

# Supporting Information

## Discovery of nitro-azolo[1,5-*a*]pyrimidines with anti-inflammatory and protective activity against LPS-induced acute lung injury

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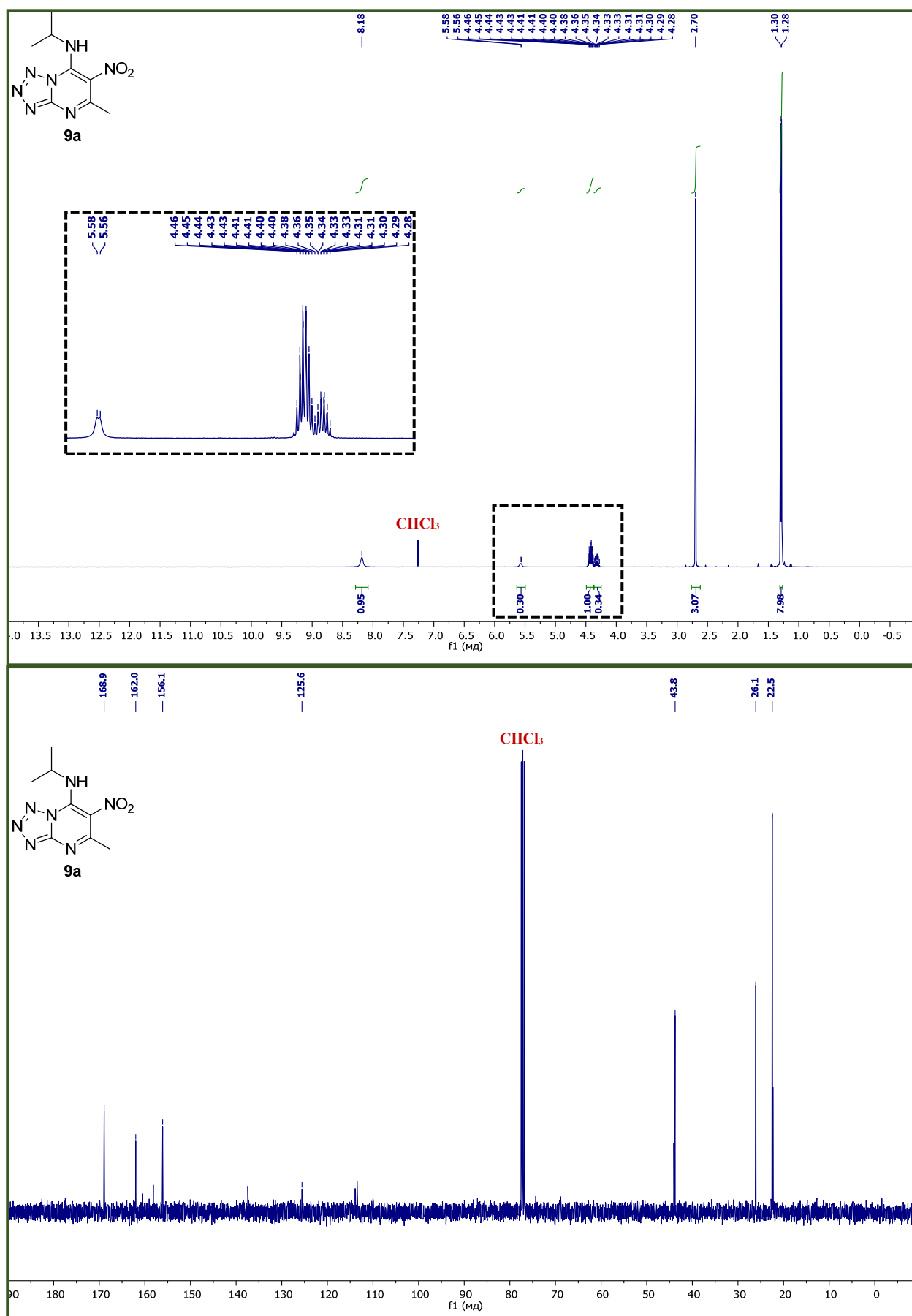
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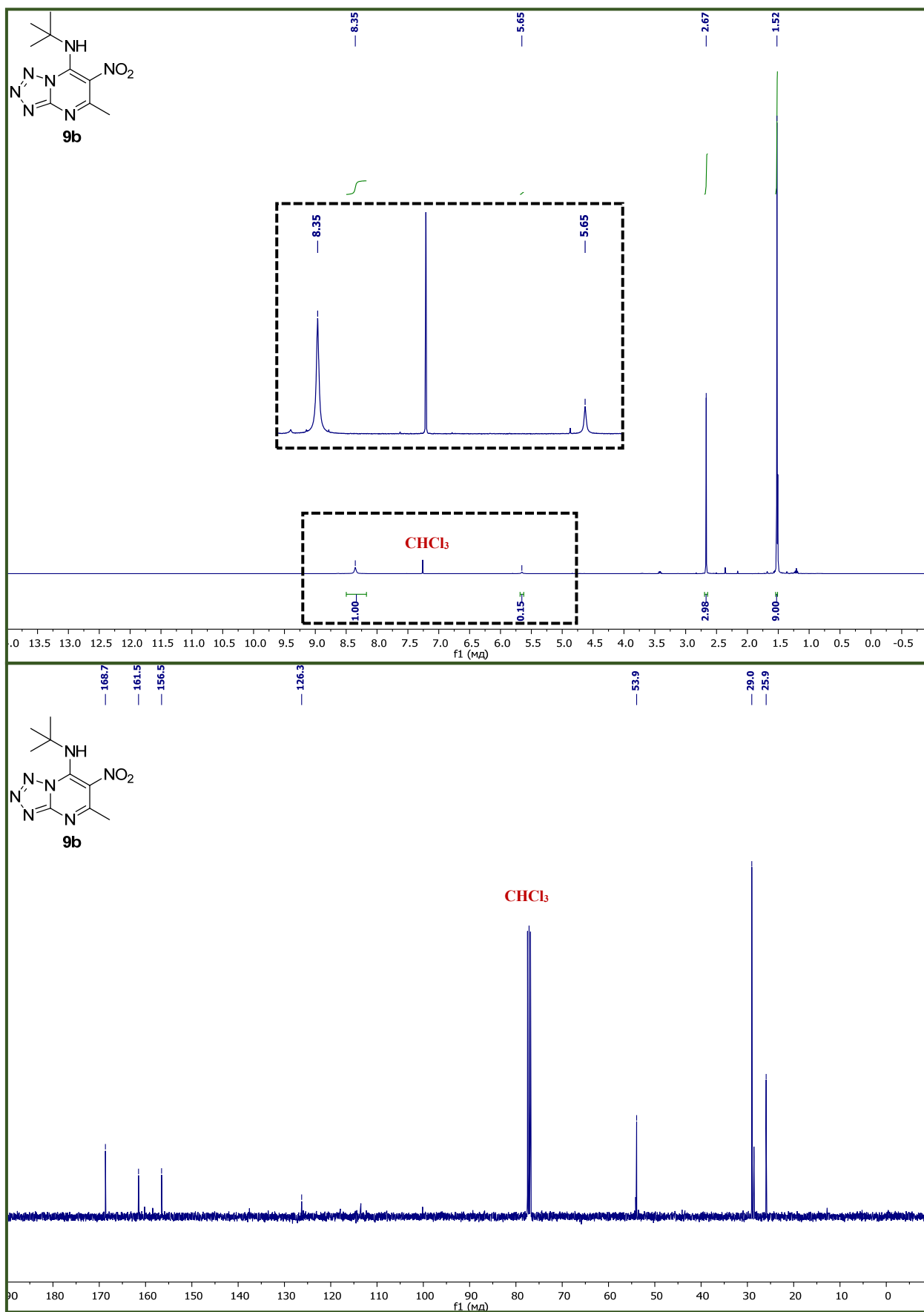
Spectra of compounds .....	2
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**Spectra of compounds**  
***N*-Isopropyl-5-methyl-6-nitrotetrazolo[1,5-*a*]pyrimidin-7-amine (9a)**



**Figure S1.** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) and <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectra of **9a**

***N*-tert-Butyl-5-methyl-6-nitrotetrazolo[1,5-*a*]pyrimidin-7-amine (9b)**



**Figure S2.** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) and <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectra of **9b**

2-[(5-Methyl-6-nitrotetrazolo[1,5-*a*]pyrimidin-7-yl)-amino]ethanol (**9c**)

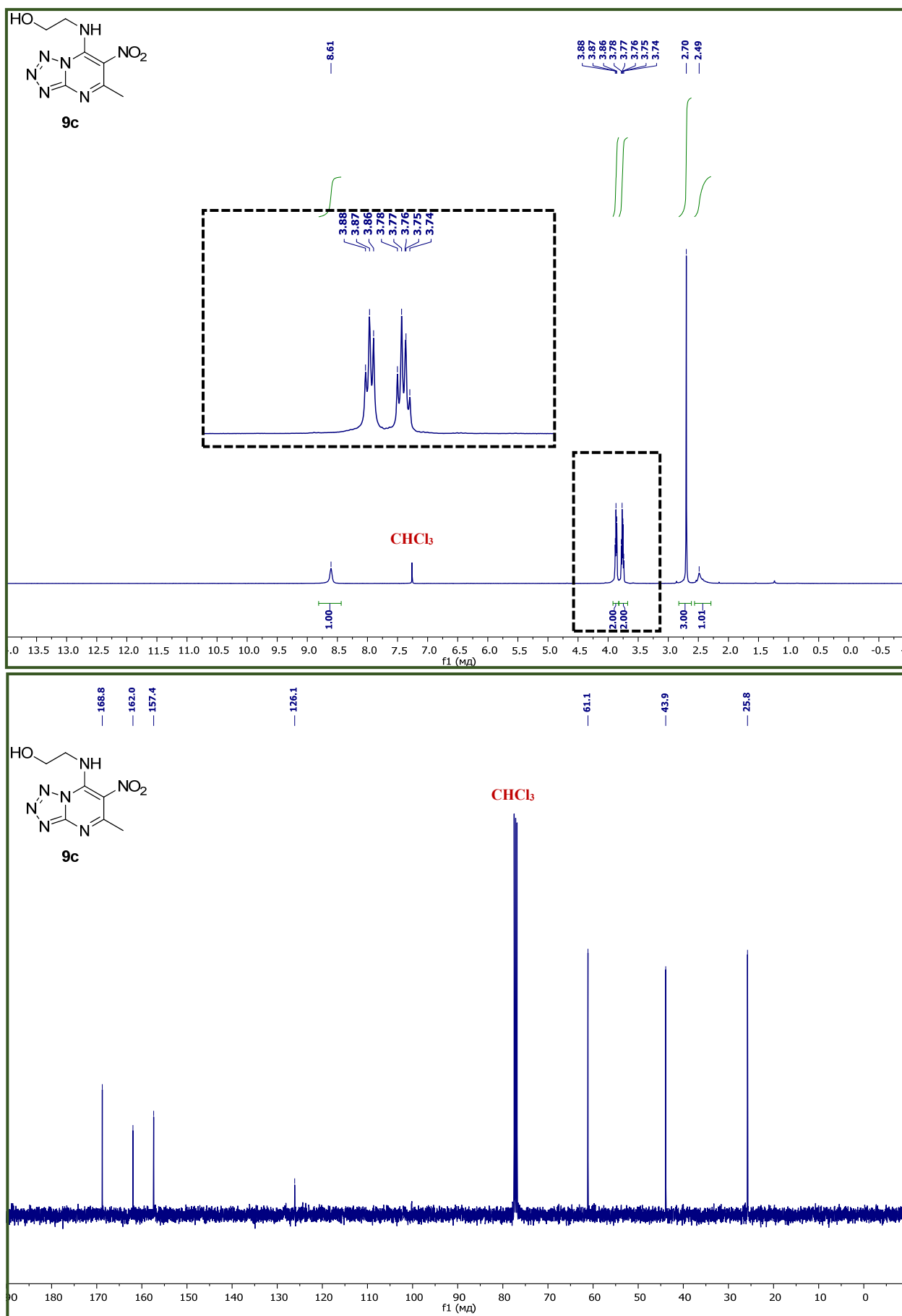


Figure S3. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) and <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectra of **9c**

3-[(5-Methyl-6-nitrotetrazolo[1,5-*a*]pyrimidin-7-yl)-amino]propanol (**9d**)

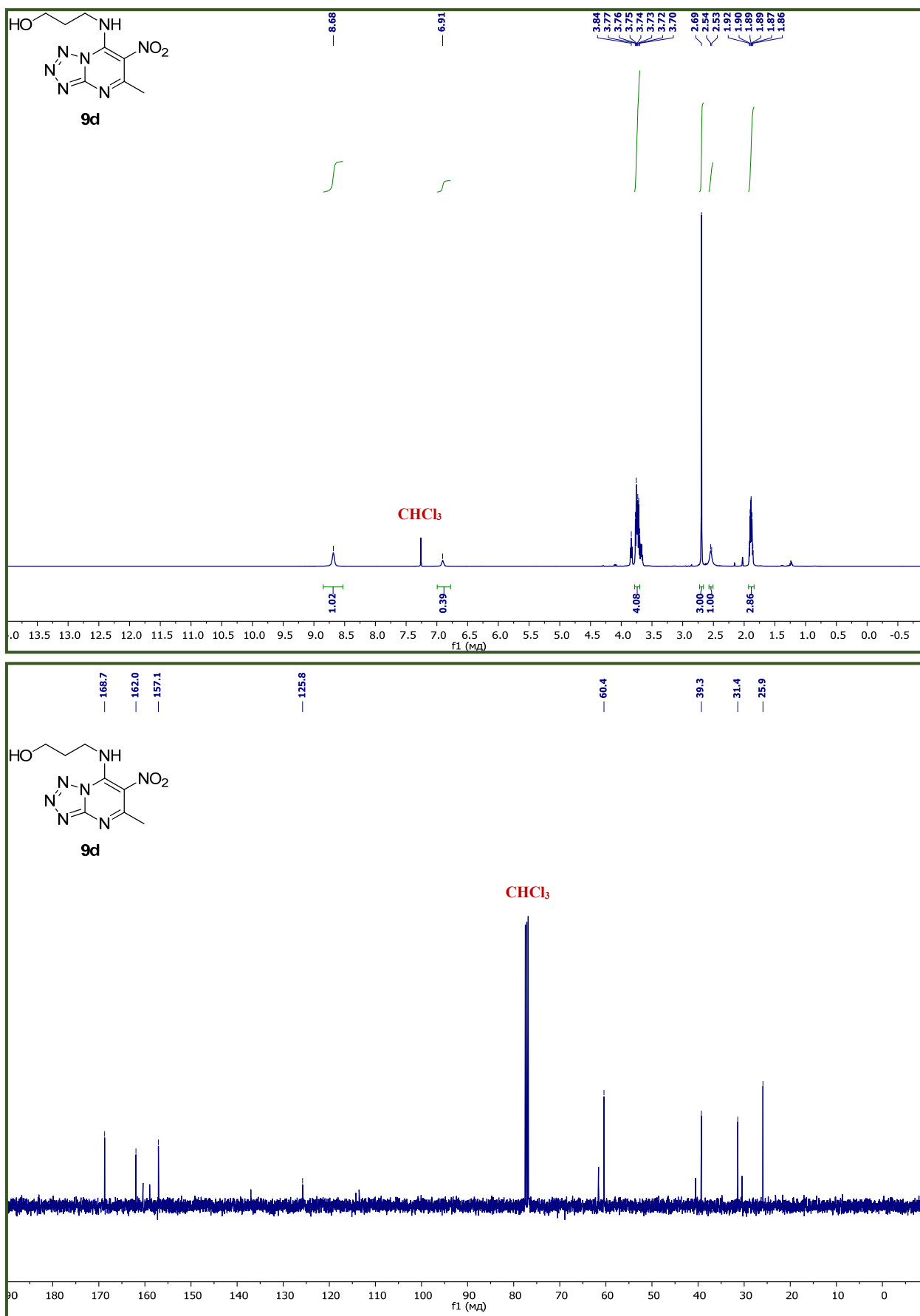
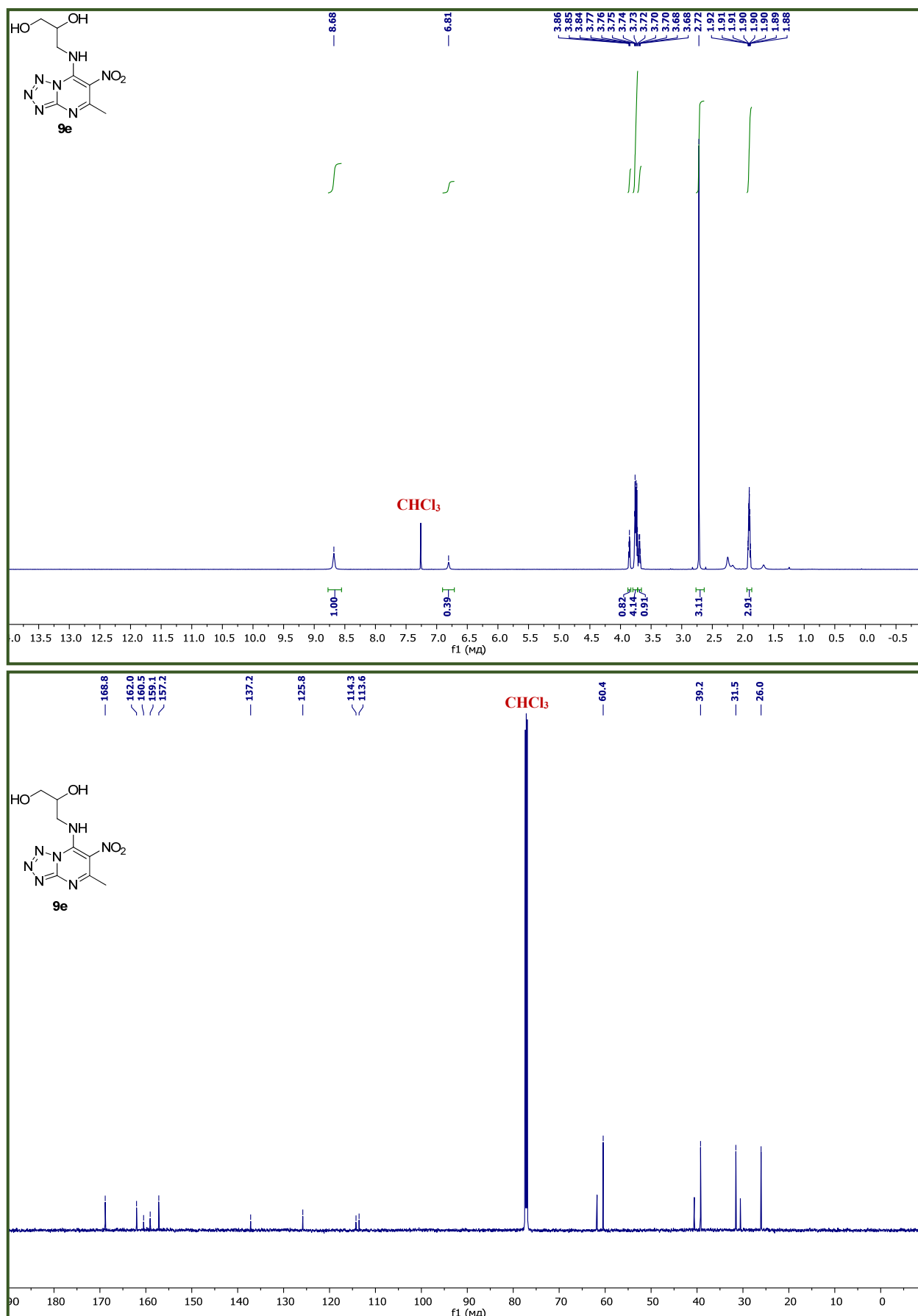


Figure S4. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) and <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectra of **9d**

**3-[(5-Methyl-6-nitrotetrazolo[1,5-*a*]pyrimidin-7-yl)-amino]propane-1,2-diol (9e)**



**Figure S5.** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) and <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectra of **9e**

N-[2-(4-Chlorophenyl)ethyl]-5-methyl-6-nitrotetrazolo-[1,5-*a*]pyrimidin-7-amine (9f)

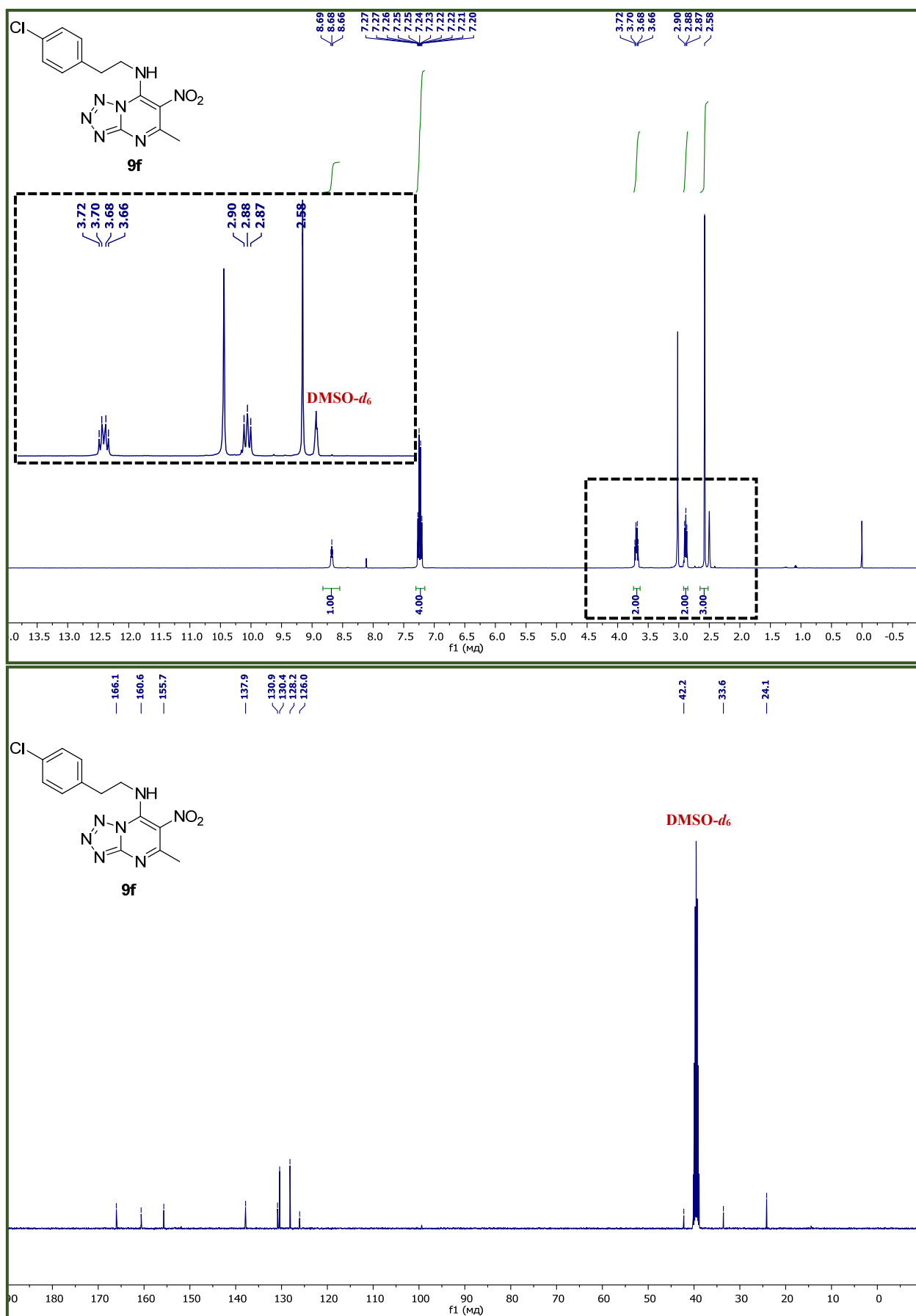


Figure S6. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) and <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) spectra of 9f

N-[2-(4-Hydroxyphenyl)ethyl]-5-methyl-6-nitrotetrazolo-[1,5-*a*]pyrimidin-7-amine (9g)

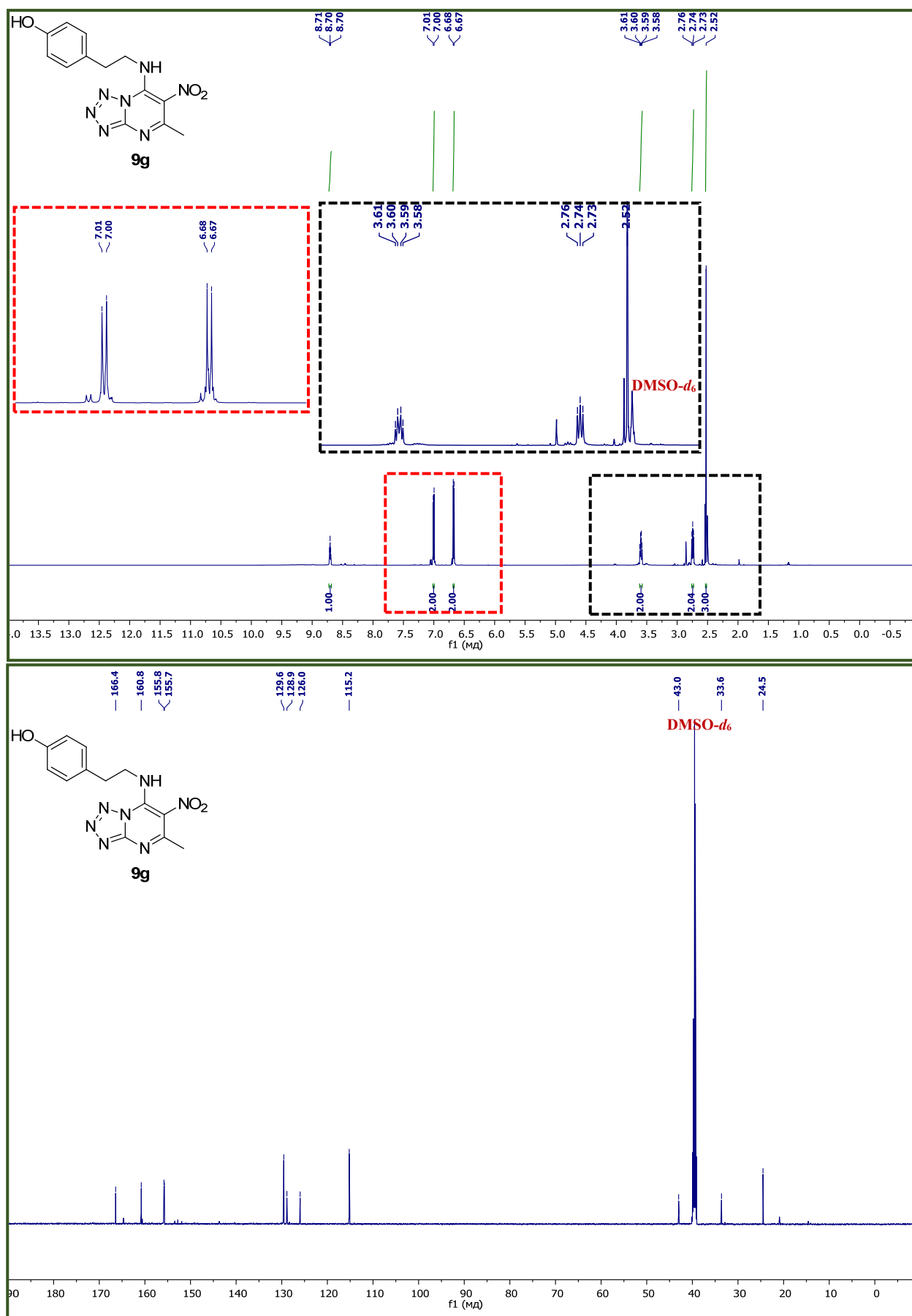
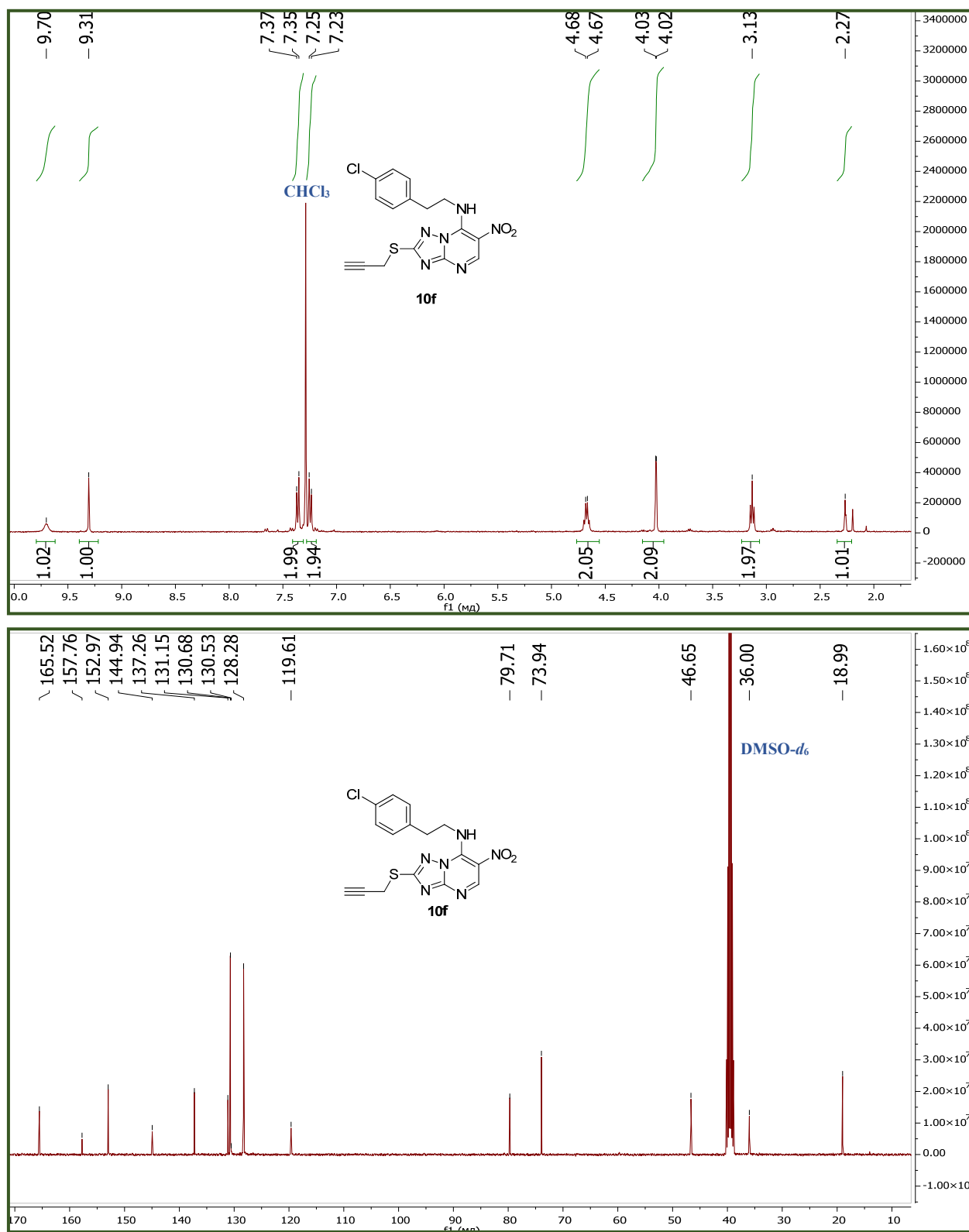


Figure S7. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) and <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) spectra of 9f



**N-(4-Chlorophenethyl)-6-nitro-2-(prop-2-yn-1-ylsulfanyl)[1,2,4]triazolo[1,5-a]pyrimidin-7-amine (10f)**



**Figure S8.** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) and <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) spectra of **10f**

4-{2-[(6-Nitro-2-(prop-2-yn-1-ylsulfany)[1,2,4]triazolo[1,5-*a*]pyrimidin-7-yl)amino]ethyl}phenol (**10g**)

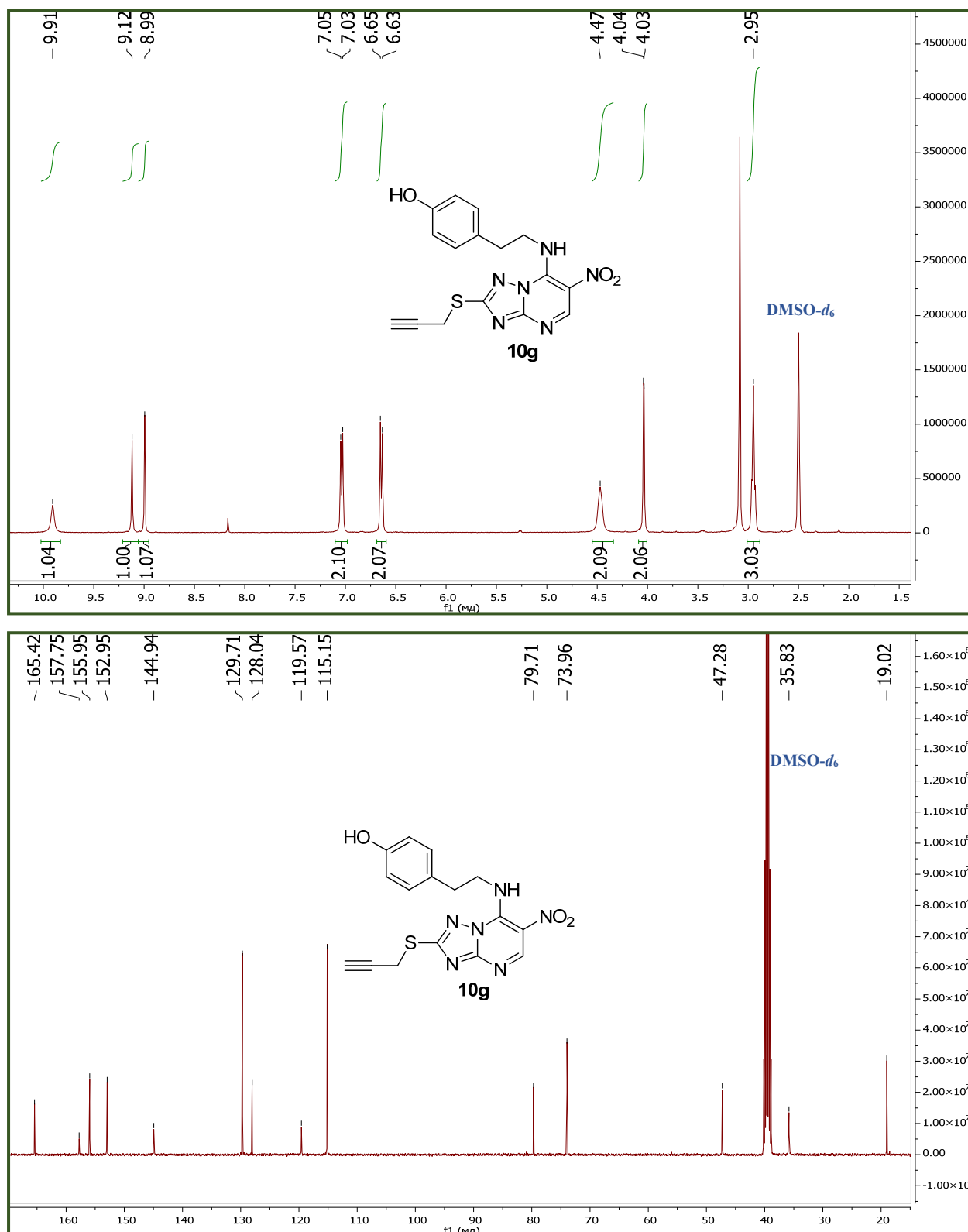
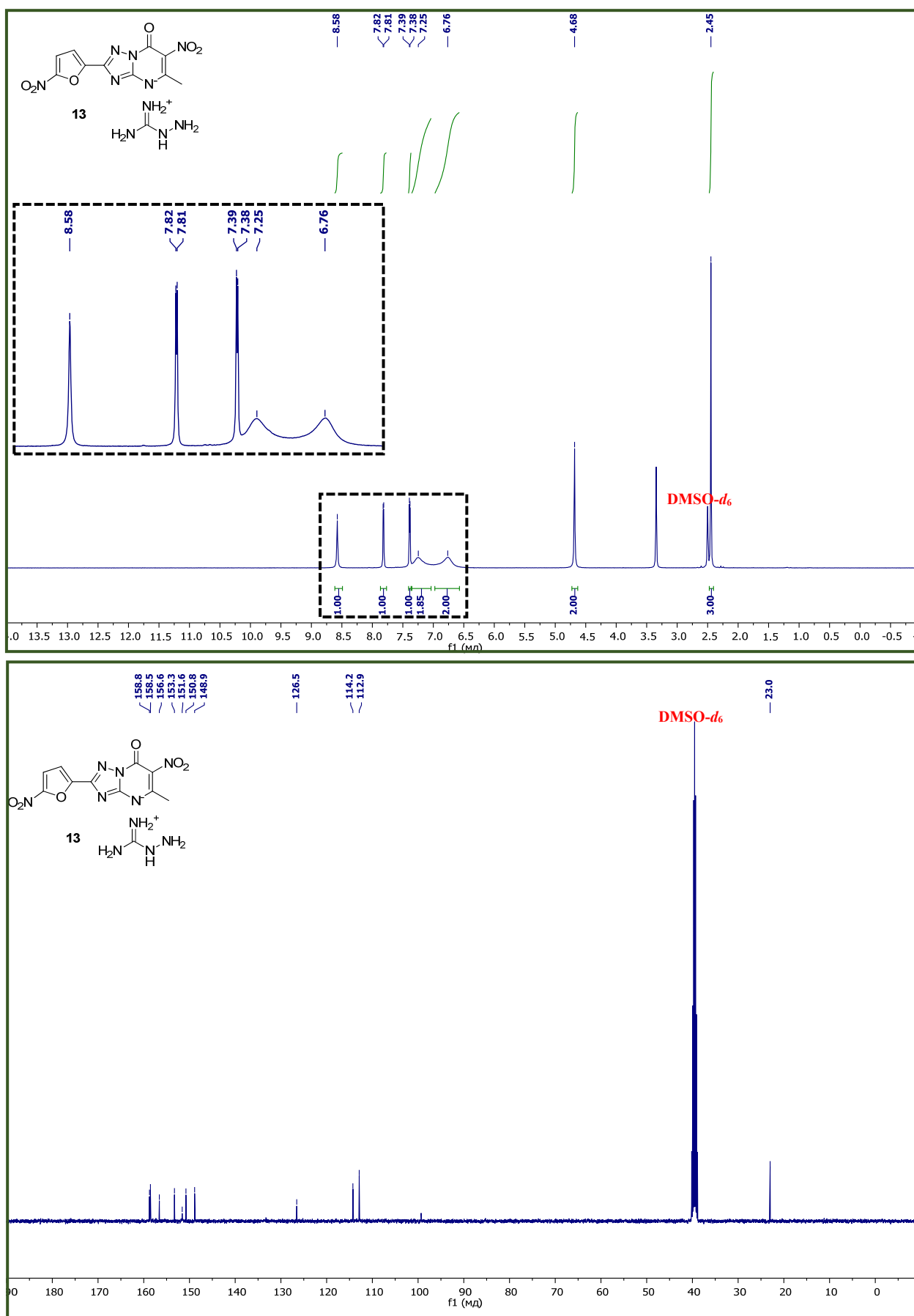


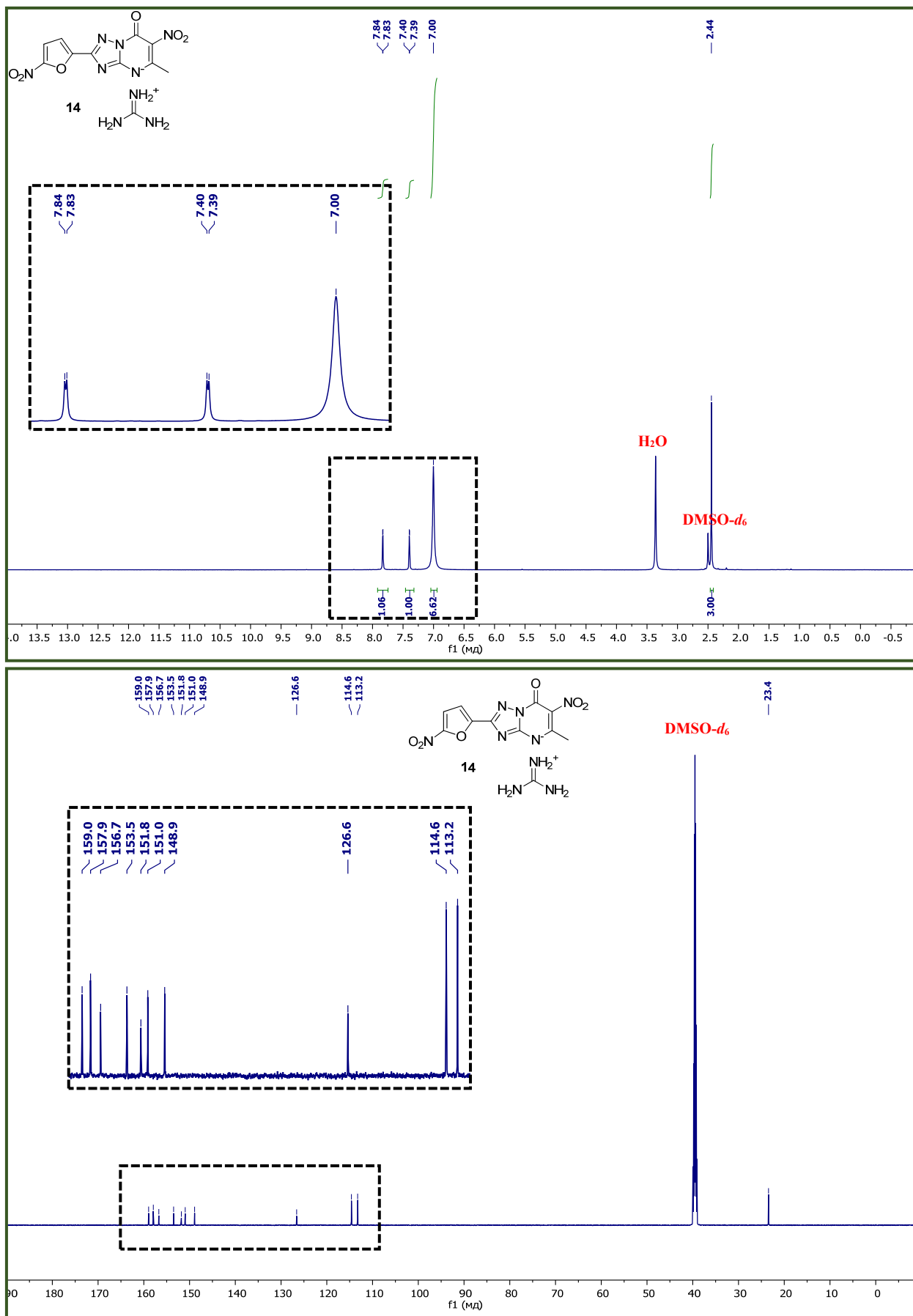
Figure S9. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) and <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) spectra of **10g**

**2-(5-Nitrofur-2-yl)-5-methyl-6-nitro-1,2,4-triazolo[1,5-*a*]pyrimidin-7-one  
aminoguanidinium salt (13)**



**Figure S10.** <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) and <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) spectra of **13**

**2-(5-Nitrofur-2-yl)-5-methyl-6-nitro-1,2,4-triazolo[1,5-*a*]pyrimidin-7-one guanidinium salt (14)**



**Figure S11.** <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) and <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) spectra of **14**