Supporting information *for*

Synthesis of functionalized 1*H*-imidazoles *via* denitrogenative transformation of 5-amino-1,2,3-triazoles

Pavel S. Gribanov, Anna N. Philippova, Diana N. Tukhvatullina, Viktoria A. Vlasova, Maxim A. Topchiy, Alexander F. Smol'yakov, Andrey F. Asachenko and Sergey N. Osipov

X-ray crystallography of 4d and 5a:

Table S1. Crystal data and structure refinement for **4d** (CCDC 2426762) and **5a** (CCDC 2426763).

Identification code	**4d**	**5a**
Empirical formula	$C_{13}H_{16}N_2O$	$C_9H_7N_5$
Formula weight	216.28	185.20
Temperature/K	120	120
Crystal system	monoclinic	monoclinic
Space group	$P2_1/n$	$P2_1/n$
a/Å	9.9055(7)	4.1391(3)
b/Å	18.8699(14)	16.4192(14)
c/Å	12.9213(10)	12.1450(9)
α/°	90	90
β/°	92.299(3)	98.262(4)
γ/°	90	90
Volume/Å^3	2413.3(3)	816.82(11)
Z	8	4
ρ_{calc}g/cm^3	1.191	1.506
μ/mm^{-1}	0.077	0.101
F(000)	928.0	384.0
Crystal size/mm^3	0.42 × 0.33 × 0.21	0.33 × 0.08 × 0.04
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.822 to 51.996	4.2 to 51.984
Index ranges	$-12 \le h \le 12$, $-23 \le k \le 23$, $-15 \le l \le 15$	$-5 \le h \le 5$, $-20 \le k \le 20$, $-13 \le l \le 14$
Reflections collected	33287	8267
Independent reflections	4736 [R_{int} = 0.0486, R_{sigma} = 0.0390]	1584 [R_{int} = 0.0338, R_{sigma} = 0.0324]
Data/restraints/parameters	4736/0/293	1584/0/127
Goodness-of-fit on F^2	1.033	1.059
Final R indexes [I>=2σ (I)]	R_1 = 0.0674, wR_2 = 0.1739	R_1 = 0.0339, wR_2 = 0.0835
Final R indexes [all data]	R_1 = 0.0843, wR_2 = 0.1842	R_1 = 0.0438, wR_2 = 0.0859
Largest diff. peak/hole / e Å^{-3}	0.98/-0.37	0.19/-0.22

NMR spectra

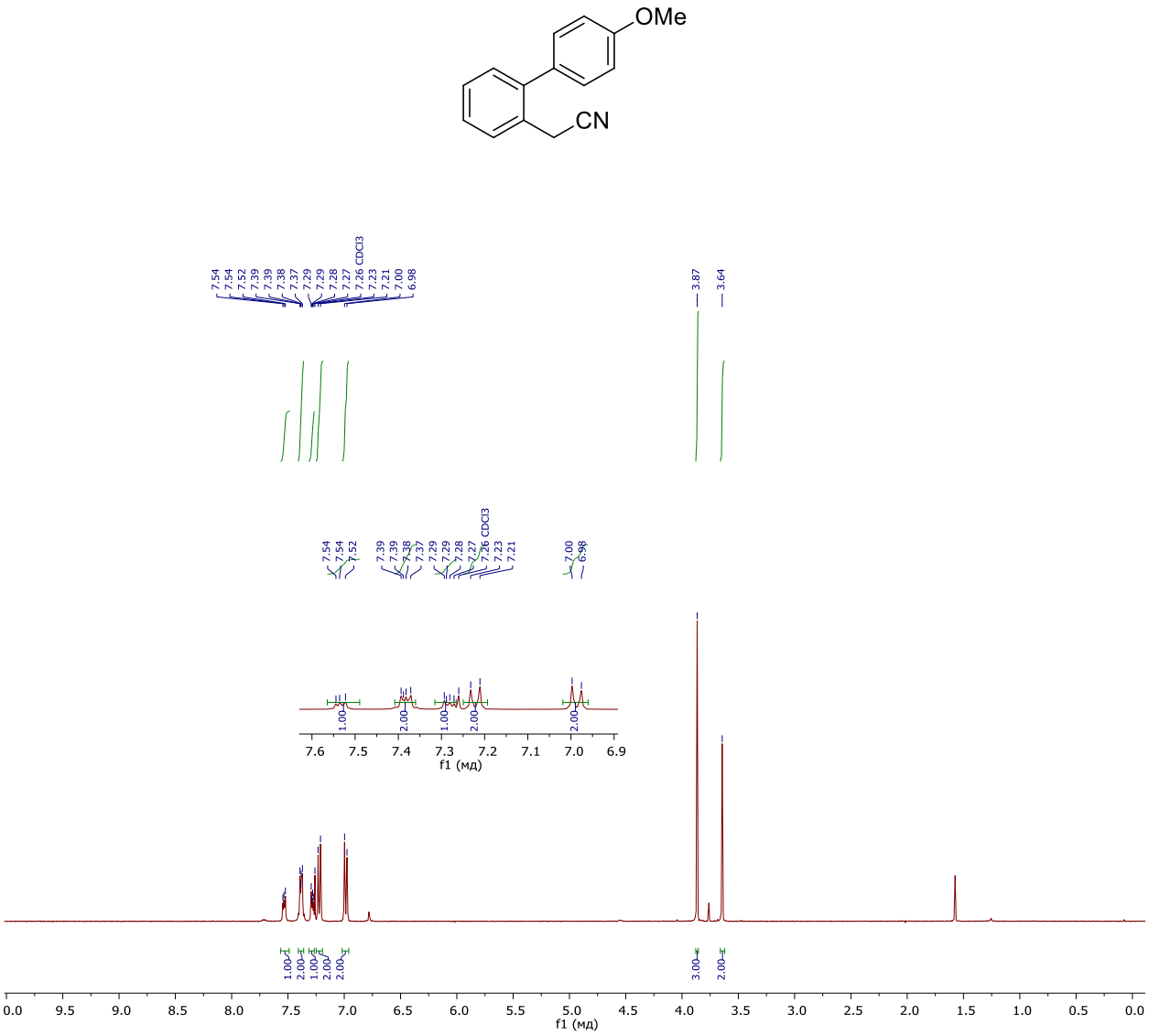


Figure S1. ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of 2-(4'-methoxy-[1,1'-biphenyl]-2-yl)acetonitrile.

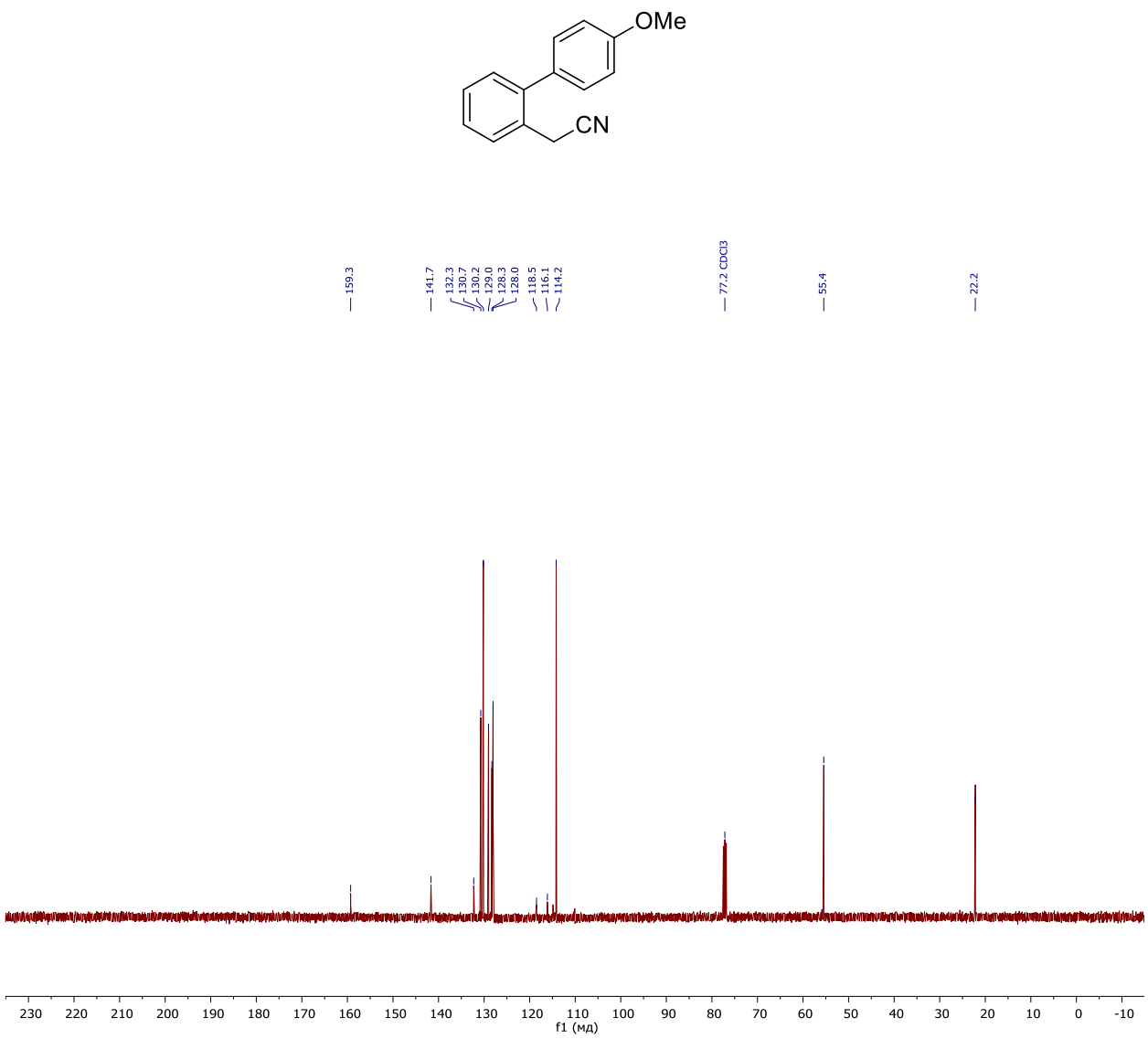


Figure S2. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of 2-(4'-methoxy-[1,1'-biphenyl]-2-yl)acetonitrile

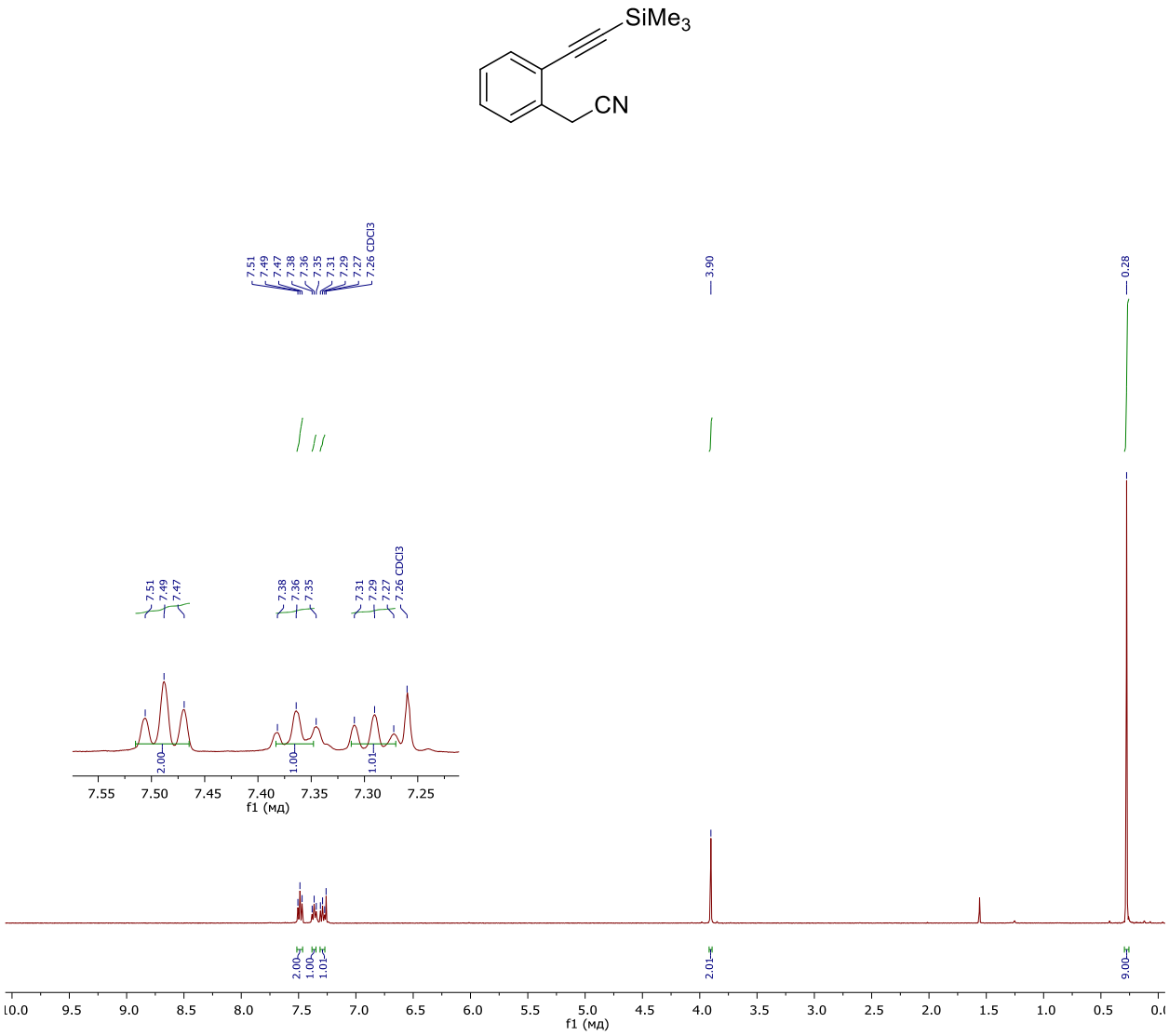


Figure S3. ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of 2-(2-((trimethylsilyl)ethynyl) phenyl)acetonitrile.

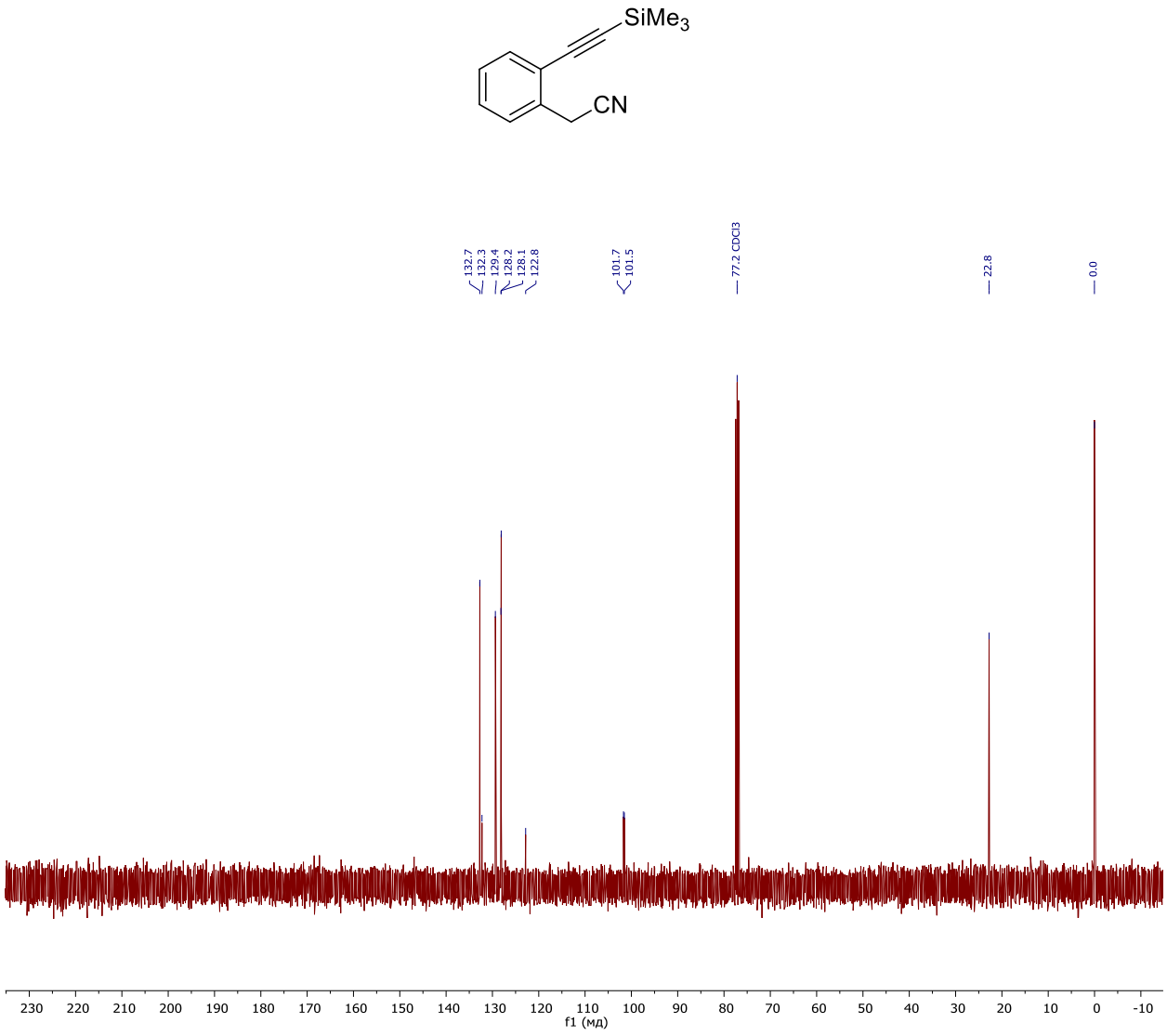


Figure S4. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of 2-(2-((trimethylsilyl)ethynyl) phenyl)acetonitrile.

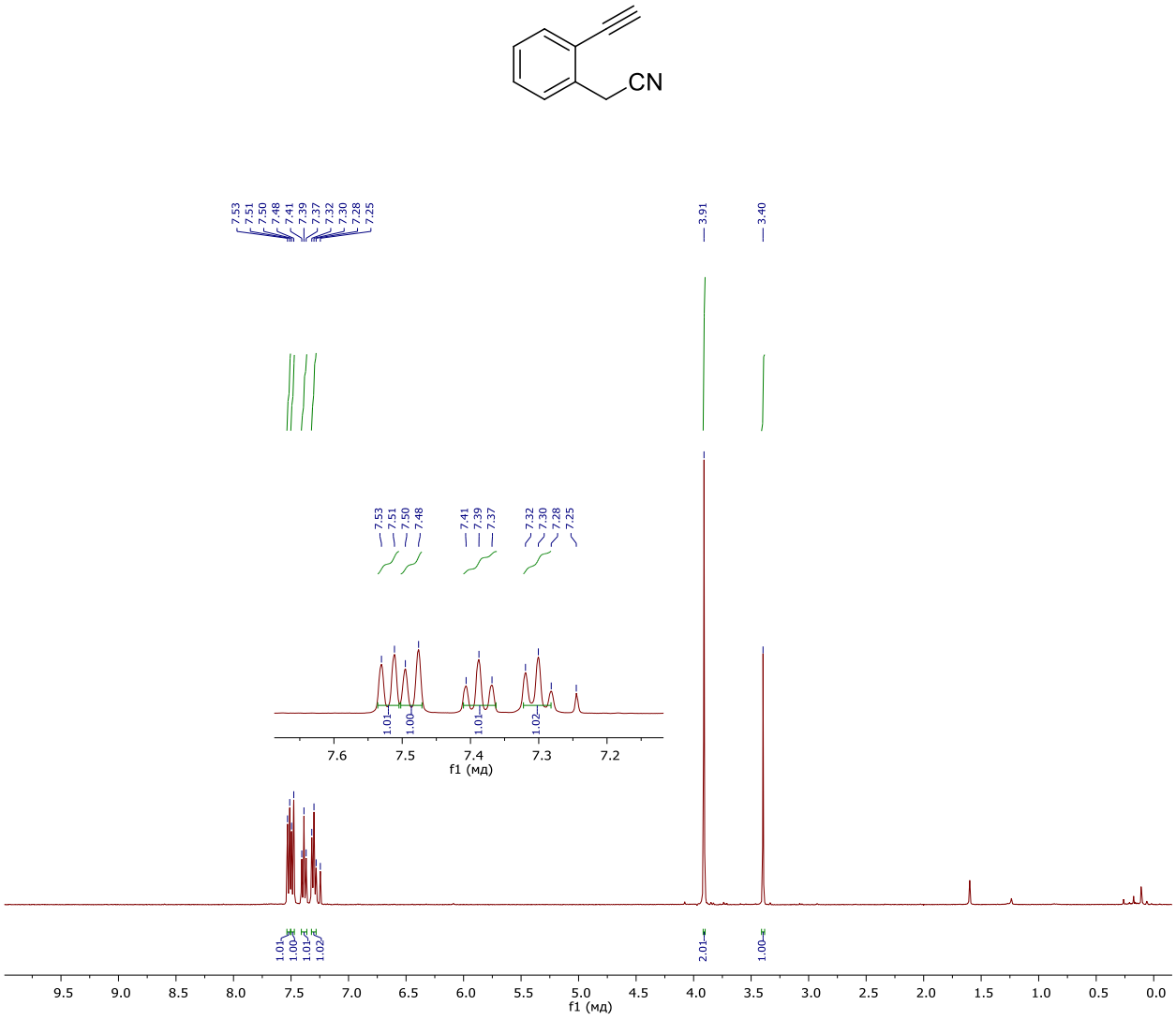


Figure S5. ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of 2-(2-ethynylphenyl)acetonitrile.

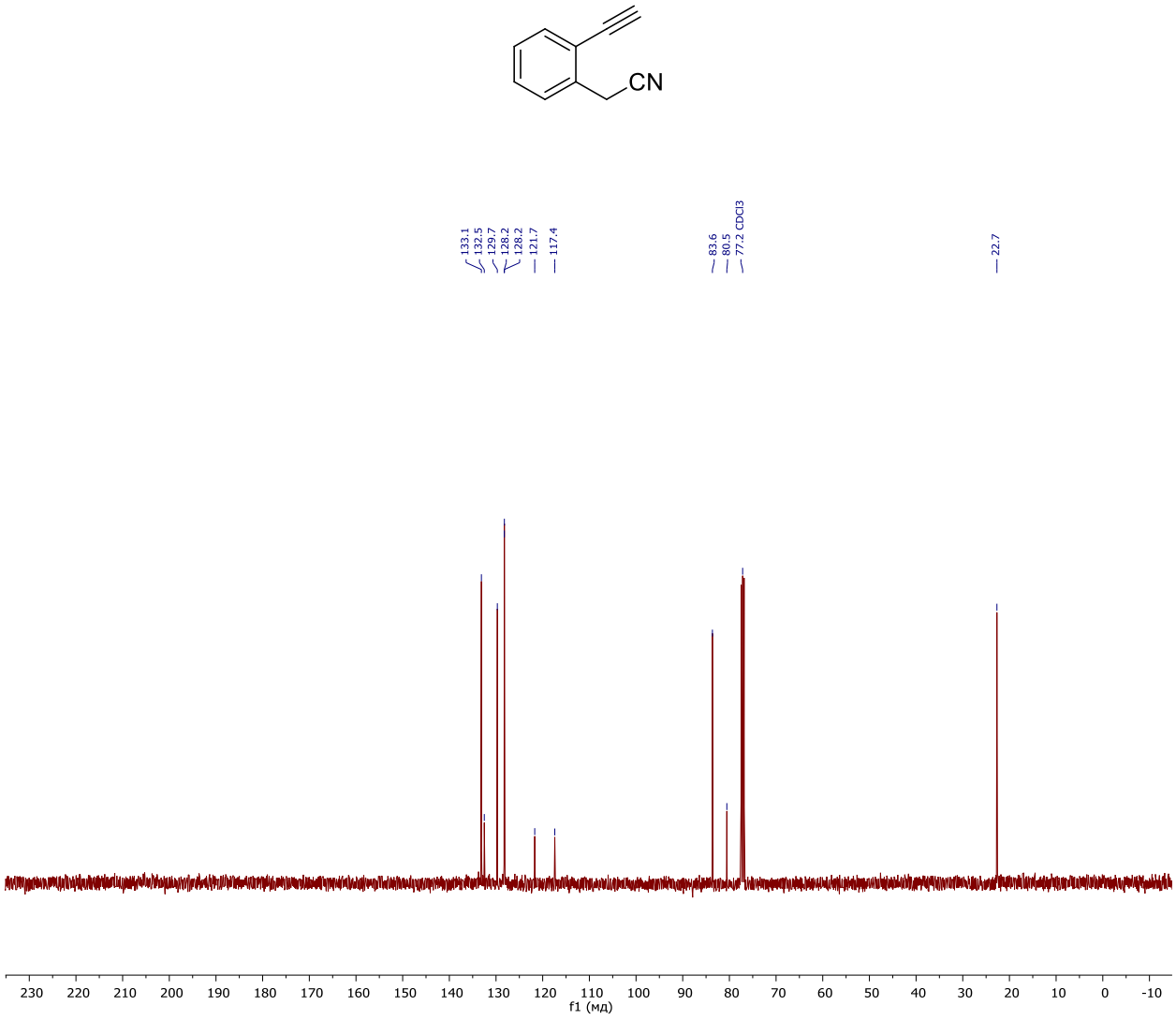


Figure S6. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of 2-(2-ethynylphenyl)acetonitrile.

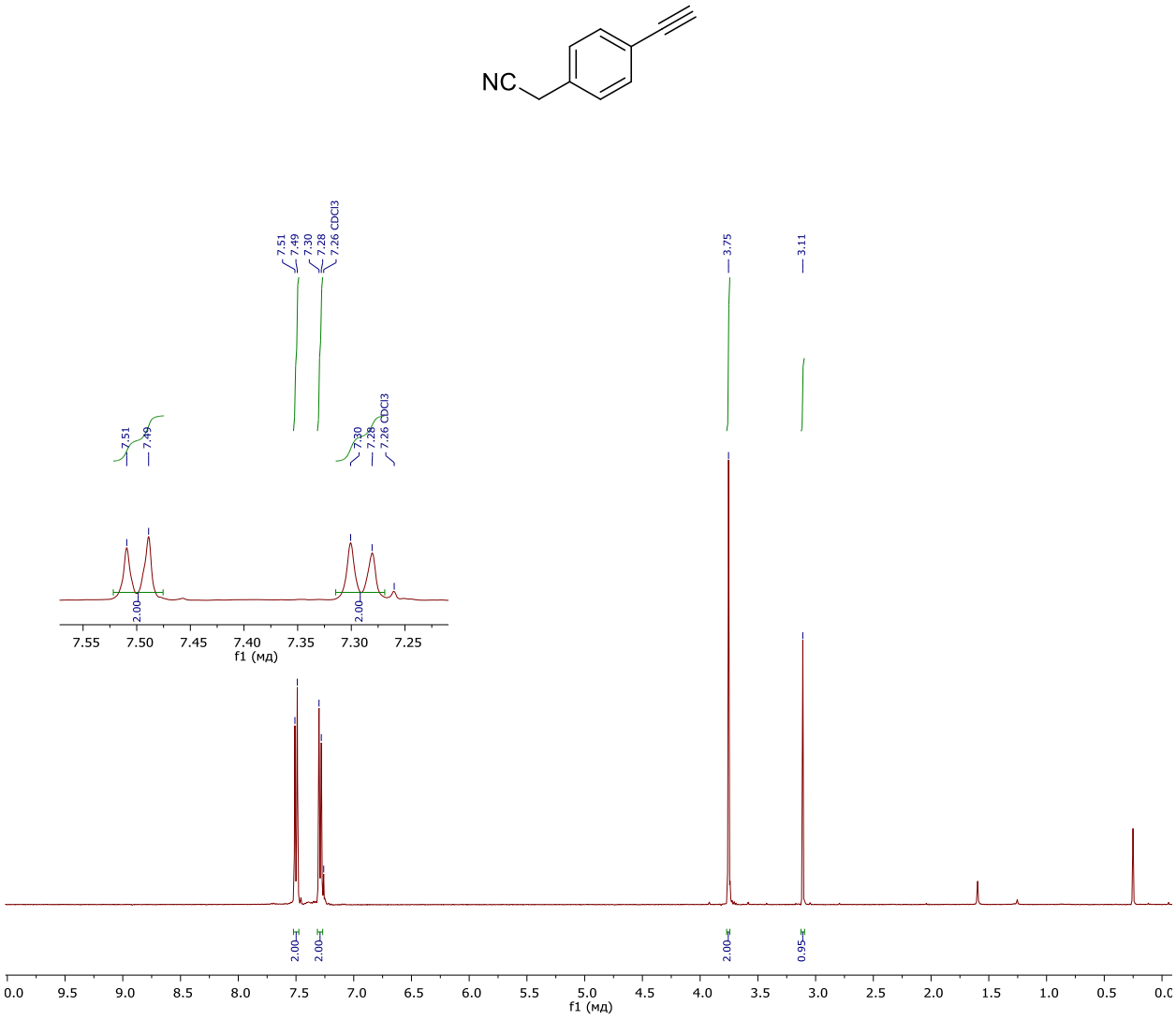


Figure S7. ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of 2-(4-ethynylphenyl)acetonitrile.

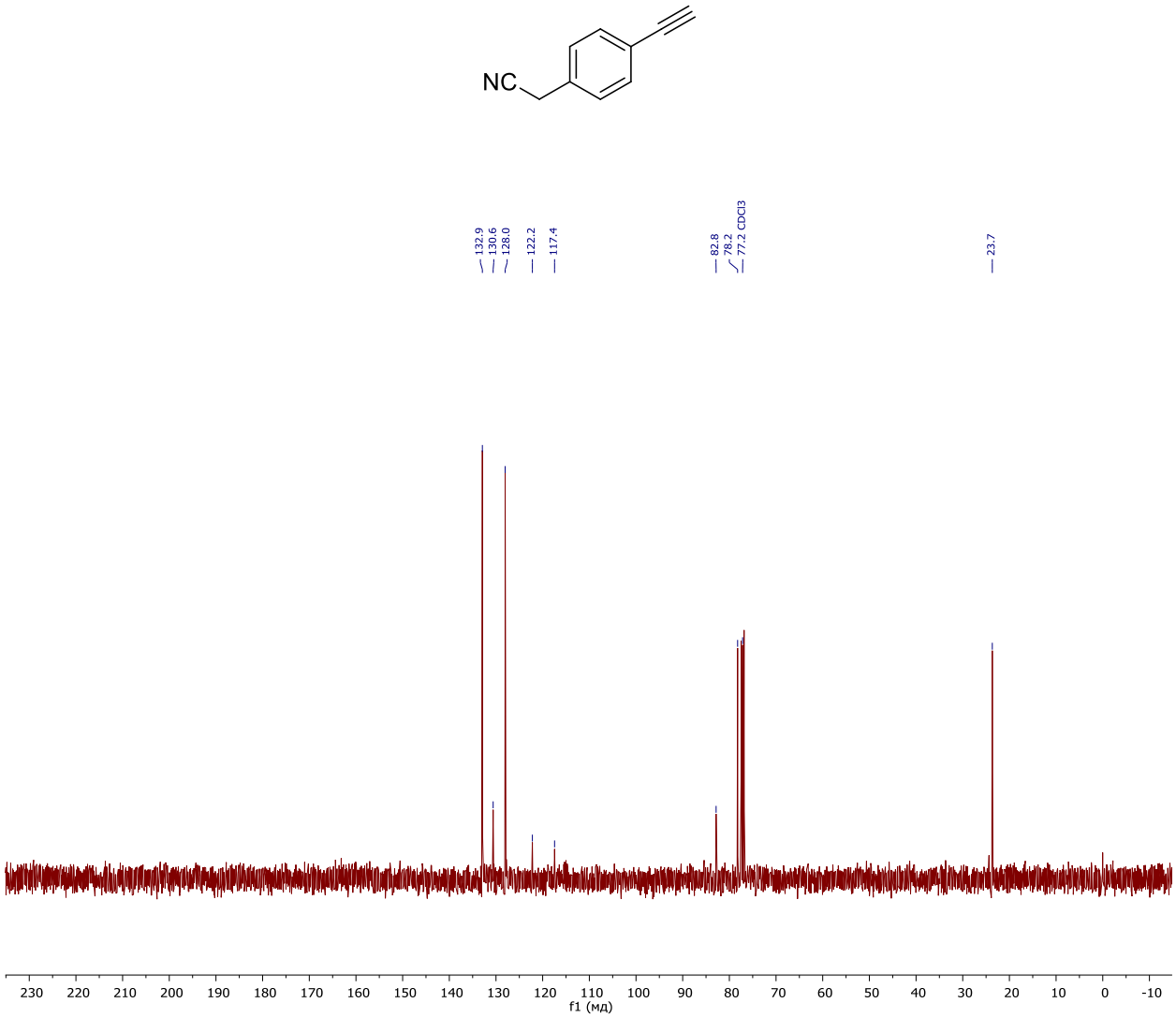


Figure S8. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of 2-(4-ethynylphenyl)acetonitrile.

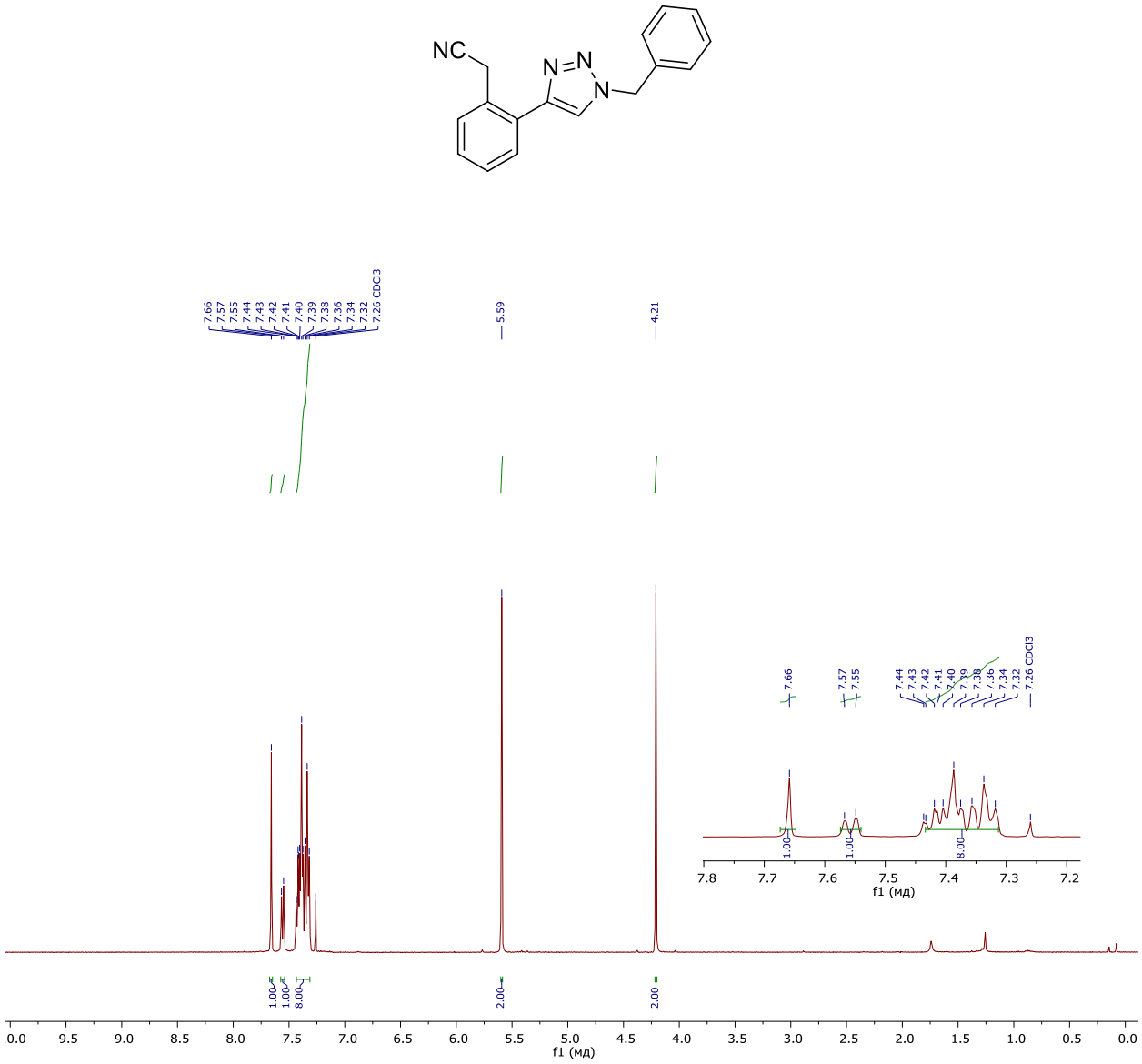


Figure S9. ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of 2-(2-(1-benzyl-1H-1,2,3-triazol-4-yl)phenyl)acetonitrile.

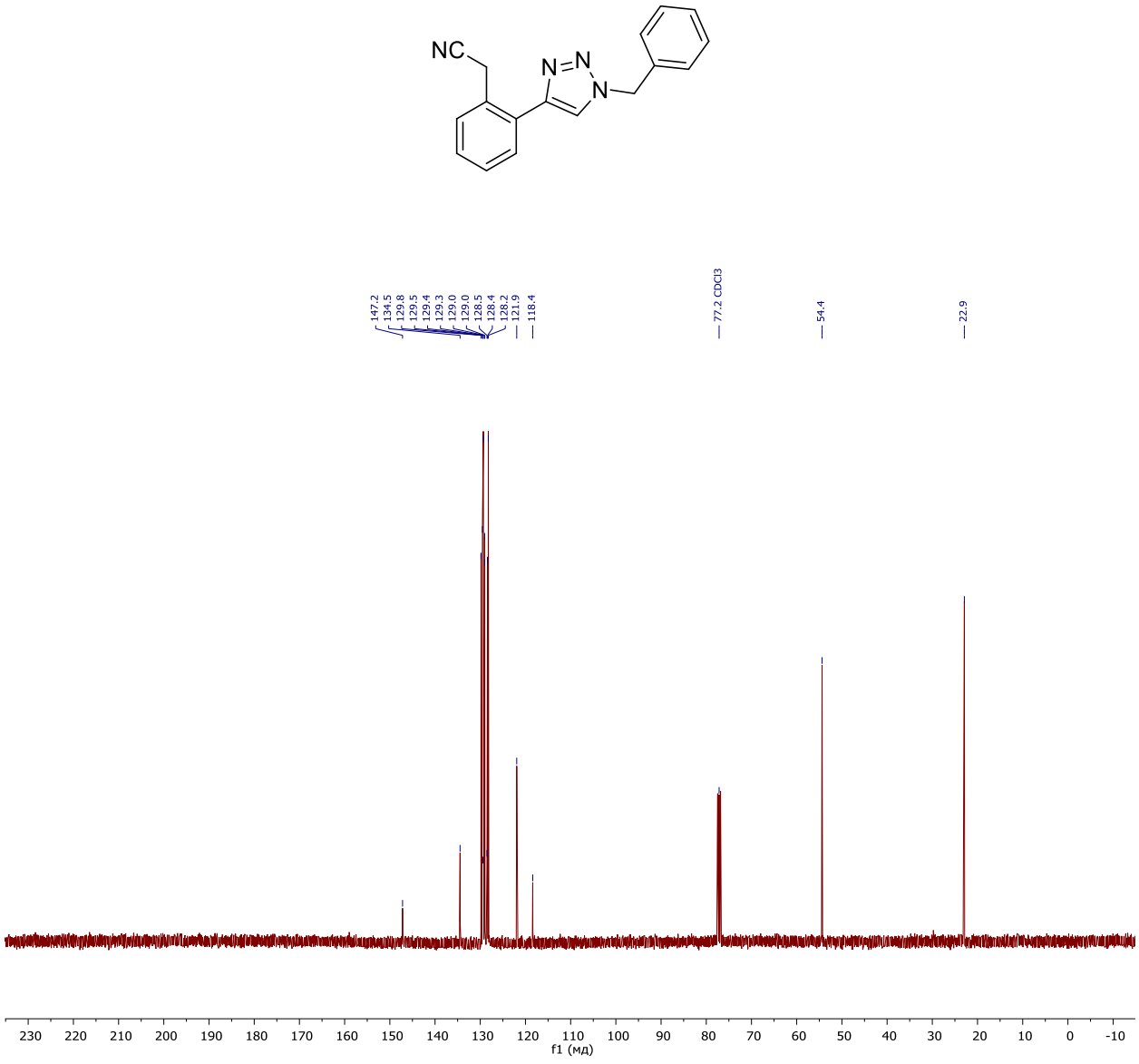


Figure S10. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of 2-(2-(1-benzyl-1H-1,2,3-triazol-4-yl)phenyl)acetonitrile.

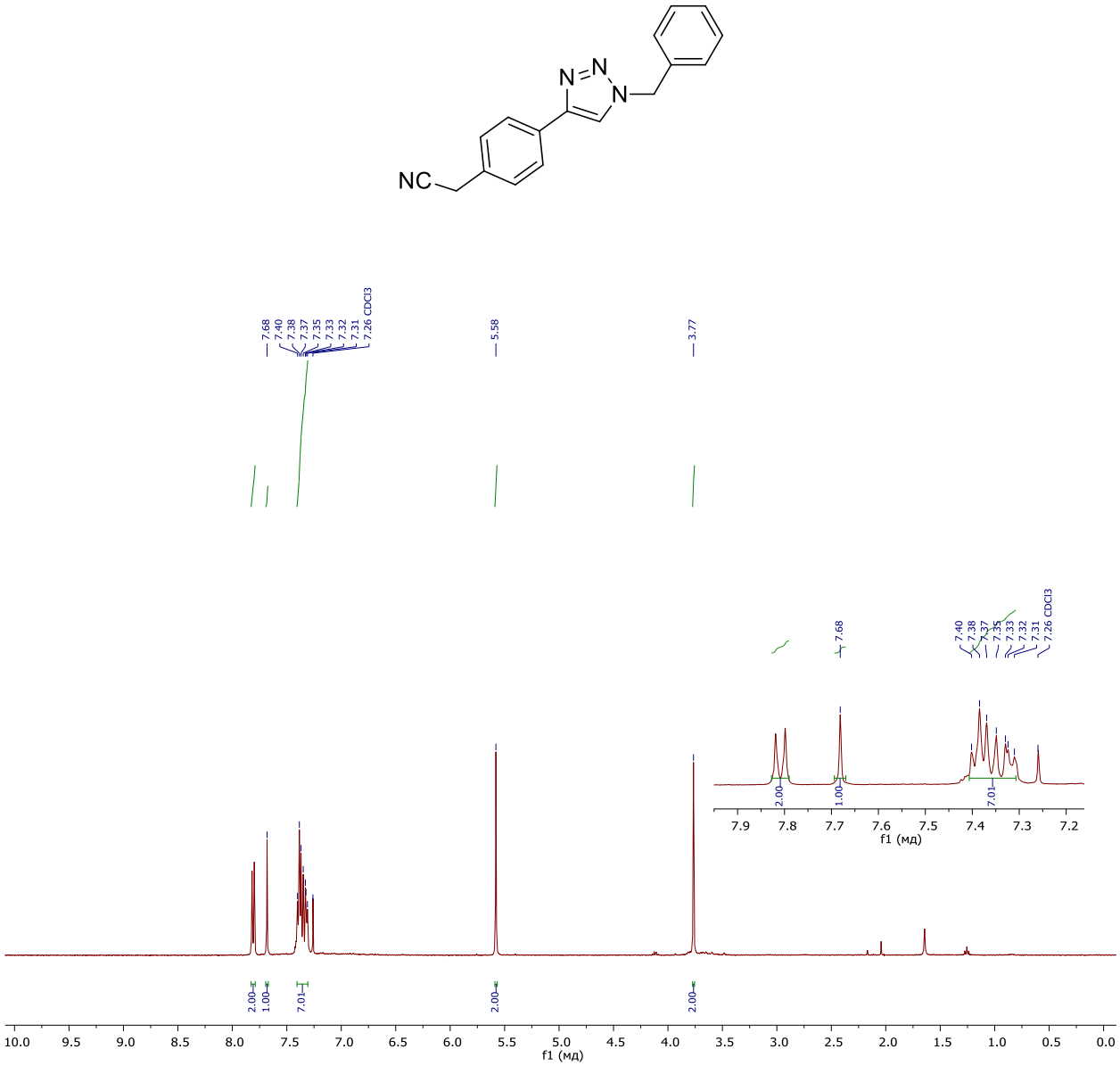


Figure S11. ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of 2-(4-(1-benzyl-1H-1,2,3-triazol-4-yl)phenyl)acetonitrile.

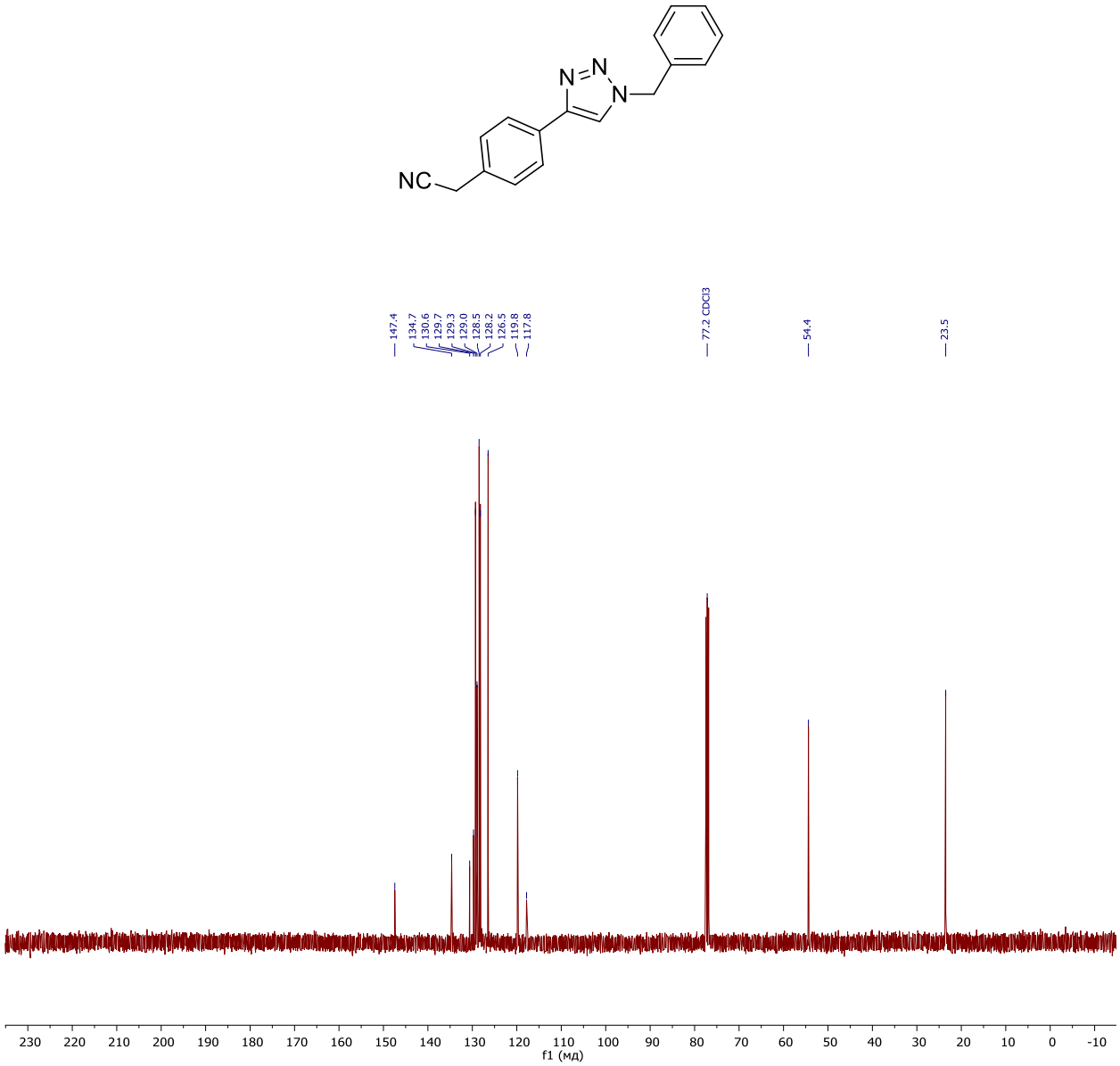


Figure S12. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of 2-(4-(1-benzyl-1H-1,2,3-triazol-4-yl)phenyl)acetonitrile.

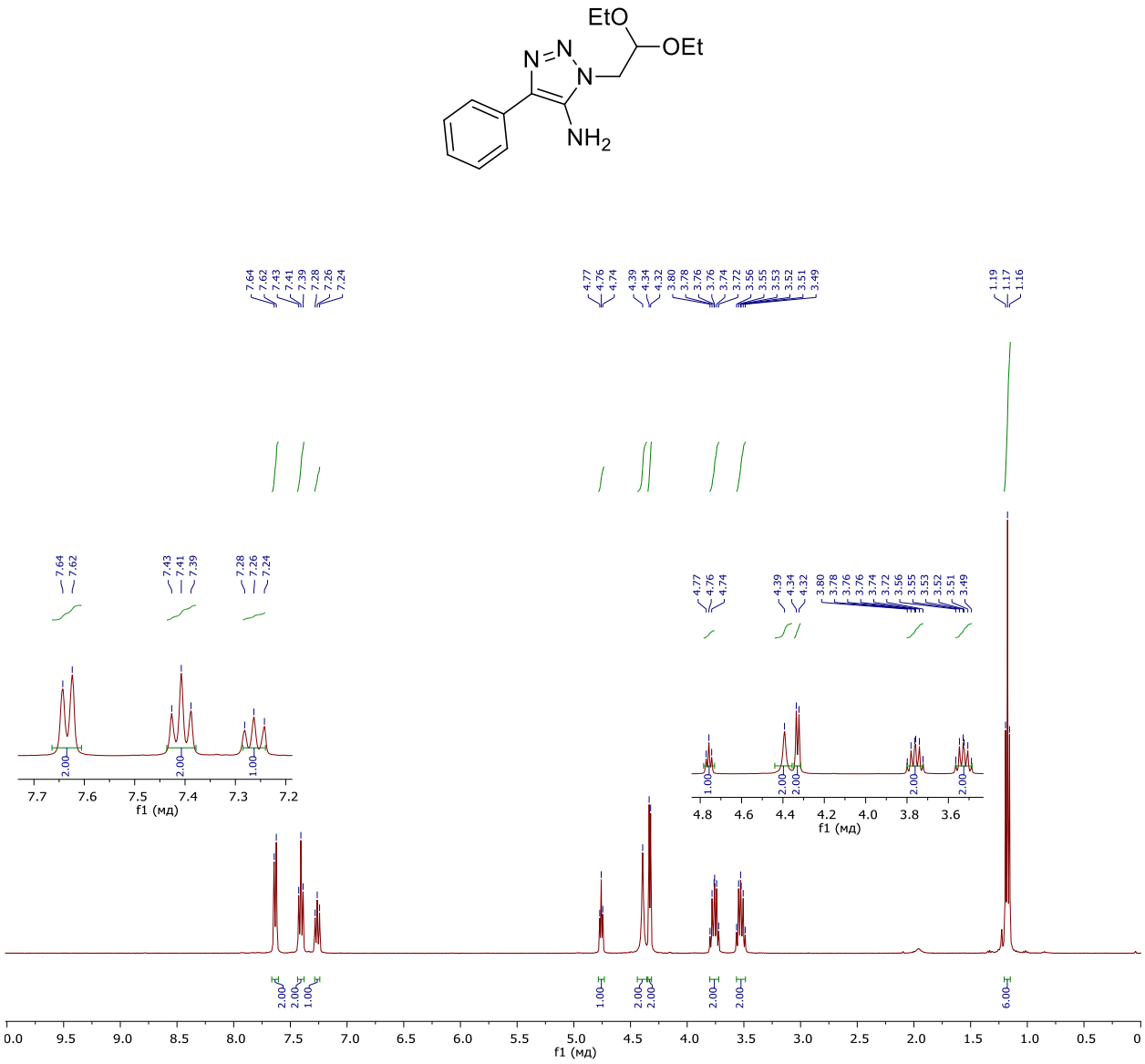


Figure S13. ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **3a**.

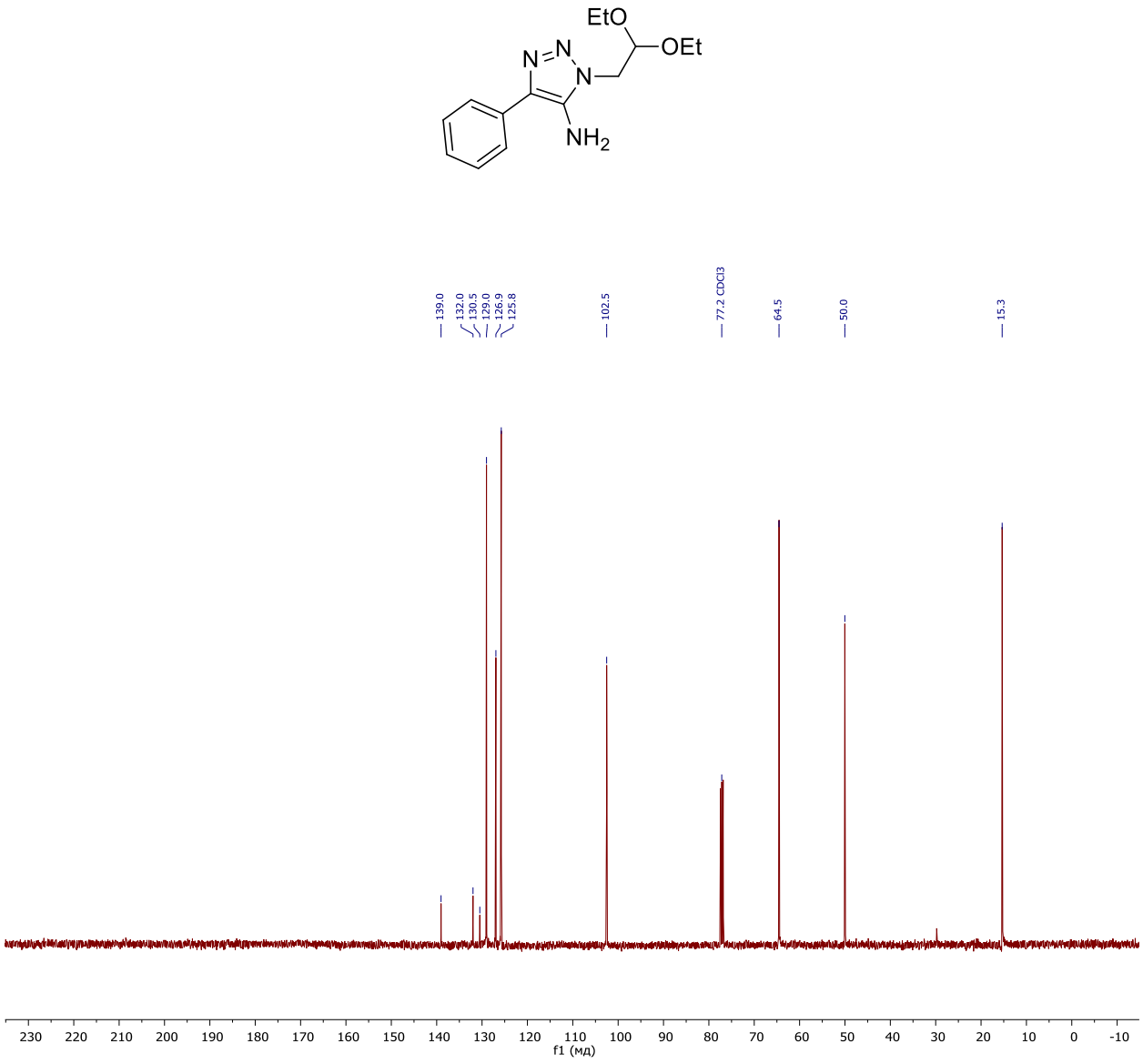


Figure S14. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of compound **3a**.

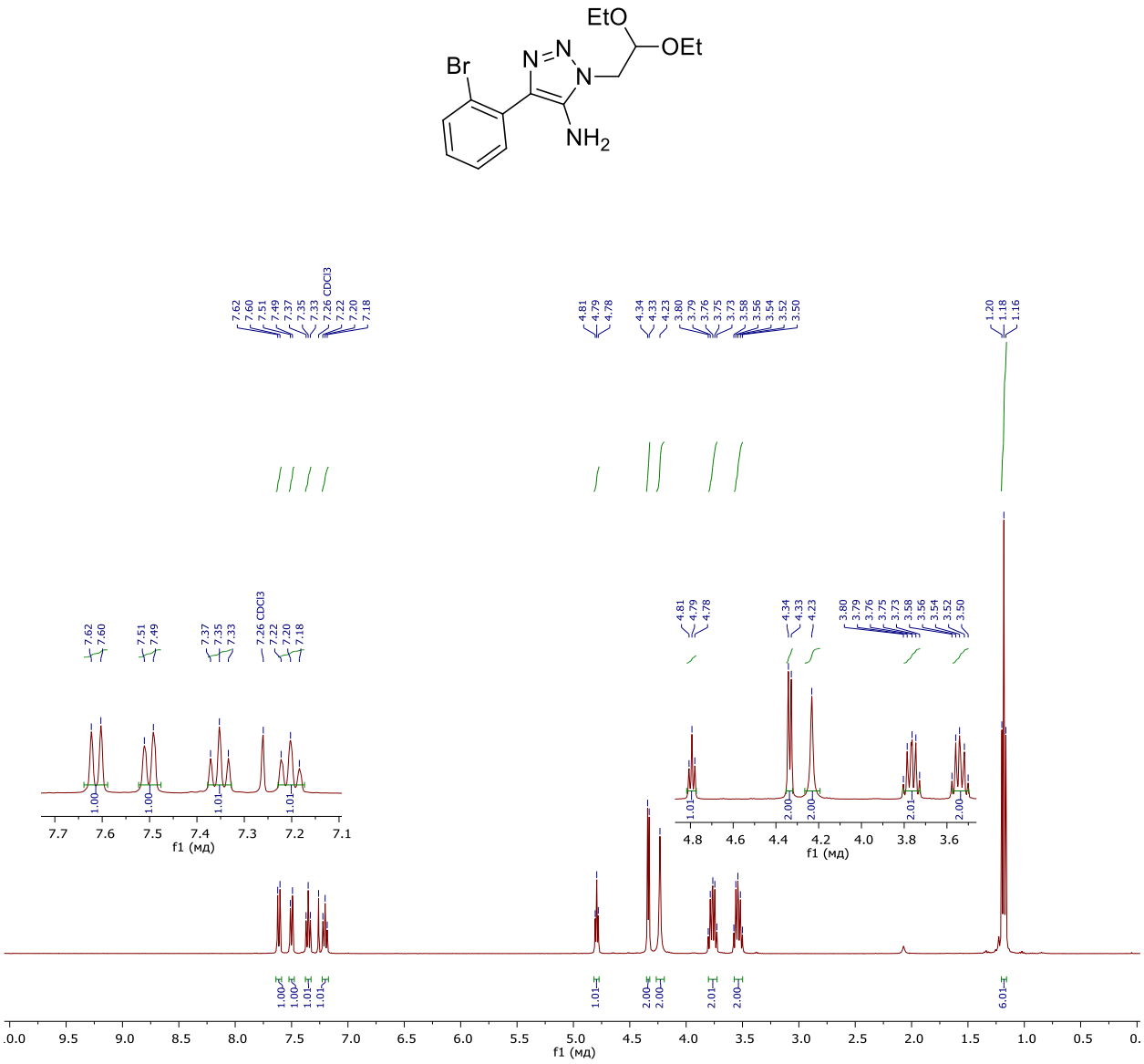


Figure S15. ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **3b**.

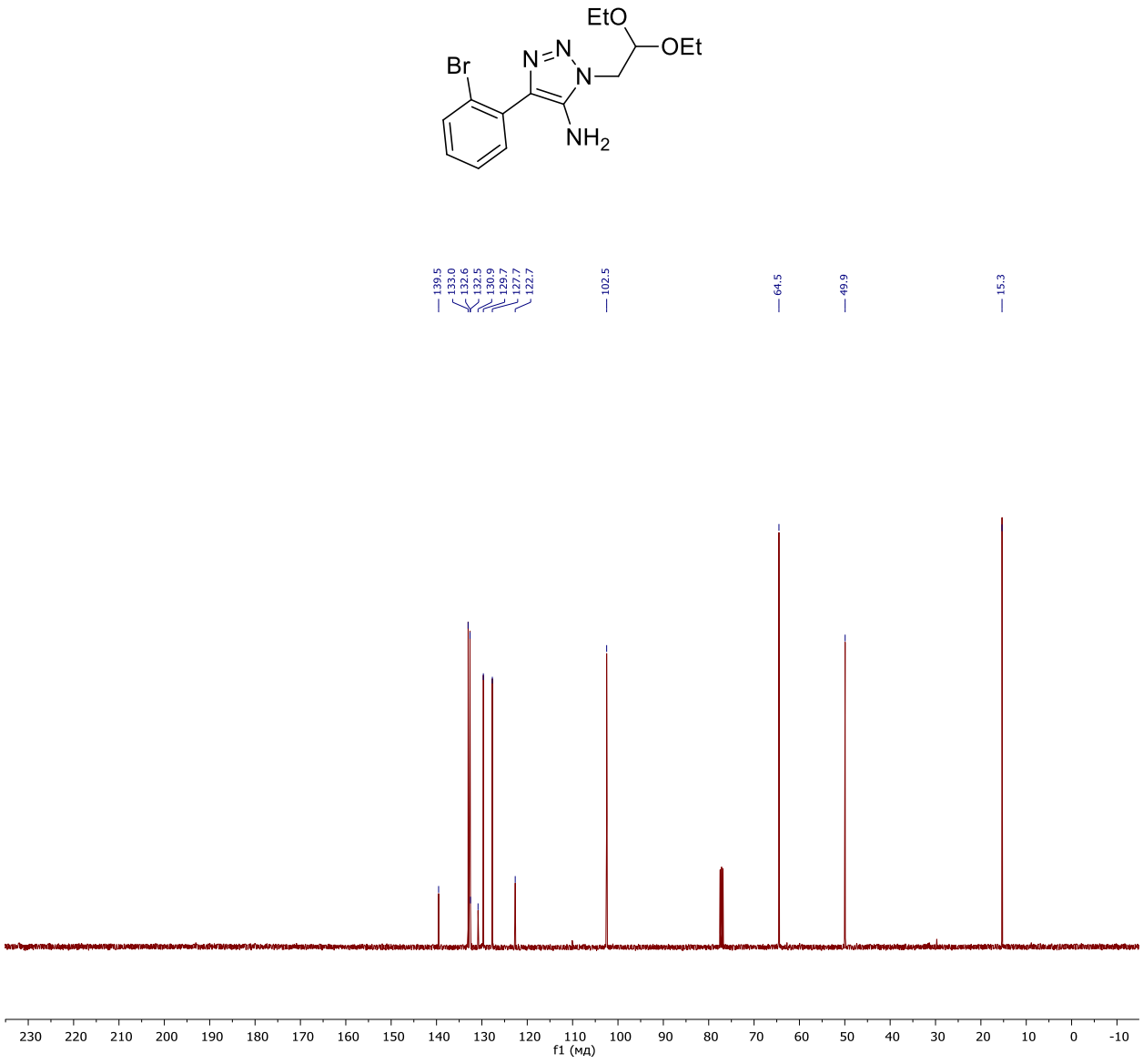


Figure S16. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of compound **3b**.

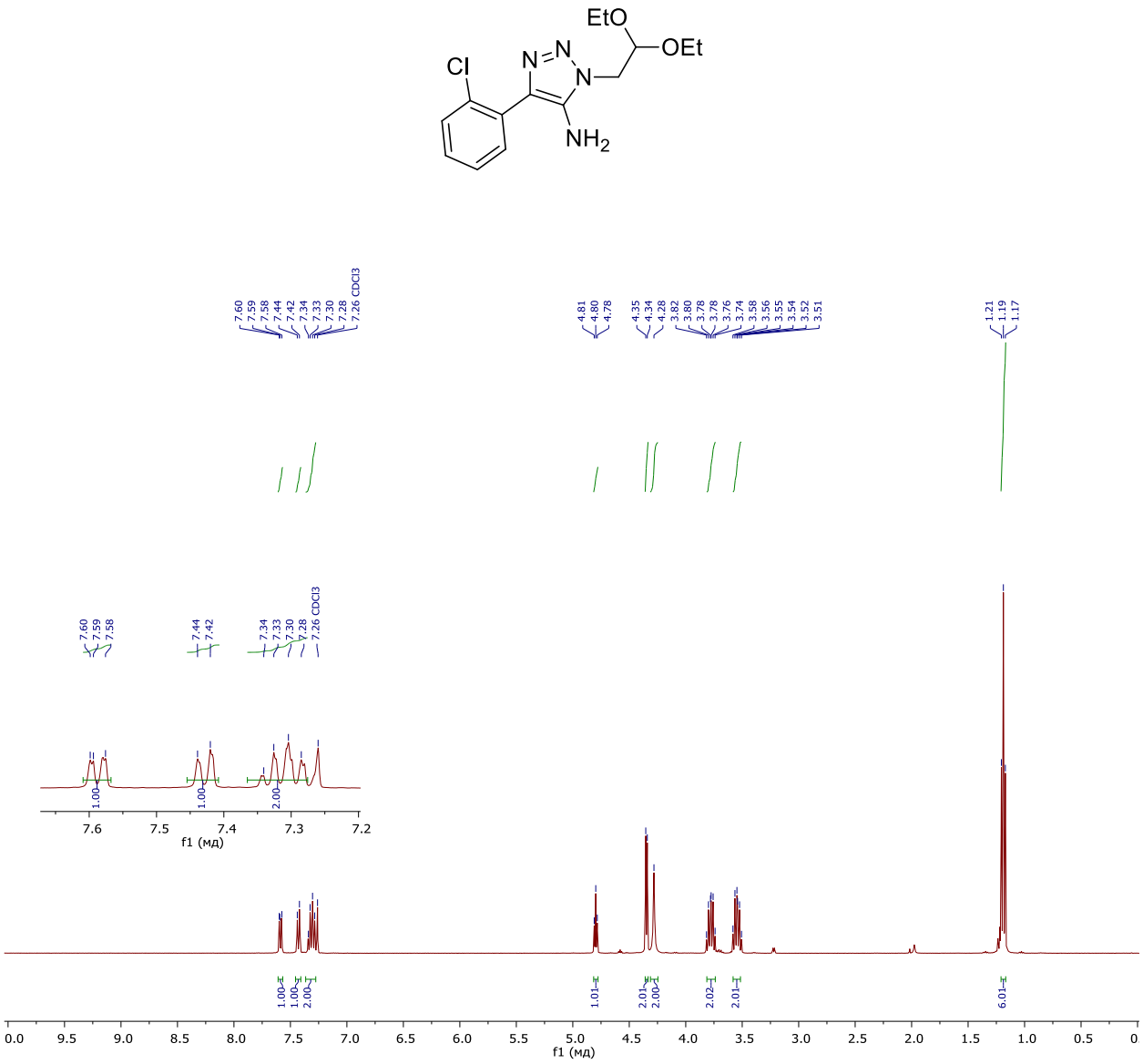


Figure S17. ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **3c**.

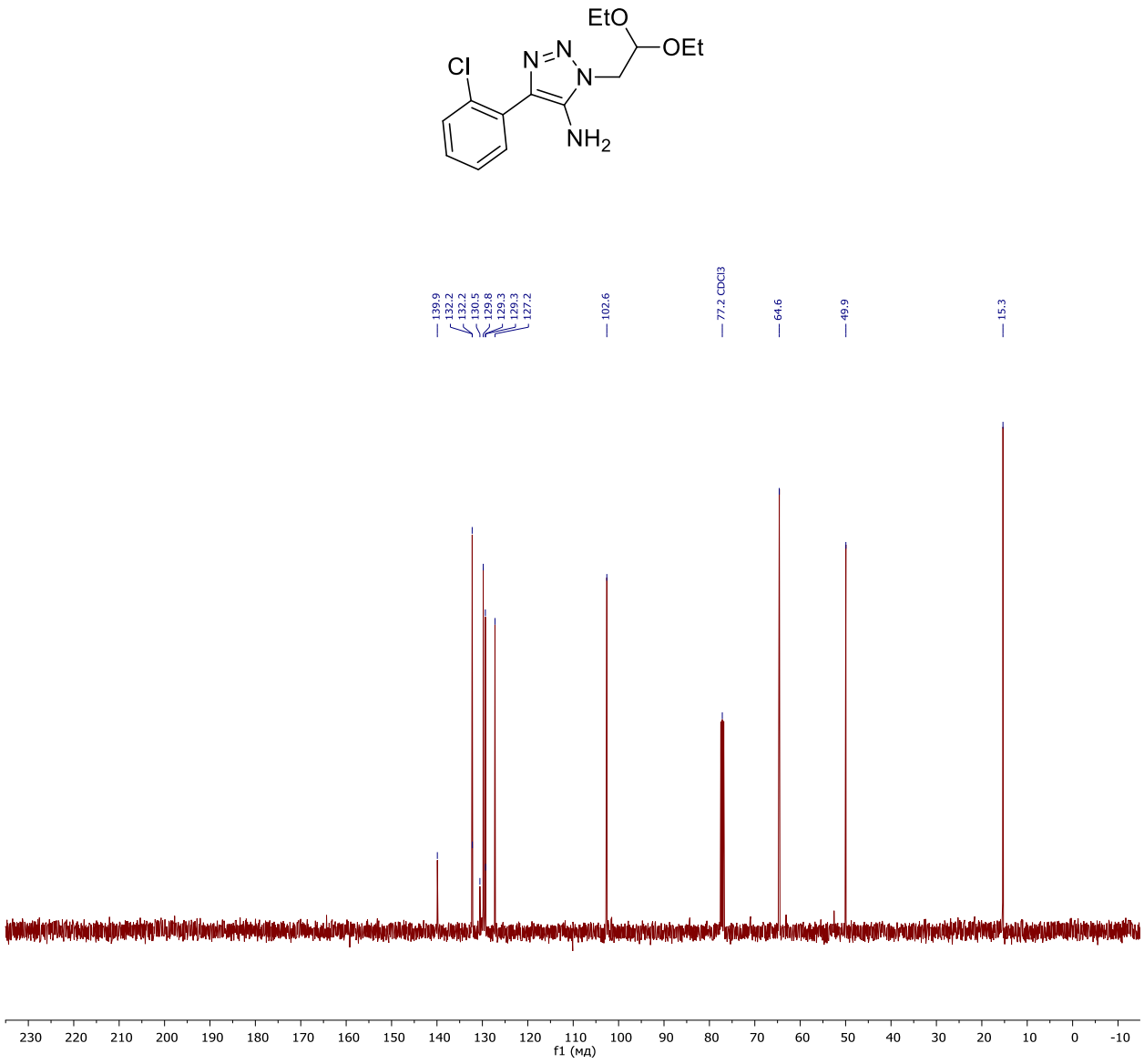


Figure S18. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of compound **3c**.

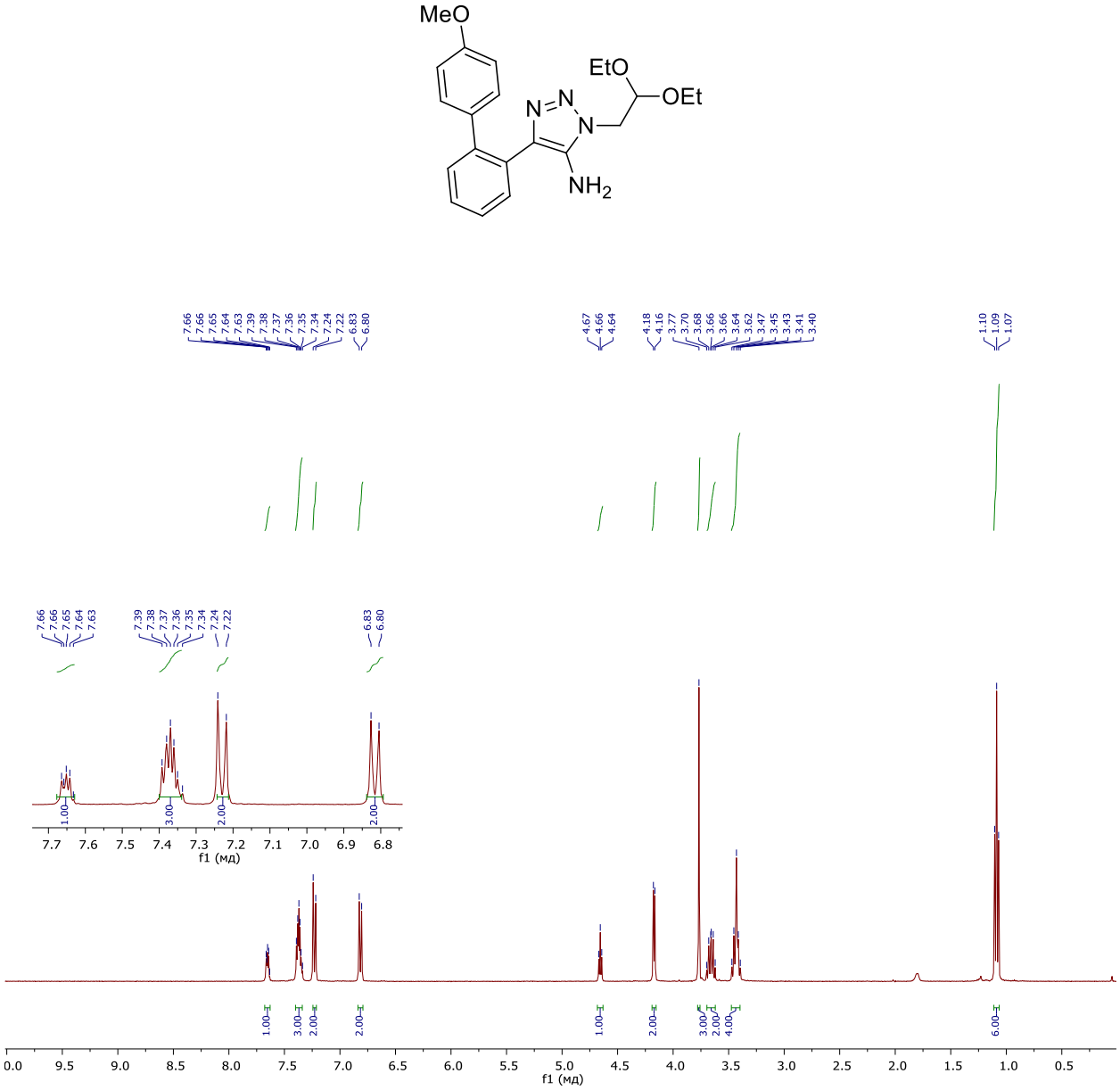


Figure 19 ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **3d**.

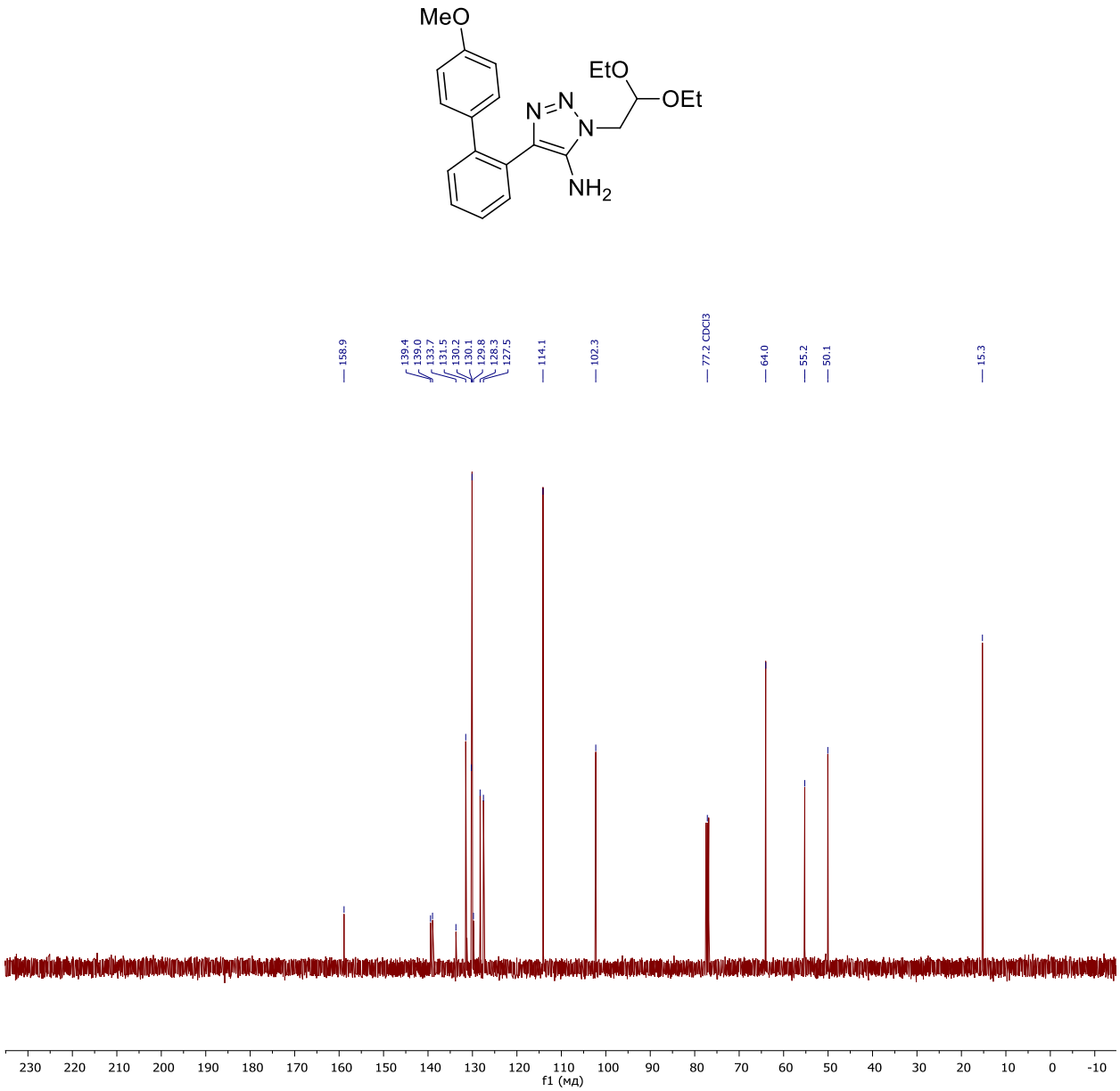


Figure S20. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of compound **3d**.

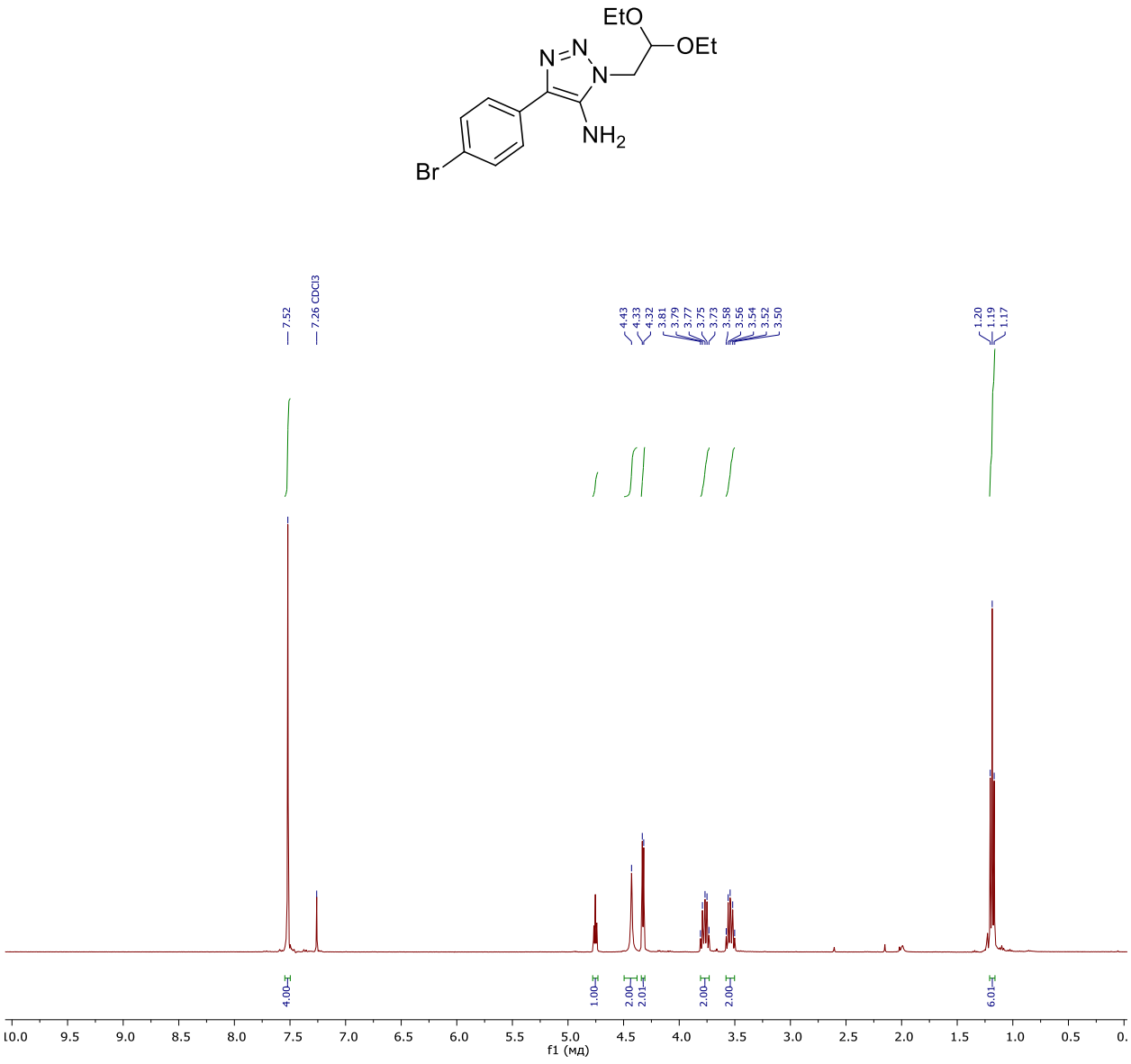


Figure S21. [1]H NMR (400 MHz, Chloroform-*d*) spectrum of compound **3e**.

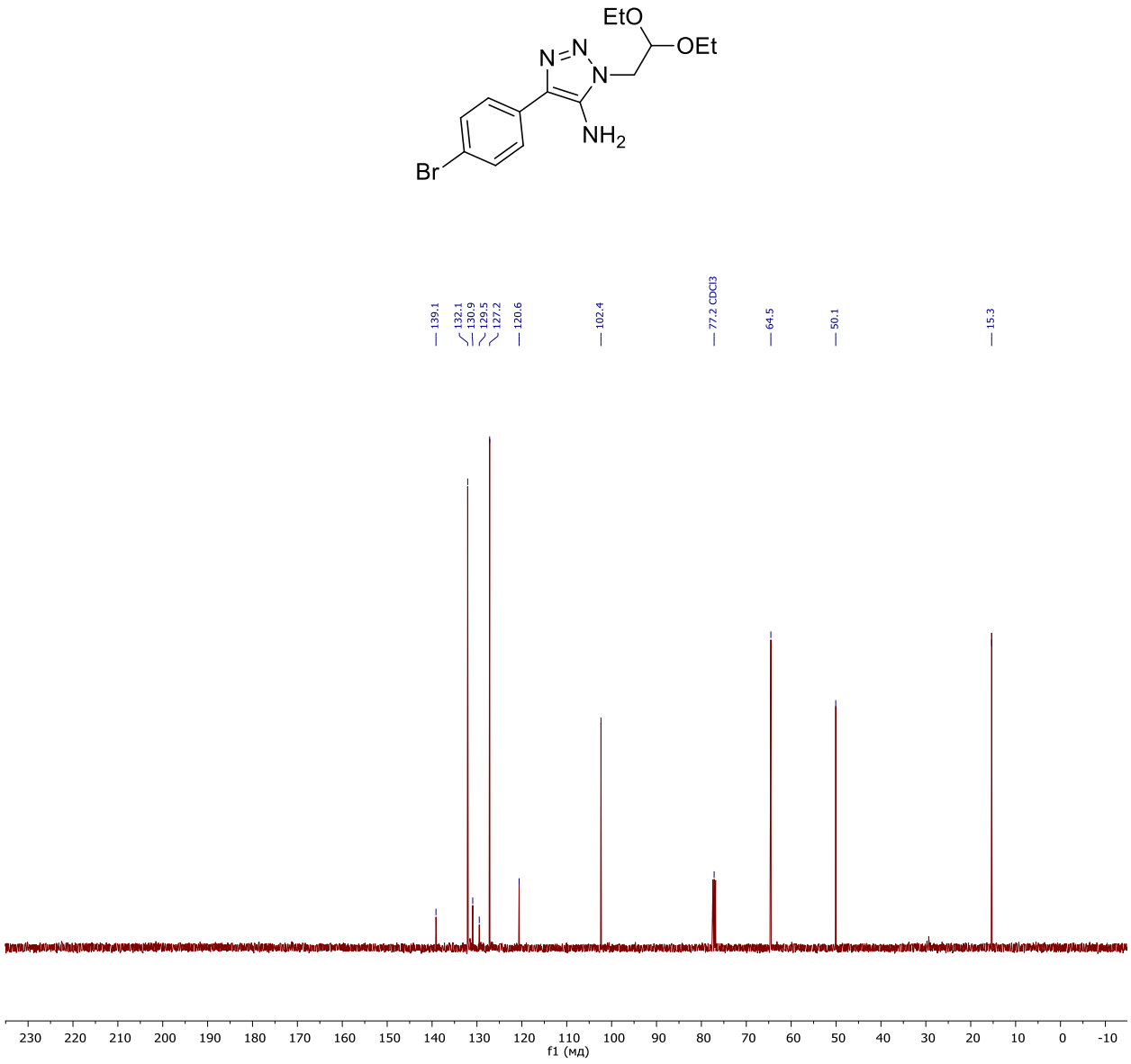


Figure S22. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of compound **3e**.

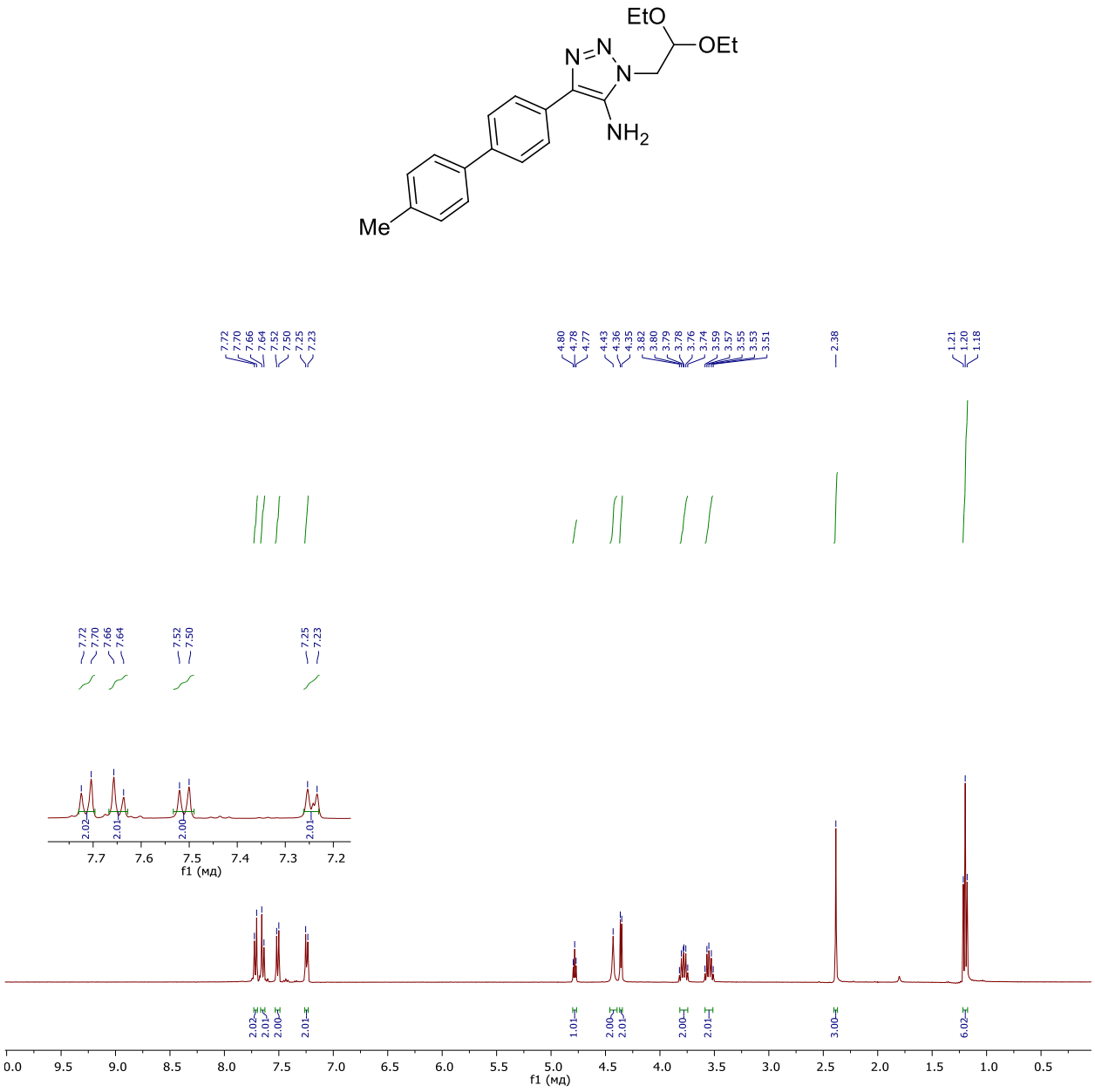


Figure S23. ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **3f**.

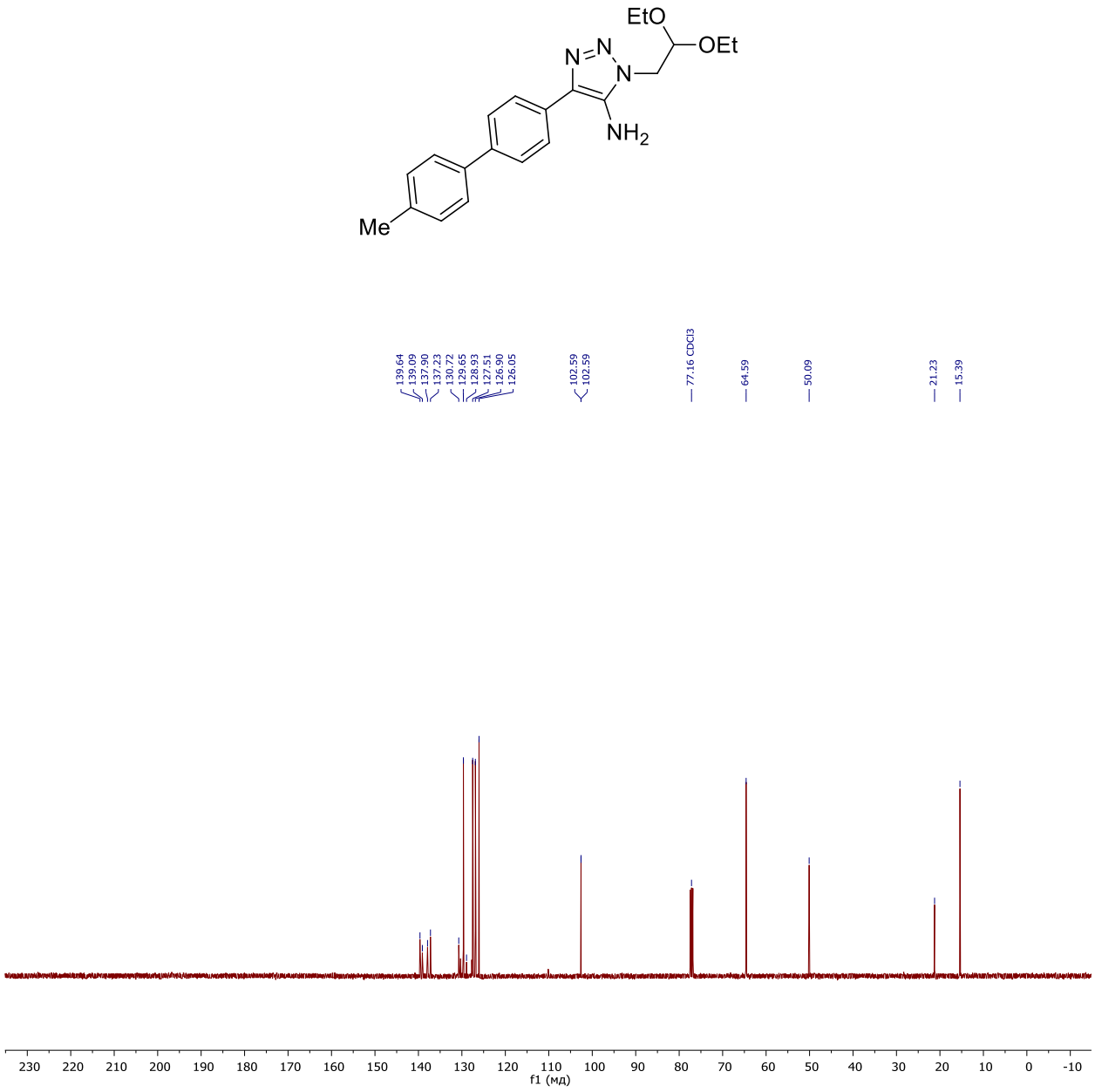


Figure S24. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of compound **3f**.

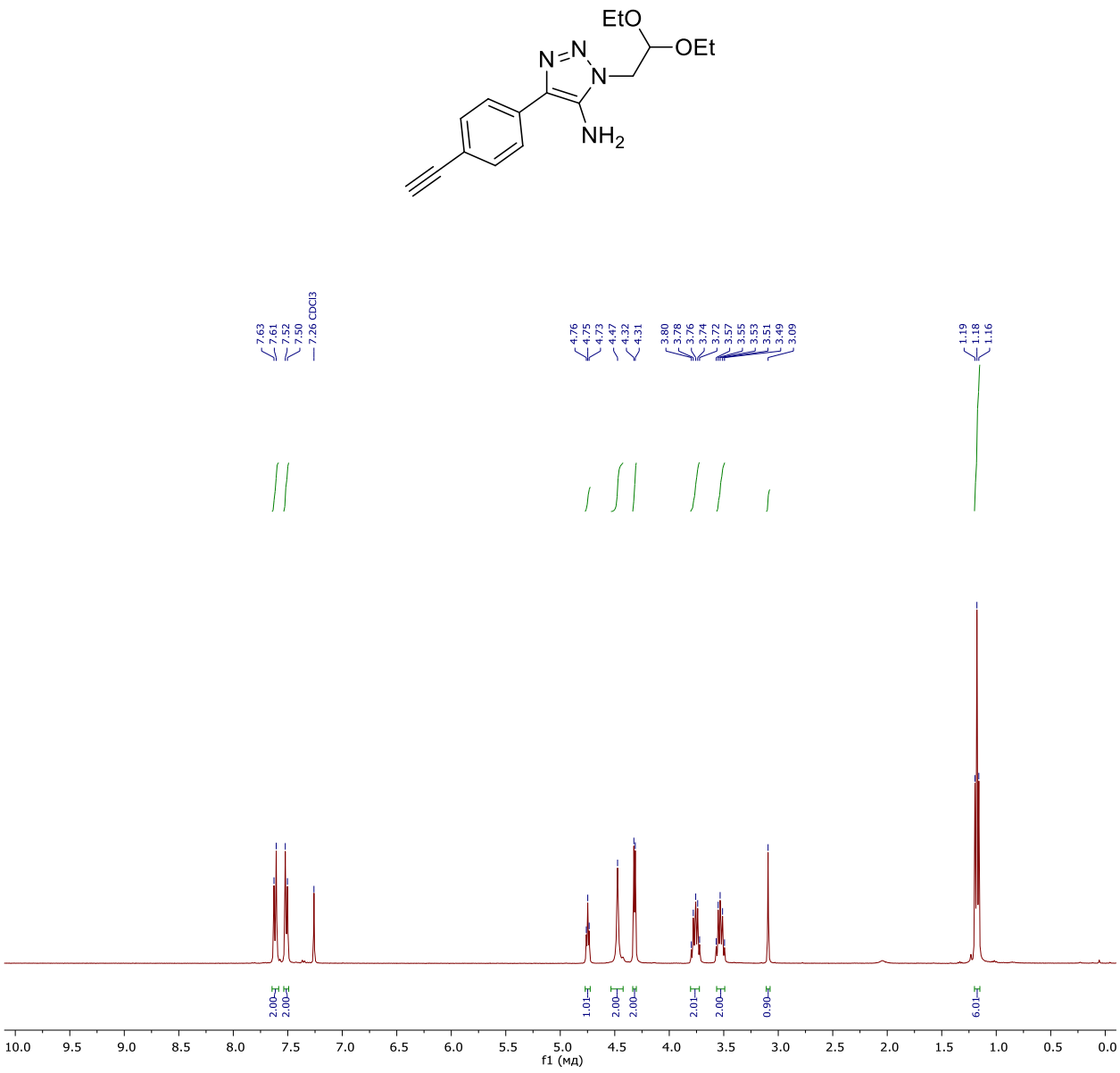


Figure 25 ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **3g**.

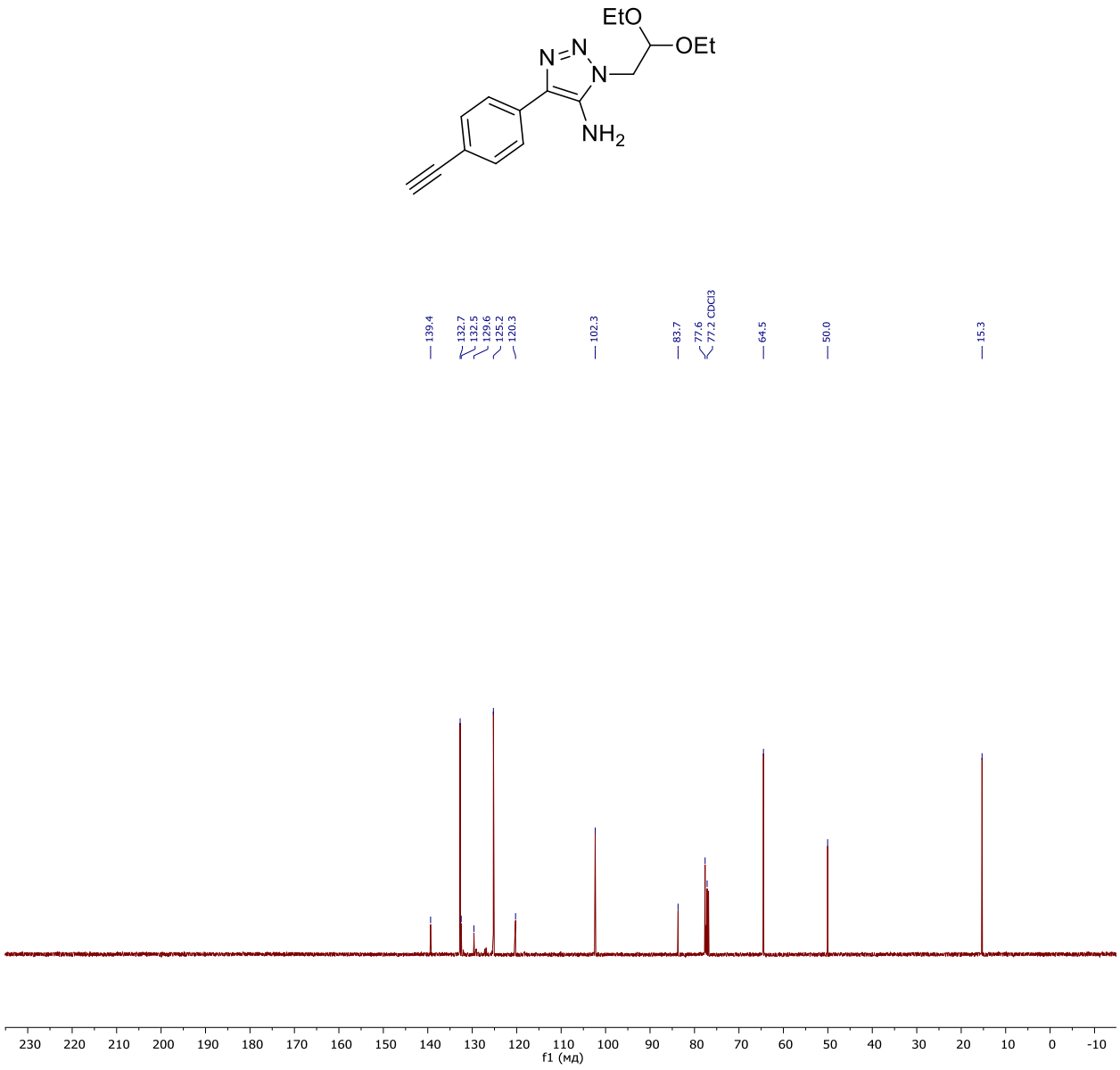


Figure S26. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of compound **3g**.

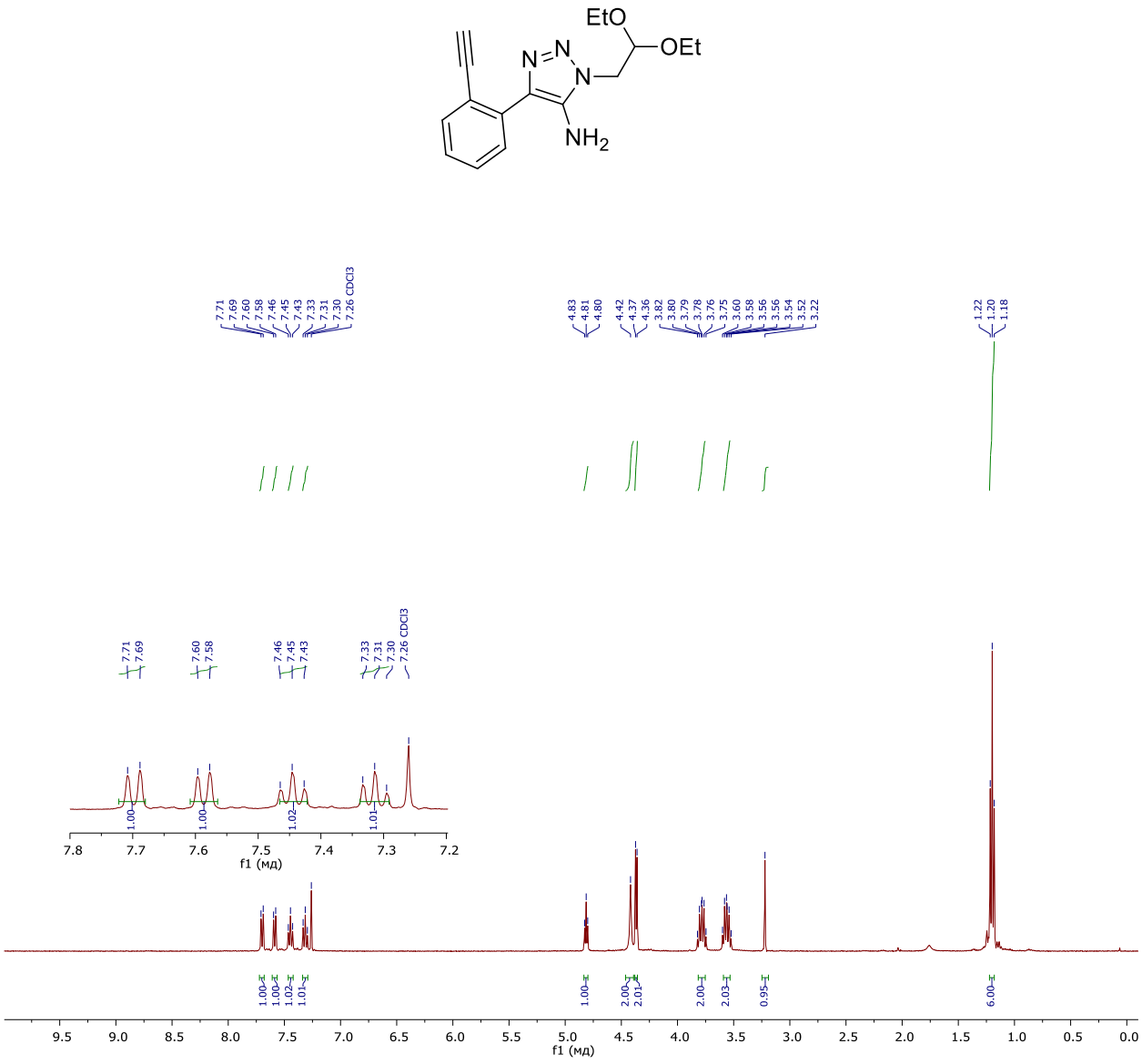


Figure 27 ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **3h**.

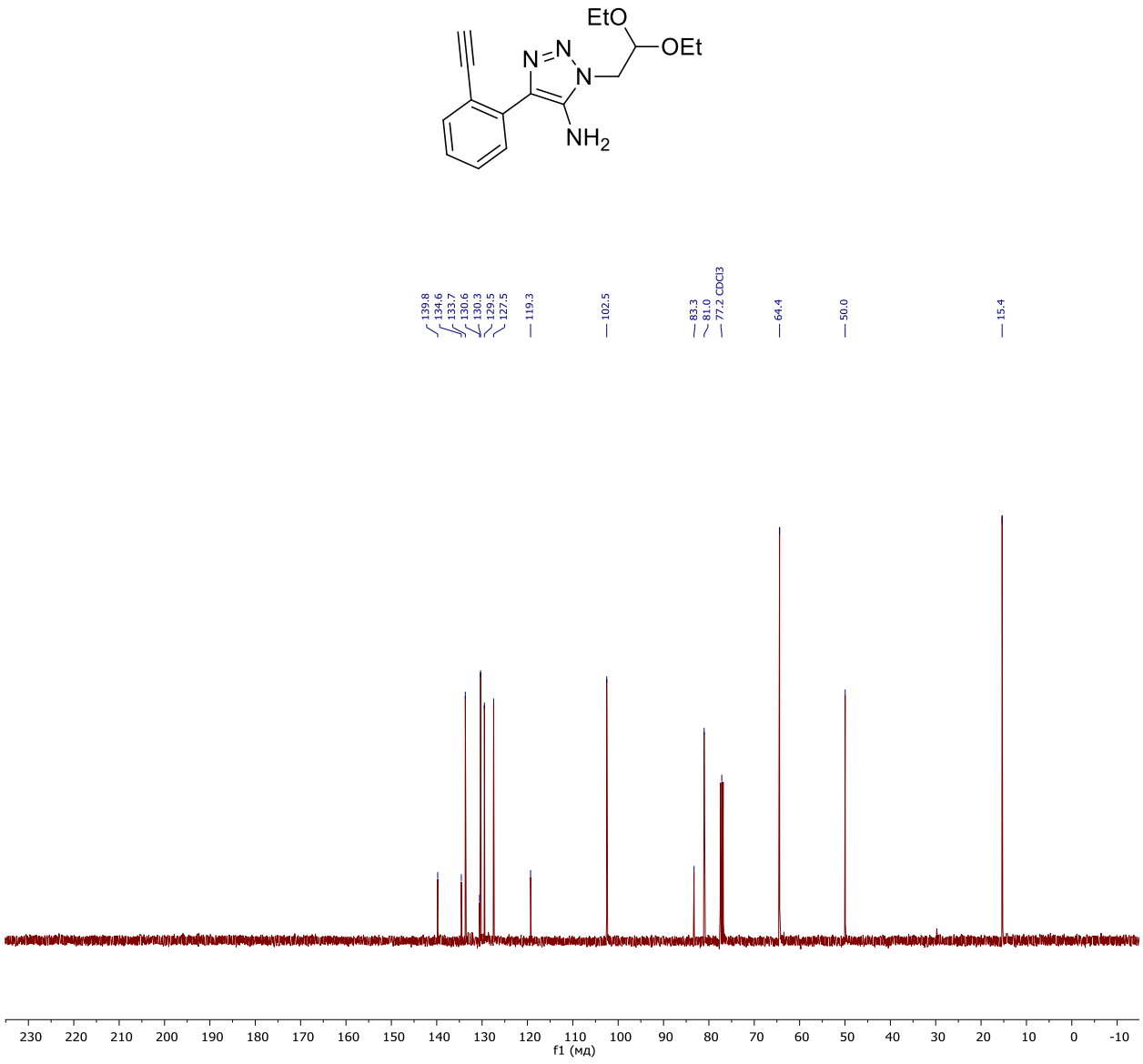


Figure S28. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of compound **3h**.

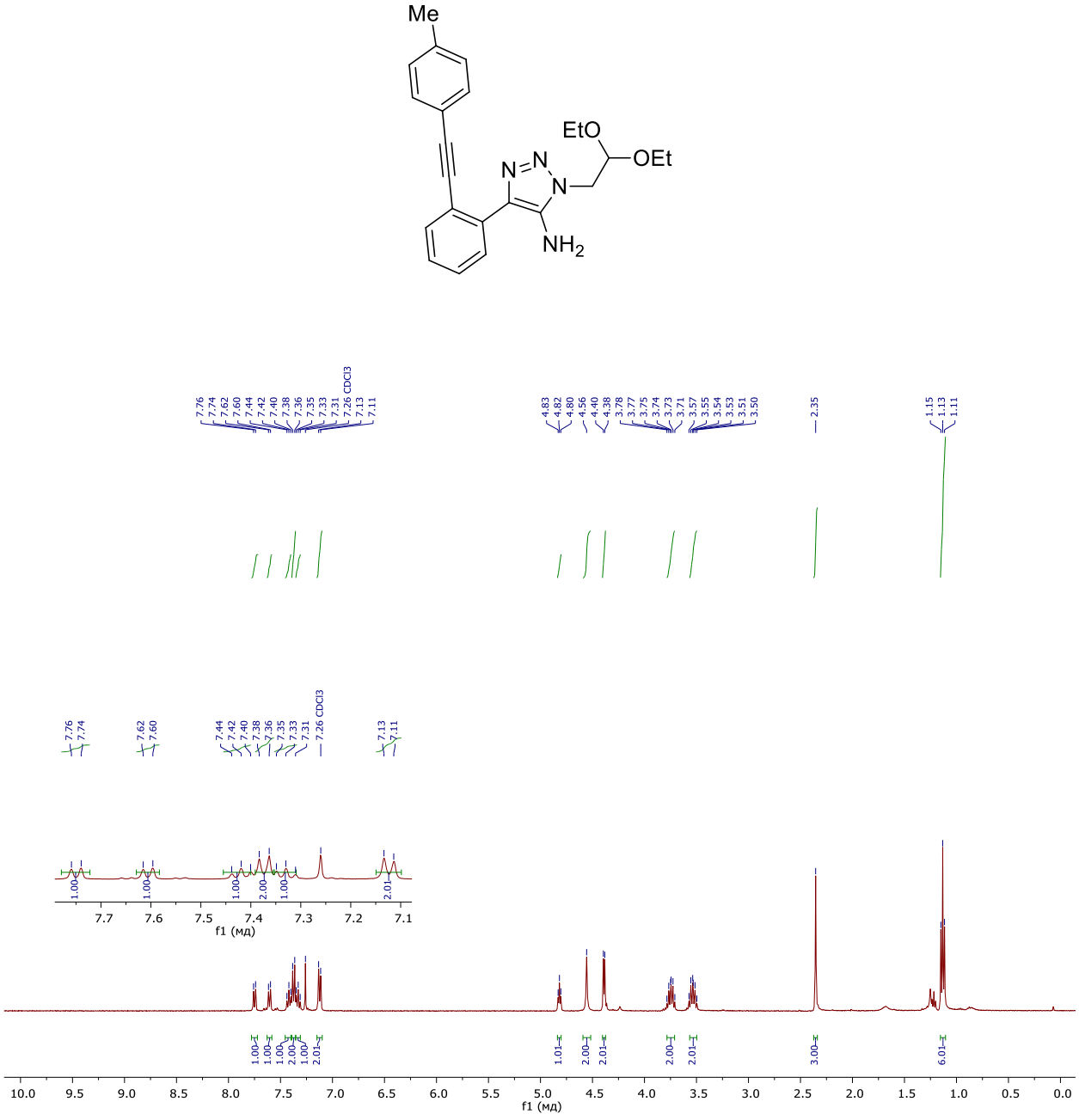


Figure 29 ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **3i**.

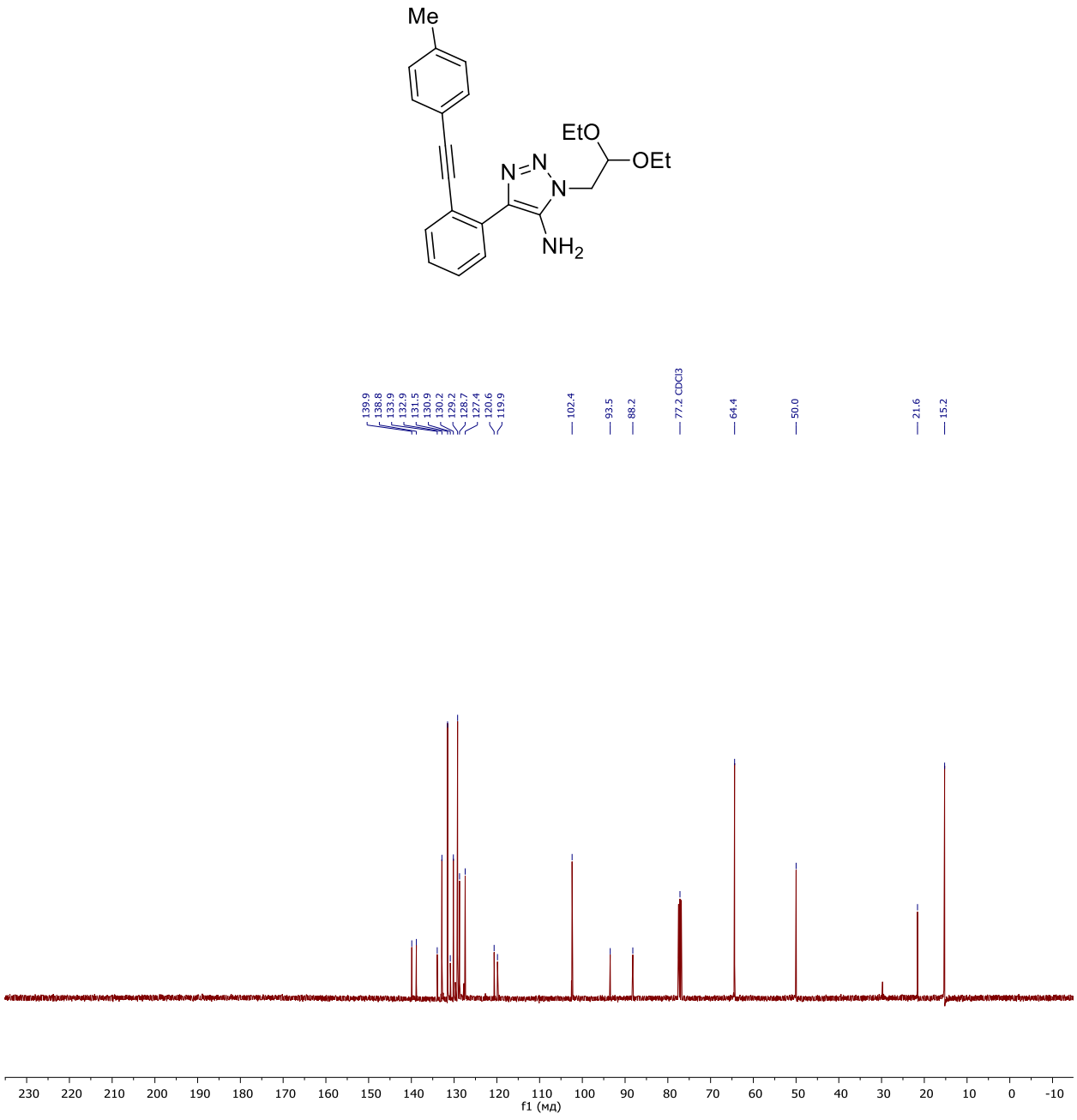


Figure S30. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of compound **3i**.

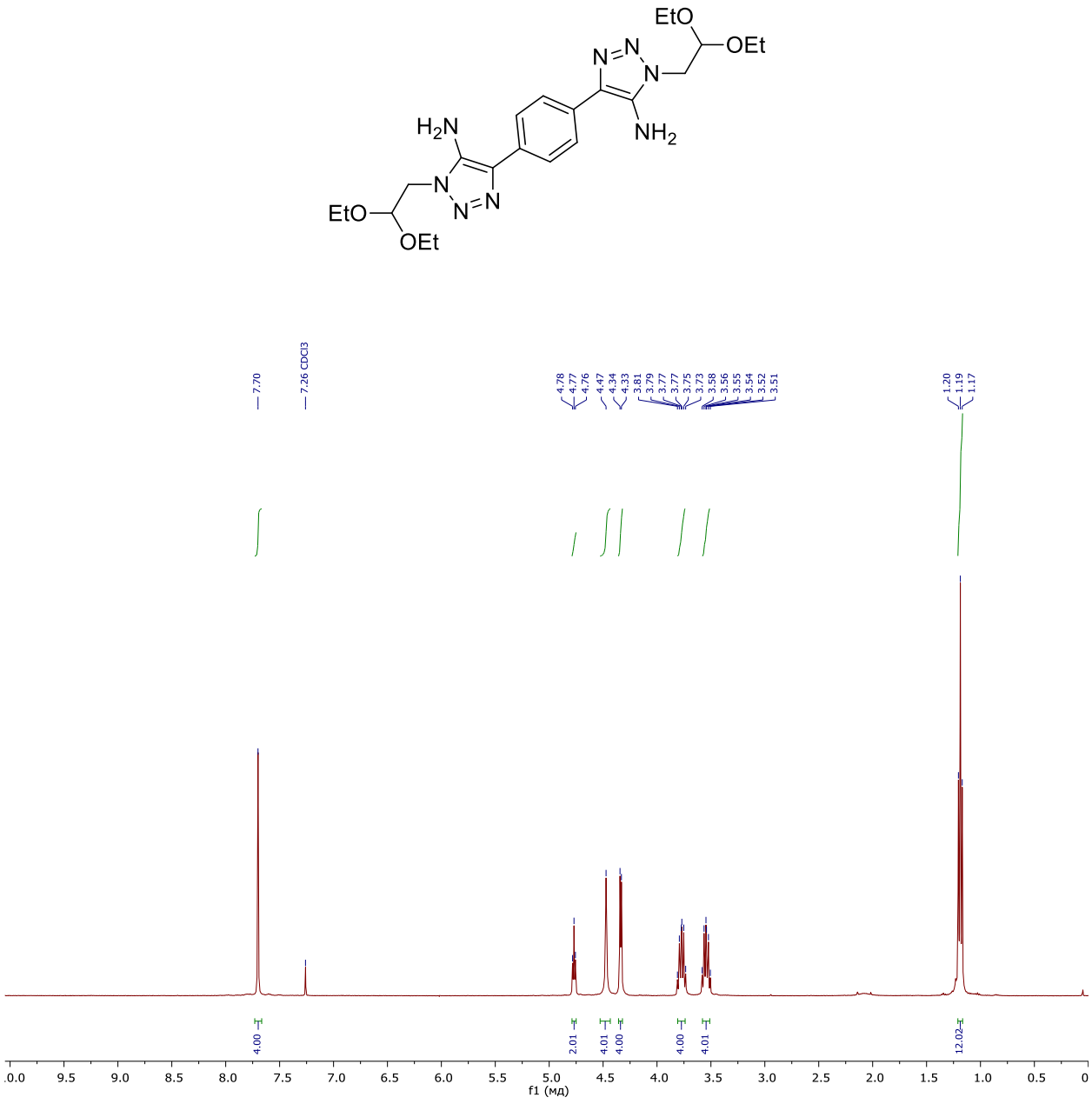


Figure 31 ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **3j**.

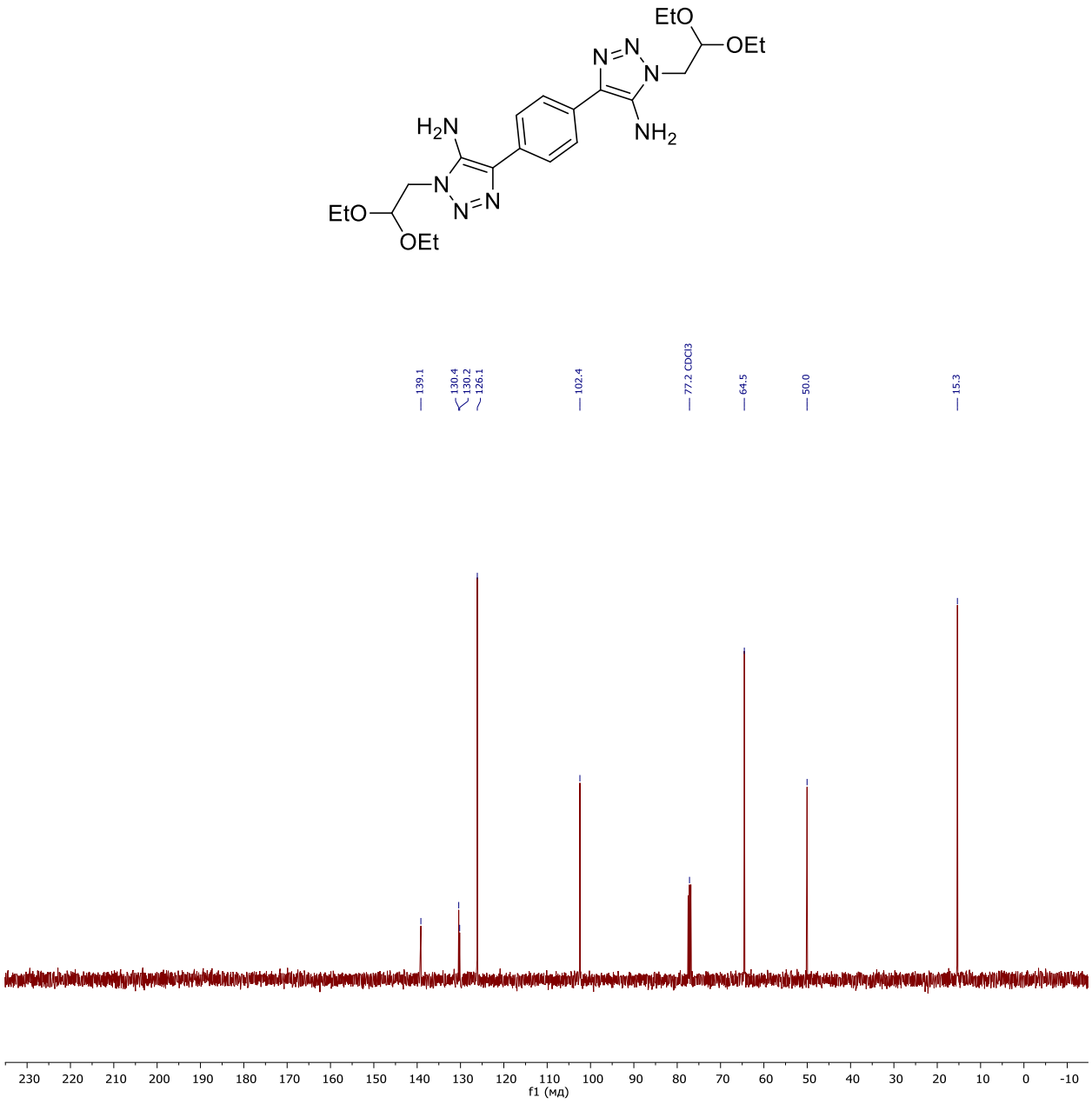


Figure S32. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of compound **3j**.

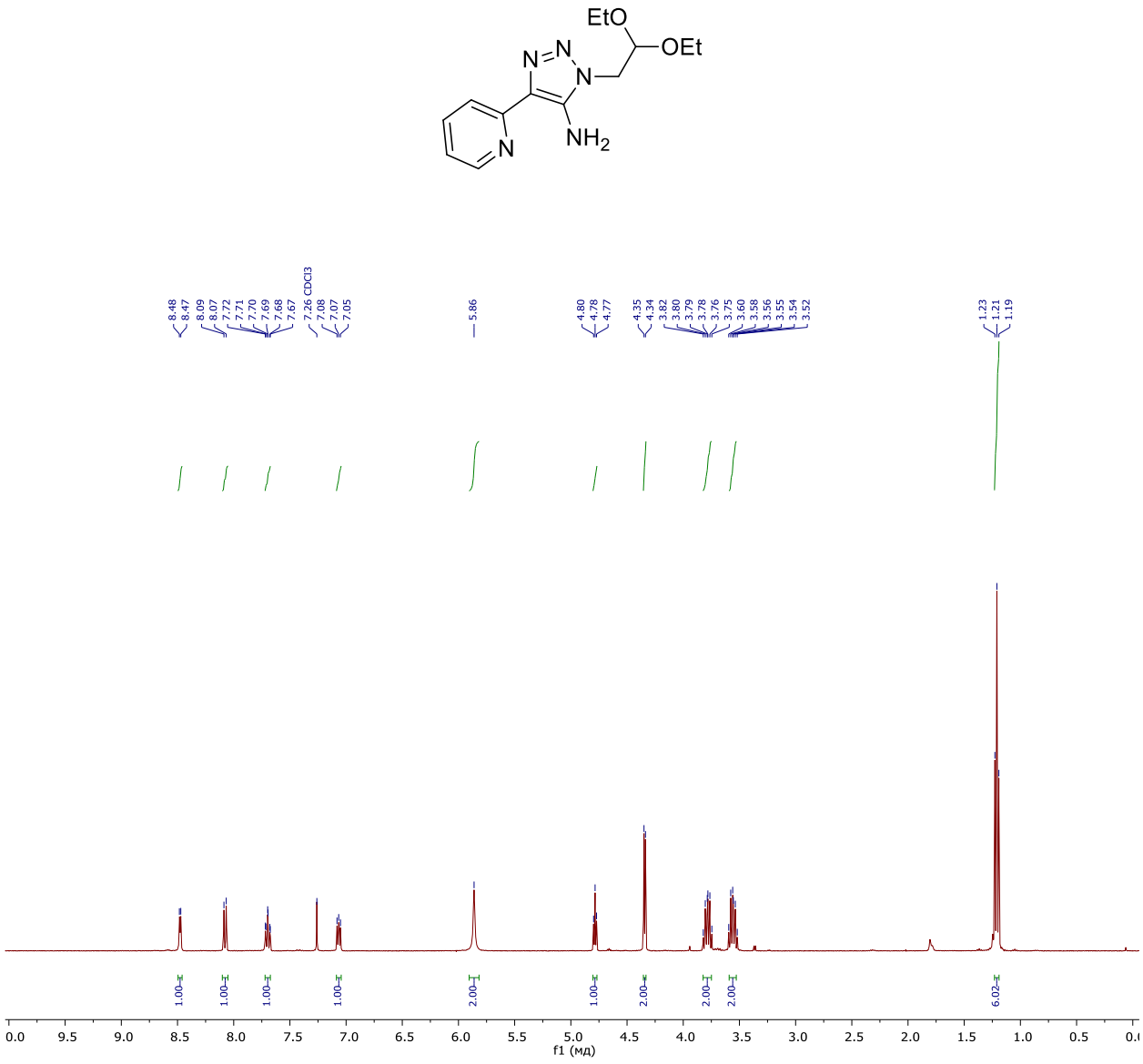


Figure S33 ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **3k**.

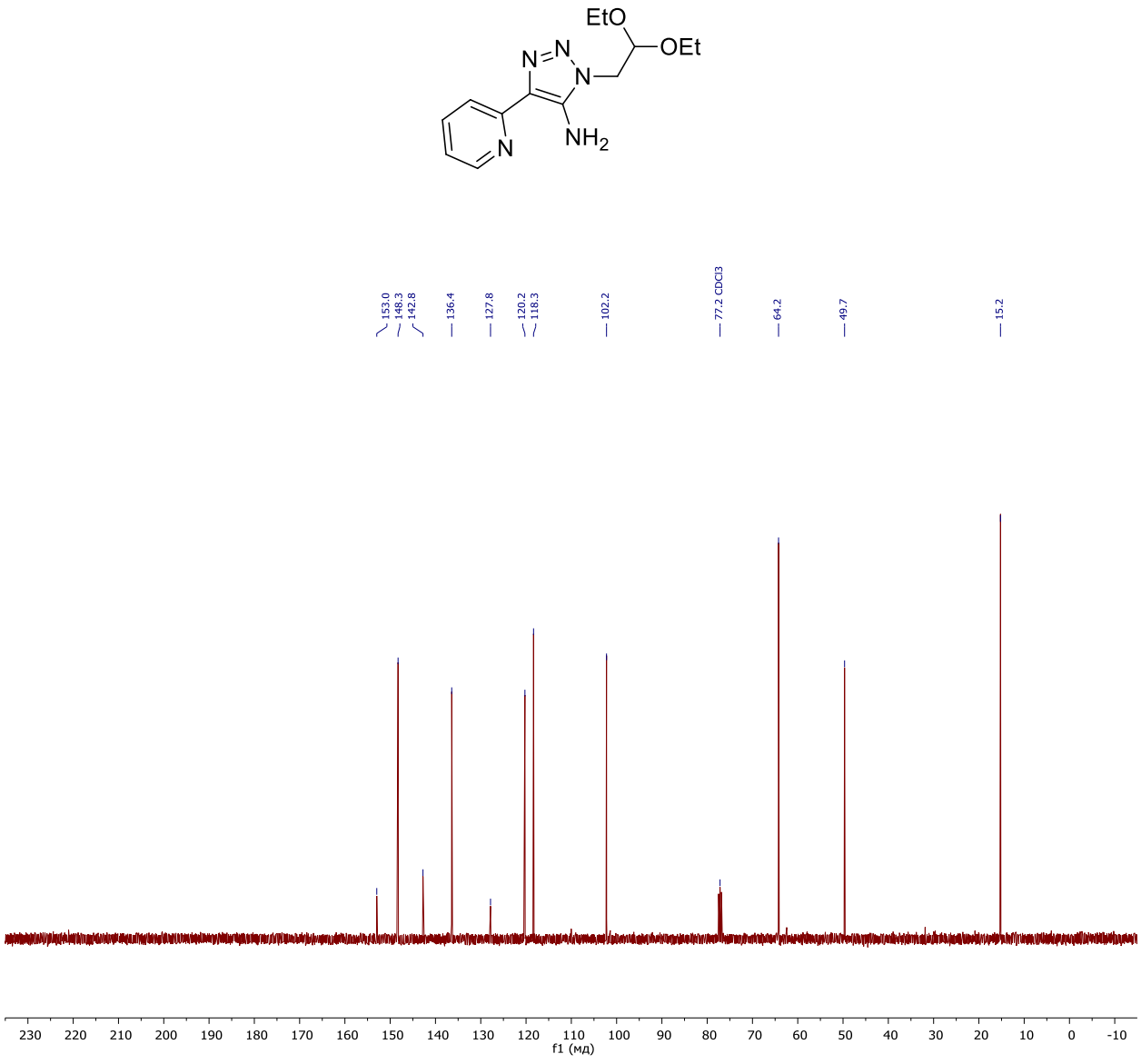


Figure S34. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of compound **3k**.

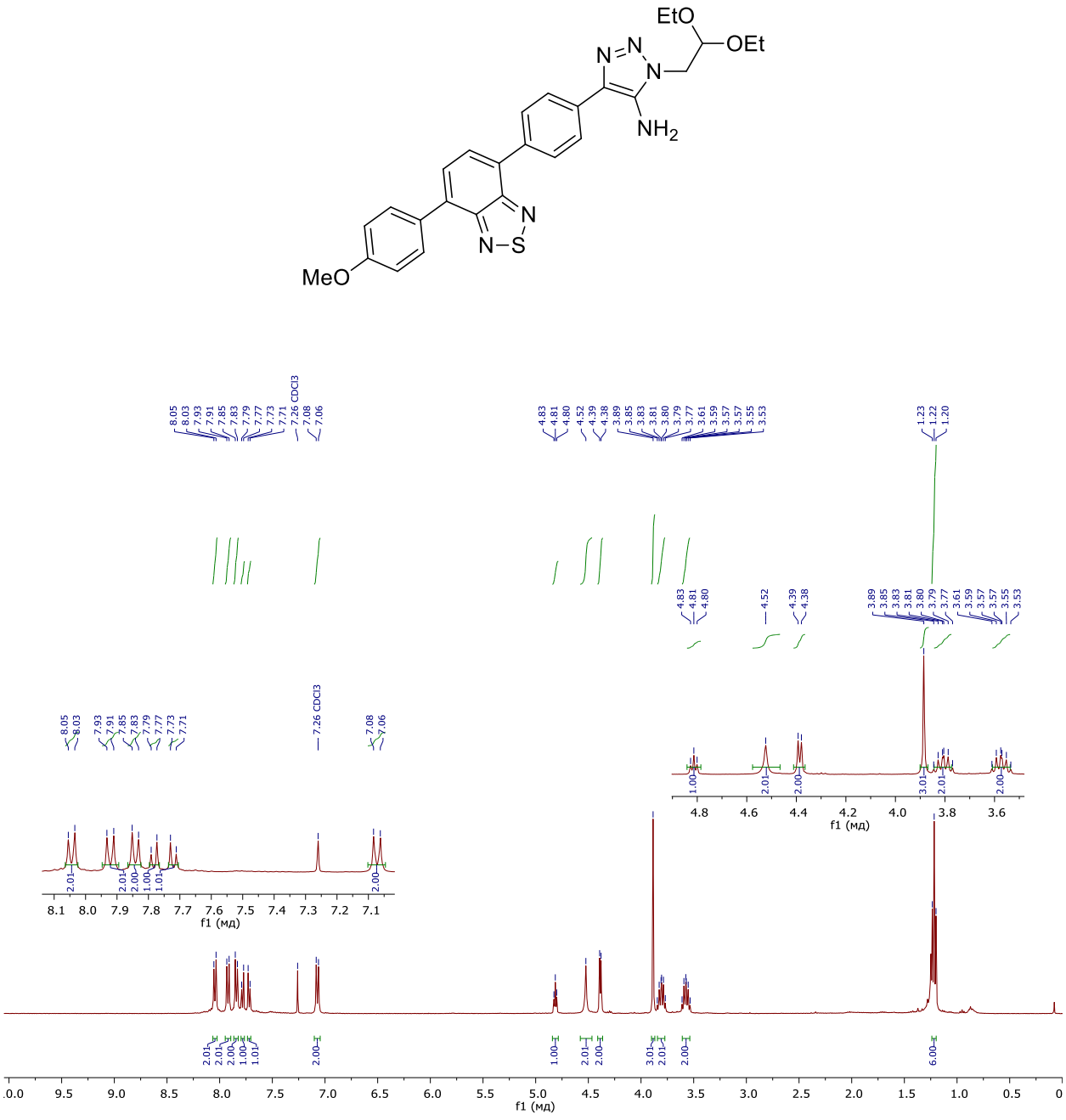


Figure S35. ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **3l**.

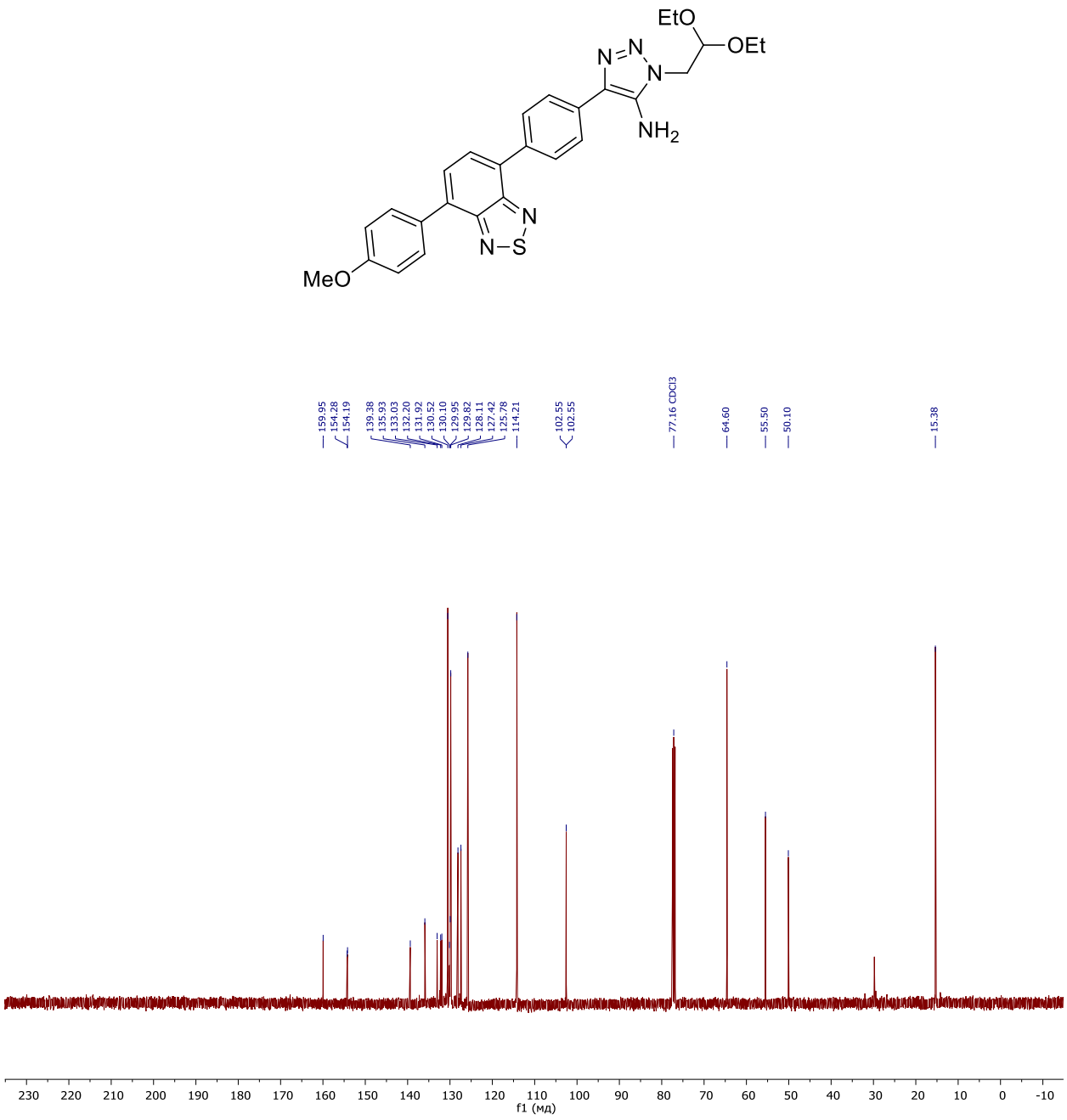


Figure S36. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of compound **3l**.

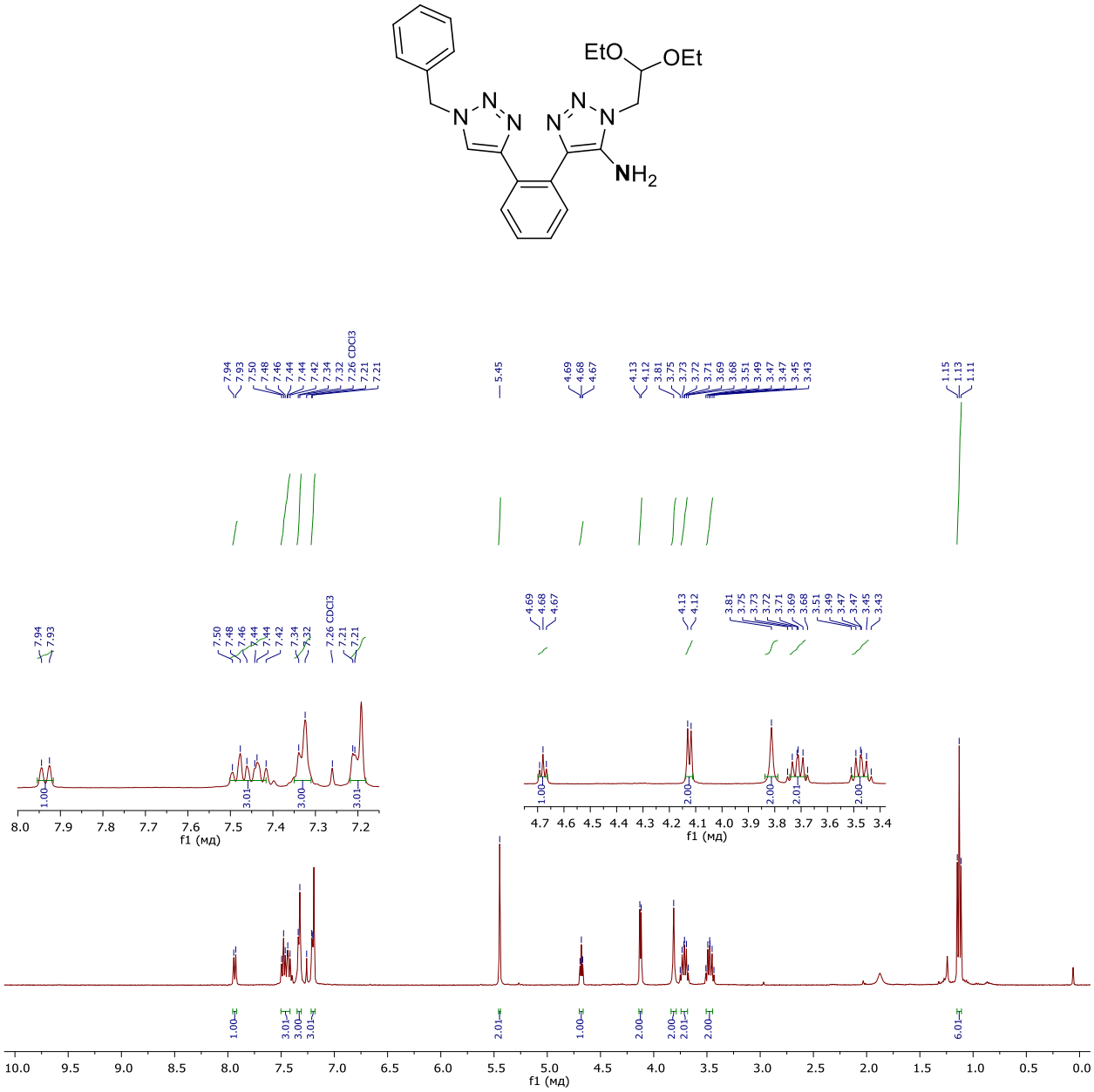


Figure S37. ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **3m**.

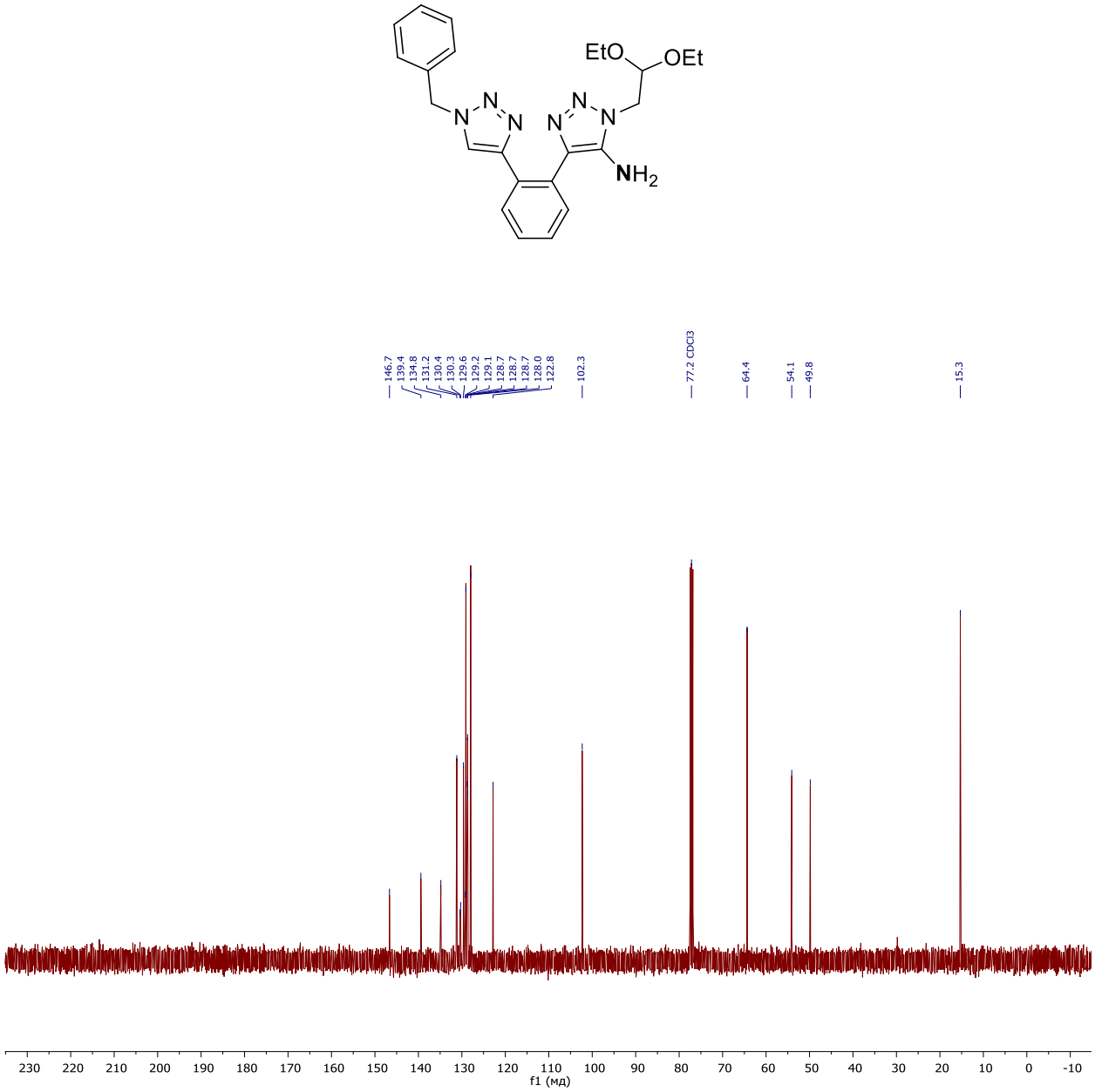


Figure S38. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of compound **3m**.

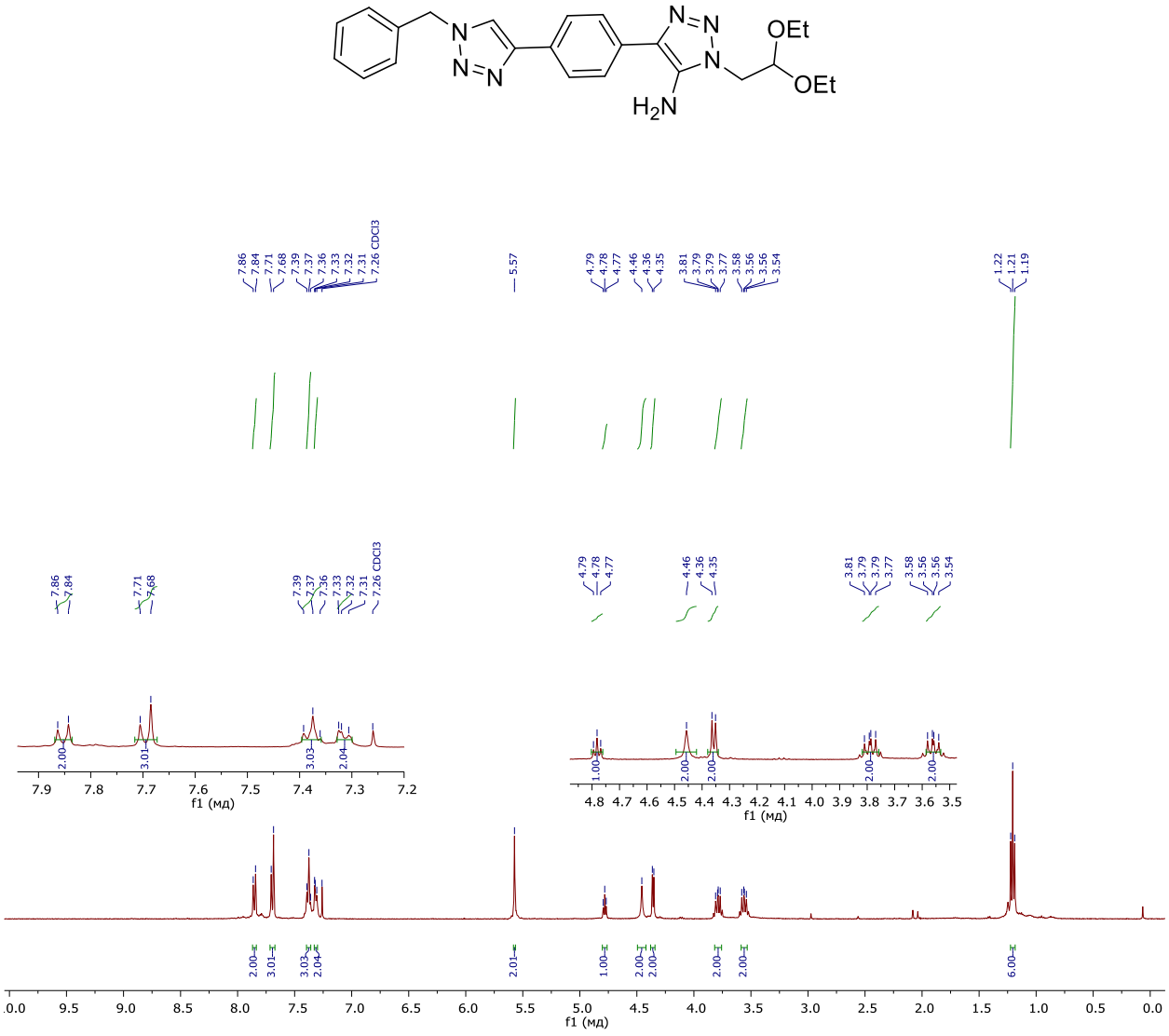


Figure S39. ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **3n**.

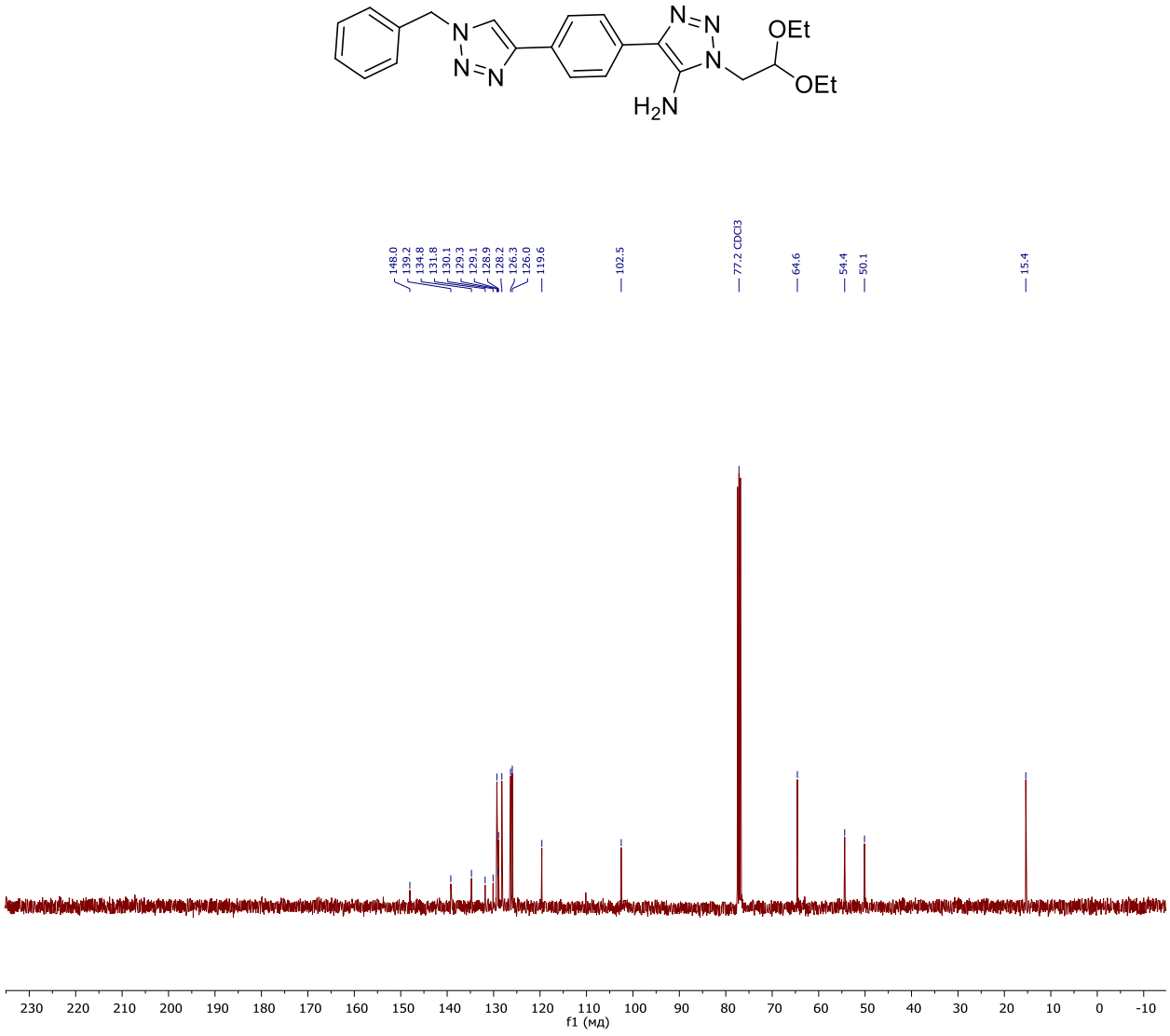


Figure S40. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of compound **3n**.

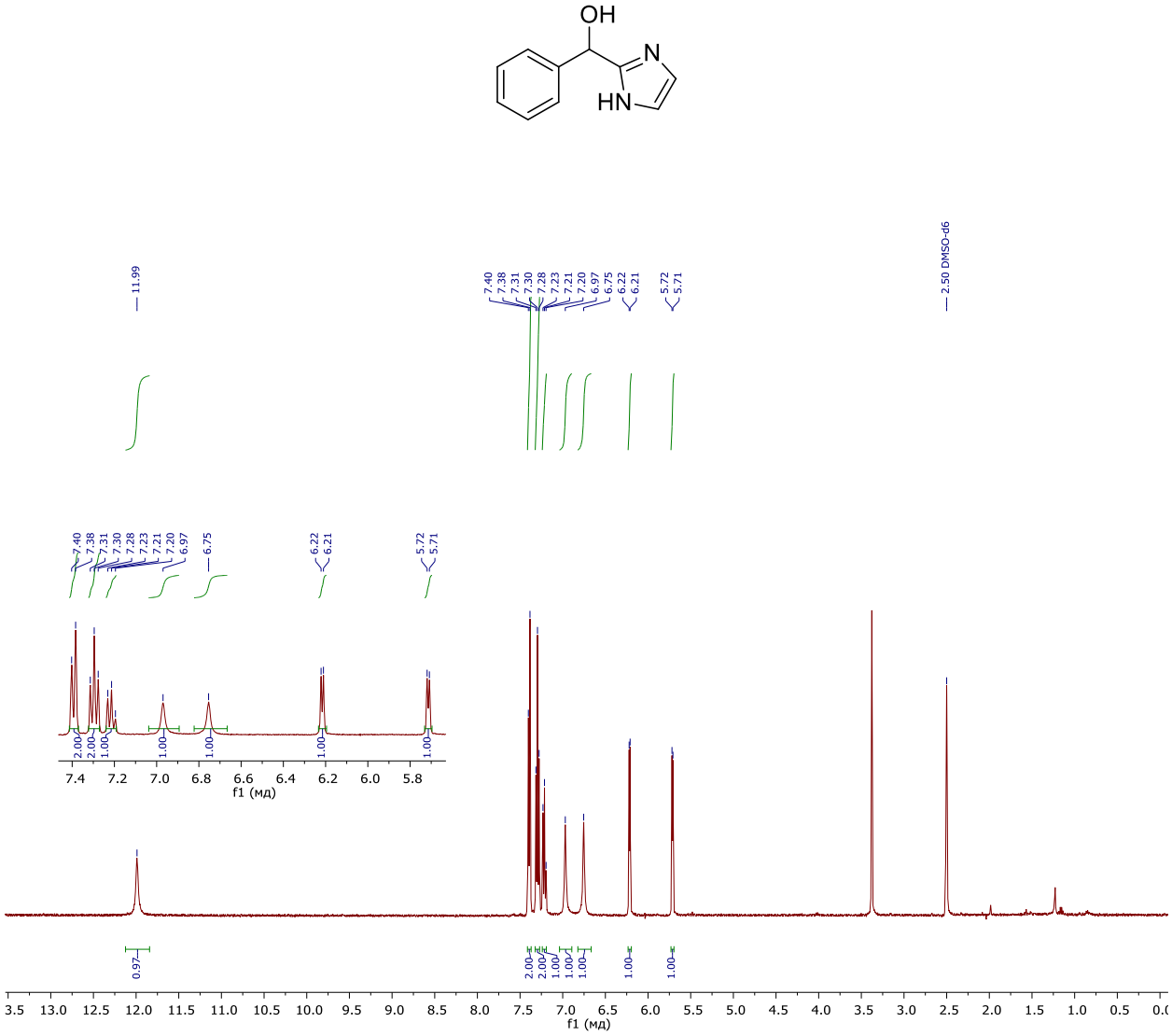


Figure S41. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **4a**.

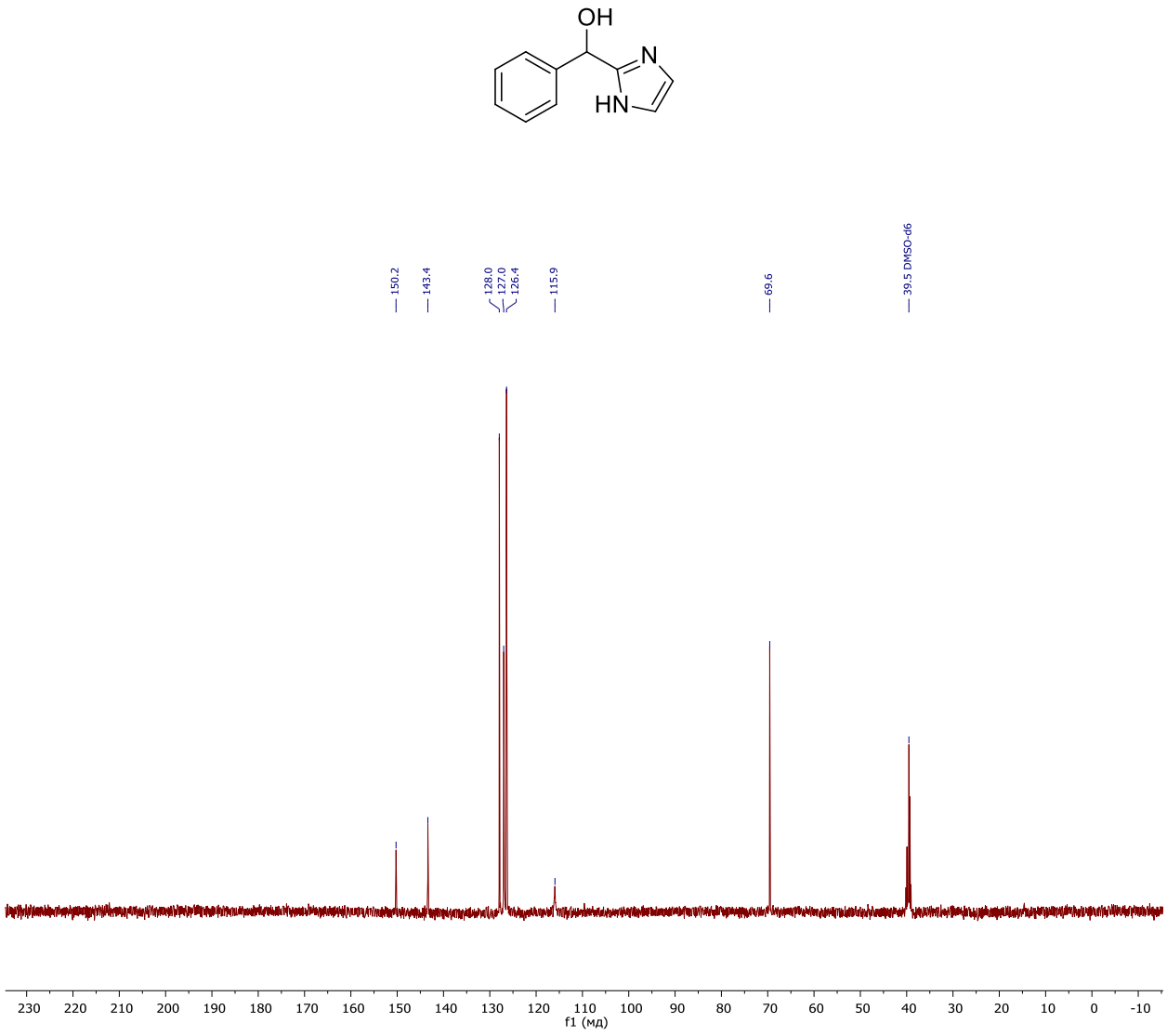


Figure S42. ^{13}C NMR (101 MHz, DMSO-d_6) spectrum of compound **4a**.

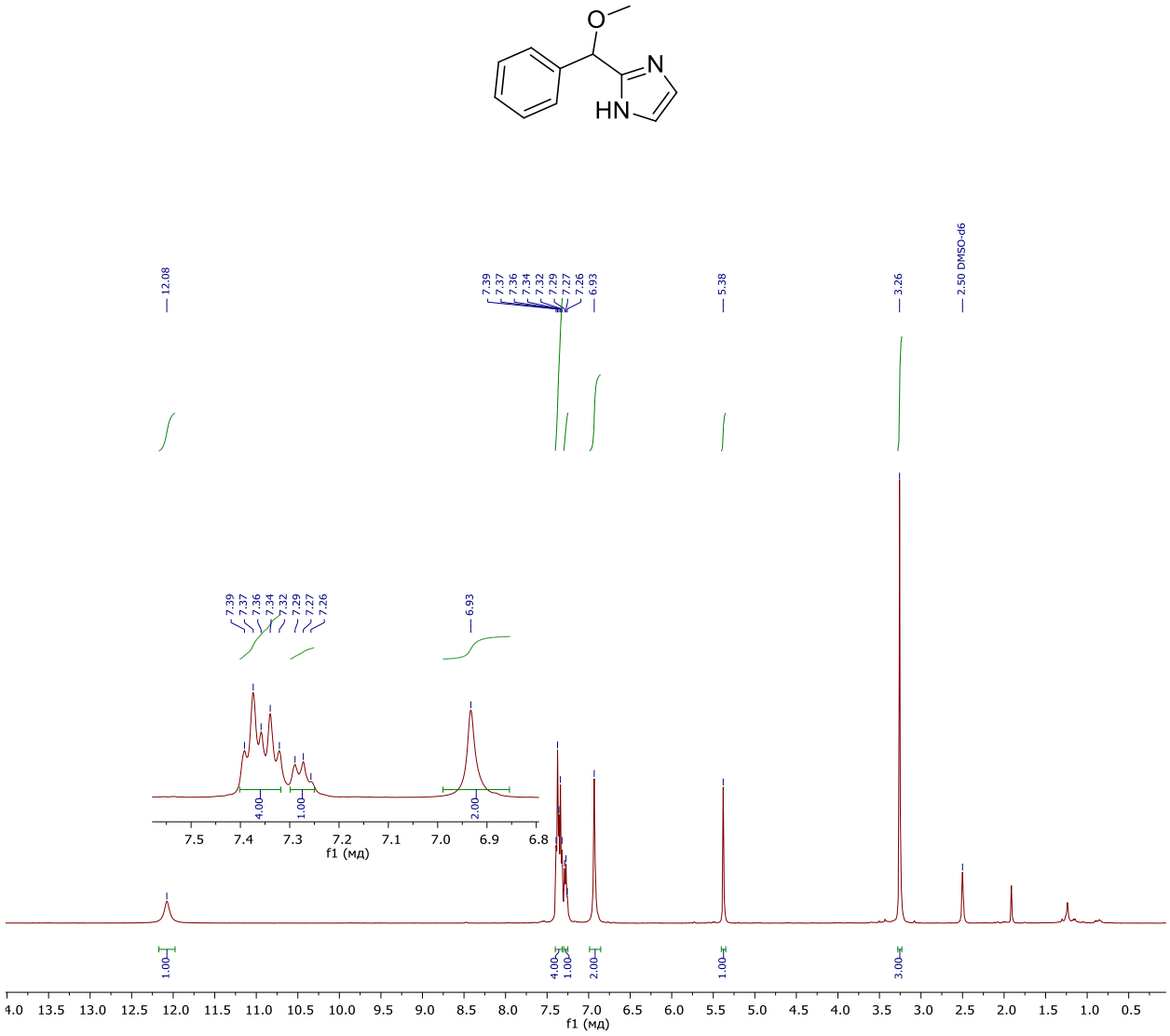


Figure 43 ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **4b**.

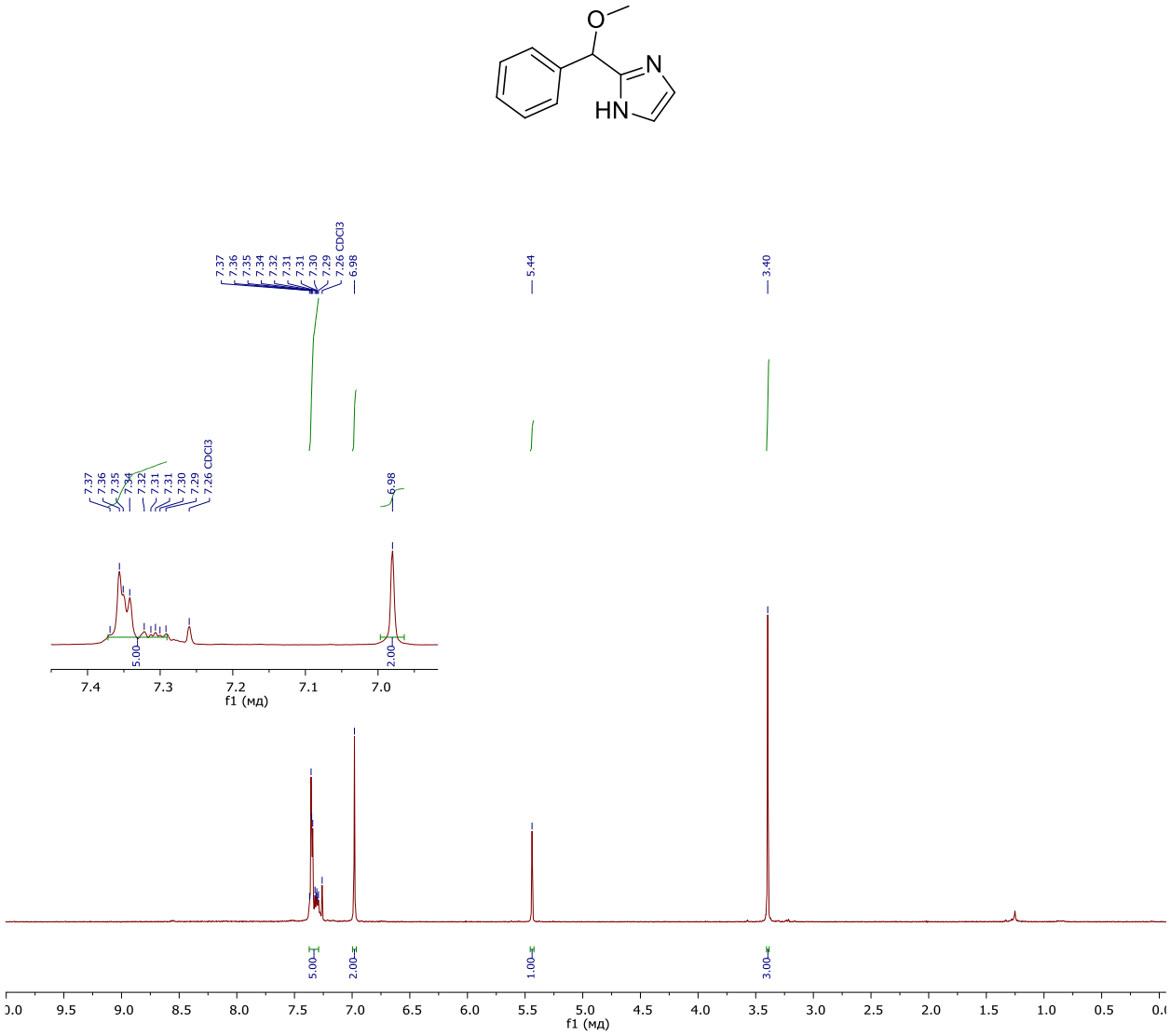


Figure 44 ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **4b**.

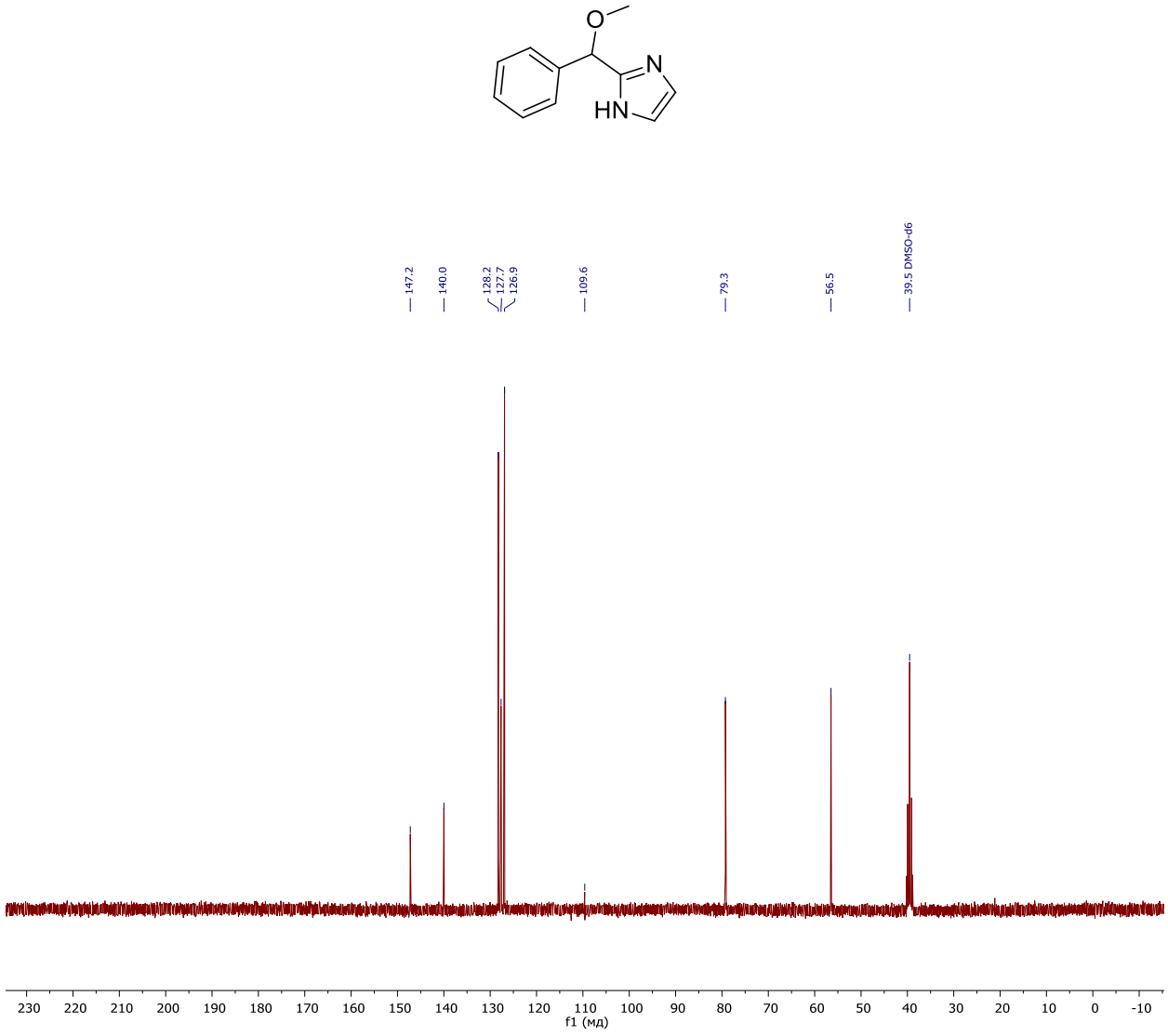


Figure S45. ^{13}C NMR (101 MHz, DMSO-d_6) spectrum of compound **4b**.

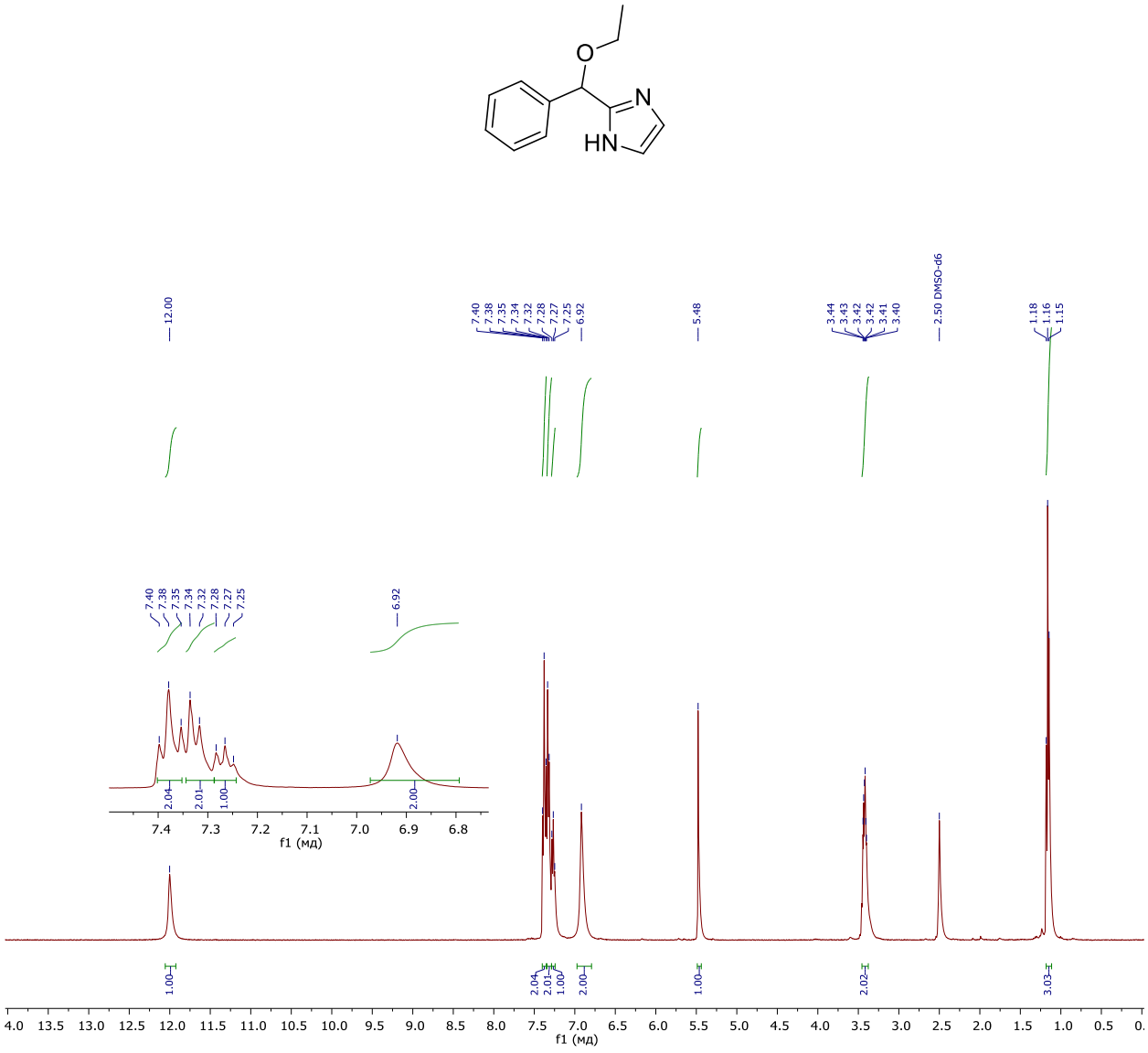


Figure 46 ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **4c**.

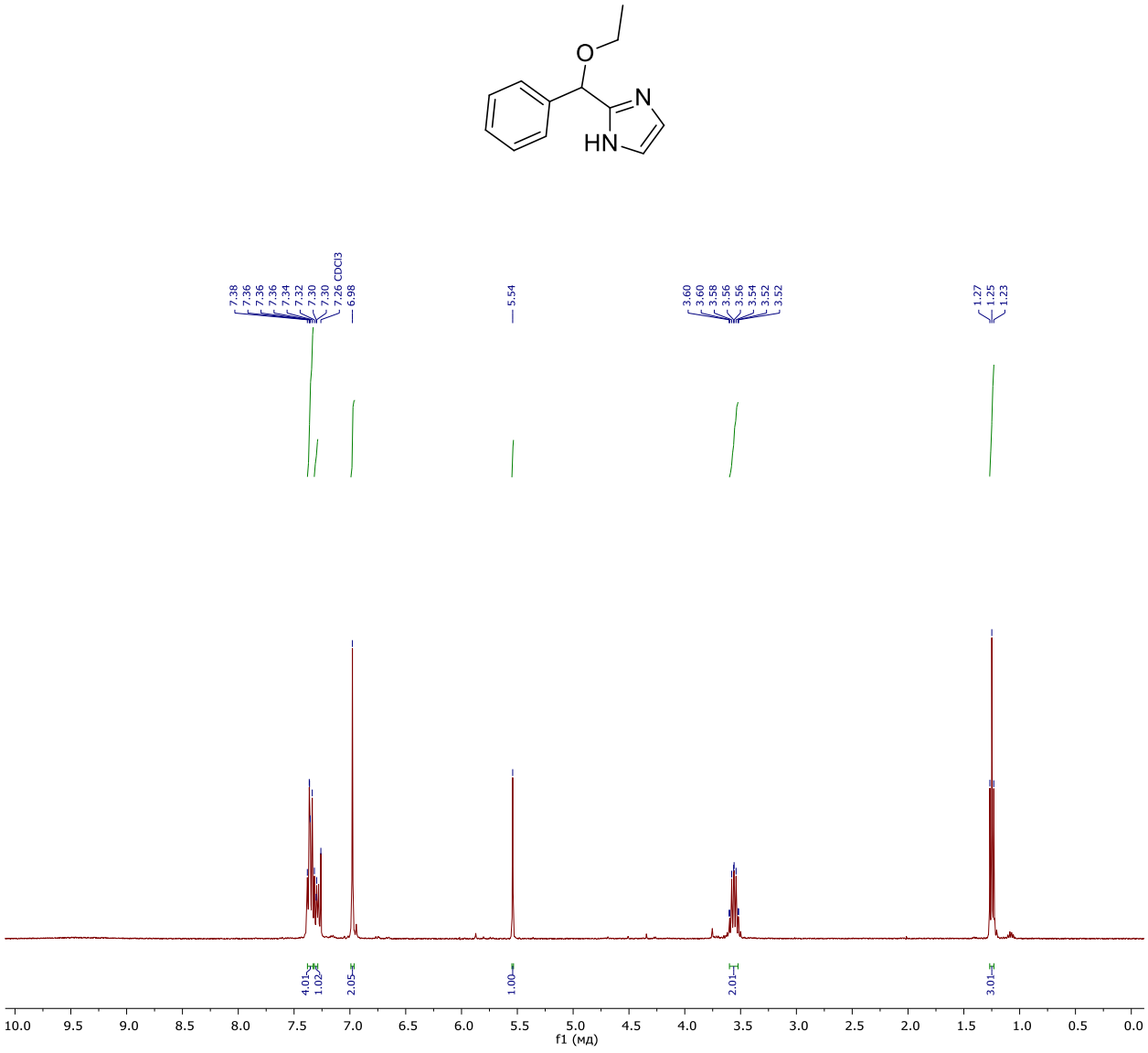


Figure 47 ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **4c**.

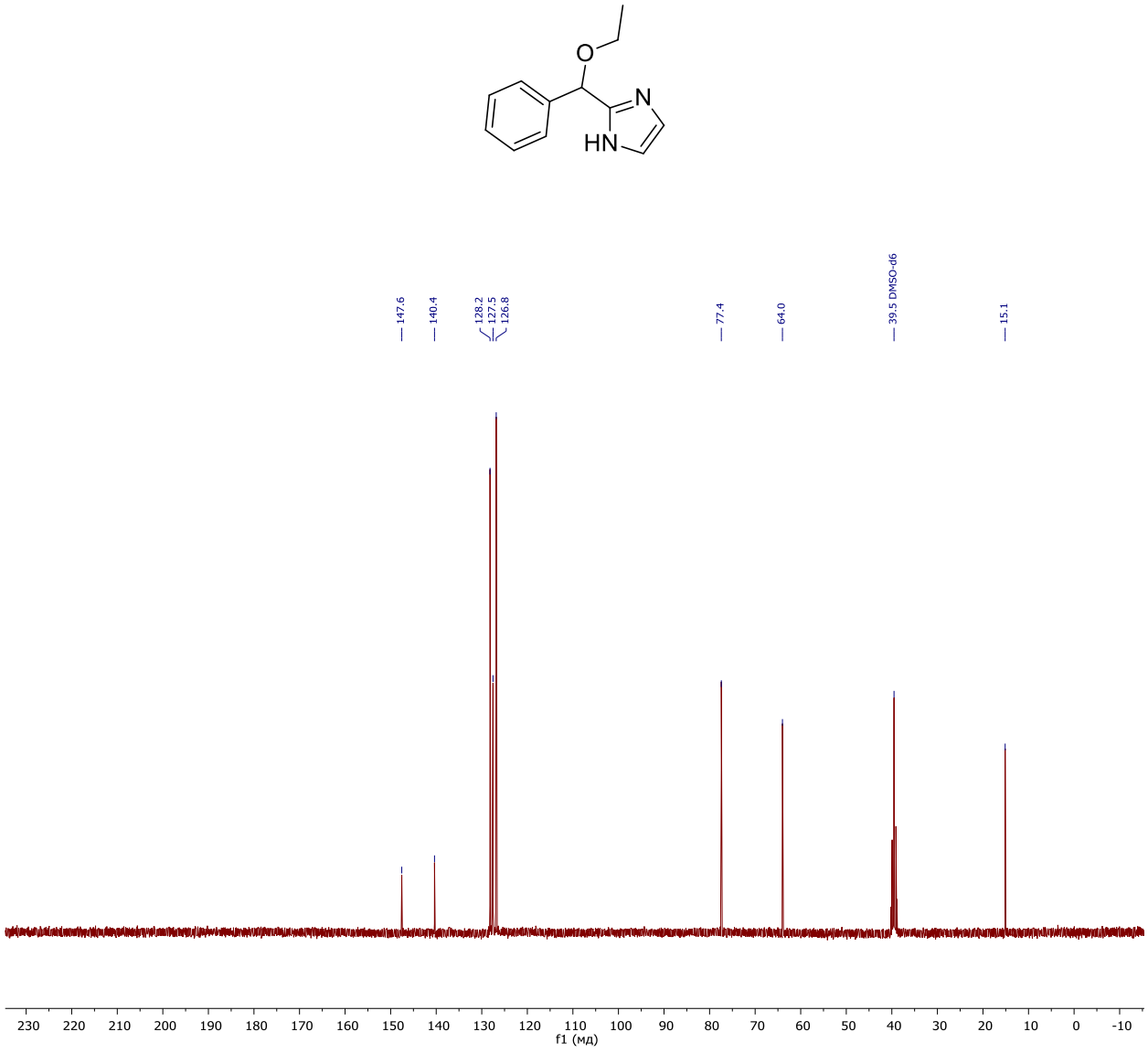


Figure S48. ^{13}C NMR (101 MHz, DMSO-d_6) spectrum of compound **4c**.

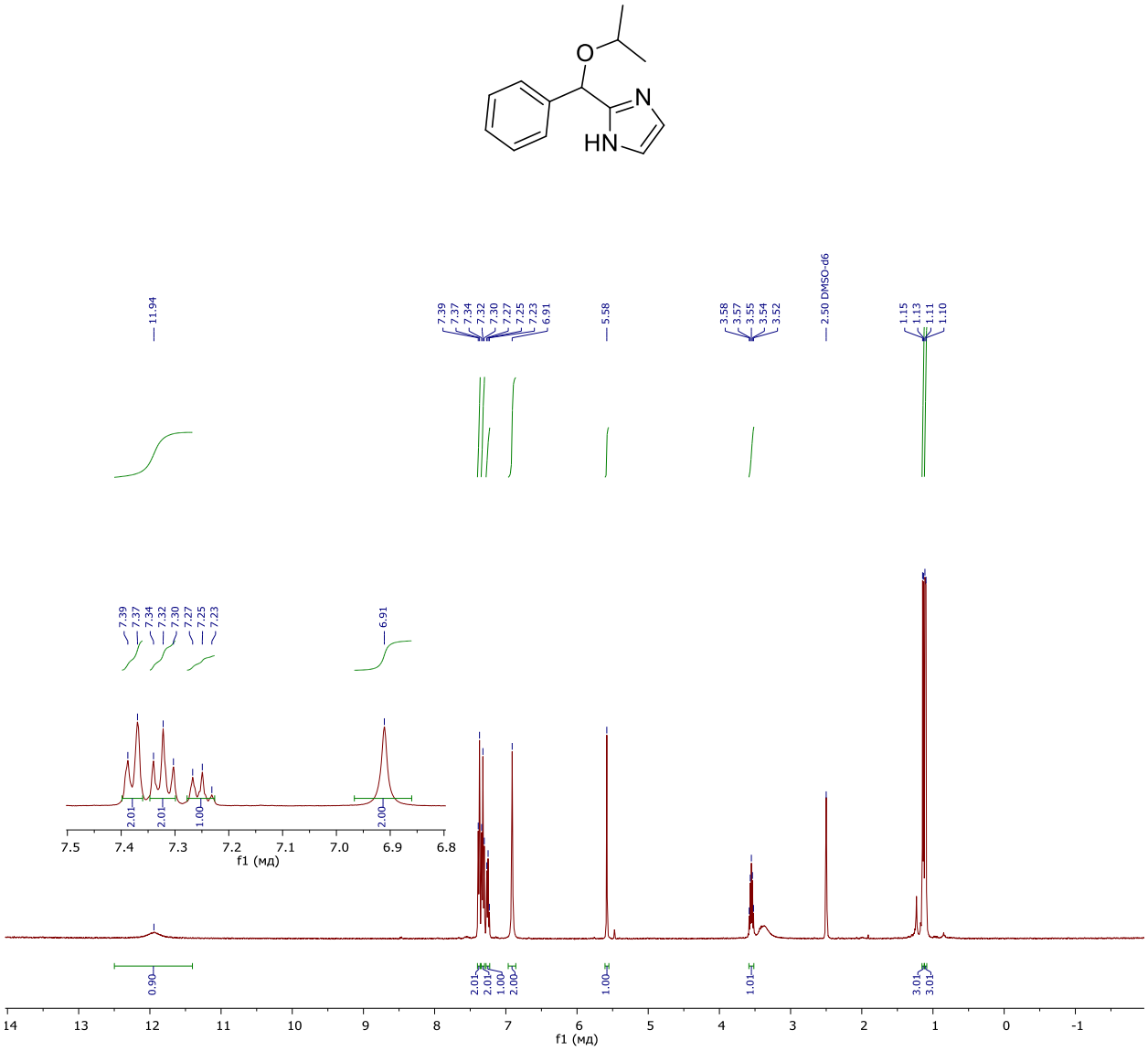


Figure S49. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **4d**.

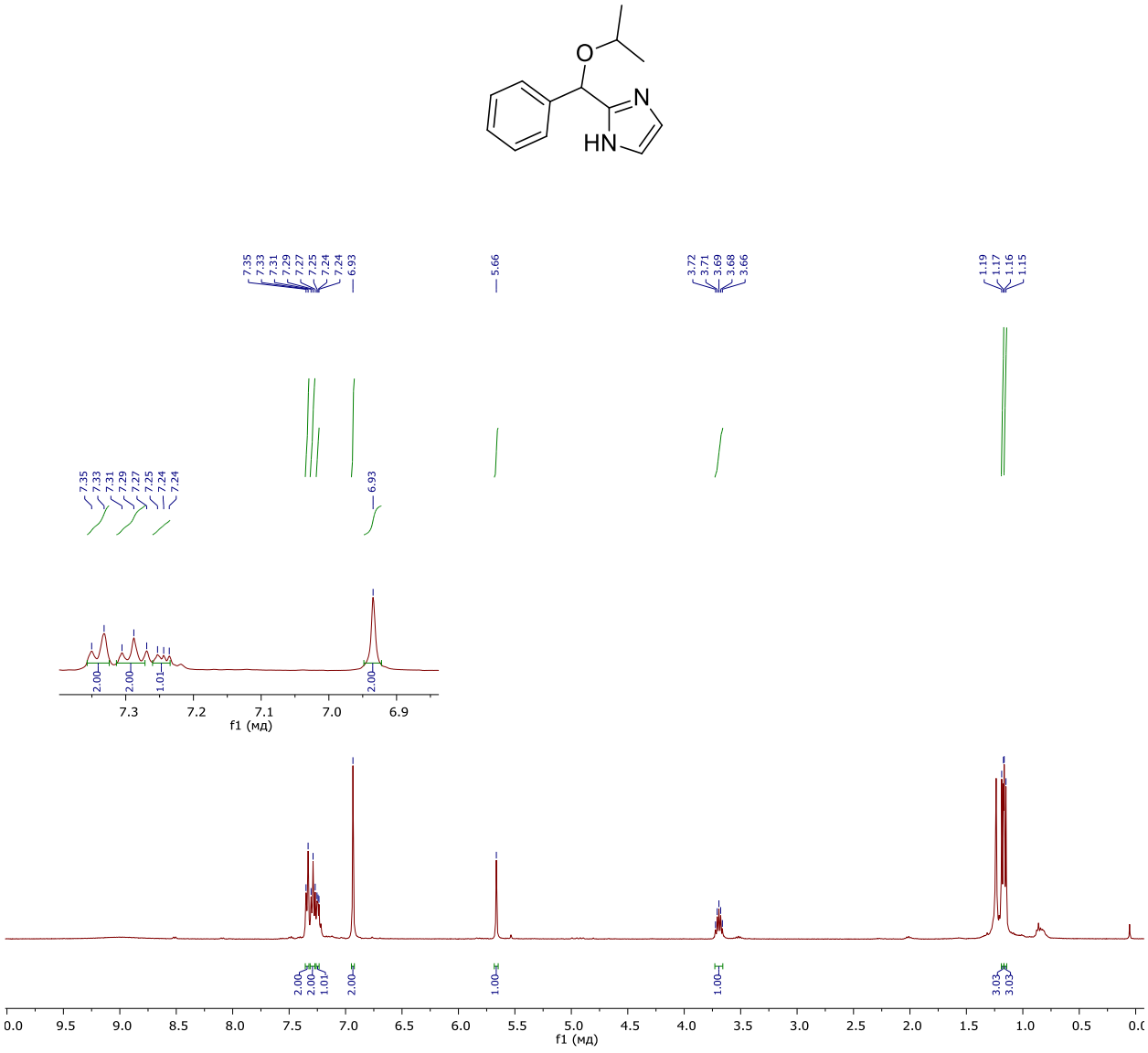


Figure S50. ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **4d**.

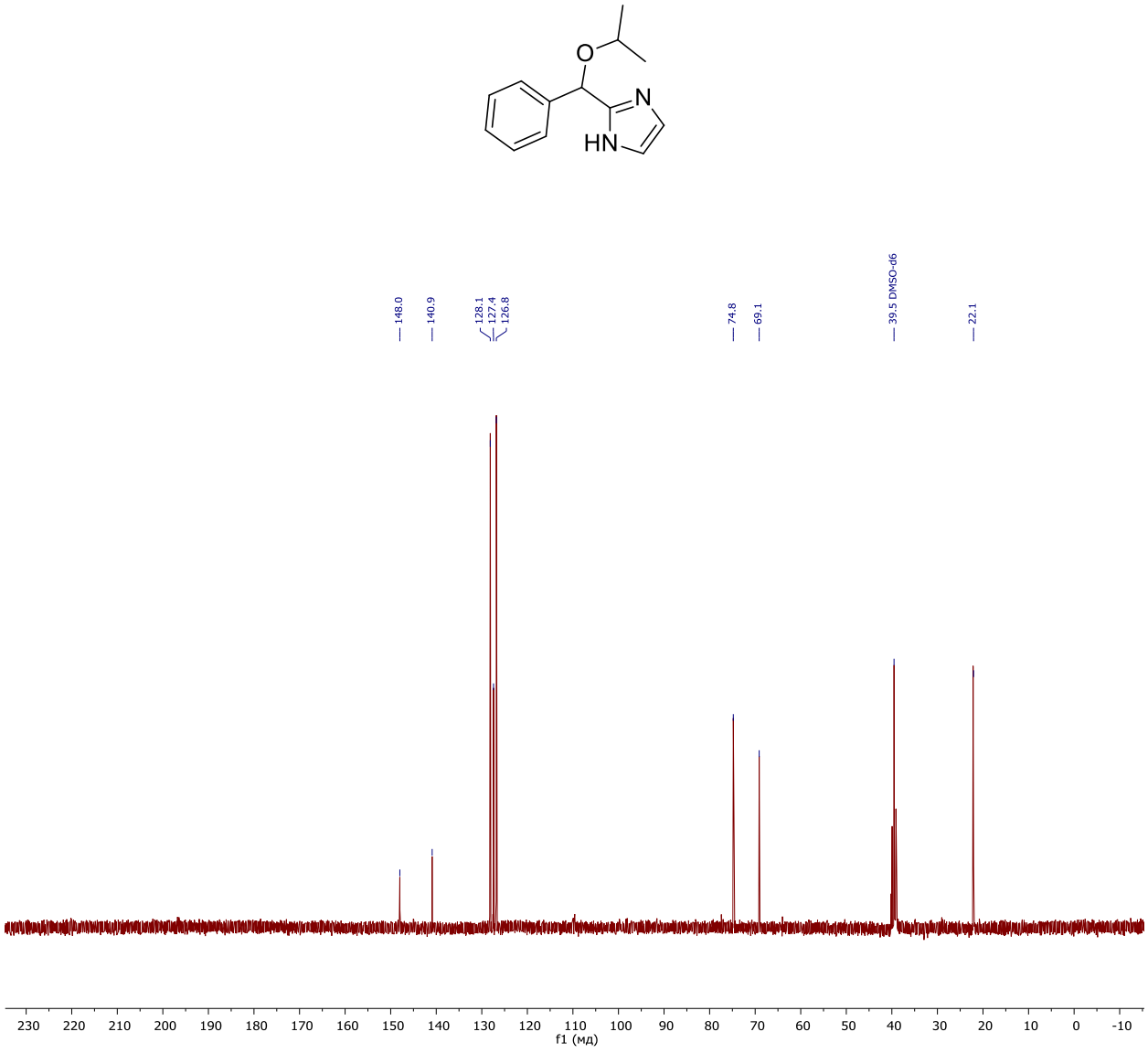


Figure S51. ^{13}C NMR (101 MHz, DMSO-d_6) spectrum of compound **4d**.

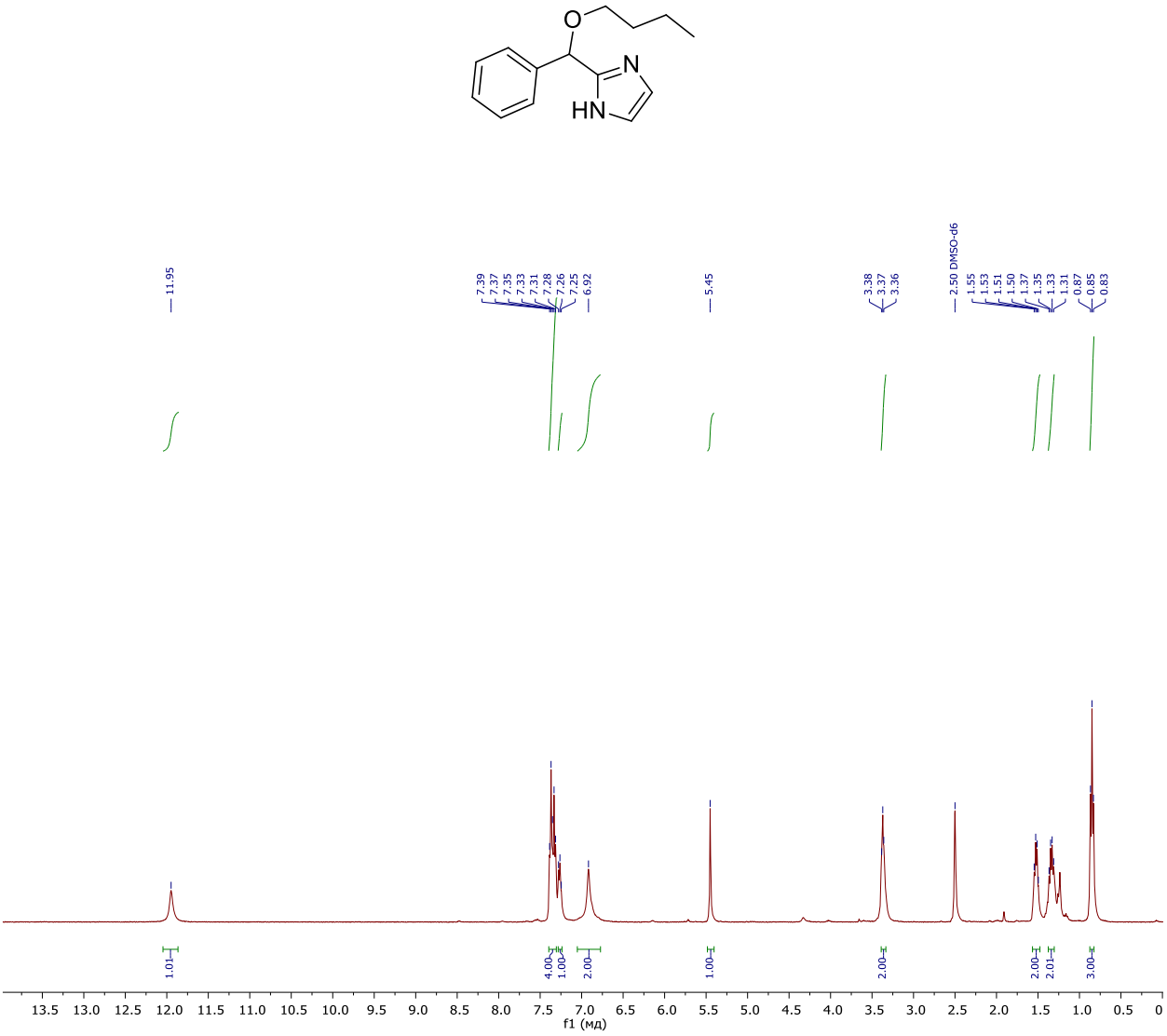


Figure S52. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **4e**.

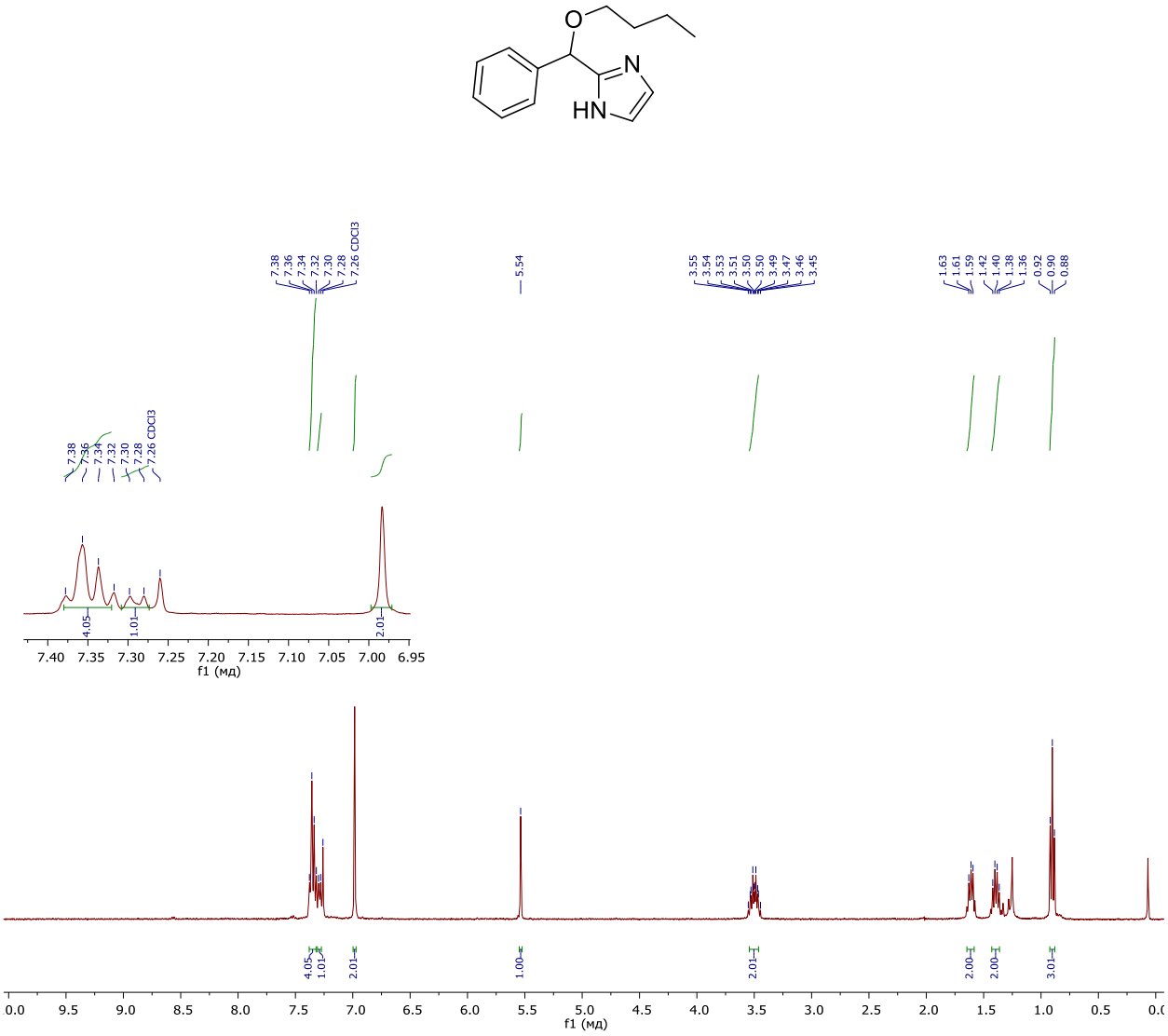


Figure S53. ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **4e**.

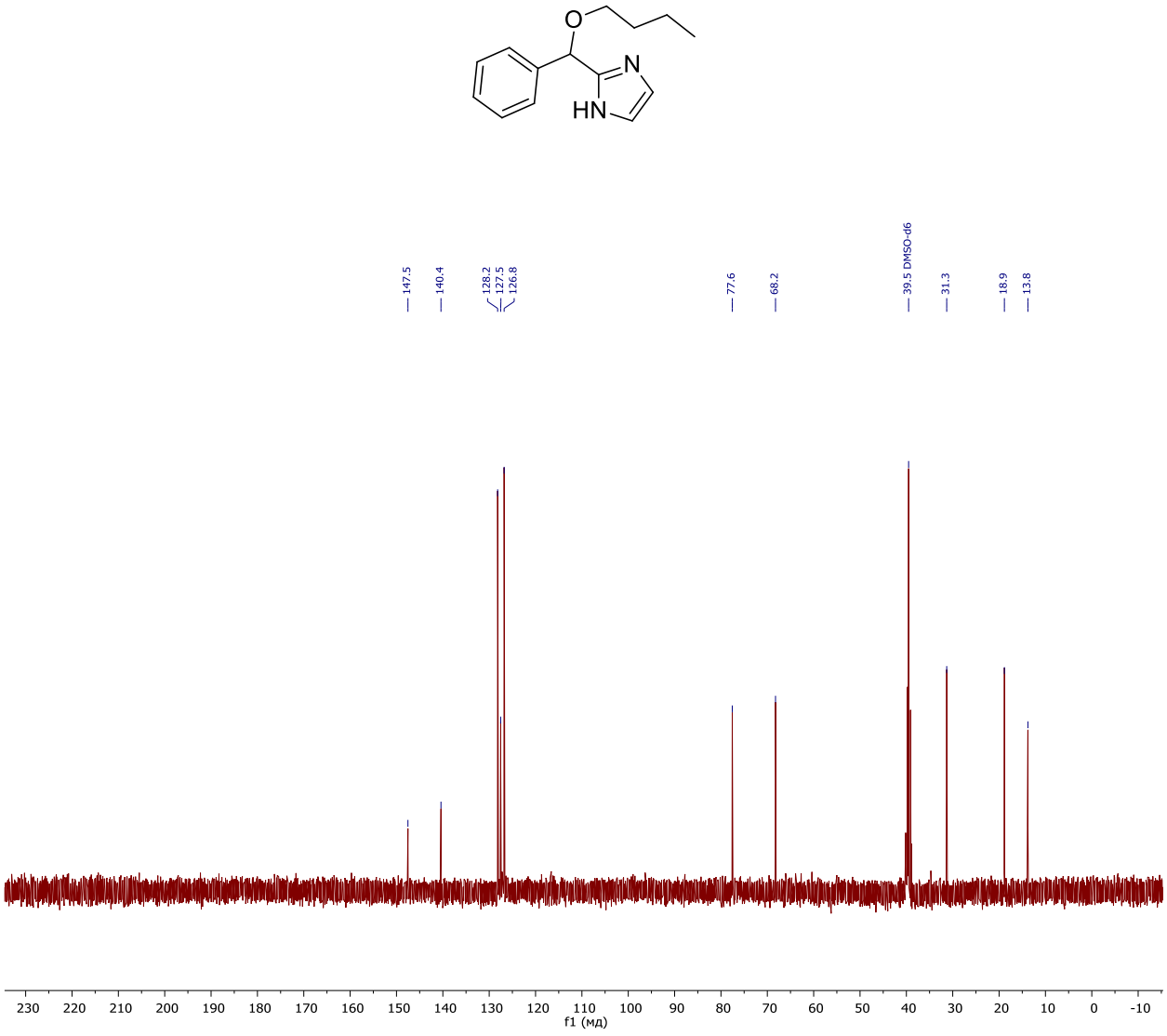


Figure S54. ^{13}C NMR (101 MHz, DMSO-d_6) spectrum of compound **4e**.

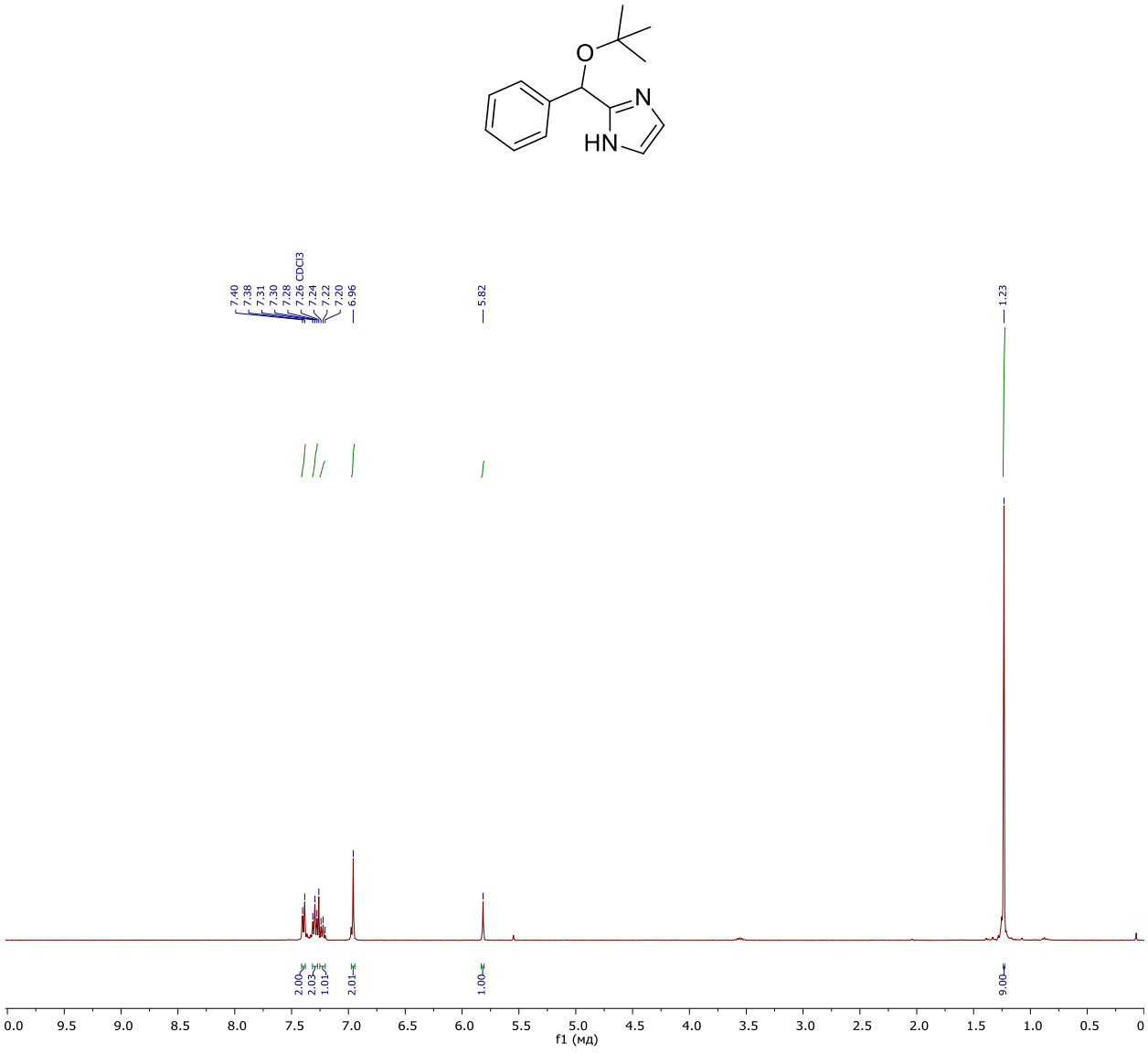


Figure S55. ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **4f**.

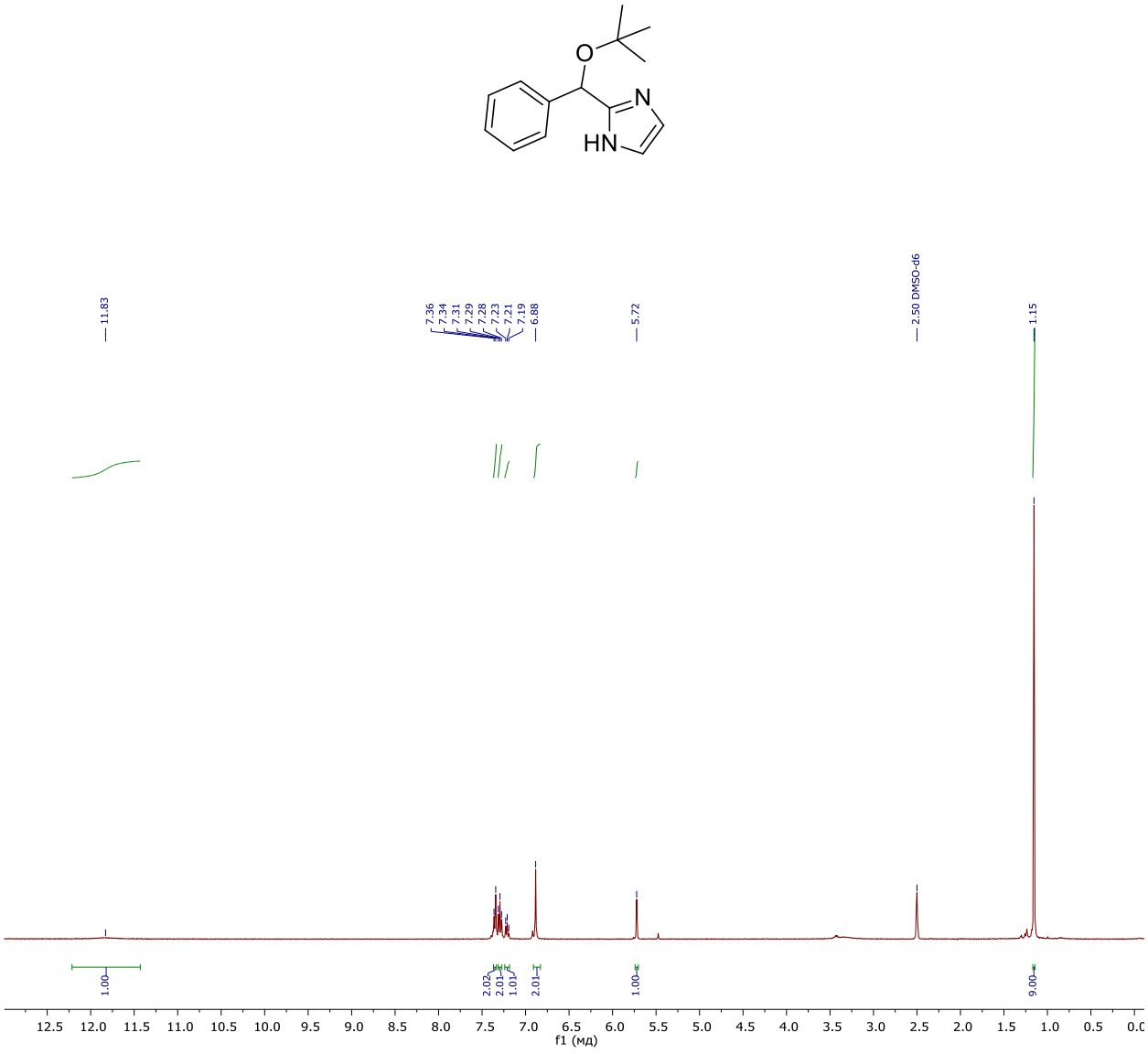


Figure S56. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **4f**.

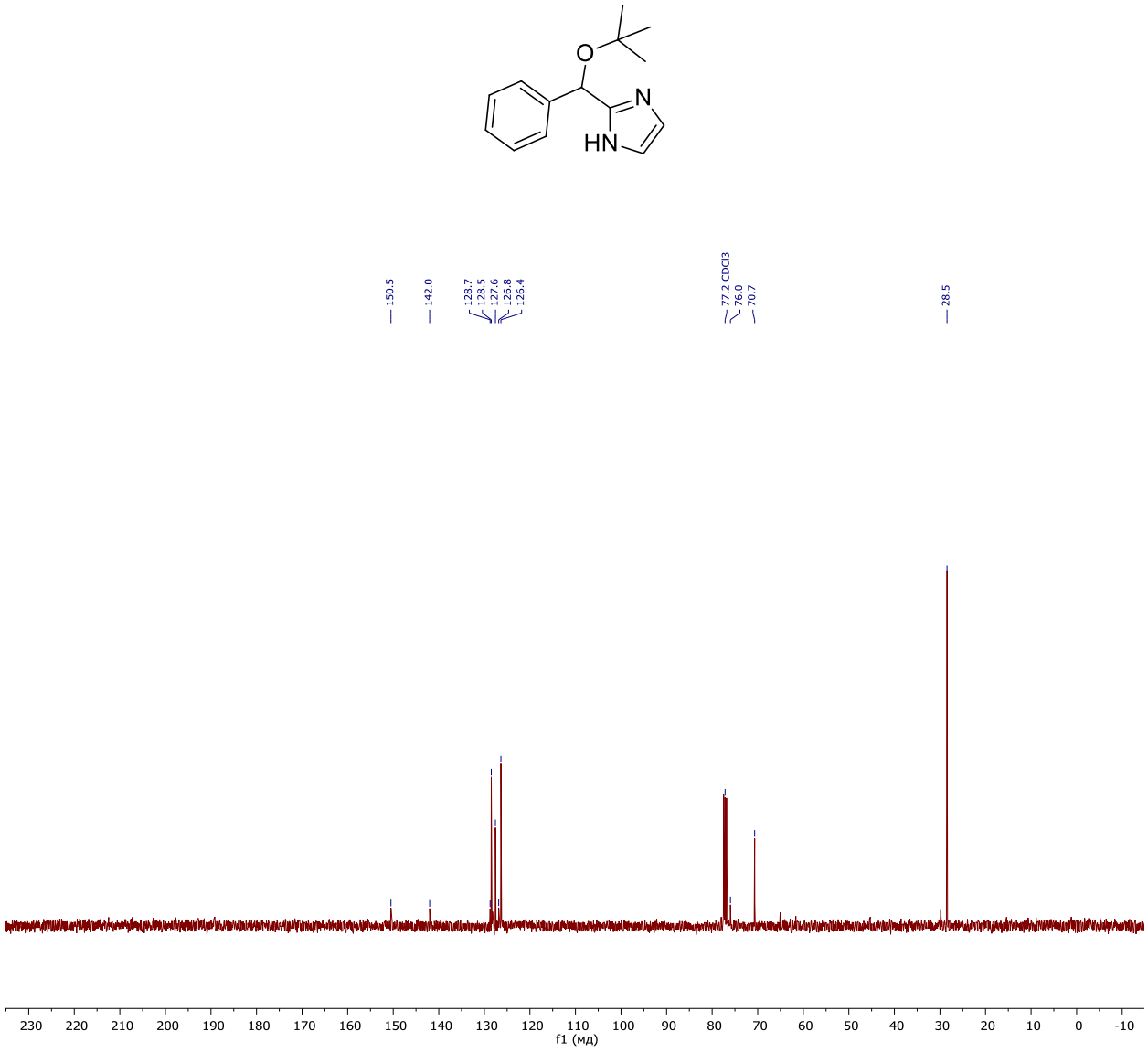


Figure S57. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of compound **4f**.

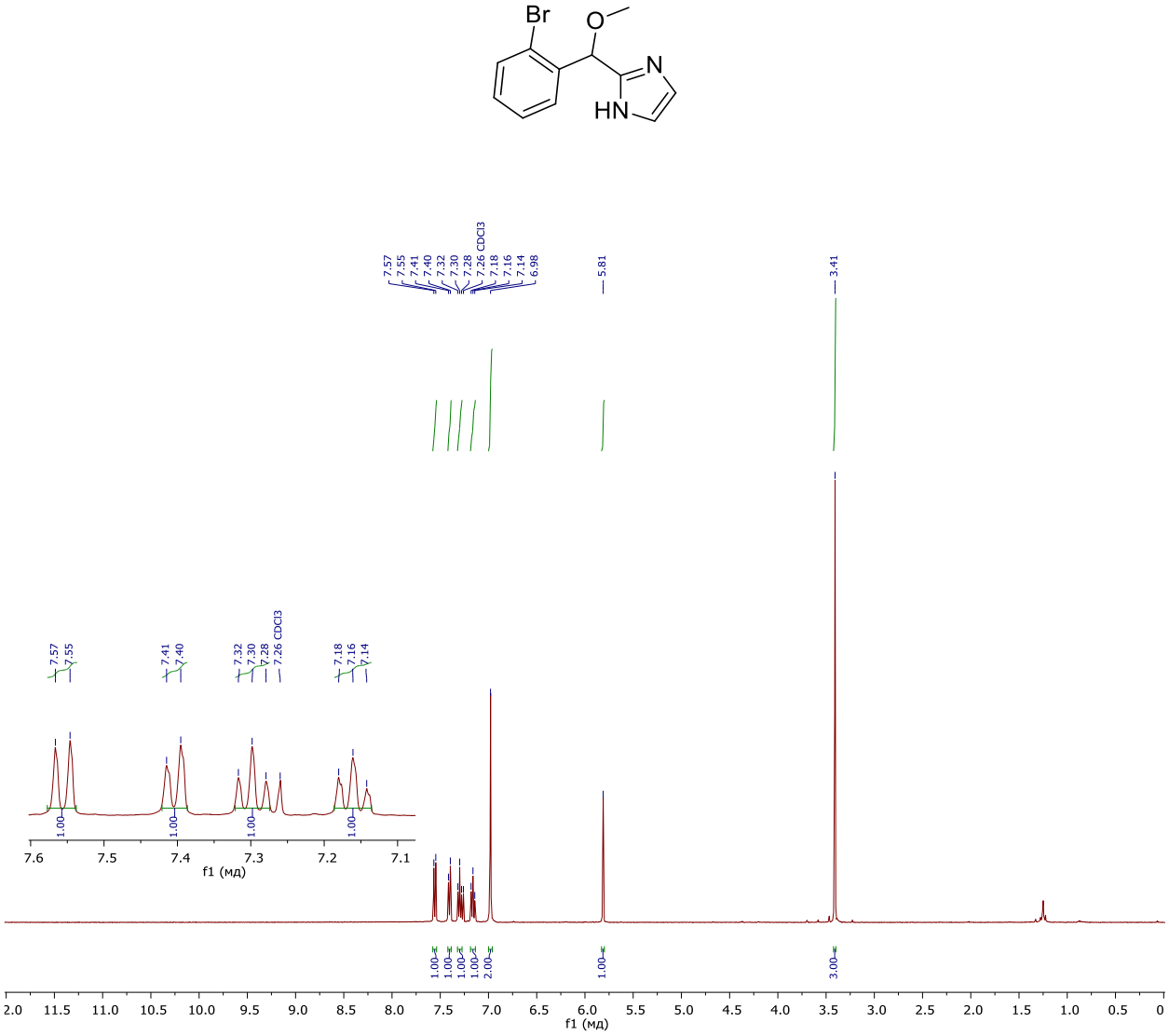


Figure S58. ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **4g**.

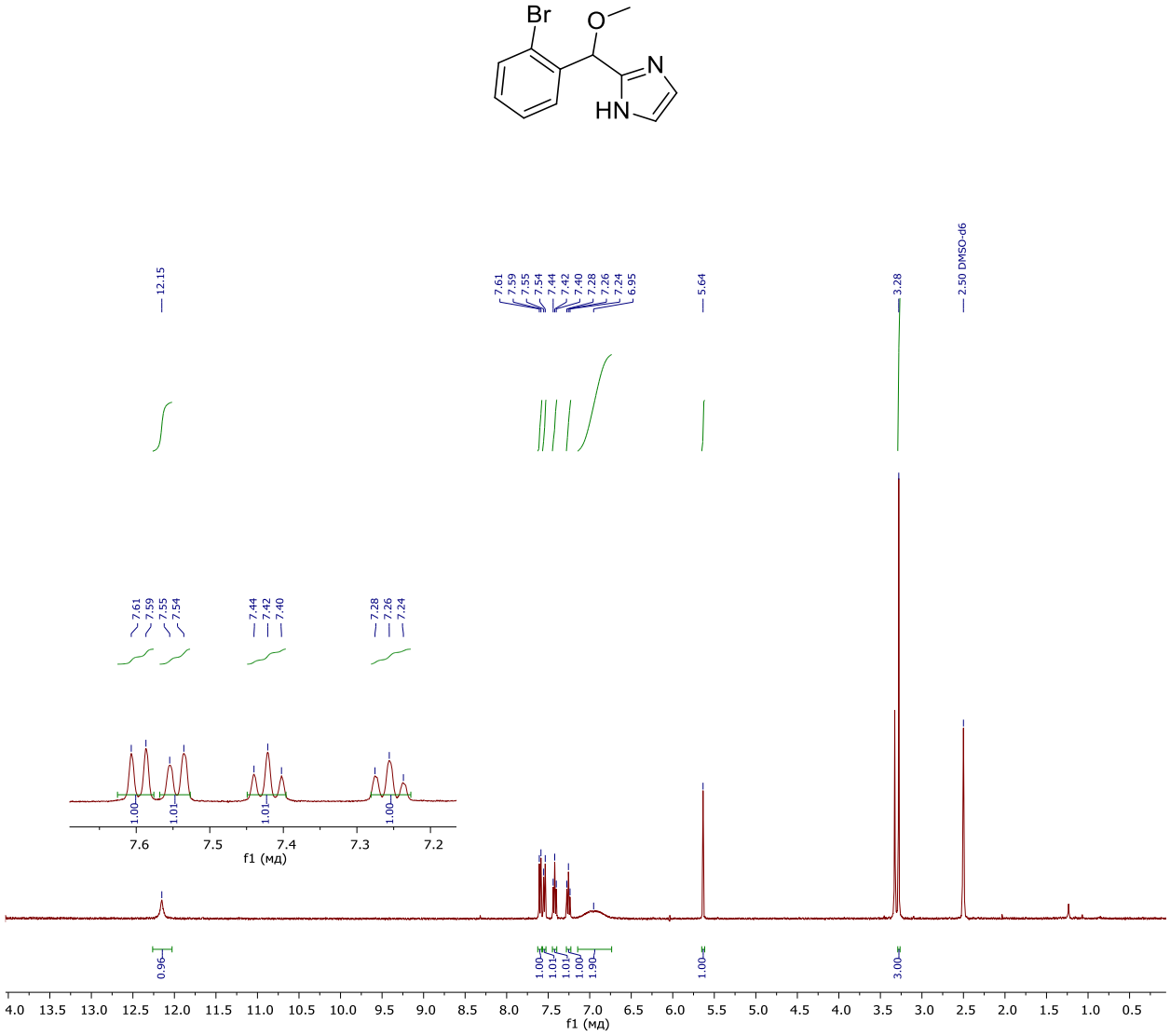


Figure S59. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **4g**.

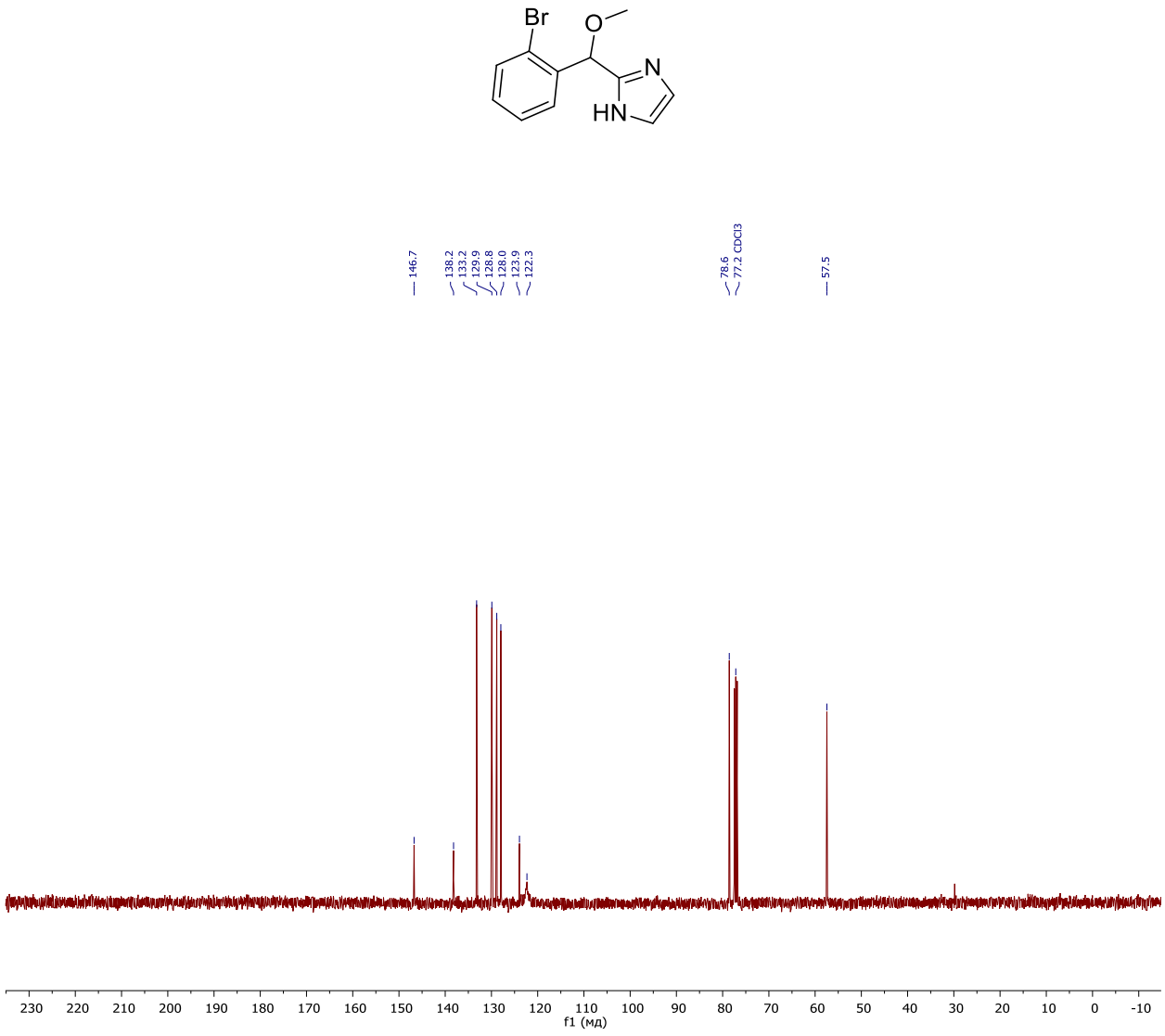


Figure S60. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of compound **4g**.

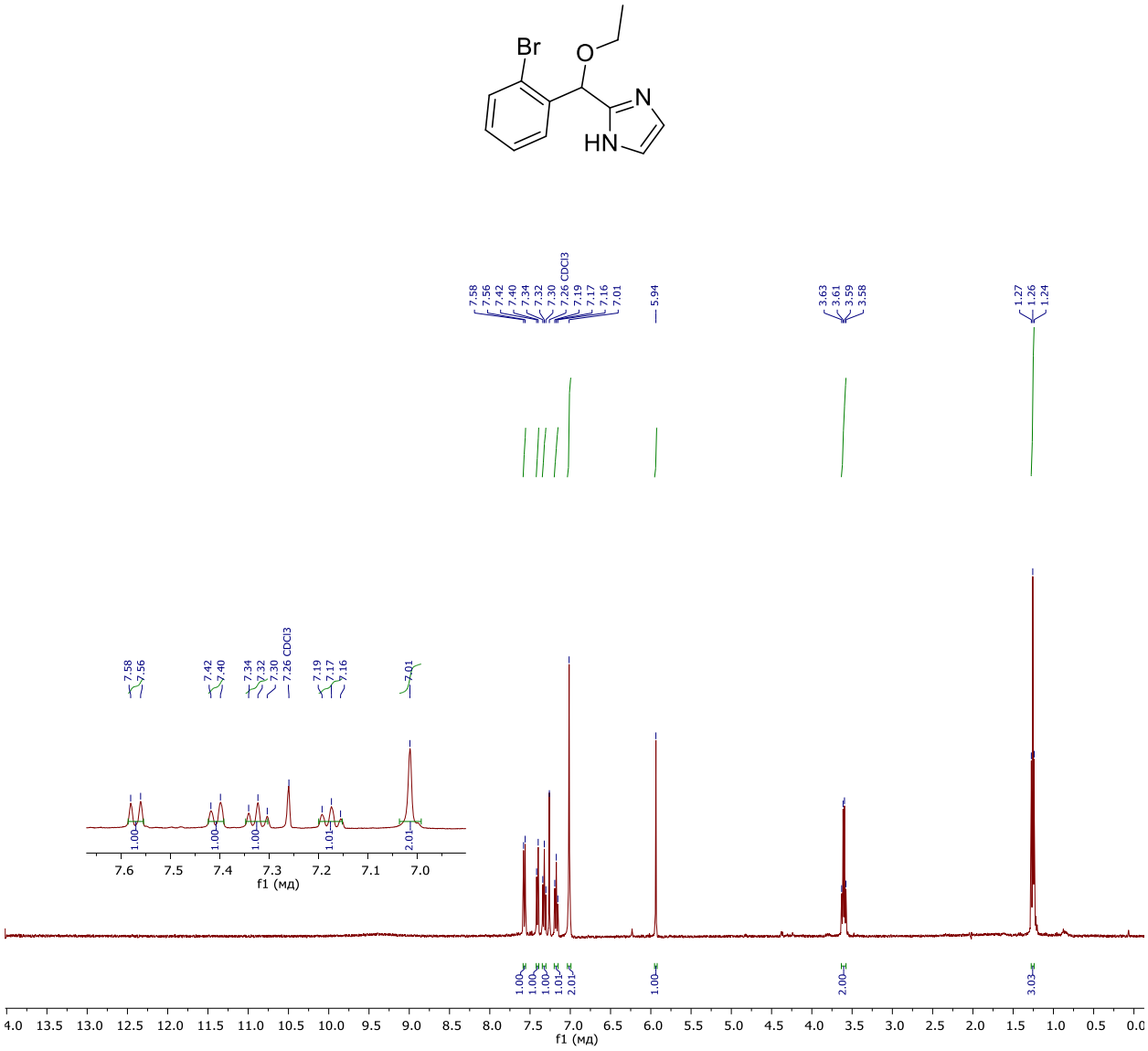


Figure S61. ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **4h**.

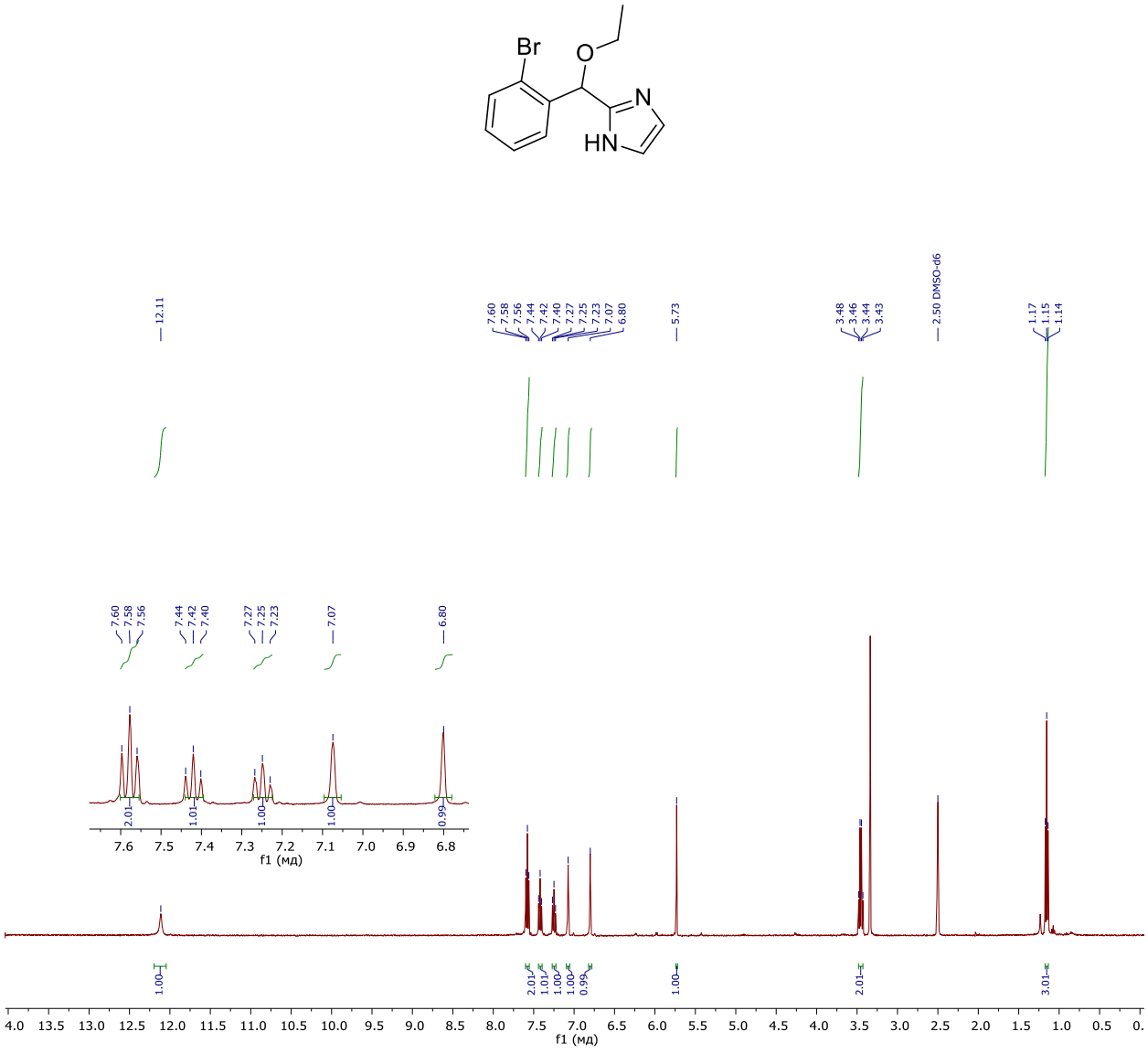


Figure S62. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **4h**.

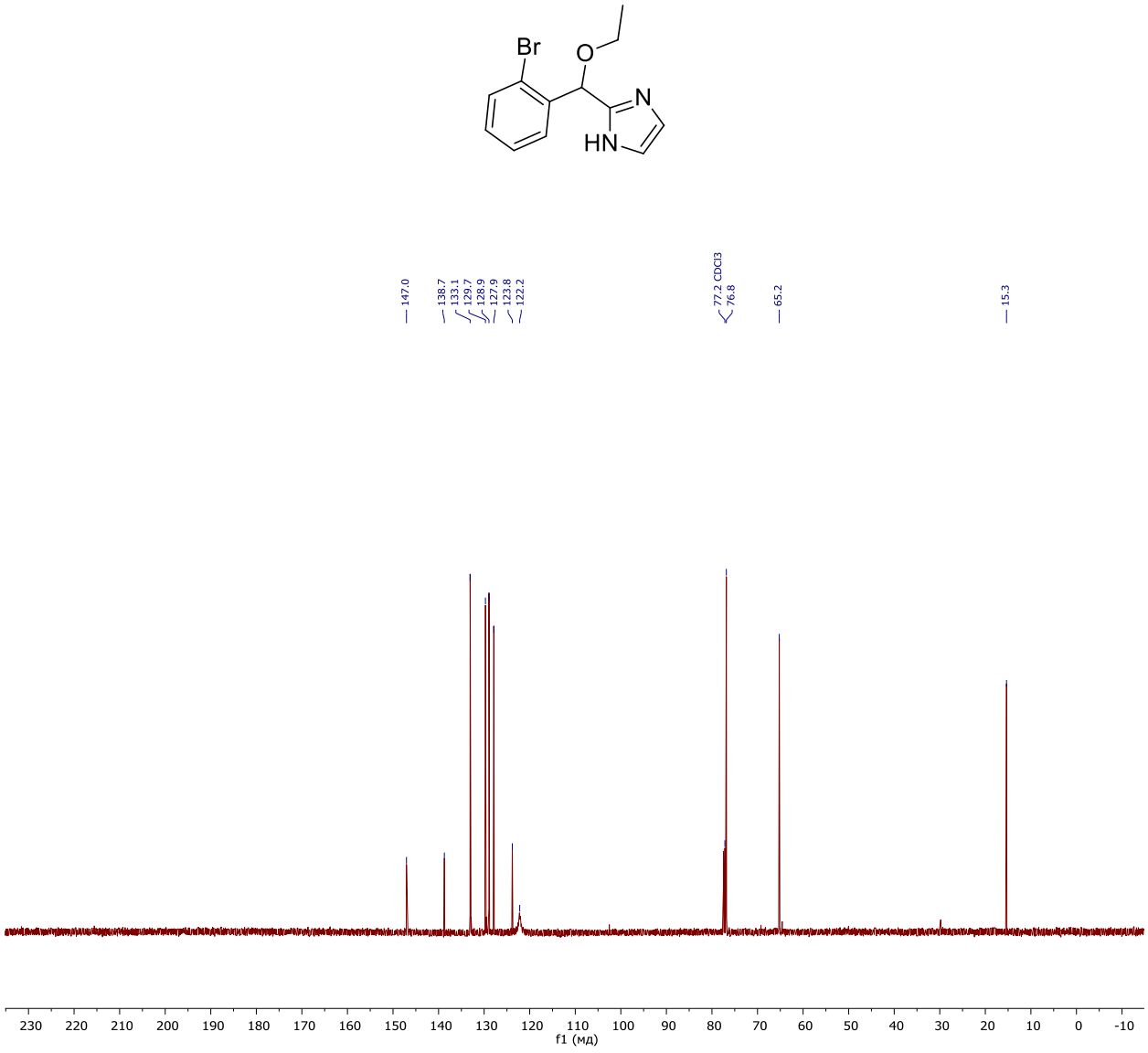


Figure S63. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of compound **4h**.

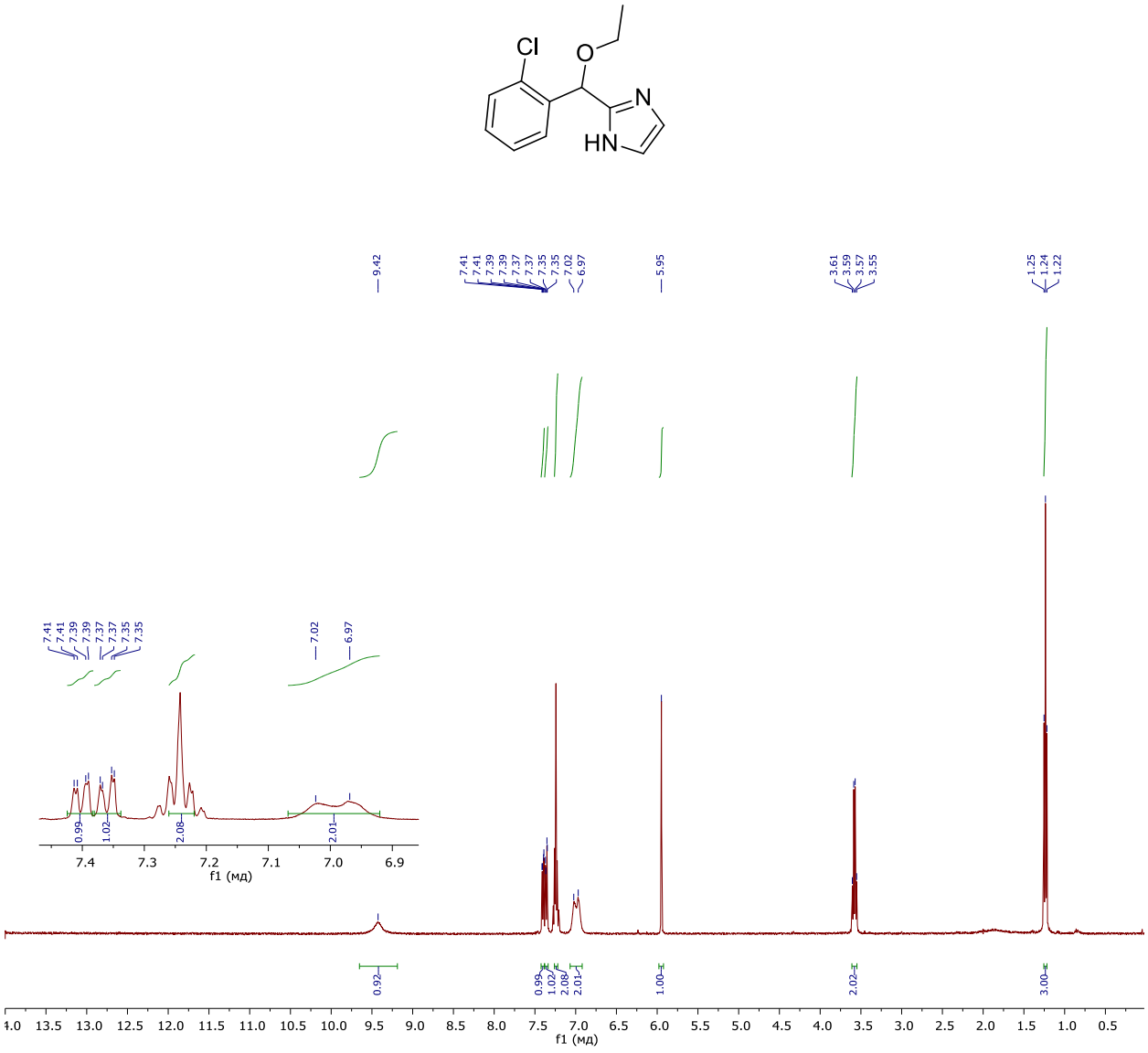


Figure S64. ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **4i**.

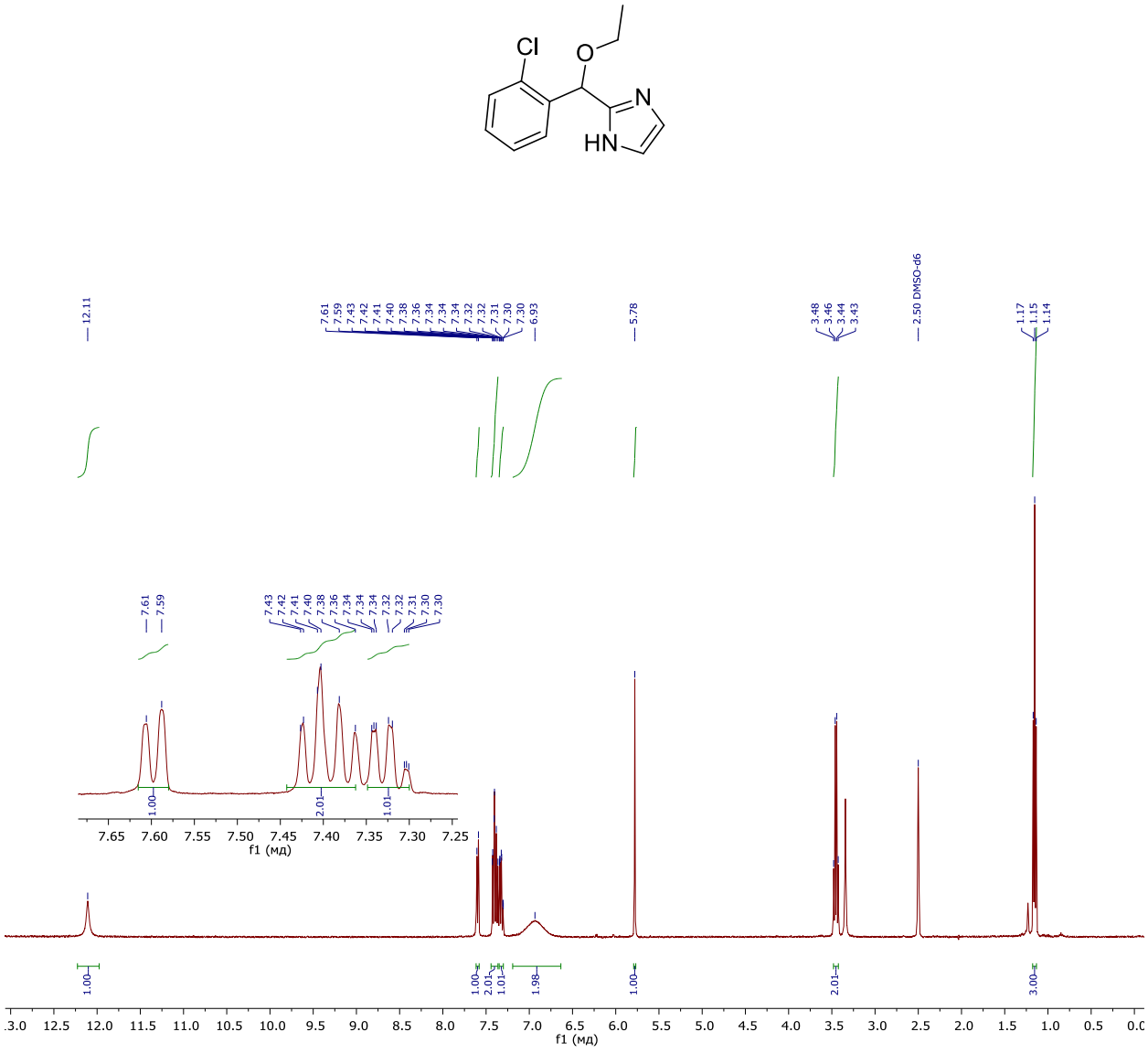


Figure S65. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **4i**.

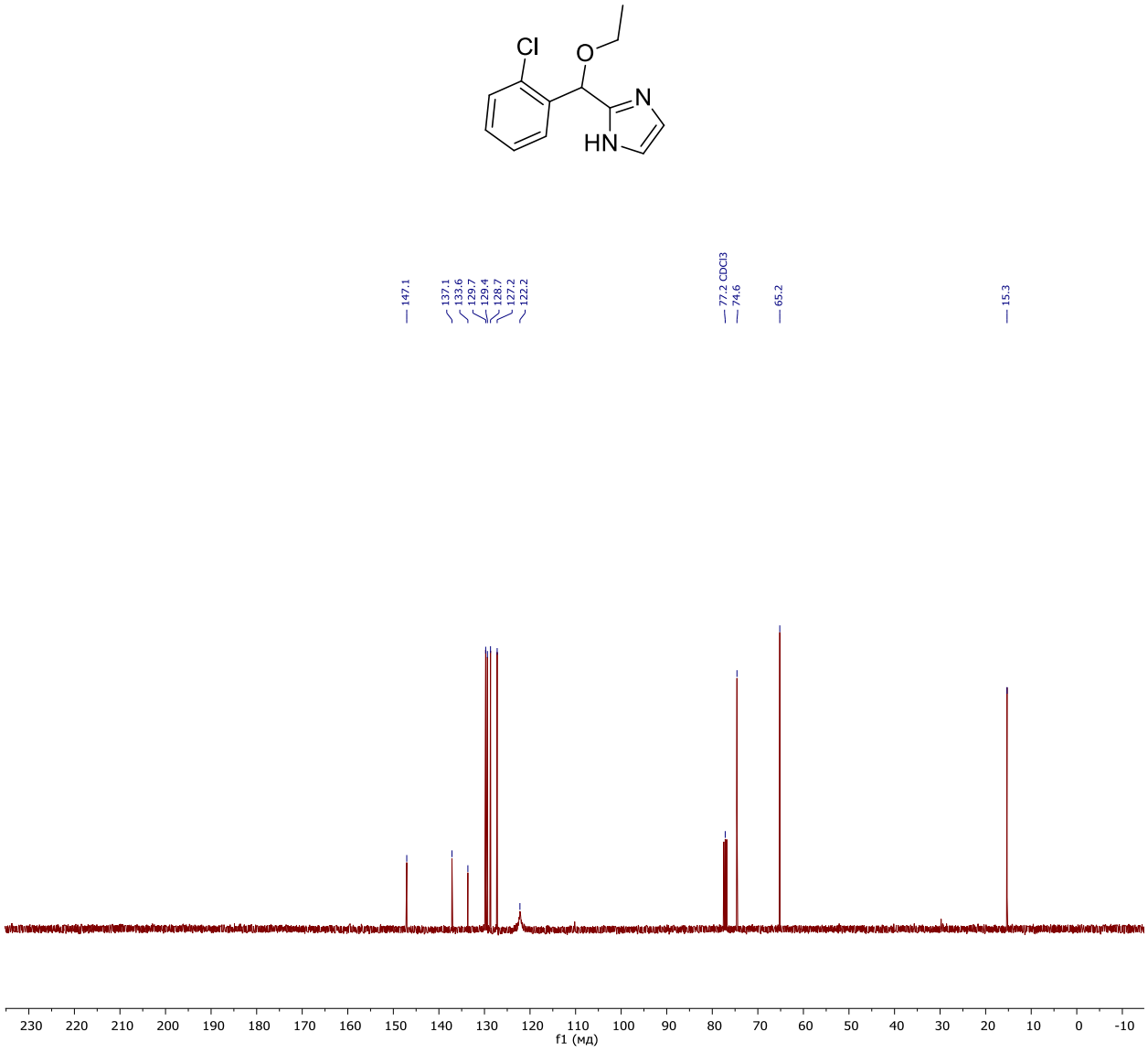


Figure S66. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of compound **4i**.

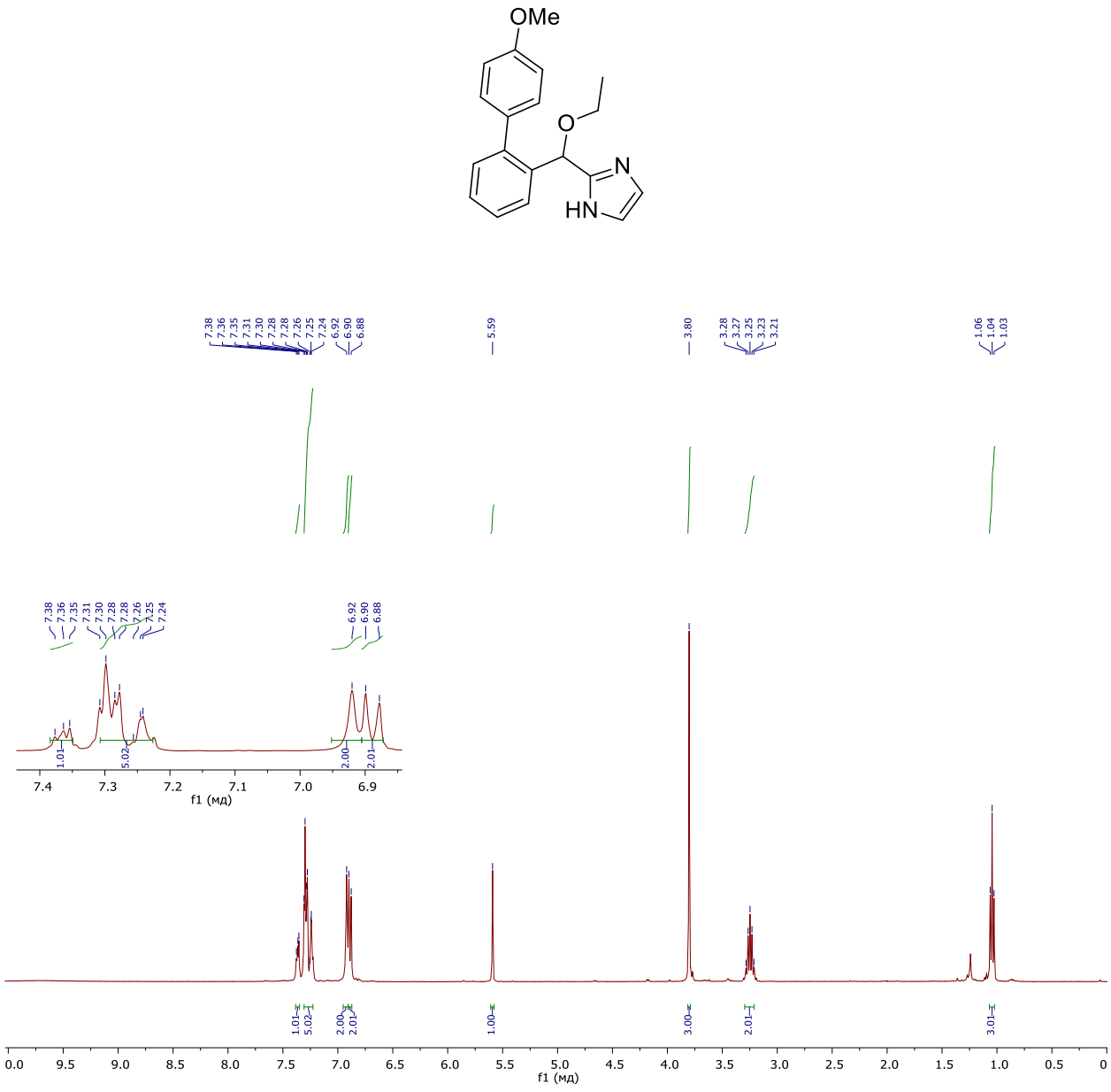


Figure S67. ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **4j**.

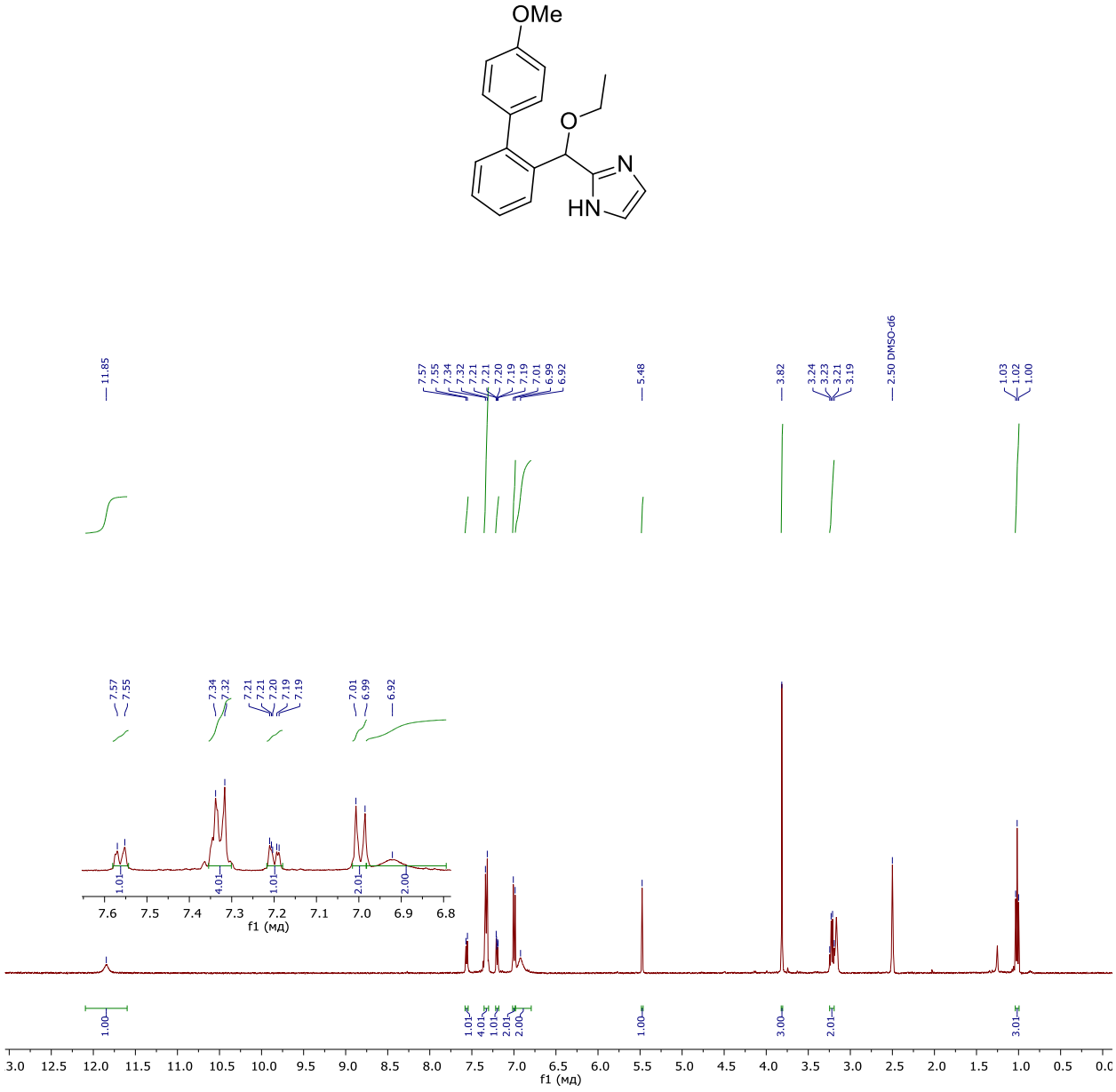


Figure S68. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **4j**.

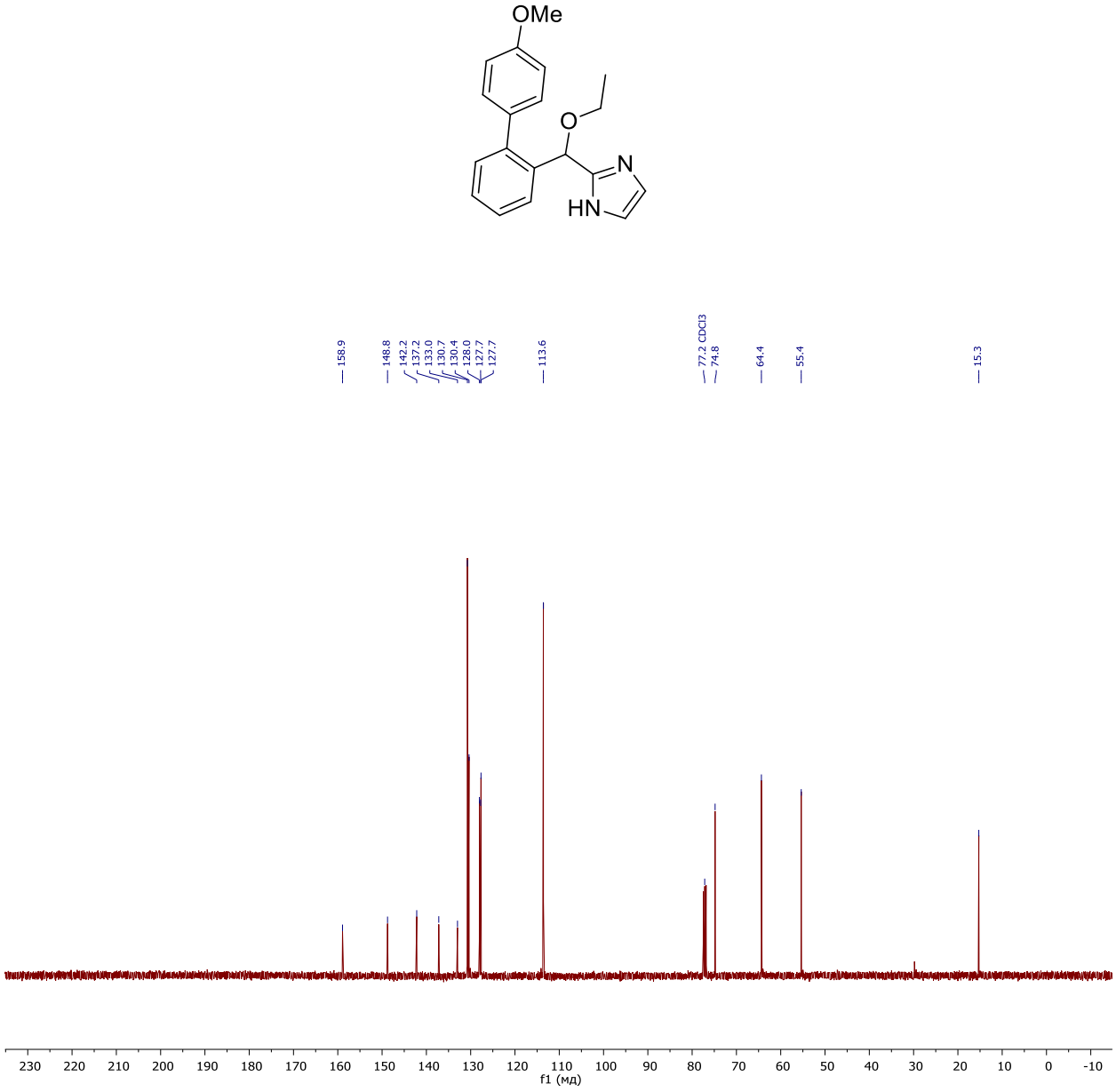


Figure S69. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of compound **4j**.

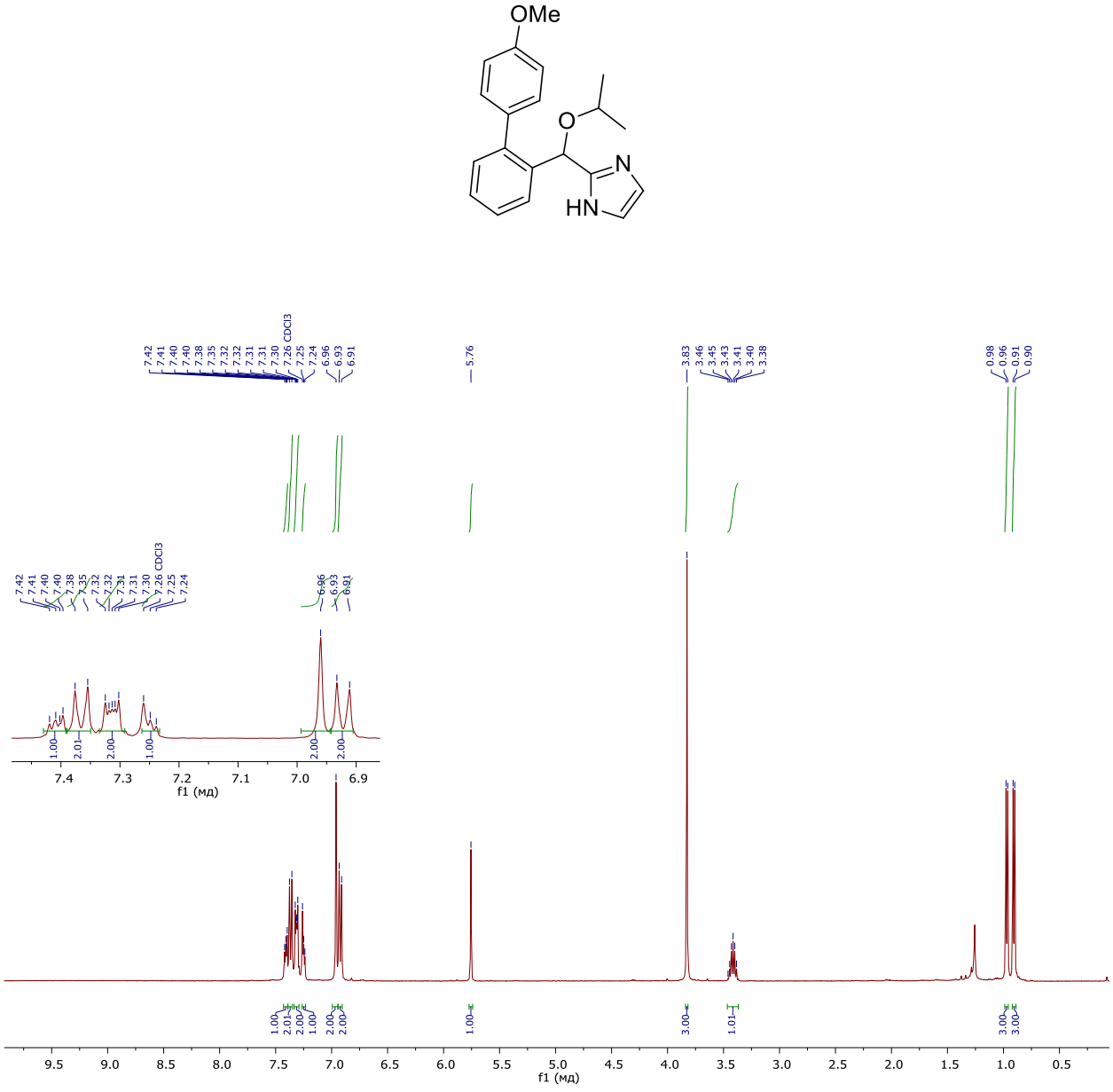


Figure S70. ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **4k**.

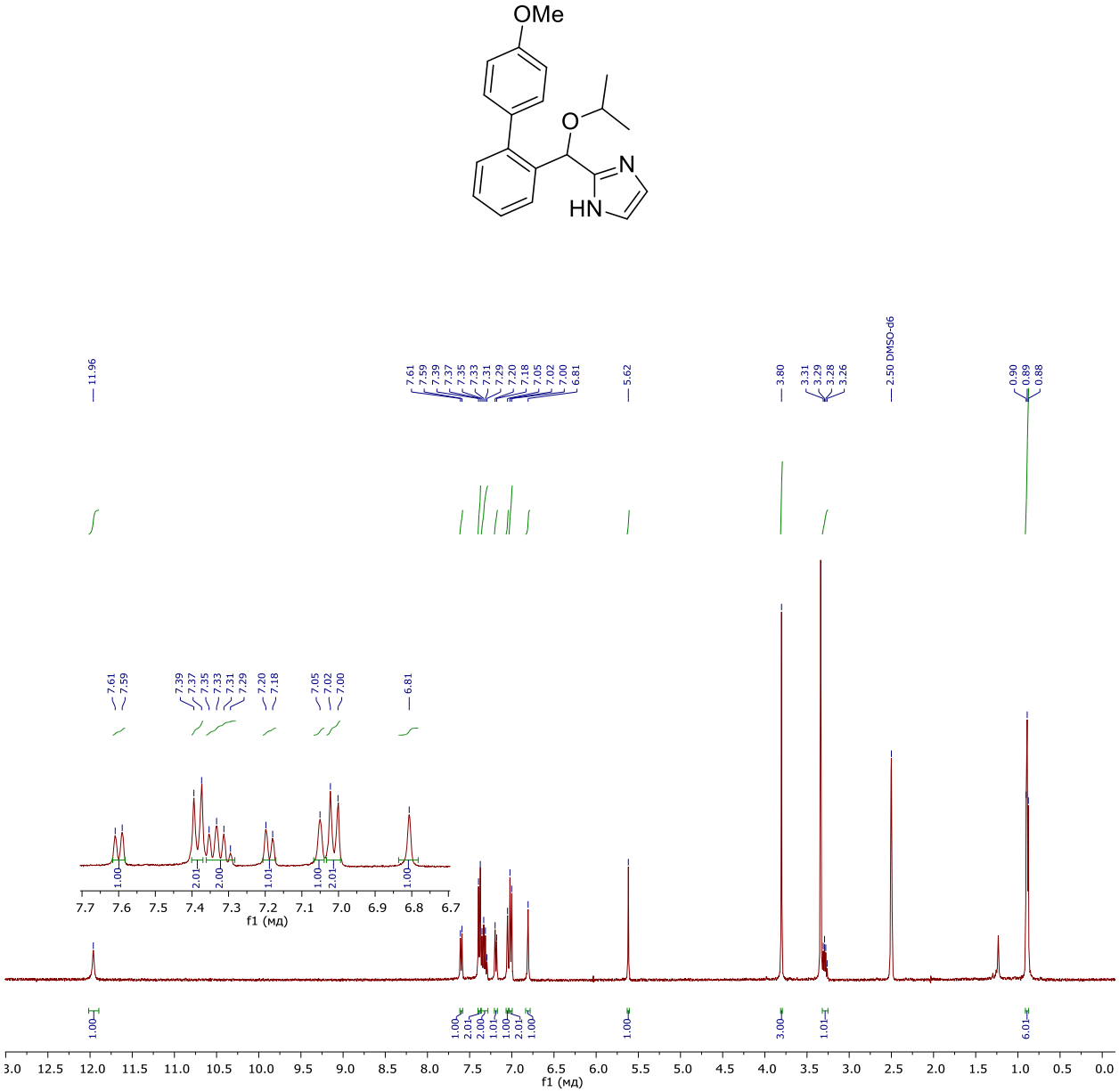


Figure S71. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **4k**.

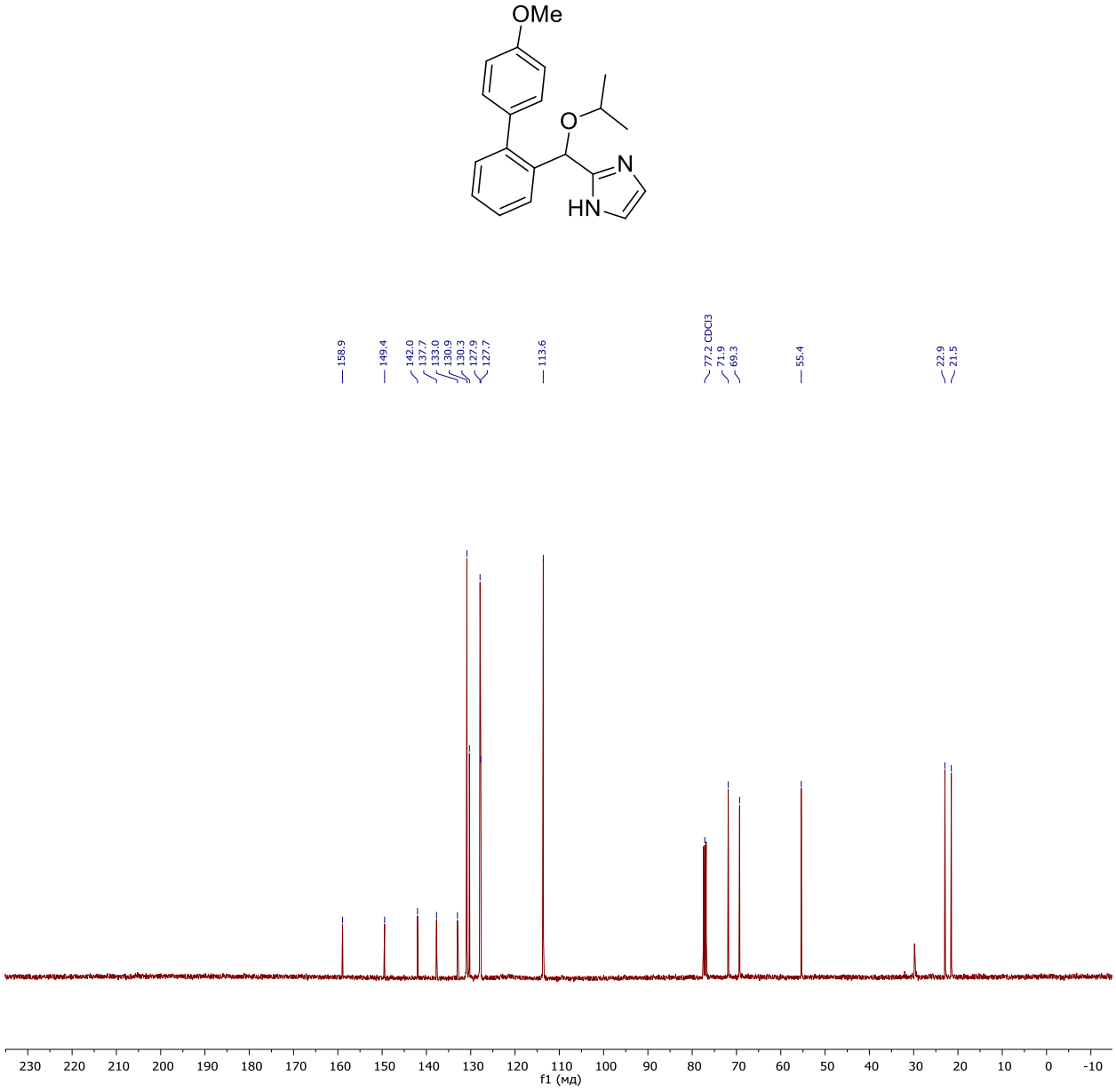


Figure S72. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of compound **4k**.

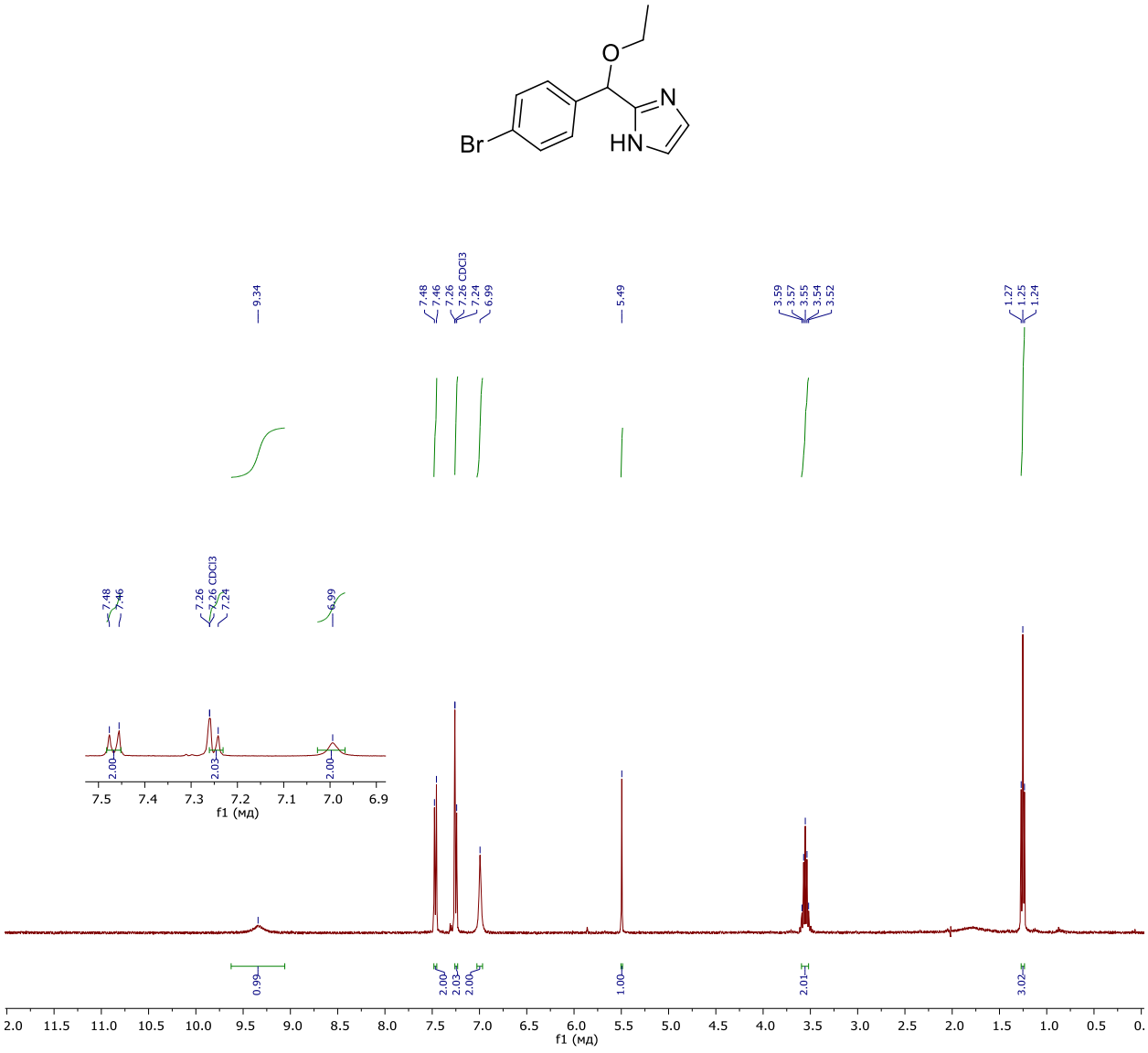


Figure S73. ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **4l**.

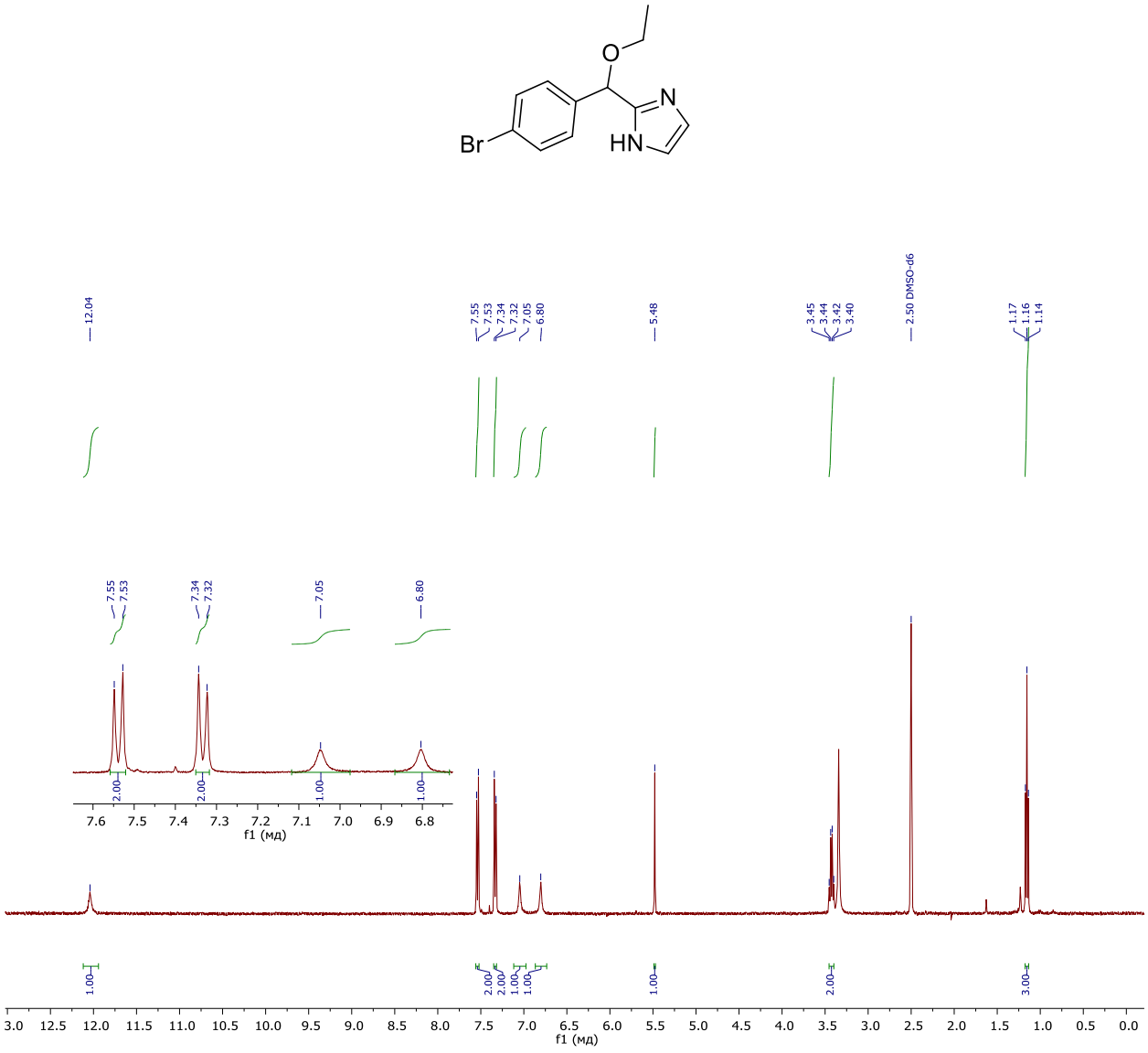


Figure S74. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **4l**.

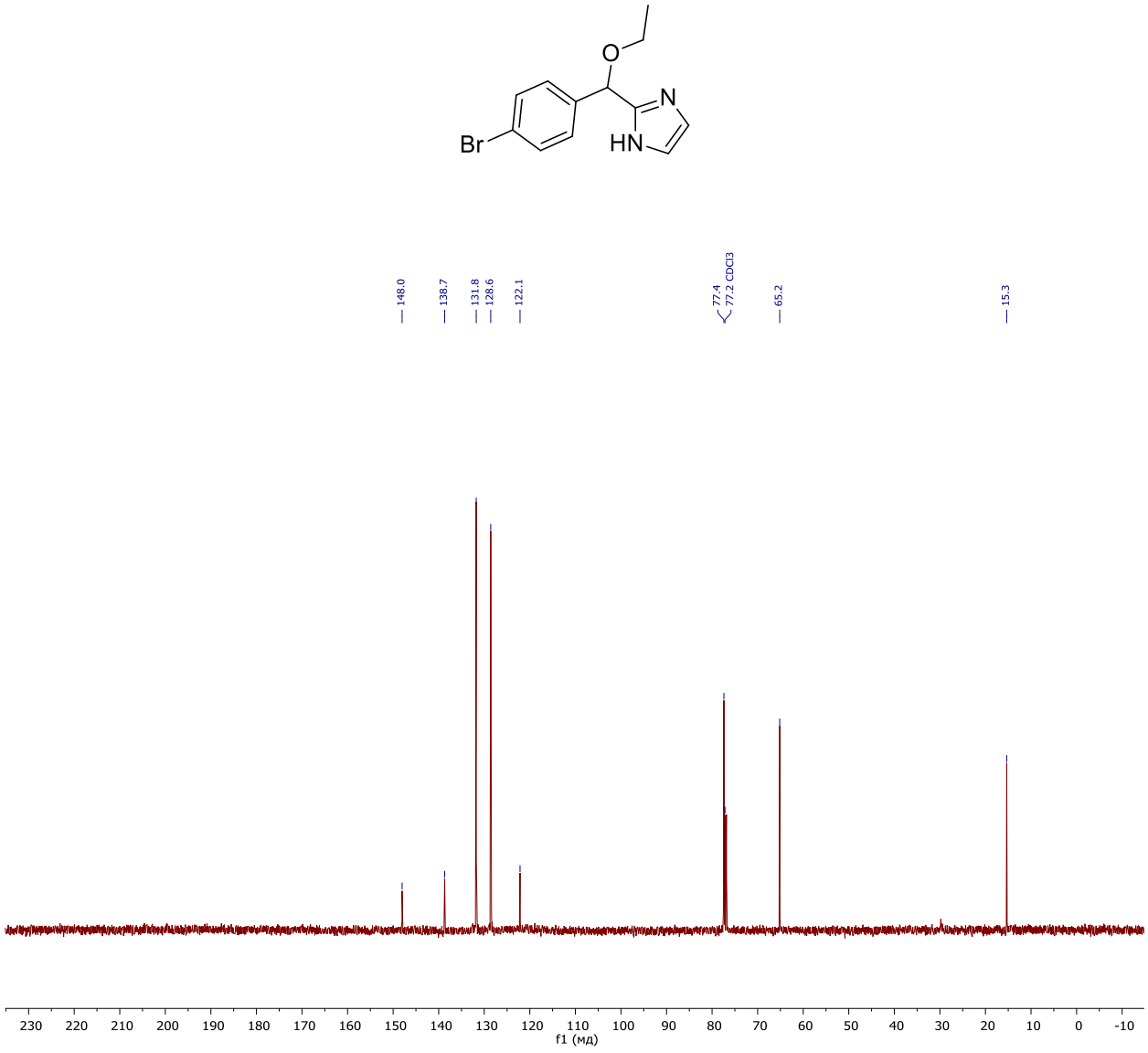


Figure S75. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of compound **4l**.

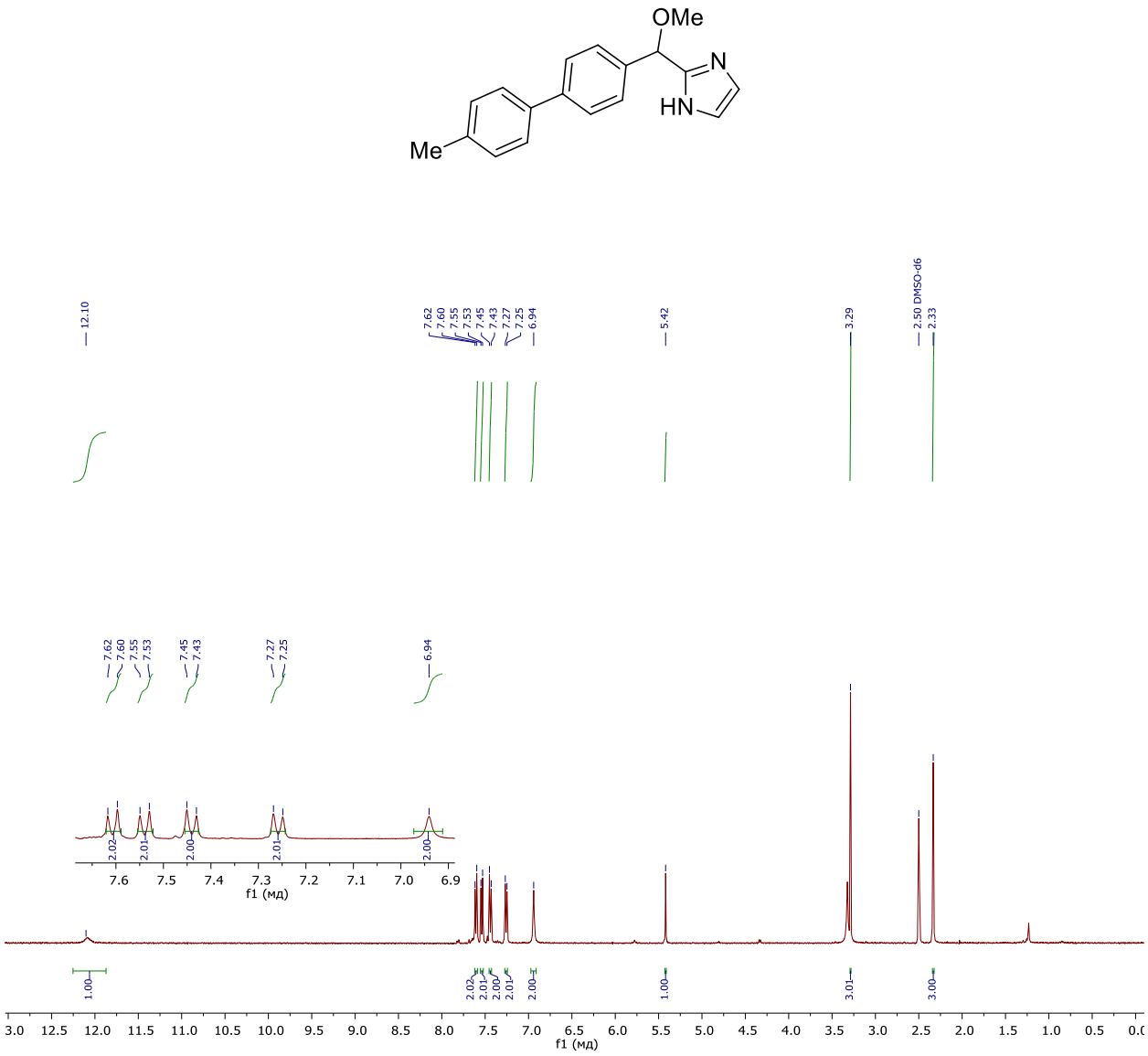


Figure S76. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **4m**.

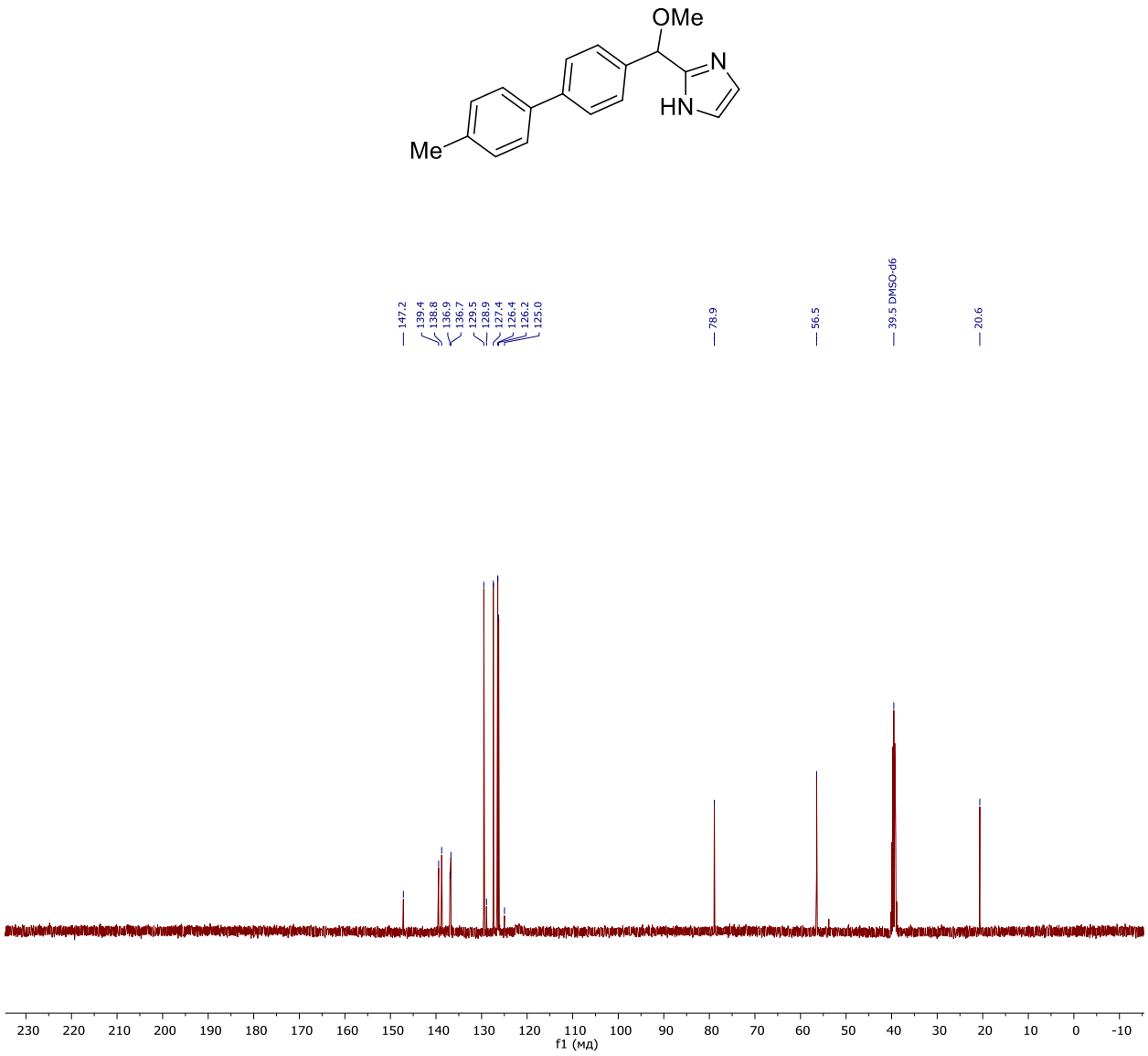


Figure S77. ^{13}C NMR (101 MHz, DMSO-d_6) spectrum of compound **4m**.

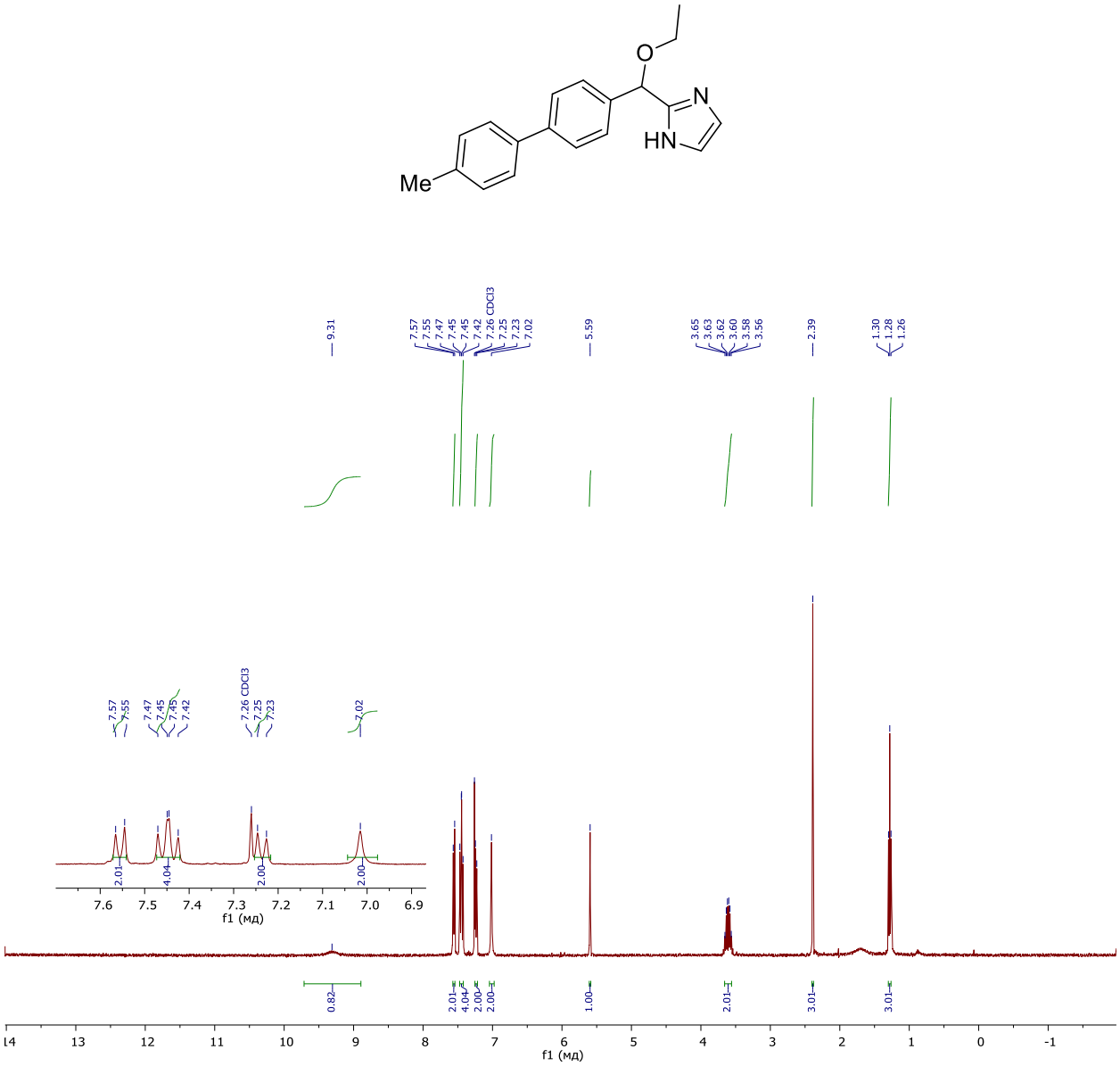


Figure S78. ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **4n**.

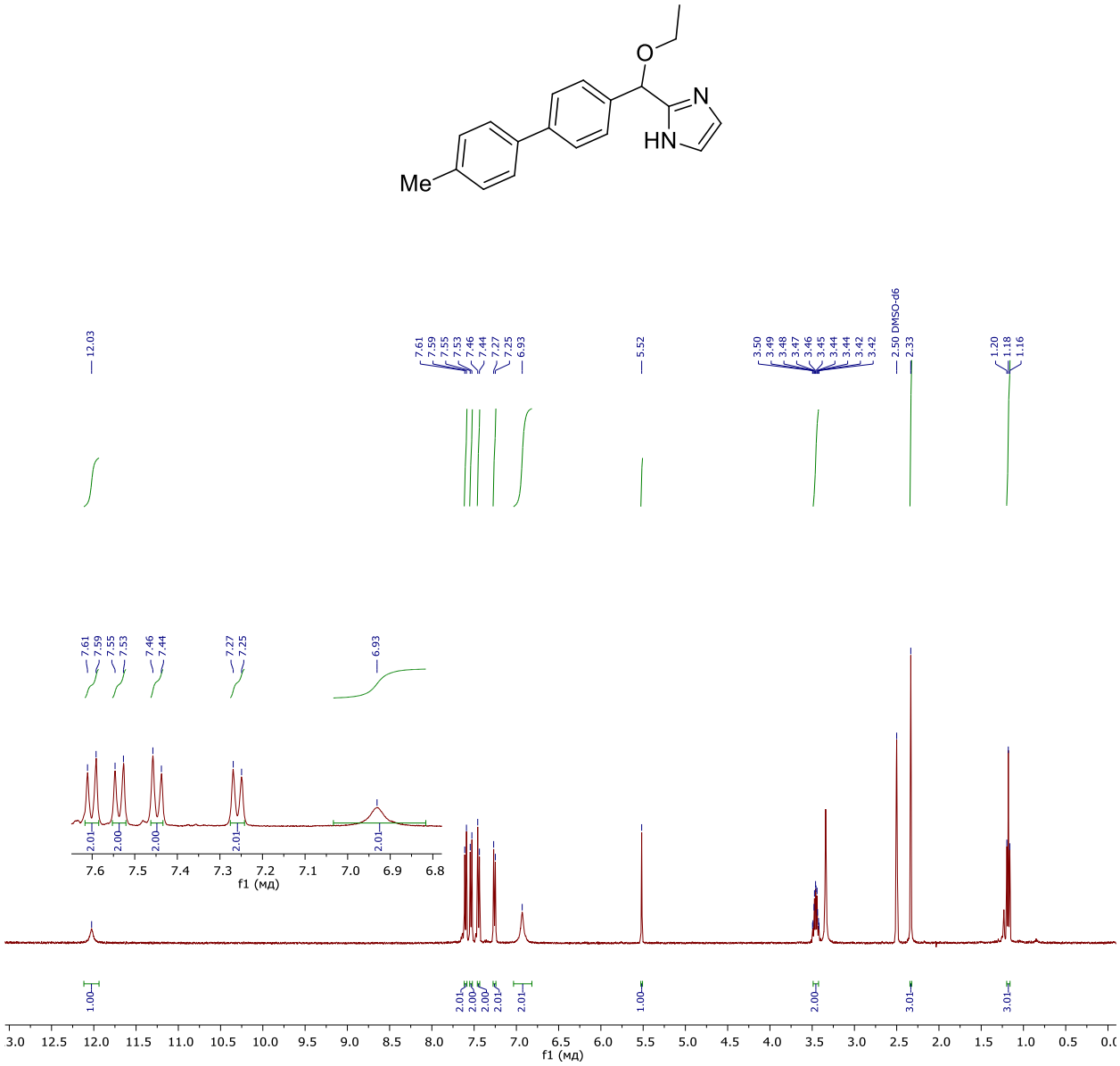


Figure S79. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **4n**.

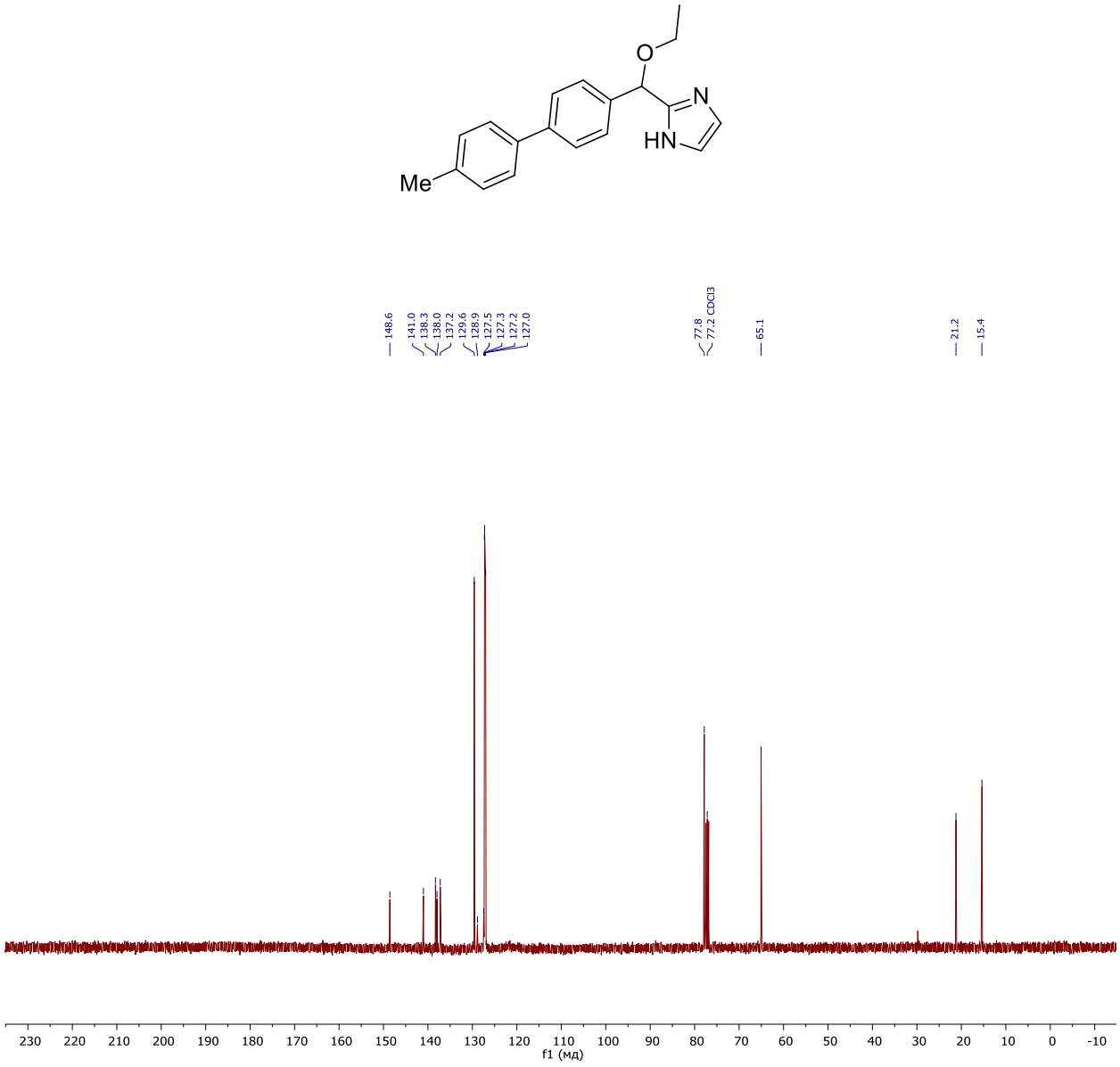


Figure S80. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of compound **4n**.

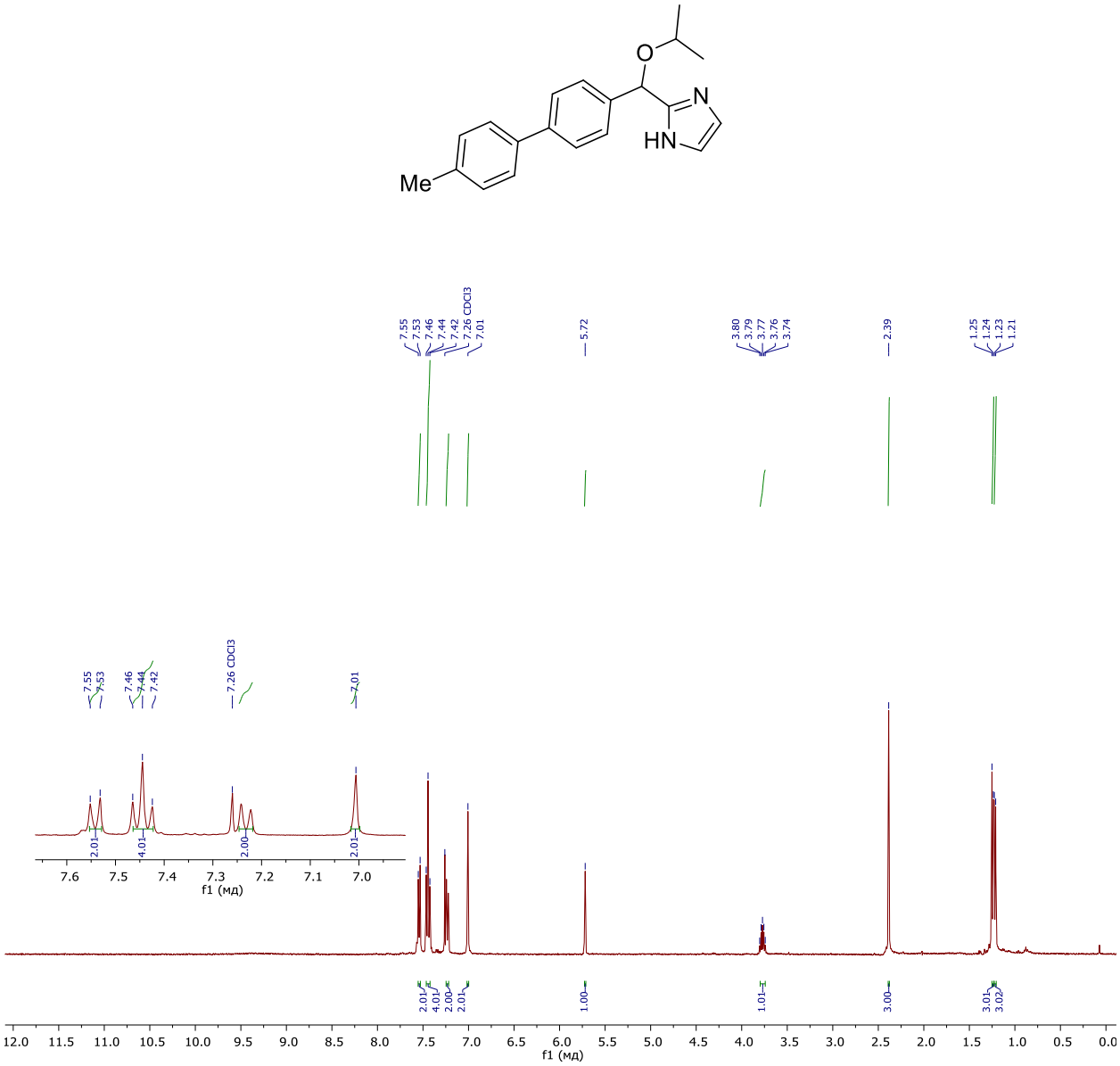


Figure S81. ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **4o**.

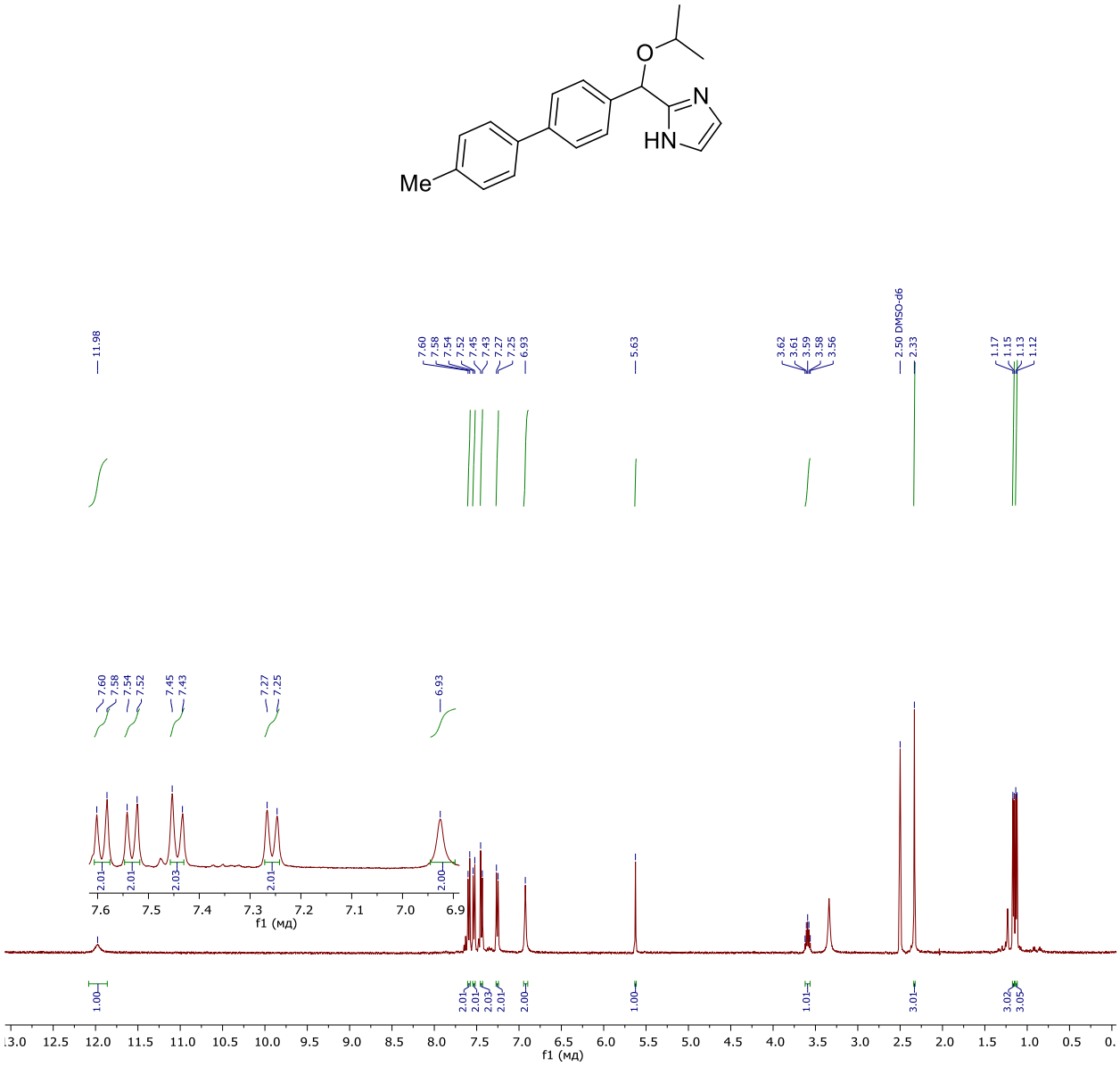


Figure S82. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **4o**.

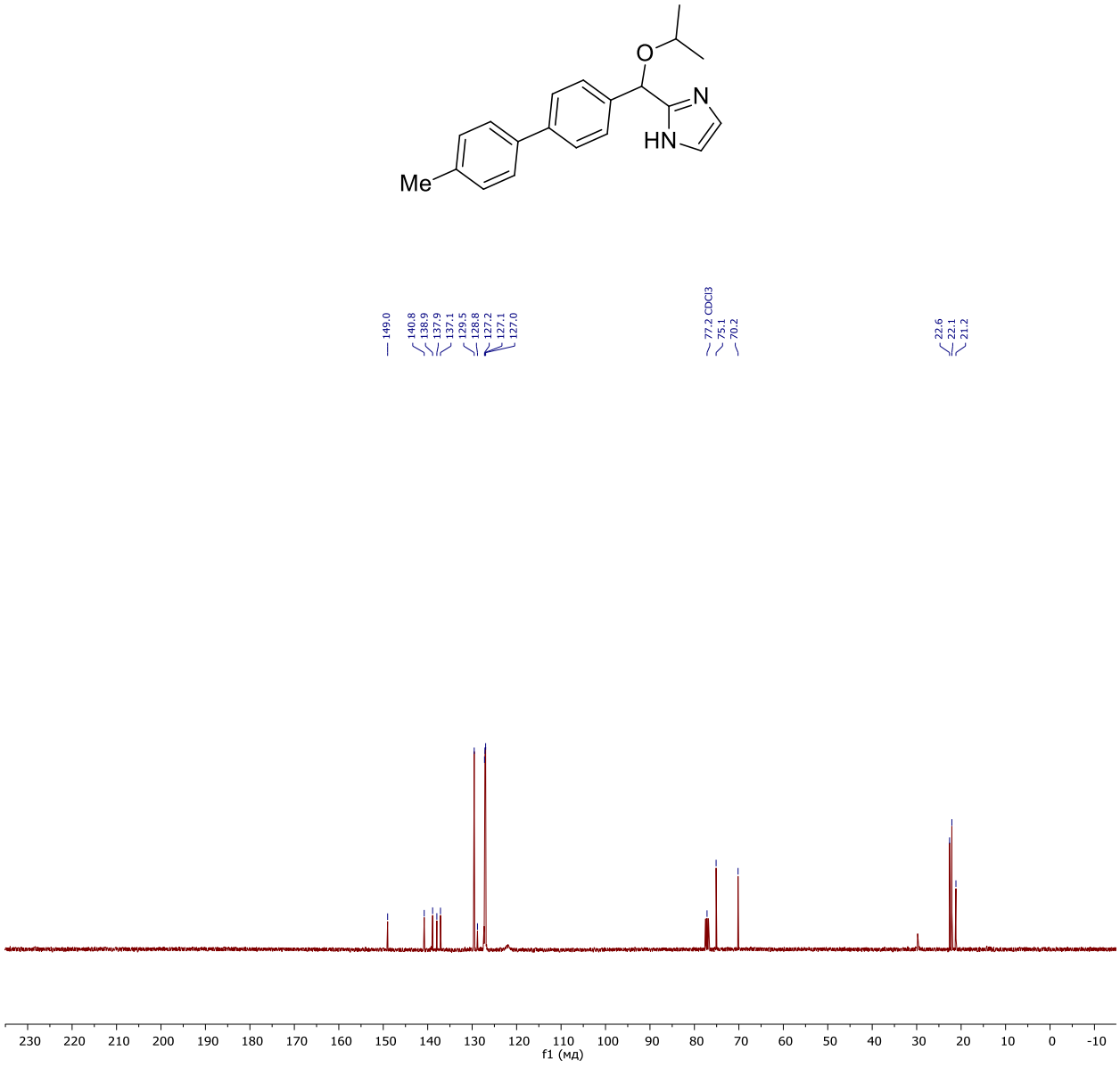


Figure S83. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of compound **4o**.

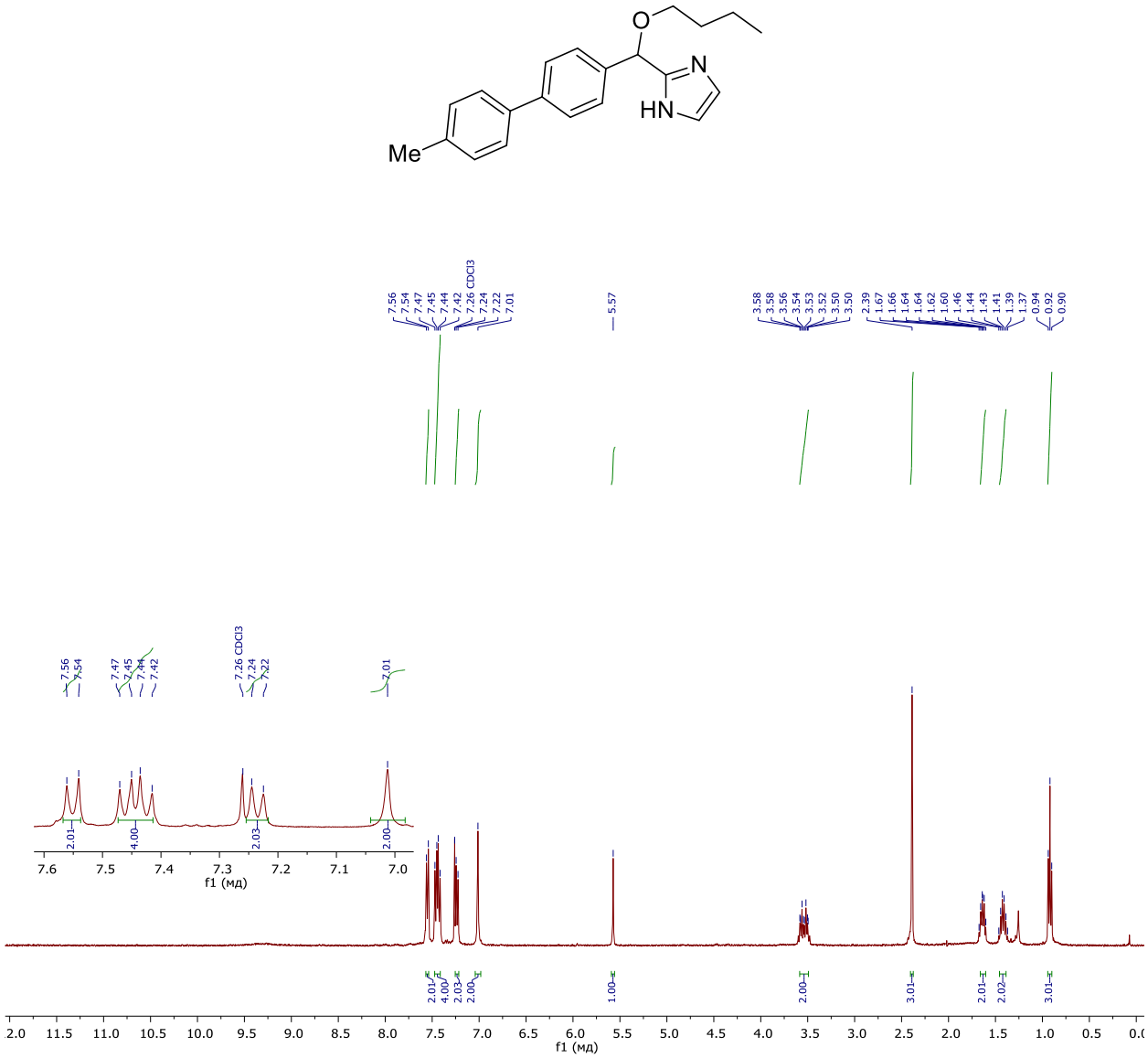


Figure S84. ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **4p**.

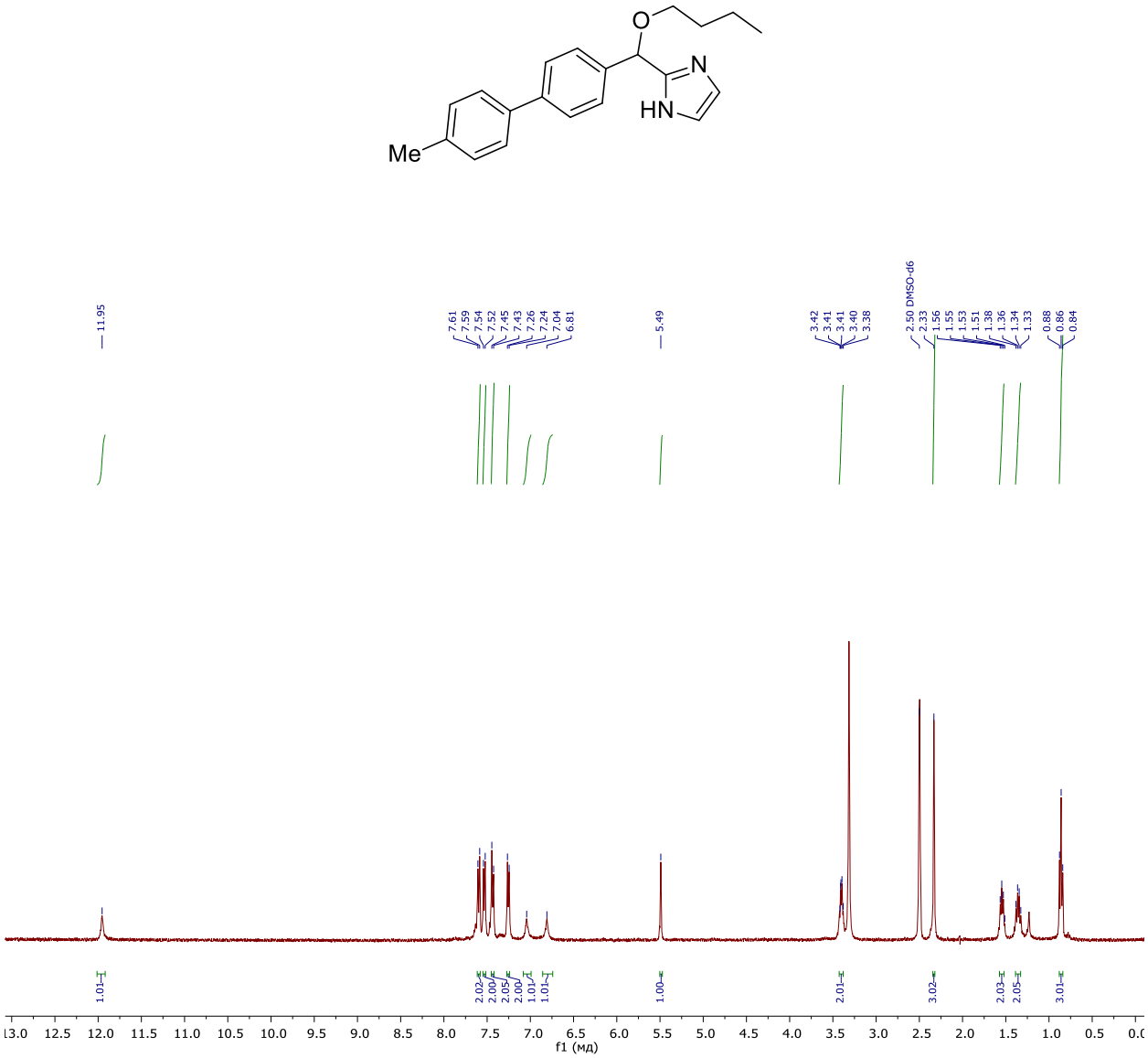


Figure S85. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **4p.**

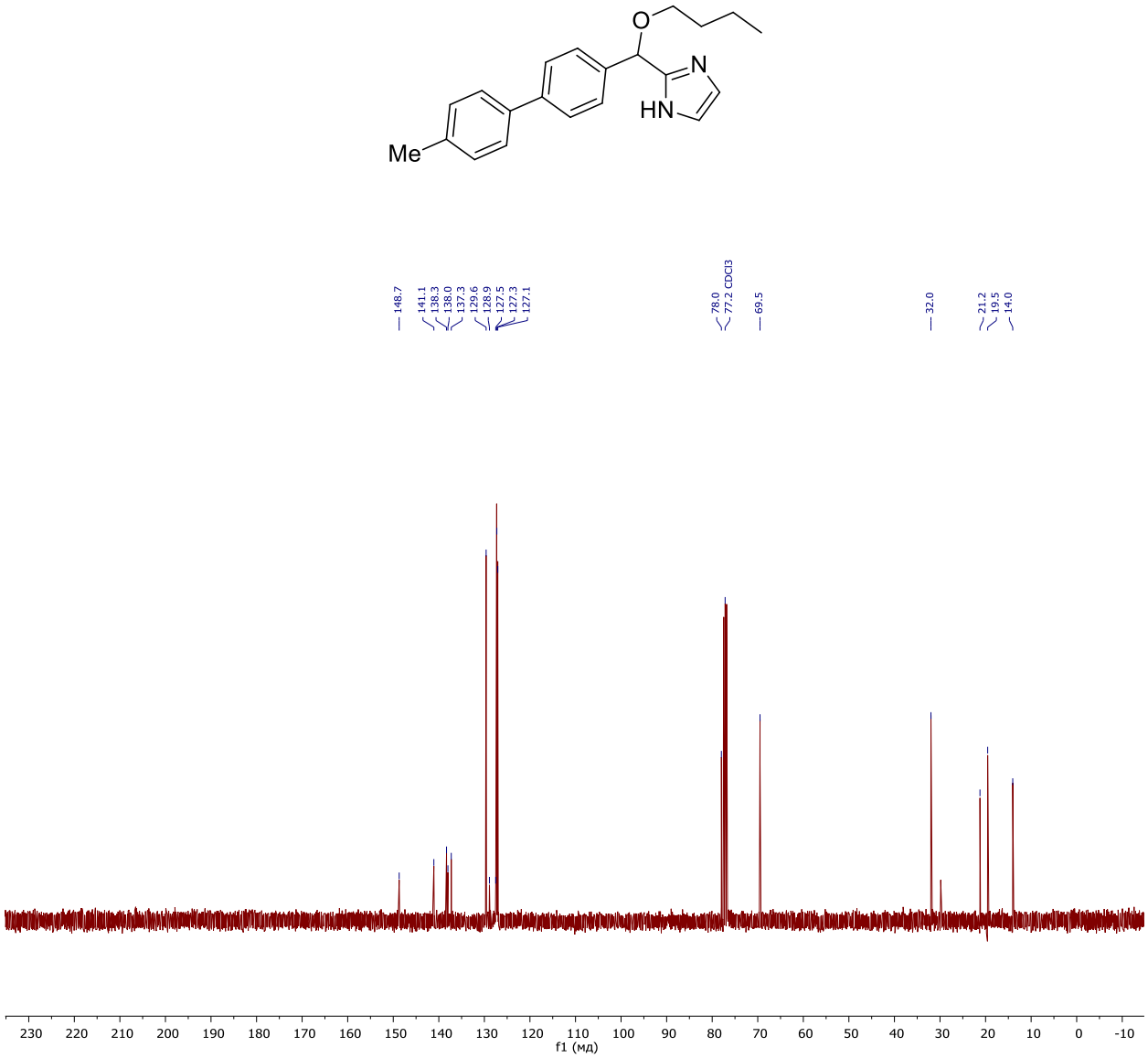


Figure S86. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of compound **4p.**

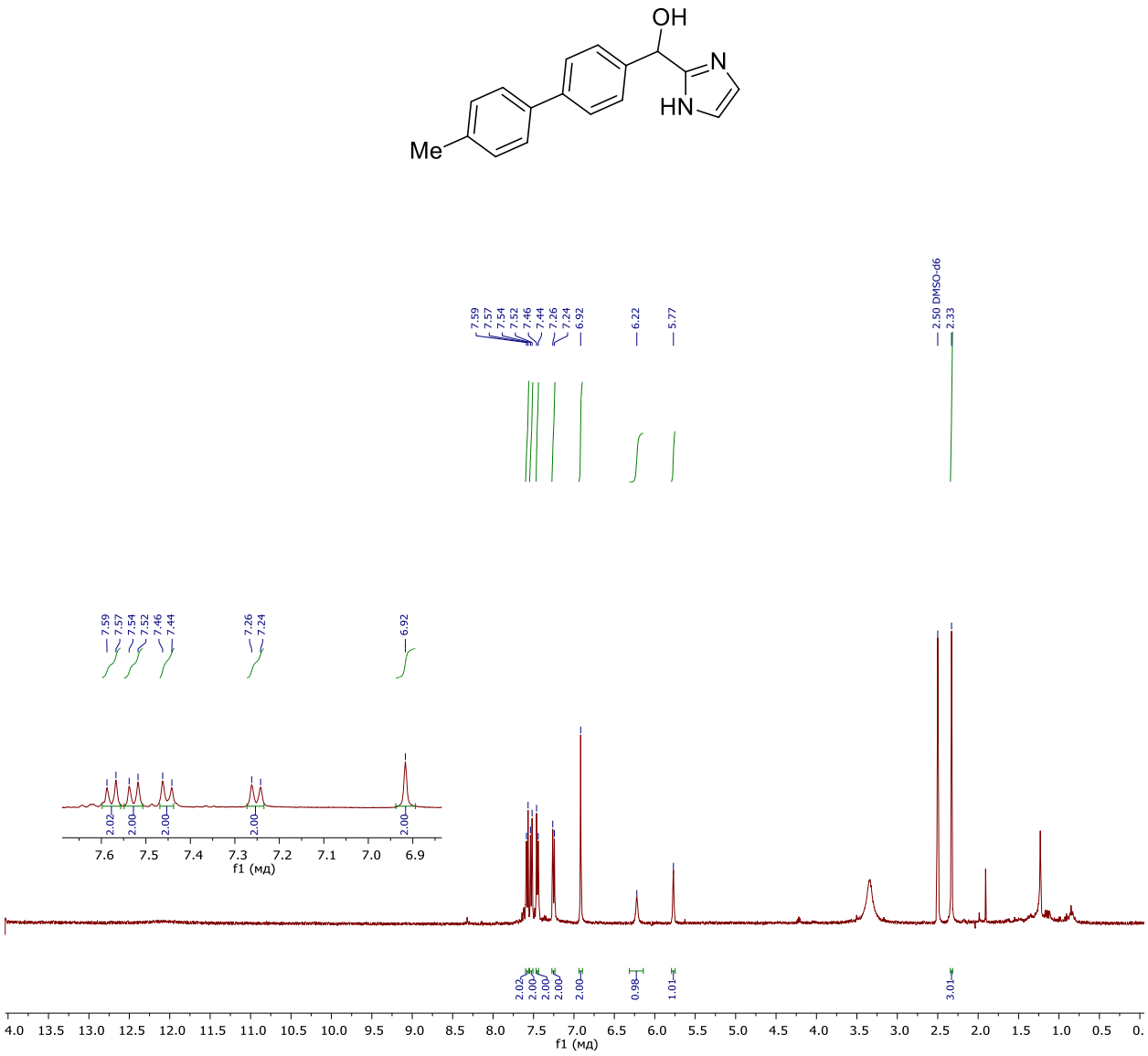


Figure S87. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **4q.**

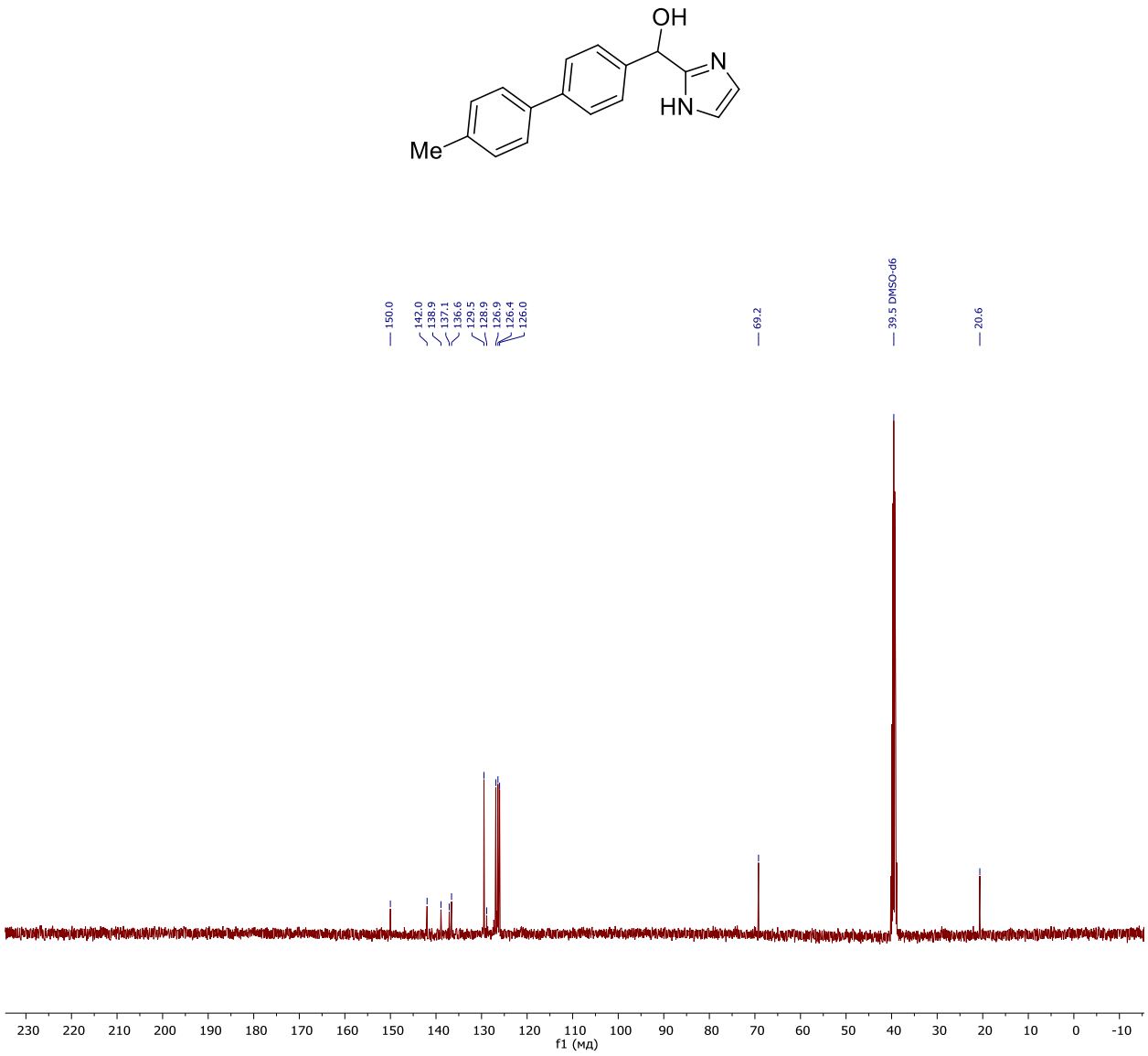


Figure S88. ^{13}C NMR (101 MHz, DMSO-d_6) spectrum of compound **4q.**

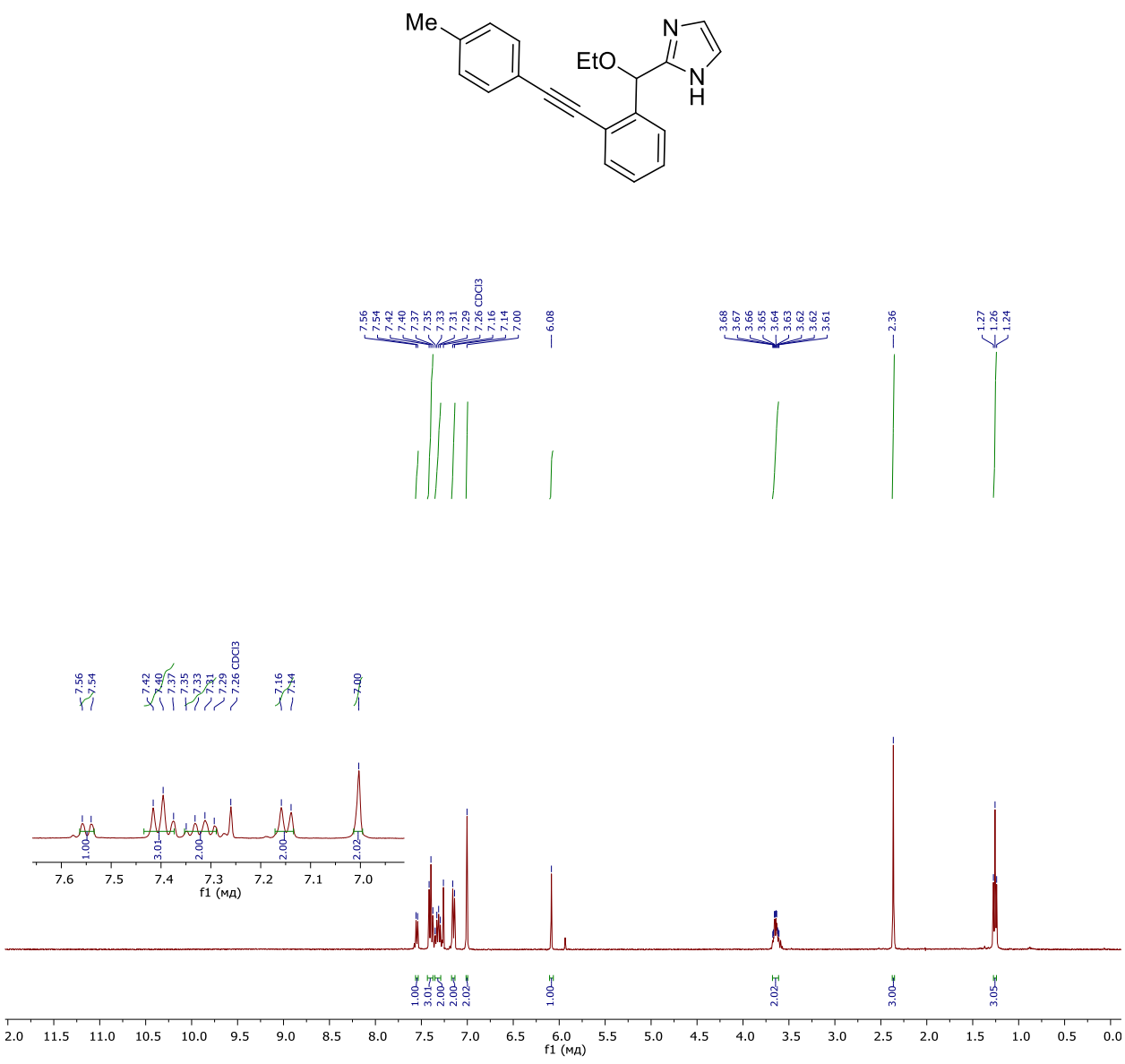


Figure S89. [1]H NMR (400 MHz, Chloroform-*d*) spectrum of compound **4r.**

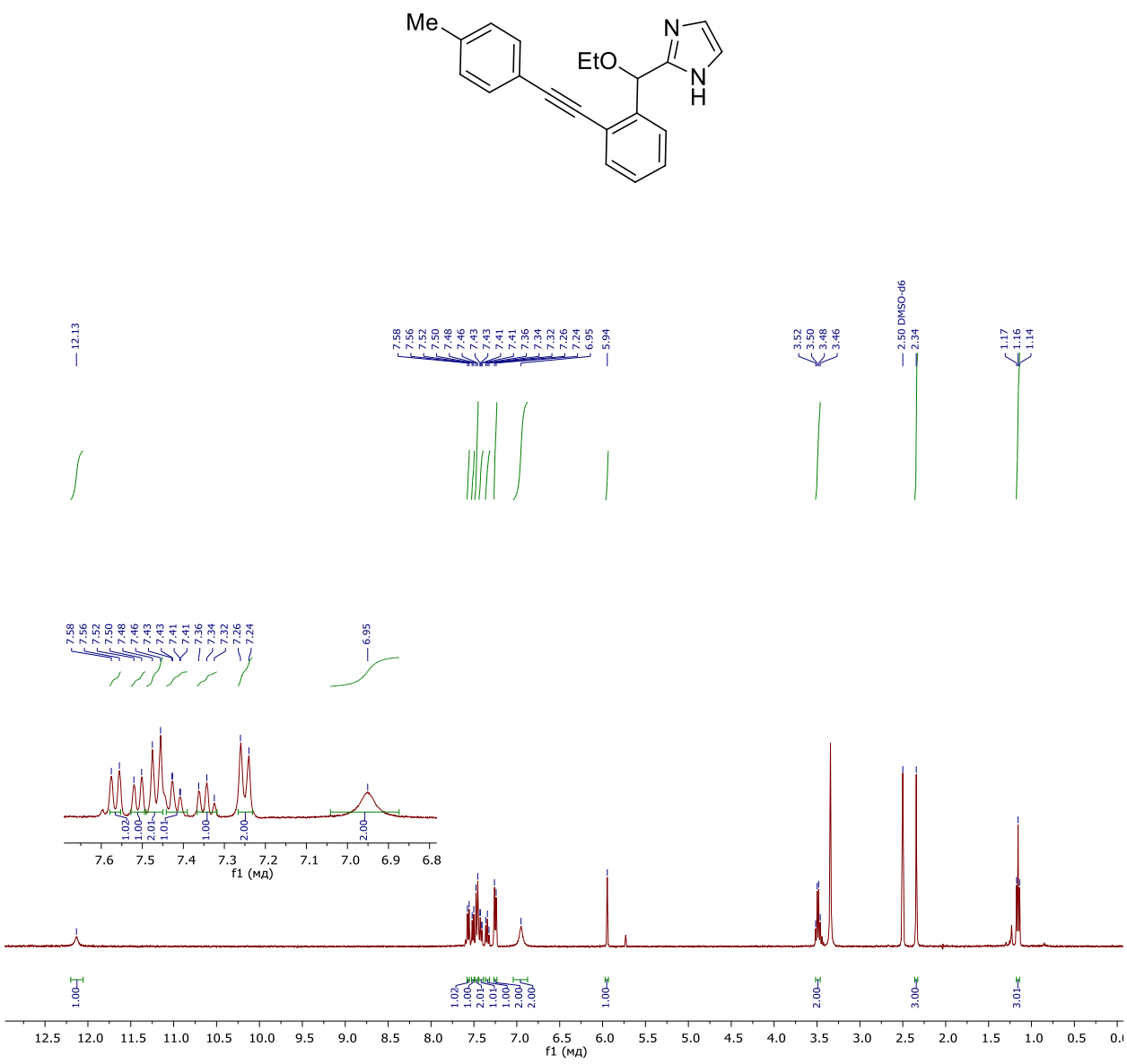


Figure S90 ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **4r.**

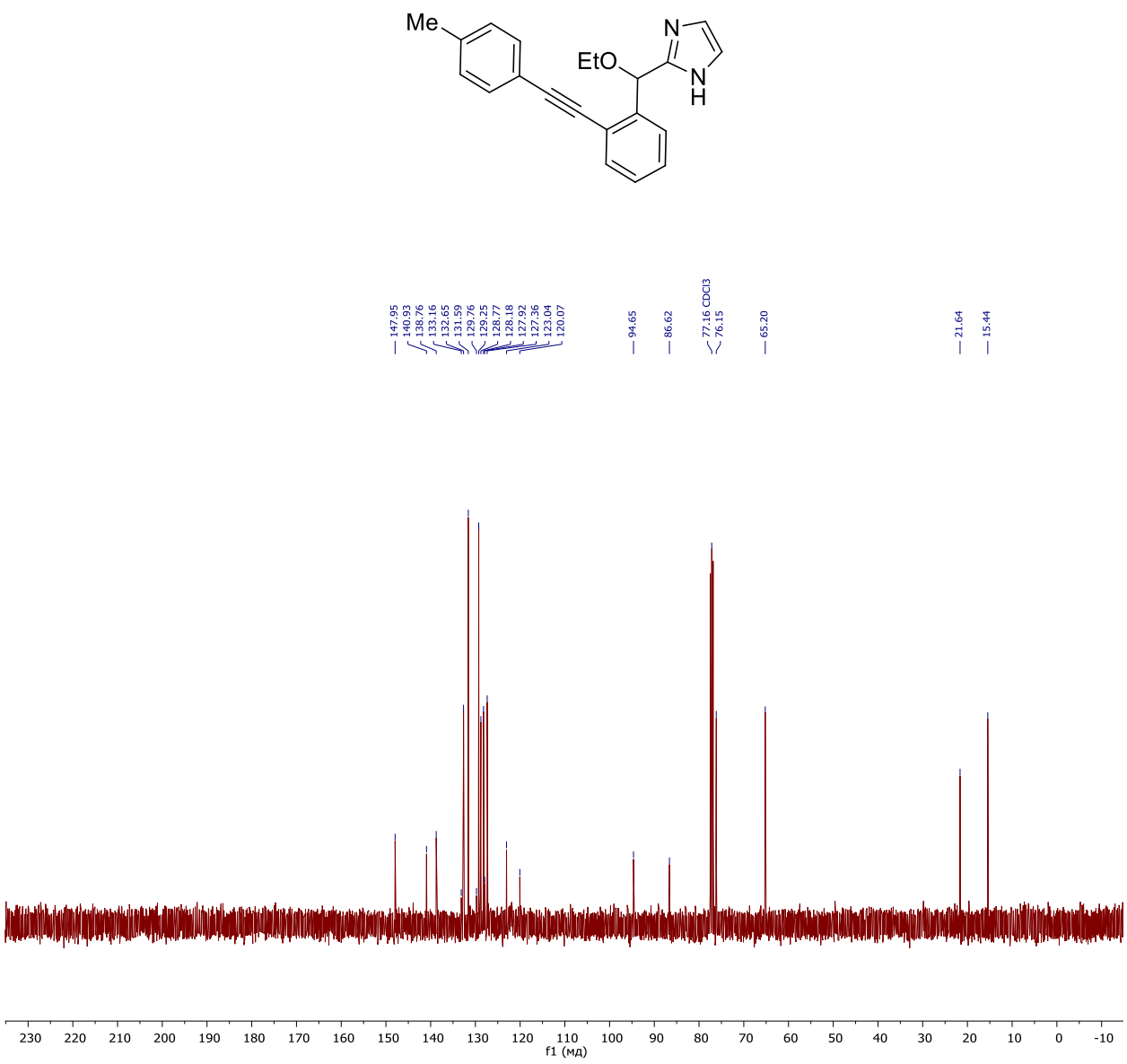


Figure S91. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of compound **4r.**

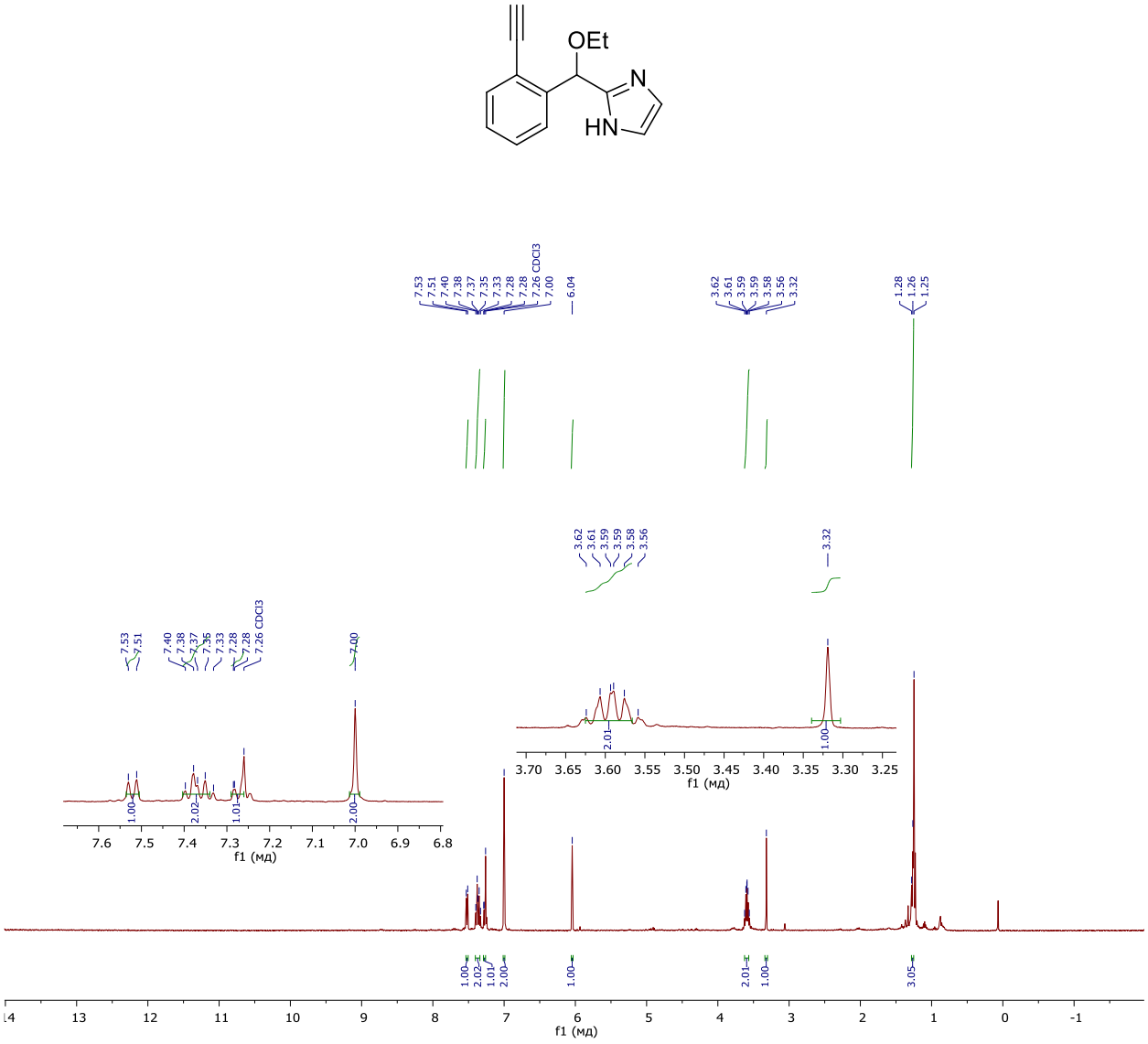


Figure S92. ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **4s.**

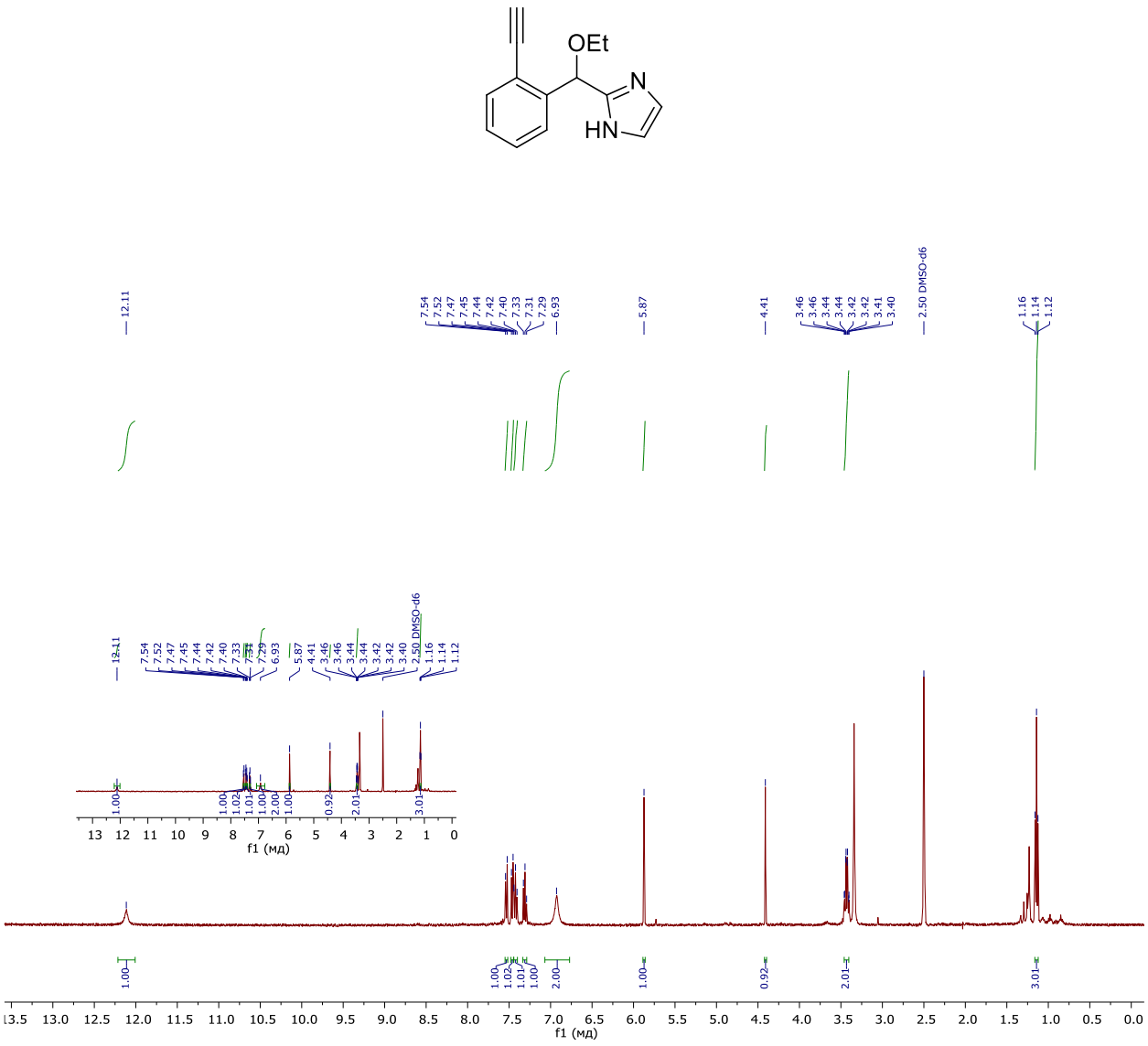


Figure S93. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **4s.**

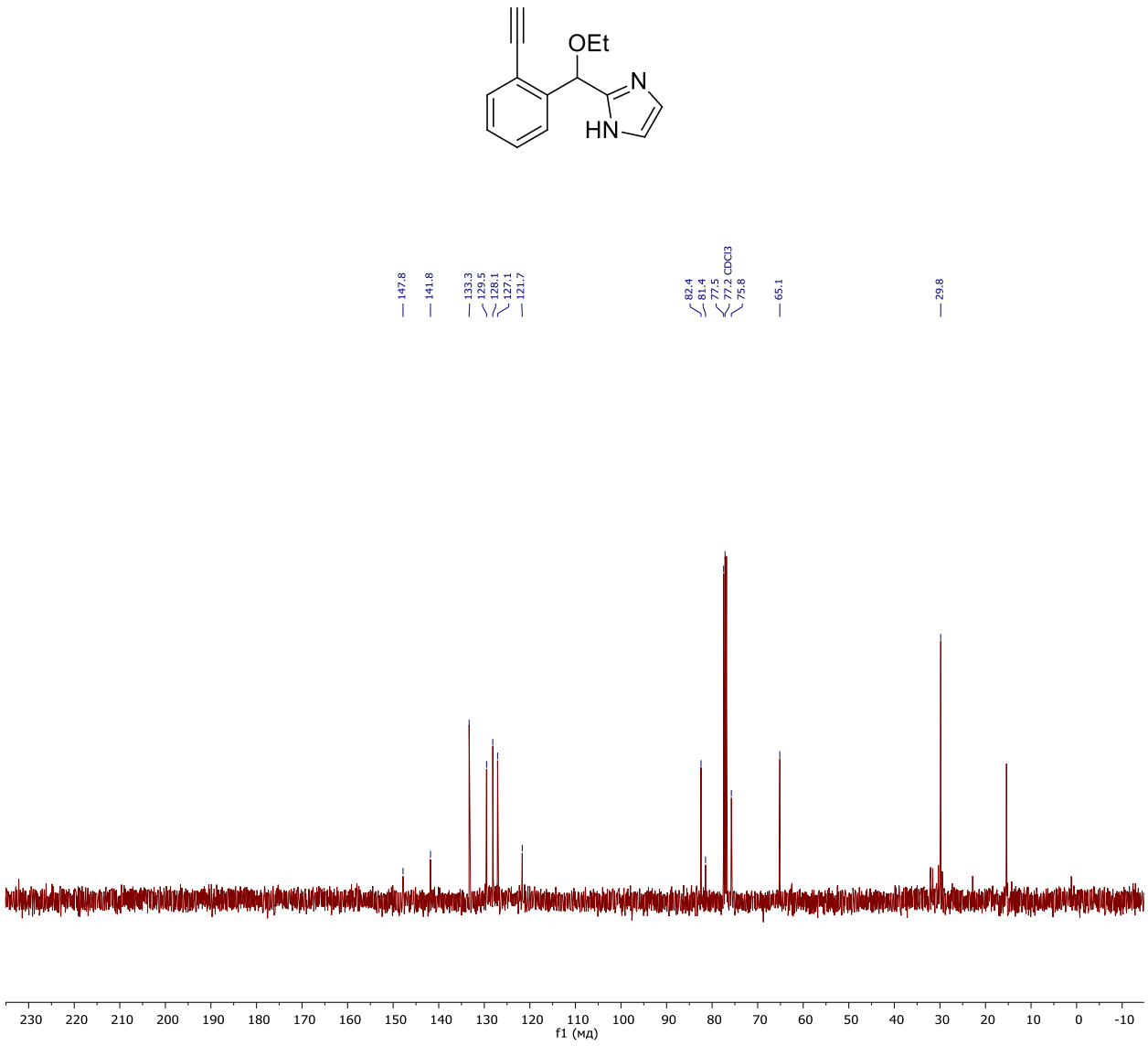


Figure S94. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of compound **4s.**

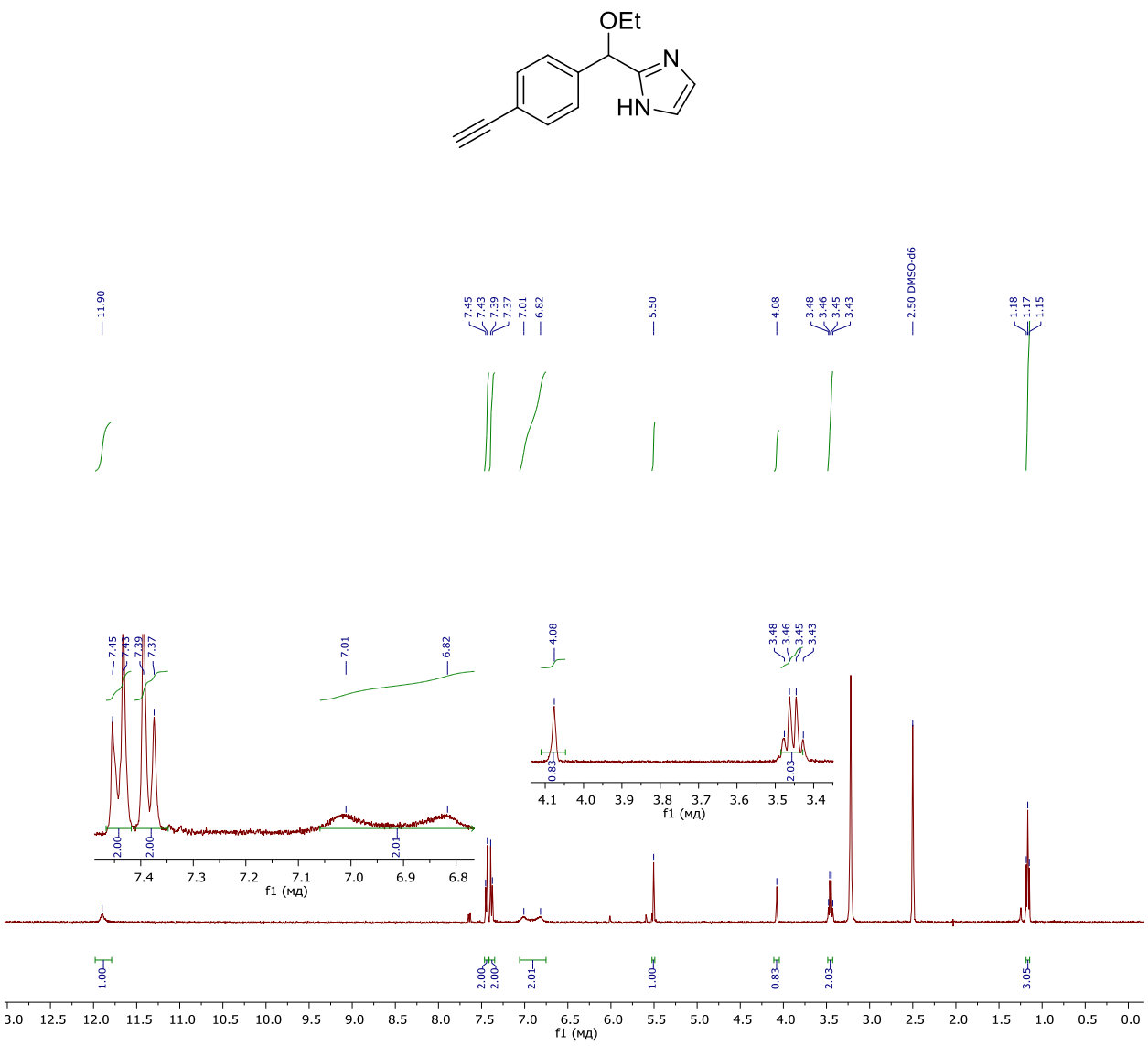


Figure S95. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **4t.**

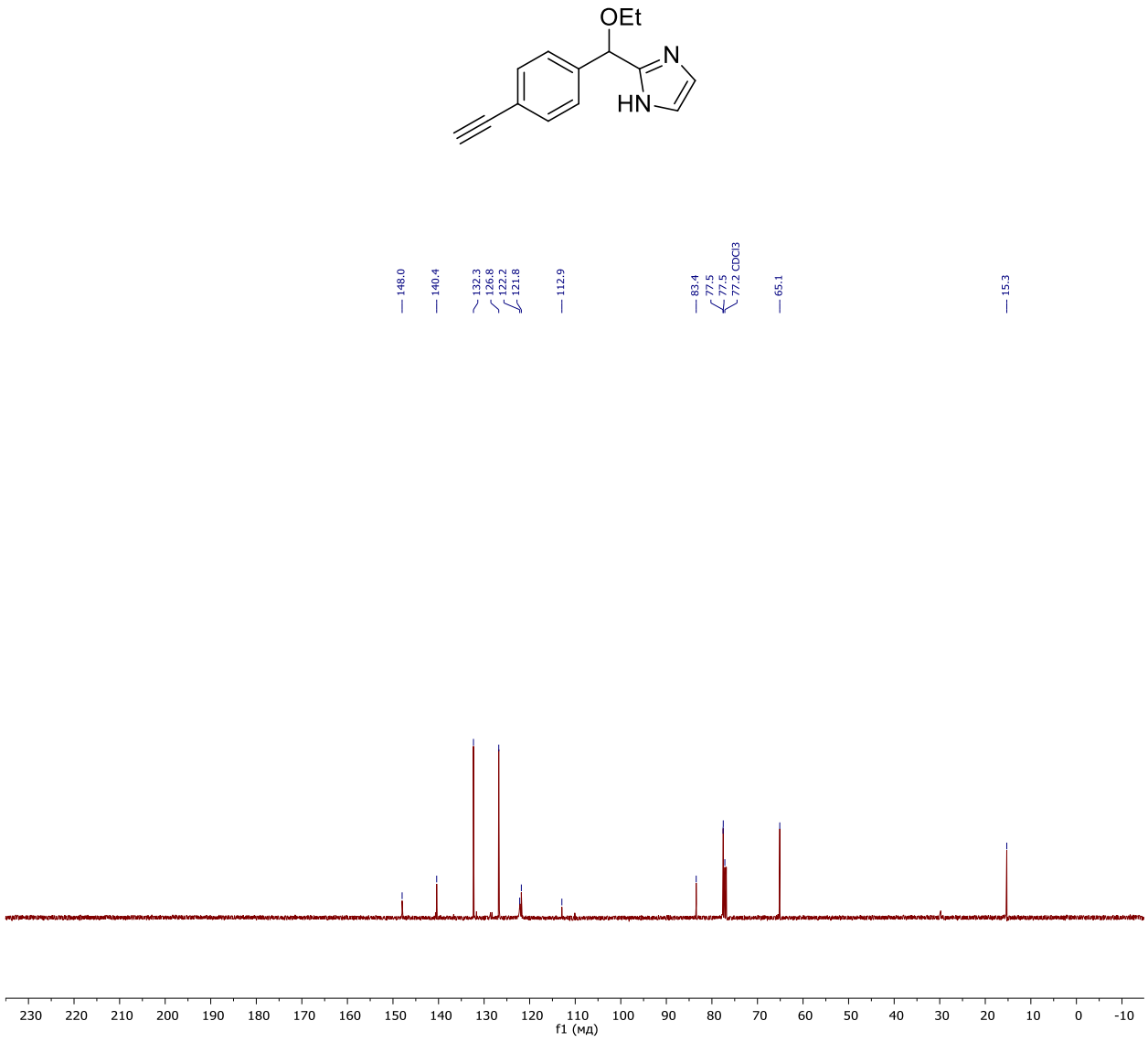


Figure S96. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of compound **4t.**

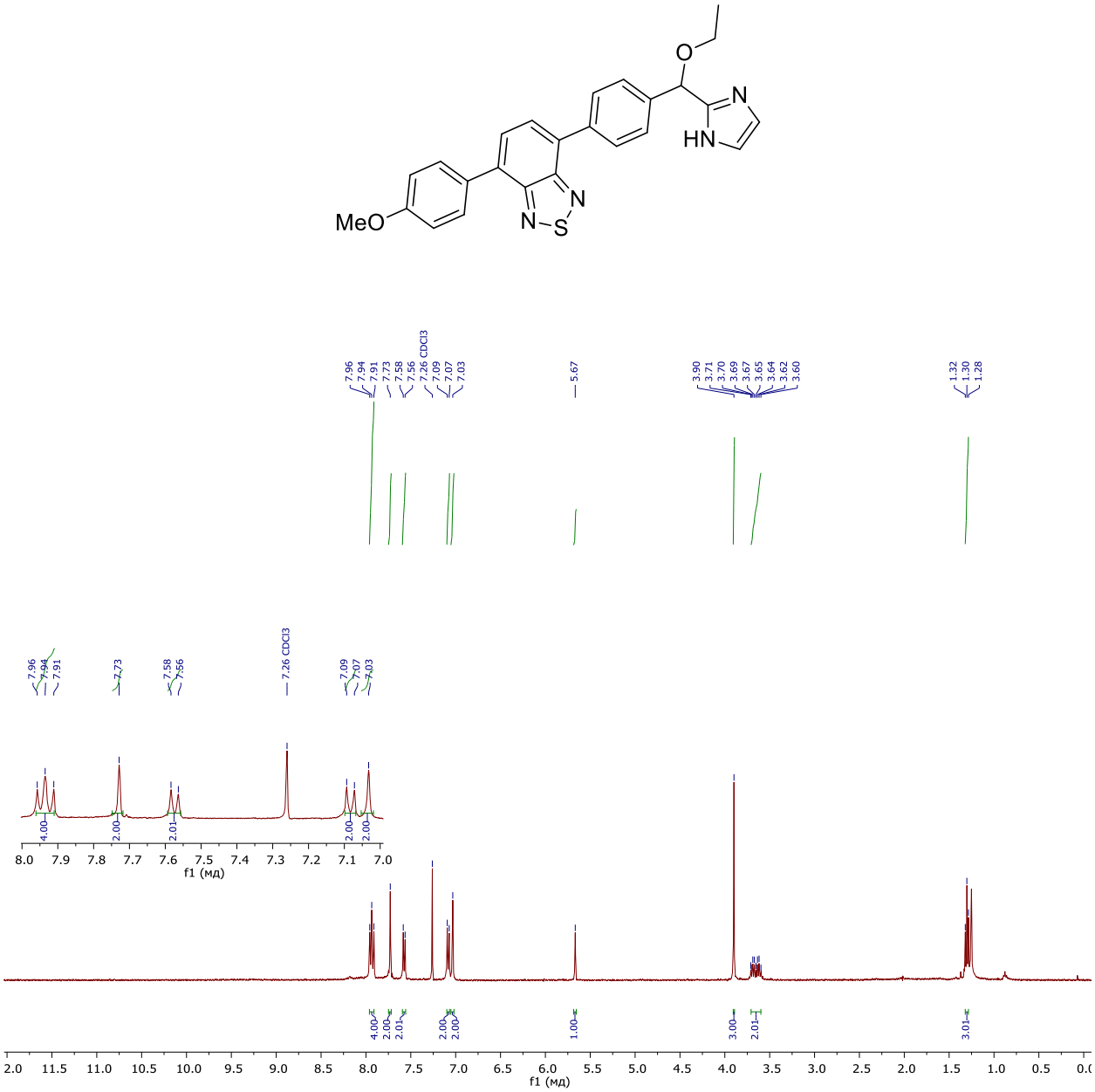


Figure S97. ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **4u.**

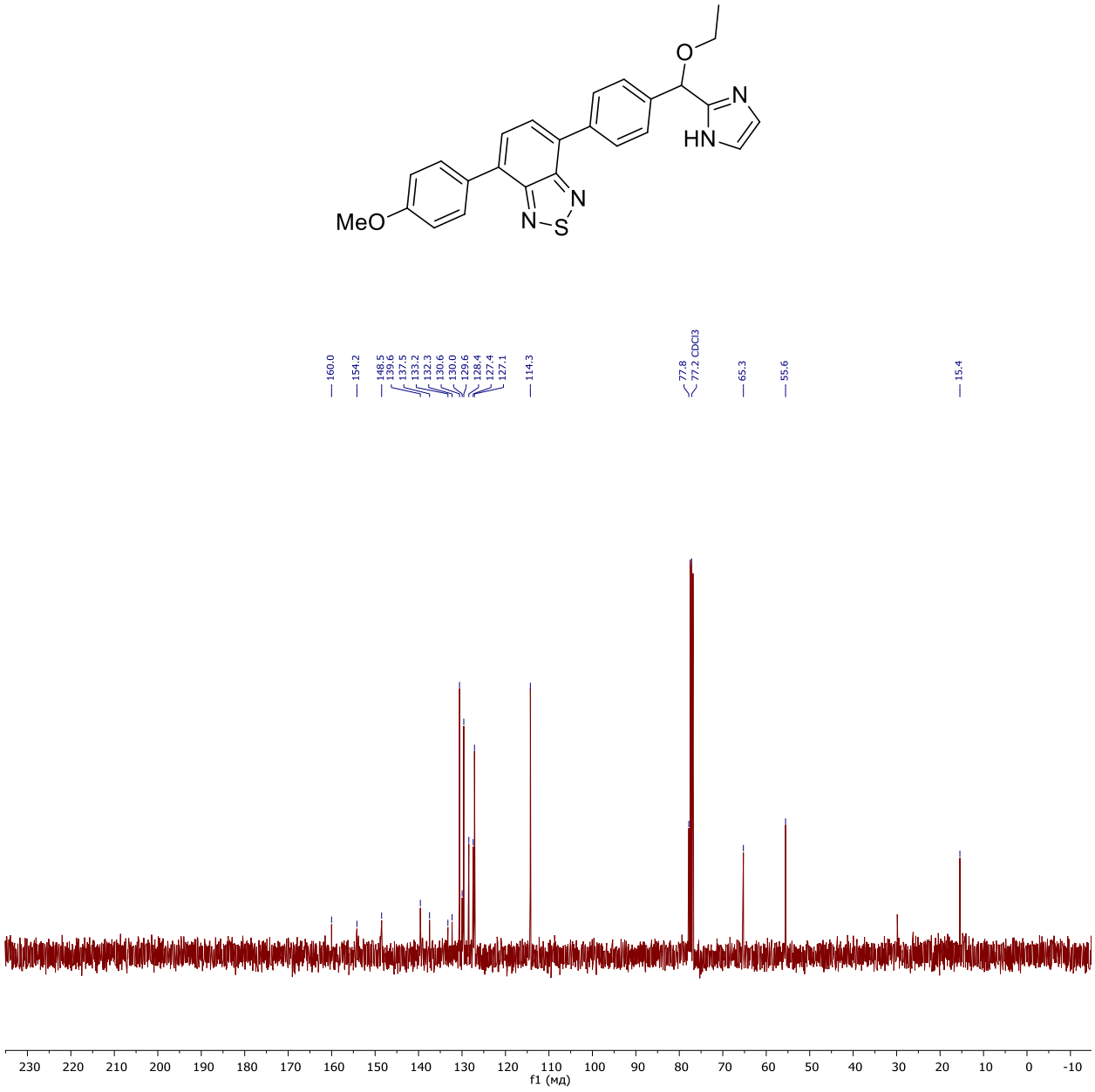


Figure S98. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of compound **4u.**

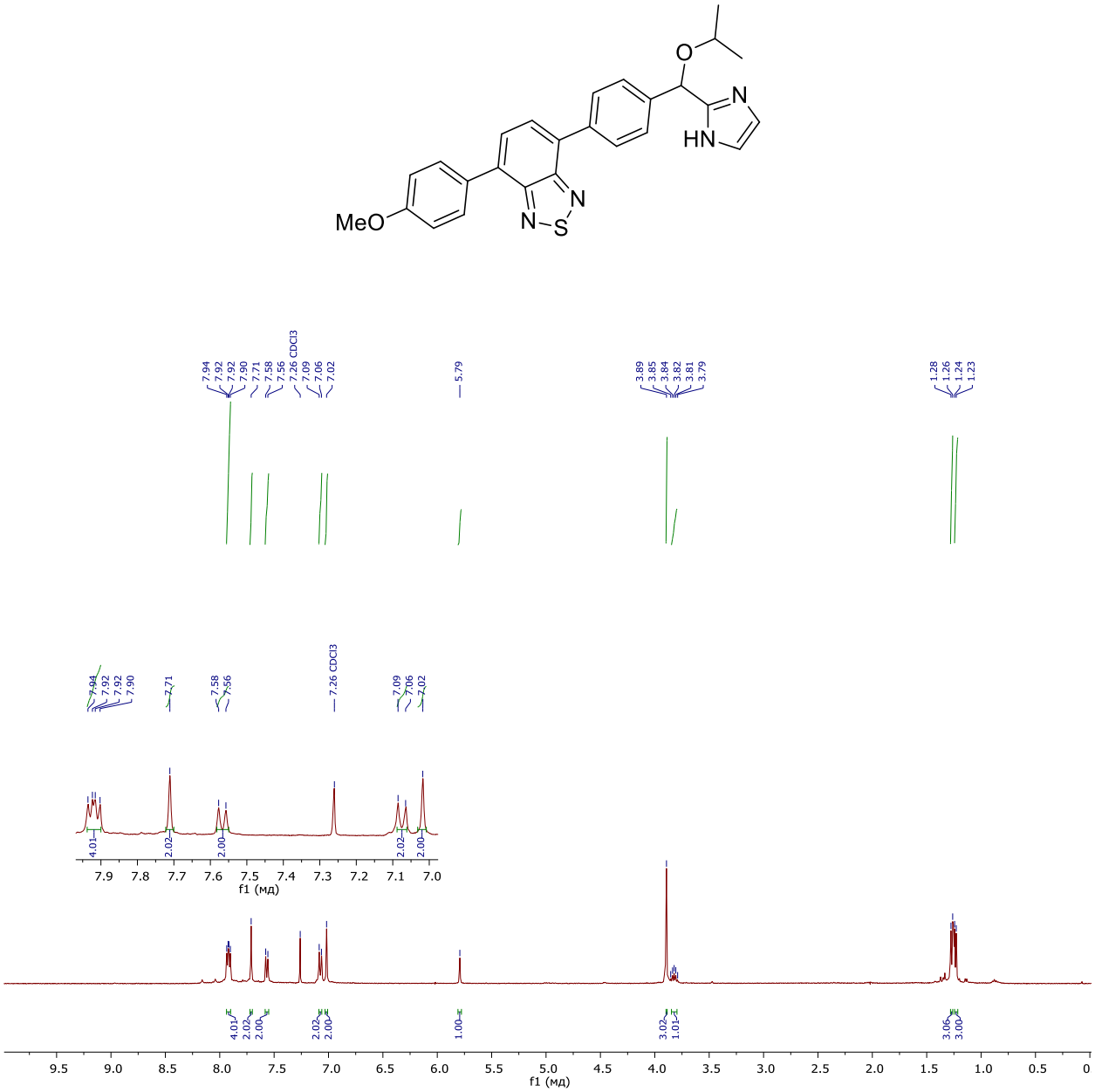


Figure S99 ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **4v.**

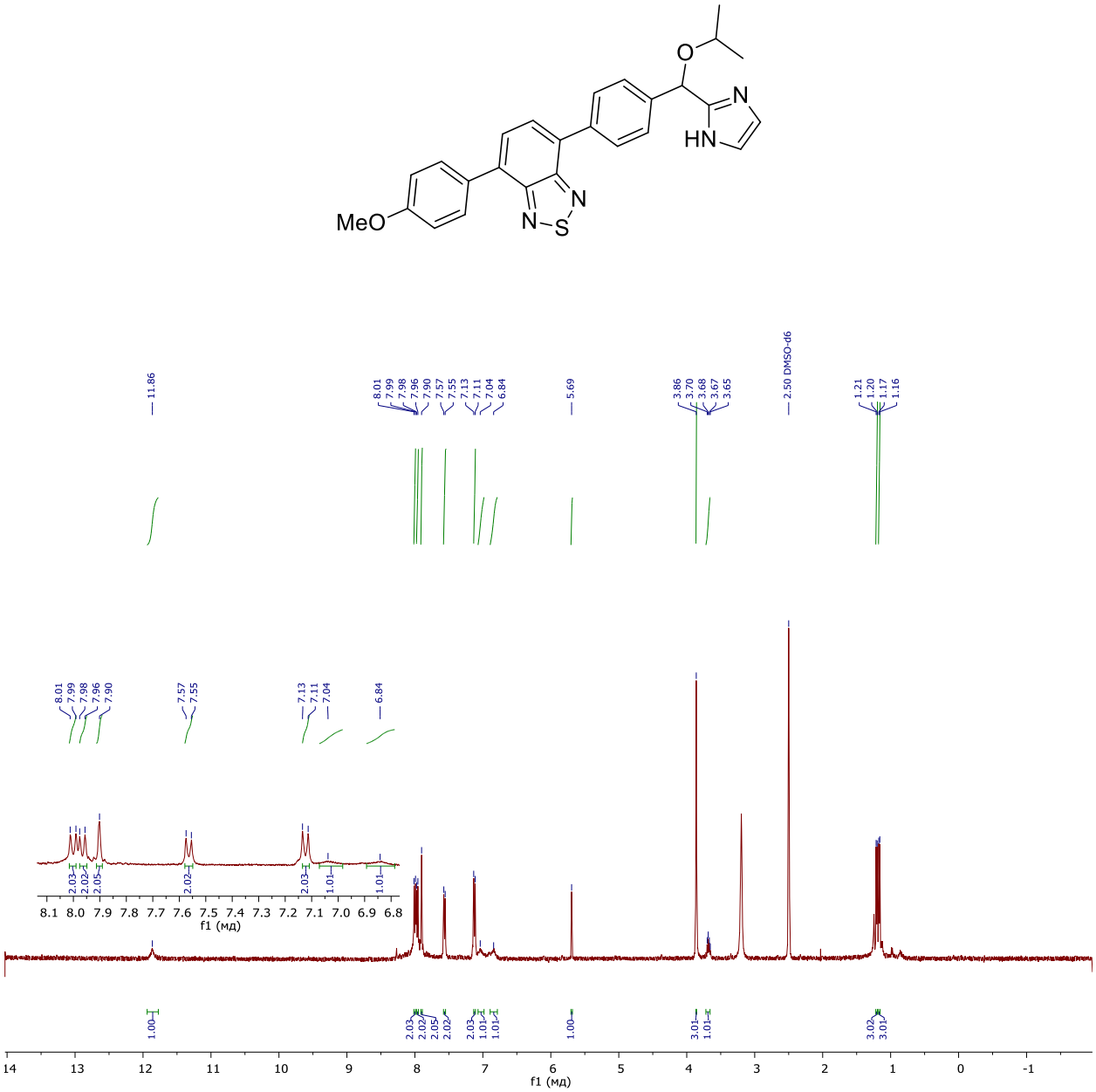


Figure S100. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **4v.**

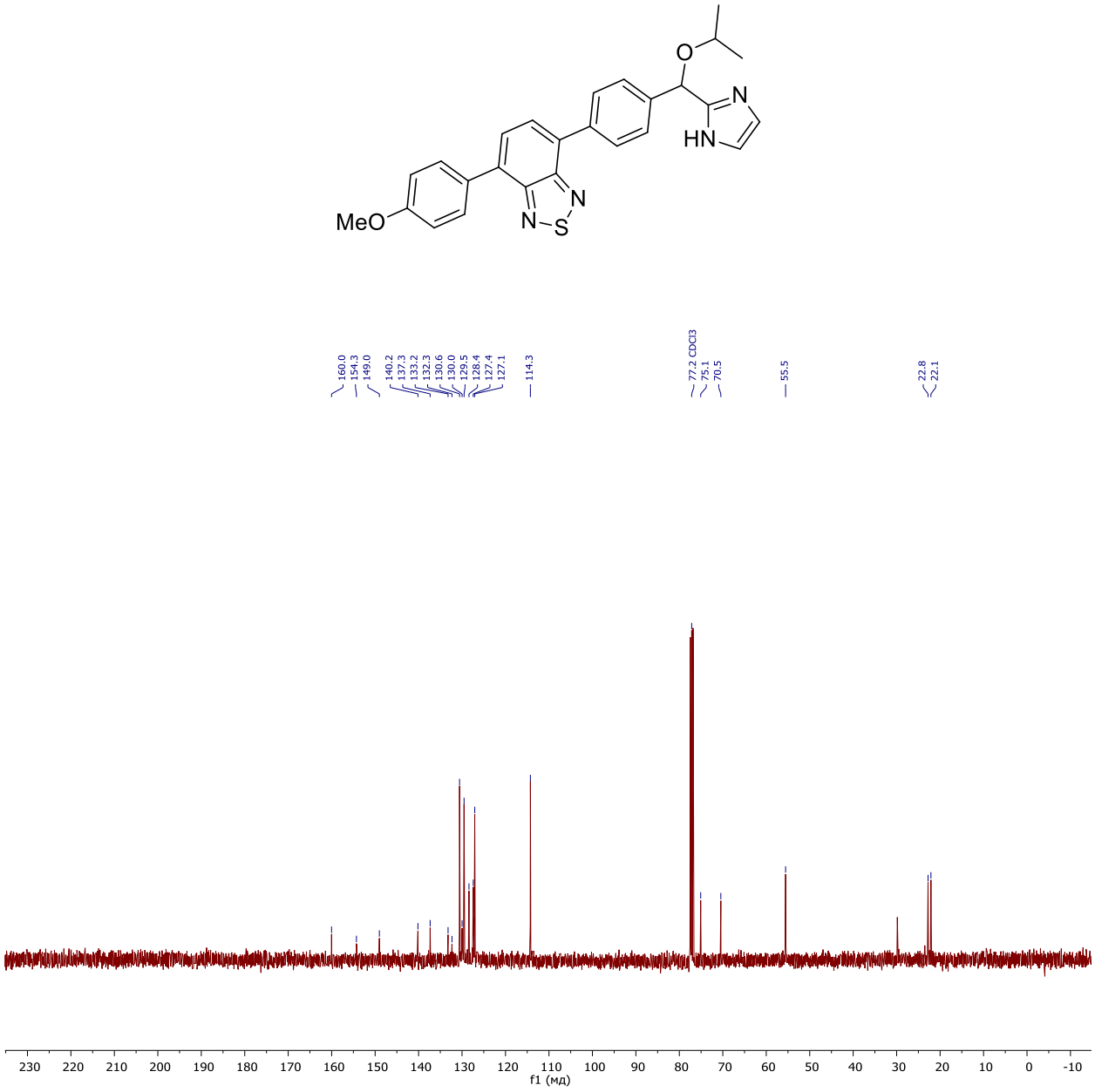


Figure S101. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of compound **4v.**

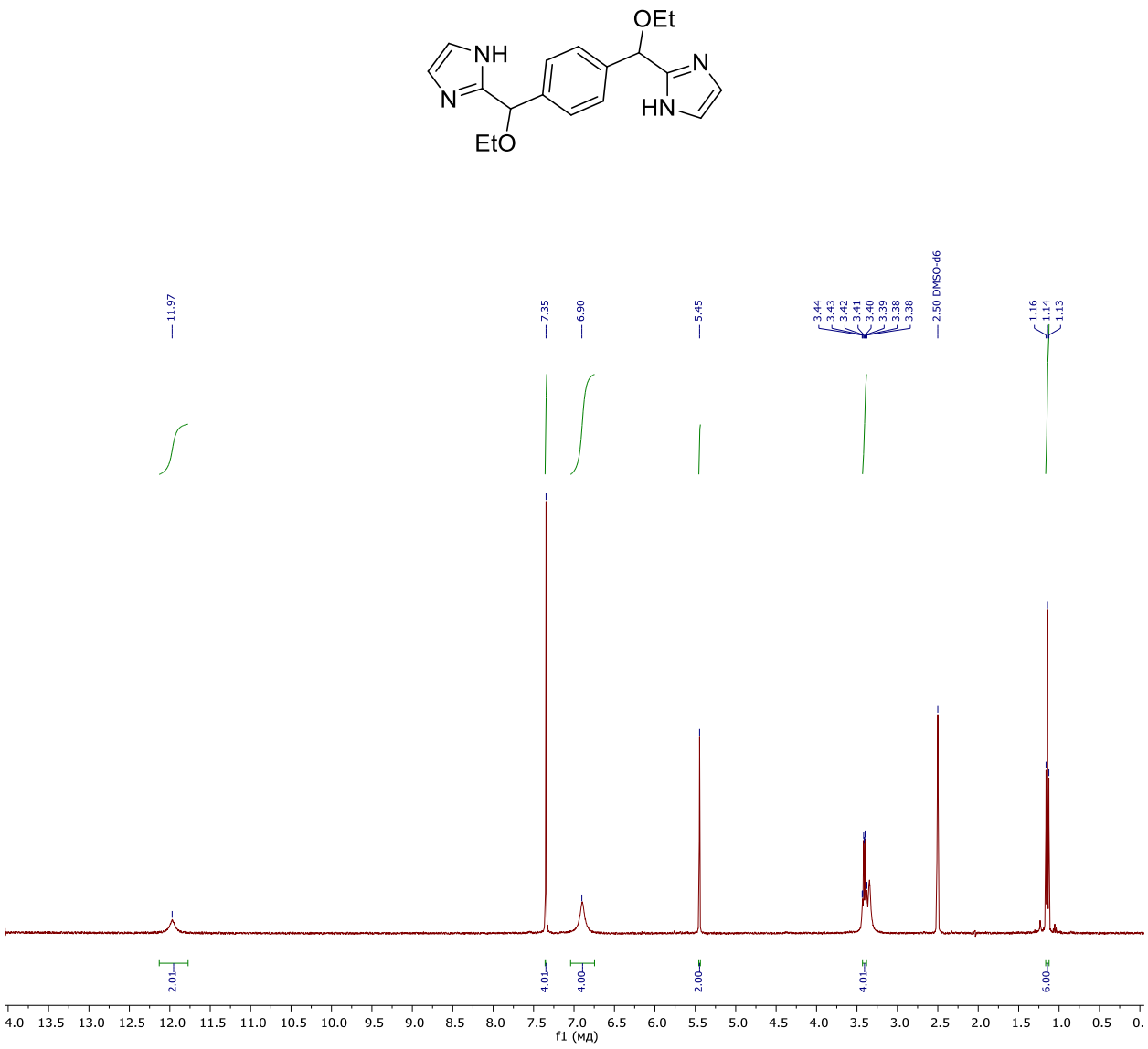


Figure S102. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **4w.**

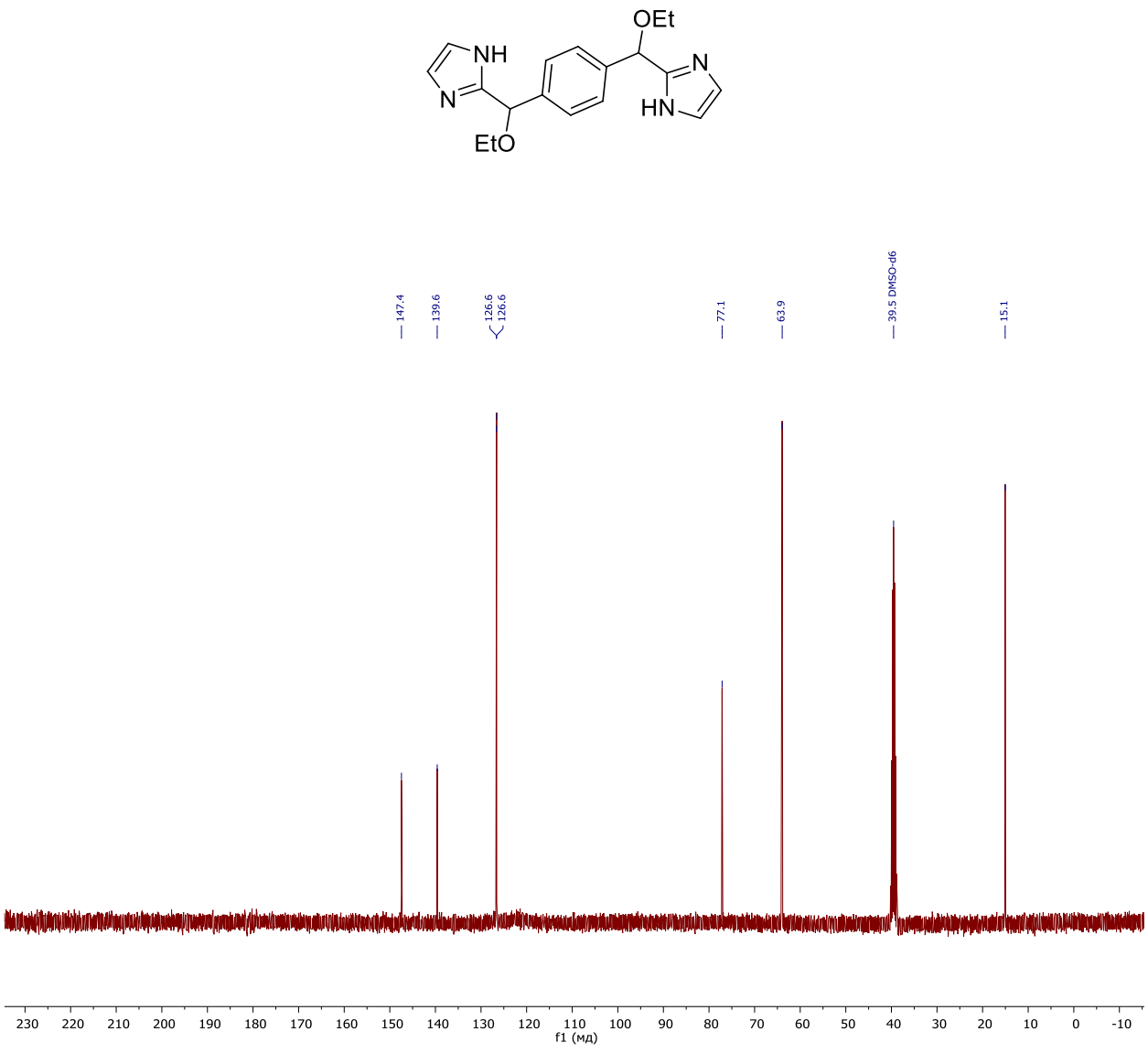


Figure S103. ^{13}C NMR (101 MHz, DMSO-d_6) spectrum of compound **4w.**

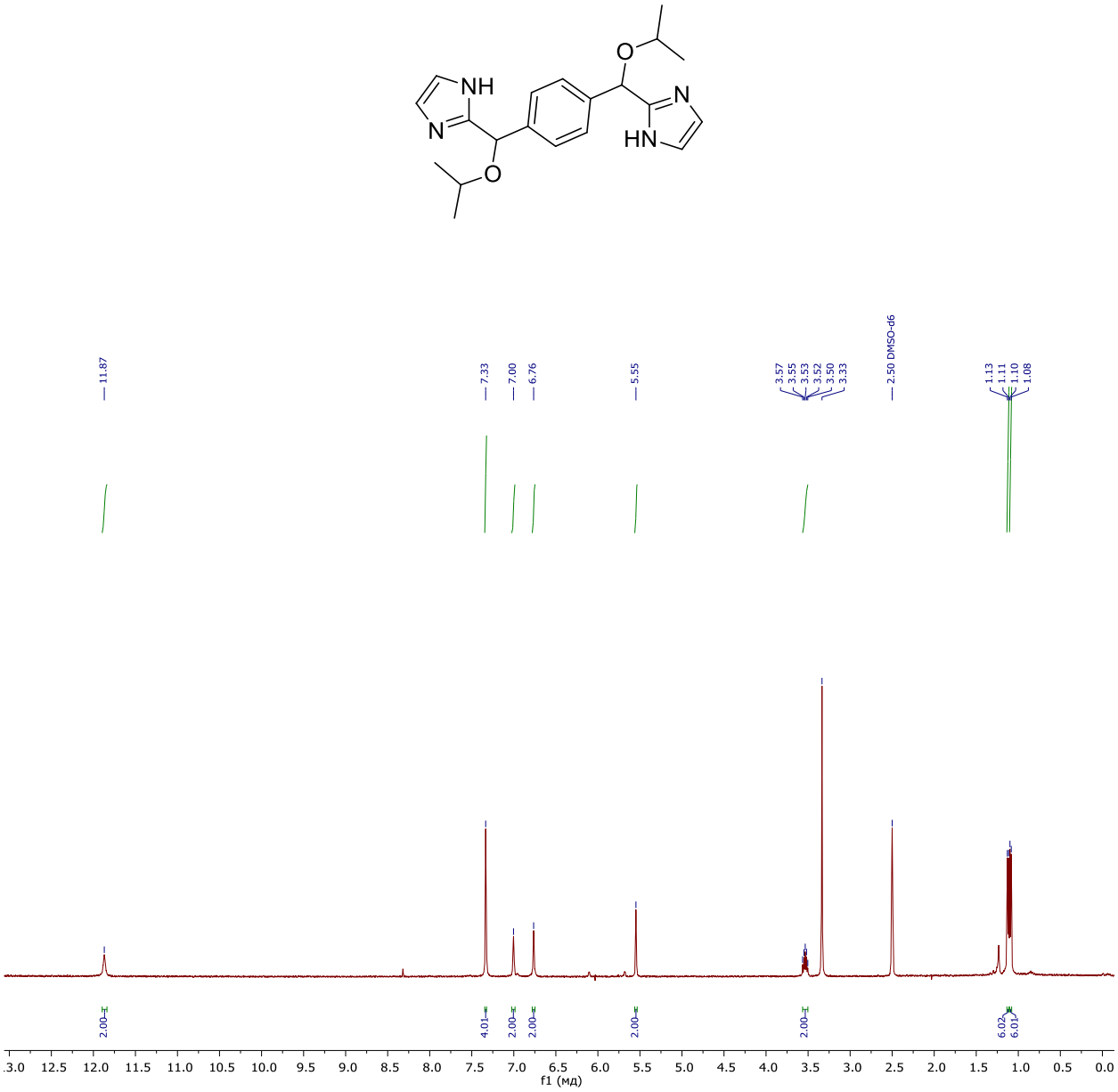


Figure S104. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **4x.**

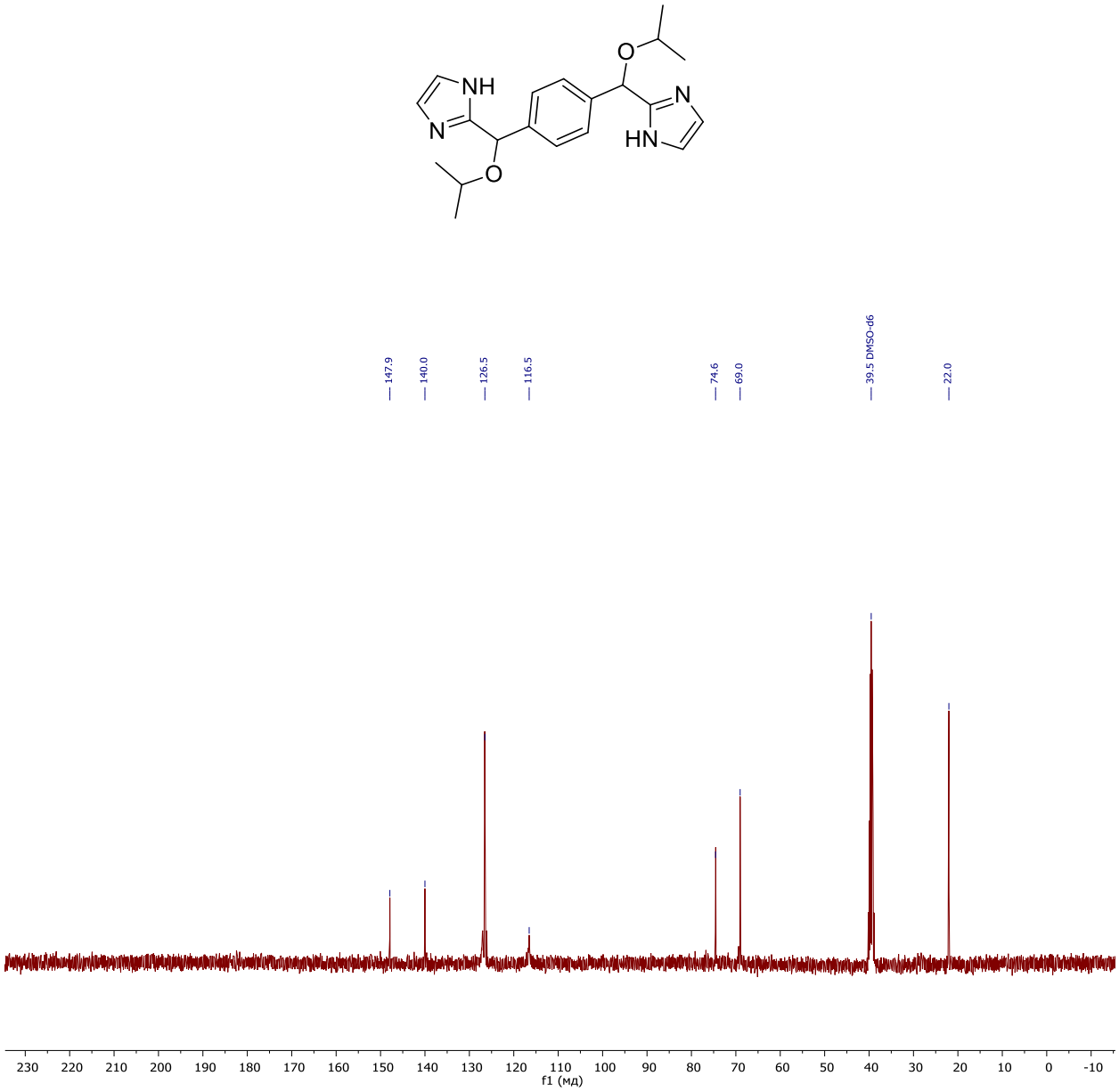


Figure S105. ^{13}C NMR (101 MHz, DMSO-d_6) spectrum of compound **4x.**

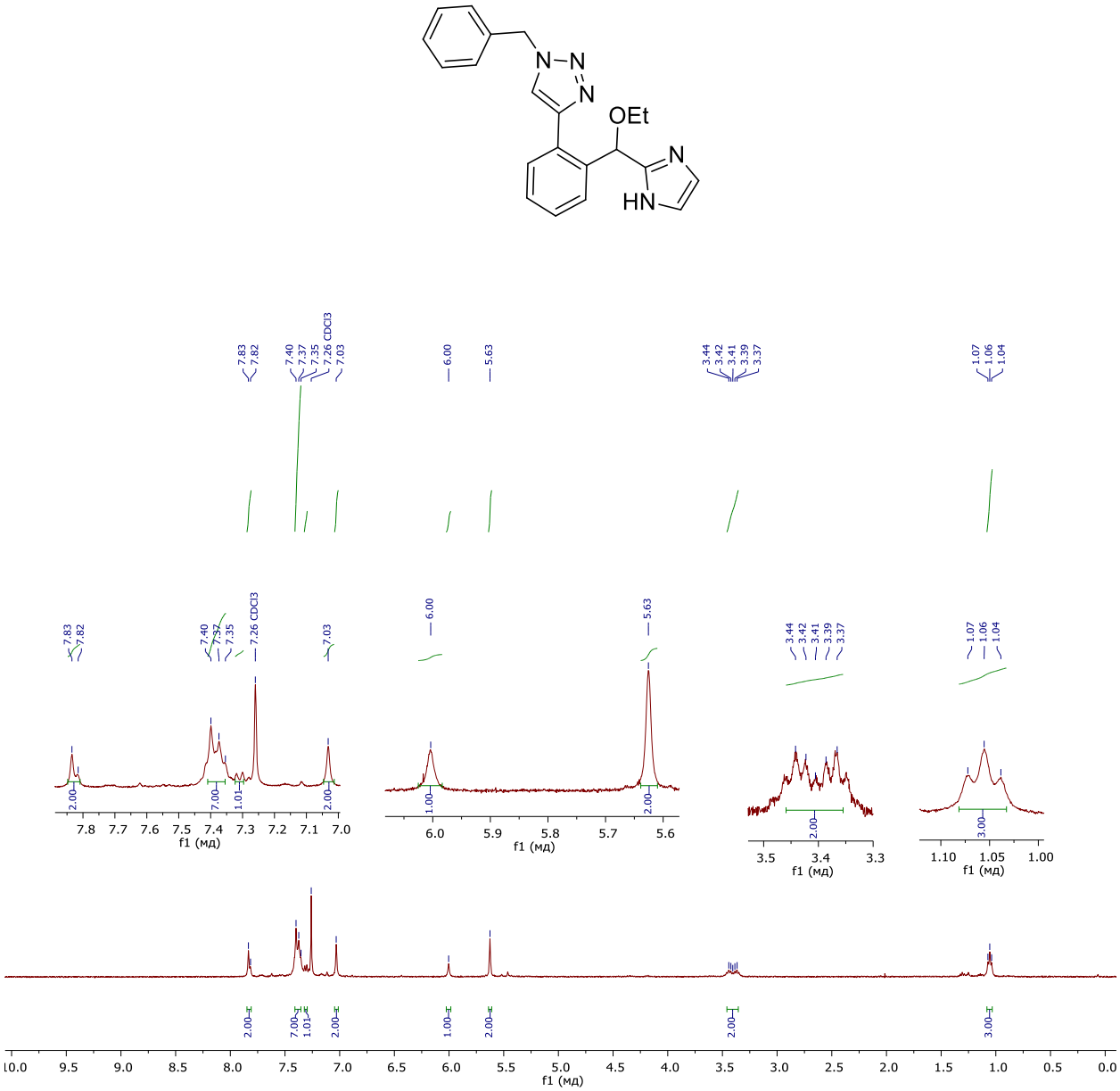


Figure S106. ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **4y.**

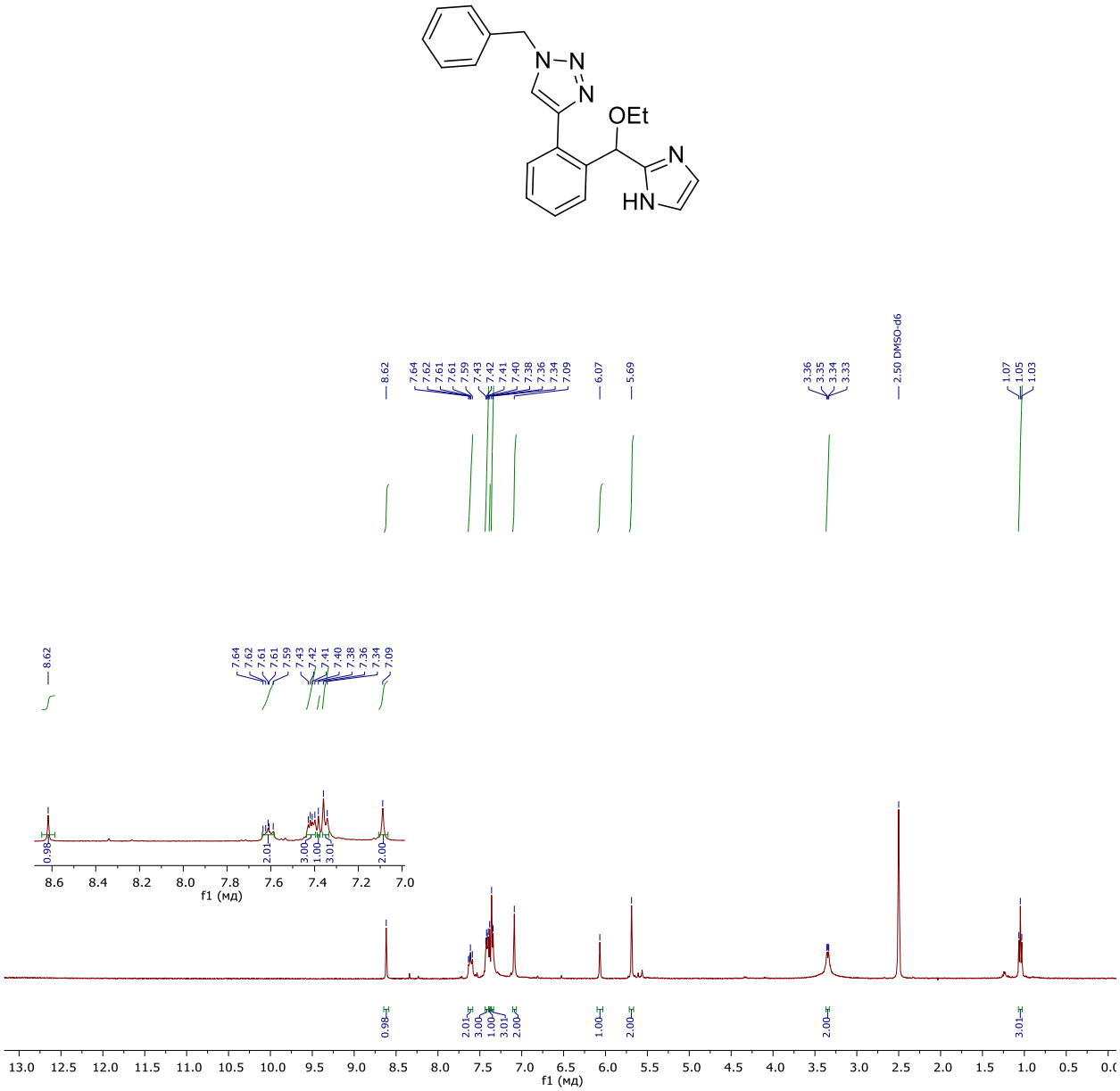


Figure S107. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **4y.**

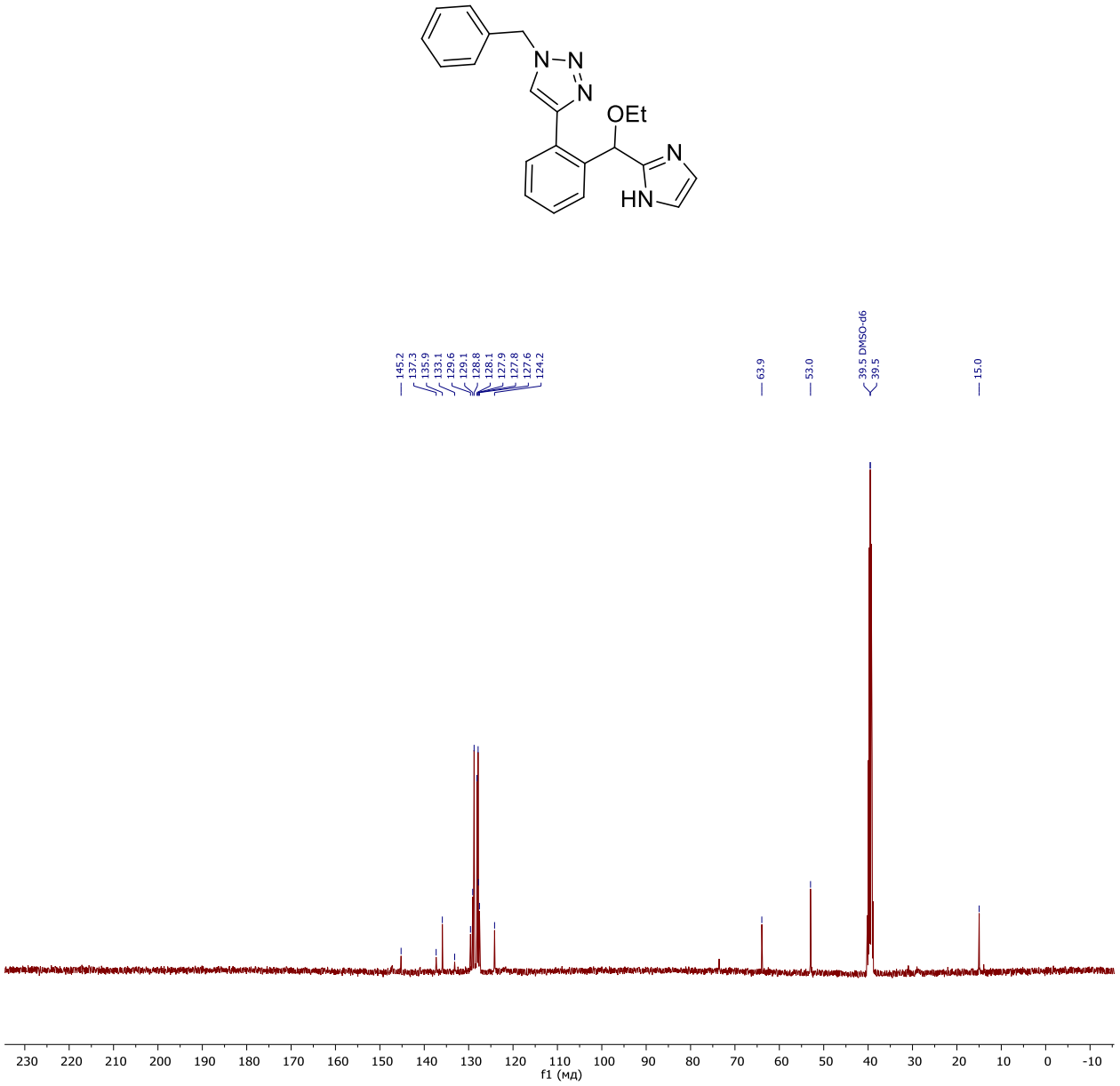


Figure S108. ^{13}C NMR (101 MHz, DMSO-d_6) spectrum of compound **4y.**

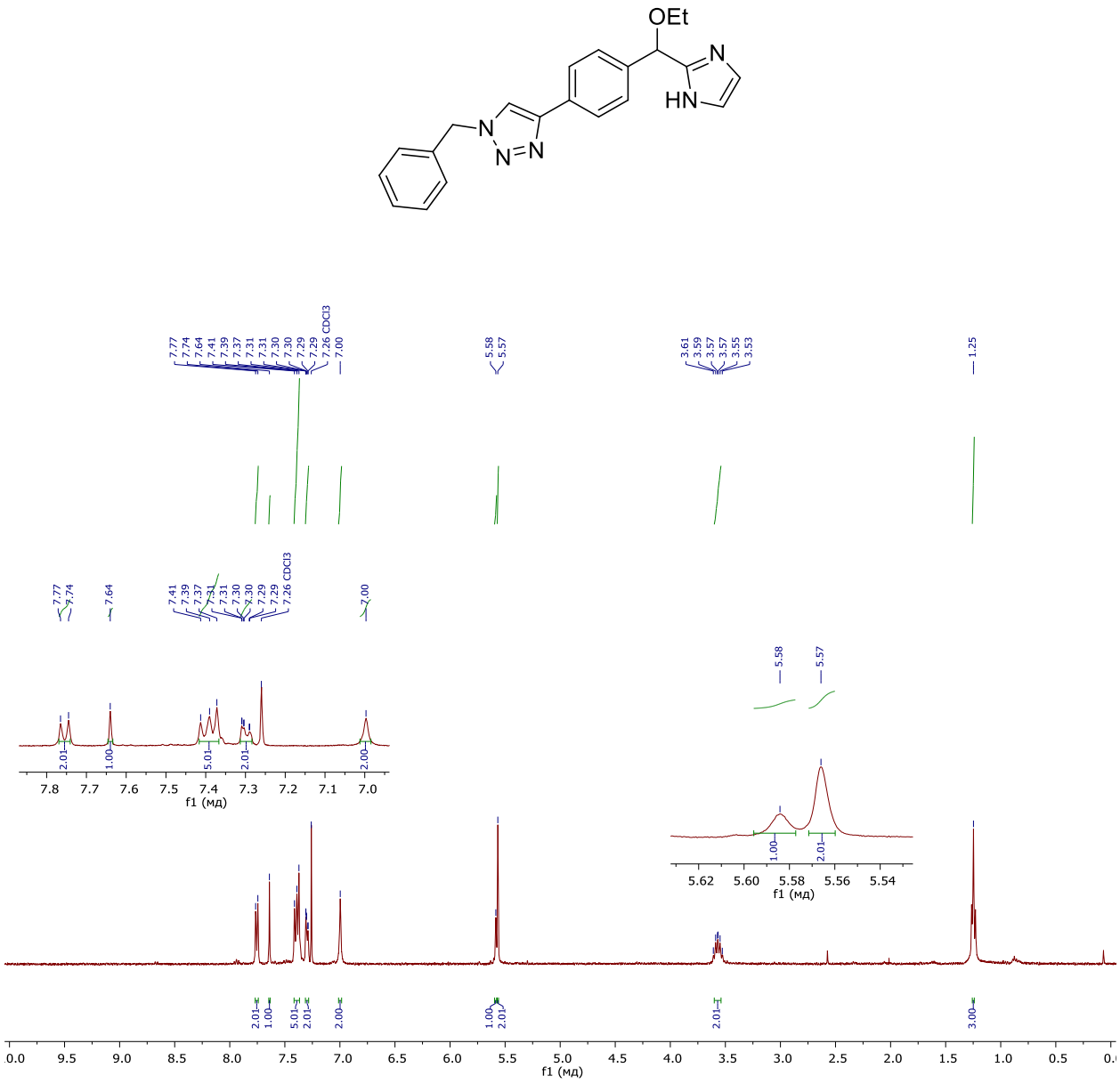


Figure S109. ^{1}H NMR (400 MHz, Chloroform-*d*) spectrum of compound **4z.**

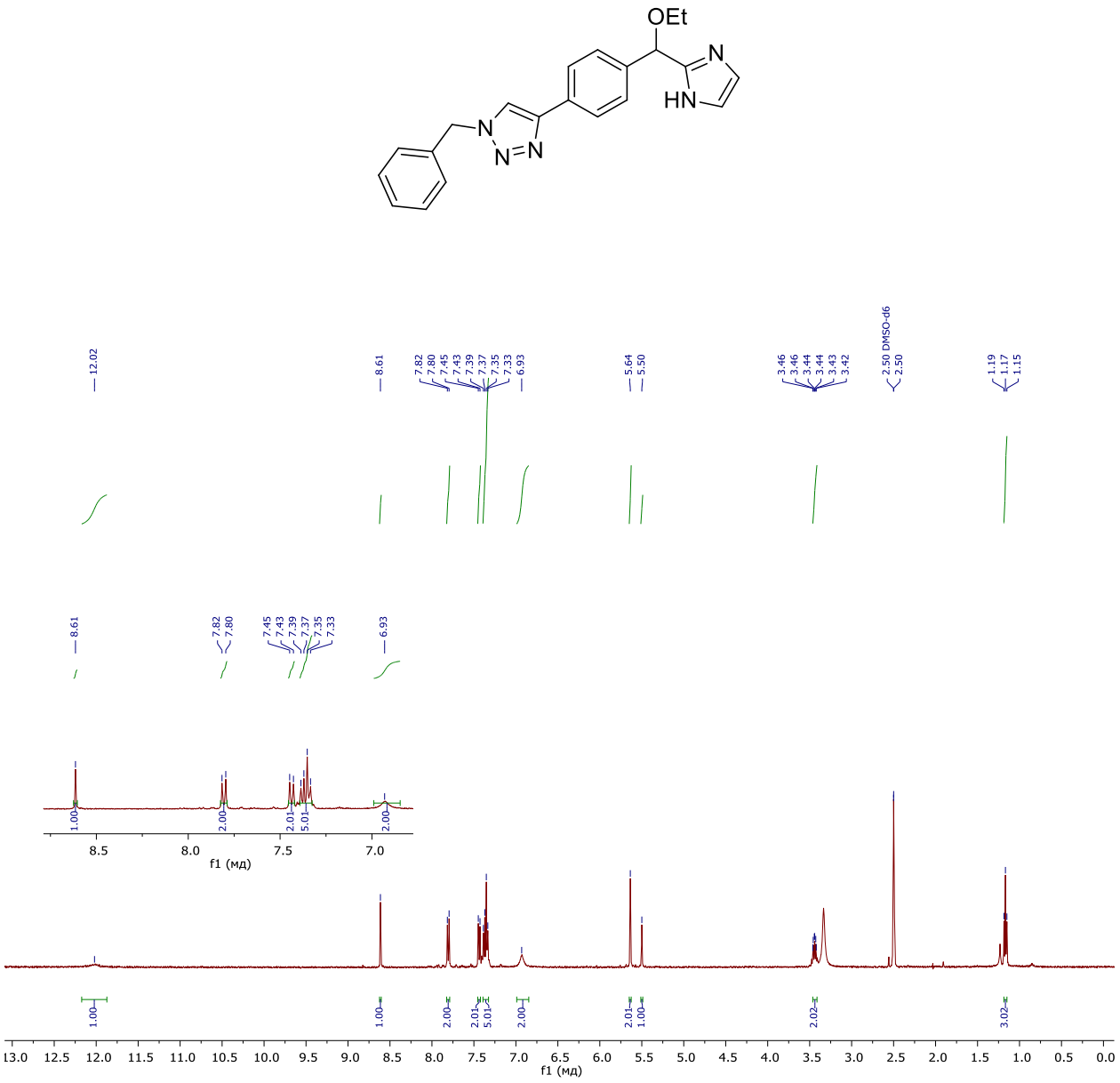


Figure S110. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **4z.**

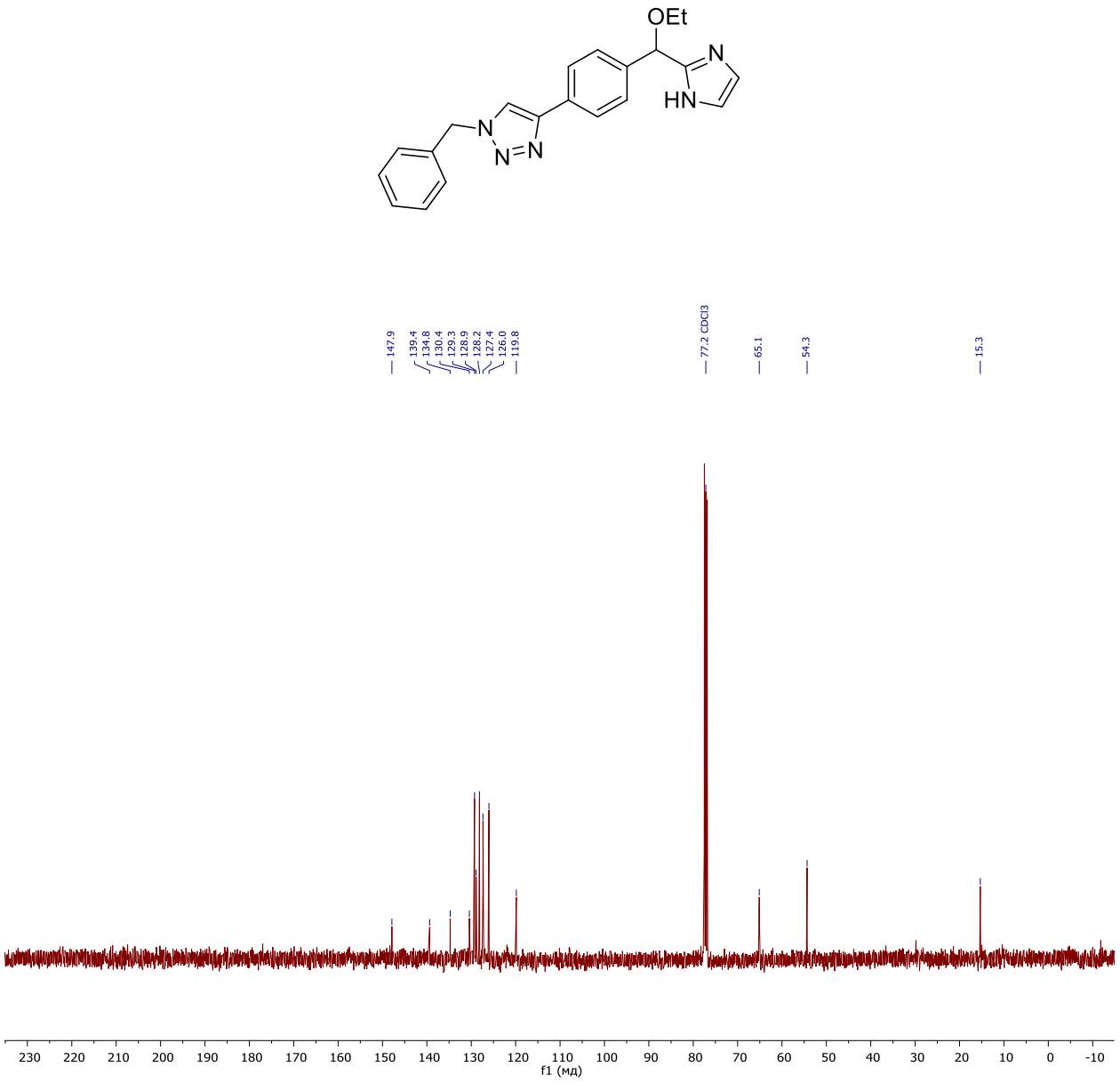


Figure S111. ^{13}C NMR (101 MHz, Chloroform-*d*) spectrum of compound **4z.**

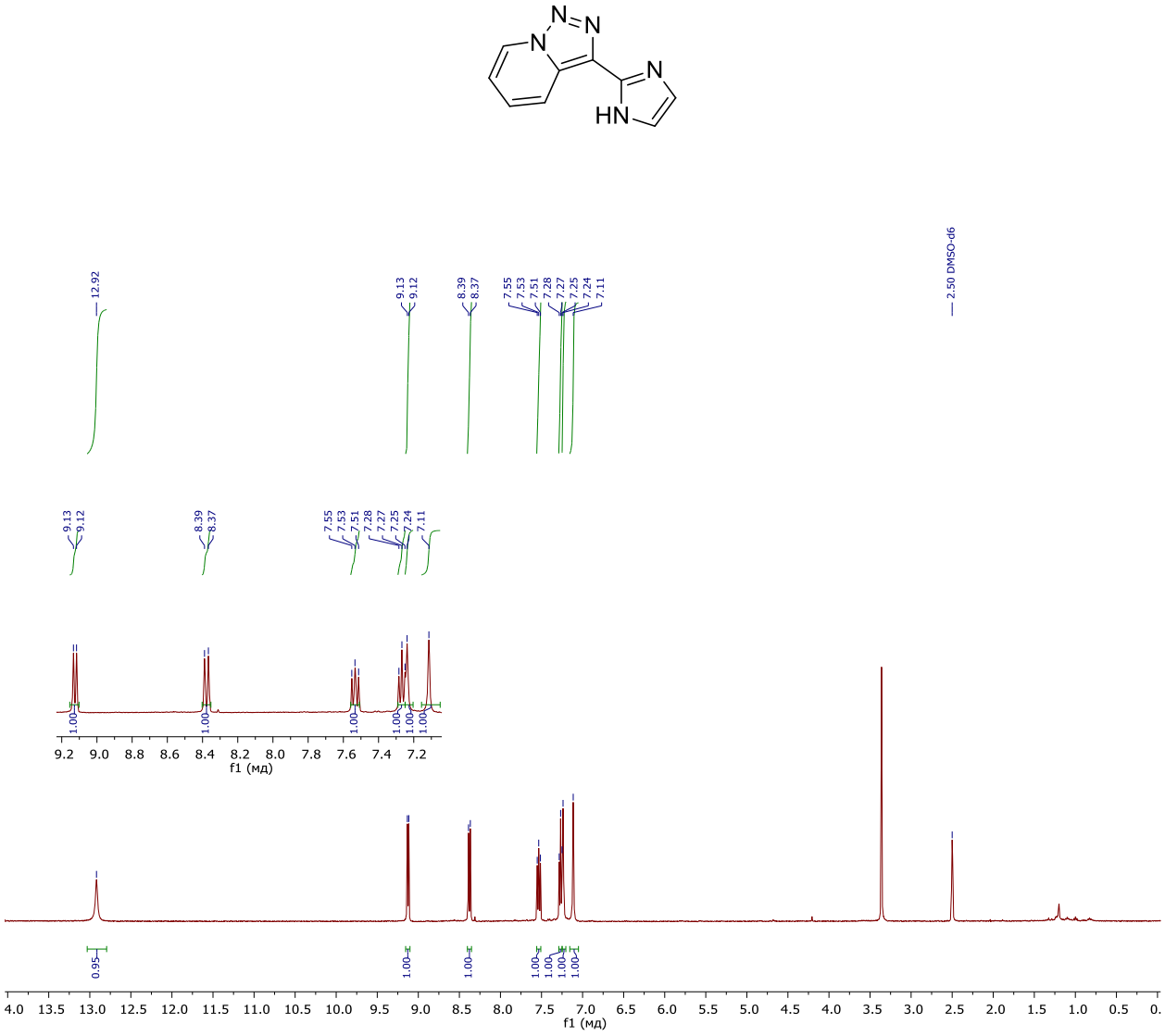


Figure S112. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **5a.**

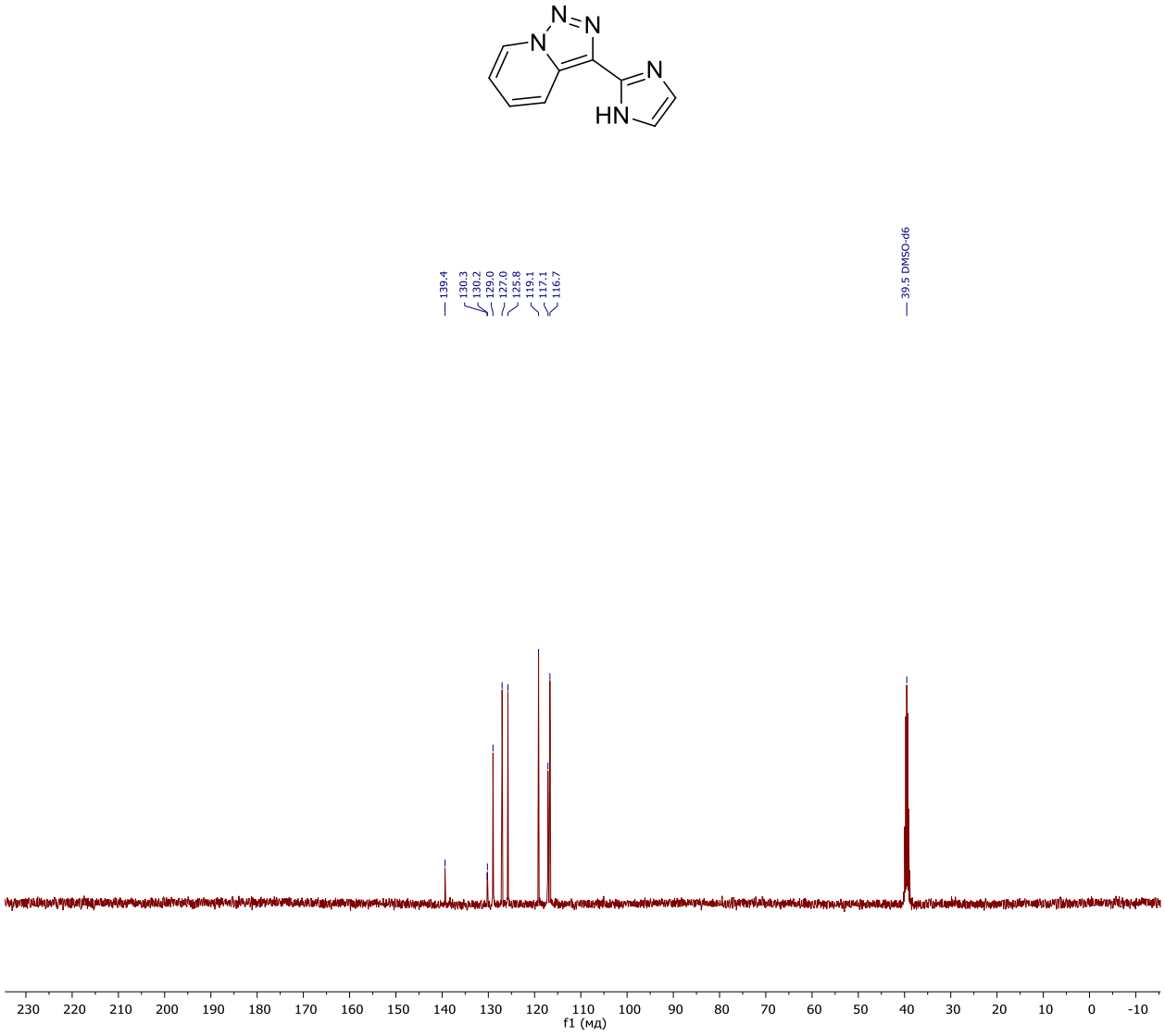


Figure S113. ^{13}C NMR (101 MHz, DMSO-d_6) spectrum of compound **5a.**