

Supplementary data for article:

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Supplementary Data

Synthesis and antioxidant activity of 1,3,4-oxadiazoles and their diacylhydrazine precursors derived from phenolic acids

Nevena Mihailović,^a Violeta Marković,^a Ivana Z. Matić,^b Nemanja S. Stanisavljević,^c Živko S. Jovanović,^c Snežana Trifunović,^d Ljubinka Joksović^{a,*}

^a Faculty of Science, Department of Chemistry, University of Kragujevac, R. Domanovića 12, 34000 Kragujevac, Serbia

^b Institute of Oncology and Radiology of Serbia, Pasterova 14, 11000 Belgrade, Serbia

^c Institute of Molecular Genetics and Genetic Engineering, University of Belgrade, Vojvode Stepe 444a, 11000 Belgrade, Serbia

^d Faculty of Chemistry, University of Belgrade, Studentski trg 12–16, 11000 Belgrade, Serbia

*Corresponding author. *E-mail address:* ljubinka@kg.ac.rs (Lj. Joksović).

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N'-Benzoyl-3-hydroxybenzohydrazide $\times 0.5 H_2O$ (**6b**): Beige powder; yield: 0.20 g (74%); mp: > 250°C; 1H NMR (200 MHz, DMSO- d_6): 6.97, (dt, 1H, $J = 7.4$ and 2.2 Hz, Ar-H); 7.30-7.34, (m, 3H, Ar-H); 7.47-7.60, (m, 3H, Ar-H); 7.92, (dd, 2H, $J = 8.0$ and 1.6 Hz, Ar-H); 9.76, (s, 1H, OH); 10.40, (d, $J = 1.0$ Hz, 1H, NH); 10.47, (d, $J = 1.0$ Hz, 1H, NH); ^{13}C NMR (50 MHz, DMSO- d_6): 114.6, 118.0, 118.8, 127.5 (2C), 128.5 (2C), 129.6, 131.8, 132.8, 134.2, 157.5, 165.9, 166.0; IR (KBr, cm^{-1}): 3245; 3067; 1614; 1586; 1508; 1476; 1307; 749; Anal. Calcd. For $C_{14}H_{12}N_2O_3 \times 0.5H_2O$ (265.27 g/mol): C, 63.39; H, 4.94; N, 10.56; Found: C, 63.42; H, 4.95; N, 10.54.

2-(5-Phenyl-1,3,4-oxadiazol-2-yl)phenol (**7a**): White powder; yield: 0.16 g (66%); mp: 158 - 159°C; 1H NMR (200 MHz, DMSO- d_6): 7.01-7.14, (m, 2H, Ar-H); 7.45-7.54, (m, 1H, Ar-H); 7.61-7.68, (m, 3H, Ar-H); 7.93, (dd, 1H, $J = 7.4$ and 1.6 Hz, Ar-H); 8.08-8.13, (m, 2H, Ar-H); 10.34, (s, 1H, OH); ^{13}C NMR (50 MHz, DMSO- d_6): 109.6, 117.3, 119.9, 123.4, 126.8 (2C), 128.9, 129.6 (2C), 132.2, 133.6, 156.5, 163.5, 163.7; IR (KBr, cm^{-1}): 3444; 3206; 1624; 1593; 1542; 1489; 1254; 1240; 709; Anal. Calcd. For $C_{14}H_{10}N_2O_2$ (238.25 g/mol): C, 70.58; H, 4.23; N, 11.76; Found: C, 70.56; H, 4.22; N, 11.74.

3-(5-Phenyl-1,3,4-oxadiazol-2-yl)phenol $\times 0.5 H_2O$ (**7b**): Beige powder; yield: 0.14 g (56%); mp: 179 - 180°C; 1H NMR (200 MHz, DMSO- d_6): 7.04, (dq, 1H, $J = 8.2$, 2.4 and 1.0 Hz, Ar-H); 7.43, (t, 1H, $J = 7.8$ Hz, Ar-H); 7.51, (t, 1H, $J = 2.0$ Hz, Ar-H); 7.57, (dt, 1H, $J = 7.8$ and 1.2 Hz, Ar-H); 7.62-7.66, (m, 3H, Ar-H); 8.09-8.14, (m, 2H, Ar-H); 10.02, (s, 1H, OH); ^{13}C NMR (50 MHz, DMSO- d_6): 113.2, 117.5, 119.3, 123.5, 124.5, 126.8 (2C), 129.5 (2C), 130.7, 132.1, 158.1, 164.0, 164.2; IR (KBr, cm^{-1}): 3263; 3051; 1604; 1562; 1550; 1459; 1227; 726; Anal. Calcd. For $C_{14}H_{10}N_2O_2 \times 0.5H_2O$ (247.25 g/mol): C, 68.01; H, 4.48; N, 11.33; Found: C, 68.04; H, 4.47; N, 11.35.

3-(5-Phenyl-1,3,4-oxadiazol-2-yl)benzene-1,2-diol (**7d**): Beige crystals; yield: 0.15 g (58%); mp: 172 - 173°C; 1H NMR (200 MHz, DMSO- d_6): 6.88, (t, 1H, $J = 7.8$ Hz, Ar-H); 7.04, (dd, 1H, $J = 7.8$ and 1.6 Hz, Ar-H); 7.39, (dd, 1H, $J = 7.8$ and 1.6 Hz, Ar-H); 7.61-7.69, (m, 3H, Ar-H); 8.09-8.14, (m, 2H, Ar-H); 9.70, (s, 1H, OH); 9.77, (s, 1H, OH); ^{13}C NMR (50 MHz, DMSO- d_6): 109.7, 118.3, 119.0, 120.1, 123.4, 126.8 (2C), 129.6 (2C), 132.2, 145.5, 146.4, 163.3, 164.0; IR (KBr, cm^{-1}): 3439; 3297; 1624; 1610; 1551; 1494; 1284; 727; Anal. Calcd. For $C_{14}H_{10}N_2O_3$ (254.24 g/mol): C, 66.14; H, 3.96; N, 11.02; Found: C, 66.15; H, 3.97; N, 11.00.

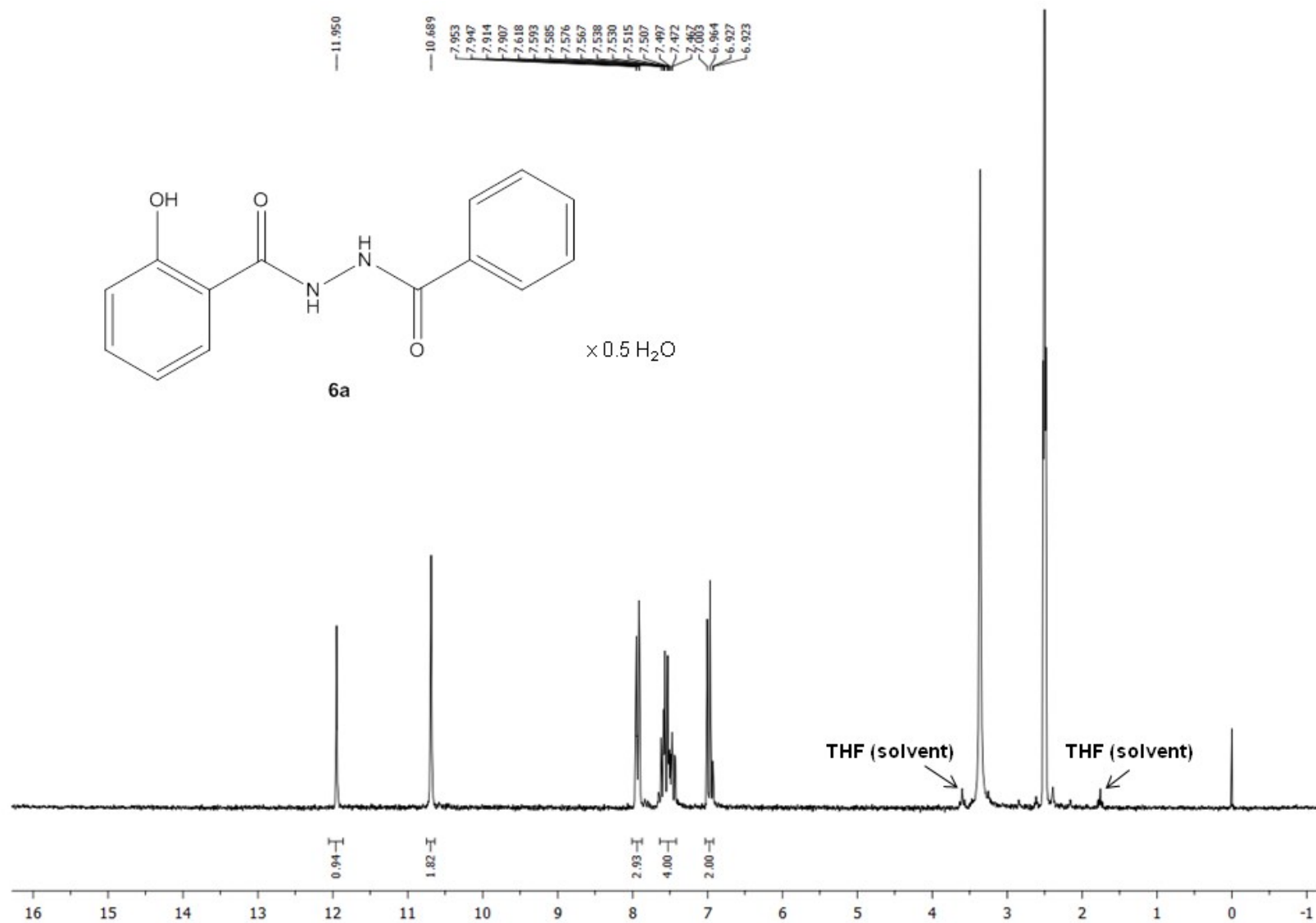


Figure S1. ^1H NMR spectrum of **6a** in DMSO-d_6 (200 MHz).

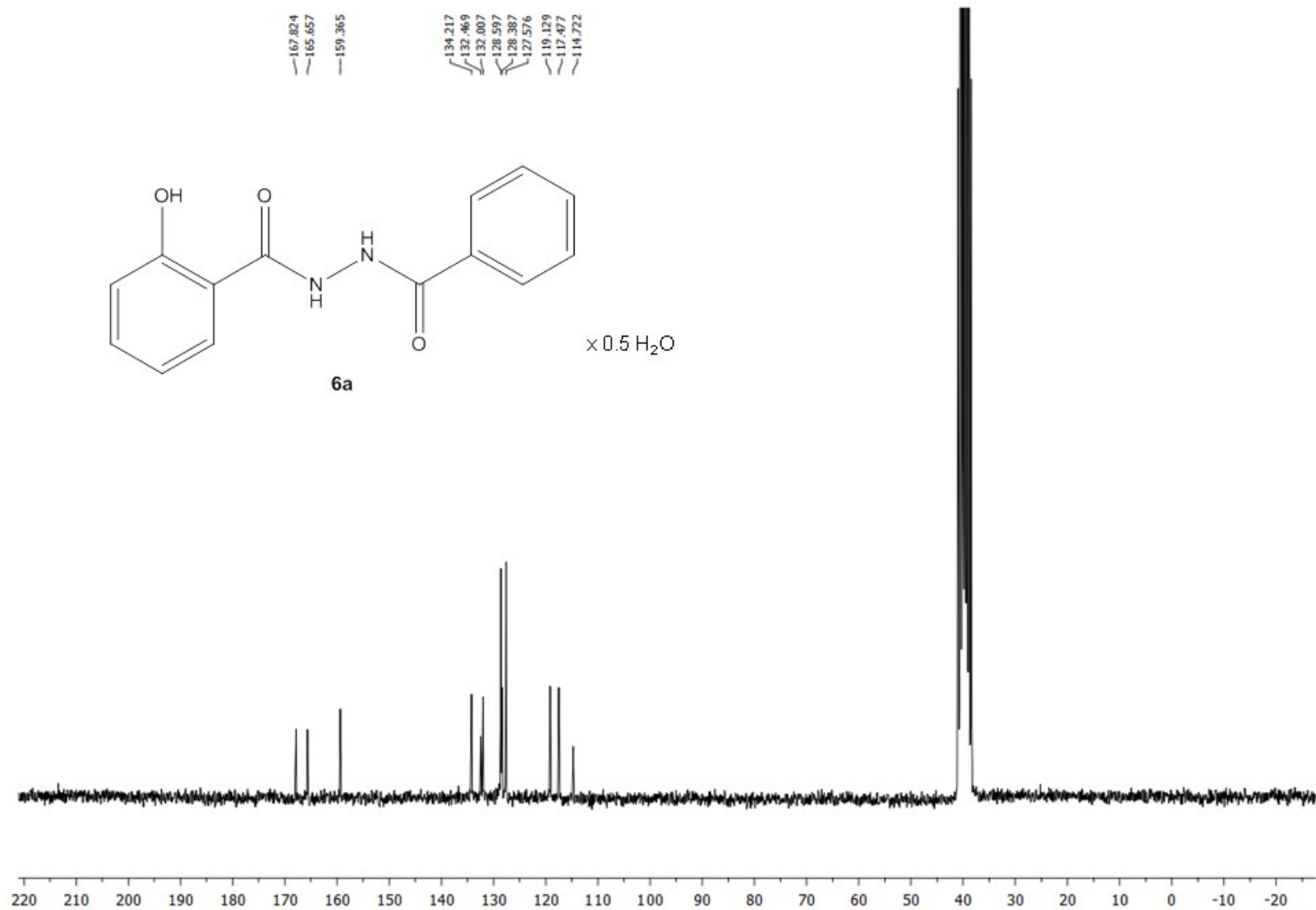


Figure S2. ^{13}C NMR spectrum of **6a** in DMSO-d_6 (50 MHz).

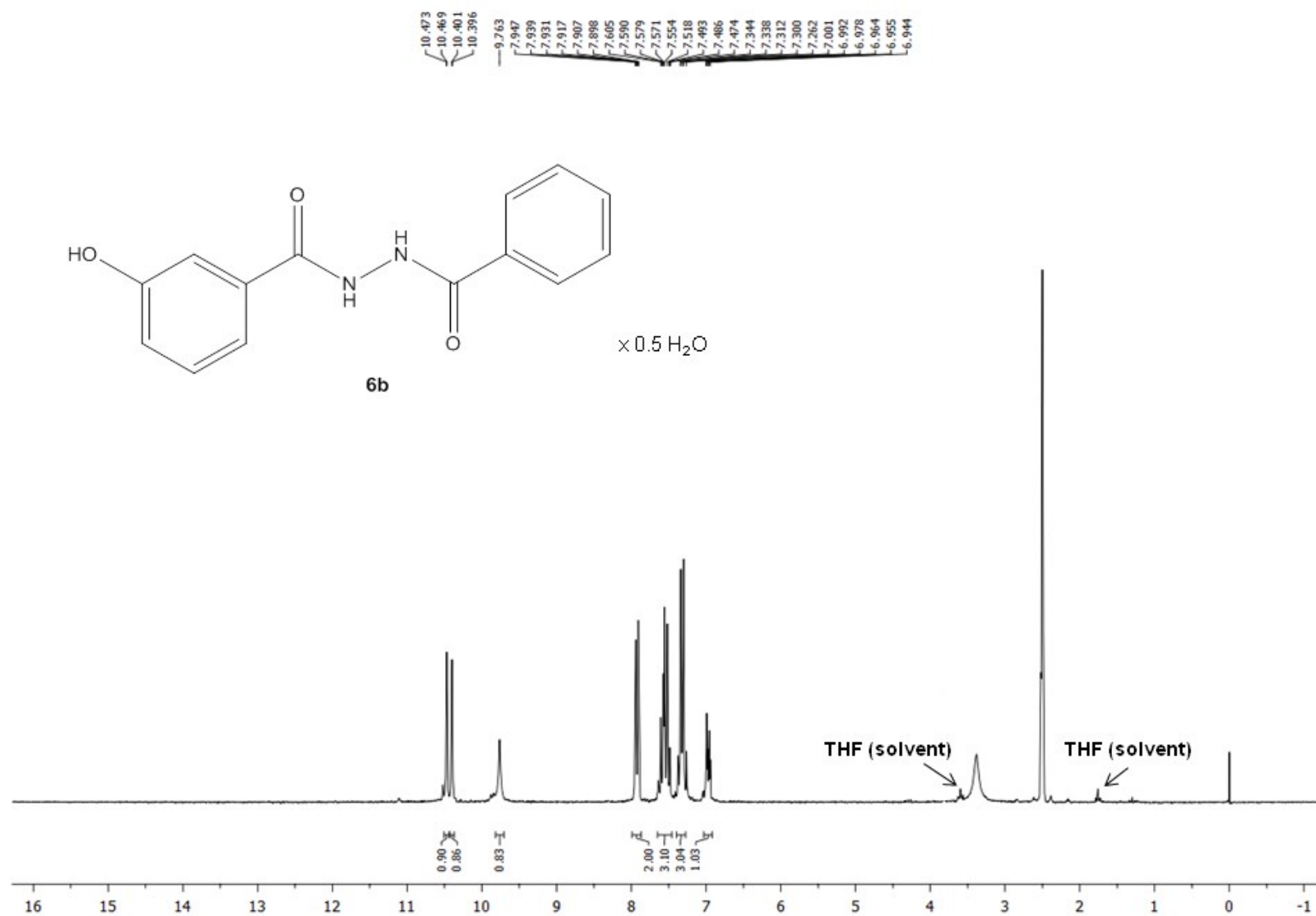


Figure S3. ¹H NMR spectrum of **6b** in DMSO-d₆ (200 MHz).

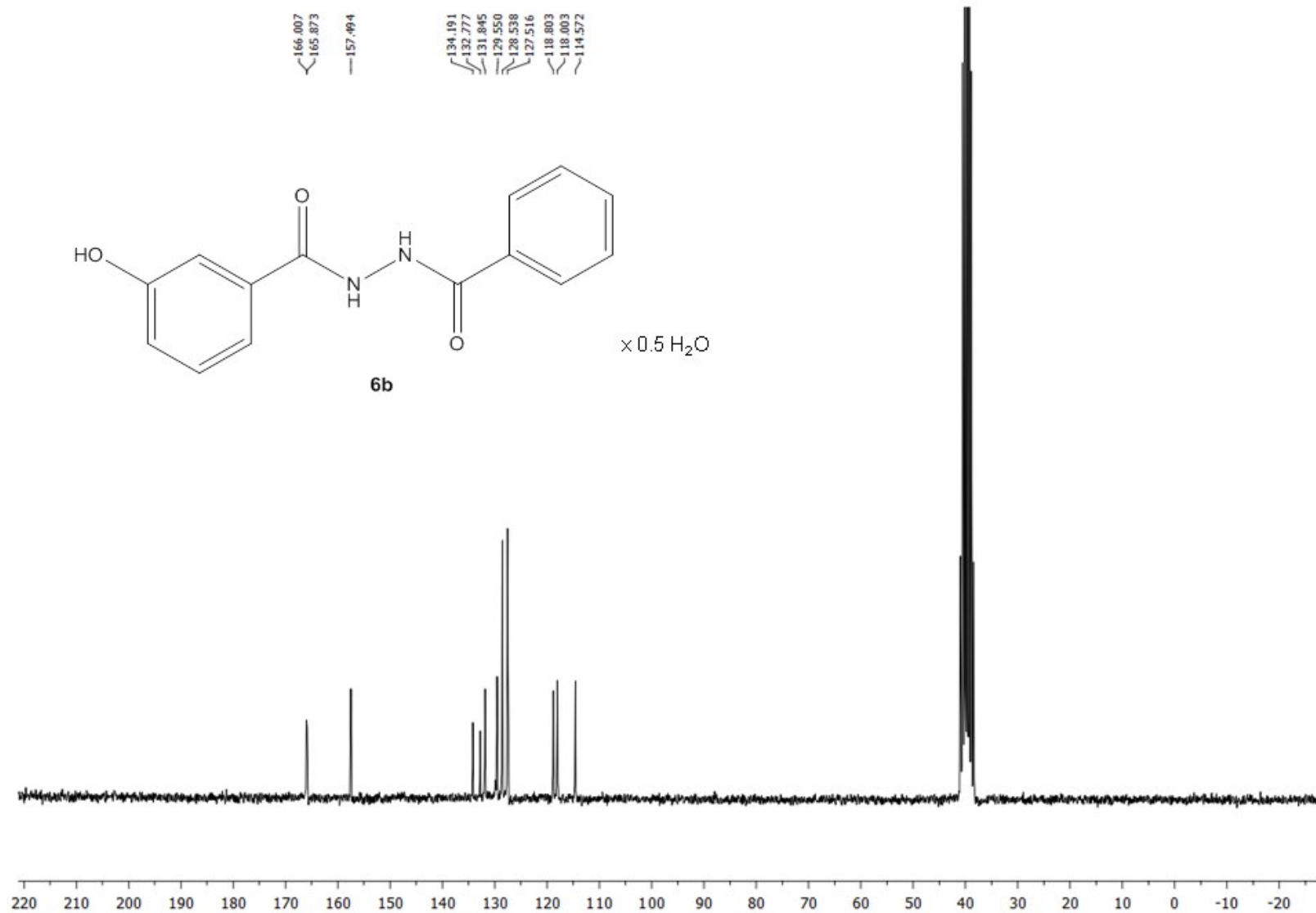


Figure S4. ¹³C NMR spectrum of **6b** in DMSO-d₆ (50 MHz).

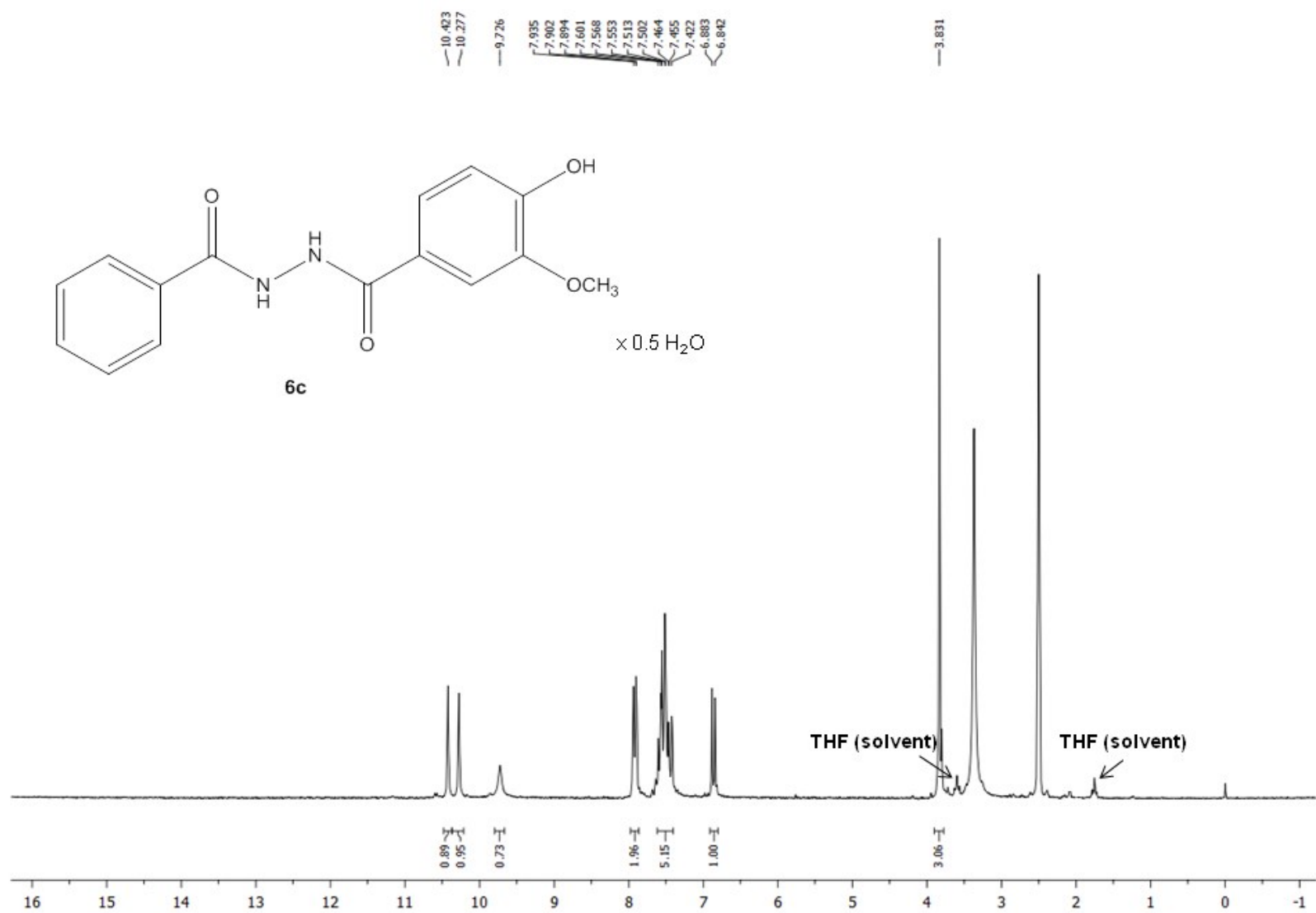


Figure S5. ¹H NMR spectrum of **6c** in DMSO-d₆ (200 MHz).

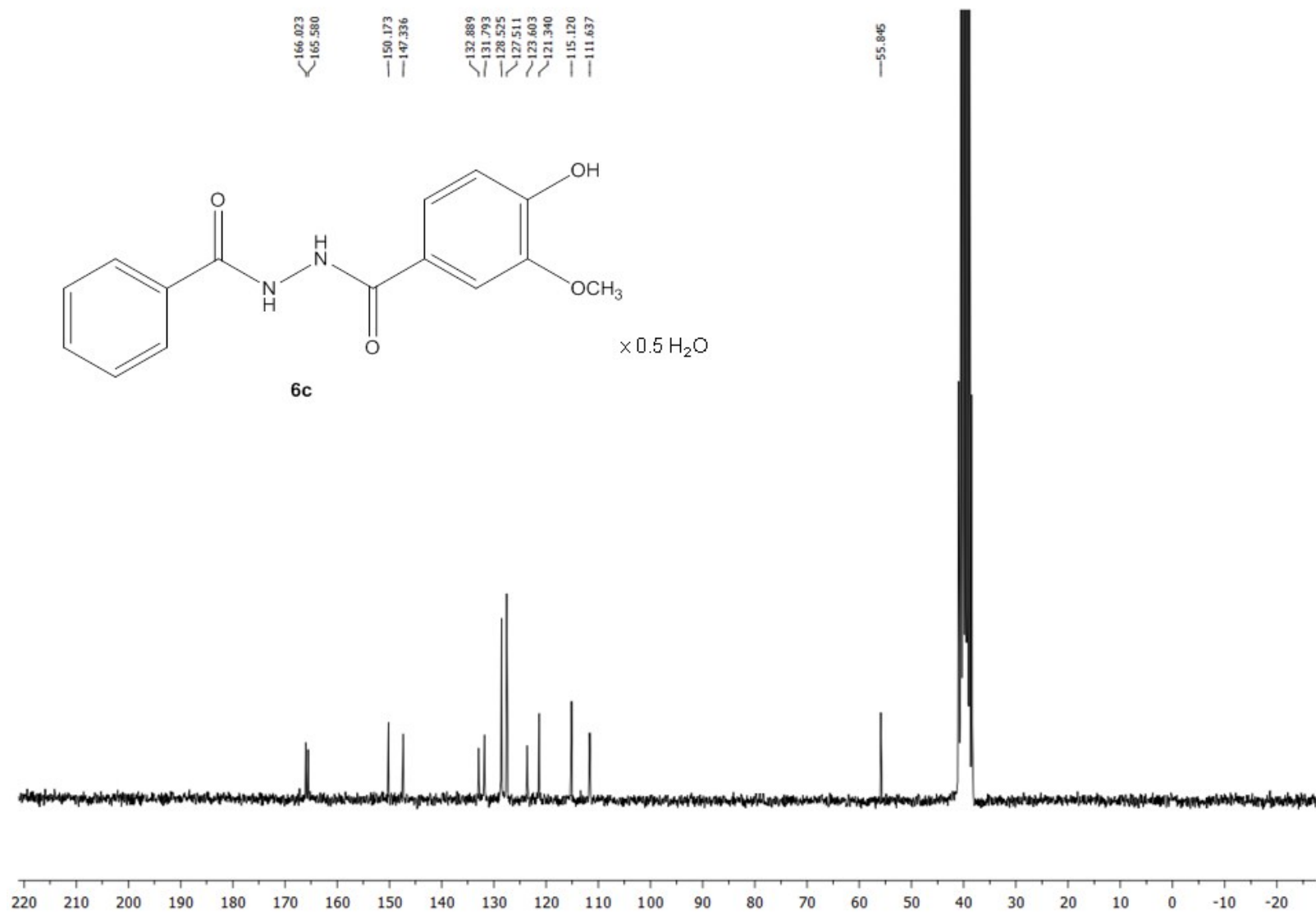


Figure S6. ¹³C NMR spectrum of **6c** in DMSO-d₆ (50 MHz).

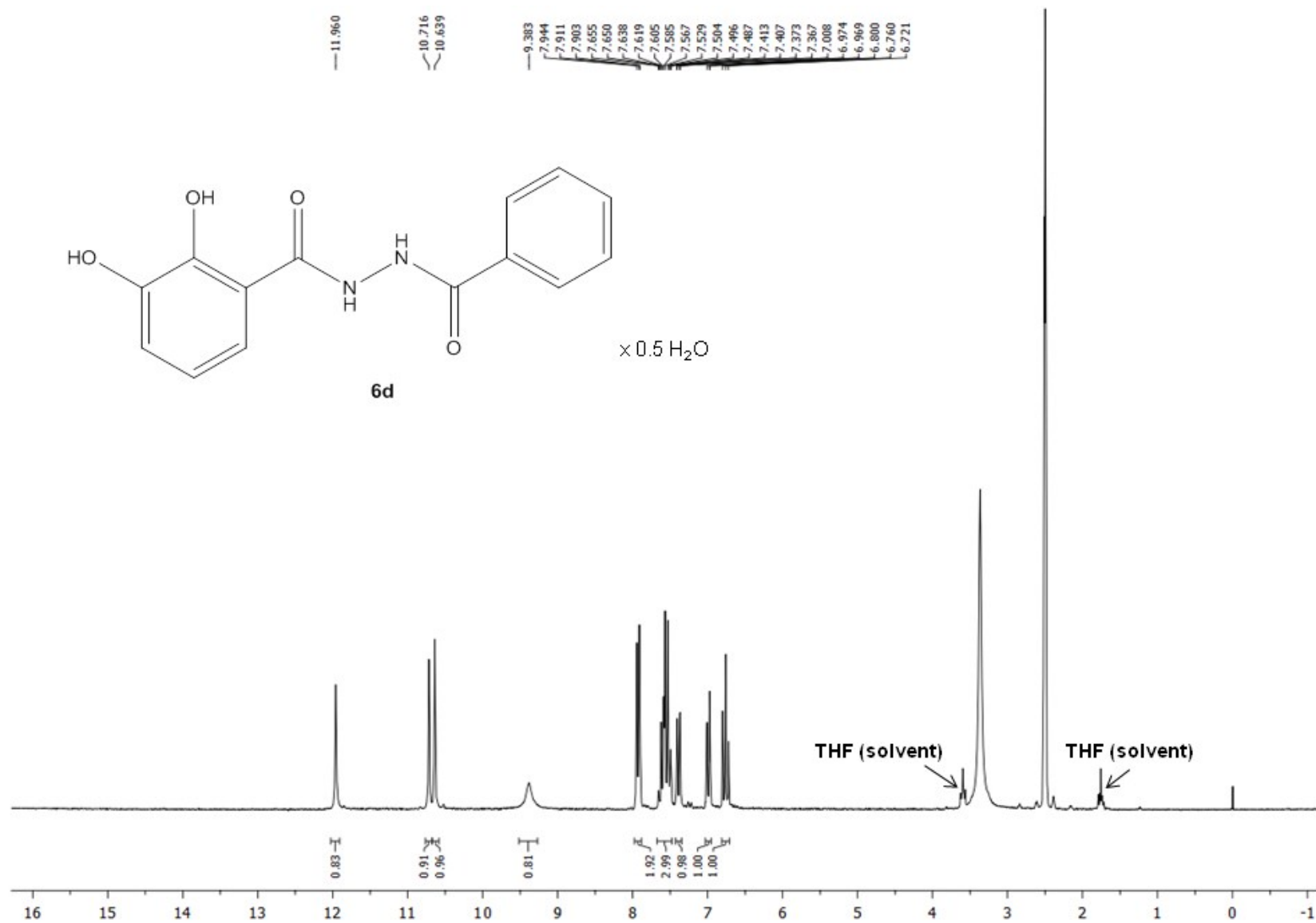


Figure S7. ^1H NMR spectrum of **6d** in DMSO- d_6 (200 MHz).

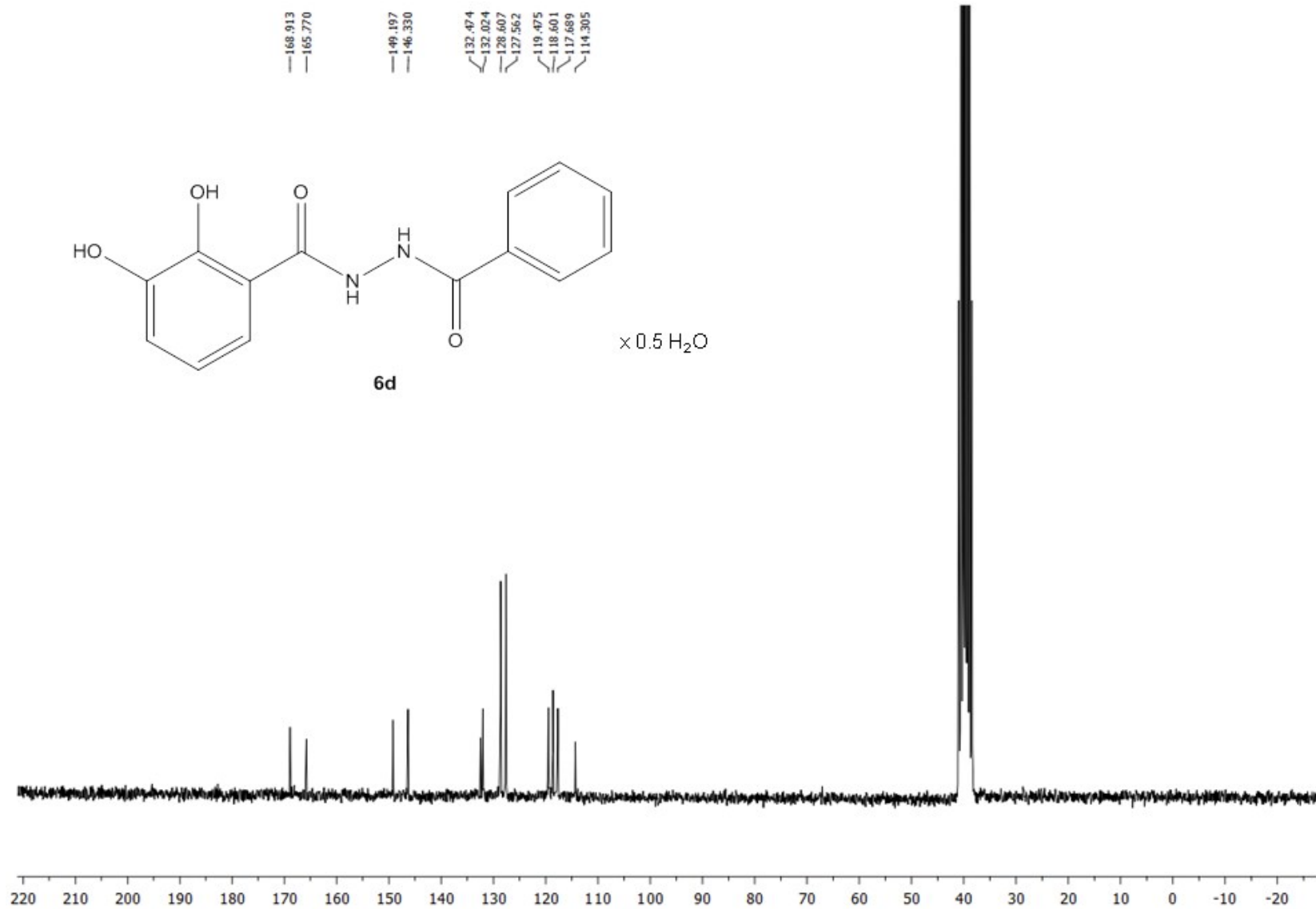


Figure S8. ^{13}C NMR spectrum of **6d** in DMSO-d_6 (50 MHz).

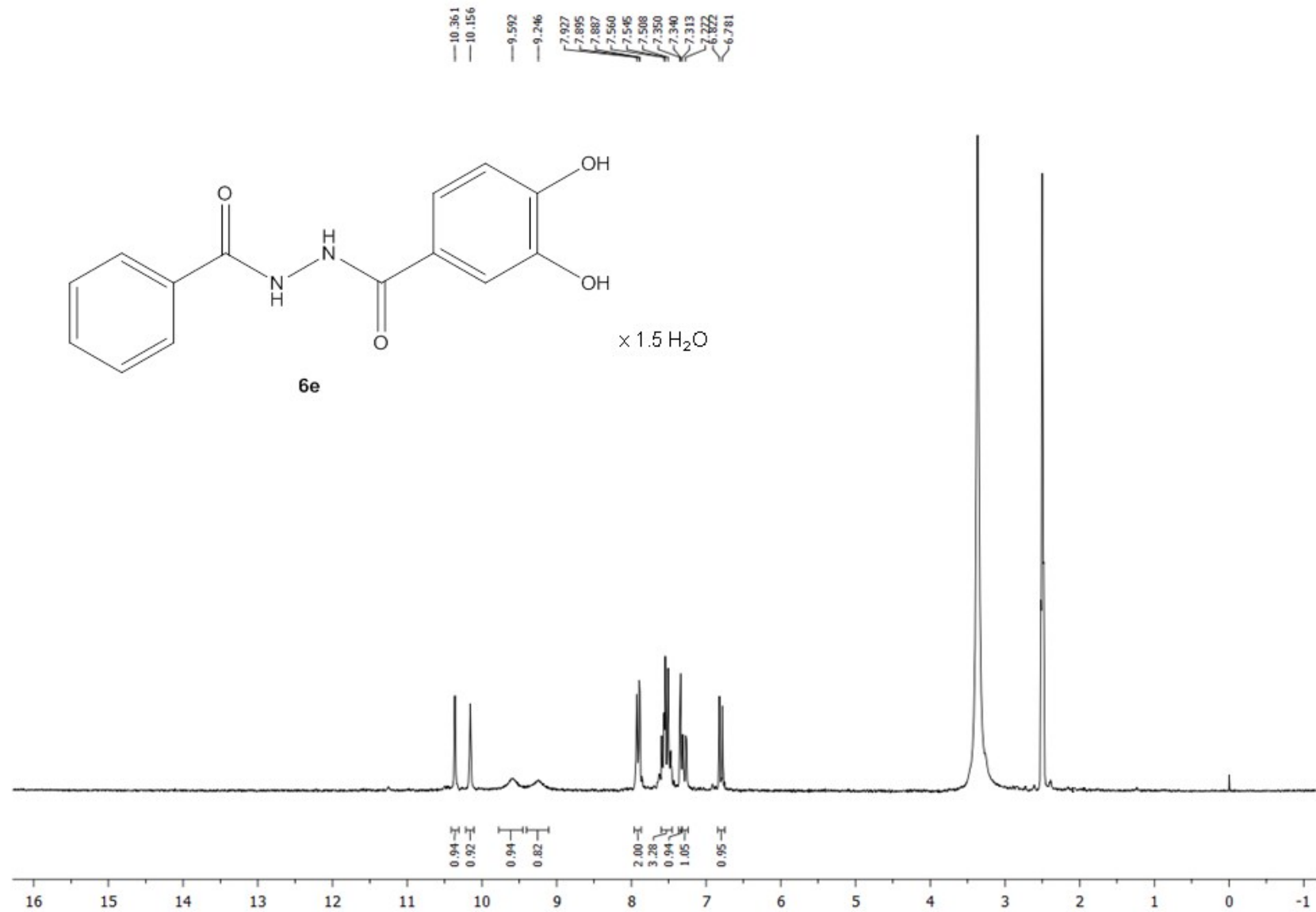


Figure S9. ^1H NMR spectrum of **6e** in DMSO-d_6 (200 MHz).

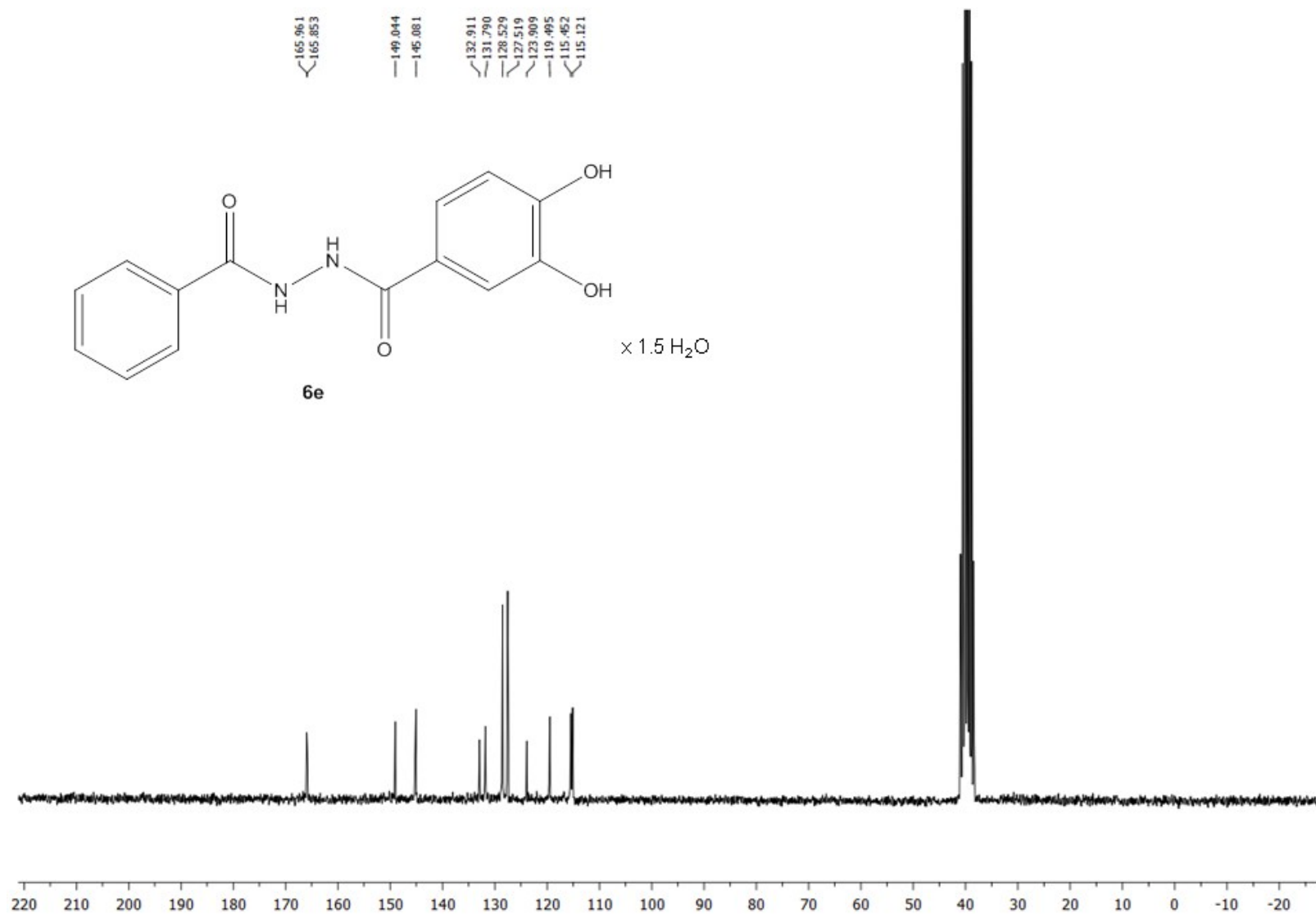


Figure S10. ^{13}C NMR spectrum of **6e** in DMSO-d_6 (50 MHz).

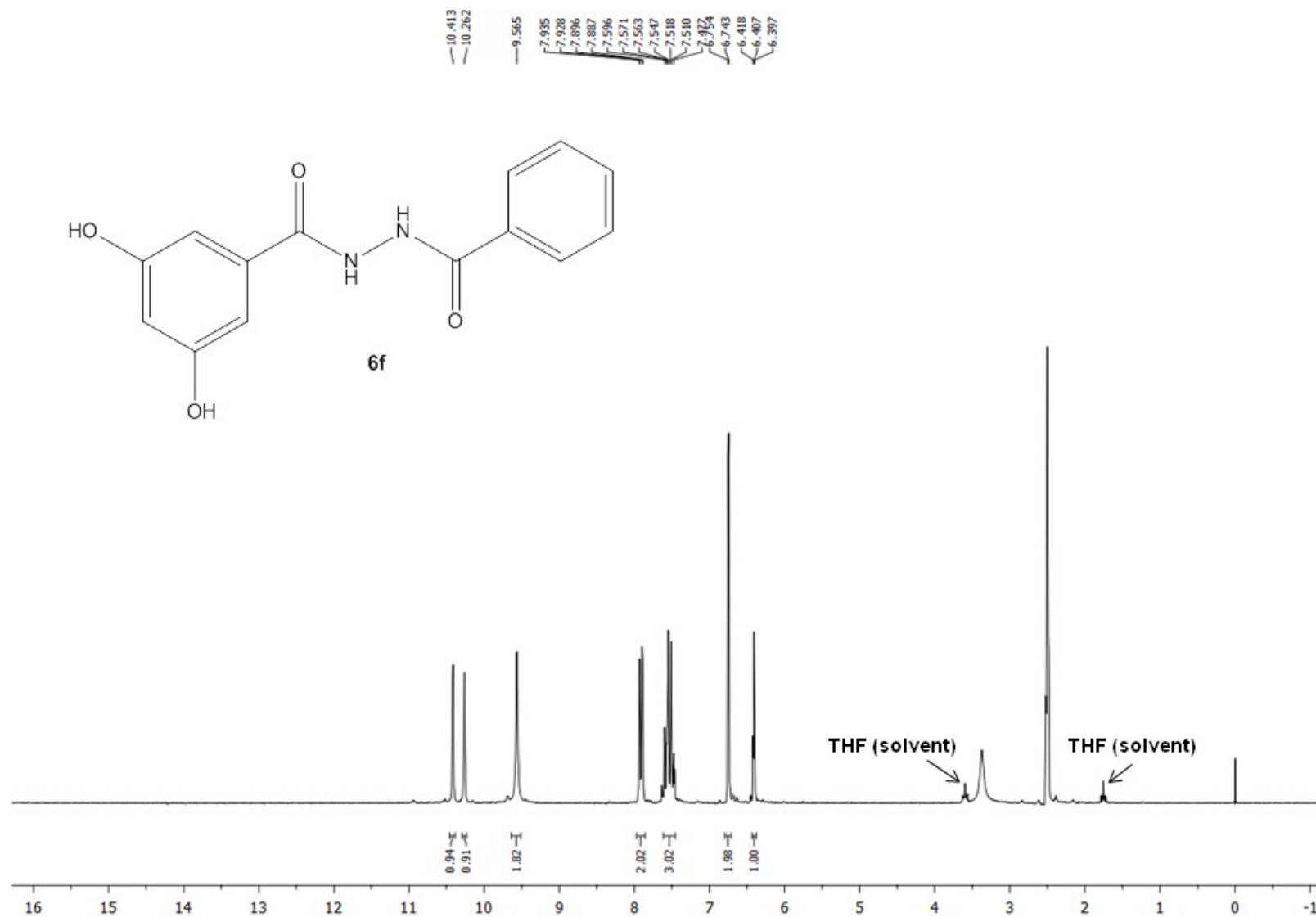


Figure S11. ^1H NMR spectrum of **6f** in DMSO-d_6 (200 MHz).

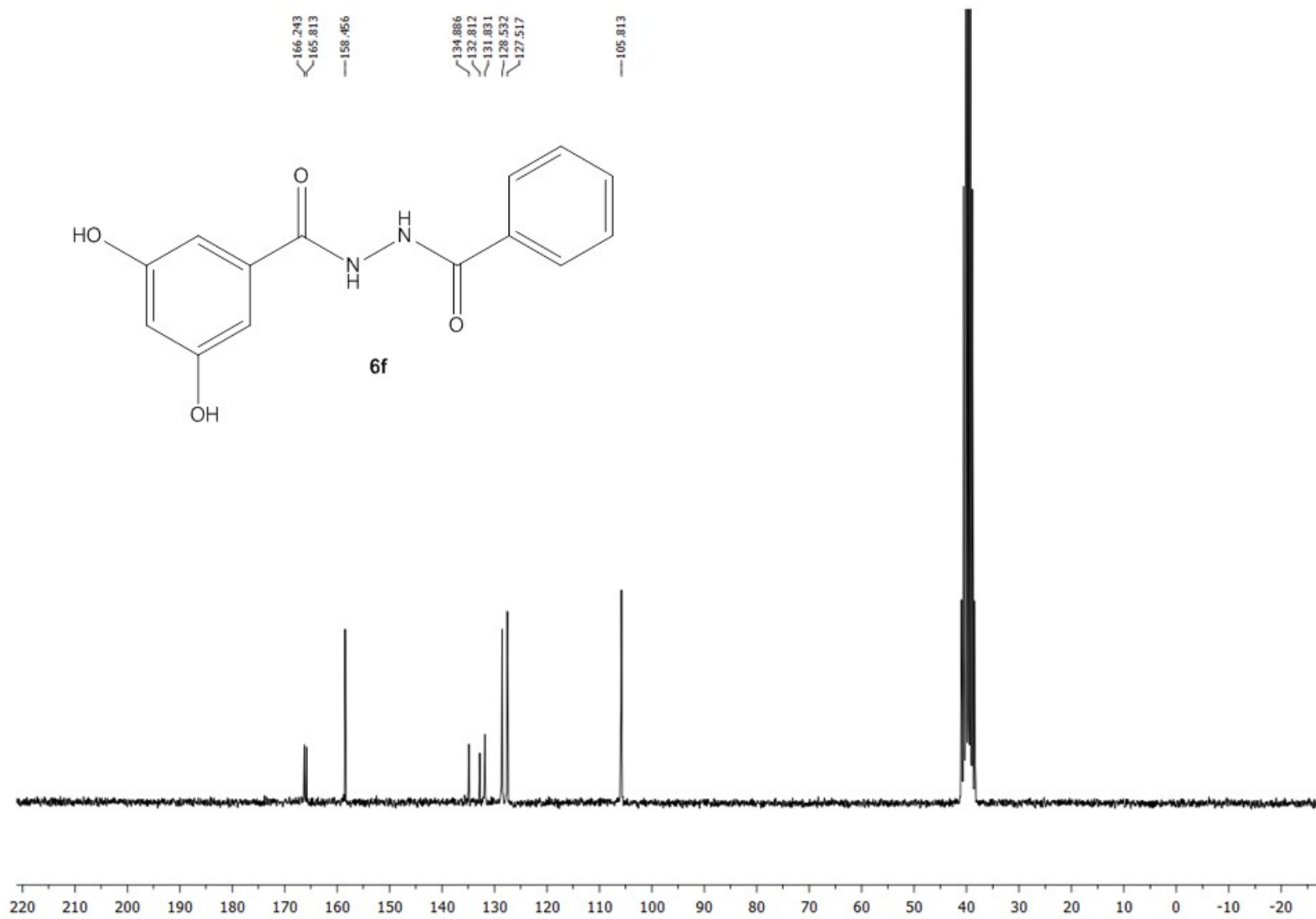


Figure S12. ^{13}C NMR spectrum of **6f** in DMSO-d_6 (50 MHz).

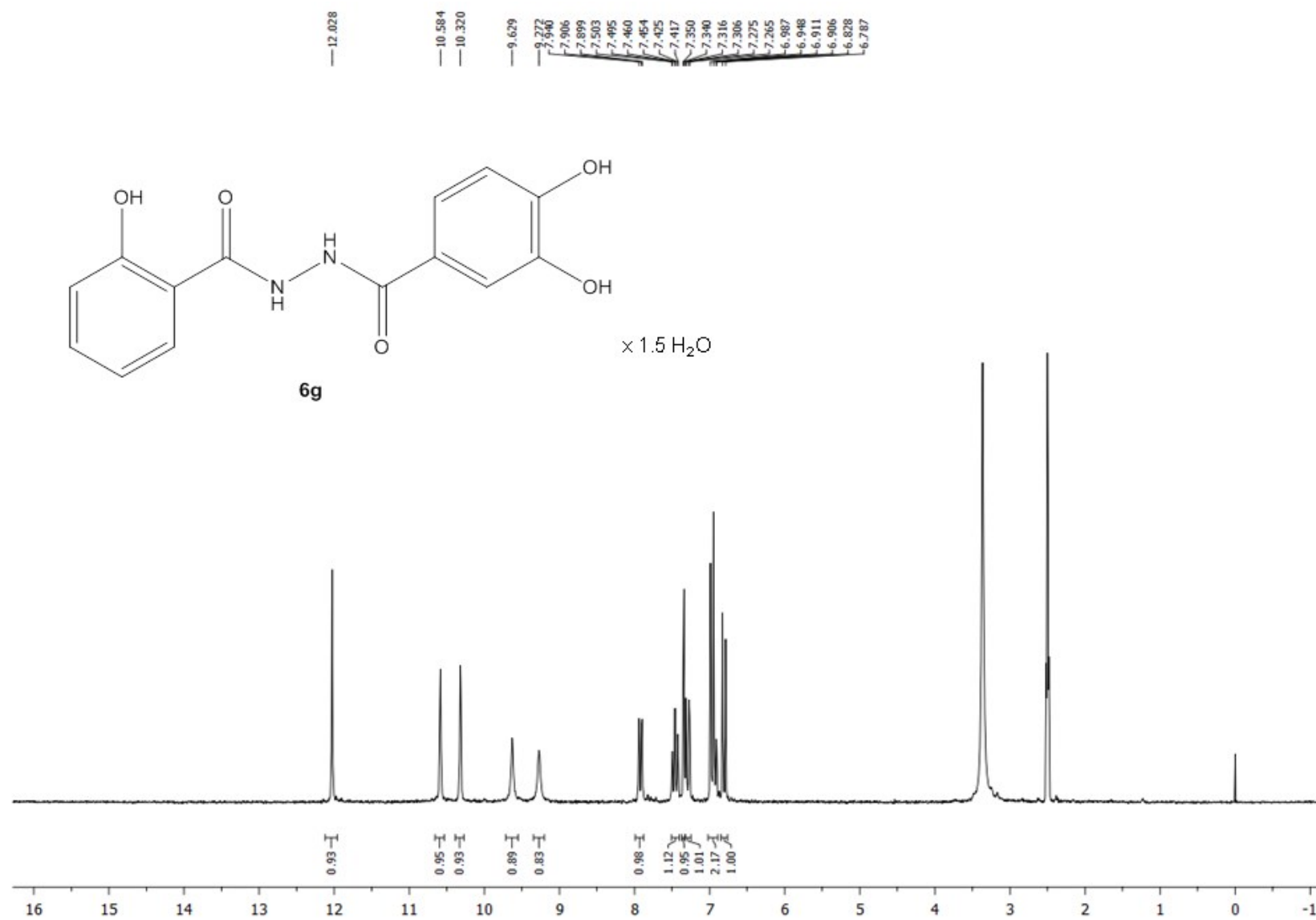


Figure S13. ¹H NMR spectrum of **6g** in DMSO-d₆ (200 MHz).

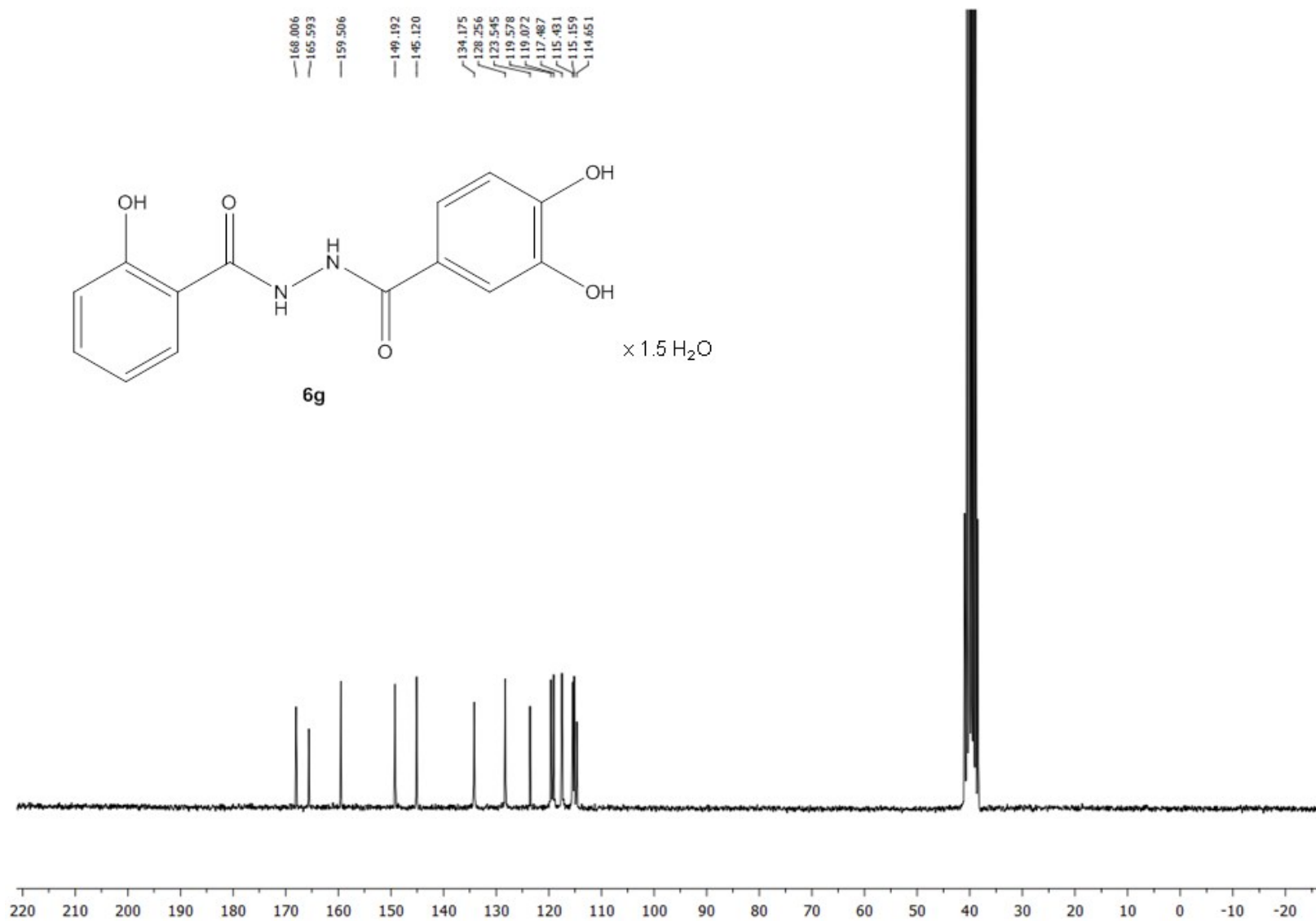


Figure S14. ^{13}C NMR spectrum of **6g** in DMSO-d_6 (50 MHz).

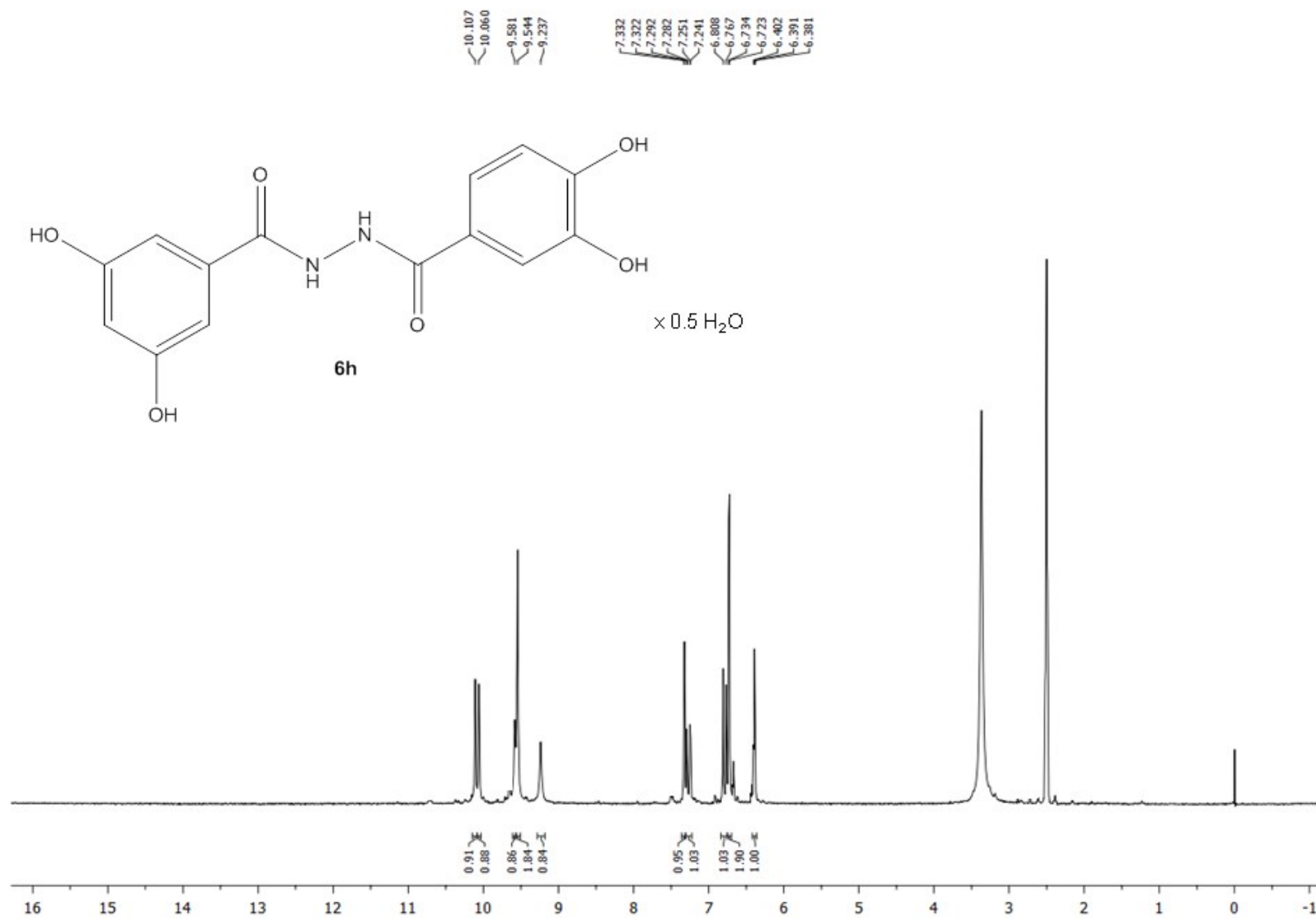


Figure S15. ¹H NMR spectrum of **6h** in DMSO-d₆ (200 MHz).

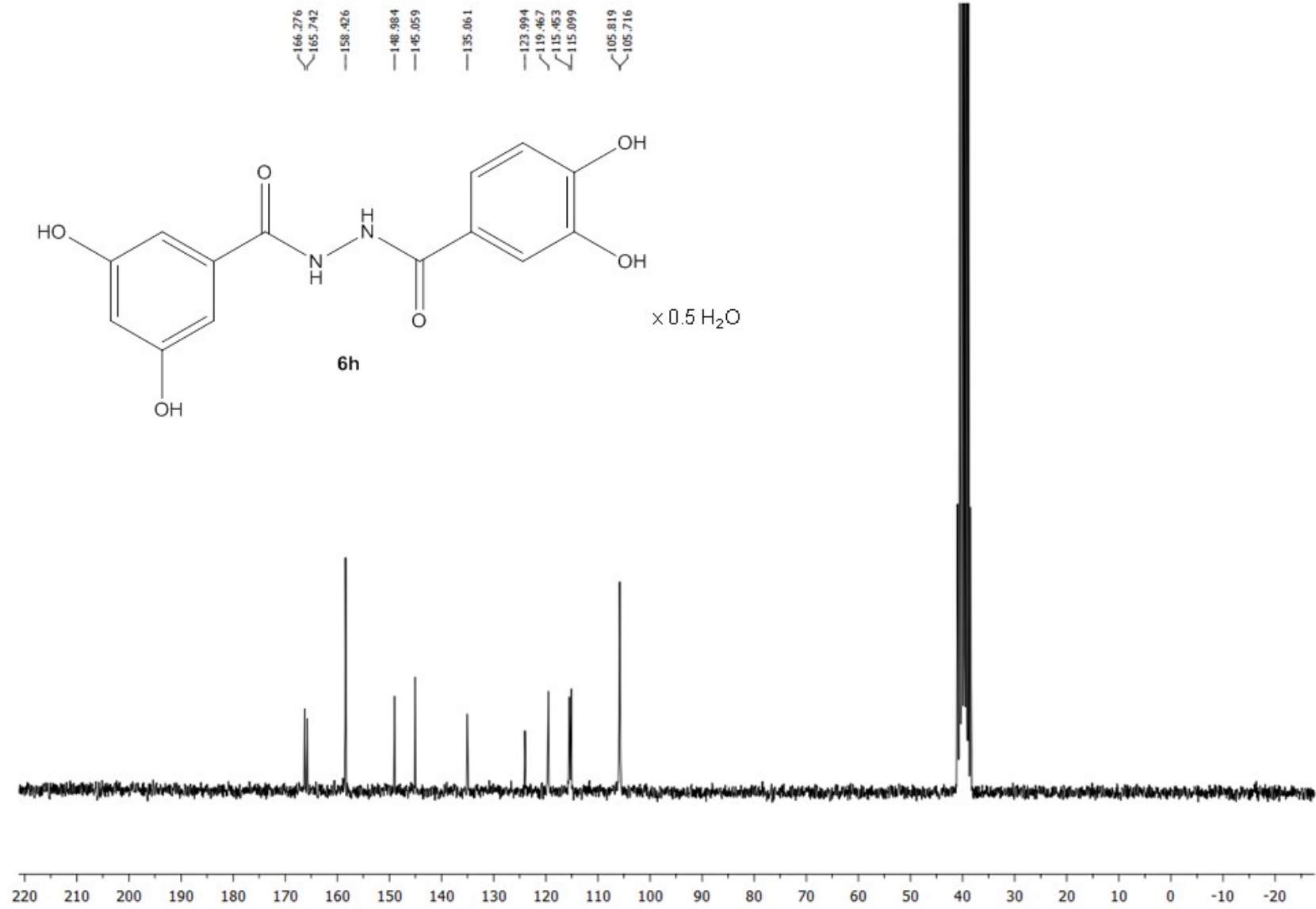


Figure S16. ^{13}C NMR spectrum of **6h** in DMSO-d_6 (50 MHz).

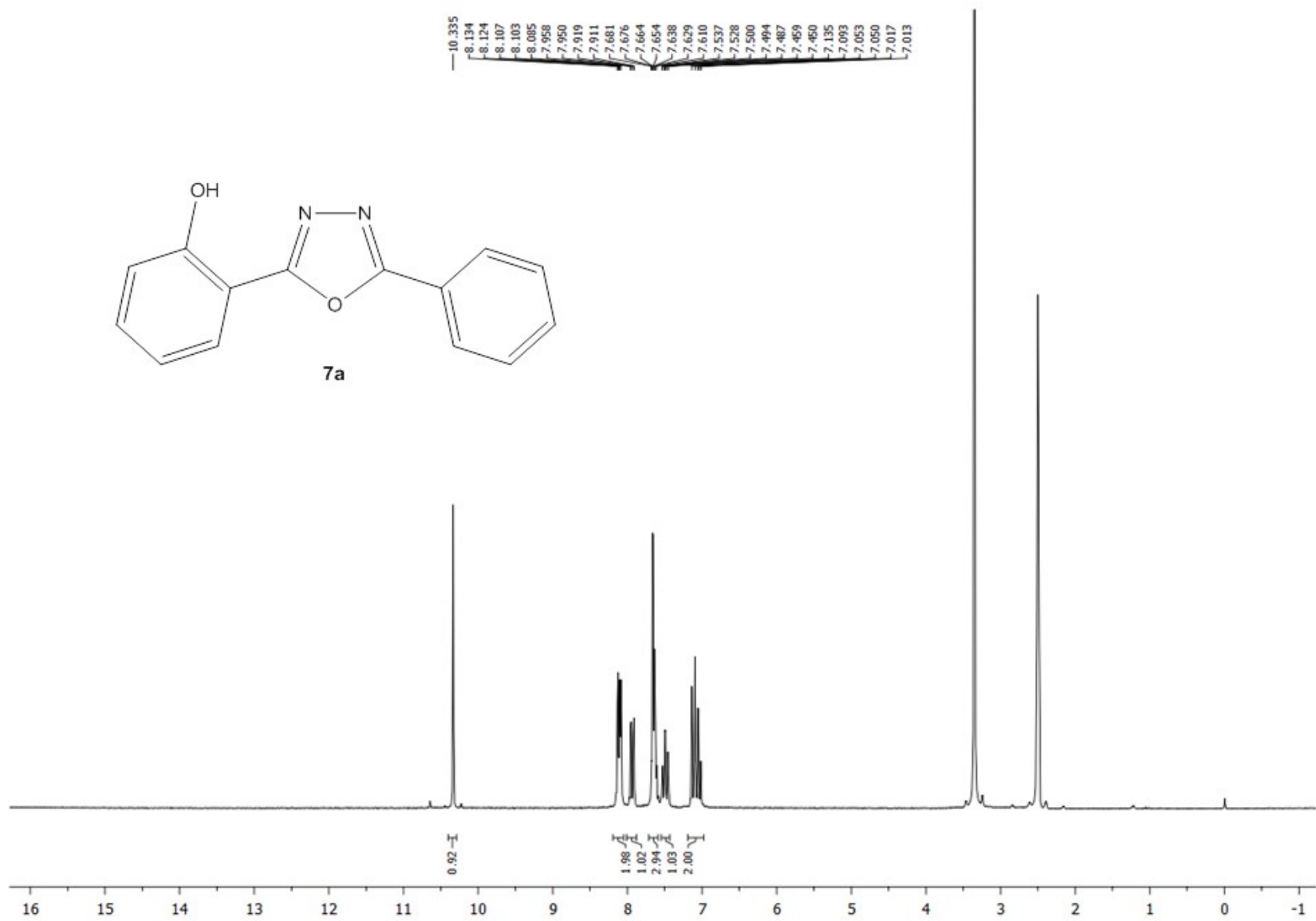


Figure S17. ¹H NMR spectrum of **7a** in DMSO-d₆ (200 MHz).

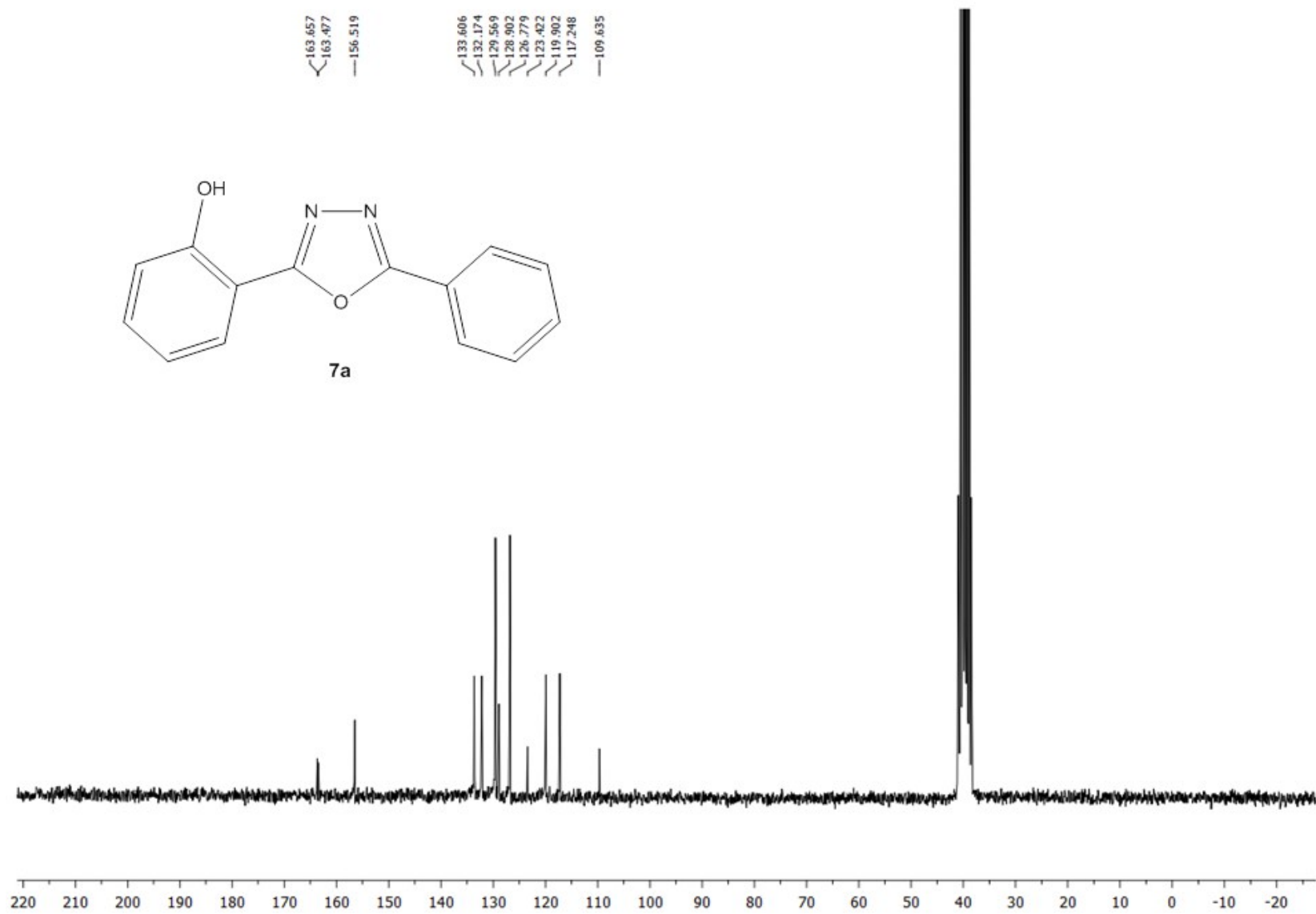


Figure S18. ^{13}C NMR spectrum of **7a** in DMSO- d_6 (50 MHz).

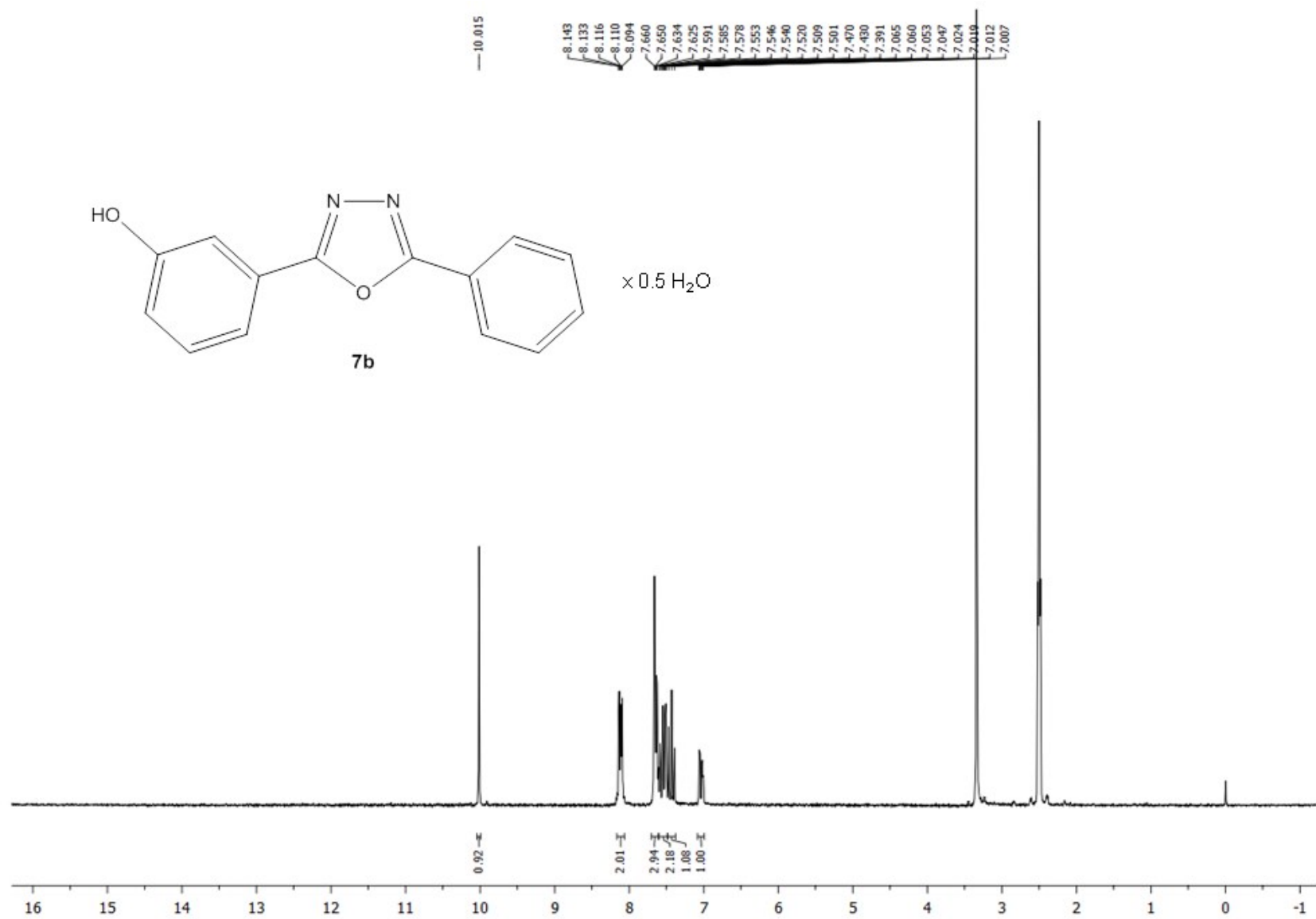


Figure S19. ¹H NMR spectrum of **7b** in DMSO-d₆ (200 MHz).

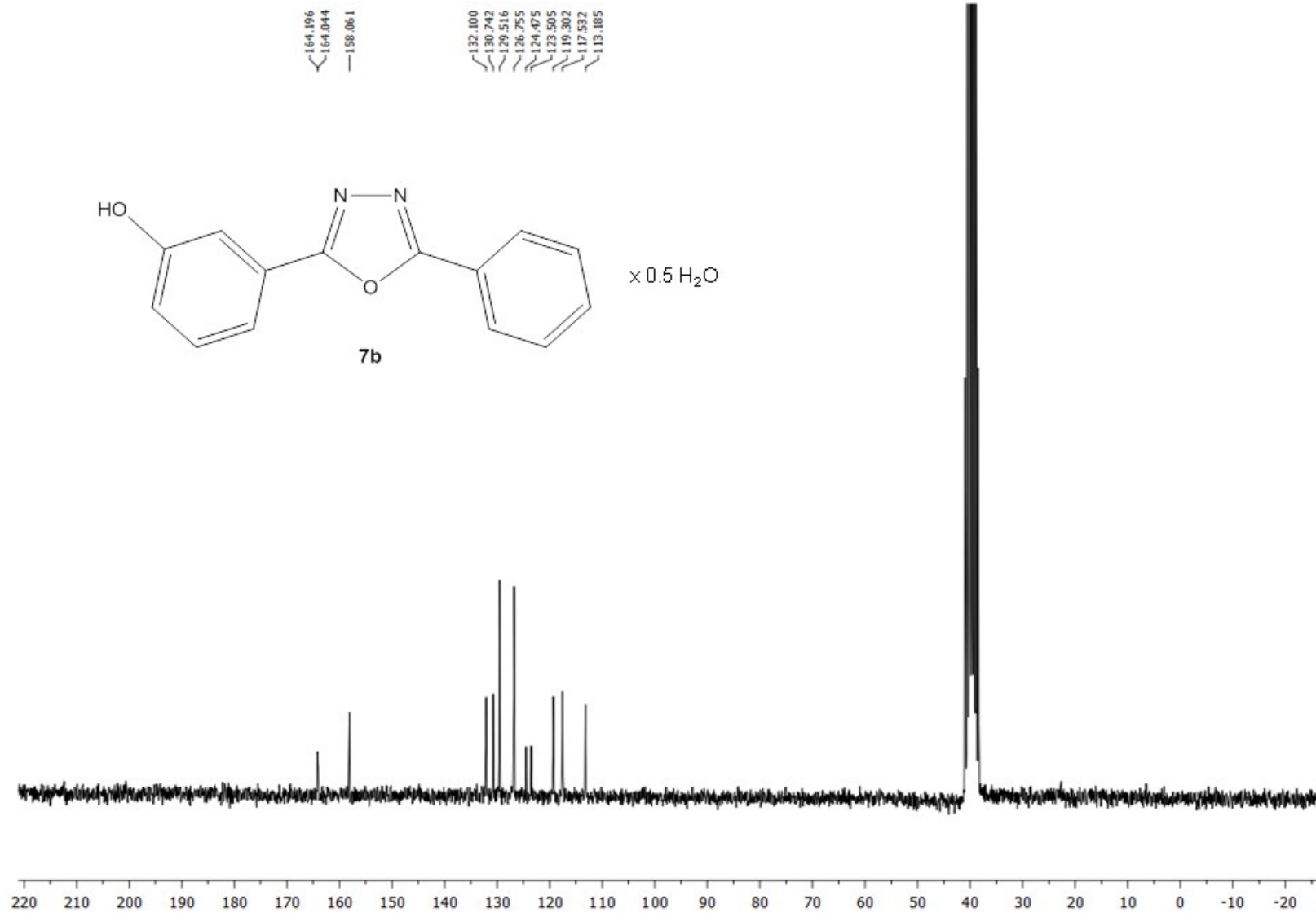


Figure S20. ^{13}C NMR spectrum of **7b** in DMSO- d_6 (50 MHz).

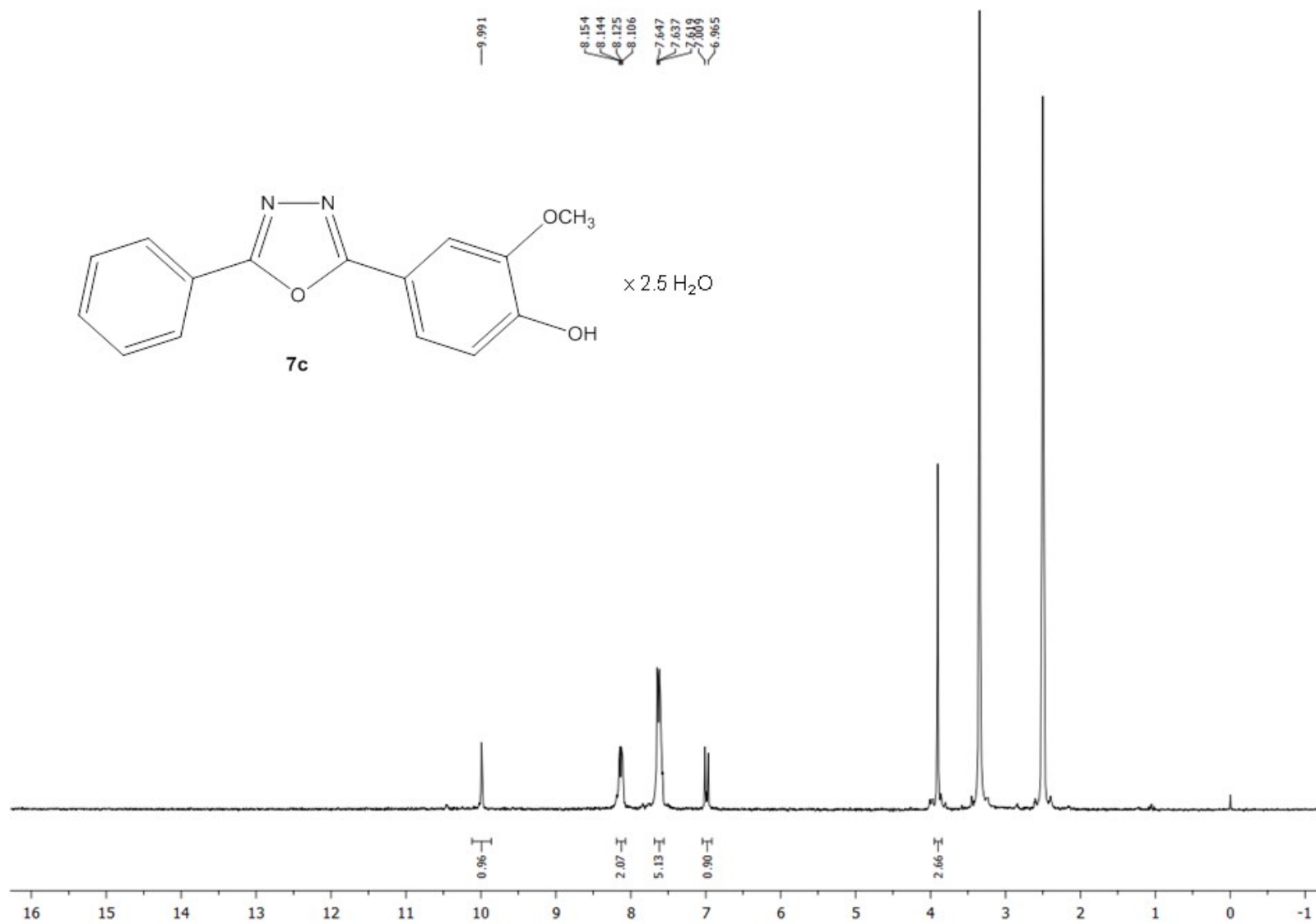


Figure S21. ^1H NMR spectrum of **7c** in DMSO-d_6 (200 MHz).

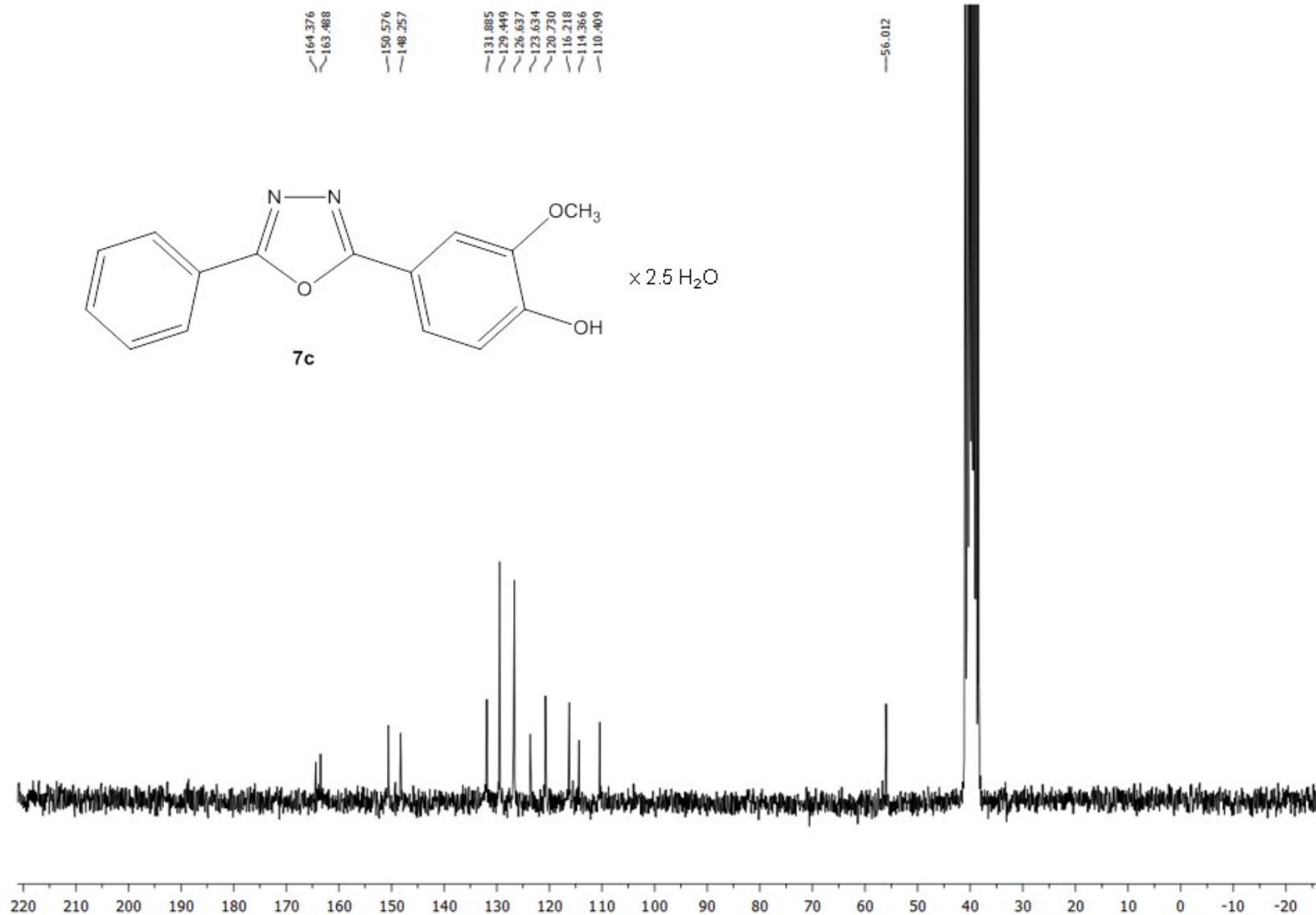


Figure S22. ¹³C NMR spectrum of **7c** in DMSO-d₆ (50 MHz).

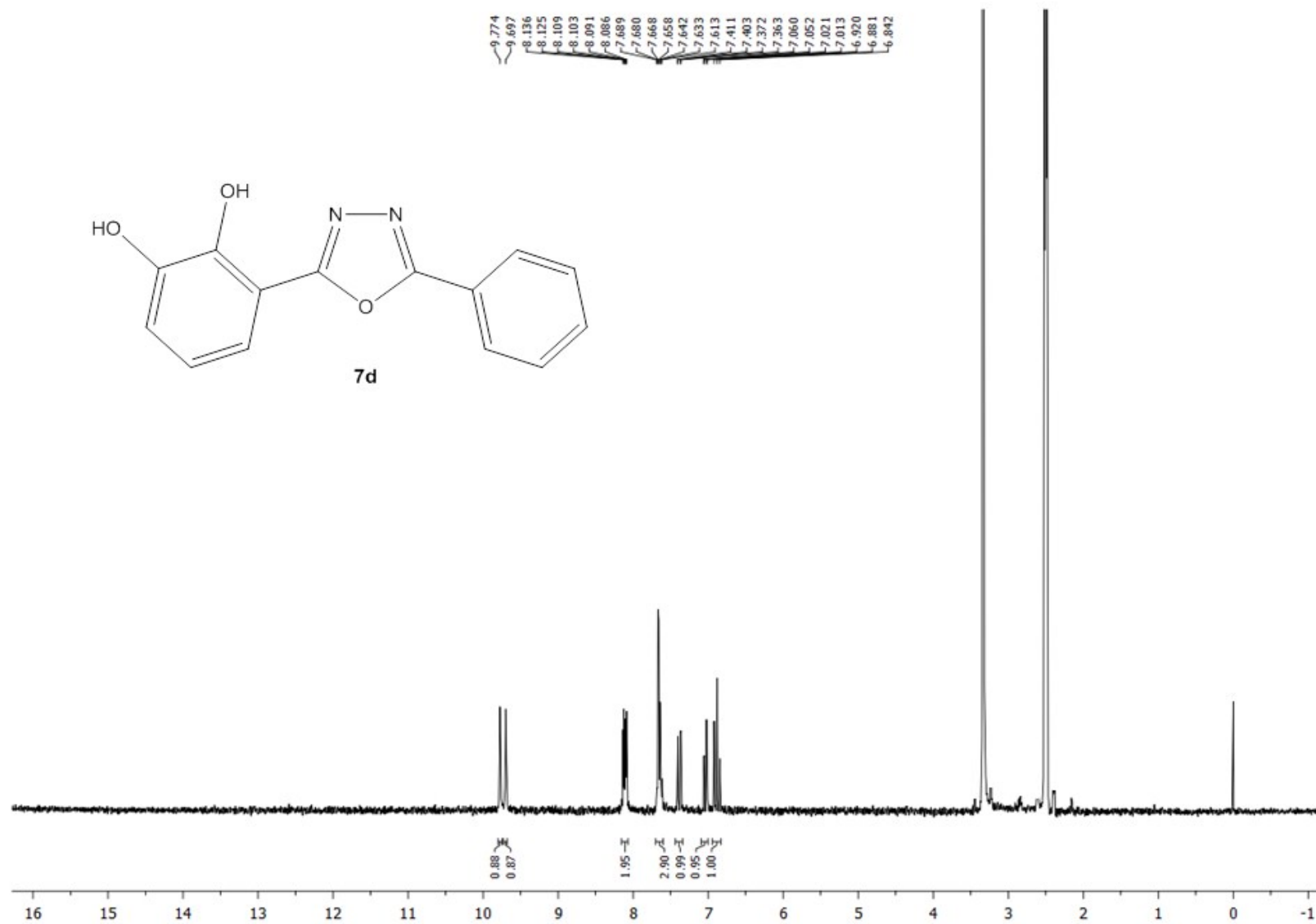


Figure S23. ¹H NMR spectrum of **7d** in DMSO-d₆ (200 MHz).

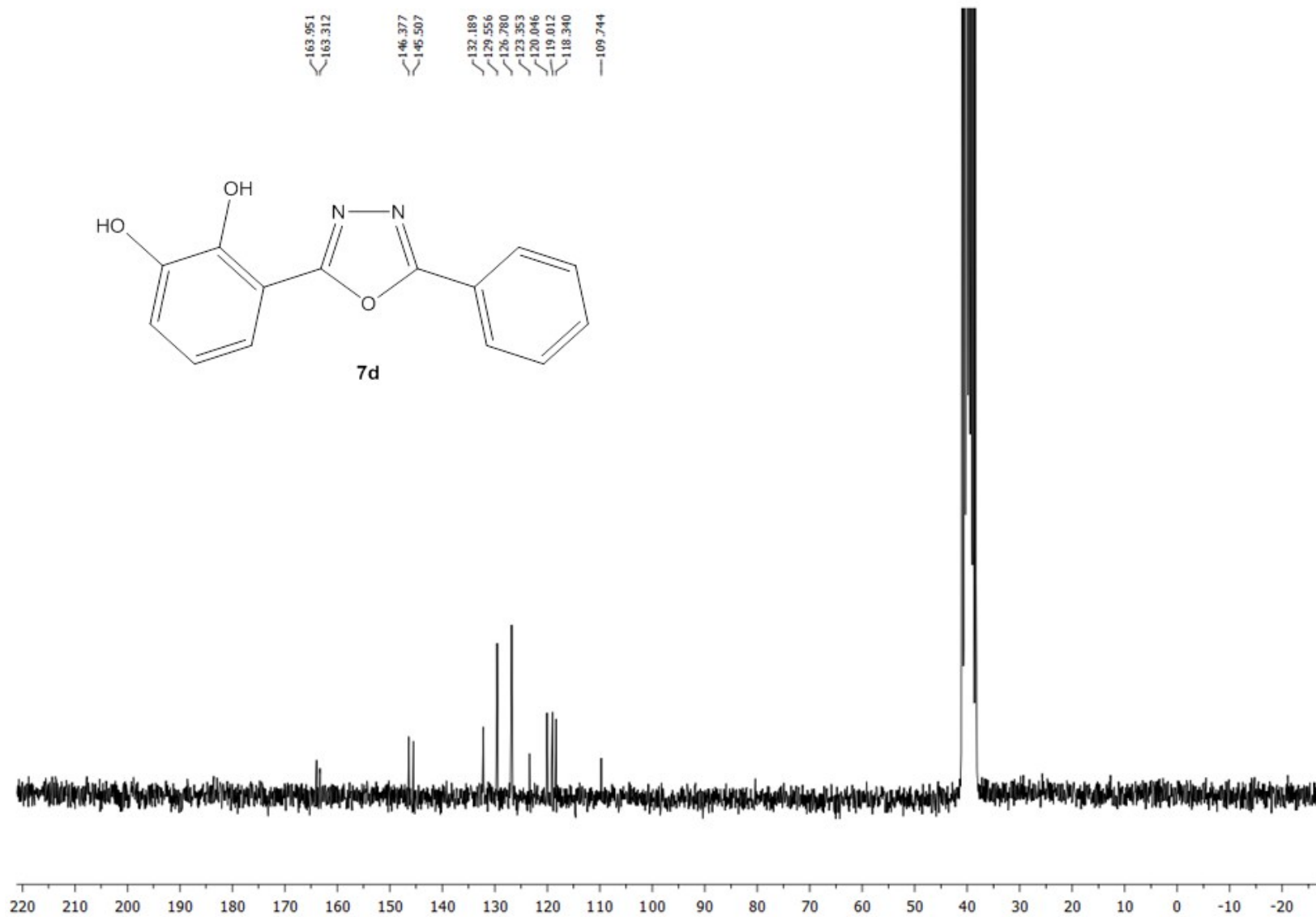


Figure S24. ^{13}C NMR spectrum of **7d** in DMSO-d_6 (50 MHz).

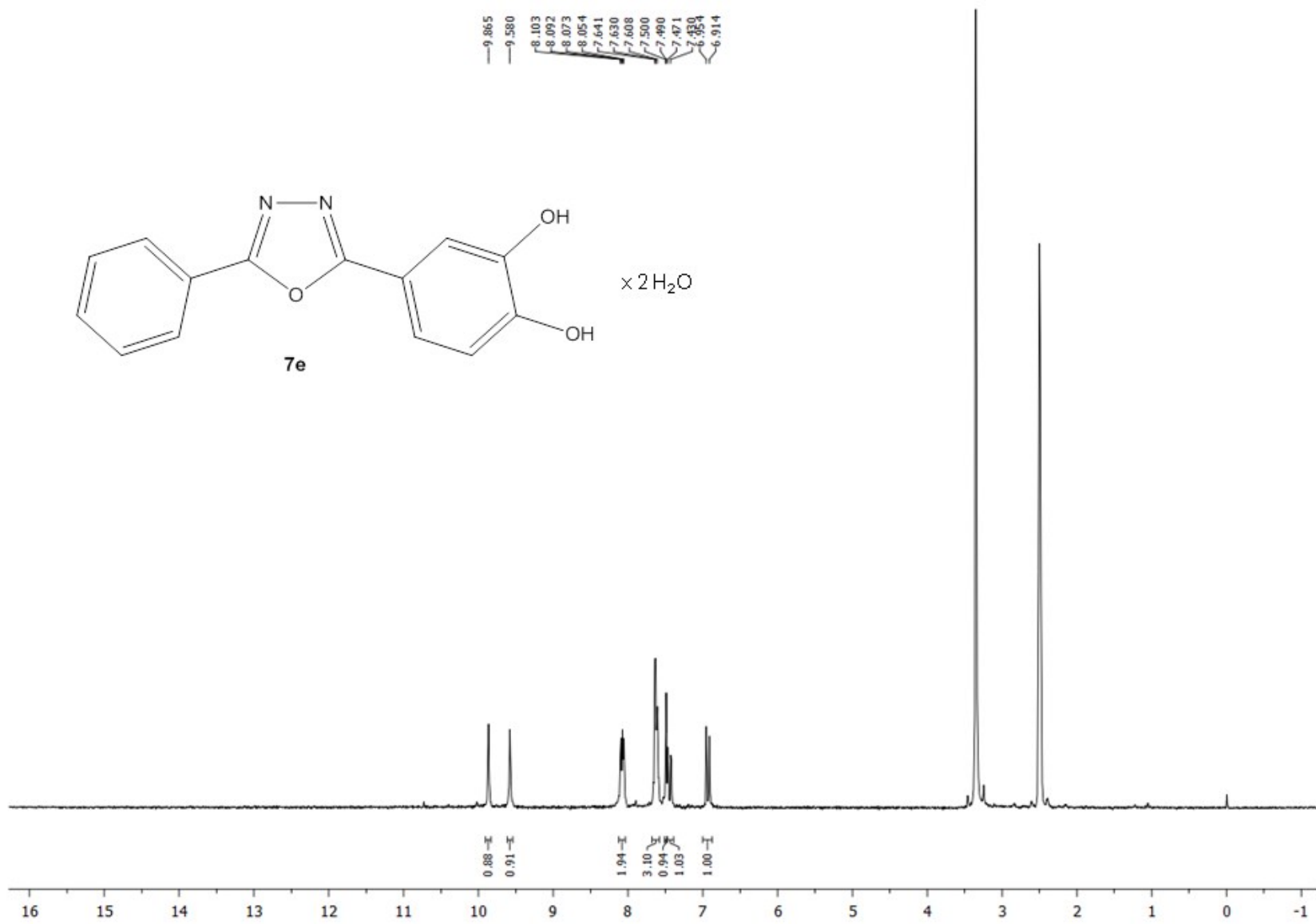


Figure S25. ¹H NMR spectrum of **7e** in DMSO-d₆ (200 MHz).

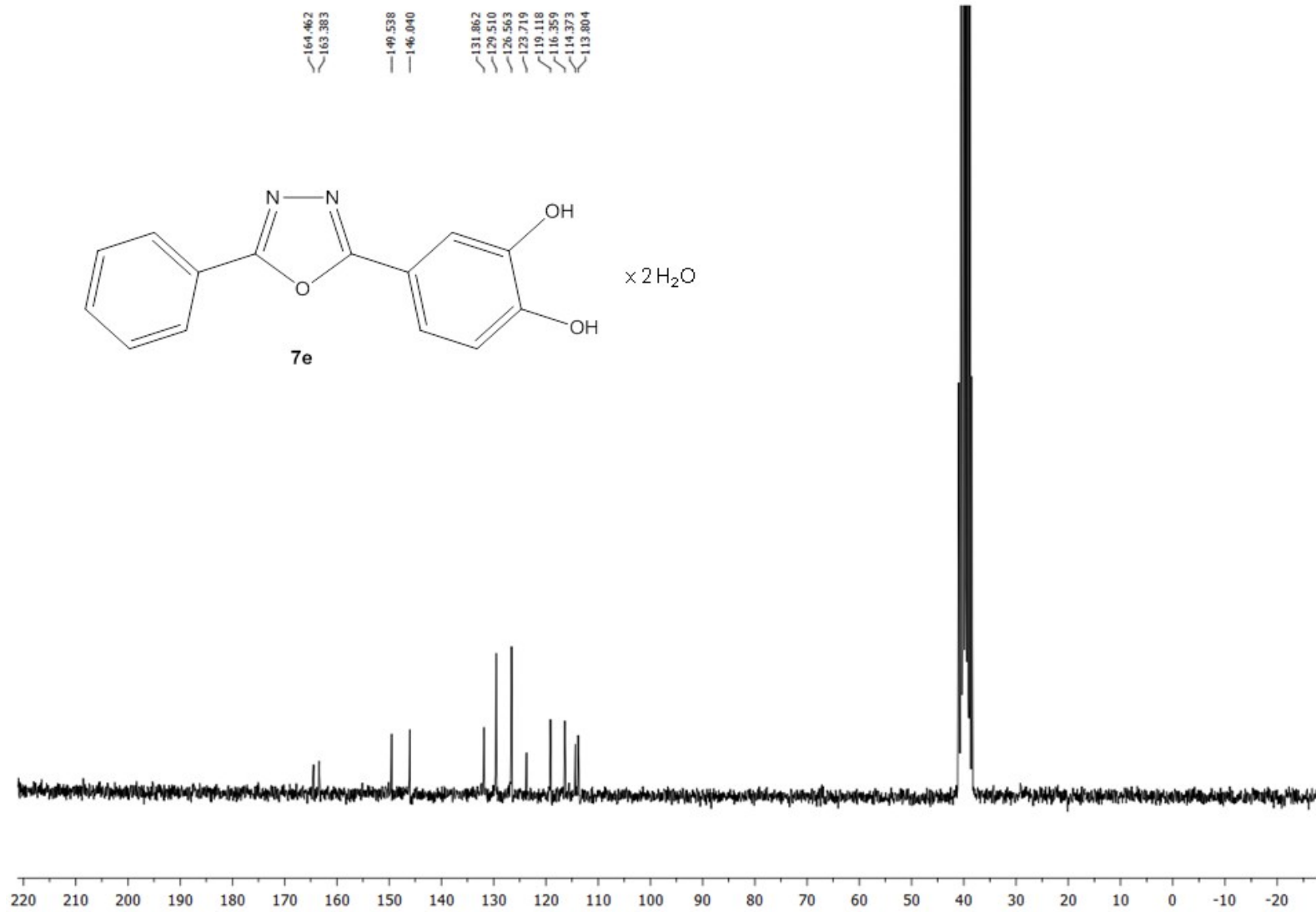


Figure S26. ^{13}C NMR spectrum of **7e** in DMSO-d_6 (50 MHz).

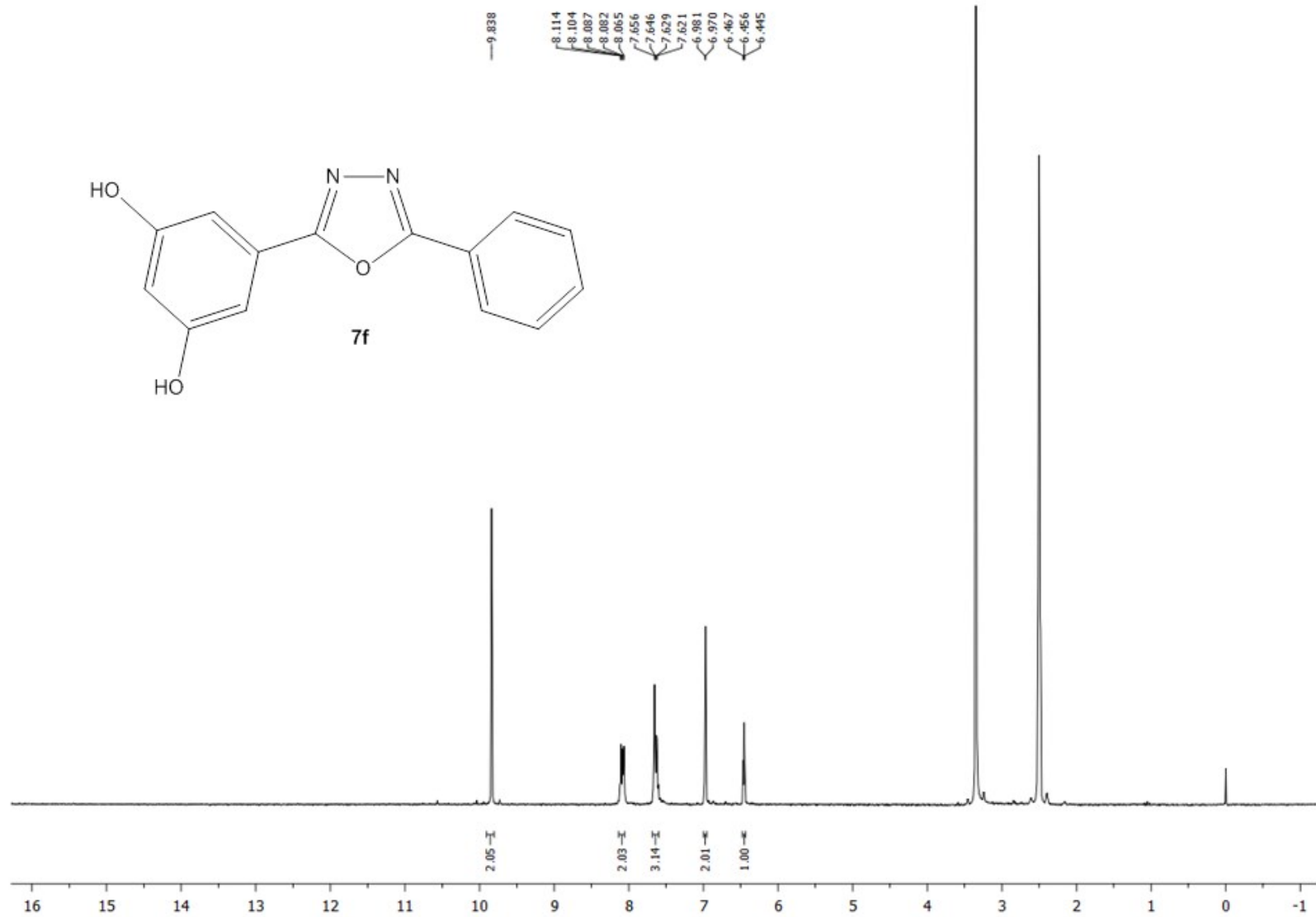


Figure S27. ¹H NMR spectrum of **7f** in DMSO-d₆ (200 MHz).

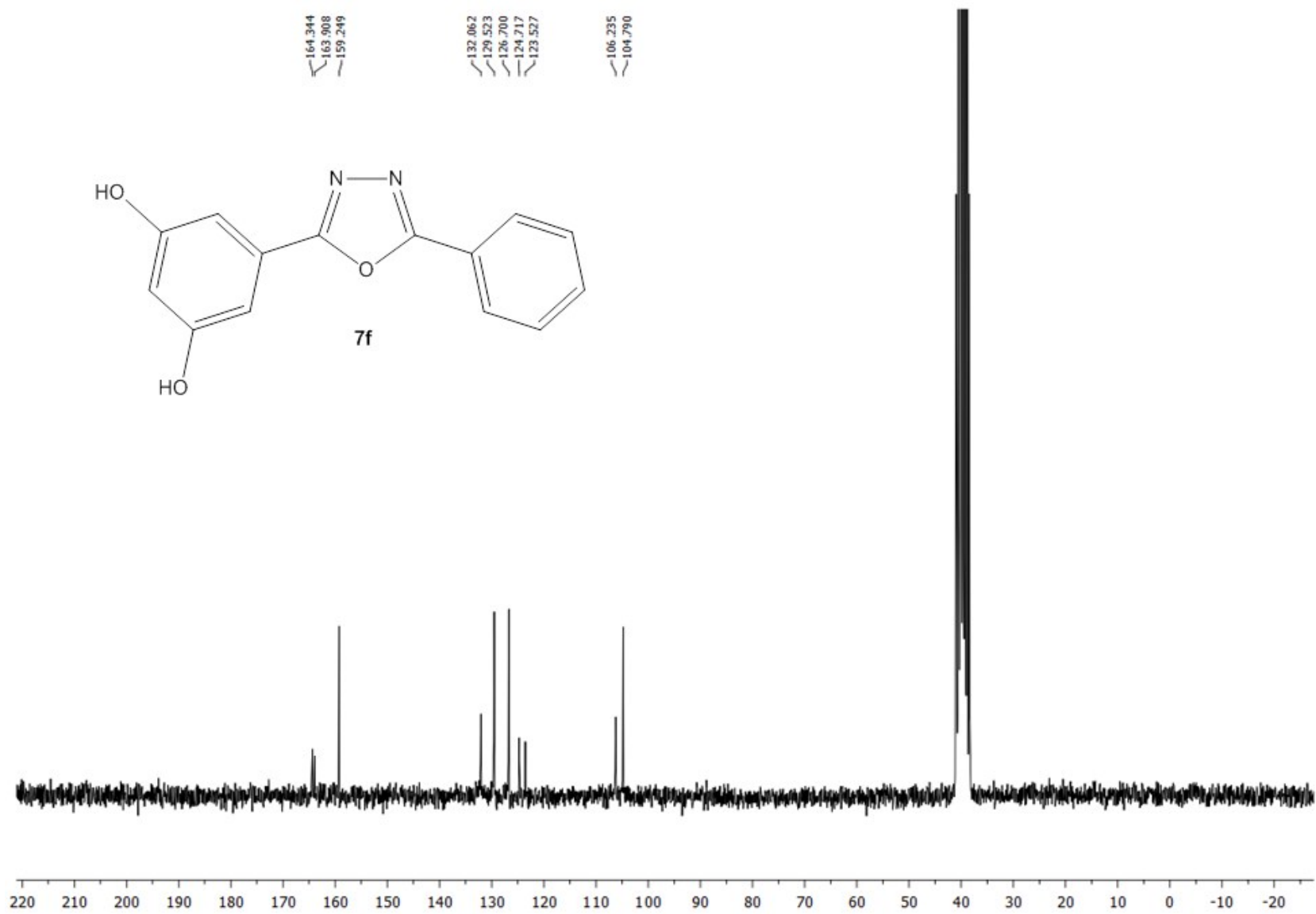


Figure S28. ¹³C NMR spectrum of **7f** in DMSO-d₆ (50 MHz).

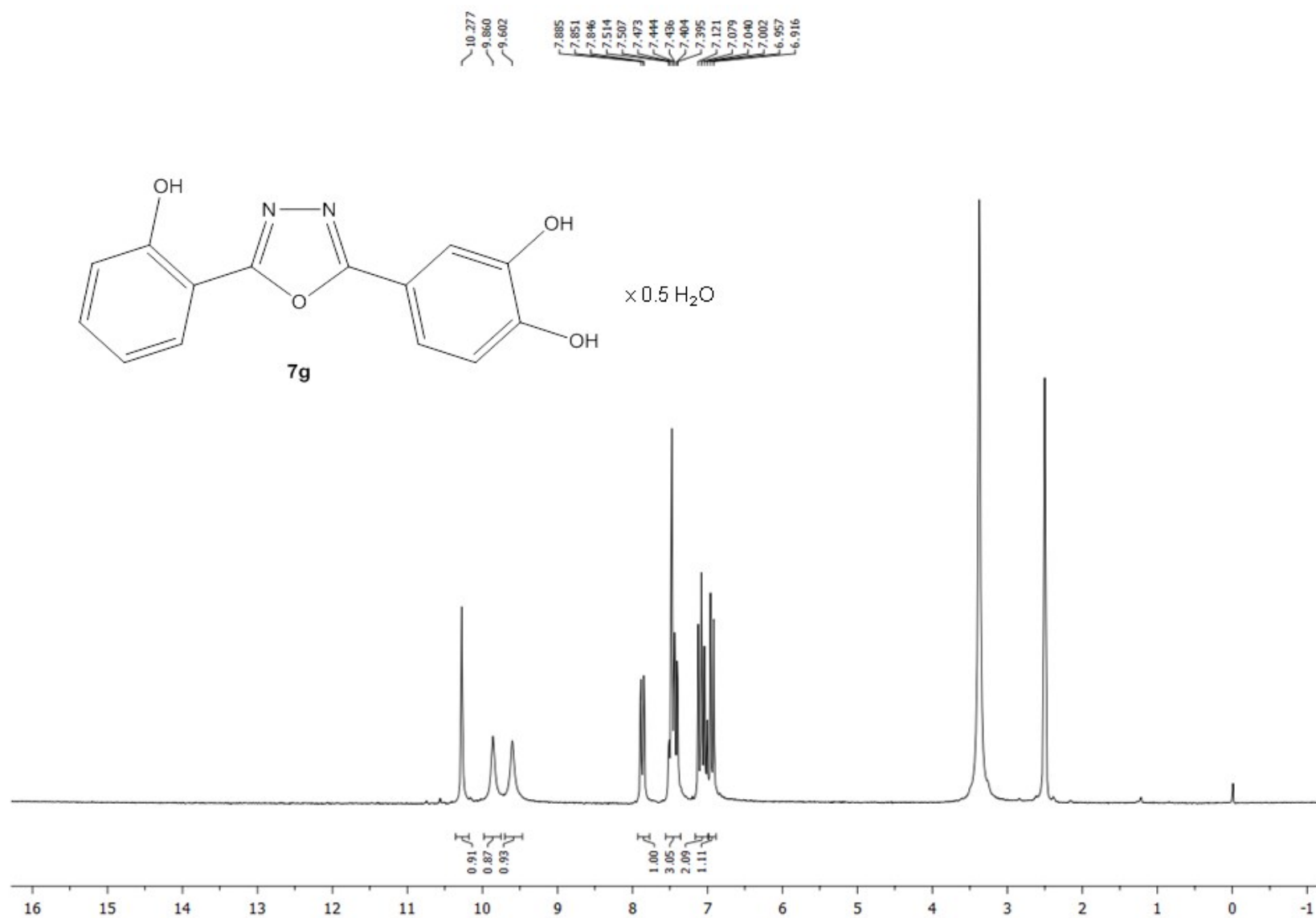


Figure S29. ^1H NMR spectrum of **7g** in DMSO-d_6 (200 MHz).

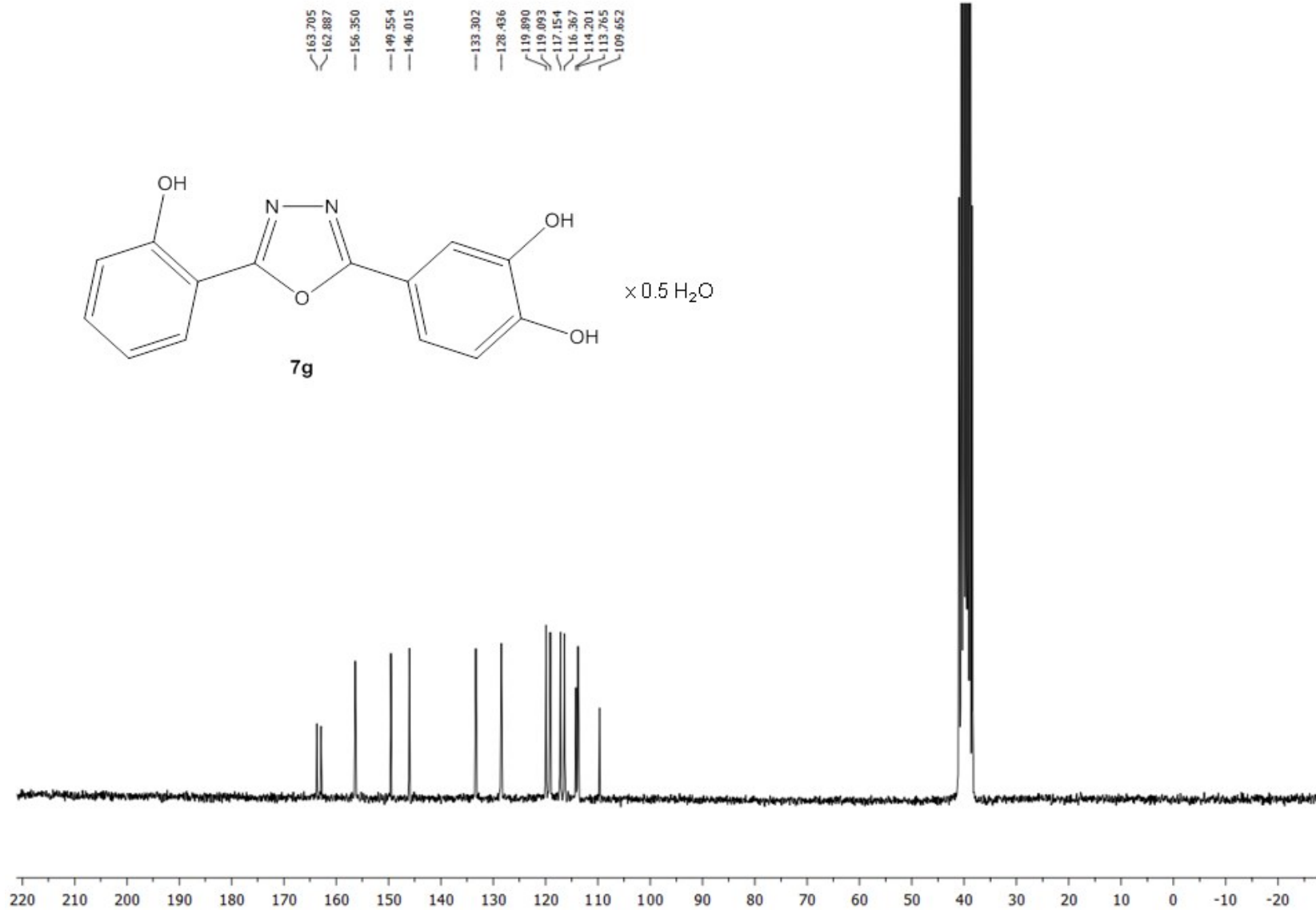


Figure S30. ^{13}C NMR spectrum of **7g** in DMSO-d_6 (50 MHz).

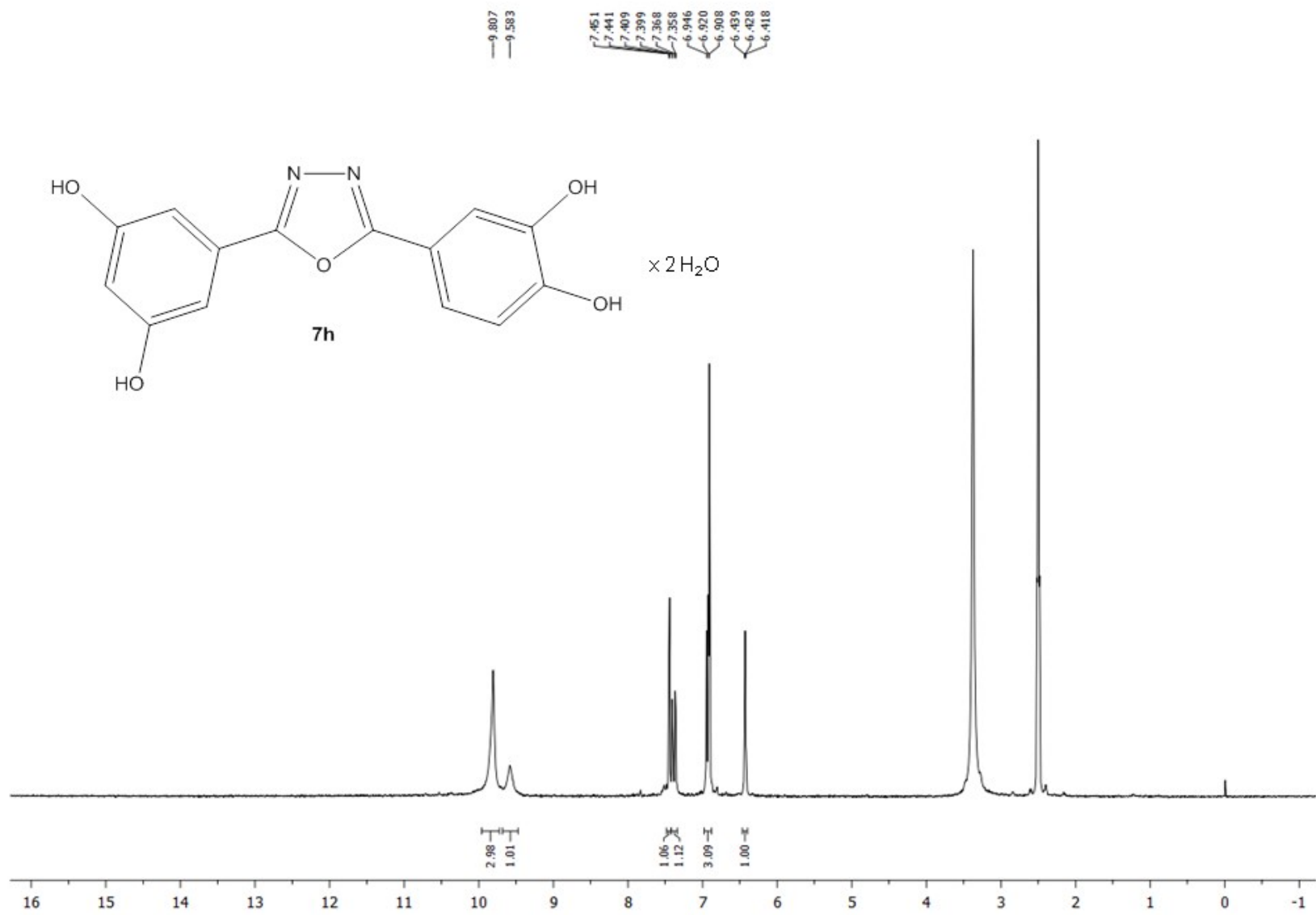


Figure S31. ^1H NMR spectrum of **7h** in DMSO-d_6 (200 MHz).

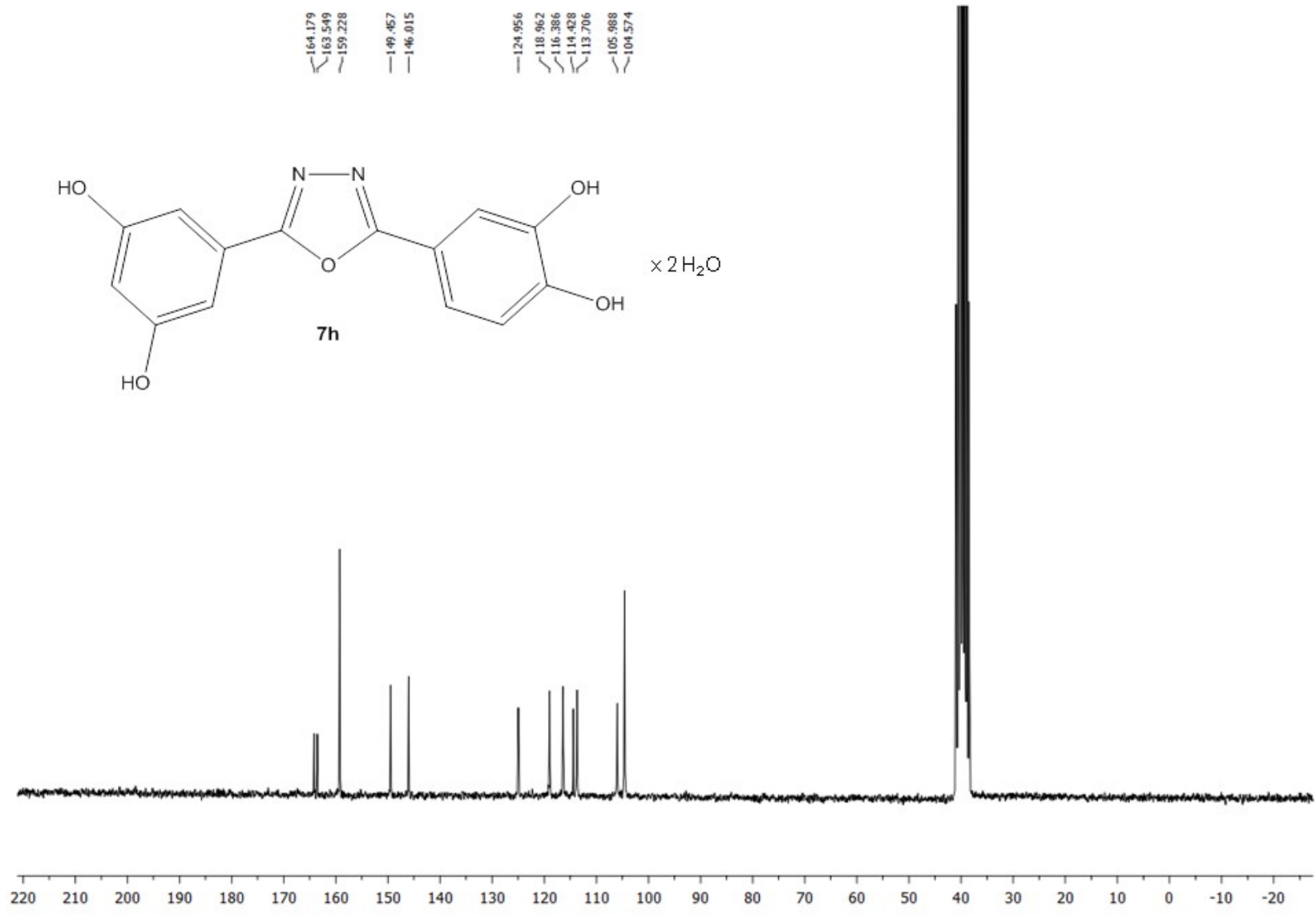


Figure S32. ^{13}C NMR spectrum of **7h** in DMSO- d_6 (50 MHz).