

Zirconium Oxide Nano-Catalyzed Synthesis of Pharmacologically Important Bis(indolyl)methanes: A Highly Efficient and Mild Approach

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Supporting Information

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SPECTRA

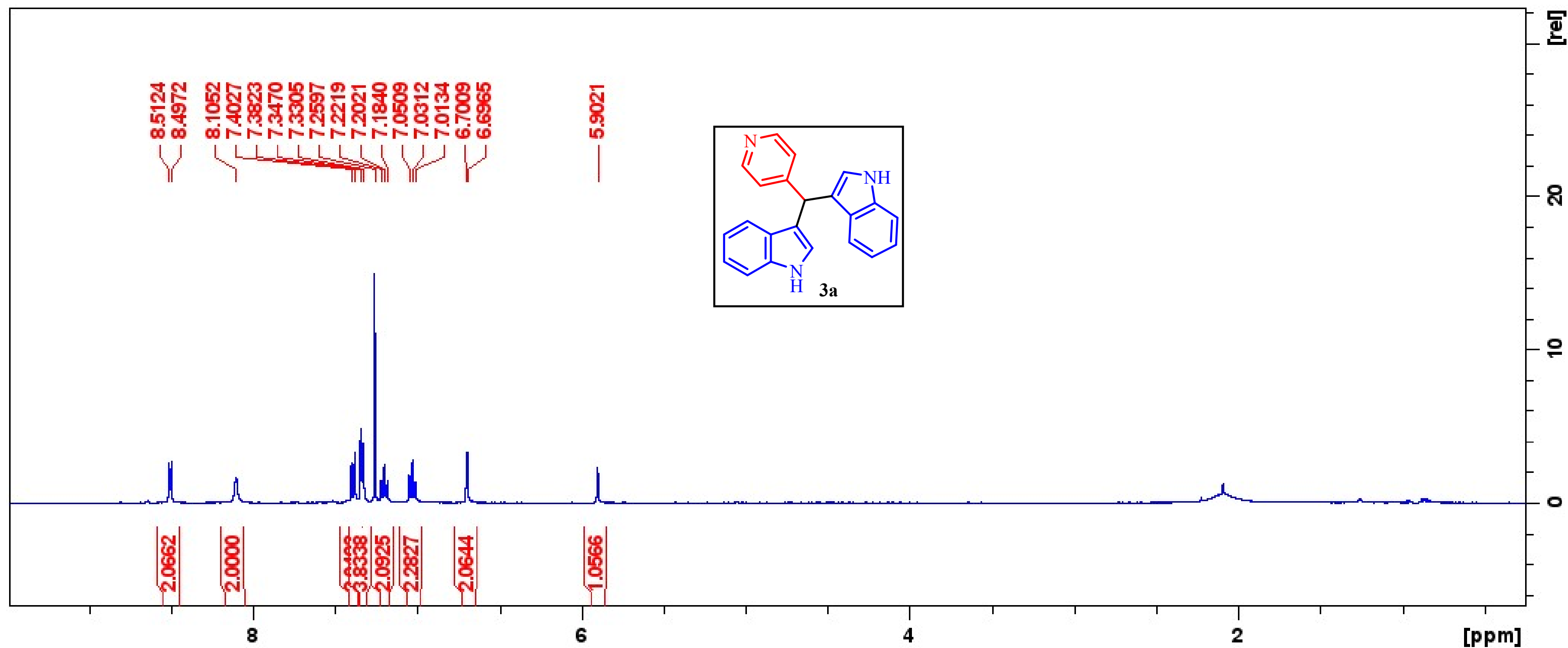


Figure 1. ¹H NMR spectrum of compound **3a**

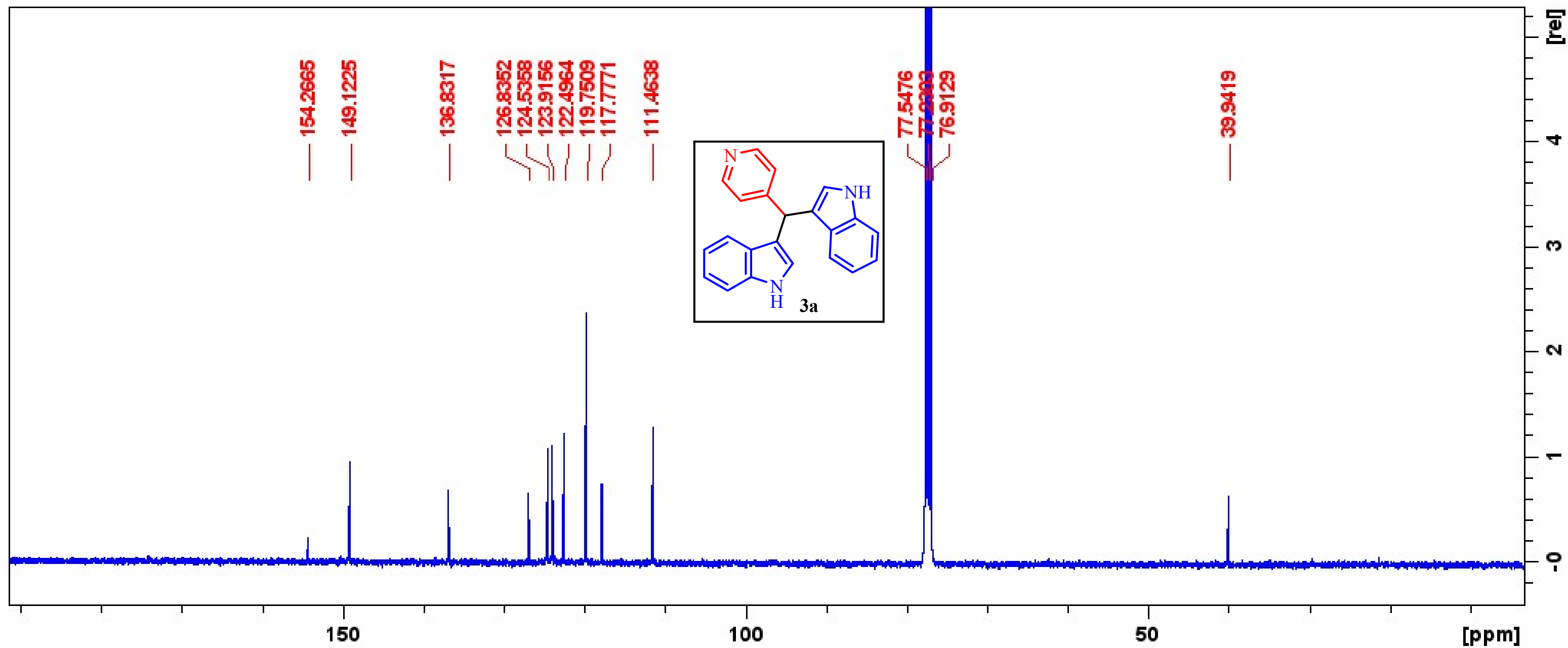


Figure 2. ¹³C NMR spectrum of compound **3a**

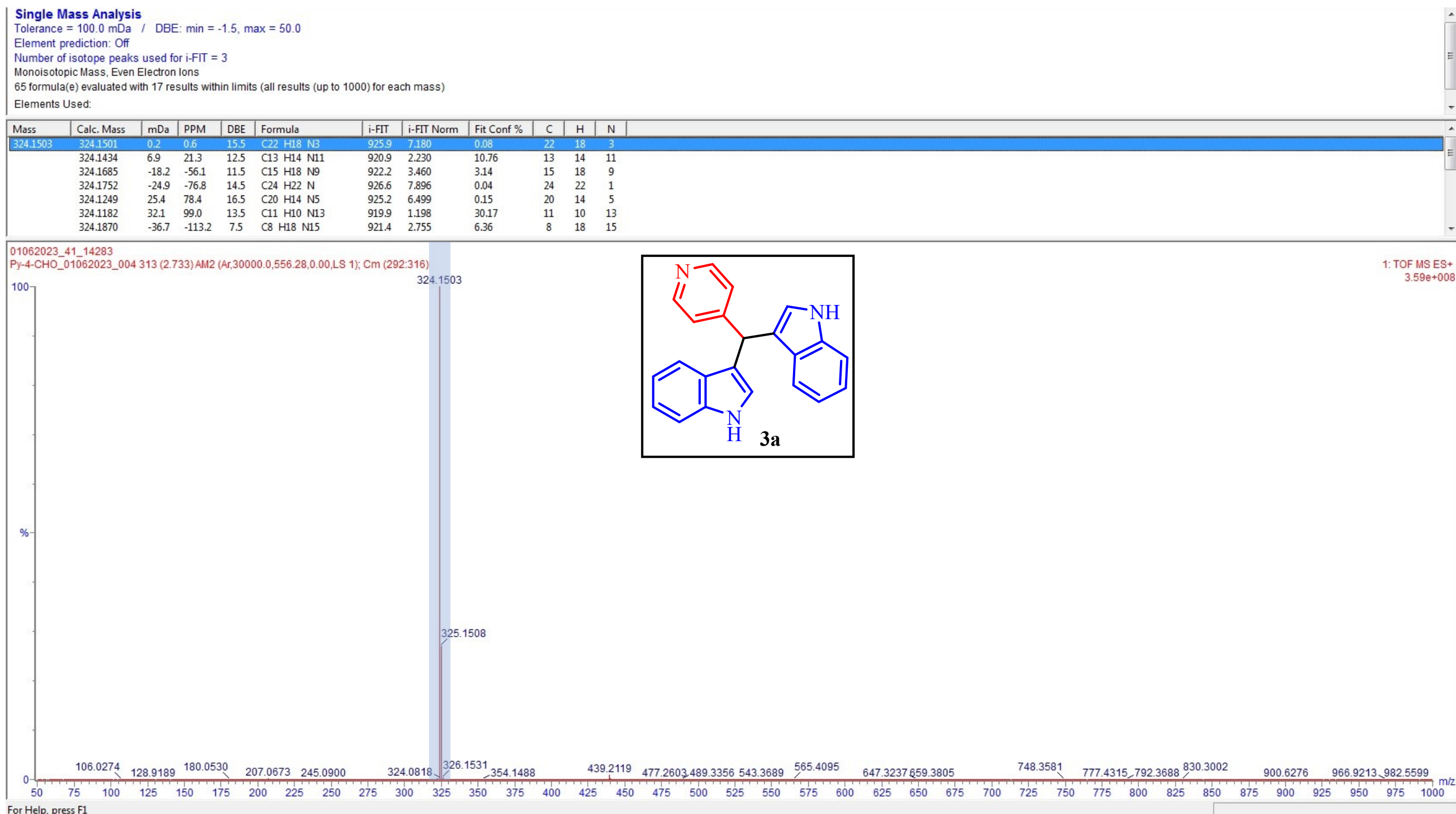


Figure 3. HRMS spectrum of compound **3a**

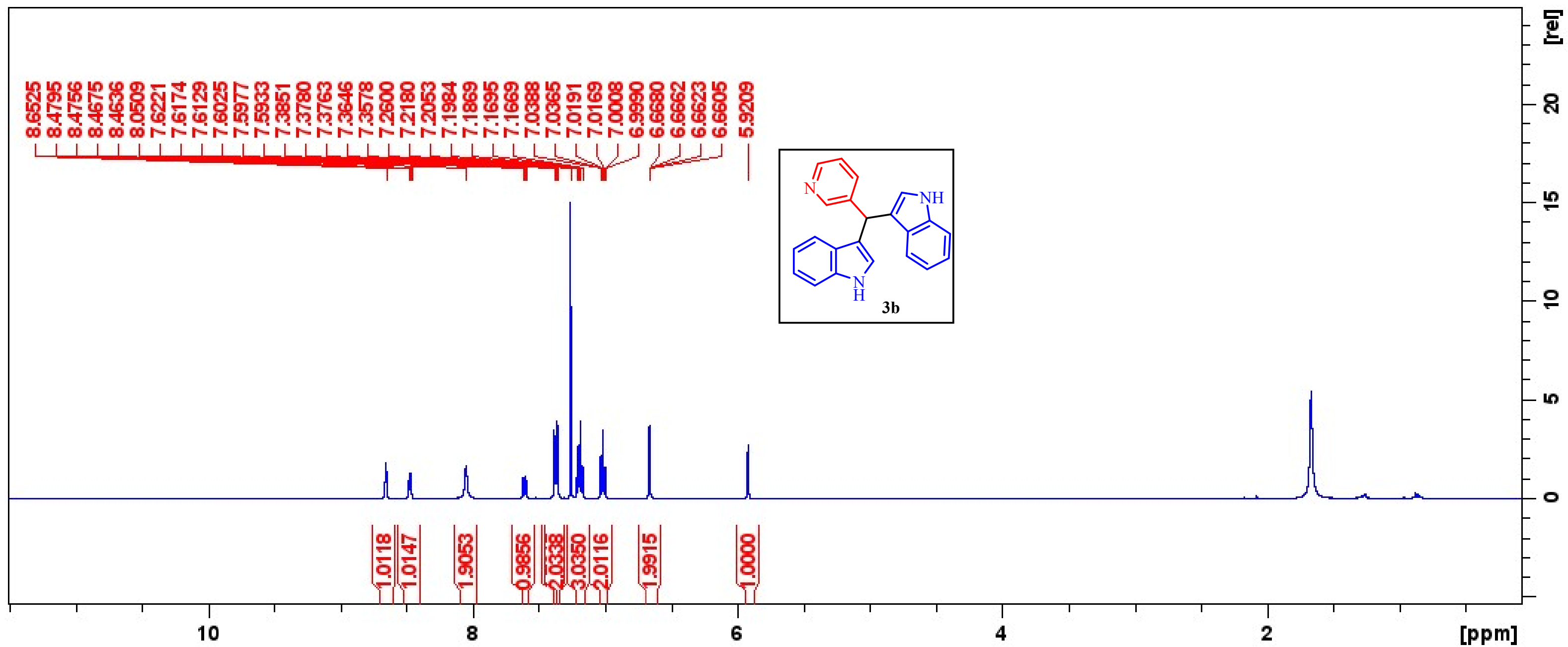


Figure 4. ^1H NMR spectrum of compound **3b**

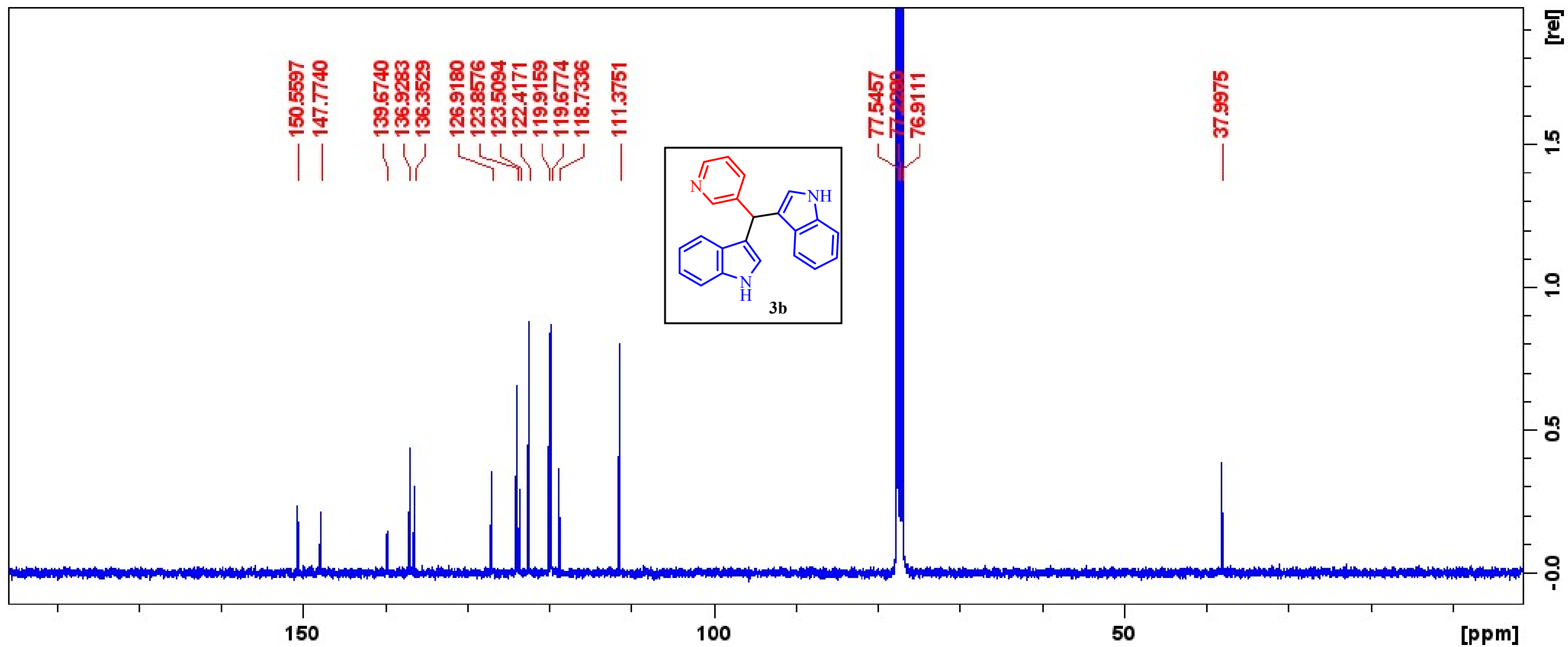


Figure 5. ¹³C NMR spectrum of compound **3b**

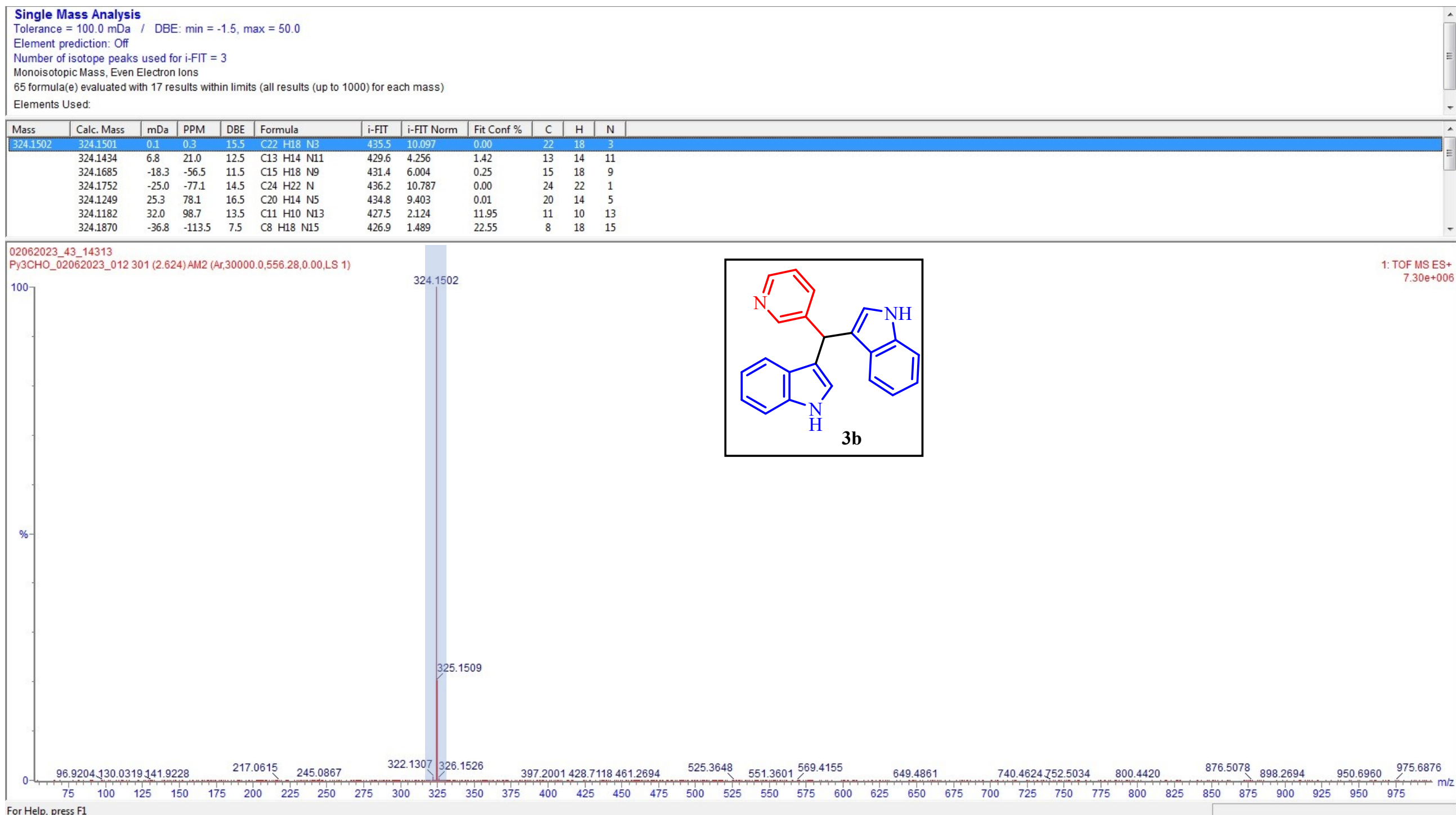


Figure 6. HRMS spectrum of compound **3b**

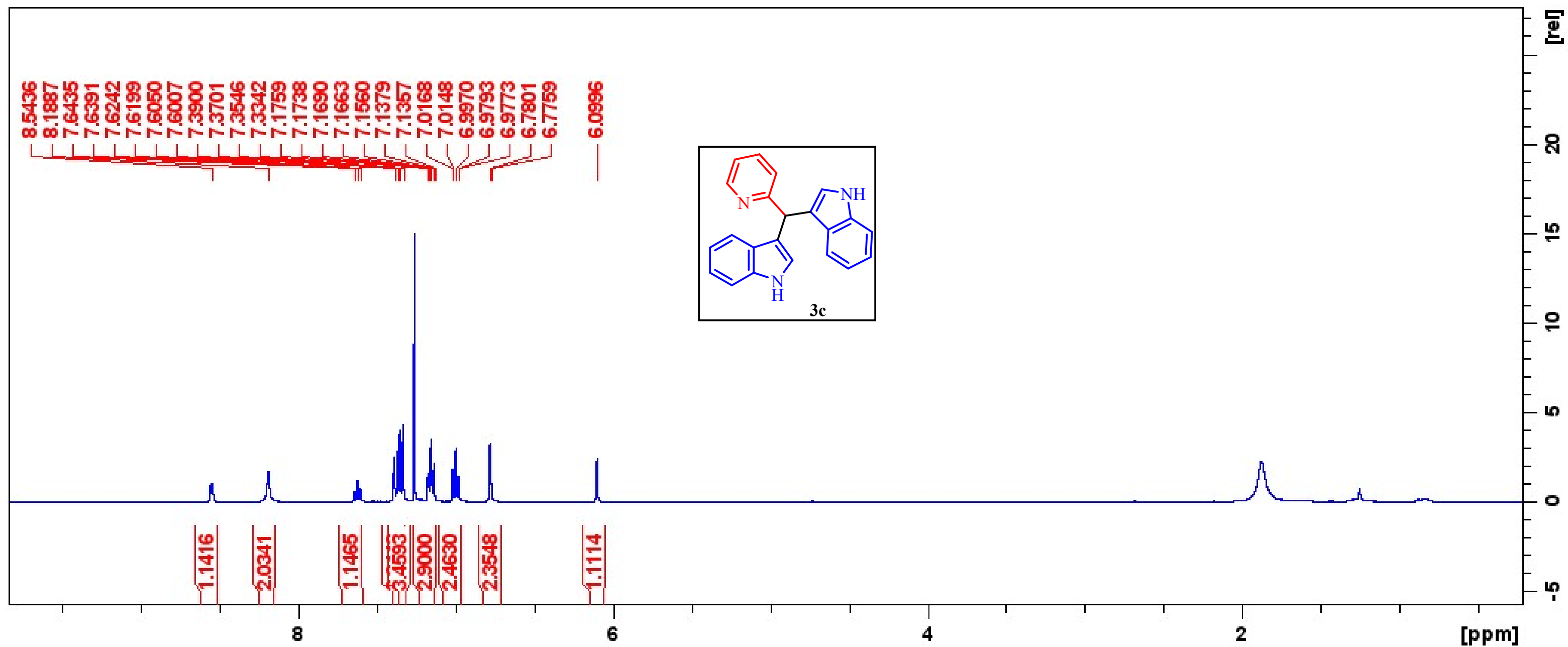


Figure 7. ¹H NMR spectrum of compound **3c**

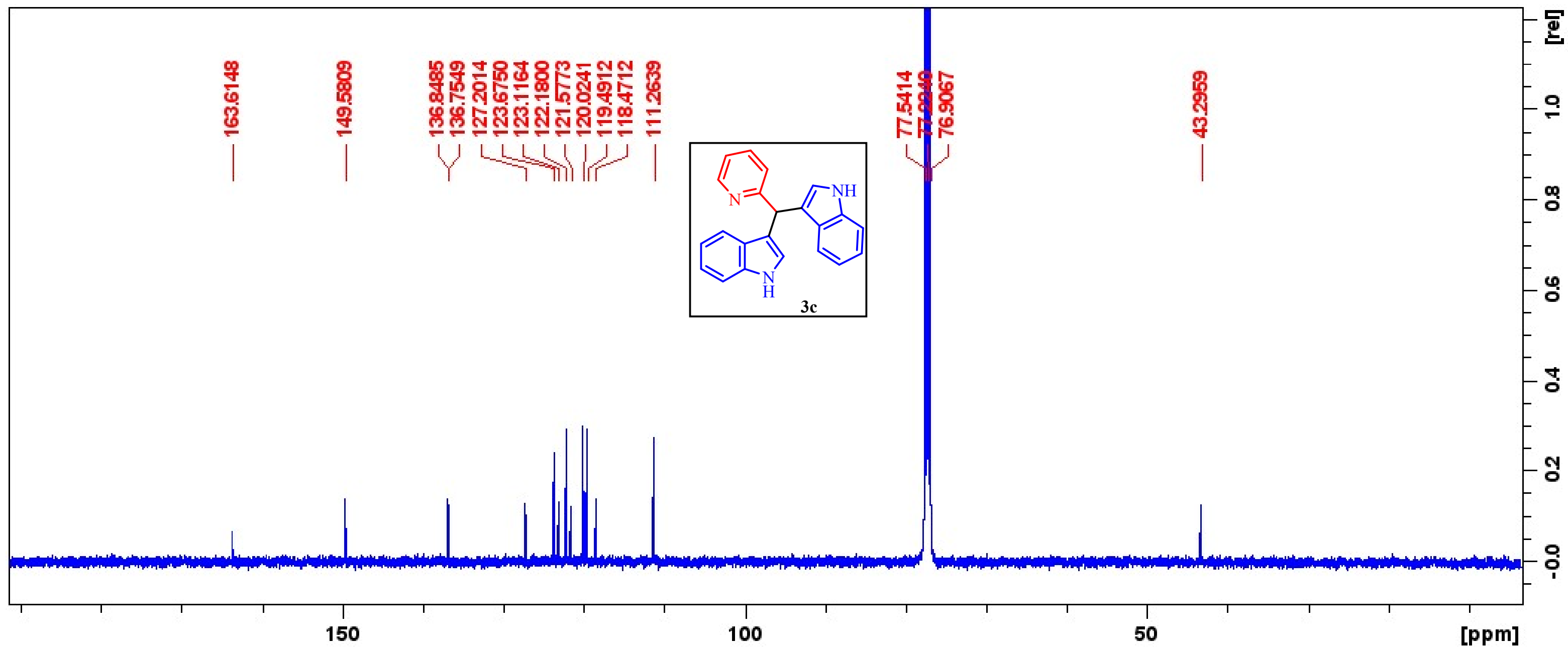


Figure 8. ¹³C NMR spectrum of compound **3c**

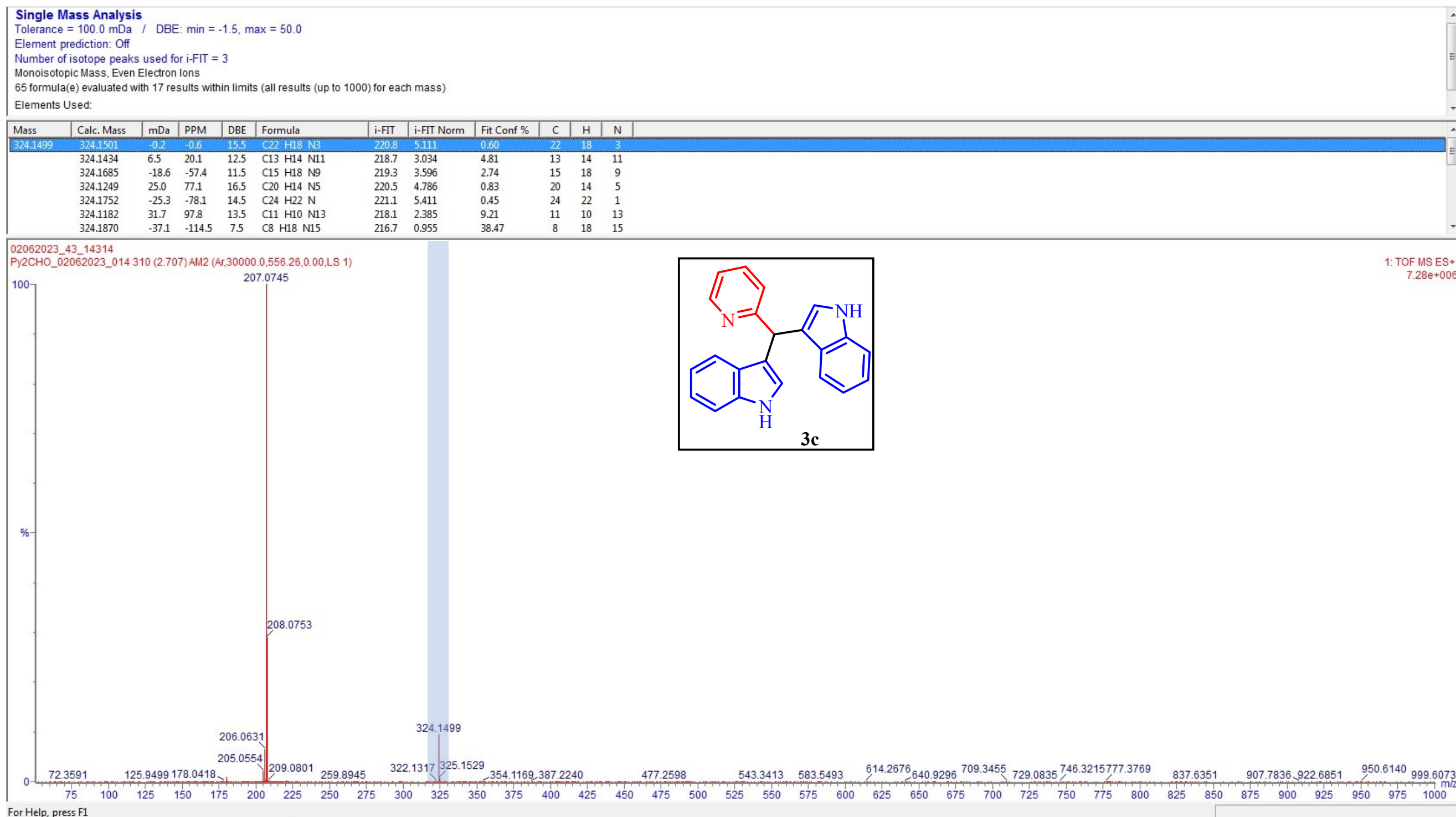


Figure 9. HRMS spectrum of compound **3c**

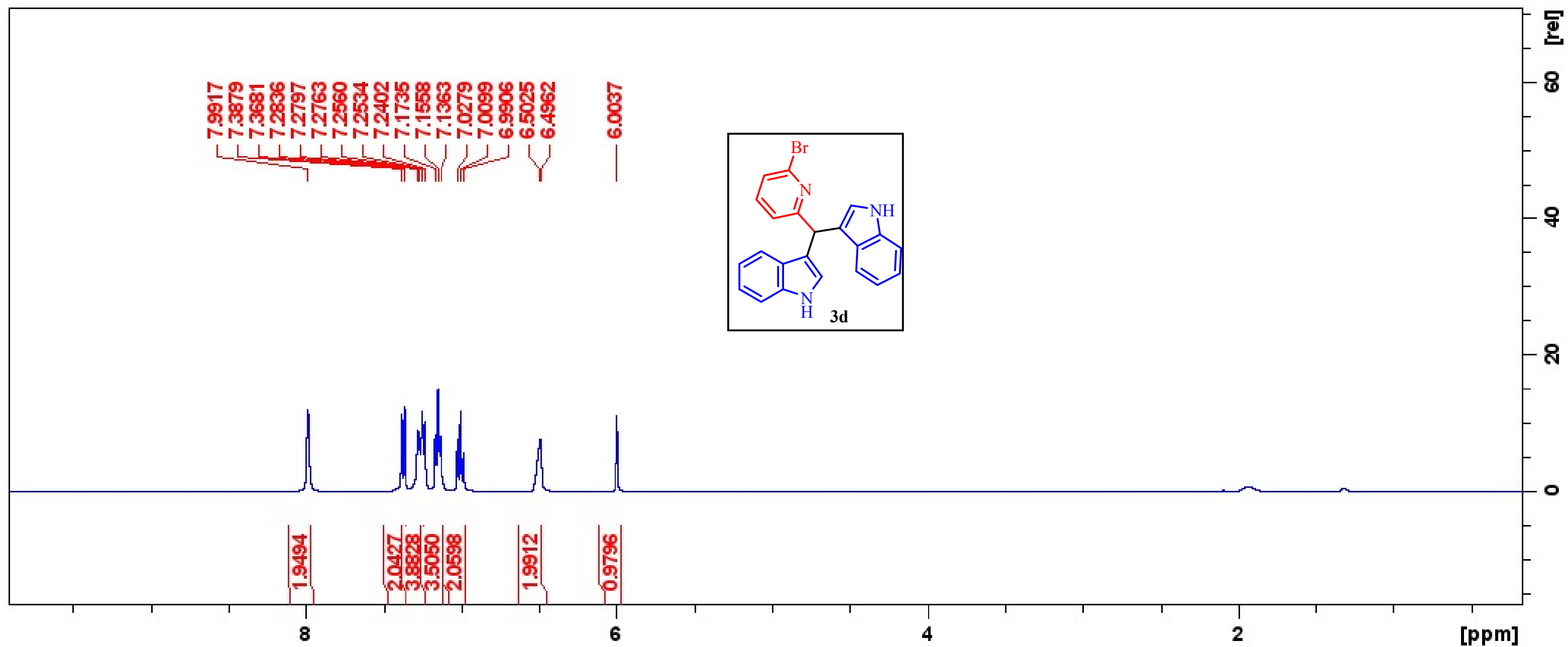


Figure 10. ¹H NMR spectrum of compound **3d**

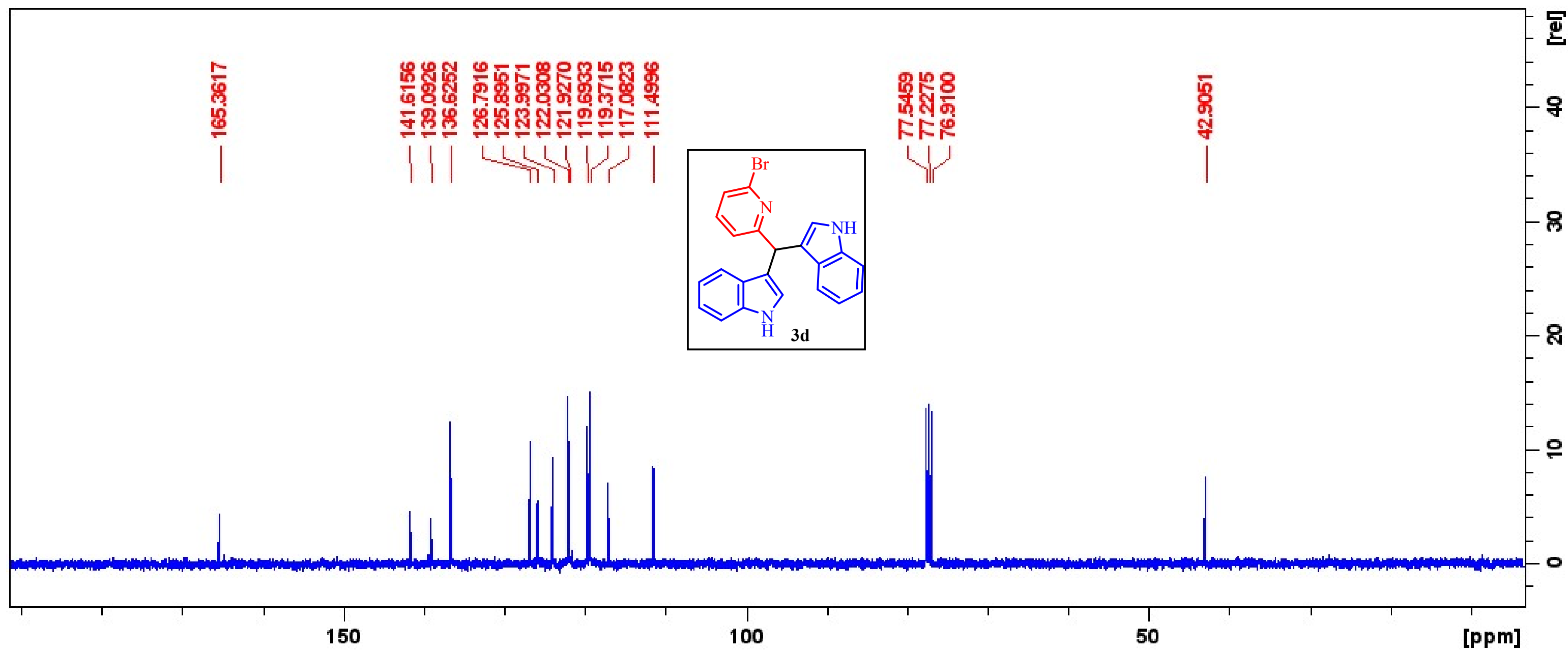


Figure 11. ¹³C NMR spectrum of compound **3d**

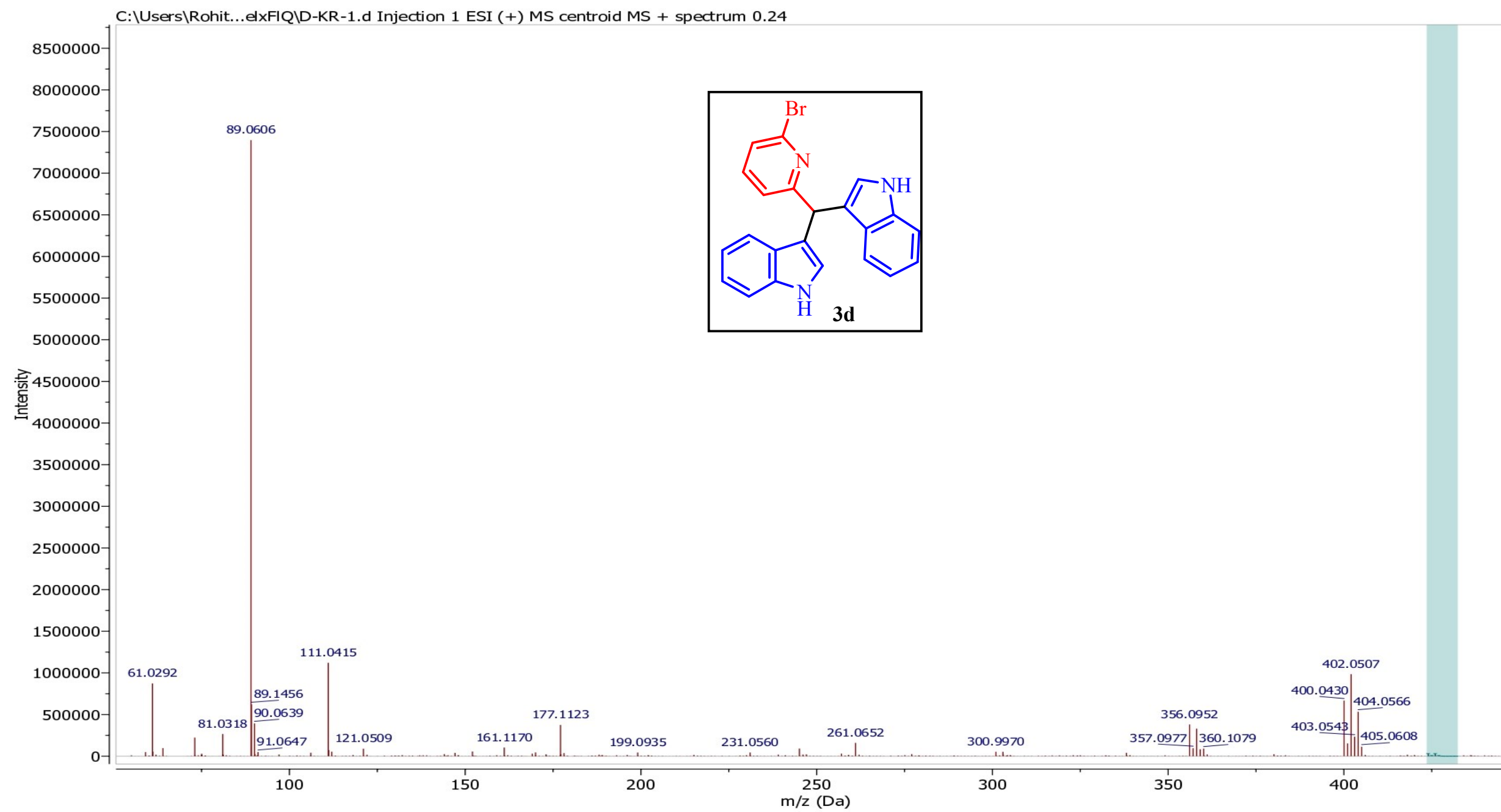


Figure 12. HRMS spectrum of compound **3d**

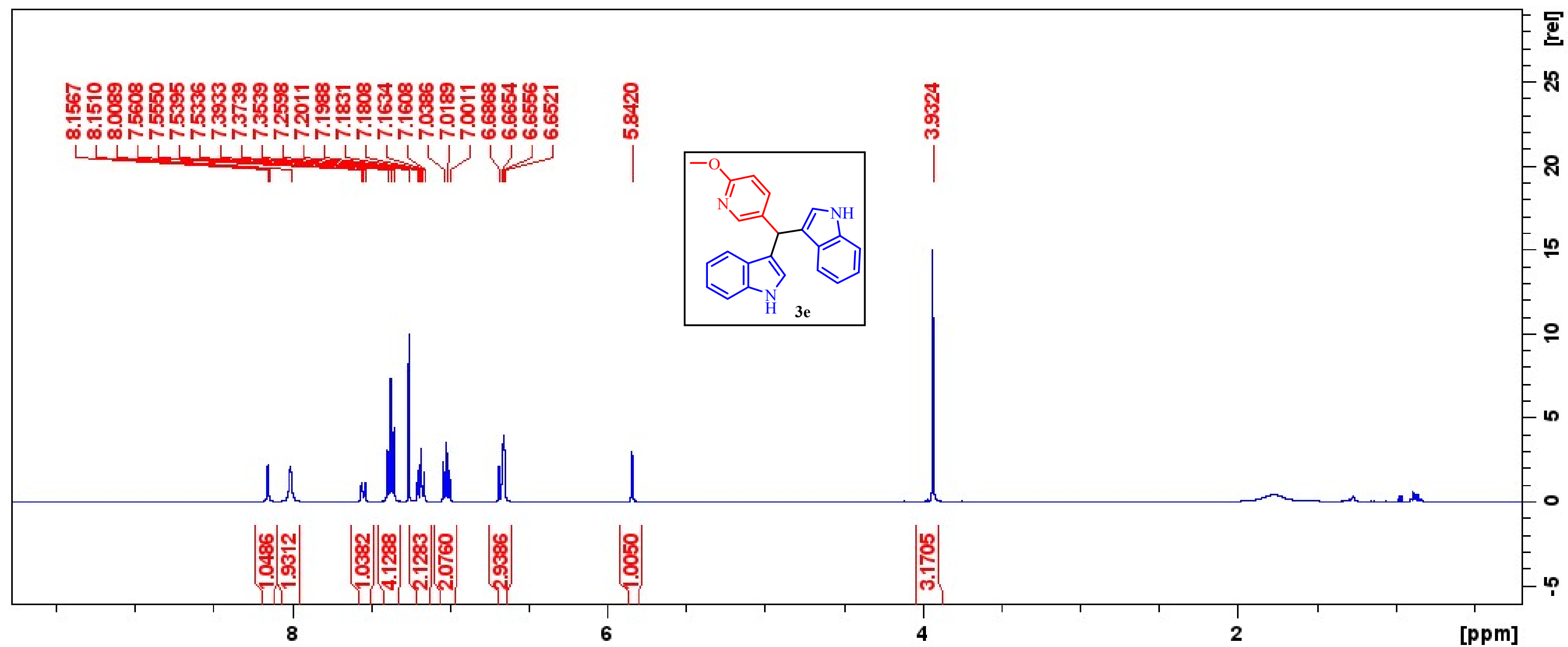


Figure 13. ¹H NMR spectrum of compound 3e

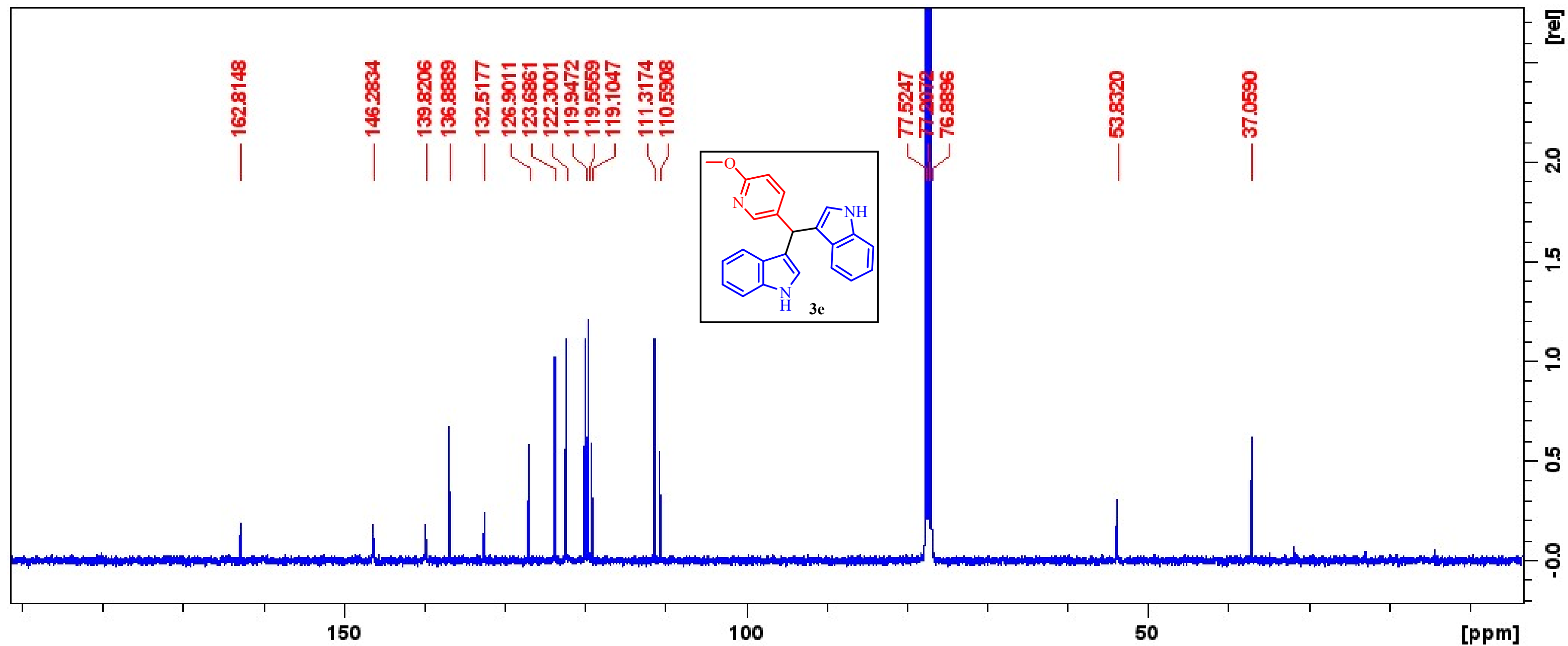


Figure 14. ¹³C NMR spectrum of compound **3e**

Single Mass Analysis

Tolerance = 100.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

771 formula(e) evaluated with 176 results within limits (all results (up to 1000) for each mass)

Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O
354.1602	354.1598	0.4	1.1	3.5	C7 H20 N11 O6	707.8	5.001	0.67	7	20	11	6
	354.1606	-0.4	-1.1	15.5	C23 H20 N3 O	710.6	7.796	0.04	23	20	3	1
	354.1611	-0.9	-2.5	8.5	C8 H16 N15 O2	708.1	5.246	0.53	8	16	15	2
	354.1585	1.7	4.8	-1.5	C6 H24 N7 O10	709.3	6.520	0.15	6	24	7	10
	354.1625	-2.3	-6.5	2.5	C11 H24 N5 O8	710.2	7.344	0.06	11	24	5	8
	354.1566	3.6	10.2	11.5	C18 H20 N5 O3	709.8	6.997	0.09	18	20	5	3
	354.1638	-3.6	-10.2	7.5	C12 H20 N9 O4	708.7	5.913	0.27	12	20	9	4

02062023_43_14310

6Me3PyCHO_02062023_008 383 (3.340)AM2 (Ar,30000.0,556.25,0.00,LS 1)

1: TOF MS ES+
4.95e+007

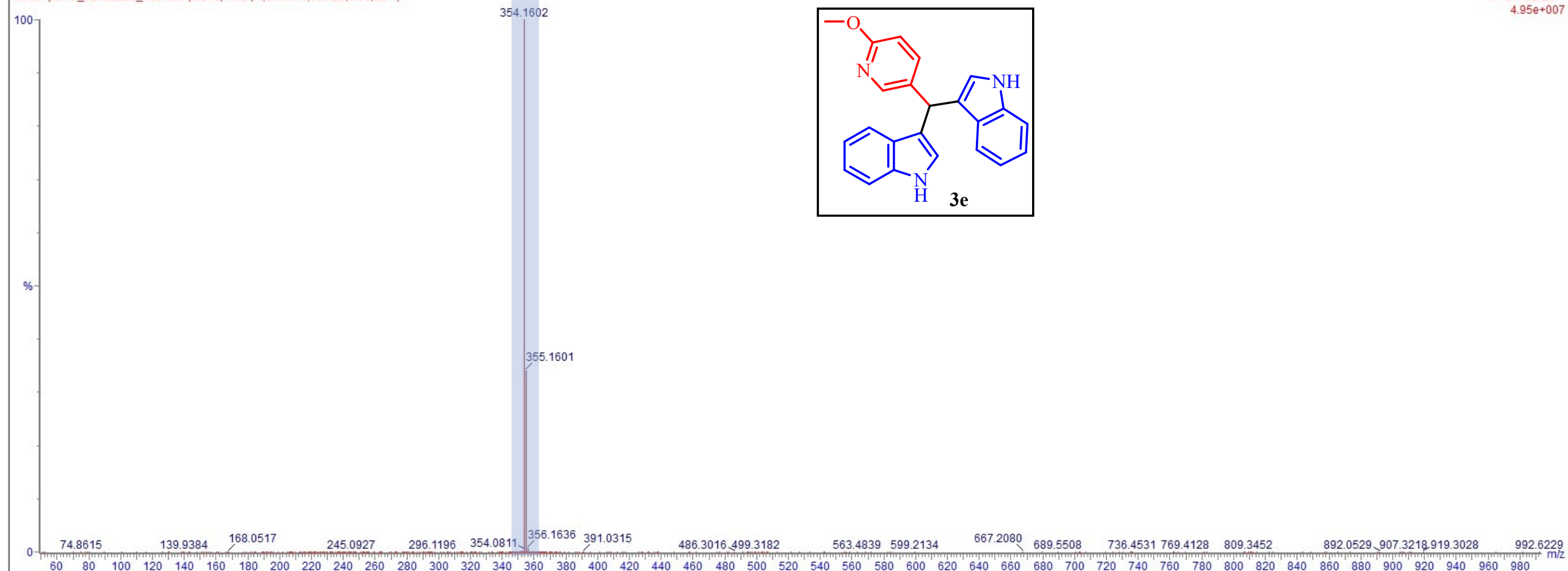


Figure 15. HRMS spectrum of compound **3e**

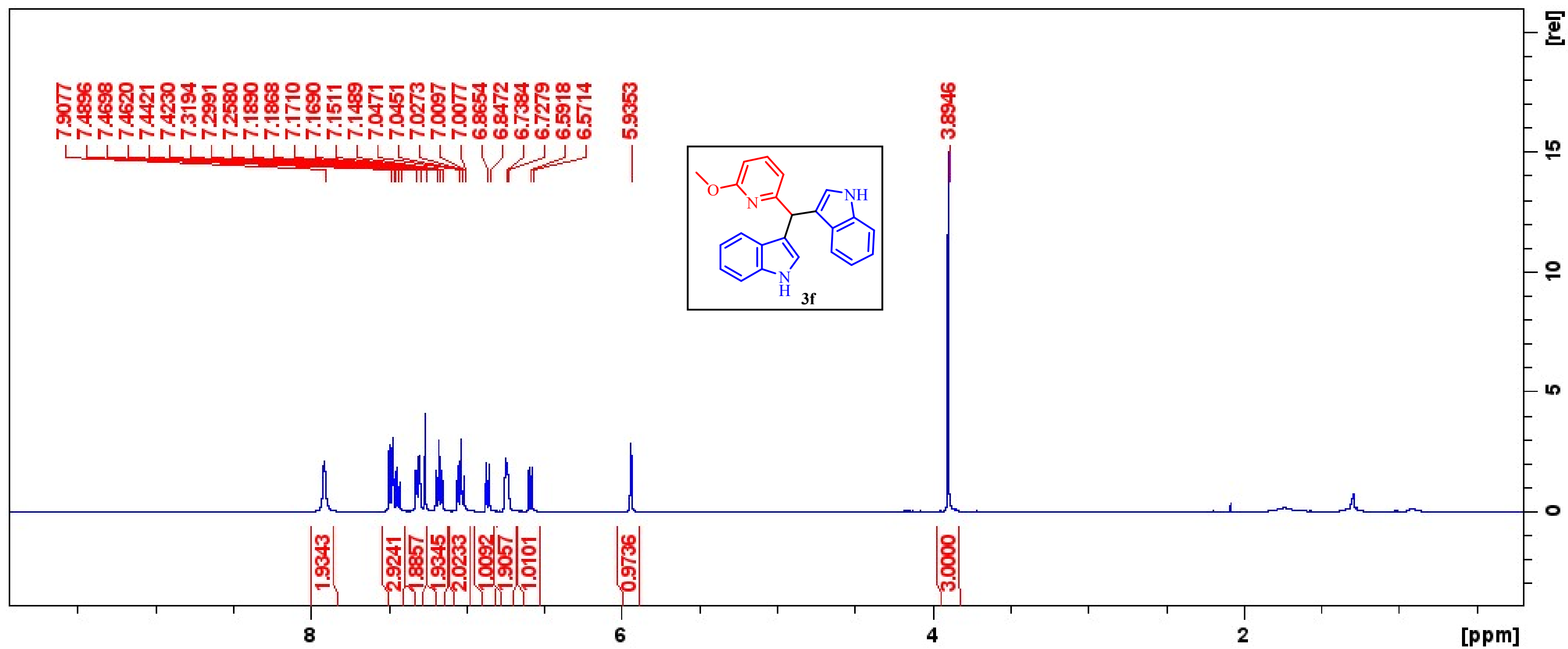


Figure 16. ¹H NMR spectrum of compound 3f

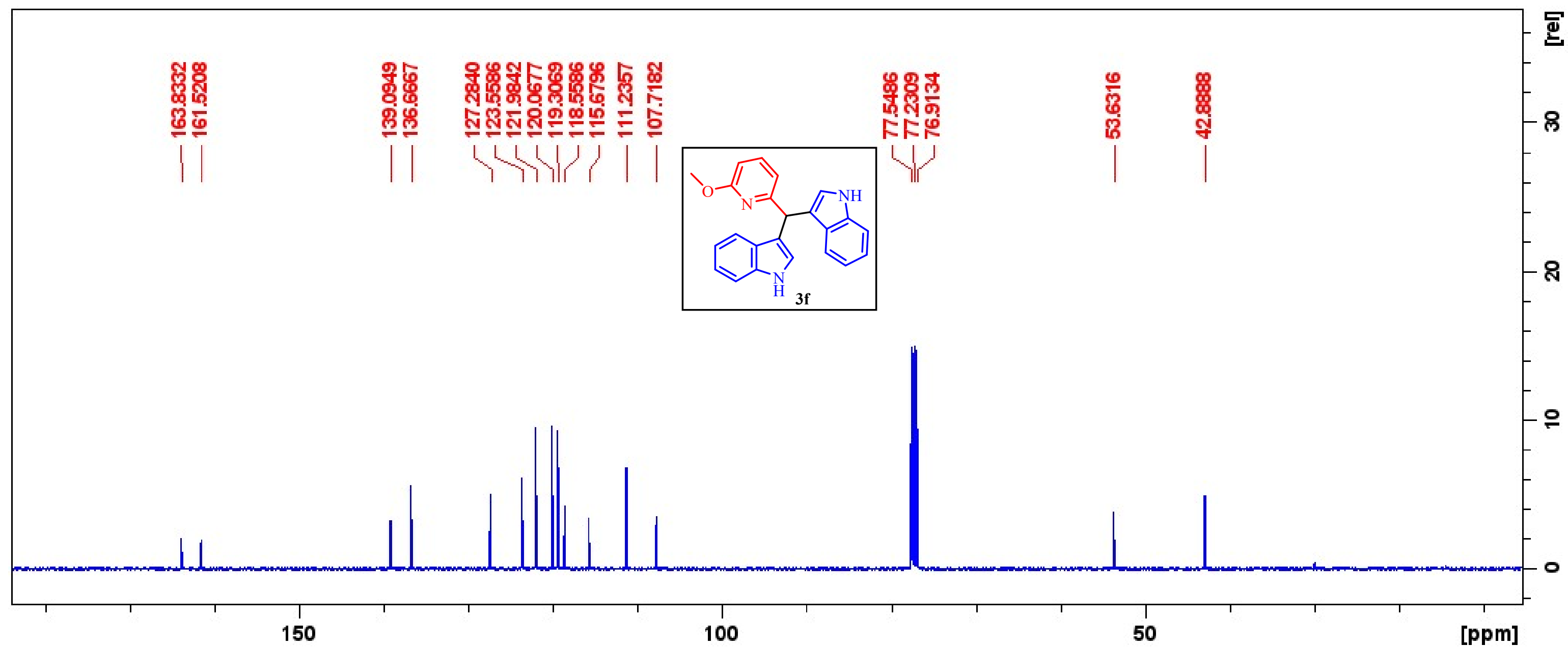


Figure 17. ¹³C NMR spectrum of compound **3f**

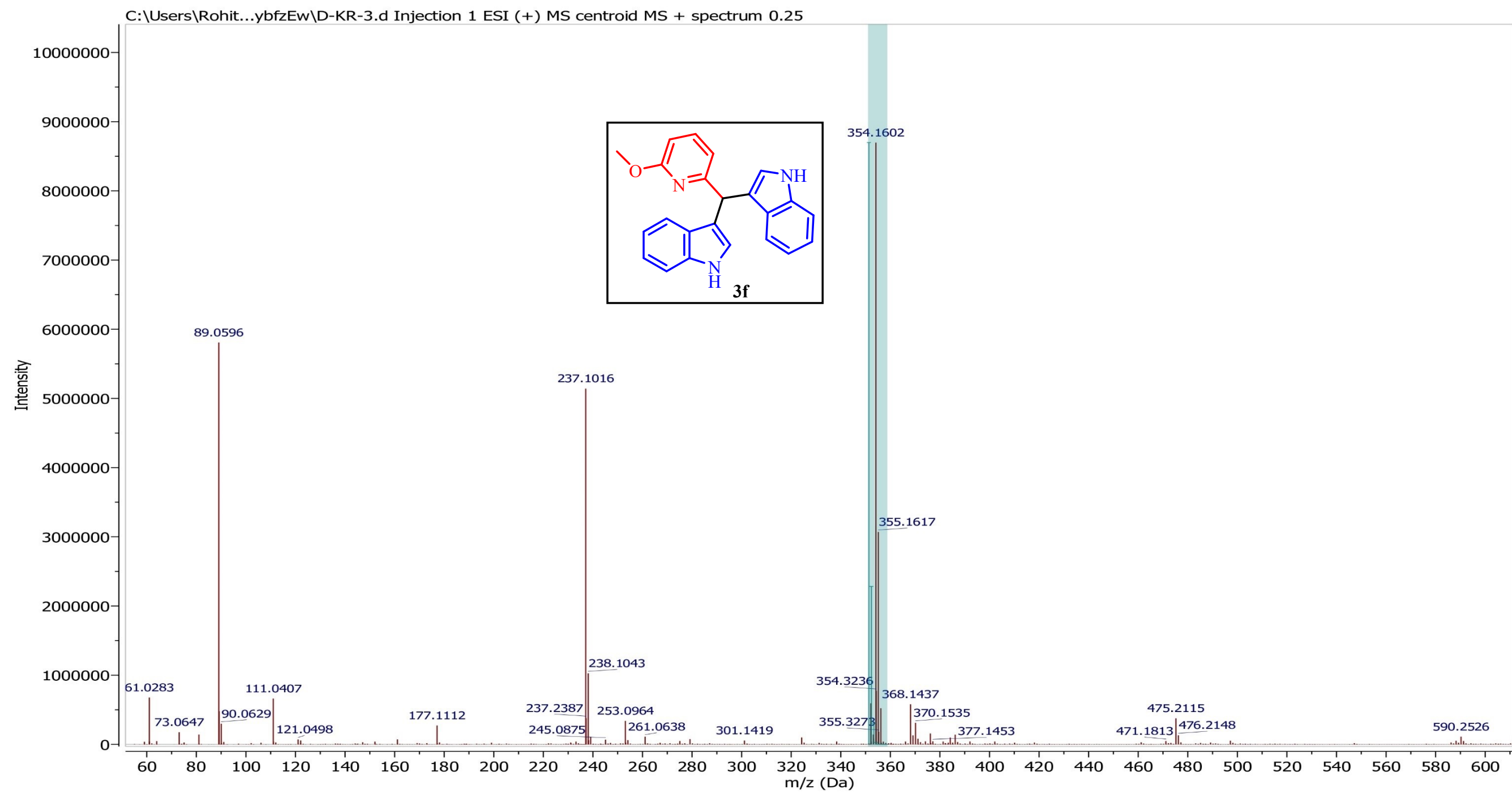


Figure 18. HRMS spectrum of compound **3f**

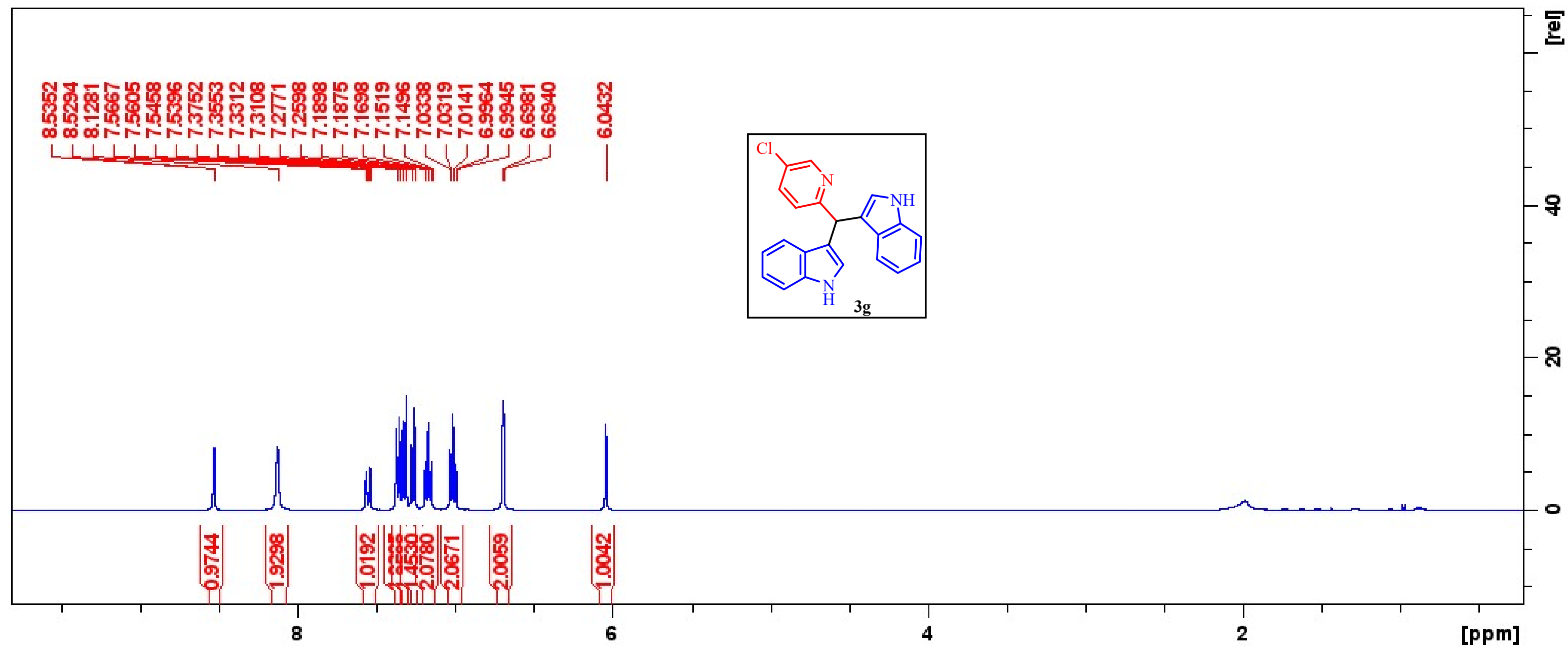


Figure 19. ¹H NMR spectrum of compound **3g**

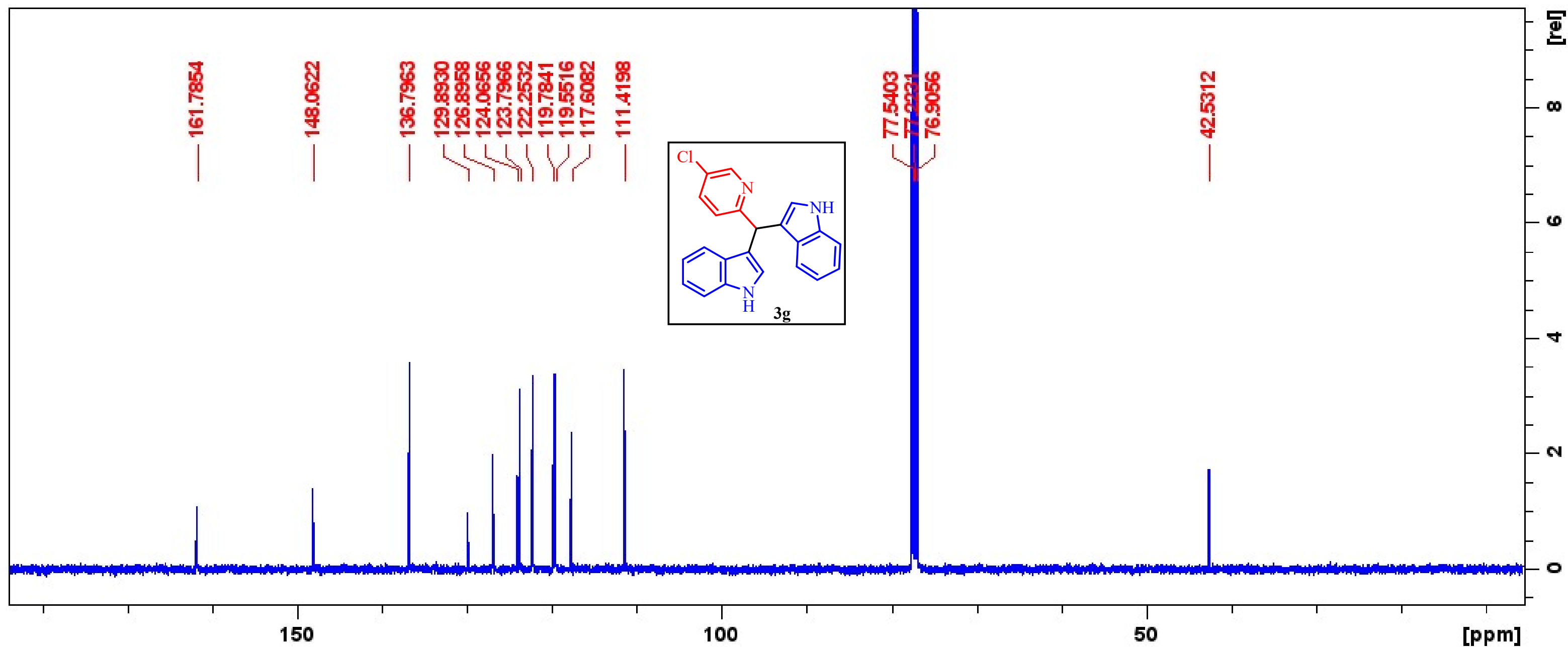


Figure 20. ^{13}C NMR spectrum of compound **3g**

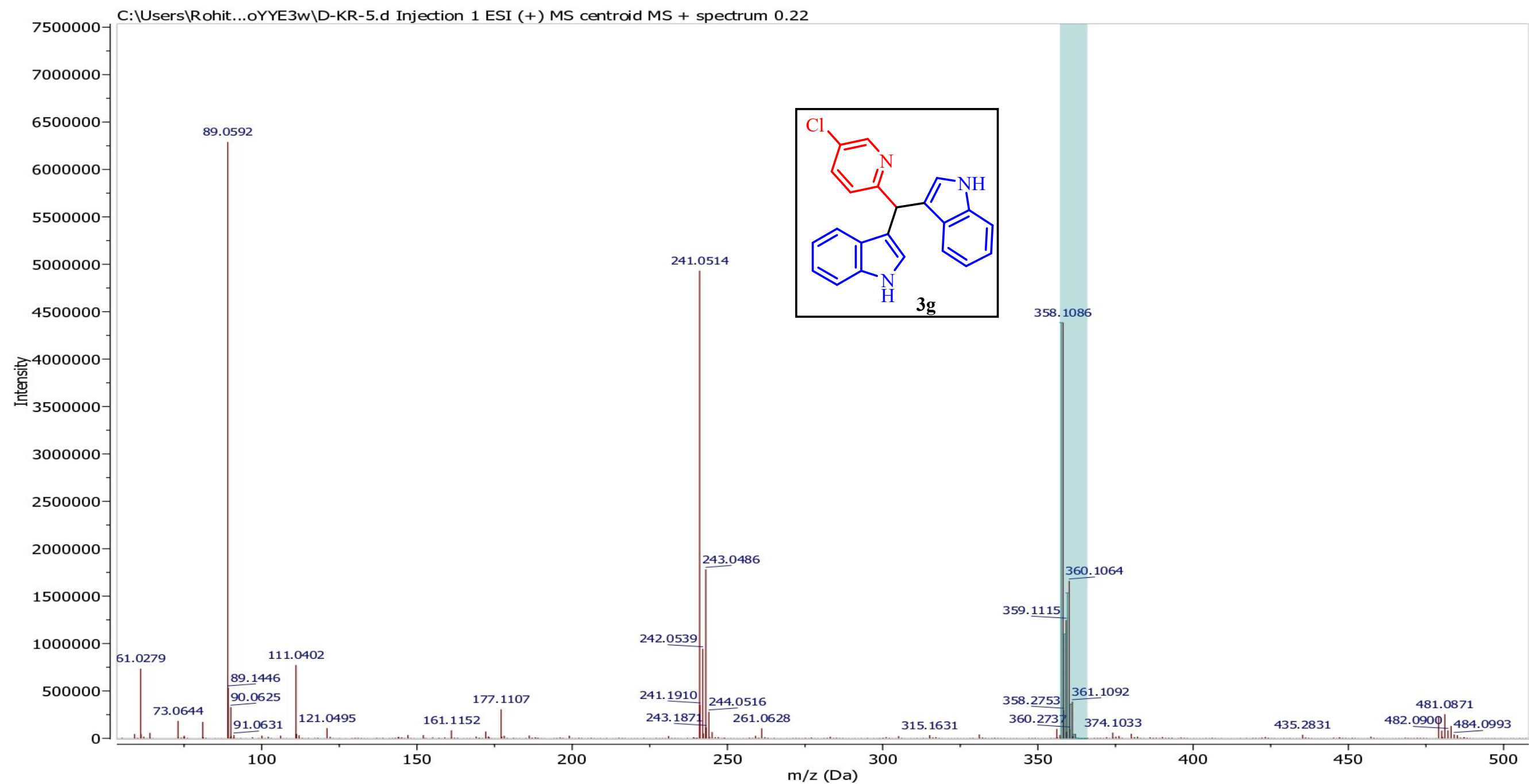


Figure 21. HRMS spectrum of compound **3g**

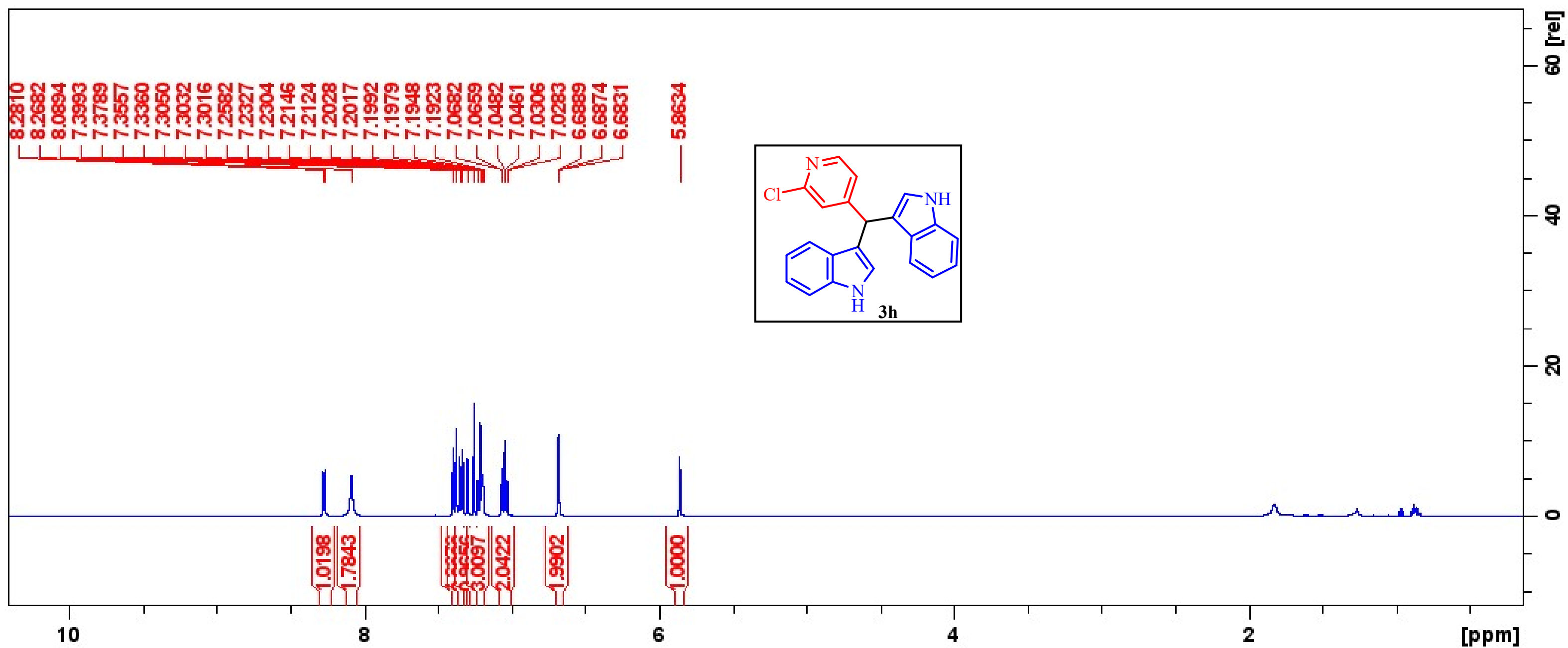


Figure 22. ¹H NMR spectrum of compound **3h**

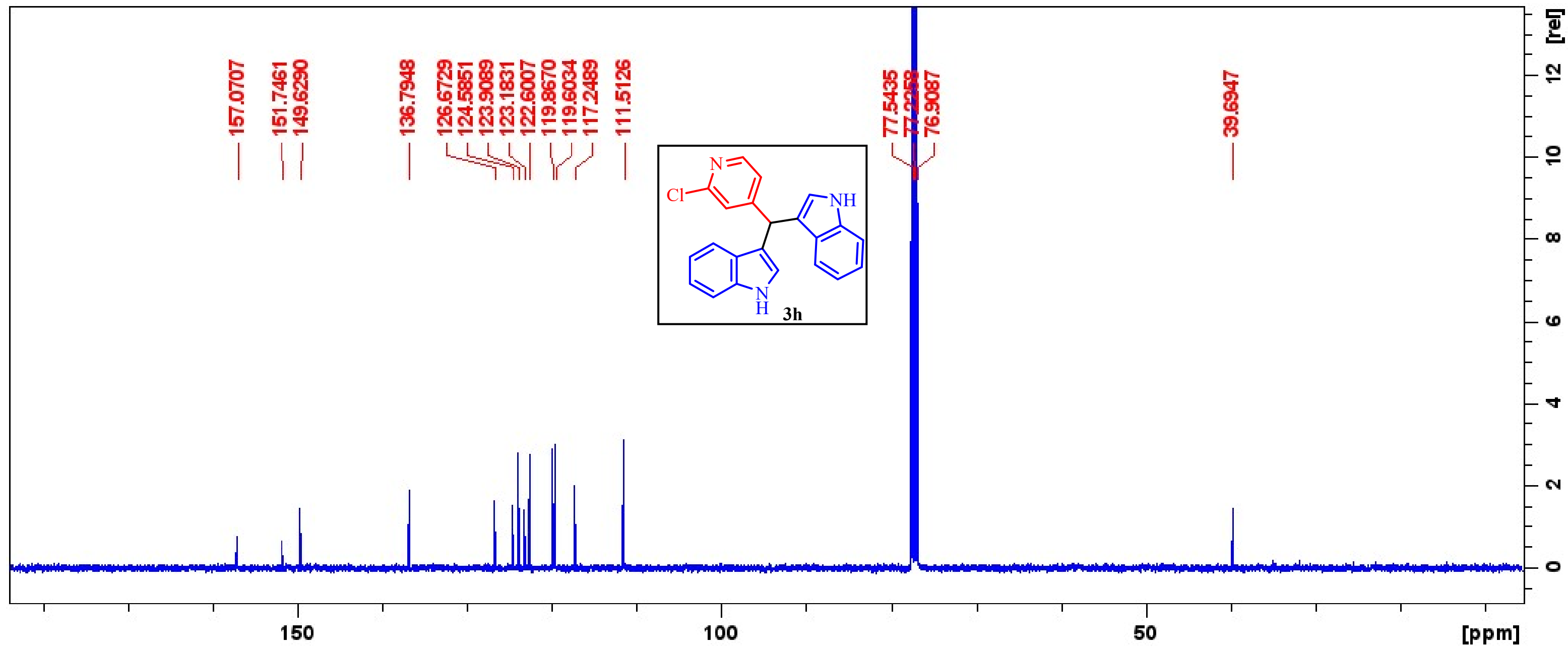


Figure 23. ^{13}C NMR spectrum of compound **3h**

Single Mass Analysis

Tolerance = 100.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

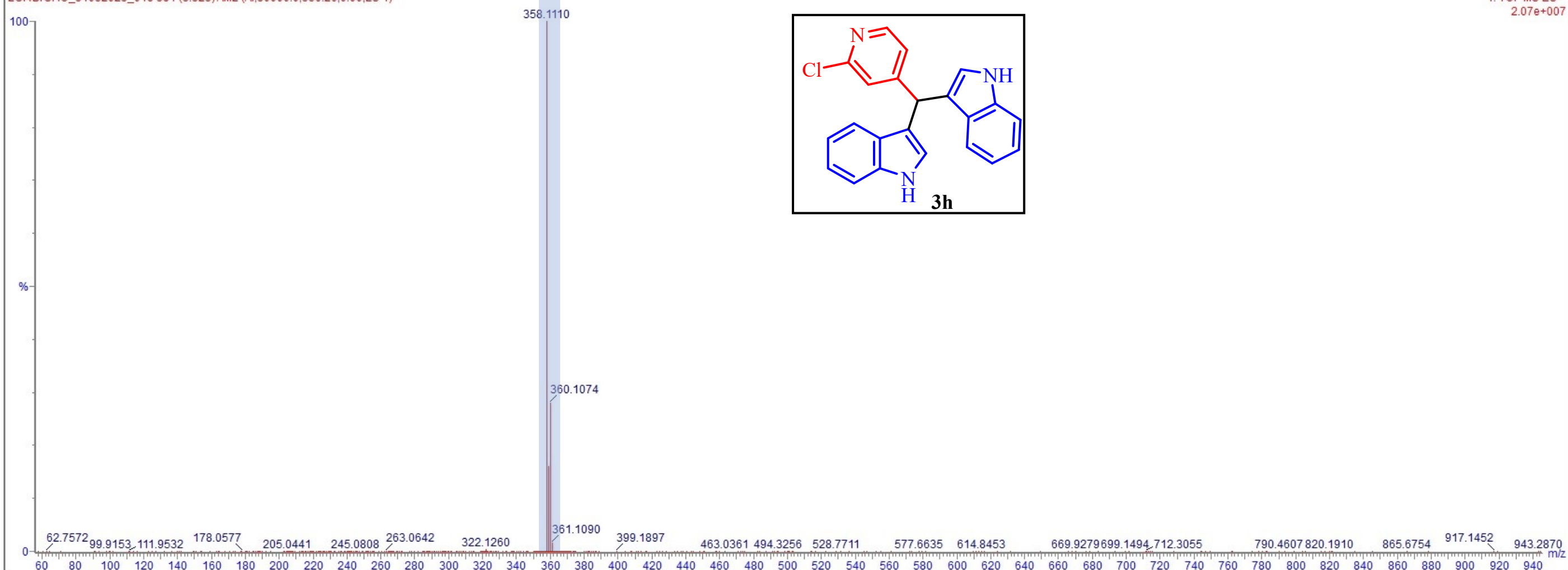
356 formula(e) evaluated with 73 results within limits (all results (up to 1000) for each mass)

Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	Cl
358.1110	358.1111	-0.1	-0.3	15.5	C22 H17 N3 Cl	553.4	6.182	0.21	22	17	3	1
358.1093		1.7	4.7	20.5	C23 H12 N5	564.7	17.494	0.00	23	12	5	
358.1129		-1.9	-5.3	10.5	C21 H22 N Cl2	556.7	9.497	0.01	21	22	1	2
358.1081		2.9	8.1	2.5	C11 H23 N7 Cl3	555.7	8.535	0.02	11	23	7	3
358.1062		4.8	13.4	7.5	C12 H18 N9 Cl2	554.3	7.081	0.08	12	18	9	2
358.1044		6.6	18.4	12.5	C13 H13 N11 Cl	548.6	1.464	23.13	13	13	11	1
358.1026		8.4	23.5	17.5	C14 H8 N13	563.6	16.472	0.00	14	8	13	

31052023_41_14257

2Cl4BrCHO_31052023_018 381 (3.323) AM2 (Ar,30000.0,556.26,0.00,LS 1)



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Figure 24. HRMS spectrum of compound **3h**

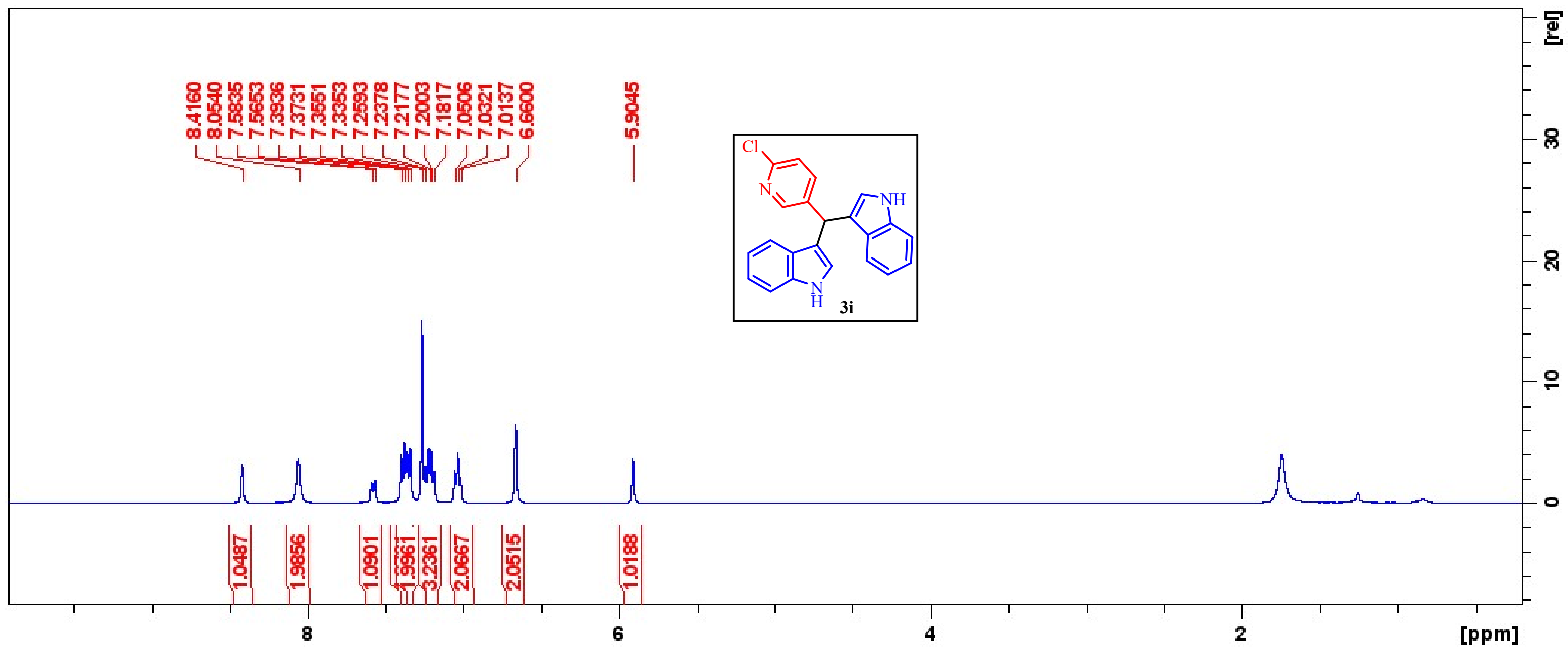


Figure 25. ¹H NMR spectrum of compound **3i**

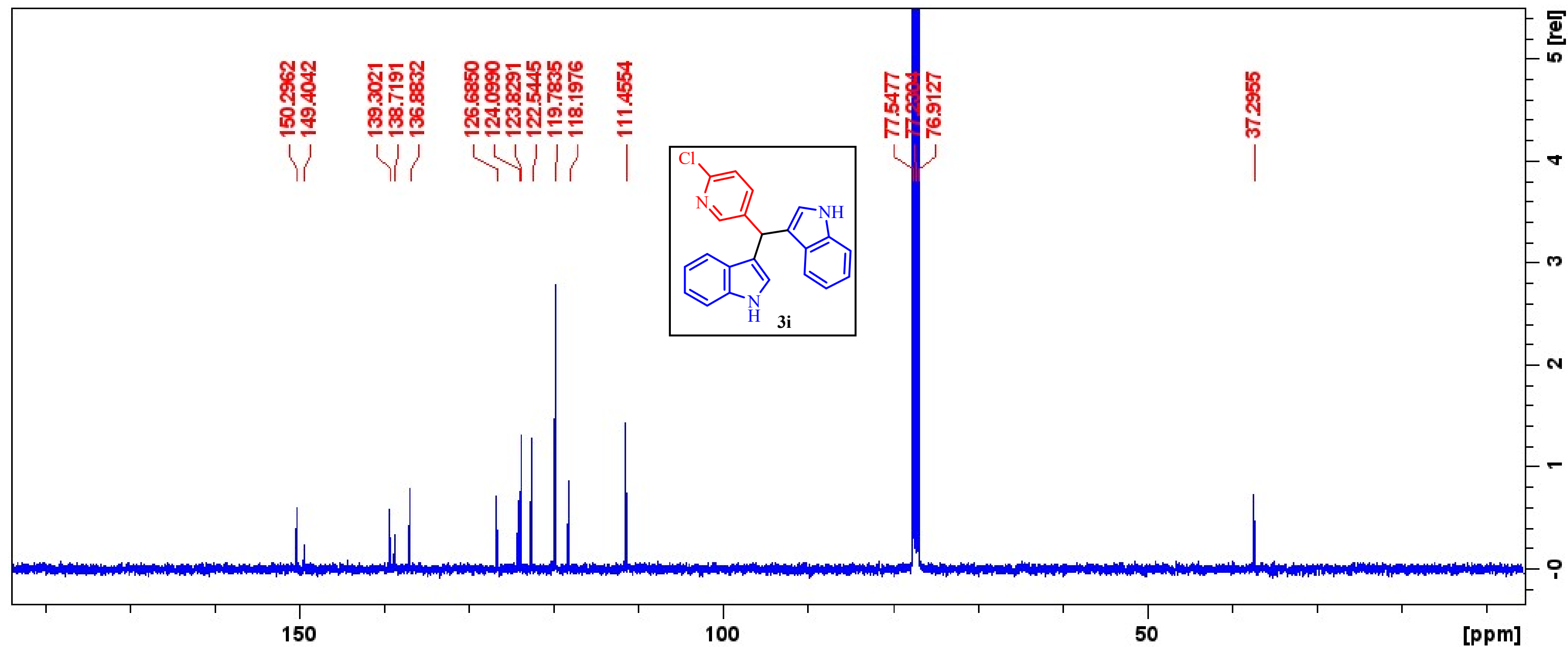


Figure 26. ^{13}C NMR spectrum of compound **3i**

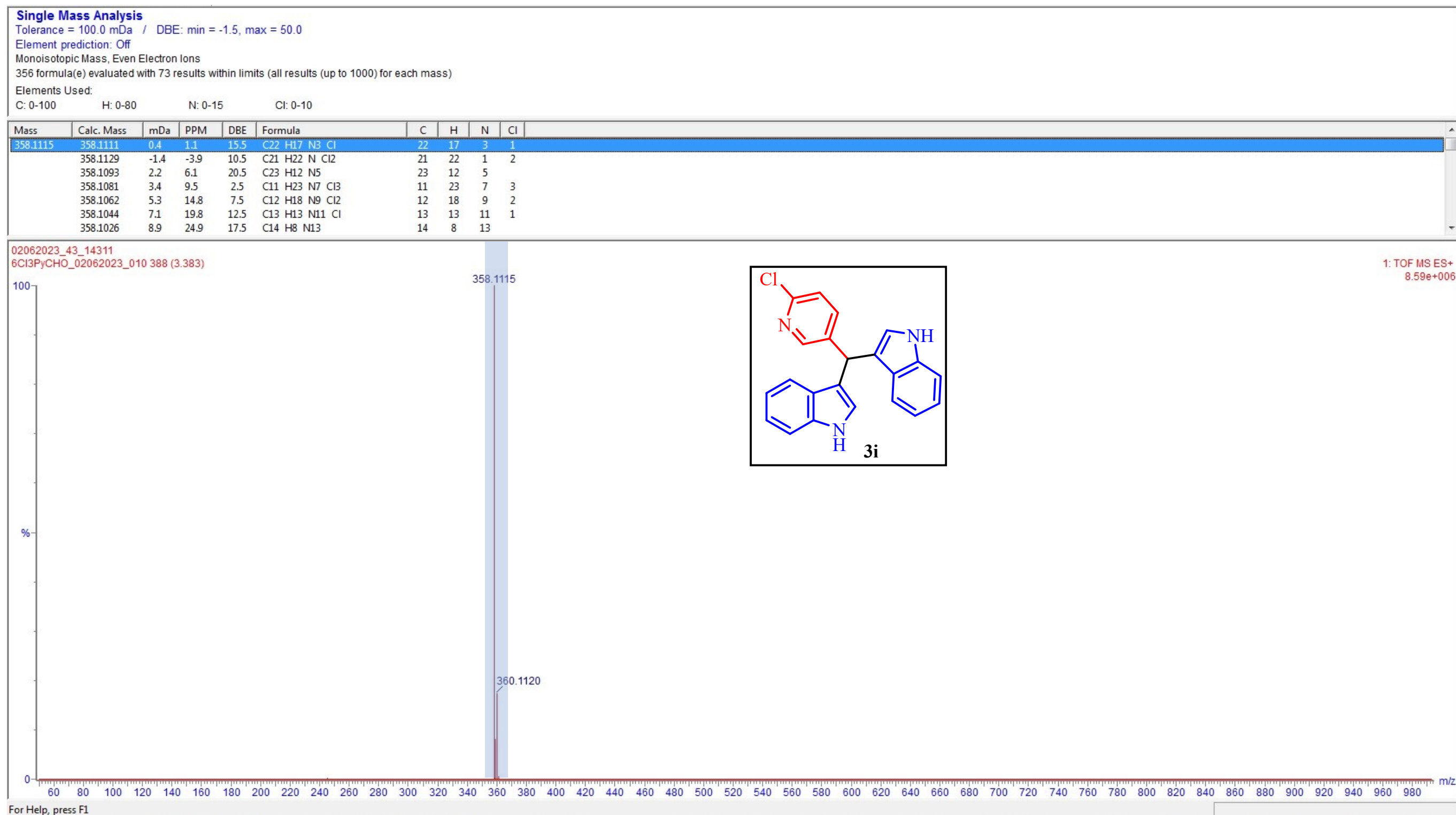


Figure 27. HRMS spectrum of compound **3i**

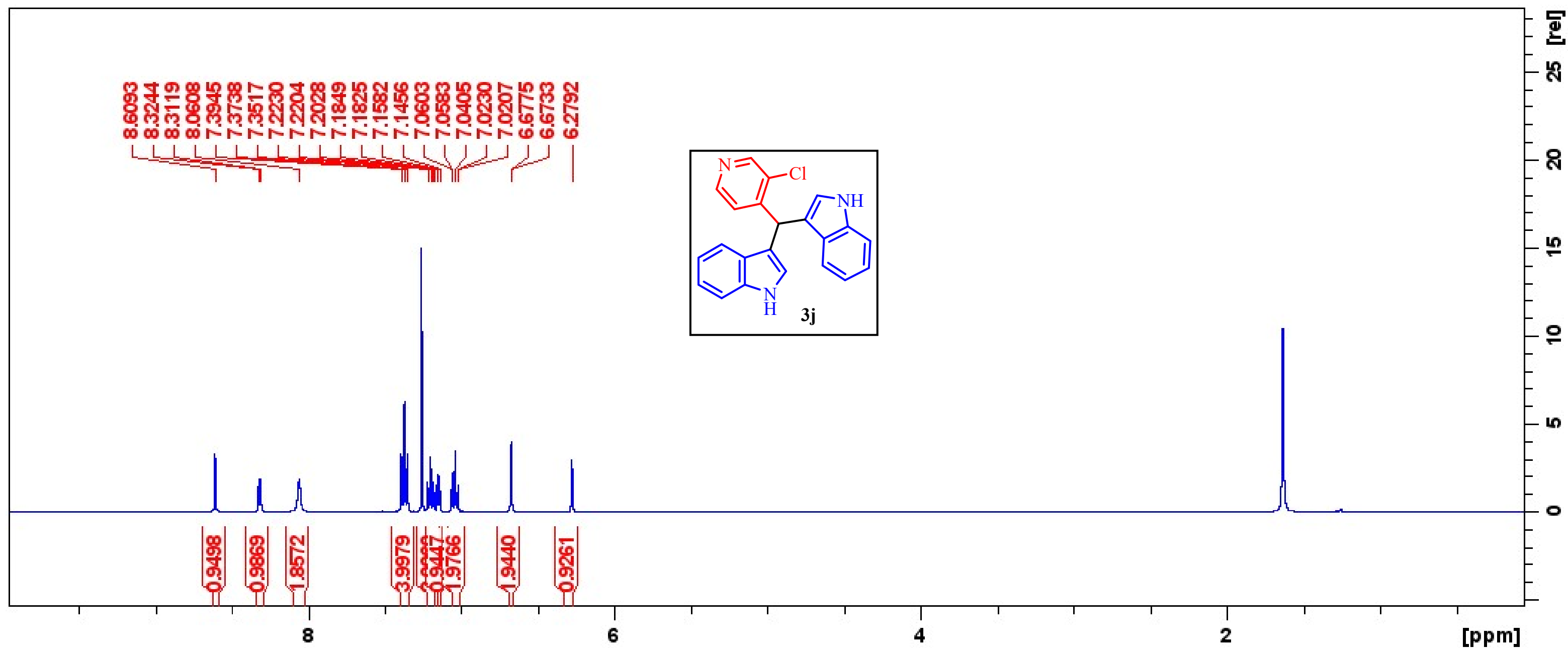


Figure 28. ¹H NMR spectrum of compound **3j**

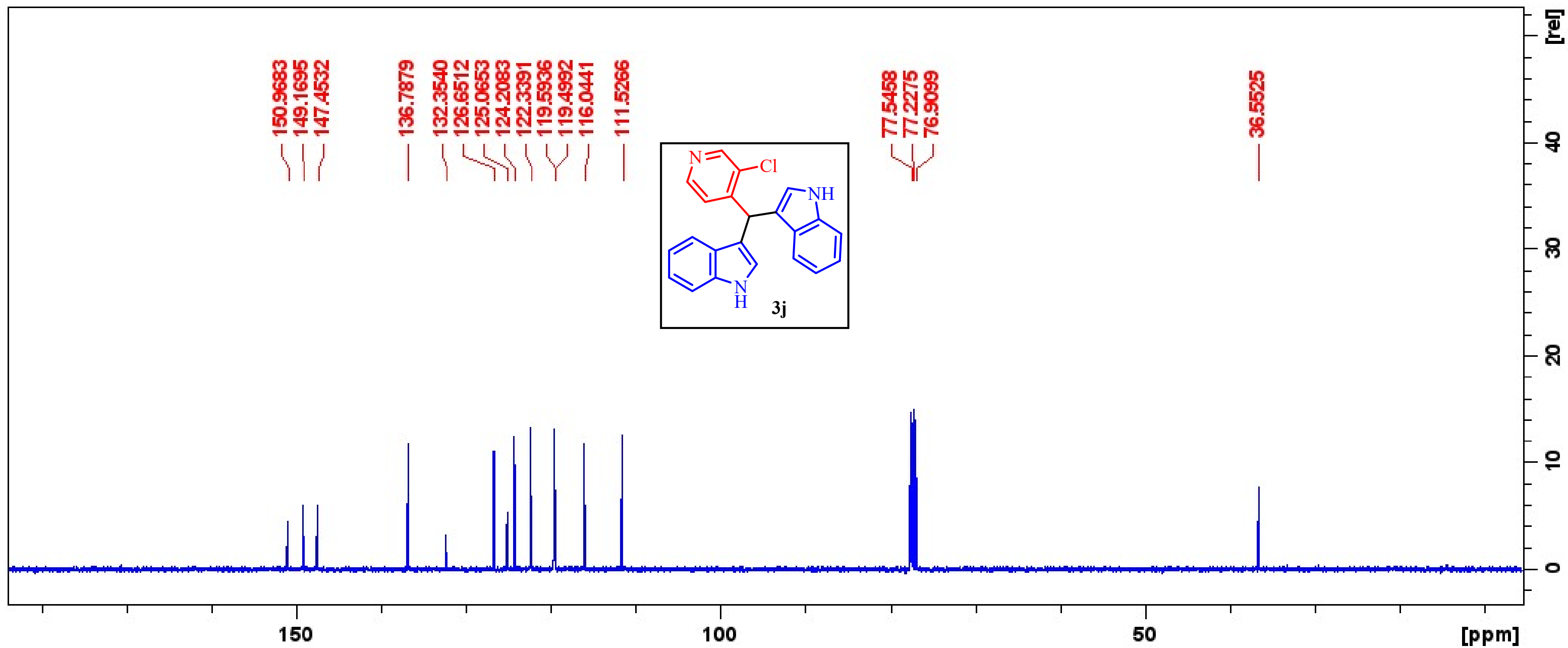


Figure 29. ¹³C NMR spectrum of compound **3j**

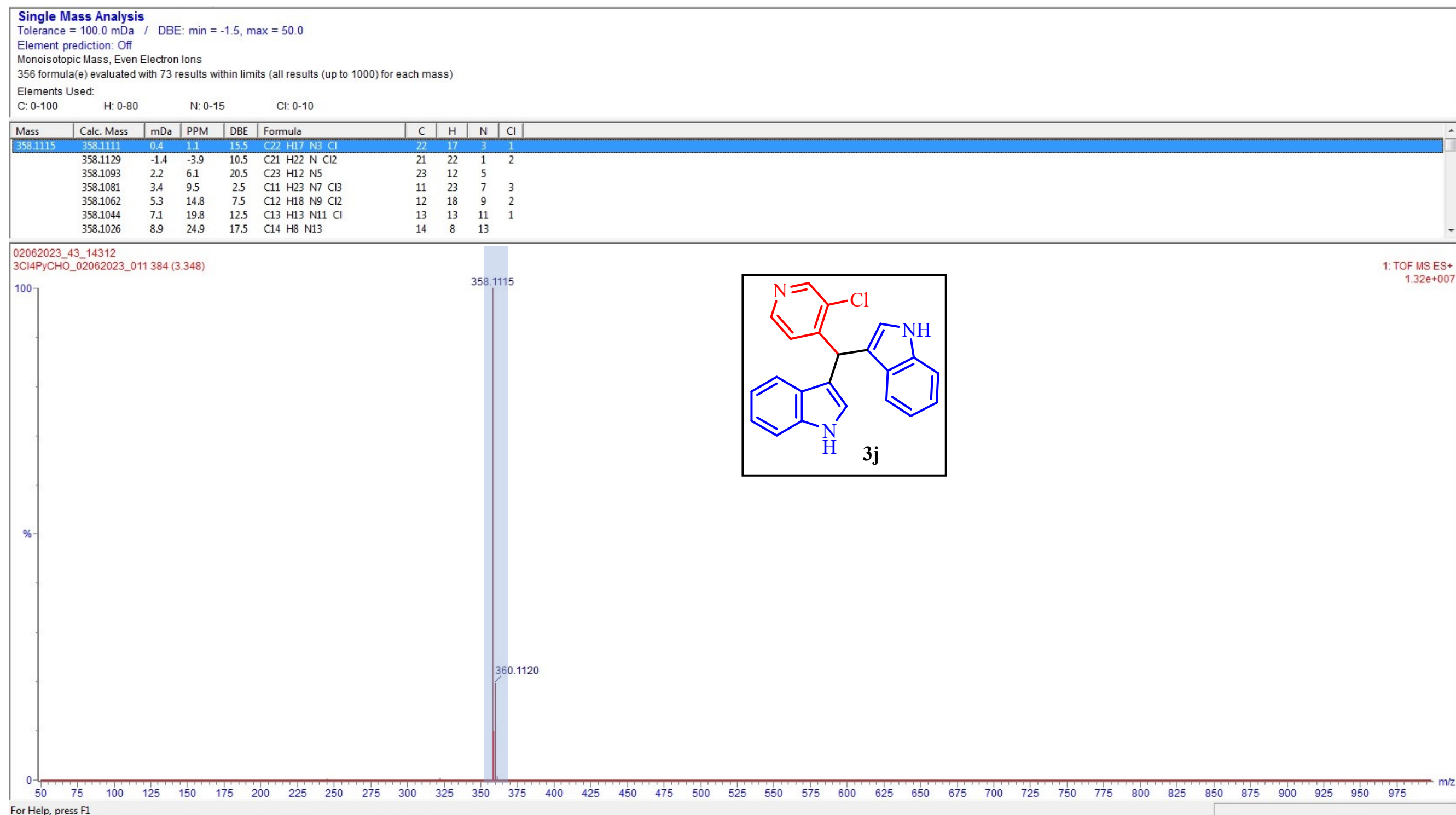


Figure 30. HRMS spectrum of compound **3j**

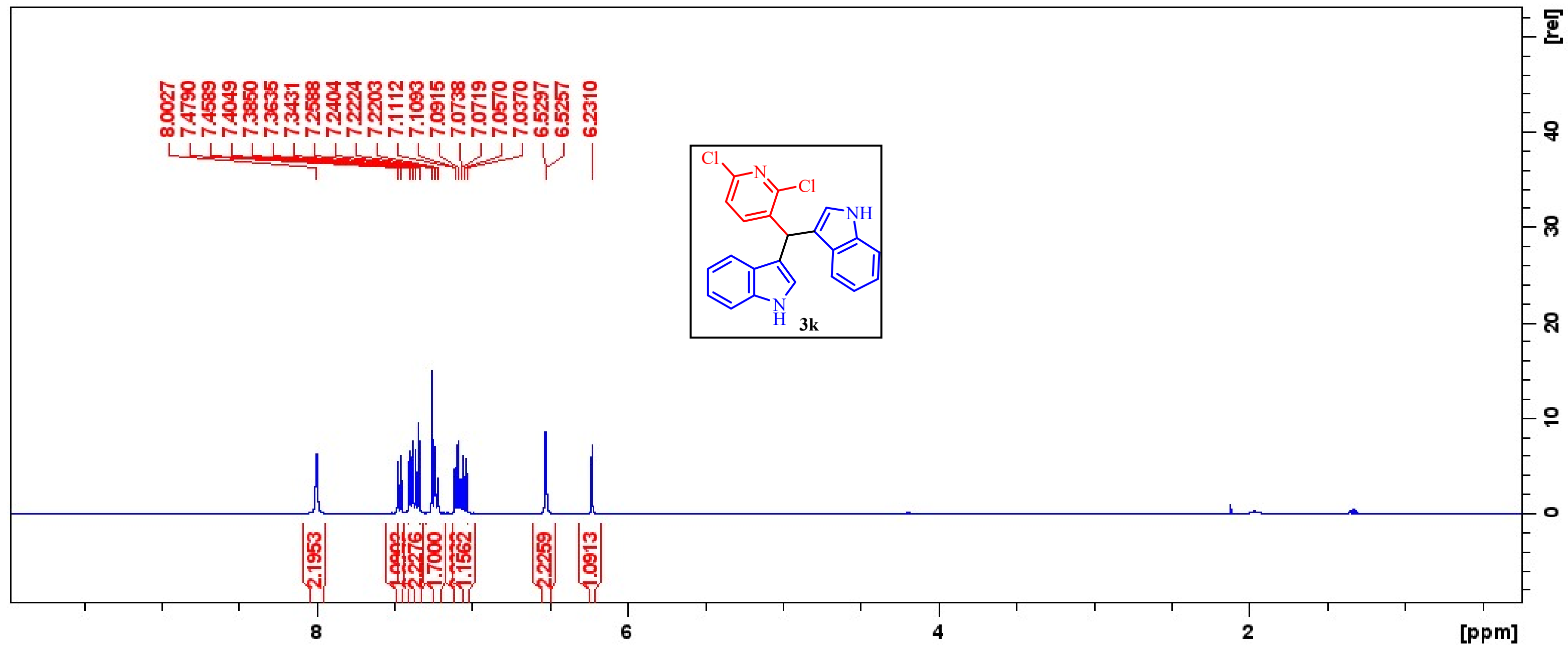


Figure 31. ¹H NMR spectrum of compound **3k**

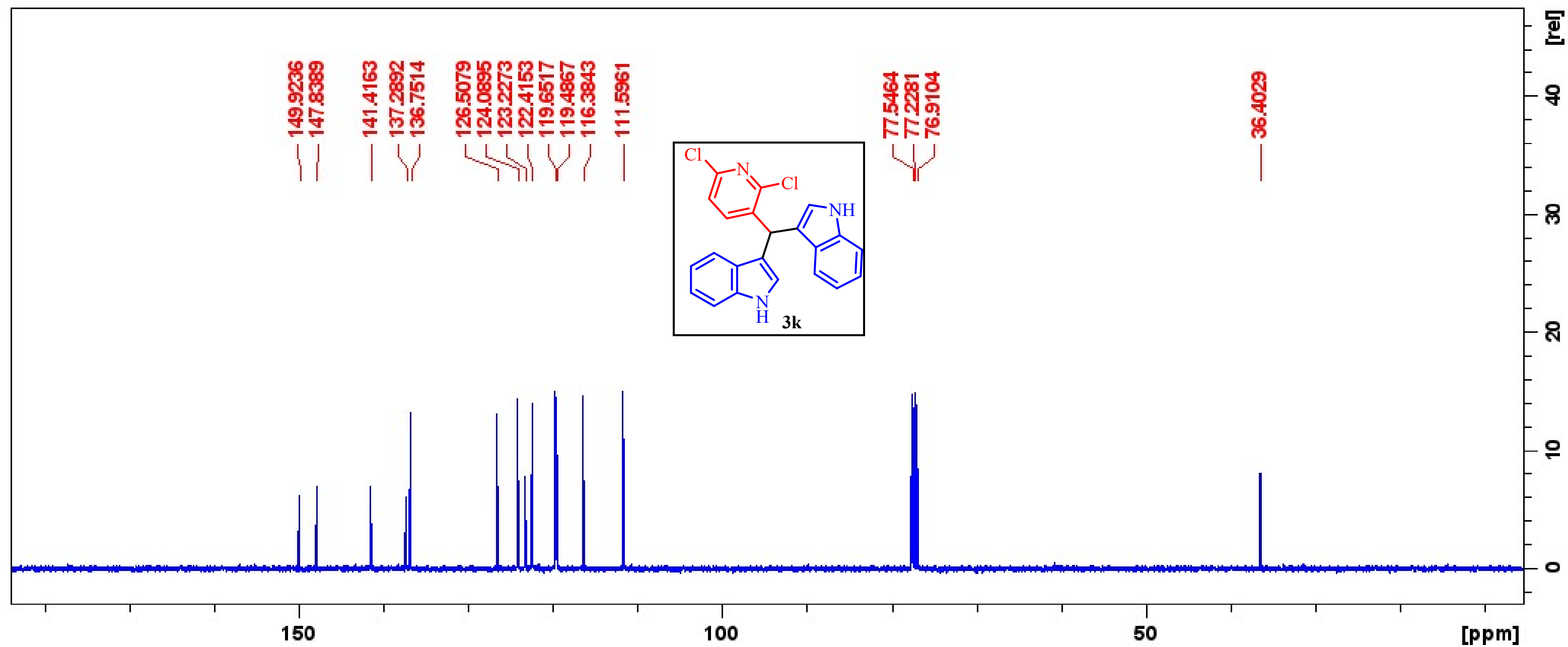


Figure 32. ¹³C NMR spectrum of compound **3k**

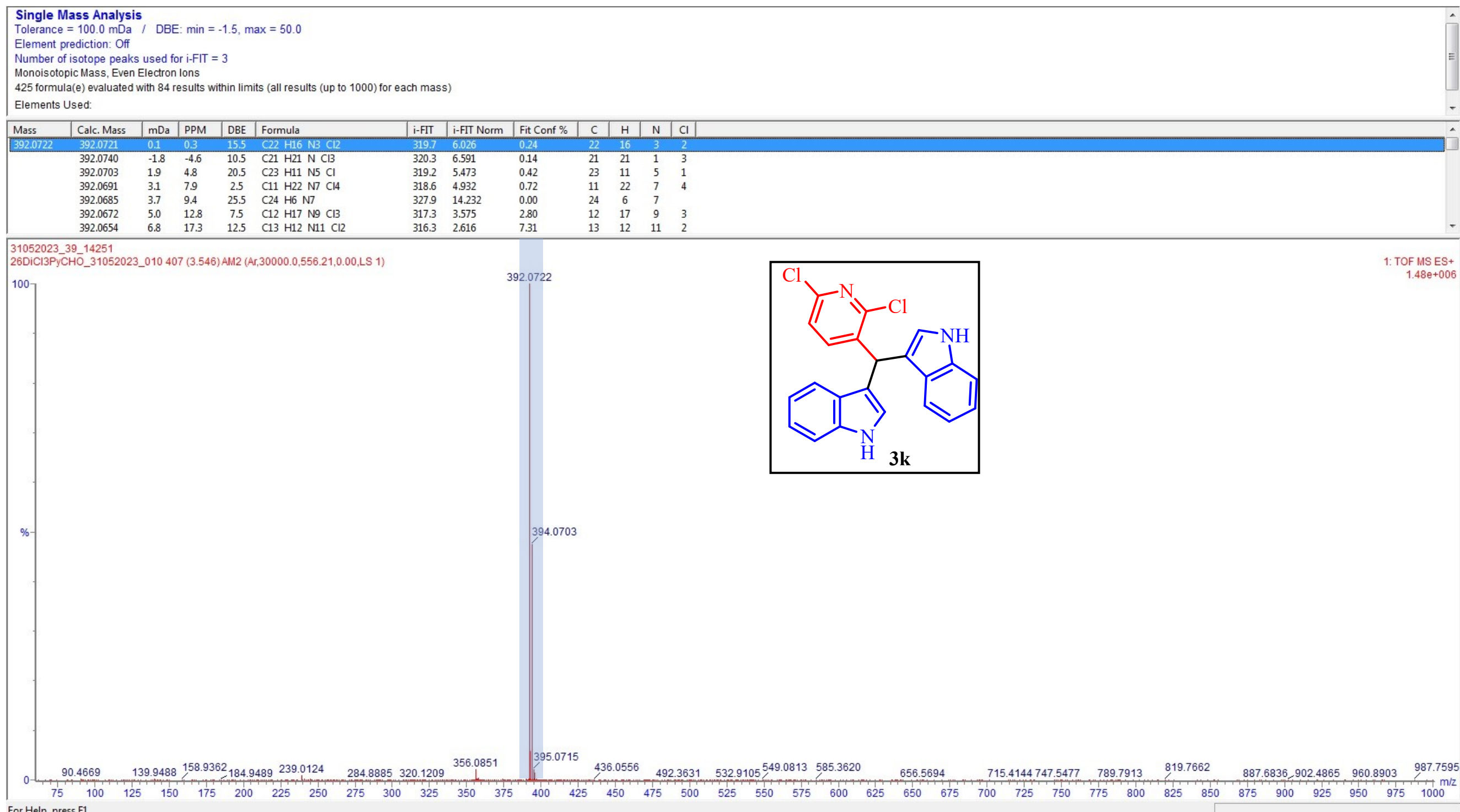


Figure 33. HRMS spectrum of compound **3k**

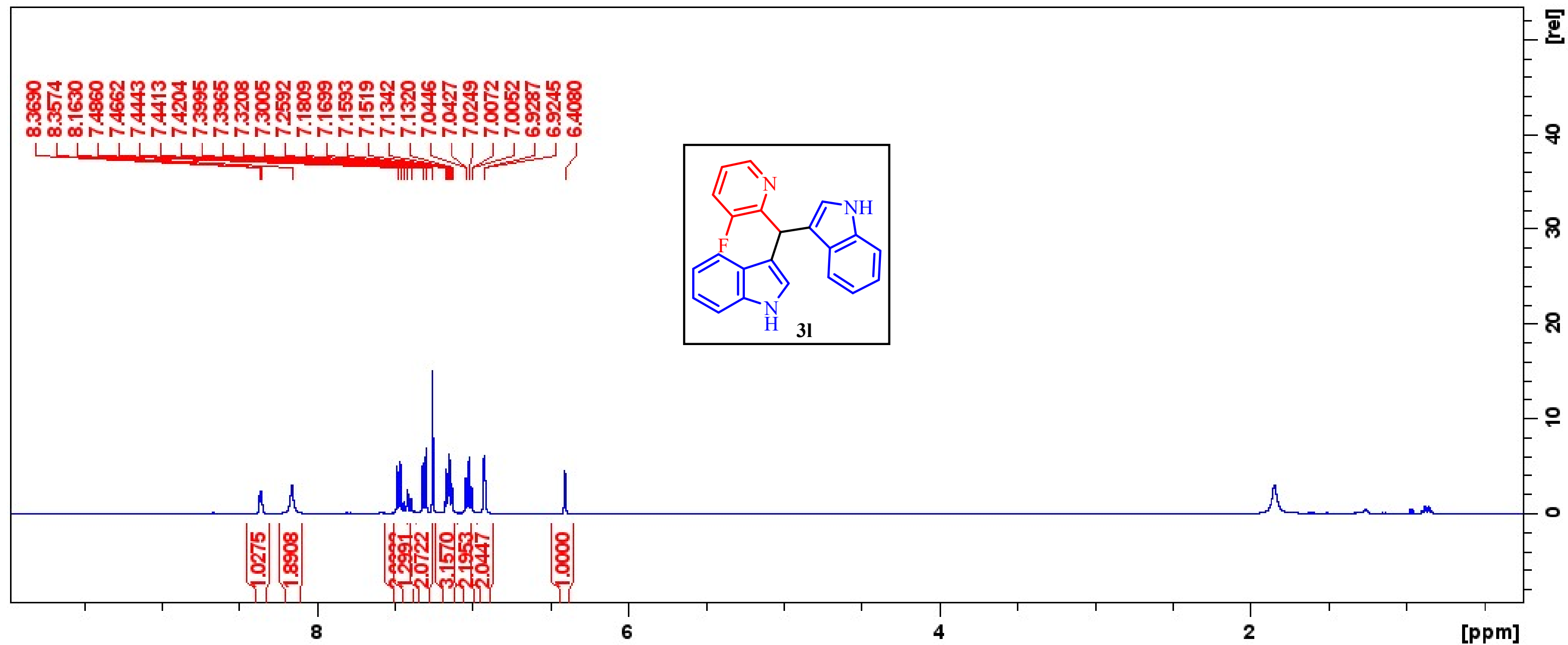


Figure 34. ¹H NMR spectrum of compound **3l**

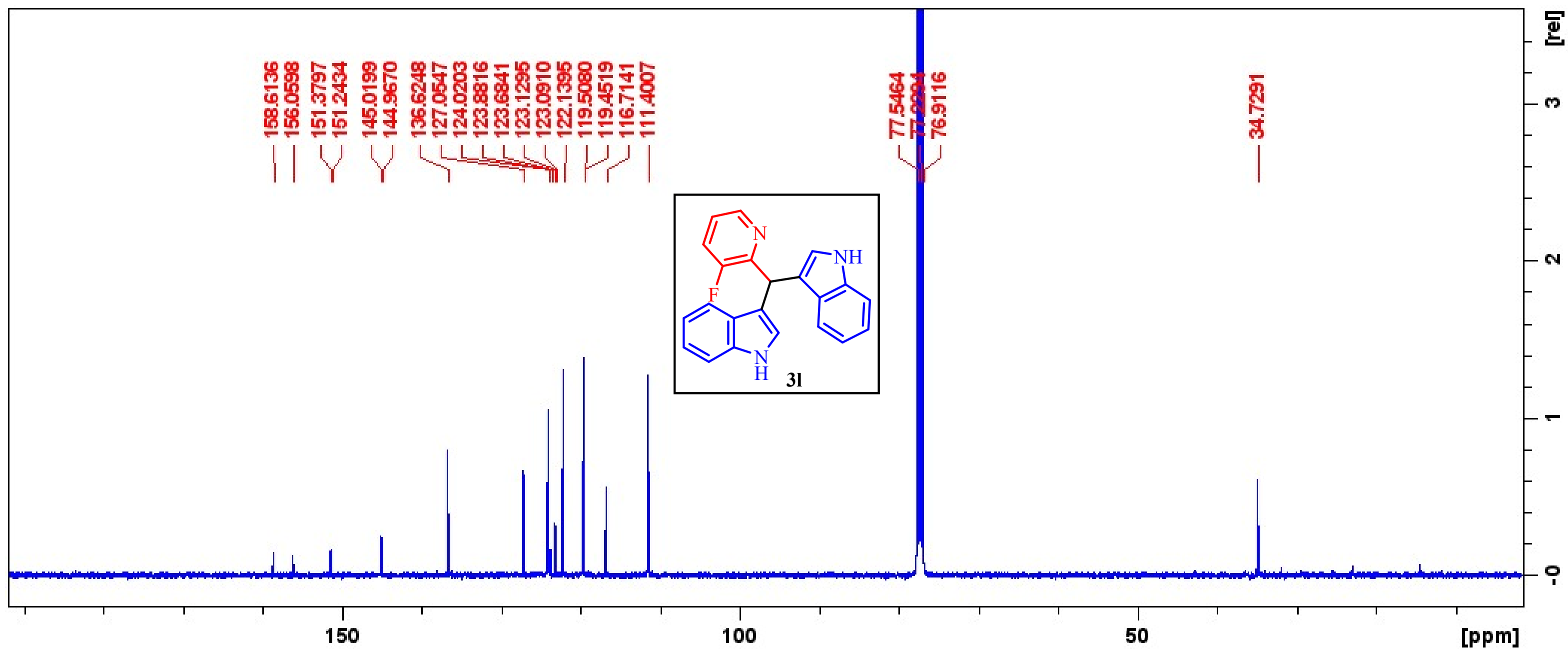


Figure 35. ¹³C NMR spectrum of compound **3l**

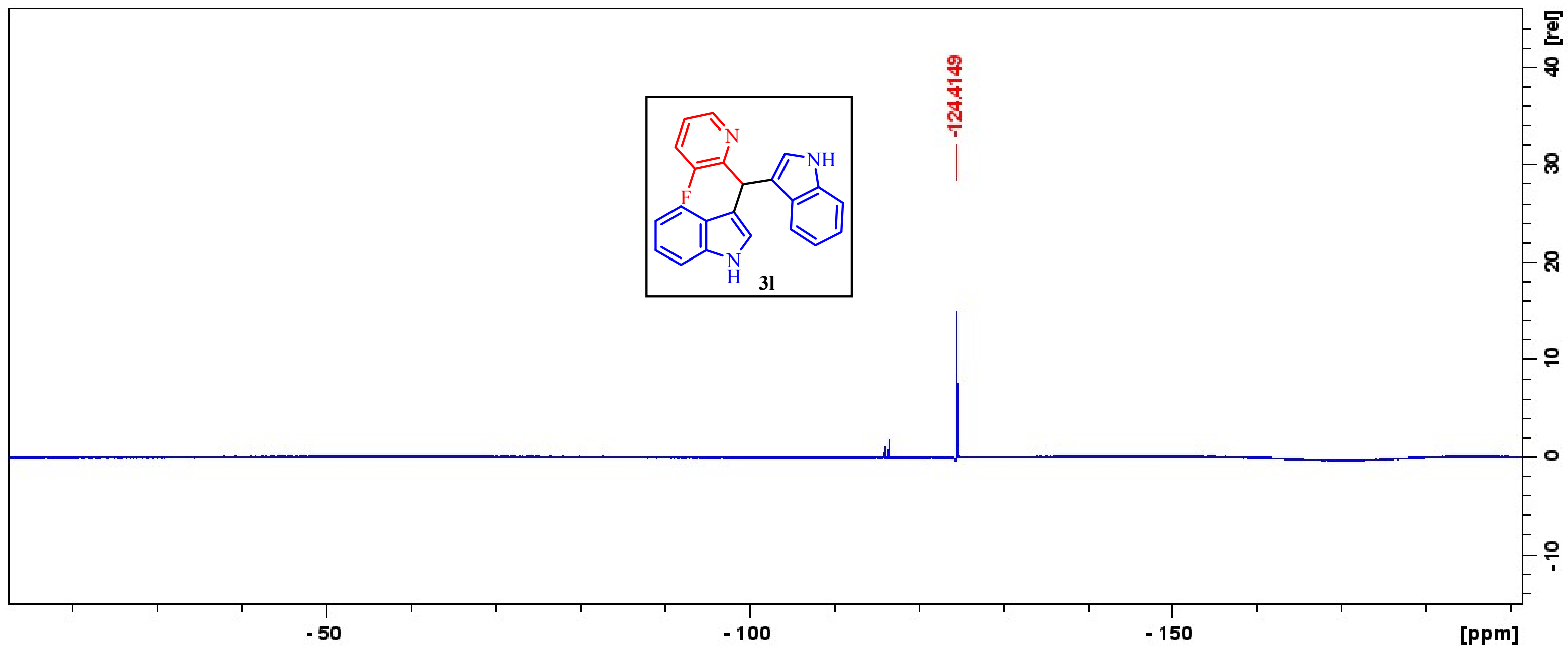


Figure 36. ^{19}F NMR spectrum of compound **3l**

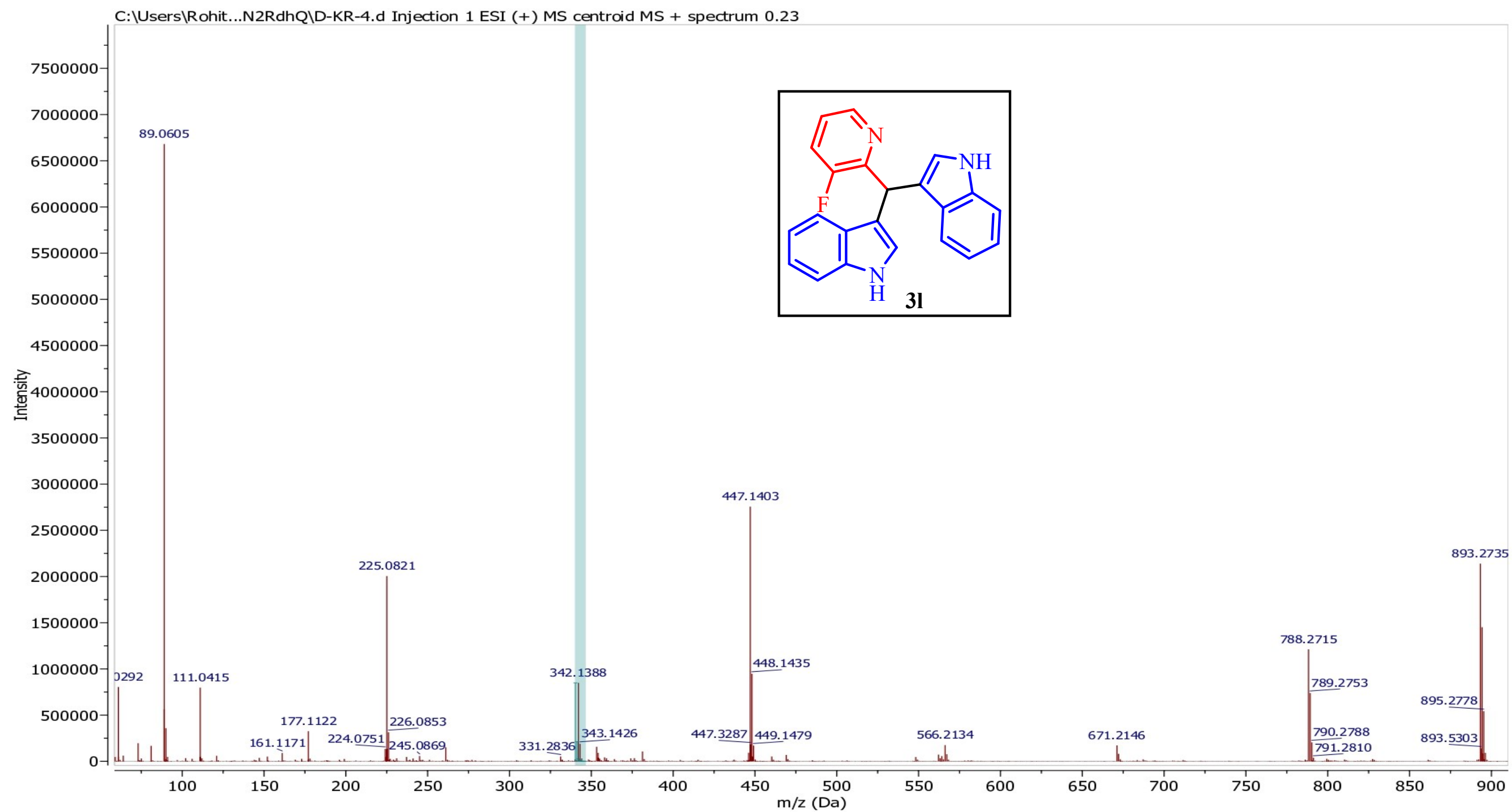


Figure 37. HRMS spectrum of compound **3l**

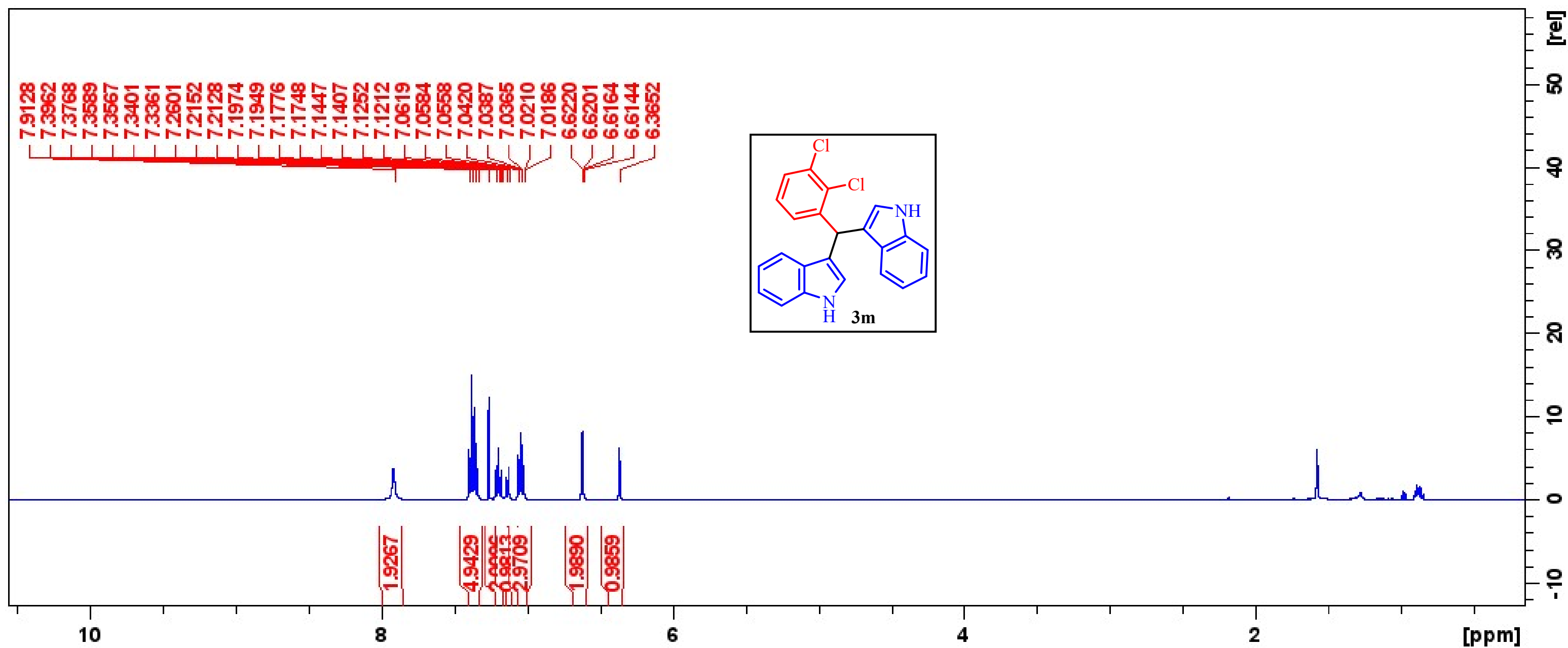


Figure 38. ¹H NMR spectrum of compound **3m**

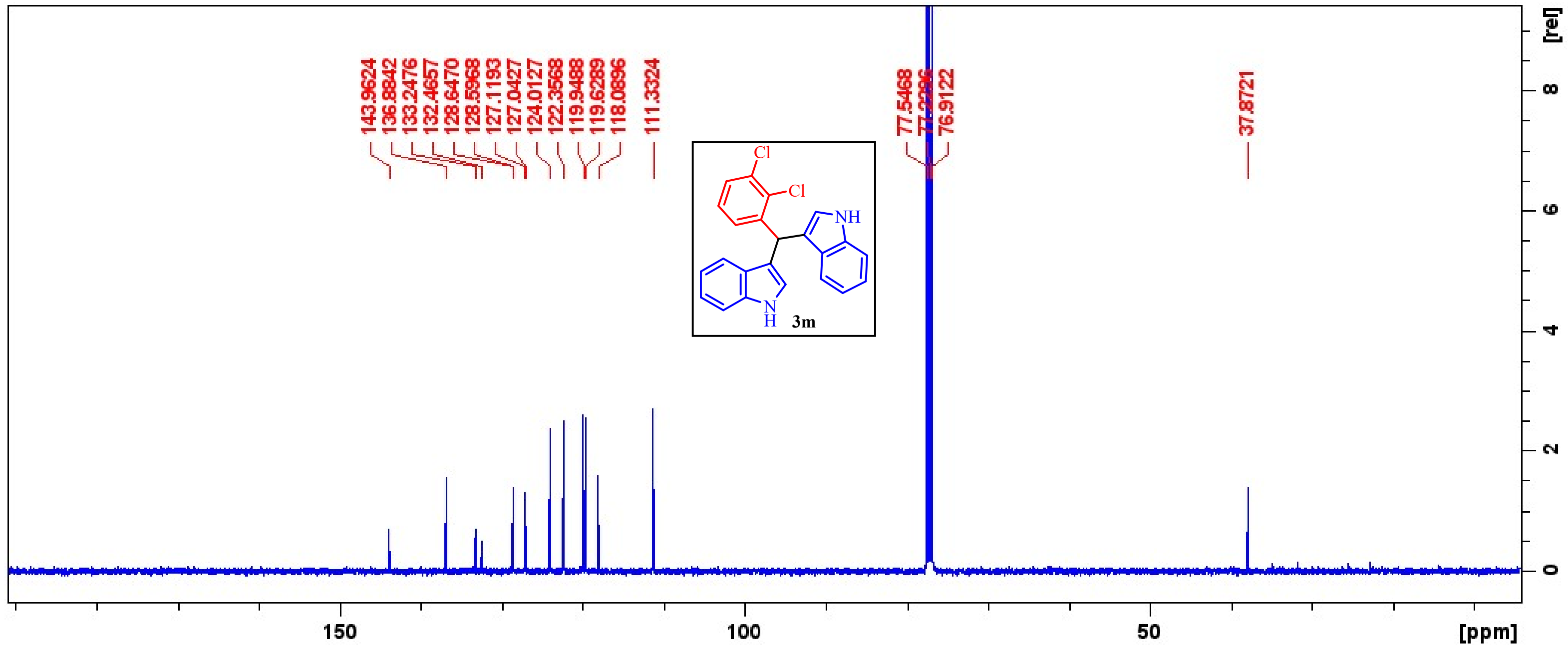


Figure 39. ^{13}C NMR spectrum of compound **3m**

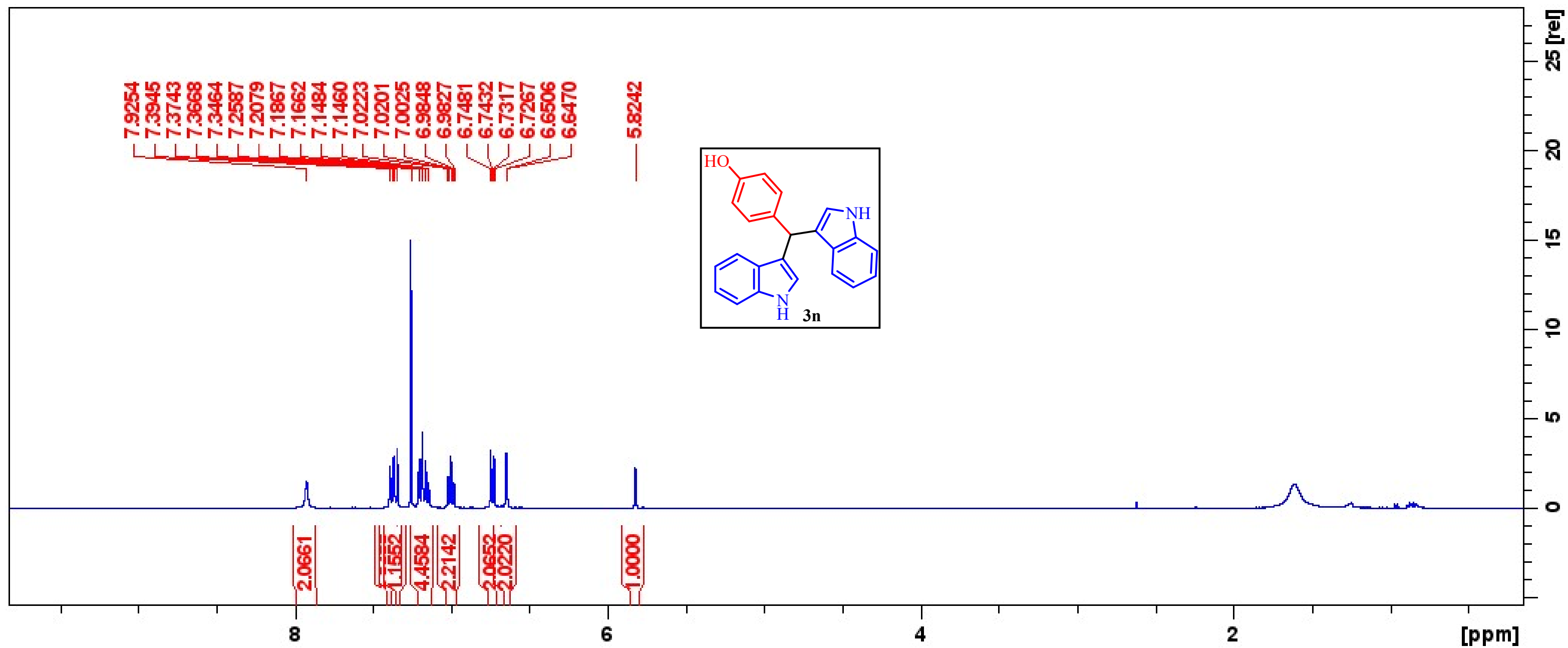


Figure 40. ^1H NMR spectrum of compound **3n**

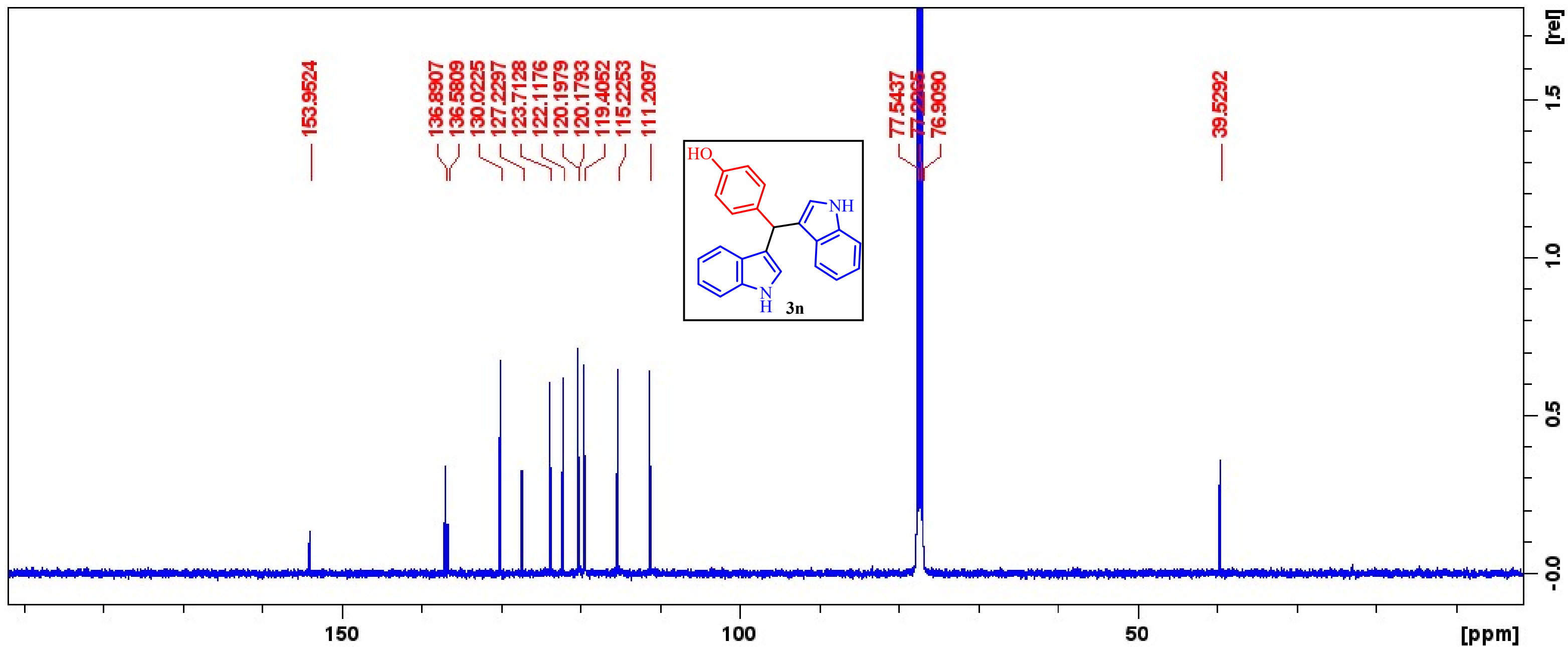


Figure 41. ^{13}C NMR spectrum of compound **3n**

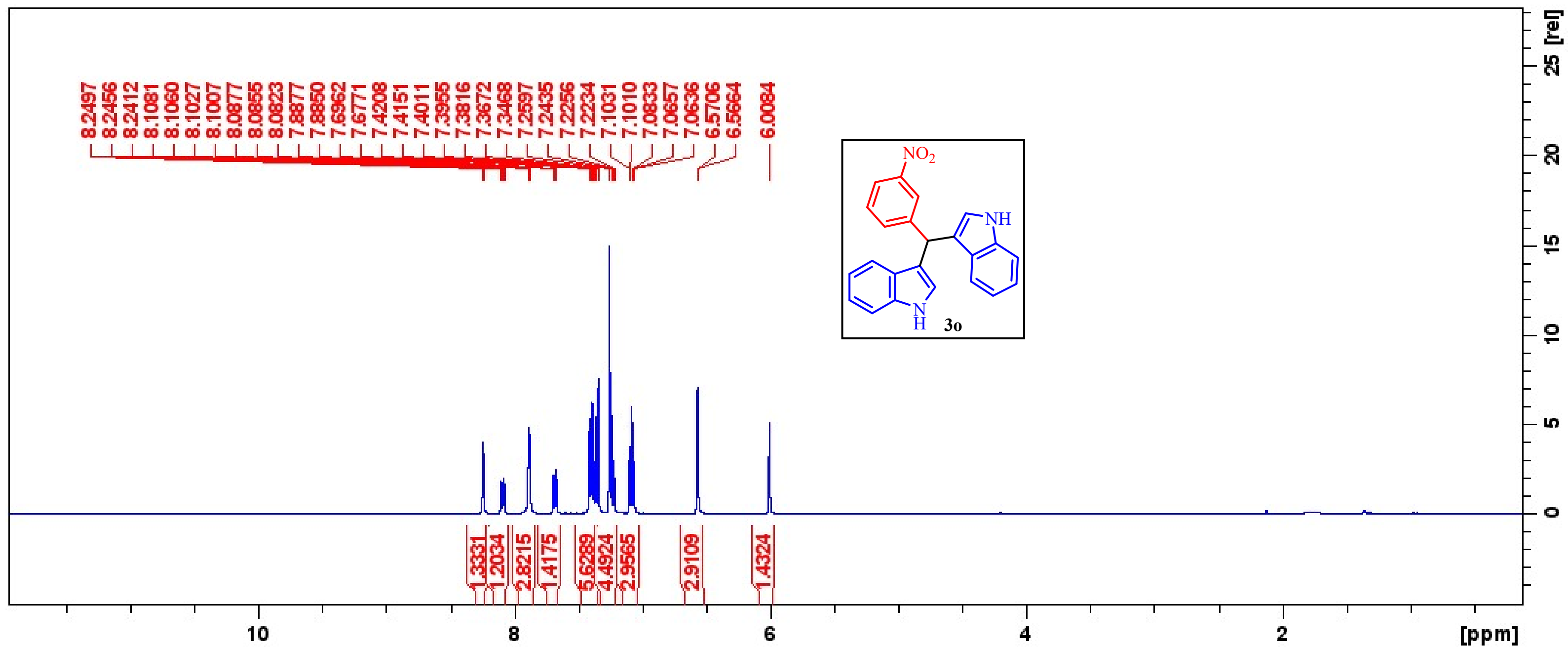


Figure 42. ¹H NMR spectrum of compound **3o**

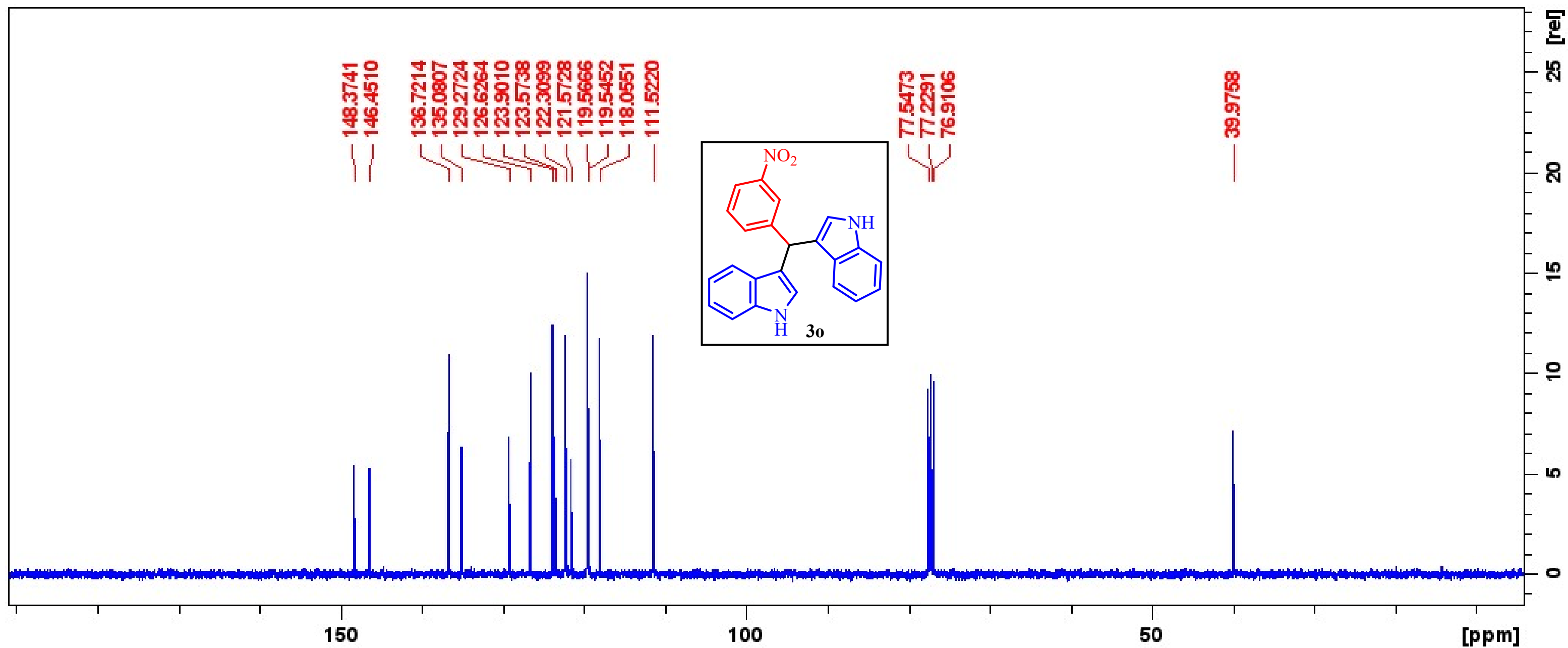


Figure 43. ^{13}C NMR spectrum of compound **3o**

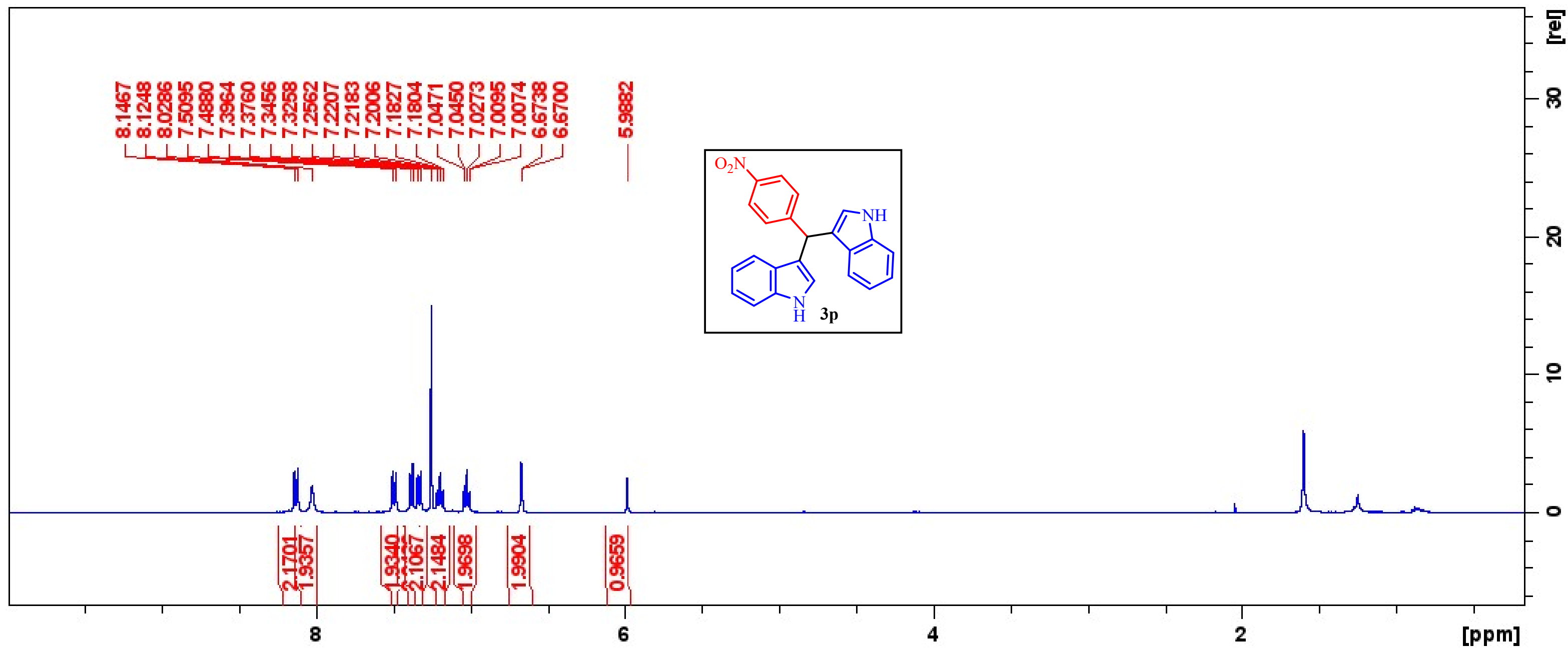


Figure 44. ^1H NMR spectrum of compound **3p**

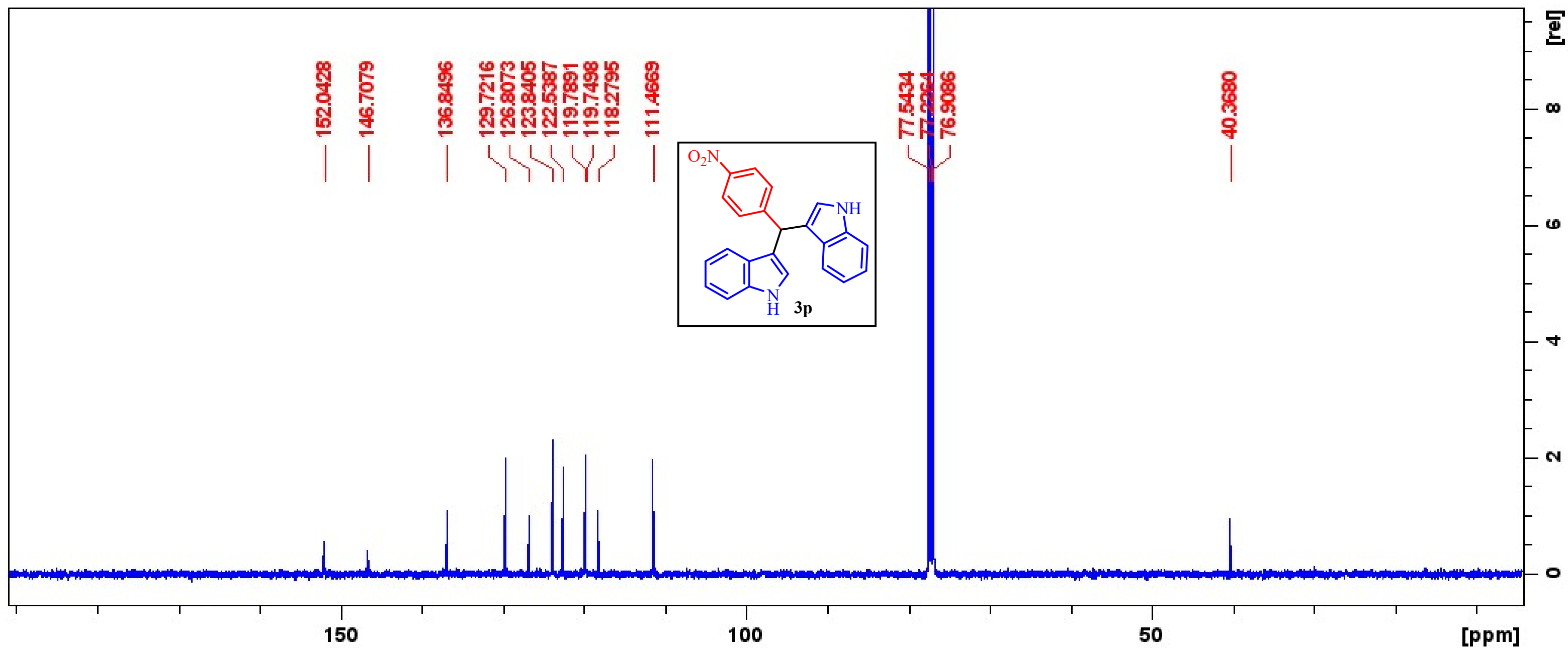


Figure 45. ^{13}C NMR spectrum of compound **3p**

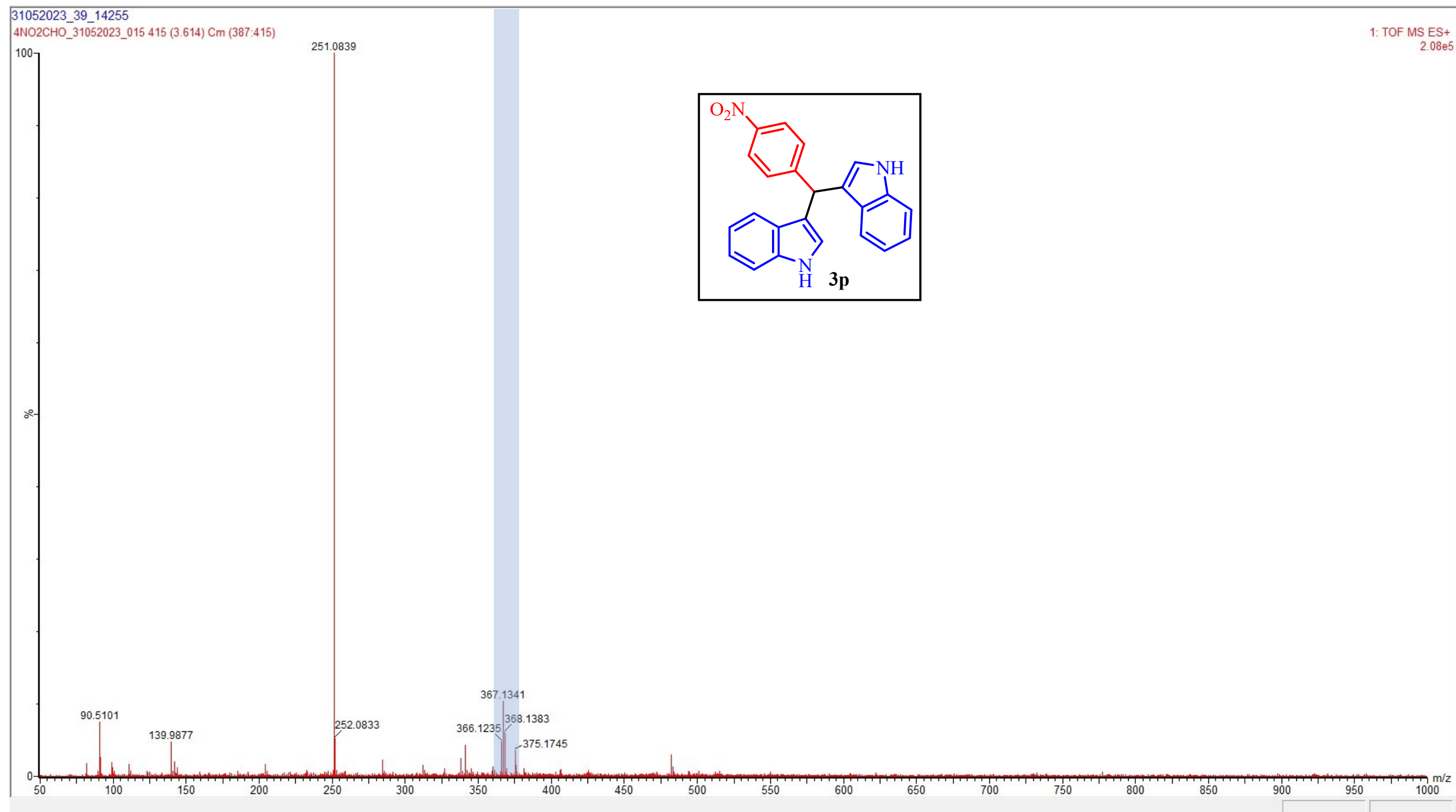


Figure 46. HRMS spectrum of compound **3p**

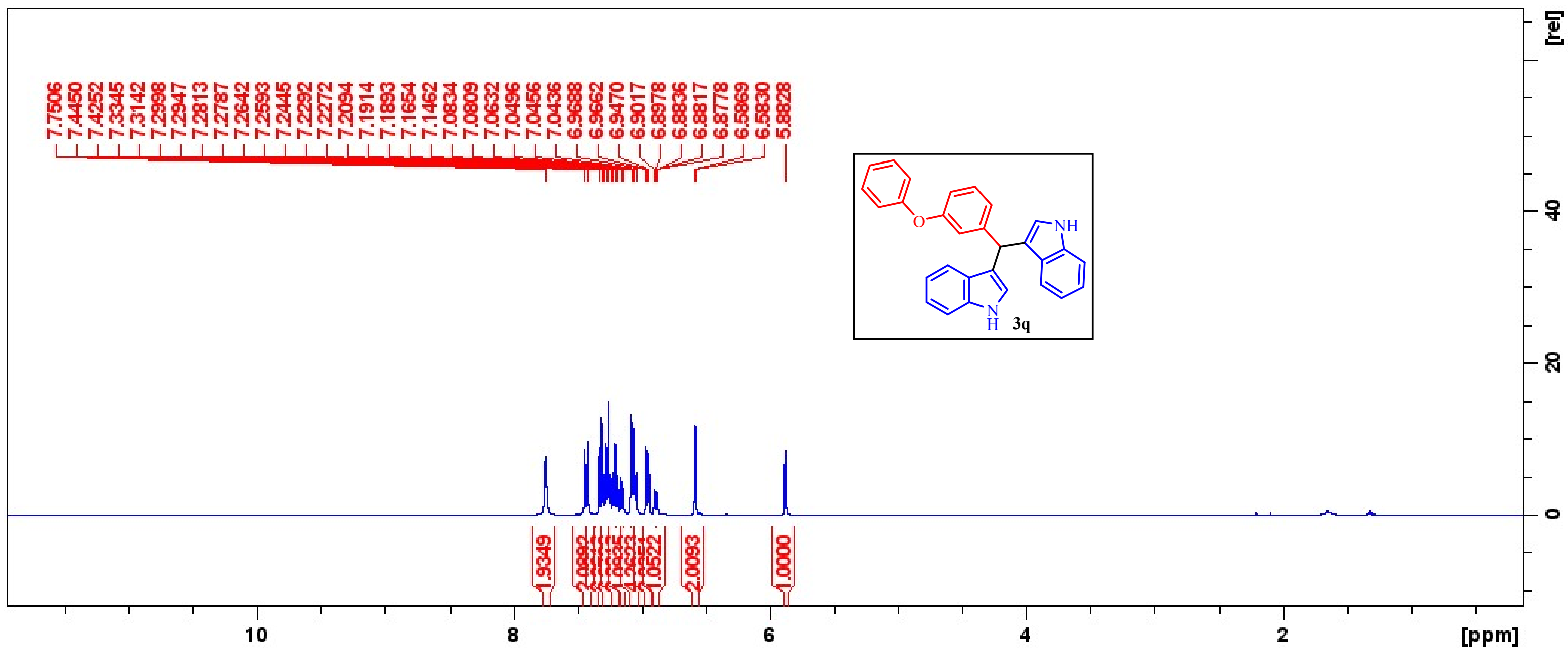


Figure 47. ^1H NMR spectrum of compound **3q**

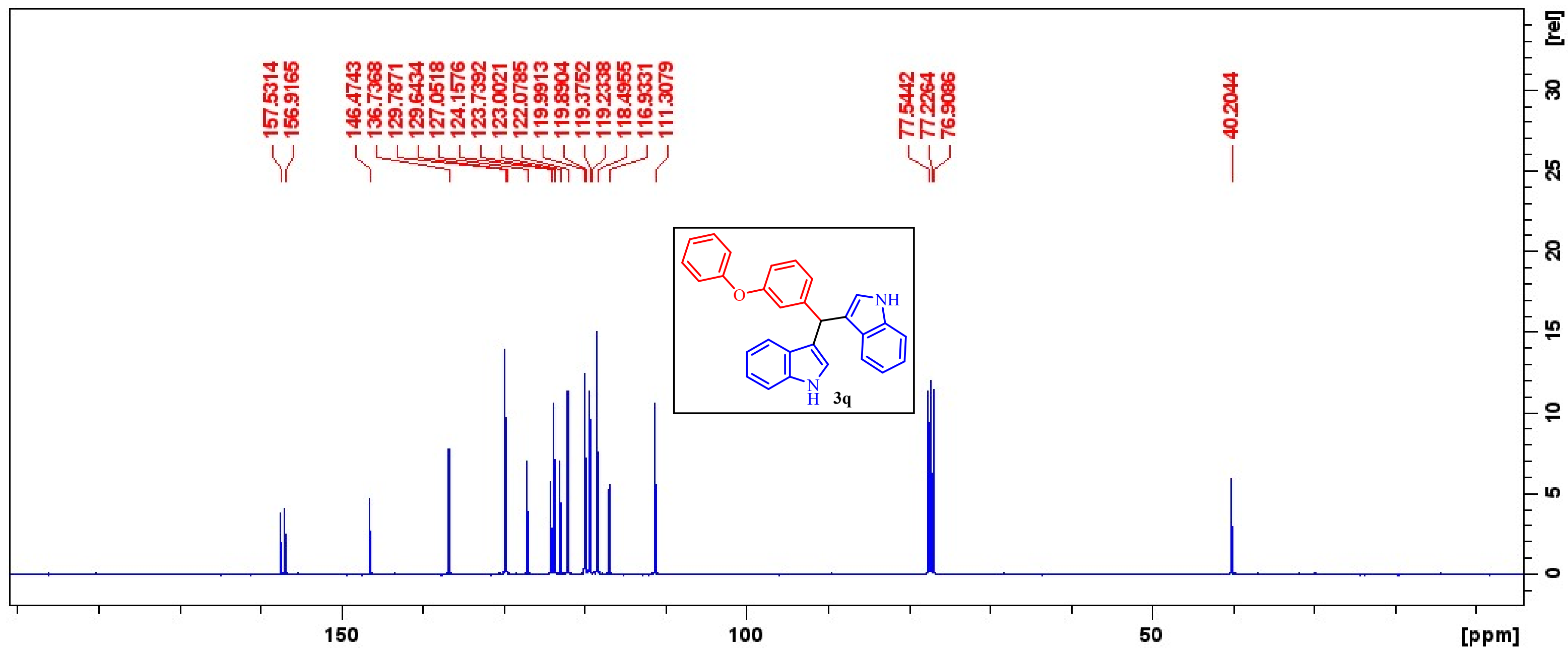


Figure 48. ^{13}C NMR spectrum of compound **3q**

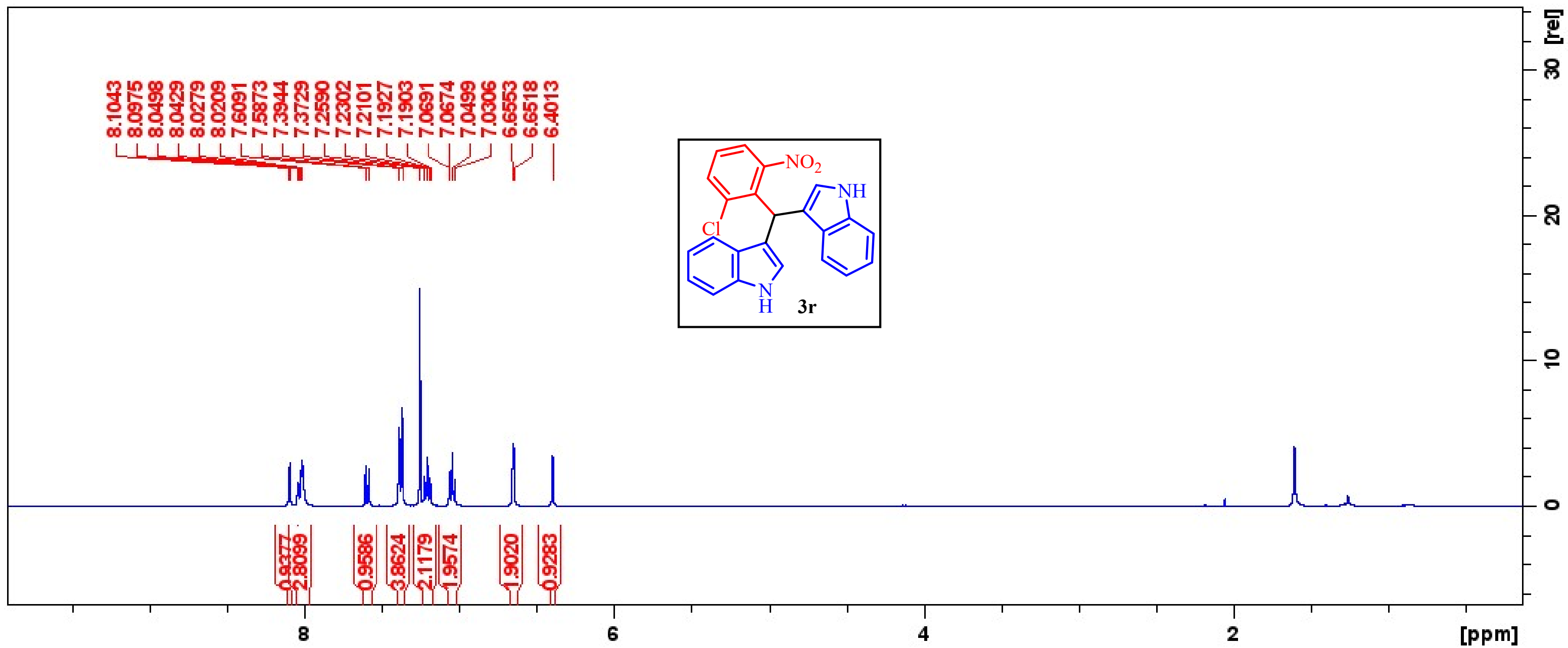


Figure 49. ¹H NMR spectrum of compound **3r**

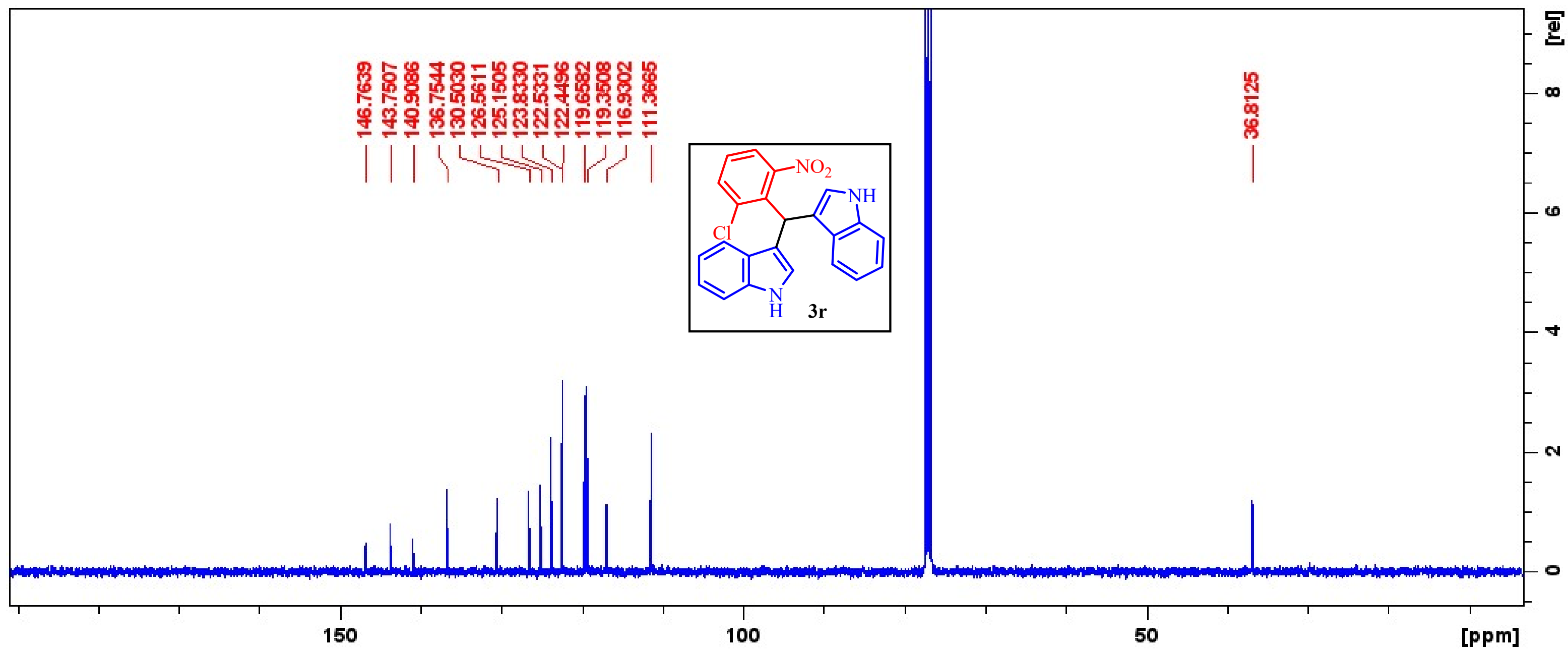


Figure 50. ¹³C NMR spectrum of compound **3r**

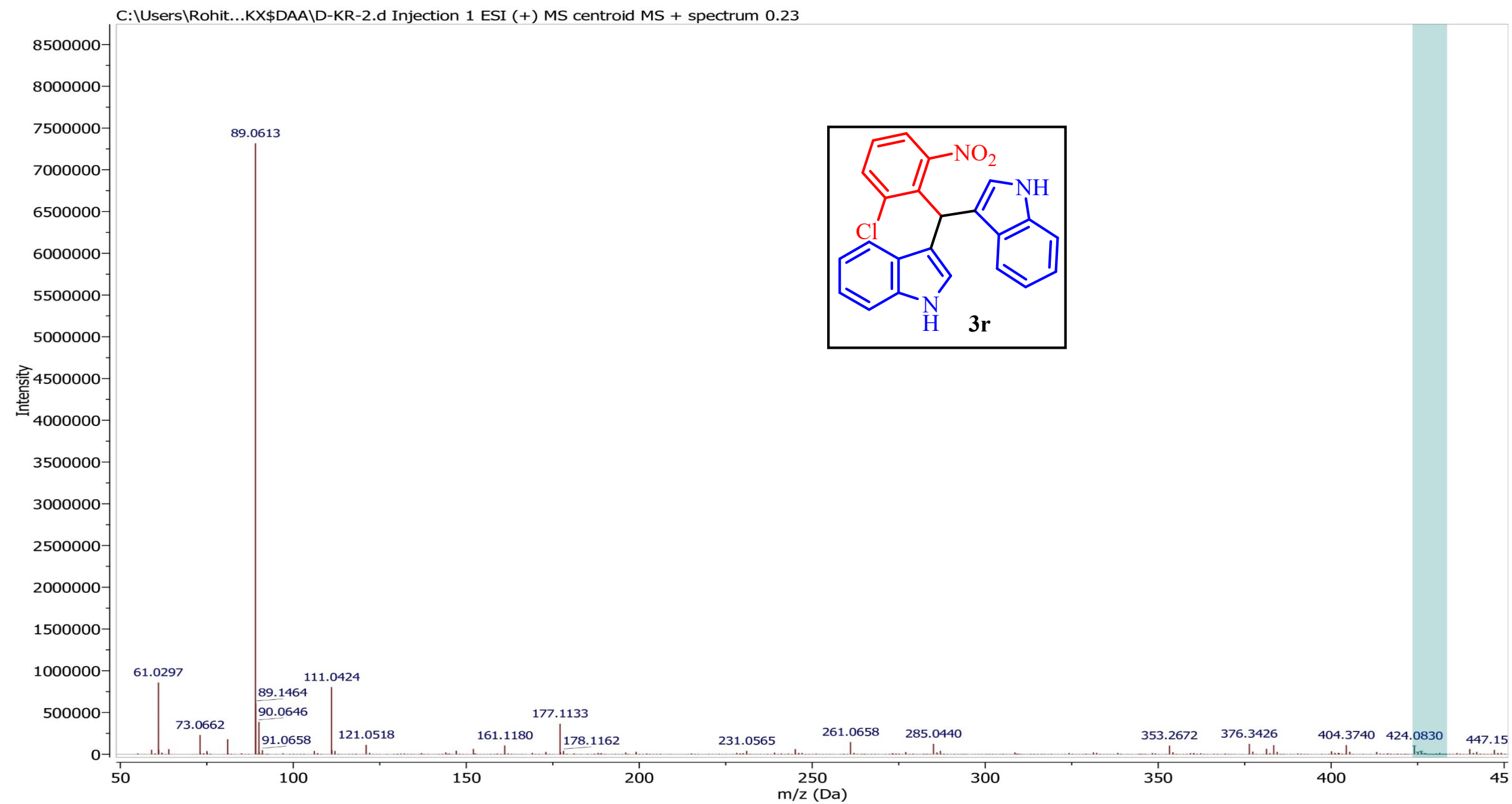


Figure 51. HRMS spectrum of compound **3r**

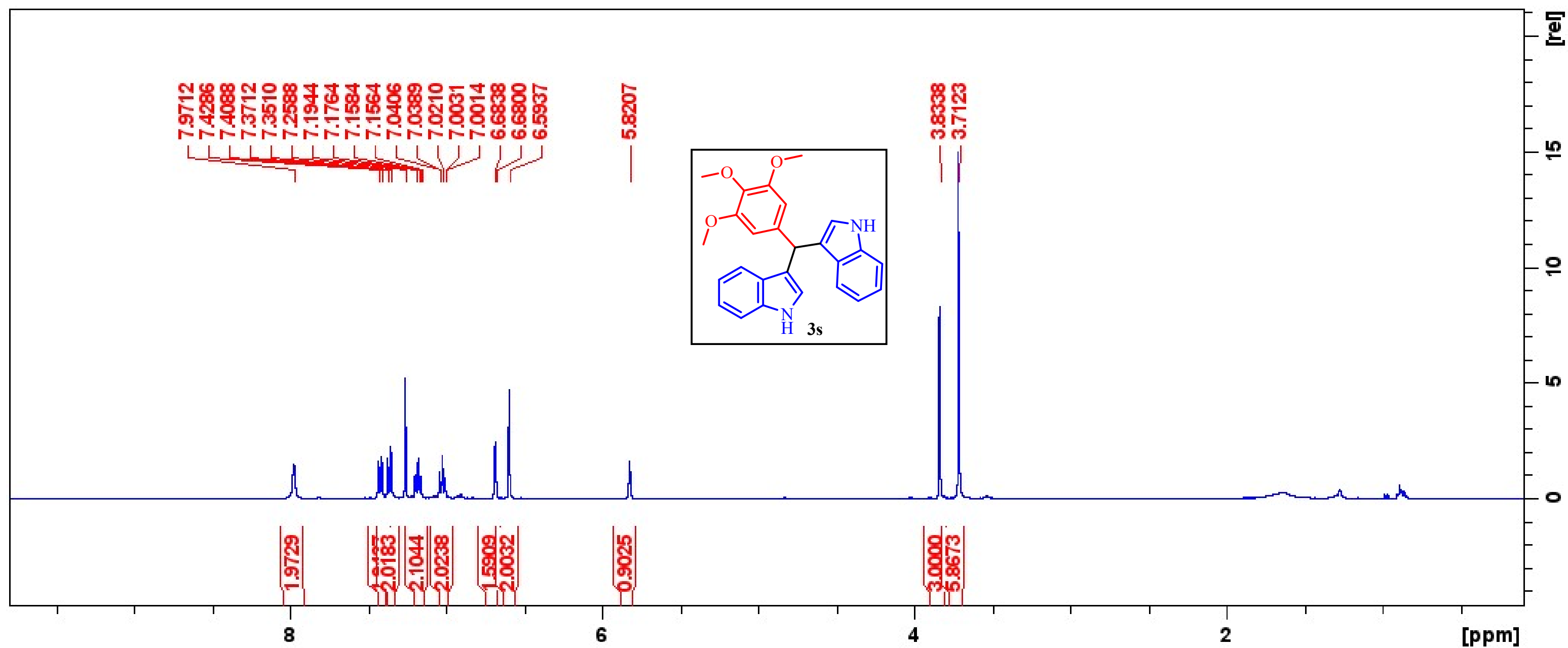


Figure 52. ^1H NMR spectrum of compound 3s

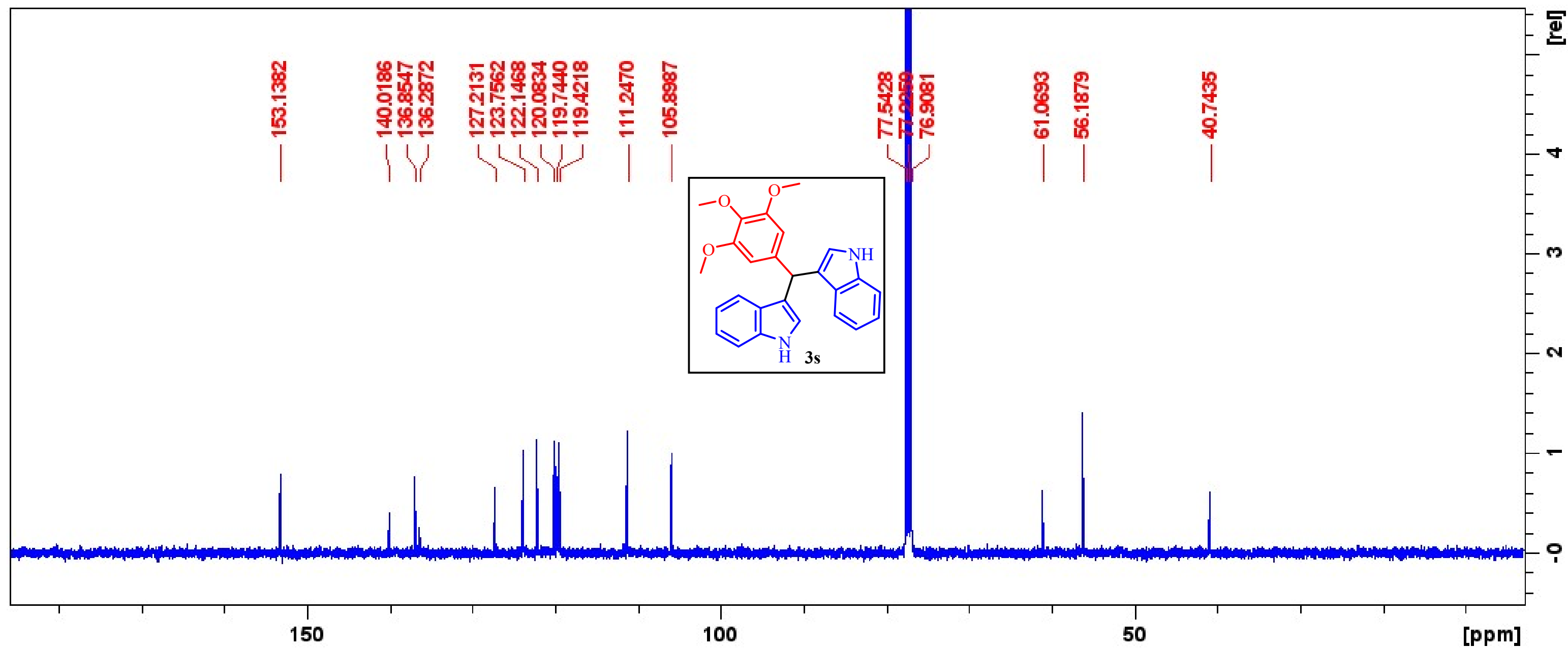


Figure 53. ^{13}C NMR spectrum of compound 3s

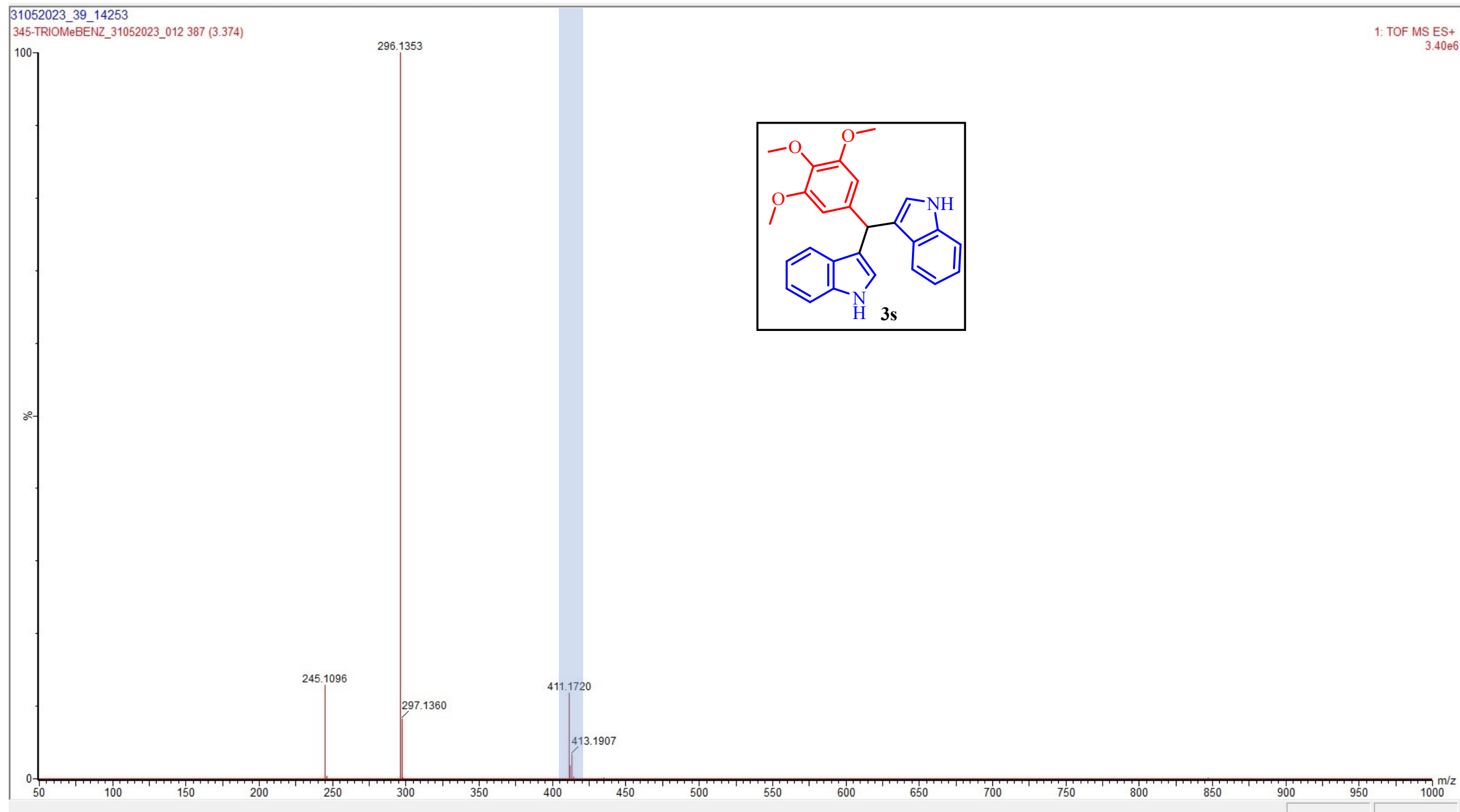


Figure 54. HRMS spectrum of compound **3s**

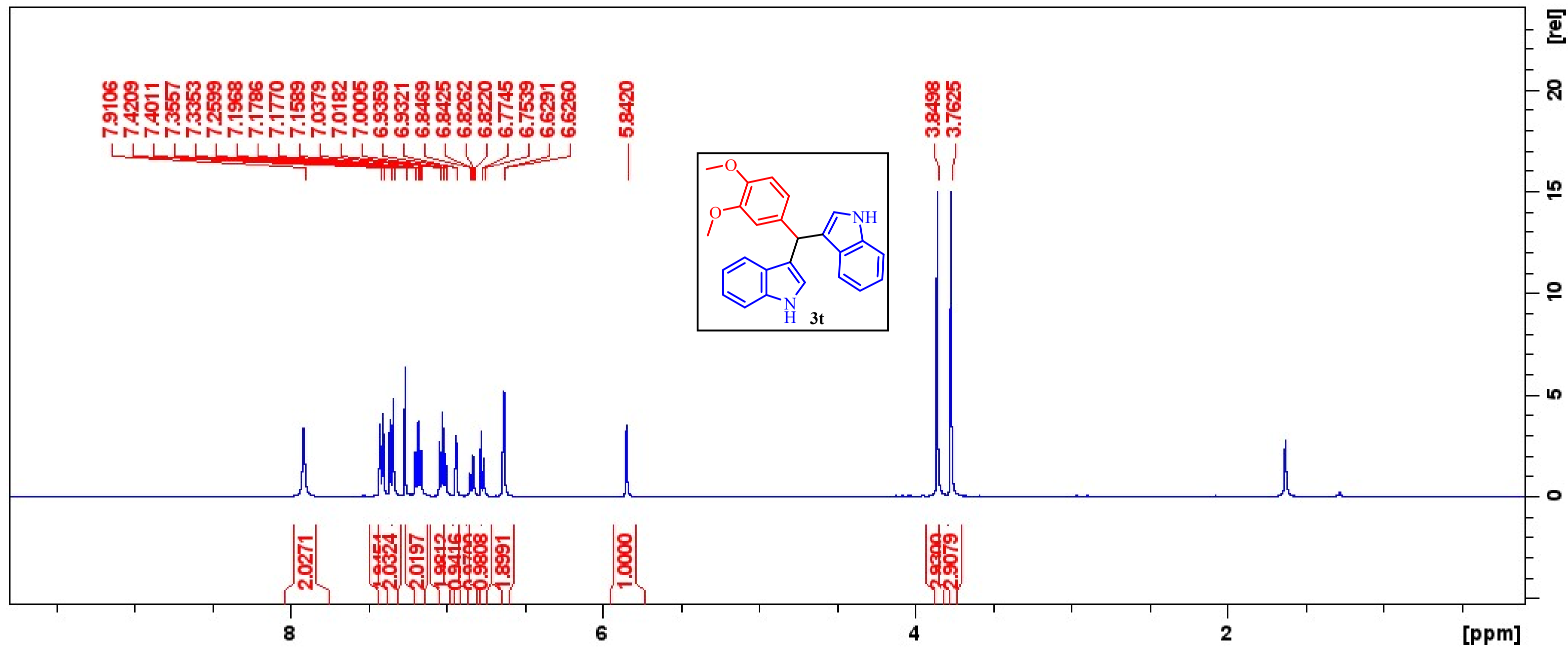


Figure 55. ^1H NMR spectrum of compound **3t**

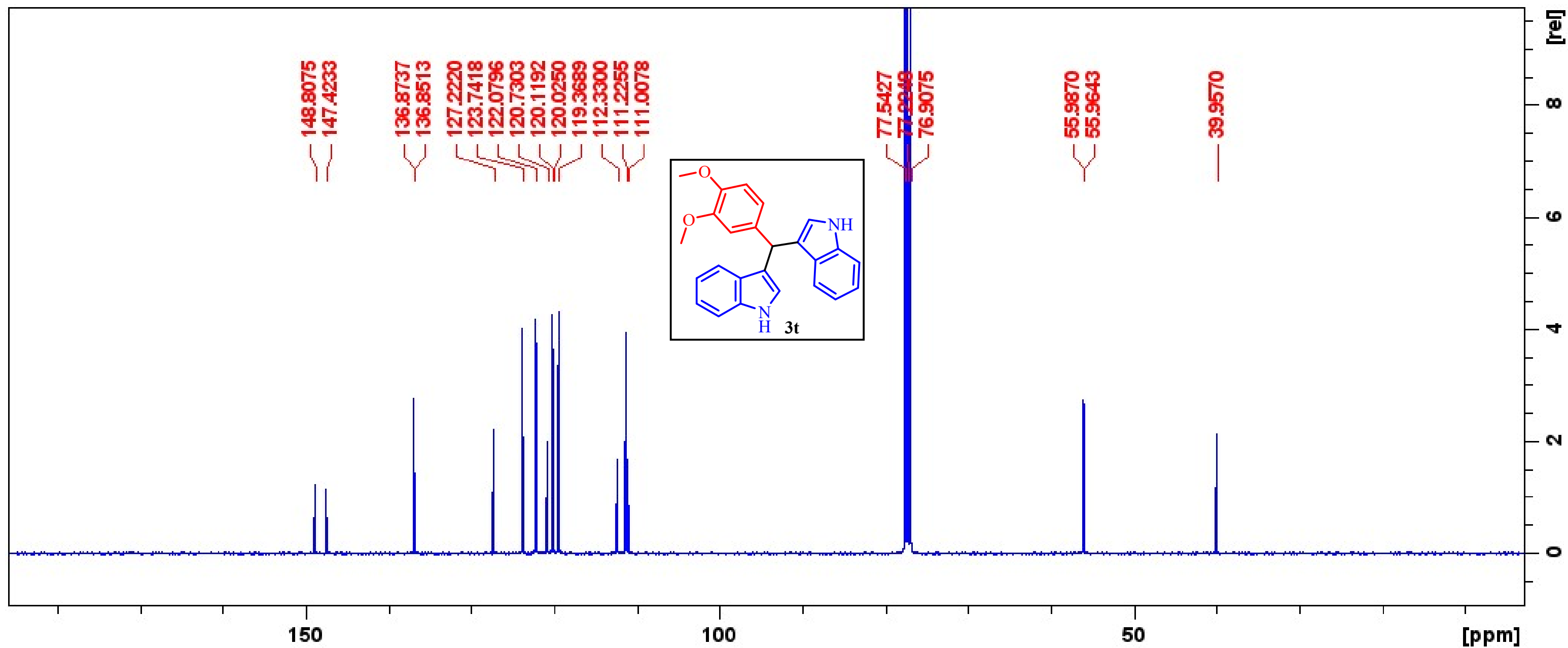


Figure 56. ^{13}C NMR spectrum of compound **3t**

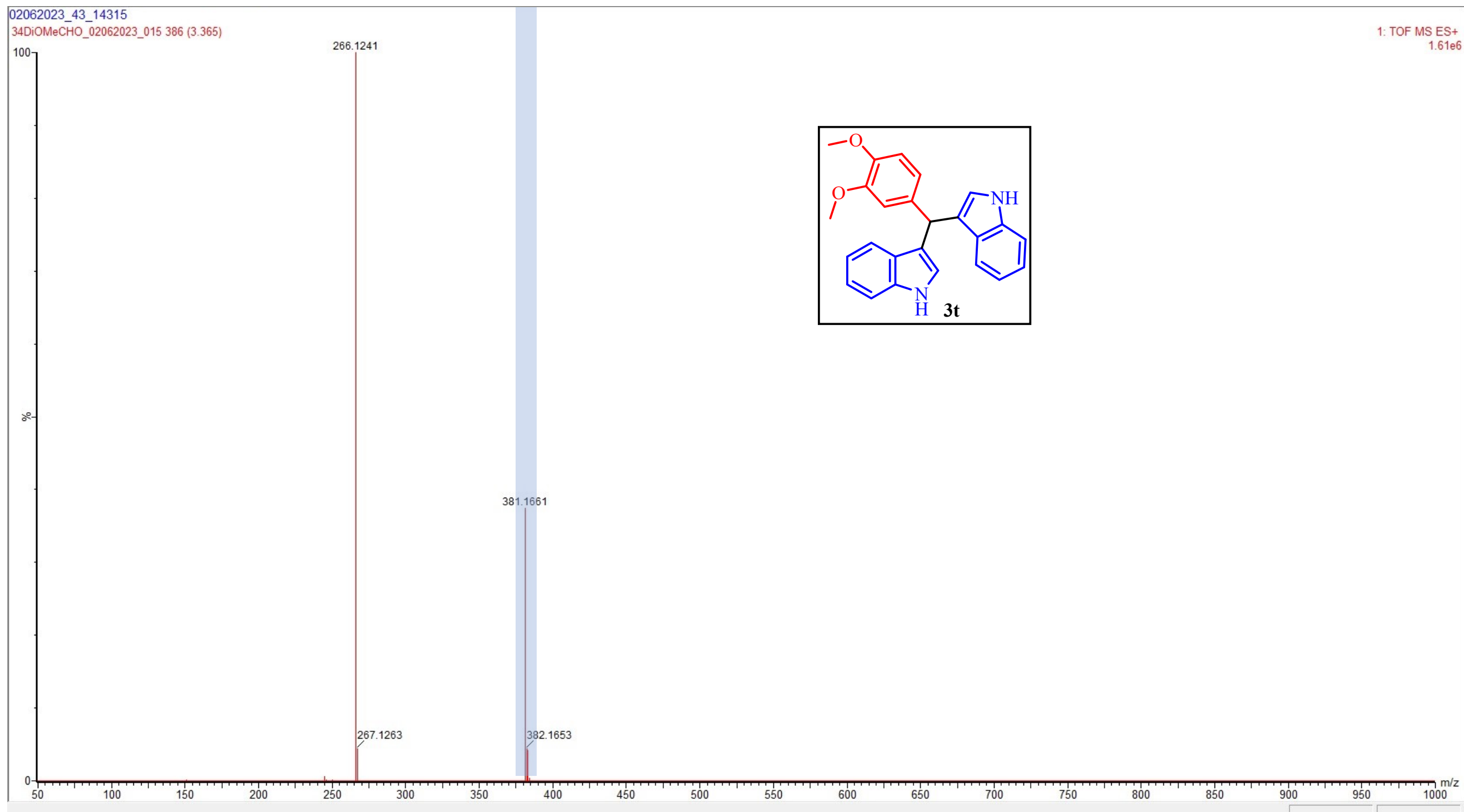


Figure 57. HRMS spectrum of compound **3t**

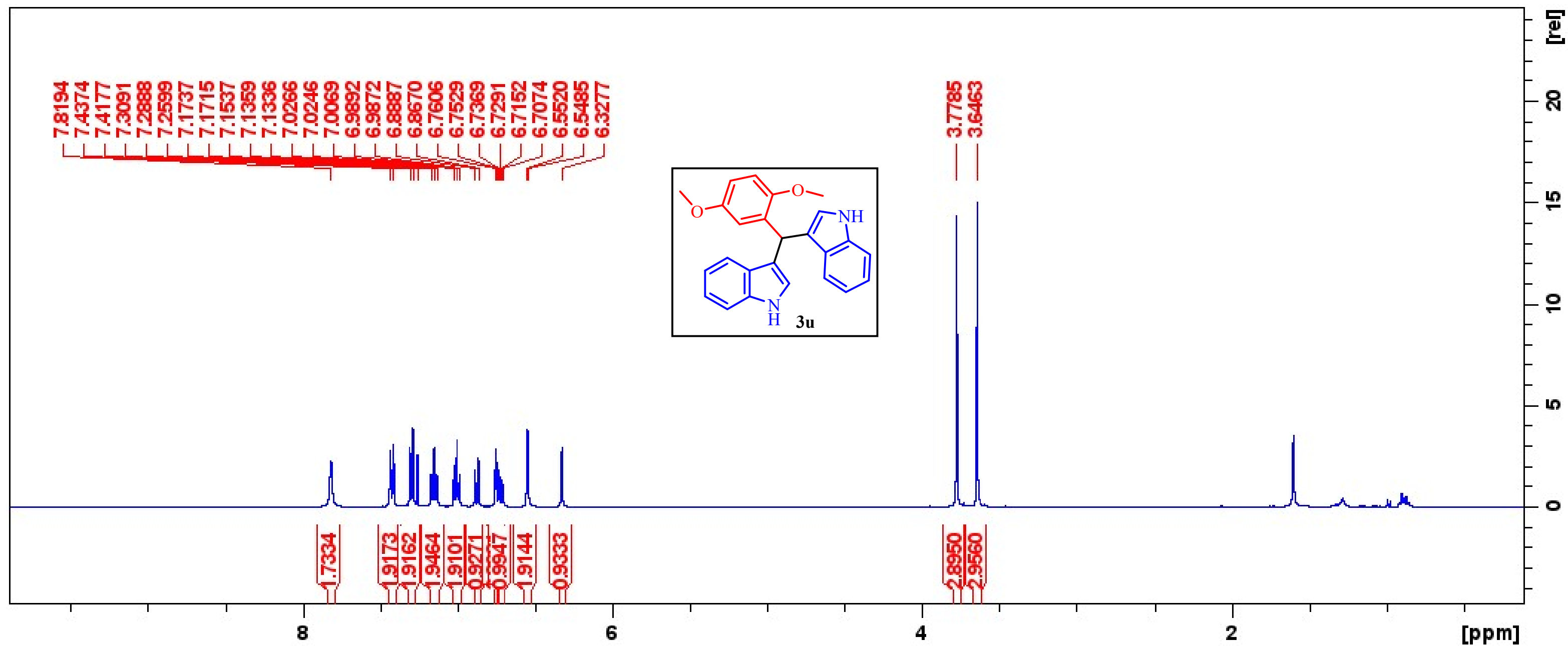


Figure 58. ^1H NMR spectrum of compound **3u**

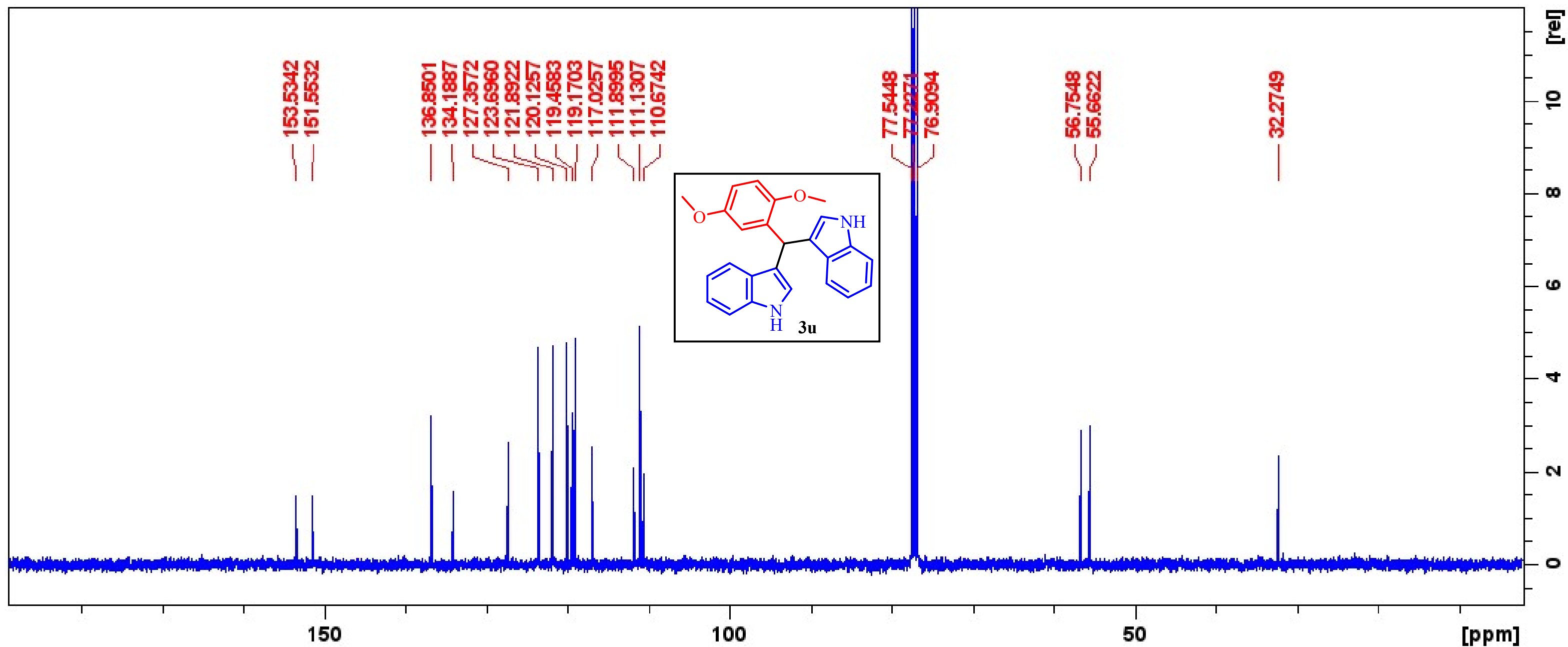


Figure 59. ^{13}C NMR spectrum of compound **3u**

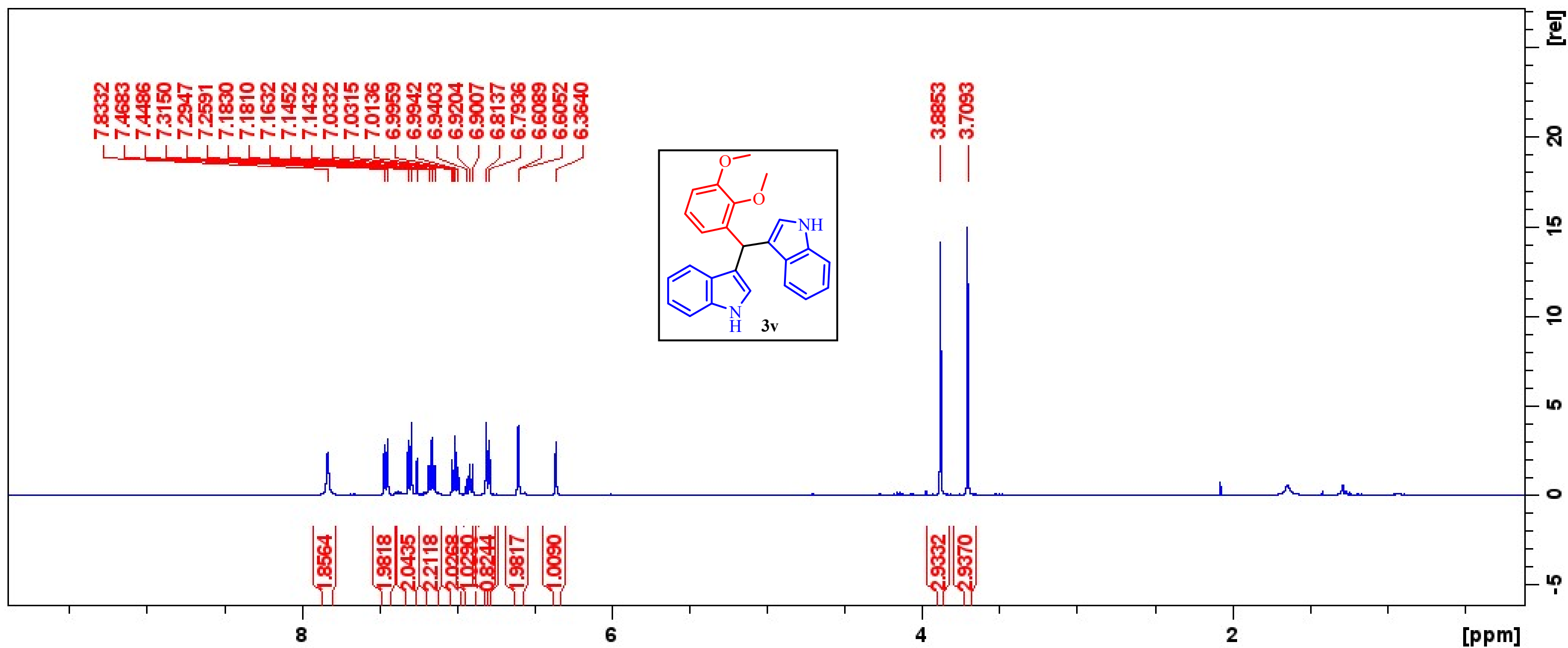


Figure 60. ¹H NMR spectrum of compound 3v

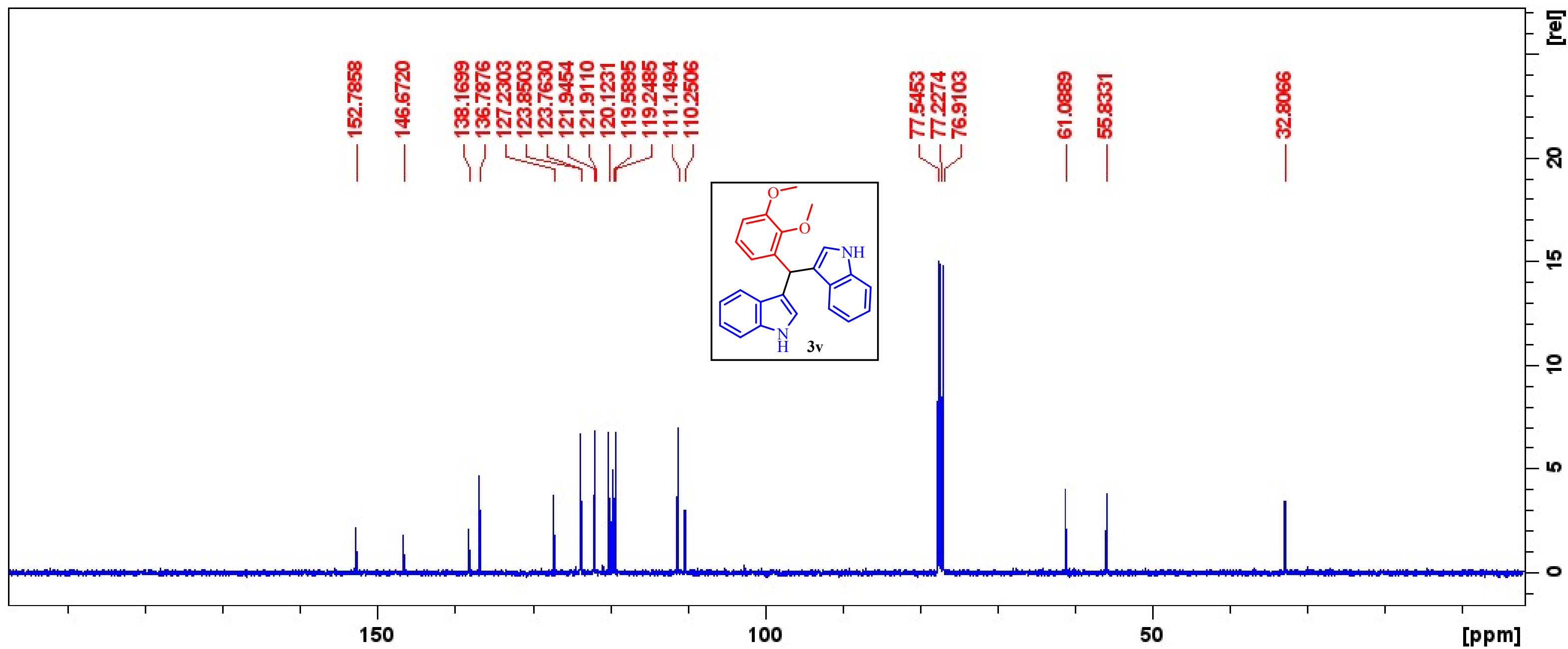


Figure 61. ¹³C NMR spectrum of compound **3v**

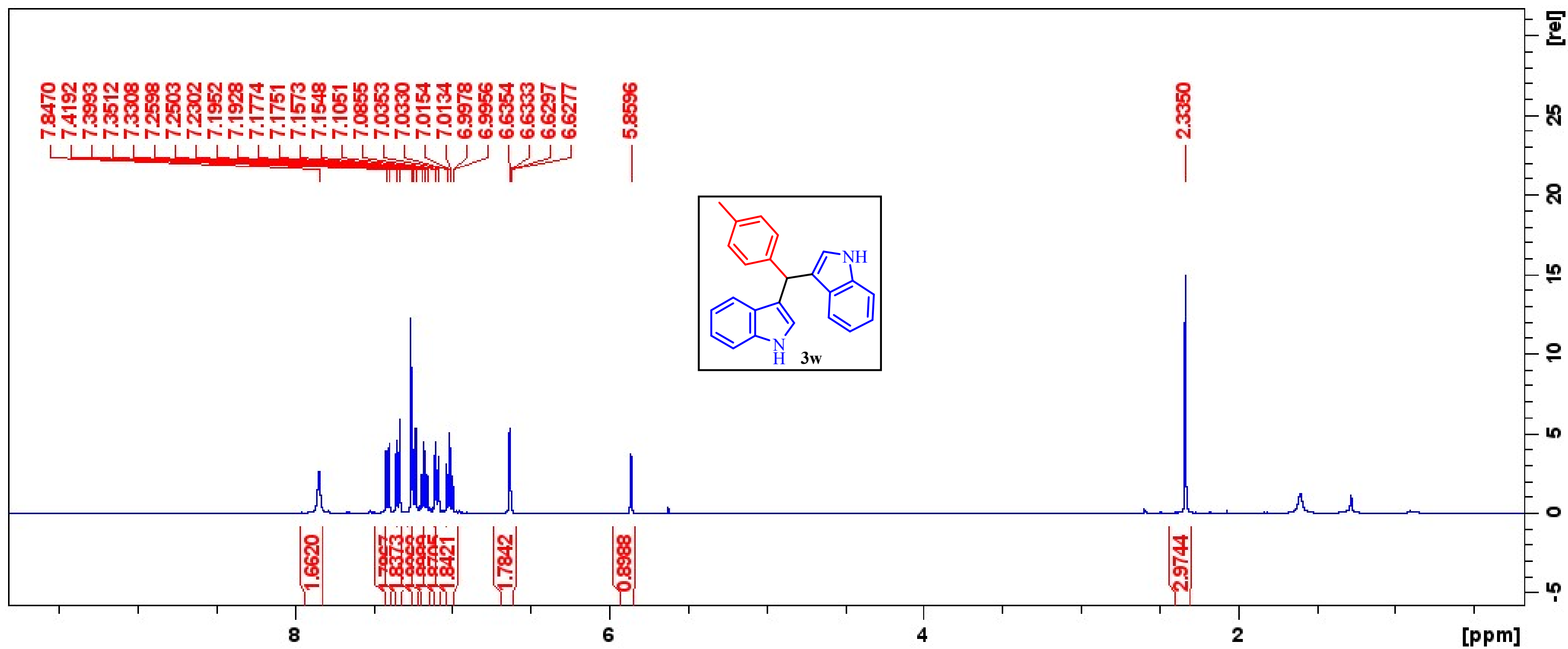


Figure 62. ¹H NMR spectrum of compound **3w**

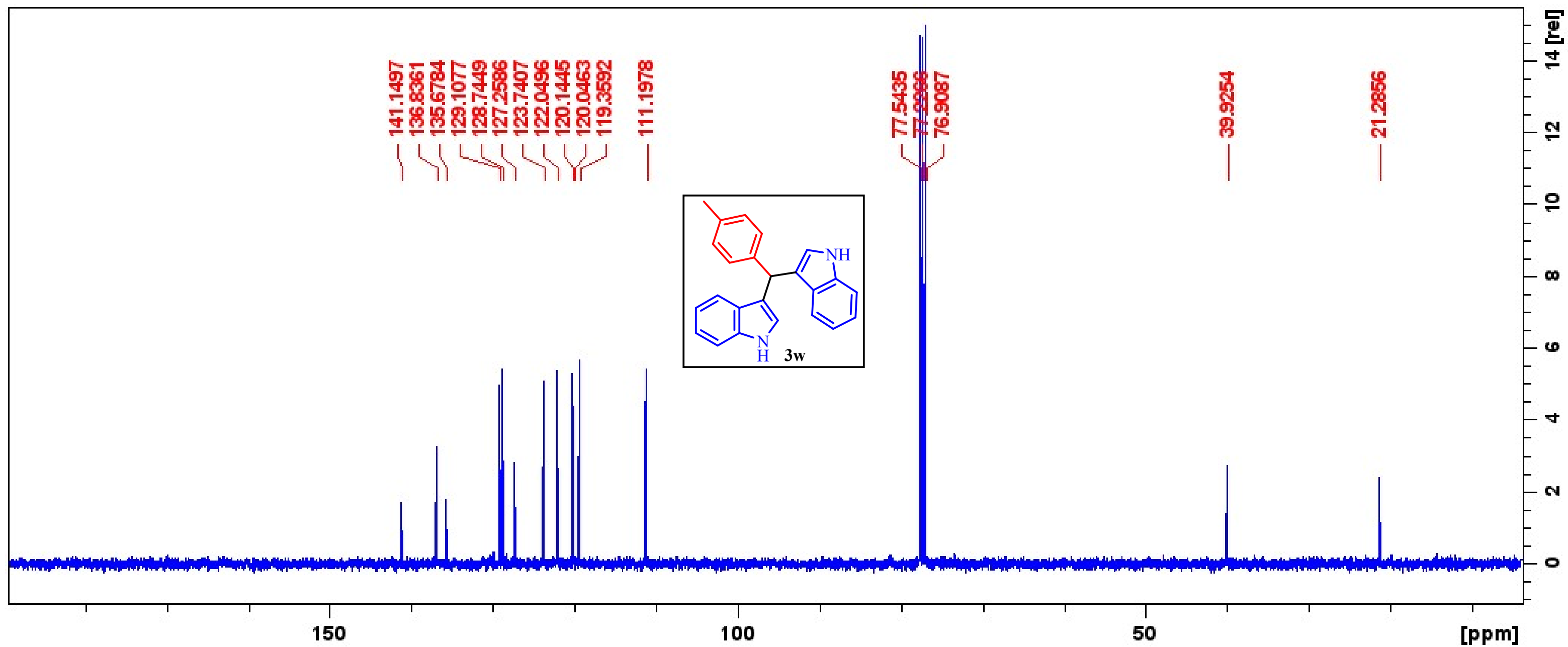


Figure 63. ¹³C NMR spectrum of compound 3w

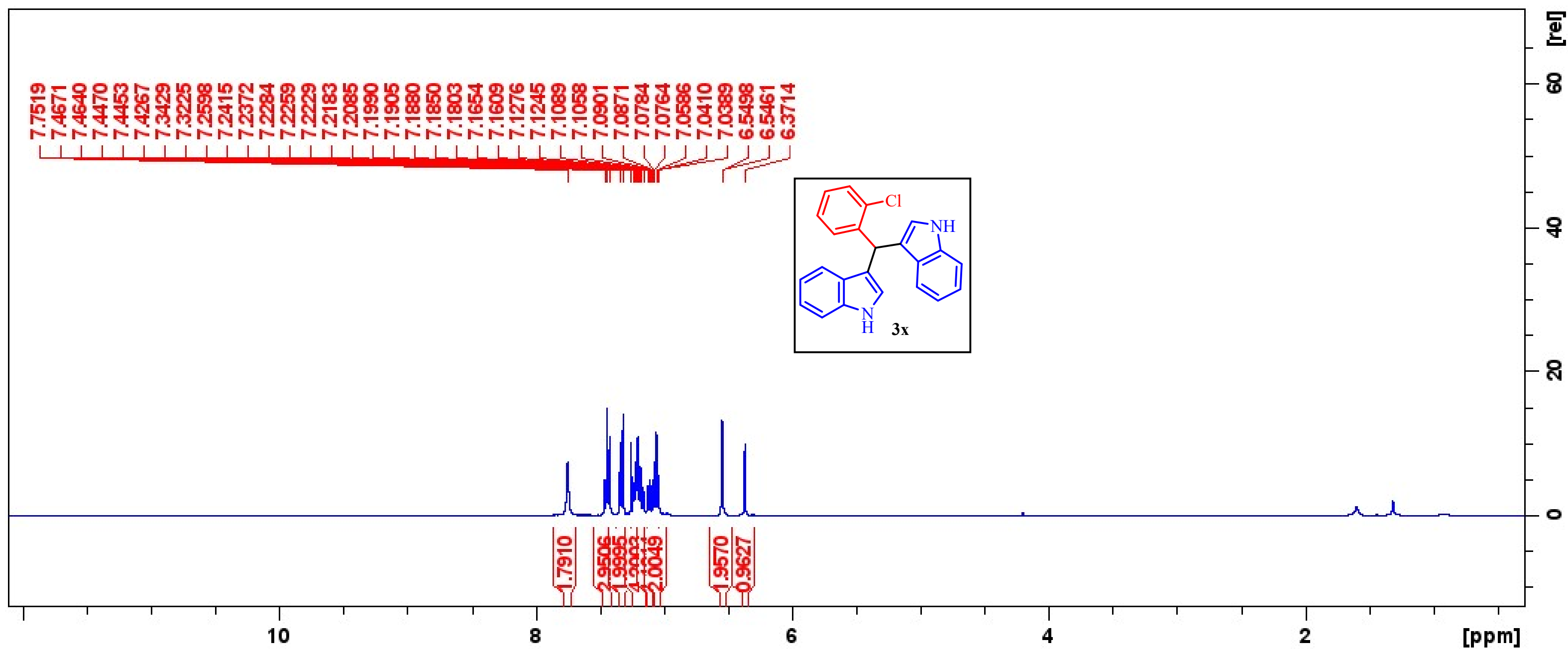


Figure 64. ^1H NMR spectrum of compound **3x**

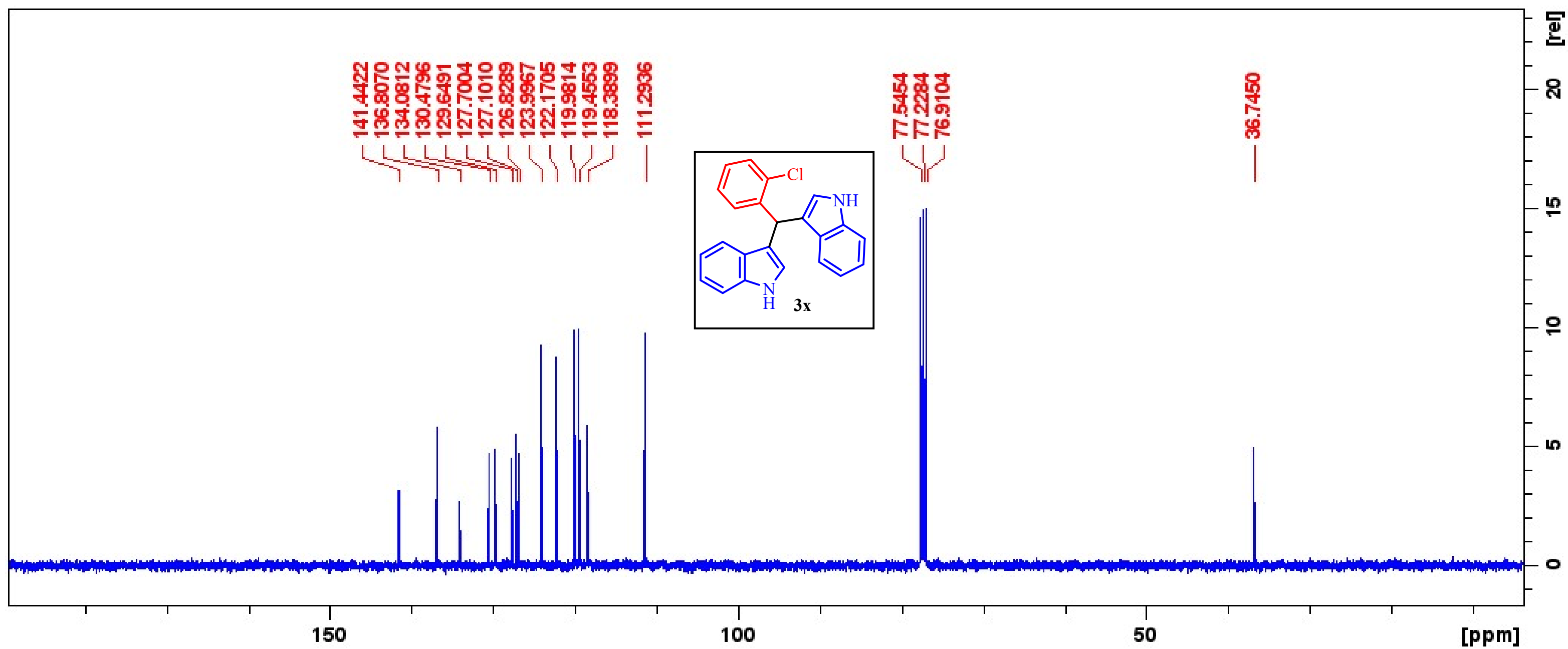


Figure 65. ^{13}C NMR spectrum of compound **3x**

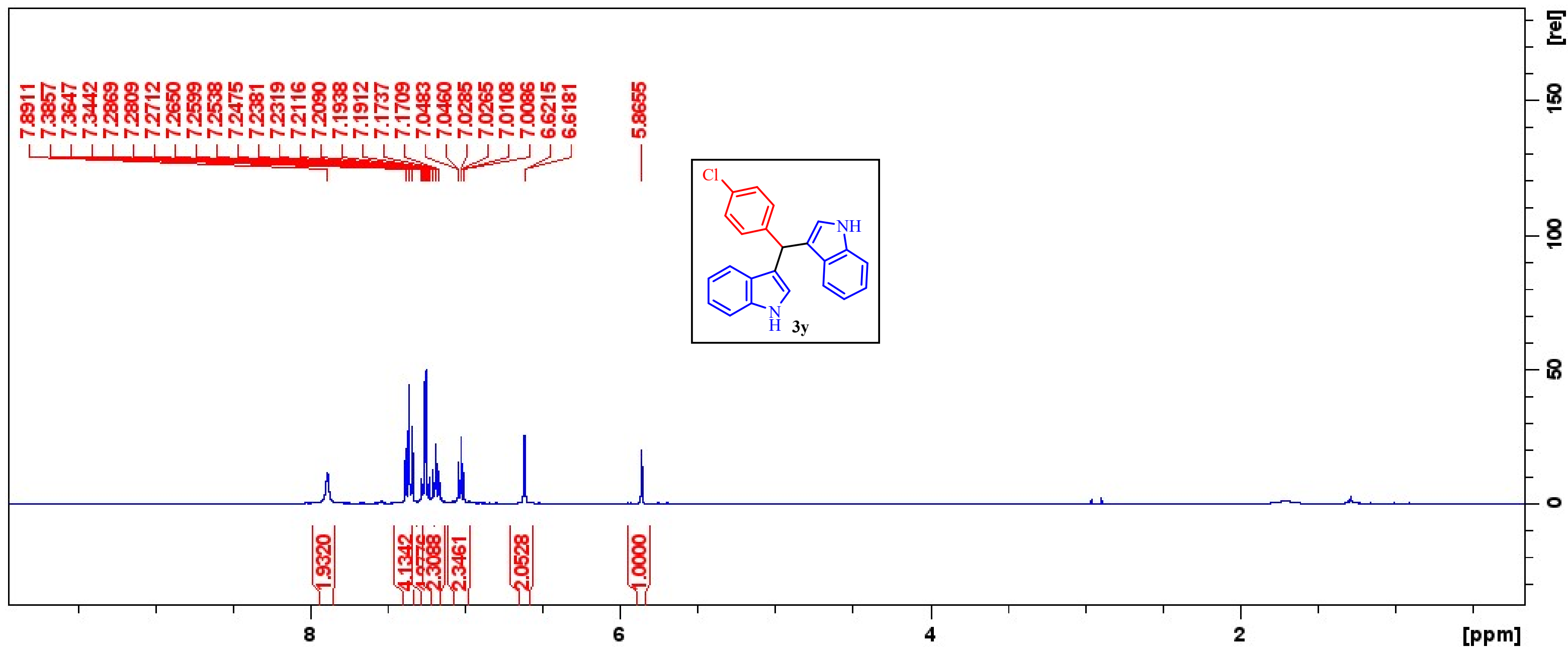


Figure 66. ^1H NMR spectrum of compound **3y**

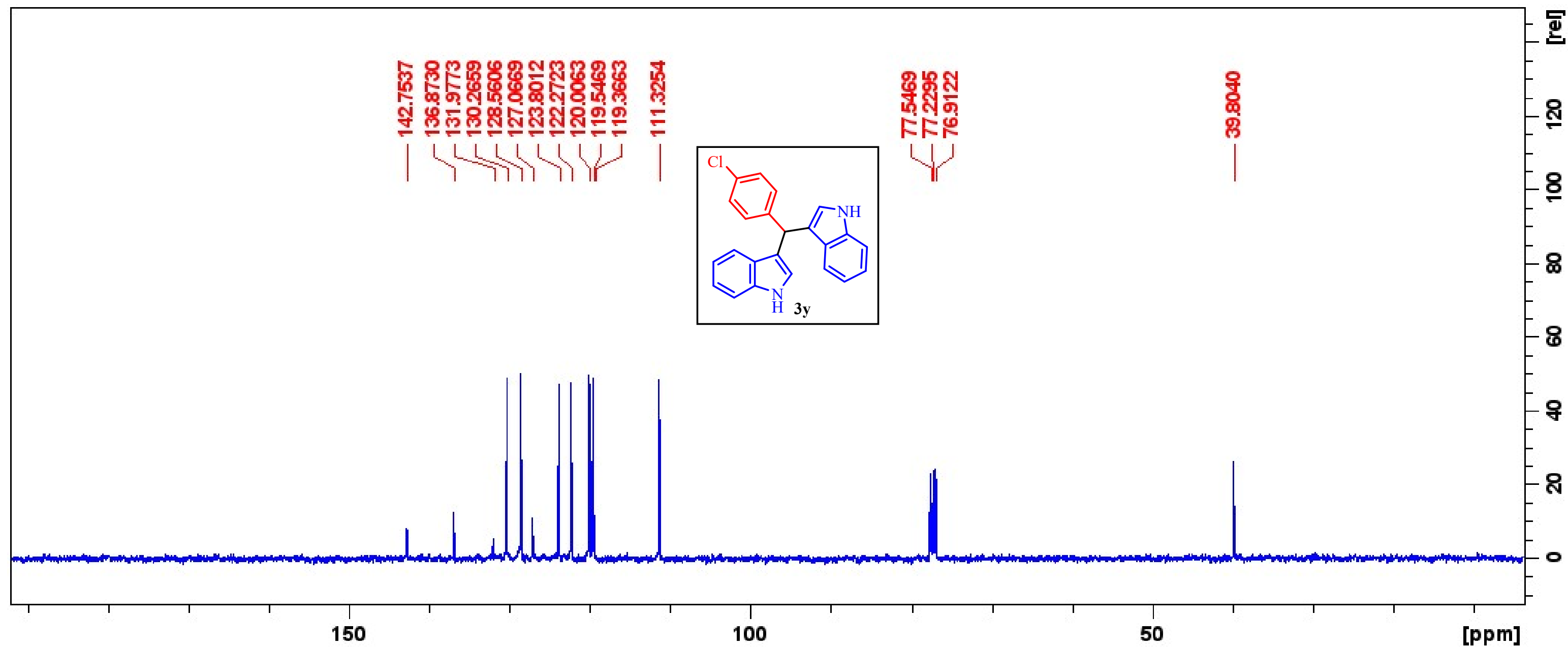


Figure 67. ¹³C NMR spectrum of compound 3y

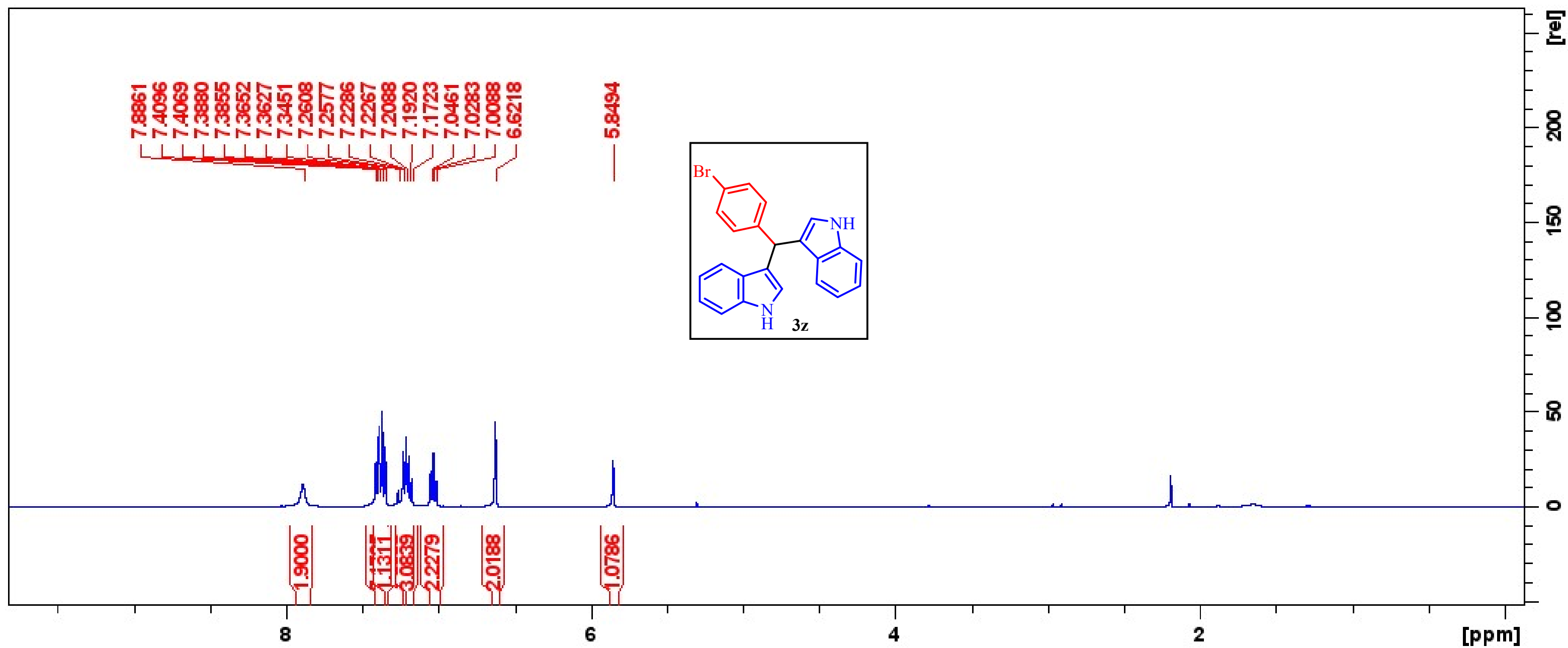


Figure 68. ¹H NMR spectrum of compound **3z**

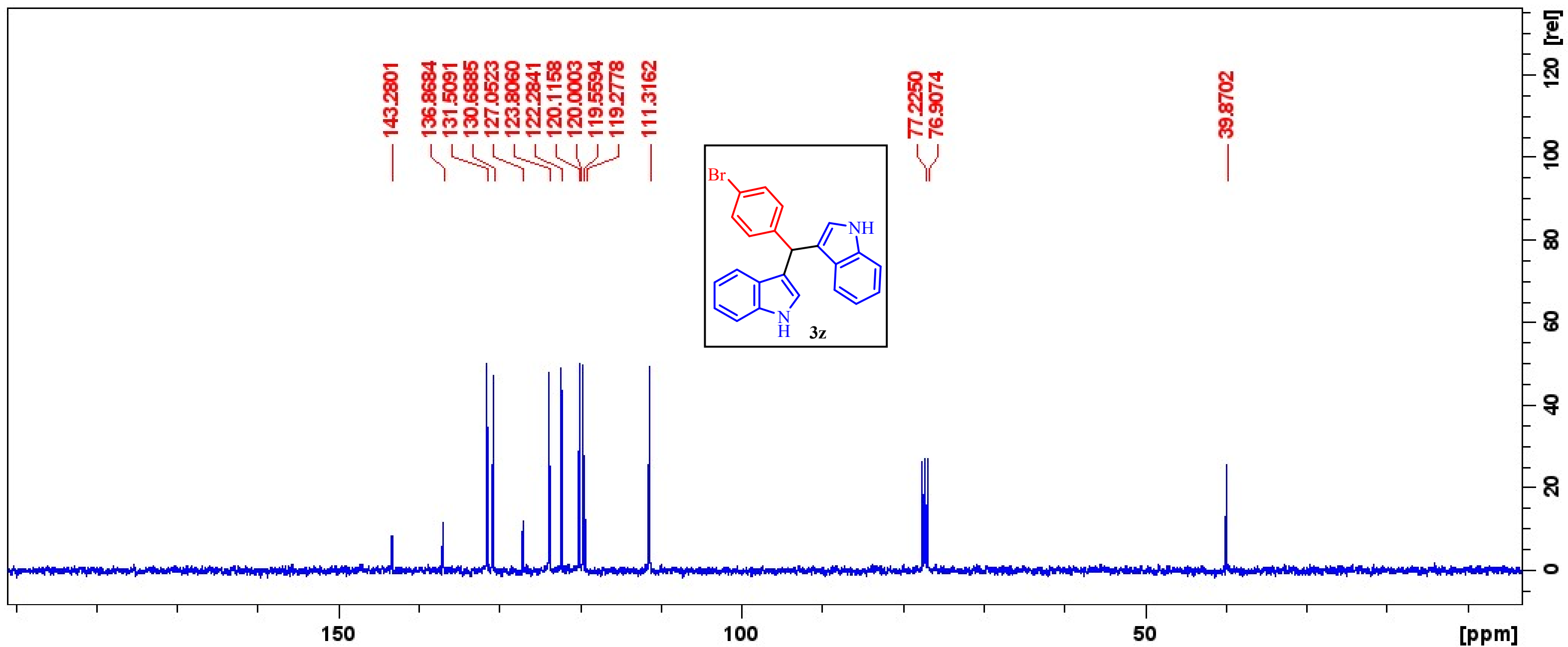


Figure 69. ¹³C NMR spectrum of compound **3z**