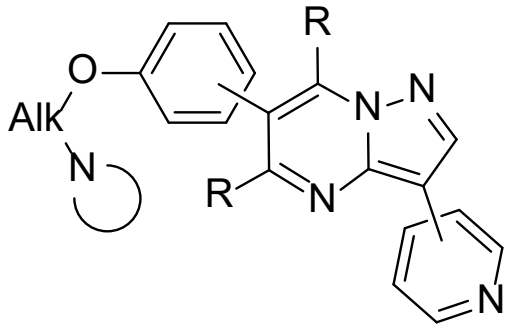
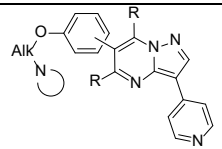
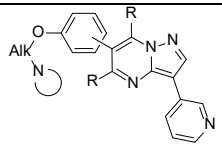
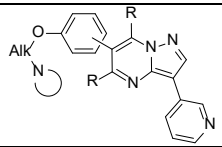
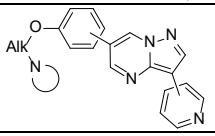
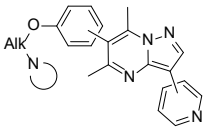
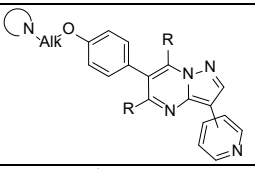
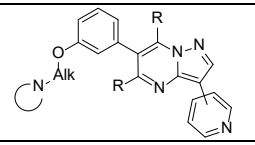
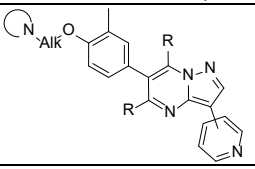
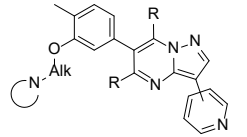
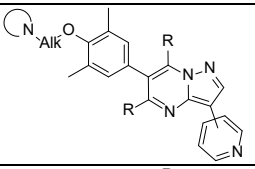
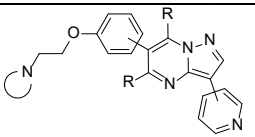
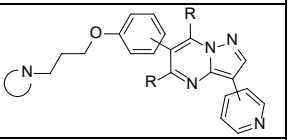
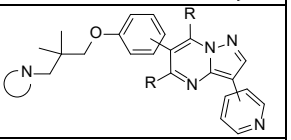
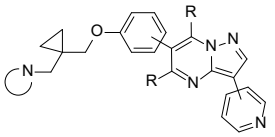
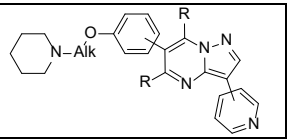
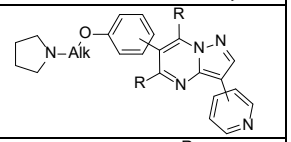
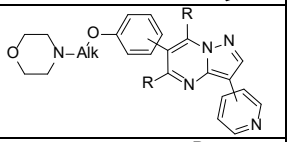
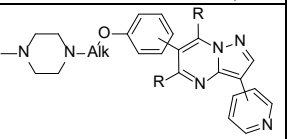
Table S1. Annotation of the structure identifier (XXXXX) for compounds that make up the target-focused library of dorsomorphin analogs.



Identifier position	Point of structure variation	Variation is realized by	Variants	Designation	Structure
First number	Nitrogen atom position in the pyridine ring	Corresponding pyridinecarboxylic acids: - 4-pyridinecarboxylic acid (isonicotinic acid) - 3-pyridinecarboxylic acid (nicotinic acid) - 2-pyridinecarboxylic acid (picolinic acid)	Nitrogen atom at position 4	4XXXX	
			Nitrogen atom at position 3	3XXXX	
			Nitrogen atom at position 2	2XXXX	
Second number	Substitution in the pyrimidine ring	Corresponding β-dicarbonyl compounds: - bromomalonic aldehyde - 3-bromoacetylacetone	No substitution at positions 5 and 7 (R = H)	X0XXX	
			Dimethyl substitution at positions 5 and 7 ($R = CH_3$)	X2XXX	

Third number	Orientation of alkylamine moiety and substitution in the phenyl ring	Corresponding bromophenols: - 4-bromophenol - 3-bromophenol - 4-bromo-2-methylphenol - 5-bromo-2-methylphenol - 4-bromo-2,6-dimethylphenol	Para-orientation of the chain, no substitution	XX<u>1</u>XX	
			Meta-orientation of the chain, no substitution	XX<u>2</u>XX	
			Para-orientation of the chain, methyl substitution	XX<u>3</u>XX	
			Meta-orientation of the chain, methyl substitution	XX<u>4</u>XX	
			Para-orientation of the chain, dimethyl substitution	XX<u>5</u>XX	
Fourth number	Length and substitution in the alkyl chain	Corresponding glycols: - ethylene glycol - 1,3-propanediol - 2,2-dimethylpropane-1,3-diol - 1,1-bis(hydroxymethyl)cyclopropane	Two-carbon chain, no substitution	XXX<u>1</u>X	
			Three-carbon chain, no substitution	XXX<u>2</u>X	
			Three-carbon chain, dimethyl substitution	XXX<u>3</u>X	
			Three-carbon chain, cyclopropyl substitution	XXX<u>4</u>X	

Fifth number	Cyclic amine moiety	Corresponding cyclic amines: - piperidine - pyrrolidine - morpholine - *N*-methylpiperazine	*N*-piperidinyl moiety	XXXX1	
			N-pyrrolidinyl moiety	XXXX2	
			N-morpholinyl moiety	XXXX3	
			N-(4-methylpiperazinyl) moiety	XXXX4	

Note. Dorsomorphin is also included in the library and designated as 40111.

Figure S1. ^{1}H NMR spectrum of **dorsomorphin**.

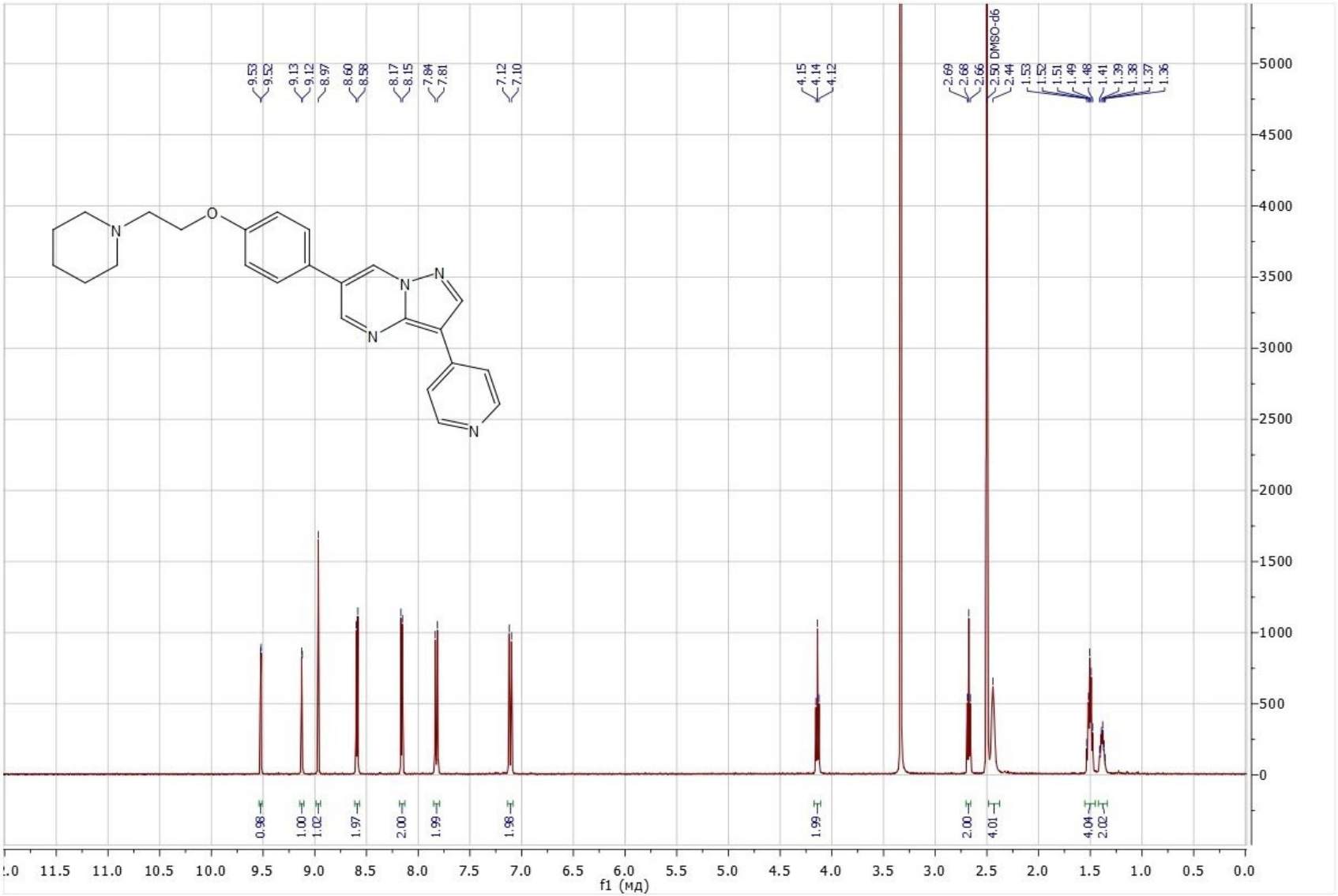


Figure S2. ^{13}C NMR spectrum of **dorsomorphin**.

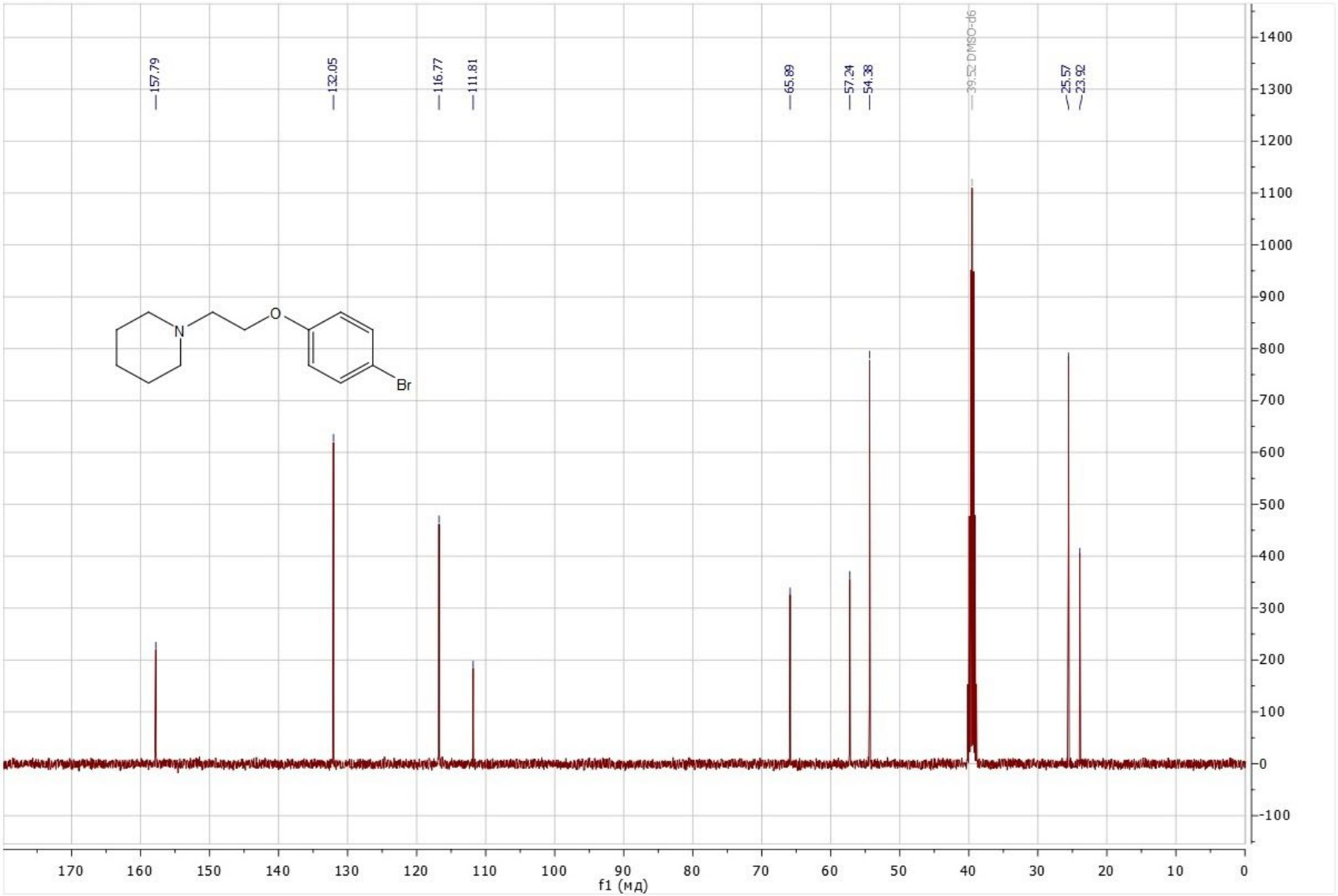


Figure S3. ^{1}H NMR spectrum of **6a**.

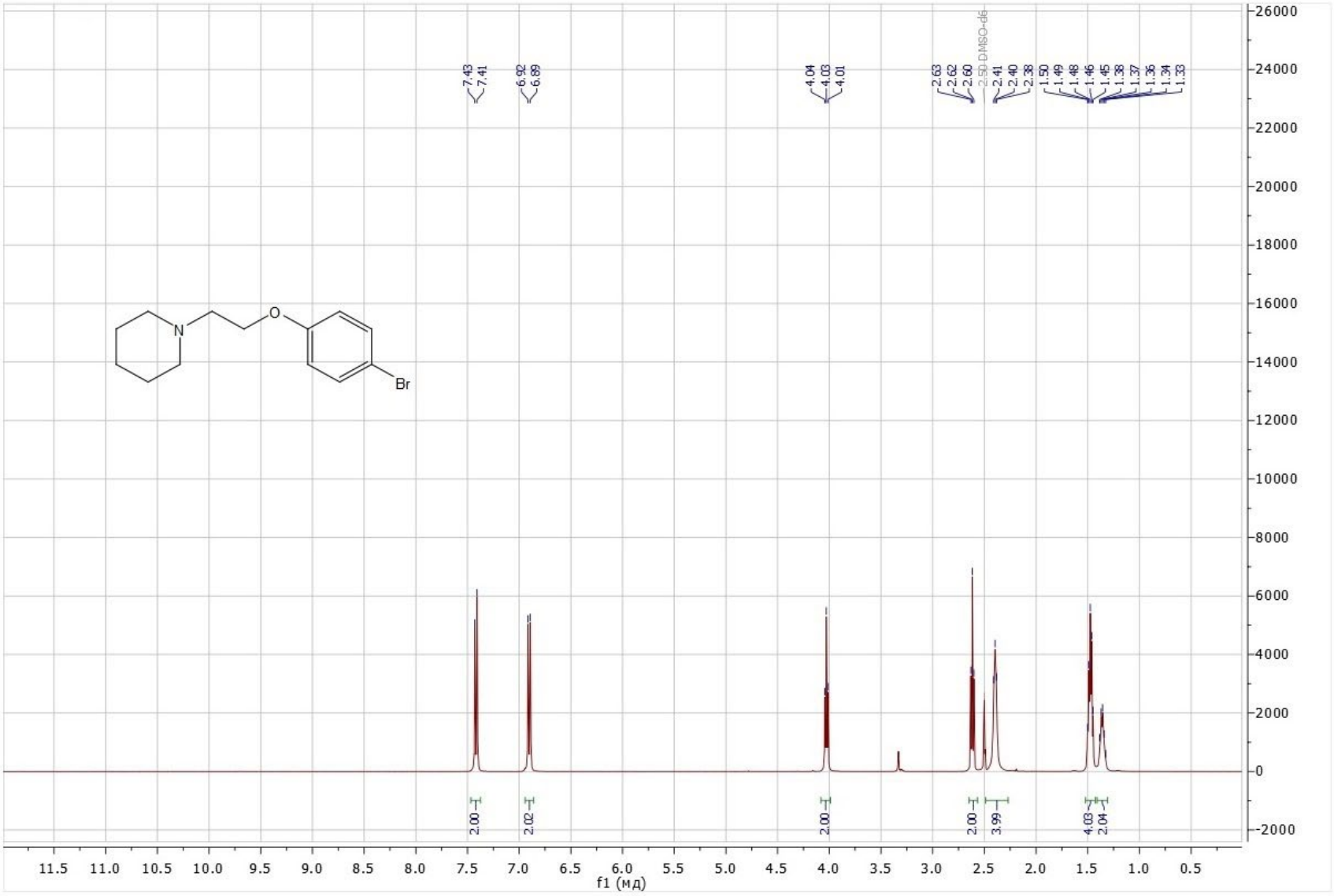


Figure S4. ^{13}C NMR spectrum of **6a**.

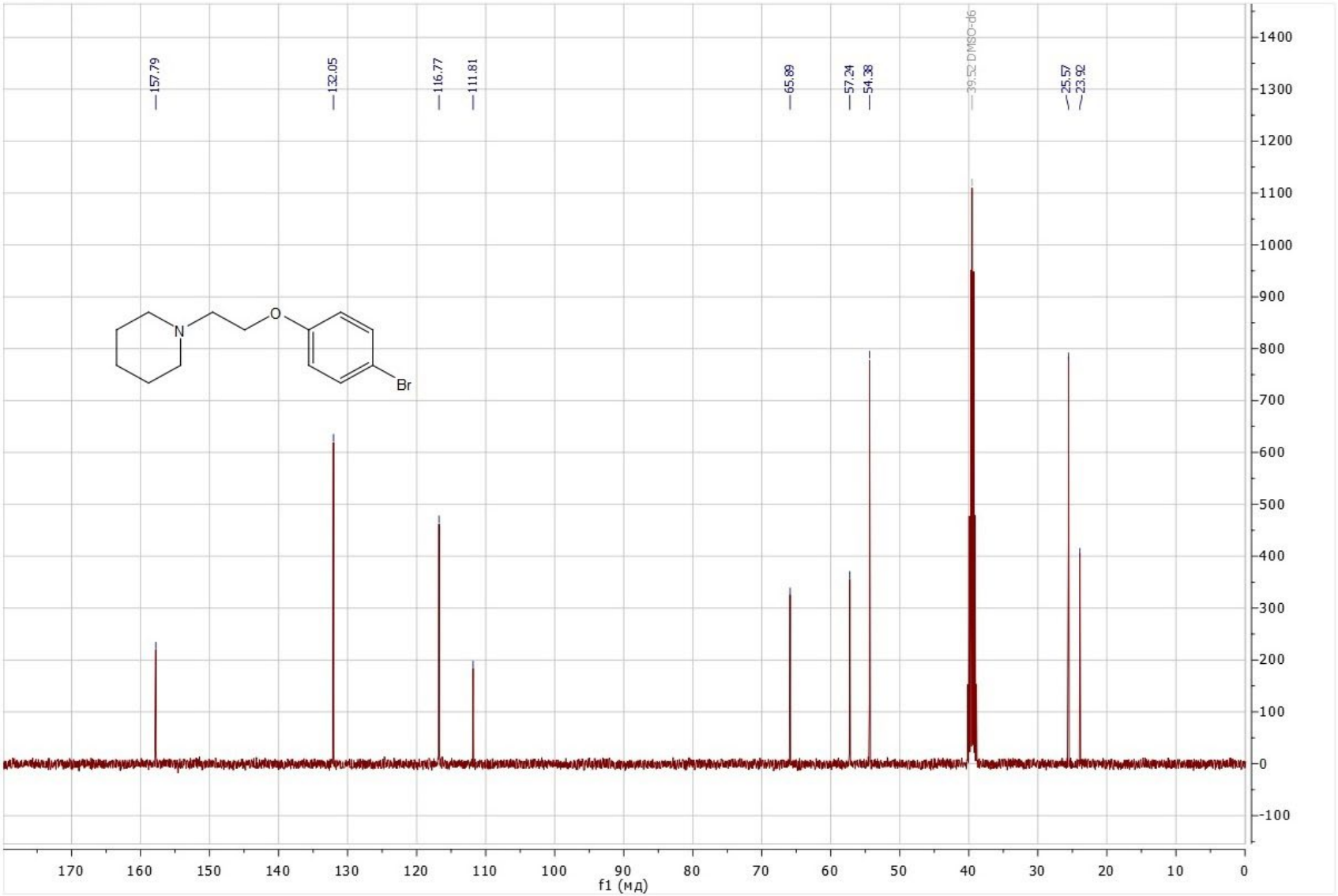


Figure S5. ^{1}H NMR spectrum of **6b**.

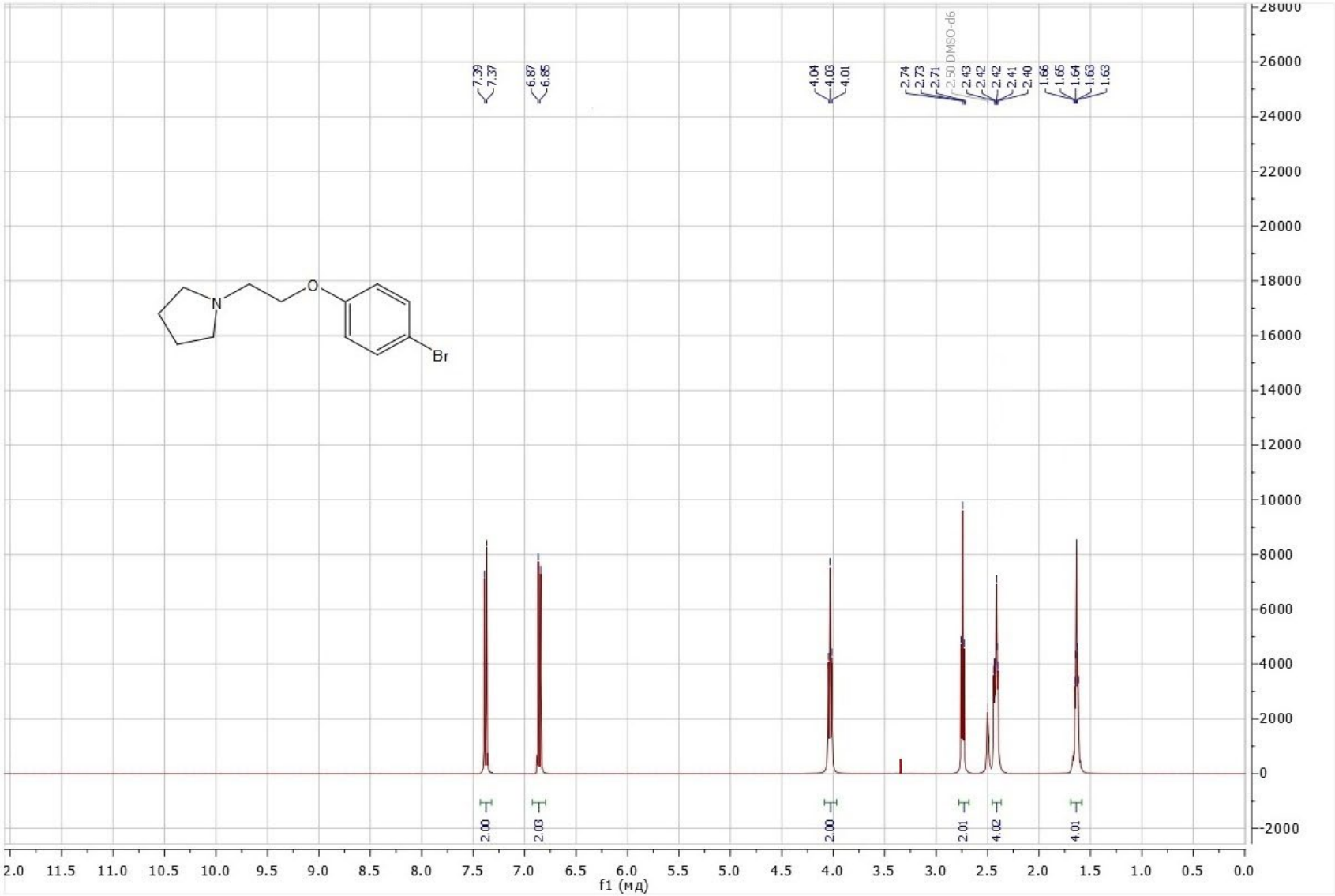


Figure S6. ^{13}C NMR spectrum of **6b**.

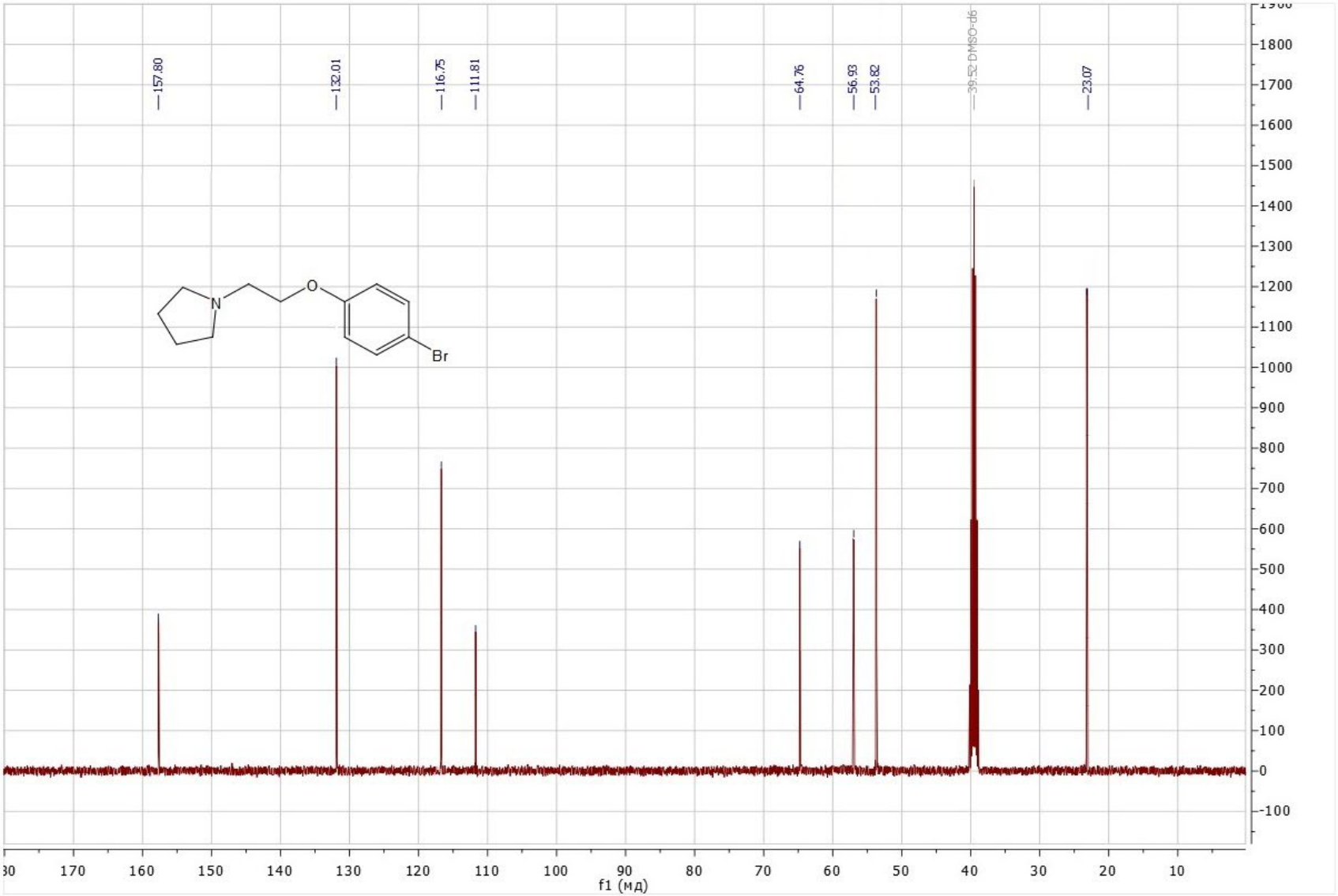


Figure S7. ^{1}H NMR spectrum of **6c**.

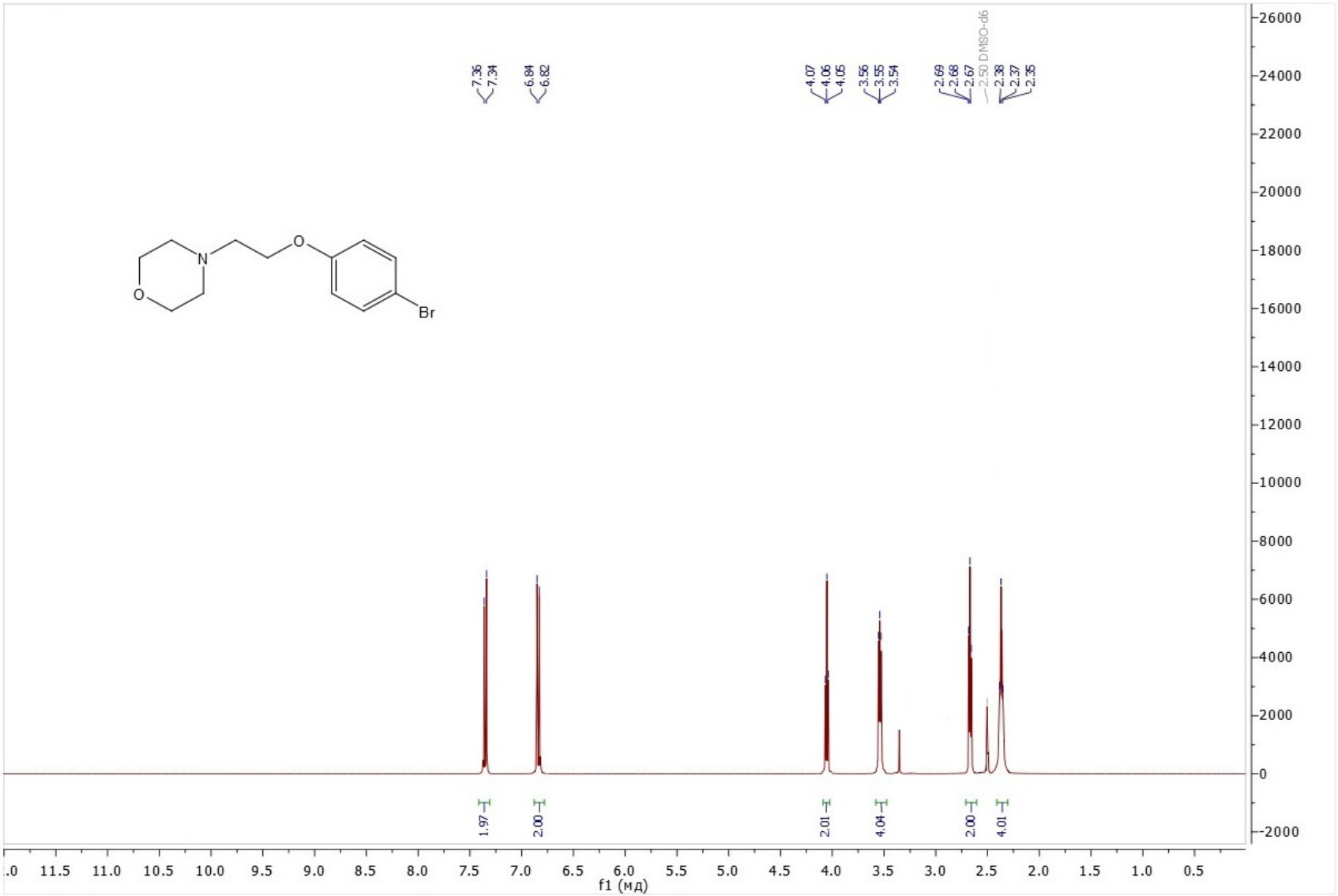


Figure S8. ^{13}C NMR spectrum of **6c**.

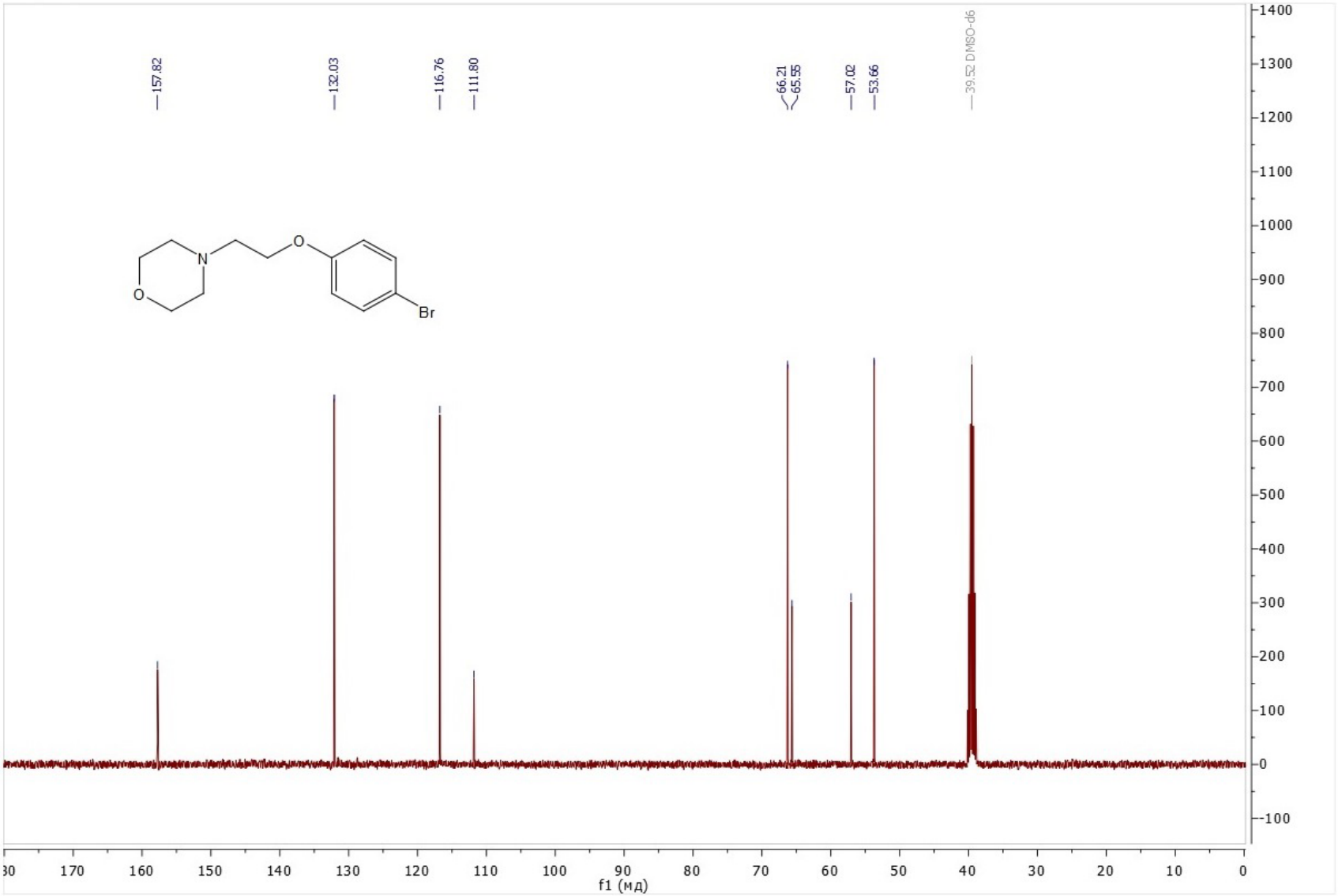


Figure S9. ^{1}H NMR spectrum of **6d**.

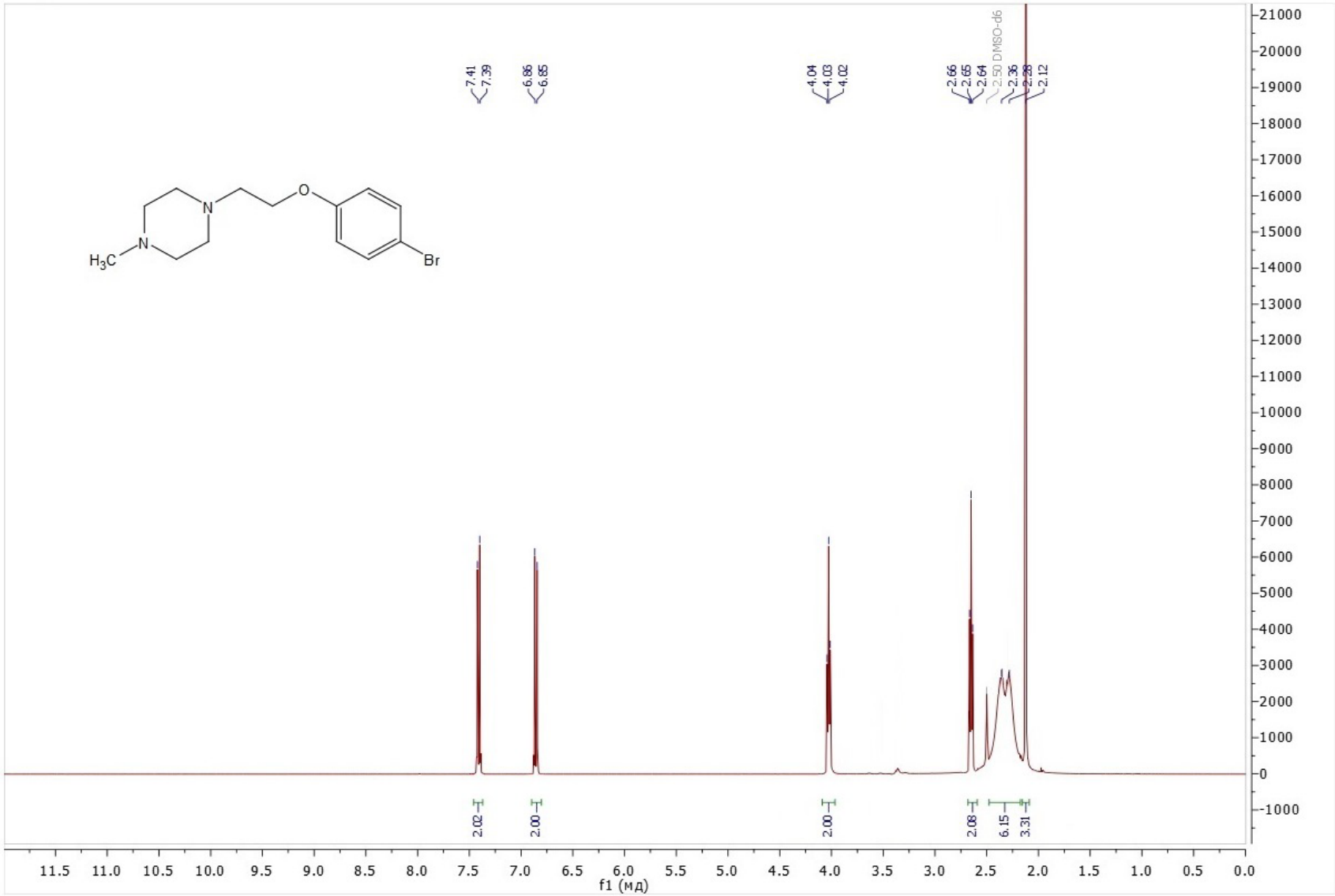


Figure S10. ^{13}C NMR spectrum of **6d**.

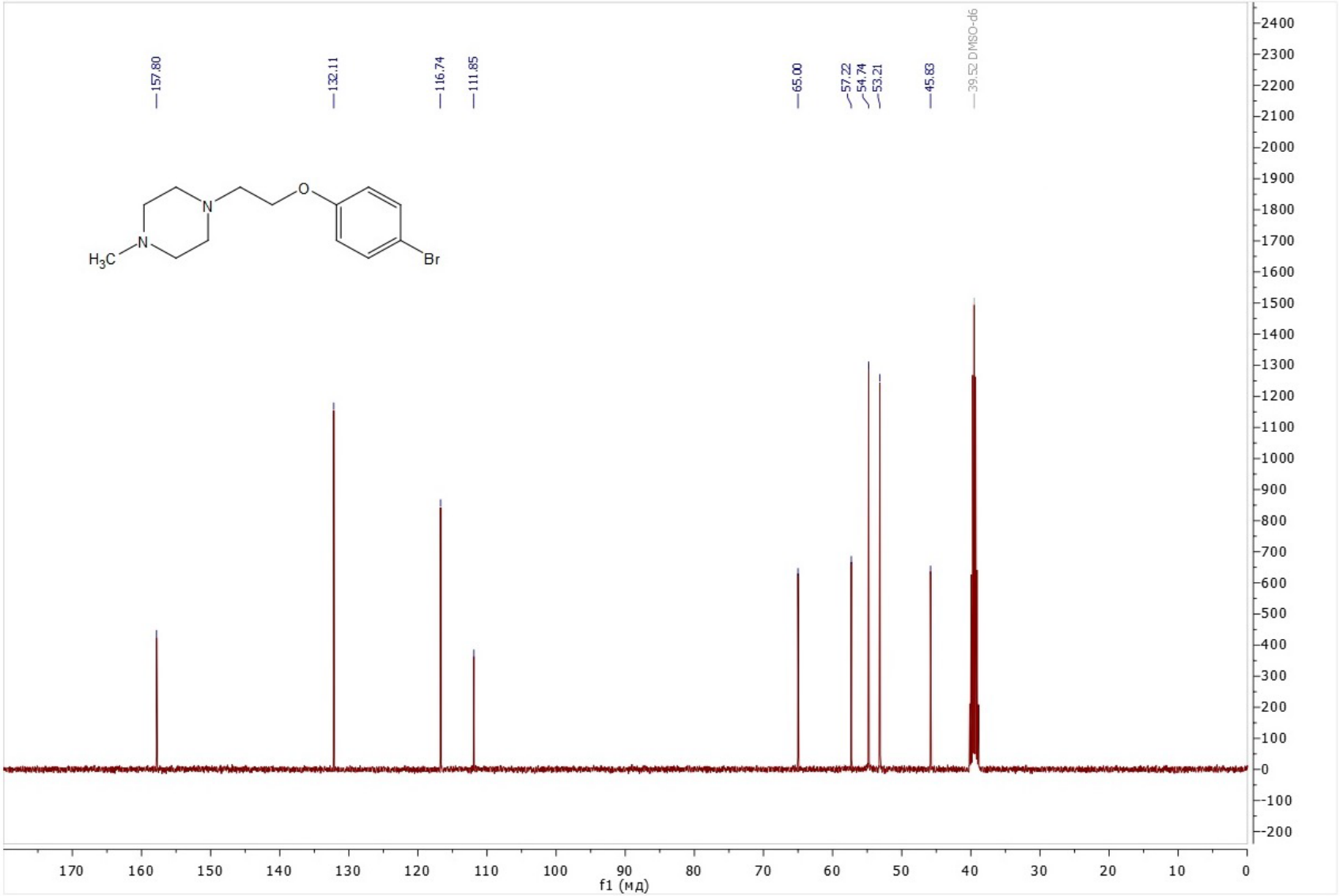


Figure S11. ^{1}H NMR spectrum of **6e**.

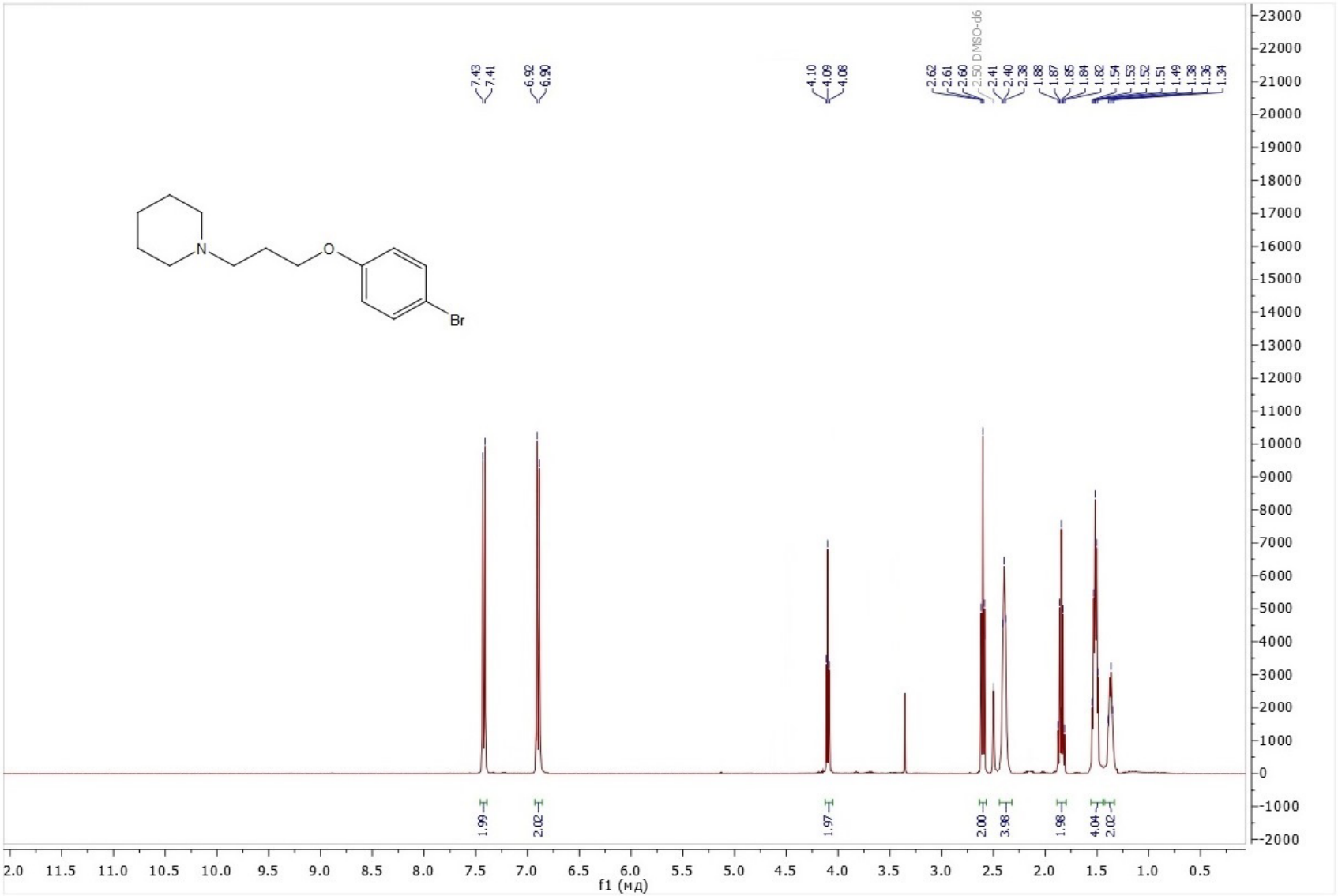


Figure S12. ^{13}C NMR spectrum of **6e**.

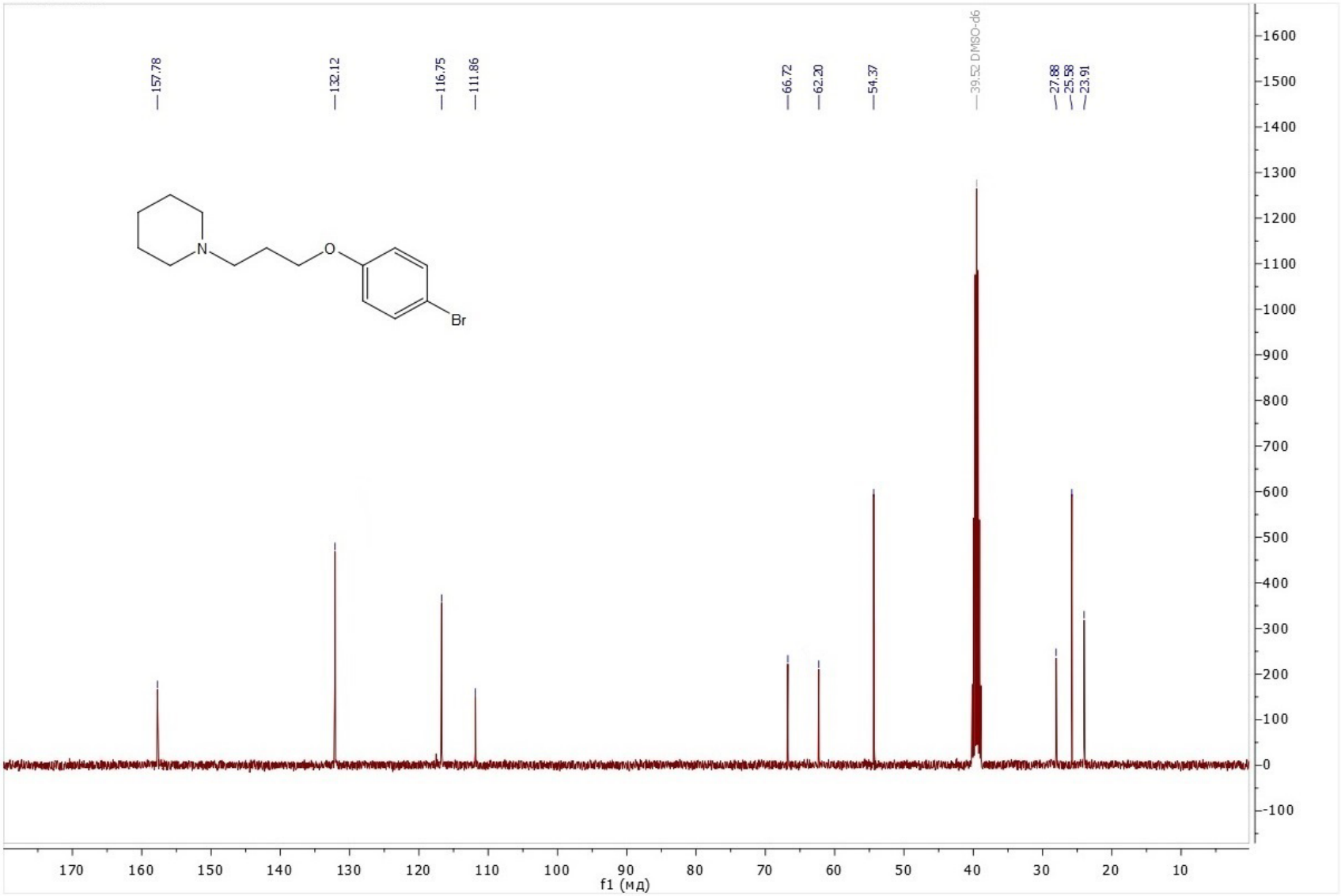


Figure S13. ^{1}H NMR spectrum of **6f**.

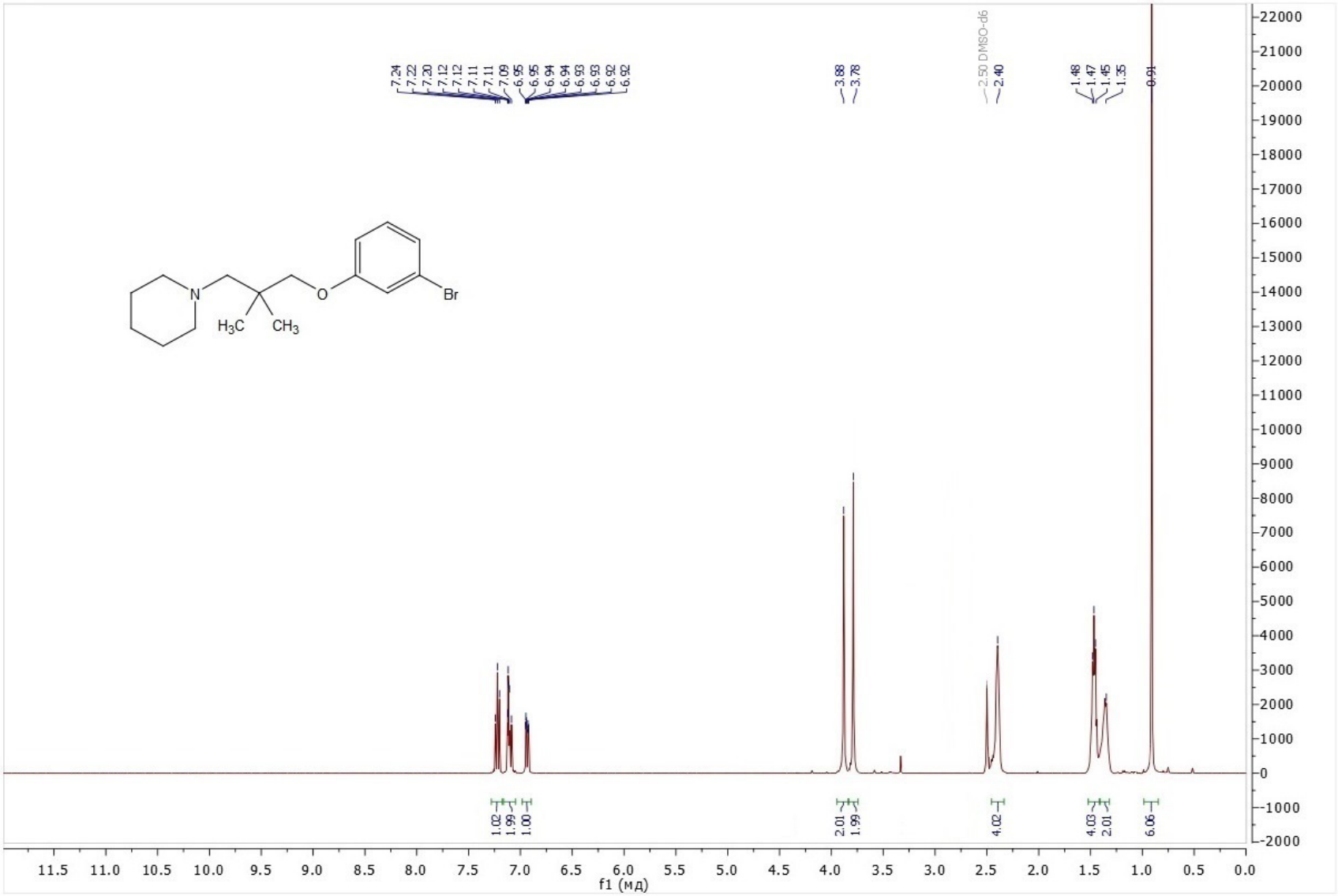


Figure S14. ^{13}C NMR spectrum of **6f**.

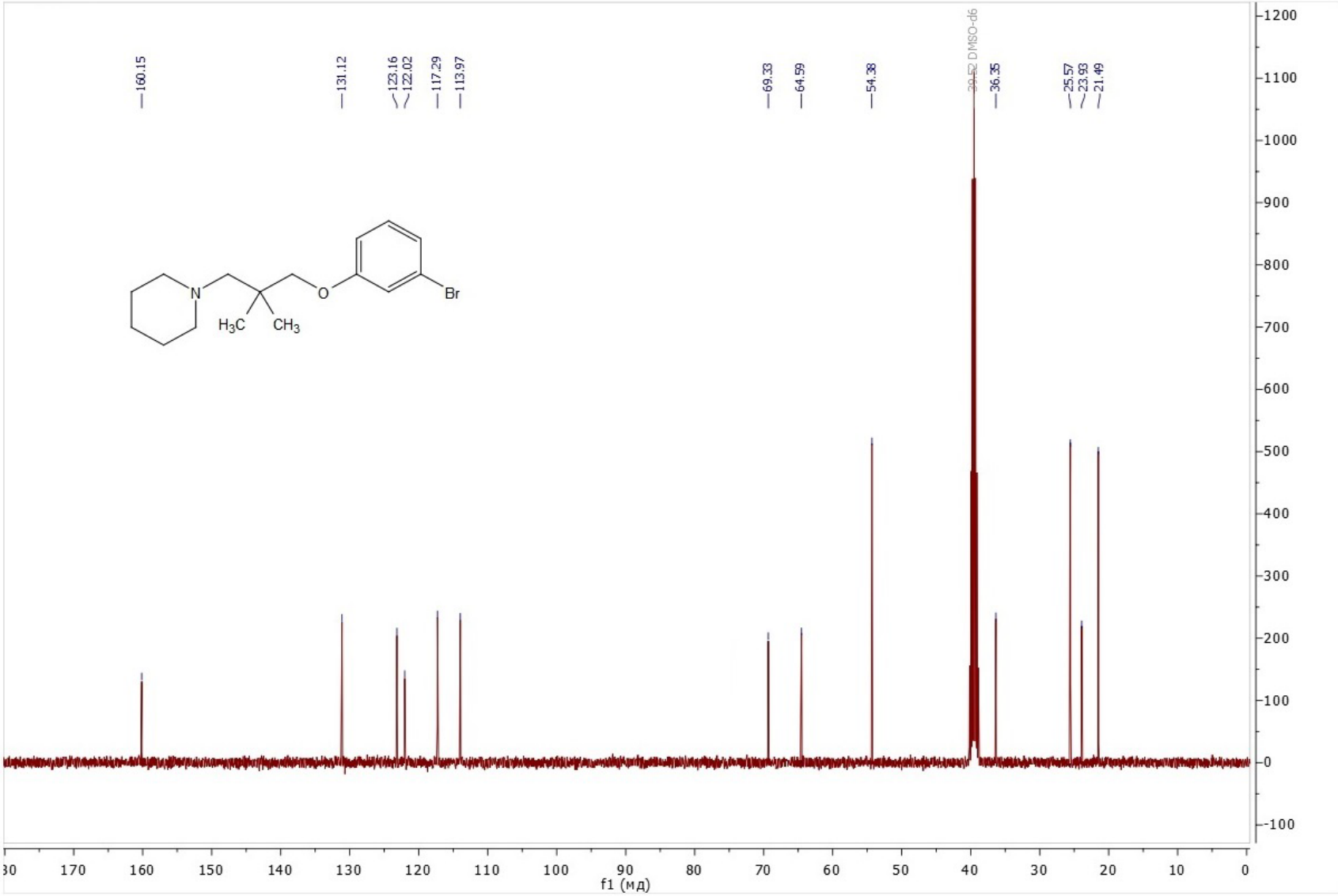


Figure S15. ^{1}H NMR spectrum of **6g**.

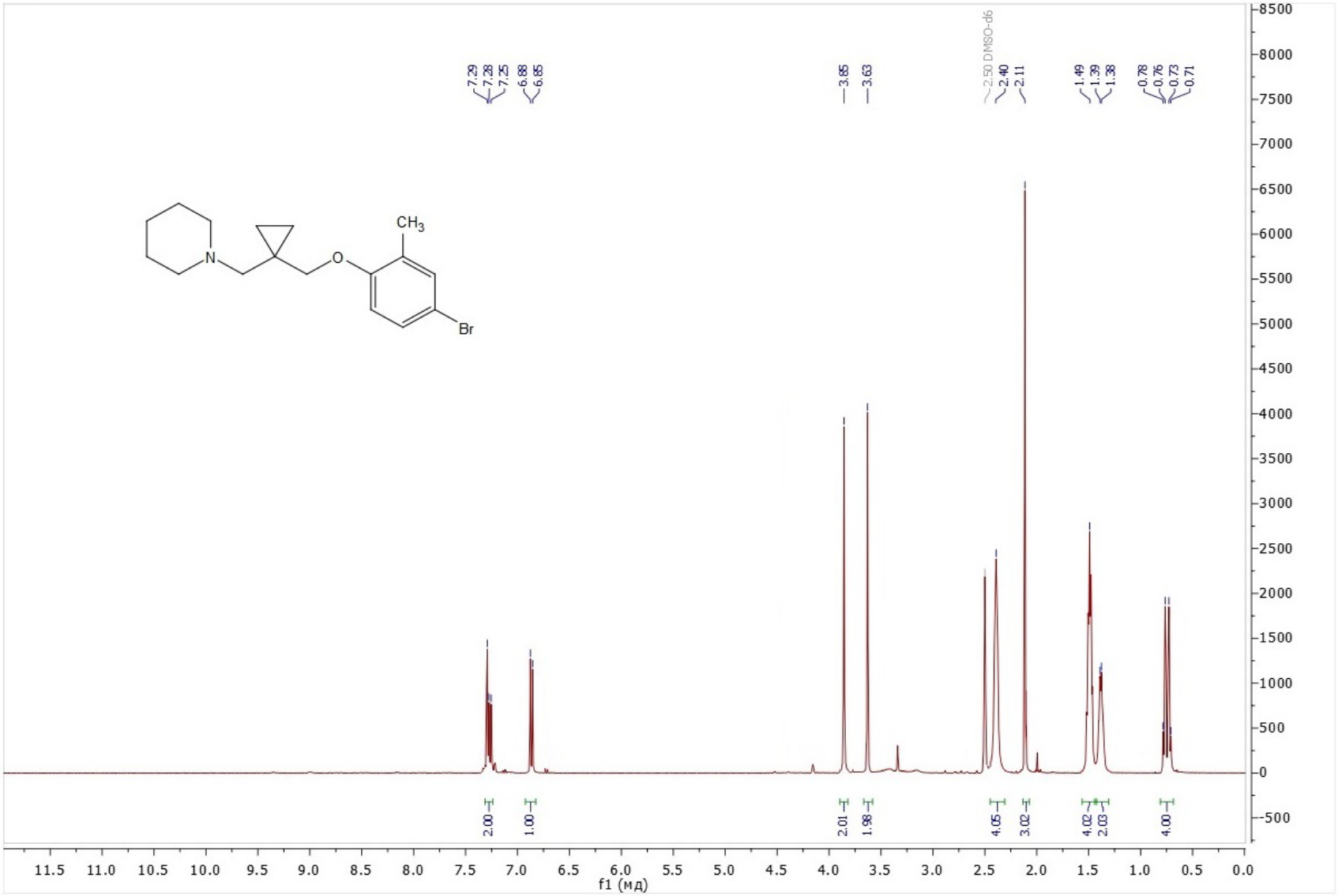


Figure S16. ^{13}C NMR spectrum of **6g**.

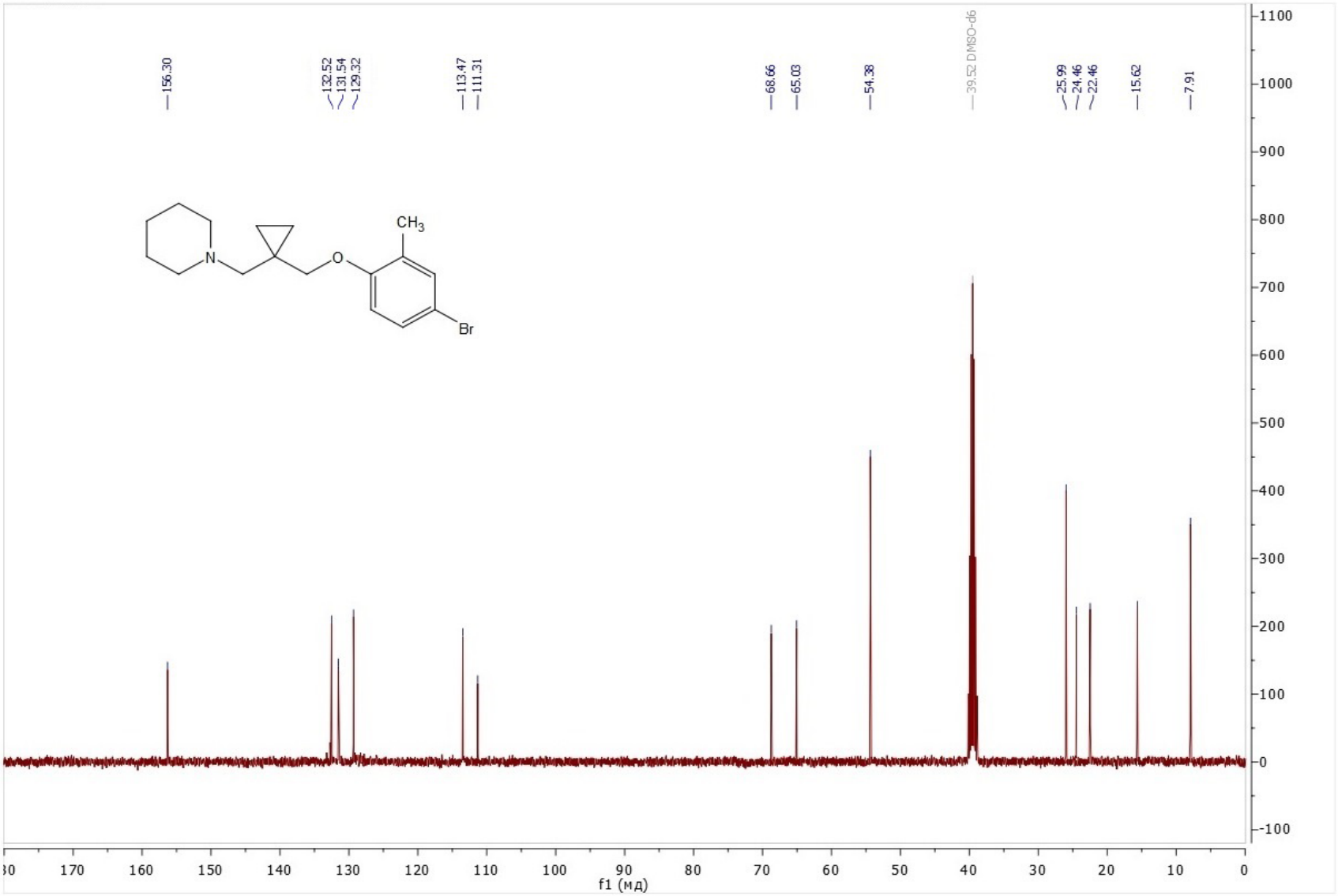


Figure S17. ^{1}H NMR spectrum of **6h**.

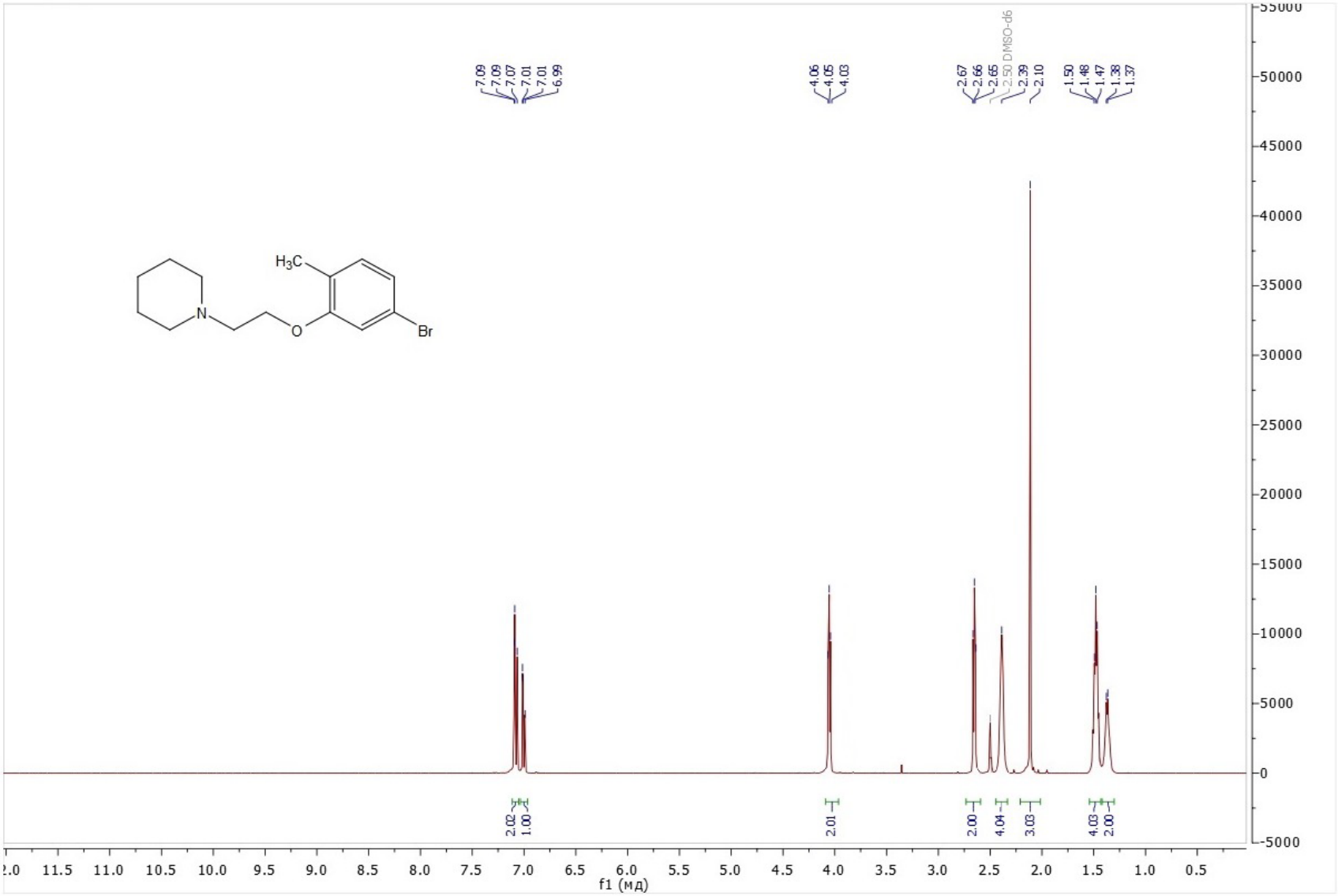


Figure S18. ^{13}C NMR spectrum of **6h**.

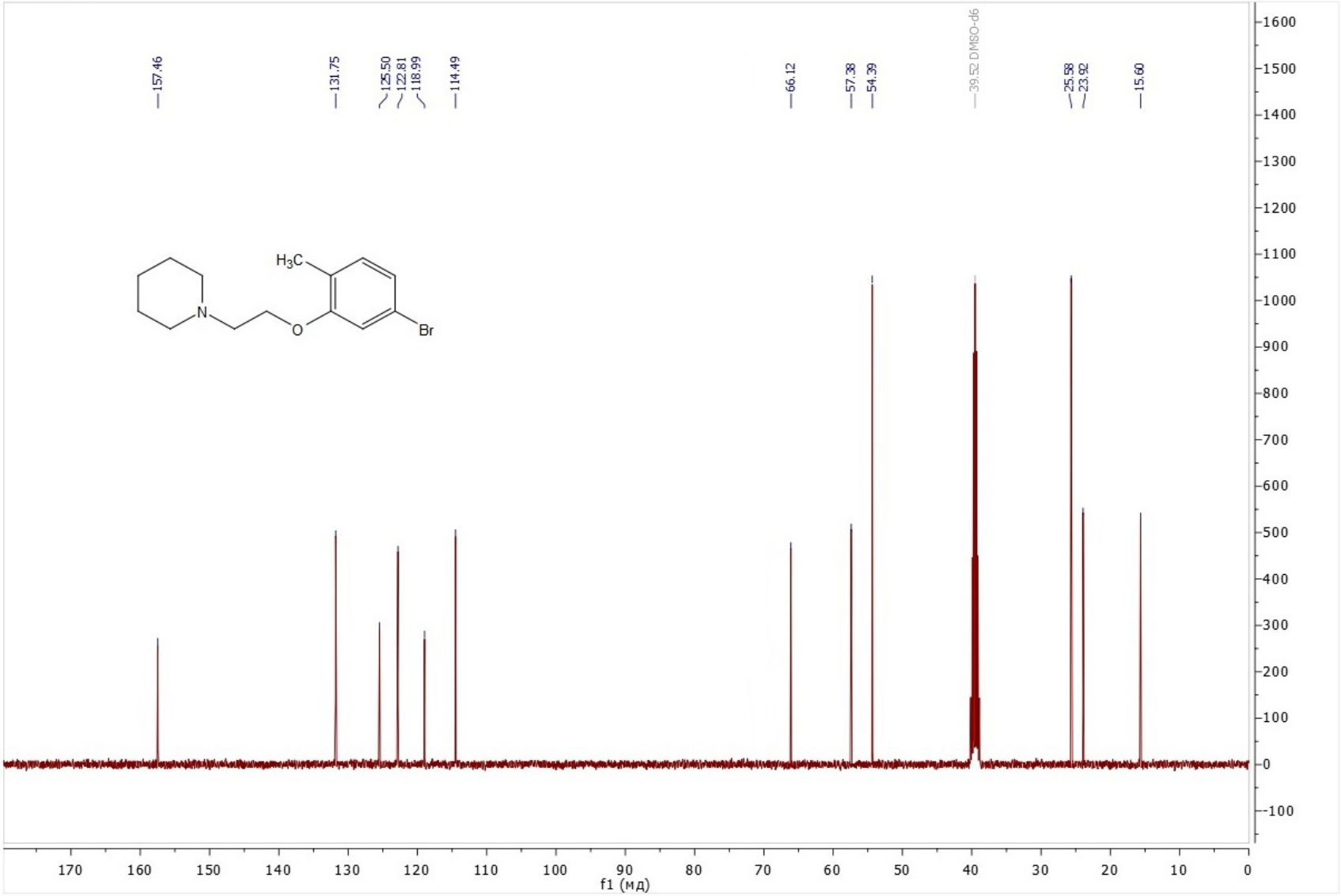


Figure S19. ^{1}H NMR spectrum of **6i**.

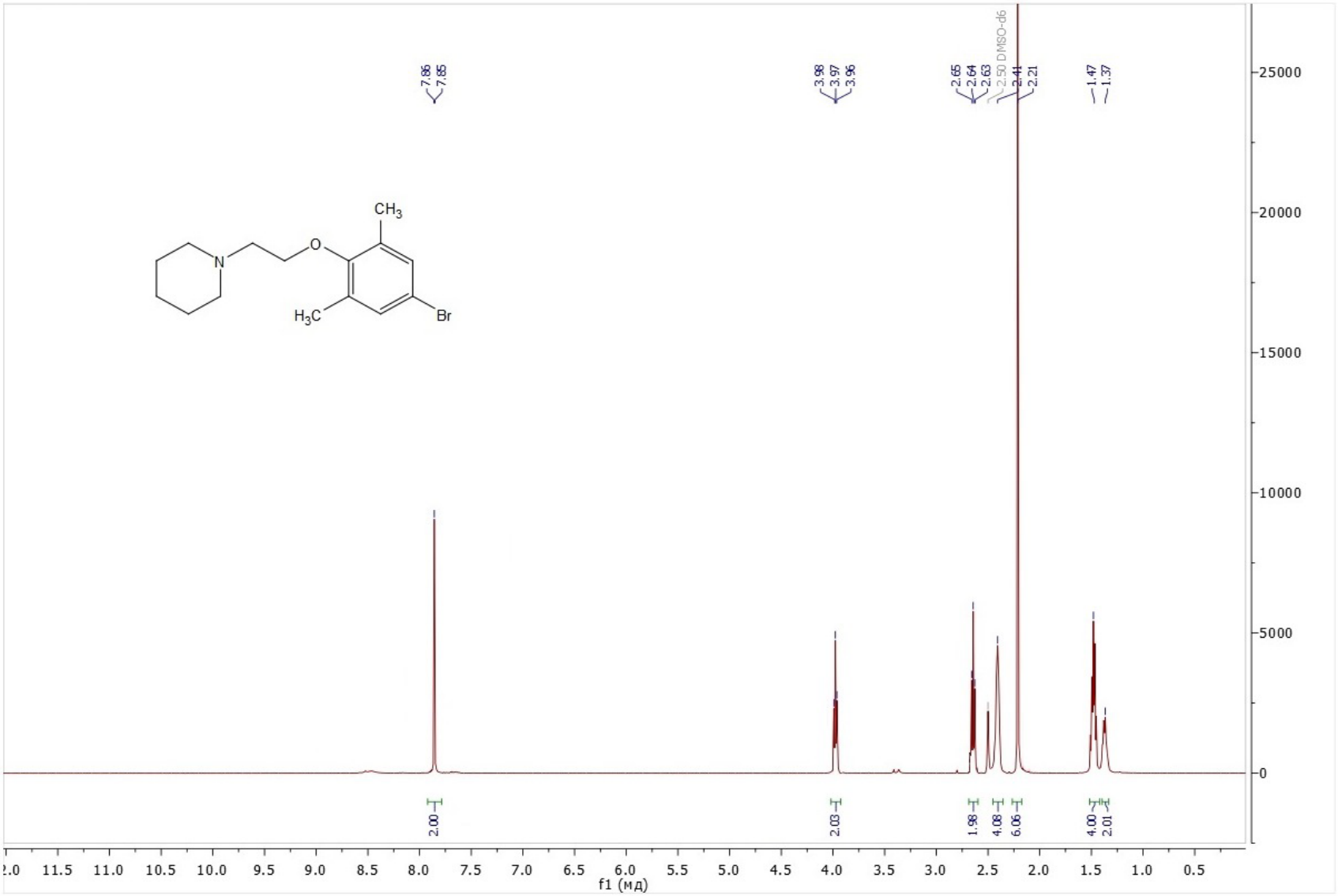


Figure S20. ^{13}C NMR spectrum of **6i**.

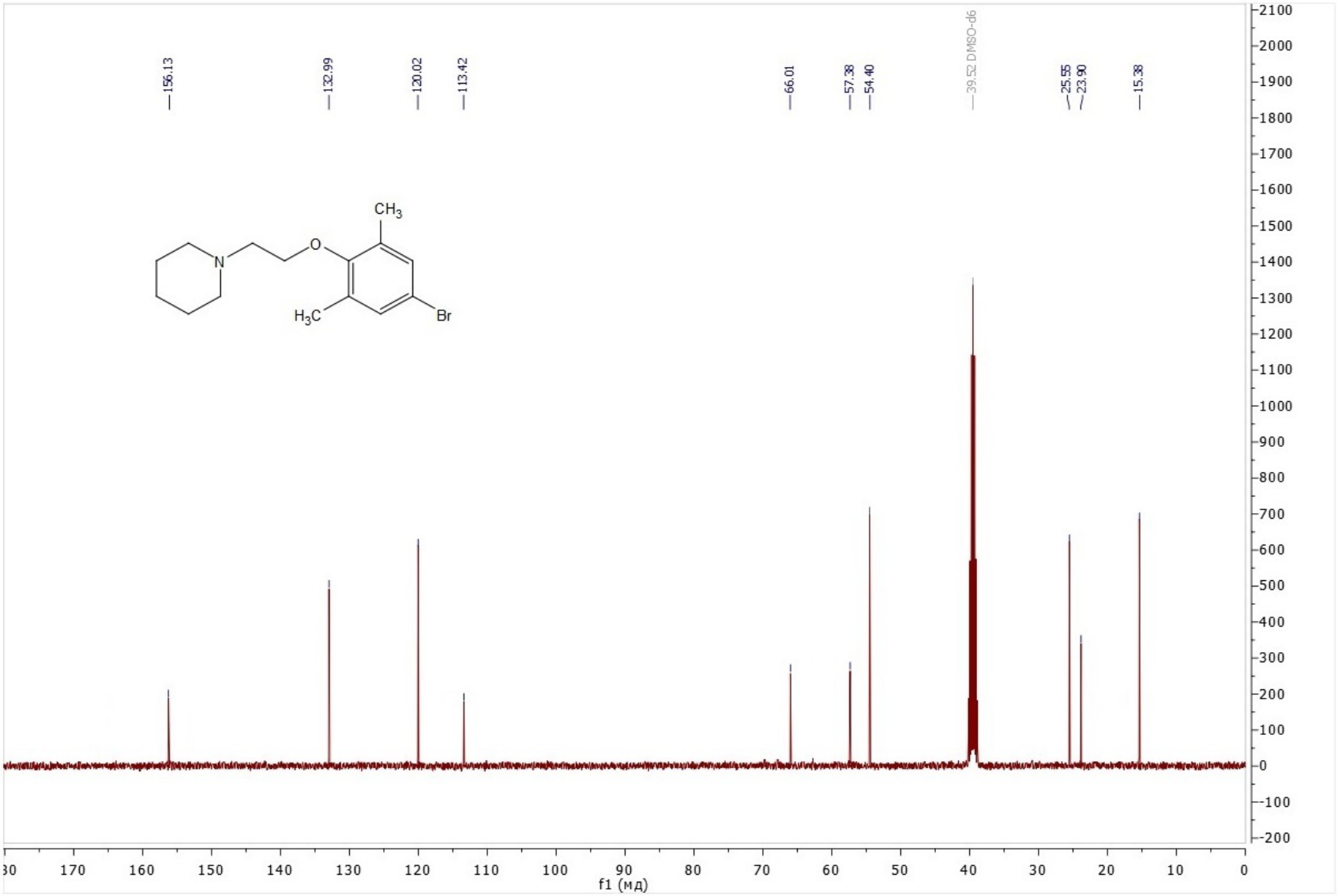


Figure S21. ^{1}H NMR spectrum of **15a**.

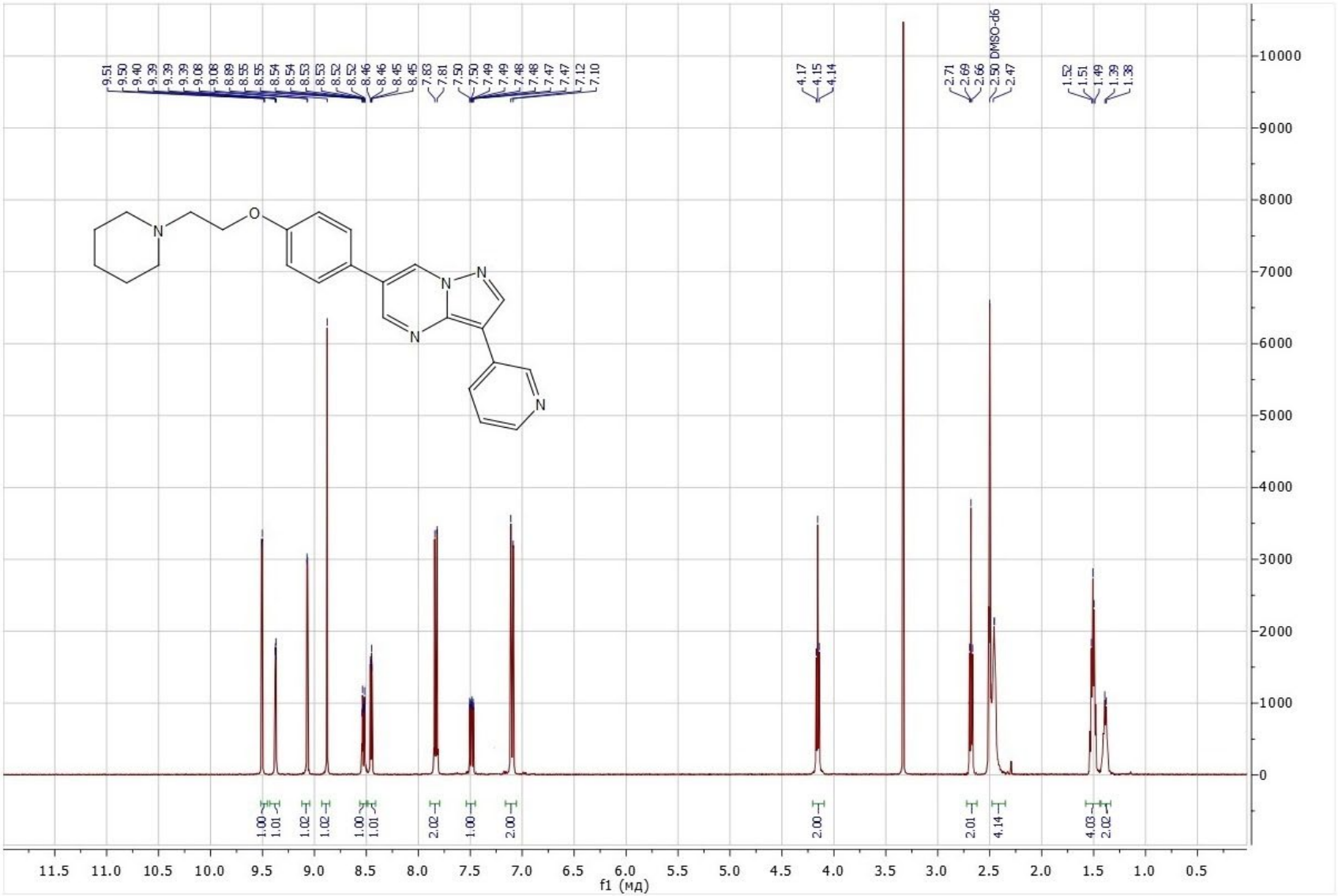


Figure S22. ^{13}C NMR spectrum of **15a**.

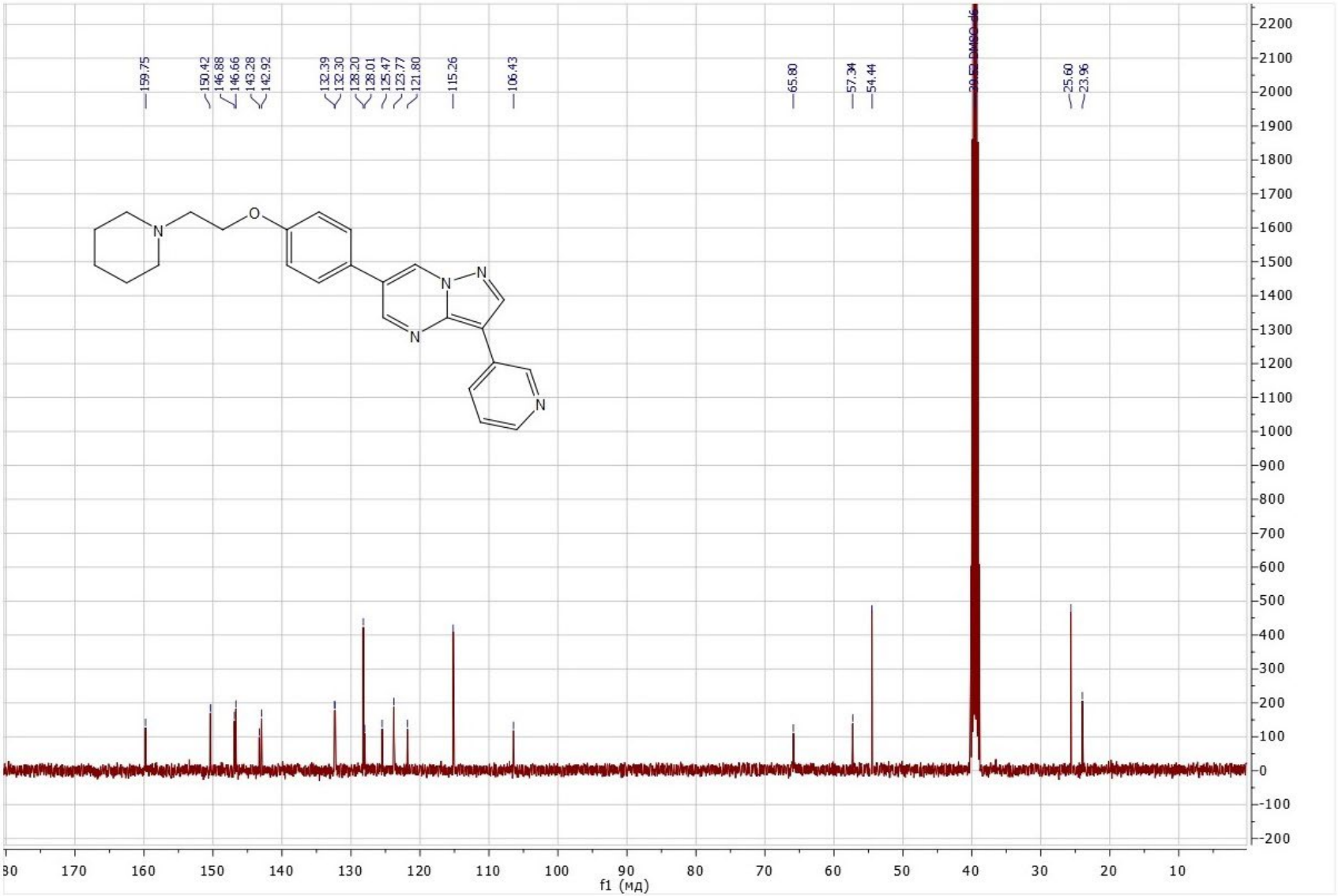


Figure S23. ^{1}H NMR spectrum of **15b**.

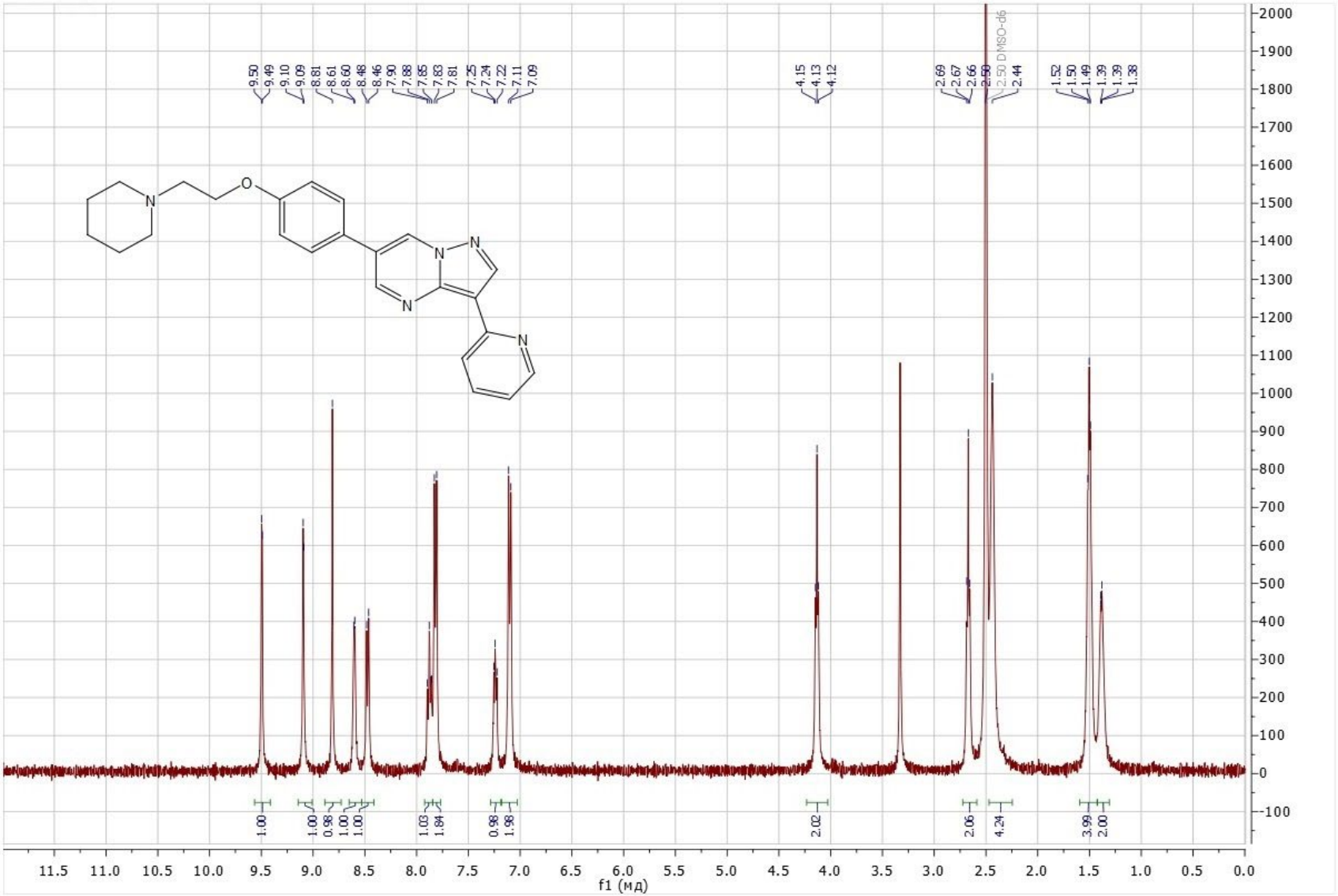


Figure S24. ^{13}C NMR spectrum of **15b**.

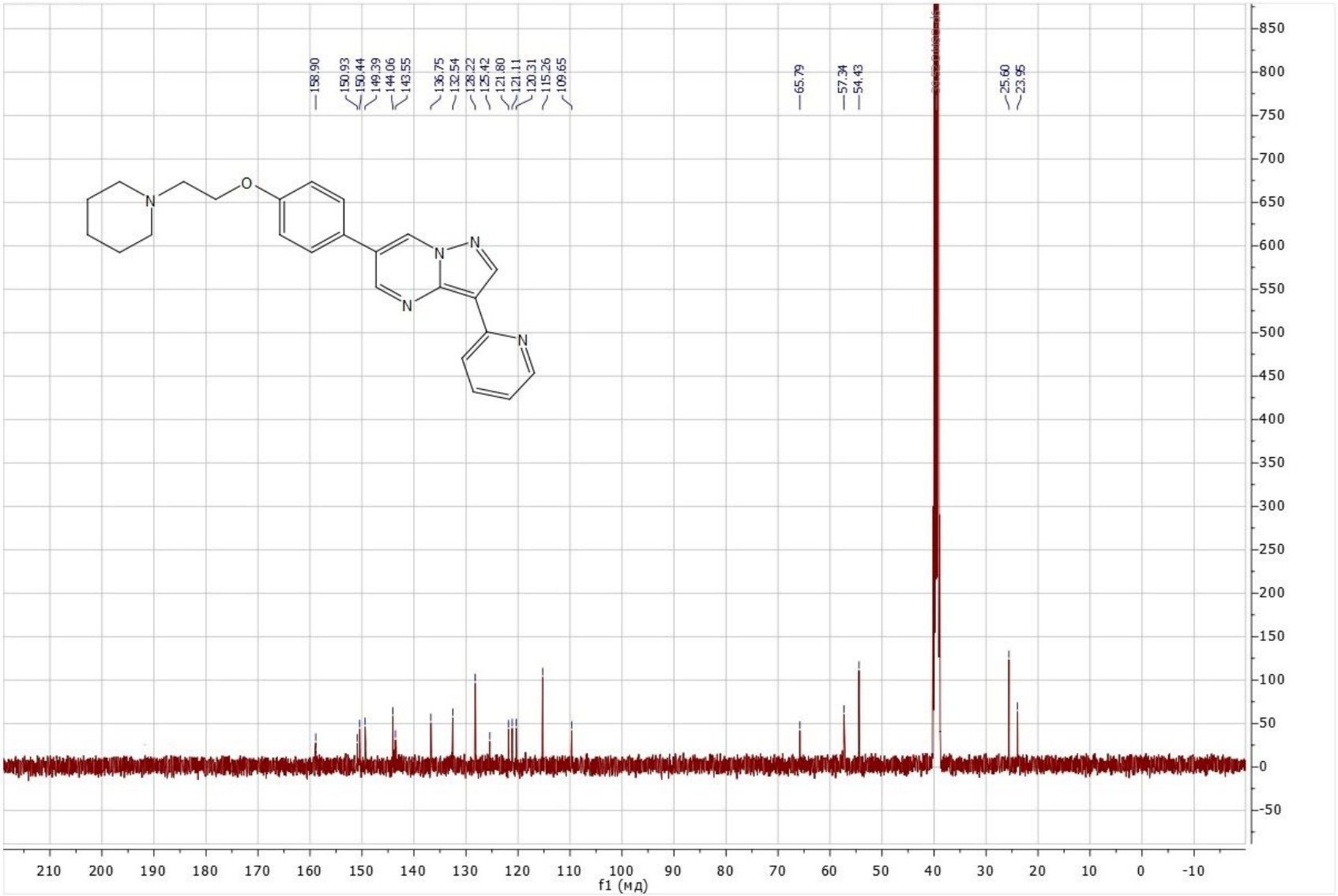


Figure S25. ^{1}H NMR spectrum of **15c**.

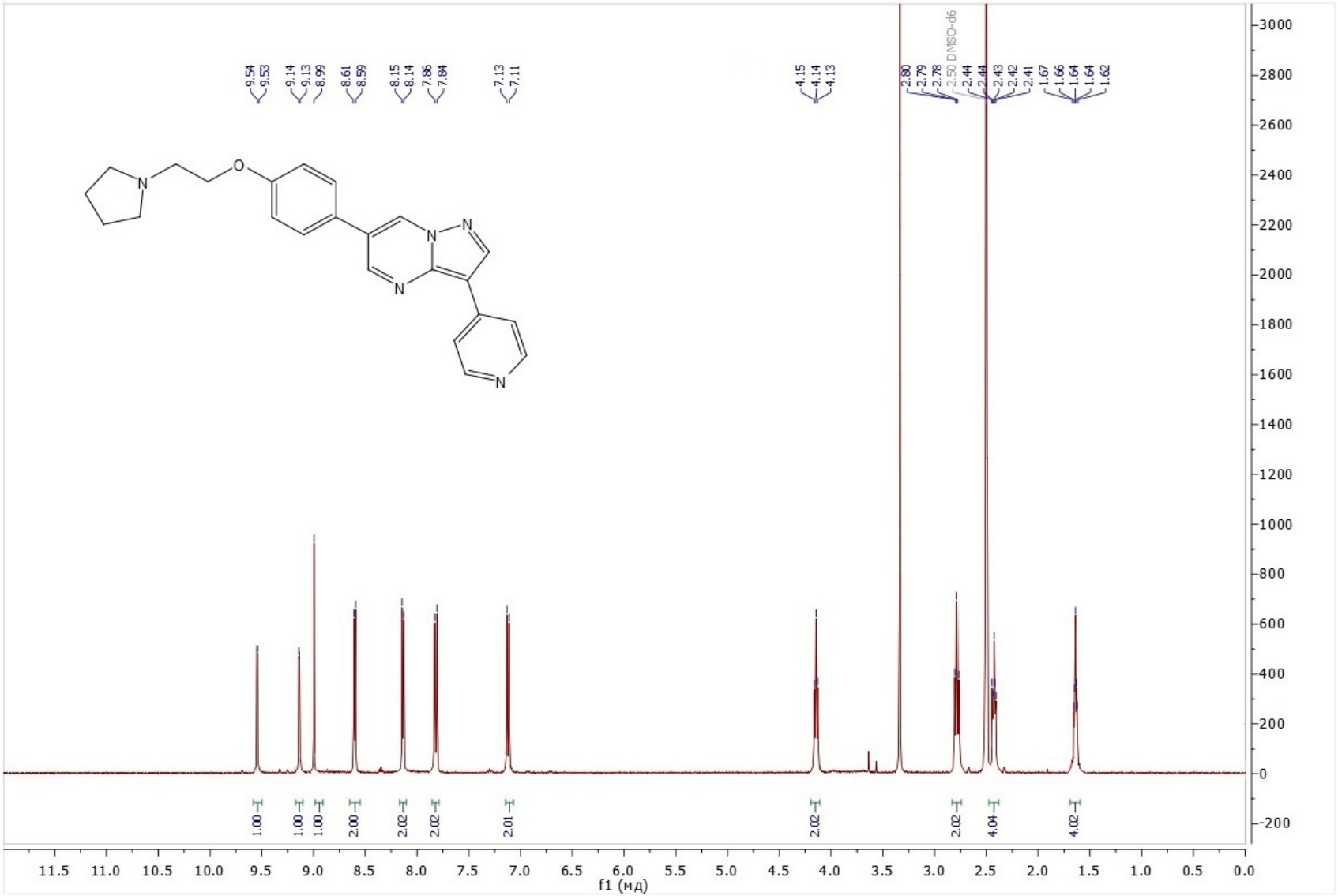


Figure S26. ^{13}C NMR spectrum of **15c**.

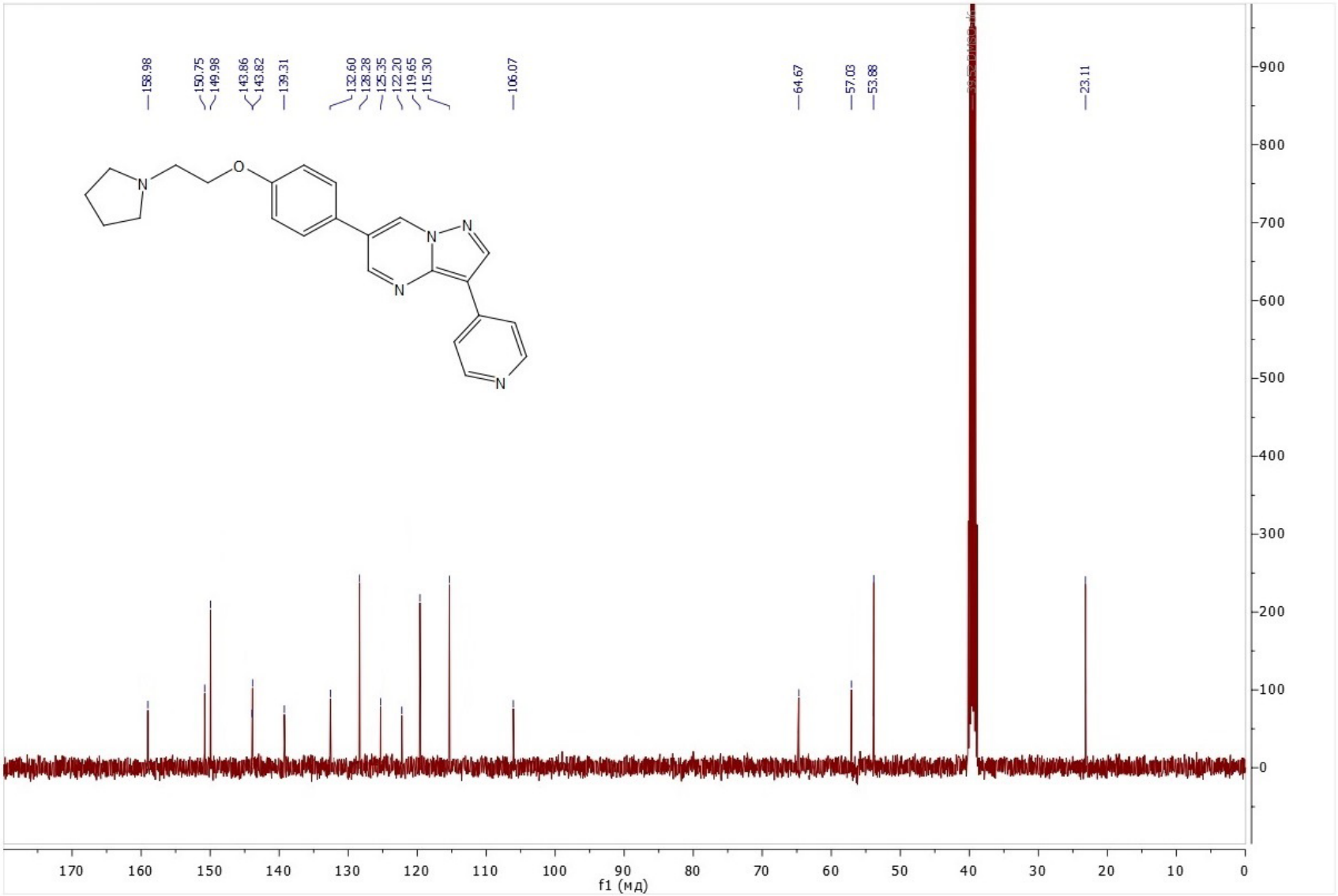


Figure S27. ^{1}H NMR spectrum of **15d**.

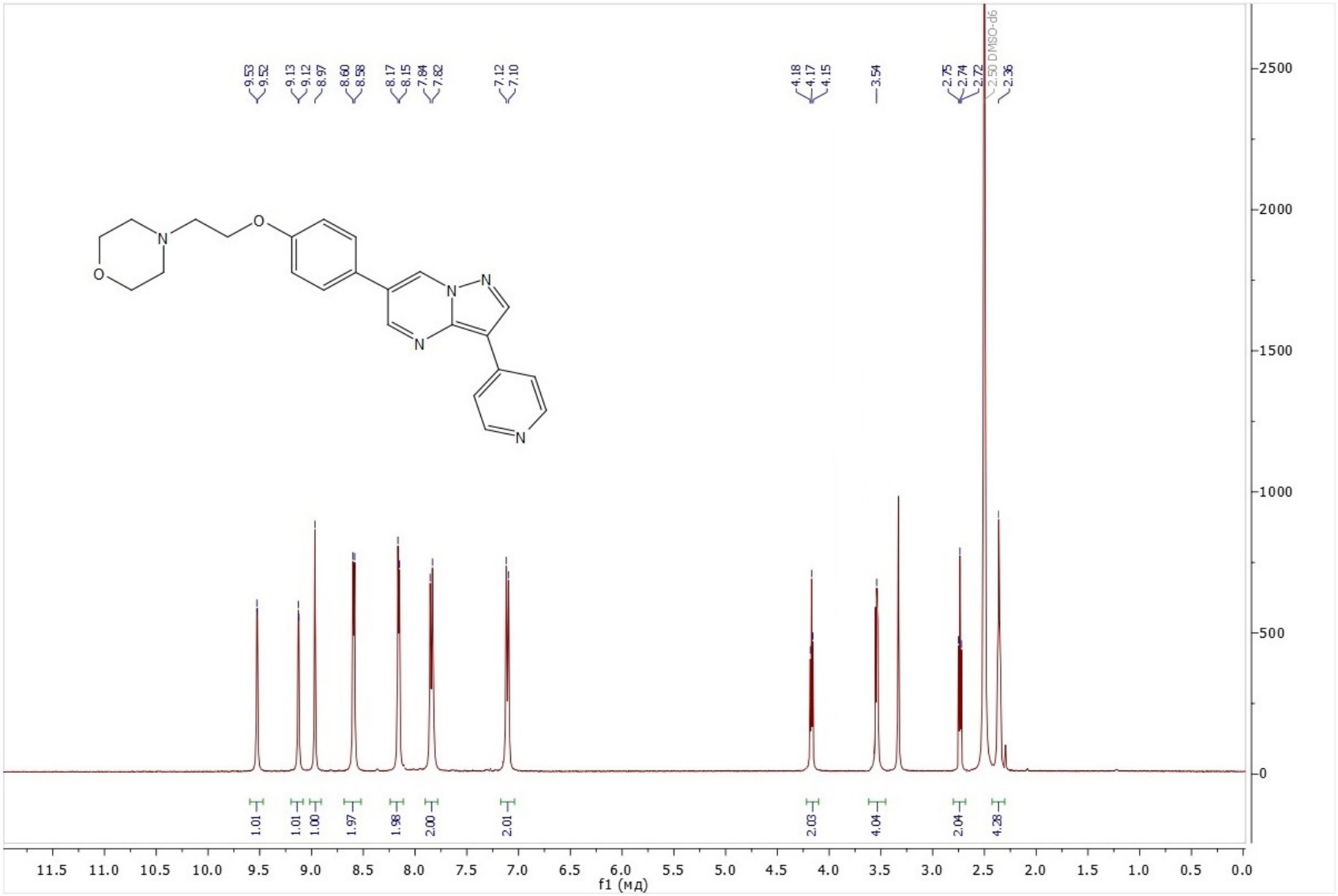


Figure S28. ^{13}C NMR spectrum of **15d**.

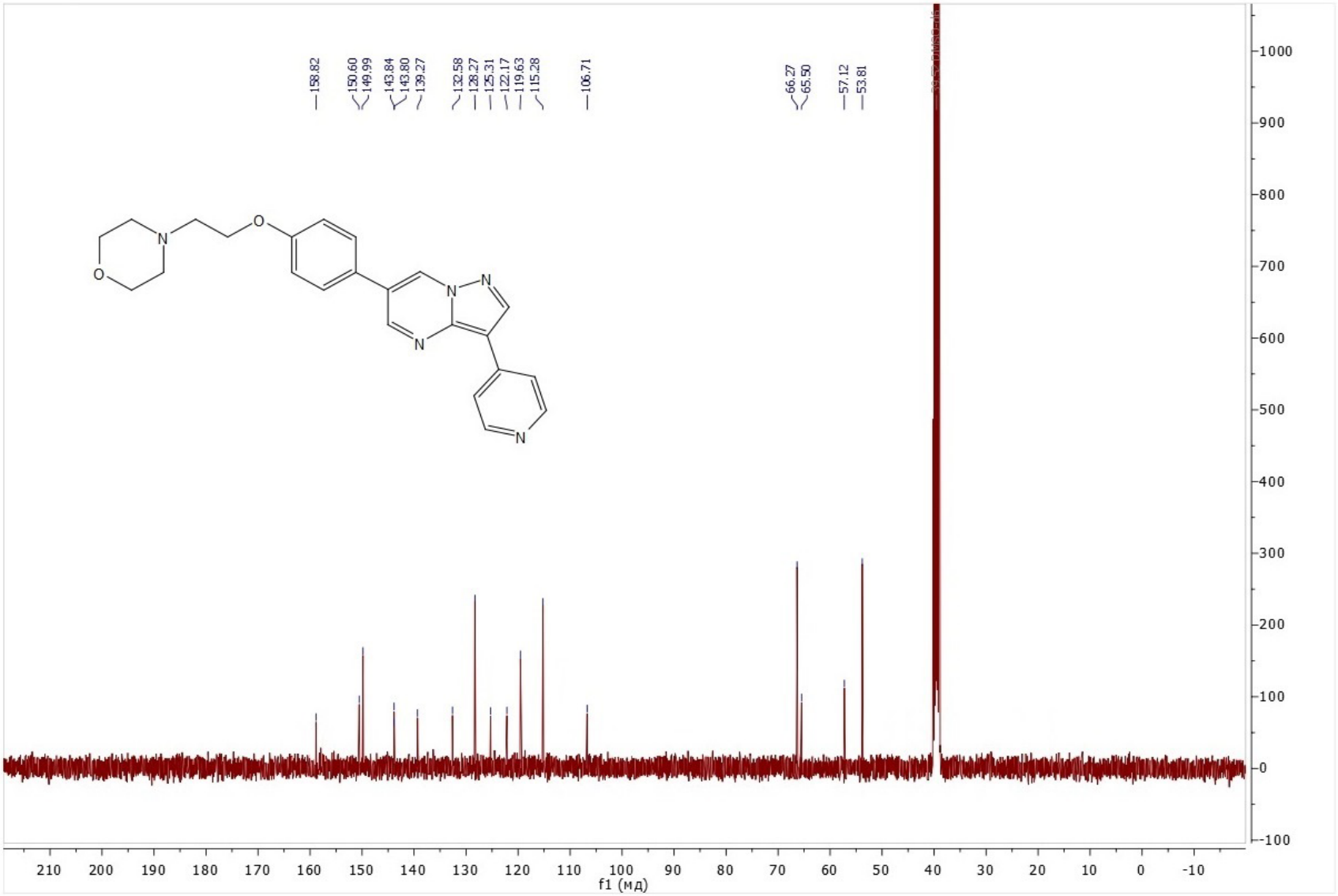


Figure S29. ^{1}H NMR spectrum of **15e**.

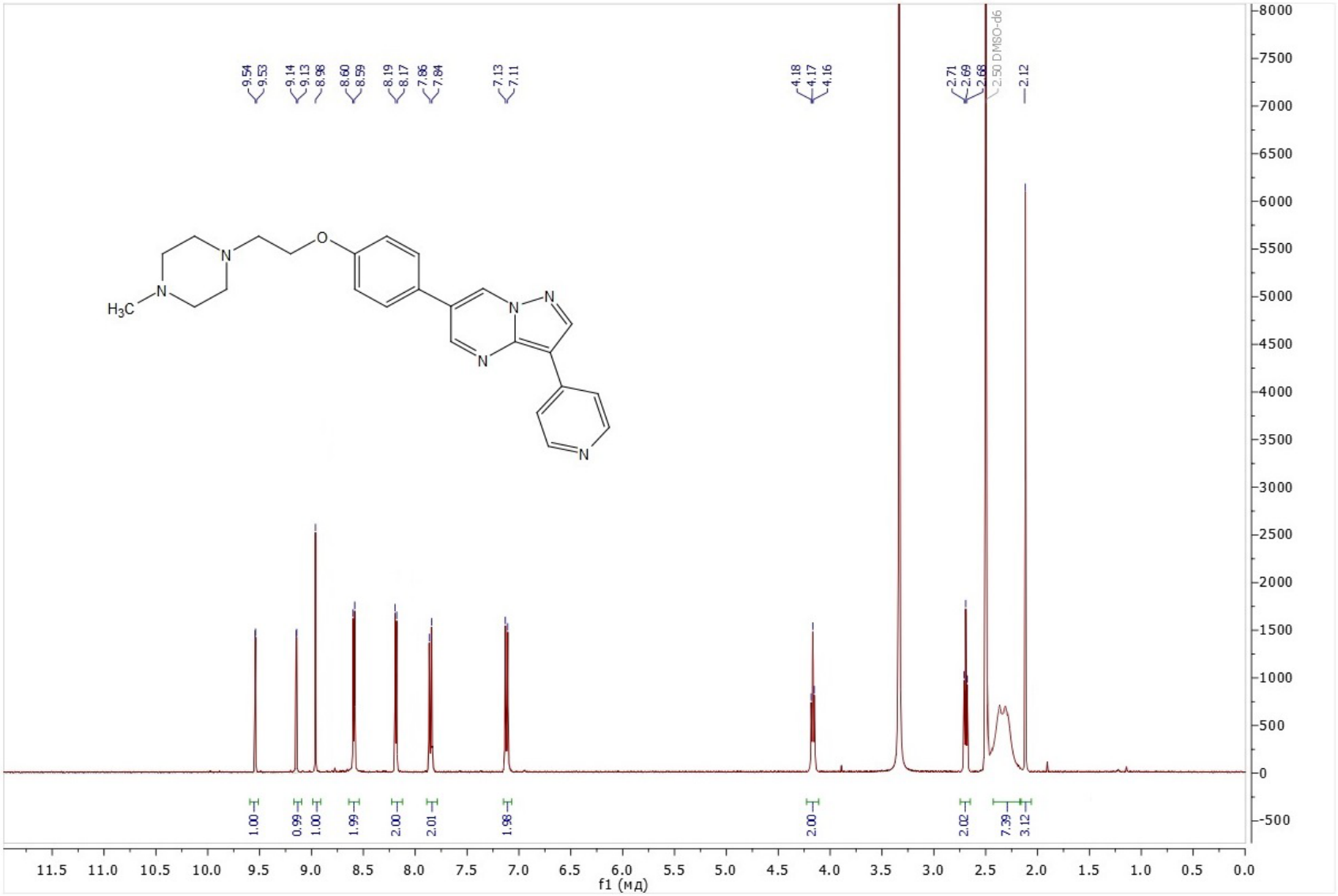


Figure S30. ^{13}C NMR spectrum of **15e**.

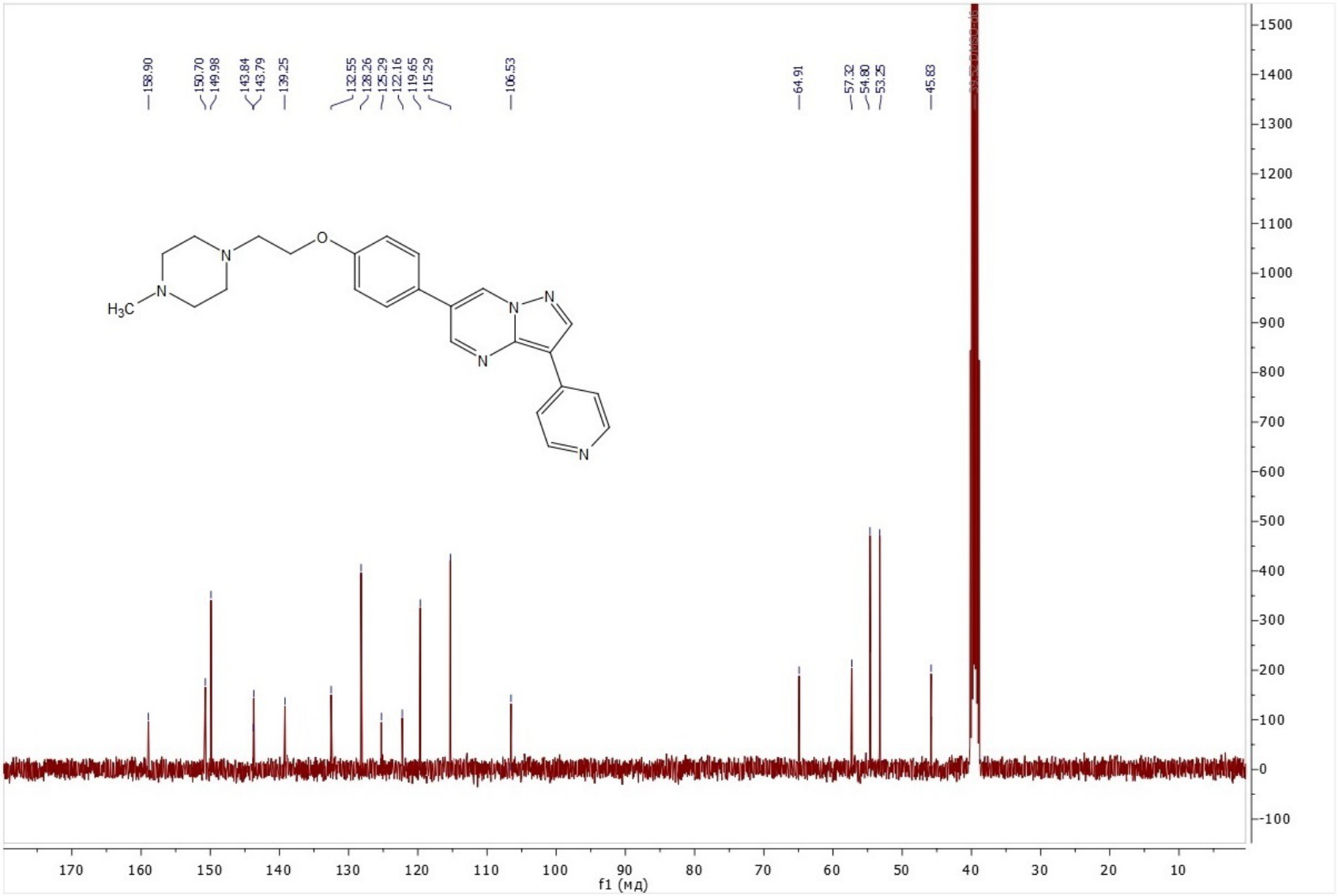


Figure S31. ^{1}H NMR spectrum of **15f**.

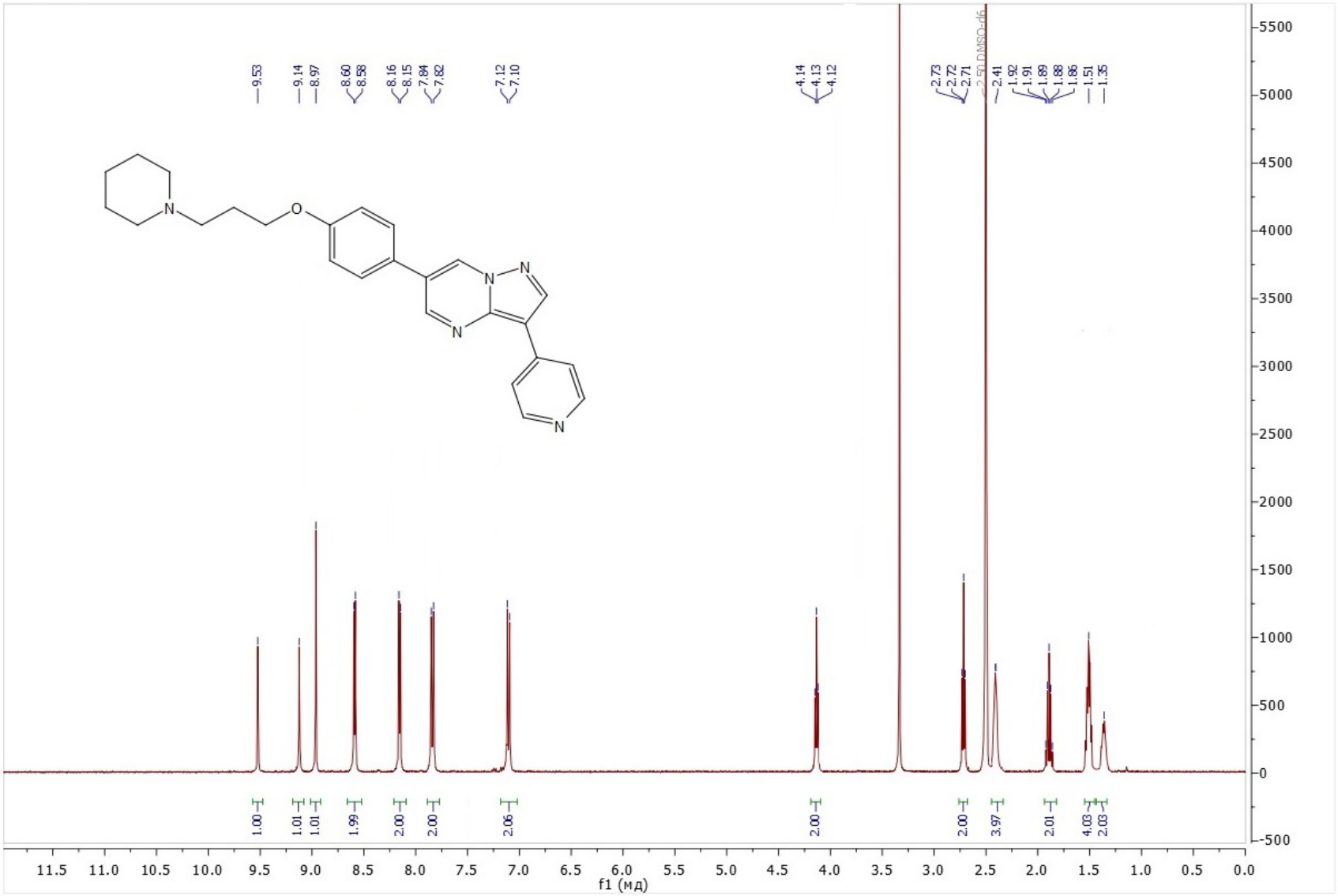


Figure S32. ^{13}C NMR spectrum of **15f**.

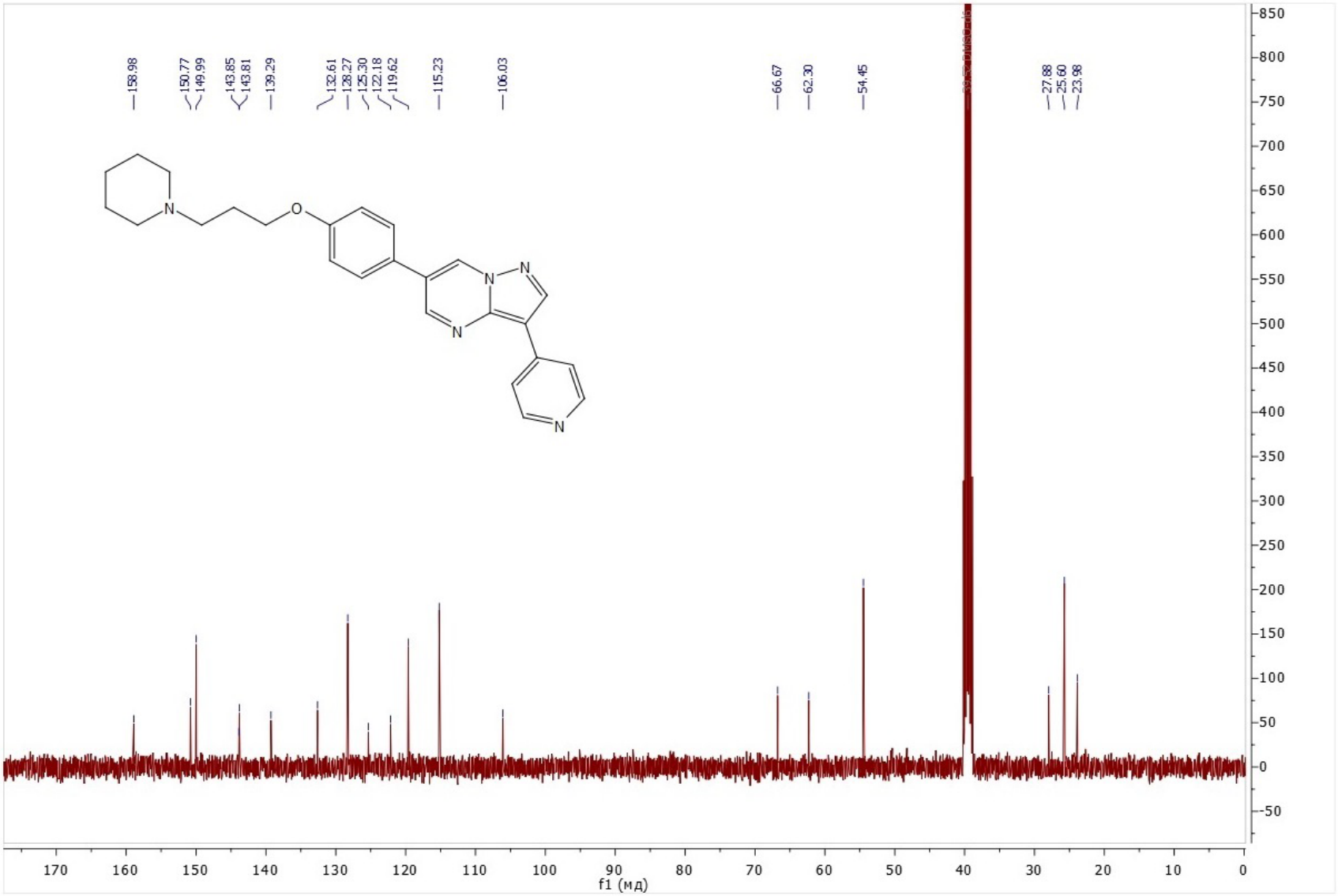


Figure S33. ^{1}H NMR spectrum of **15g**.

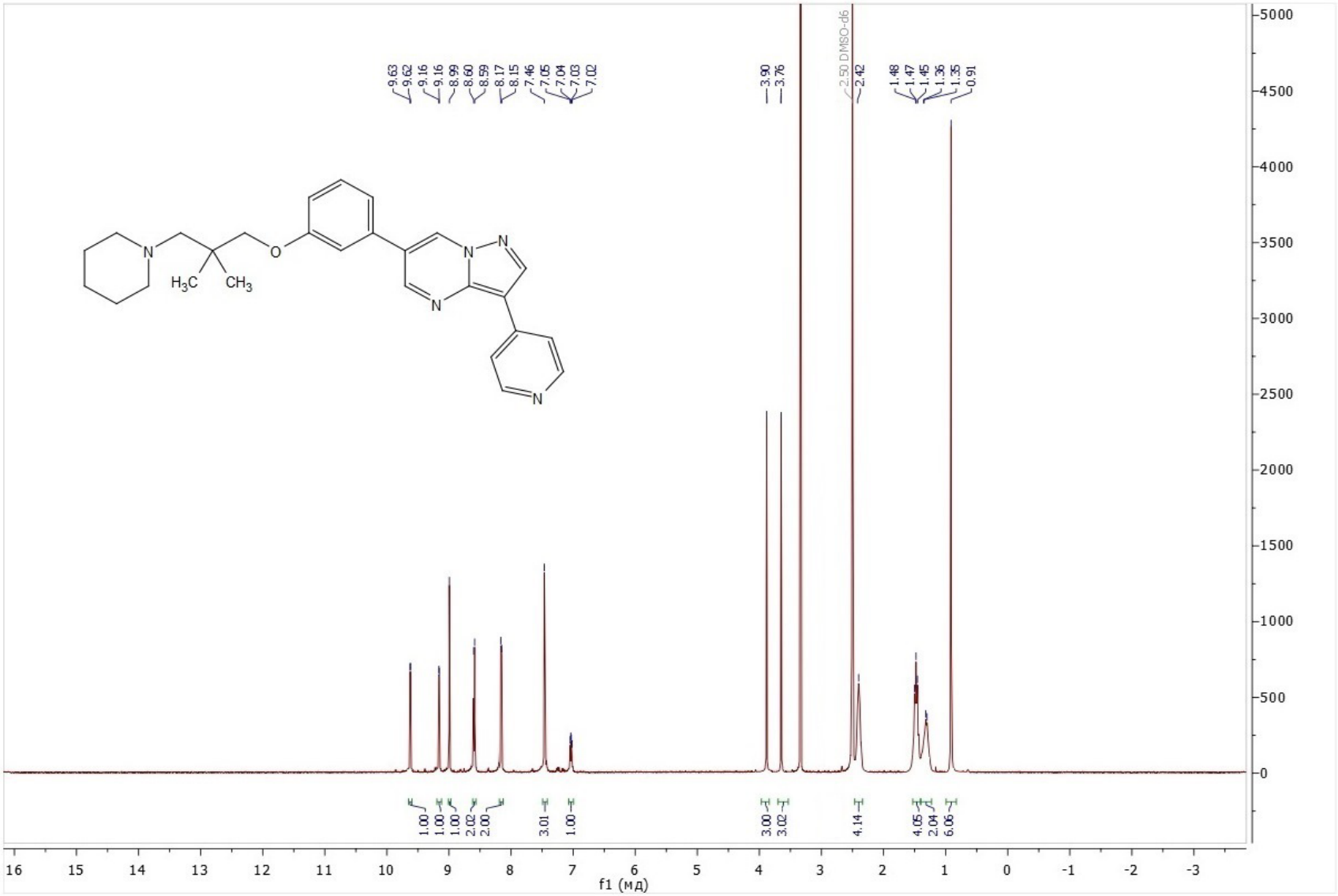


Figure S34. ^{13}C NMR spectrum of **15g**.

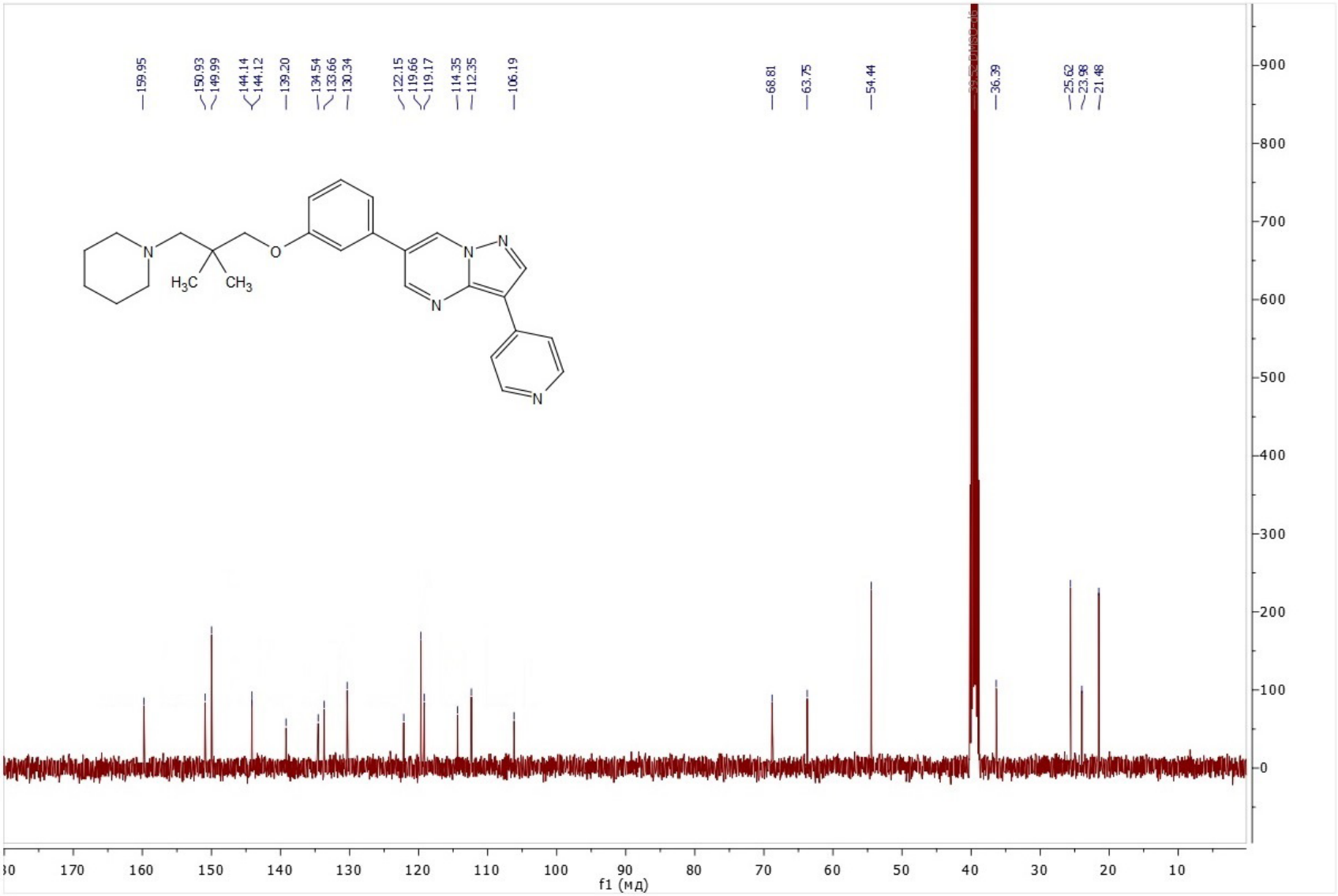


Figure S35. ^{1}H NMR spectrum of **15h**.

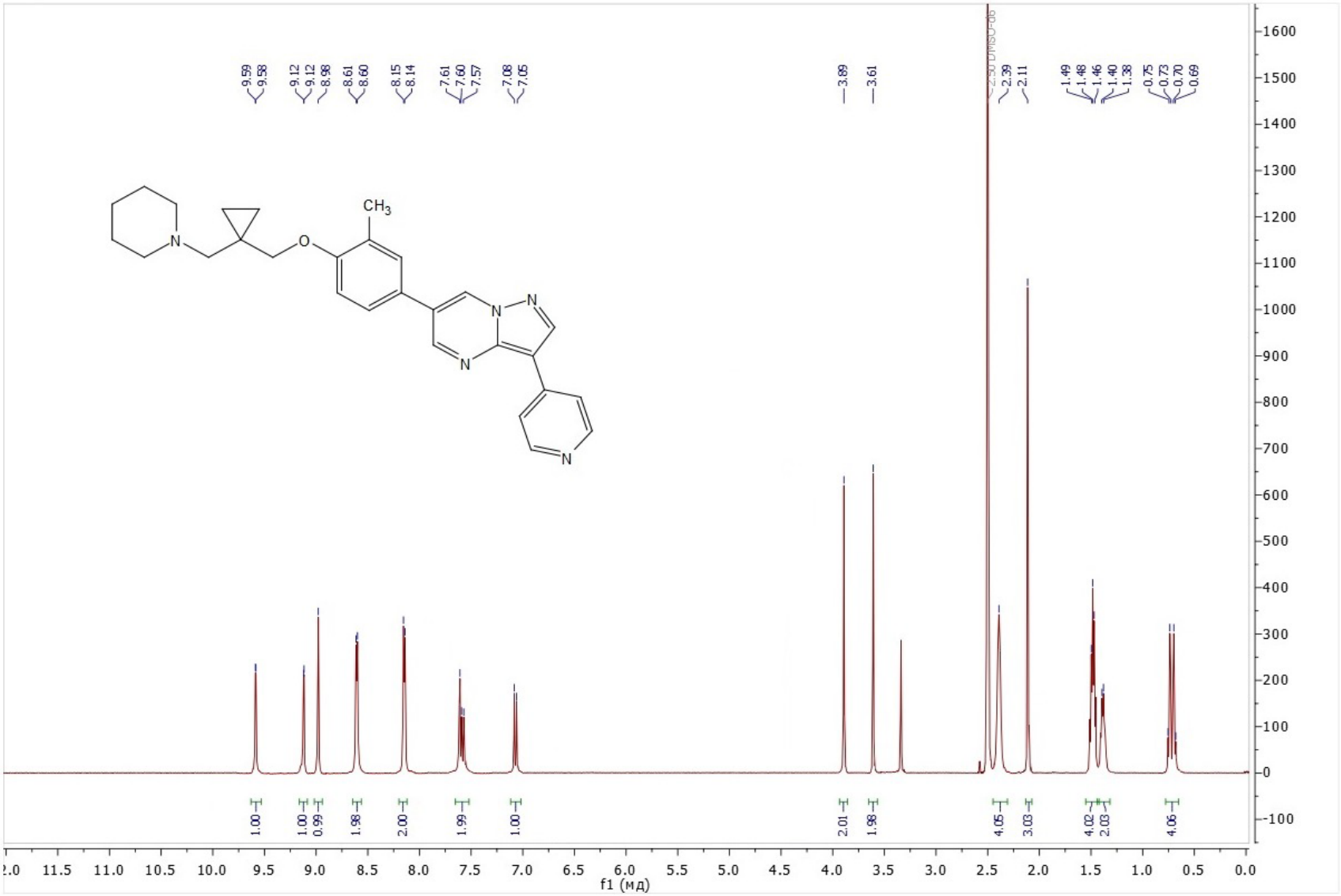


Figure S36. ^{13}C NMR spectrum of **15h**.

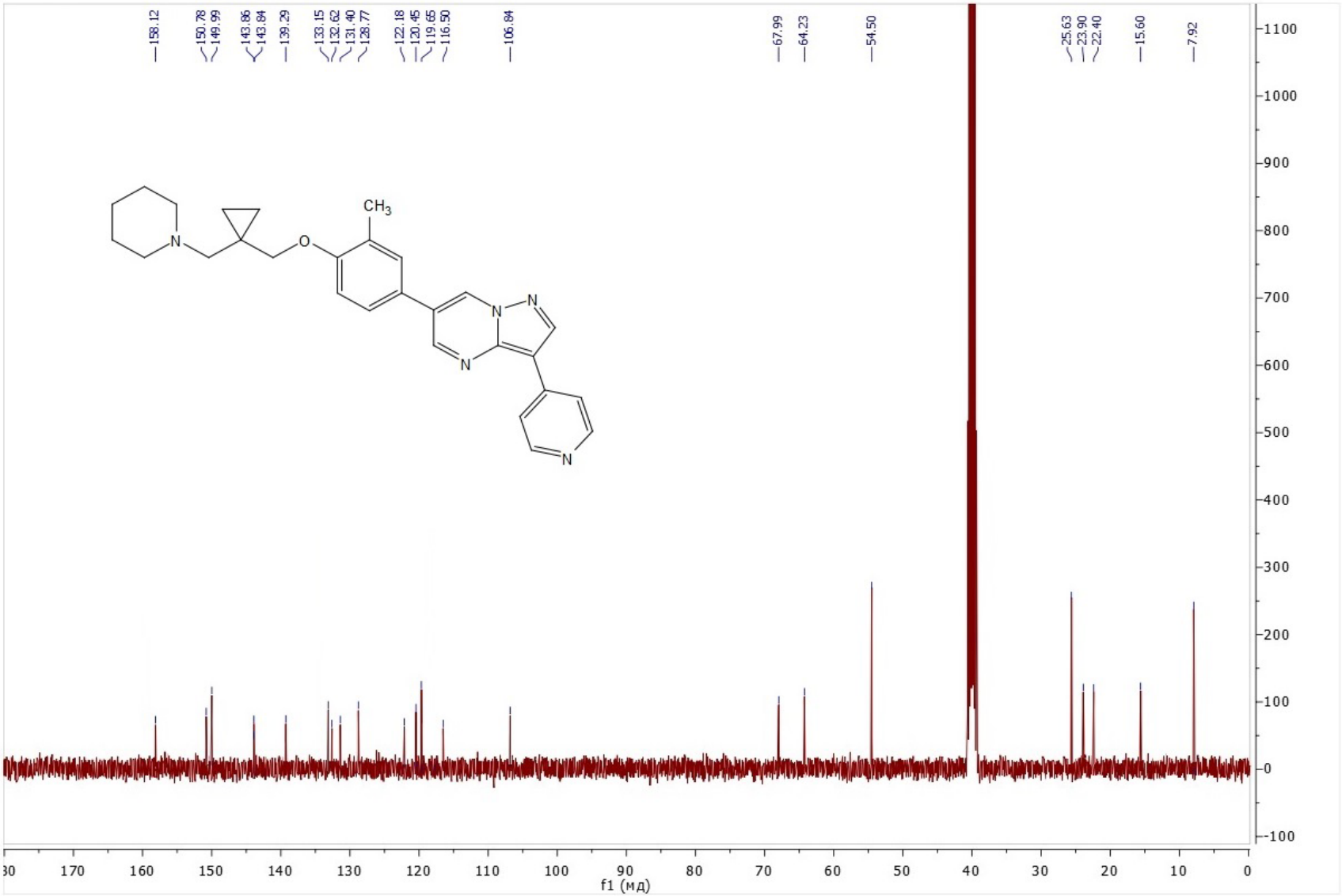


Figure S37. ^{1}H NMR spectrum of **15i**.

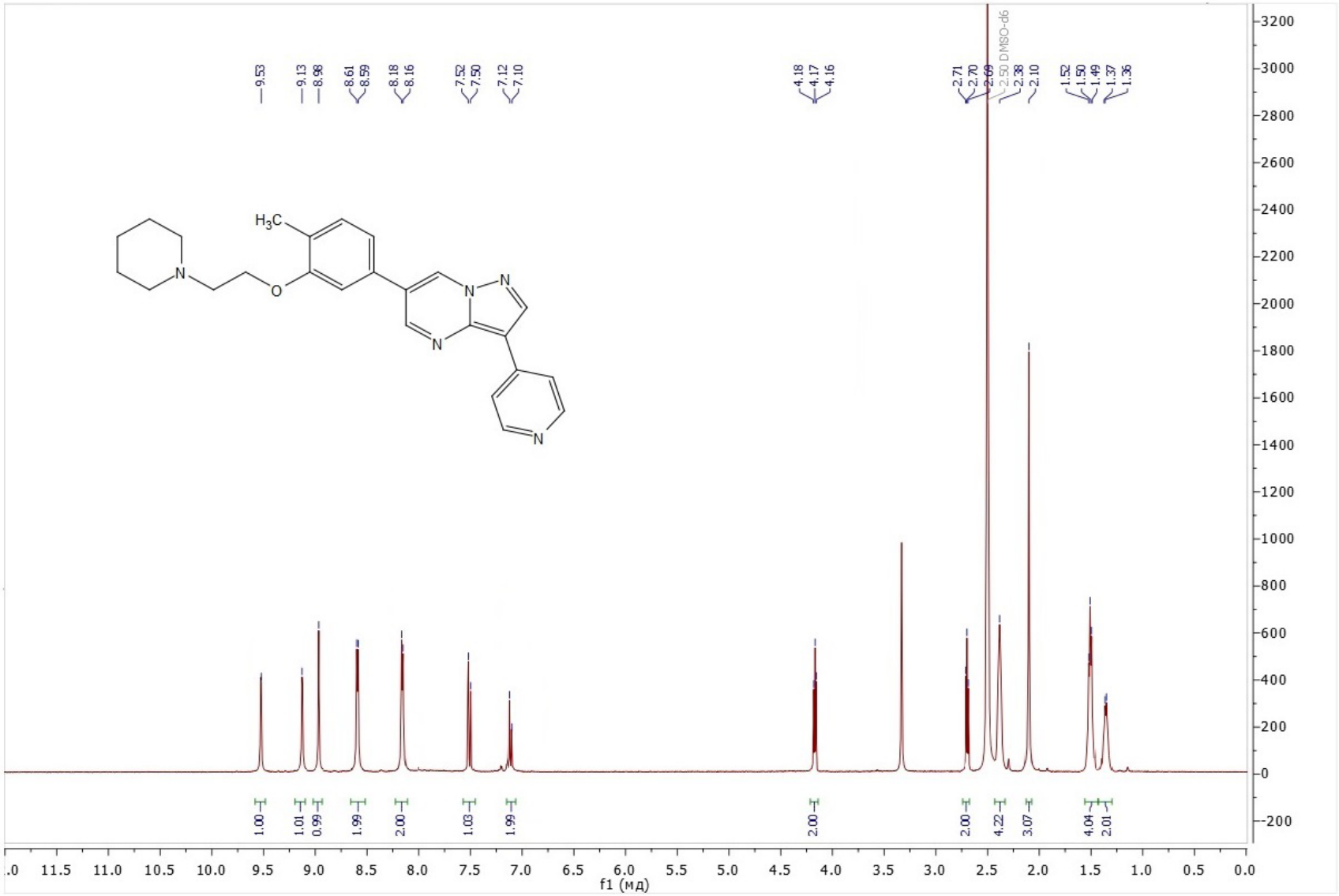


Figure S38. ^{13}C NMR spectrum of **15i**.

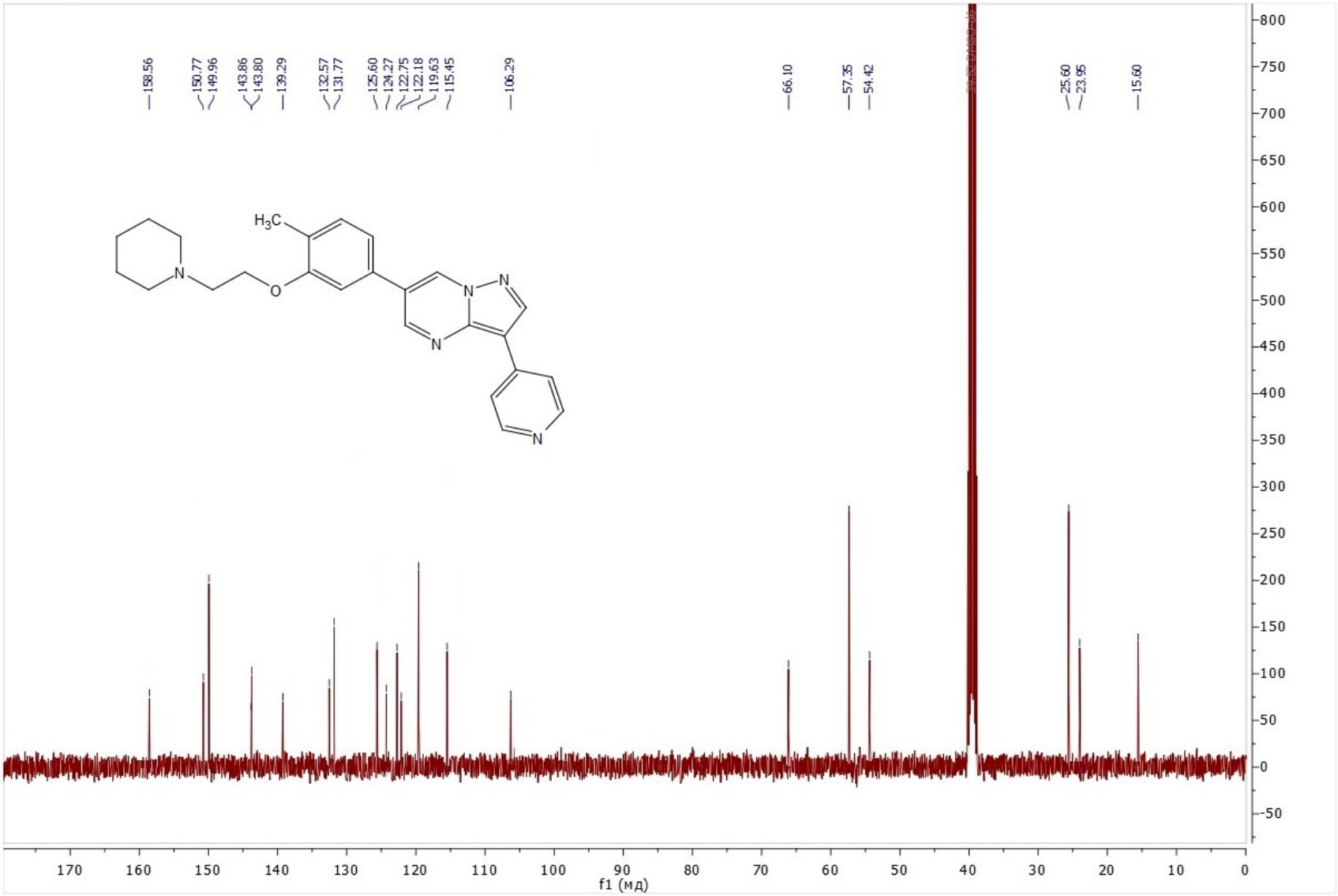


Figure S39. ^{1}H NMR spectrum of **15j**.

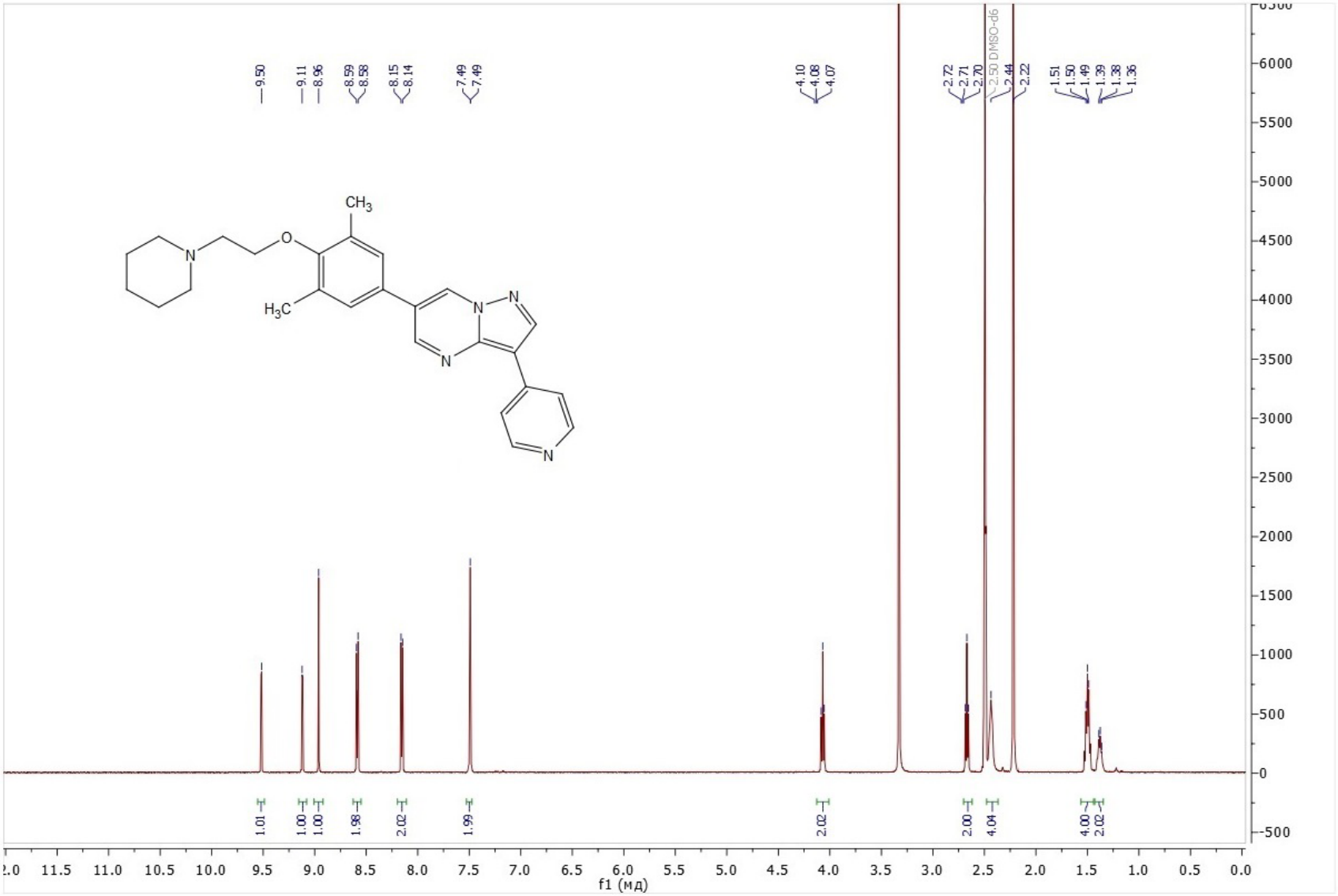


Figure S40. ^{13}C NMR spectrum of **15j**.

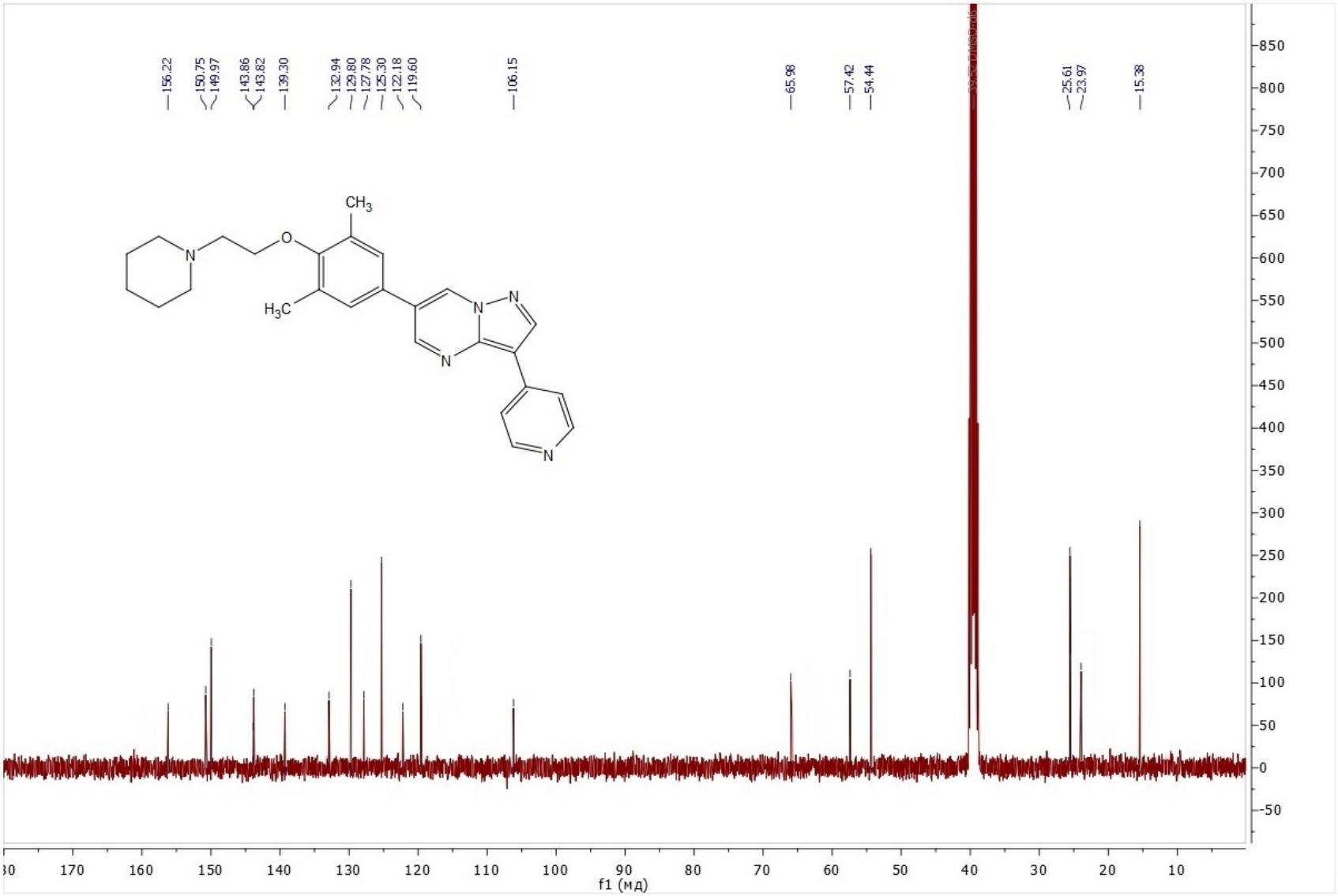


Figure S41. ^{1}H NMR spectrum of **15k**.

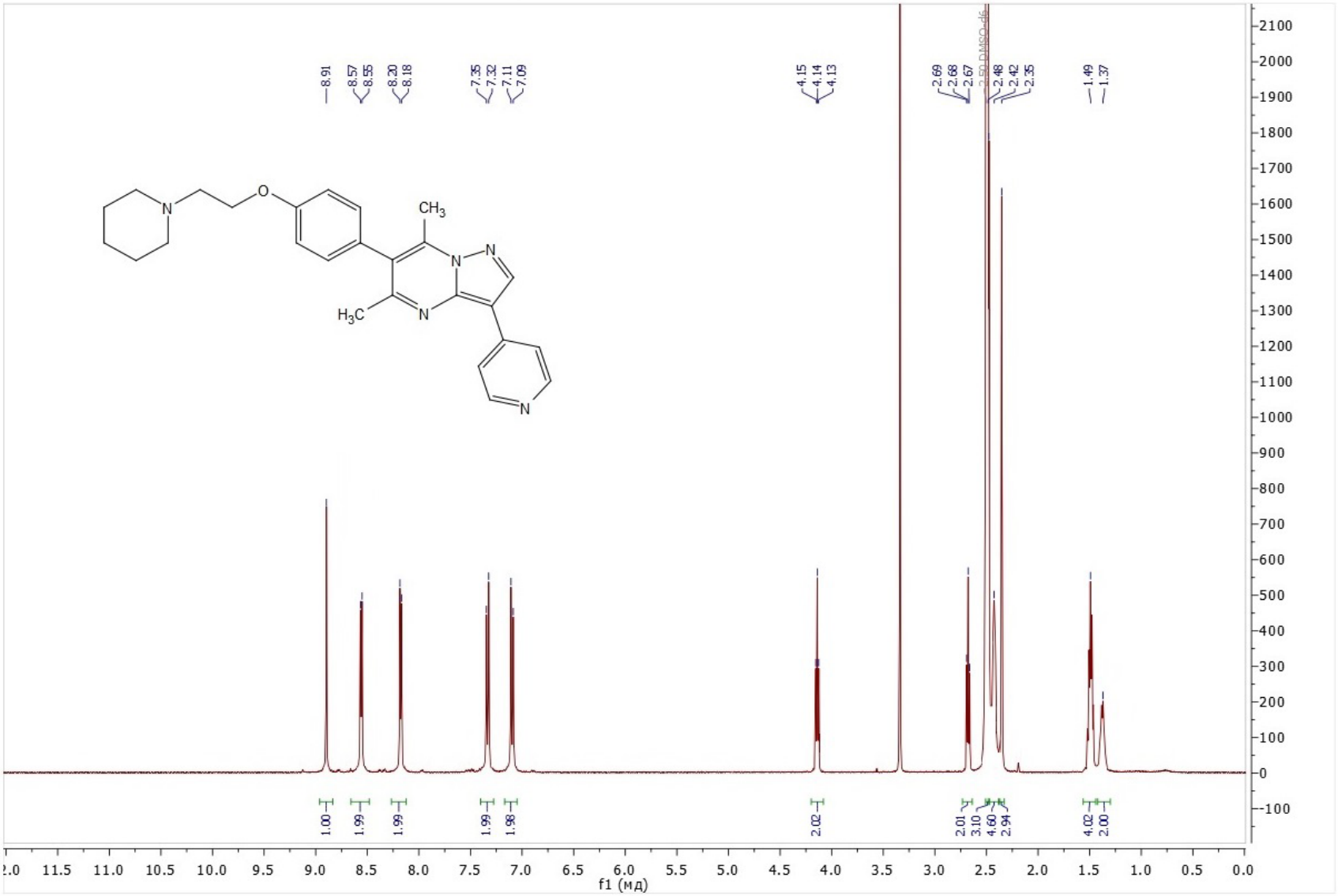


Figure S42. ^{13}C NMR spectrum of **15k**.

