

Biological Activity of Amidino Substituted Imidazo [4,5-*b*]pyridines

Ida Boček Pavlinac¹, Katarina Zlatić², Leentje Persoons³, Dirk Daelemans³, Mihajlo Banjanac⁴, Vedrana Radovanović⁴, Kristina Butković⁵, Marijeta Kralj², and Marijana Hranjec^{1*}

¹Faculty of Chemical Engineering and Technology, University of Zagreb, 10000 Zagreb, Croatia; ²Division of Molecular Medicine, Institute Ruđer Bošković, 10000 Zagreb, Croatia;

³KU Leuven Department of Microbiology, Immunology and Transplantation, Laboratory of Virology and Chemotherapy, Rega Institute, 3000 Leuven, Belgium;

⁴Pharmacology *in vitro*, Selvita Ltd., 10000 Zagreb, Croatia;

⁵Chemistry, Selvita Ltd., 10000 Zagreb, Croatia;

Content

Figures S1-S30: NMR spectra of prepared compounds

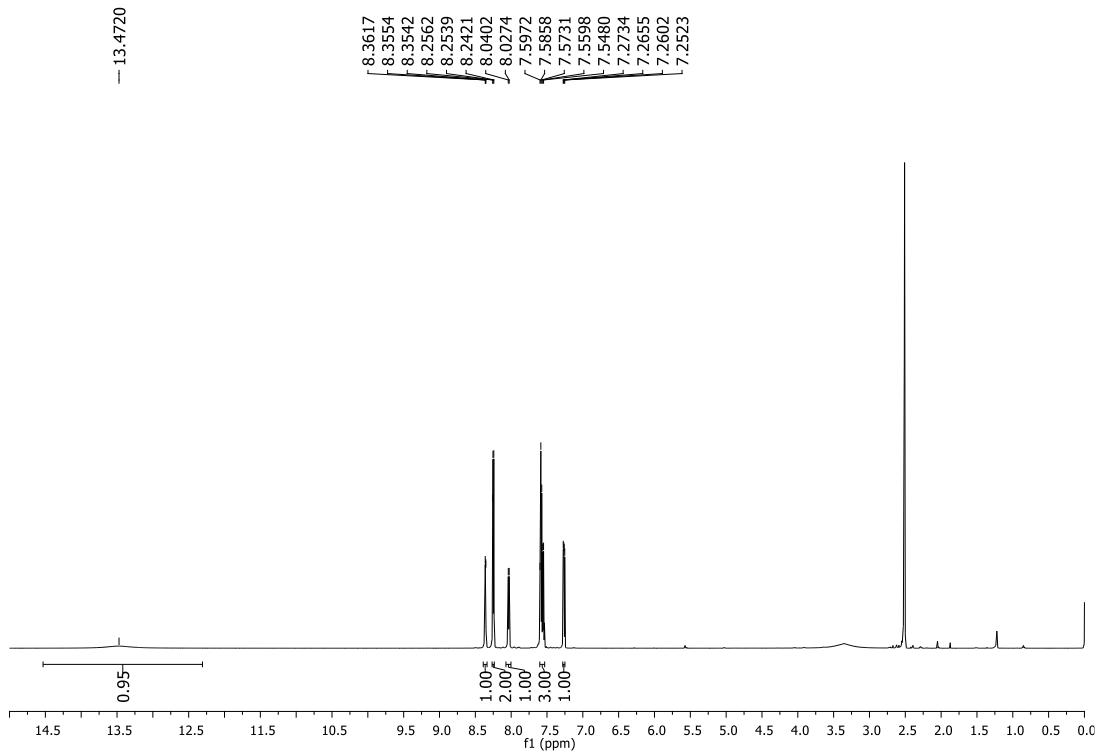


Figure S1. ^1H NMR spectrum (DMSO- d_6 , 300 MHz) of 2-phenyl-1*H*-imidazo[4,5-*b*]pyridine **5**

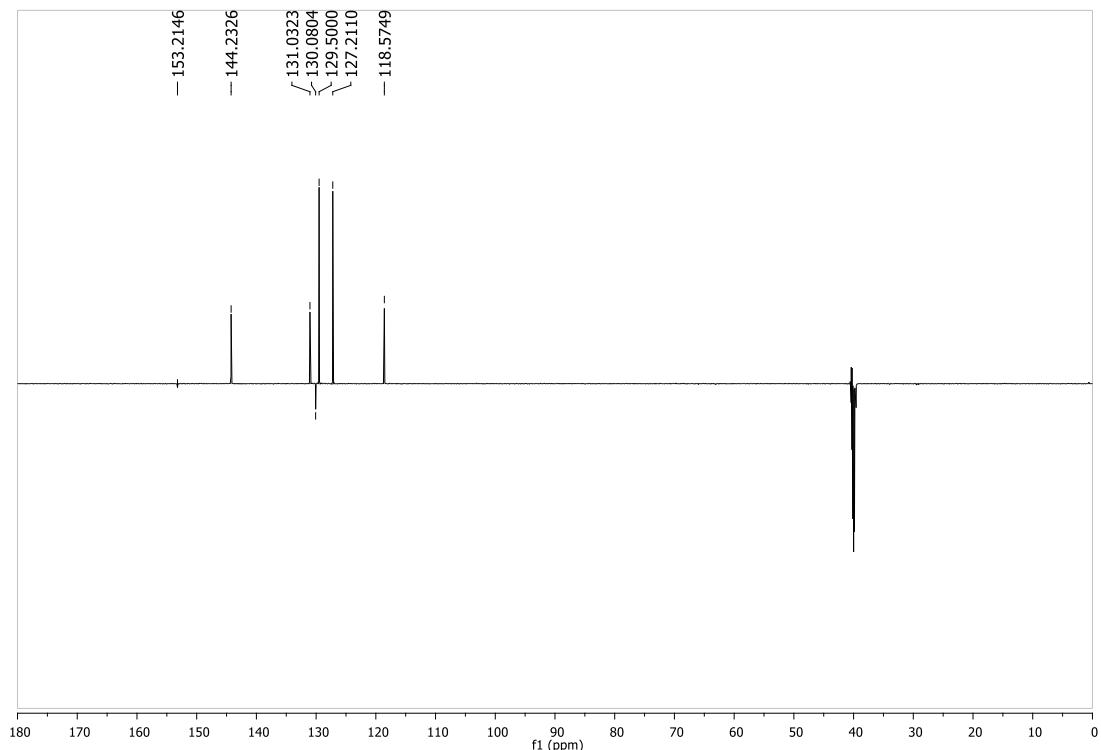


Figure S2. ^{13}C NMR spectrum (DMSO- d_6 , 75 MHz) of 2-phenyl-1*H*-imidazo[4,5-*b*]pyridine **5**

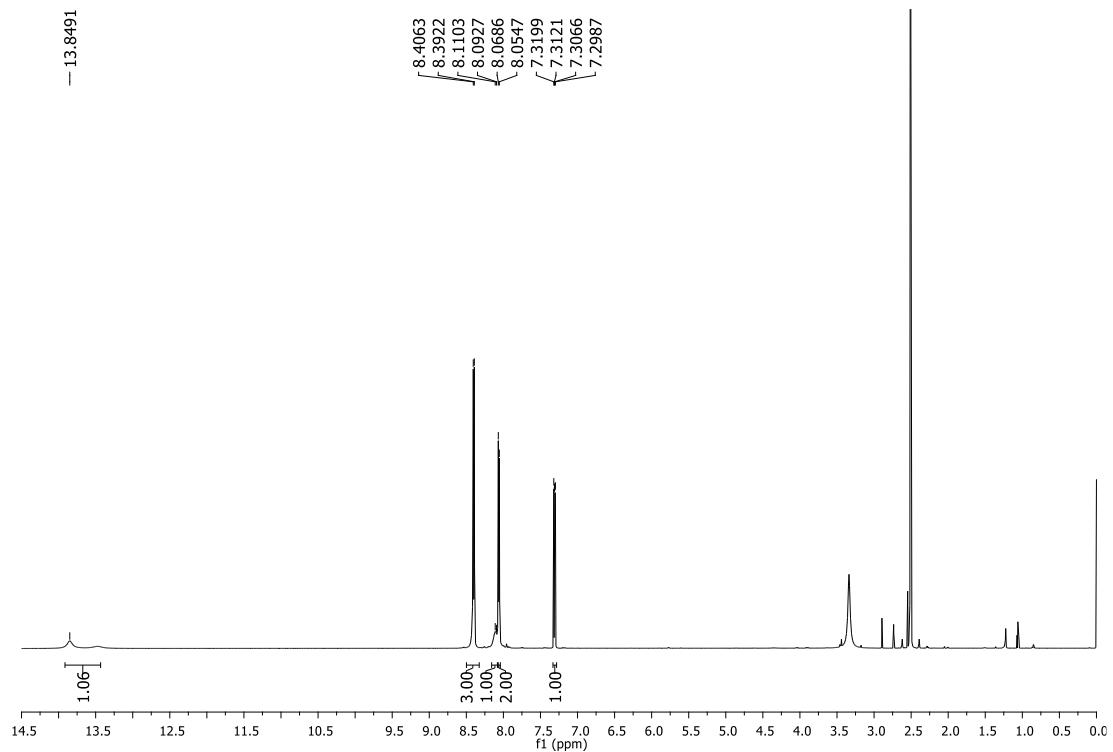


Figure S3. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of 4-(1*H*-imidazo[4,5-*b*]pyridin-2-yl)benzonitrile **6**

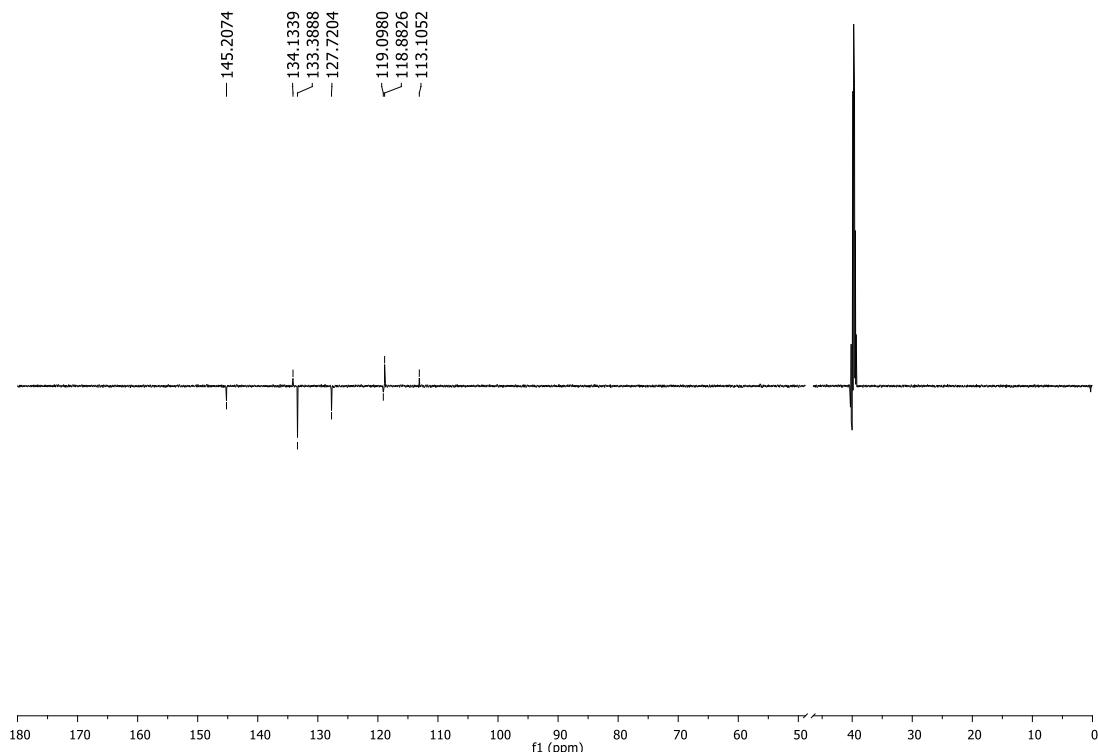


Figure S4. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of 4-(1*H*-imidazo[4,5-*b*]pyridin-2-yl)benzonitrile **6**

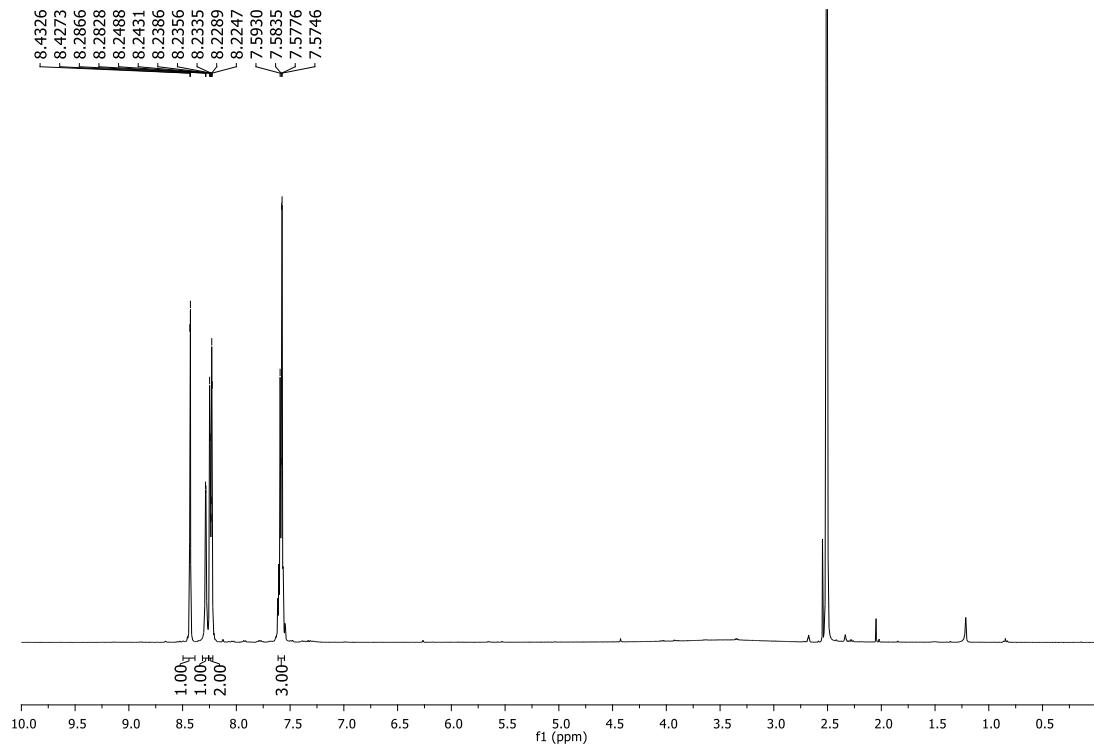


Figure S5. ^1H NMR spectrum (DMSO- d_6 , 400 MHz) of 6-bromo-2-phenyl-1*H*-imidazo[4,5-*b*]pyridine **7**

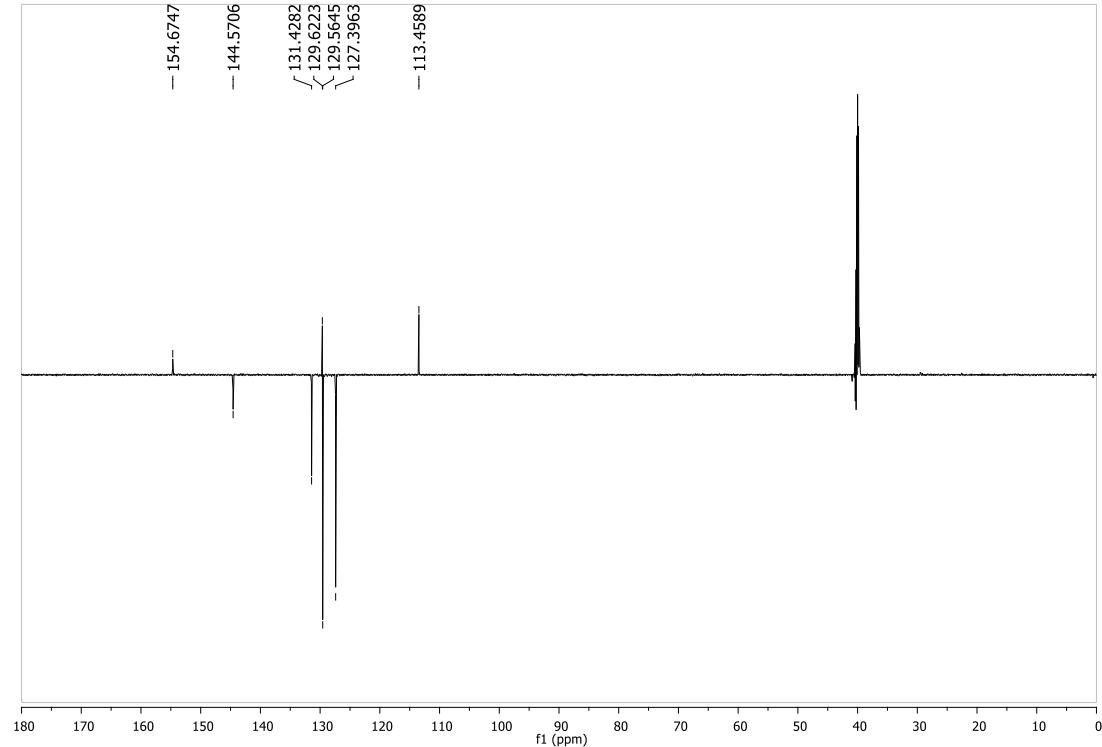


Figure S6. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of 6-bromo-2-phenyl-1*H*-imidazo[4,5-*b*]pyridine **7**

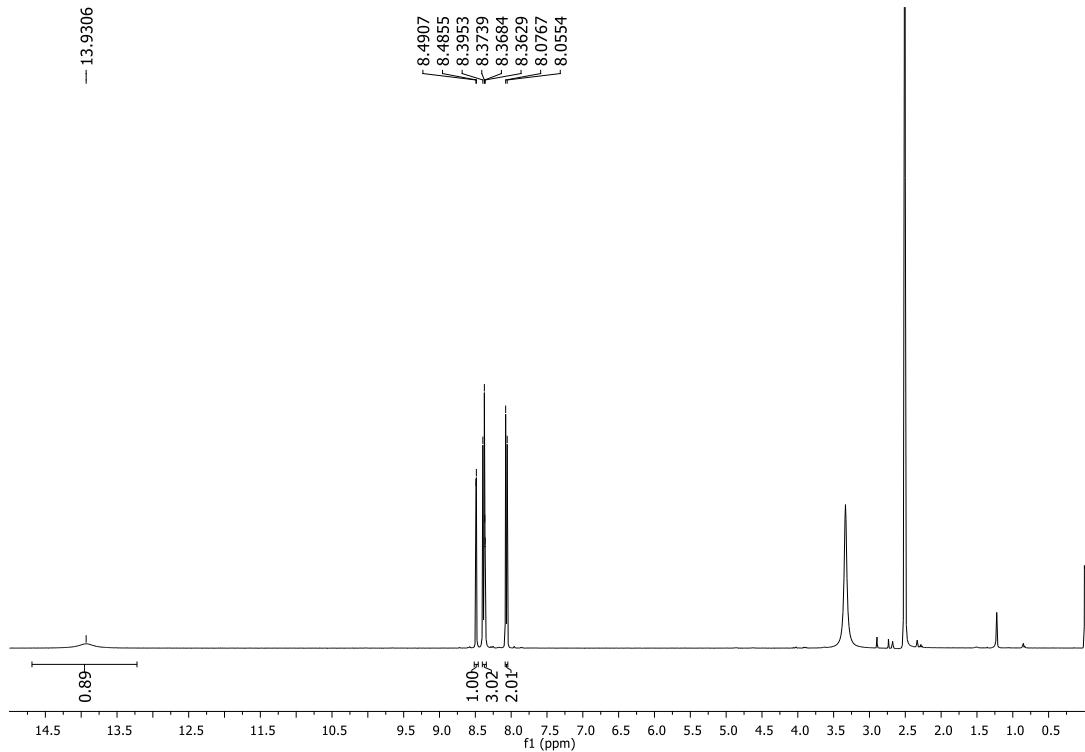


Figure S7. ¹H NMR spectrum (DMSO-*d*₆, 600 MHz) of 4-(6-bromo-1*H*-imidazo[4,5-*b*]pyridin-2-yl)benzonitrile **8**

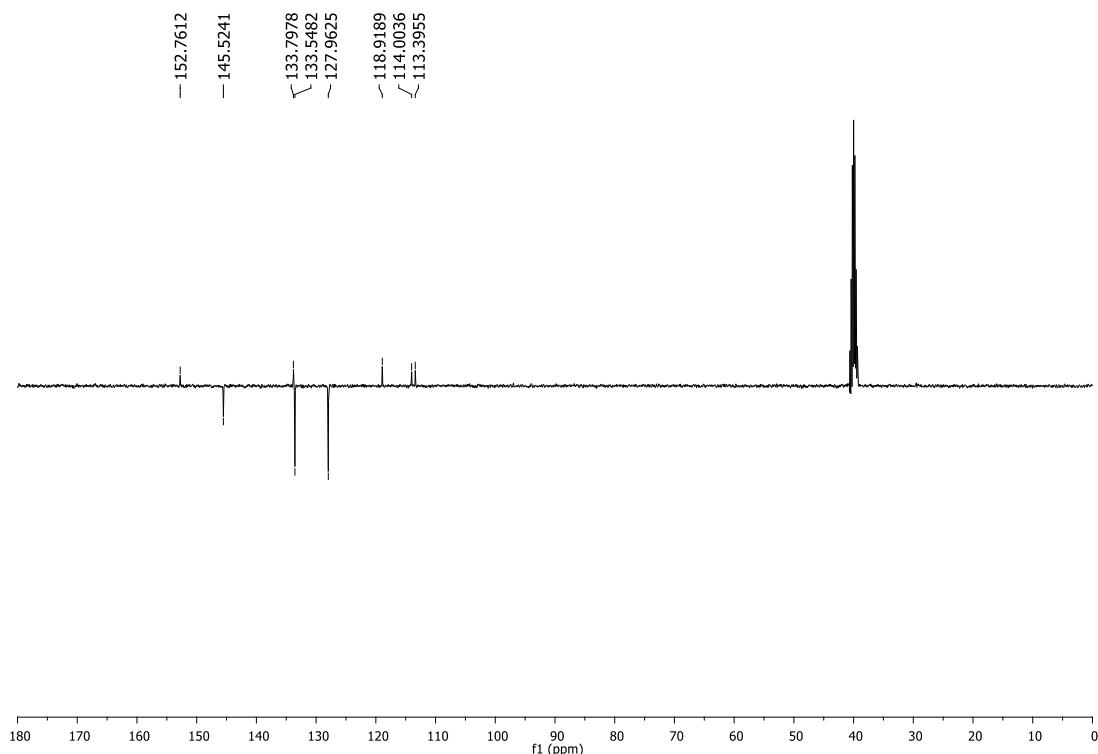


Figure S8. ¹³C NMR spectrum (DMSO-*d*₆, 101 MHz) of 4-(6-bromo-1*H*-imidazo[4,5-*b*]pyridin-2-yl)benzonitrile **8**

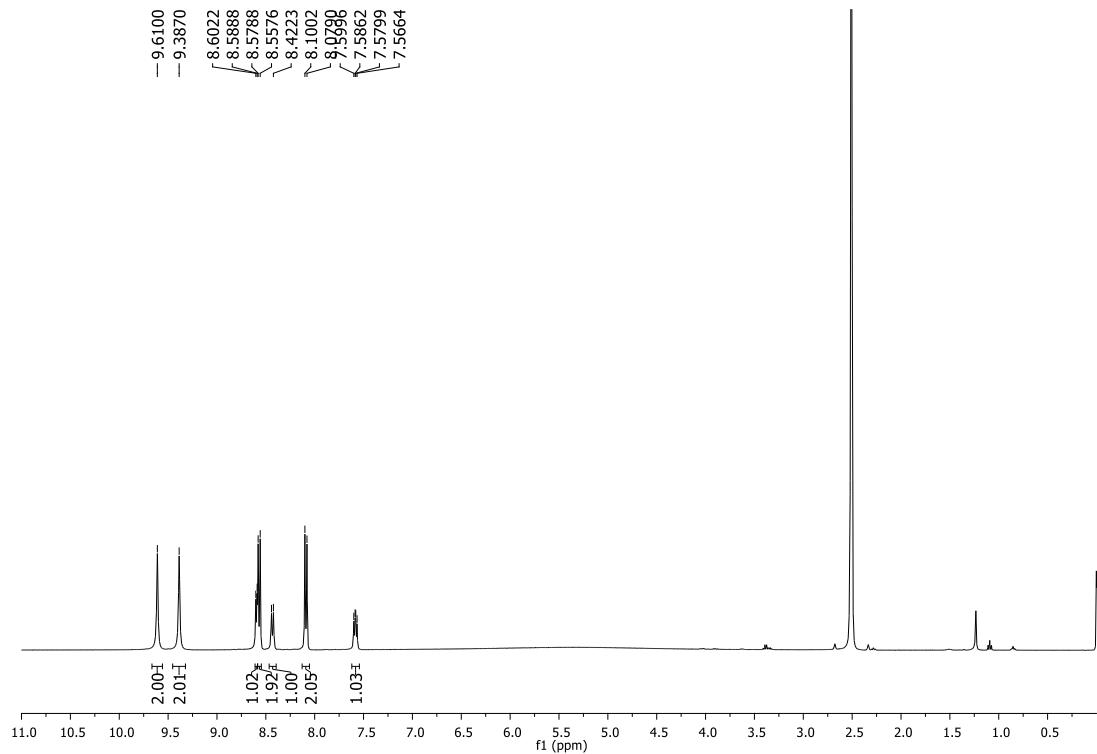


Figure S9. ^1H NMR spectrum (DMSO- d_6 , 400 MHz) of 4-(1*H*-imidazo[4,5-*b*]pyridin-2-yl)benzimidamide hydrochloride **9**

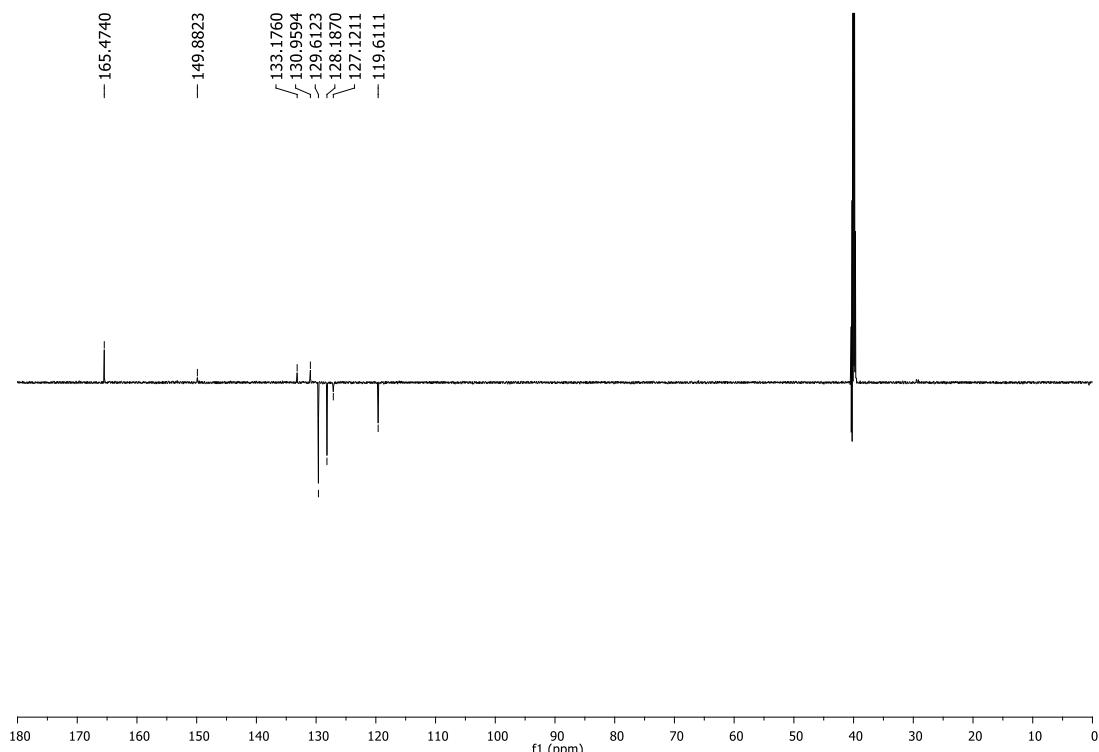


Figure S10. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of 4-(1*H*-imidazo[4,5-*b*]pyridin-2-yl)benzimidamide hydrochloride **9**

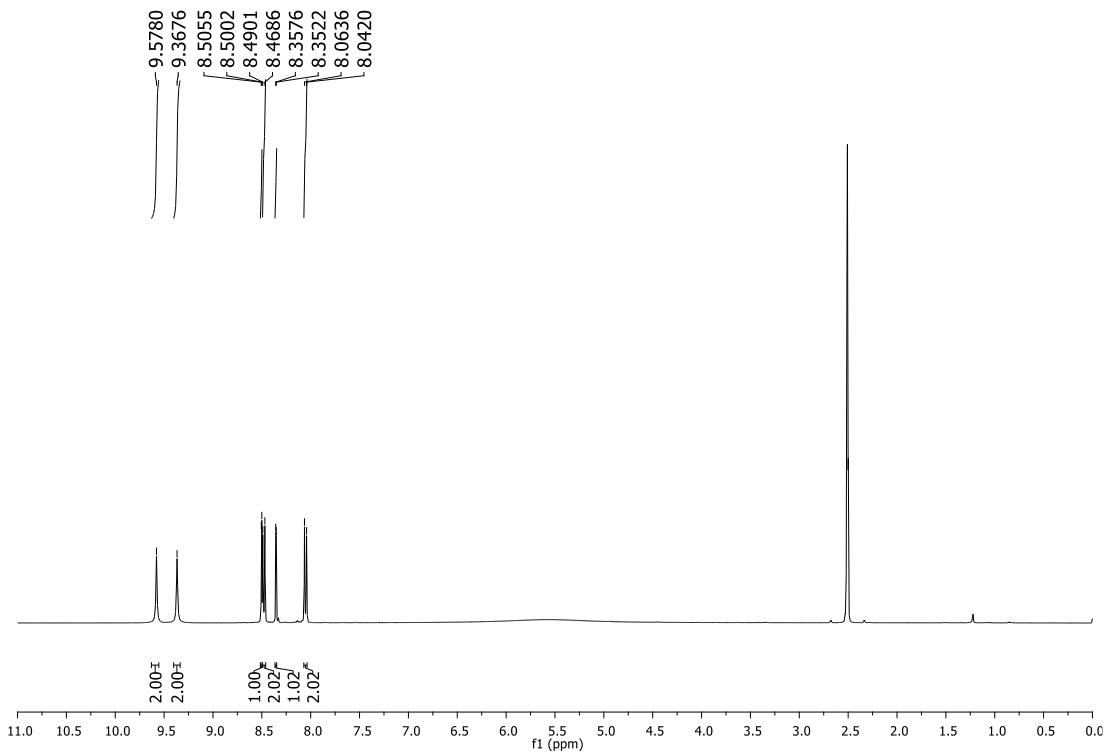


Figure S11. ^1H NMR spectrum (DMSO- d_6 , 400 MHz) of 4-(6-bromo-1*H*-imidazo[4,5-*b*]pyridin-2-yl)benzimidamide hydrochloride **10**

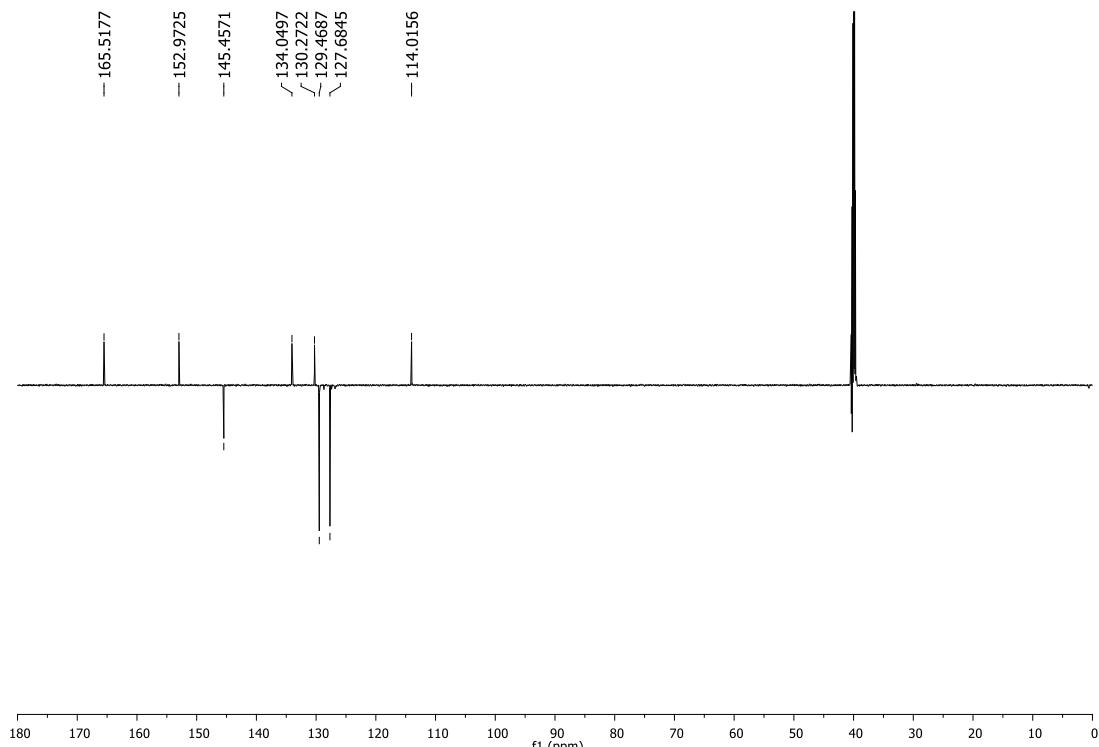


Figure S12. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of 4-(6-bromo-1*H*-imidazo[4,5-*b*]pyridin-2-yl)benzimidamide hydrochloride **10**

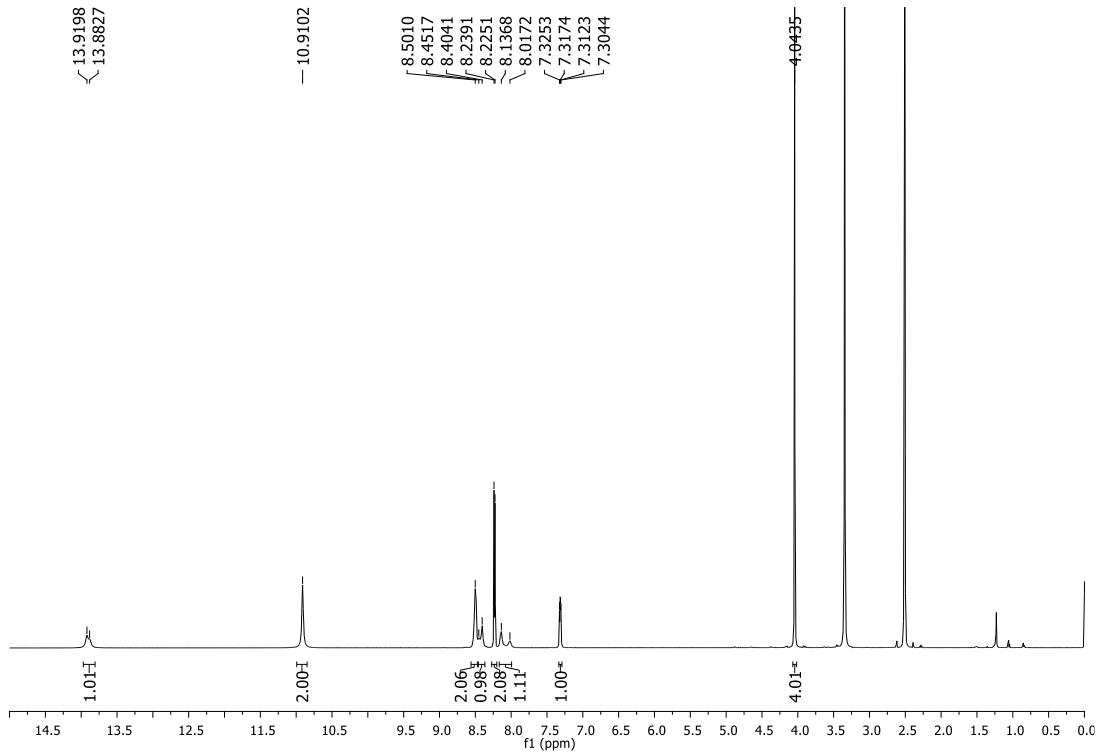


Figure S13. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of 2-(4-(4,5-dihydro-1*H*-imidazol-2-yl)phenyl)-1*H*-imidazo[4,5-*b*]pyridine hydrochloride **11**

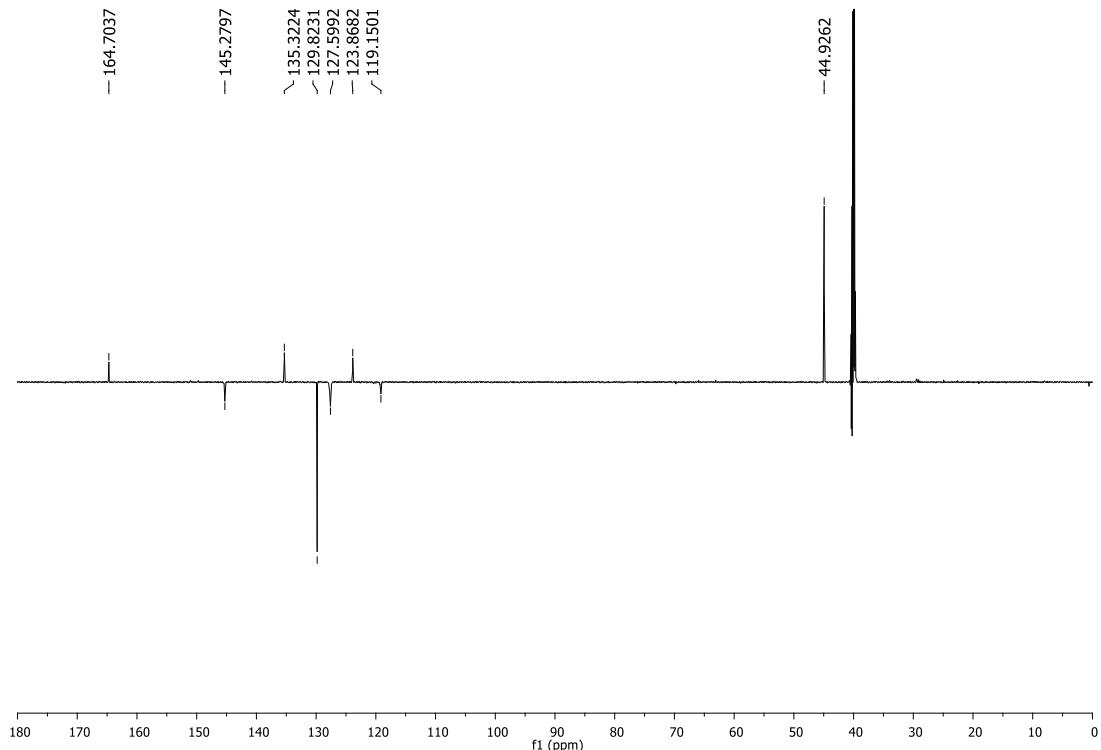


Figure S14. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of 2-(4-(4,5-dihydro-1*H*-imidazol-2-yl)phenyl)-1*H*-imidazo[4,5-*b*]pyridine hydrochloride **11**

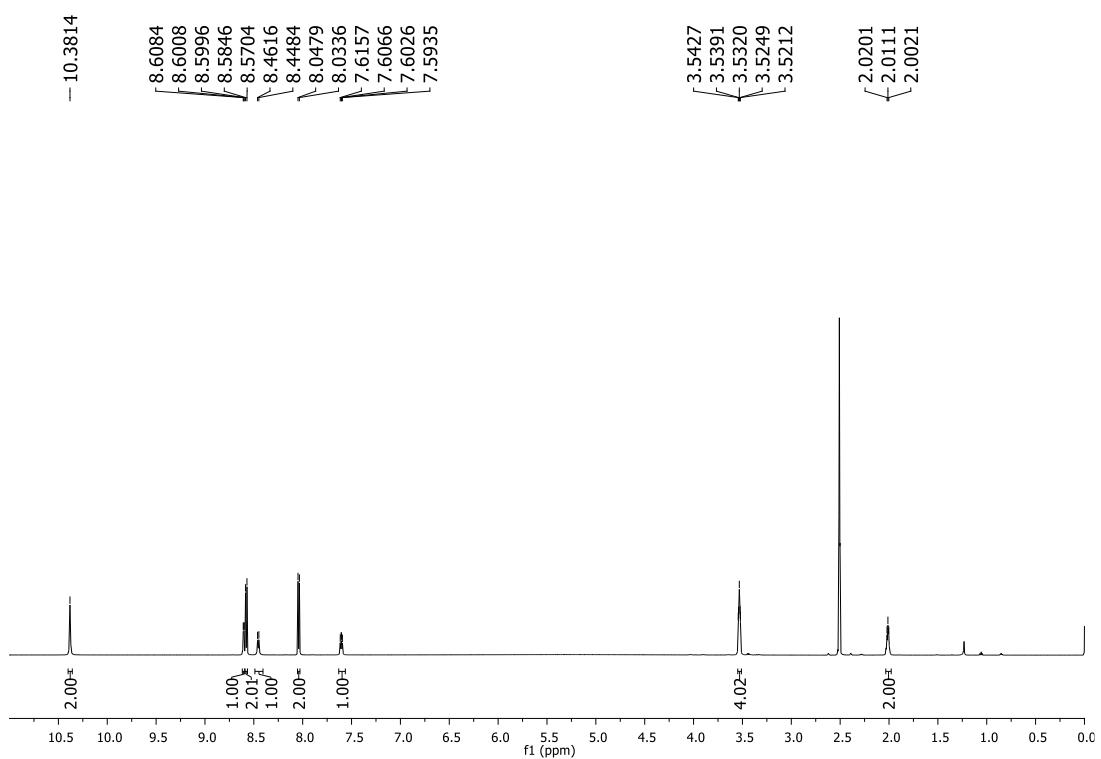


Figure S15. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of 2-(4-(1*H*-imidazo[4,5-*b*]pyridin-2-yl)phenyl)-3,4,5,6-tetrahydropyrimidin-1-i um chloride **12**

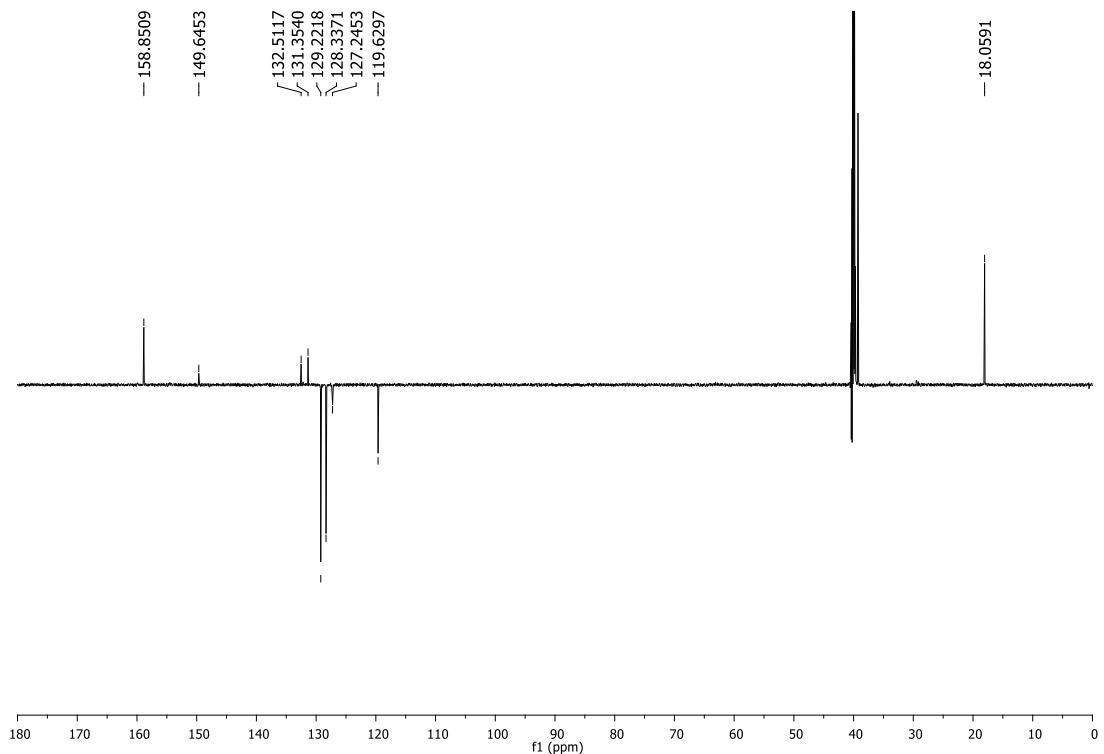


Figure S16. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of 2-(4-(1*H*-imidazo[4,5-*b*]pyridin-2-yl)phenyl)-3,4,5,6-tetrahydropyrimidin-1-i um chloride **12**

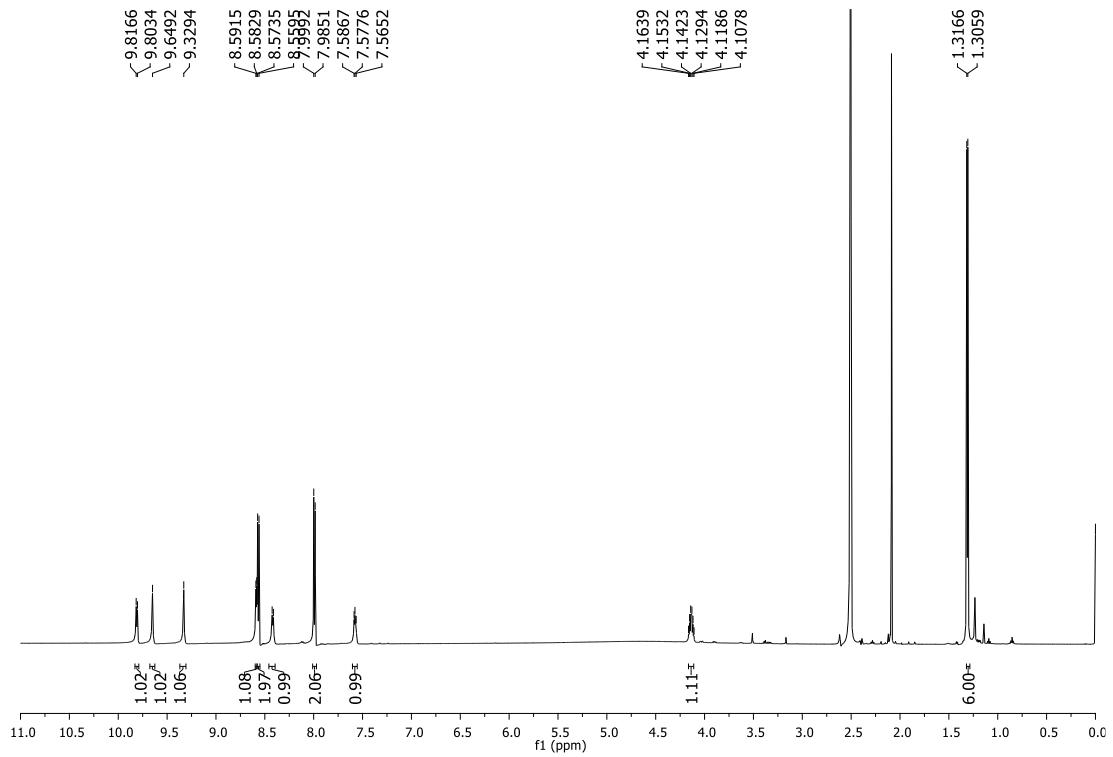


Figure S17. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of 4-(1*H*-imidazo[4,5-*b*]pyridin-2-yl)-*N*-isopropylbenzimidamide hydrochloride **13**

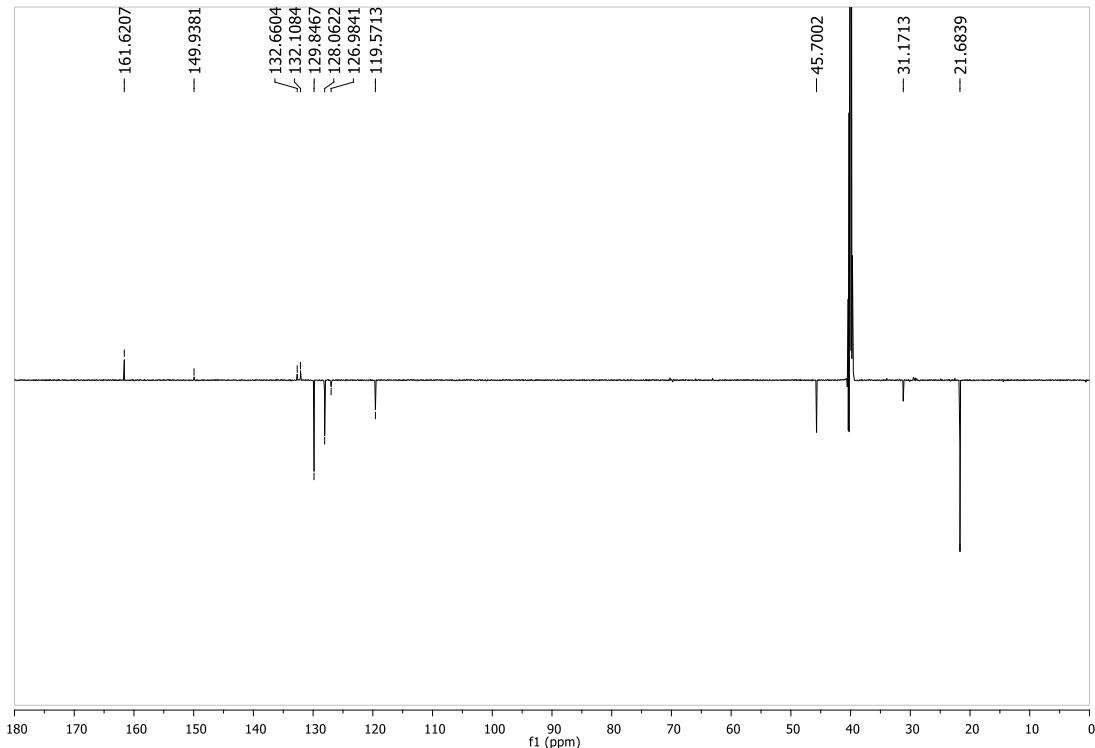


Figure S18. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of 4-(1*H*-imidazo[4,5-*b*]pyridin-2-yl)-*N*-isopropylbenzimidamide hydrochloride **13**

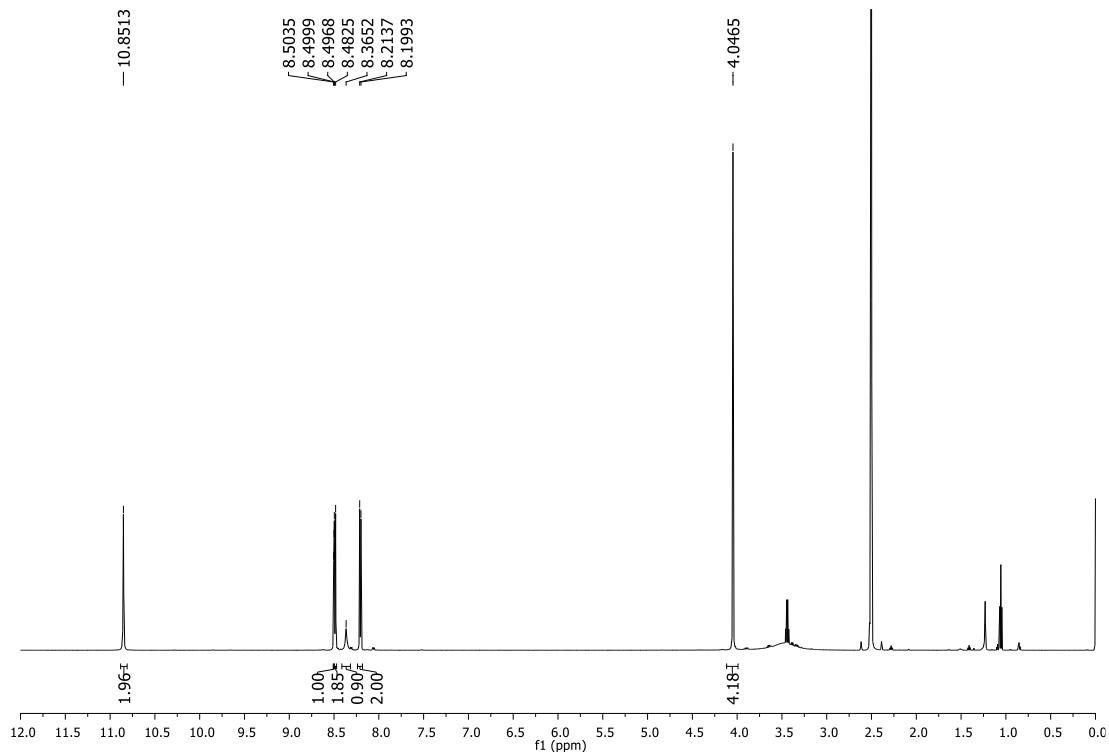


Figure S19. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of 6-bromo-2-(4-(4,5-dihydro-1*H*-imidazol-2-yl)phenyl)-1*H*-imidazo[4,5-*b*]pyridine hydrochloride **14**

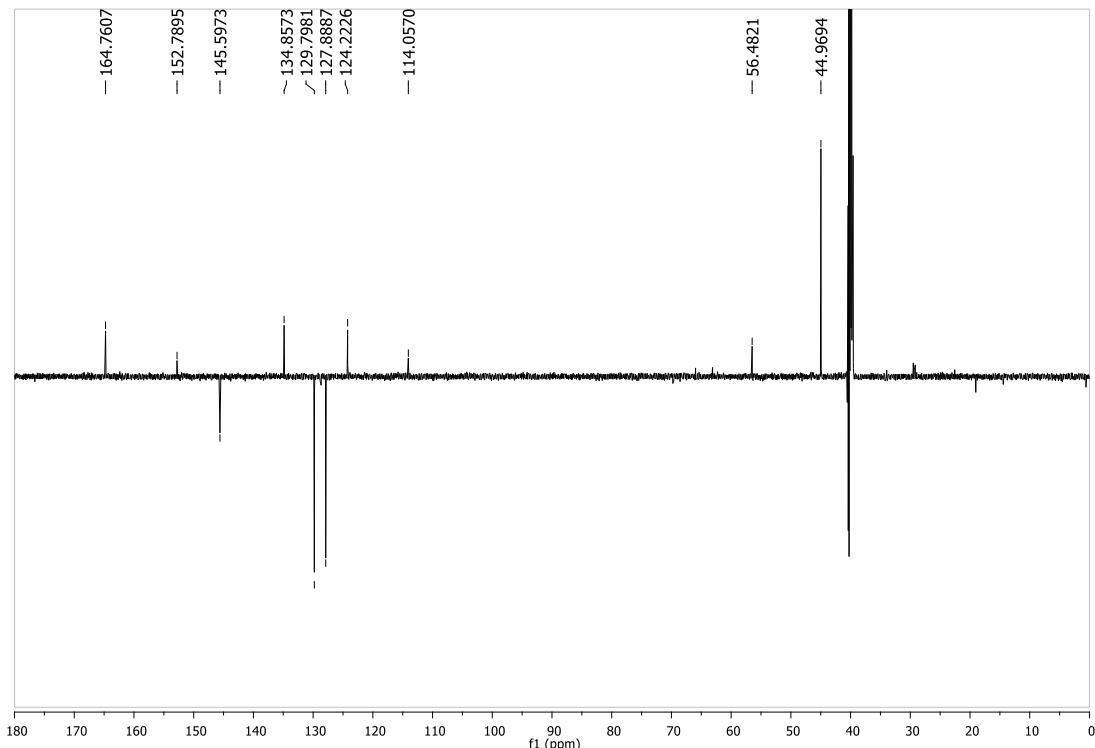


Figure S20. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of 6-bromo-2-(4-(4,5-dihydro-1*H*-imidazol-2-yl)phenyl)-1*H*-imidazo[4,5-*b*]pyridine hydrochloride **14**

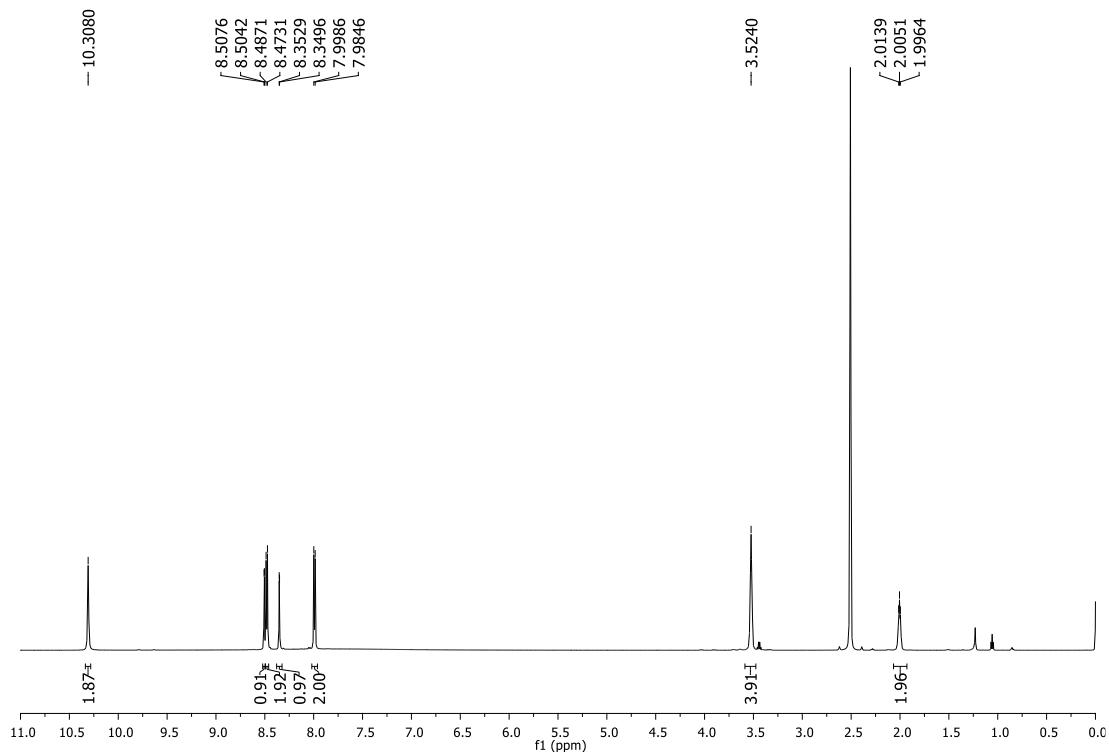


Figure S21. ¹H NMR spectrum (DMSO-*d*₆, 600 MHz) of 6-bromo-2-(4-(1,4,5,6-tetrahydropyrimidin-2-yl)phenyl)-1*H*-imidazo[4,5-*b*]pyridine hydrochloride **15**

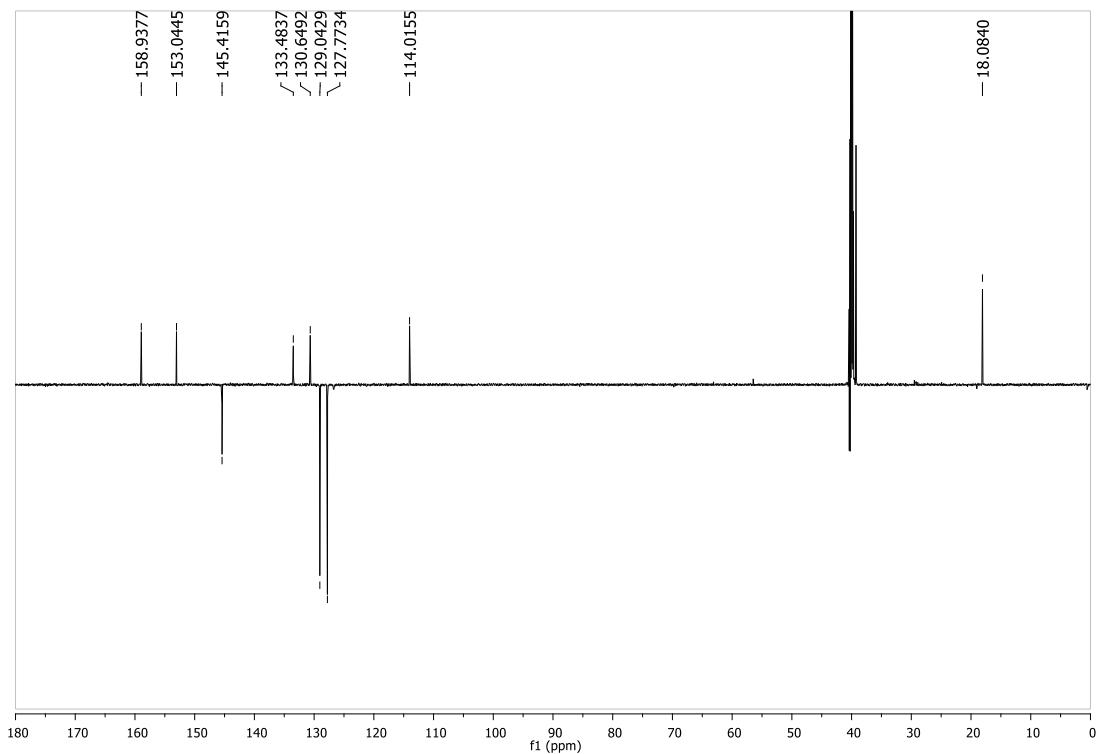


Figure S22. ¹³C NMR spectrum (DMSO-*d*₆, 151 MHz) of 6-bromo-2-(4-(1,4,5,6-tetrahydropyrimidin-2-yl)phenyl)-1*H*-imidazo[4,5-*b*]pyridine hydrochloride **15**

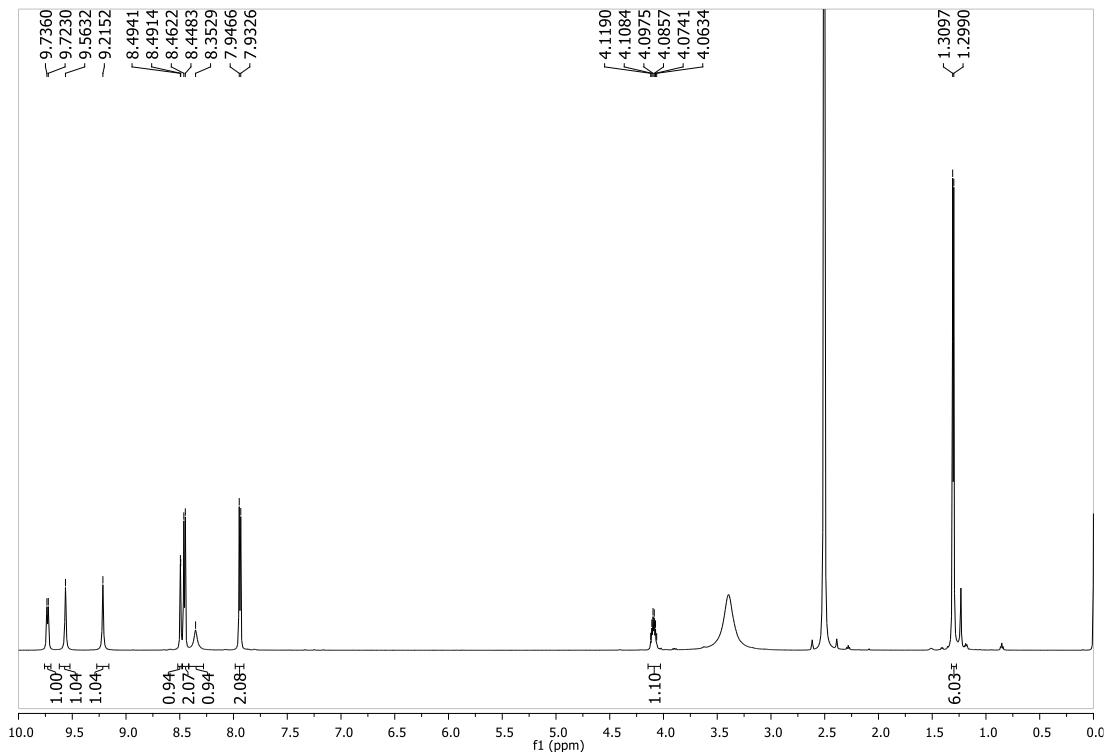


Figure S23. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of 4-(6-bromo-1*H*-imidazo[4,5-*b*]pyridin-2-yl)-*N*-isopropylbenzimidamide hydrochloride **16**

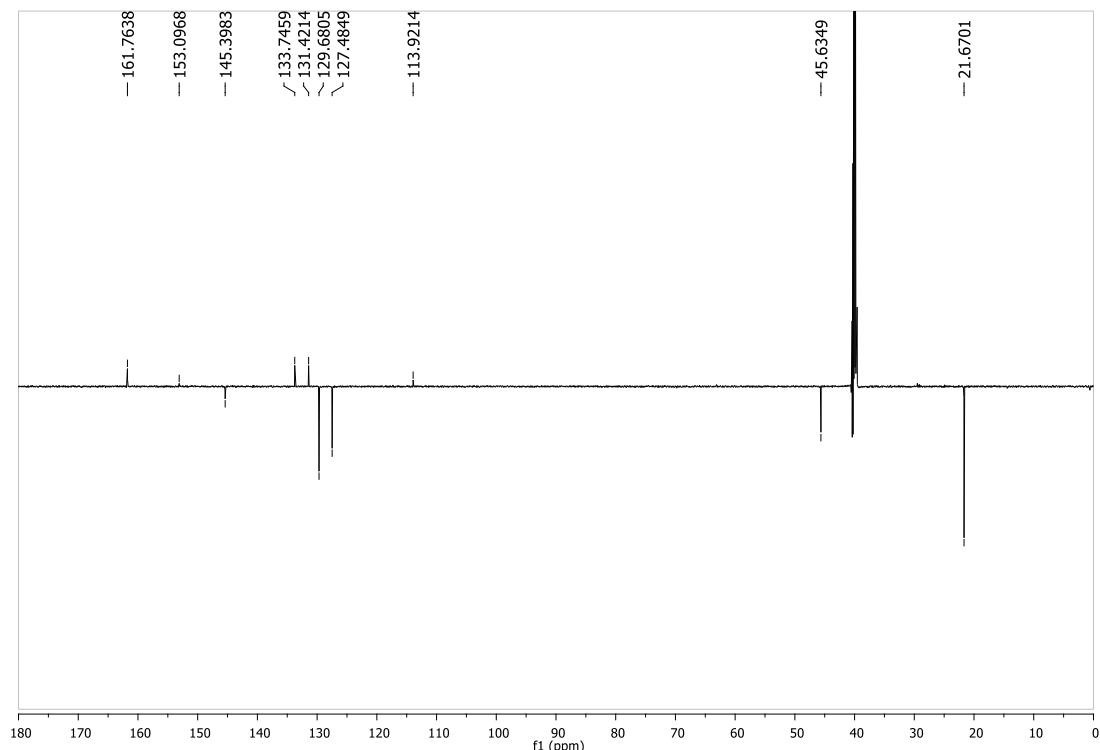


Figure S24. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of 4-(6-bromo-1*H*-imidazo[4,5-*b*]pyridin-2-yl)-*N*-isopropylbenzimidamide hydrochloride **16**

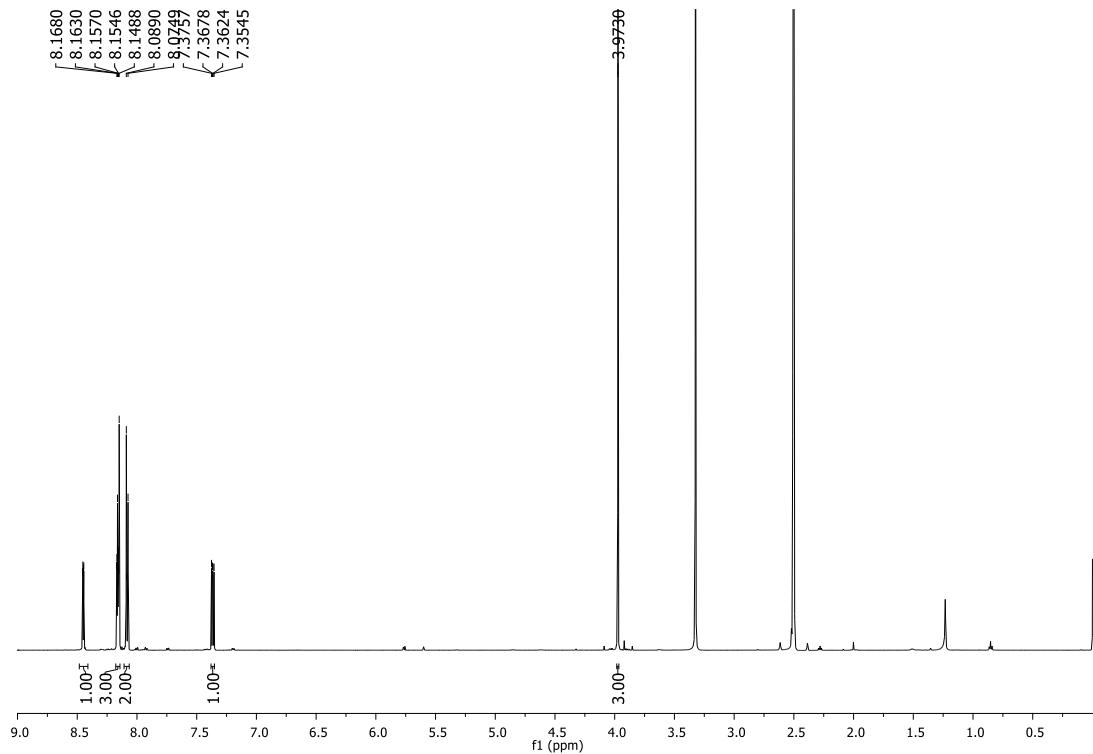


Figure S25. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of 4-(3-methyl-3*H*-imidazo[4,5-*b*]pyridin-2-yl)benzonitrile **17**

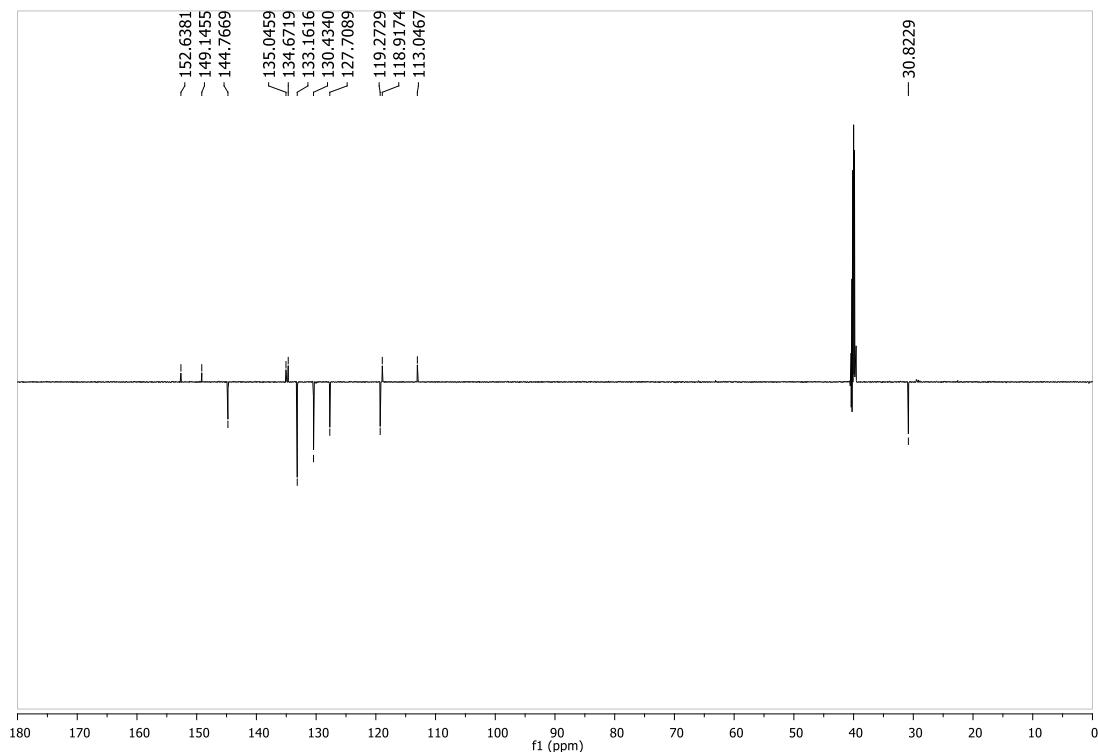


Figure S26. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of 4-(3-methyl-3*H*-imidazo[4,5-*b*]pyridin-2-yl)benzonitrile **17**

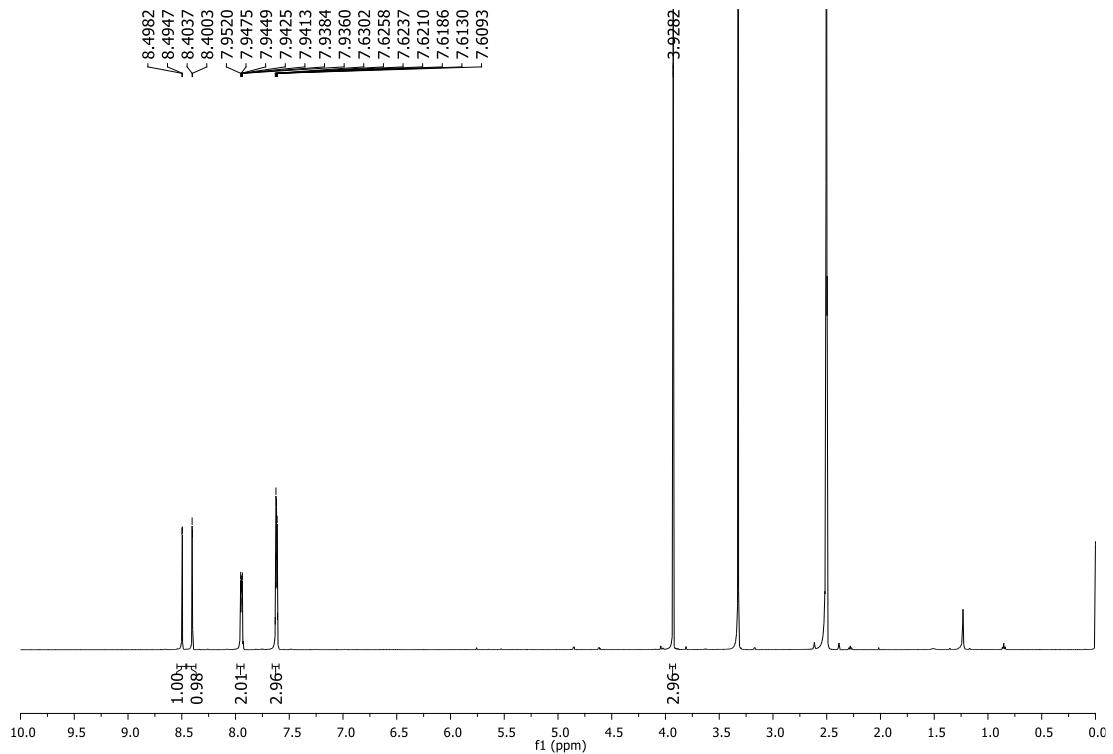


Figure S27. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of 6-bromo-3-methyl-2-phenyl-3*H*-imidazo[4,5-*b*]pyridine **18**

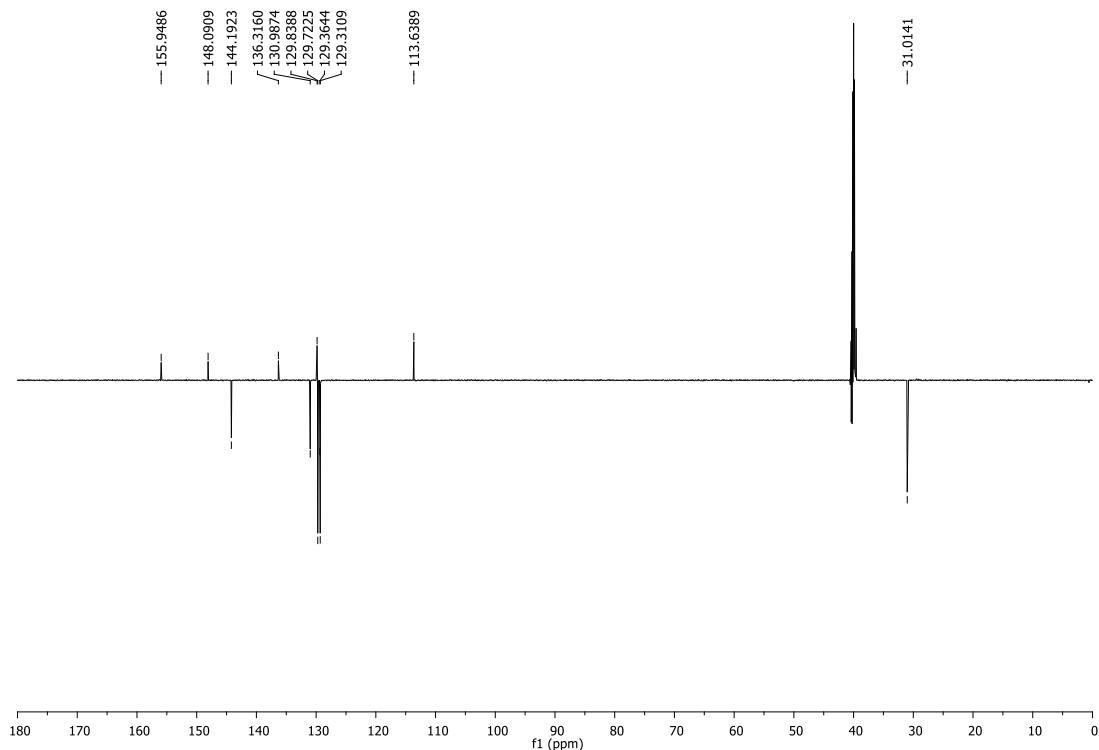


Figure S28. ^{13}C NMR spectrum (DMSO- d_6 , 75 MHz) of 6-bromo-3-methyl-2-phenyl-3*H*-imidazo[4,5-*b*]pyridine **18**

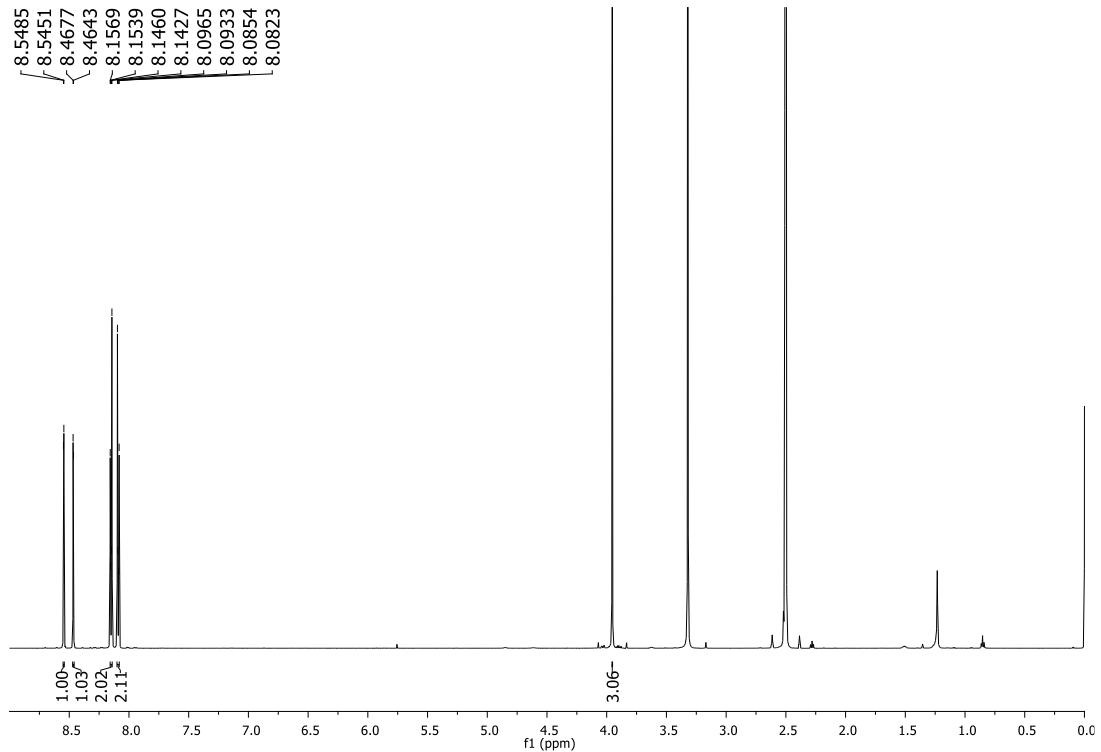


Figure S29. ^1H NMR spectrum (DMSO- d_6 , 600 MHz) of 4-(6-bromo-3-methyl-3*H*-imidazo[4,5-*b*]pyridin-2-yl)benzonitrile **19**

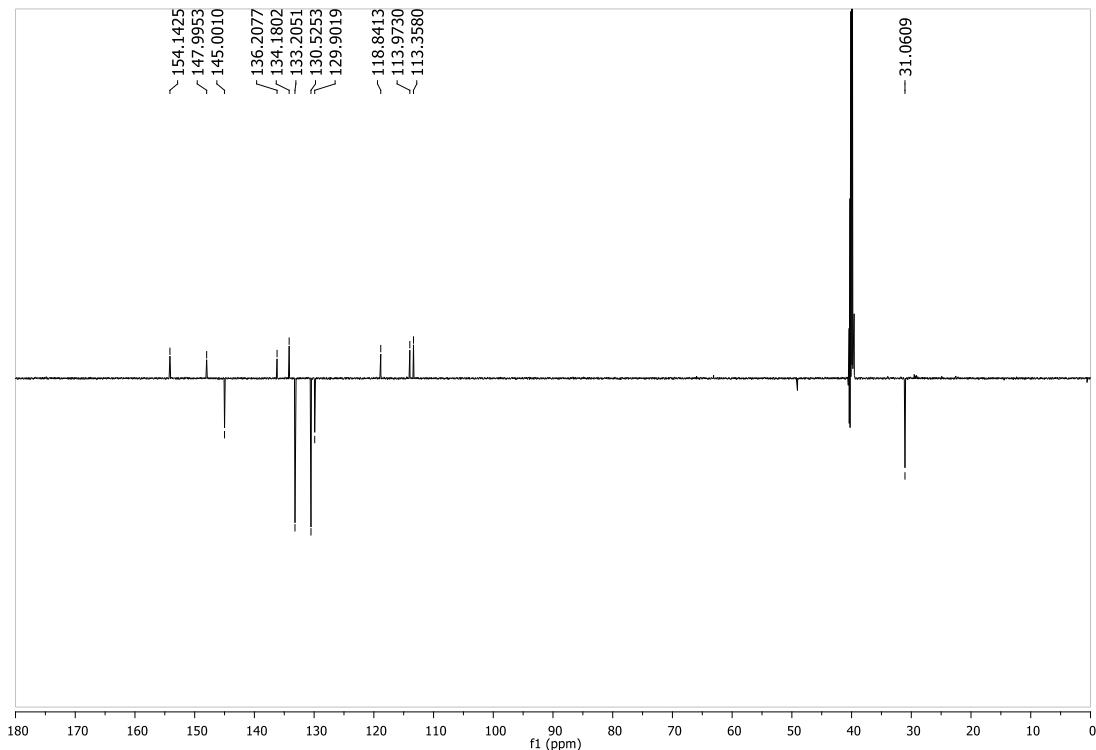


Figure S30. ^{13}C NMR spectrum (DMSO- d_6 , 151 MHz) of 4-(6-bromo-3-methyl-3*H*-imidazo[4,5-*b*]pyridin-2-yl)benzonitrile **19**