

Synthesis, antiprotozoal activity, and cheminformatic analysis of 2-phenyl-2*H*-indazole derivatives

Karen Rodríguez-Villar ¹, Lilián Yépez-Mulia ², Miguel Cortés-Gines ³, Jacobo David Aguilera-Perdomo ³, Edgar A. Quintana-Salazar ³, Kevin Samael Olascoaga Del Angel ⁴, Francisco Cortés-Benítez ³, Juan Francisco Palacios-Espinosa ³, Olivia Soria-Arteche ³ and Jaime Pérez-Villanueva ^{3,*}

¹ Doctorado en Ciencias Biológicas y de la Salud, Universidad Autónoma Metropolitana (UAM), Ciudad de México 04960, Mexico; qkarenrodv@hotmail.com

² Unidad de Investigación Médica en Enfermedades Infecciosas y Parasitarias, UMAE Hospital de Pediatría, Centro Médico Siglo XXI, Instituto Mexicano del Seguro Social, Ciudad de México 06720, Mexico; lilianyopez@yahoo.com

³ Departamento de Sistemas Biológicos, División de Ciencias Biológicas y de la Salud, Universidad Autónoma Metropolitana-Xochimilco (UAM-X), Ciudad de México 04960, Mexico; mcortes@pharmometrica.com.mx (M.C.-G.); jacoboaaguilera.96@gmail.com (J.D.A.-P); edgarqsl2811@gmail.com (E.A.Q.-S); jcortesb@correo.xoc.uam.mx (F.C.-B); jpalacios@correo.xoc.uam.mx (J.F.P.-E.); soriao@correo.xoc.uam.mx (O.S.-A.);

⁴ Doctorado en Biología experimental, Universidad Autónoma Metropolitana (UAM), Ciudad de México 04960, Mexico; olaskuaga@gmail.com

* Correspondence: jpvillanueva@correo.xoc.uam.mx; Tel.: +525 54 83 72 59; fax: +525 55 94 79 29.

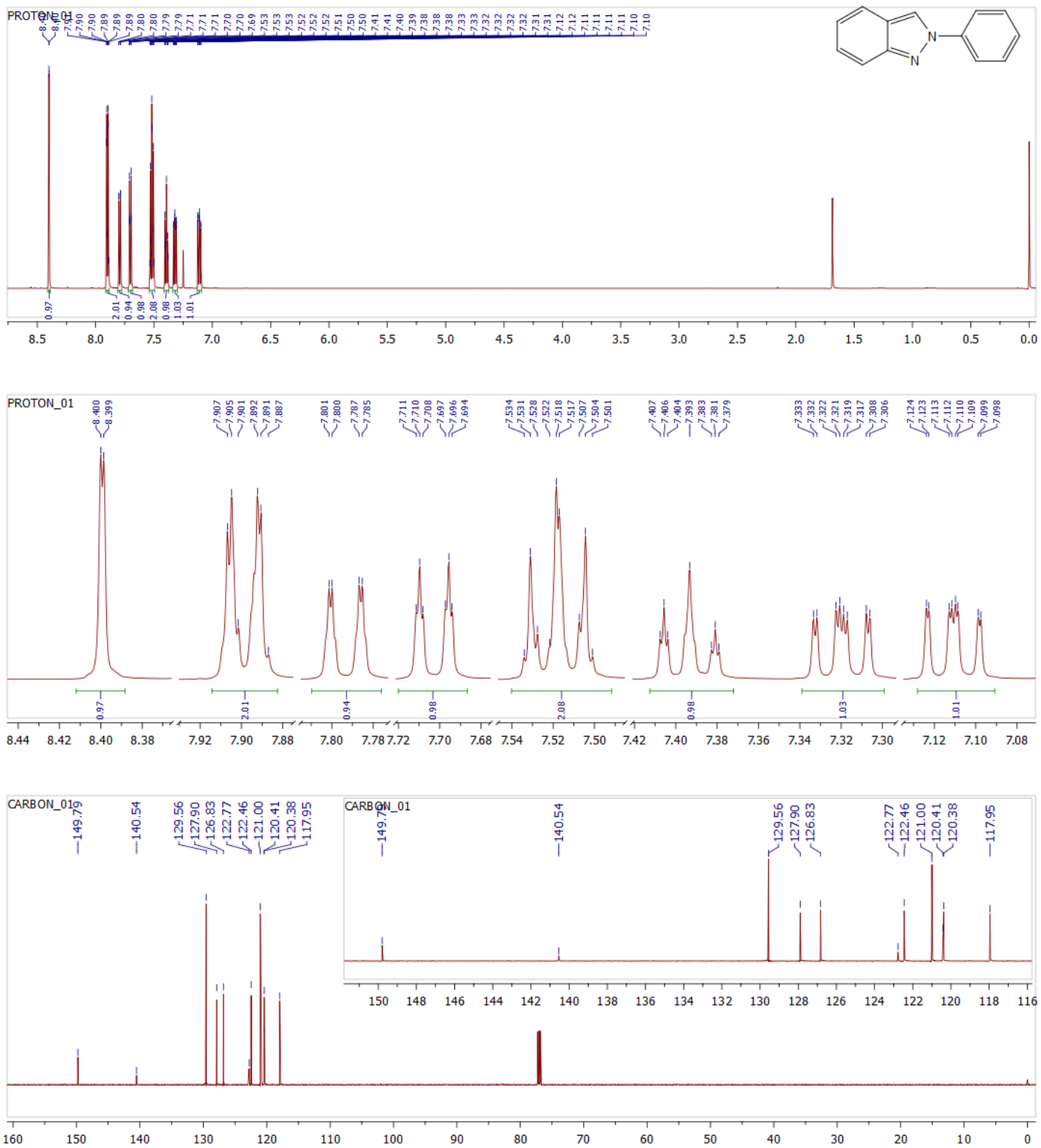


Figure S1. ¹H NMR (600 MHz, CDCl₃) and ¹³C NMR (151 MHz, CDCl₃) for 2-phenyl-2H-indazole (**1**).

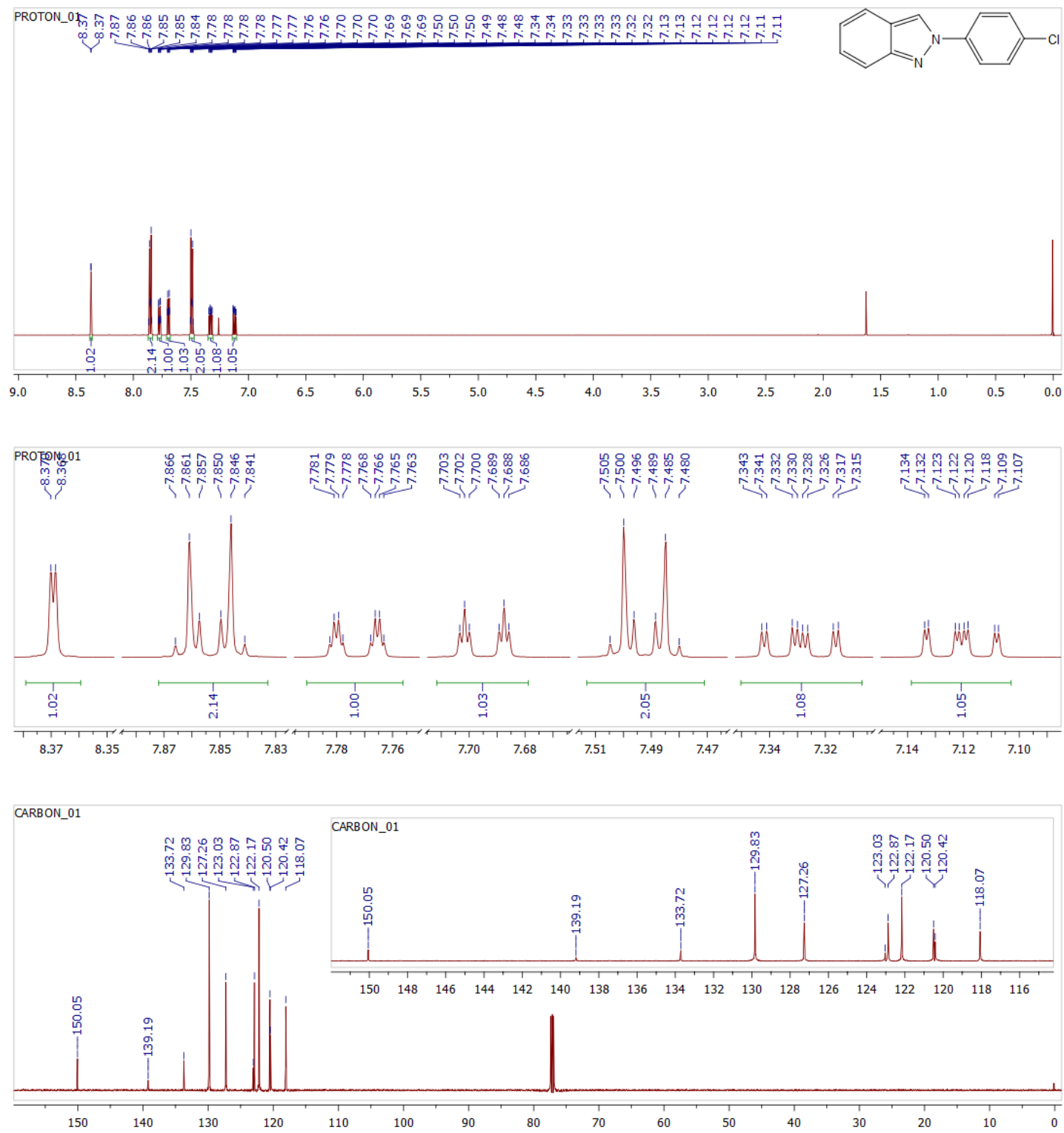


Figure S2. ¹H NMR (600 MHz, CDCl₃) and ¹³C NMR (151 MHz, CDCl₃) for 2-(4-chlorophenyl)-2H-indazole (2)

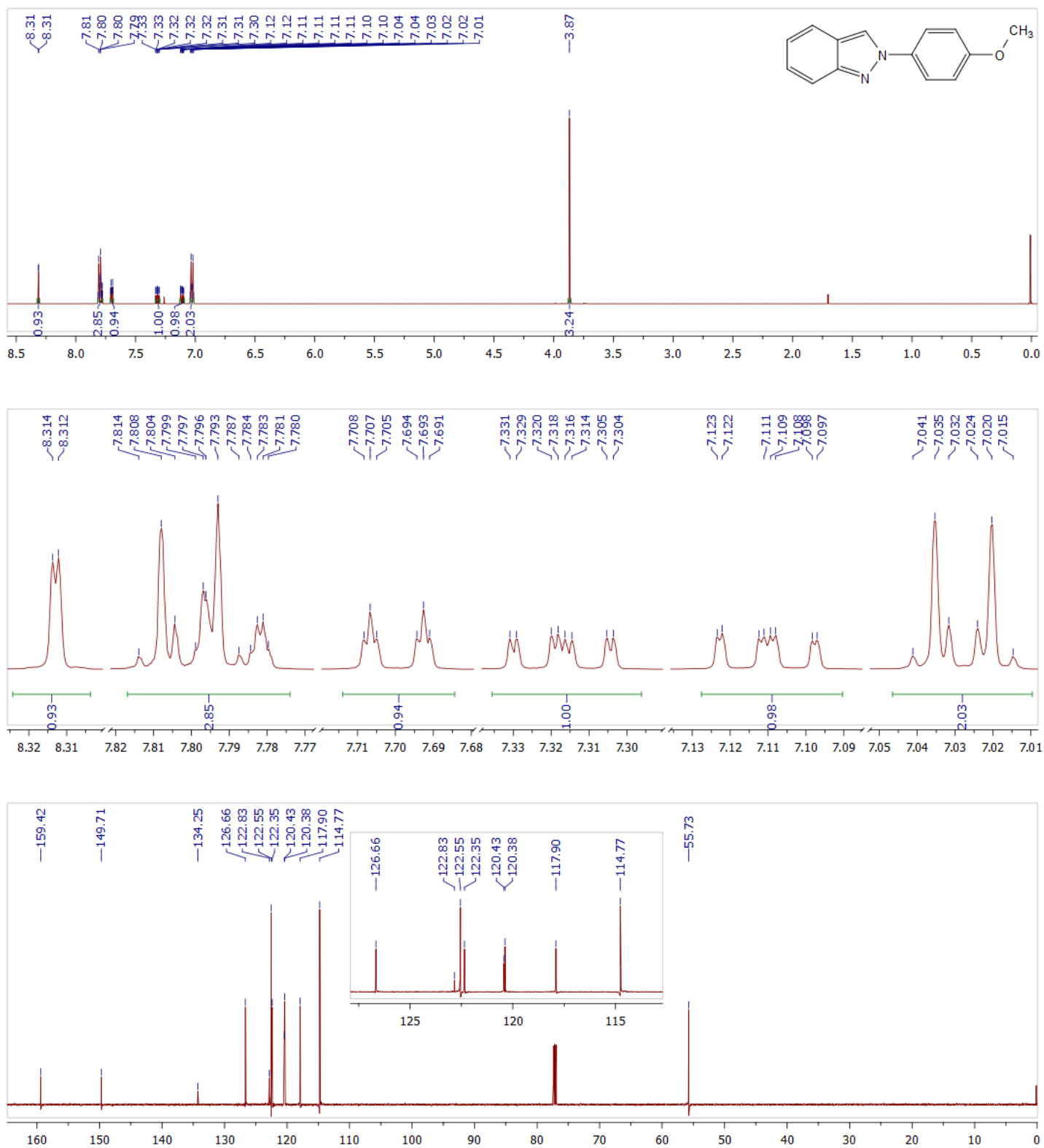


Figure S3. ¹H NMR (600 MHz, CDCl₃) and ¹³C NMR (151 MHz, CDCl₃) for 2-(4-methoxyphenyl)-2H-indazole (**3**).

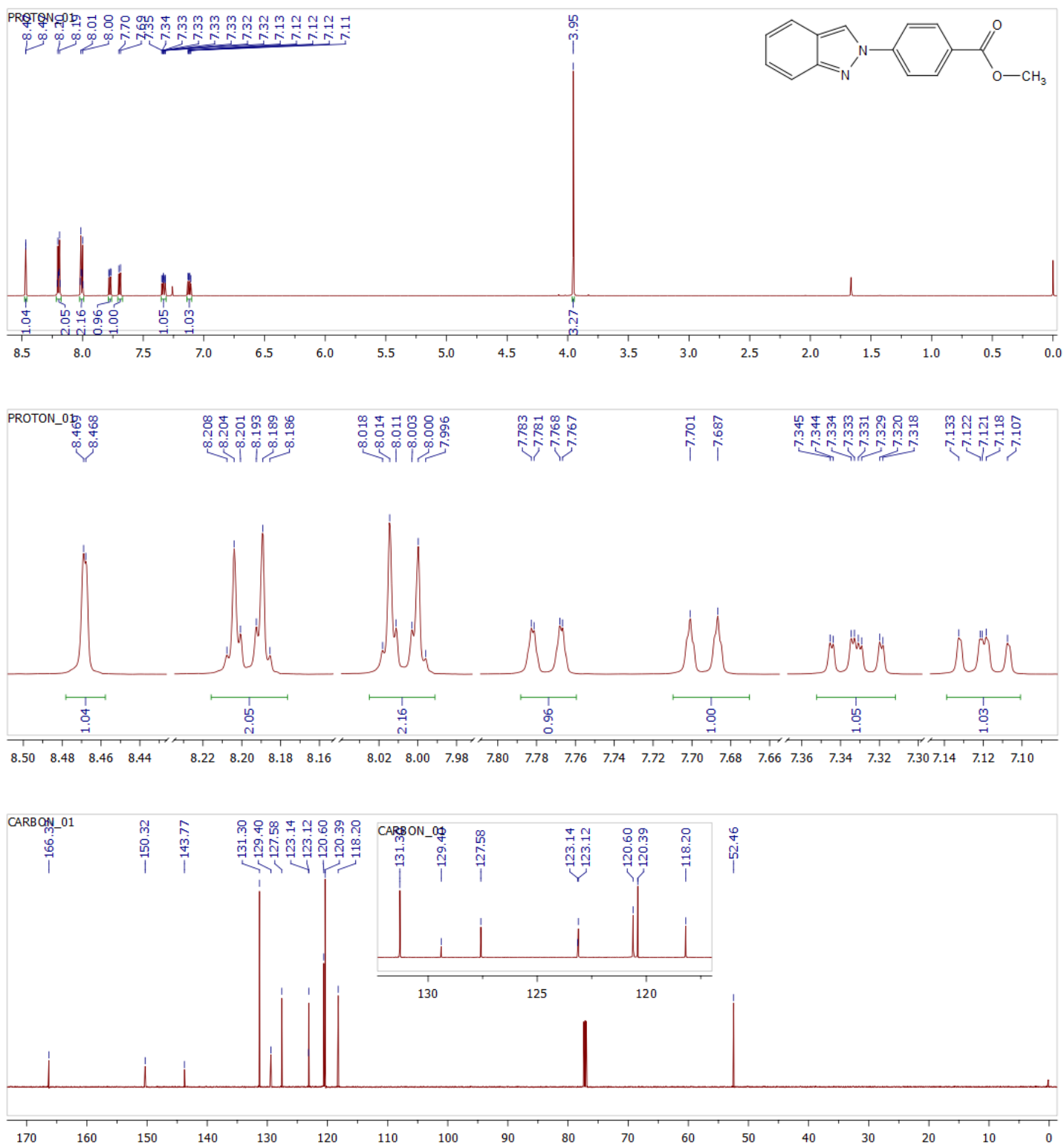


Figure S4. ¹H NMR (600 MHz, CDCl₃) and ¹³C NMR (151 MHz, CDCl₃) for methyl 4-(2*H*-indazol-2-yl)benzoate (**4**).

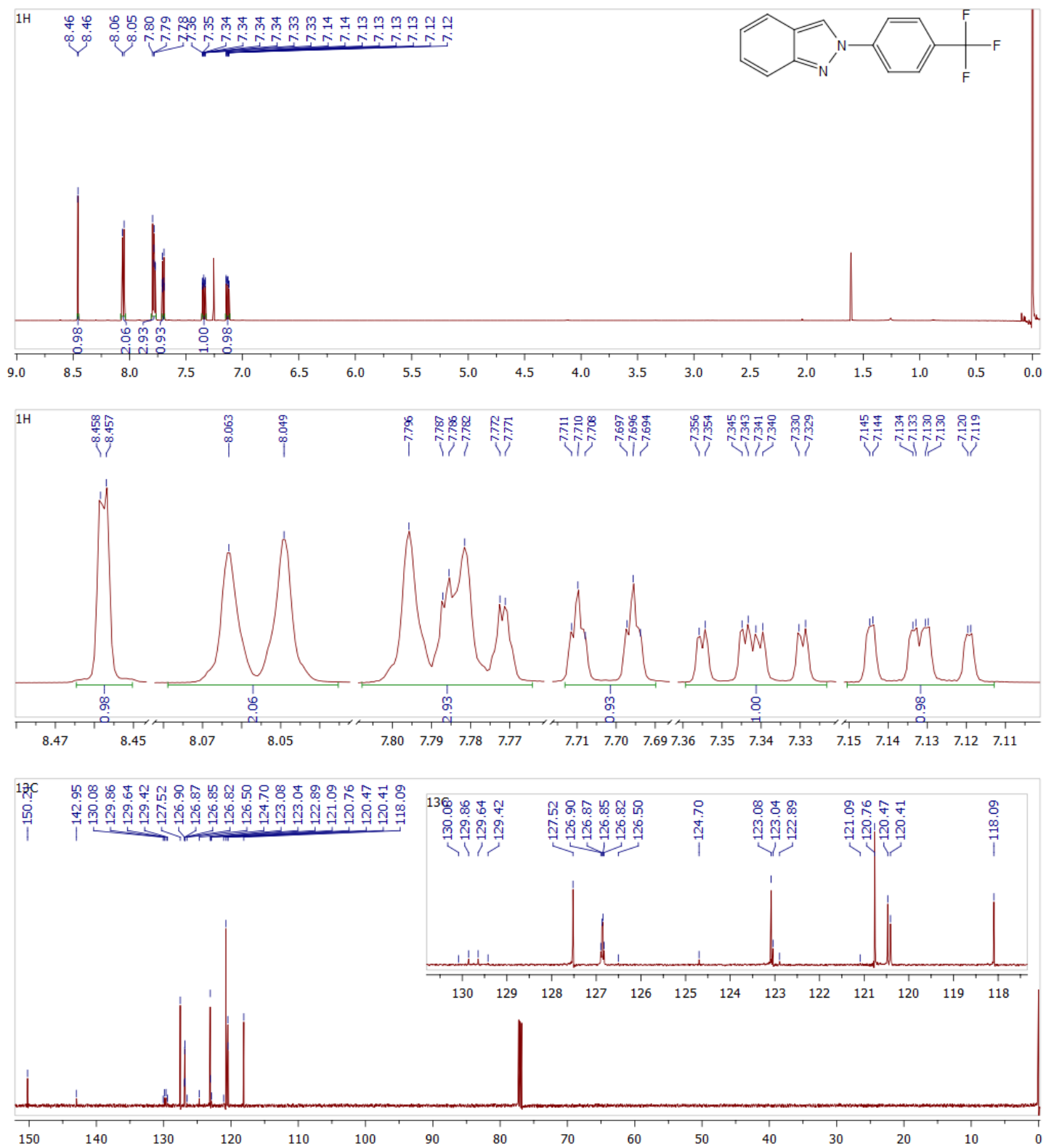


Figure S6. ¹H NMR (600 MHz, CDCl₃) and ¹³C NMR (151 MHz, CDCl₃) for 2-[4-(trifluoromethyl)phenyl]-2H-indazole (6).

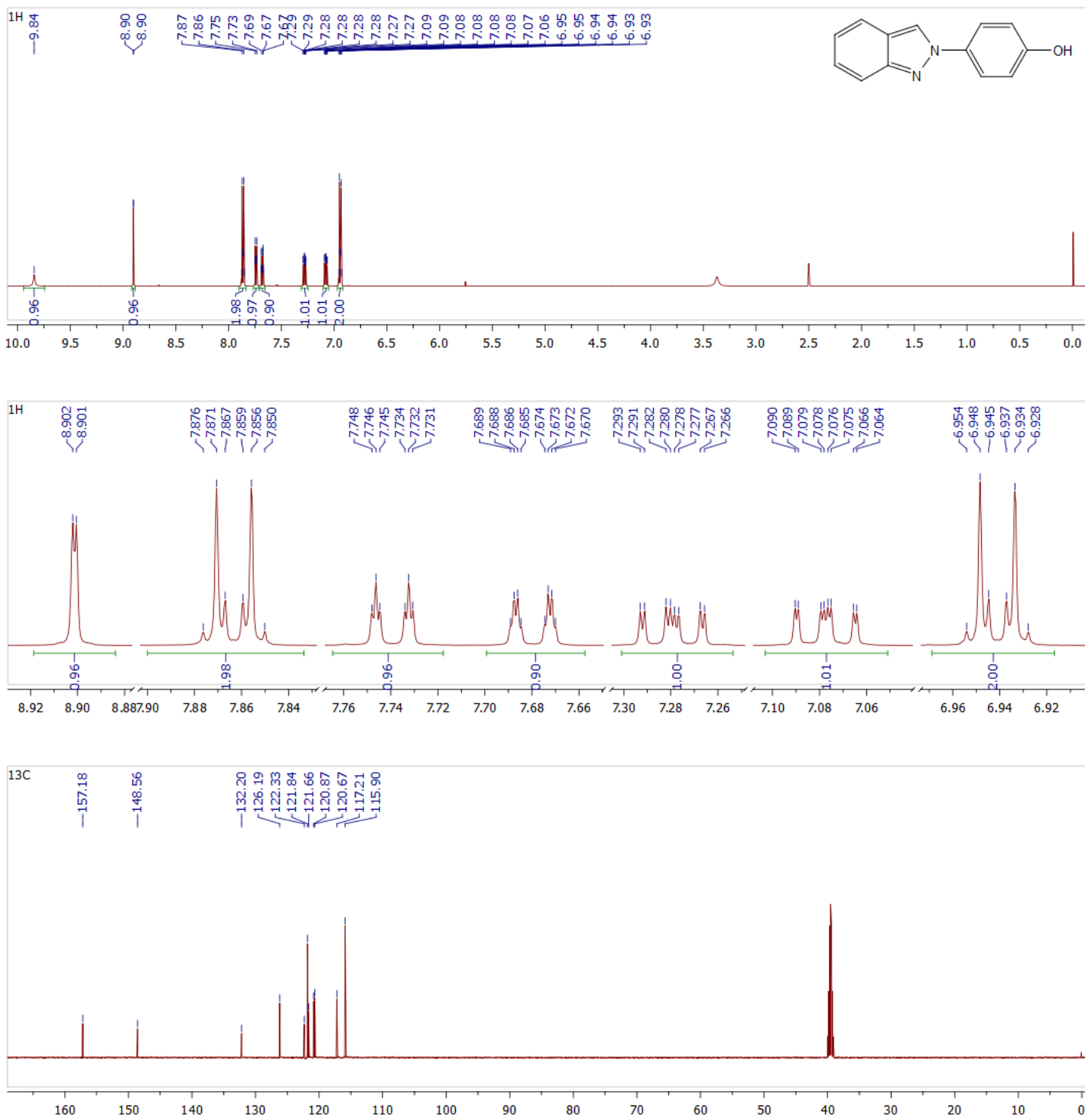


Figure S7. ¹H NMR (600 MHz, DMSO-*d*₆) and ¹³C NMR (151 MHz, DMSO-*d*₆) for 4-(2*H*-indazol-2-yl)phenol (**7**).

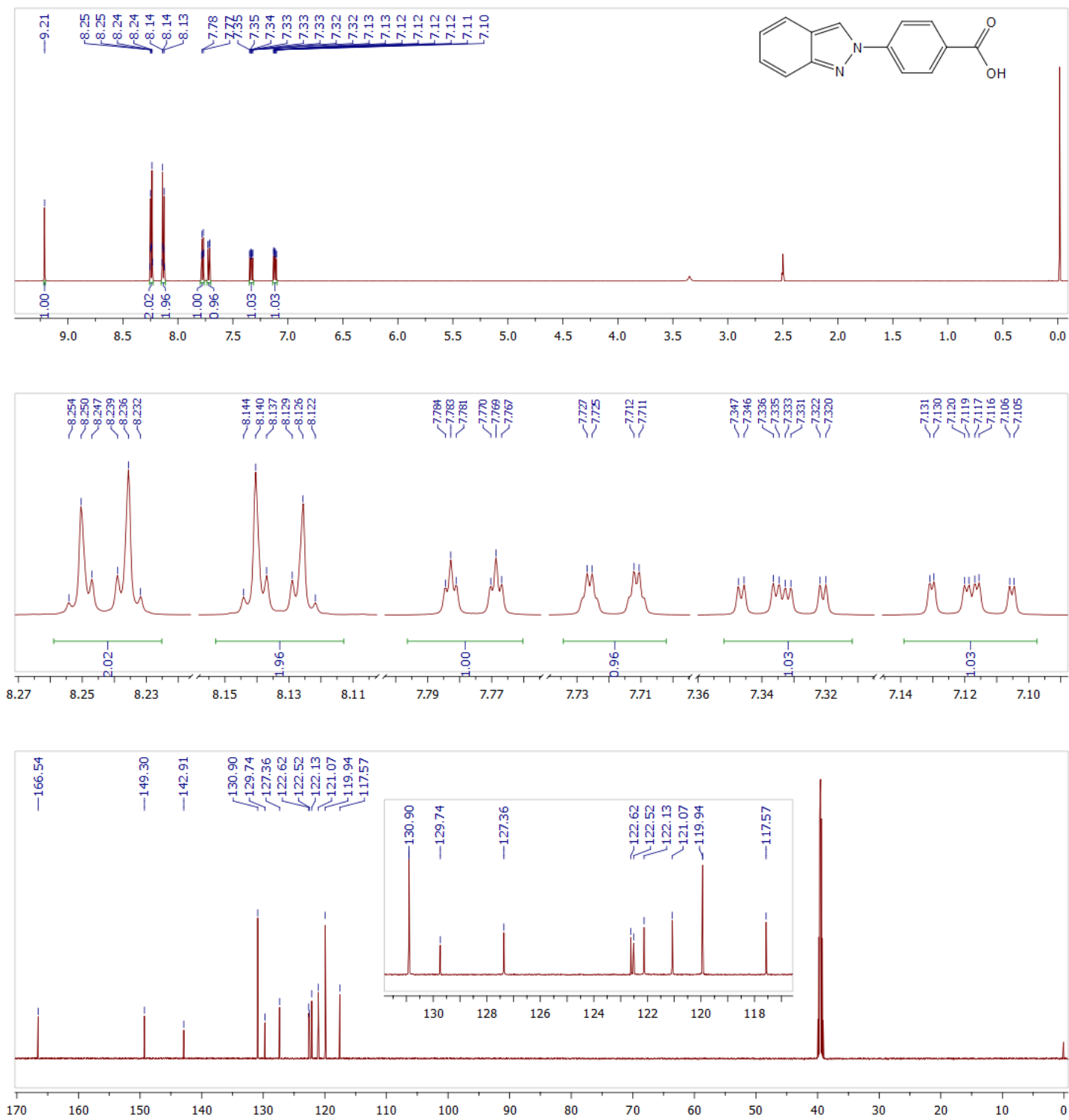


Figure S8. ¹H NMR (600 MHz, DMSO-*d*₆) and ¹³C NMR (151 MHz, DMSO-*d*₆) for 4-(2*H*-indazol-2-yl) benzoic acid (**8**).

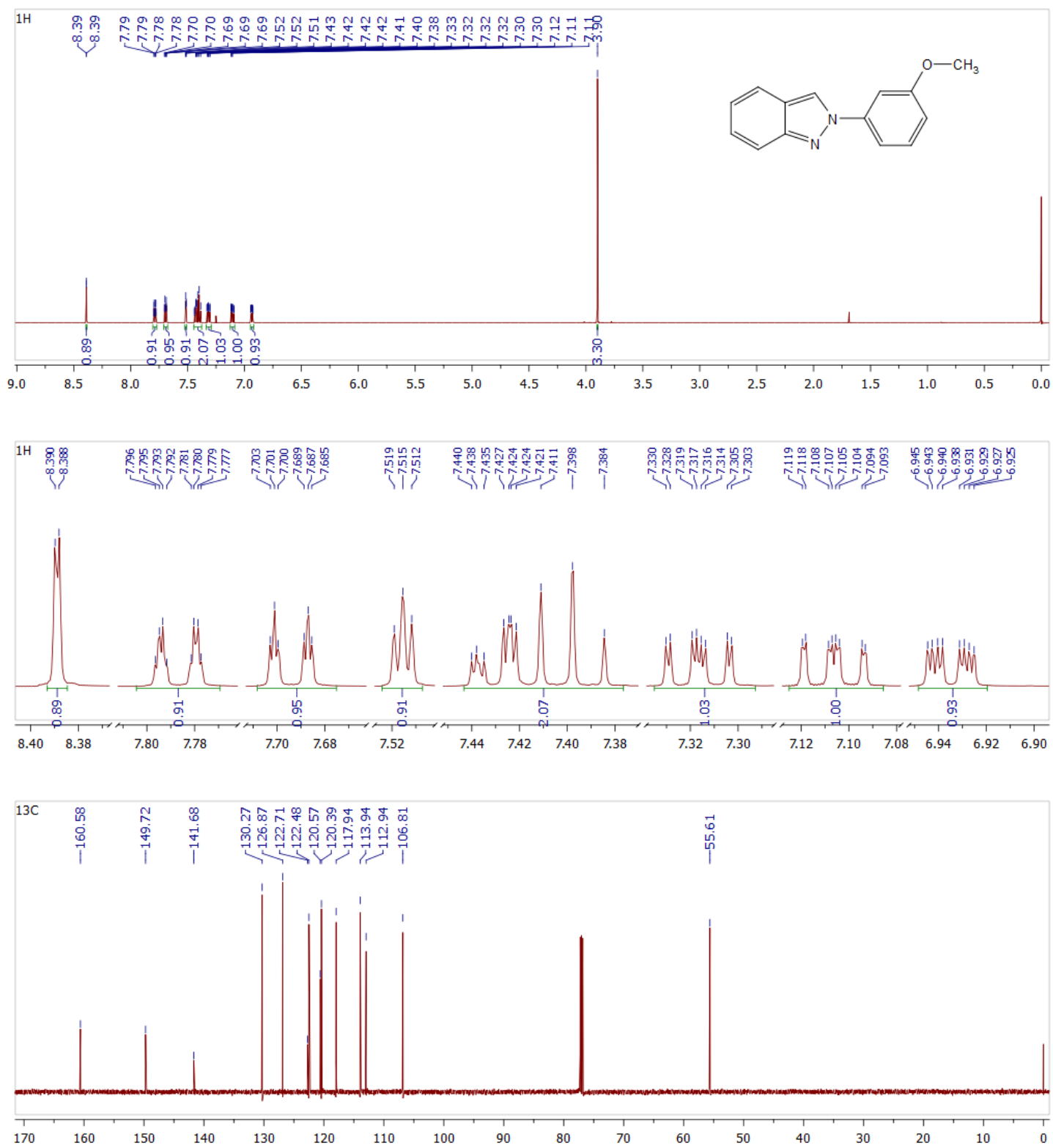


Figure S10. ¹H NMR (600 MHz, CDCl₃) and ¹³C NMR (151 MHz, CDCl₃) for 2-(3-methoxyphenyl)-2H-indazole (**10**).

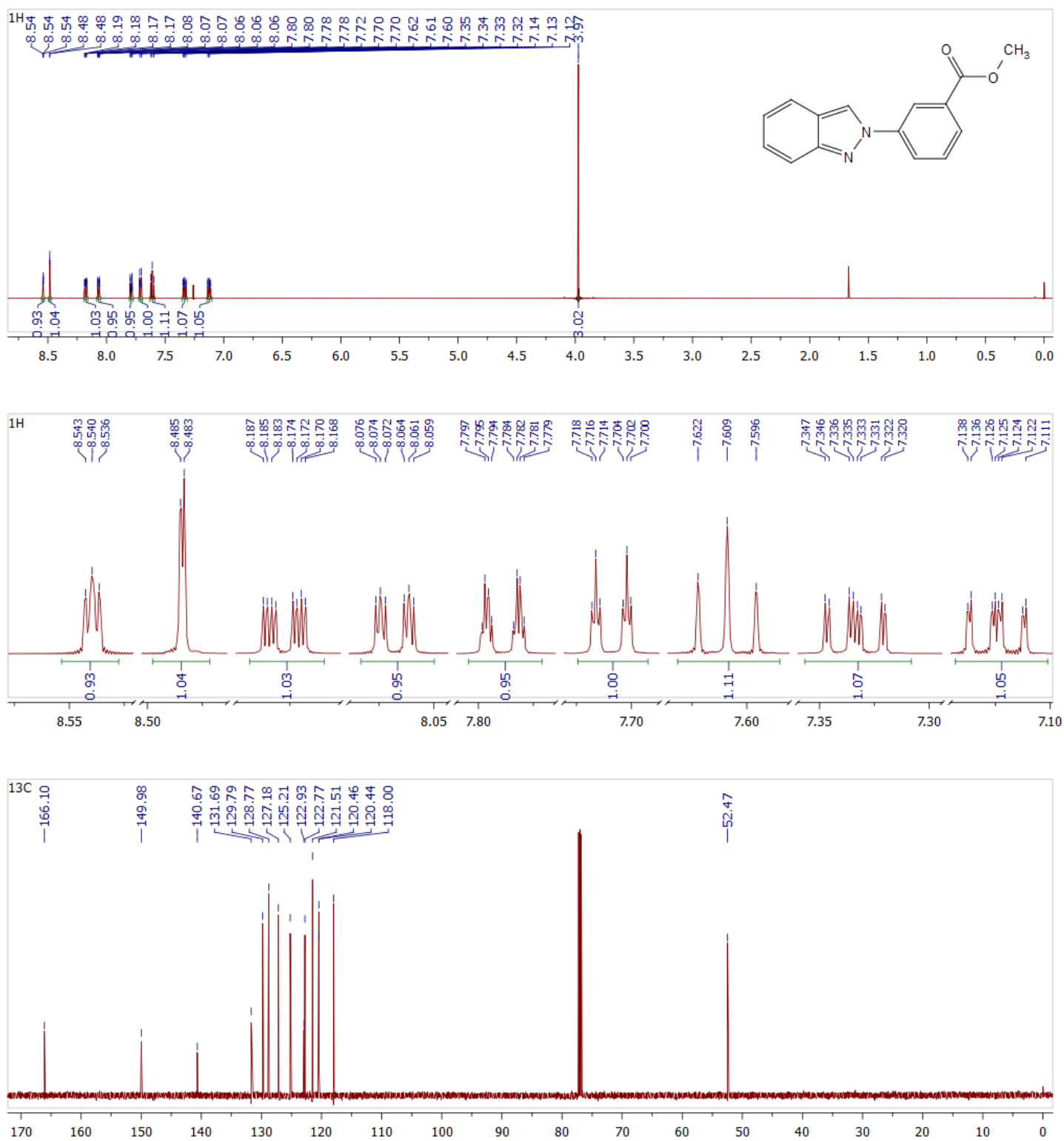


Figure S11. ¹H NMR (600 MHz, CDCl₃) and ¹³C NMR (151 MHz, CDCl₃) for methyl 3-(2H-indazol-2-yl)benzoate (11).

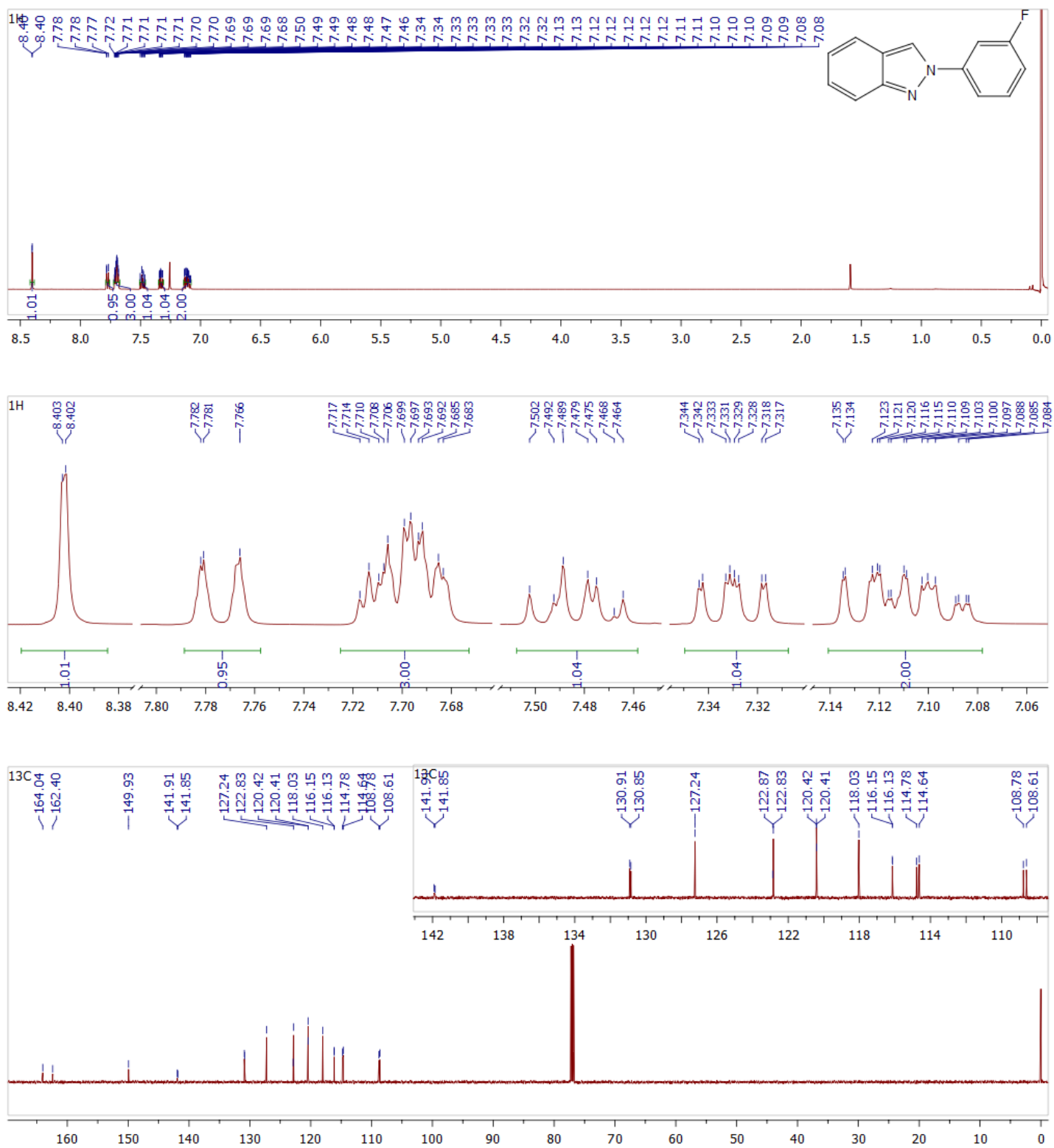


Figure S12. ¹H NMR (600 MHz, CDCl₃) and ¹³C NMR (151 MHz, CDCl₃) for 2-(3-fluorophenyl)-2H-indazole (**12**).

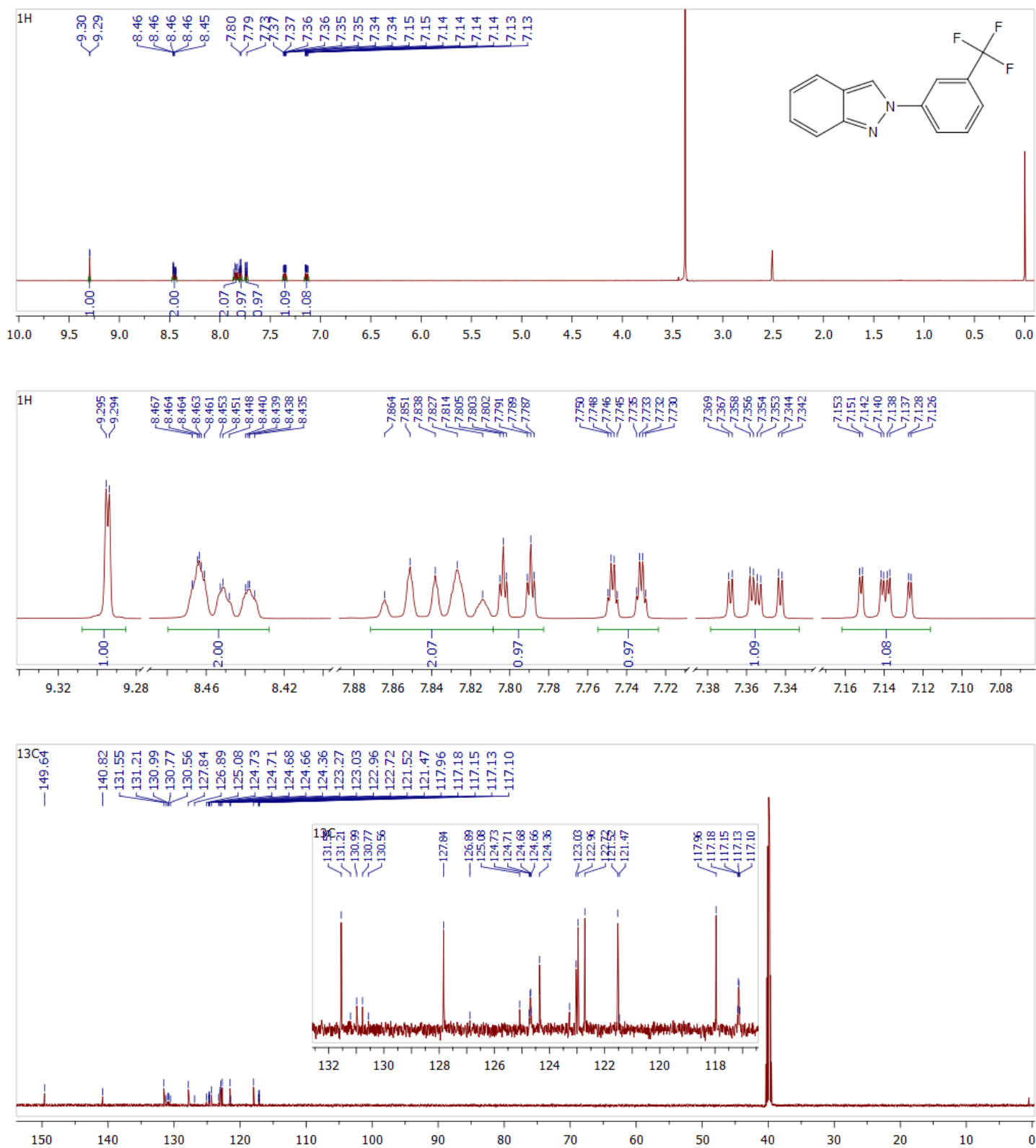


Figure S13. ¹H NMR (600 MHz, DMSO-*d*₆) and ¹³C NMR (151 MHz, DMSO-*d*₆) for 2-[3-(trifluoromethyl)phenyl]-2H-indazole (**13**).

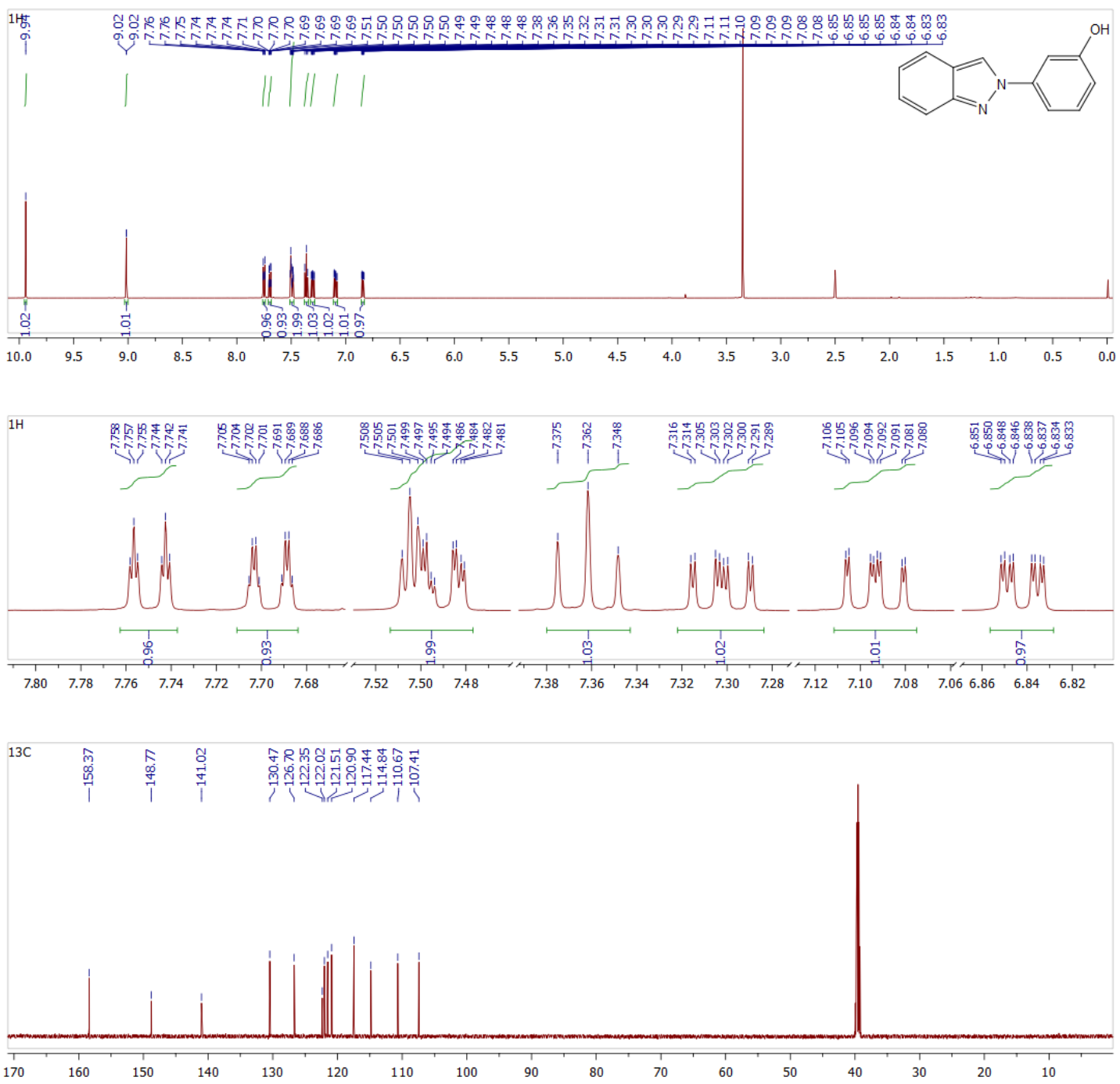


Figure S14. ¹H NMR (600 MHz, DMSO-*d*₆) and ¹³C NMR (151 MHz, DMSO-*d*₆) for 3-(2H-indazol-2-yl)phenol (**14**).

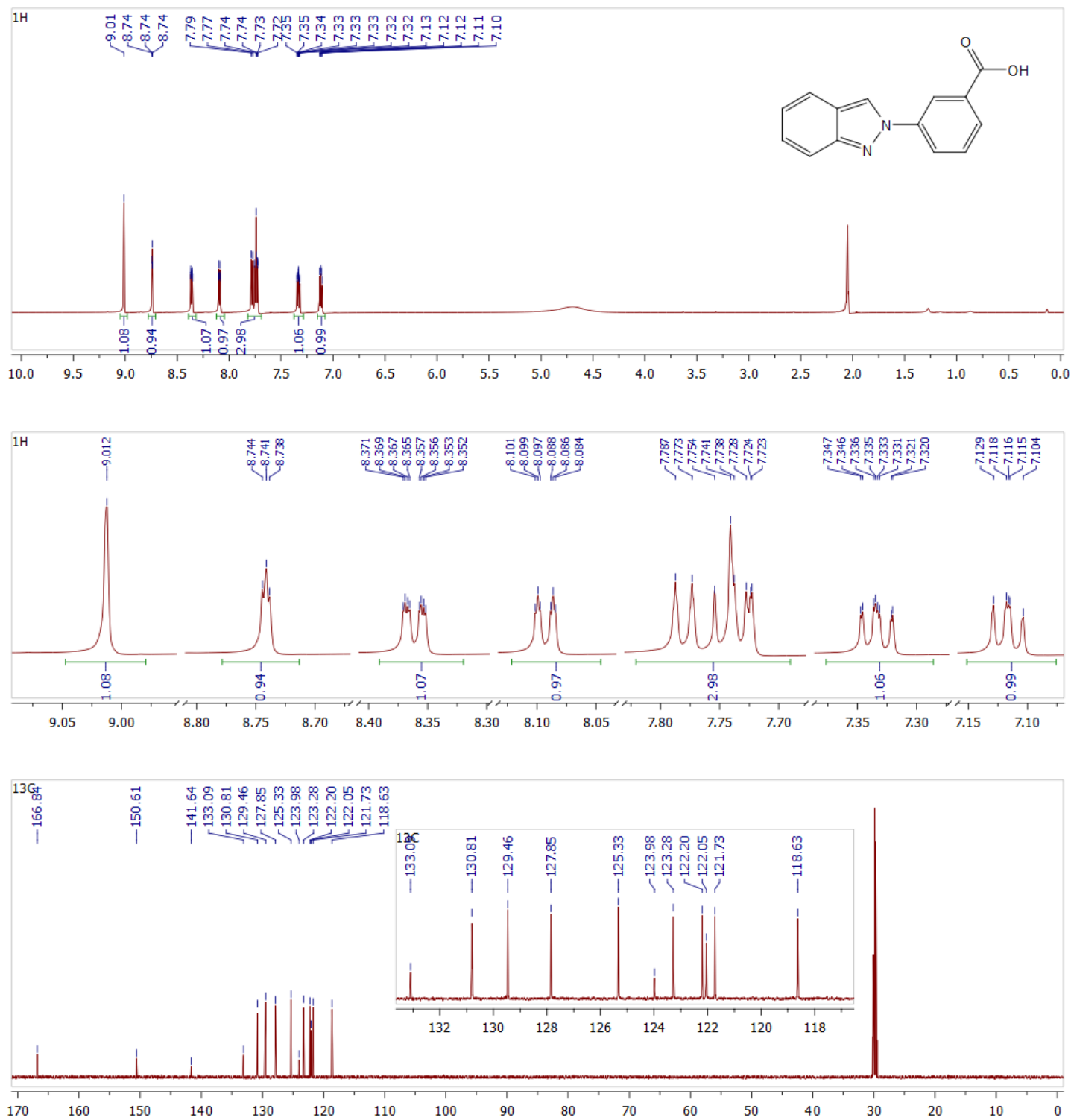


Figure S15. ¹H NMR (600 MHz, acetone-*d*₆) and ¹³C NMR (151 MHz, acetone-*d*₆) for 3-(2*H*-indazol-2-yl)benzoic acid (15).

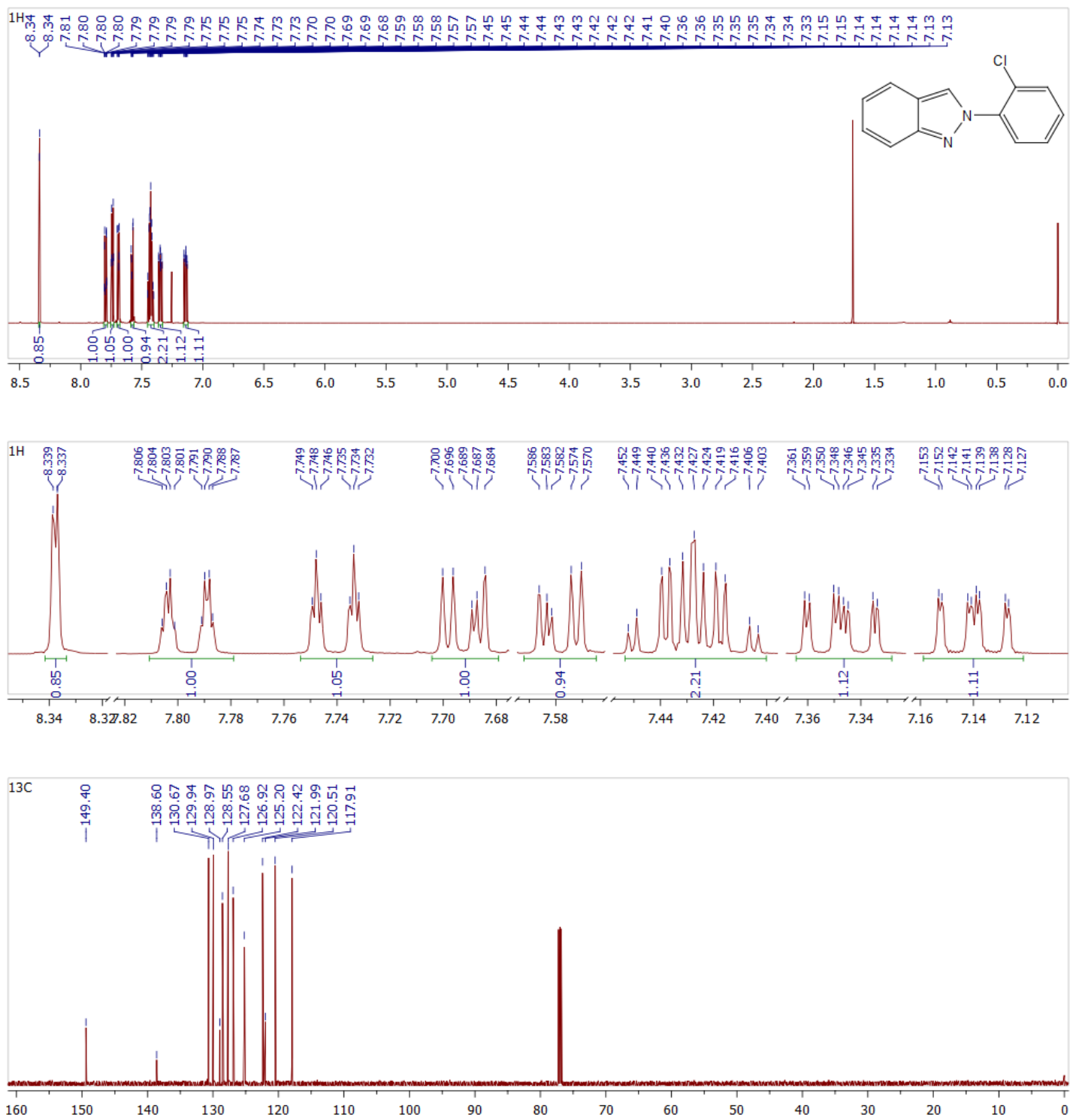


Figure S16. ¹H NMR (600 MHz, CDCl₃) and ¹³C NMR (151 MHz, CDCl₃) for 2-(2-chlorophenyl)-2H-indazole (**16**).

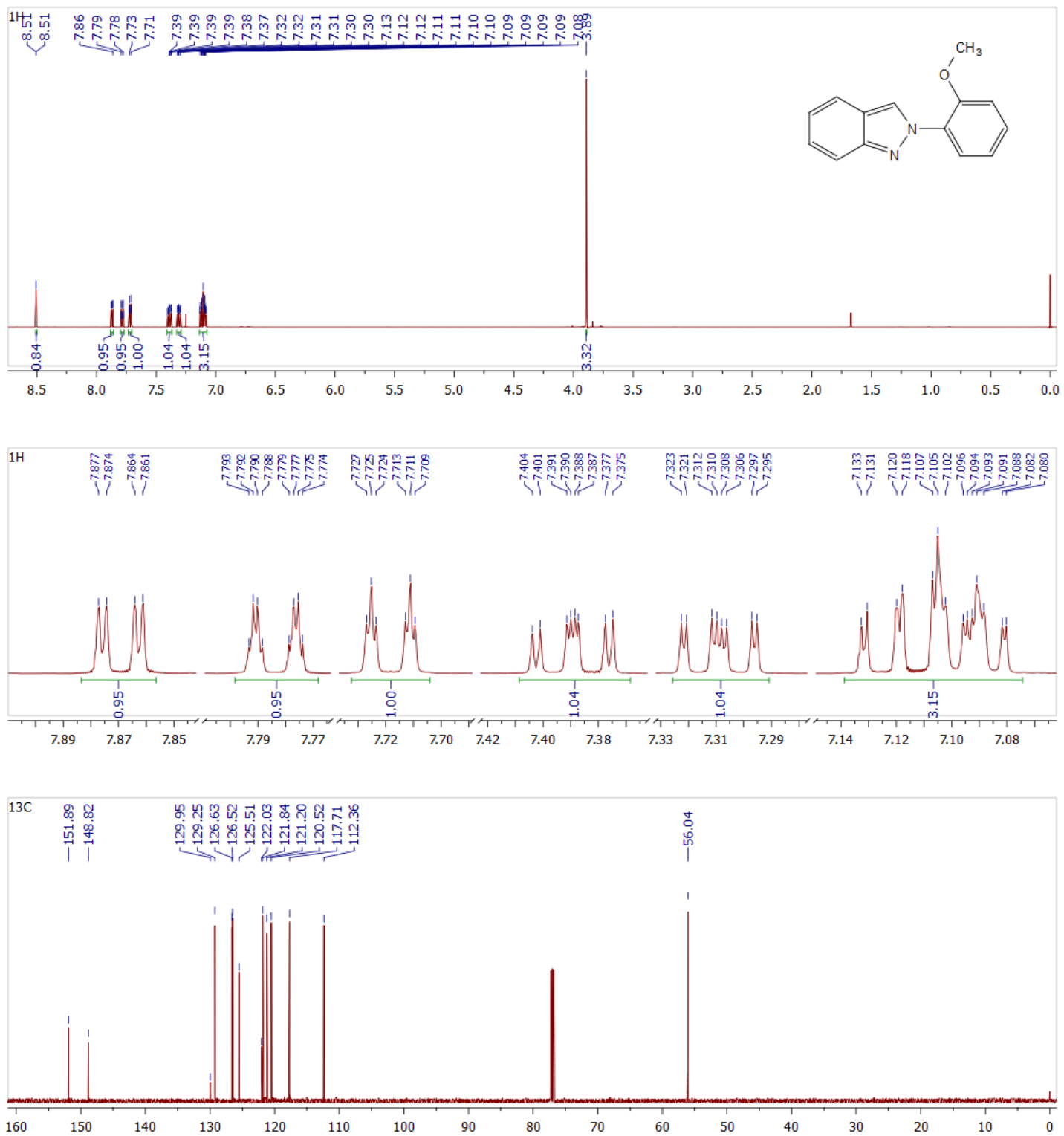


Figure S17. ¹H NMR (600 MHz, CDCl₃) and ¹³C NMR (151 MHz, CDCl₃) for 2-(2-methoxyphenyl)-2H-indazole (**17**).

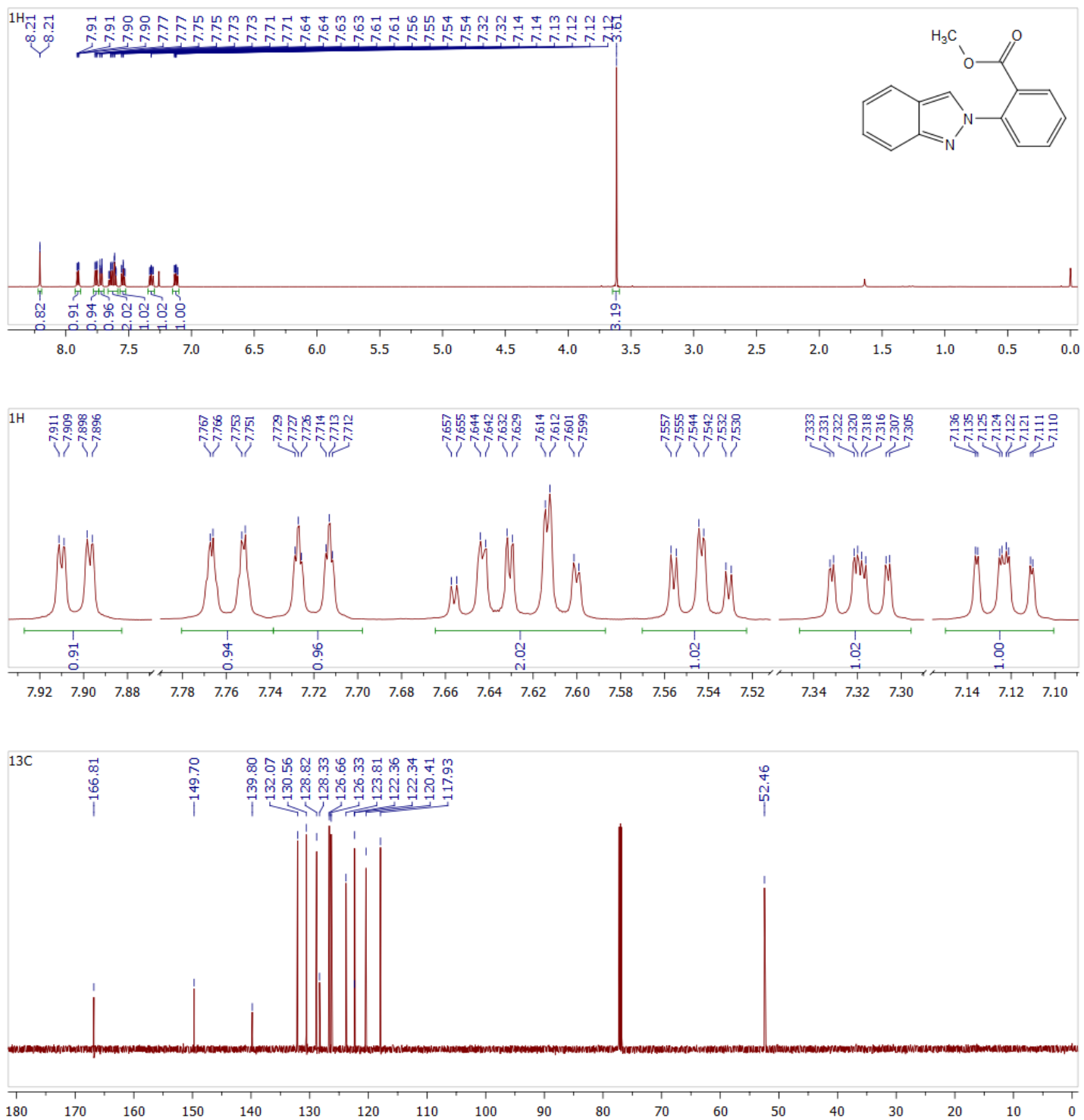


Figure S18. ¹H NMR (600 MHz, CDCl₃) and ¹³C NMR (151 MHz, CDCl₃) for methyl 2-(2H-indazol-2-yl)benzoate (**18**).

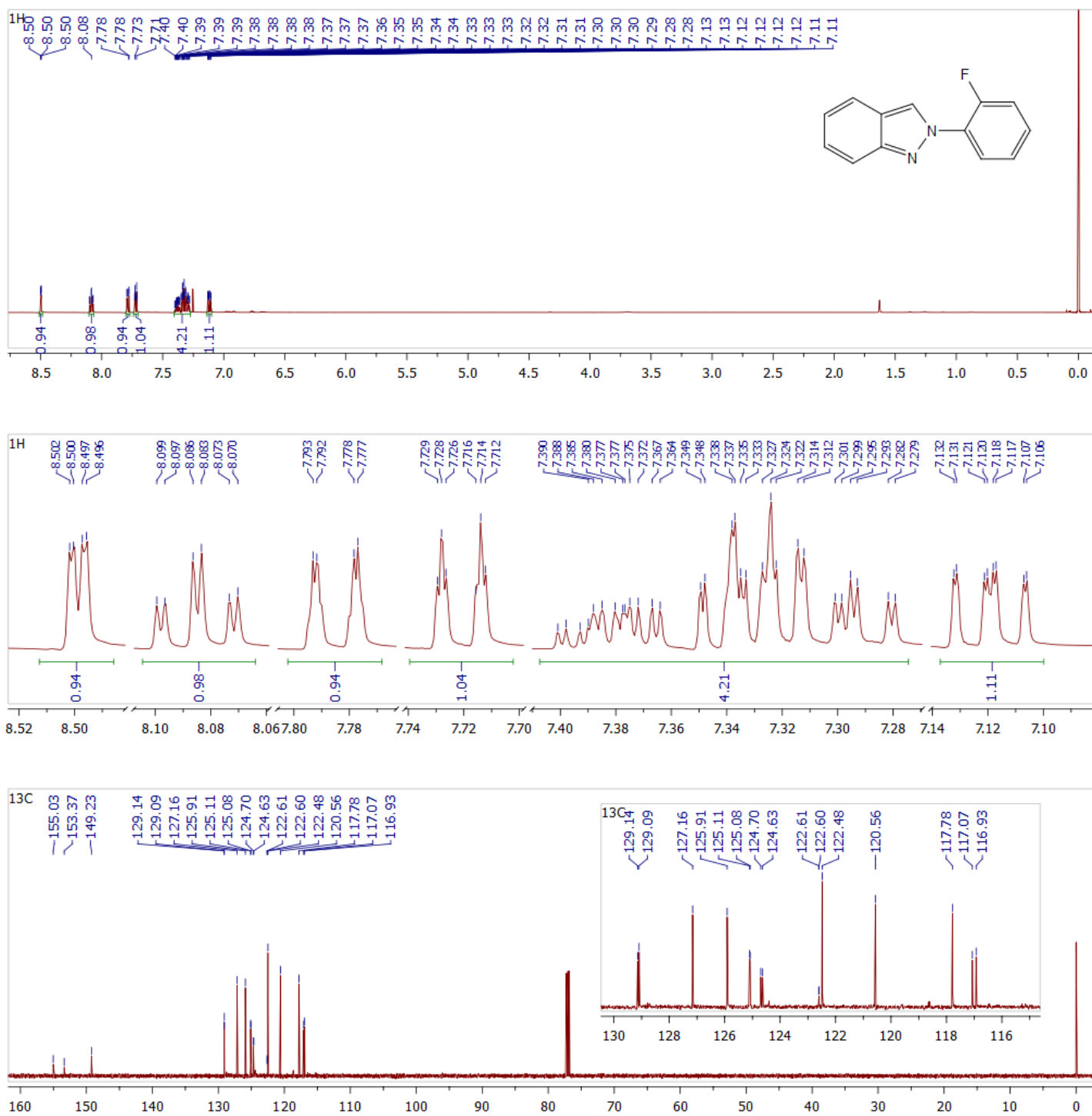


Figure S19. ¹H NMR (600 MHz, CDCl₃) and ¹³C NMR (151 MHz, CDCl₃) for 2-(2-fluorophenyl)-2H-indazole (**19**).

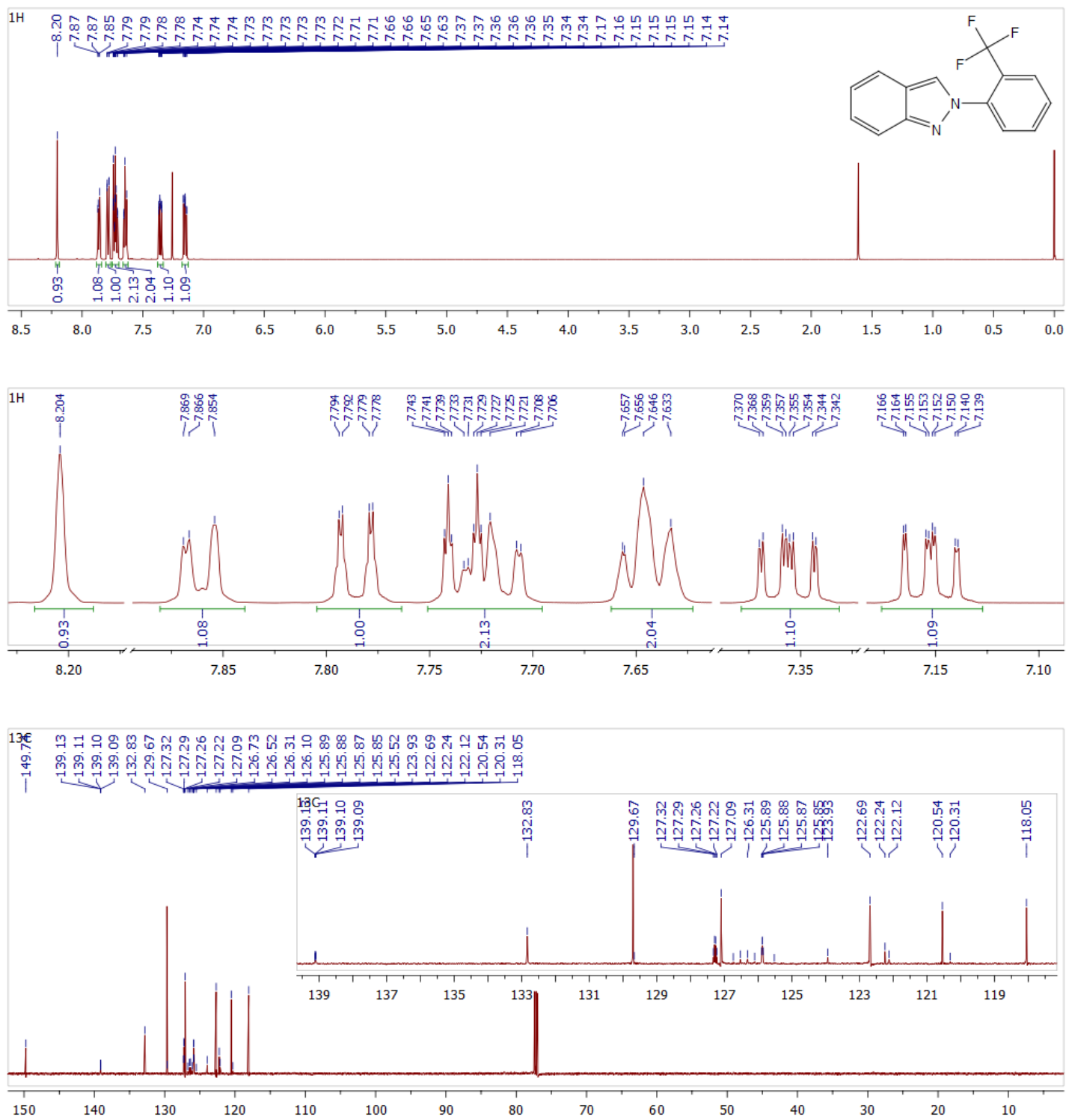


Figure S20. ¹H NMR (600 MHz, CDCl₃) and ¹³C NMR (151 MHz, CDCl₃) for 2-[2-(trifluoromethyl)phenyl]-2H-indazole (20).

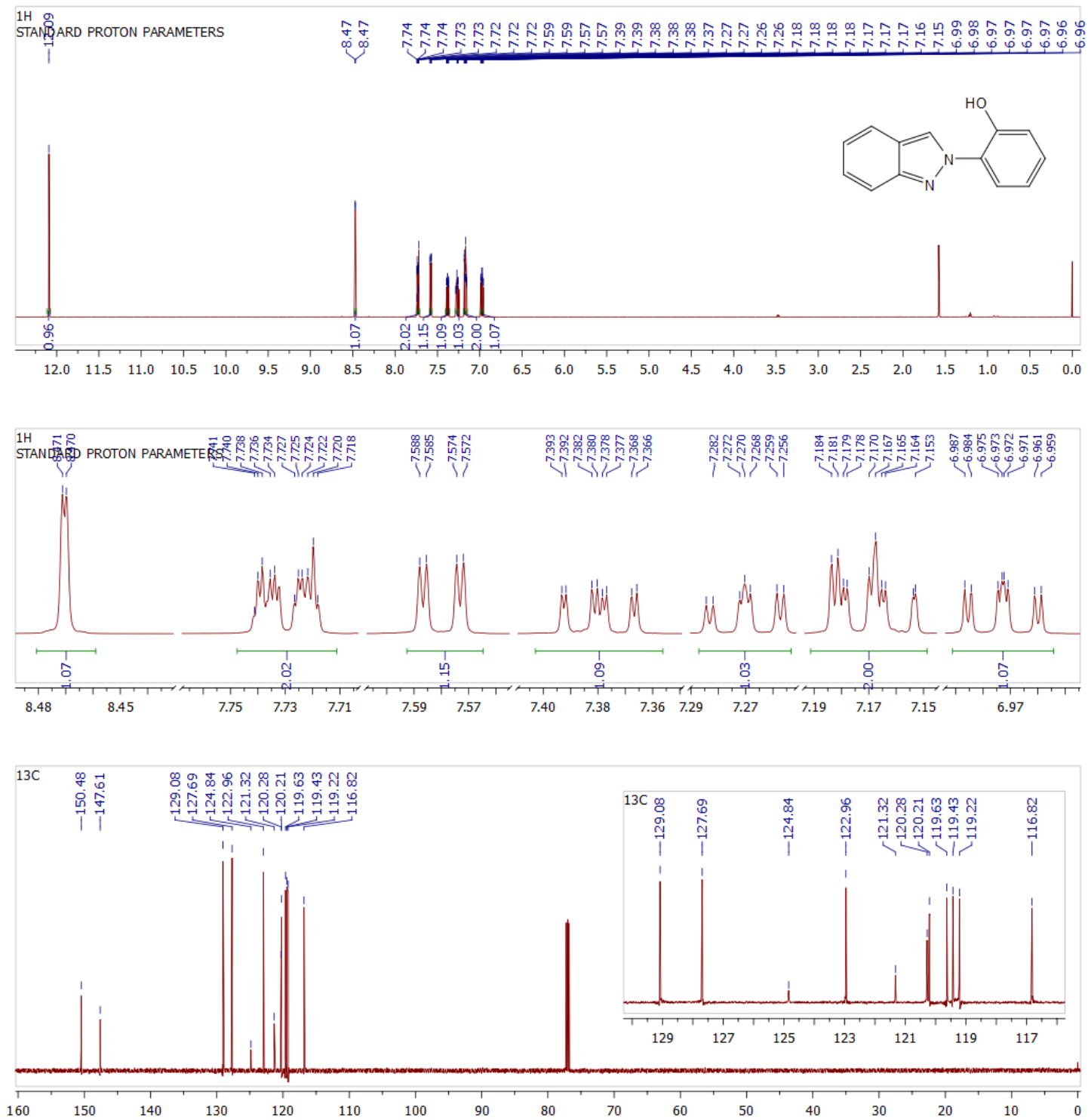


Figure S21. ¹H NMR (600 MHz, CDCl₃) and ¹³C NMR (151 MHz, CDCl₃) for 2-(2*H*-indazol-2-yl)phenol (**21**).

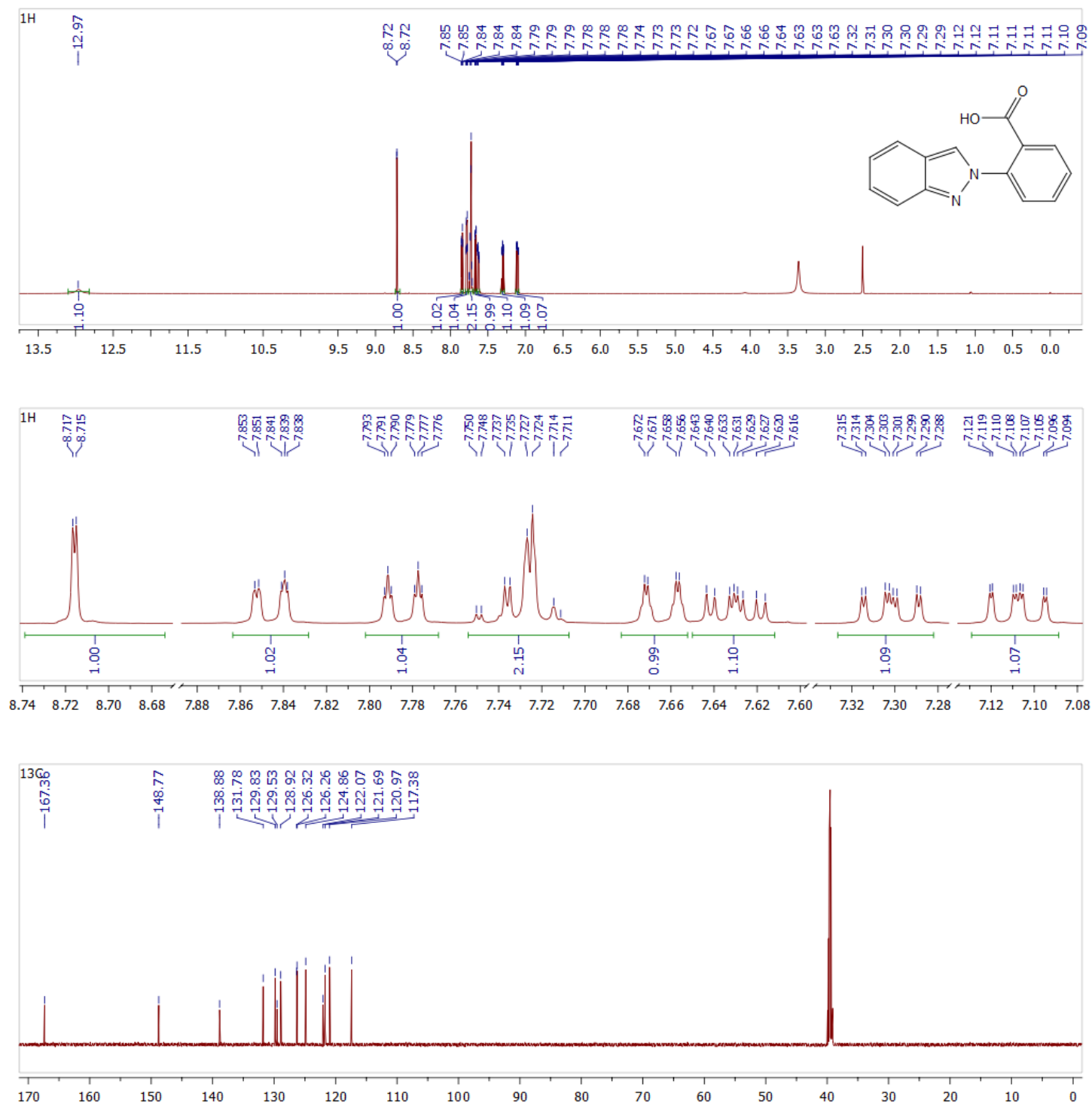


Figure S22. ¹H NMR (600 MHz, DMSO-*d*₆) and ¹³C NMR (151 MHz, DMSO-*d*₆) for 2-(2*H*-indazol-2-yl)benzoic acid (**22**).

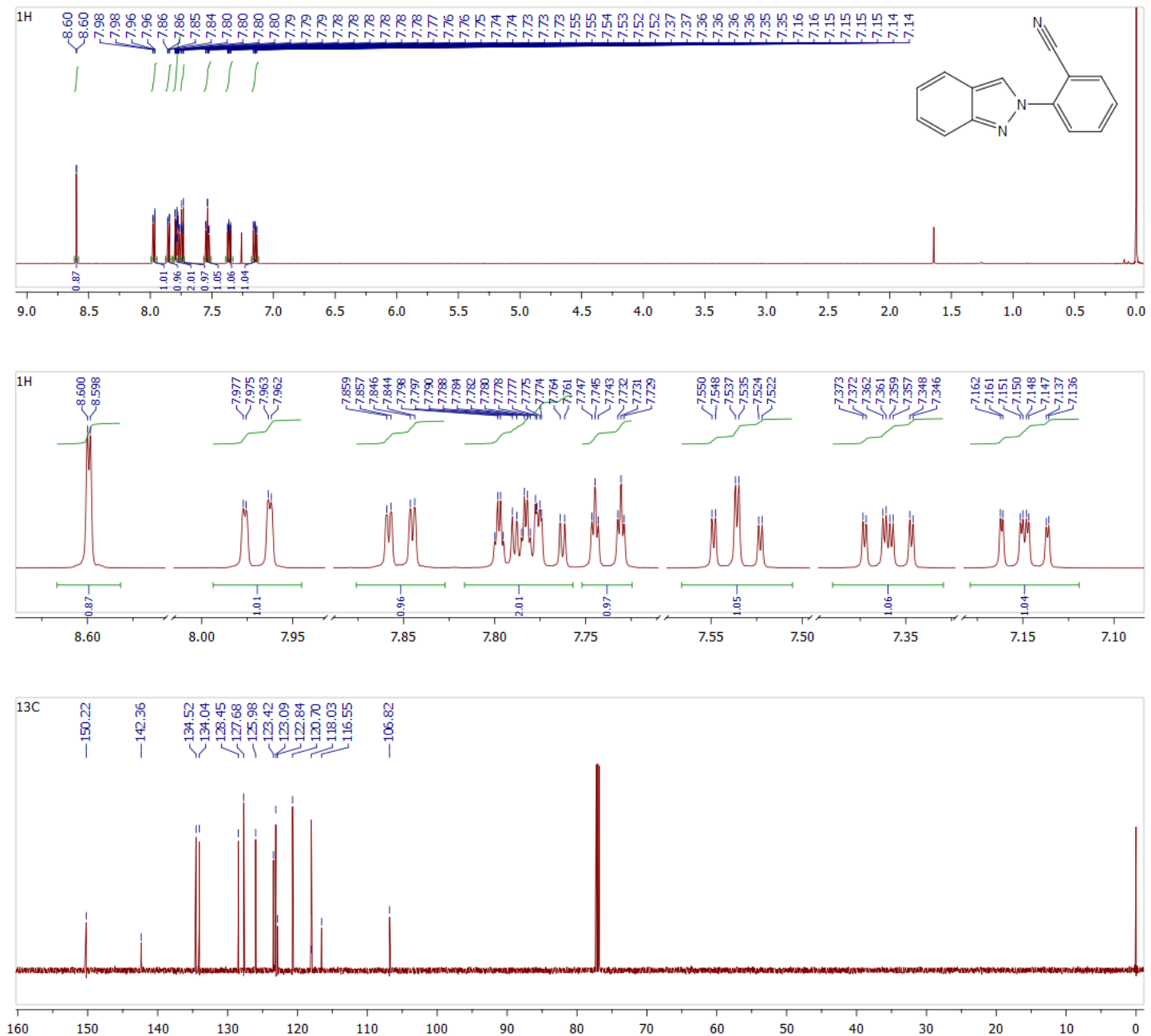


Figure S23. ¹H NMR (600 MHz, CDCl₃) and ¹³C NMR (151 MHz, CDCl₃) for 2-(2*H*-indazol-2-yl)benzotrile (**18a**).