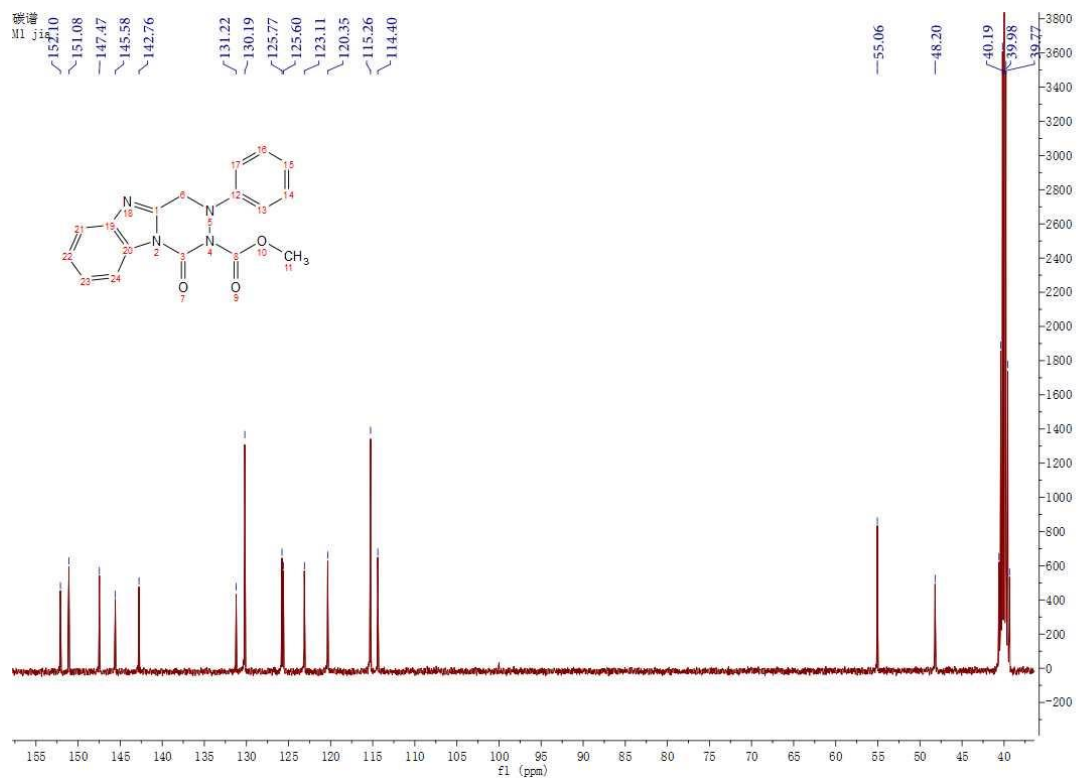
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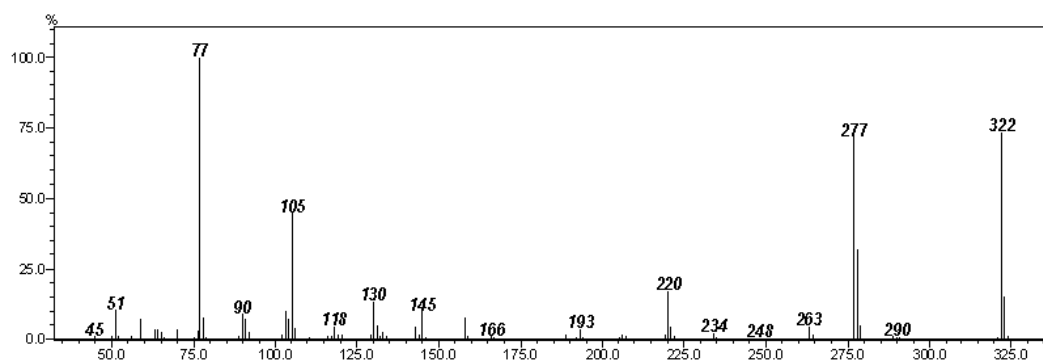
¹H NMR spectra of compound 4a



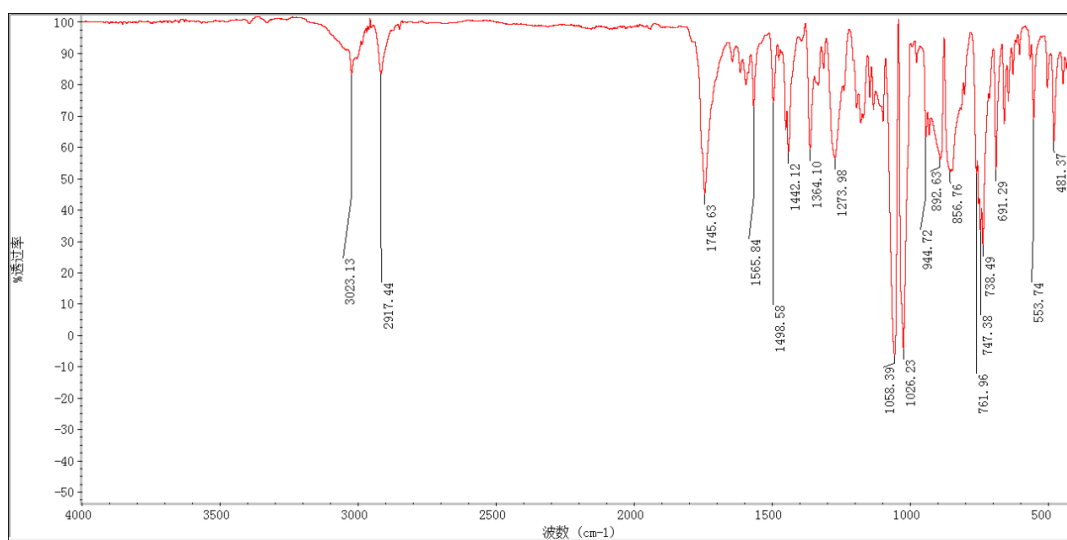
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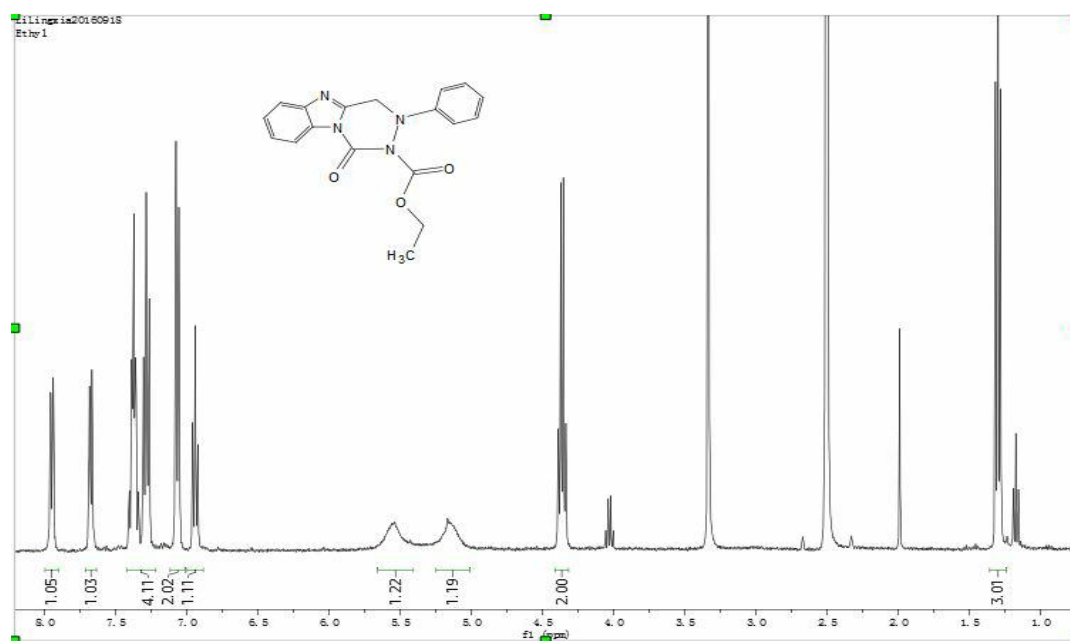
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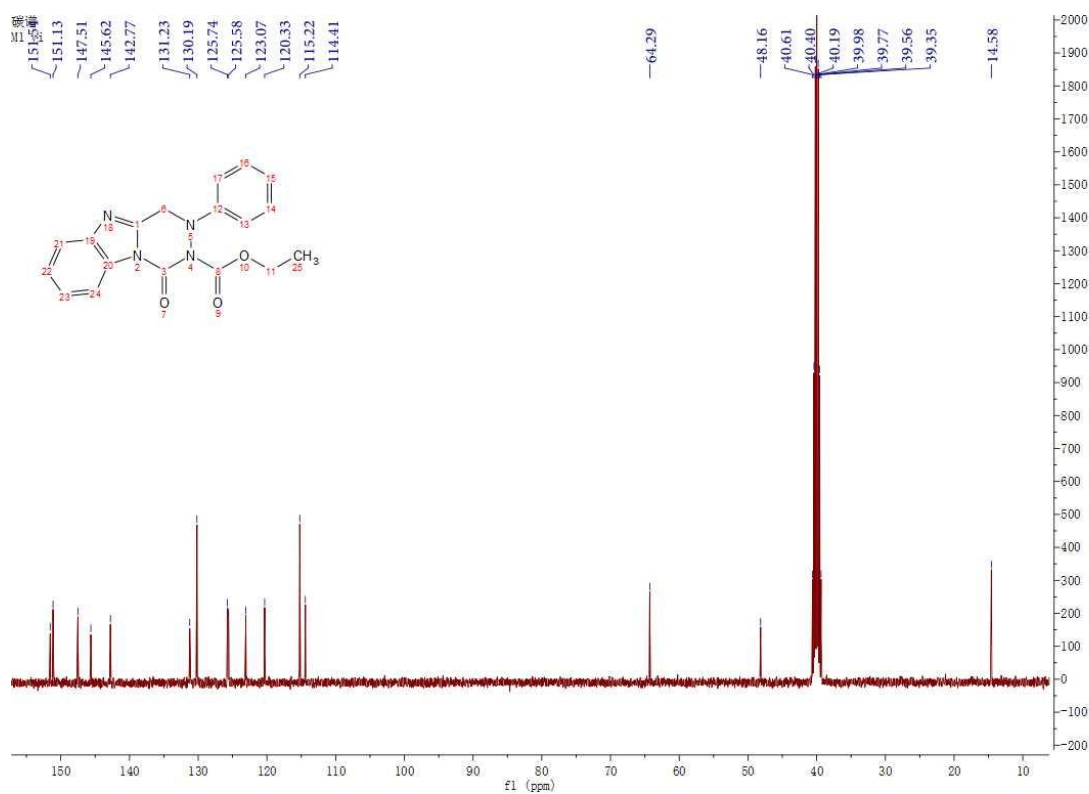
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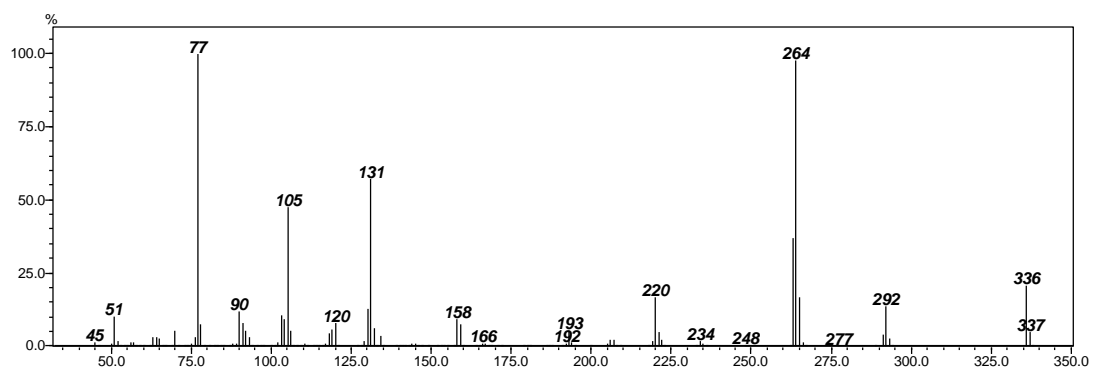
4. ^1H NMR spectra of compound **4b**



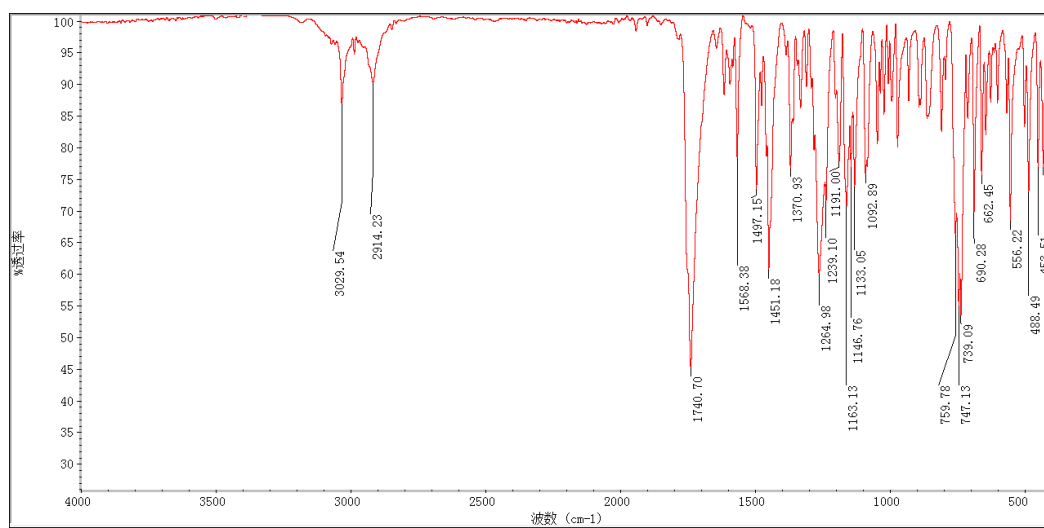
5. ^{13}C NMR spectra of compound **4b**



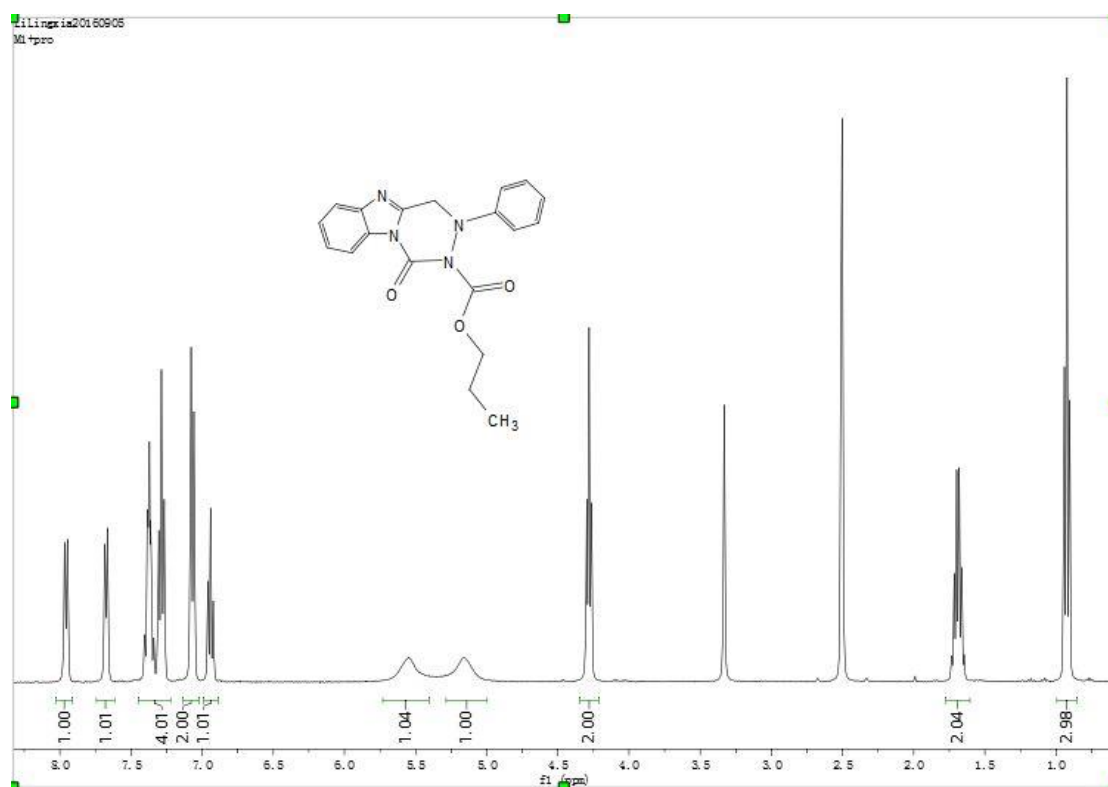
6. EI-MS spectra of compound 4b



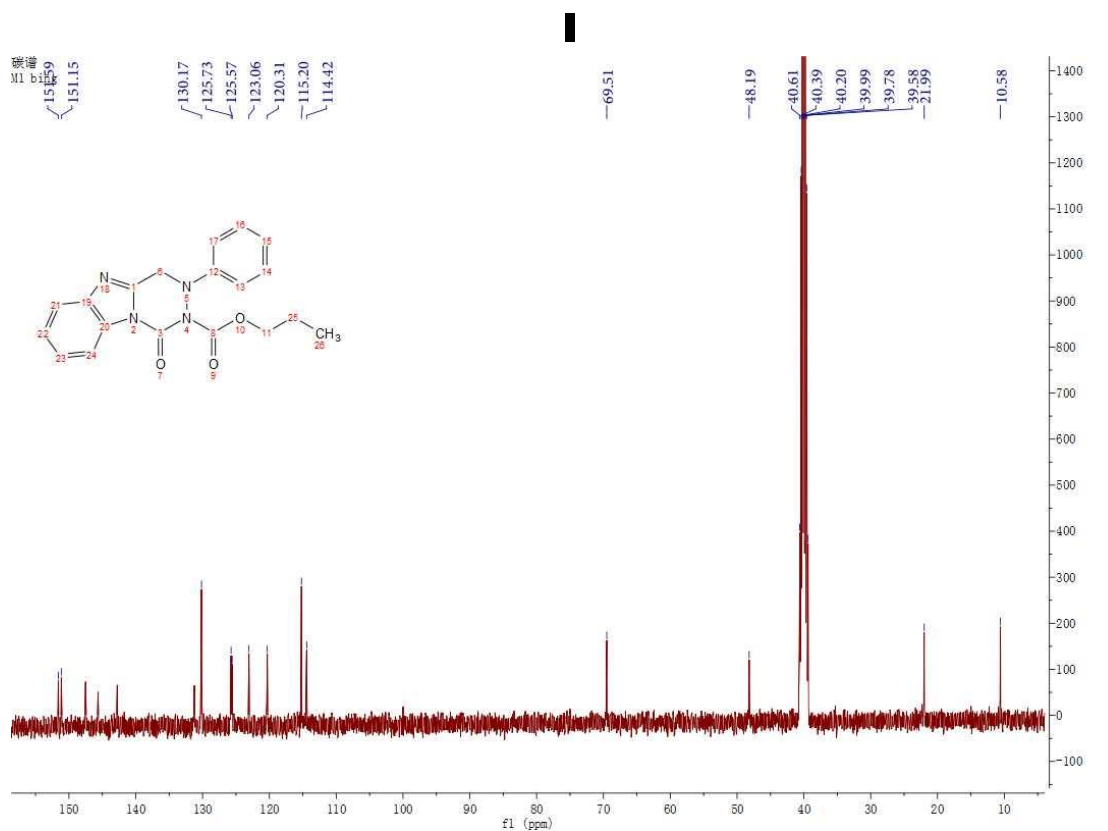
7. FT-IR spectra of compound 4b



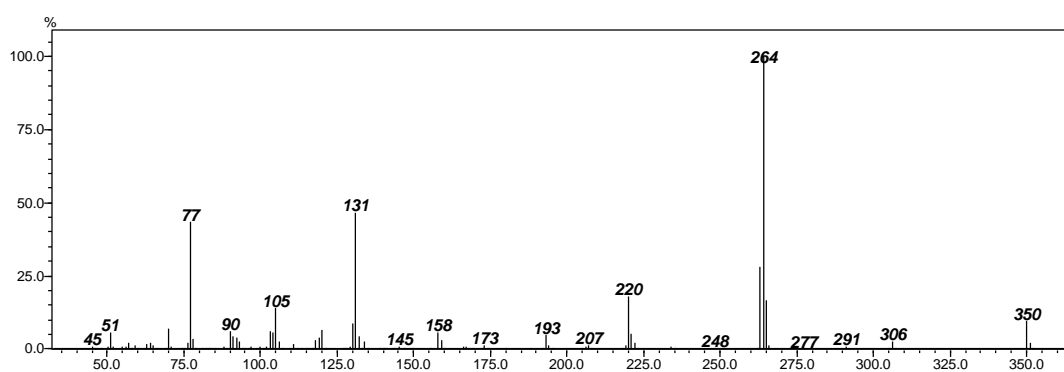
8. ¹H NMR spectra of compound 4c



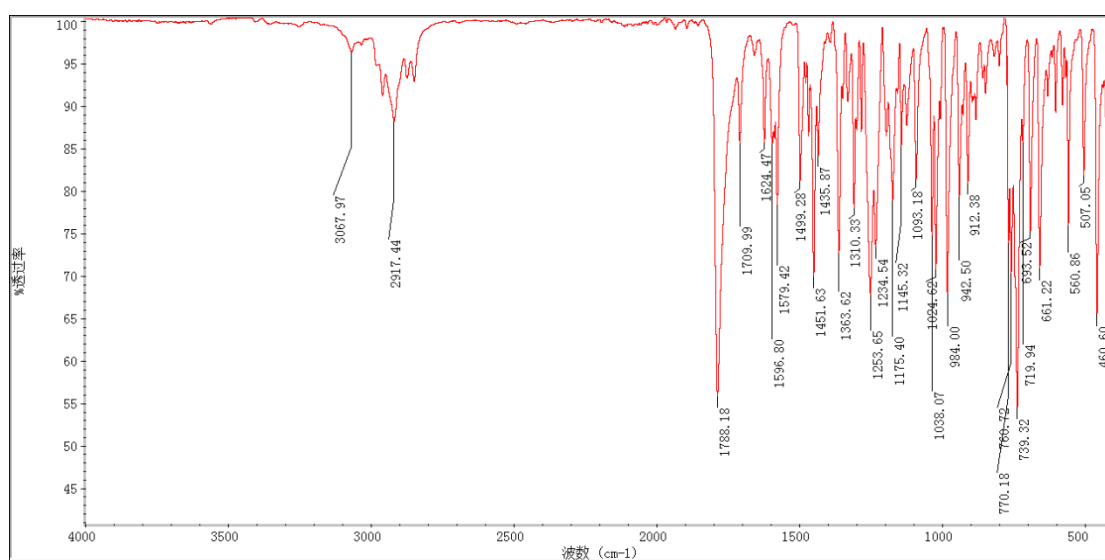
9. ¹³C NMR spectra of compound 4c



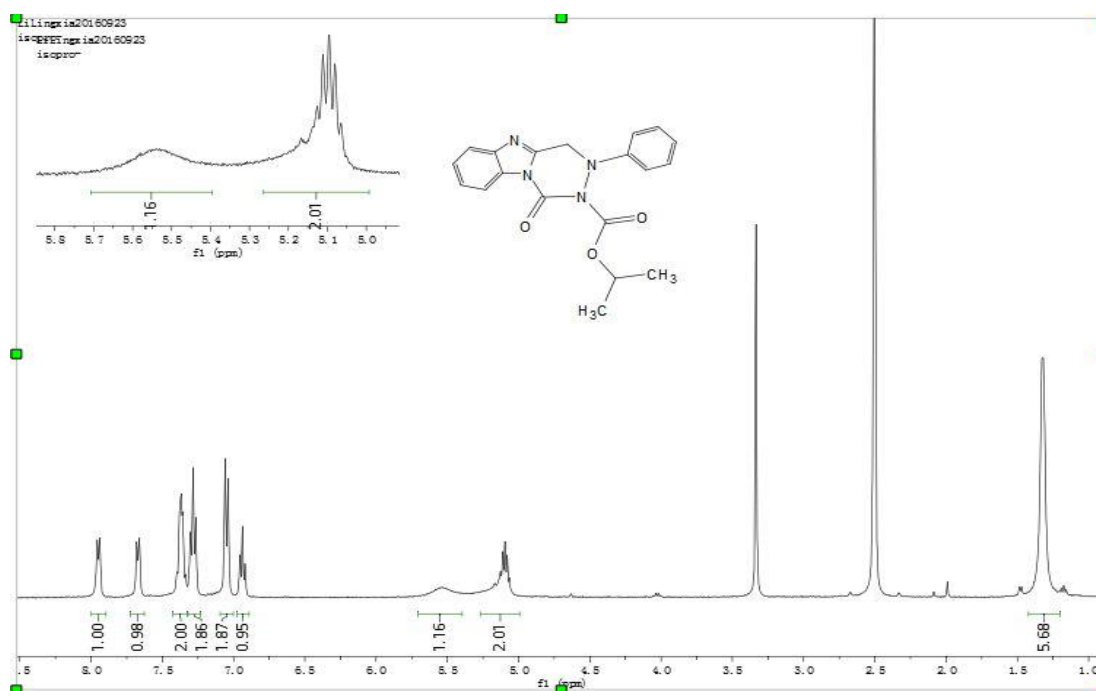
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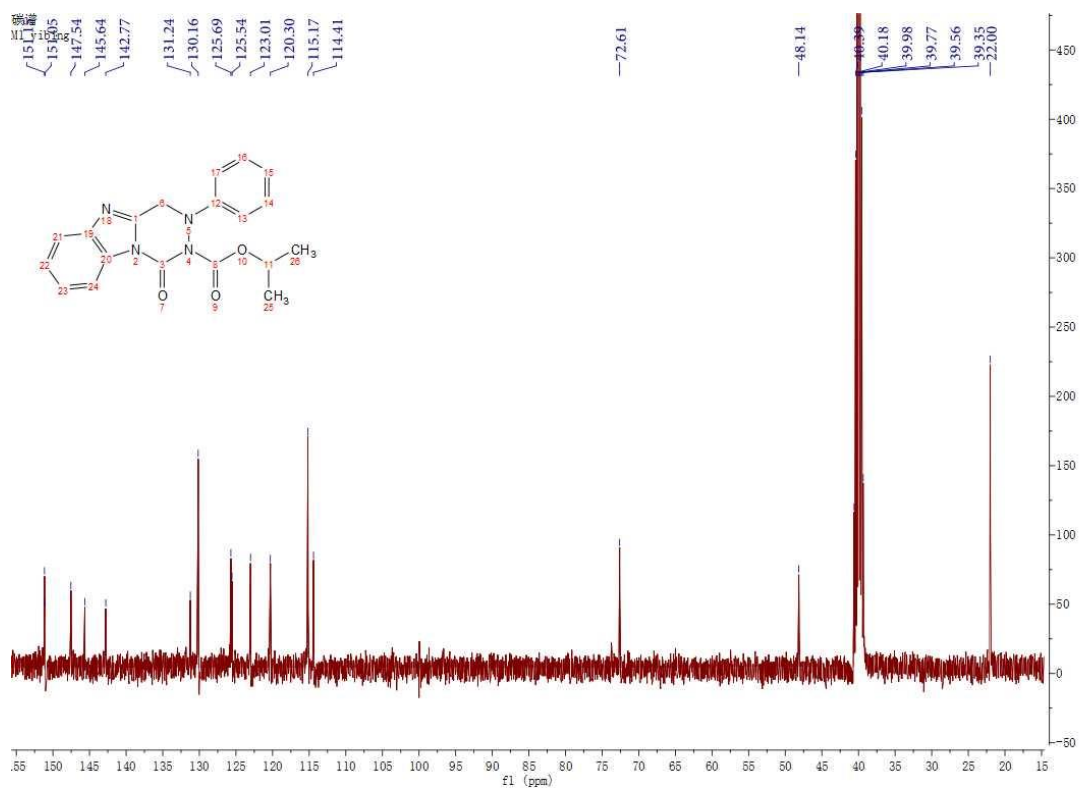
11. FT-IR spectra of compound 4c



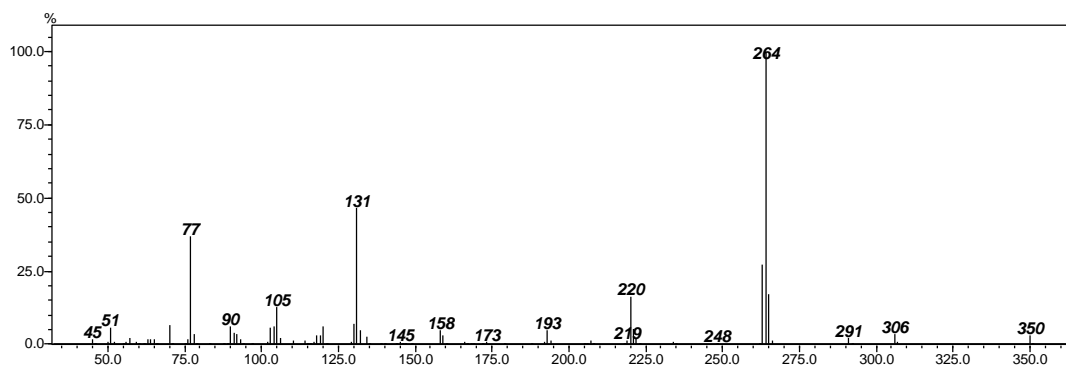
12. ¹H NMR spectra of compound 4d



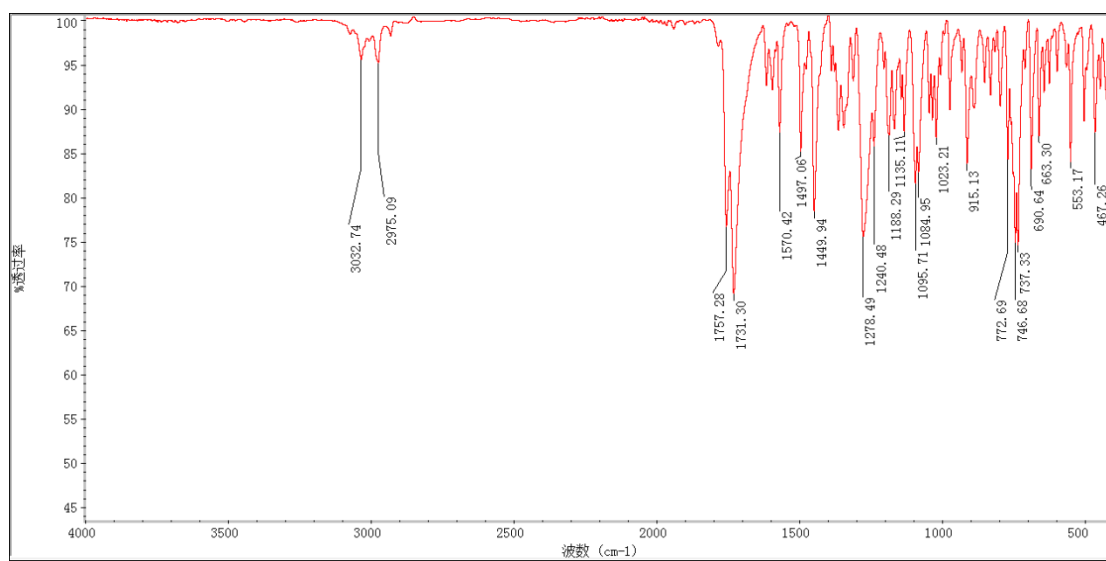
13. ¹³C NMR spectra of compound 4d



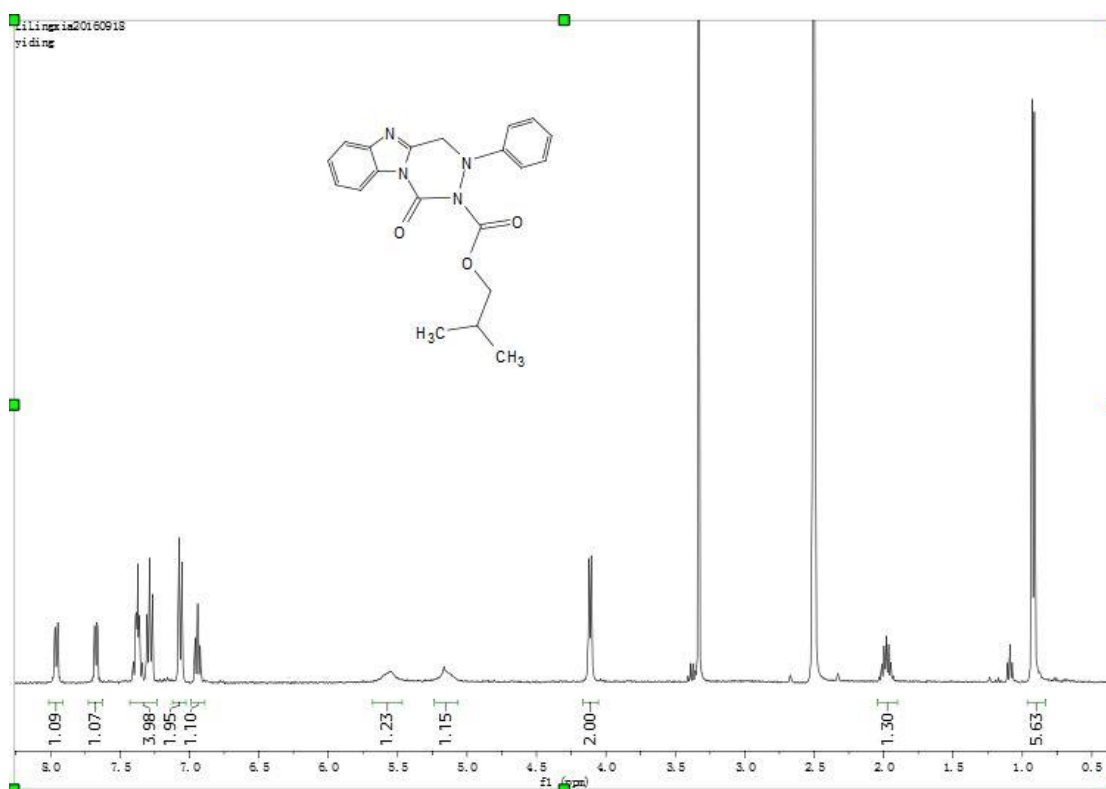
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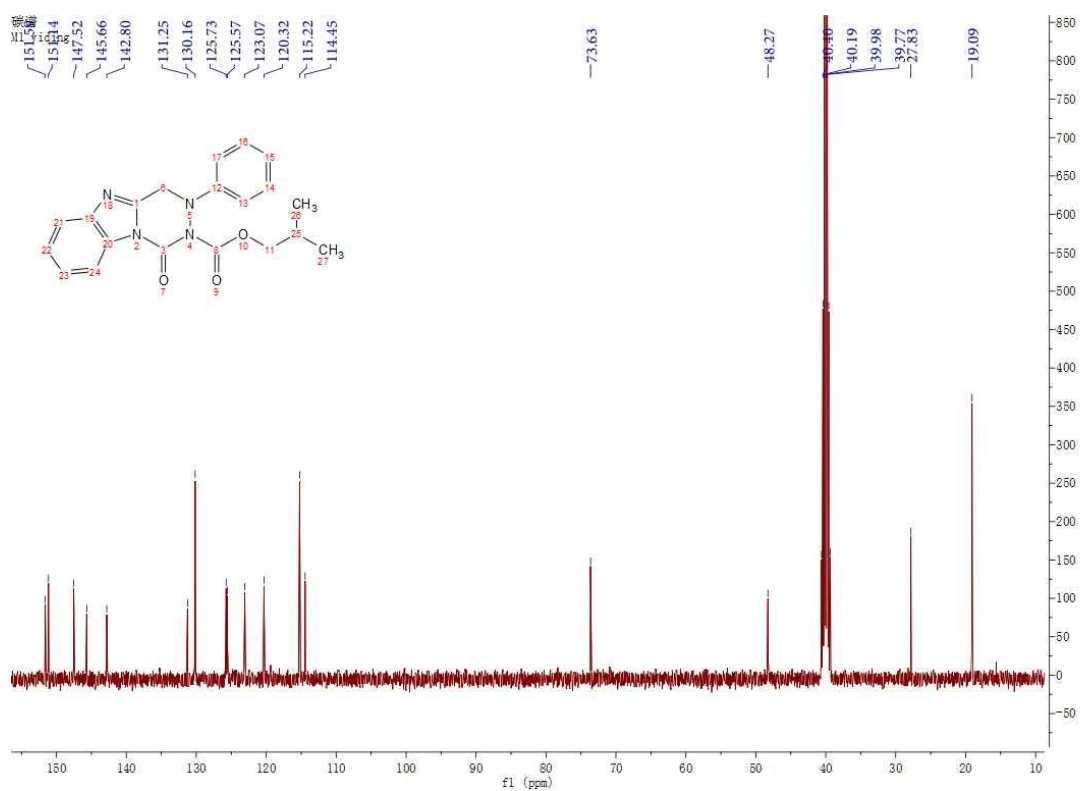
15. FT-IR spectra of compound 4d



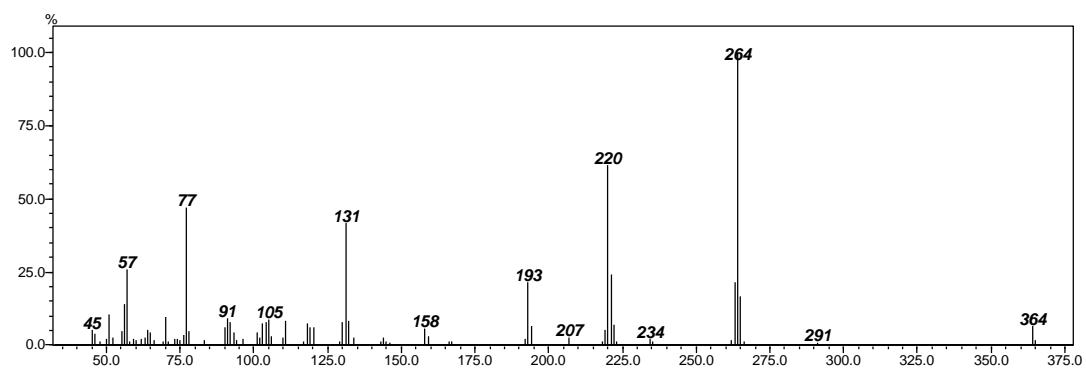
16. ¹H NMR spectra of compound 4e



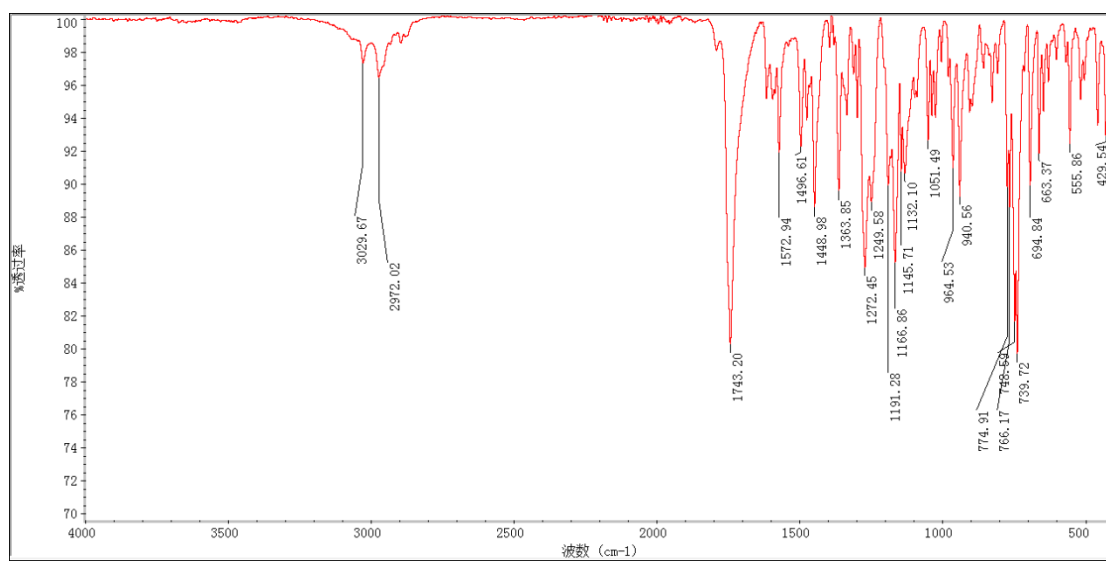
17. ¹³C NMR spectra of compound 4e



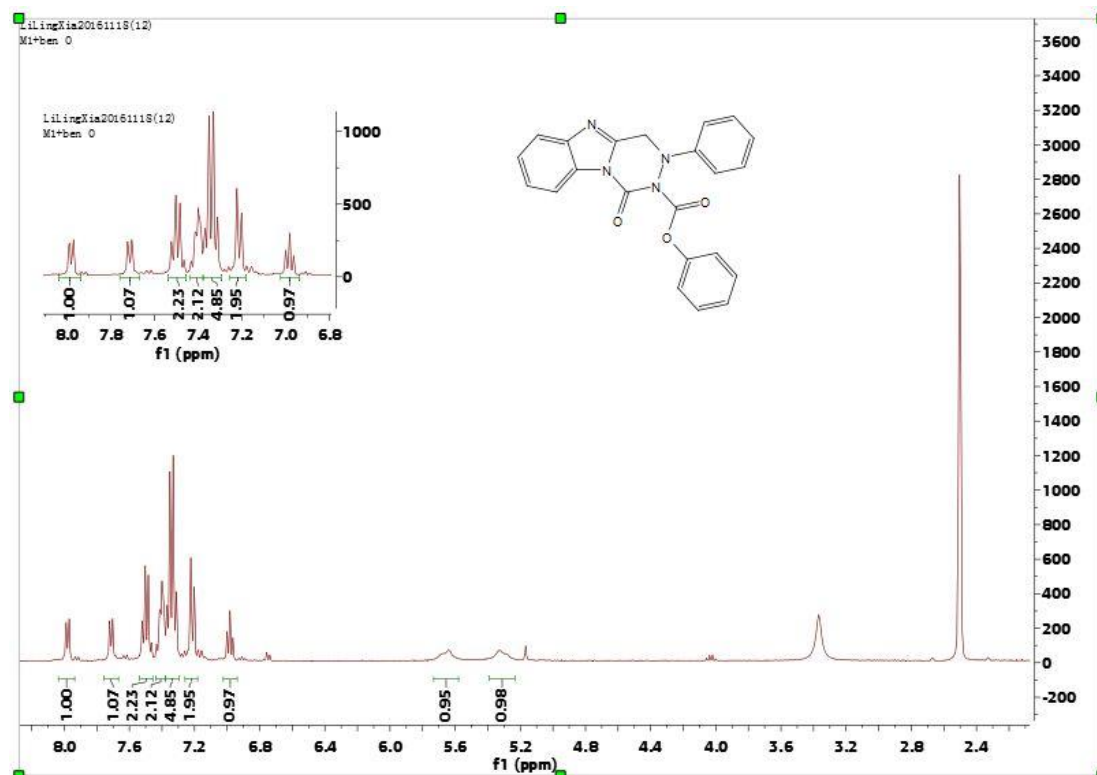
18. EI-MS spectra of compound 4e



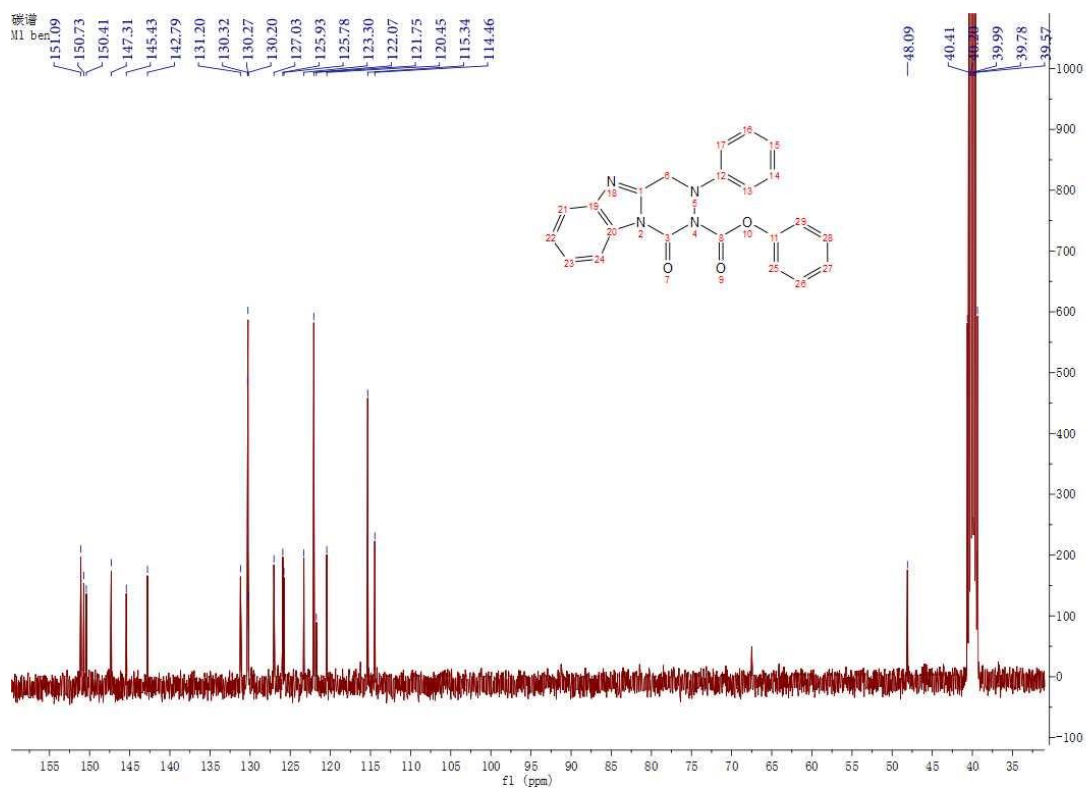
19. FT-IR spectra of compound 4e



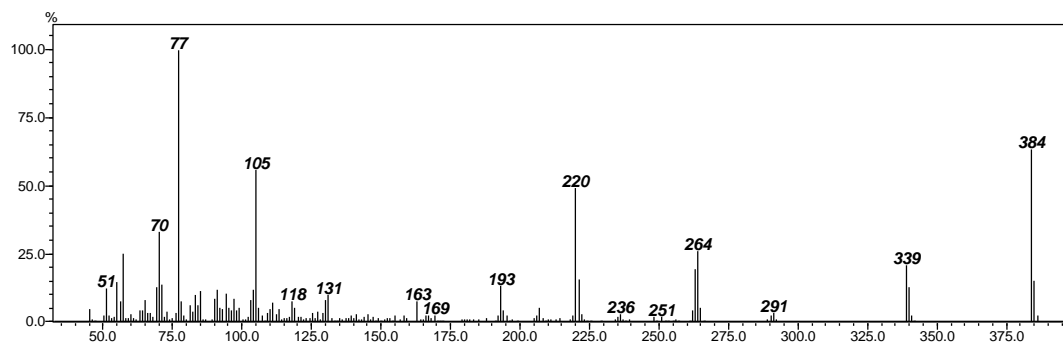
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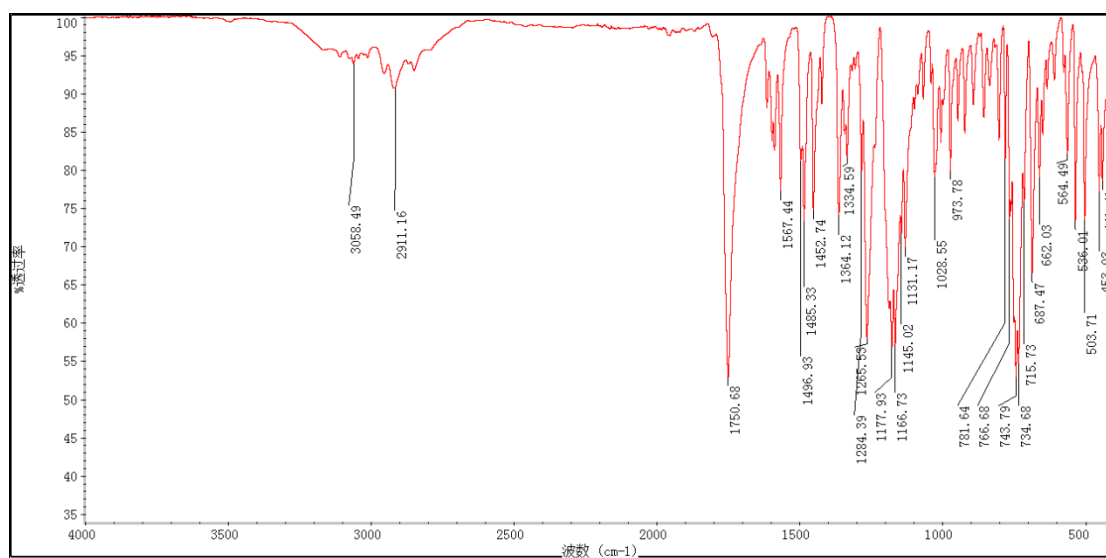
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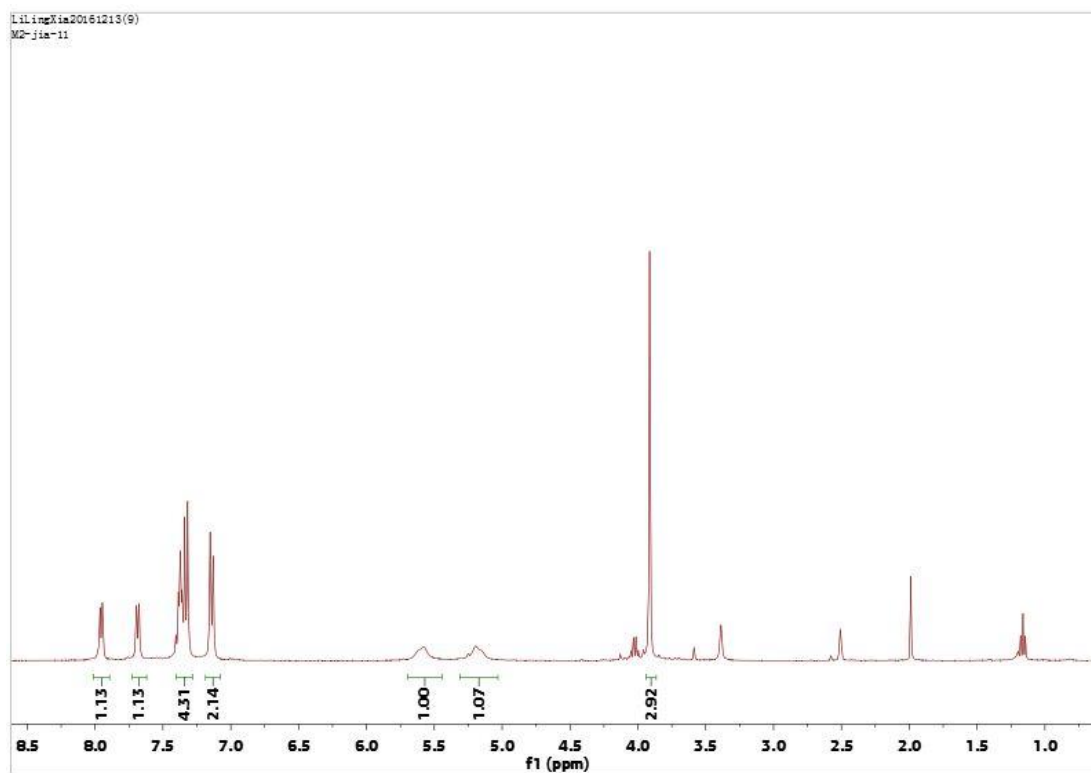
22. EI-MS spectra of compound 4f



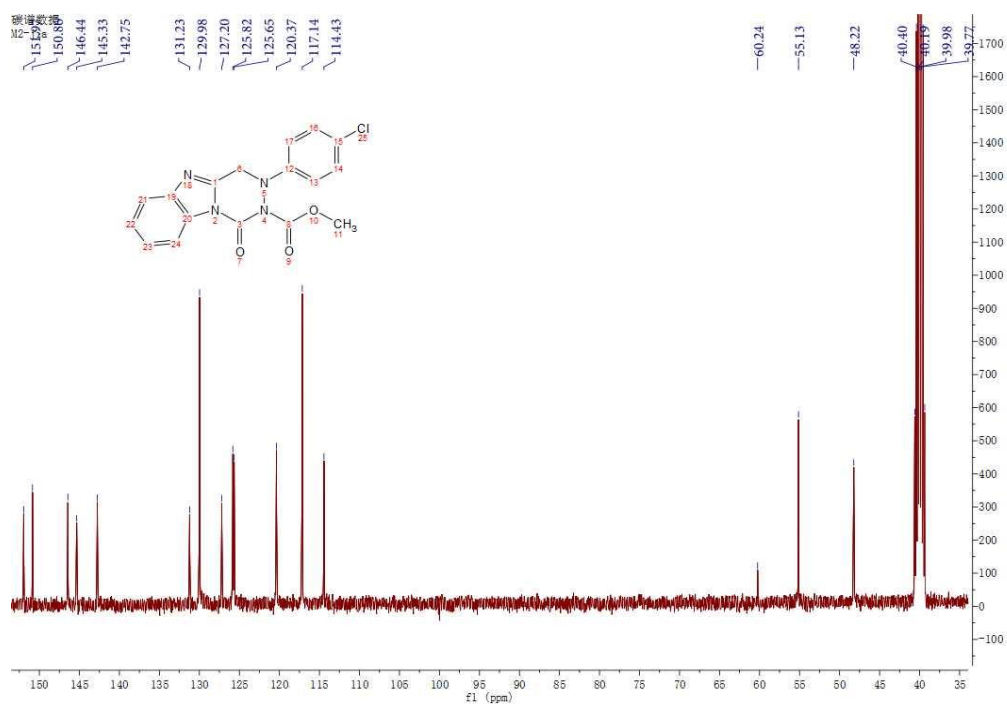
23. FT-IR spectra of compound 4f



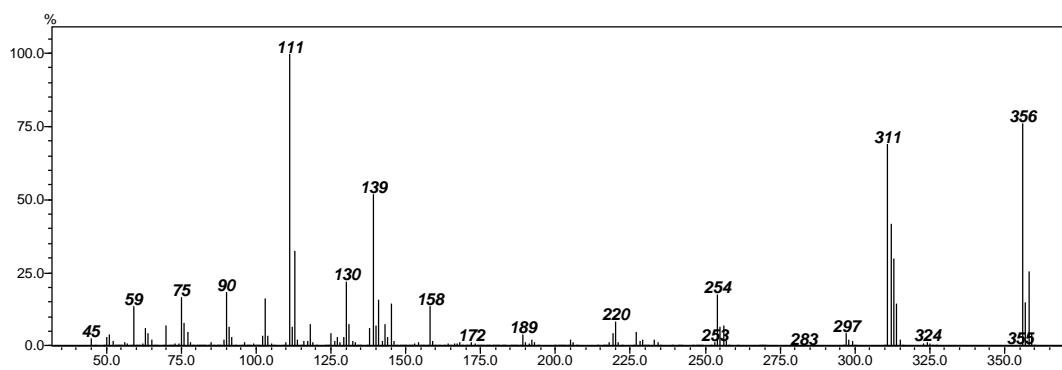
24. ¹H NMR spectra of compound 4g



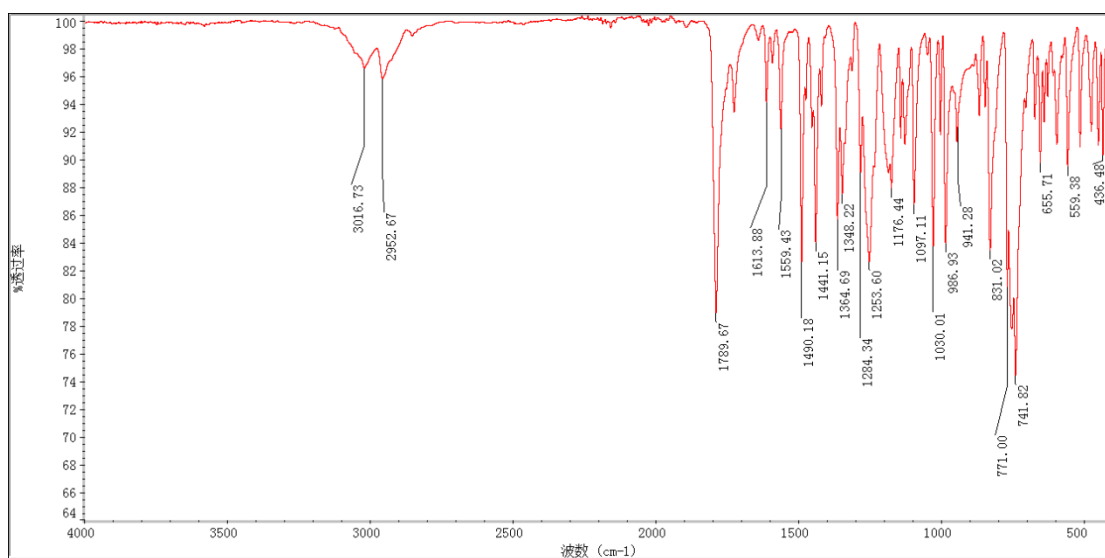
25. ^{13}C NMR spectra of compound **4g**



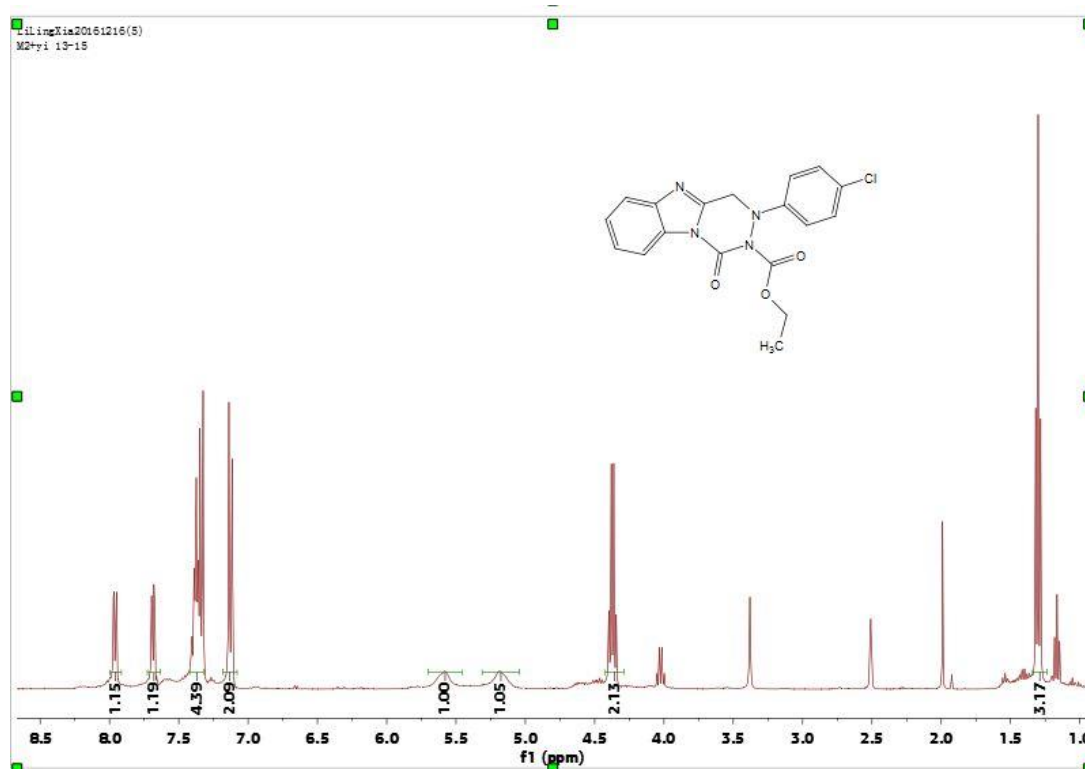
26. EI-MS spectra of compound **4g**



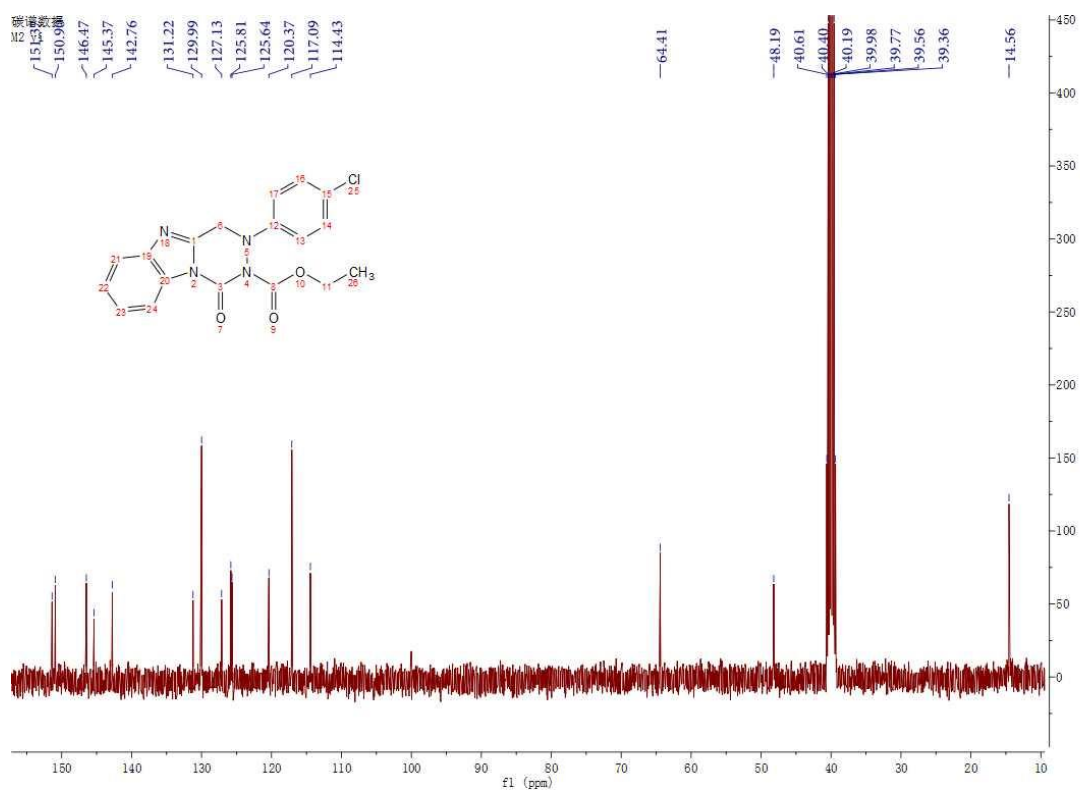
27. FT-IR spectra of compound 4g



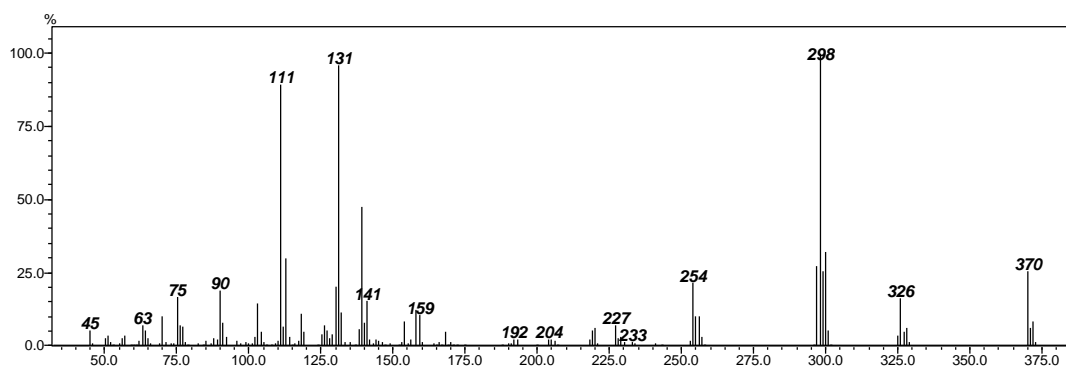
28. ¹H NMR spectra of compound 4h



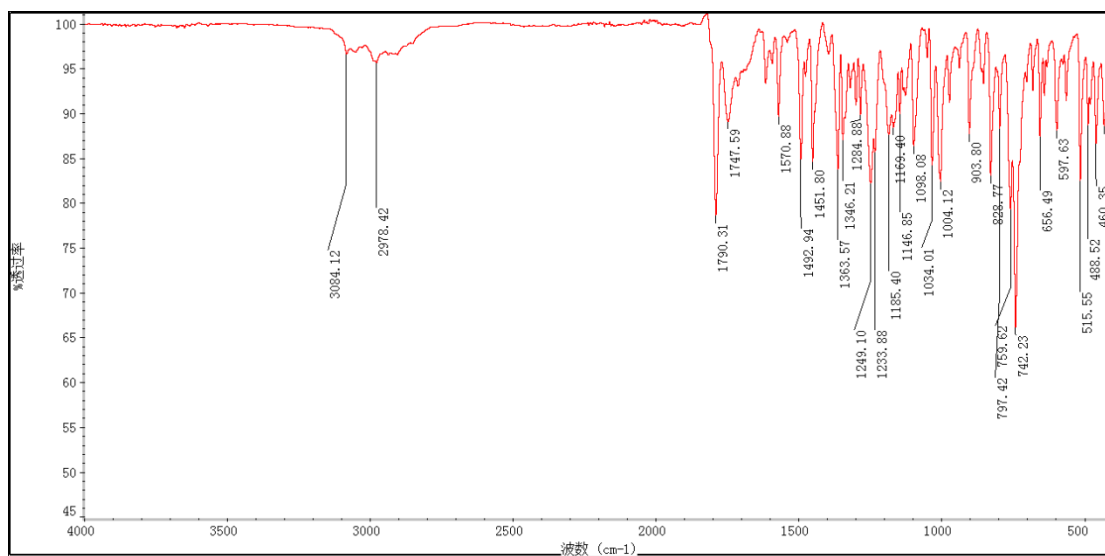
29. ¹³C NMR spectra of compound 4h



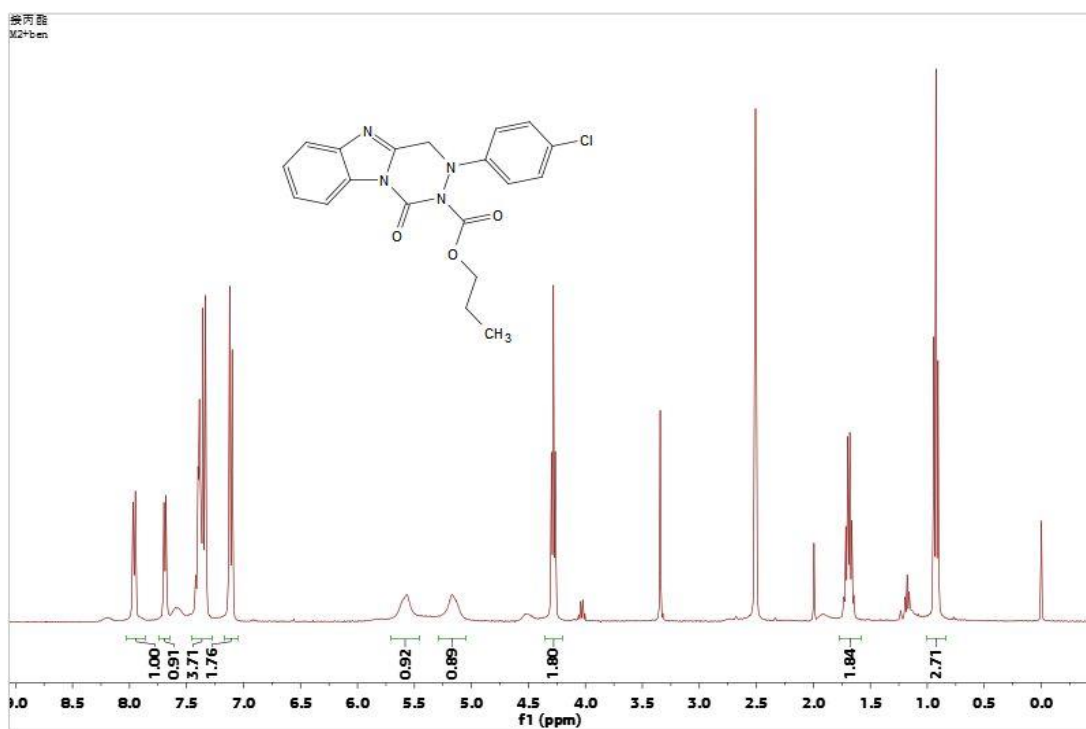
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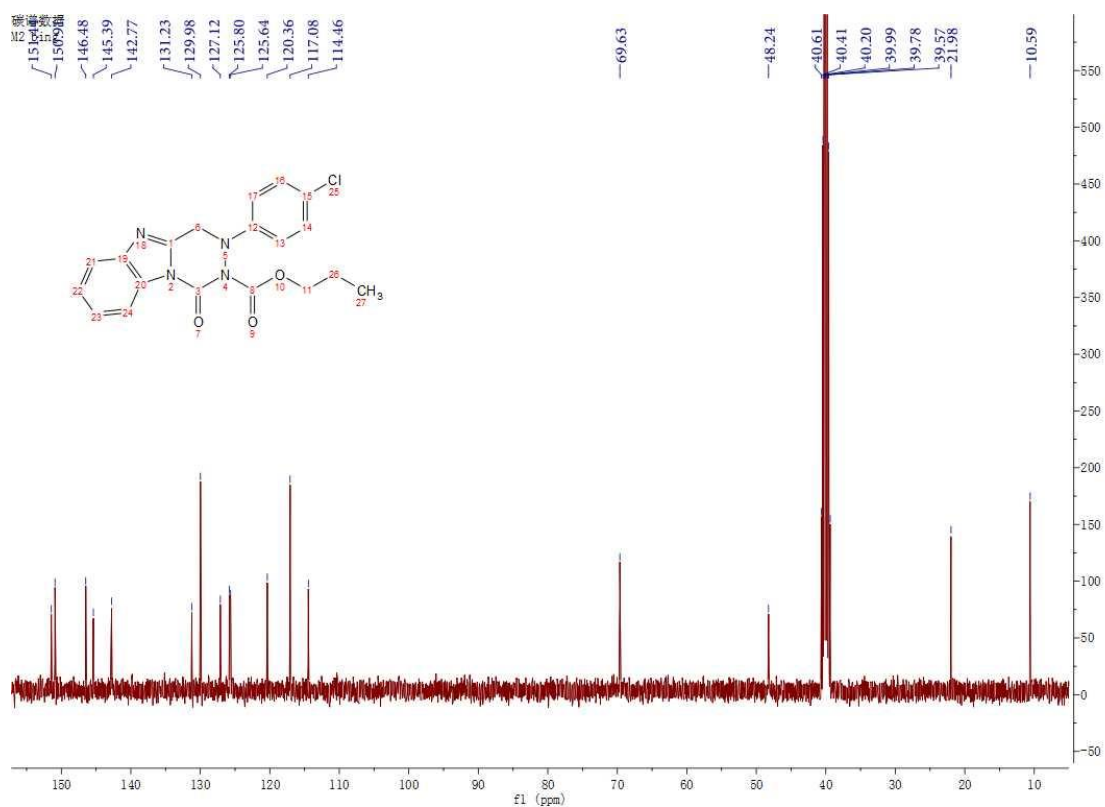
31. FT-IR spectra of compound 4h



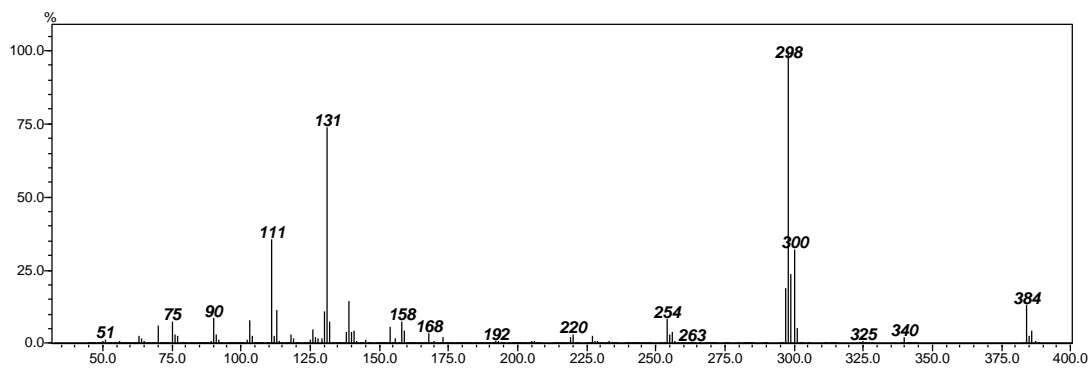
32. ¹H NMR spectra of compound 4i



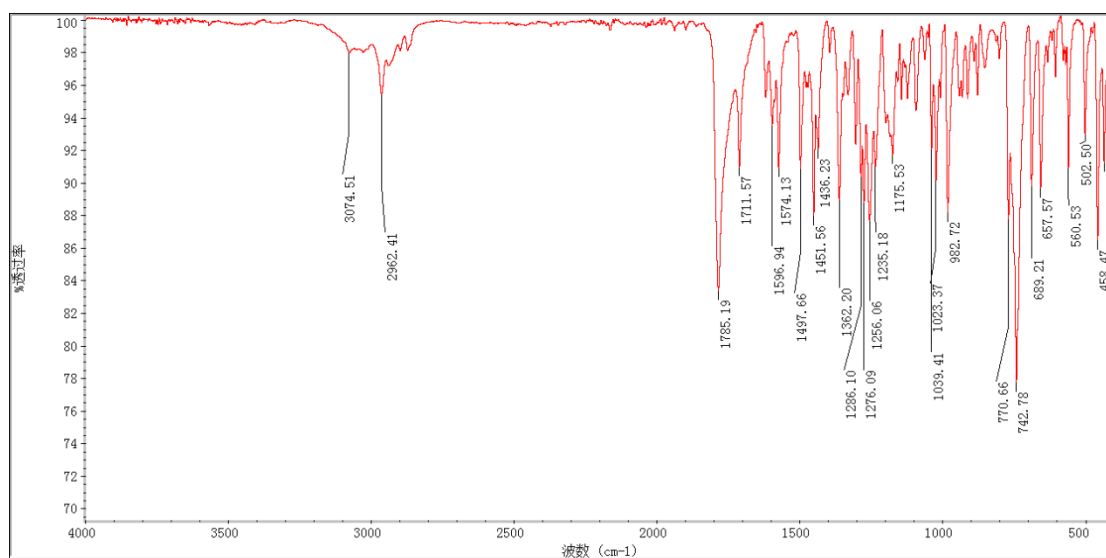
33. ¹³C NMR spectra of compound **4i**



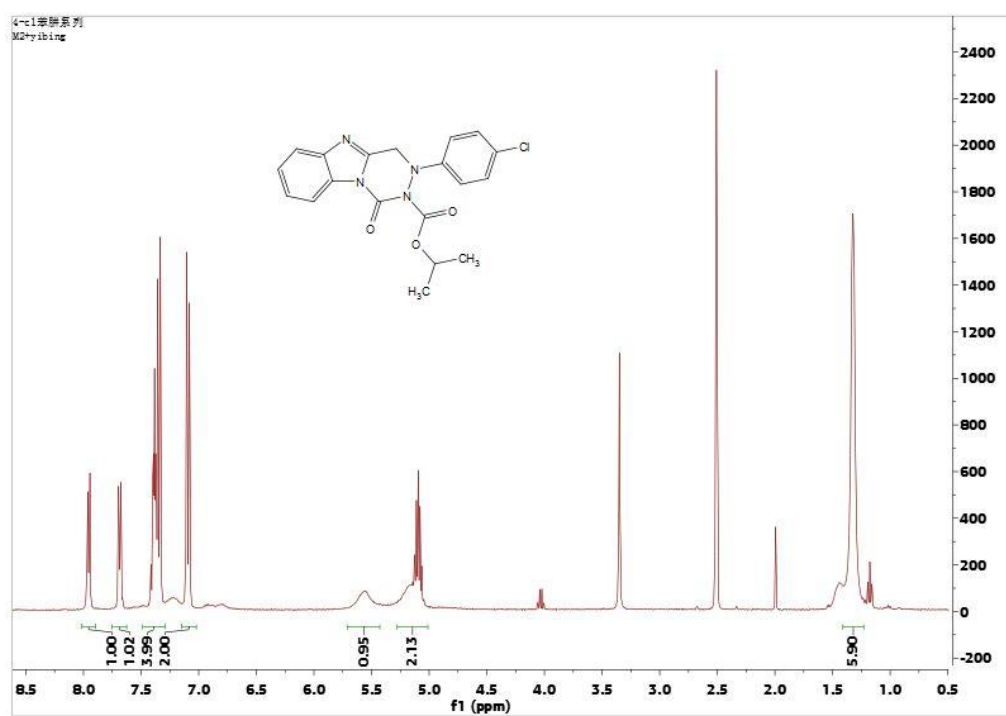
34. EI-MS spectra of compound **4i**



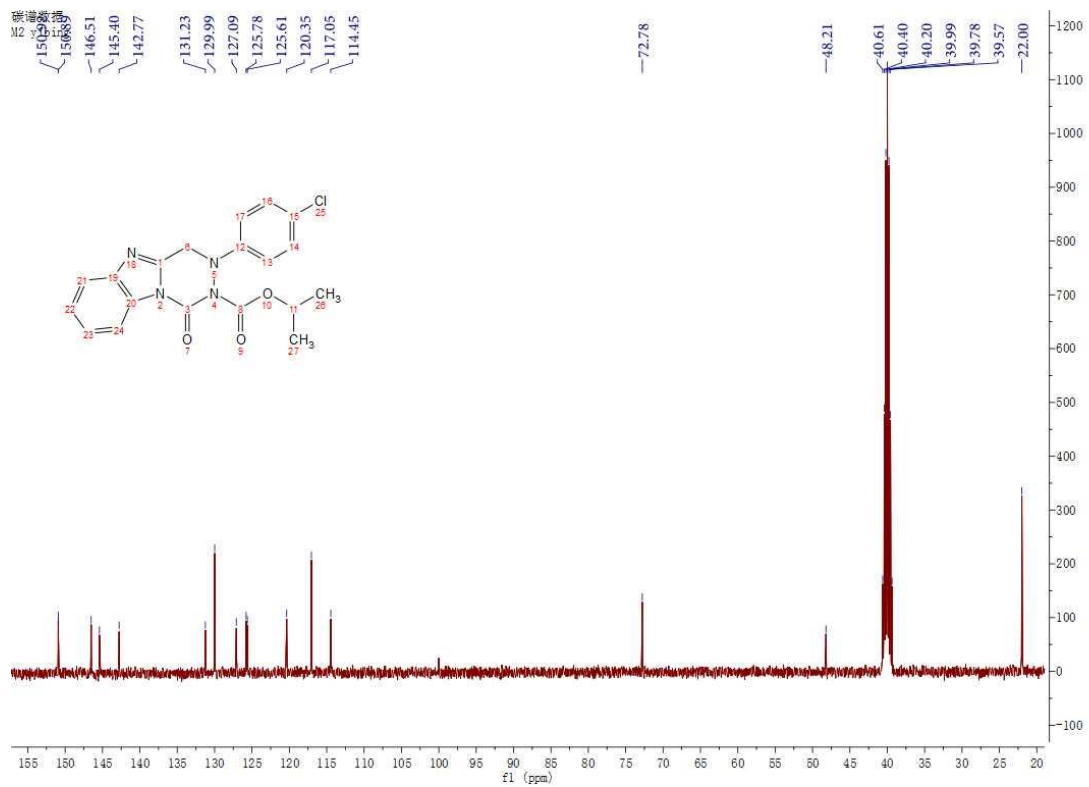
35. FT-IR spectra of compound 4i



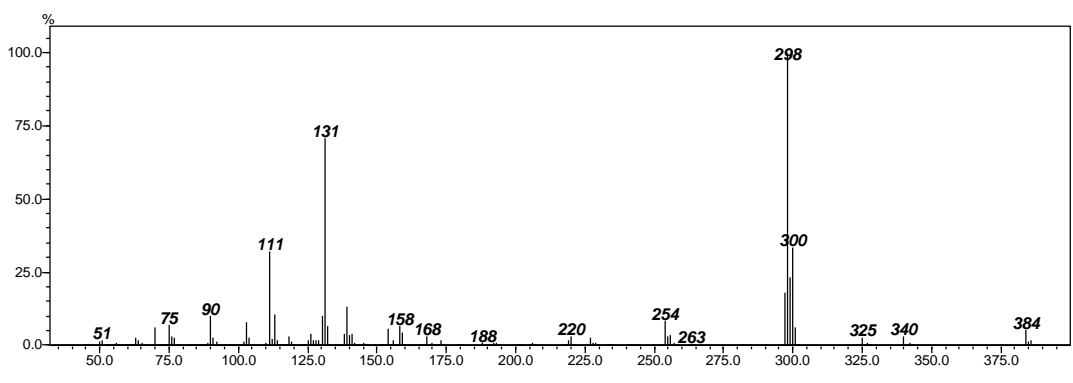
36. ¹H NMR spectra of compound 4j



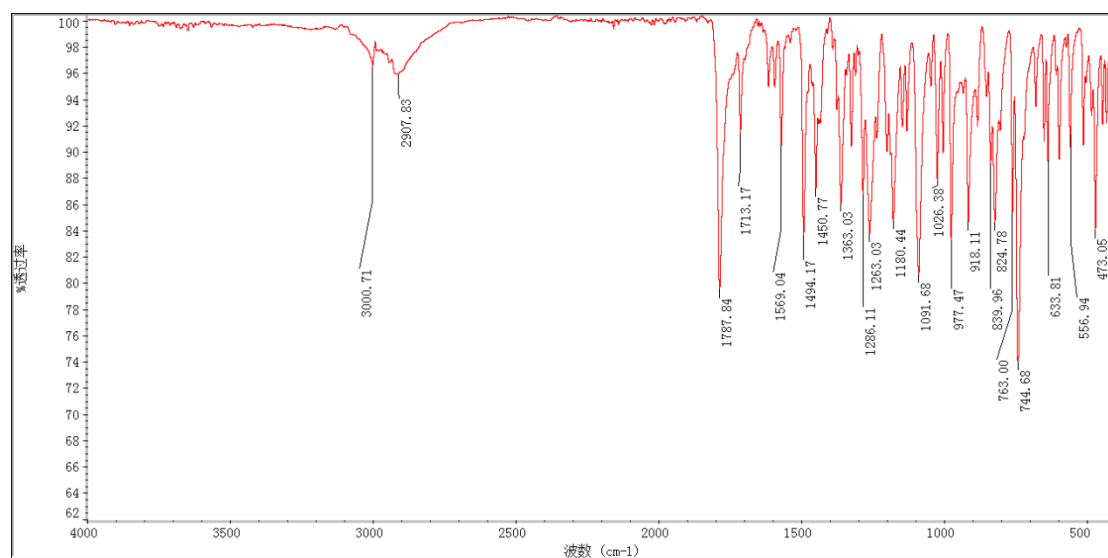
37. ¹³C NMR spectra of compound 4j



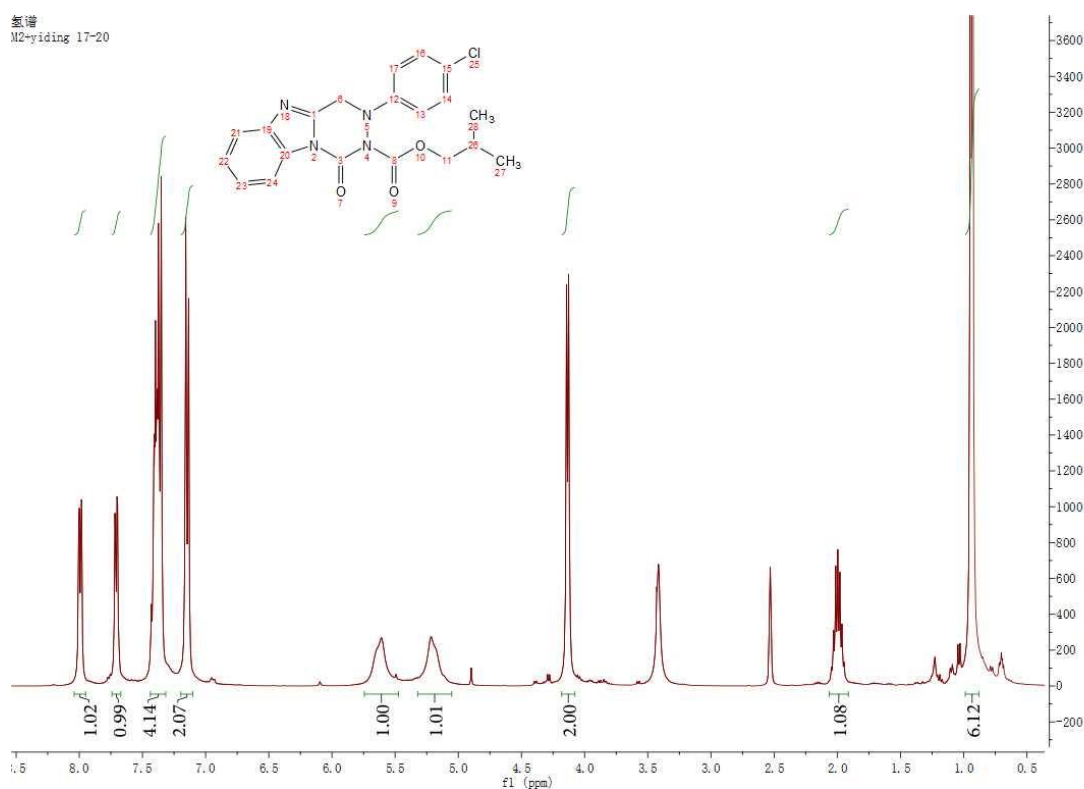
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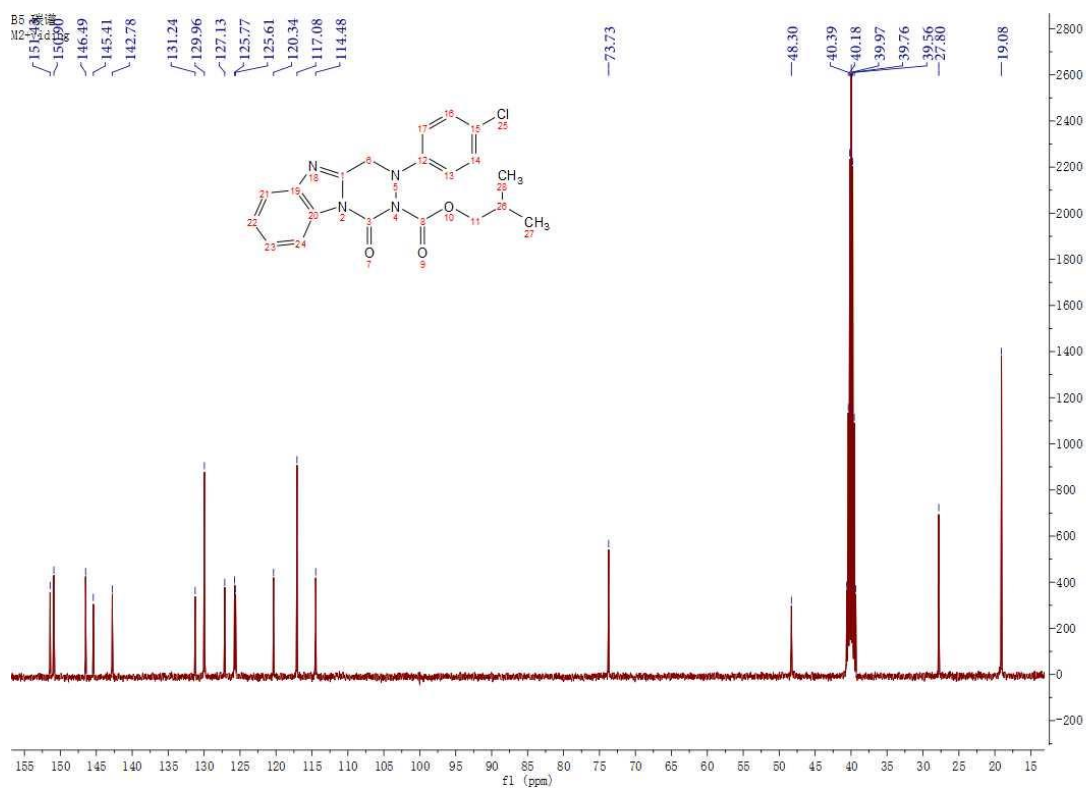
39. FT-IR spectra of compound 4j



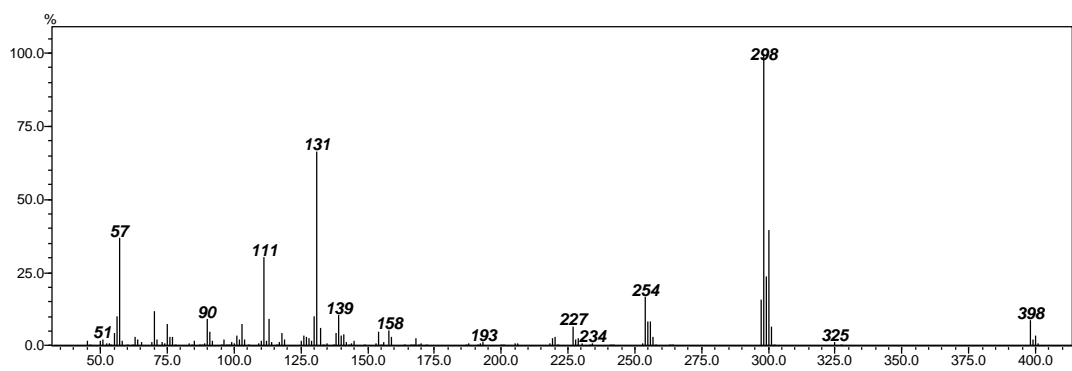
40. ¹H NMR spectra of compound 4k



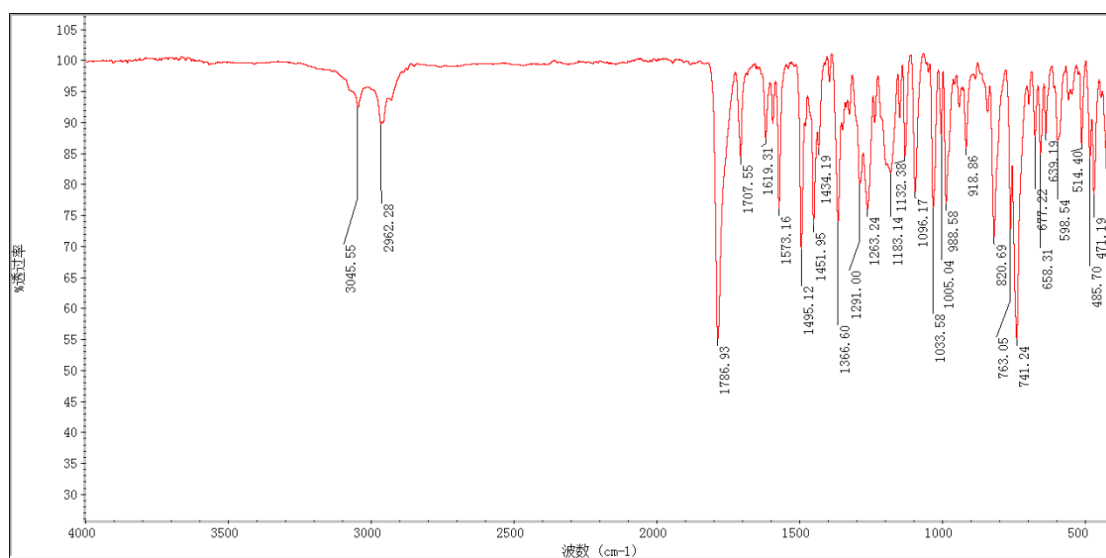
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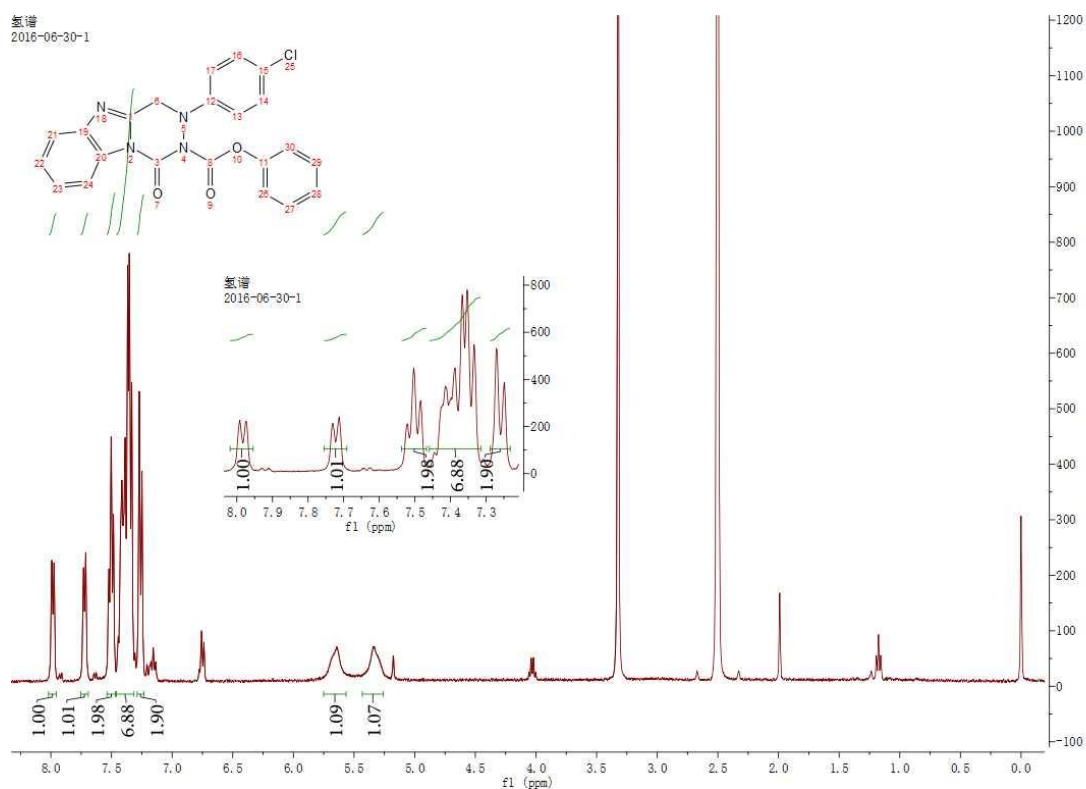
42. EI-MS spectra of compound 4k



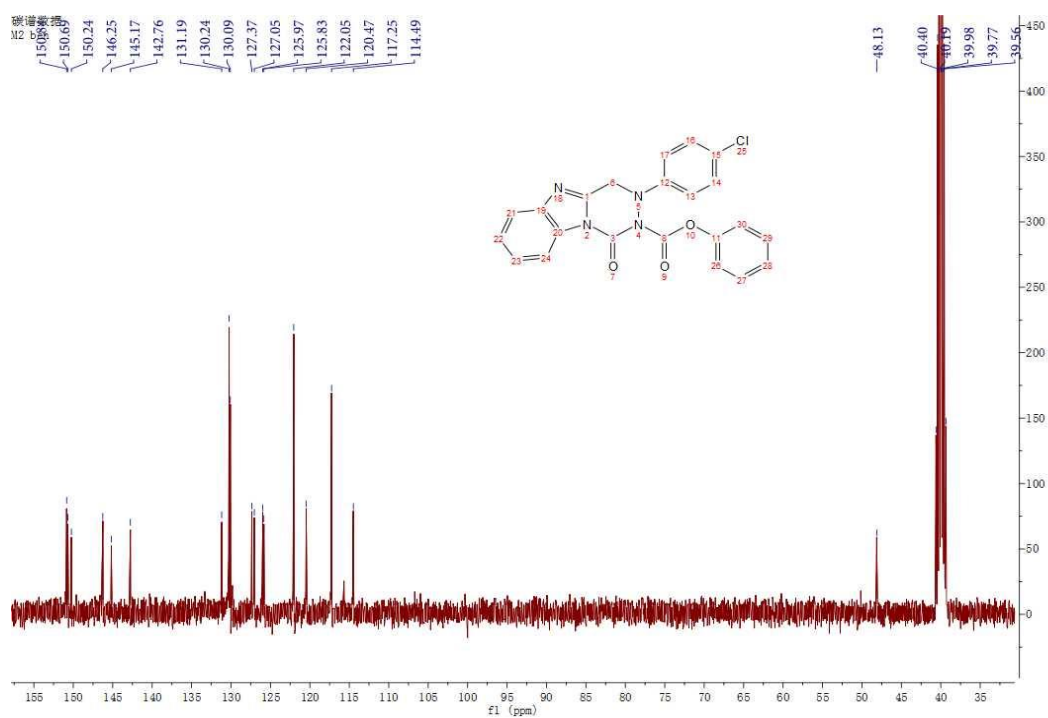
43. FT-IR spectra of compound 4k



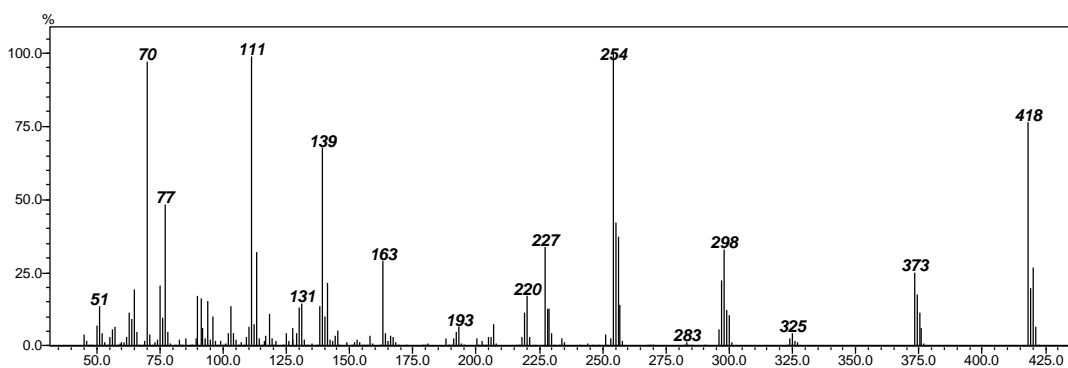
44. ¹H NMR spectra of compound 4l



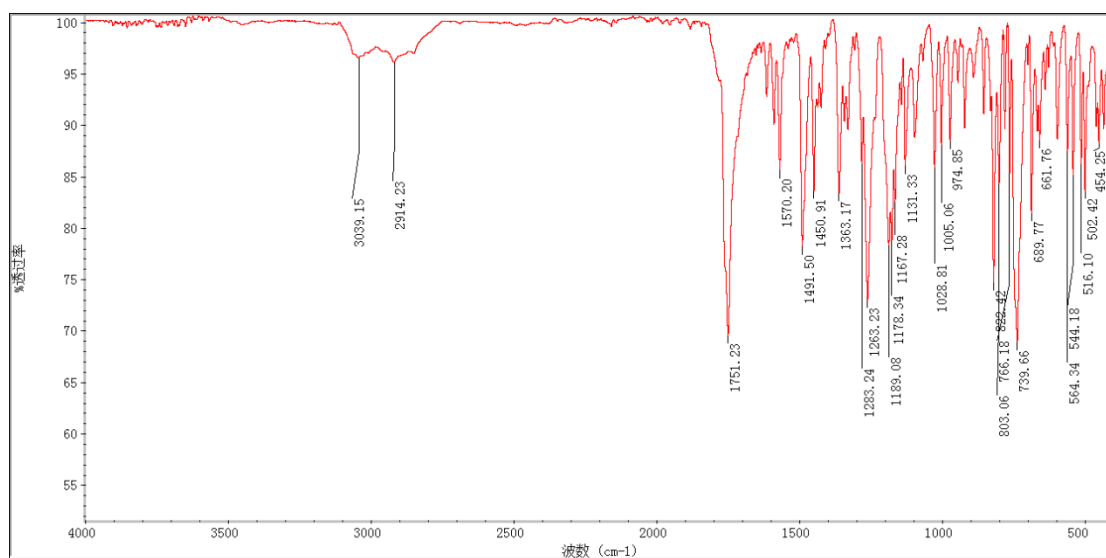
45. ^{13}C NMR spectra of compound 41



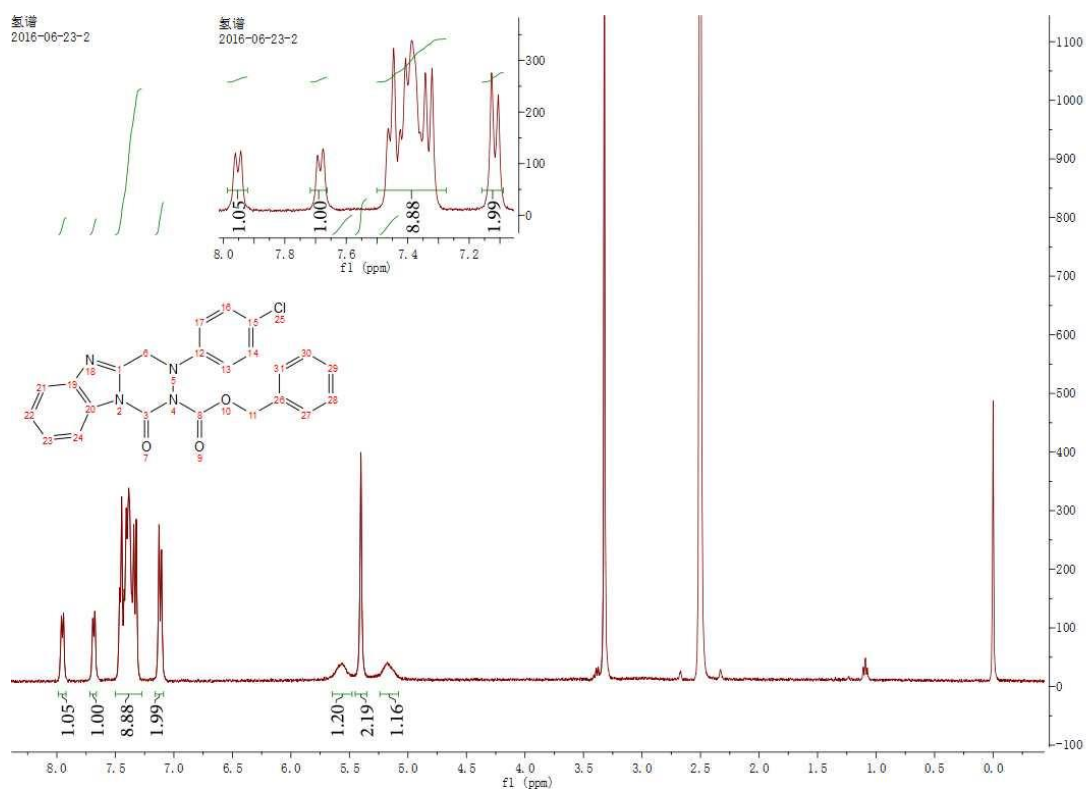
46. EI-MS spectra of compound 41



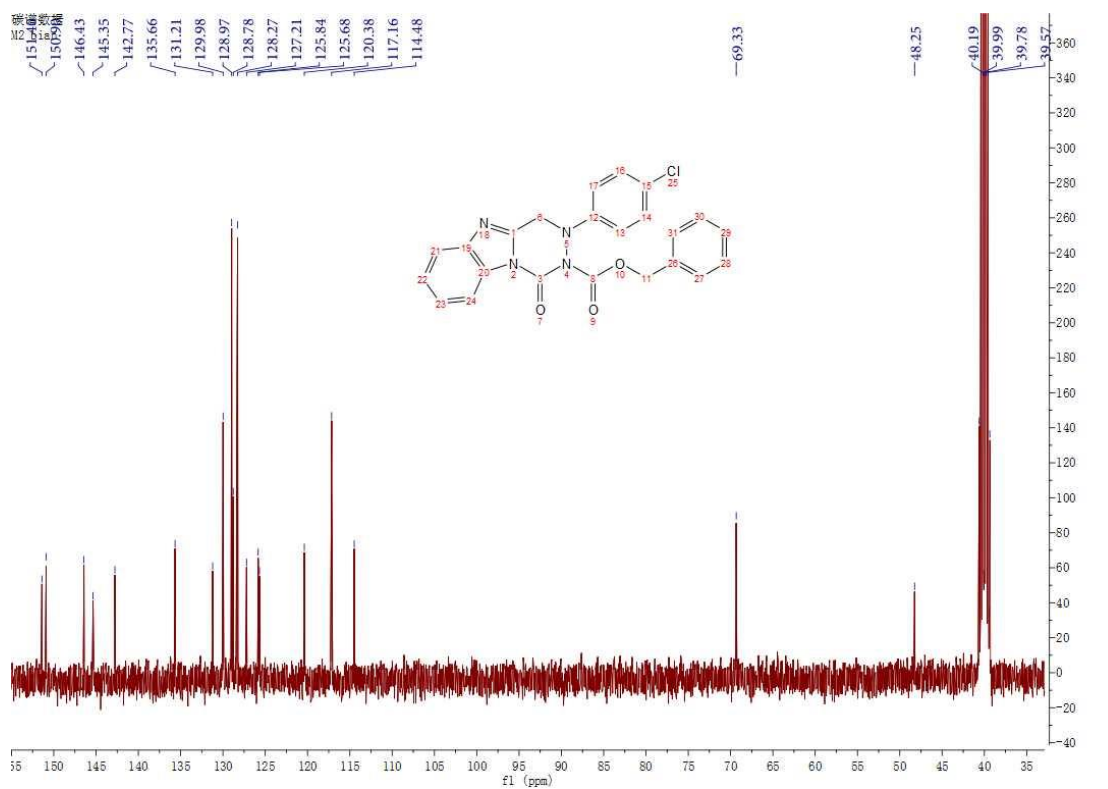
47. FT-IR spectra of compound 4l



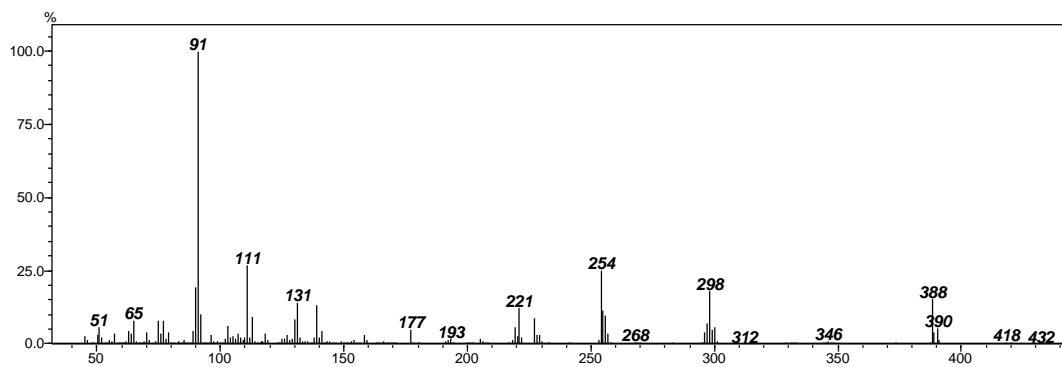
48. ¹H NMR spectra of compound 4m



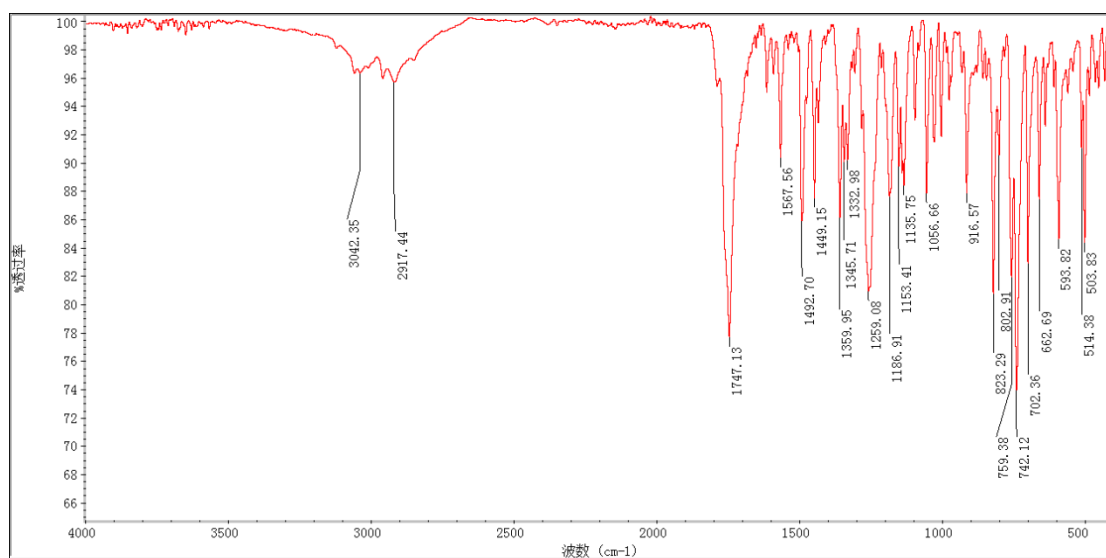
49. ^{13}C NMR spectra of compound **4m**



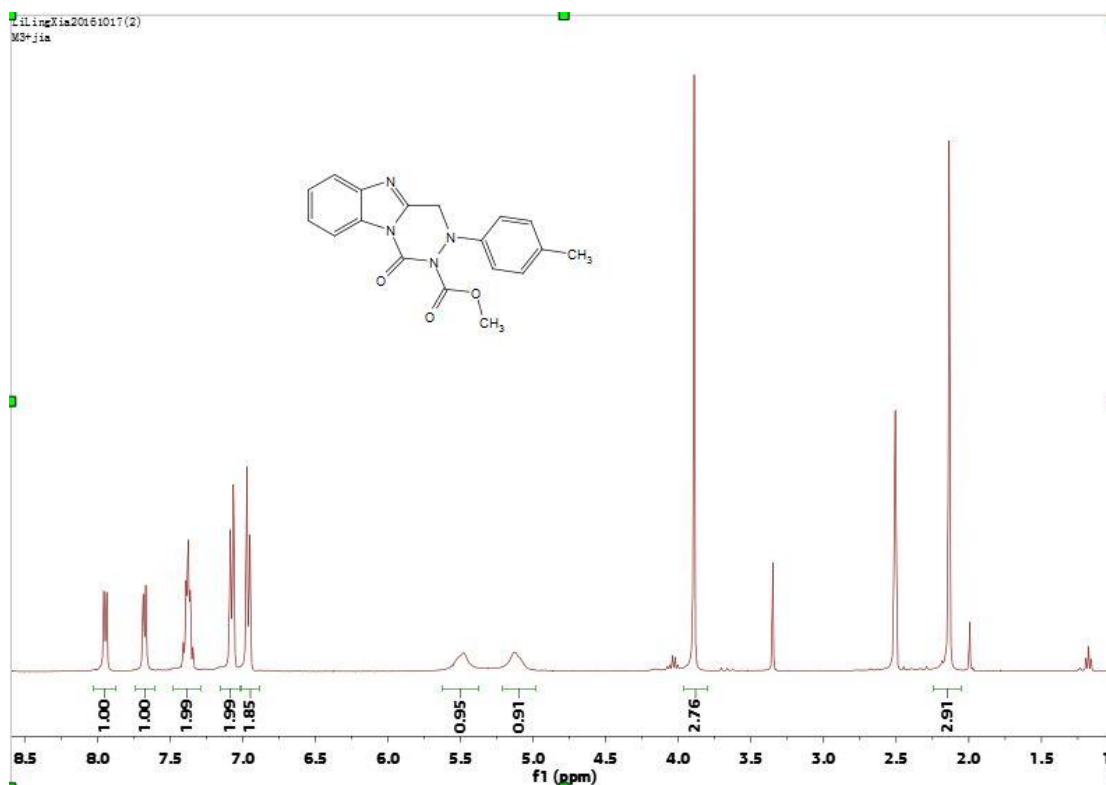
50. EI-MS spectra of compound **4m**



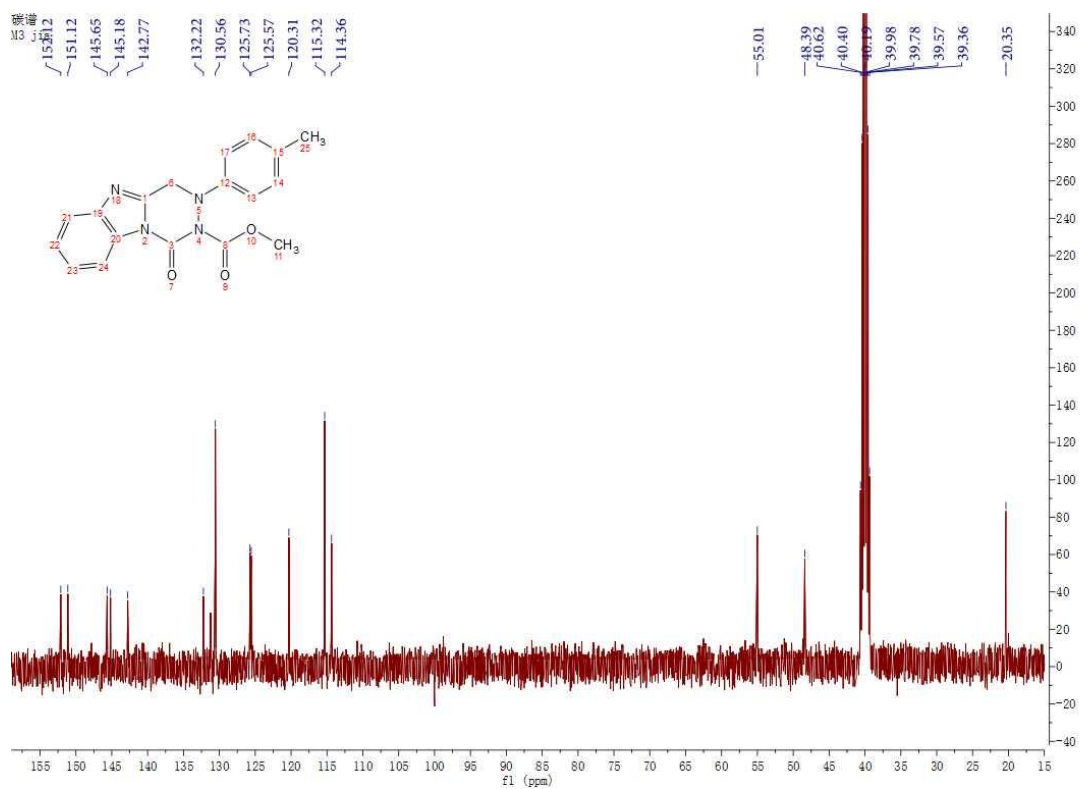
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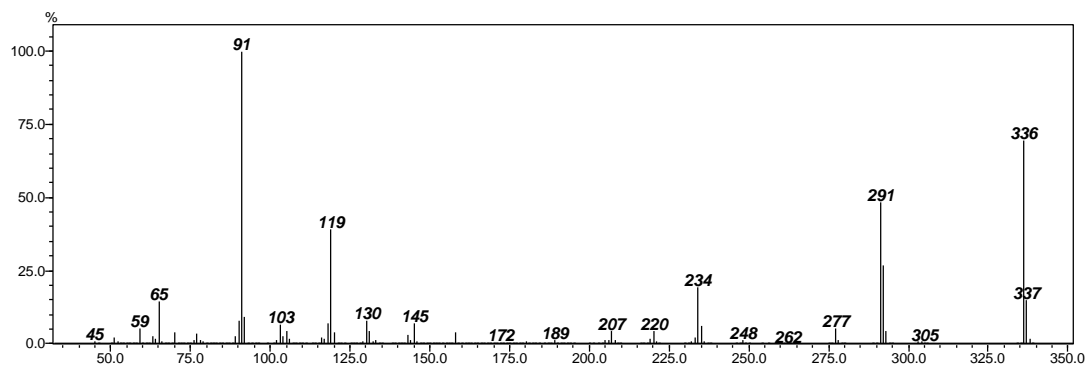
52. ¹H NMR spectra of compound 4n



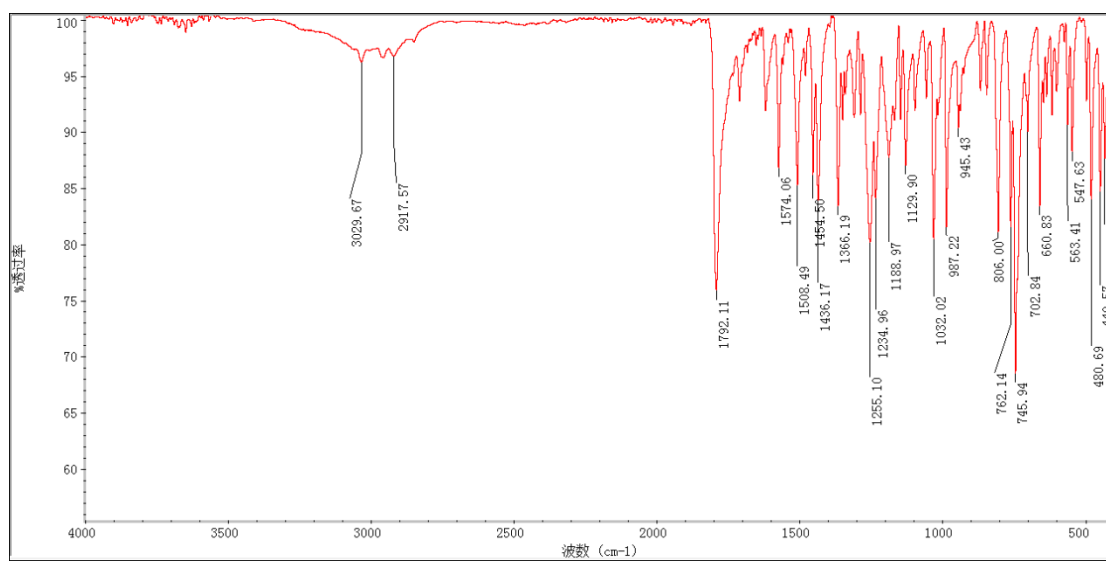
53. ^{13}C NMR spectra of compound **4n**



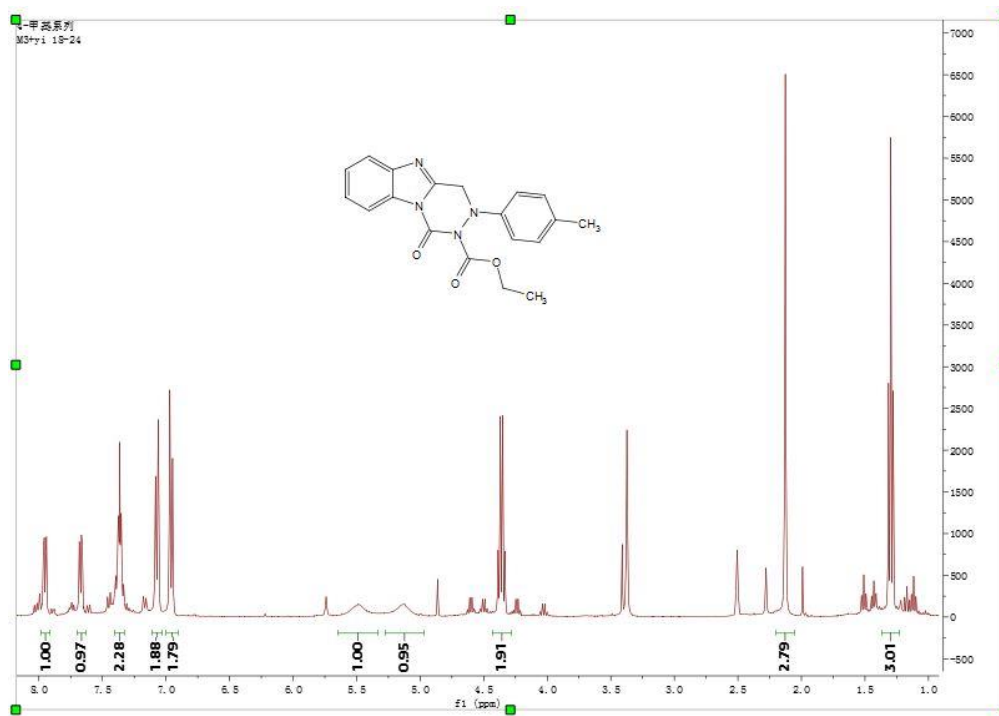
54. EI-MS spectra of compound **4n**



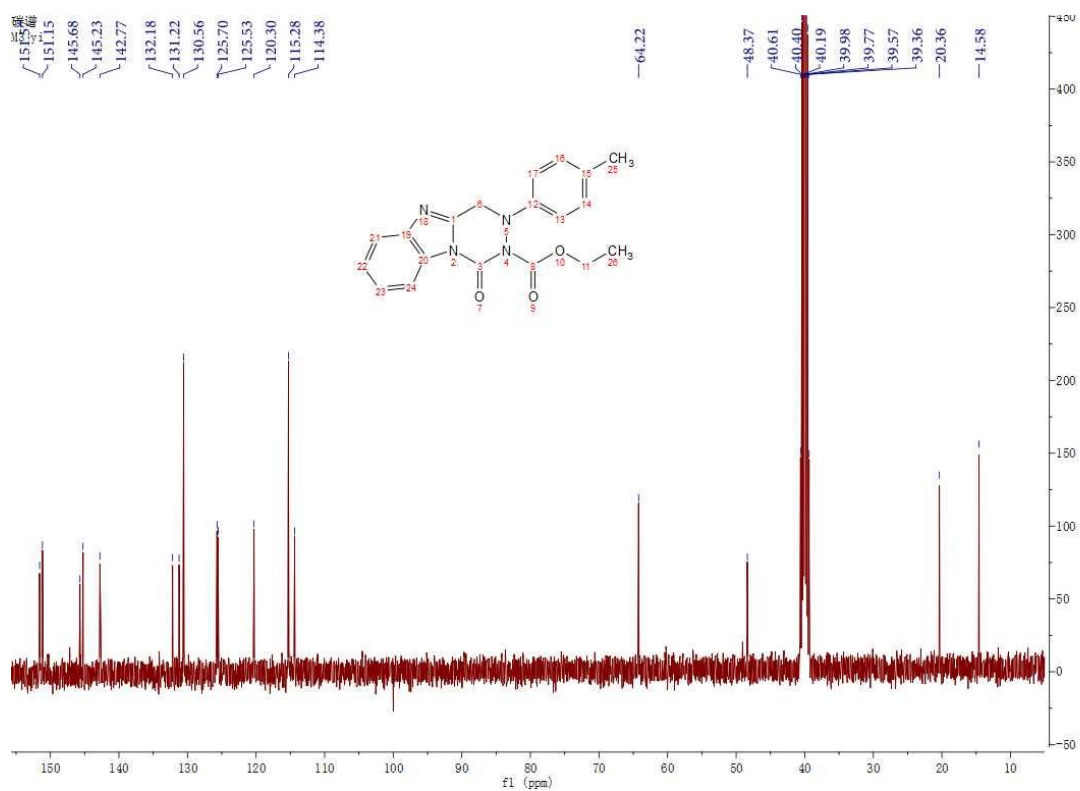
55. FT-IR spectra of compound **4n**



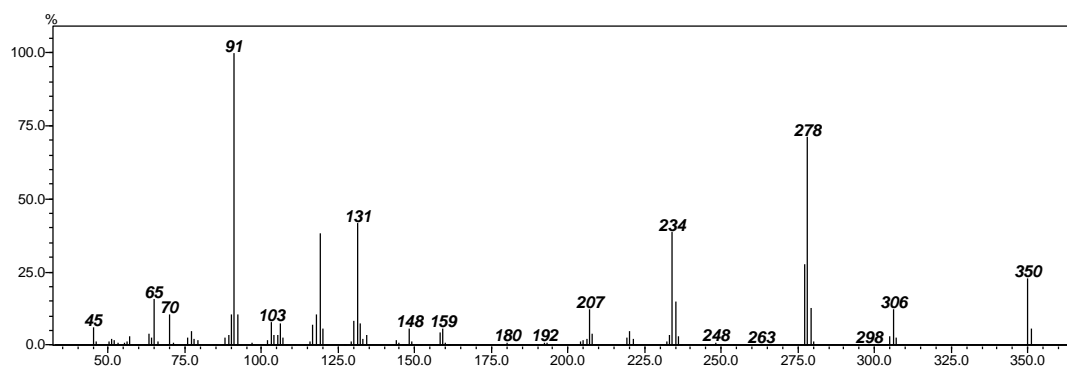
56. ¹H NMR spectra of compound **4o**



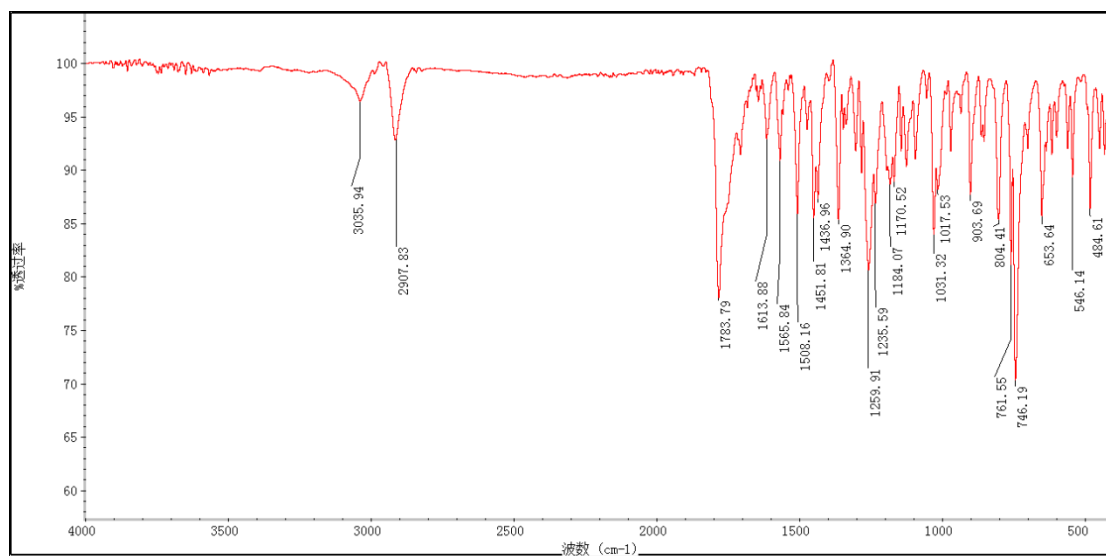
57. ^{13}C NMR spectra of compound **4o**



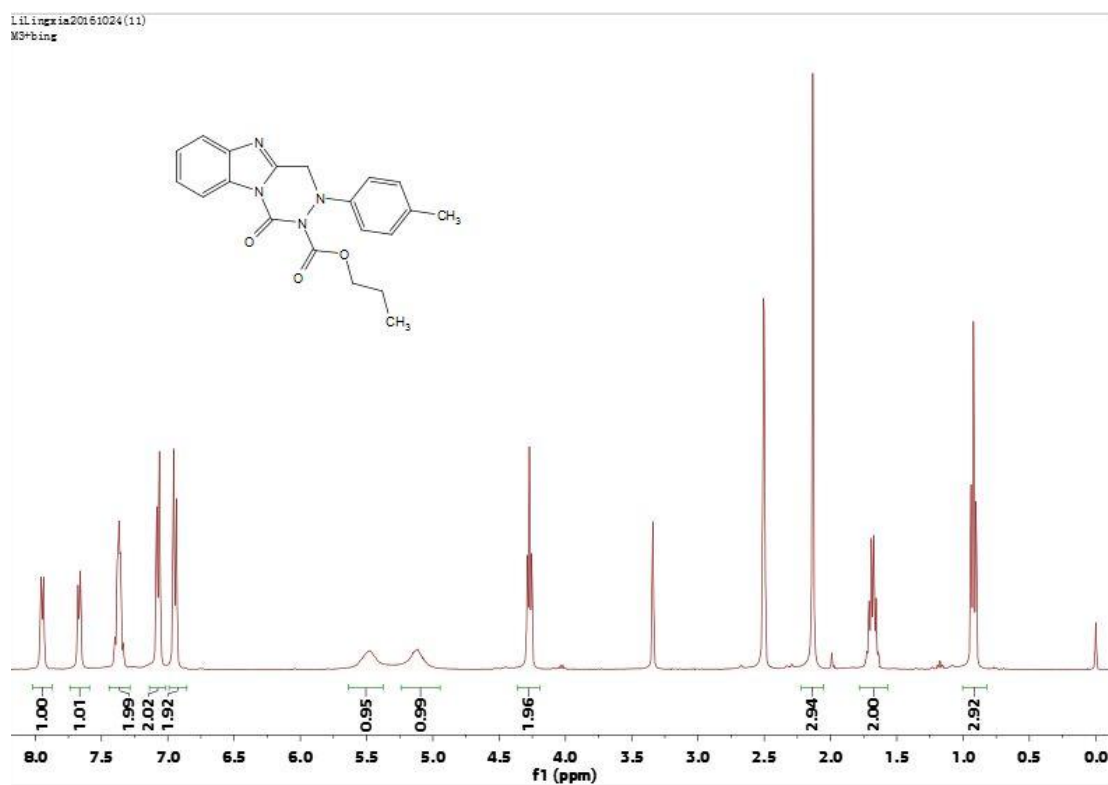
58. EI-MS spectra of compound **4o**



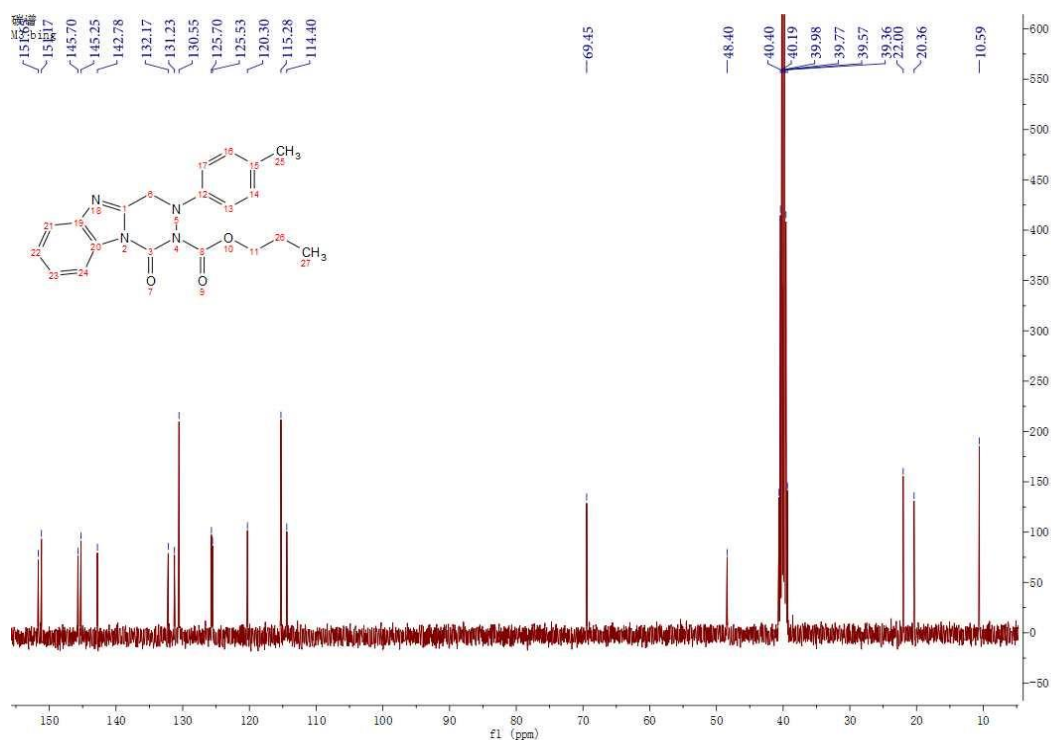
59. FT-IR spectra of compound 4o



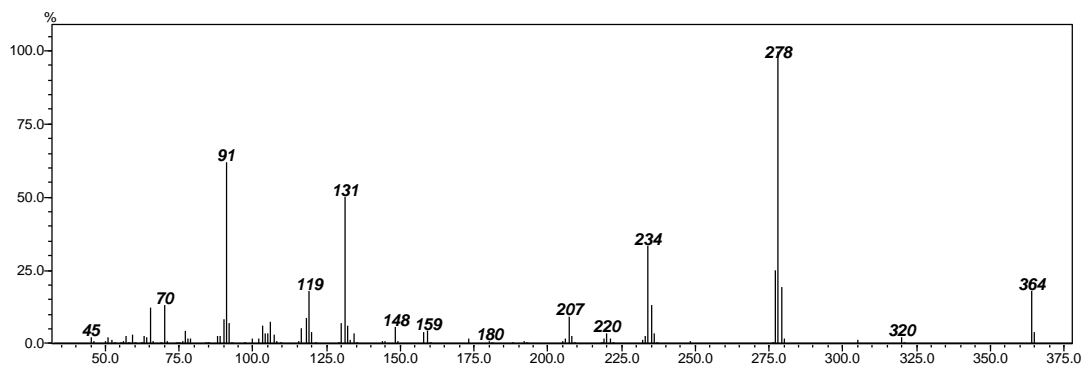
60. ¹H NMR spectra of compound 4p



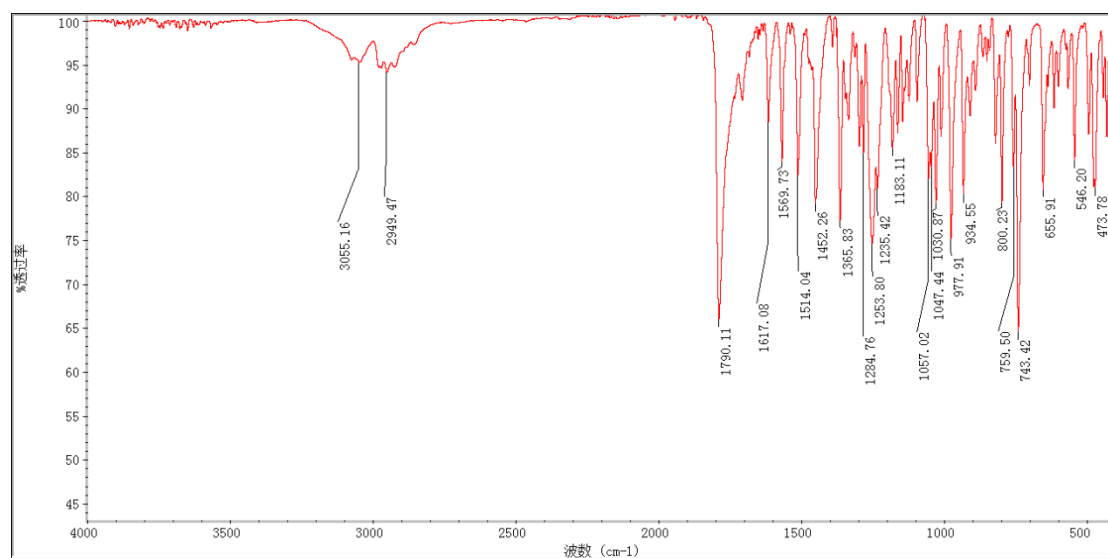
61. ¹³C NMR spectra of compound 4p



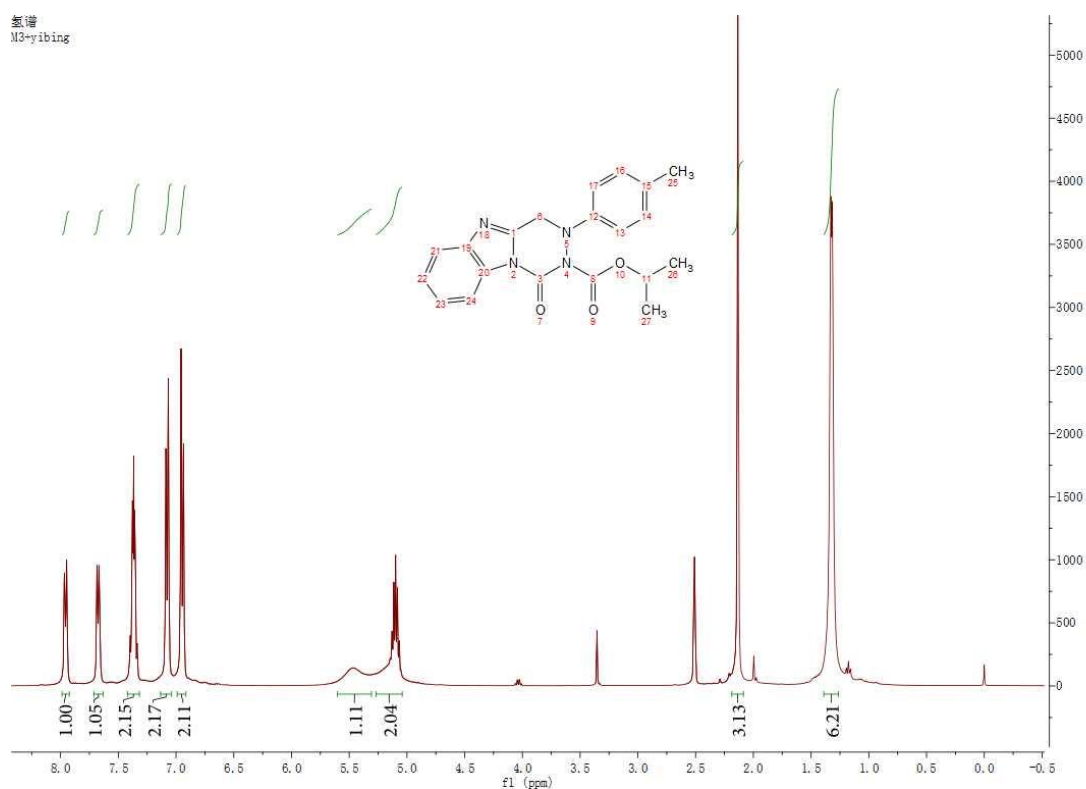
62. EI-MS spectra of compound 4p



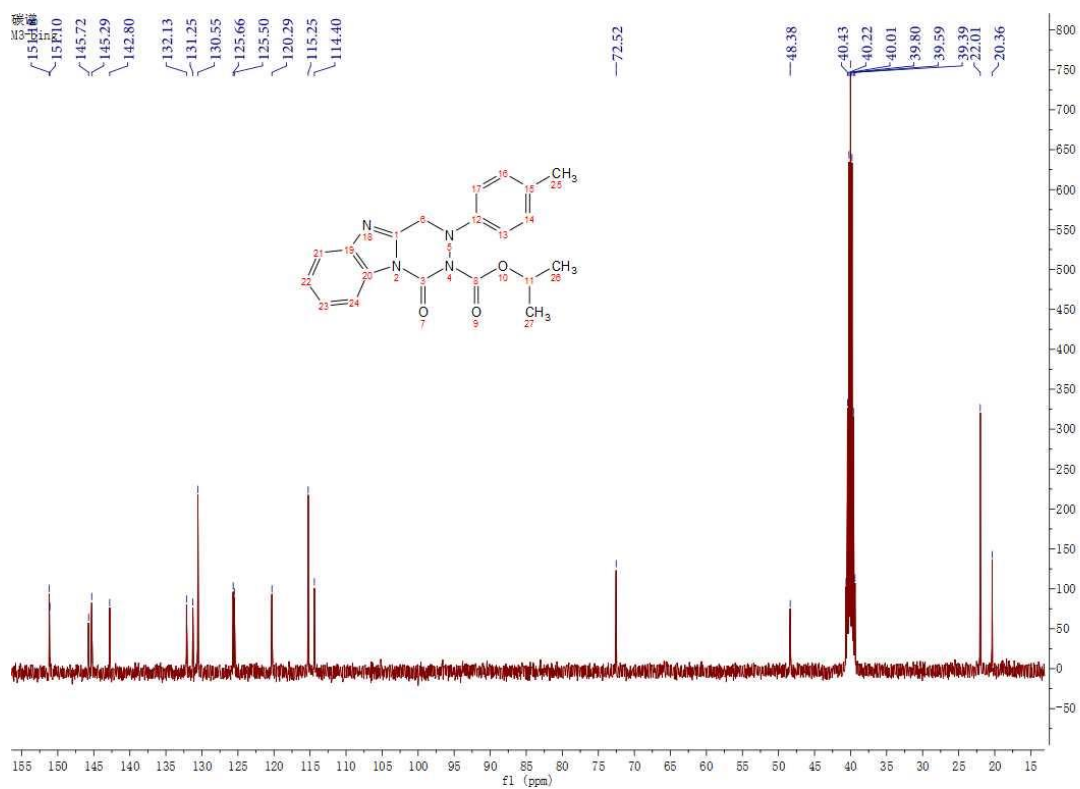
63. FT-IR spectra of compound 4p



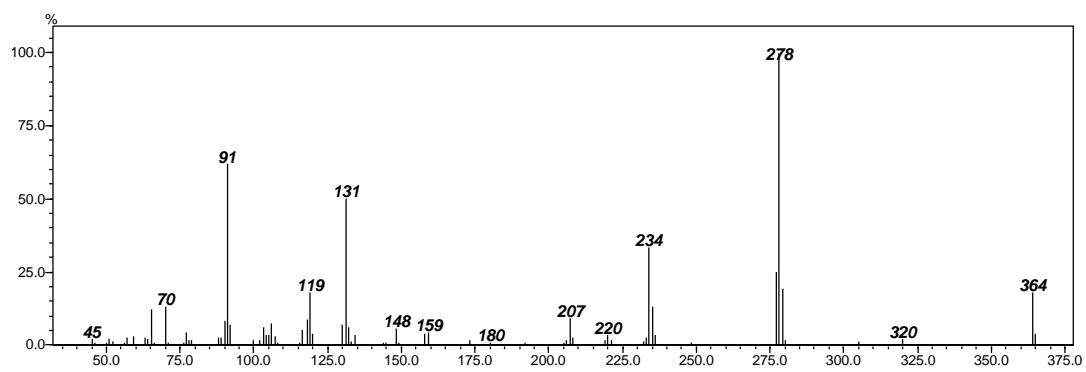
64. ¹H NMR spectra of compound 4q



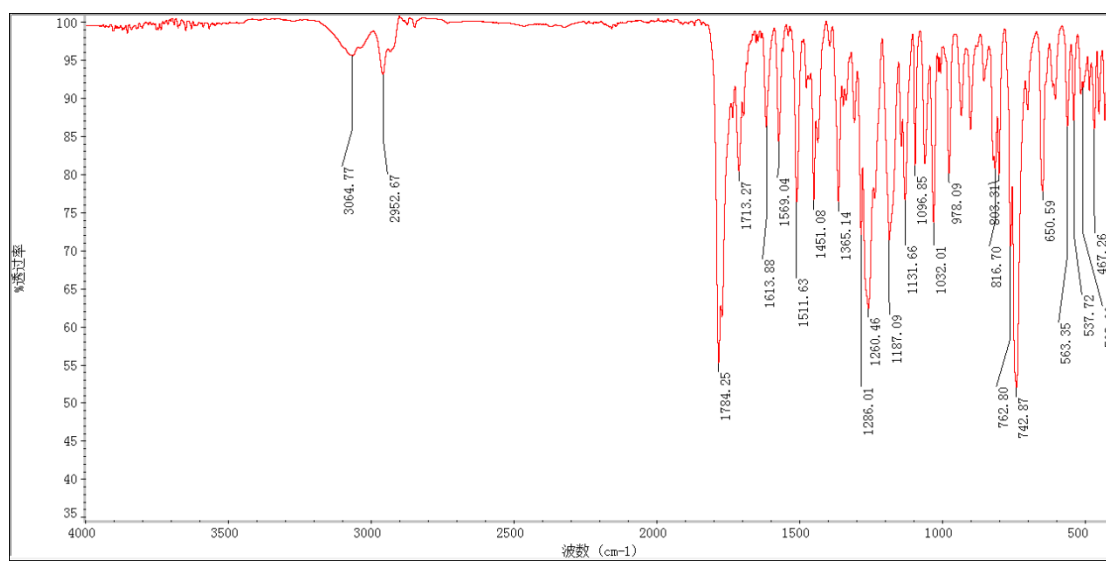
65. ^{13}C NMR spectra of compound **4q**



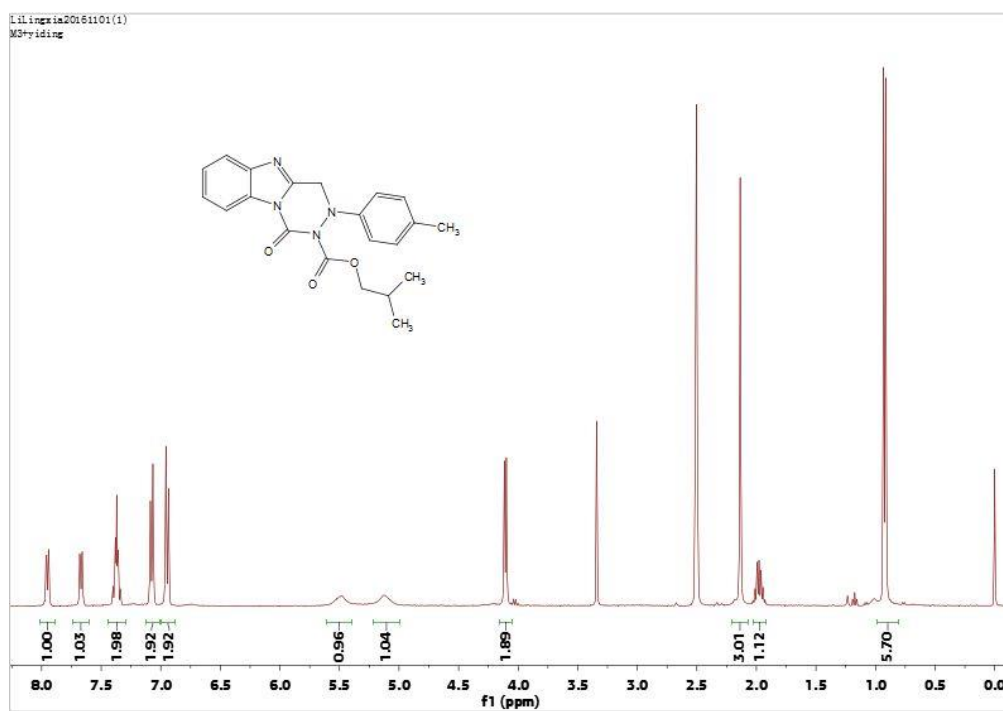
66. EI-MS spectra of compound **4q**



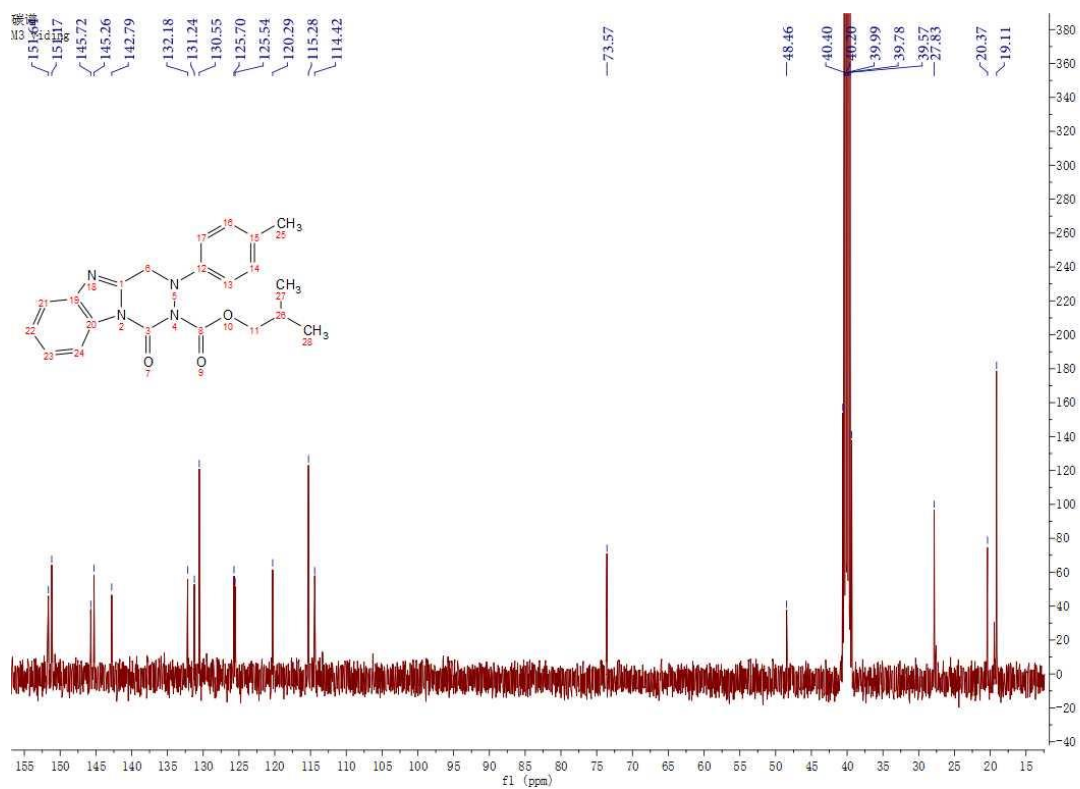
67. FT-IR spectra of compound 4q



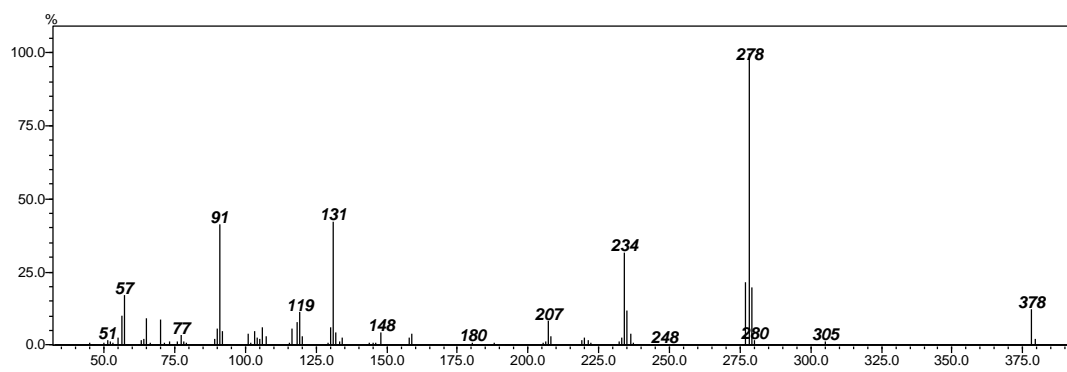
68. ¹H NMR spectra of compound 4r



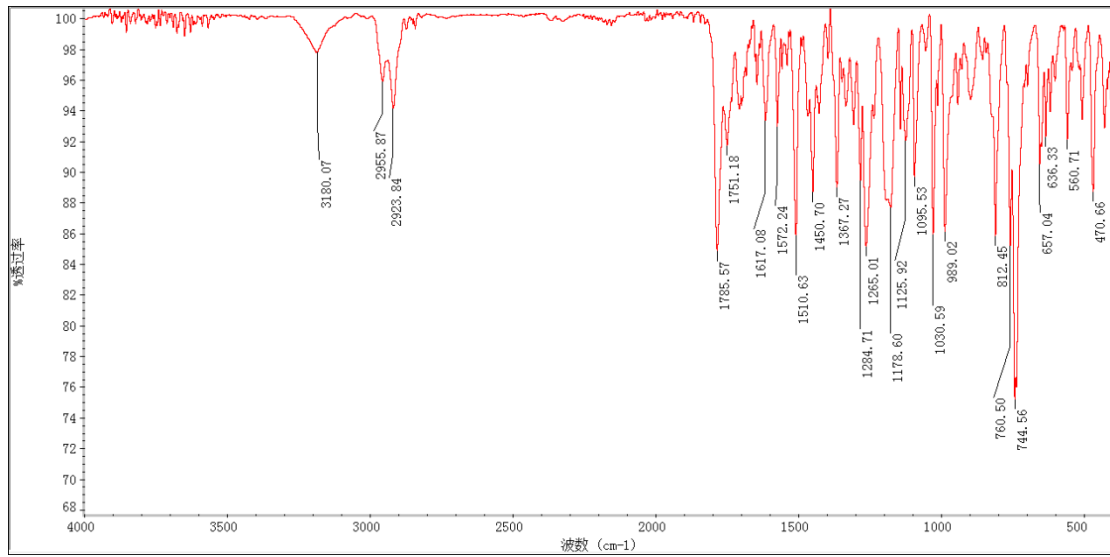
69. ^{13}C NMR spectra of compound **4r**



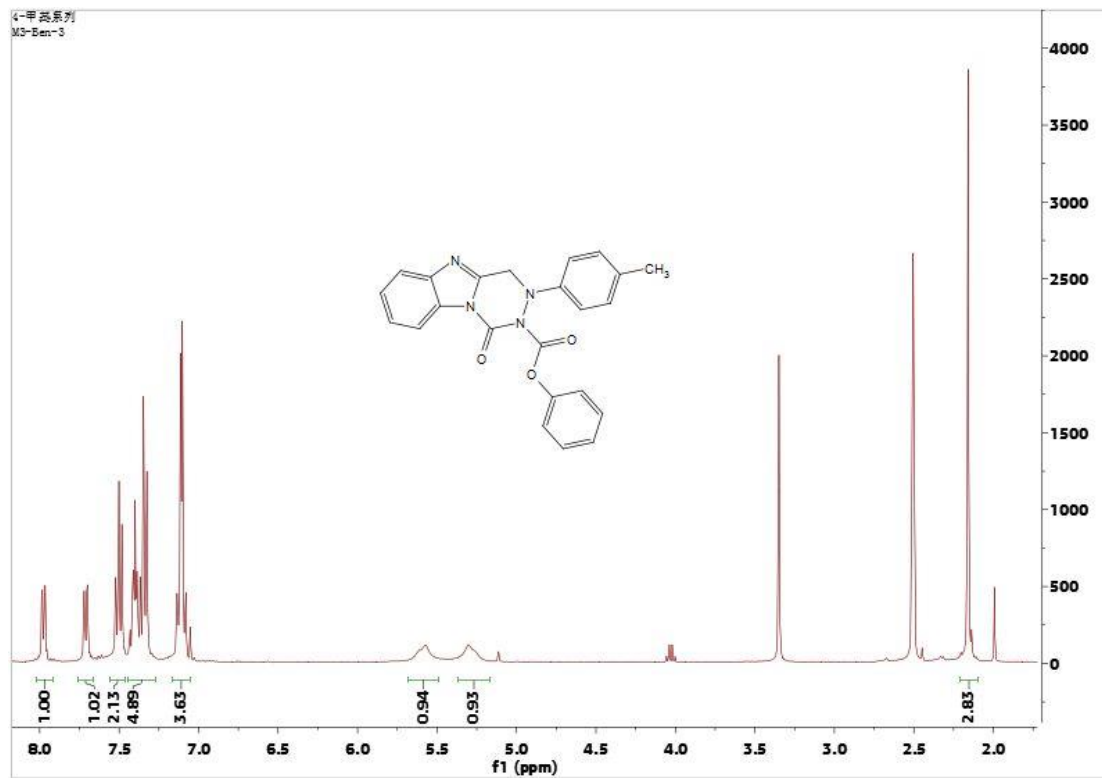
70. EI-MS spectra of compound **4r**



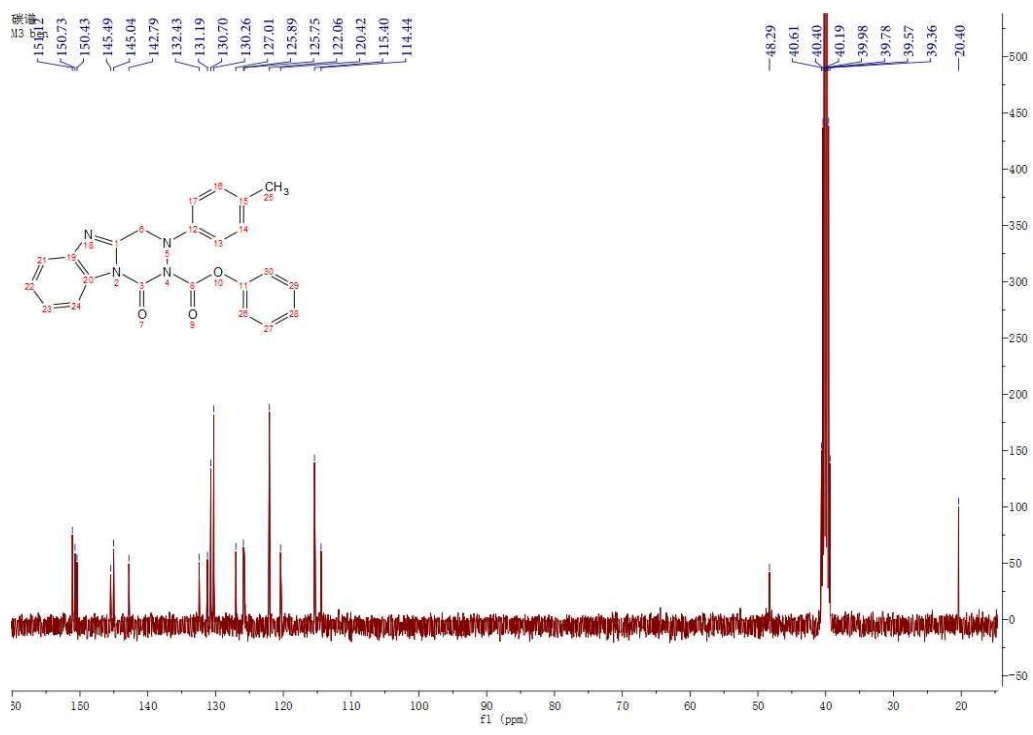
71. FT-IR spectra of compound **4r**



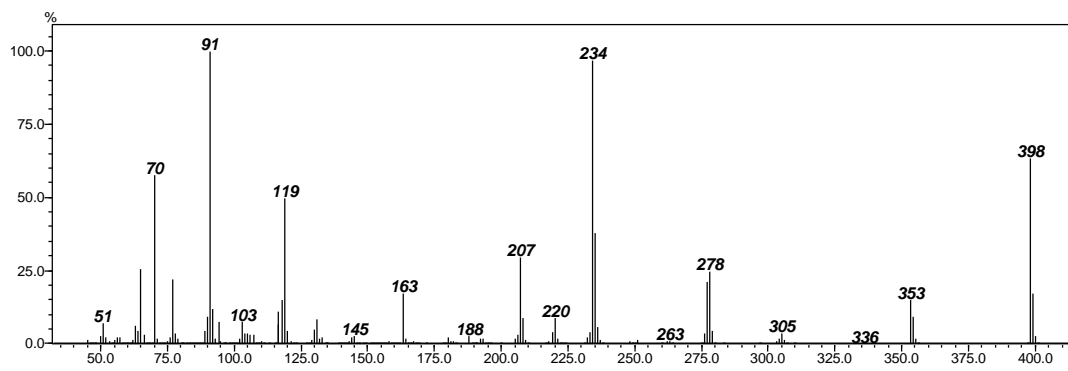
72. ¹H NMR spectra of compound 4s



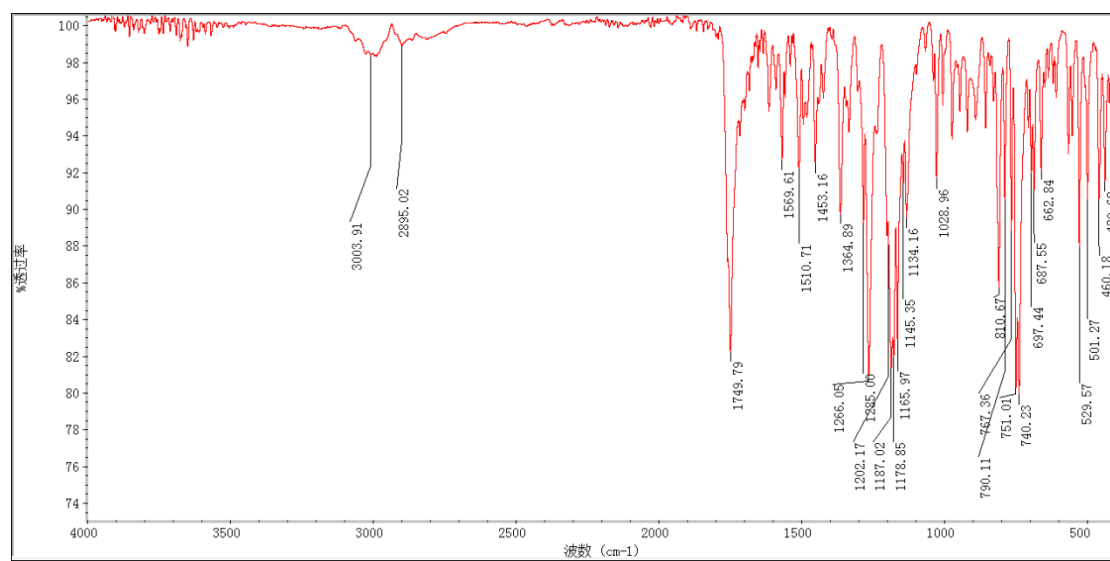
73. ¹³C NMR spectra of compound 4s



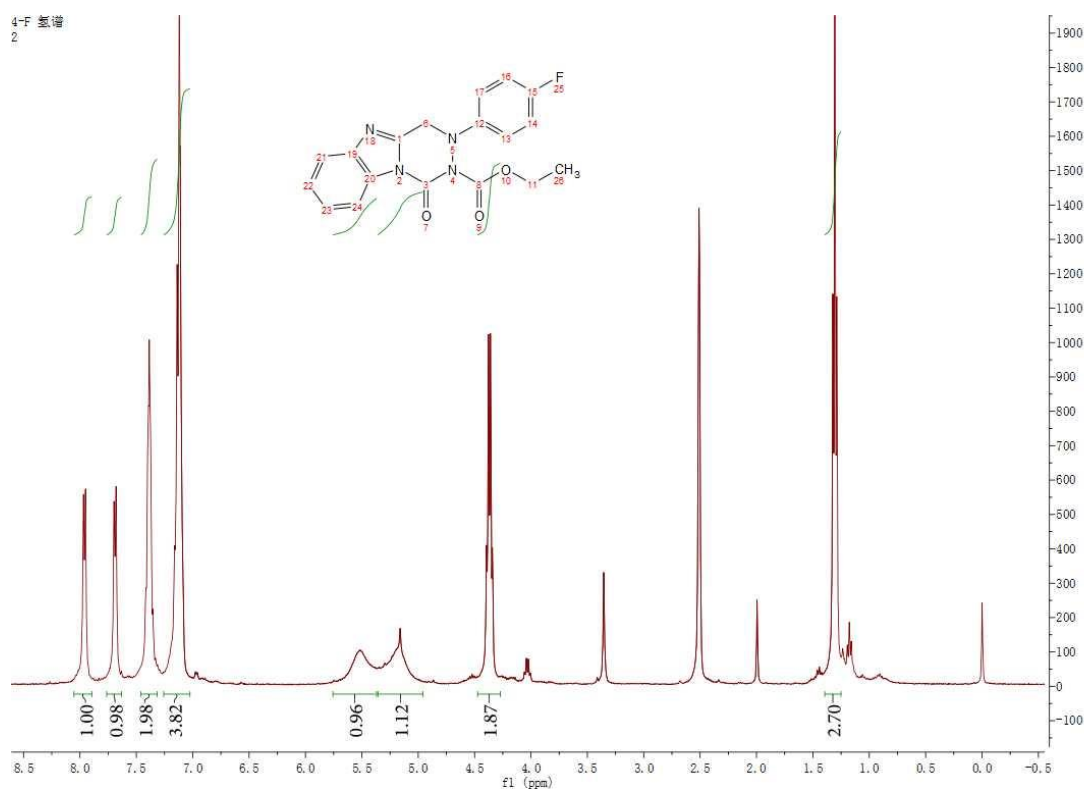
74. EI-MS spectra of compound 4s



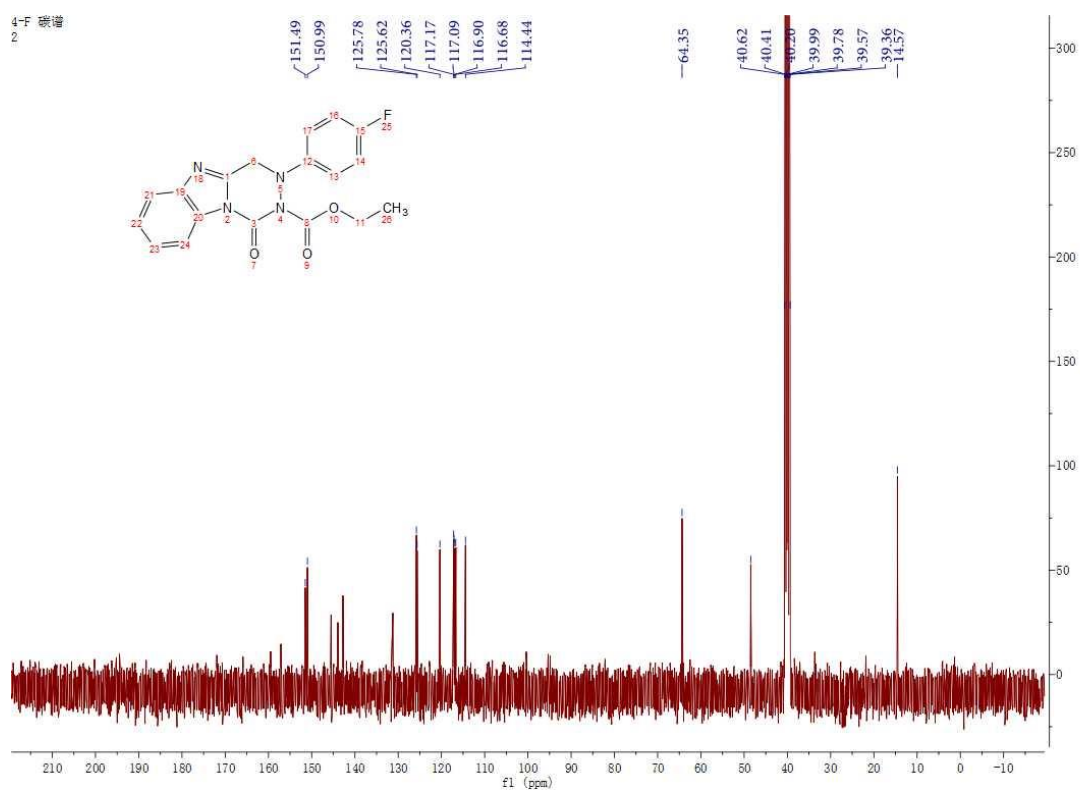
75. FT-IR spectra of compound 4s



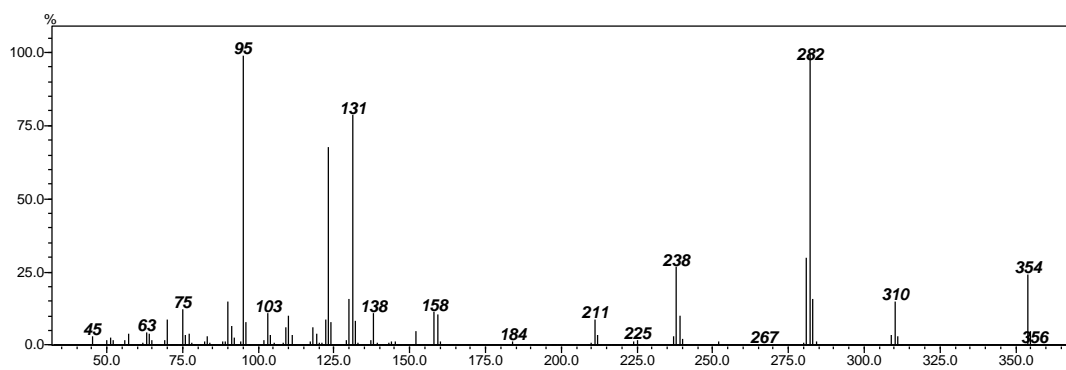
76. ¹H NMR spectra of compound 4t



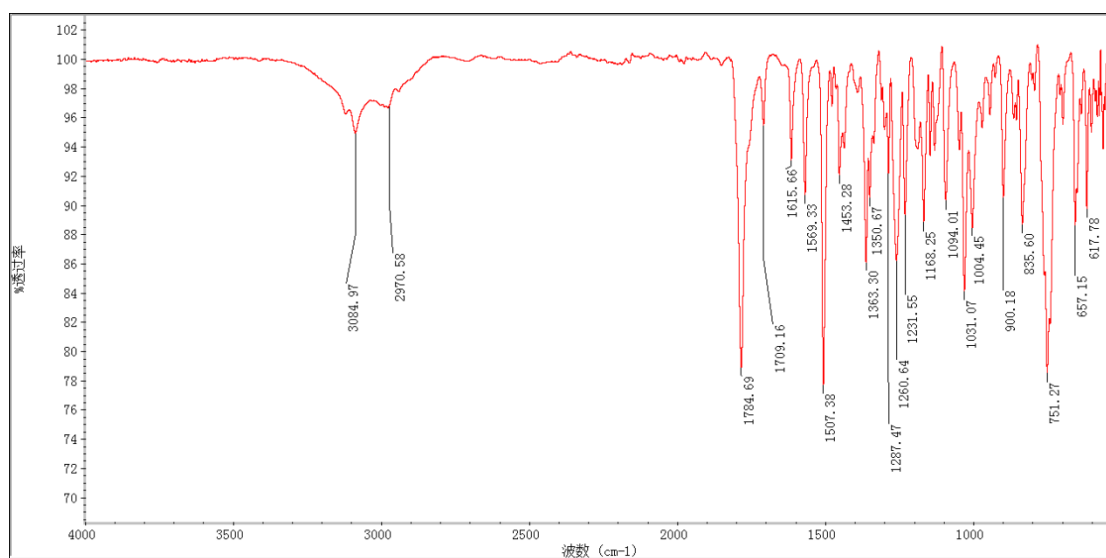
77. ^{13}C NMR spectra of compound **4t**



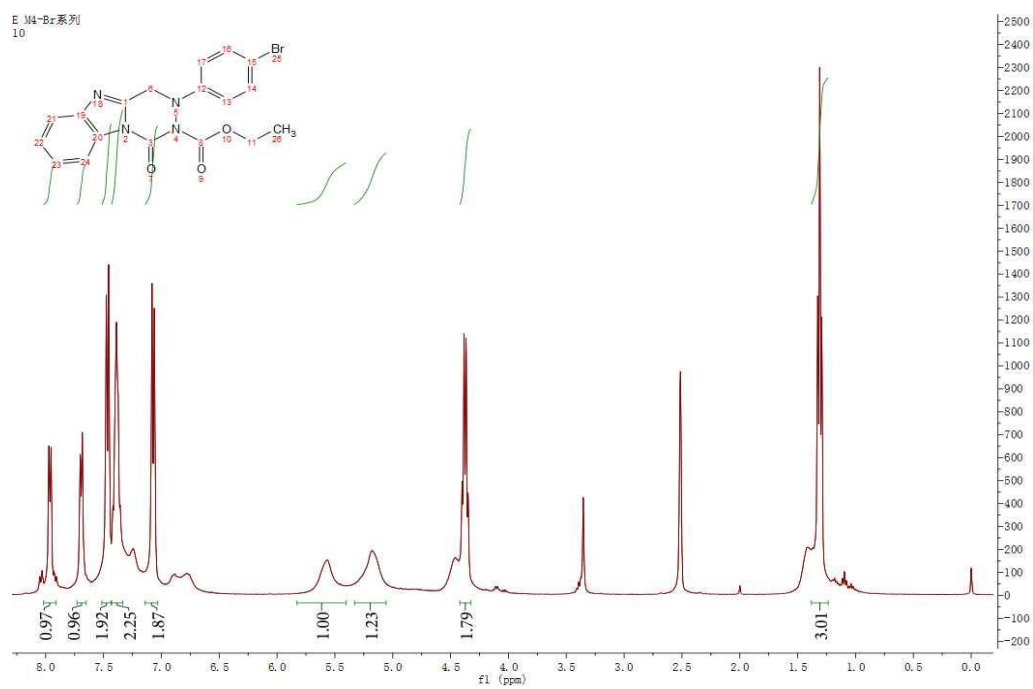
78. EI-MS spectra of compound **4t**



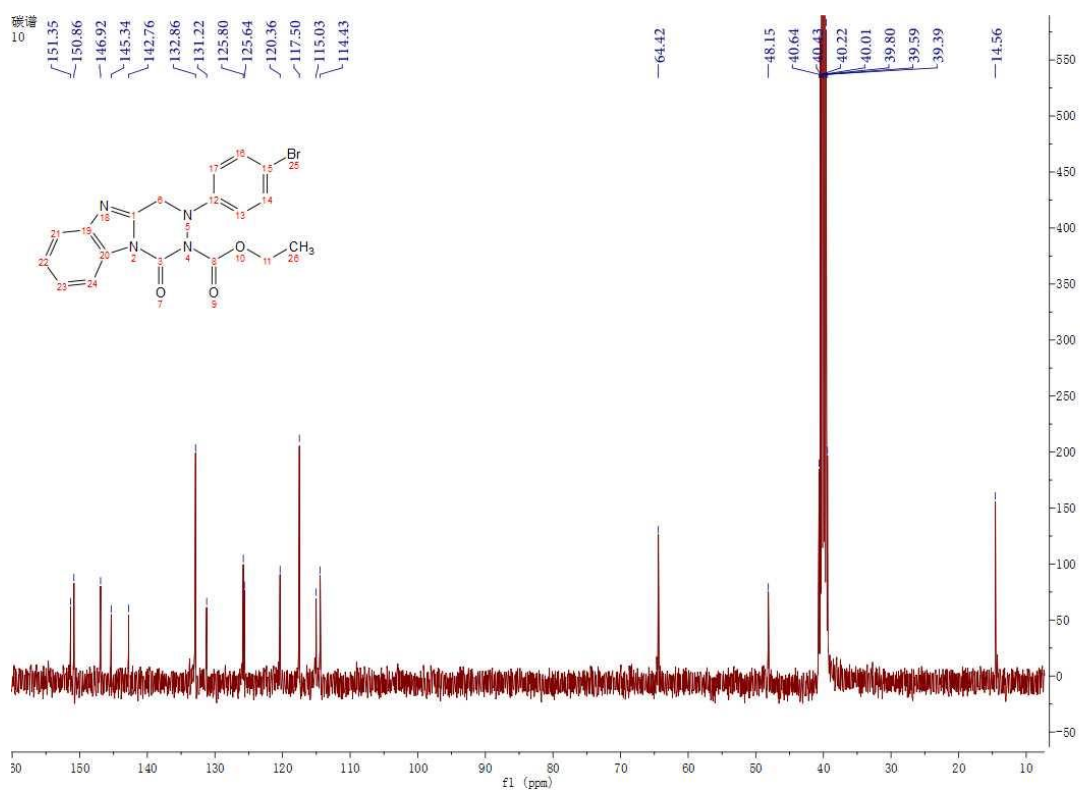
79. FT-IR spectra of compound **4t**



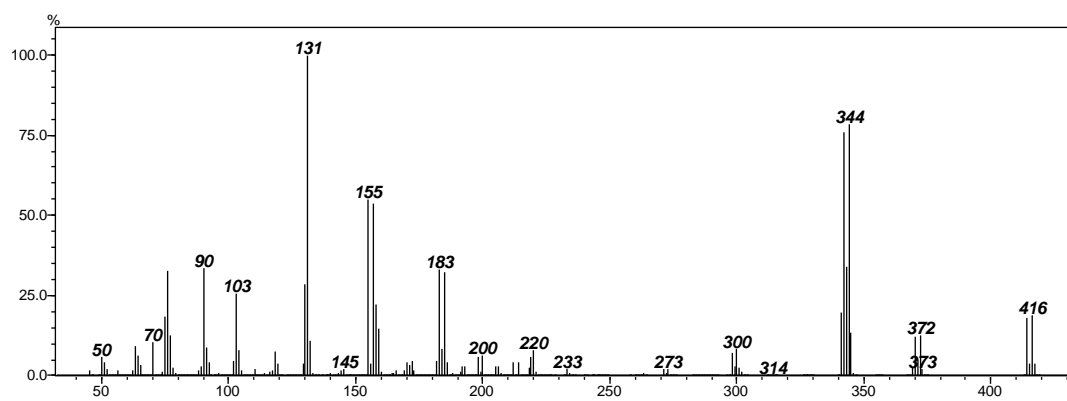
80. ¹H NMR spectra of compound **4u**



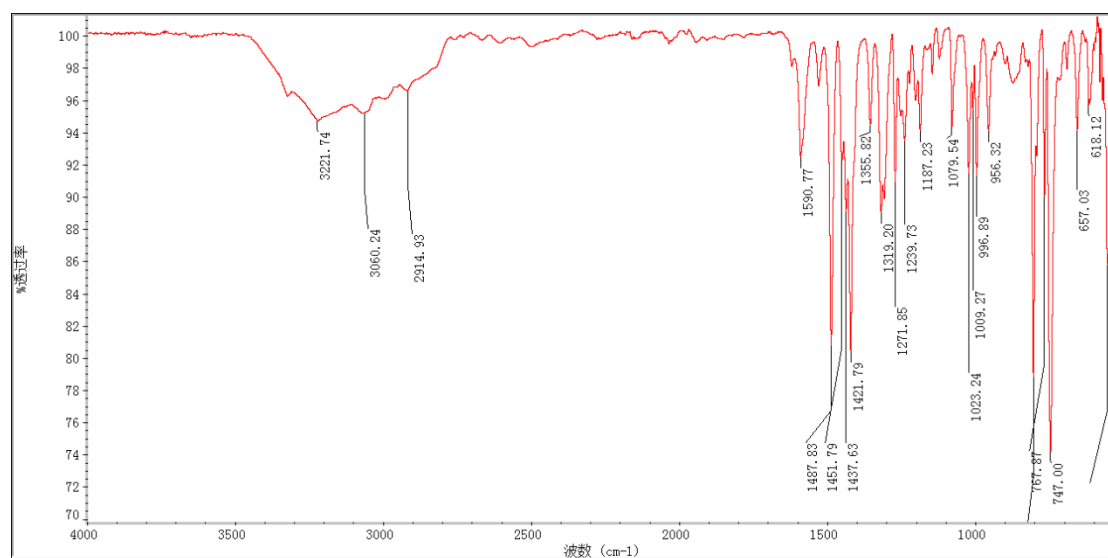
81. ^{13}C NMR spectra of compound **4u**



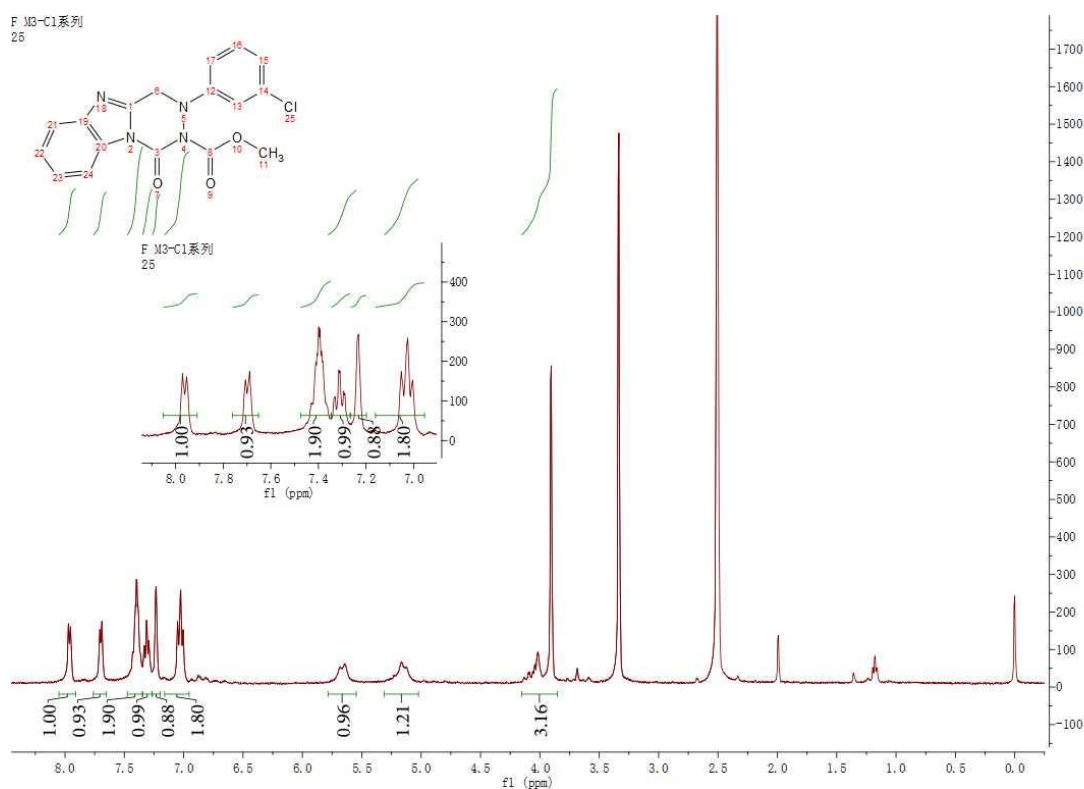
82. EI-MS spectra of compound **4u**



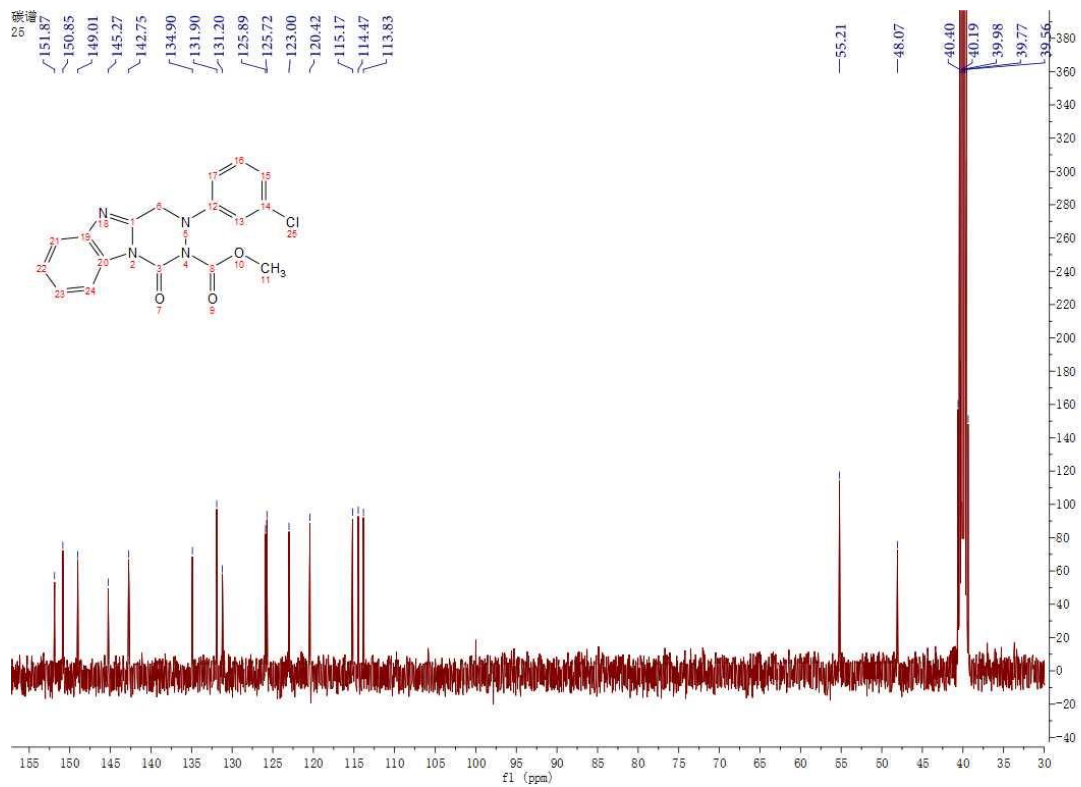
83. FT-IR spectra of compound 4u



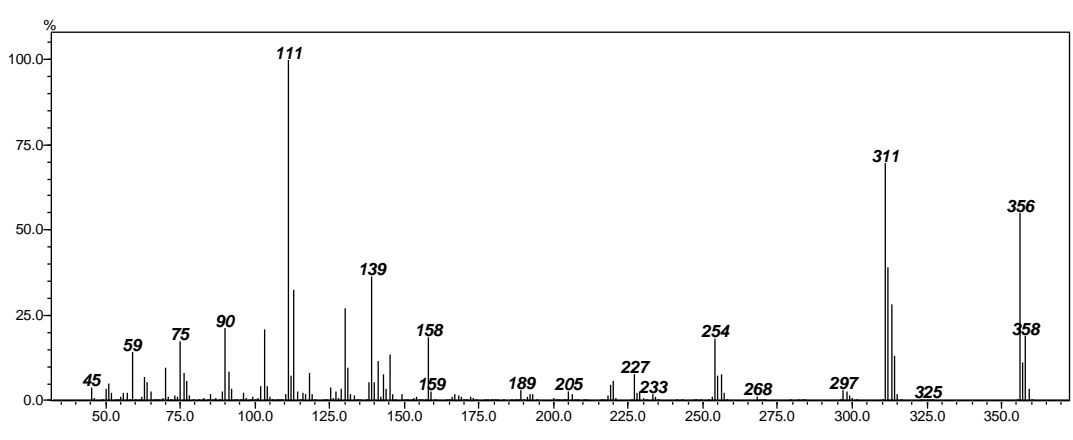
84. ¹H NMR spectra of compound 4v



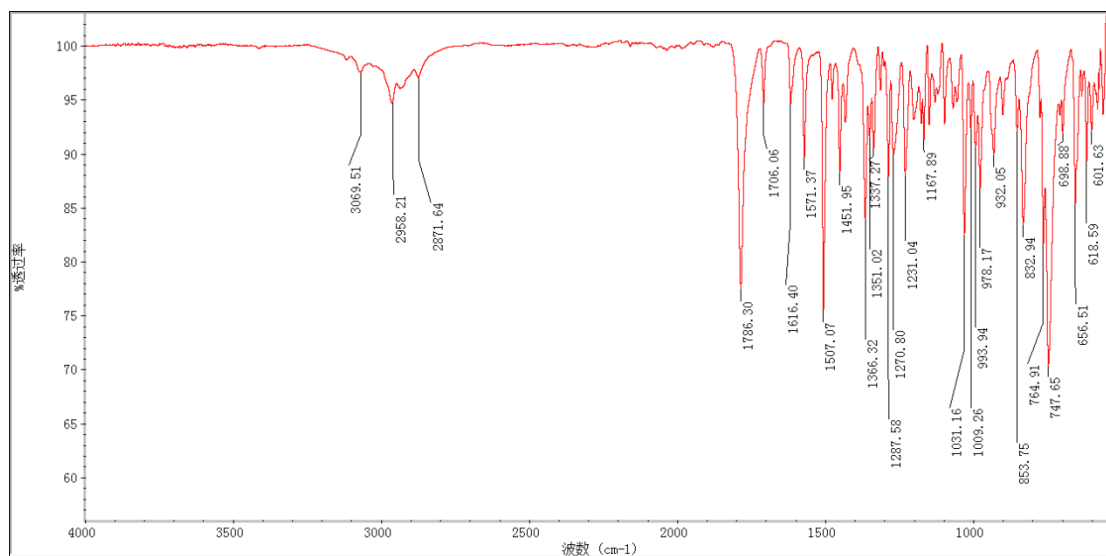
85. ¹³C NMR spectra of compound 4v



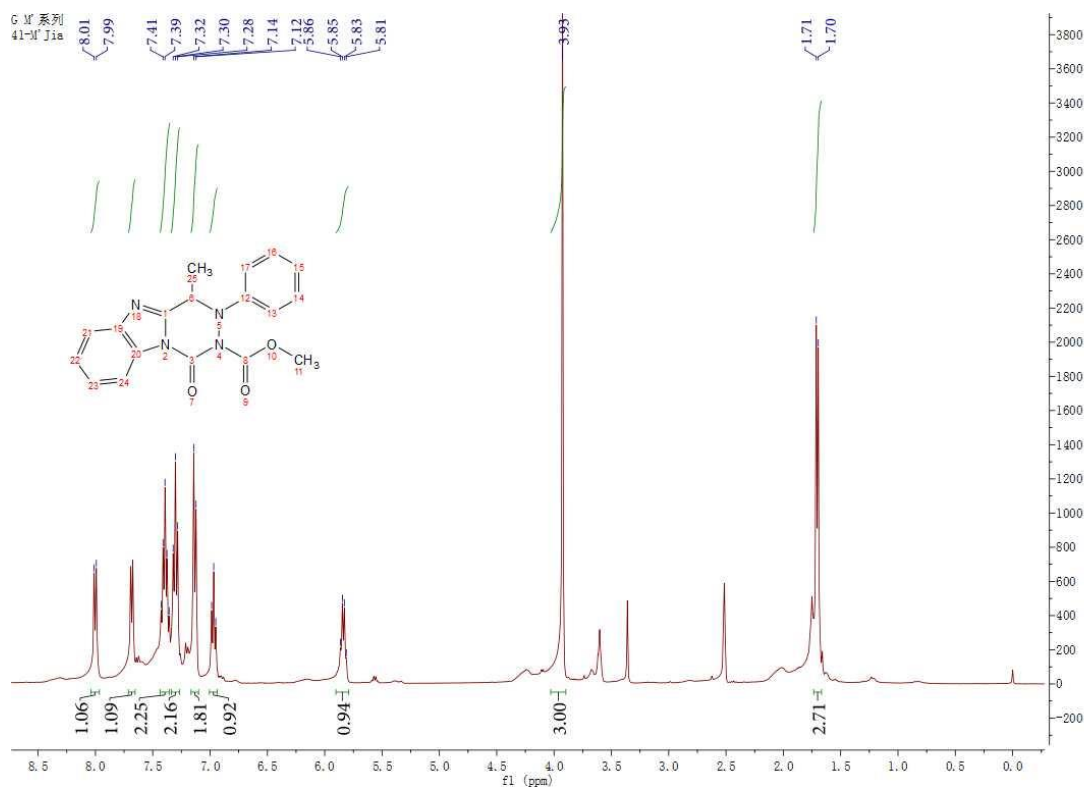
86. EI-MS spectra of compound 4v



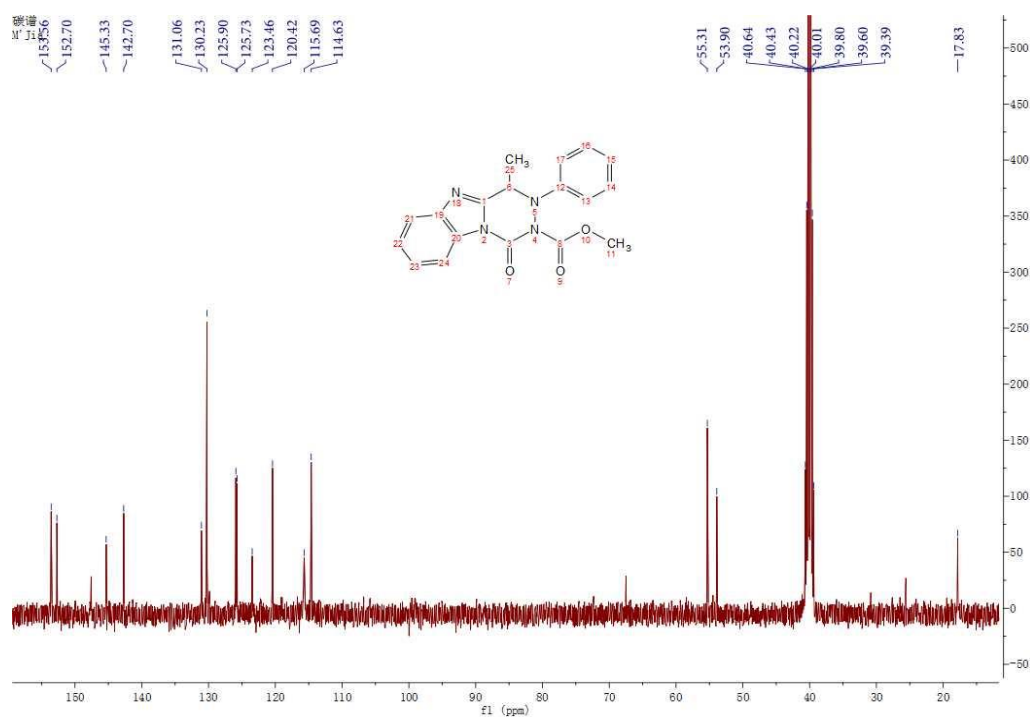
87. FT-IR spectra of compound 4v



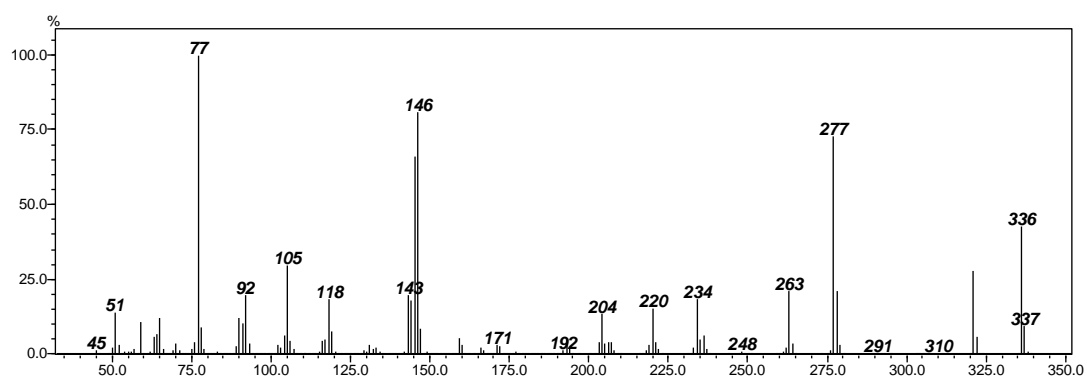
88. ¹H NMR spectra of compound 4w



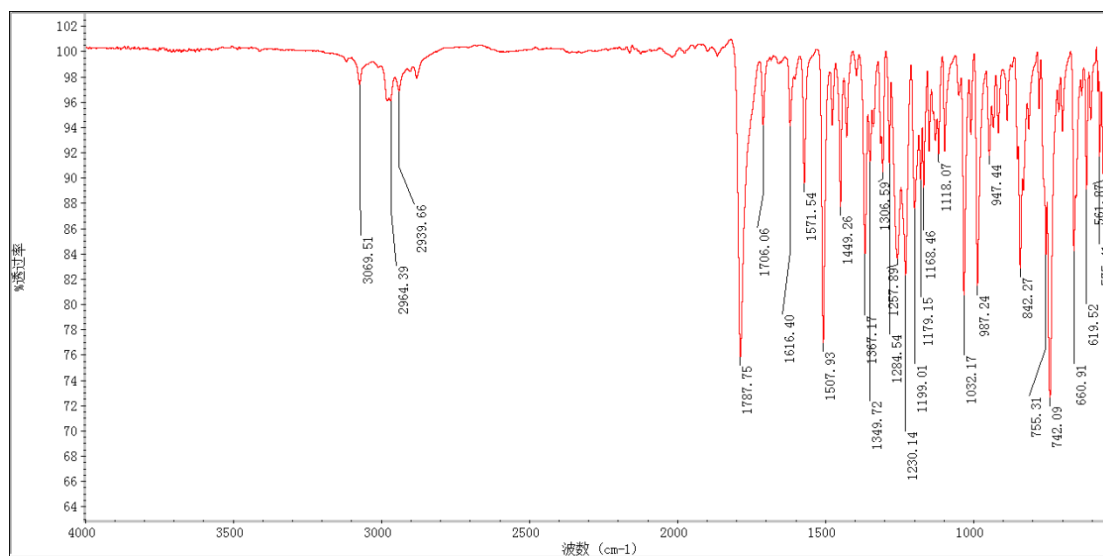
89. ^{13}C NMR spectra of compound 4w



90. EI-MS spectra of compound 4w



91. FT-IR spectra of compound 4w



92. Selected geometric parameters of compound 4n.

Bond Lengths			
Bond	Dist. (Å)	Bond	Dist. (Å)
O1–C9	1.202(2)	C1–C2	1.396(3)
O2–C10	1.190(2)	C1–C6	1.397(3)
O3–C10	1.327(2)	C2–C3	1.377(3)
O3–C11	1.460(3)	C3–C4	1.395(3)
N1–C1	1.410(2)	C4–C5	1.390(3)
N1–C7	1.293(2)	C5–C6	1.391(3)
N2–C6	1.406(2)	C7–C8	1.490(2)
N2–C7	1.401(2)	C12–C13	1.390(3)
N2–C9	1.402(2)	C12–C17	1.398(3)
N3–N4	1.423(2)	C13–C14	1.394(3)
N3–C8	1.471(2)	C14–C15	1.390(3)
N3–C12	1.440(2)	C15–C16	1.390(3)
N4–C9	1.408(2)	C16–C17	1.389(3)
N4–C10	1.417(2)	C15–C18	1.513(3)
Bond Angles			
Angle	(°)	Angle	(°)
C10–O3–C11	116.59(16)	N1–C7–N2	114.06(13)
C1–N1–C7	104.51(14)	N1–C7–C8	131.16(14)

C6–N2–C7	105.60(13)	N2–C7–C8	114.78(14)
C6–N2–C9	128.08(13)	N3–C8–C7	107.83(12)
C7–N2–C9	125.77(13)	O1–C9–N2	122.52(15)
N4–N3–C8	109.18(12)	O1–C9–N4	125.60(17)
N4–N3–C12	112.75(12)	N2–C9–N4	111.86(13)
C8–N3–C12	118.51(13)	O2–C10–O3	126.63(17)
N3–N4–C9	119.26(14)	O2–C10–N4	123.85(16)
N3–N4–C10	118.07(13)	O3–C10–N4	109.53(14)
C9–N4–C10	122.54(13)	N3–C12–C13	121.63(15)
N1–C1–C2	128.83(17)	N3–C12–C17	120.24(14)
N1–C1–C6	111.04(15)	C13–C12–C17	118.00(14)
C2–C1–C6	120.12(16)	C12–C13–C14	120.41(17)
C1–C2–C3	117.69(19)	C13–C14–C15	122.23(18)
C2–C3–C4	121.5(2)	C14–C15–C16	116.66(16)
C3–C4–C5	122.05(18)	C14–C15–C18	122.36(16)
C4–C5–C6	115.81(18)	C16–C15–C18	120.98(17)
N2–C6–C1	104.76(13)	C15–C16–C17	122.10(17)
N2–C6–C5	132.38(17)	C12–C17–C16	120.59(16)
C1–C6–C5	122.84(17)		

93. Hydrogen bonding data for compound **4n** (Å, °).

D–H...A	d(D–H)	d(H...A)	d(D...A)	∠(DHA)
C8–H8B...O3 ^a	0.9700	2.500	3.385(3)	152.00
C17–H17...N4	0.9300	2.4500	2.761(3)	100

Symmetry code for compound **4n**: (a) $-x, -y, -z$.

94. Selected distances between hydrogen and carbon atoms for compound **4n** (Å).

Bond	Dist. (Å)	Bond	Dist. (Å)
H3...C12	3.4404(23)	H4...C12	3.5022(26)
H3...C13	3.8177(27)	H4...C13	3.1355(26)
H3...C14	3.8124(31)	H4...C14	3.1414(26)
H3...C15	3.4249(26)	H4...C15	3.5343(29)
H3...C16	2.9135(24)	H4...C16	3.8278(32)

H3...C17	2.8950(24)	H4...C17	3.8172(29)
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