

Supplementary Material

New derivatives of 5-substituted uracils: potential agents with a wide spectrum of biological activity

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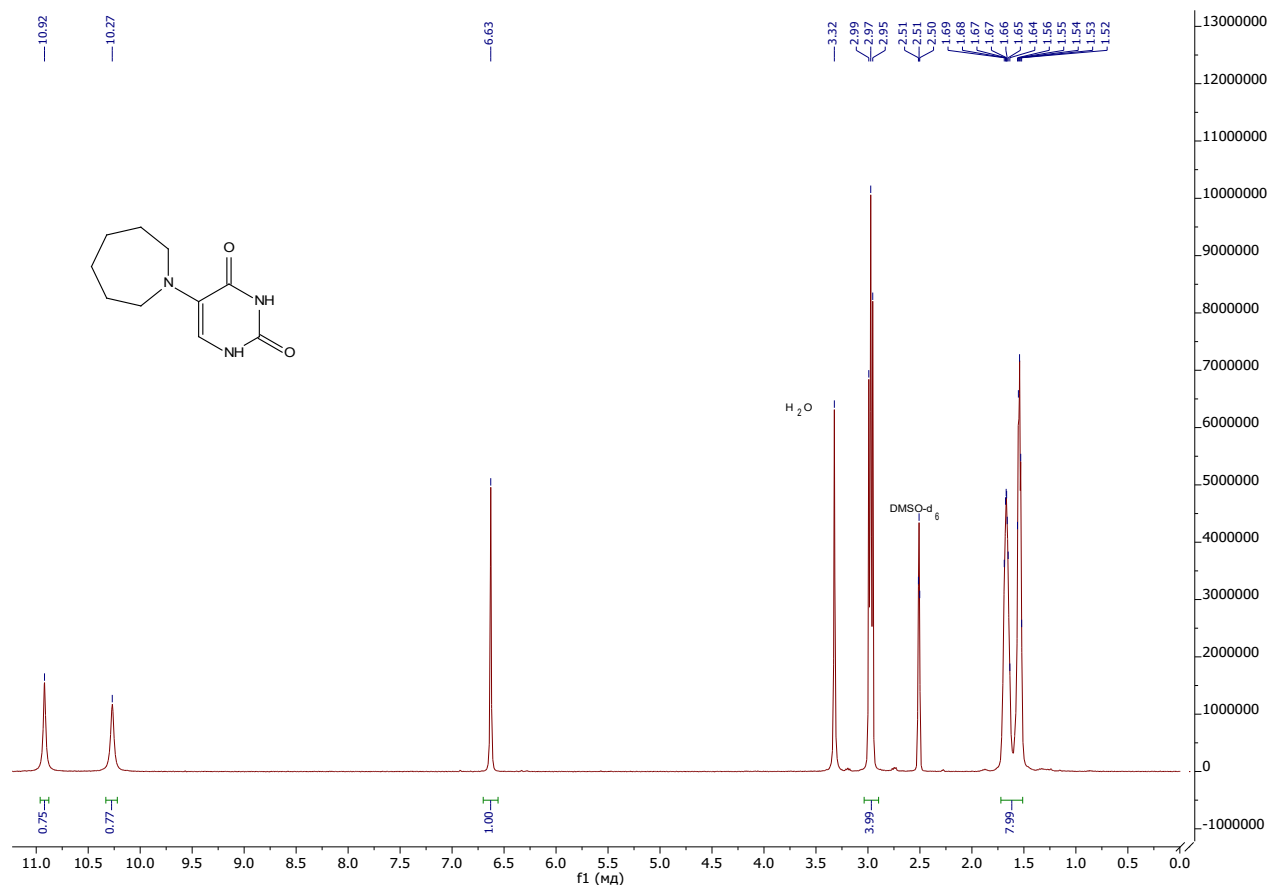


Figure S1 ¹H NMR spectrum of compound **2a** in DMSO-*d*₆

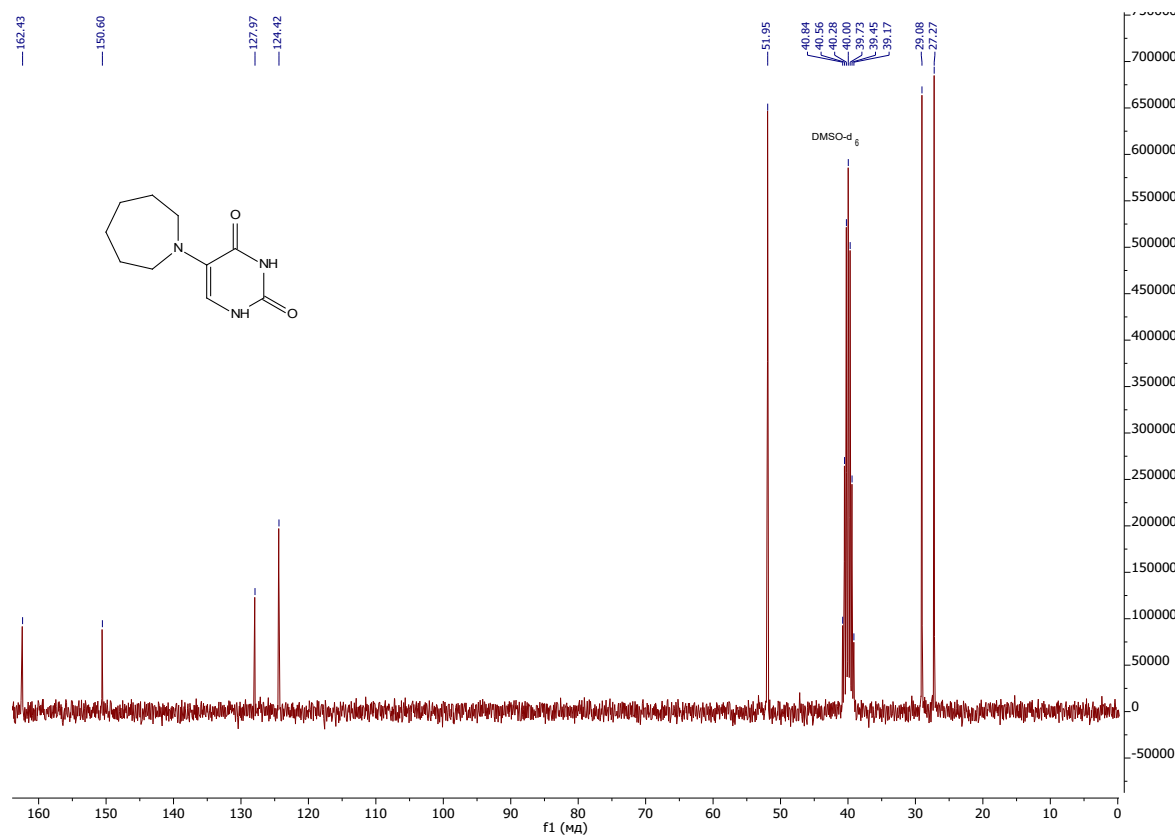


Figure S2 ¹³C NMR spectrum of compound **2a** in DMSO-*d*₆

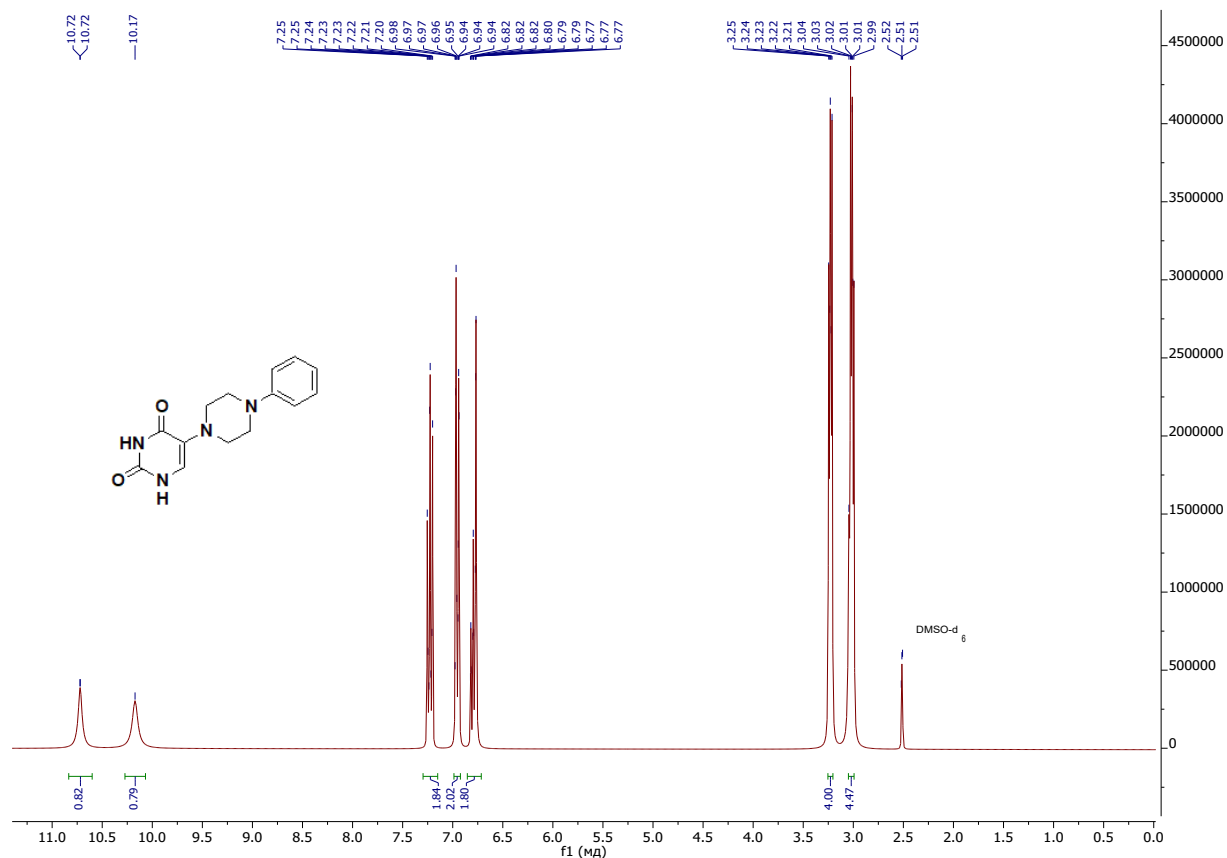


Figure S3 ¹H NMR spectrum of compound **2b** in DMSO-*d*₆ at 400 MHz.

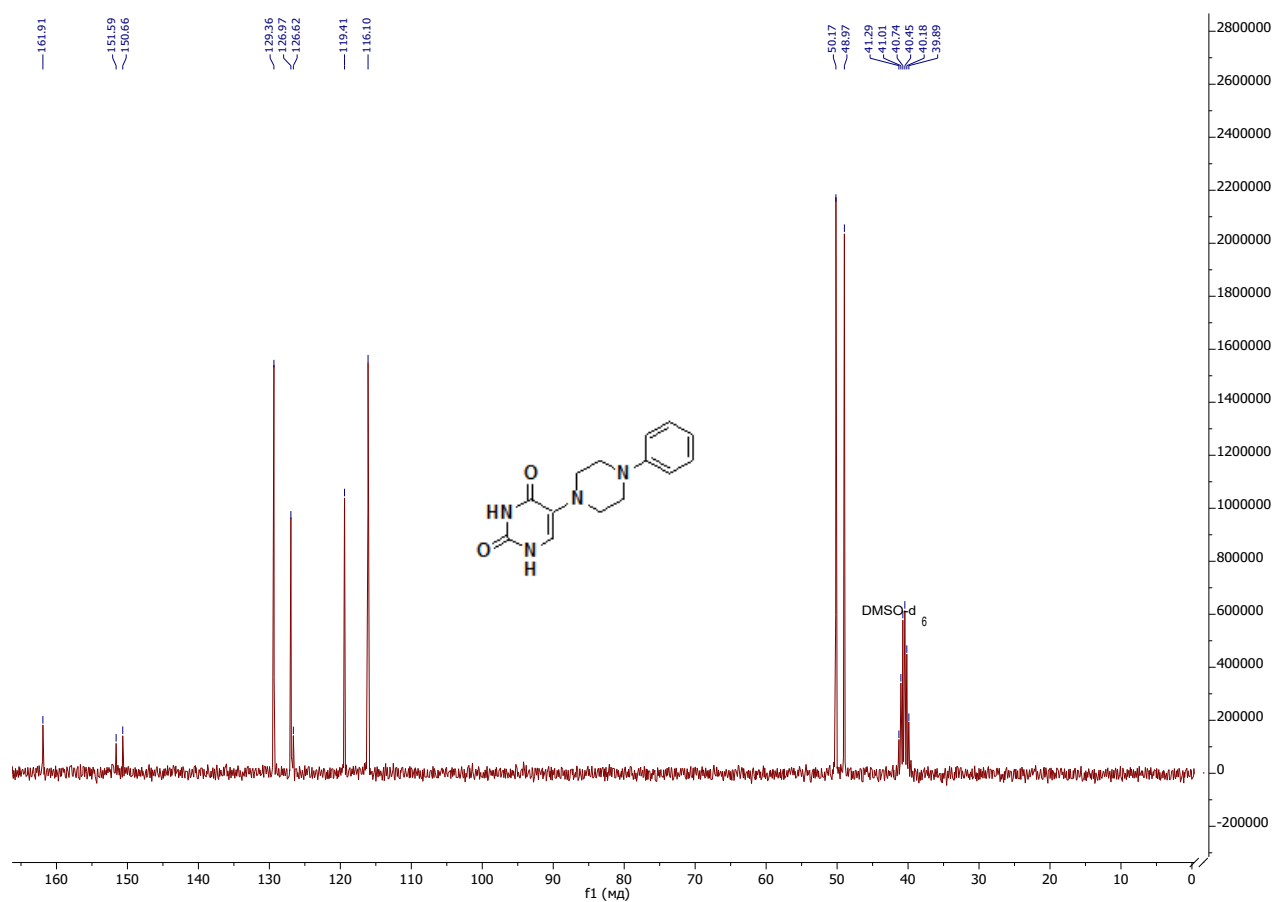


Figure S4 ¹³C NMR spectrum of compound **2b** in DMSO-*d*₆ at 100 MHz.

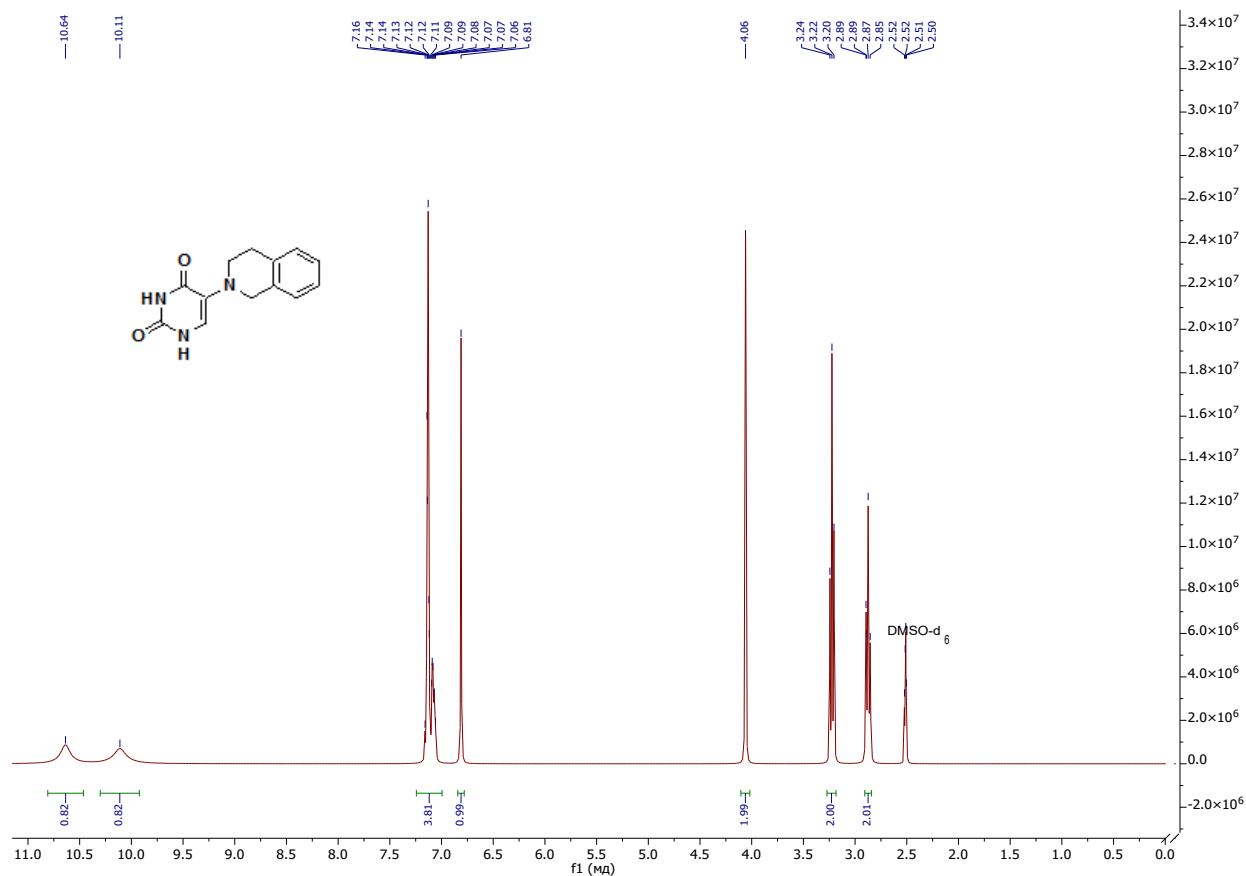


Figure S5 ¹H NMR spectrum of compound **2c** in DMSO-*d*₆ at 400 MHz.

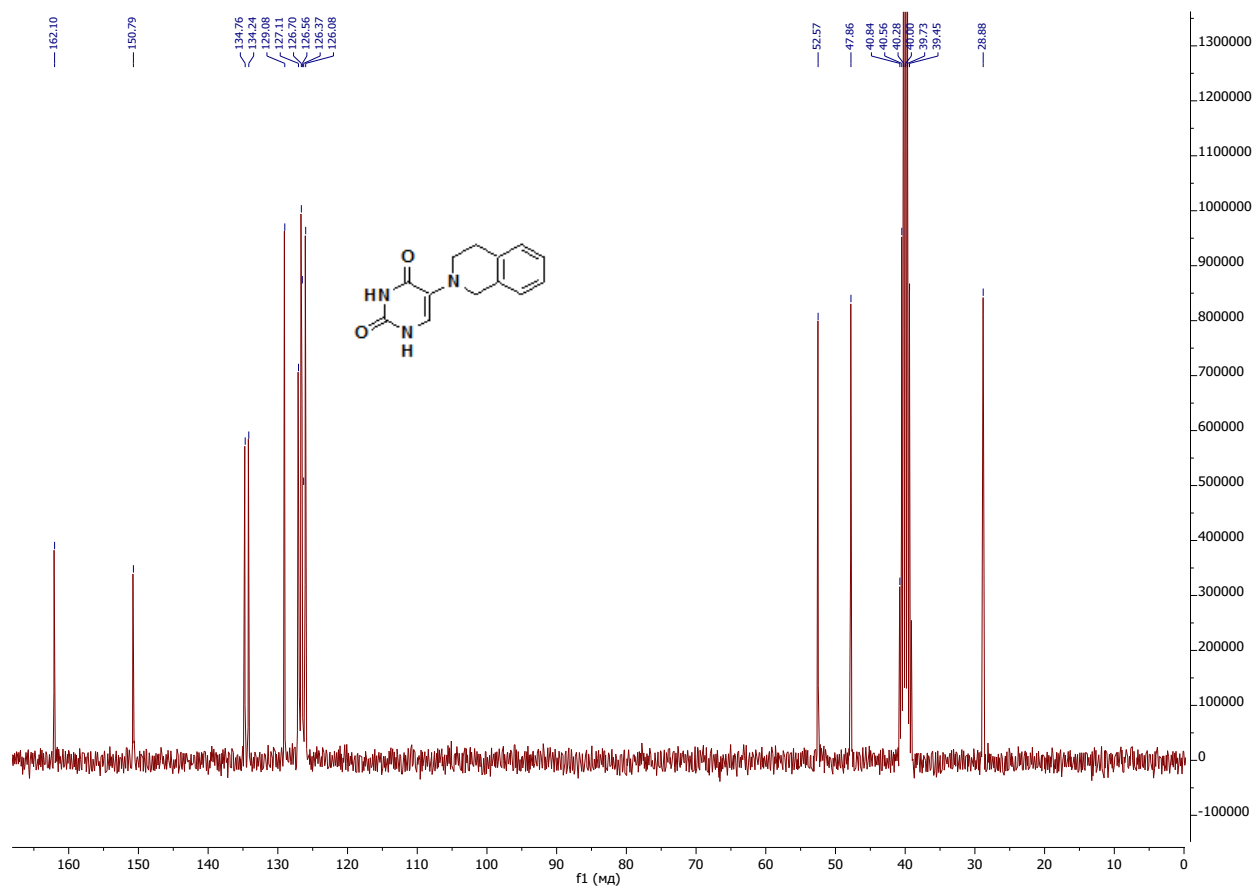


Figure S6 ¹³C NMR spectrum of compound **2c** in DMSO-*d*₆ at 100 MHz.

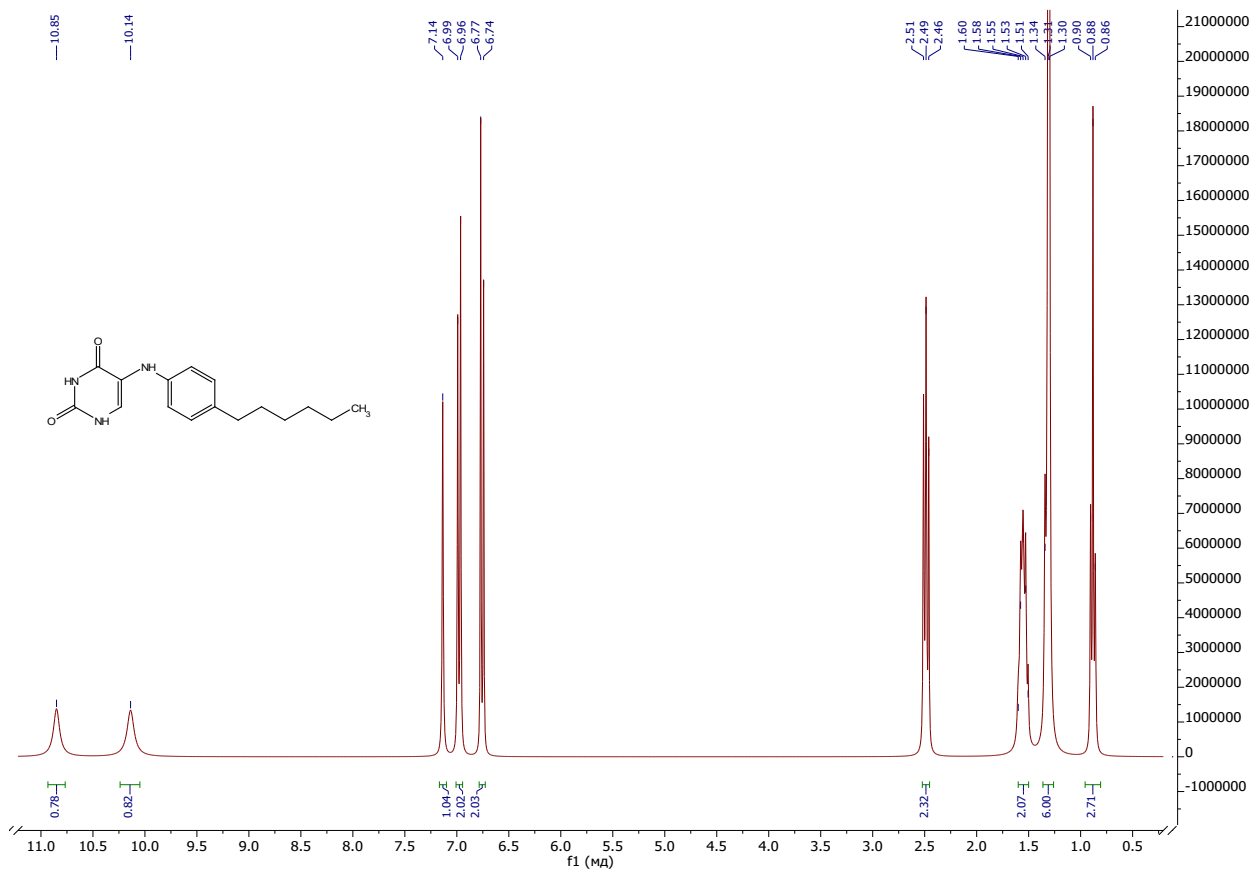


Figure S7 ¹H NMR spectrum of compound **2d** in DMSO-*d*₆ at 400 MHz.

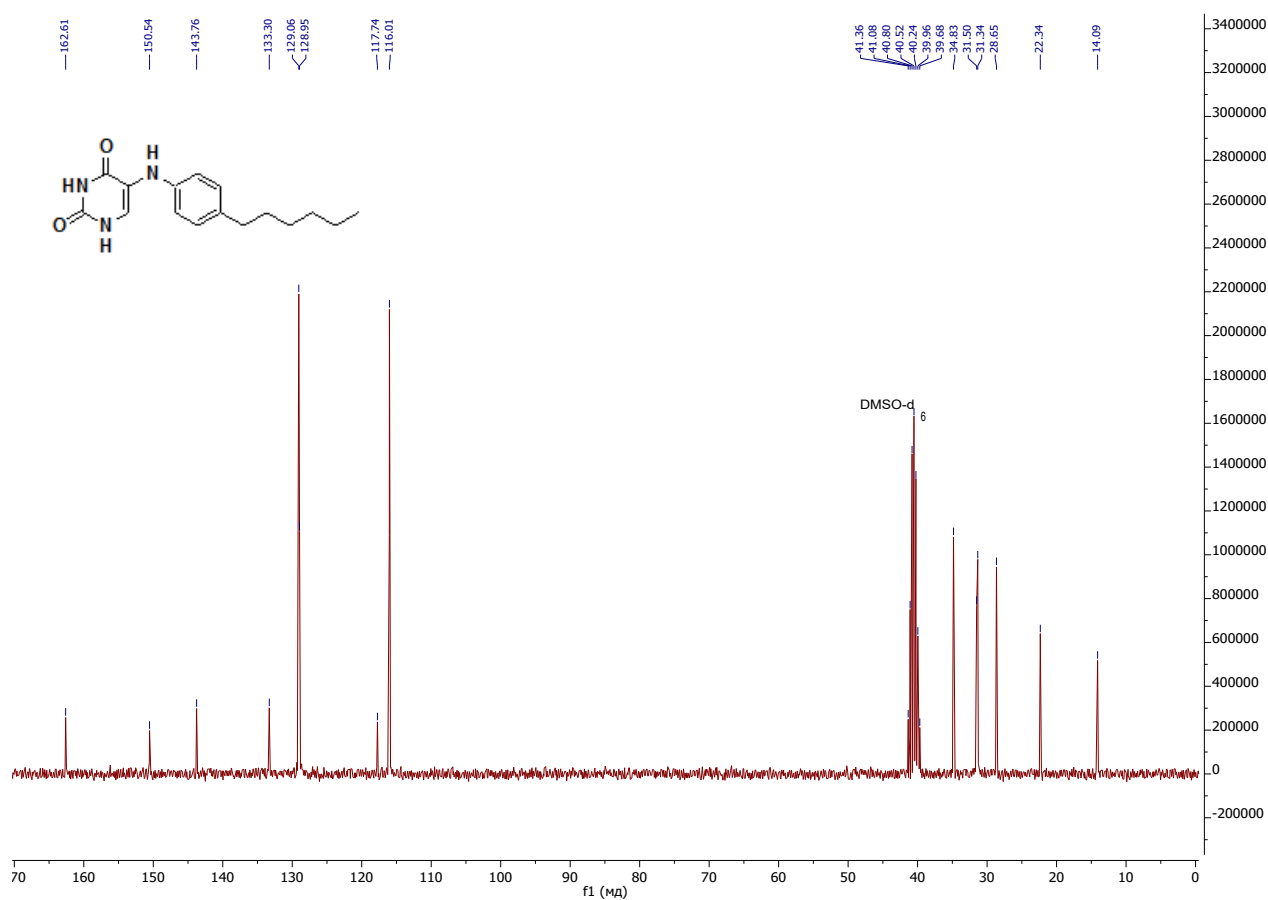


Figure S8 ¹³C NMR spectrum of compound **2d** in DMSO-*d*₆ at 100 MHz.

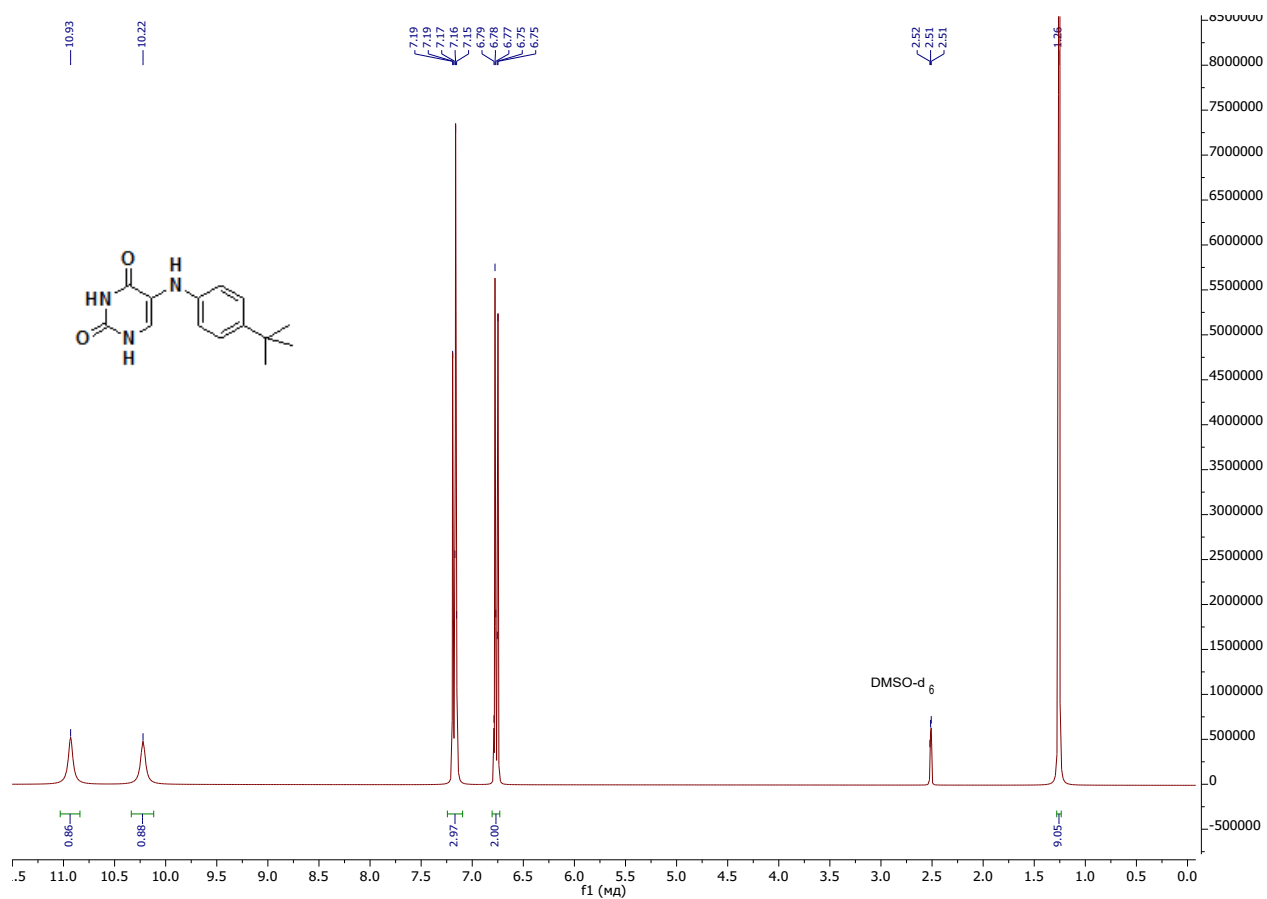


Figure S9 ¹H NMR spectrum of compound **2e** in DMSO-*d*₆ at 400 MHz.

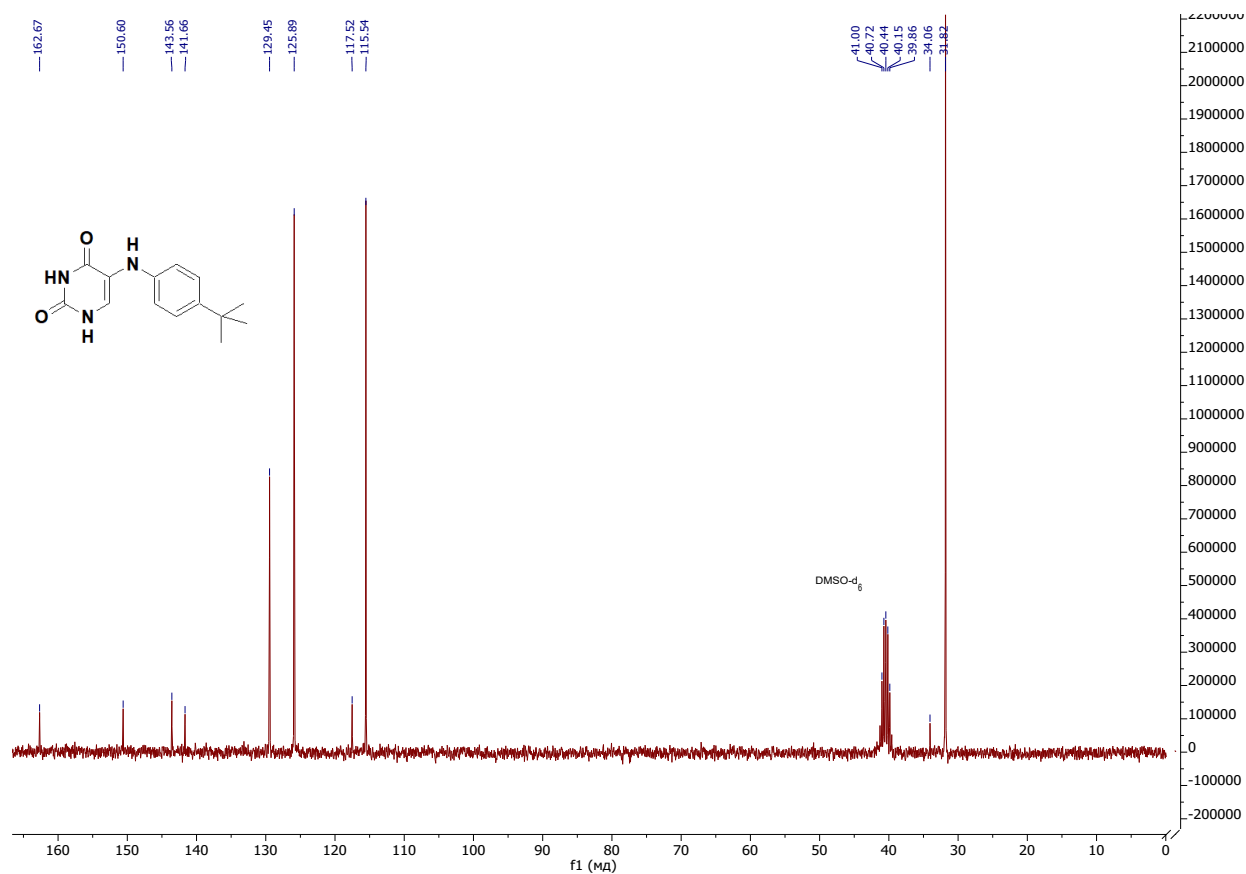


Figure S10 ¹³C NMR spectrum of compound **2e** in DMSO-*d*₆ at 100 MHz.

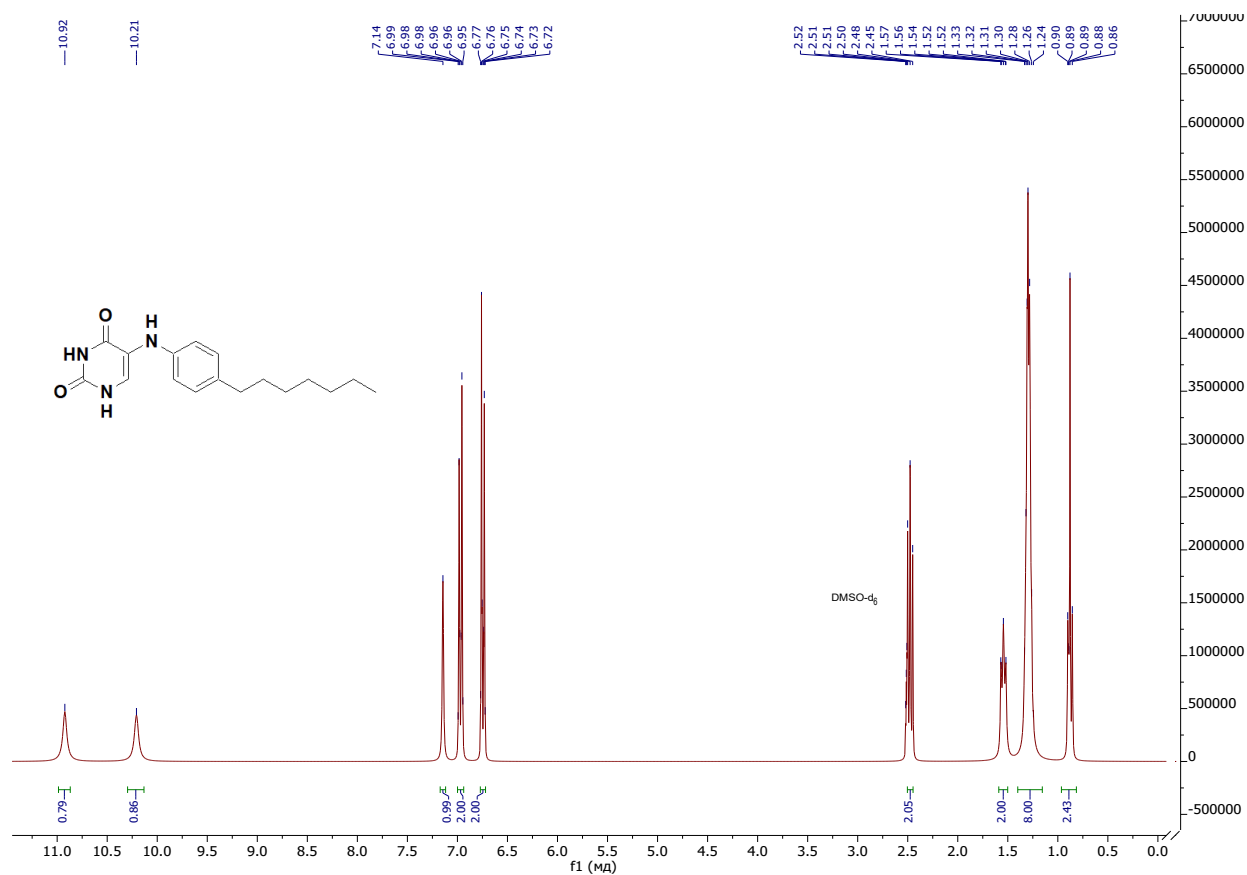


Figure S11 ¹H NMR spectrum of compound **2f** in DMSO-*d*₆ at 400 MHz.

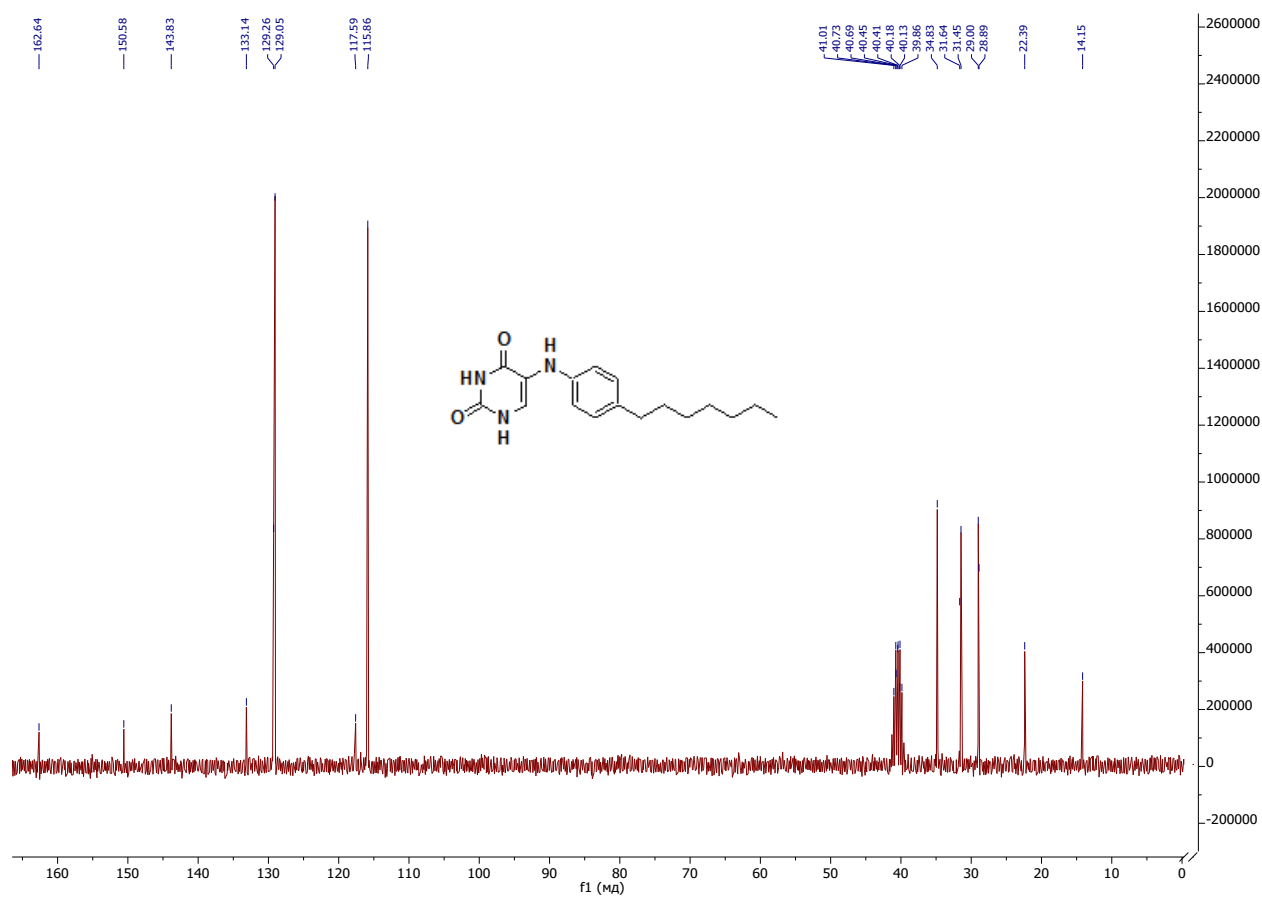


Figure S12 ¹³C NMR spectrum of compound **2f** in DMSO-*d*₆ at 100 MHz.

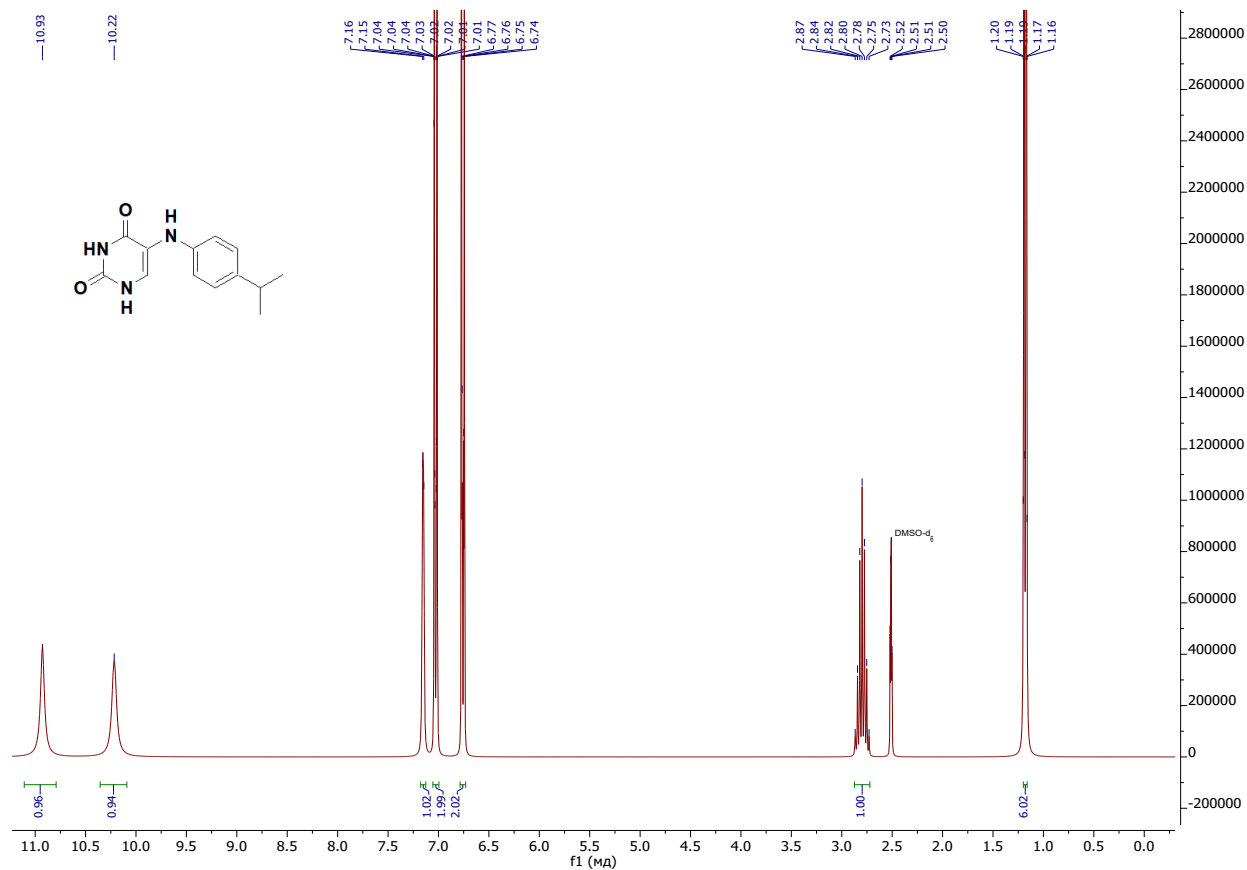


Figure S13 ¹H NMR spectrum of compound **2g** in DMSO-*d*₆ at 400 MHz.

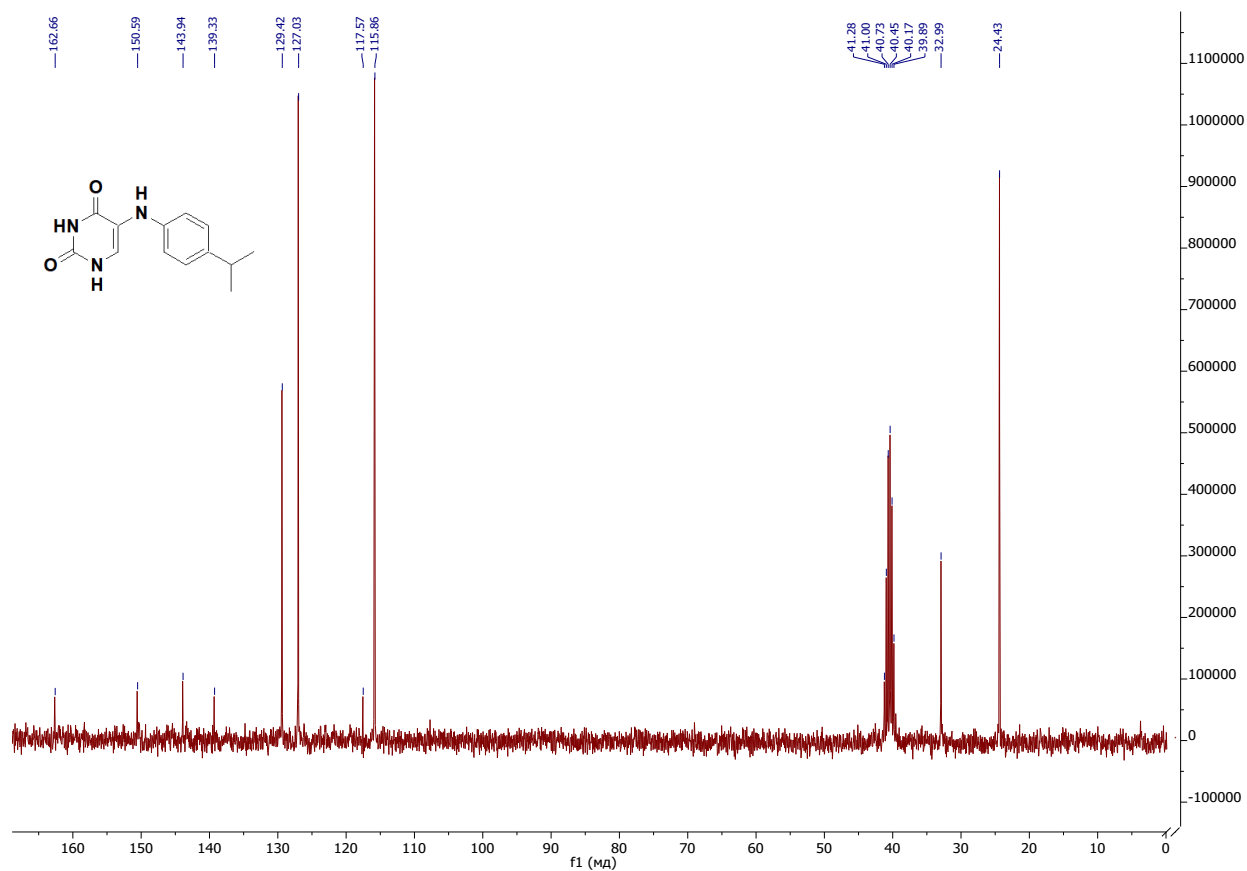


Figure S14 ¹³C NMR spectrum of compound **2g** in DMSO-*d*₆ at 100 MHz.

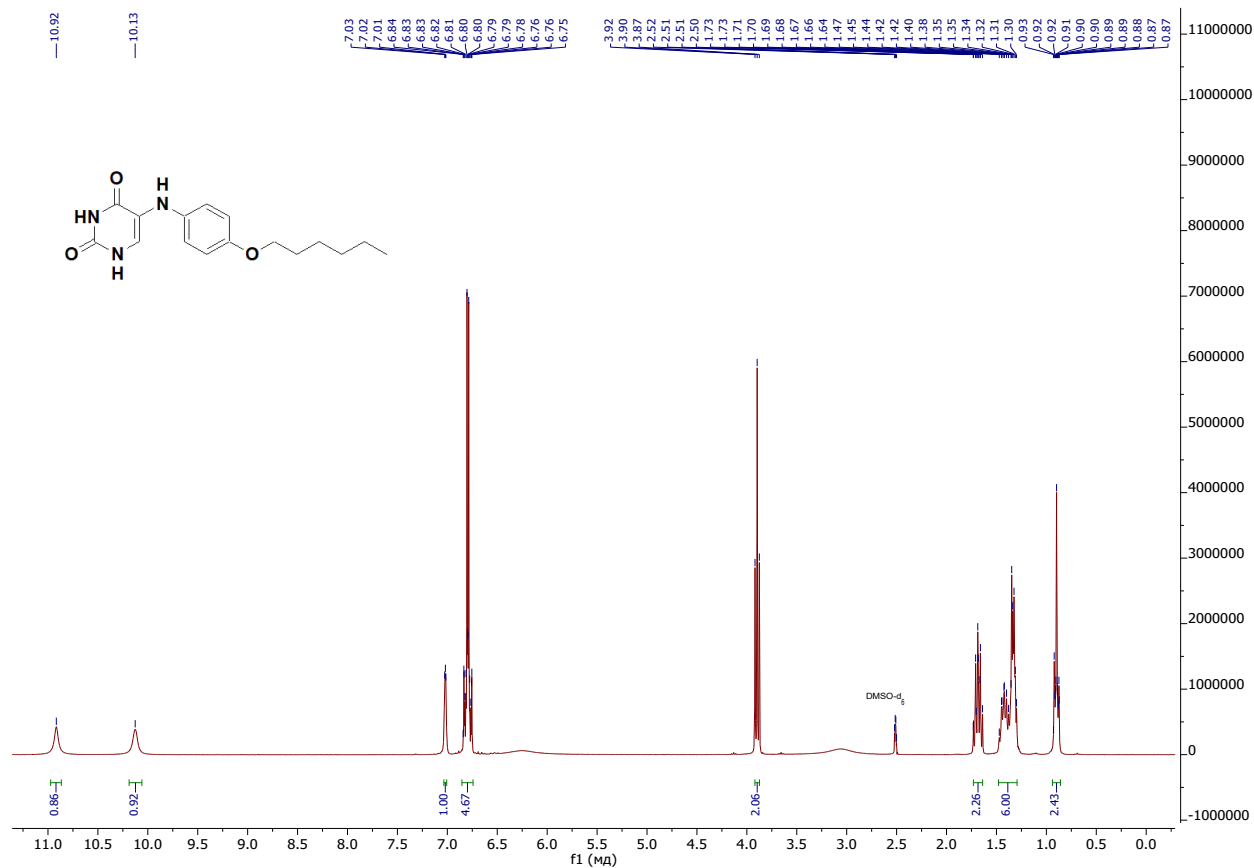


Figure S15 ¹H NMR spectrum of compound **2h** in DMSO-*d*₆ at 400 MHz.

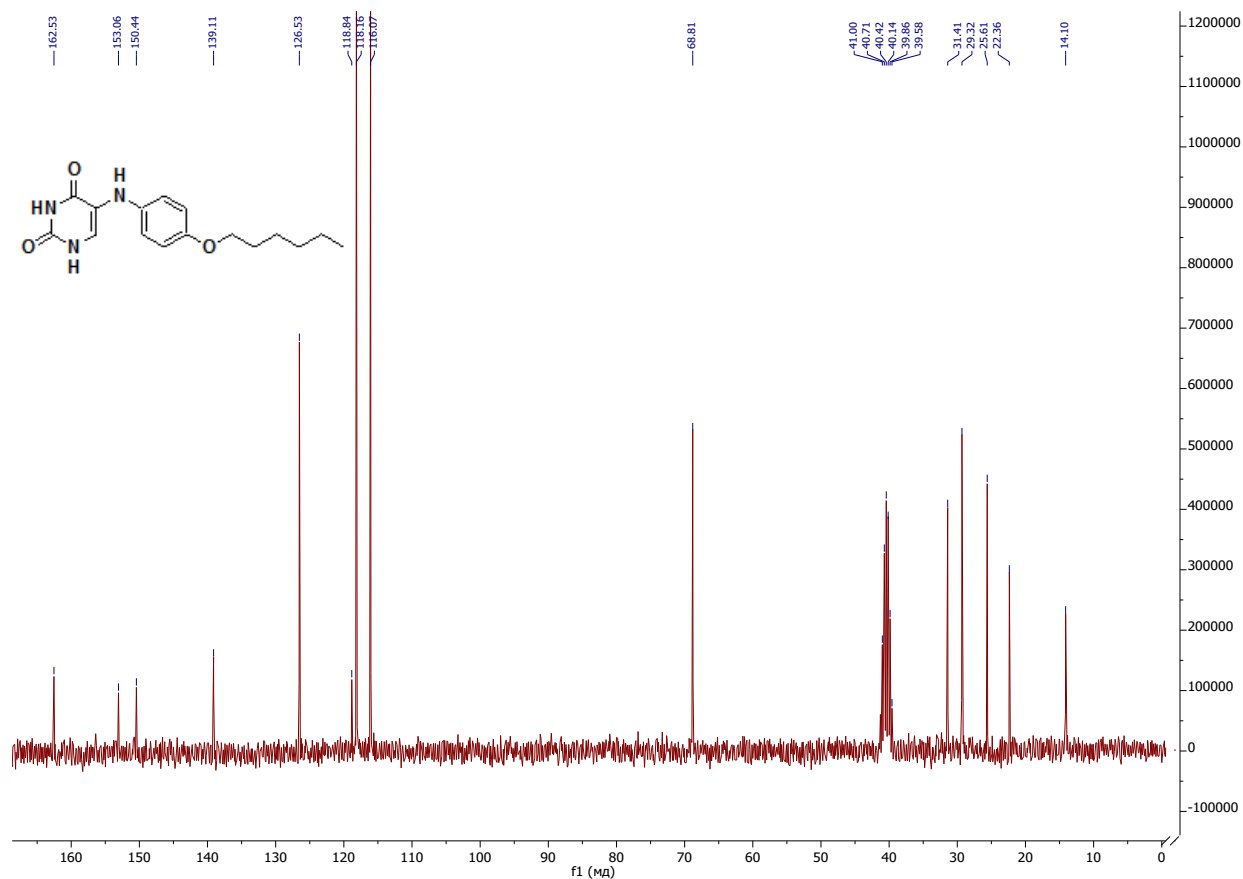


Figure S16 ¹³C NMR spectrum of compound **2h** in DMSO-*d*₆ at 100 MHz.

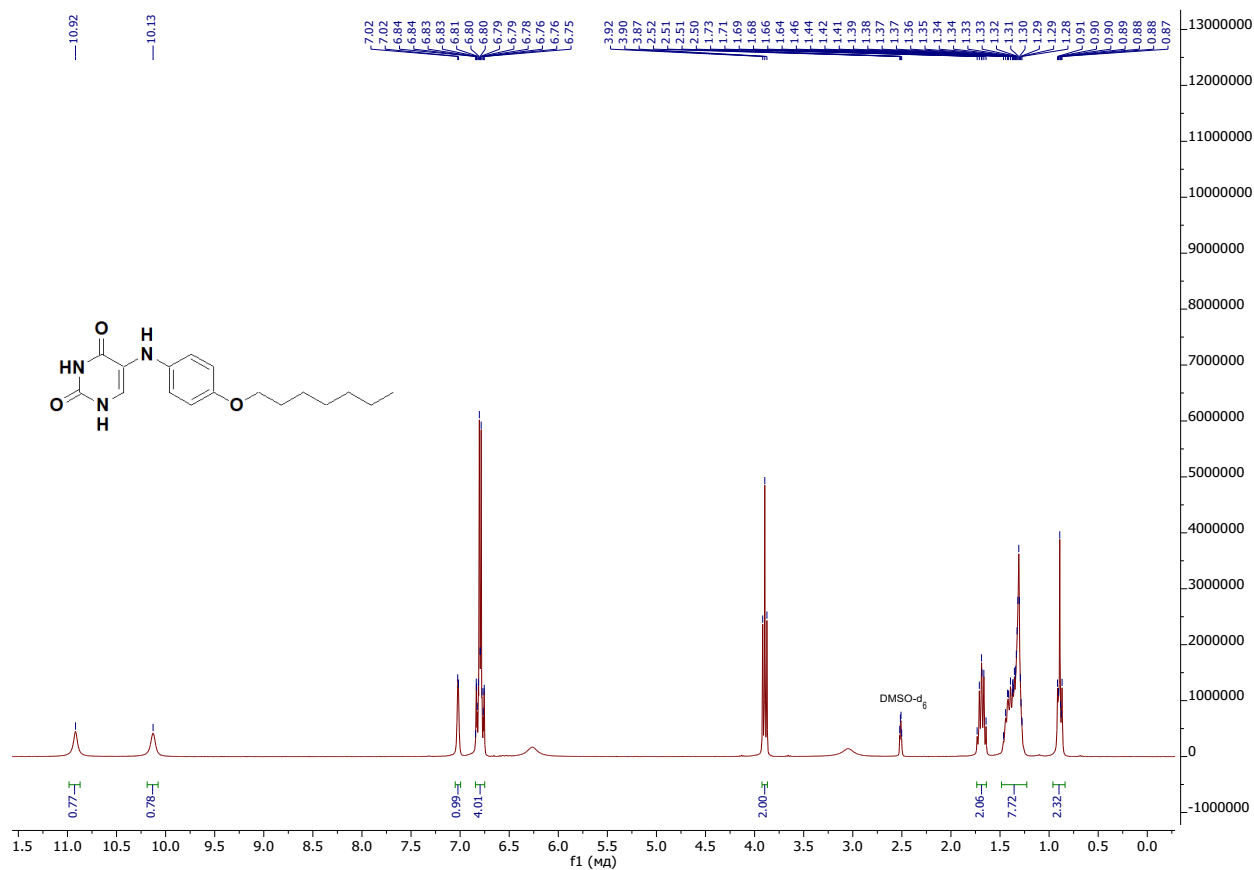


Figure S17 ¹H NMR spectrum of compound **2i** in DMSO-*d*₆ at 400 MHz.

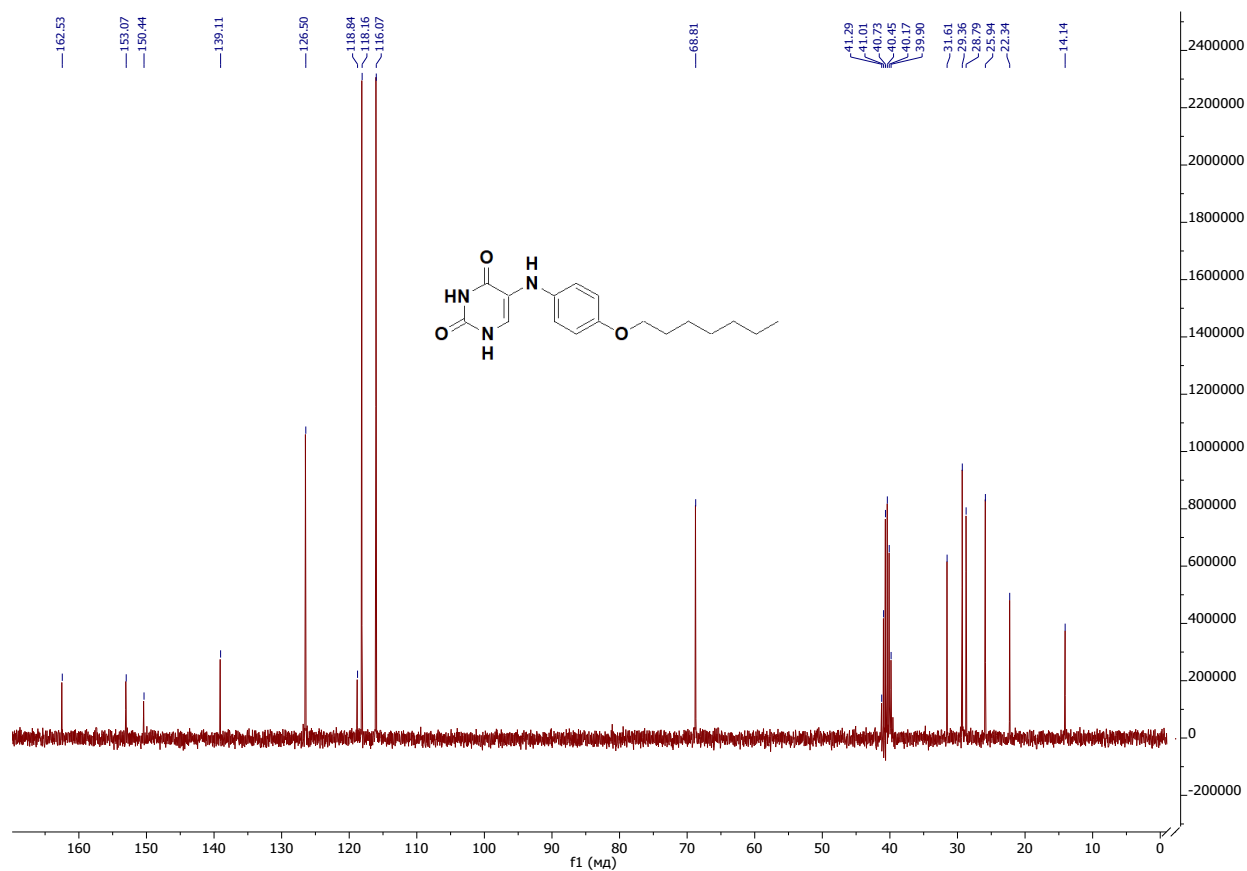


Figure S18 ¹³C NMR spectrum of compound **2i** in DMSO-*d*₆ at 100 MHz.

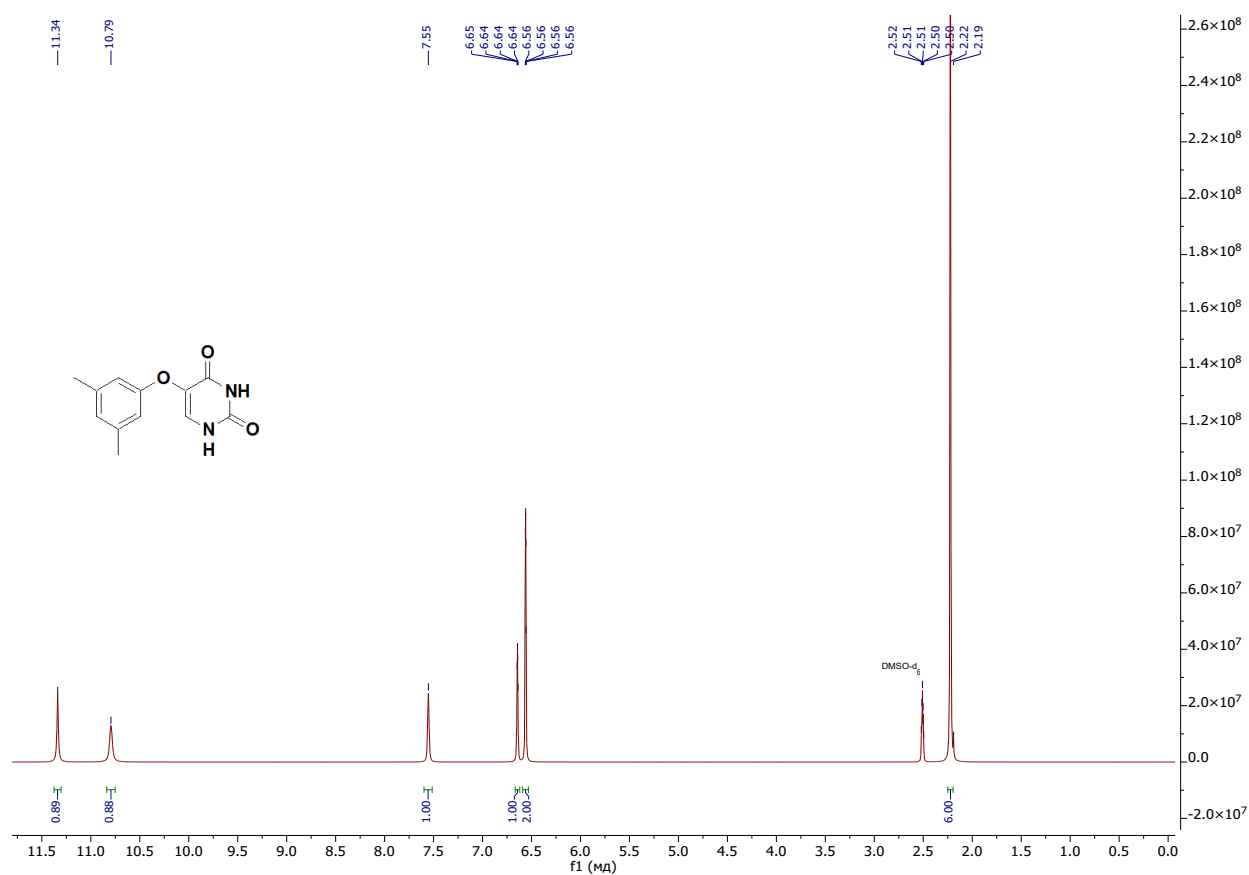


Figure S19 ¹H NMR spectrum of compound **5a** in DMSO-*d*₆ at 400 MHz.

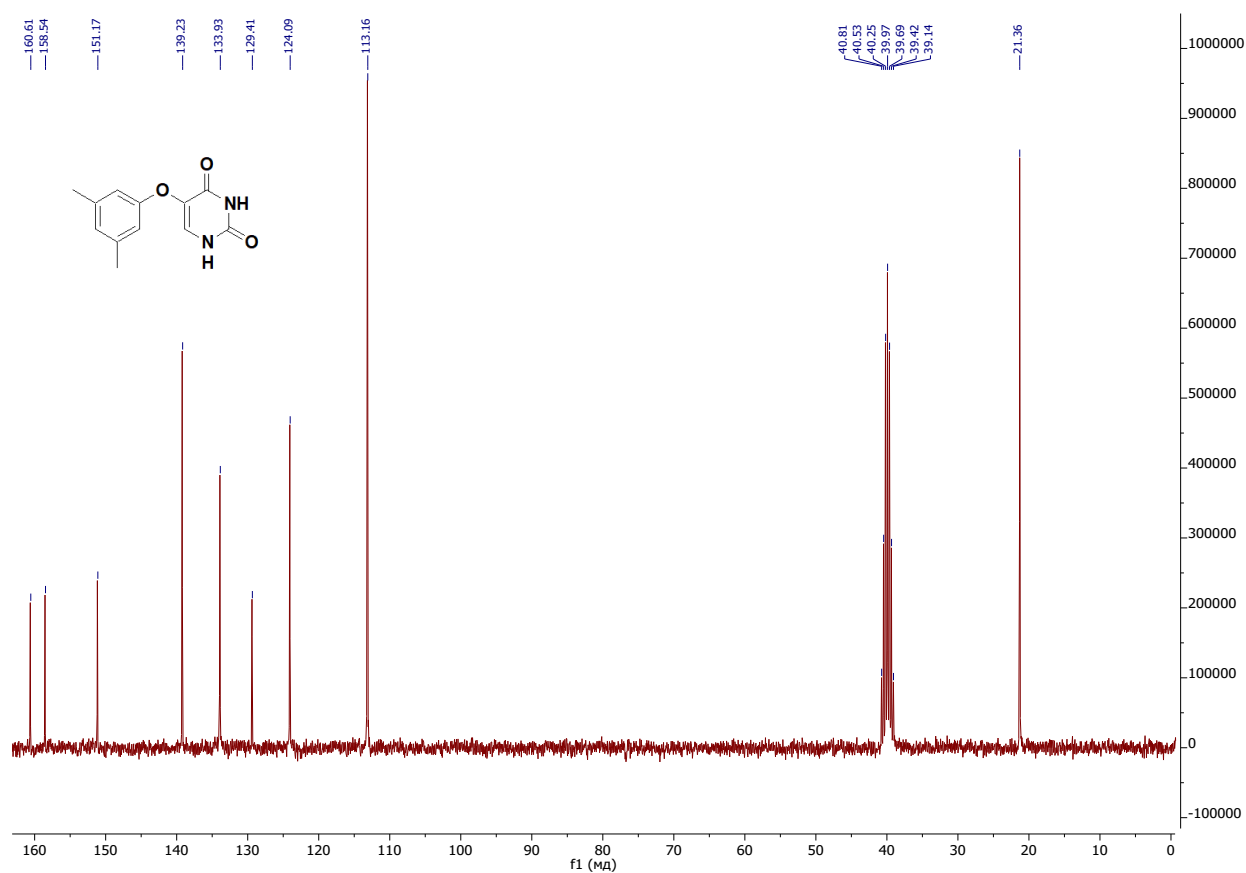


Figure S20 ¹³C NMR spectrum of compound **5a** in DMSO-*d*₆ at 100 MHz.

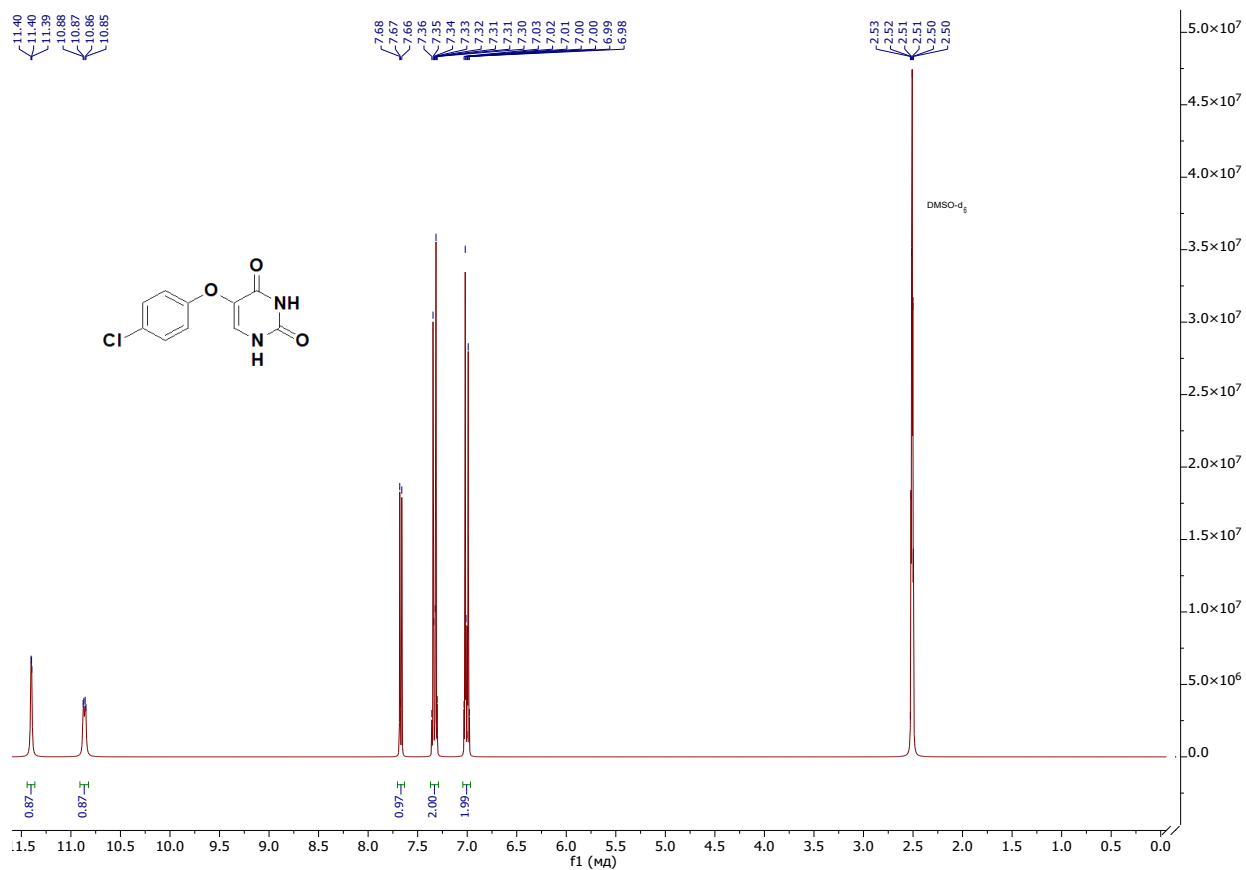


Figure S23 ¹H NMR spectrum of compound **5c** in DMSO-*d*₆ at 400 MHz.

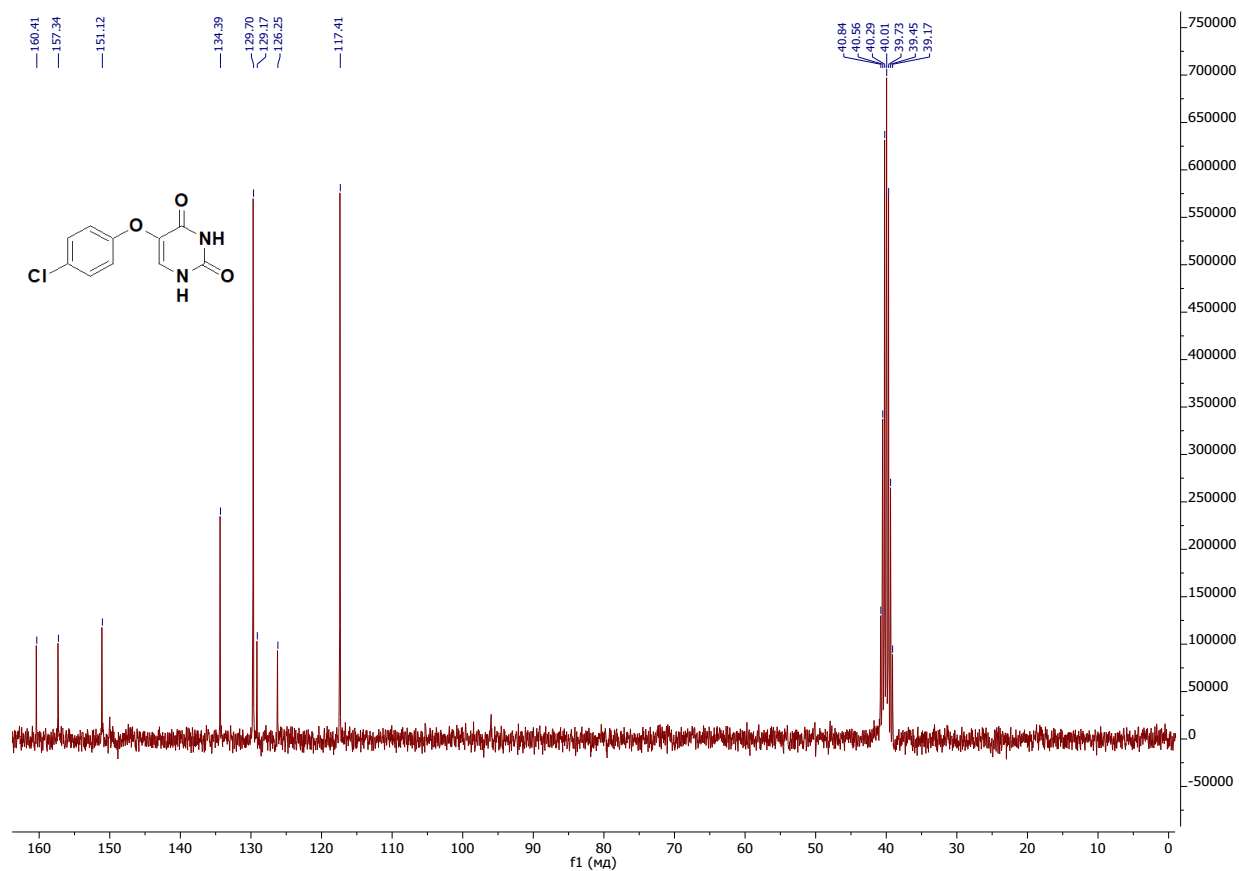


Figure S24 ¹³C NMR spectrum of compound **5c** in DMSO-*d*₆ at 100 MHz.

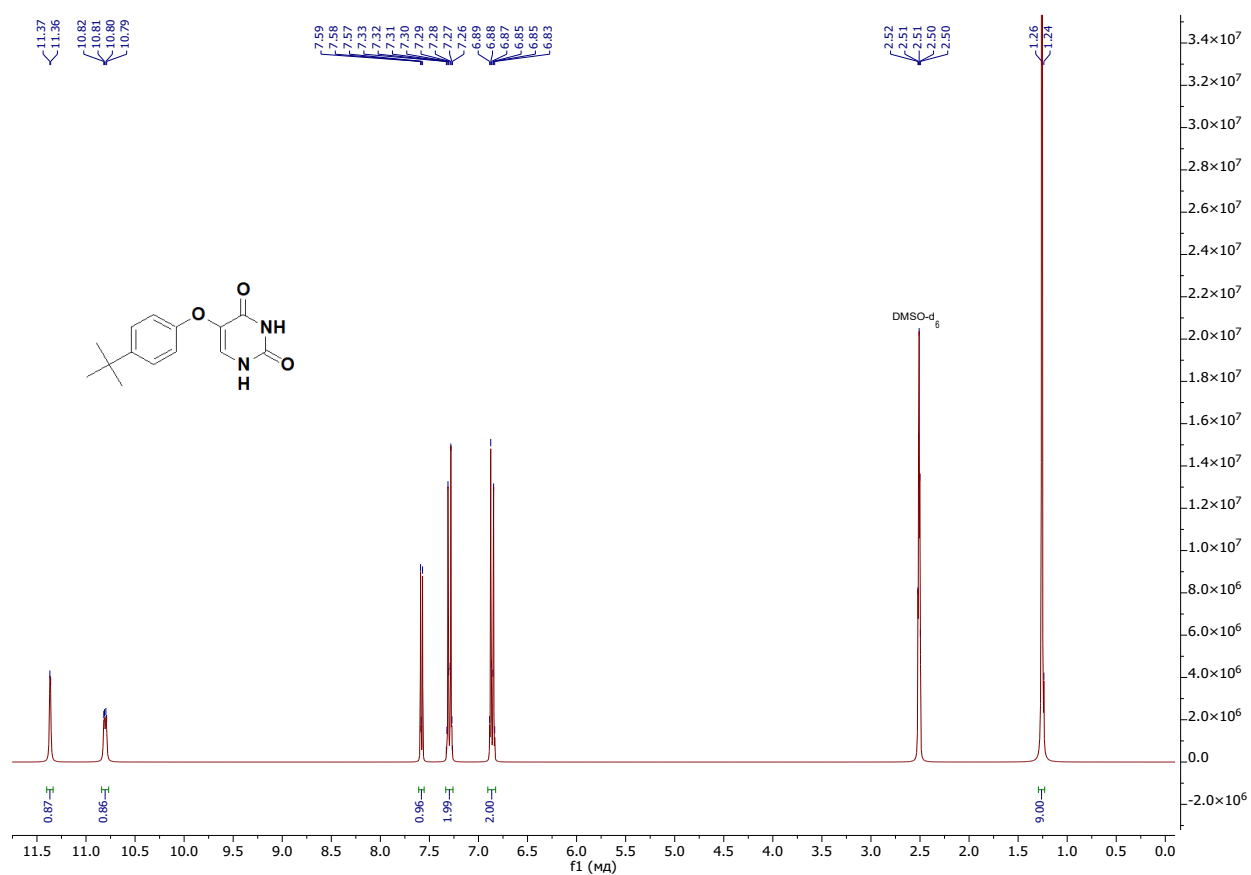


Figure S25 ¹H NMR spectrum of compound **5d** in DMSO-*d*₆ at 400 MHz.

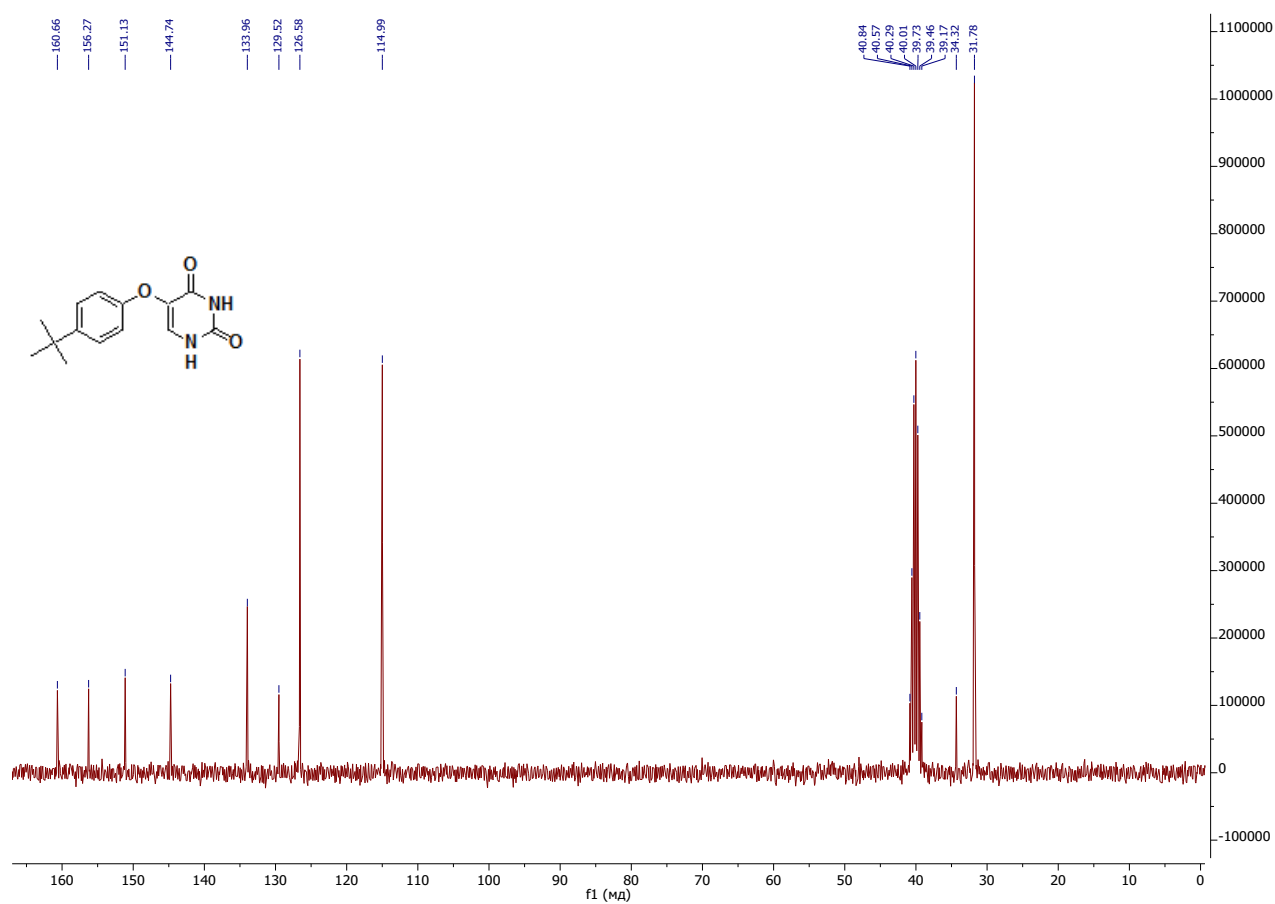


Figure S26 ¹³C NMR spectrum of compound **5d** in DMSO-*d*₆ at 100 MHz.

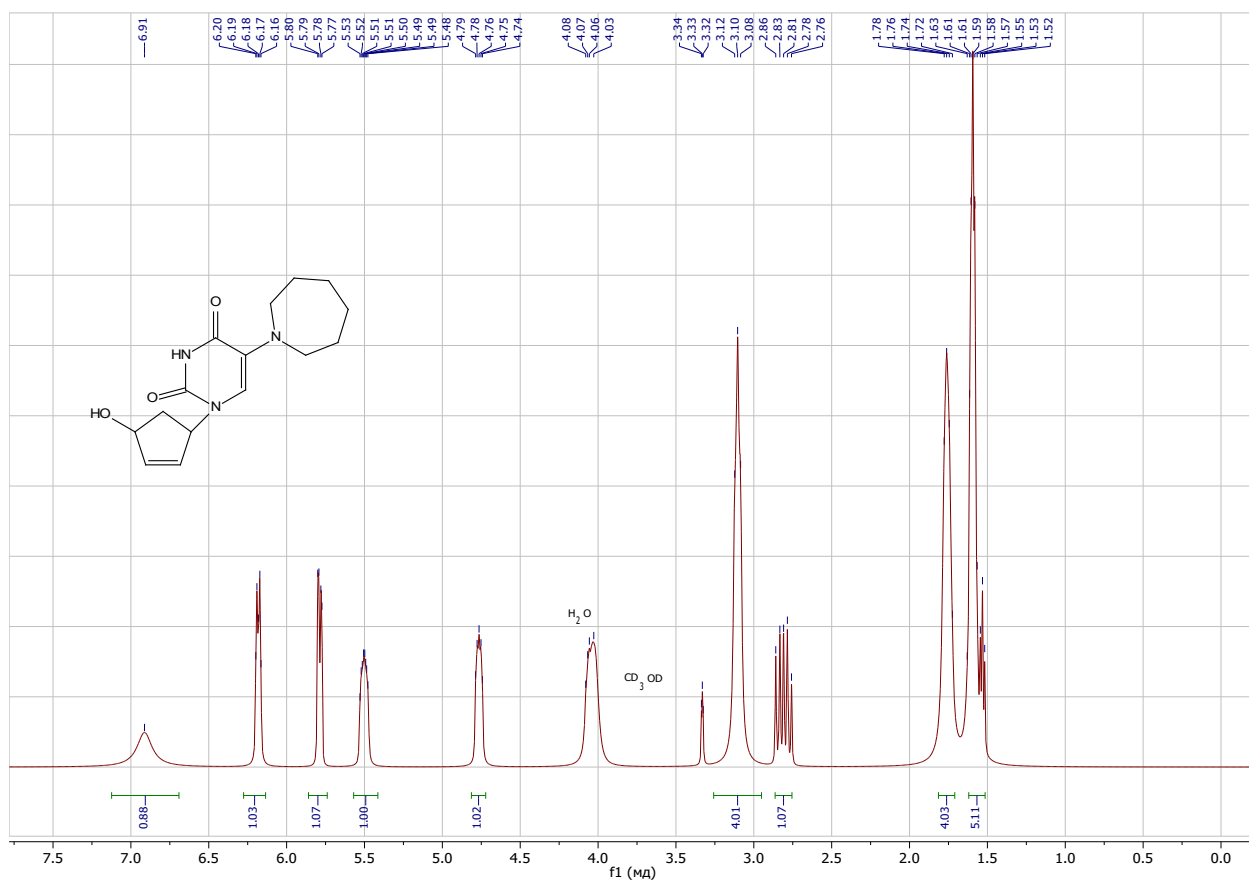


Figure S27 ¹H NMR spectrum of compound **3a** in CDCl₃ at 400 MHz.

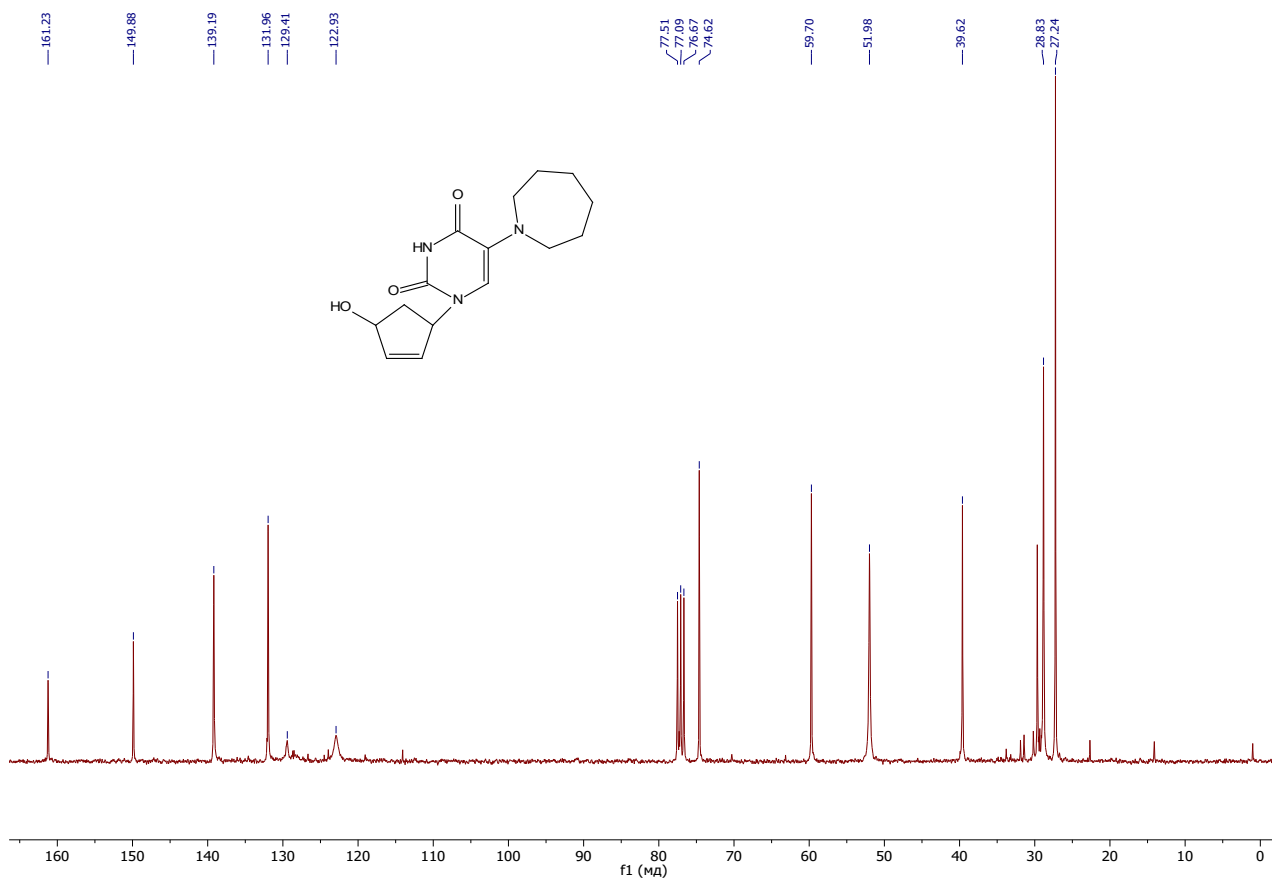


Figure S28 ¹³C NMR spectrum of compound **3a** in CDCl₃ at 100 MHz.

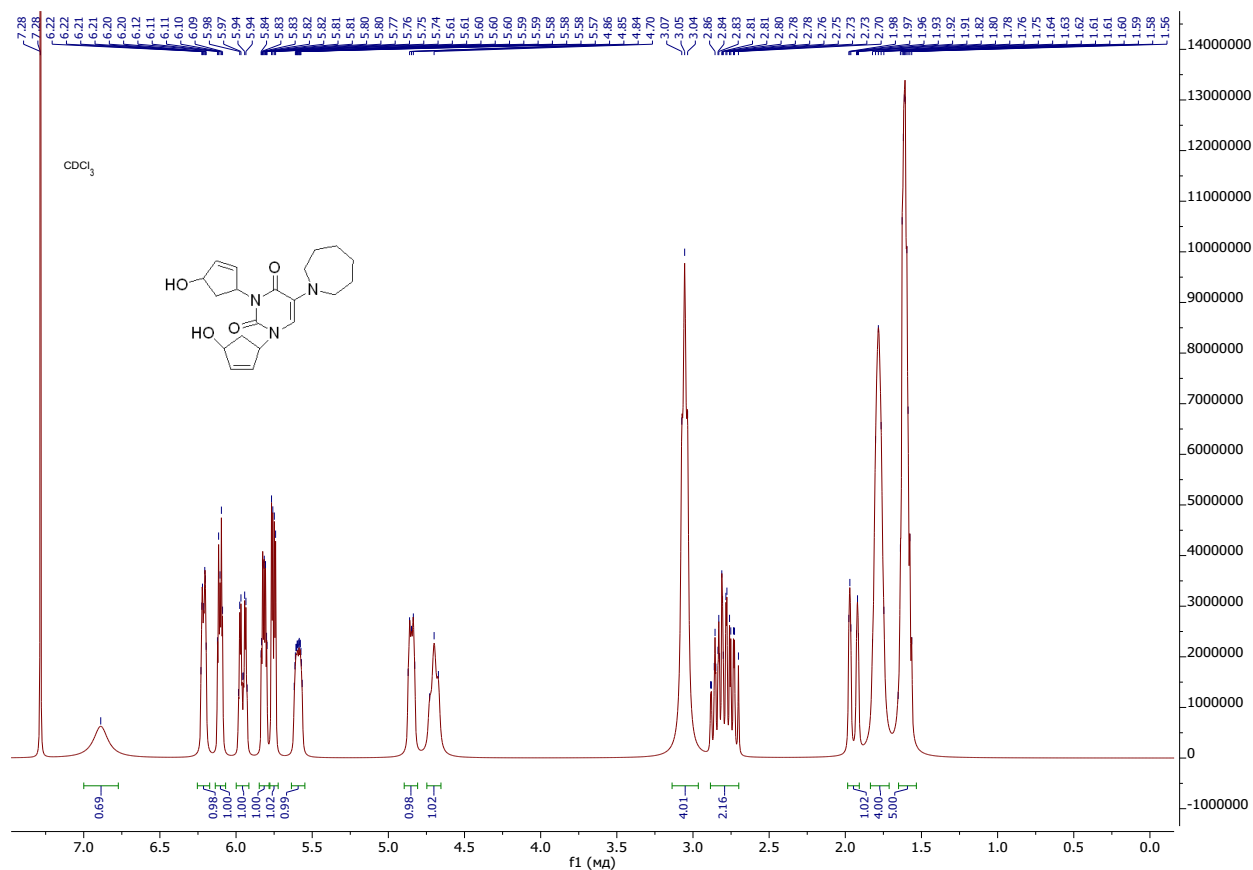


Figure S29 ^1H NMR spectrum of compound **4a** in CDCl_3 at 400 MHz.

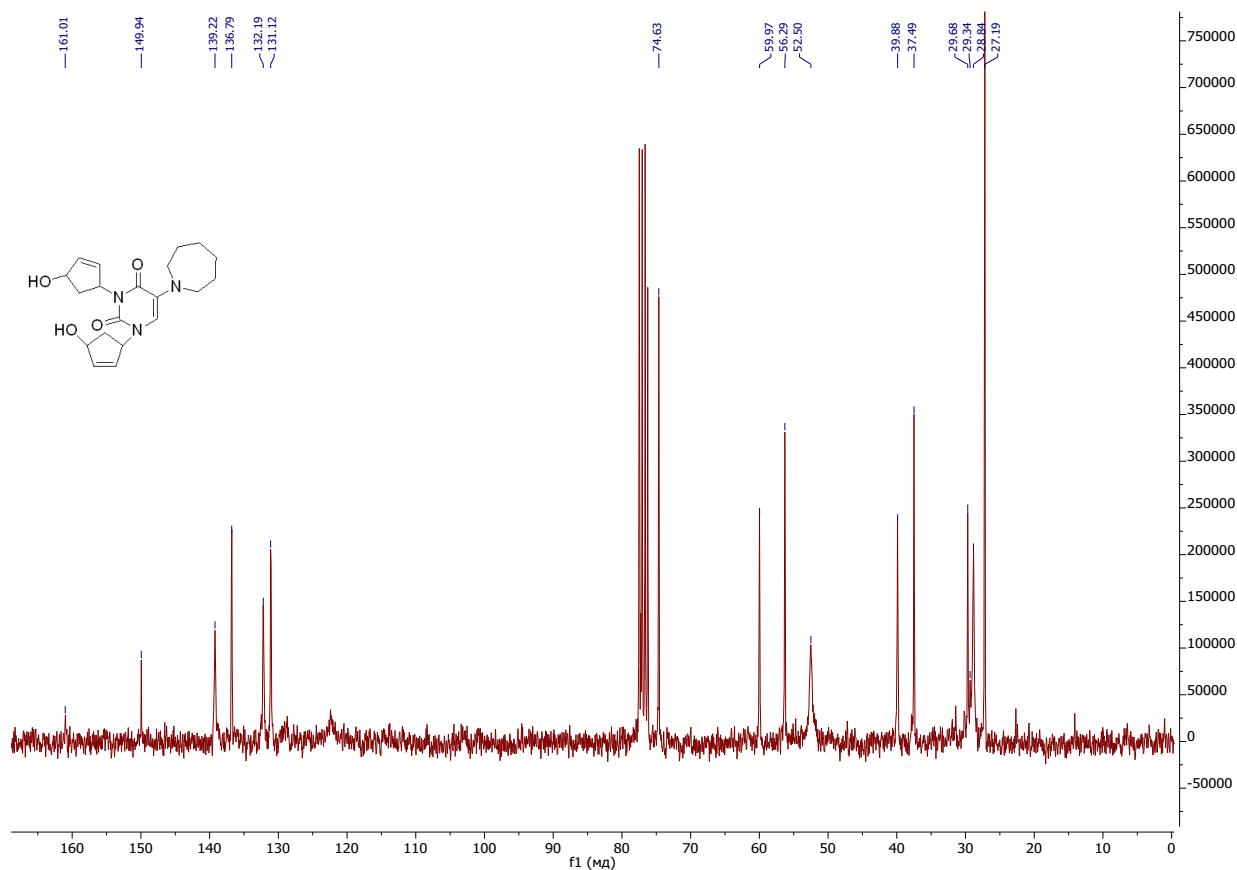


Figure S30 ^{13}C NMR spectrum of compound **4a** in CDCl_3 at 100 MHz.

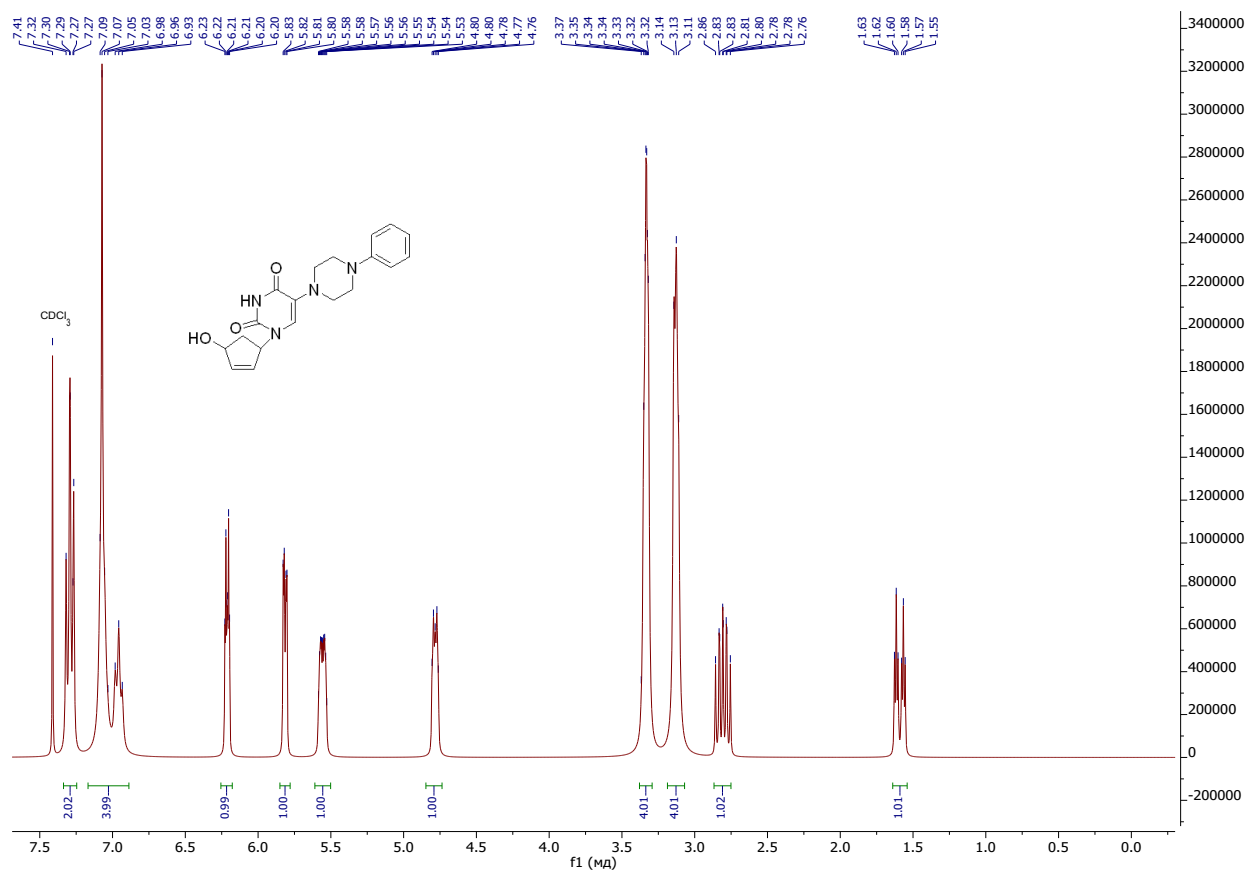


Figure S31 ^1H NMR spectrum of compound **3b** in CDCl_3 at 400 MHz.

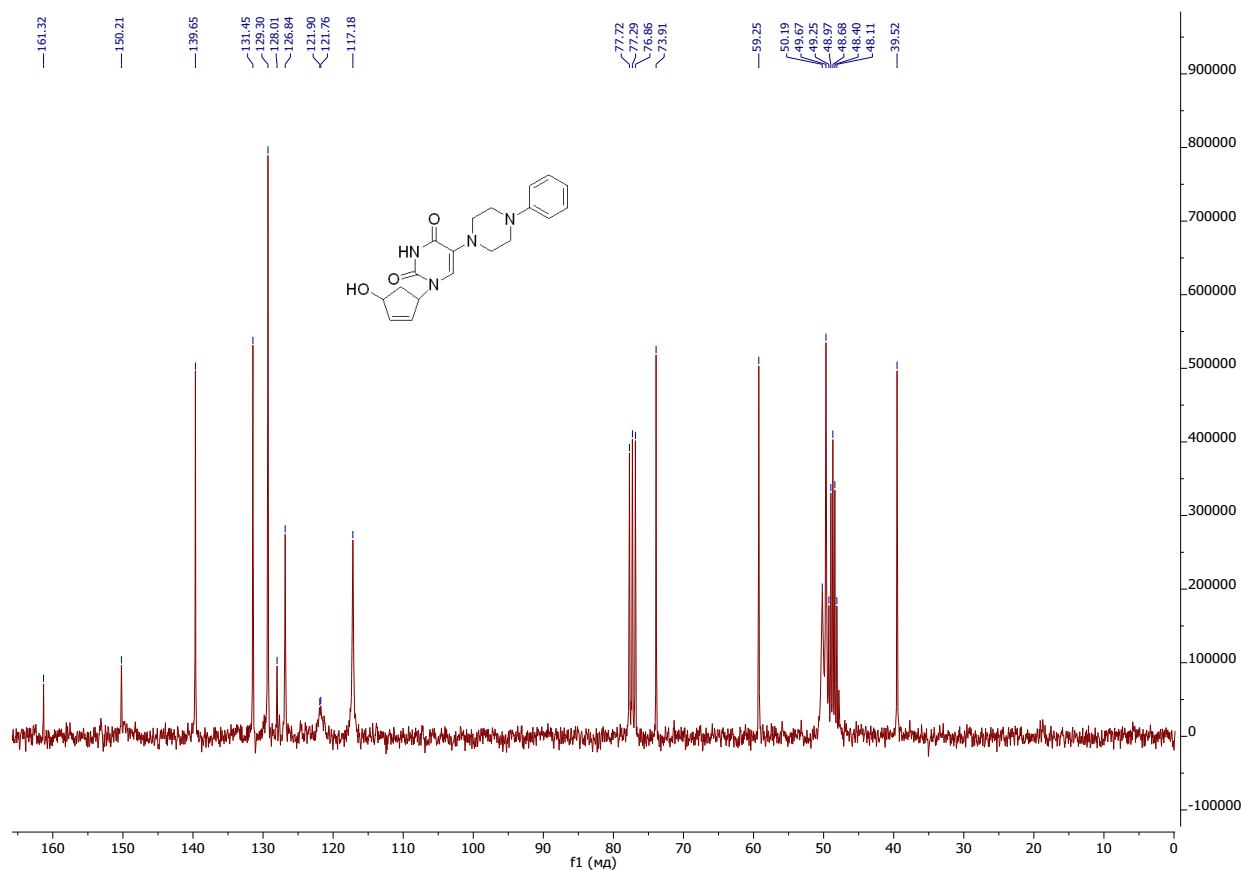


Figure S32 ^{13}C NMR spectrum of compound **3b** in $\text{CDCl}_3:\text{CD}_3\text{OD}$ at 100 MHz.

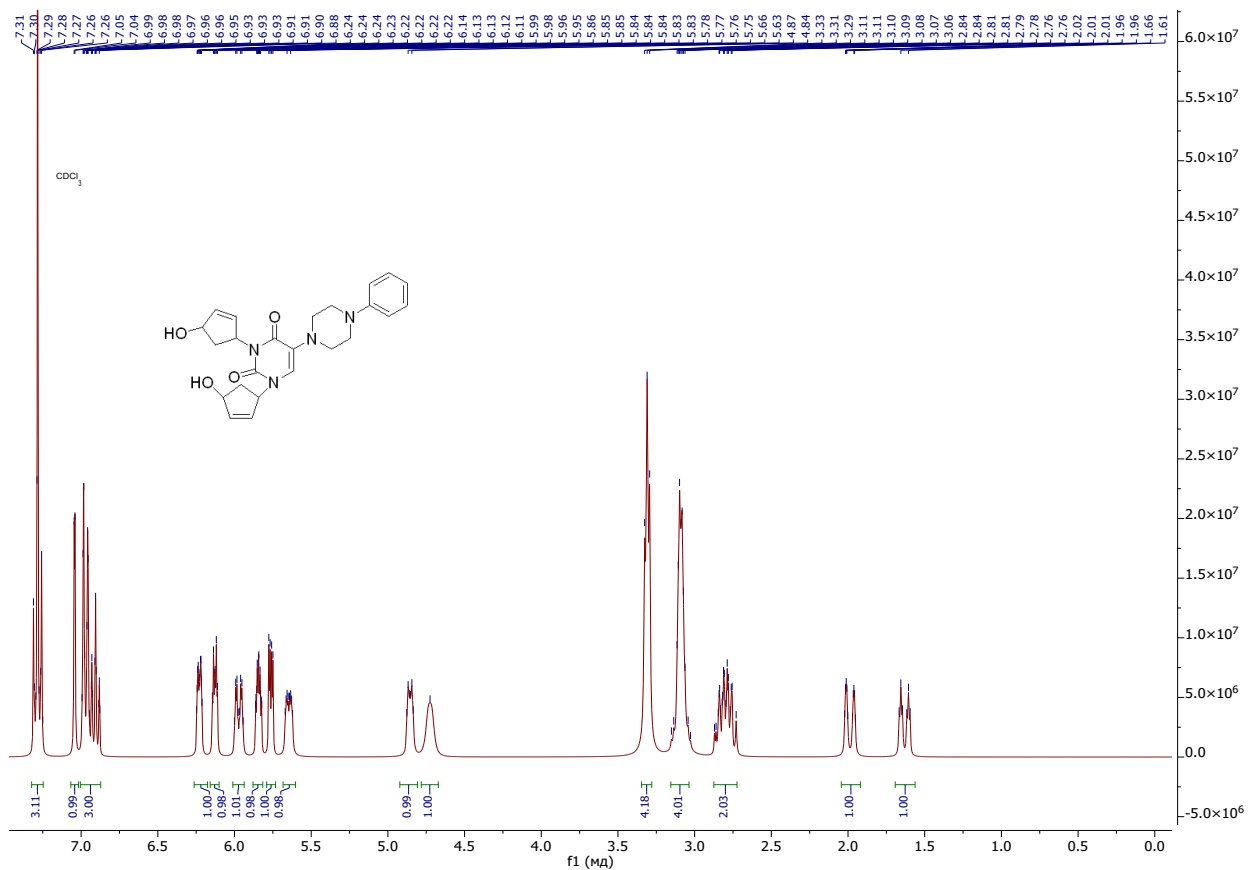


Figure S33 ^1H NMR spectrum of compound **4b** in CDCl_3 at 400 MHz.

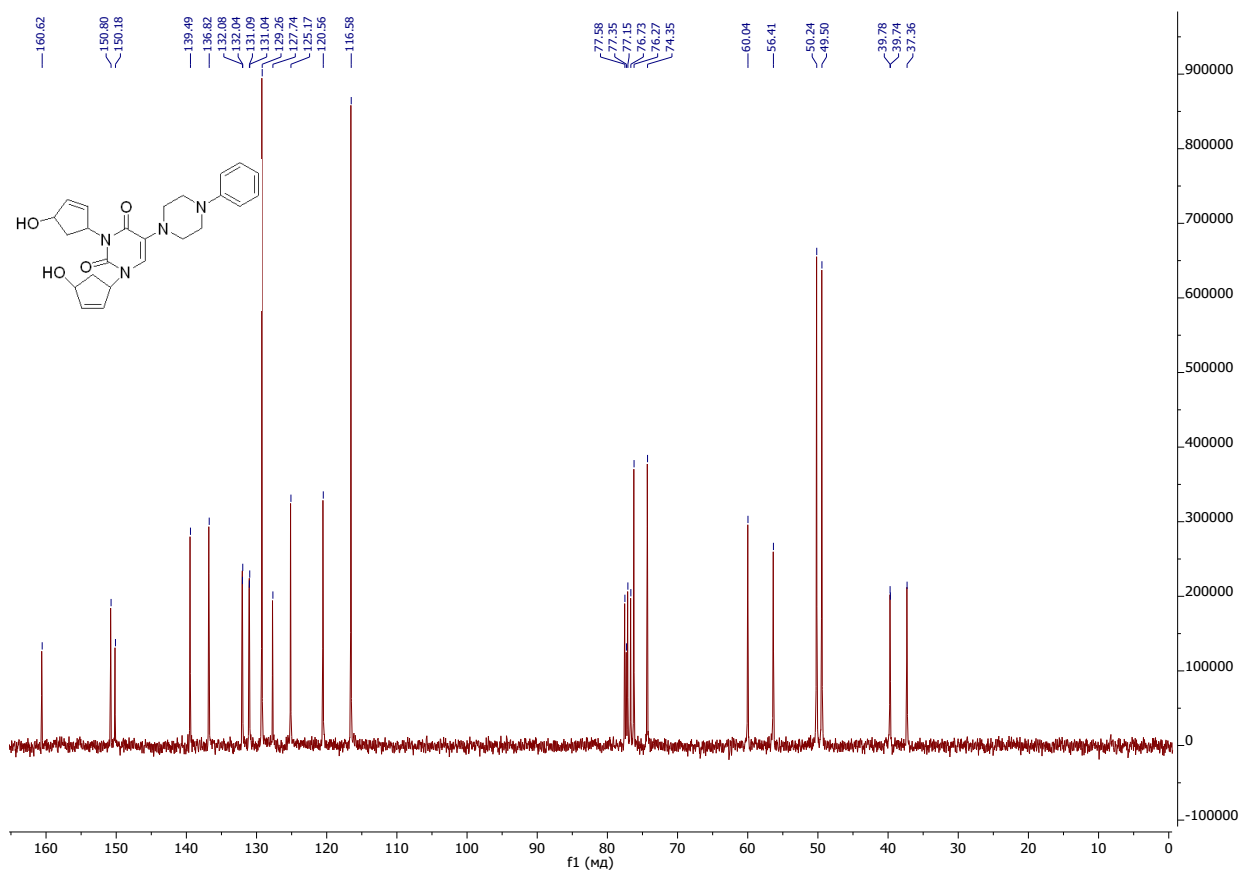


Figure S34 ^{13}C NMR spectrum of compound **4b** in CDCl_3 at 100 MHz.

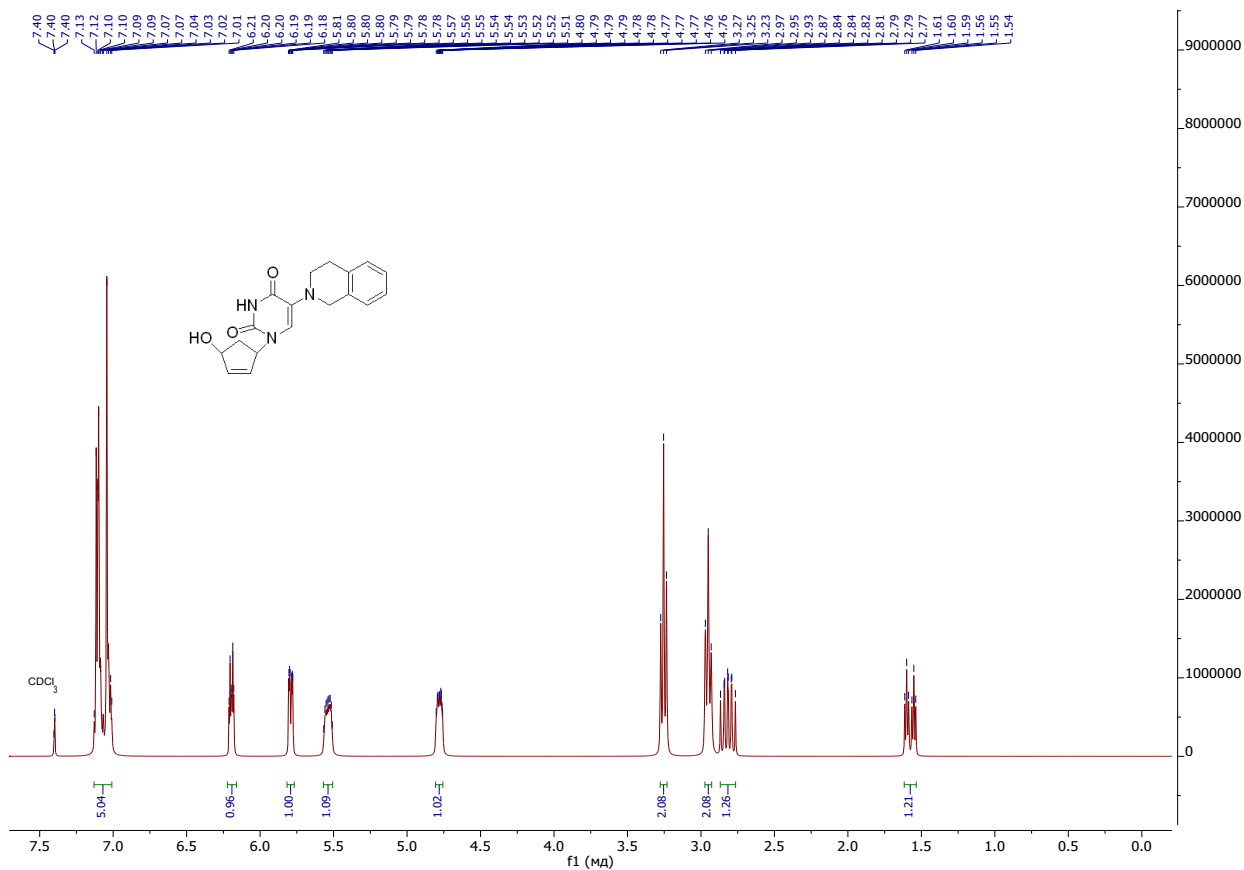


Figure S35 ^1H NMR spectrum of compound **3c** in $\text{CDCl}_3:\text{CD}_3\text{OD}$ at 400 MHz.

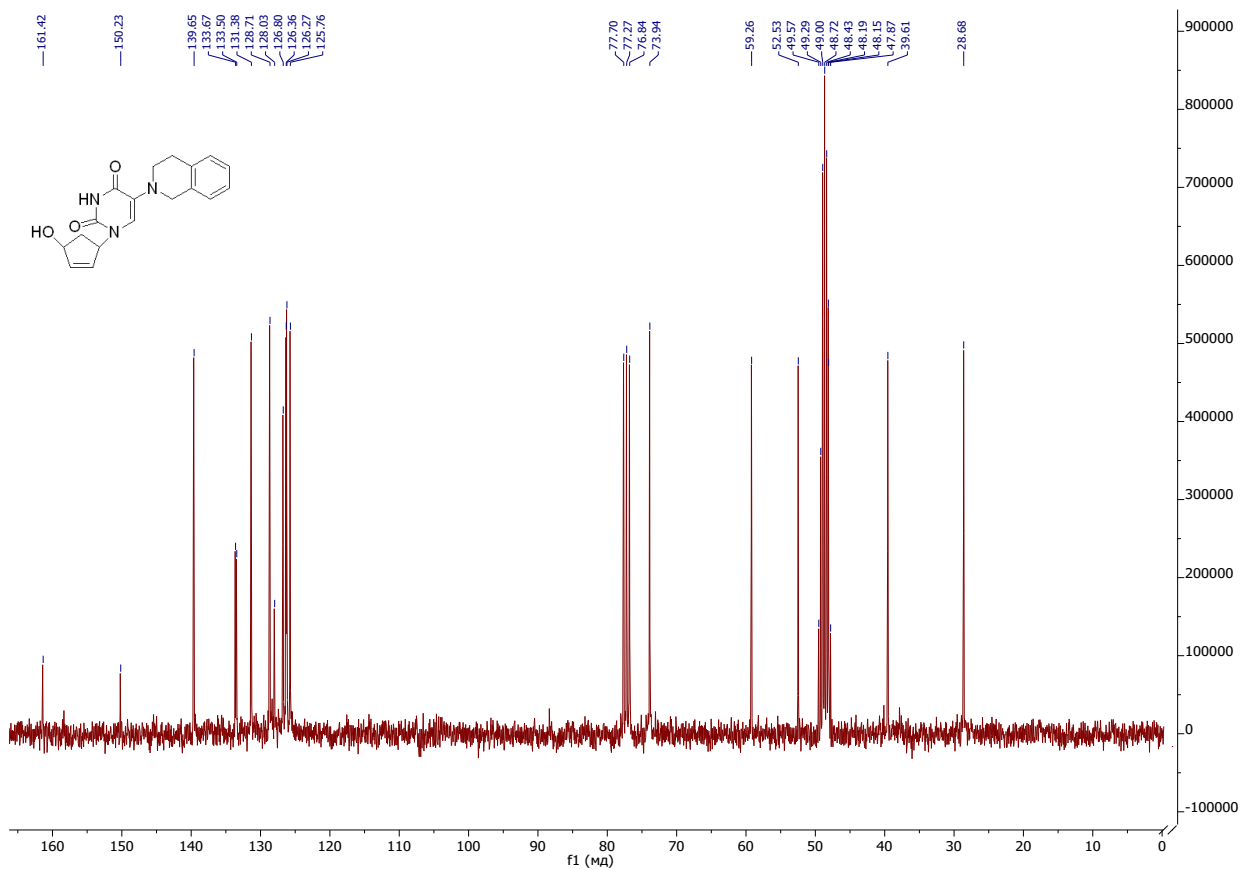


Figure S36 ^{13}C NMR spectrum of compound **3c** in $\text{CDCl}_3:\text{CD}_3\text{OD}$ at 100 MHz.

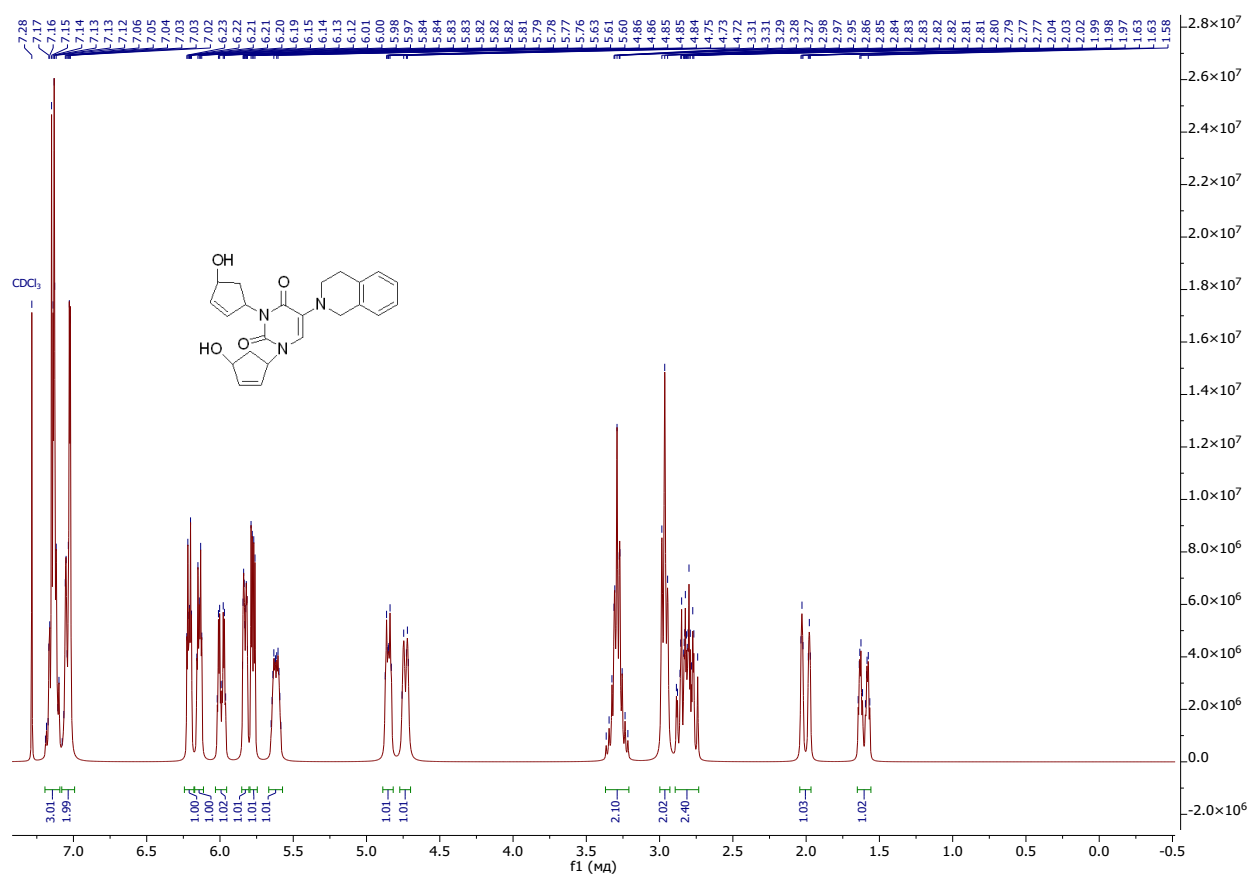


Figure S37 ¹H NMR spectrum of compound **4c** in CDCl₃ at 400 MHz.

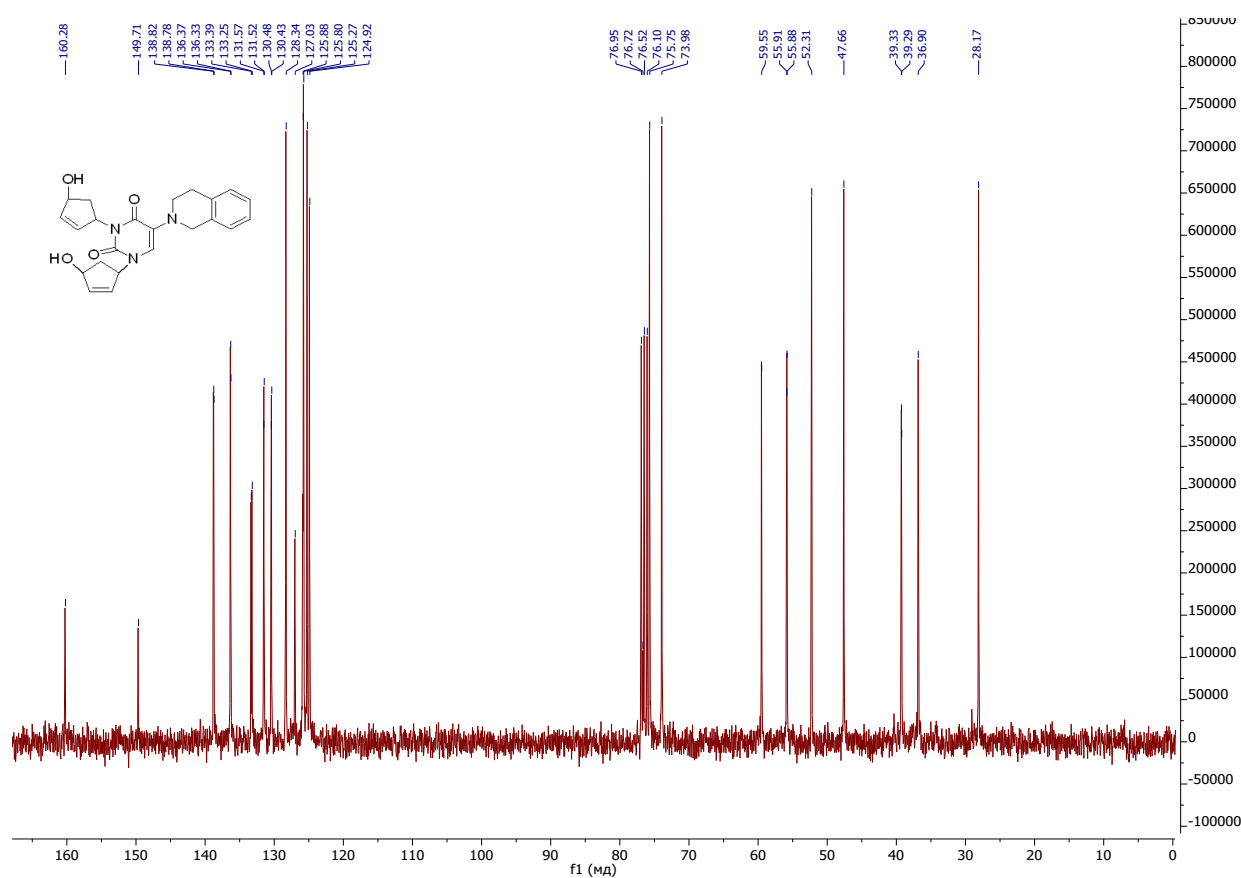


Figure S38 ¹³C NMR spectrum of compound **4c** in CDCl₃ at 100 MHz.

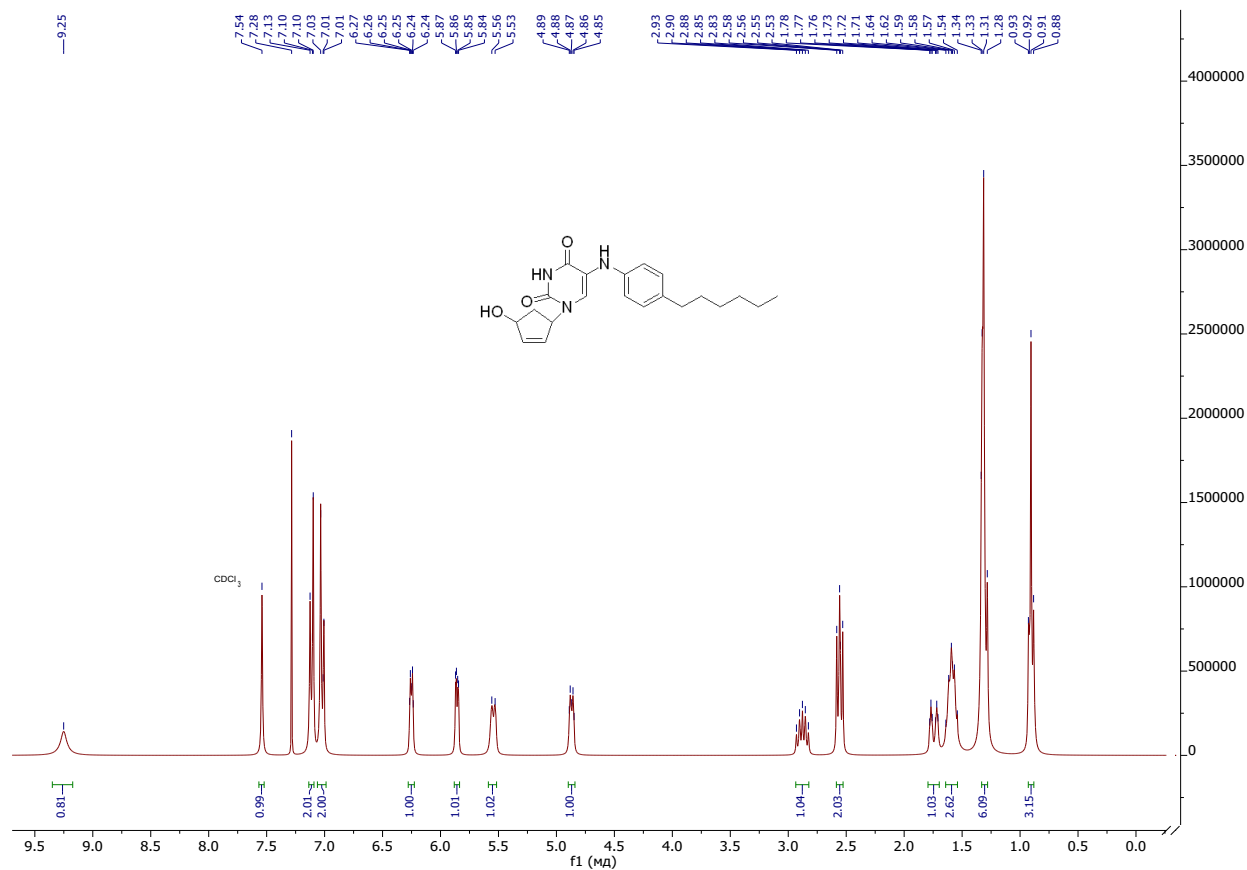


Figure S39 ¹H NMR spectrum of compound **3d** in CDCl₃ at 400 MHz.

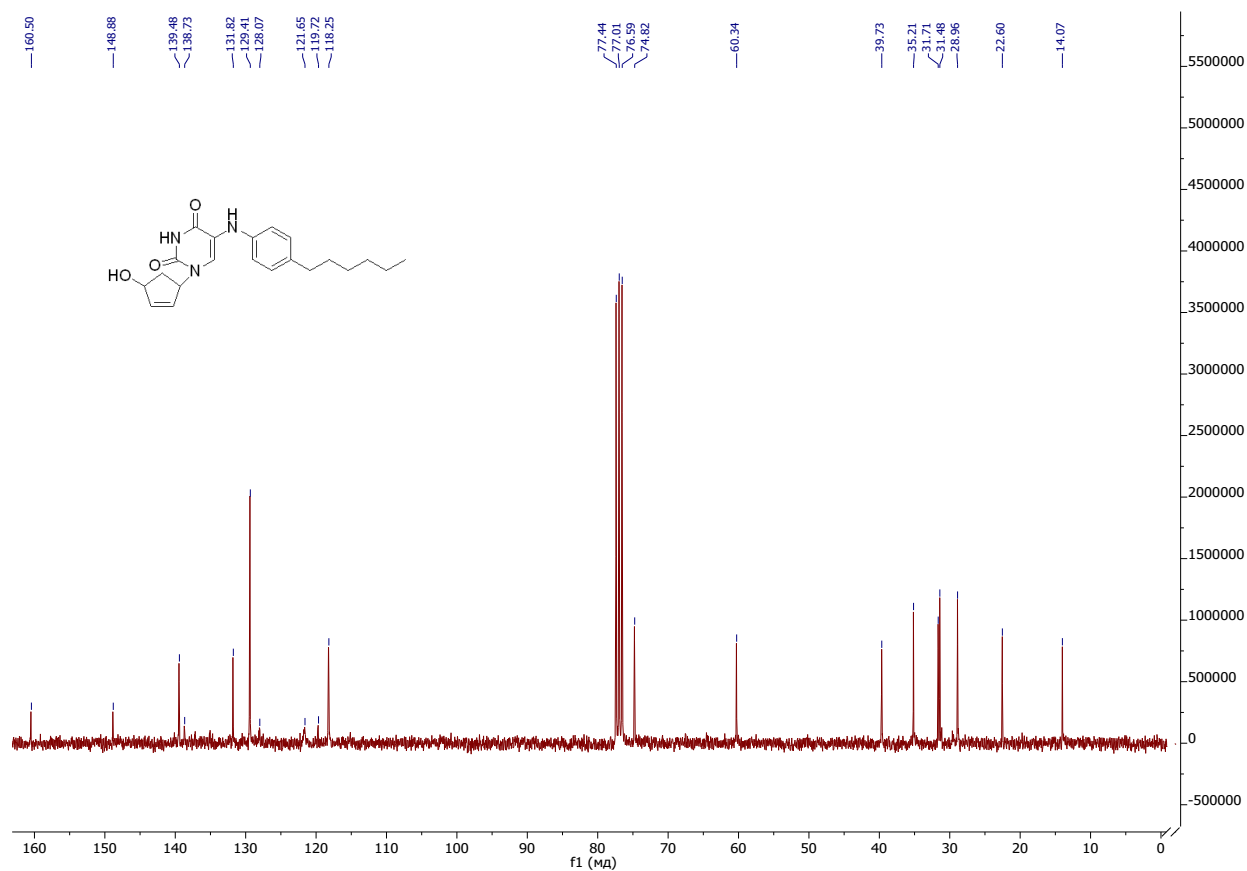


Figure S40 ¹³C NMR spectrum of compound **3d** in CDCl₃ at 100 MHz.

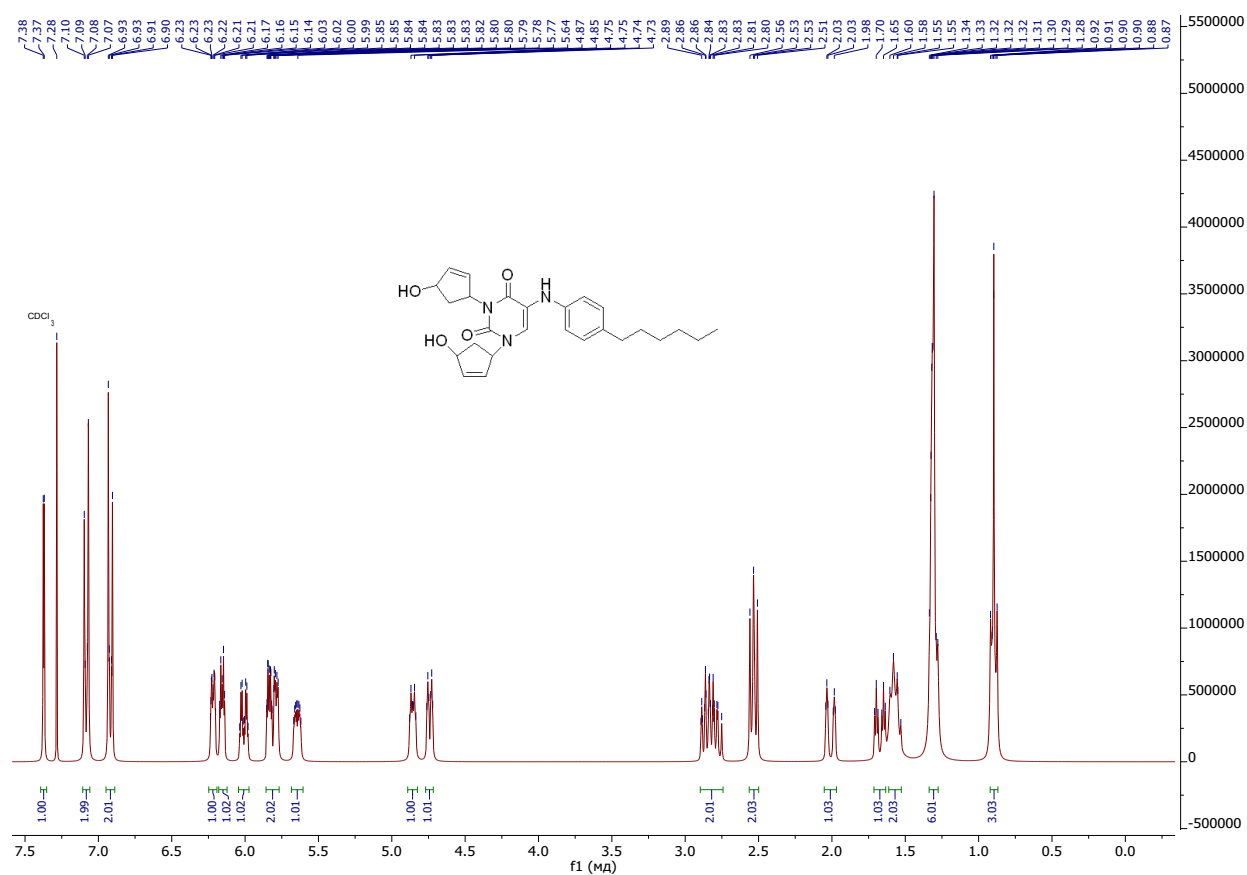


Figure S41 ¹H NMR spectrum of compound **4d** in CDCl₃ at 400 MHz.

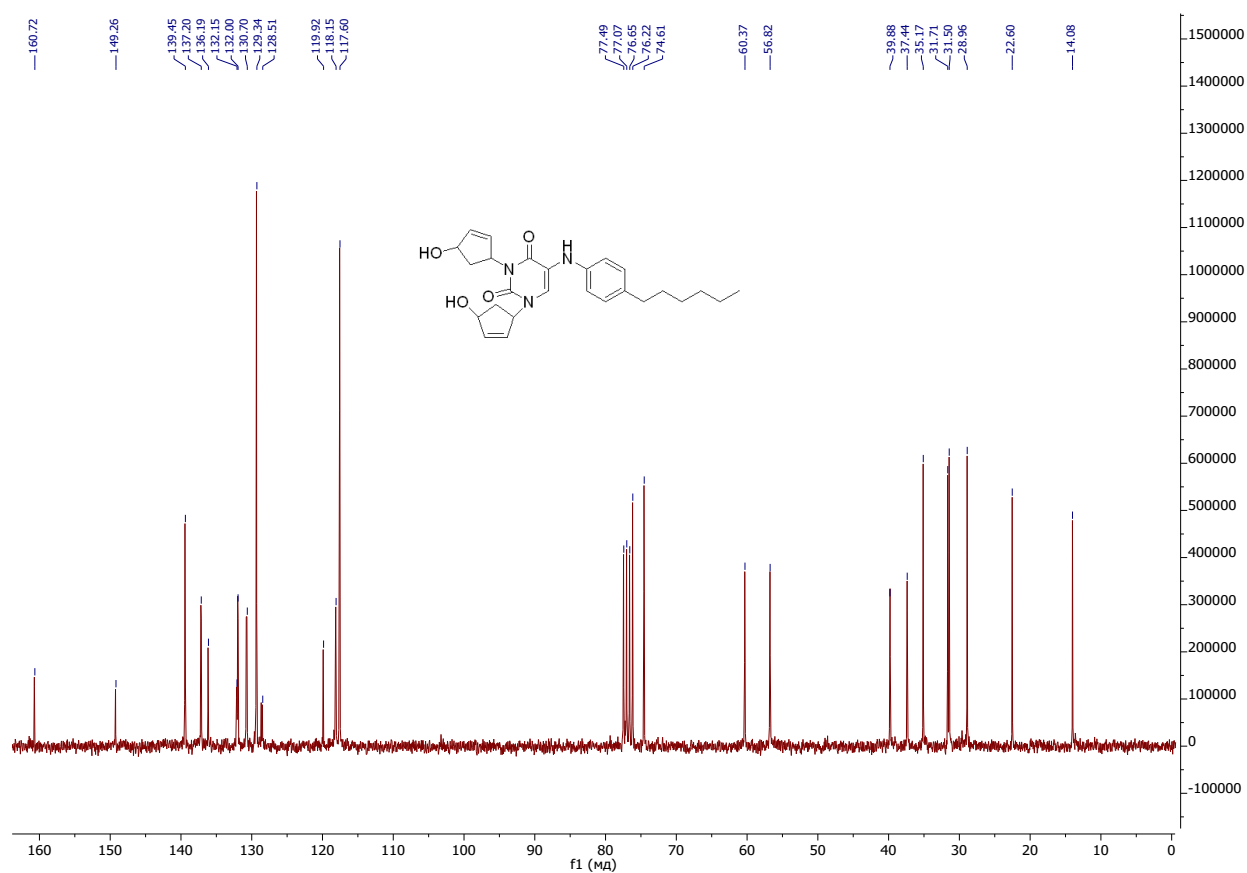


Figure S42 ¹³C NMR spectrum of compound **4d** in CDCl₃ at 100 MHz.

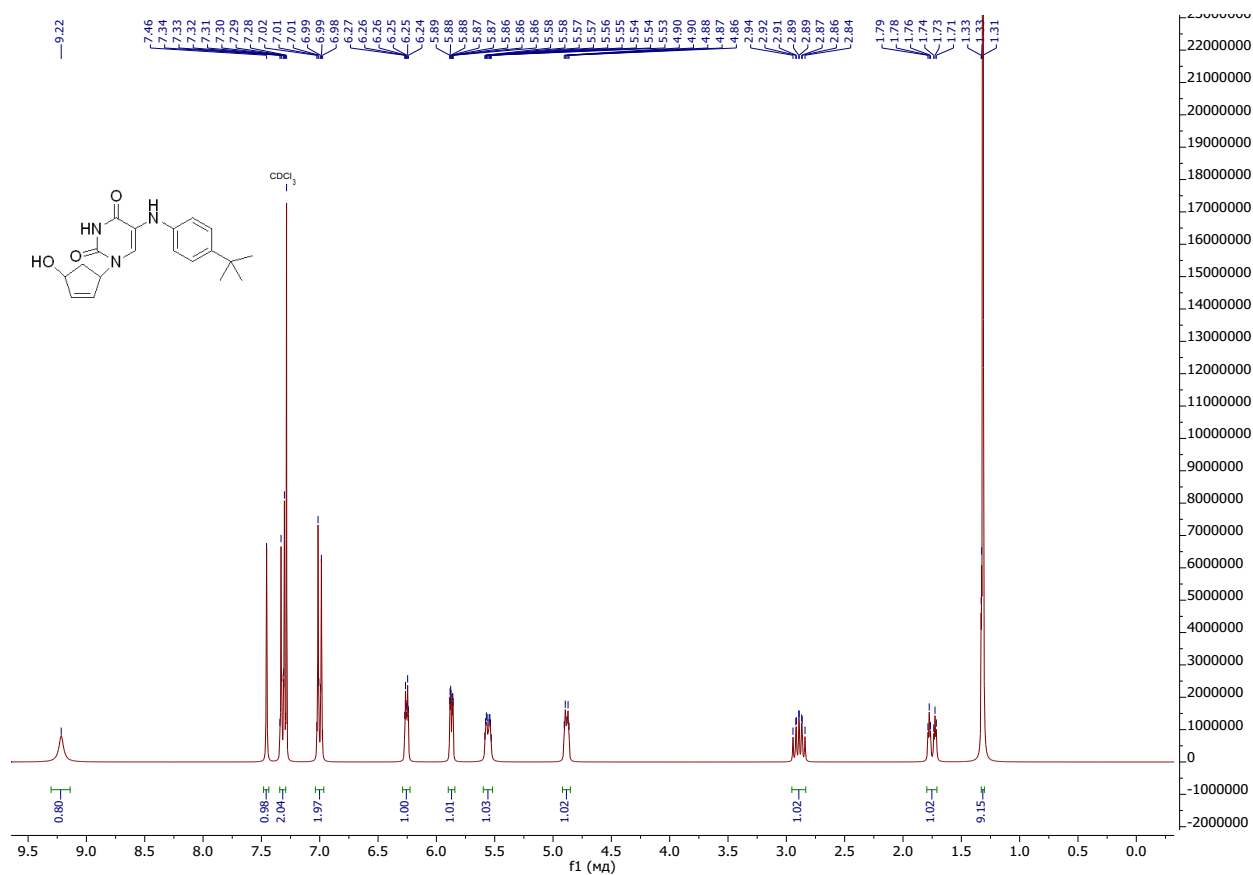


Figure S43 ¹H NMR spectrum of compound **3e** in CDCl₃ at 400 MHz.

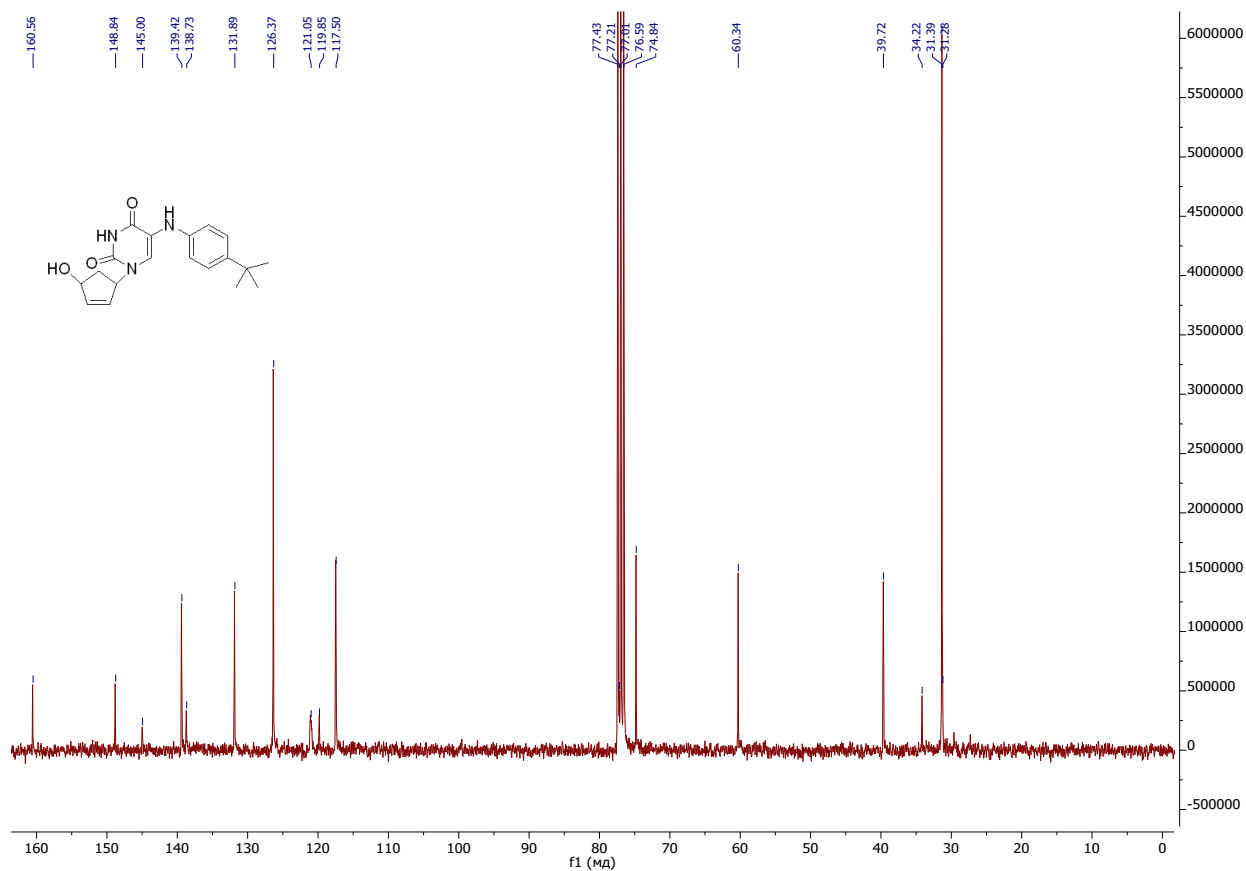


Figure S44 ¹³C NMR spectrum of compound **3e** in CDCl₃ at 100 MHz.

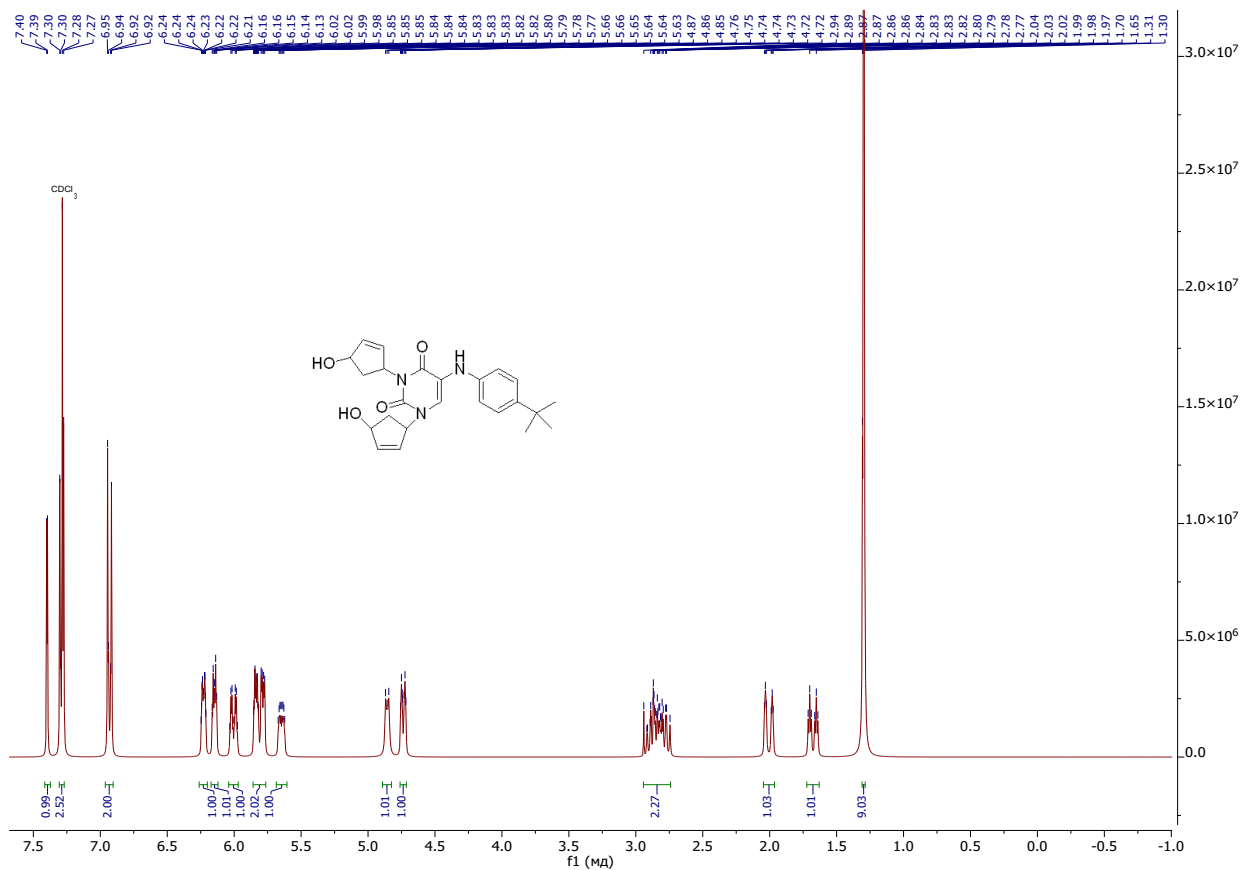


Figure S45 ^1H NMR spectrum of compound **4e** in CDCl_3 at 400 MHz.

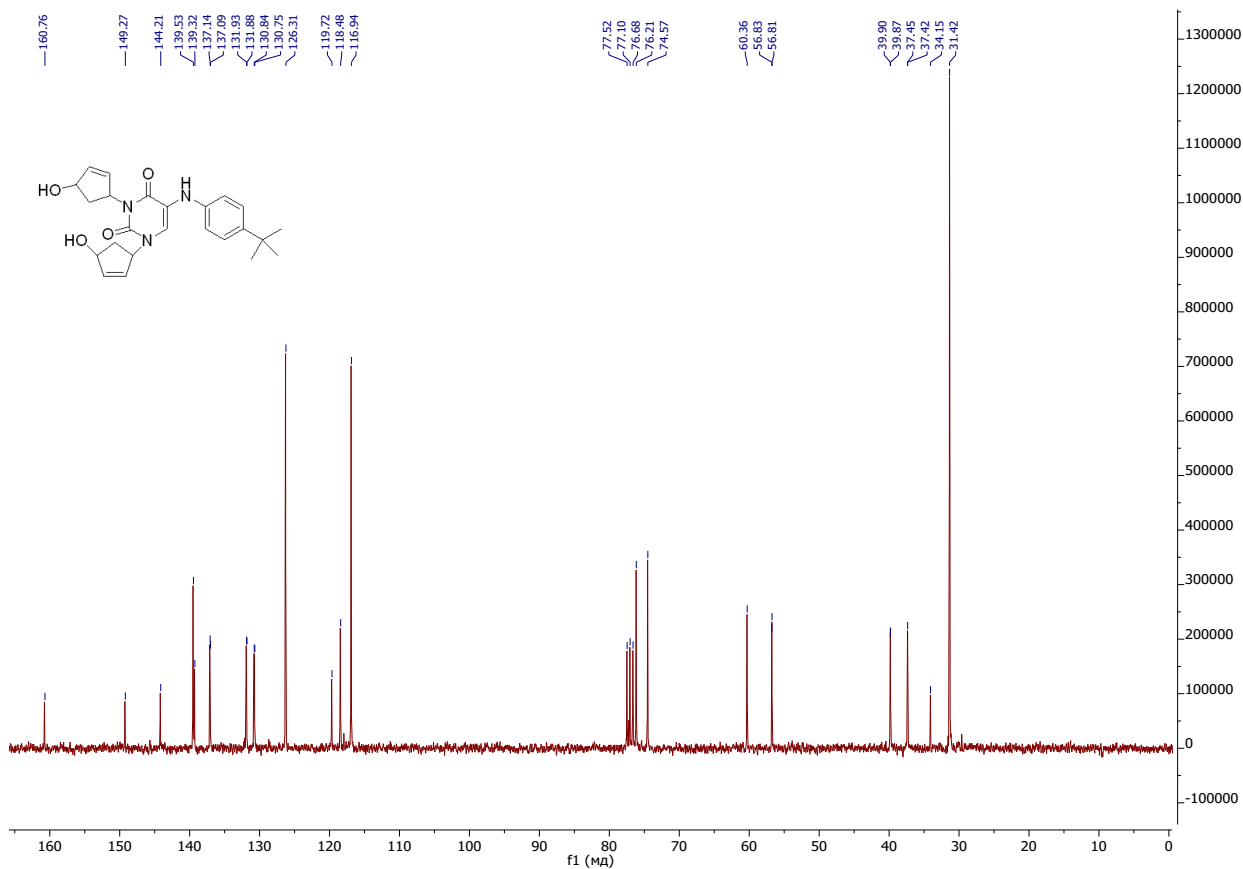


Figure S46 ^{13}C NMR spectrum of compound **4e** in CDCl_3 at 100 MHz.

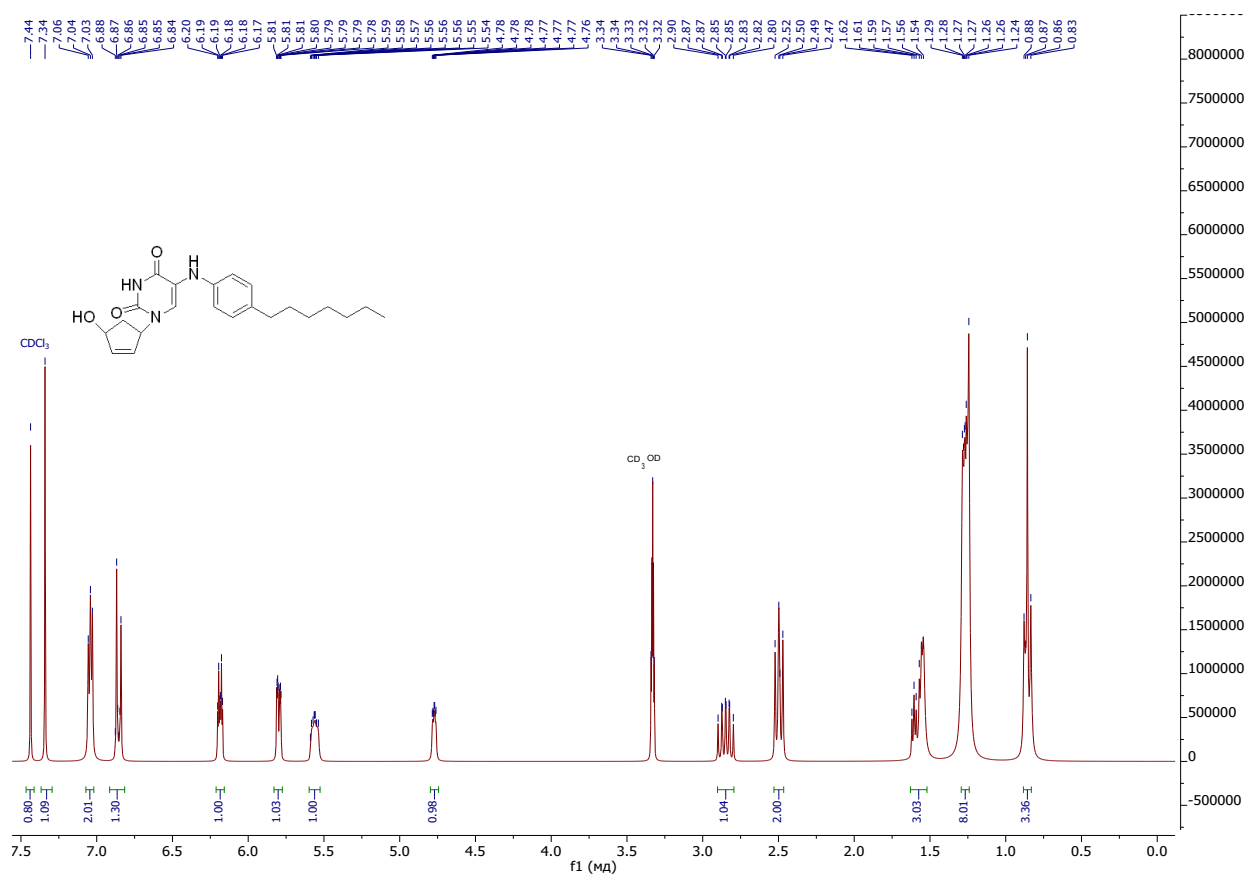


Figure S47 ¹H NMR spectrum of compound **3f** in CDCl₃:CD₃OD at 400 MHz.

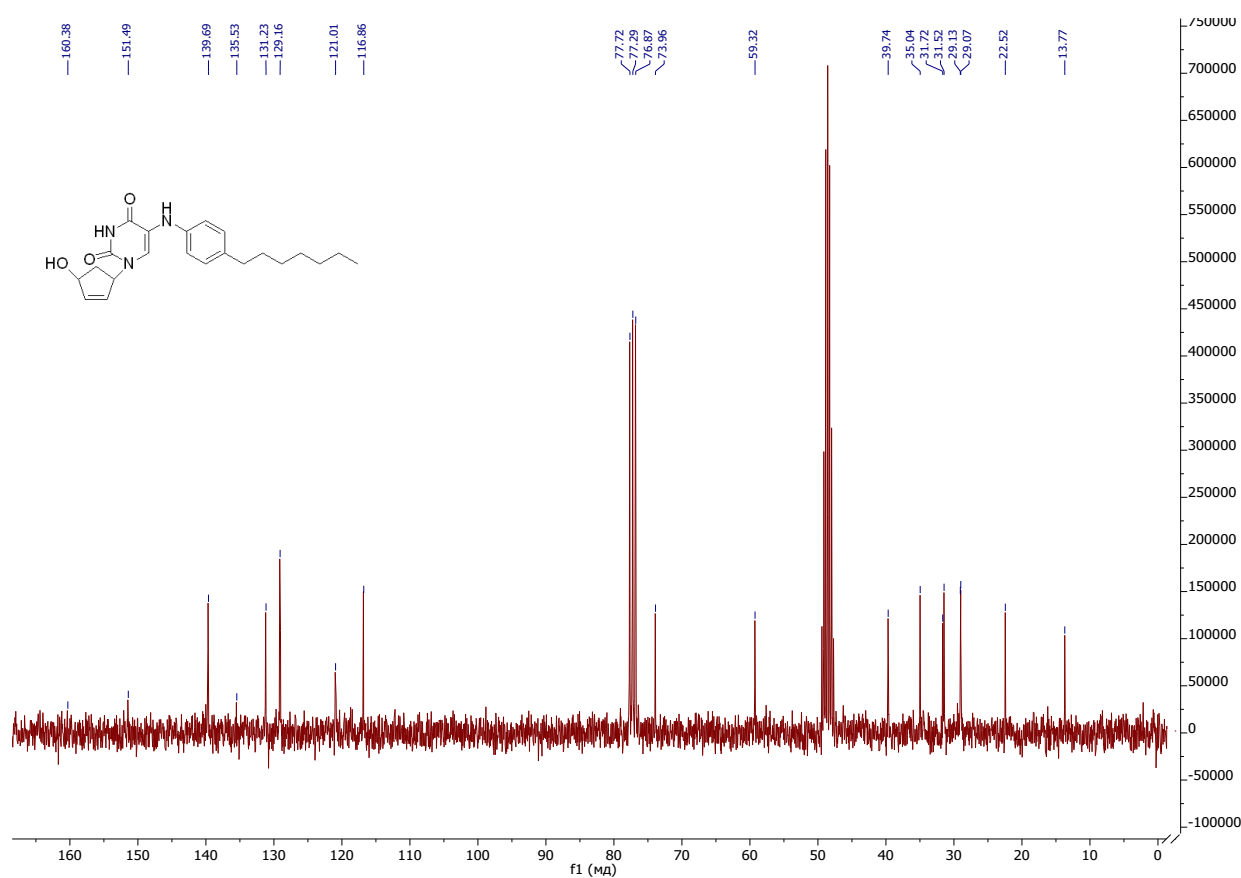


Figure S48 ¹³C NMR spectrum of compound **3f** in CDCl₃:CD₃OD at 100 MHz.

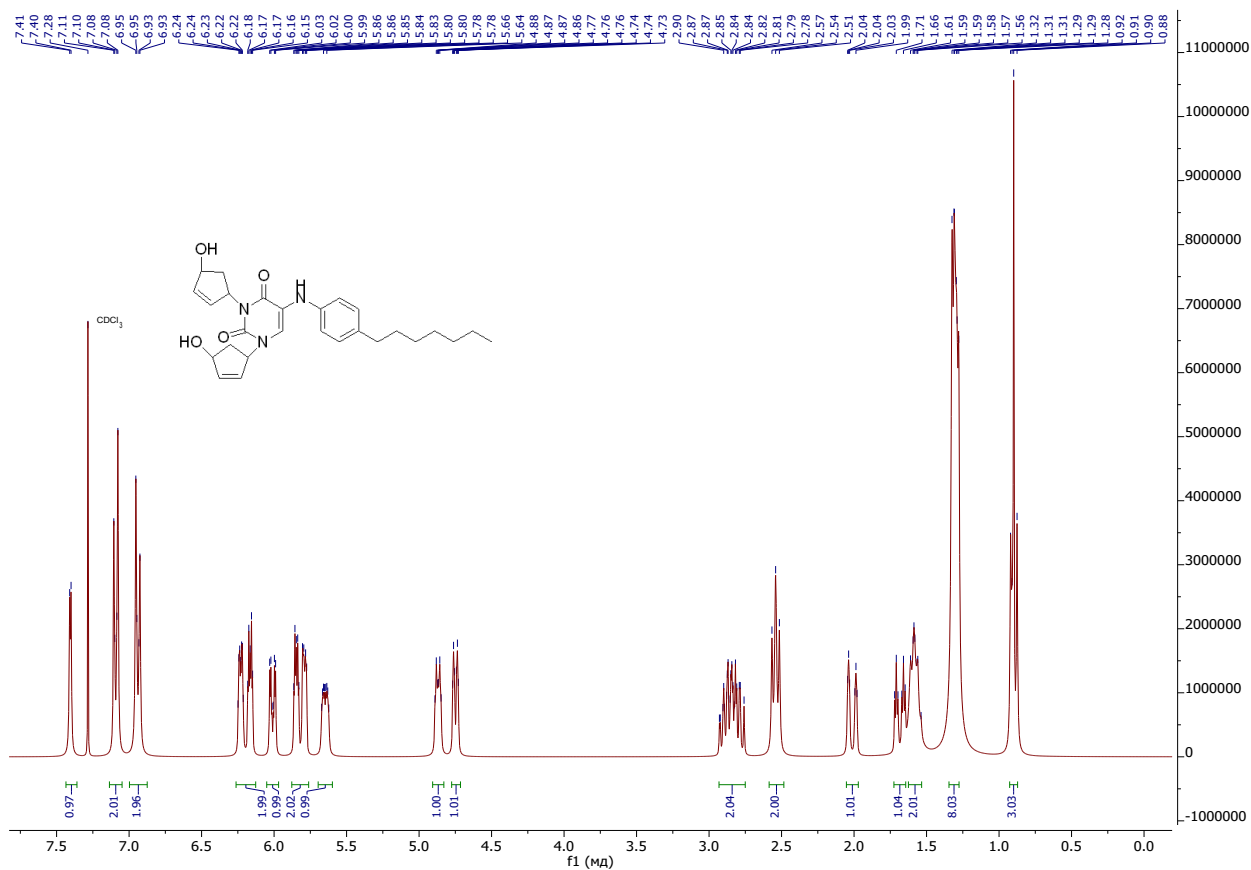


Figure S49 ^1H NMR spectrum of compound **4f** in CDCl_3 at 400 MHz.

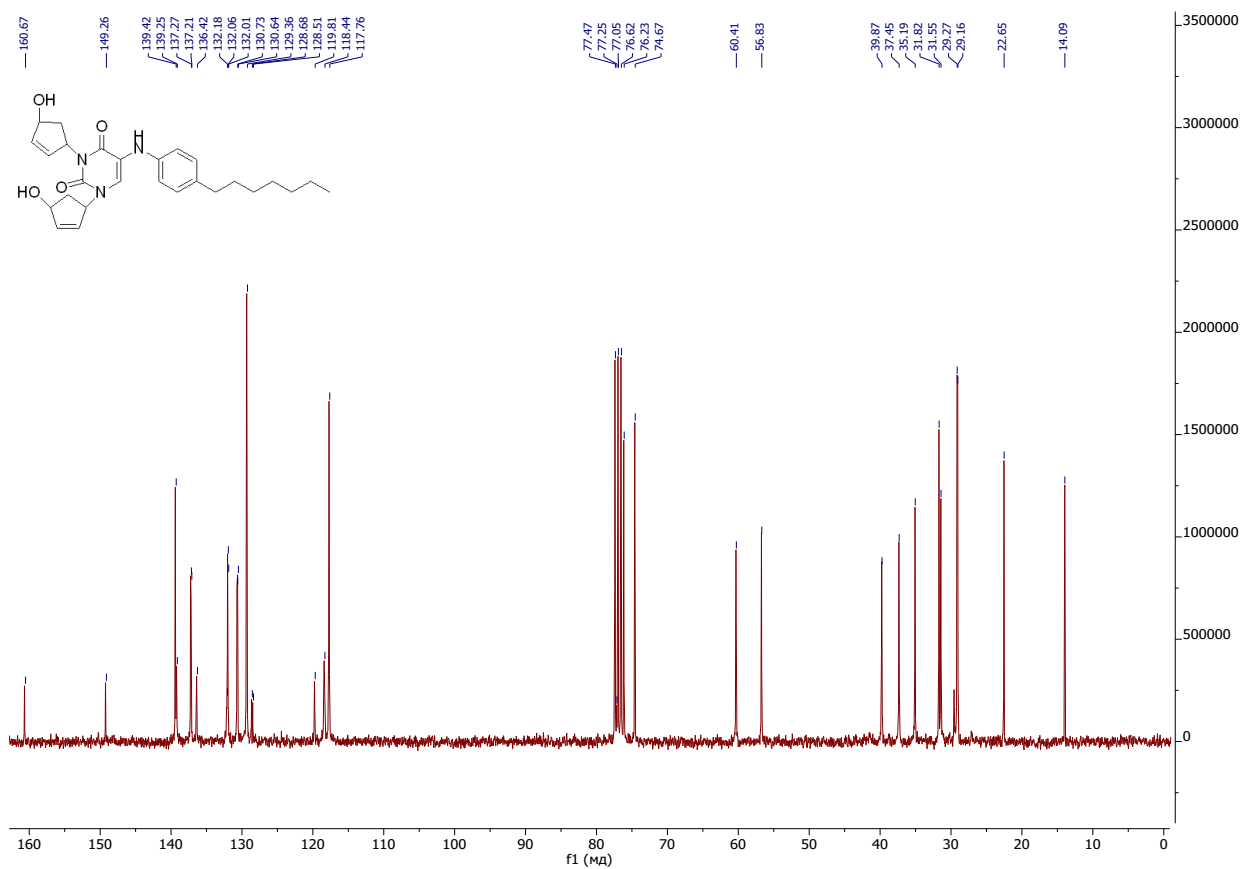


Figure S50 ^{13}C NMR spectrum of compound **4f** in CDCl_3 at 100 MHz.

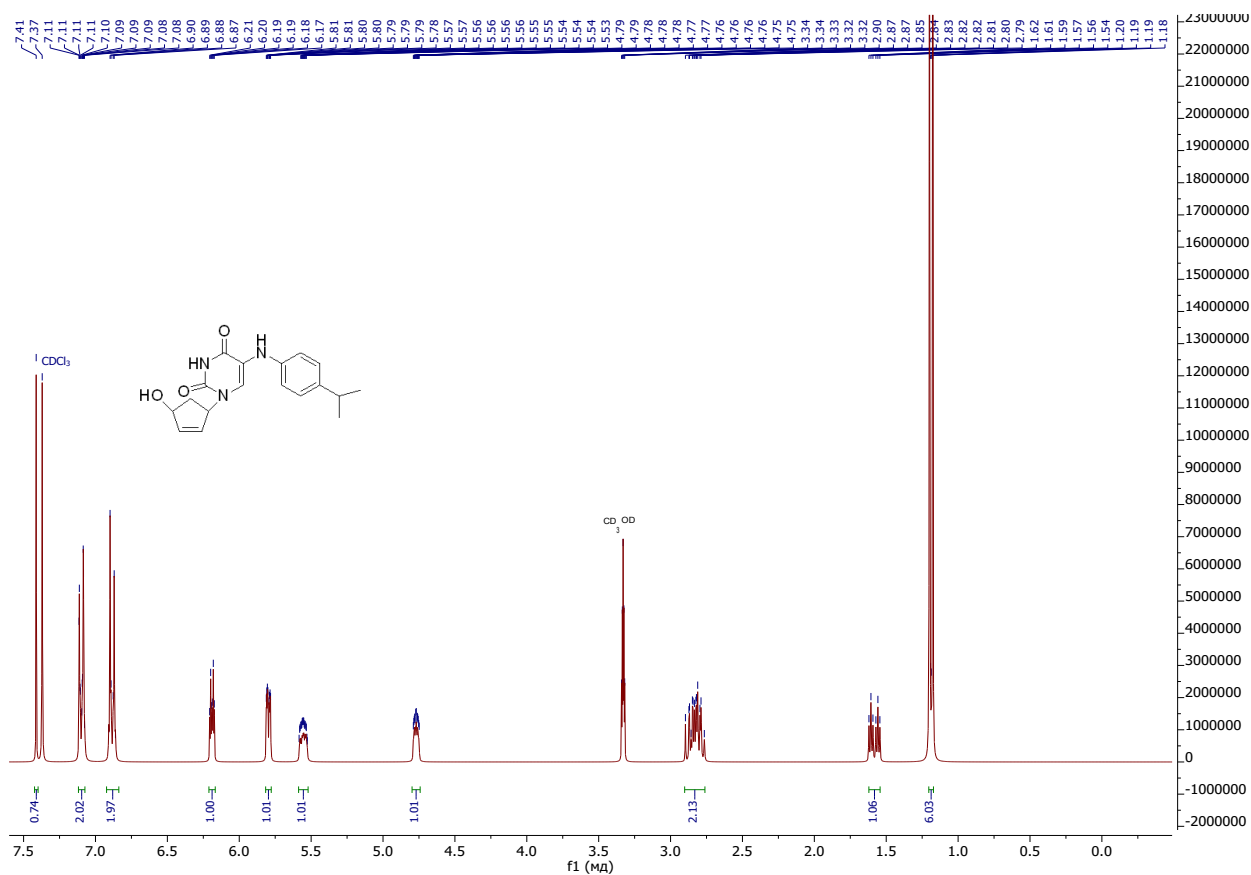


Figure S51 ^1H NMR spectrum of compound **3g** in $\text{CDCl}_3:\text{CD}_3\text{OD}$ at 400 MHz.

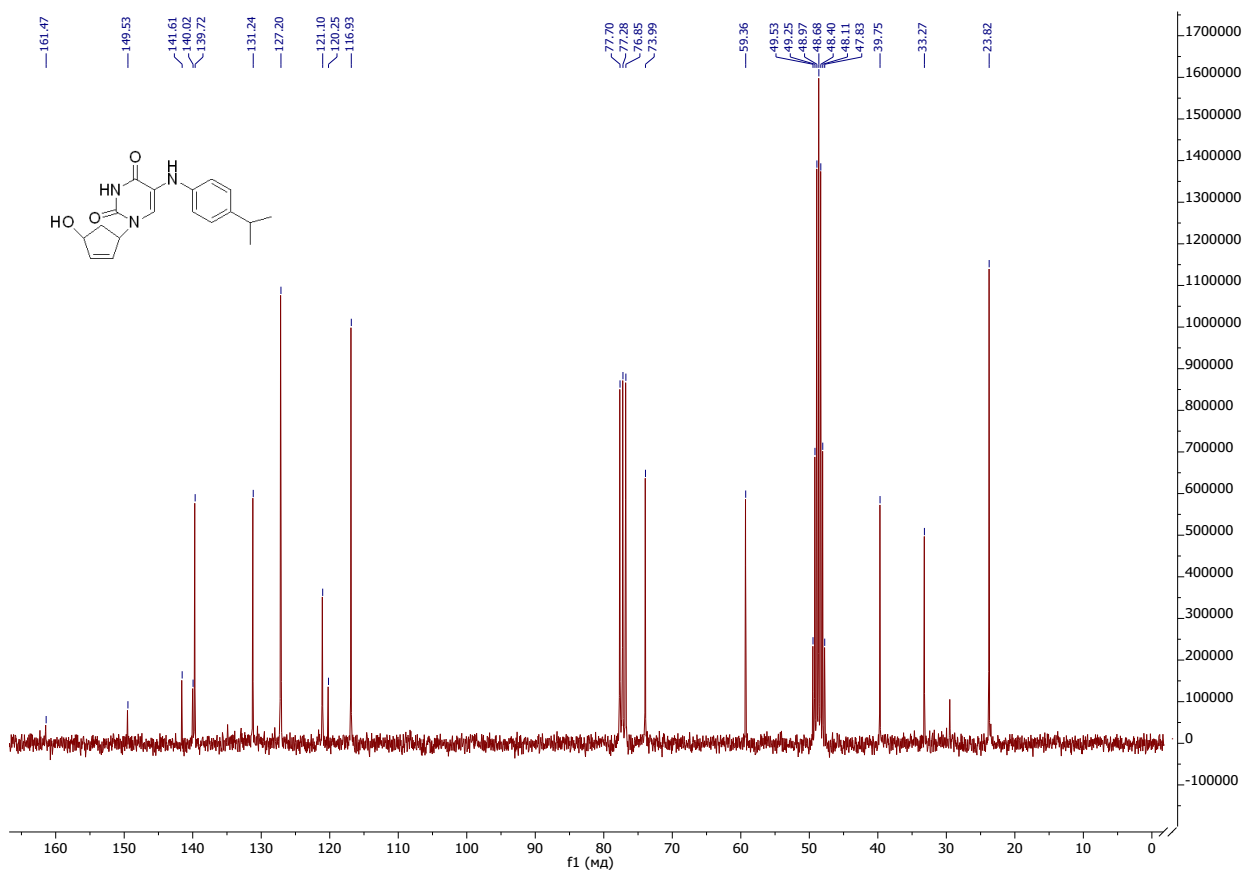


Figure S52 ^{13}C NMR spectrum of compound **3g** in $\text{CDCl}_3\text{:CD}_3\text{OD}$ at 100 MHz.

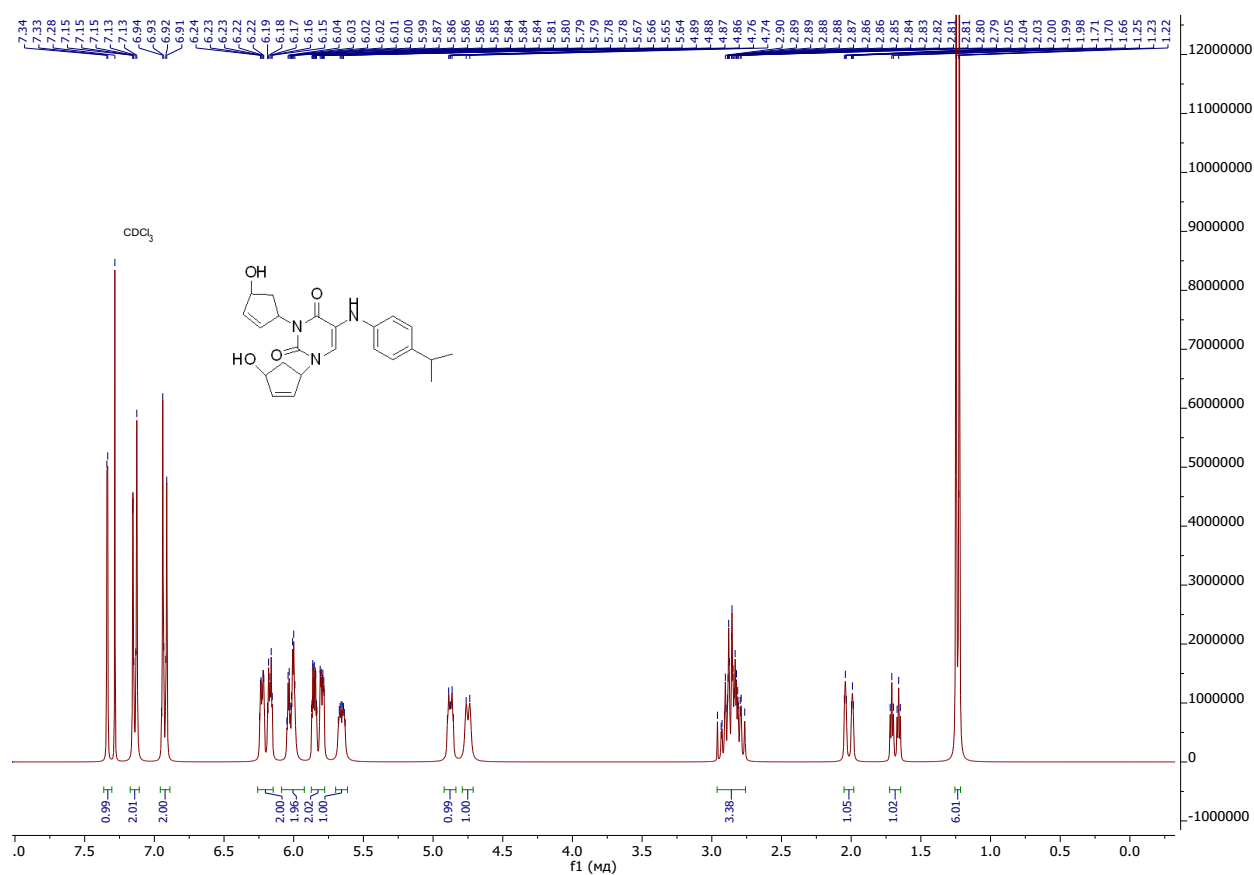


Figure S53 ¹H NMR spectrum of compound **4g** in CDCl₃ at 400 MHz.

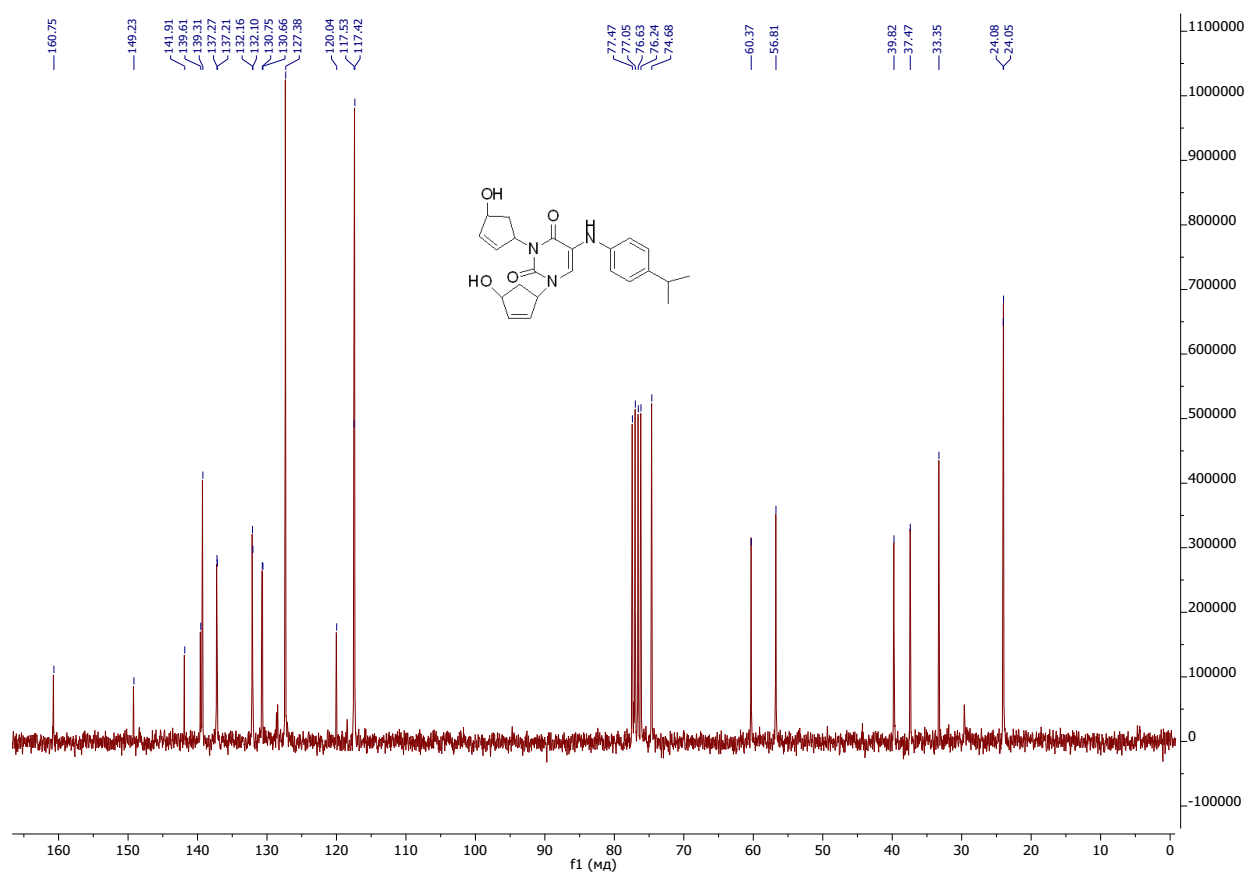


Figure S54 ¹³C NMR spectrum of compound **4g** in CDCl₃ at 100 MHz.

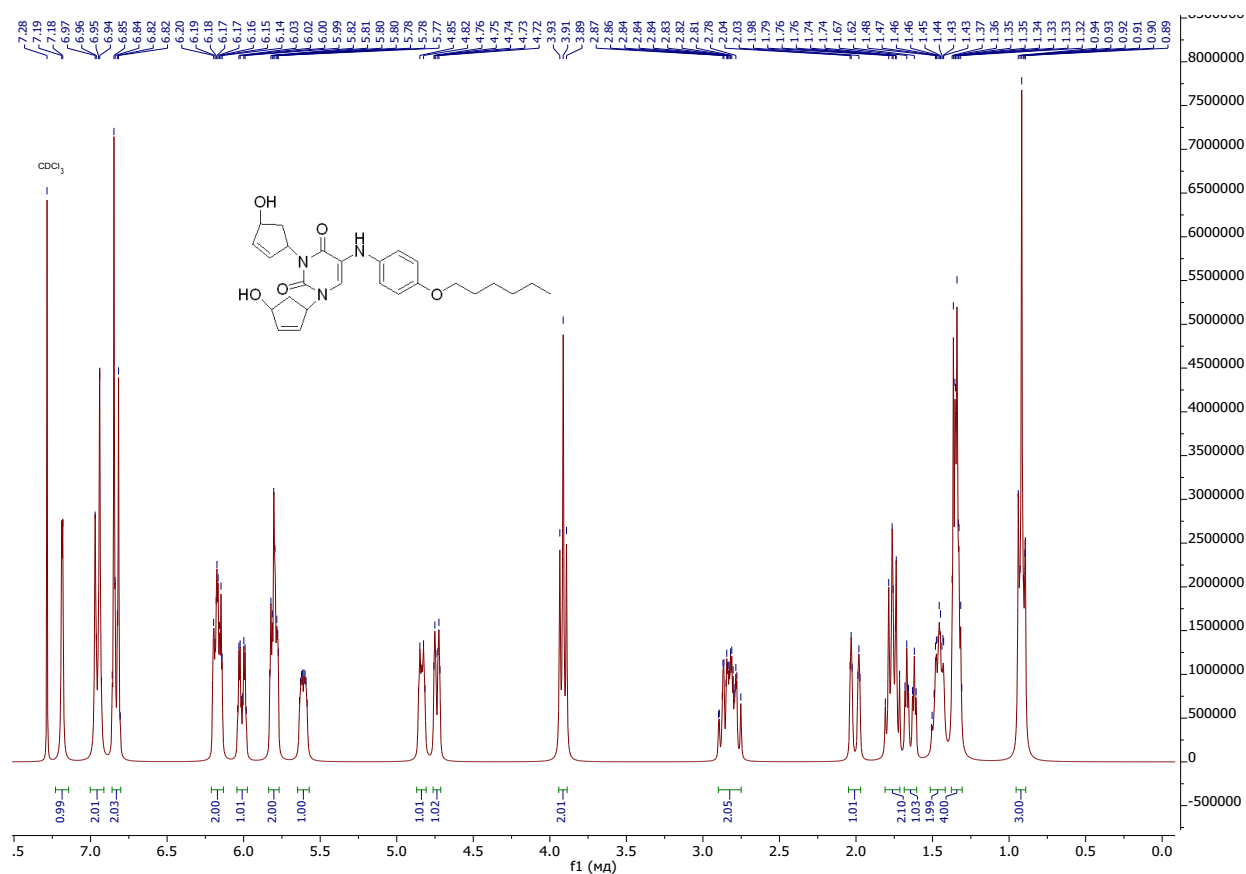


Figure S57 ¹H NMR spectrum of compound **4h** in CDCl₃ at 400 MHz.

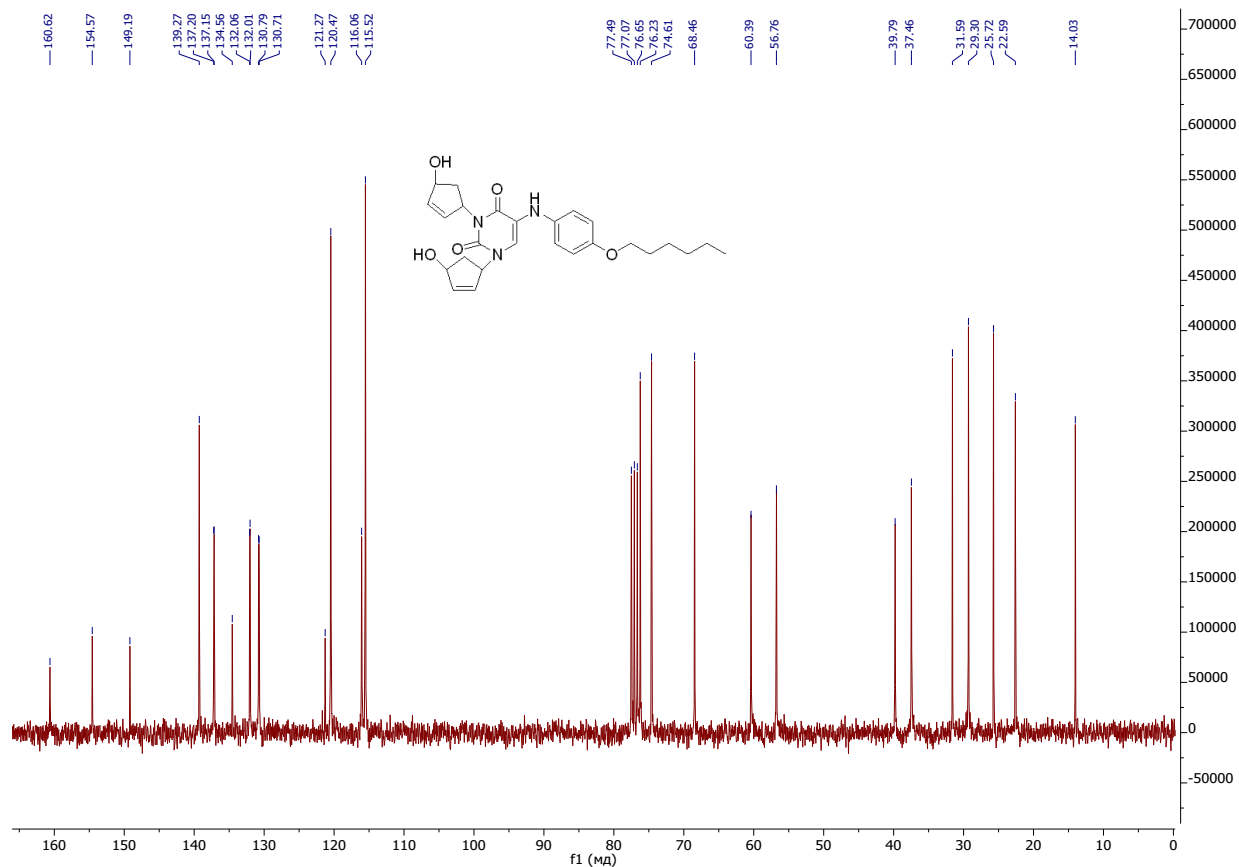


Figure S58 ¹³C NMR spectrum of compound **4h** in CDCl₃ at 100 MHz.

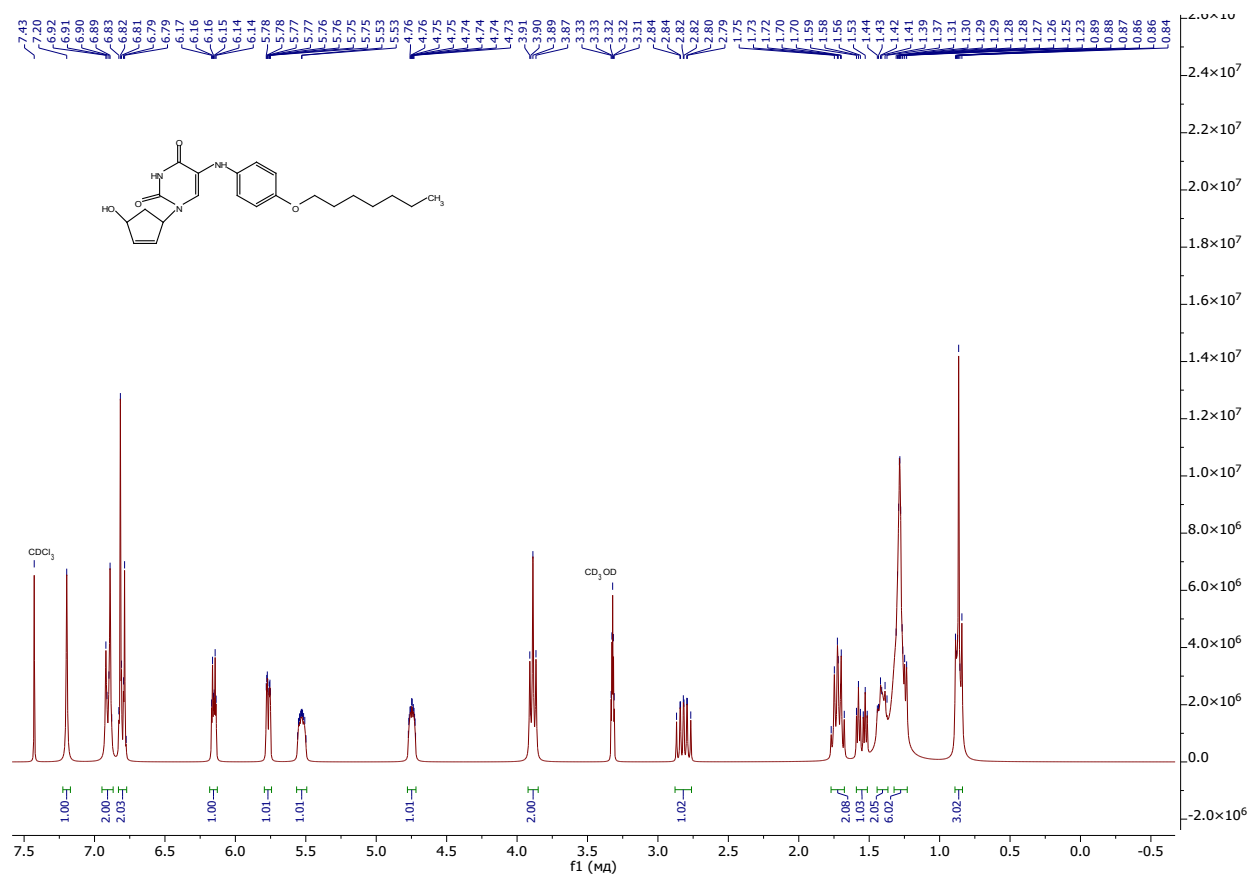


Figure S59 ¹H NMR spectrum of compound **3i** in CDCl₃:CD₃OD at 400 MHz.

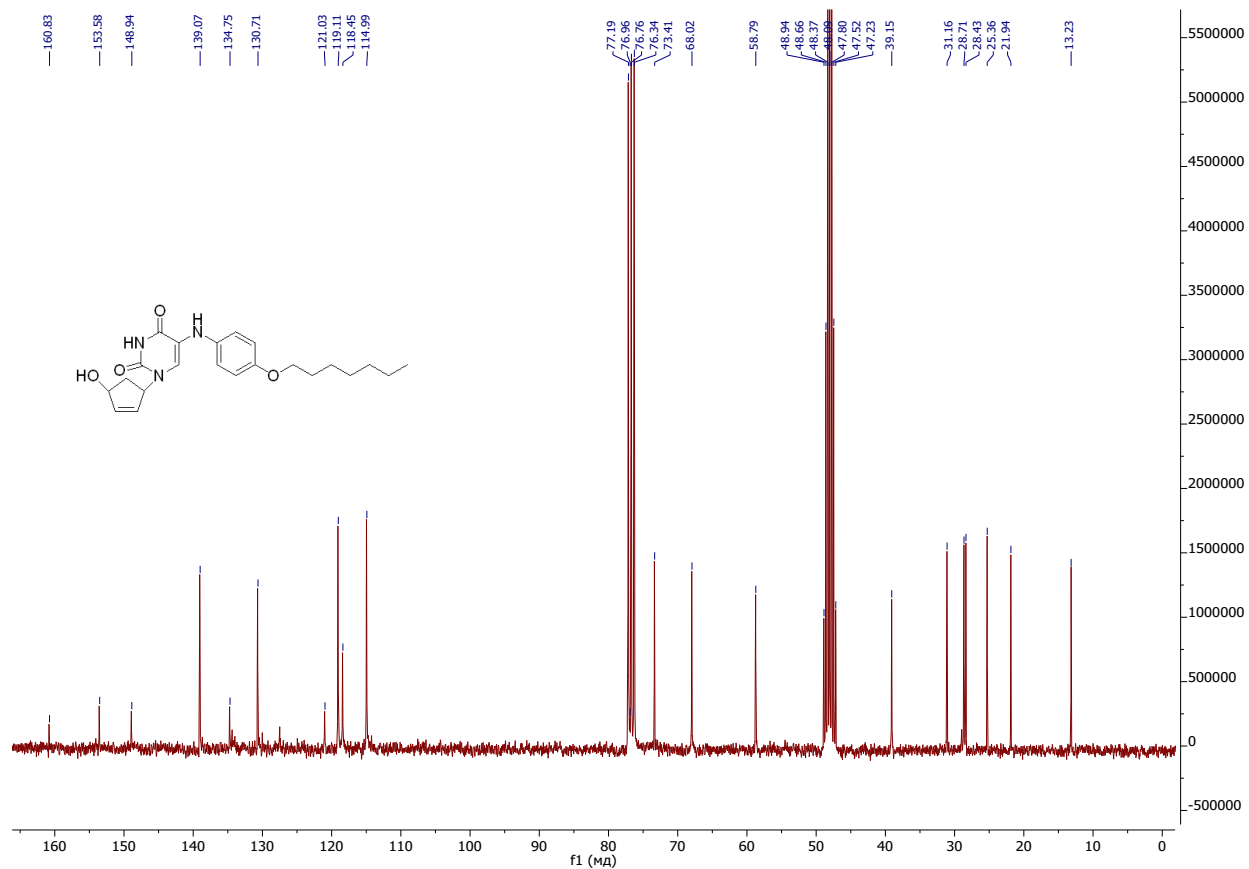
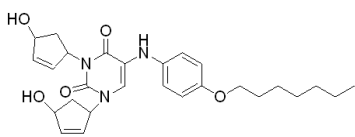


Figure S60 ¹³C NMR spectrum of compound **3i** in CDCl₃:CD₃OD at 100 MHz.



Chemical structure of compound 10: CCCCCCCCOc1ccc(NC(=O)N2C(=O)C3C(O)C=C(C2O3)C1

¹H NMR spectrum (bottom) in CDCl₃ (ppm):

- 7.692, 7.650, 7.608, 7.572, 7.420, 6.793 (aromatic protons)
- 5.991, 5.625 (NH)
- 3.926, 3.923, 3.696 (OCH₂)
- 3.126, 2.916, 2.862, 2.854, 2.549, 2.207 (CH₂ groups)
- 1.354 (CH₃)

¹³C NMR spectrum (top) in CDCl₃ (ppm):

- 160.07, 154.11, 146.66 (amide carbonyls)
- 138.59, 138.77, 136.72, 133.96, 131.70, 131.64, 130.20, 130.11 (aromatic carbons)
- 120.84, 120.06, 115.28, 114.99 (aromatic carbons)
- 76.92, 76.50, 76.08, 75.72, 74.20, 67.93 (solvent and CDCl₃)
- 59.91, 56.25 (NH)
- 39.26, 39.23, 36.96 (OCH₂)
- 31.26, 29.16, 28.62, 28.54, 25.49, 22.07 (CH₂ groups)
- 13.54 (CH₃)

Figure S62 ^{13}C NMR spectrum of compound **4i** in CDCl_3 at 100 MHz.

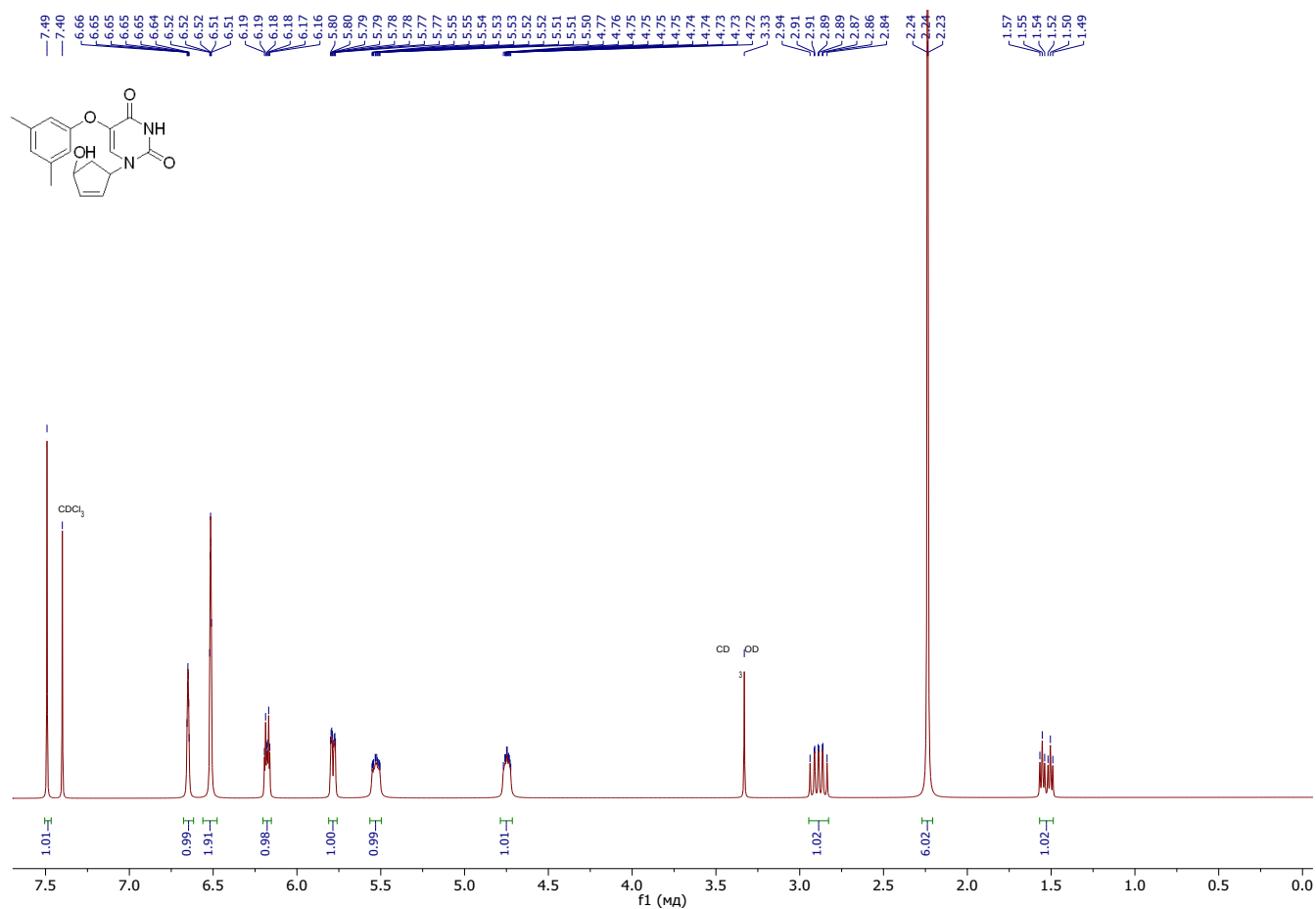


Figure S63 ¹H NMR spectrum of compound **10a** in CDCl₃:CD₃OD at 400 MHz.

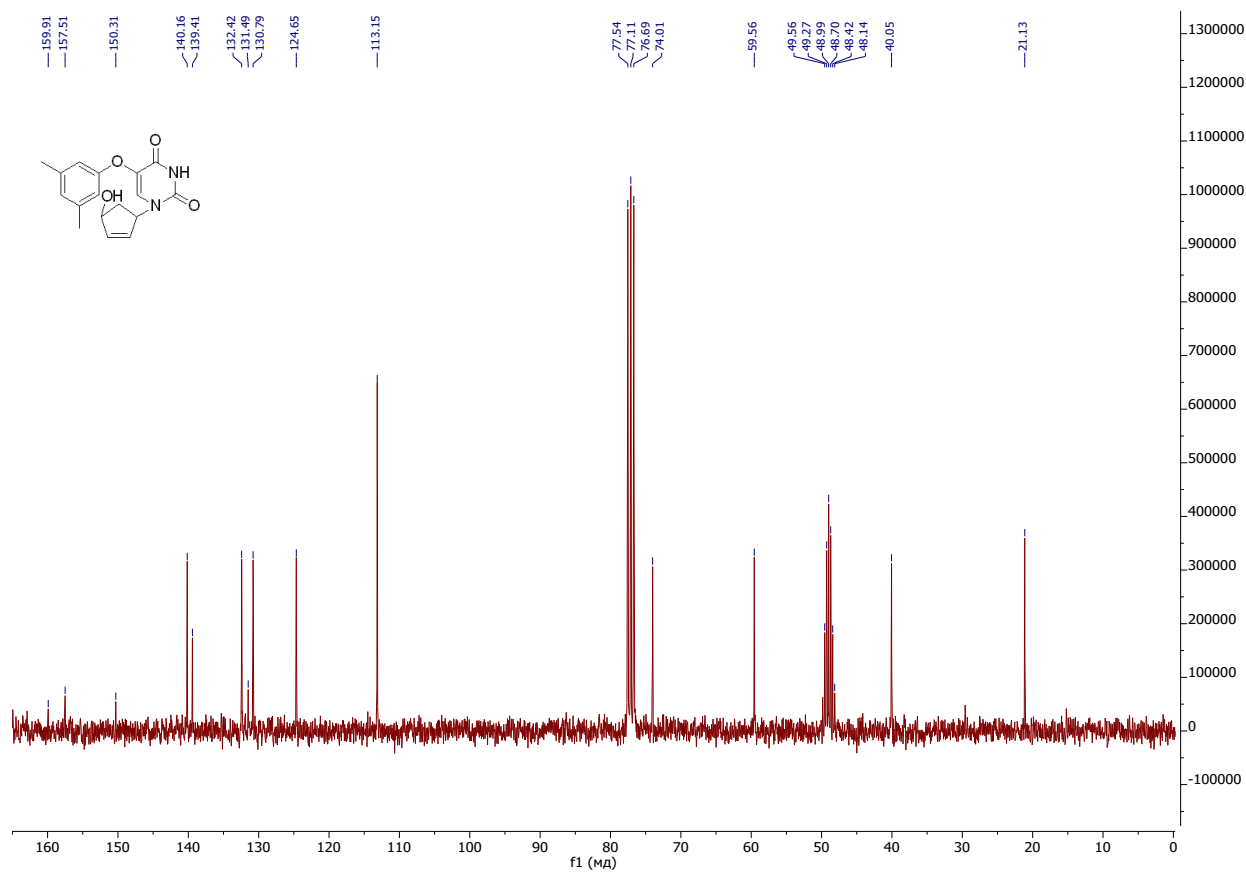


Figure S64 ¹³C NMR spectrum of compound **10a** in CDCl₃:CD₃OD at 100 MHz.

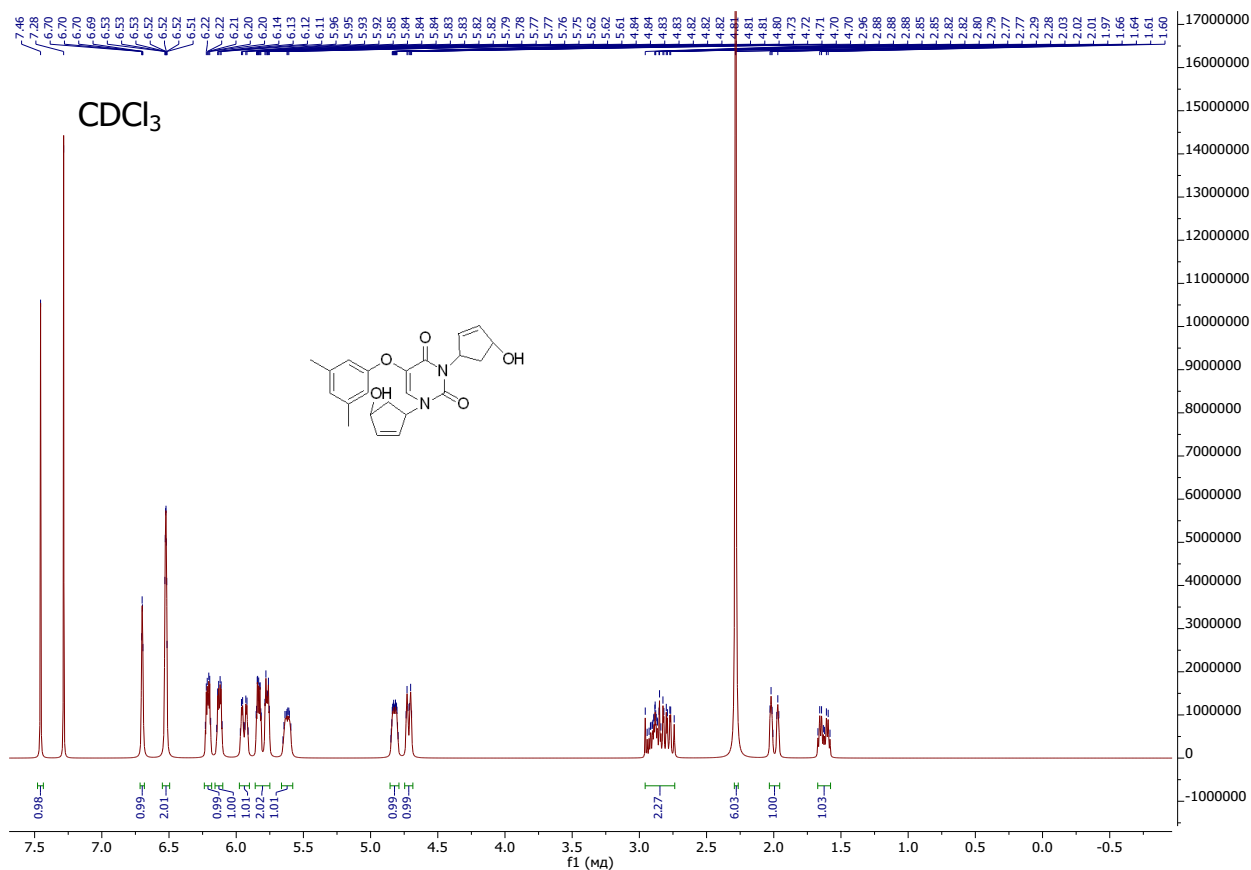


Figure S65 ^1H NMR spectrum of compound **11a** in CDCl_3 at 400 MHz.

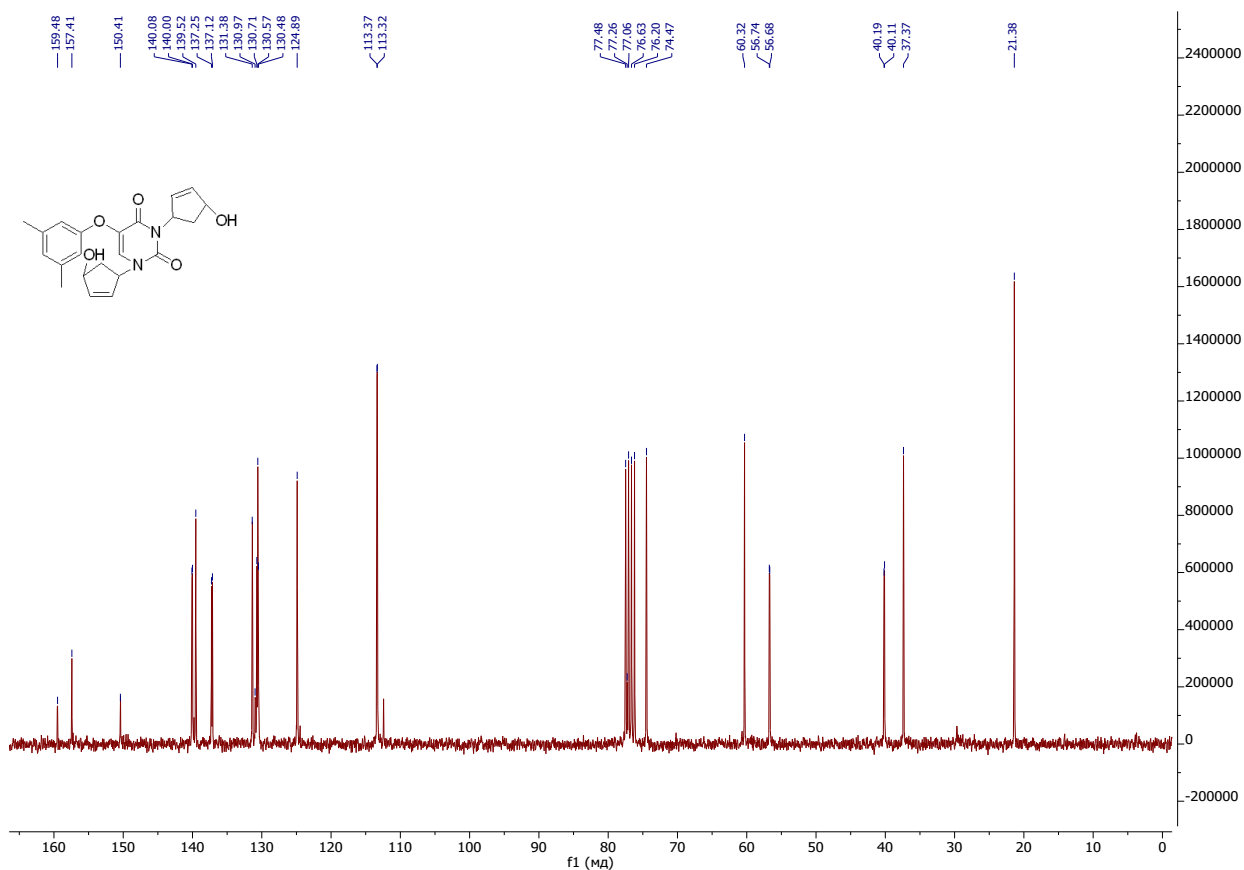


Figure S66 ^{13}C NMR spectrum of compound **11a** in CDCl_3 at 100 MHz.

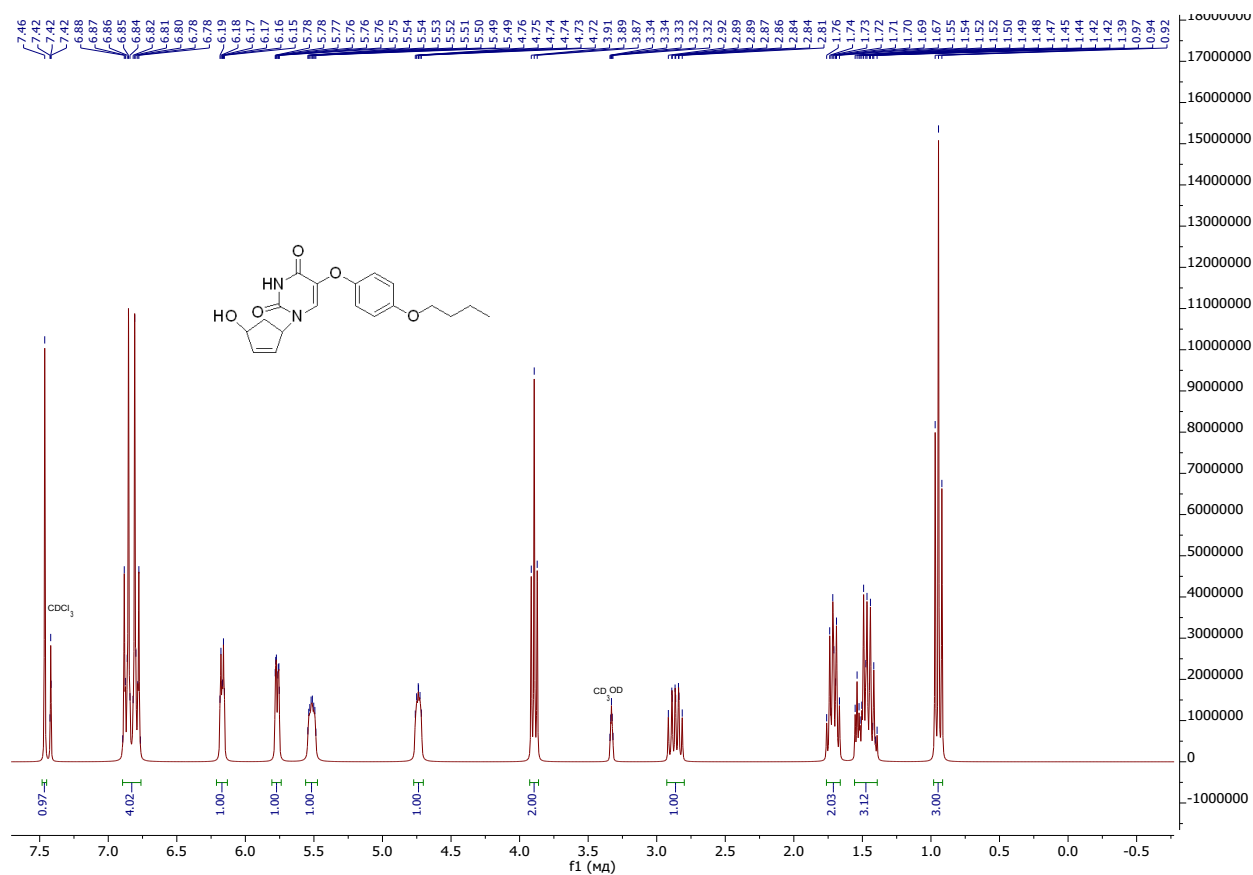


Figure S67 ¹H NMR spectrum of compound **10b** in CDCl₃:CD₃OD at 400 MHz.

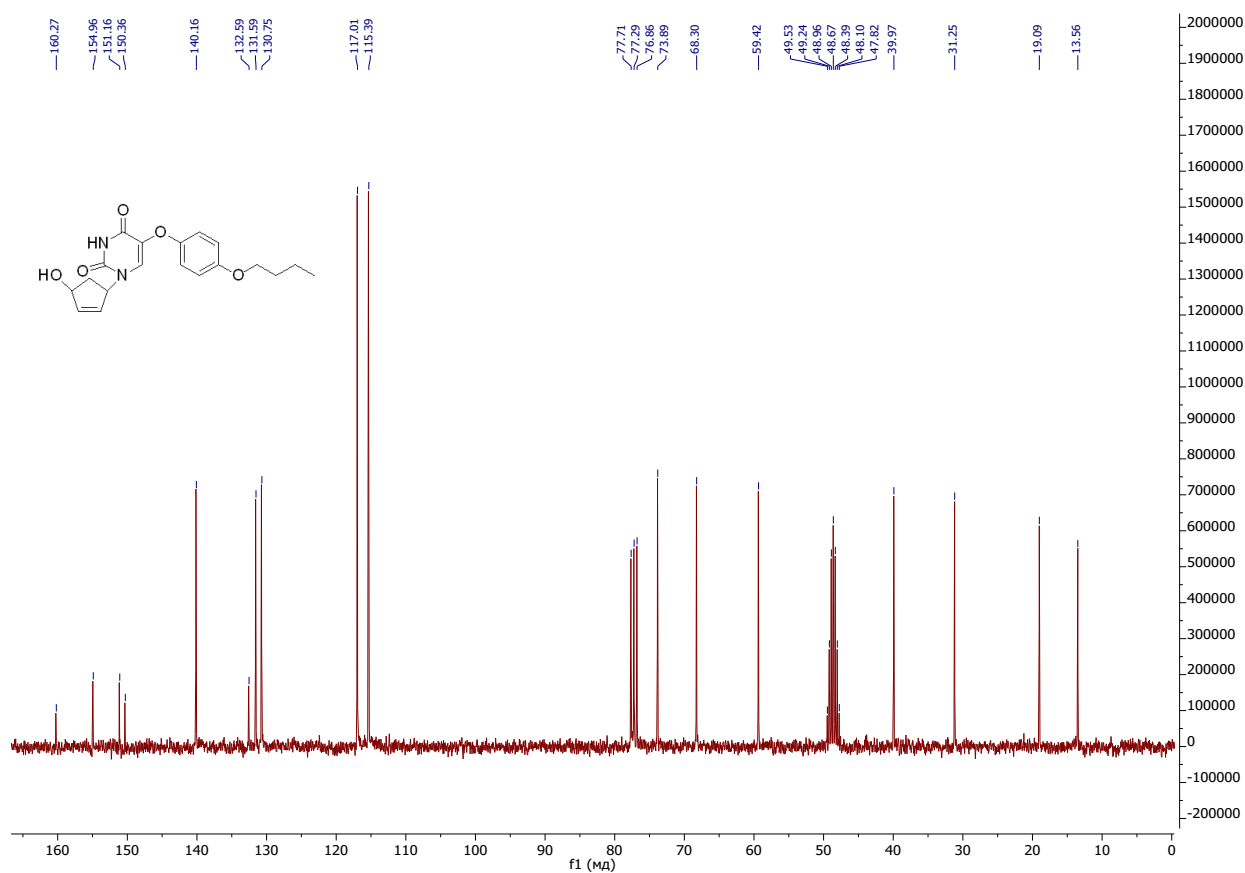
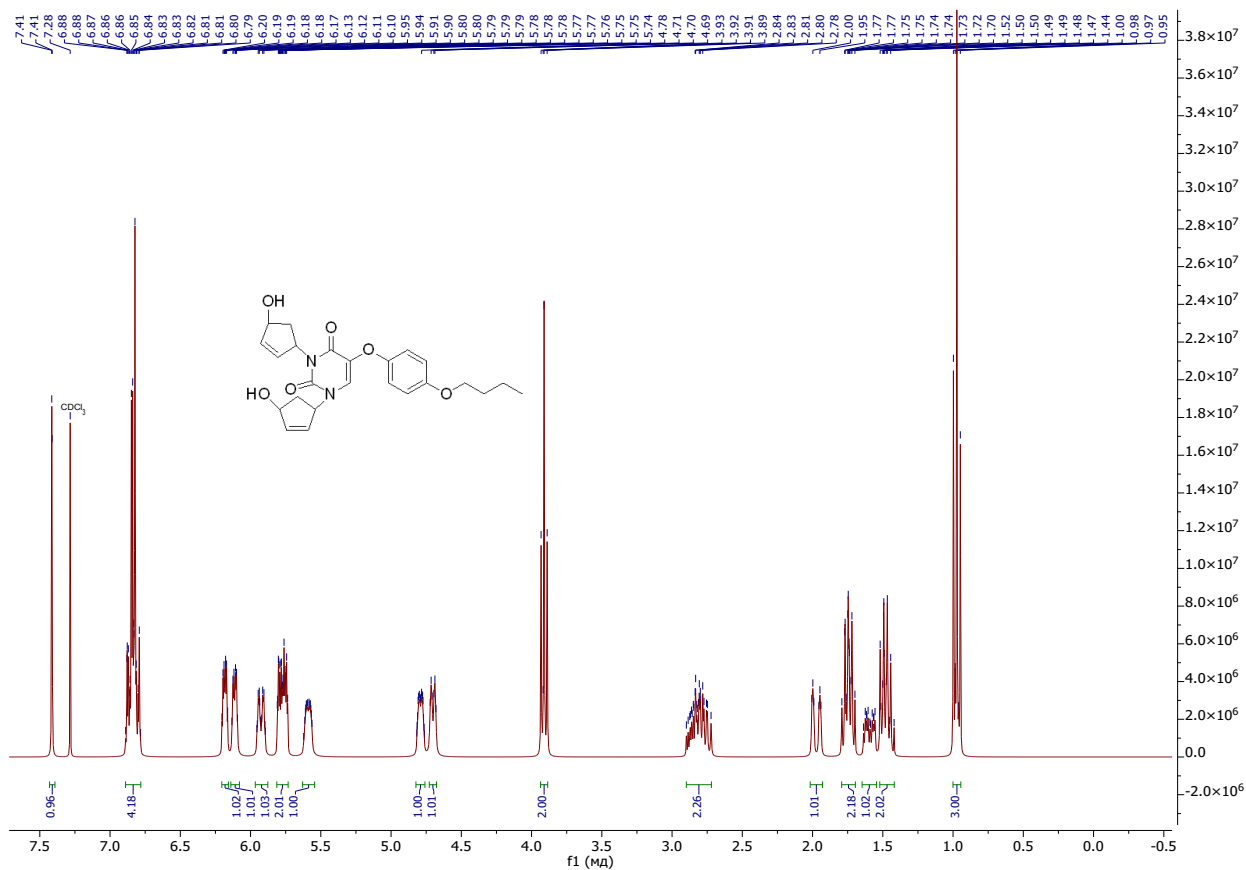


Figure S68 ¹³C NMR spectrum of compound **10b** in CDCl₃:CD₃OD at 100 MHz.



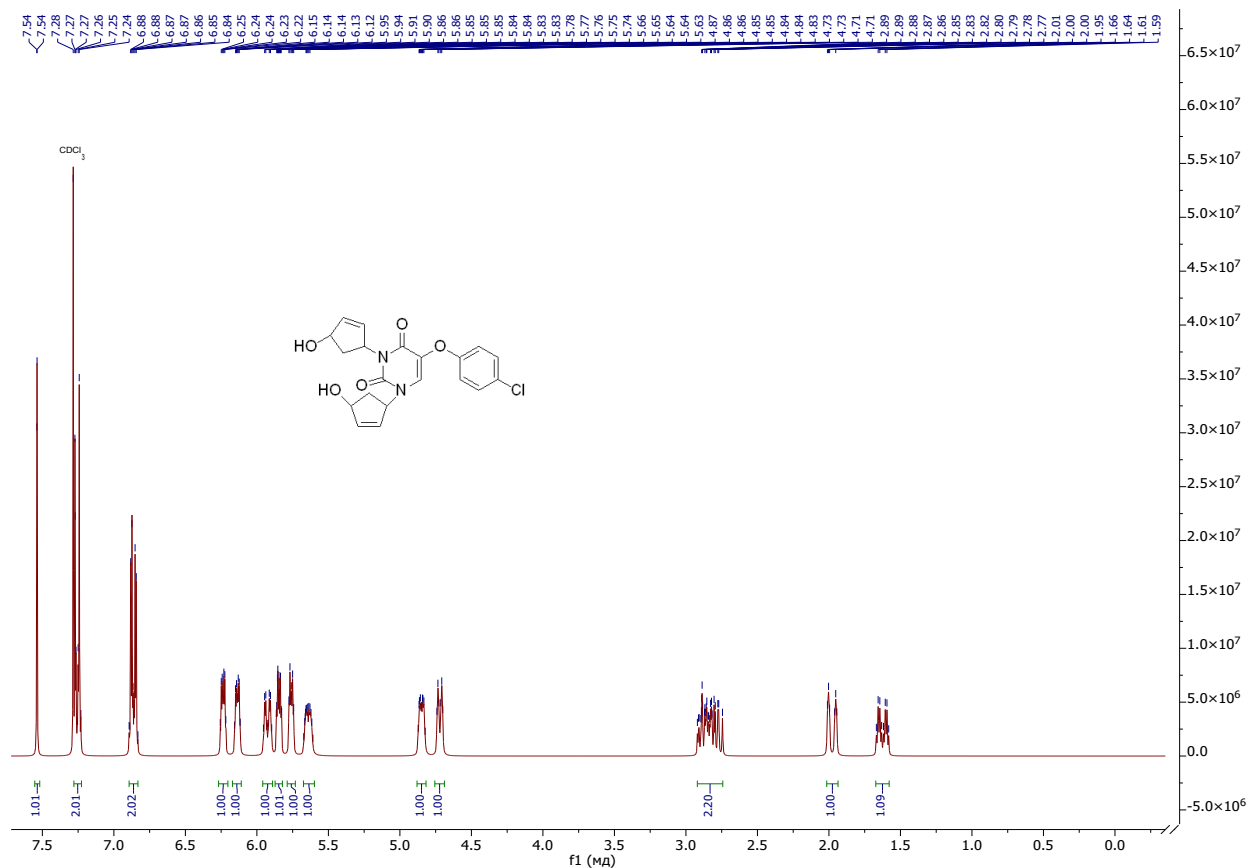


Figure S73 ¹H NMR spectrum of compound **11c** in CDCl₃ at 400 MHz.

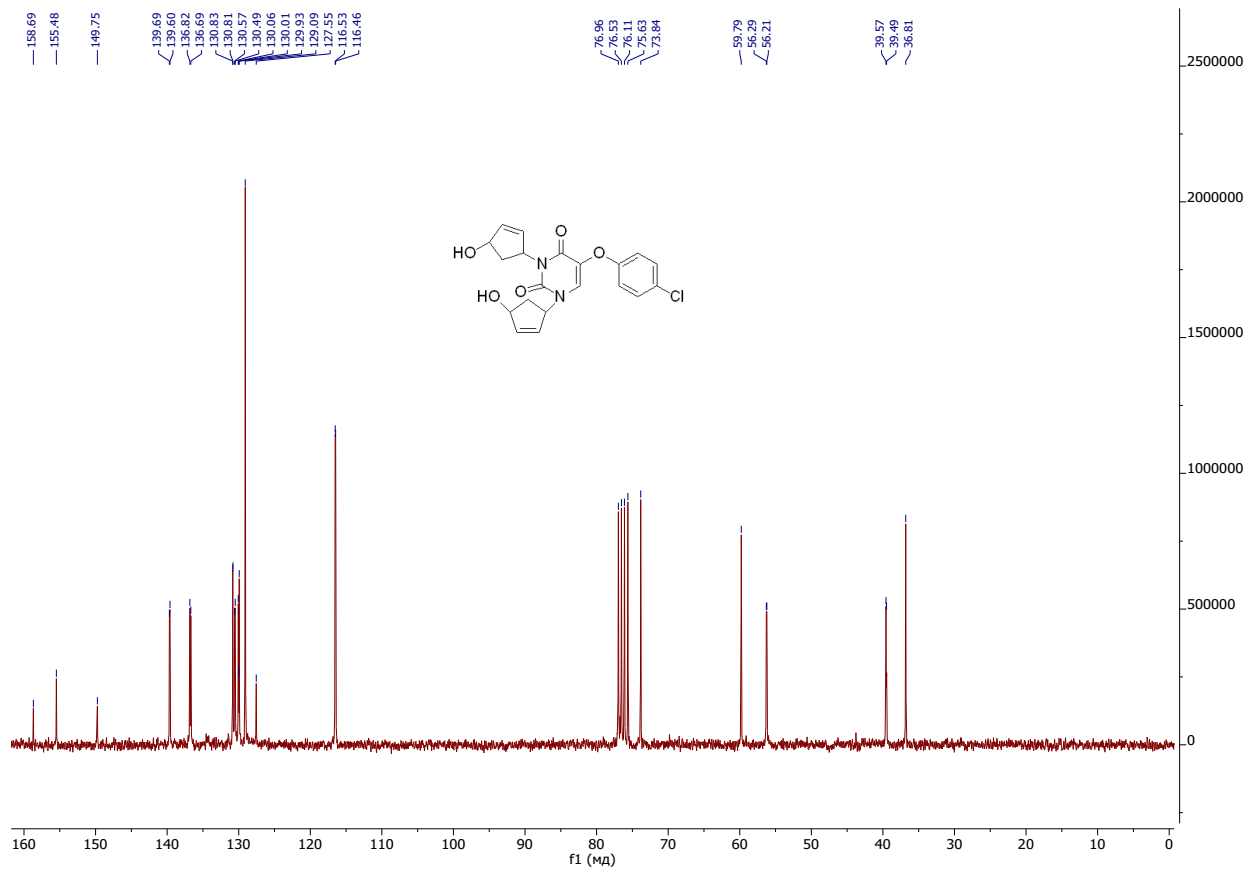
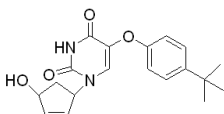


Figure S74 ¹³C NMR spectrum of compound **11c** in CDCl₃ at 100 MHz.



Chemical structure of compound 10 is shown. The ^{13}C NMR spectrum (f1 (MMA)) displays peaks corresponding to the structure, with labeled chemical shifts (ppm) as follows:

- 160.24
- 155.34
- 150.43
- 145.65
- 140.20
- 132.67
- 131.54
- 130.74
- 126.32
- 114.86
- 77.68
- 77.25
- 76.82
- 73.92
- 59.43
- 49.57
- 49.28
- 49.00
- 48.72
- 48.43
- 48.15
- 47.86
- 40.03
- 34.05
- 31.23

Figure S76 ^{13}C NMR spectrum of compound **10d** in $\text{CDCl}_3:\text{CD}_3\text{OD}$ at 100 MHz.

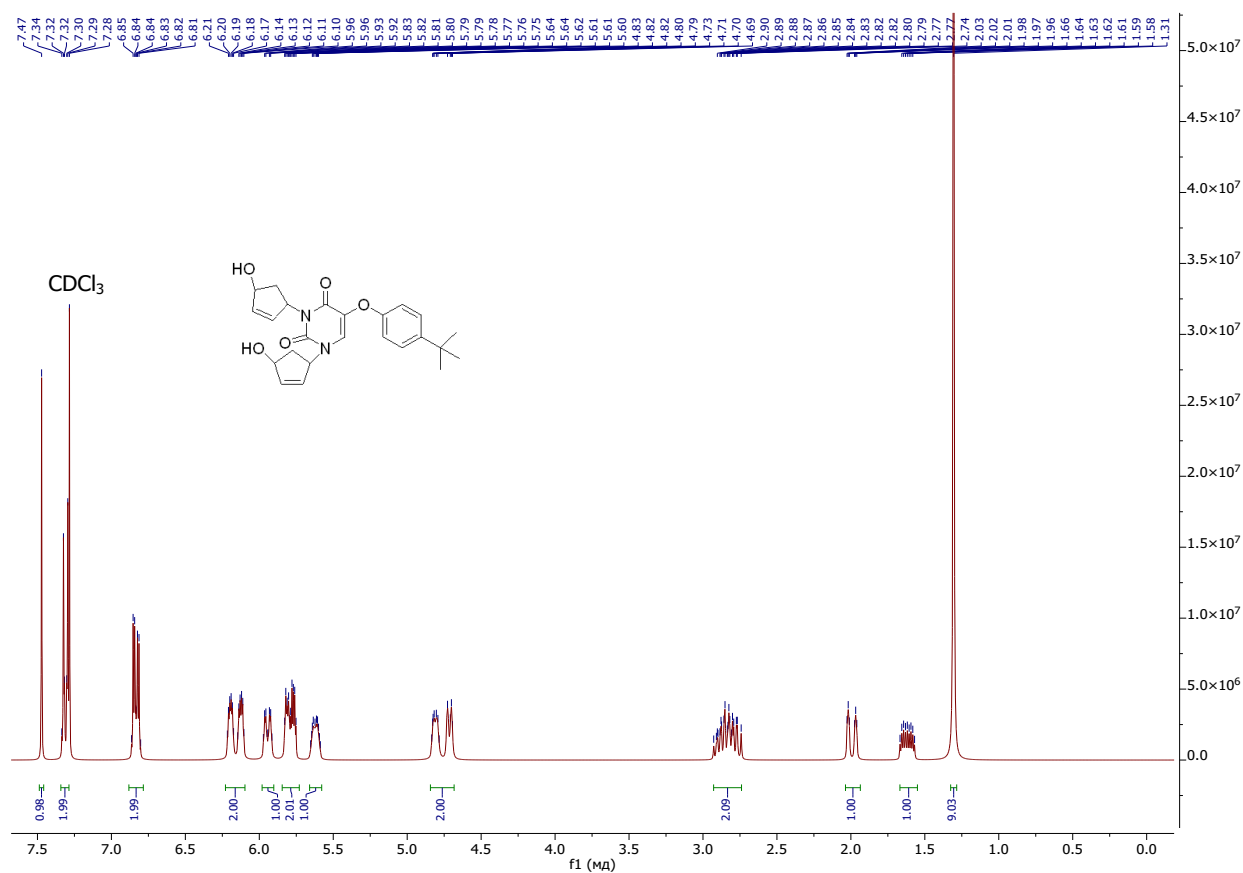


Figure S77 ¹H NMR spectrum of compound **11d** in CDCl₃ at 400 MHz.

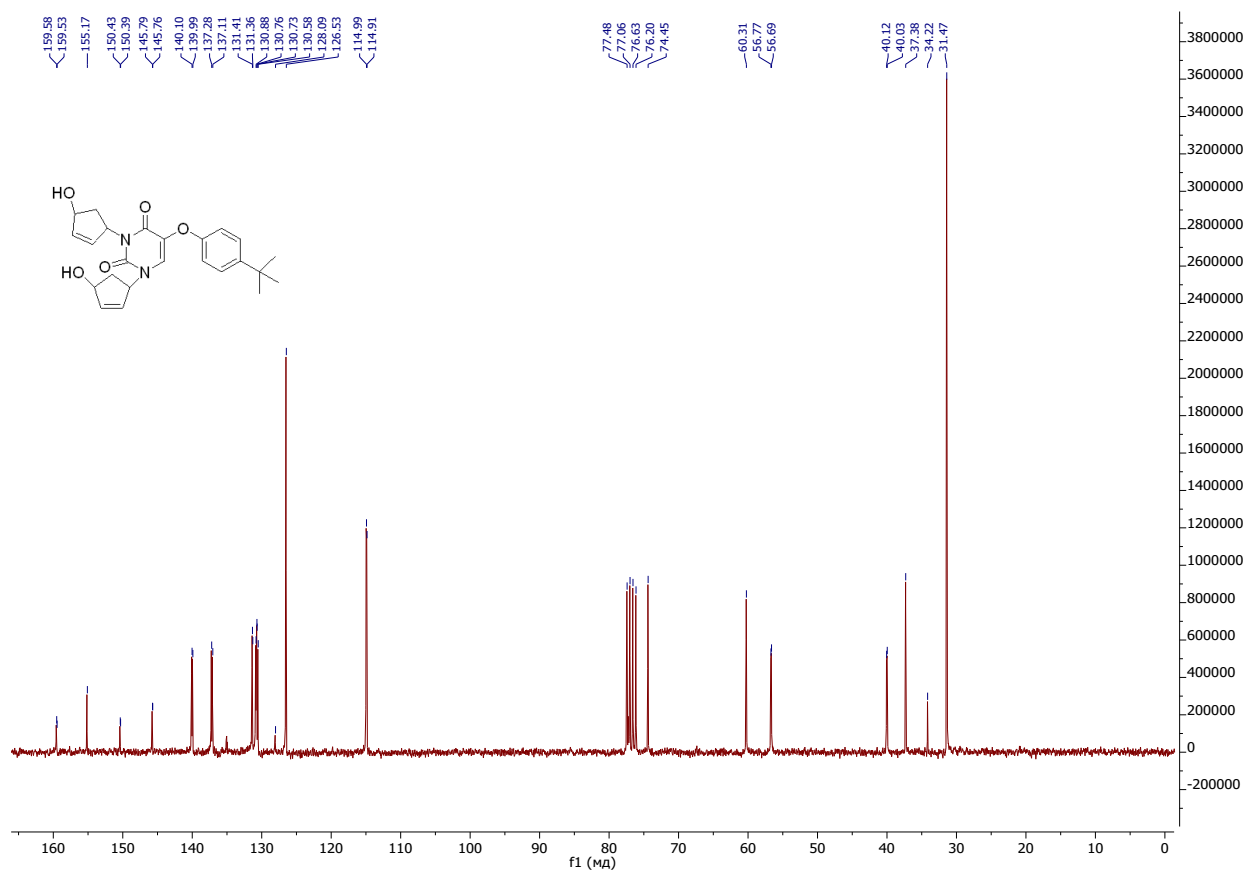


Figure S78 ¹³C NMR spectrum of compound **11d** in CDCl₃ at 100 MHz.