

Supporting Information

The Ugi Reaction in the Synthesis of Pyrrolo[3,4-*c*]pyridine Derivatives

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^1H , ^{13}C NMR spectra

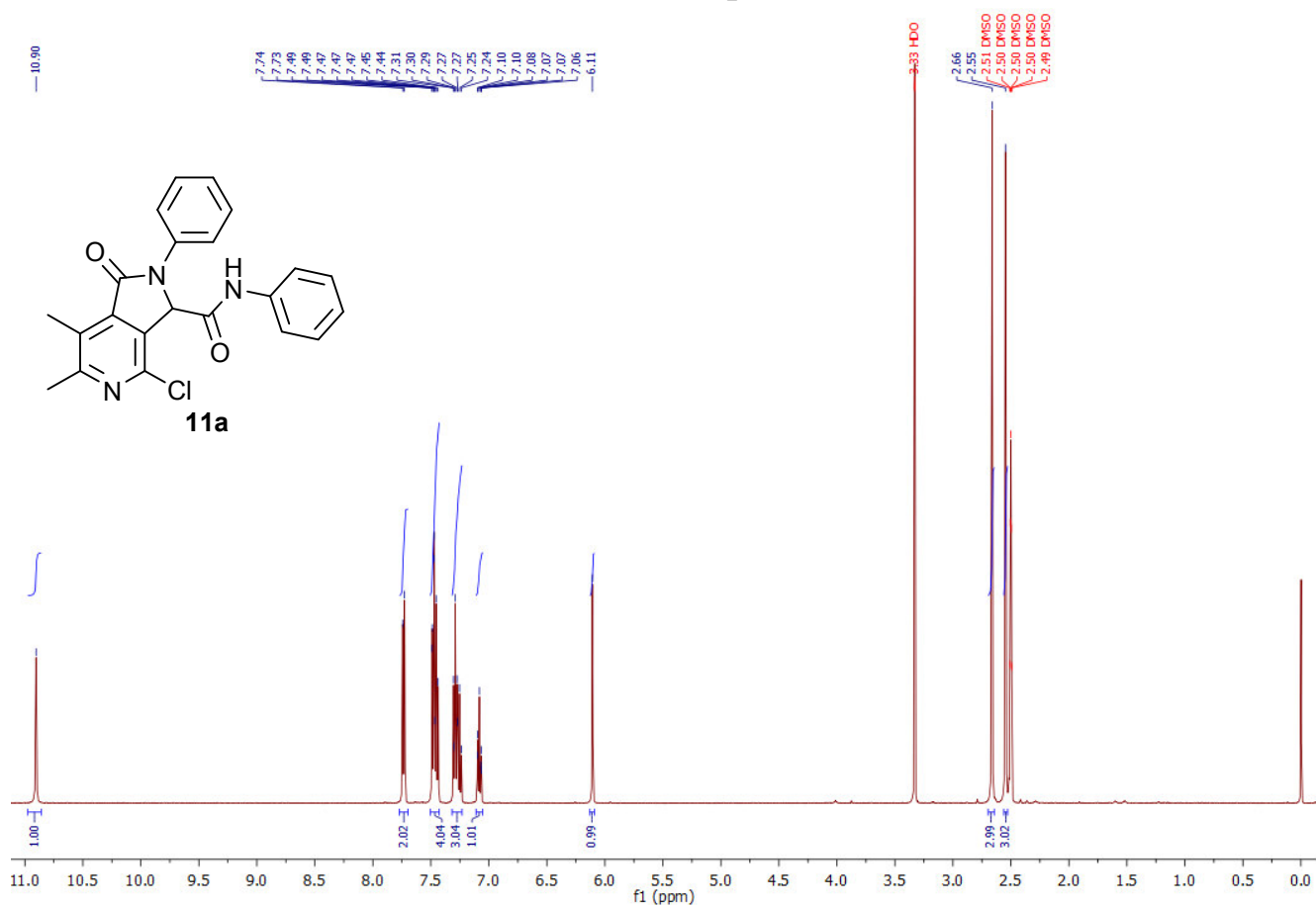


Fig. 1. ^1H -NMR-spectrum of **11a** (500 MHz, $\text{DMSO}-d_6$)

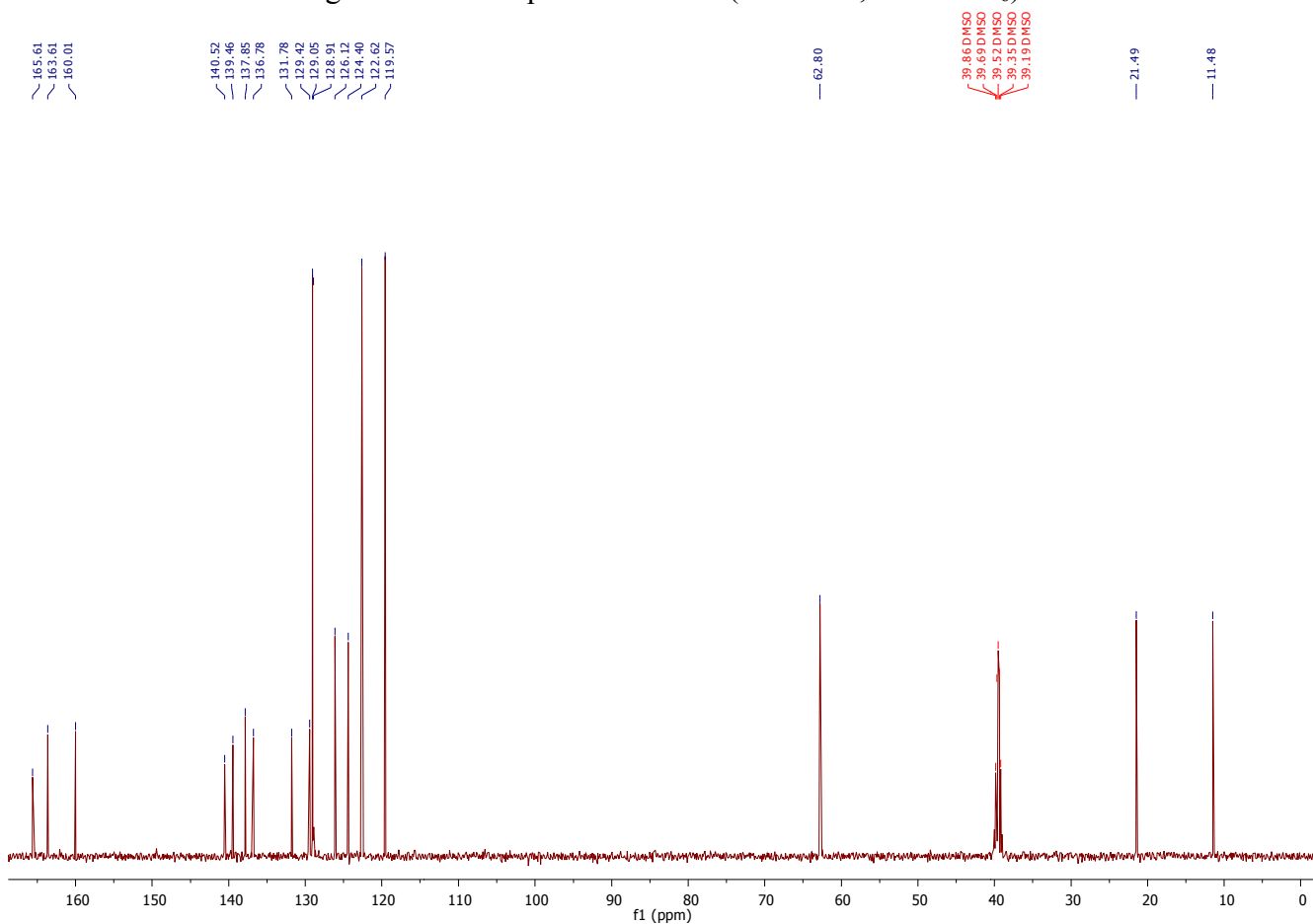


Fig. 2. ^{13}C -NMR-spectrum of **11a** (126 MHz, $\text{DMSO}-d_6$)

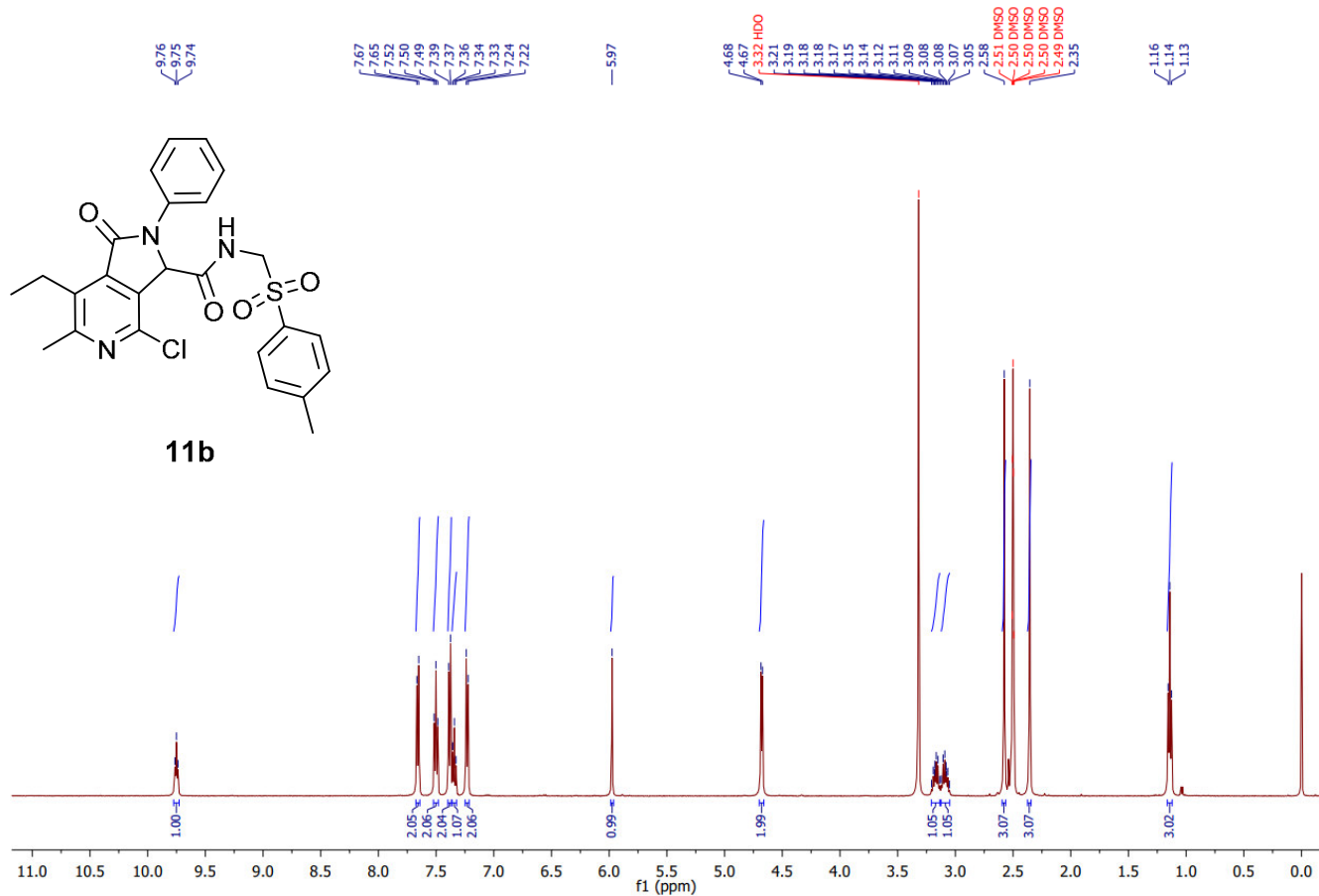


Fig. 3. ¹H-NMR-spectrum of **11b** (500 MHz, DMSO-*d*₆)

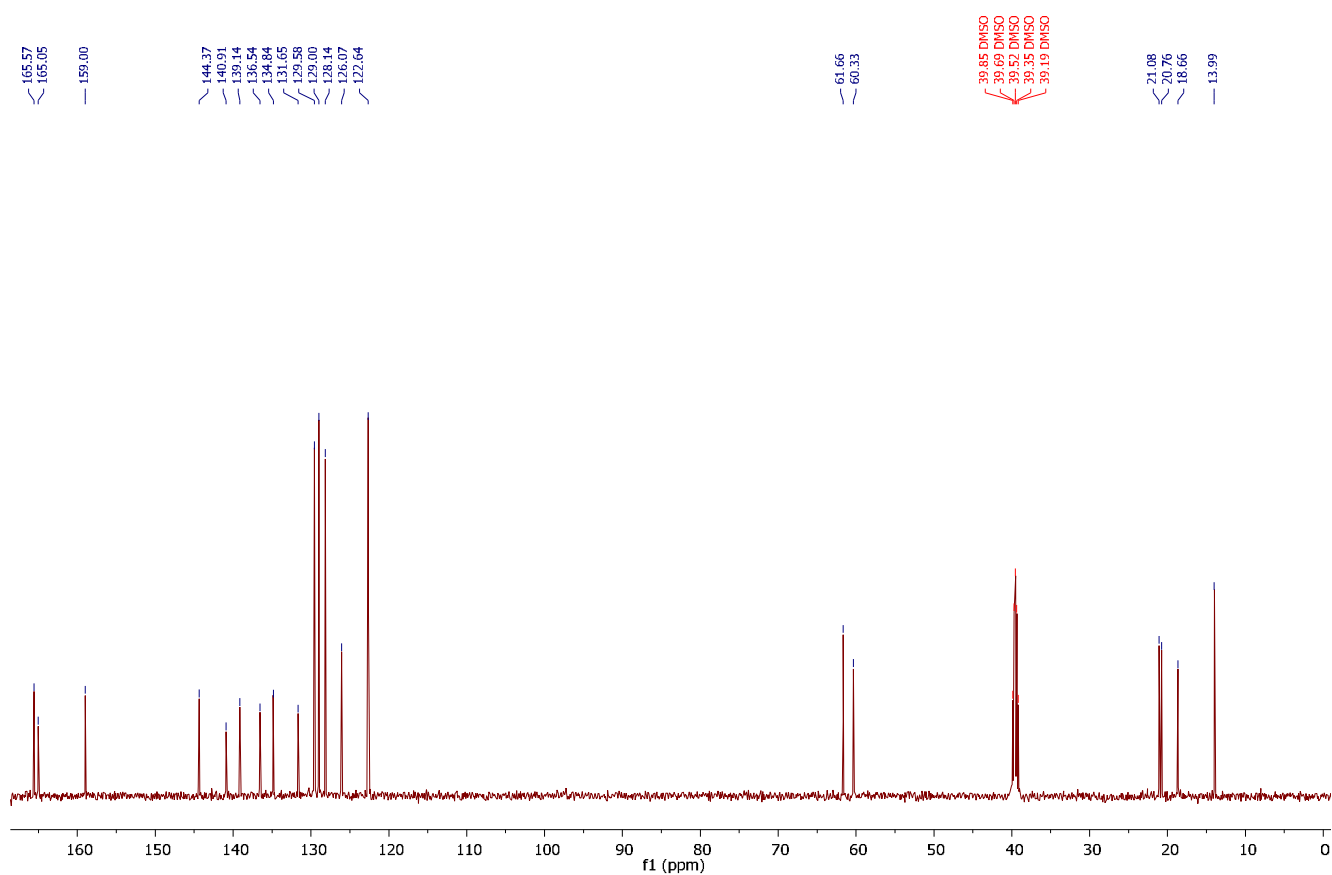


Fig. 4. ¹³C-NMR-spectrum of **11b** (126 MHz, DMSO-*d*₆)

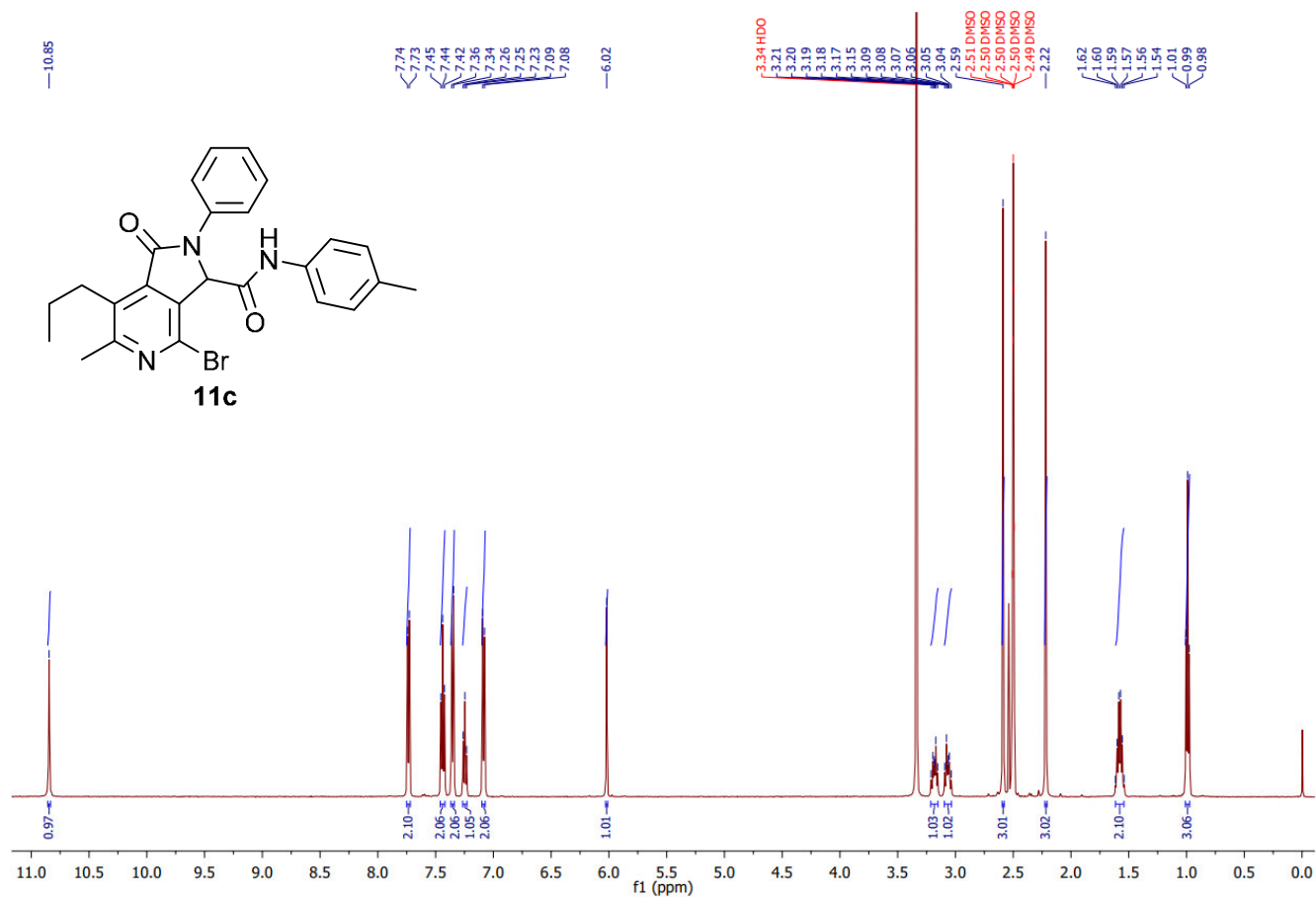


Fig. 5. ¹H-NMR-spectrum of **11c** (500 MHz, DMSO-*d*₆)

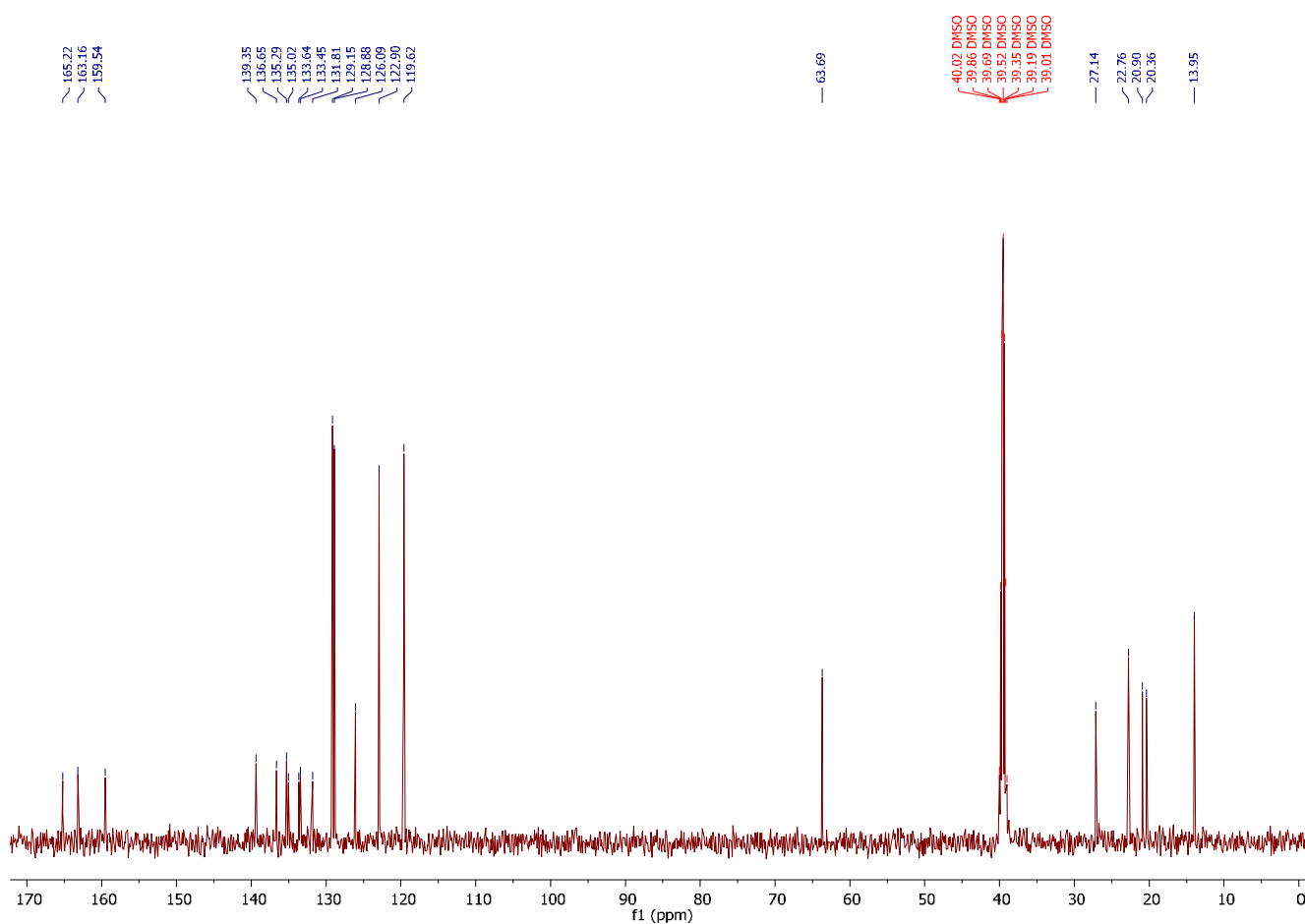


Fig. 6. ¹³C-NMR-spectrum of **11c** (126 MHz, DMSO-*d*₆)

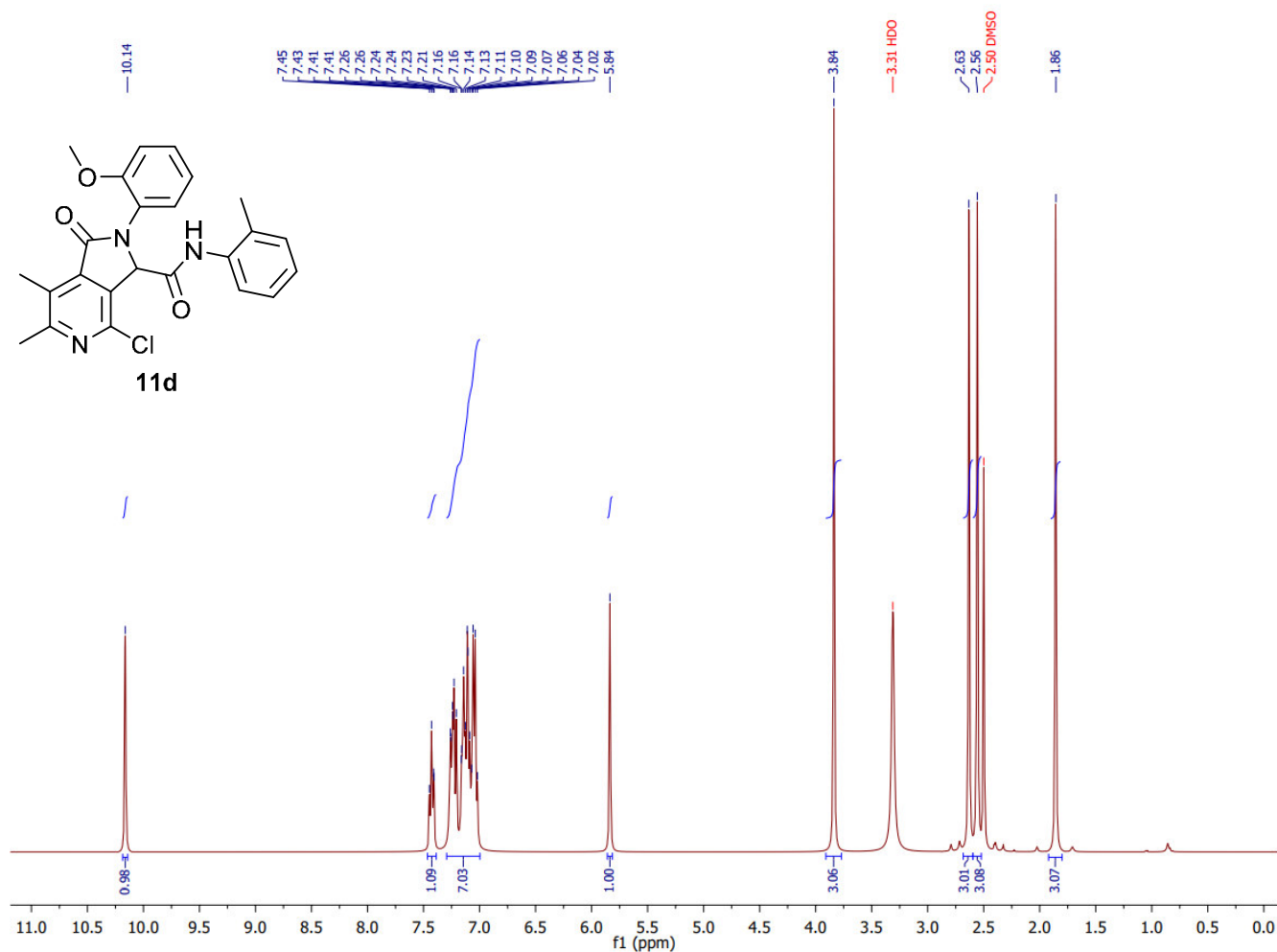


Fig. 7. ¹H-NMR-spectrum of **11d** (400 MHz, DMSO-*d*₆)

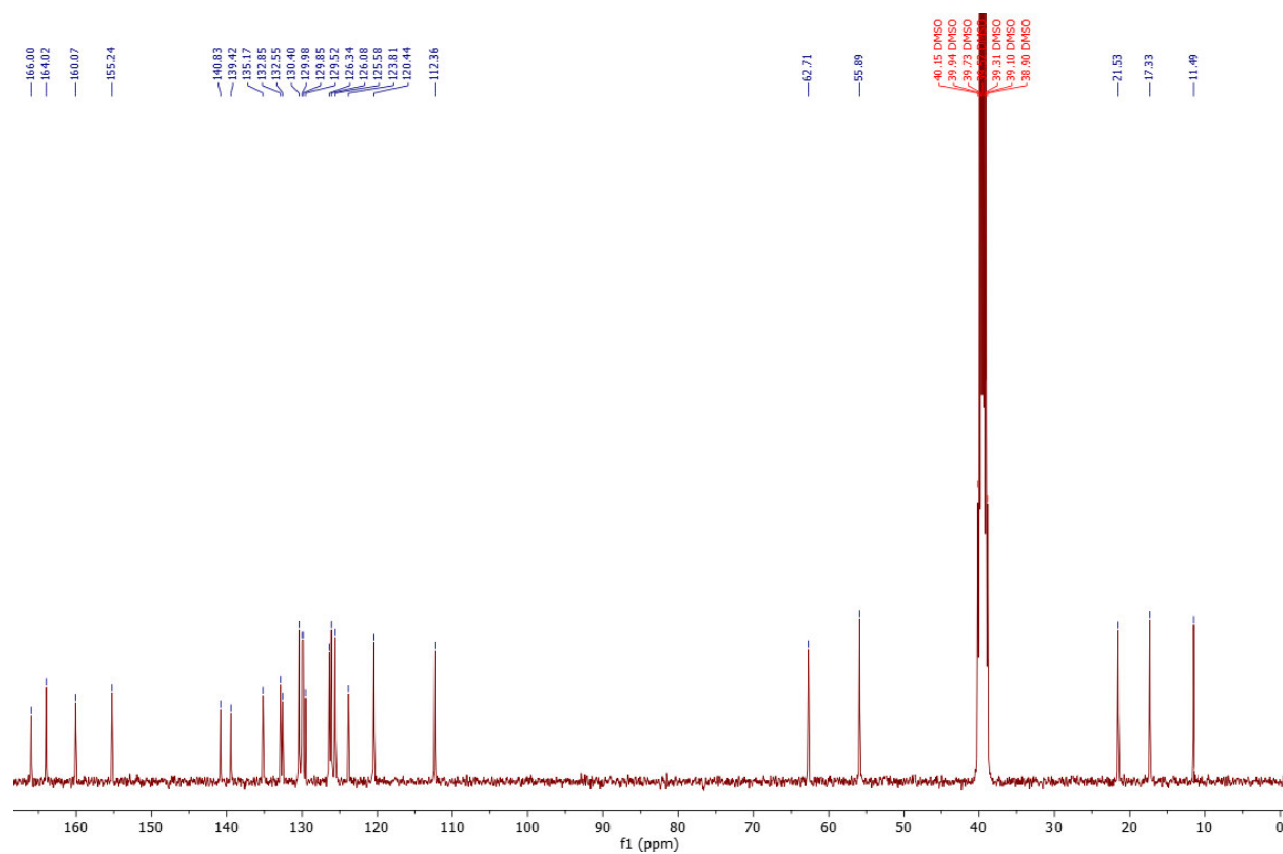


Fig. 8. ¹³C-NMR-spectrum of **11d** (101 MHz, DMSO-*d*₆)

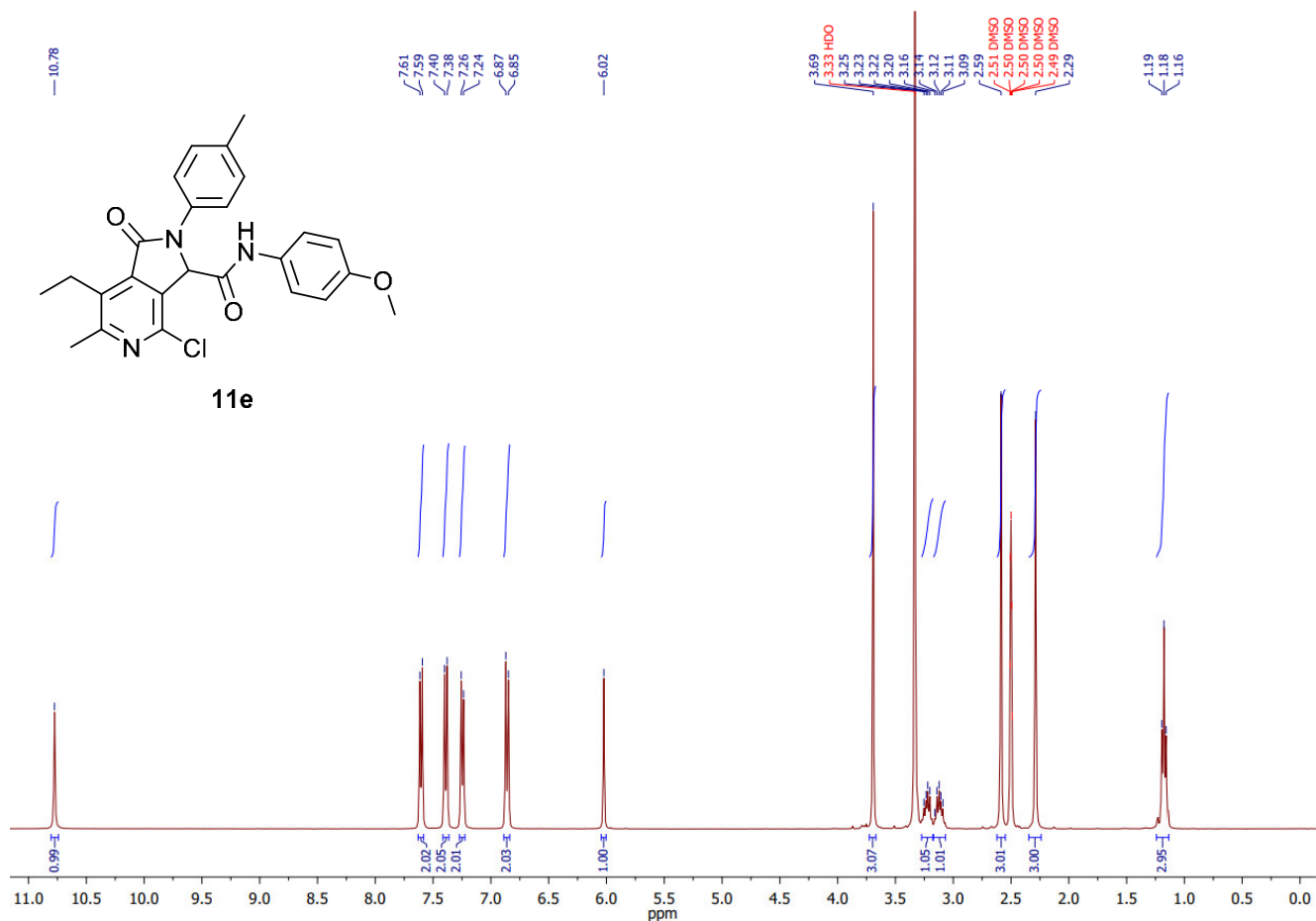


Fig. 9. ^1H -NMR-spectrum of **11e** (400 MHz, $\text{DMSO}-d_6$)

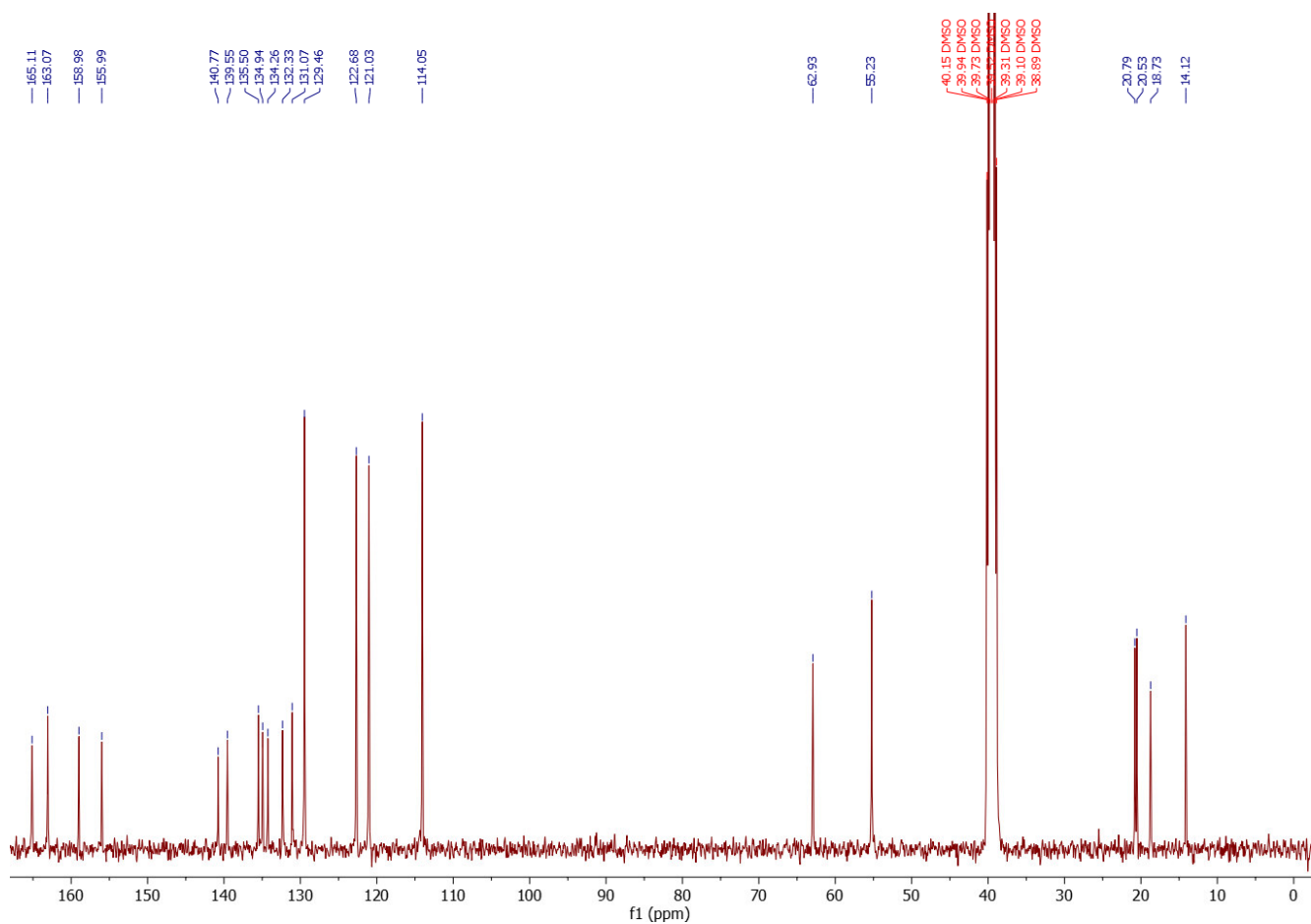


Fig. 10. ^{13}C -NMR-spectrum of **11e** (101 MHz, $\text{DMSO}-d_6$)

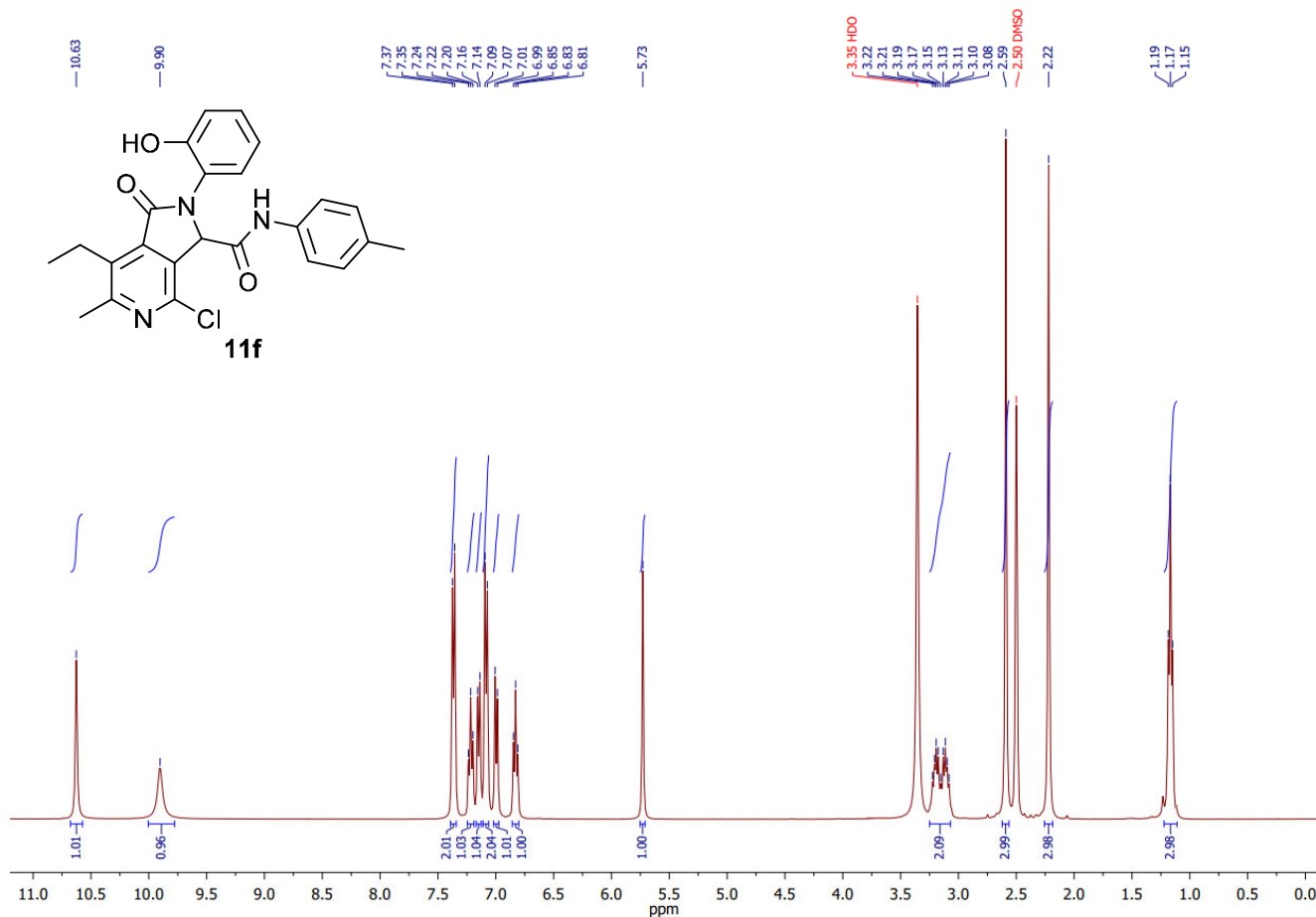


Fig. 11. ¹H-NMR-spectrum of **11f** (400 MHz, DMSO-*d*₆)

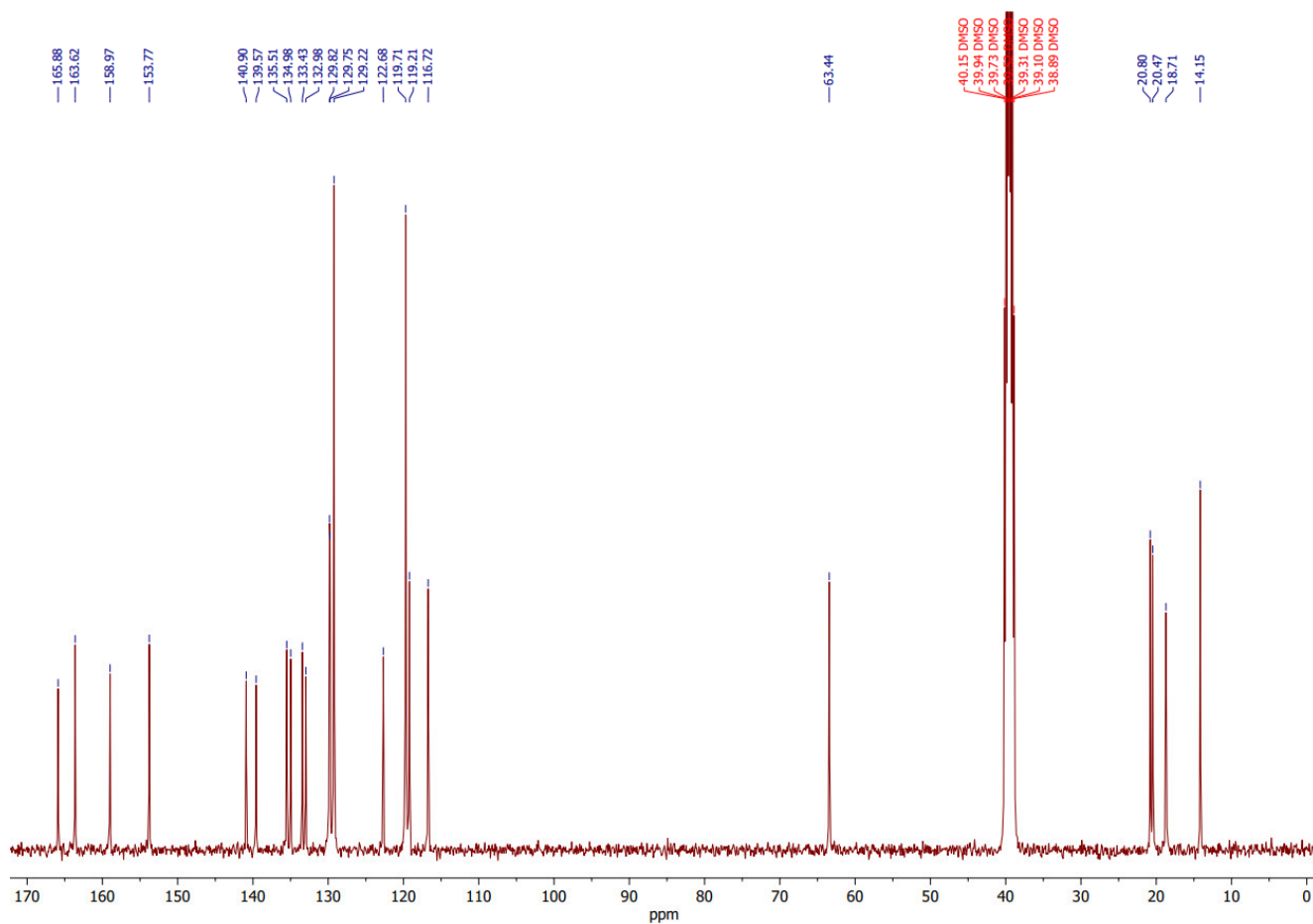


Fig. 12. ¹³C-NMR-spectrum of **11f** (101 MHz, DMSO-*d*₆)

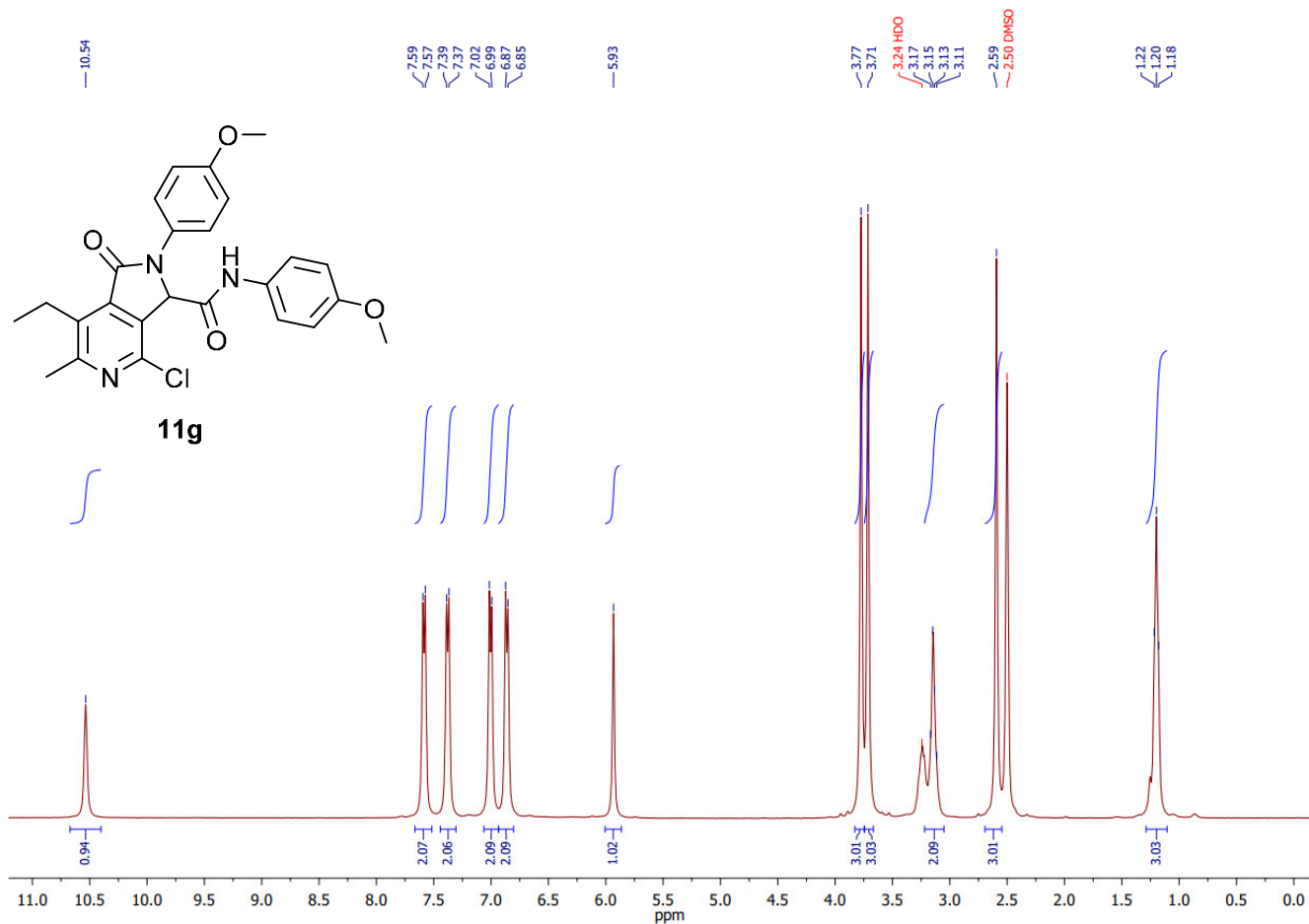


Fig. 13. ¹H-NMR-spectrum of **11g** (400 MHz, DMSO-*d*₆)

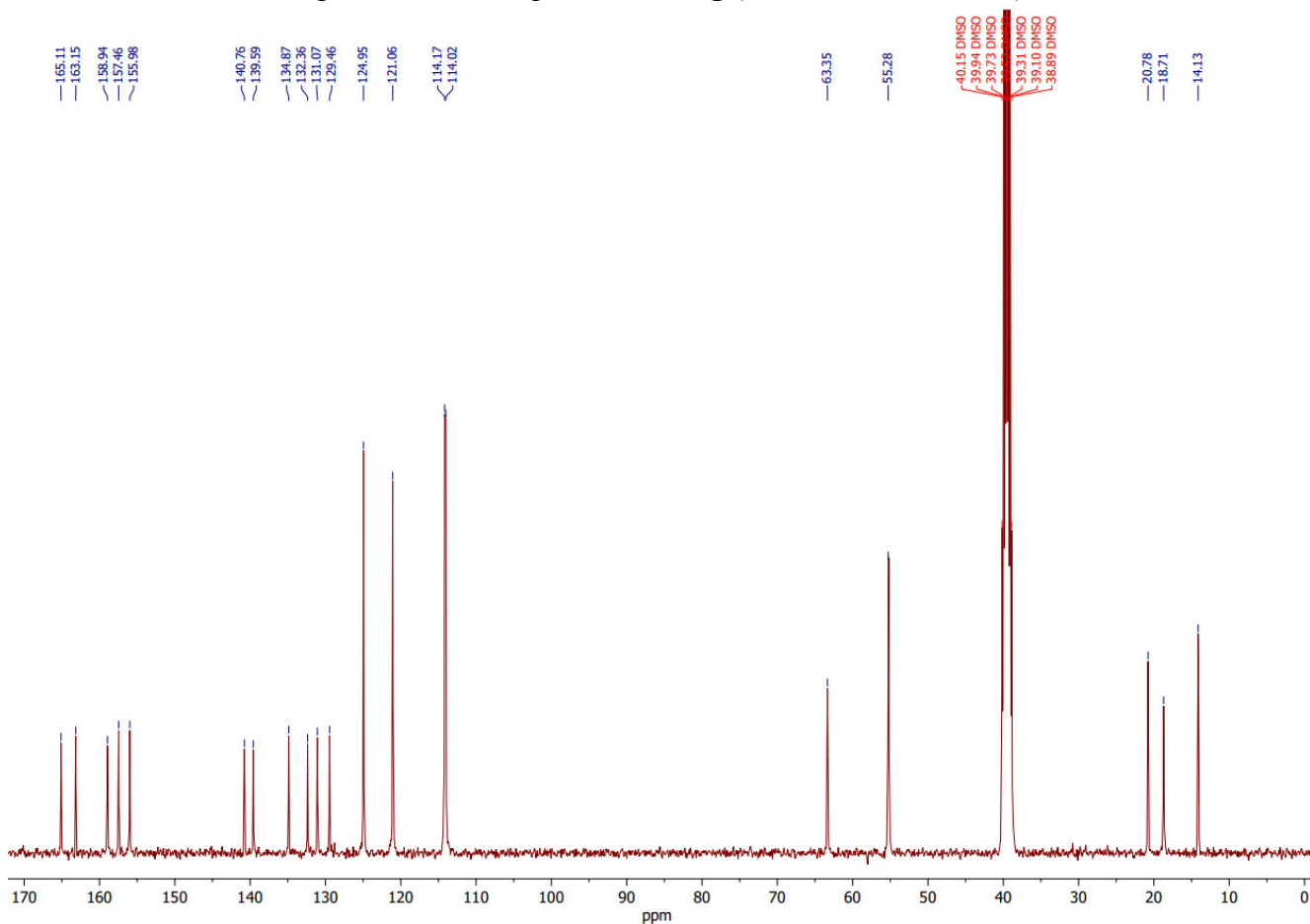


Fig. 14. ¹³C-NMR-spectrum of **11g** (101 MHz, DMSO-*d*₆)

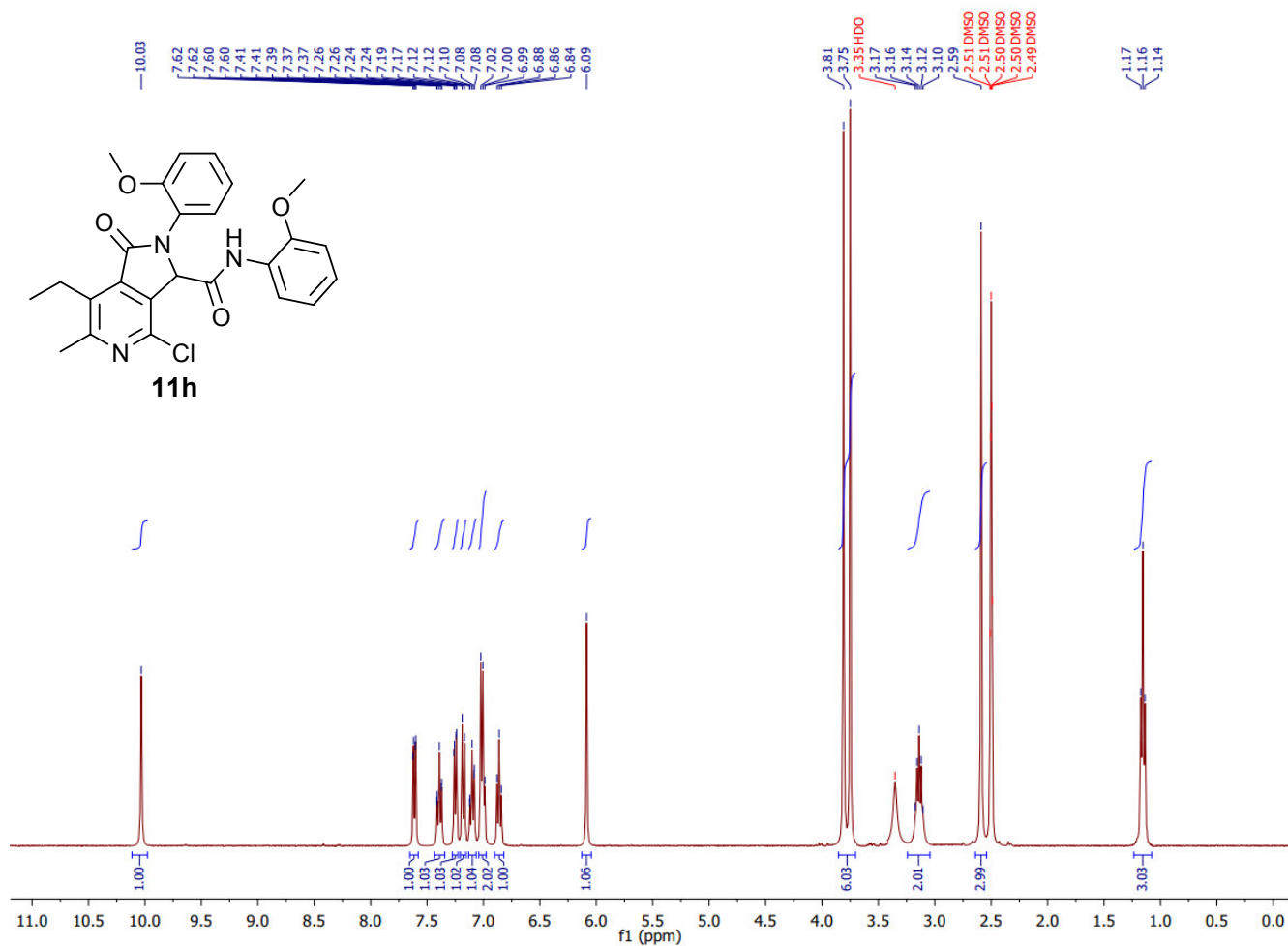


Fig. 15. ¹H-NMR-spectrum of **11h** (400 MHz, DMSO-*d*₆)

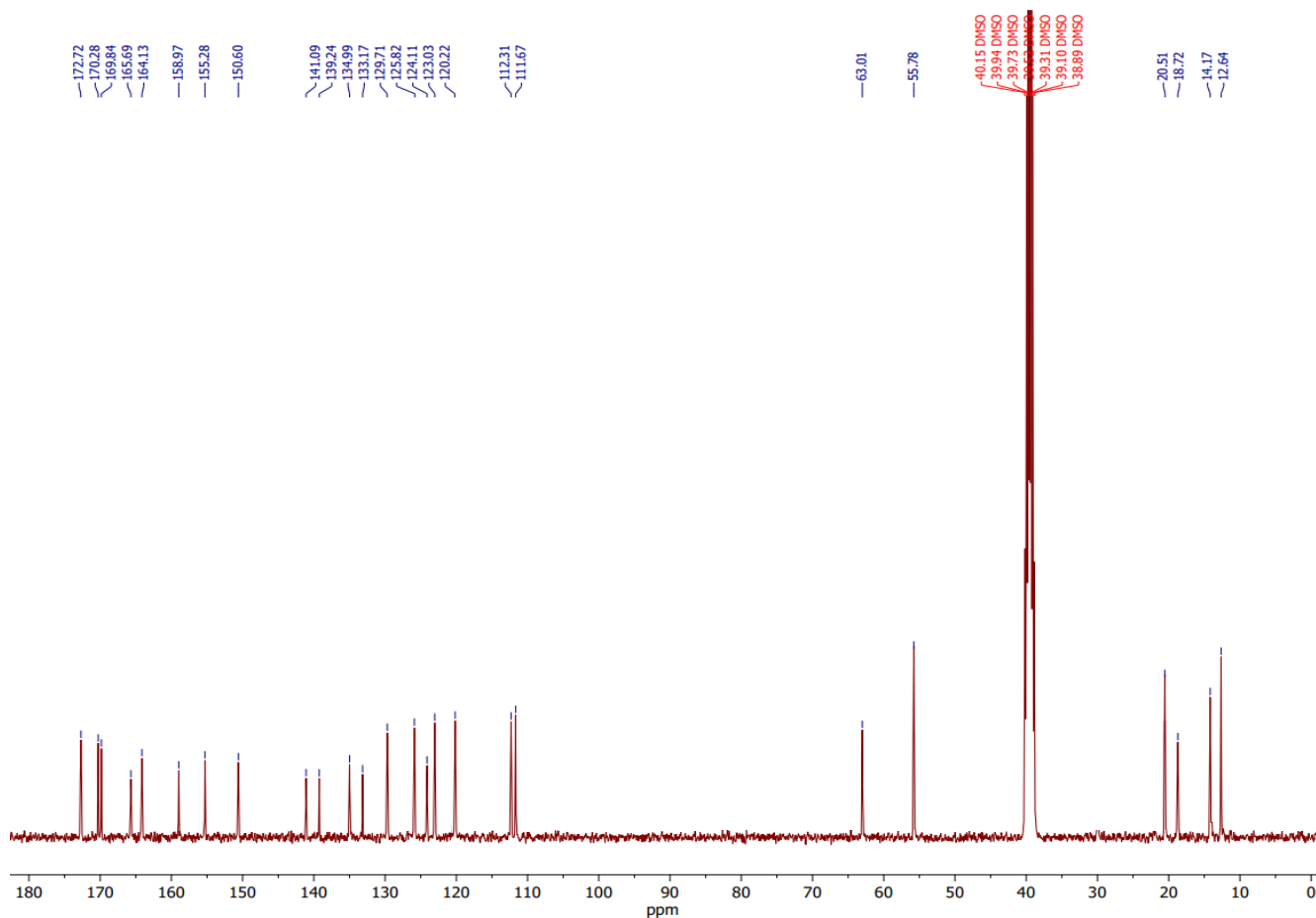


Fig. 16. ¹³C-NMR-spectrum of **11h** (101 MHz, DMSO-*d*₆)

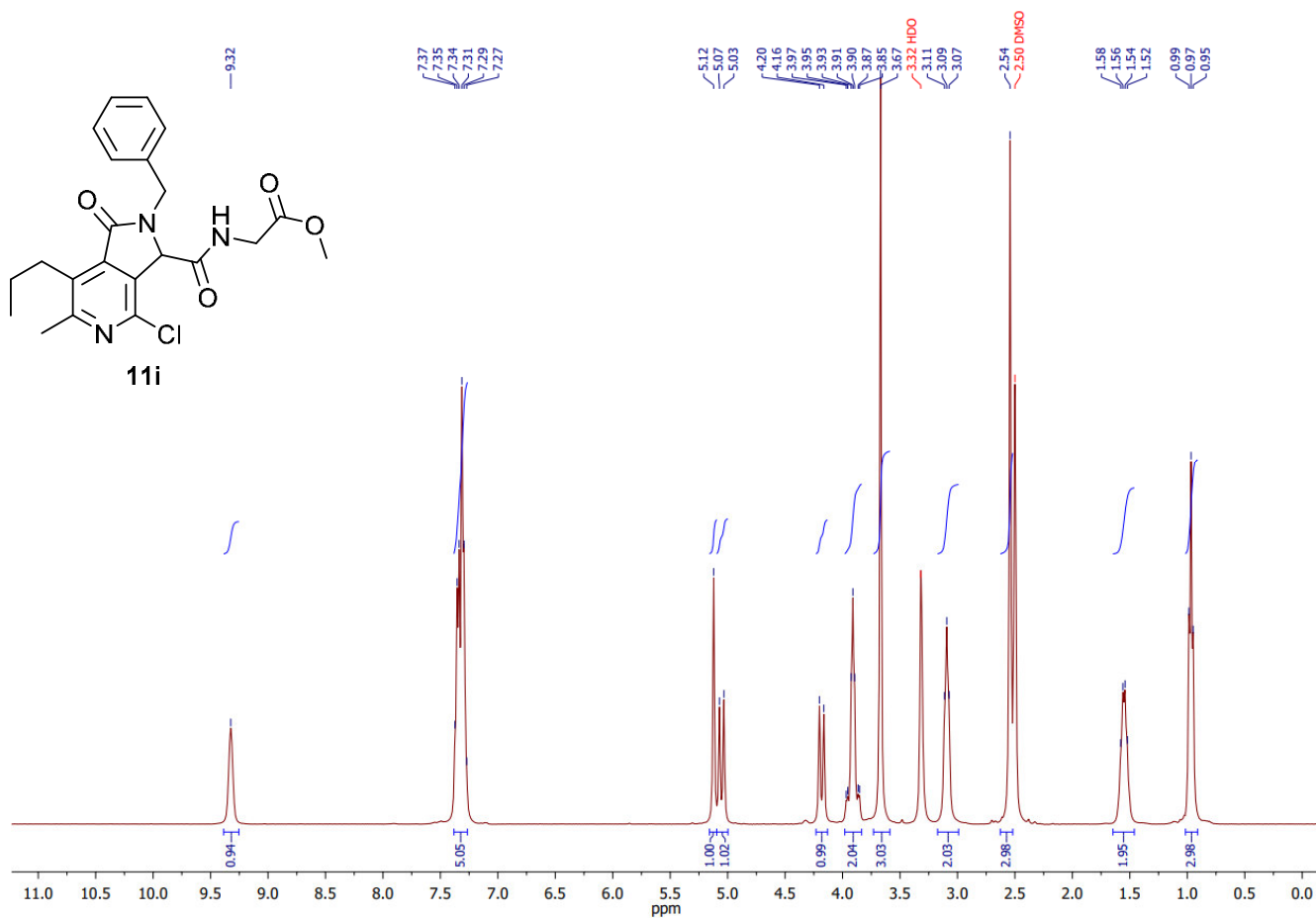


Fig. 17. ^1H -NMR-spectrum of **11i** (400 MHz, $\text{DMSO}-d_6$)

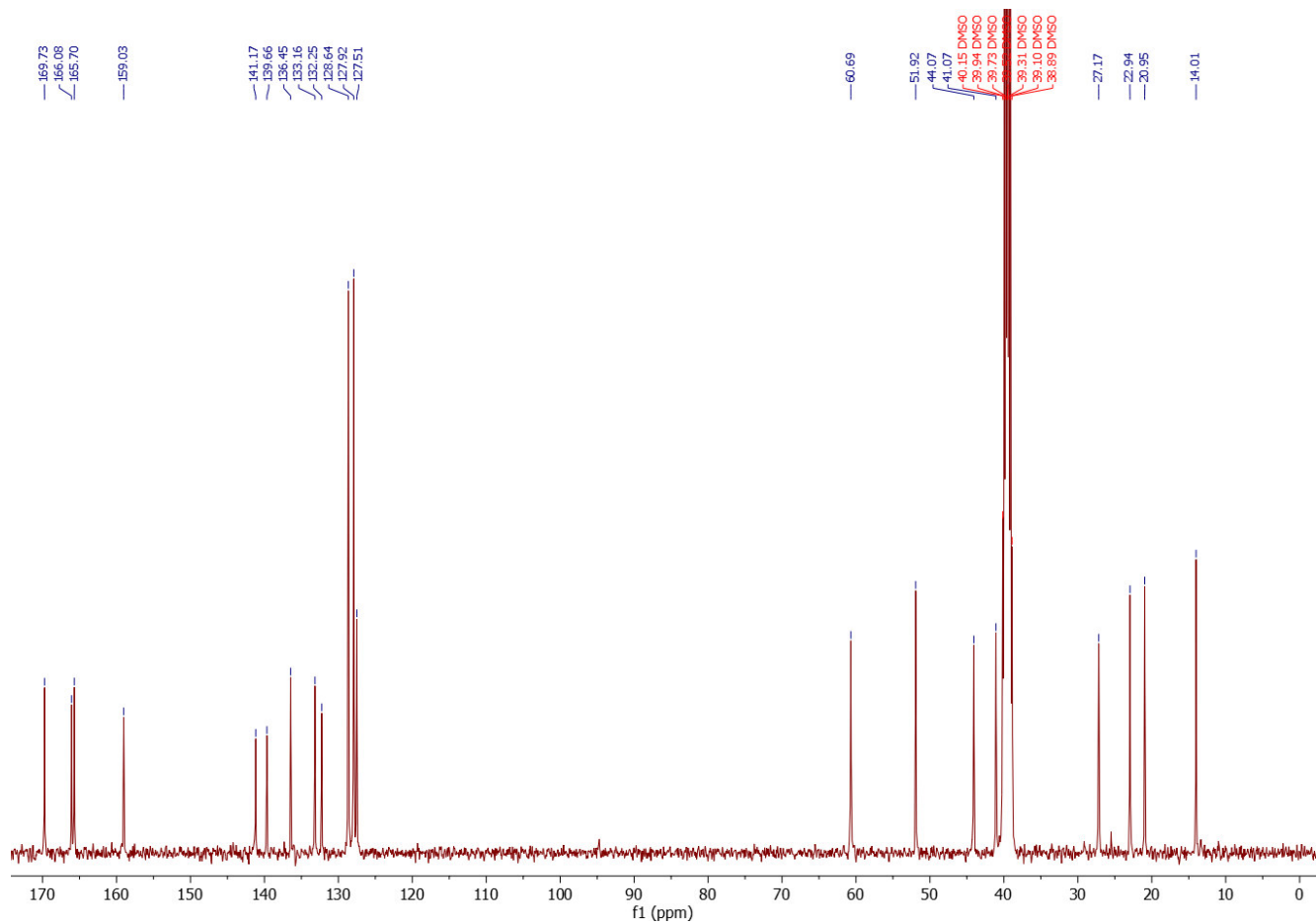


Fig. 18. ^{13}C -NMR-spectrum of **11i** (101 MHz, $\text{DMSO}-d_6$)

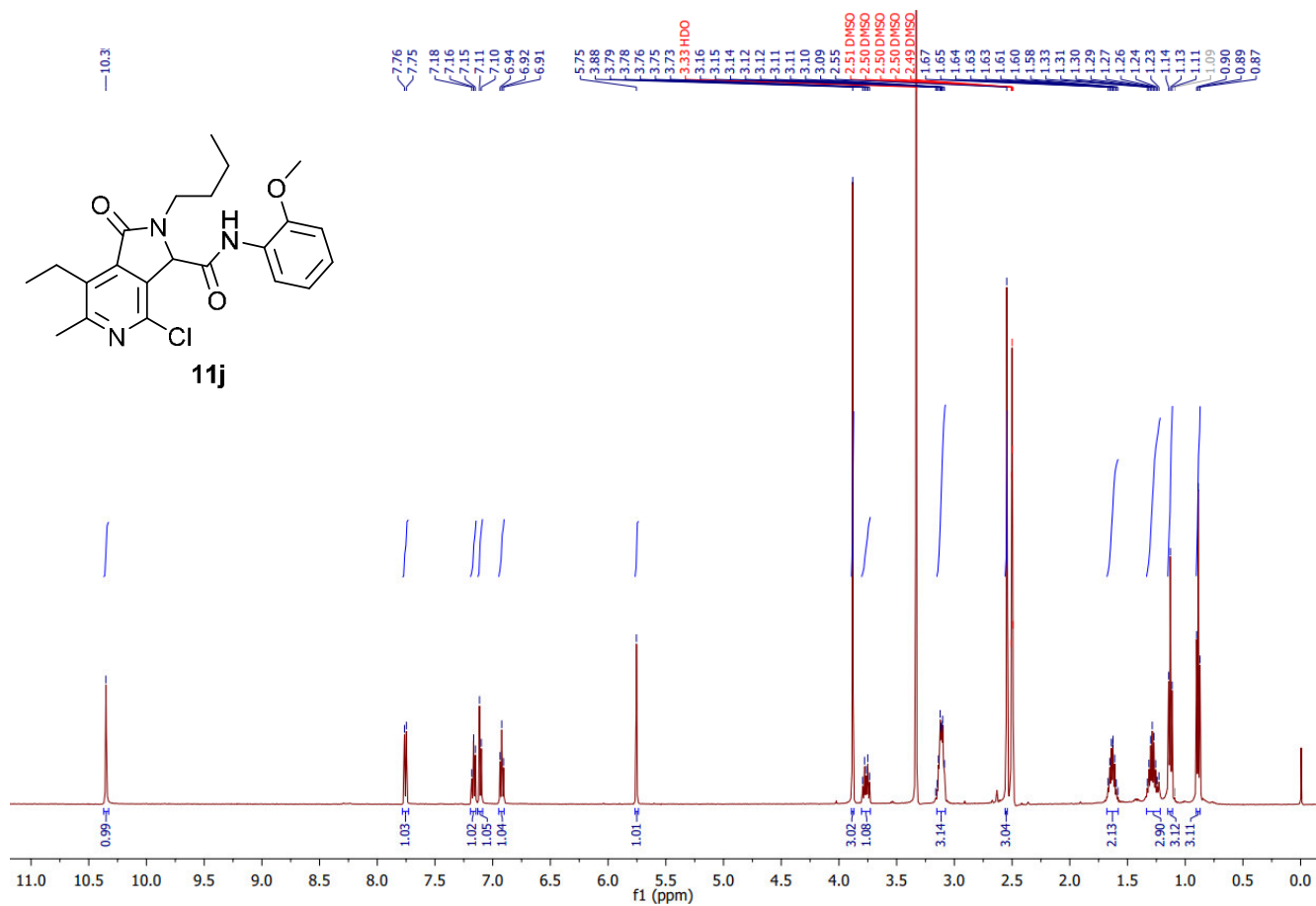


Fig. 19. ¹H-NMR-spectrum of **11j** (500 MHz, DMSO-*d*₆)

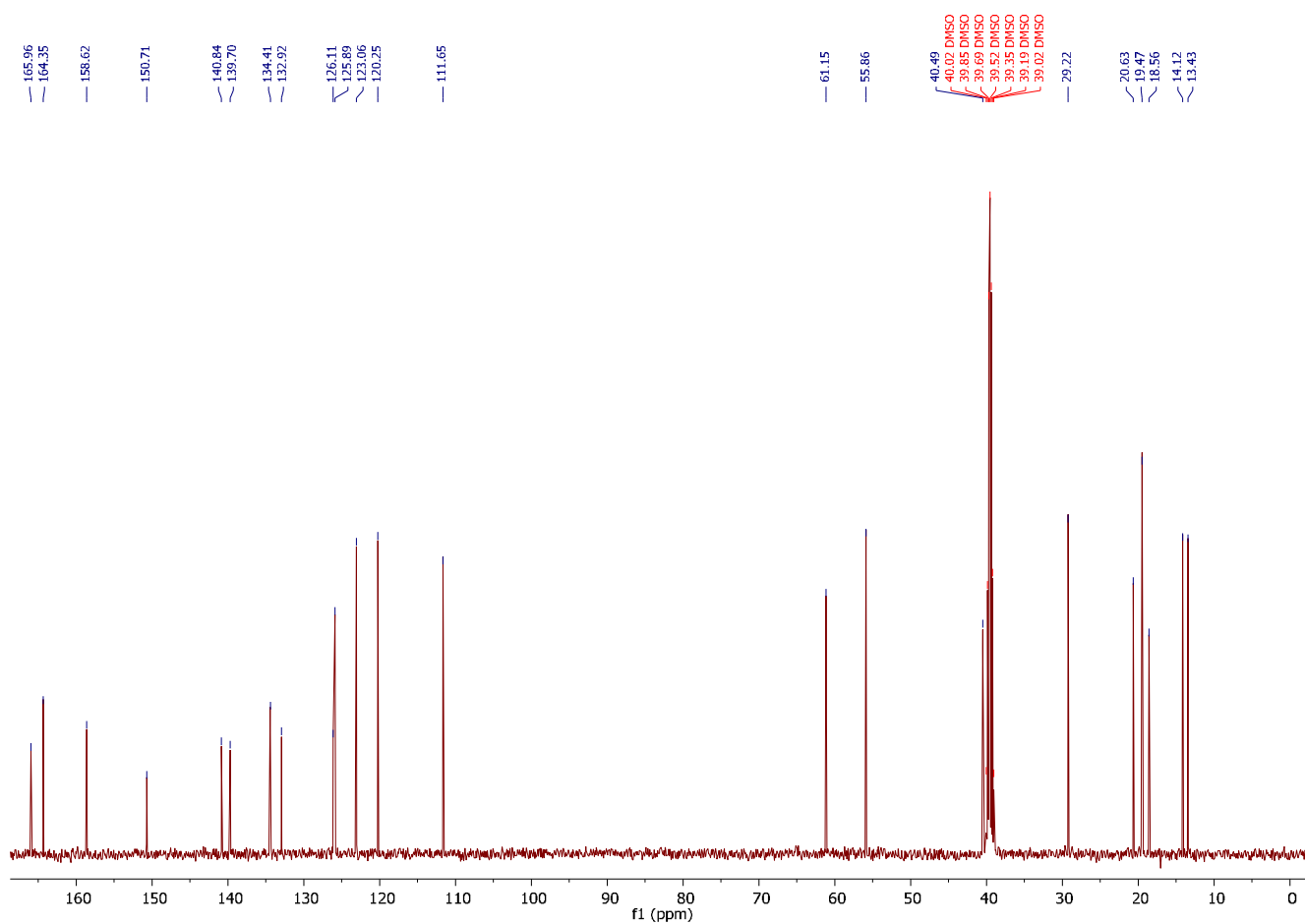


Fig. 20. ¹³C-NMR-spectrum of **11j** (126 MHz, DMSO-*d*₆)

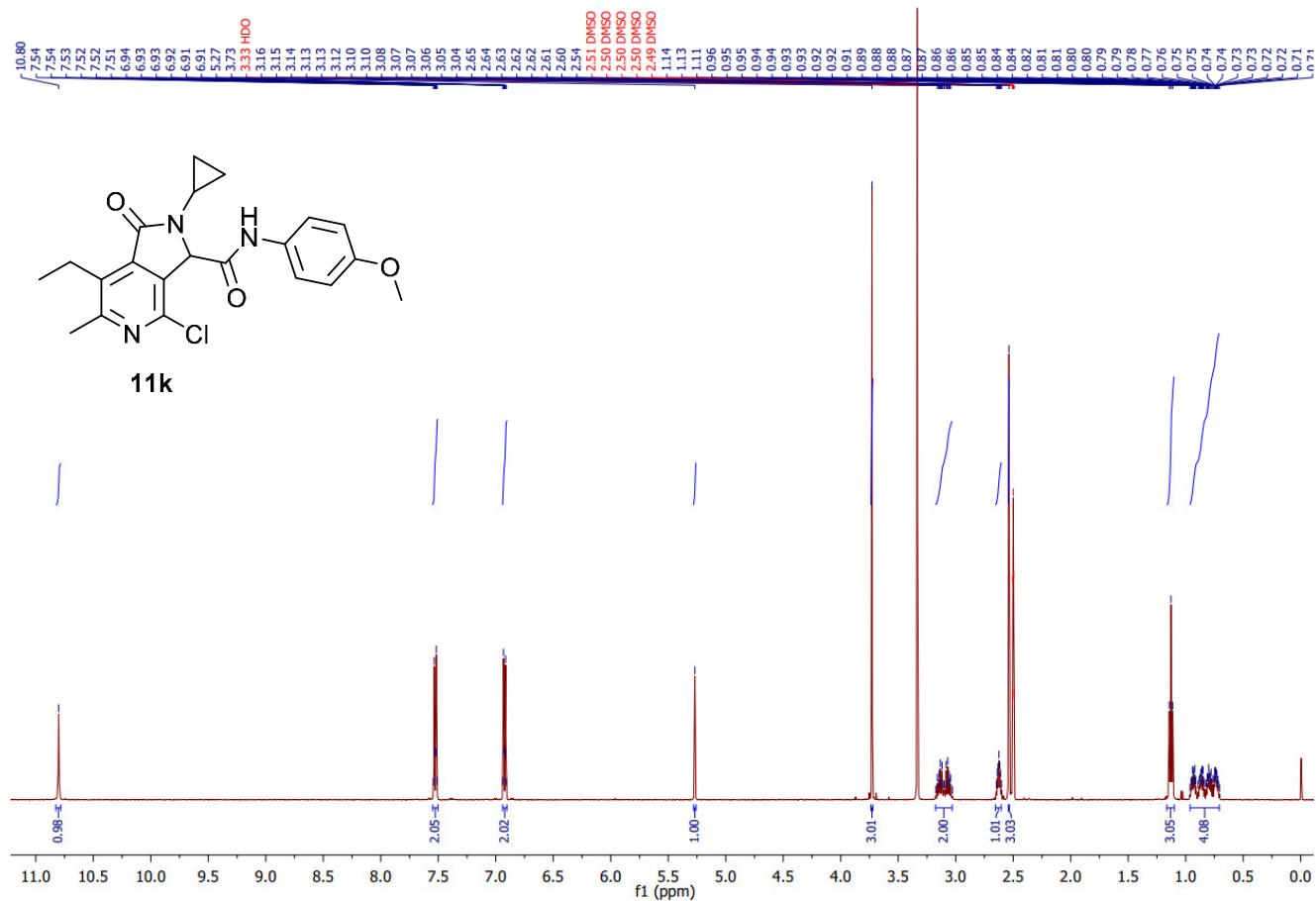


Fig. 21. ¹H-NMR-spectrum of **11k** (500 MHz, DMSO-*d*₆)

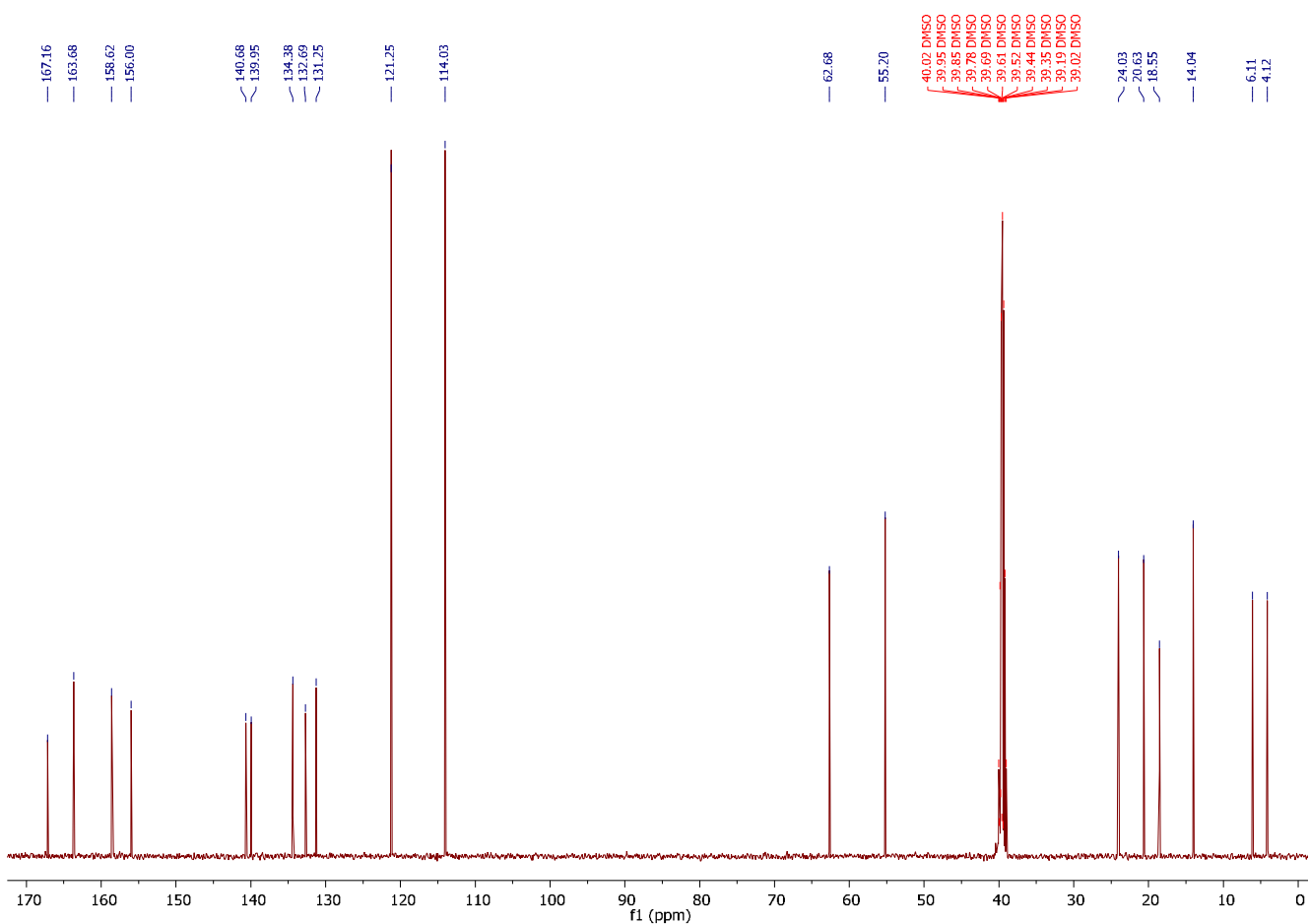


Fig. 22. ¹³C-NMR-spectrum of **11k** (126 MHz, DMSO-*d*₆)

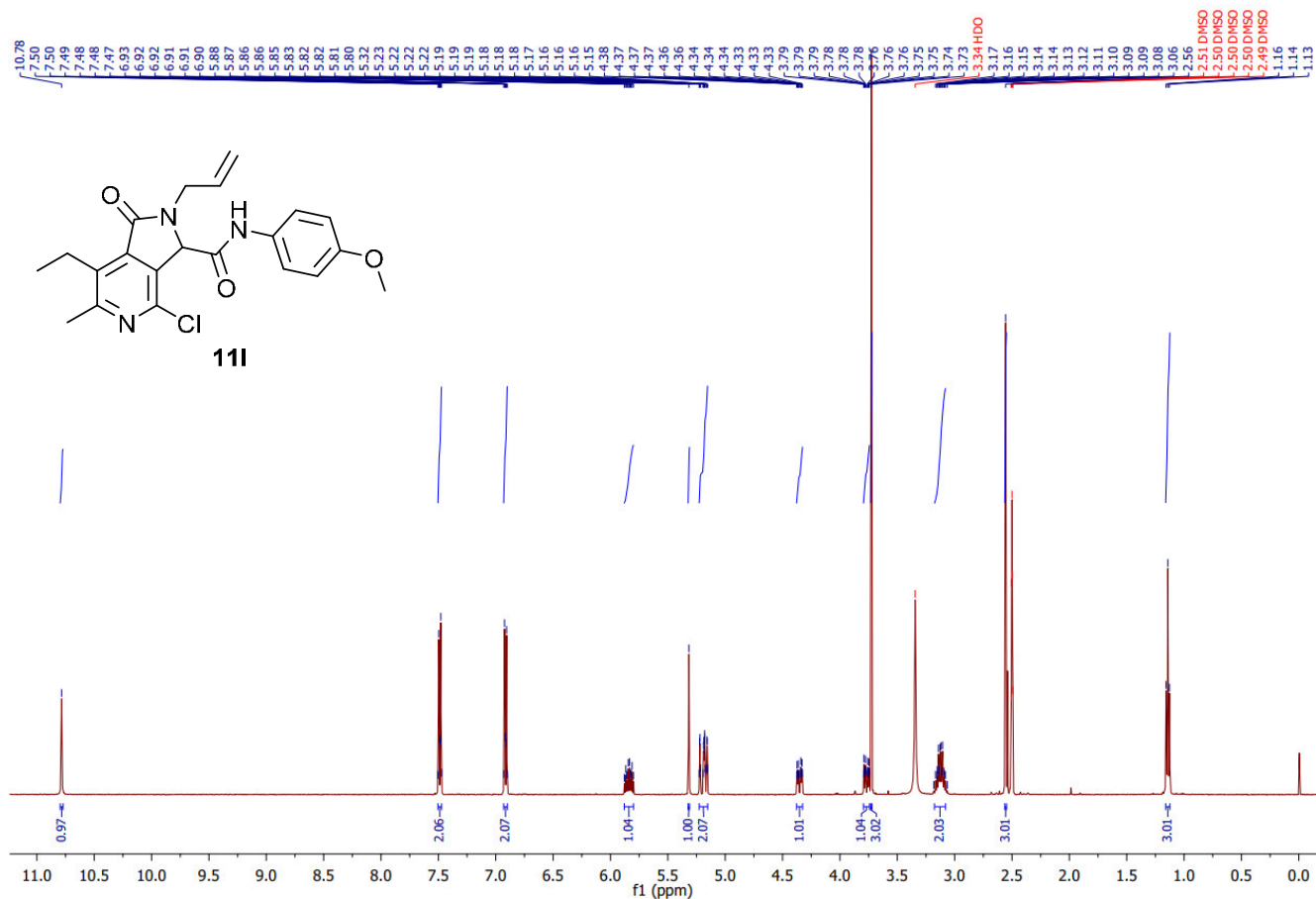


Fig. 23. ¹H-NMR-spectrum of **11l** (500 MHz, DMSO-*d*₆)

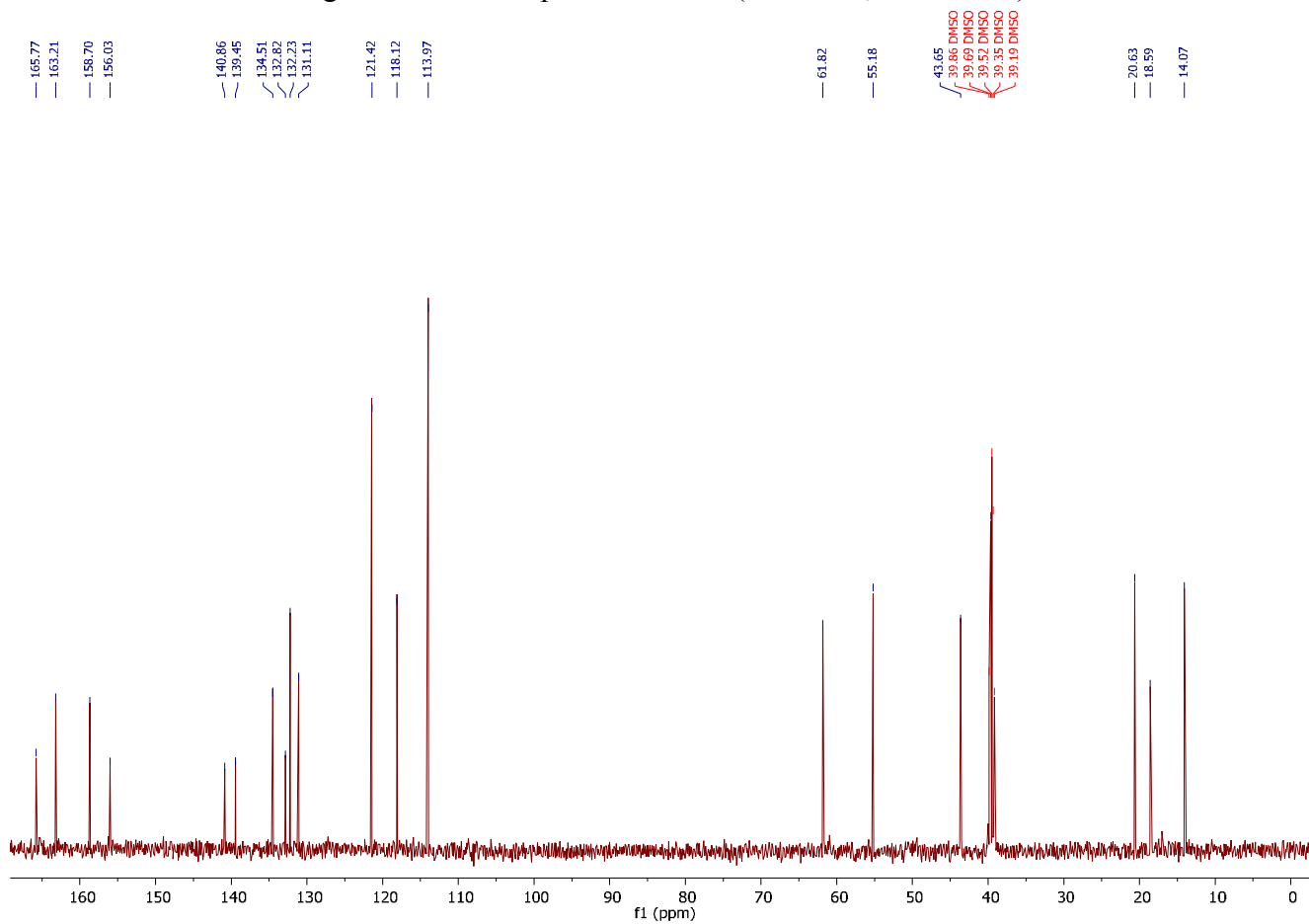


Fig. 24. ¹³C-NMR-spectrum of **11l** (126 MHz, DMSO-*d*₆)

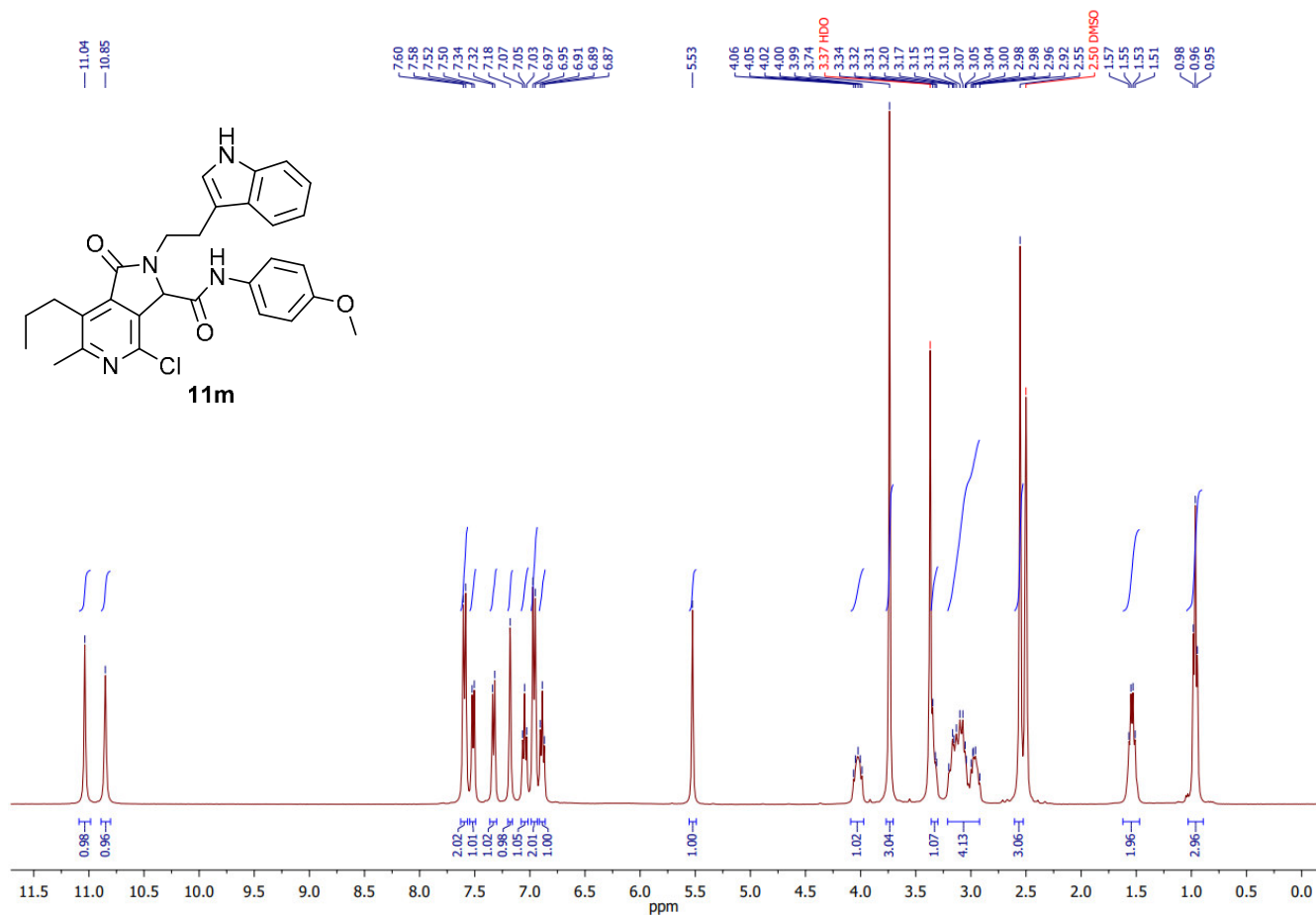


Fig. 25. ^1H -NMR-spectrum of **11m** (400 MHz, $\text{DMSO}-d_6$)

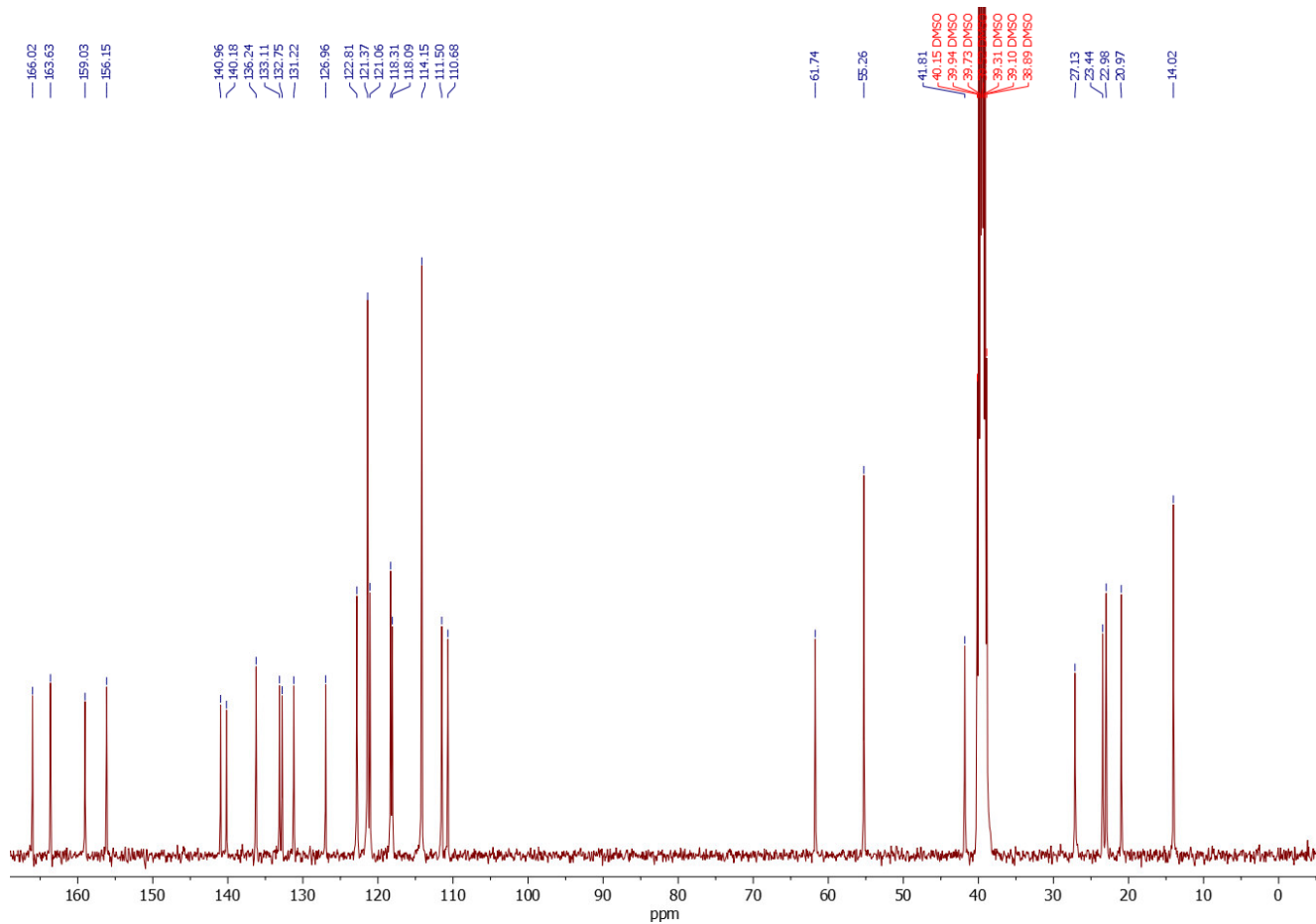


Fig. 26. ^{13}C -NMR-spectrum of **11m** (101 MHz, $\text{DMSO}-d_6$)

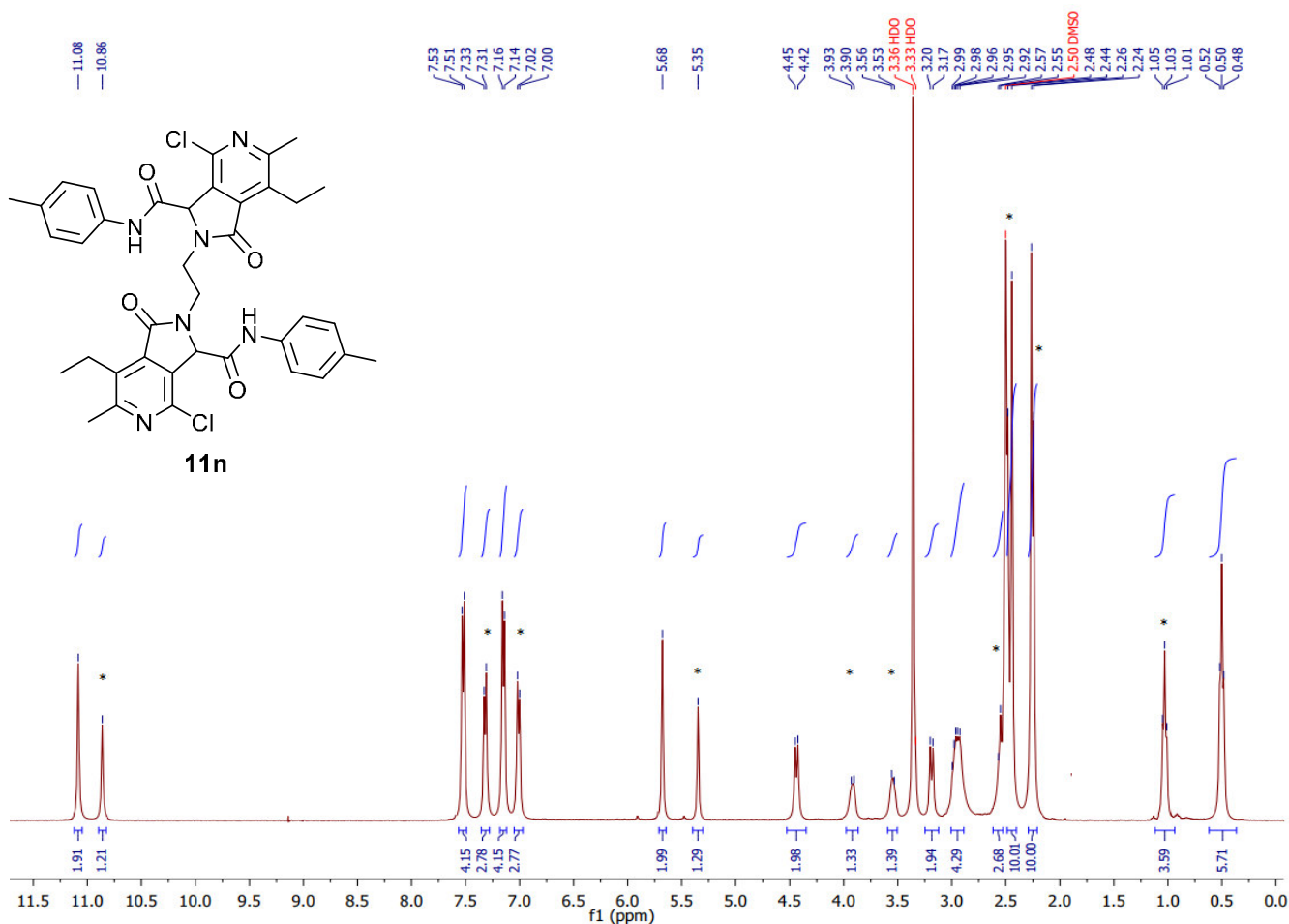


Fig. 27. ¹H-NMR-spectrum of **11n** (400 MHz, DMSO-*d*₆)

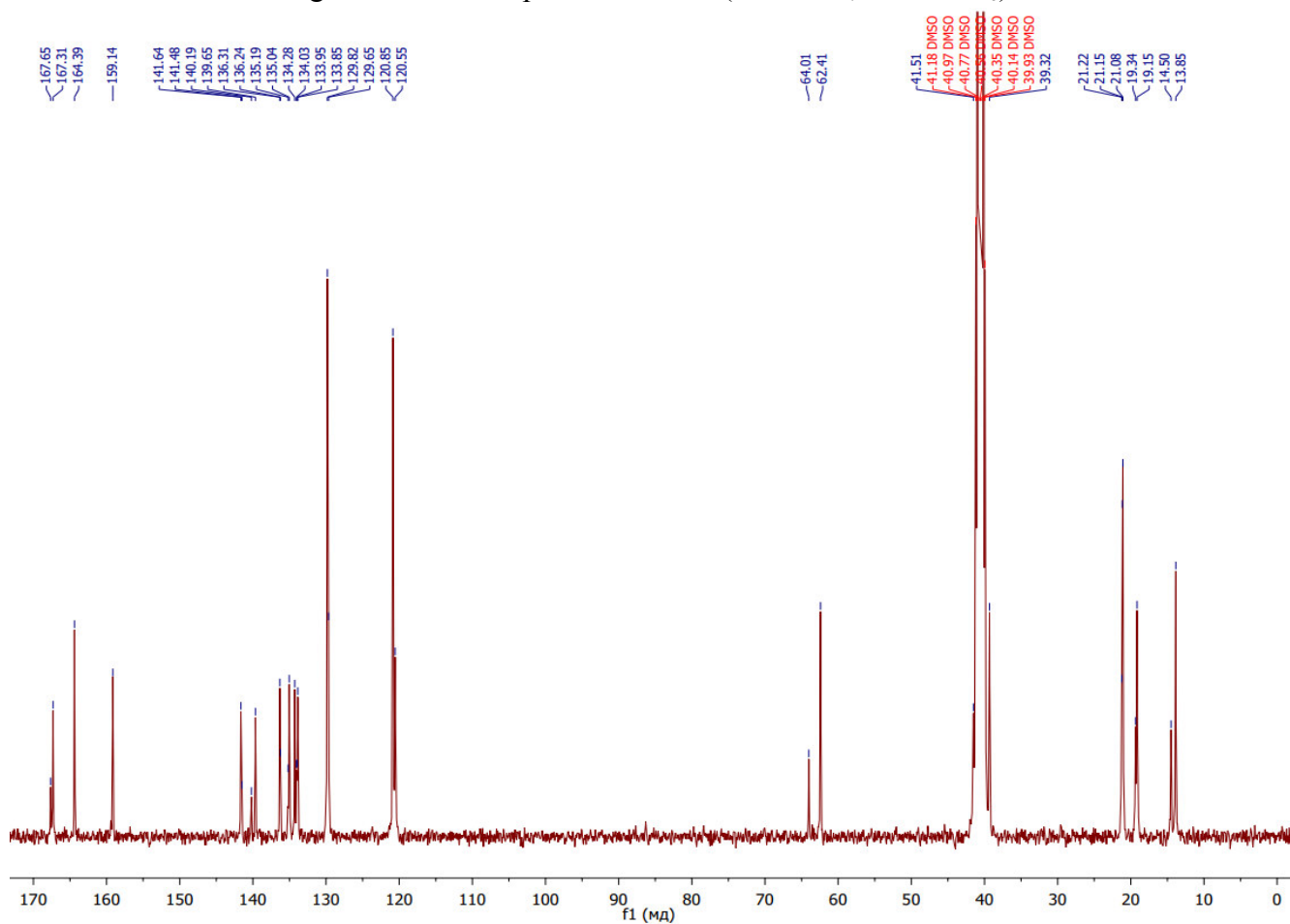


Fig. 28. ¹³C-NMR-spectrum of **11n** (101 MHz, DMSO-*d*₆)

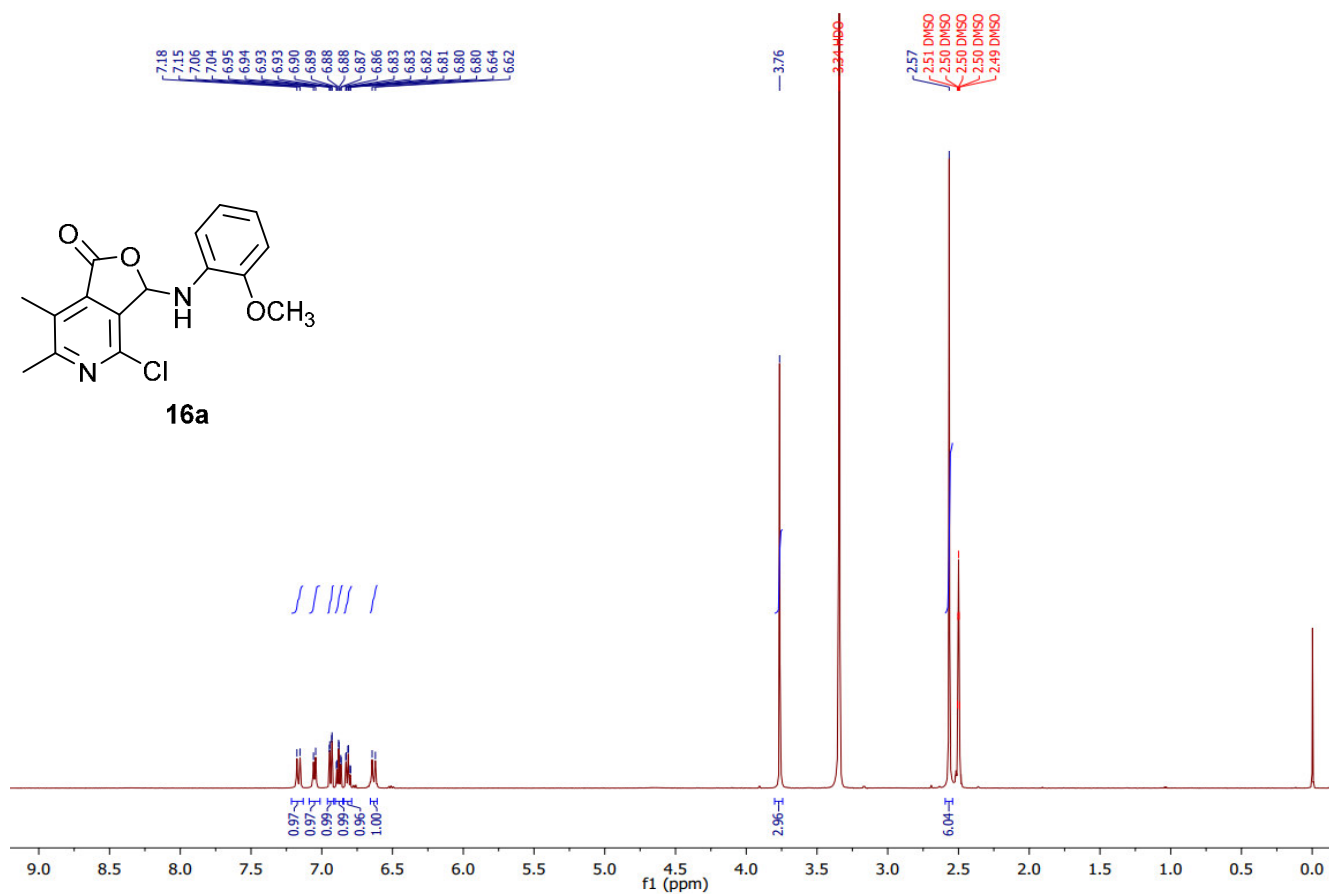


Fig. 29. ¹H-NMR-spectrum of **16a** (500 MHz, DMSO-*d*₆)

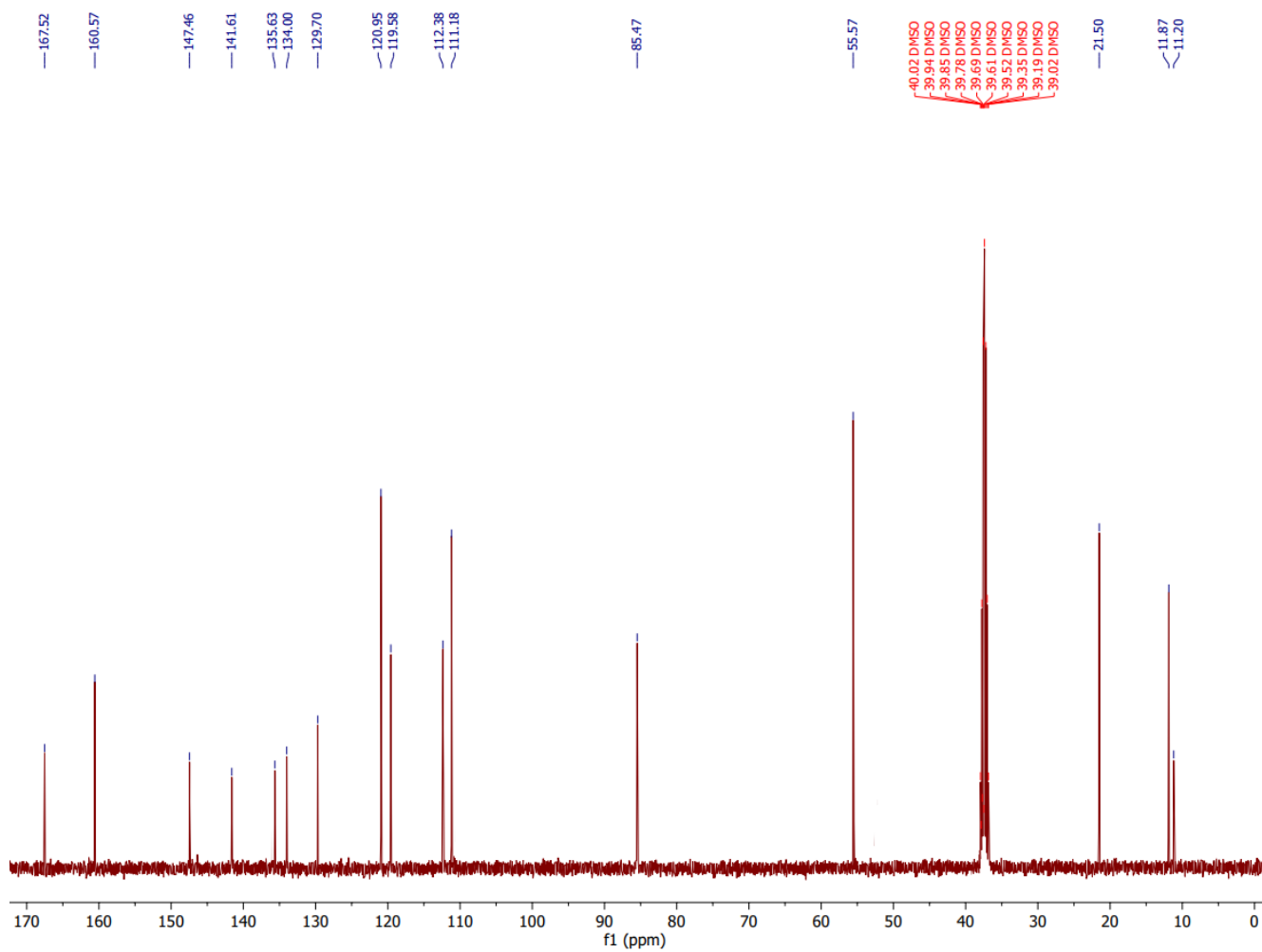


Fig. 30. ¹³C-NMR-spectrum of **16a** (126 MHz, DMSO-*d*₆)

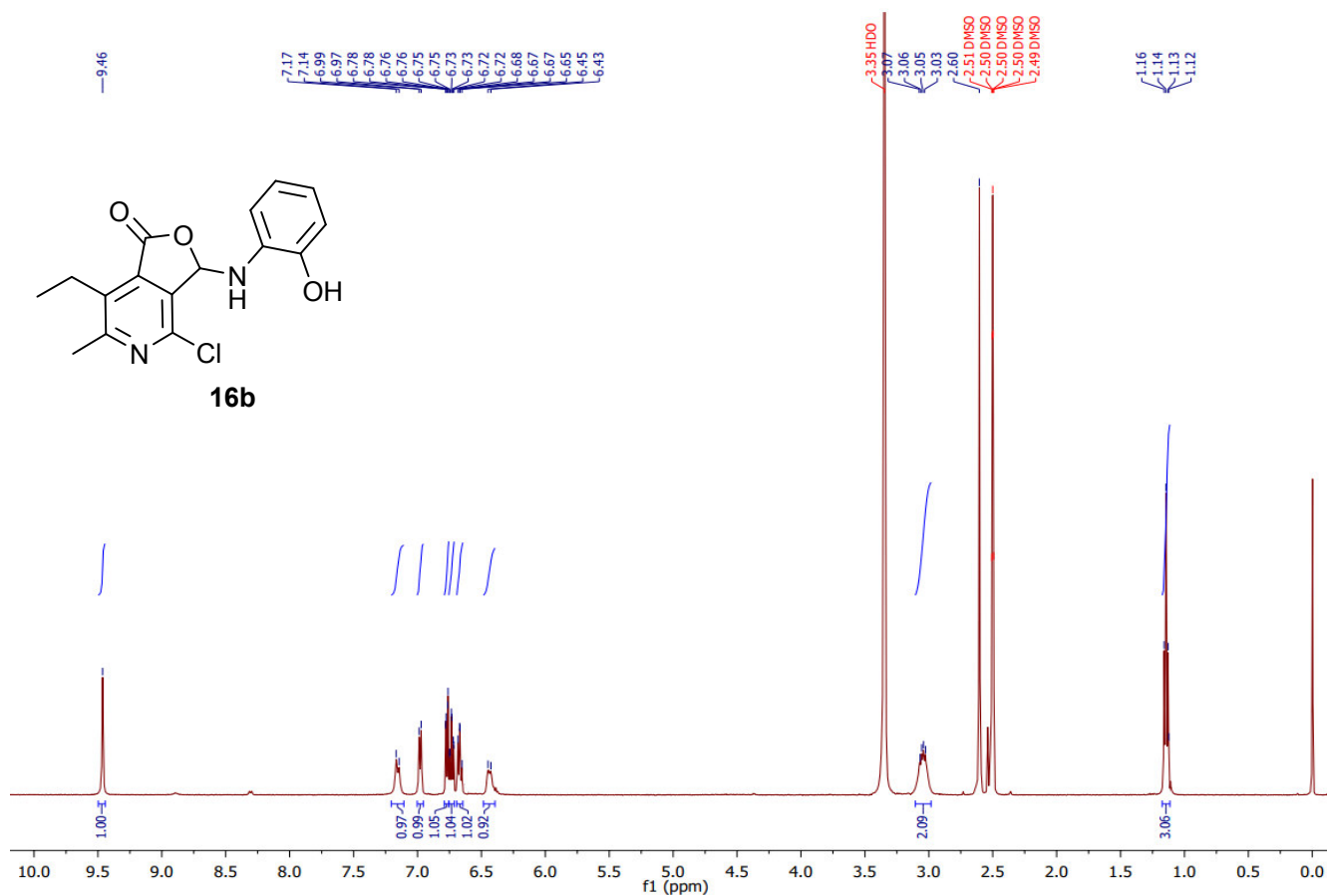


Fig. 31. ^1H -NMR-spectrum of **16b** (500 MHz, DMSO- d_6)

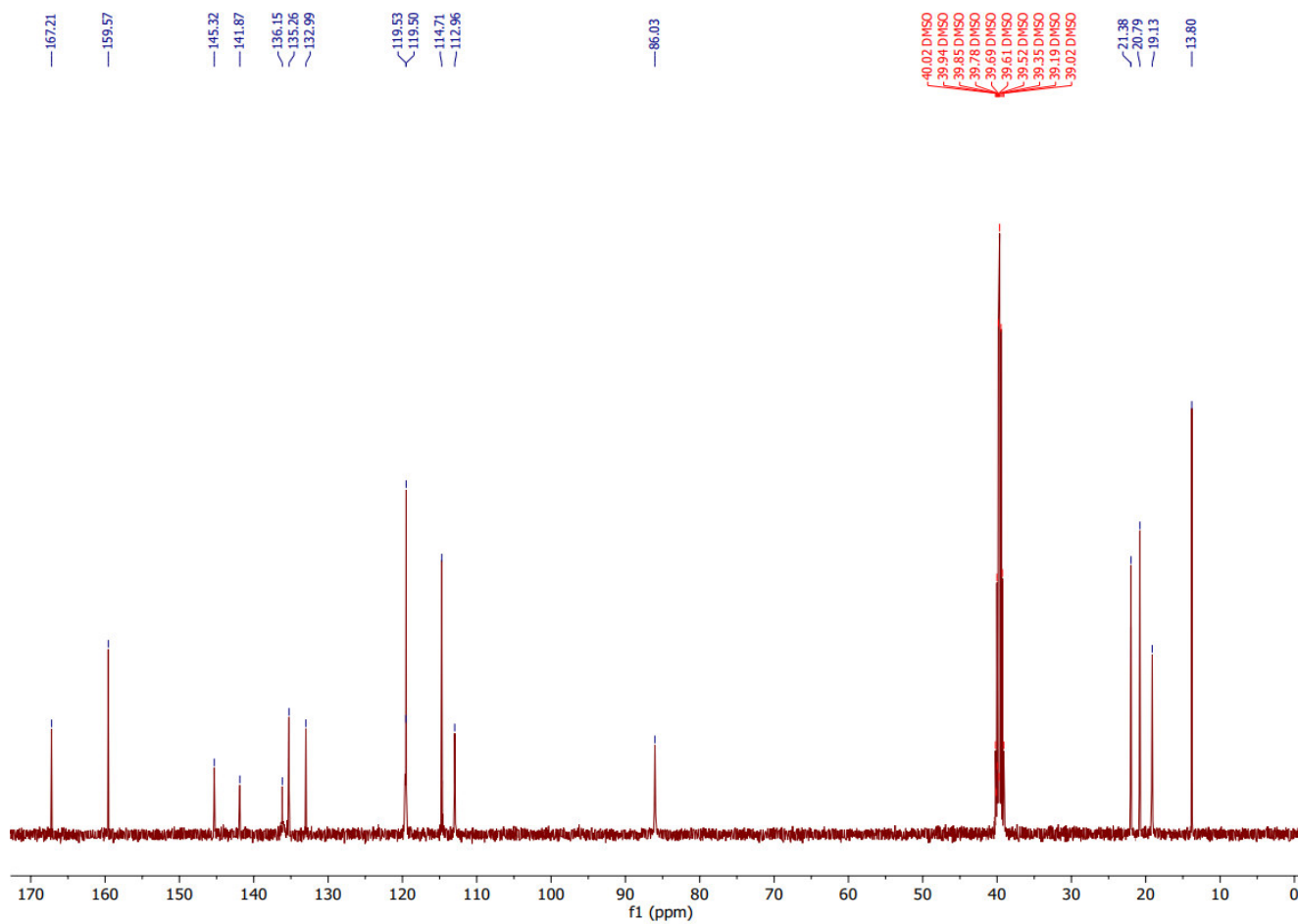


Fig. 32. ^{13}C -NMR-spectrum of **16b** (126 MHz, DMSO- d_6)

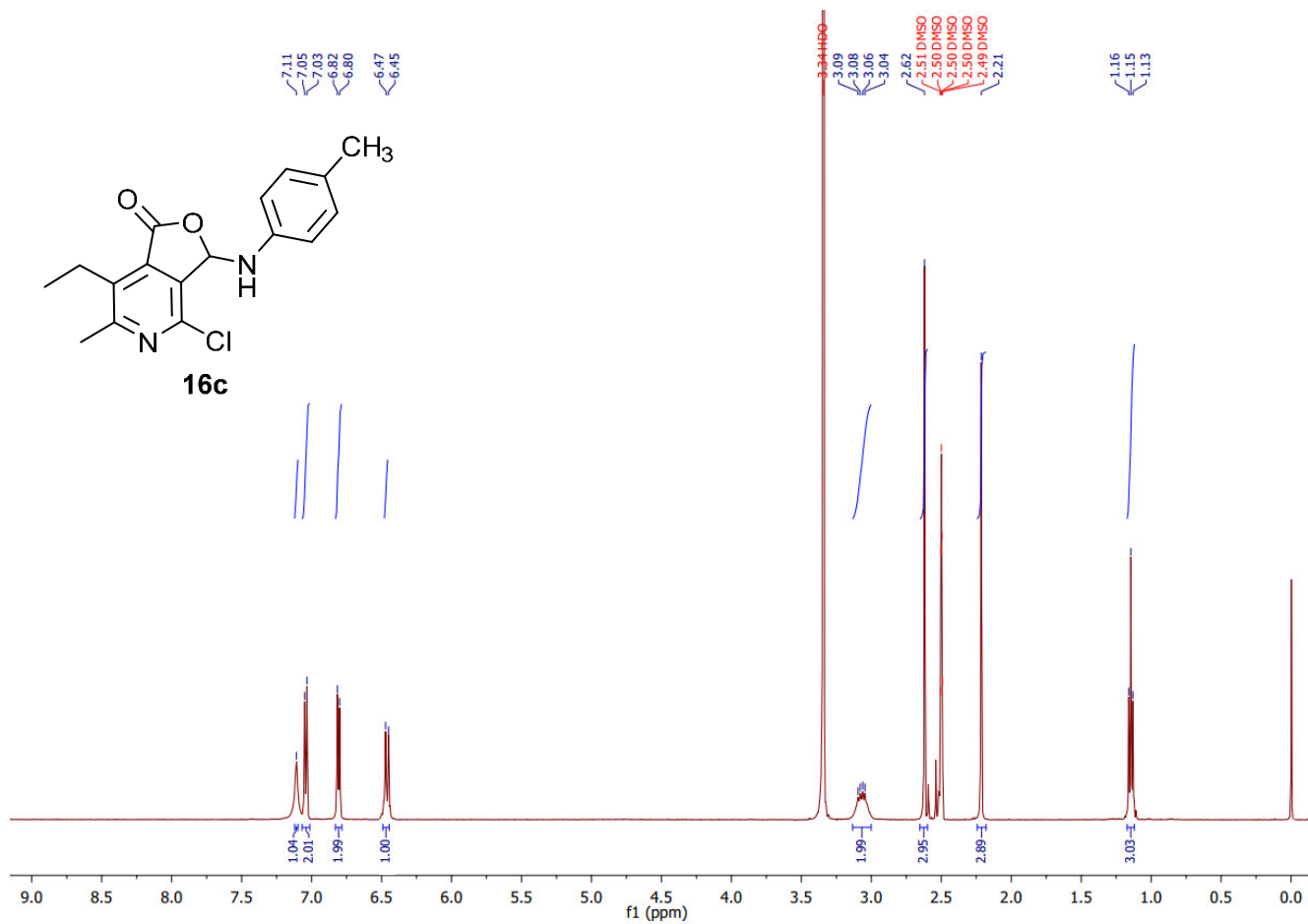


Fig. 33. ¹H-NMR-spectrum of **16c** (500 MHz, DMSO-*d*₆)

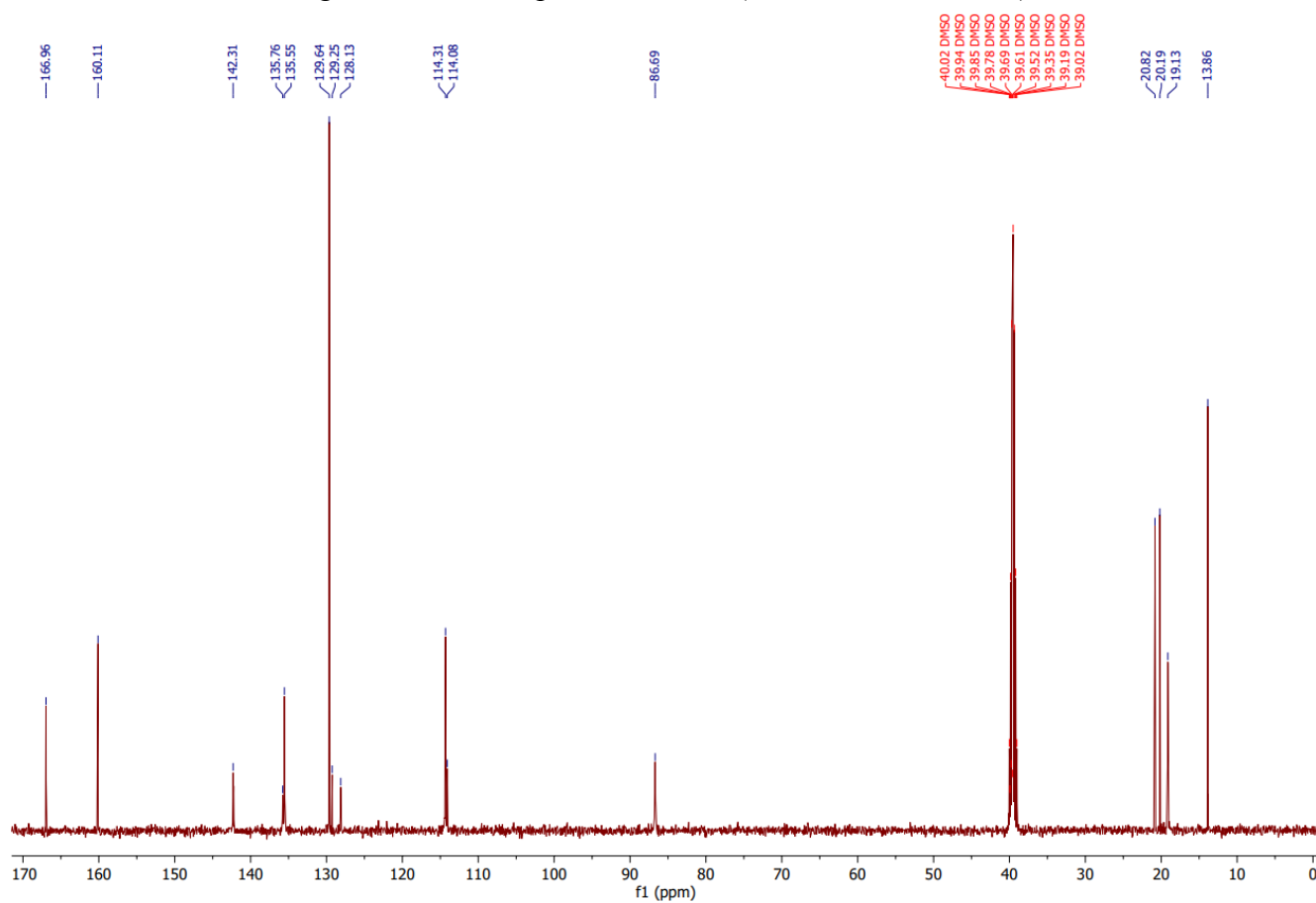


Fig. 34. ¹³C-NMR-spectrum of **16c** (126 MHz, DMSO-*d*₆)

2. Crystal data

Table 1. Crystal data and structure refinement for **11i**.

Identification code	25bel_SF1171	
Empirical formula	C ₂₂ H ₂₄ Cl N ₃ O ₄	
Formula weight	429.89	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /c	
Unit cell dimensions	a = 17.5537(7) Å	a = 90°.
	b = 14.0149(6) Å	b = 90.9271(14)°.
	c = 8.5784(3) Å	g = 90°.
Volume	2110.12(14) Å ³	
Z	4	
Density (calculated)	1.353 Mg/m ³	
Absorption coefficient	0.215 mm ⁻¹	
F(000)	904	
Crystal size	0.150 x 0.080 x 0.050 mm ³	
Theta range for data collection	1.859 to 30.551°.	
Index ranges	-25 ≤ h ≤ 25, -20 ≤ k ≤ 19, -12 ≤ l ≤ 12	
Reflections collected	33689	
Independent reflections	6457 [R(int) = 0.0406]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.6847	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	6457 / 0 / 278	
Goodness-of-fit on F ²	1.067	
Final R indices [I > 2σ(I)]	R1 = 0.0594, wR2 = 0.1295	
R indices (all data)	R1 = 0.0741, wR2 = 0.1372	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.366 and -0.459 e.Å ⁻³	

Table 2. Hydrogen bonds for **11i** [E and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(3)-H(3)...N(1)#1	0.87(3)	2.11(3)	2.959(2)	164(2)

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+3/2,z-1/2