

Iodine Catalyzed Synthesis of Imidazo[1,2-*a*]Pyrazine and Imidazo[1,2-*a*]Pyridine Derivatives and their Anticancer activity

Rajavenkatesh Krishnamoorthy*^a, Parthiban Anaikutti*^b

^aOrganic and Bioorganic Chemistry Laboratory, CSIR-Central Leather Research Institute (CSIR- CLRI), Adyar, Chennai, Tamil Nadu, - 600020, India.

^bCentre for GMP, National Institute of Pharmaceutical Education and Research (NIPER-G), Guwahati, Assam- 781101, India.

Corresponding authors

Dr. A. PARTHIBAN

Centre for GMP

National Institute of Pharmaceutical Education and Research, Guwahati

Assam. Mobile: +91- 9843080794

Email: parthichem84@gmail.com

parthiban@niperguwahati.in

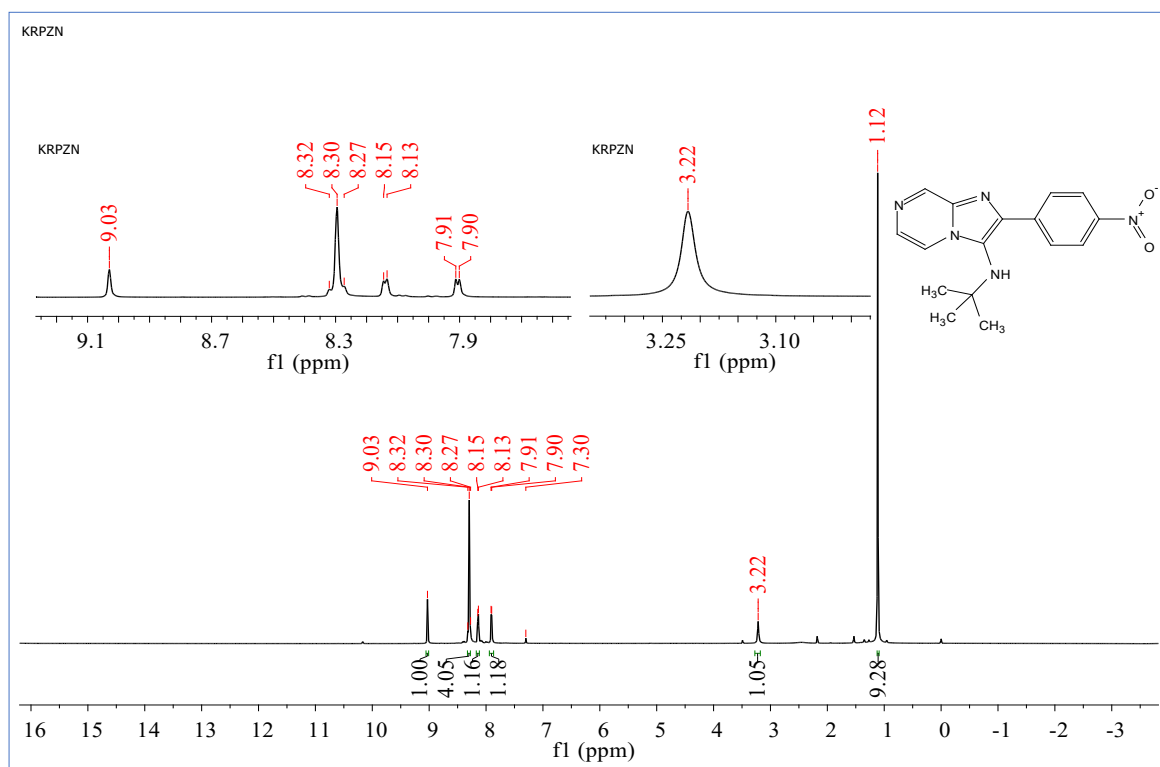
Dr. K. RAJAVENKATESH

Organic and Bioorganic Chemistry Laboratory,

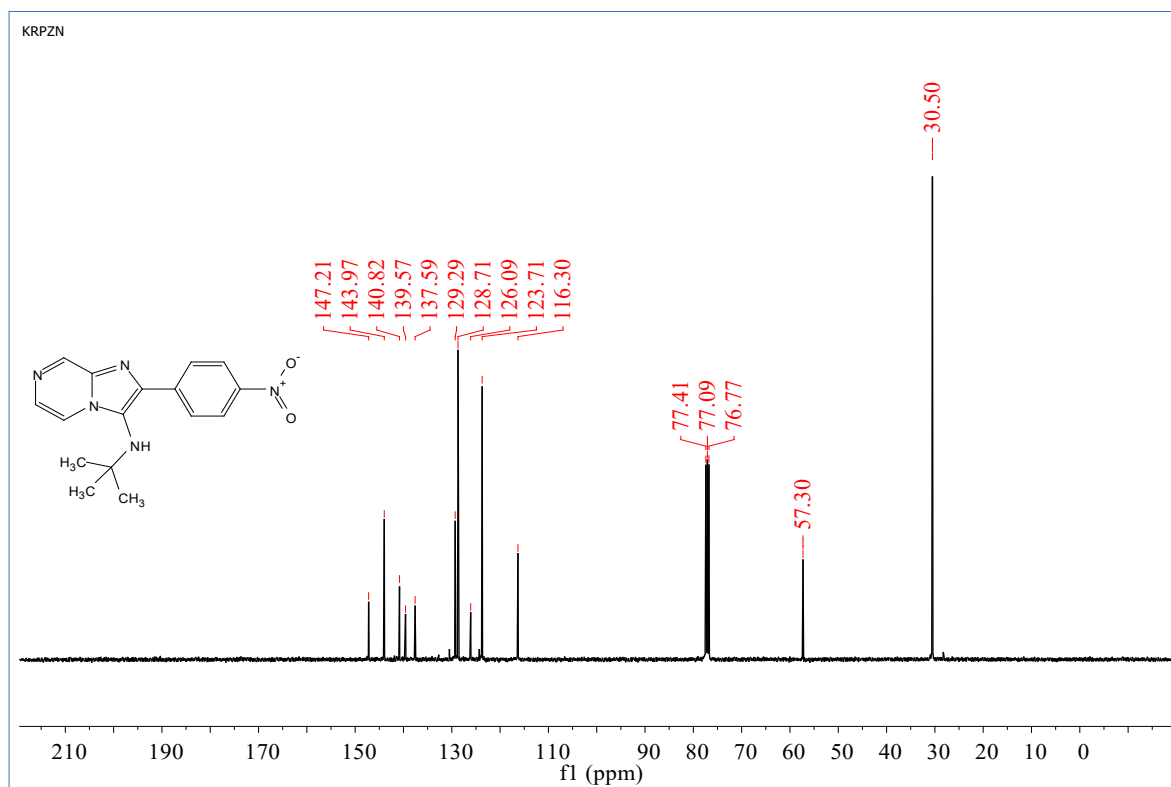
CSIR-CLRI,

Adyar, Chennai-600020, Tamilnadu, India.

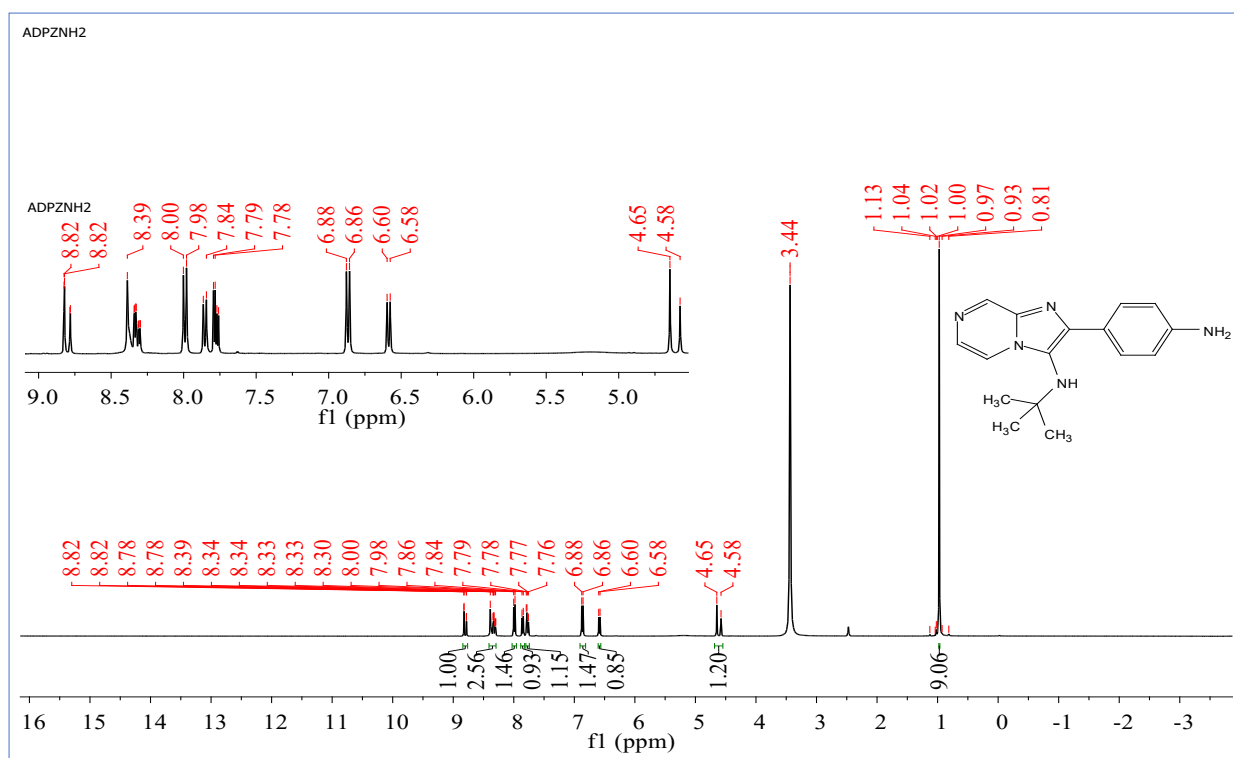
Email: krajavenkateshcmp5@gmail.com /rajavenkateshk2@gmail.com



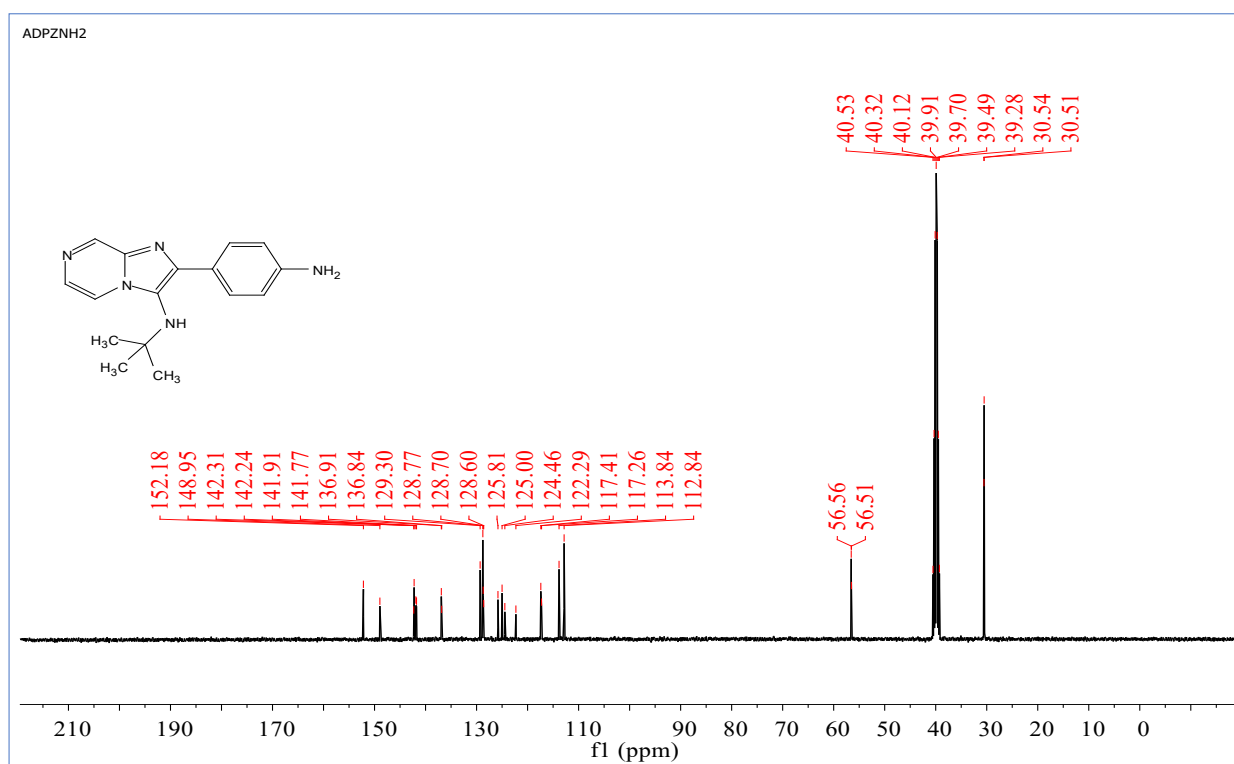
Supplementary Fig. 1 400 MHz (CDCl₃) ¹H NMR spectrum of N-(tert-butyl)-2-(4-nitrophenyl)imidazo[1,2-a]pyrazin-3-amine (10a).



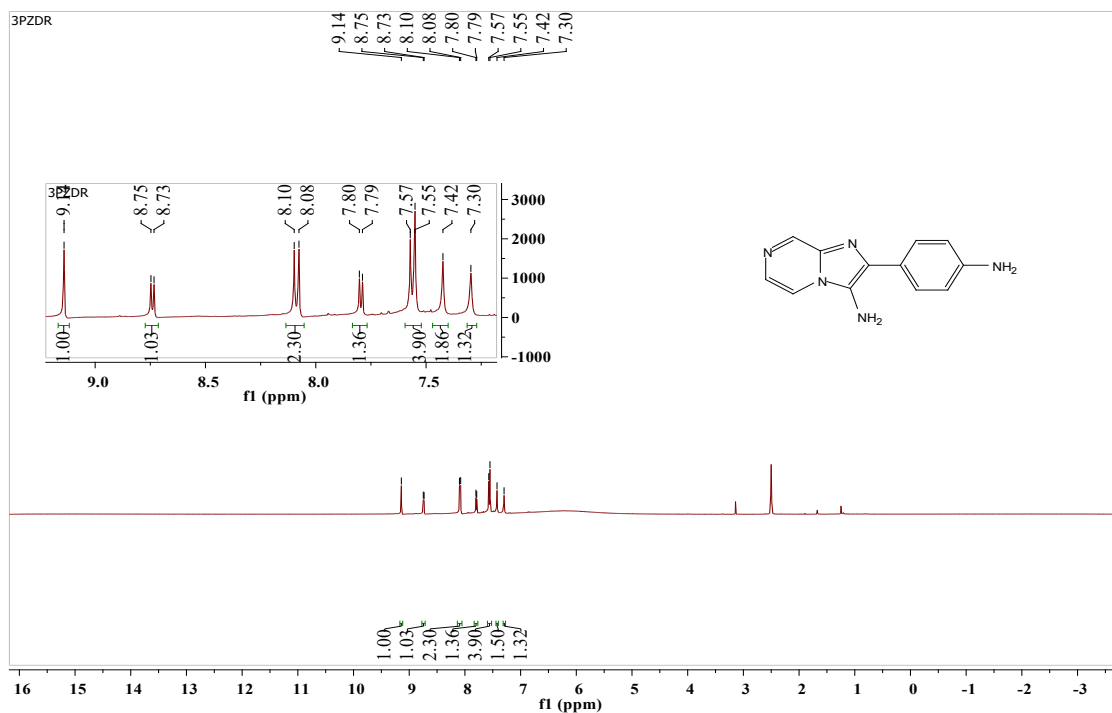
Supplementary Fig. 2 100 MHz (CDCl₃) ¹³C NMR spectrum of N-(tert-butyl)-2-(4-nitrophenyl)imidazo[1,2-a]pyrazin-3-amine (10a).



Supplementary Fig. 3 400 MHz (DMSO-d₆) ¹H NMR spectrum of 2-(4-aminophenyl)-N-(tert-butyl)imidazo[1,2-a]pyrazin-3-amine (**10b**).

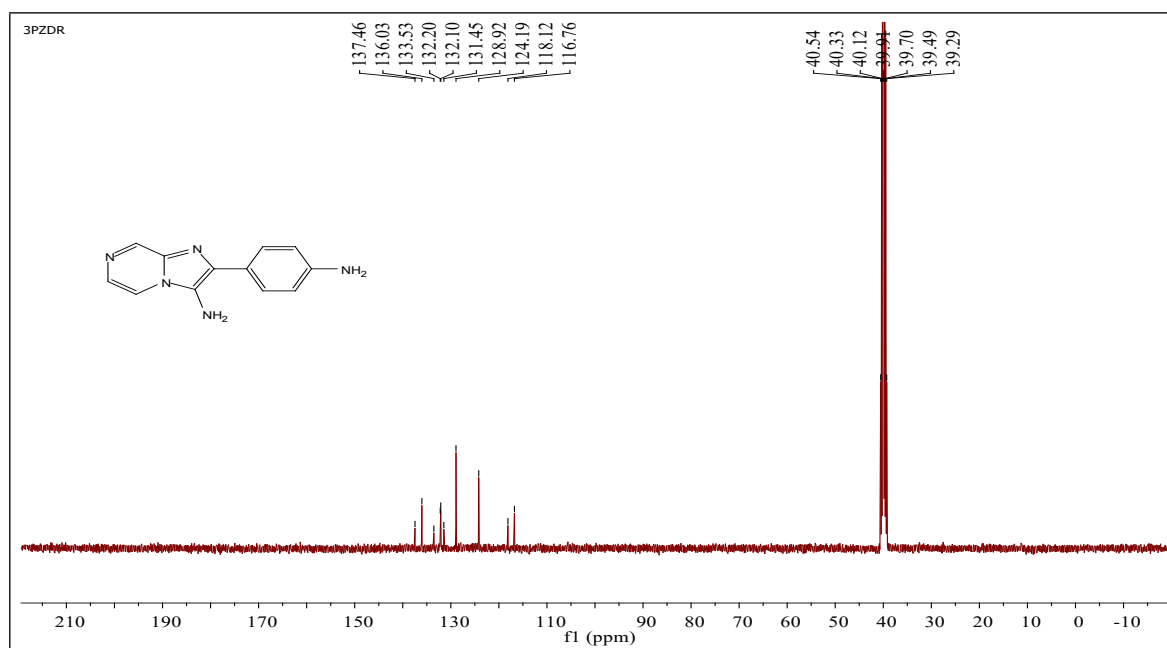


Supplementary Fig. 4 100 MHz (DMSO-d₆) ¹³C NMR spectrum of 2-(4-aminophenyl)-N-(tert-butyl)imidazo[1,2-a]pyrazin-3-amine (**10b**).

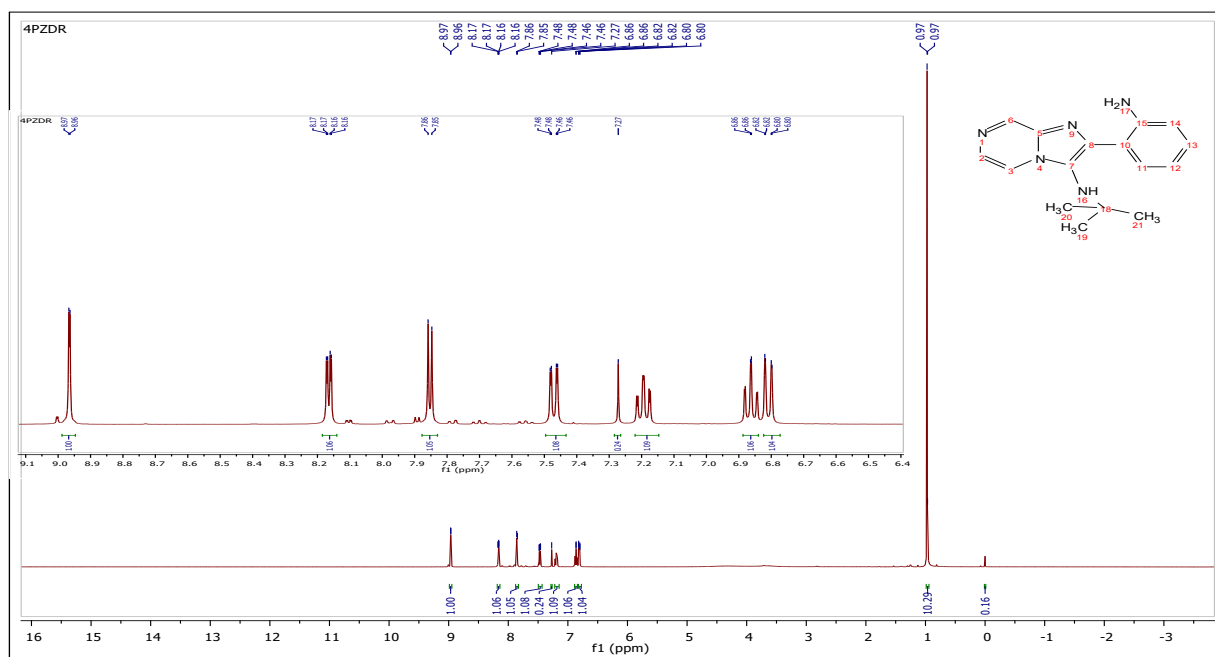


Sup

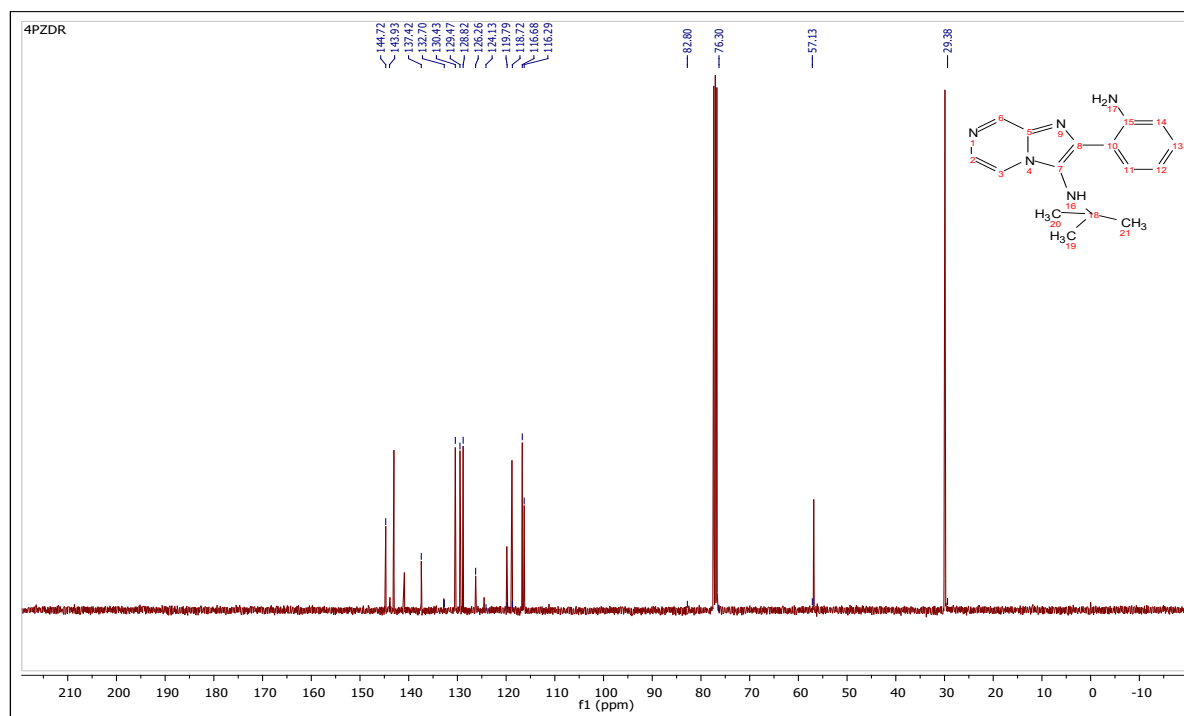
plementary Fig. 7 400 MHz (DMSO-d₆) ¹H NMR spectrum of 2-(4-aminophenyl)imidazo[1,2-a]pyrazin-3-amine (10d).



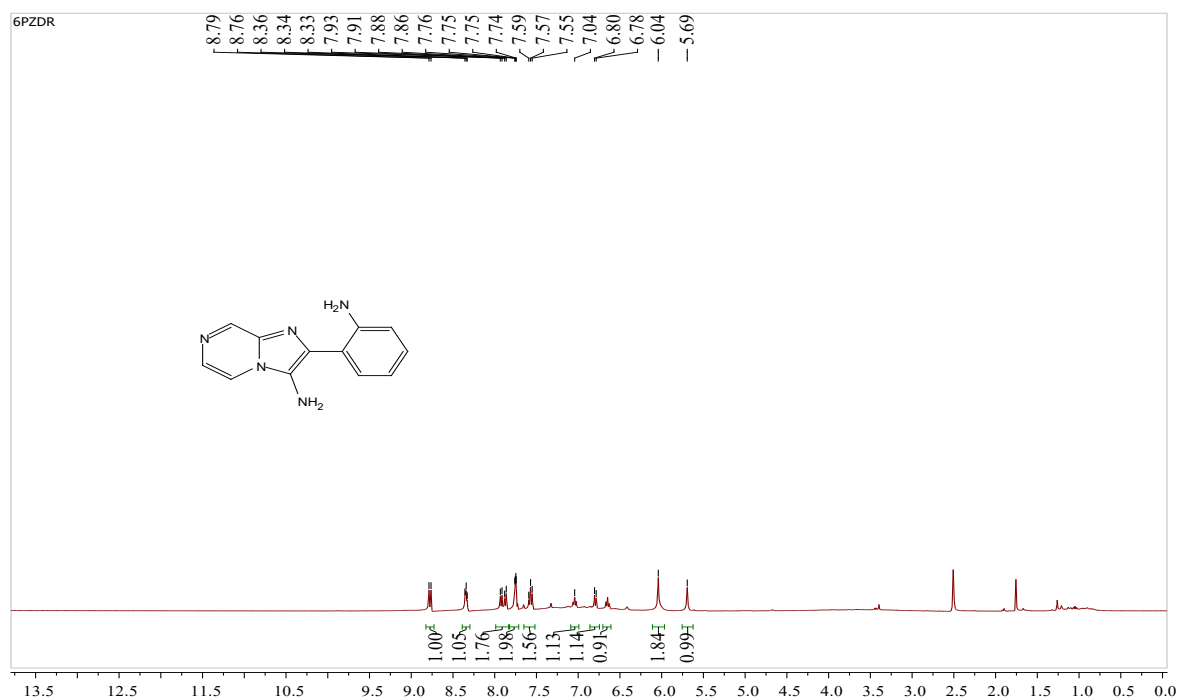
Supplementary Fig. 8 100 MHz (DMSO-d₆) ¹³C NMR spectrum of 2-(4-aminophenyl)imidazo[1,2-a]pyrazin-3-amine (10d).



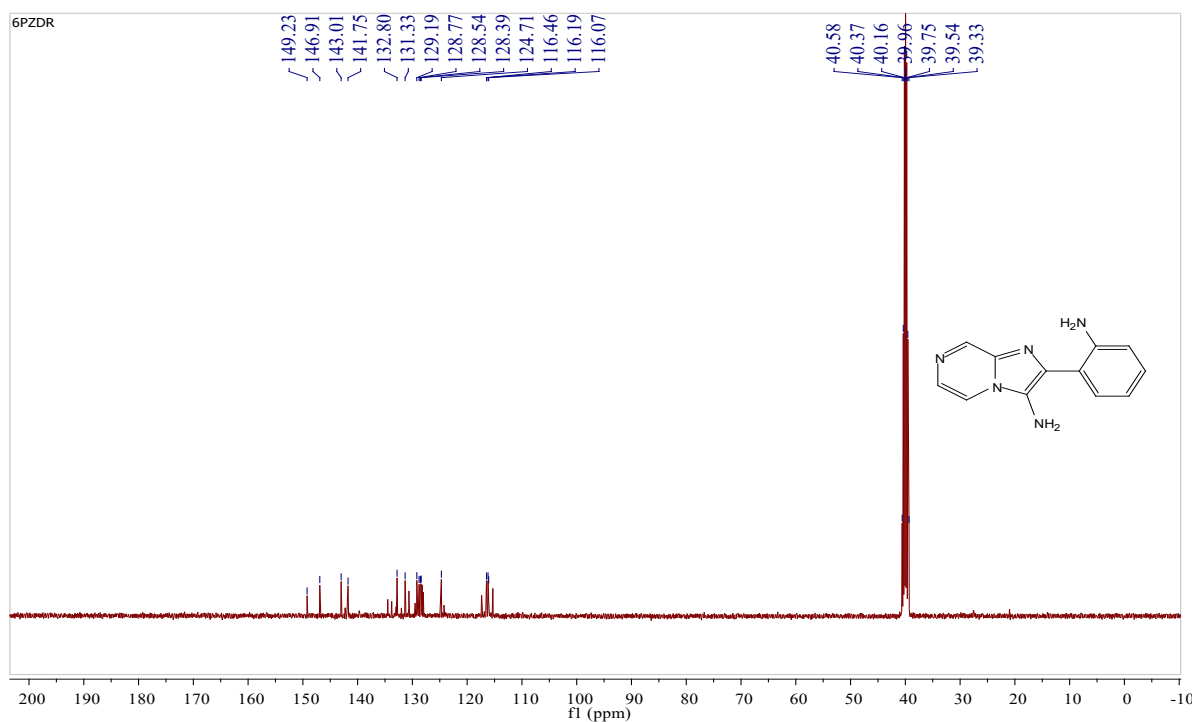
Supplementary Fig. 11 400 MHz (CDCl_3) ^1H NMR spectrum of 2-(2-aminophenyl)-N-(tert-butyl)imidazo[1,2-a]pyrazin-3-amine (10f).



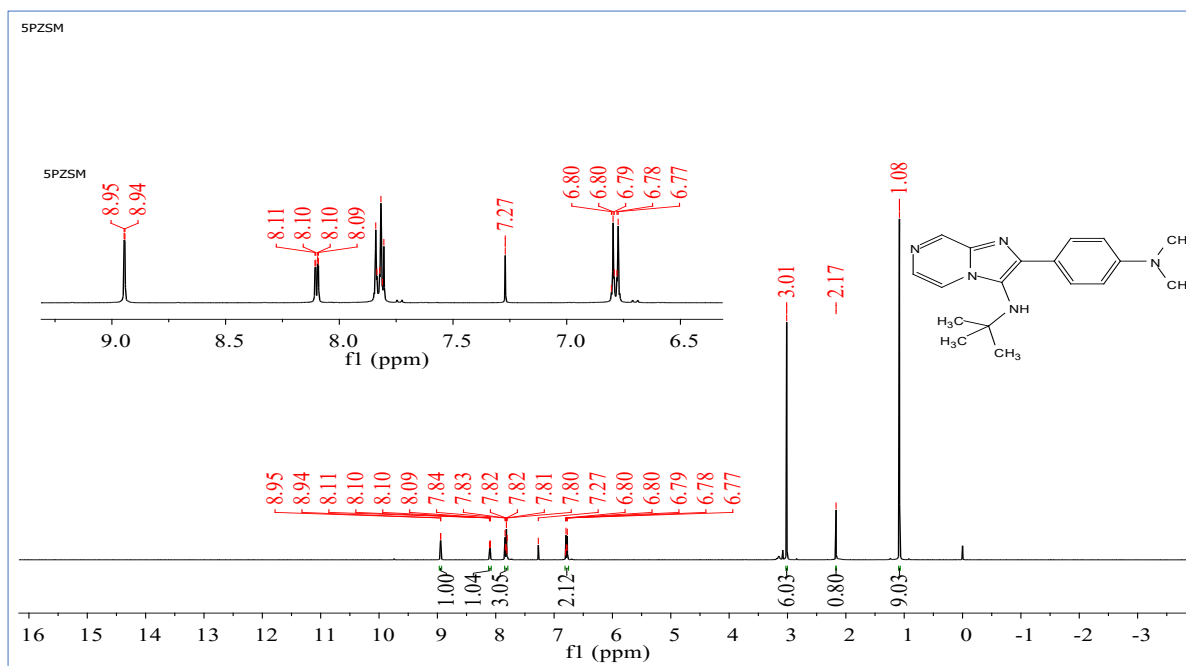
Supplementary Fig. 12 100 MHz (CDCl_3) ^{13}C NMR spectrum of 2-(2-aminophenyl)-N-(tert-butyl)imidazo[1,2-a]pyrazin-3-amine (10f).



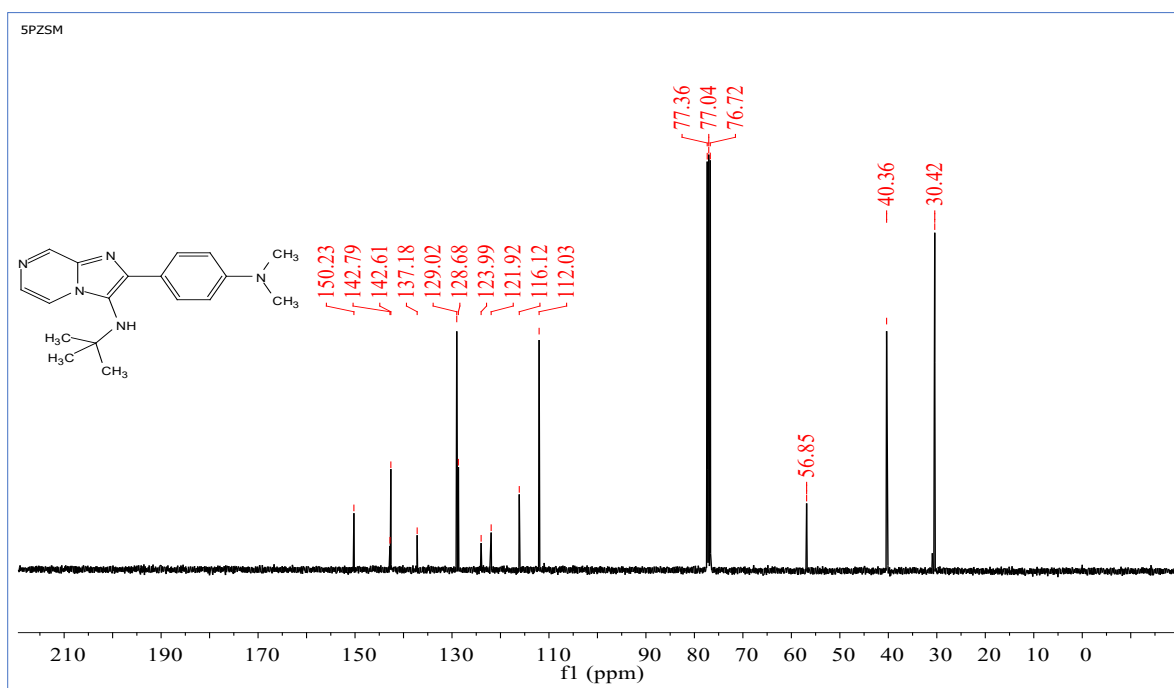
Supplementary Fig. 13 400 MHz (DMSO-d₆) ¹H NMR spectrum of 2-(2-aminophenyl)imidazo[1,2-a]pyrazin-3-amine (10g).



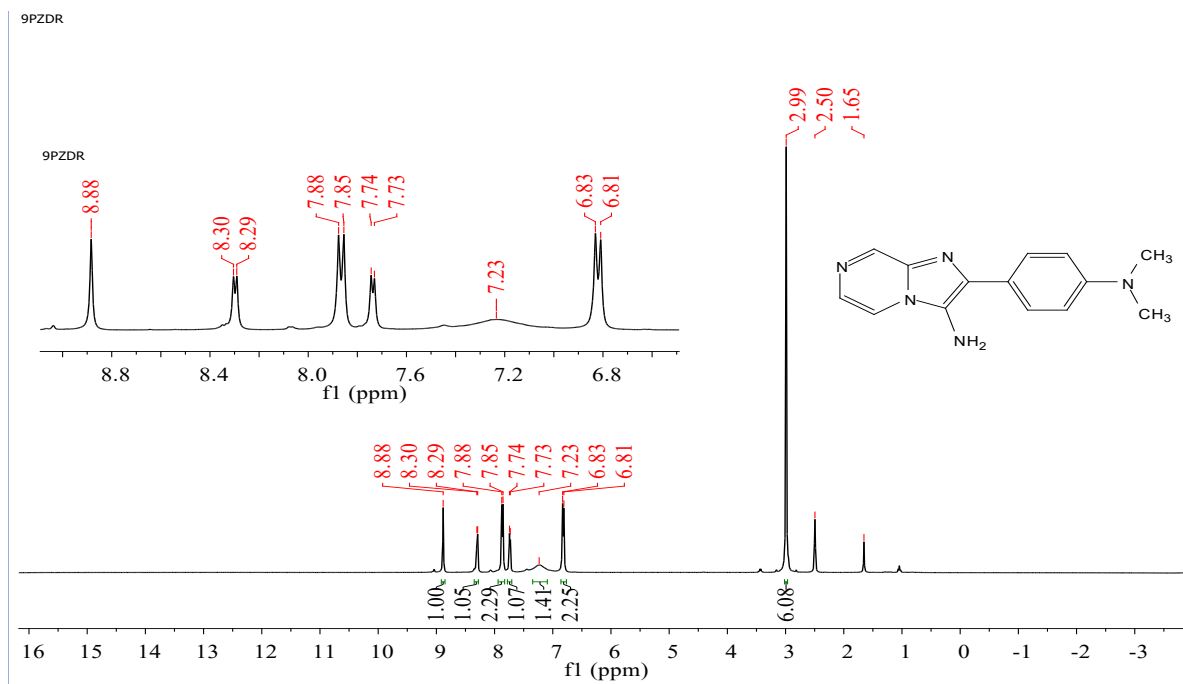
Supplementary Fig. 14 100 MHz (DMSO-d₆) ¹³C NMR spectrum of 2-(2-aminophenyl)imidazo[1,2-a]pyrazin-3-amine (10g).



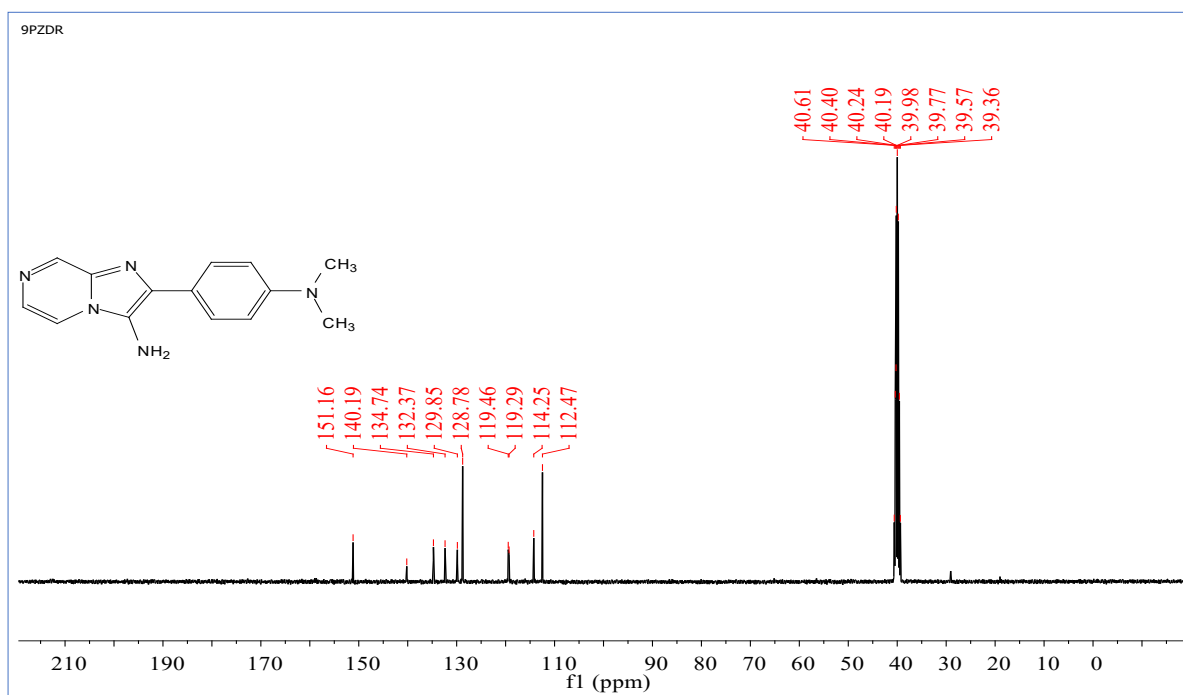
Supplementary Fig. 15 400 MHz (CDCl₃) ¹H NMR spectrum of N-(tert-butyl)-2-(4-(dimethylamino)phenyl)imidazo[1,2-a]pyrazin-3-amine (10h).



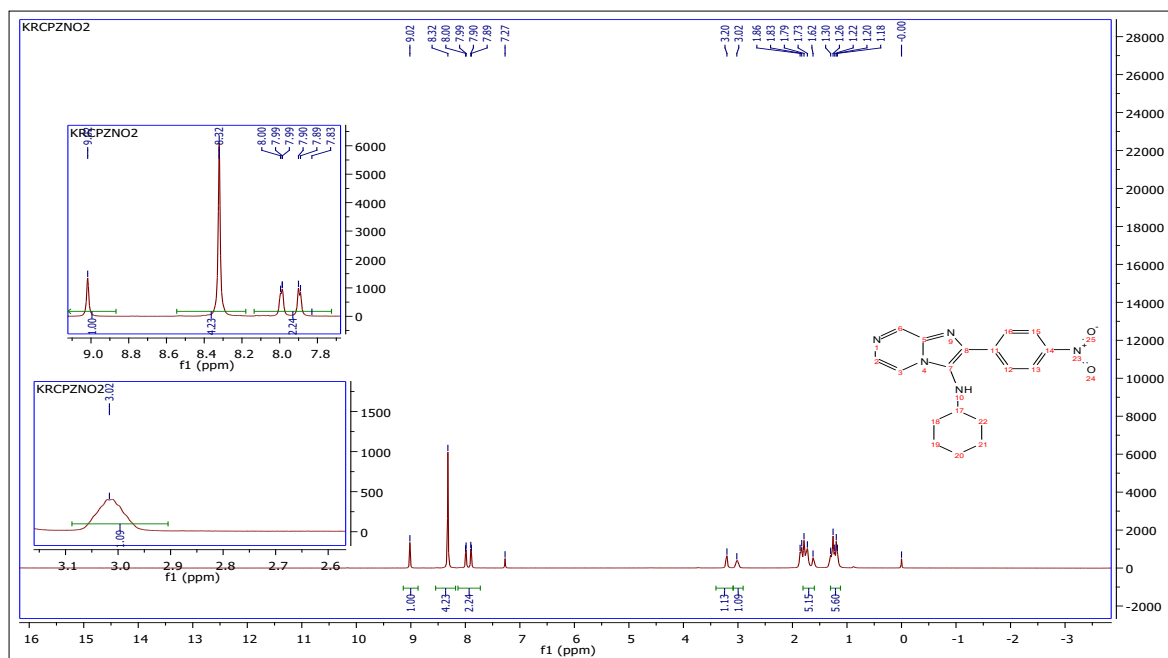
Supplementary Fig. 16 100 MHz (CDCl₃) ¹³C NMR spectrum of N-(tert-butyl)-2-(4-(dimethylamino)phenyl)imidazo[1,2-a]pyrazin-3-amine (10h).



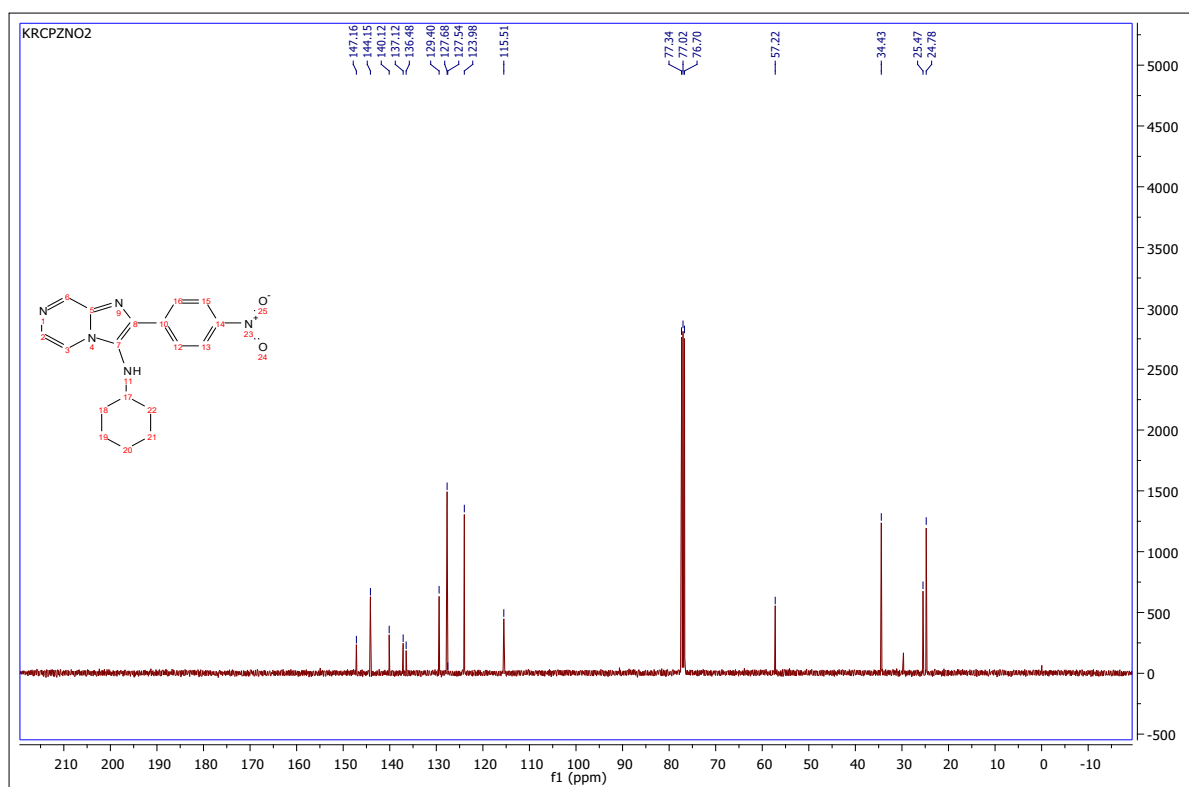
Supplementary Fig. 17 400 MHz (DMSO- d_6) ^1H NMR spectrum of 2-(4-(dimethylamino)phenyl)imidazo[1,2-a]pyrazin-3-amine (10i).



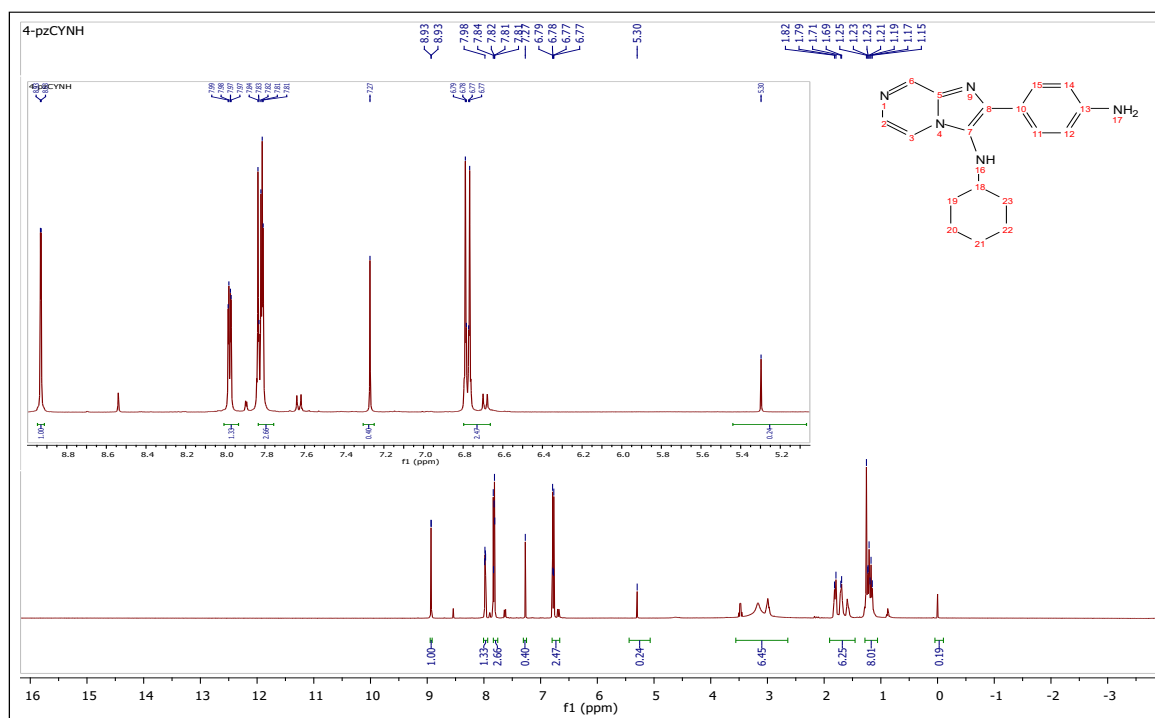
Supplementary Fig. 18 100 MHz (DMSO- d_6) ^{13}C NMR spectrum of 2-(4-(dimethylamino)phenyl)imidazo[1,2-a]pyrazin-3-amine (10i).



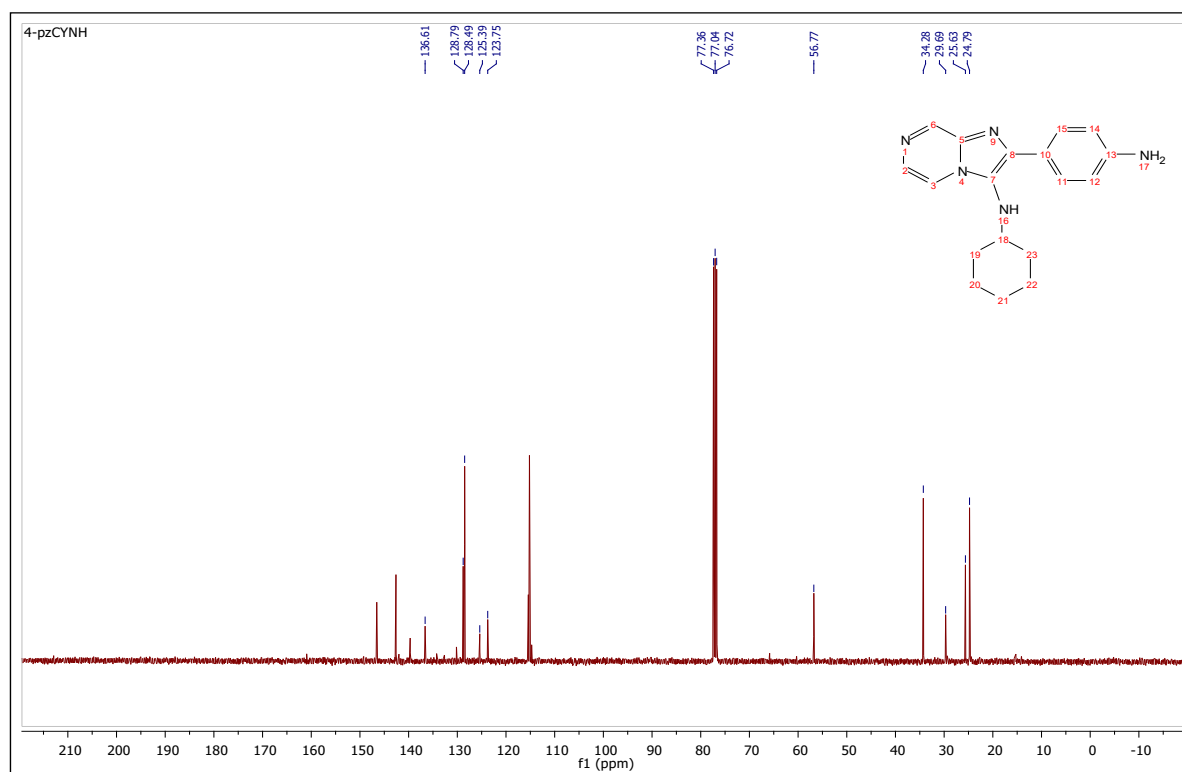
Supplementary Fig. 19 400 MHz (CDCl₃) ¹H NMR spectrum of N-cyclohexyl-2-(4-nitrophenyl)imidazo[1,2-a]pyrazin-3-amine (10j).



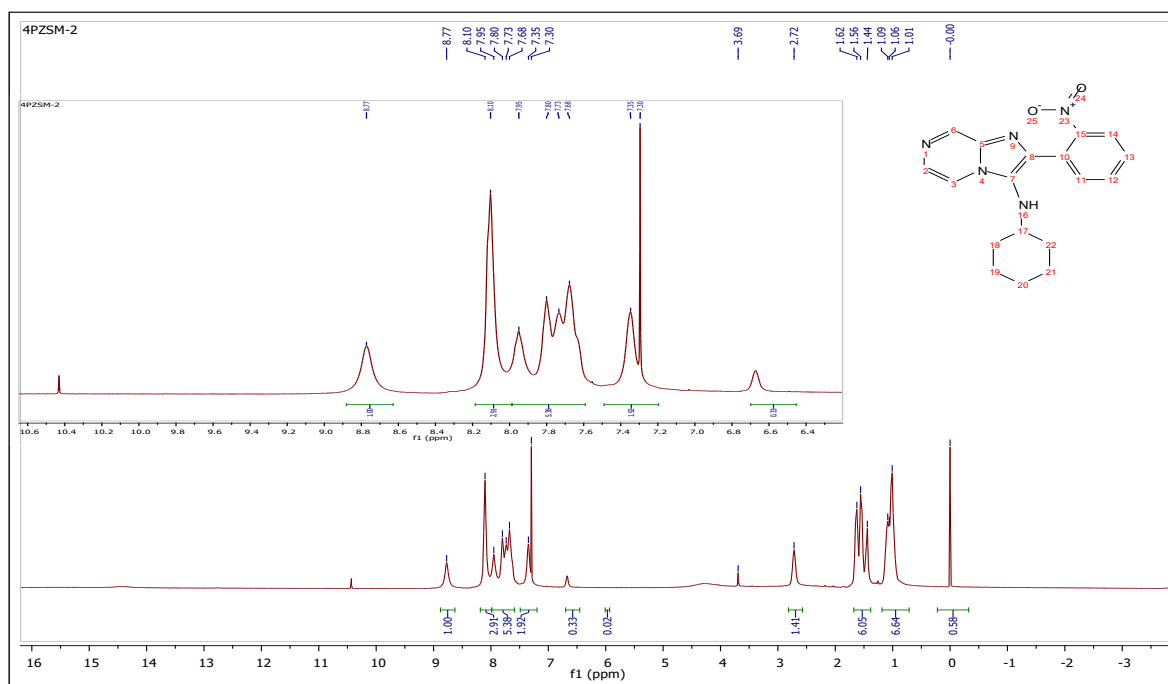
Supplementary Fig. 20 100 MHz (CDCl₃) ¹³C NMR spectrum of N-cyclohexyl-2-(4-nitrophenyl)imidazo[1,2-a]pyrazin-3-amine (10j).



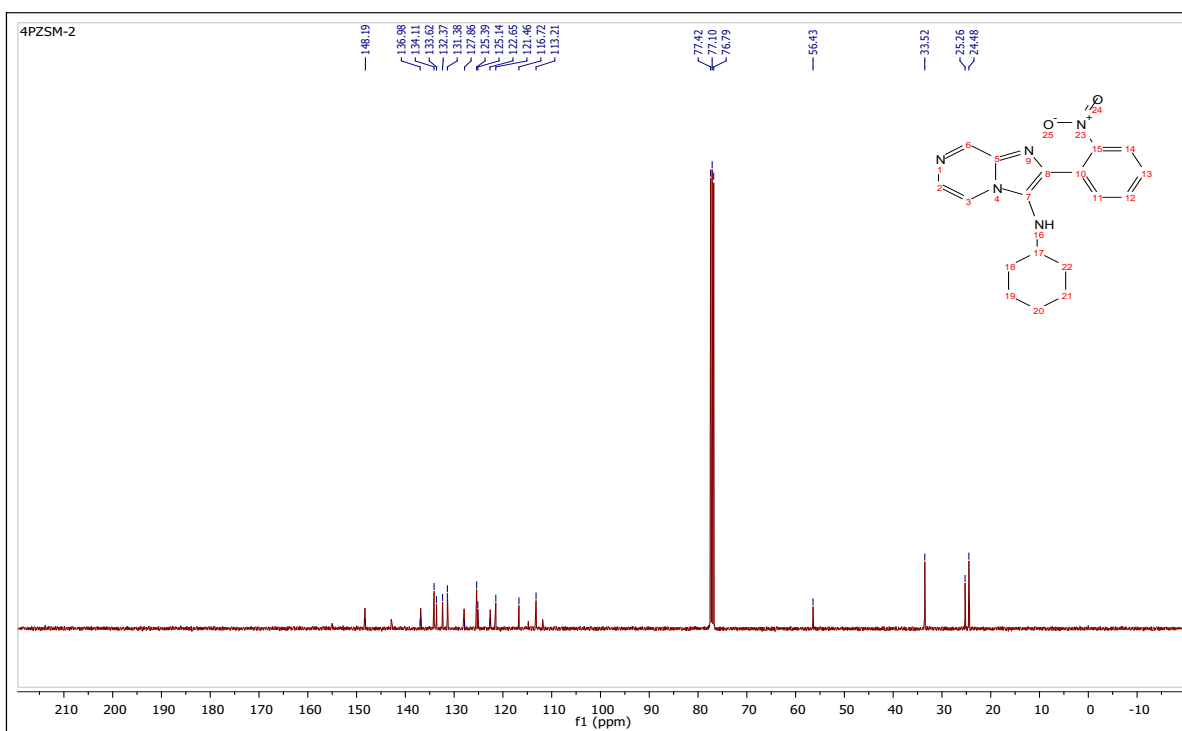
Supplementary Fig. 21 400 MHz (CDCl₃) ¹H NMR spectrum of 2-(4-aminophenyl)-N-cyclohexylimidazo[1,2-a]pyrazin-3-amine (10k).



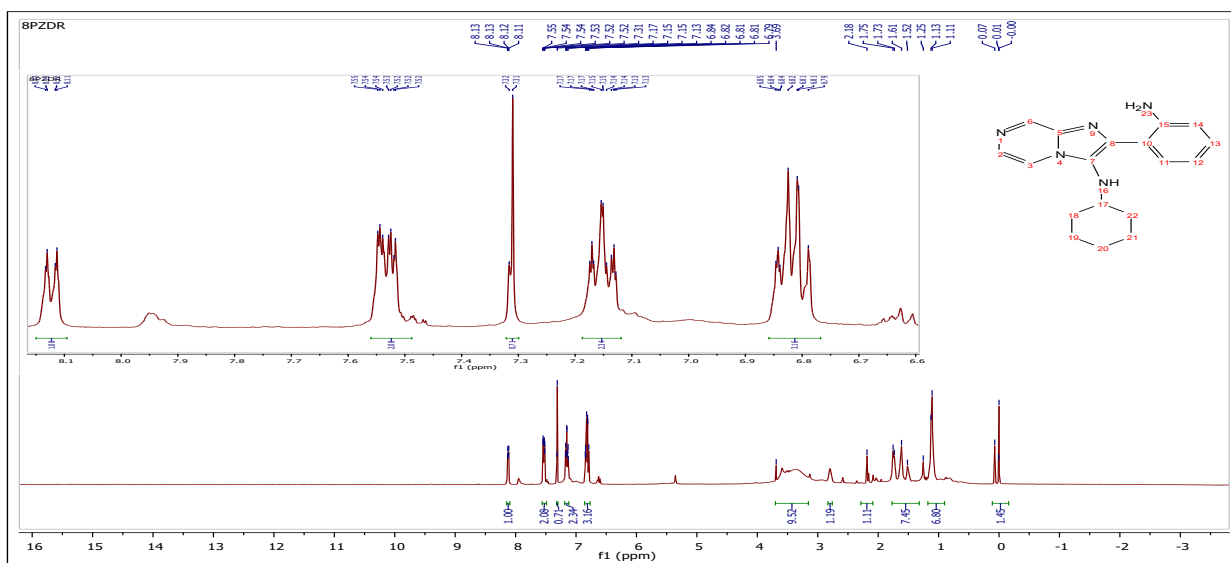
Supplementary Fig. 22 100 MHz (CDCl₃) ¹³C NMR spectrum of 2-(4-aminophenyl)-N-cyclohexylimidazo[1,2-a]pyrazin-3-amine (10k).

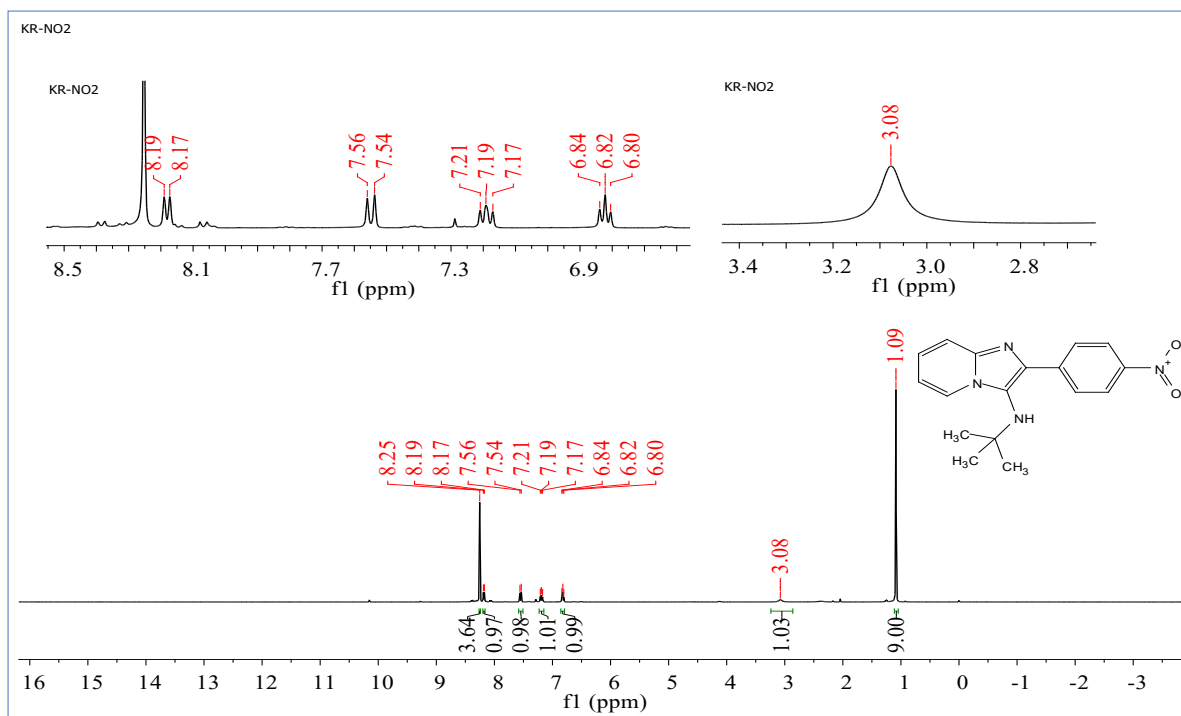


Supplementary Fig. 23 400 MHz (CDCl₃) ¹H NMR spectrum of N-cyclohexyl-2-(2-nitrophenyl)imidazo[1,2-a]pyrazin-3-amine (10).

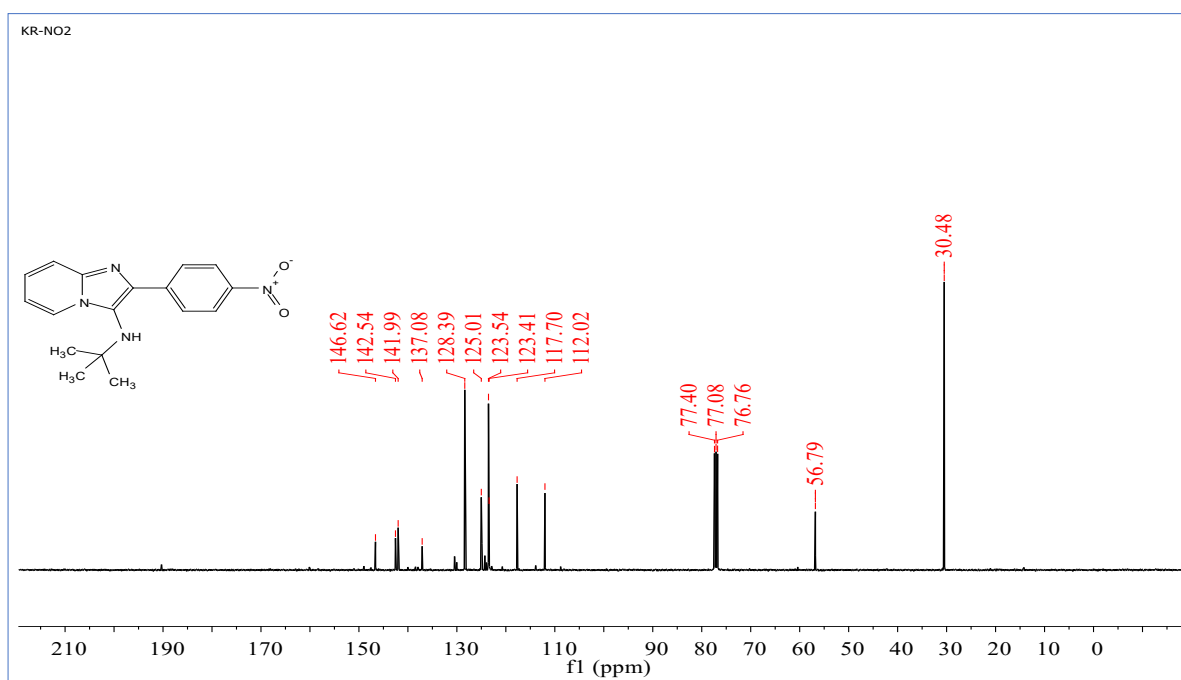


Supplementary Fig. 24 100 MHz (CDCl₃) ¹³C NMR spectrum of N-cyclohexyl-2-(2-nitrophenyl)imidazo[1,2-a]pyrazin-3-amine (10).

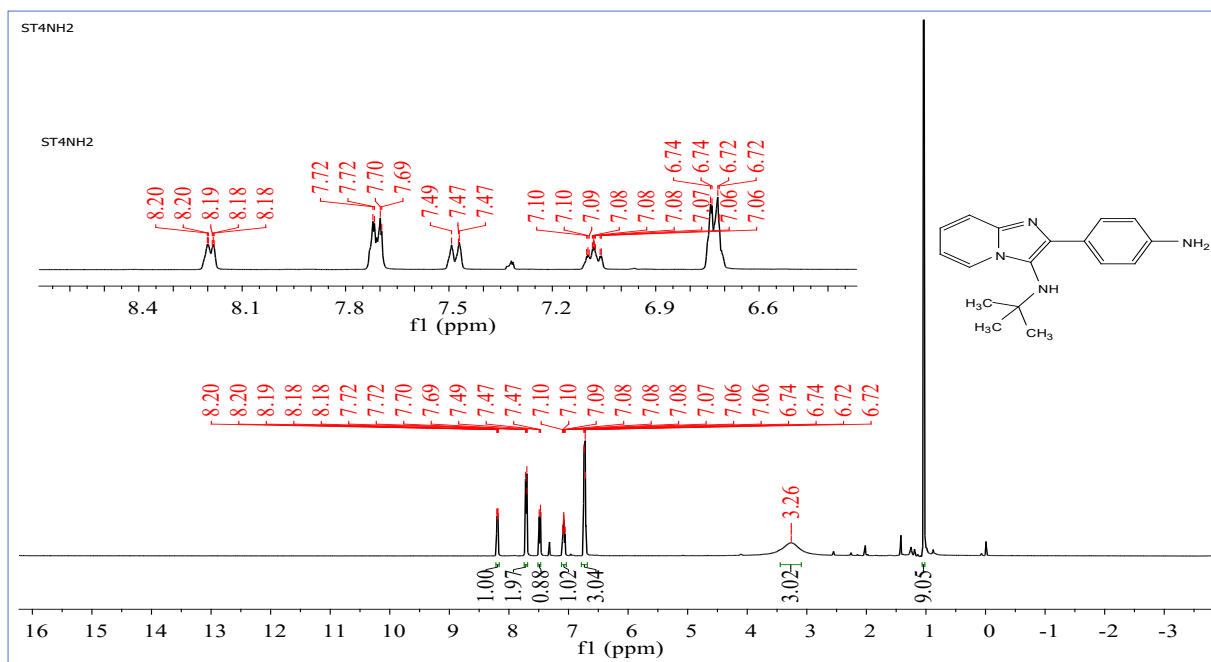




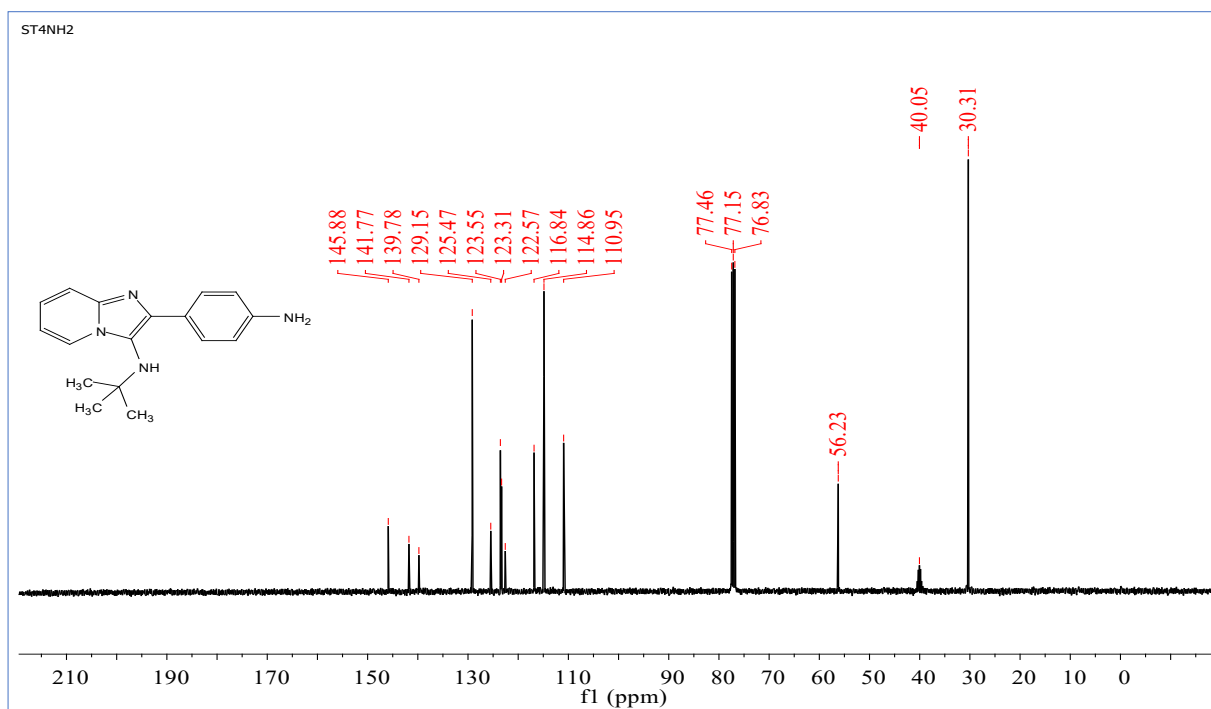
Supplementary Fig. 27 400 MHz (CDCl₃) ¹H NMR spectrum of N-(tert-butyl)-2-(4-nitrophenyl)imidazo[1,2-a]pyridin-3-amine (12a).



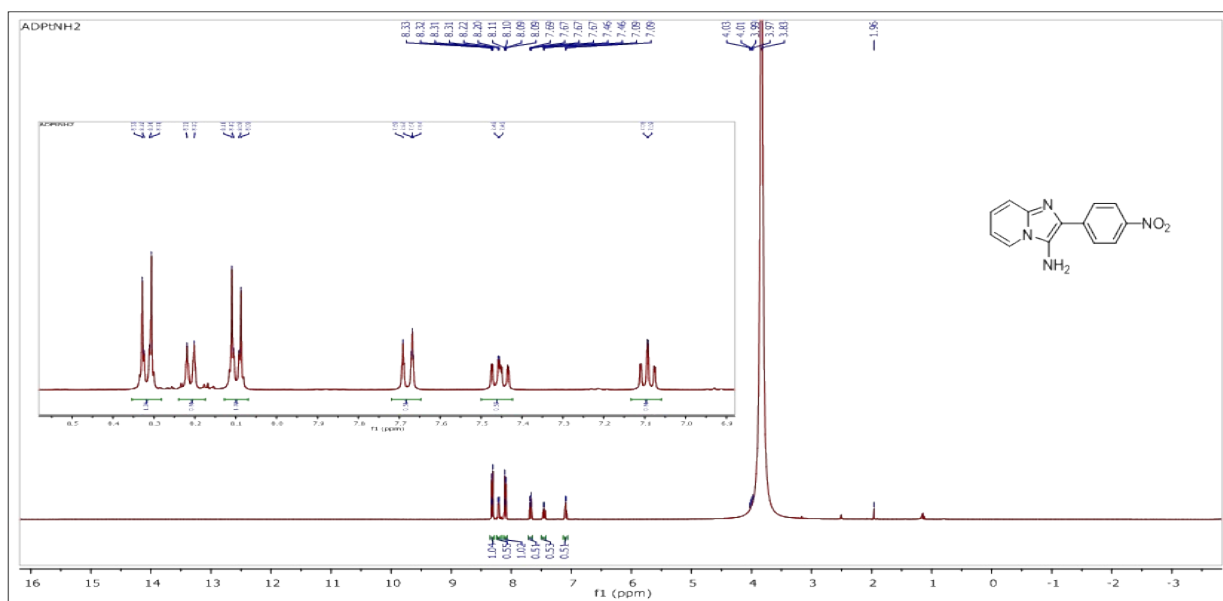
Supplementary Fig. 28 100 MHz (CDCl₃) ¹³C NMR spectrum of N-(tert-butyl)-2-(4-nitrophenyl)imidazo[1,2-a]pyridin-3-amine (12a).



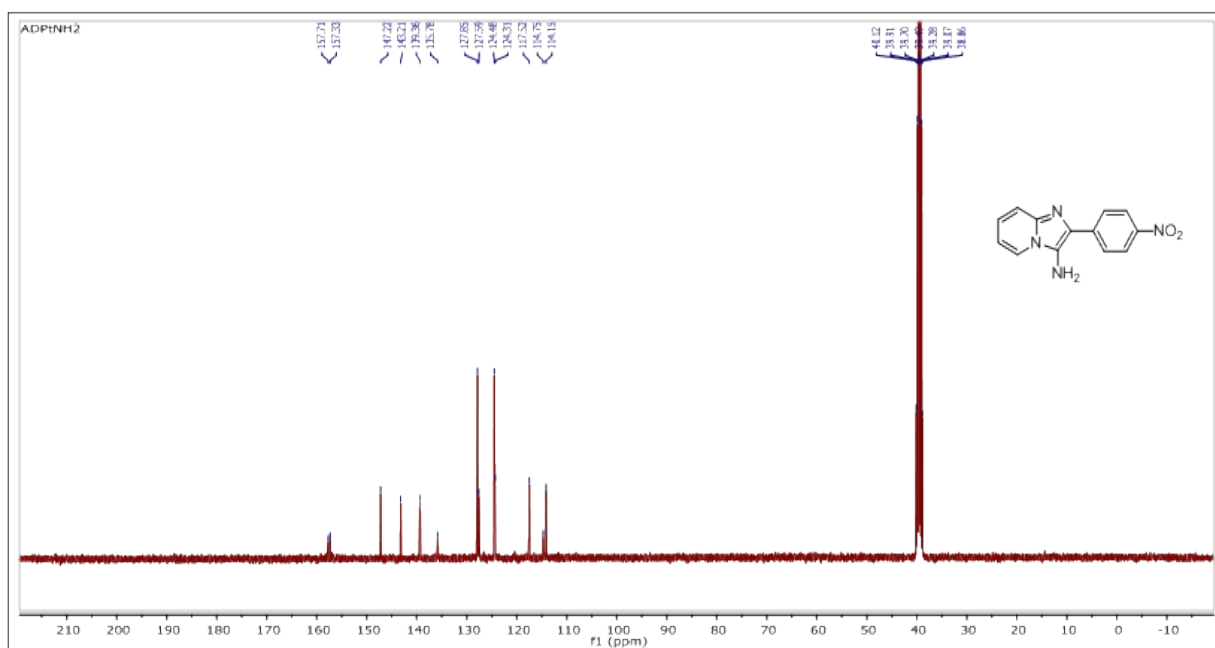
Supplementary Fig. 29 400 MHz (DMSO-d₆) ¹H NMR spectrum of 2-(4-aminophenyl)-N-(tert-butyl)imidazo[1,2-a]pyridin-3-amine (12b).



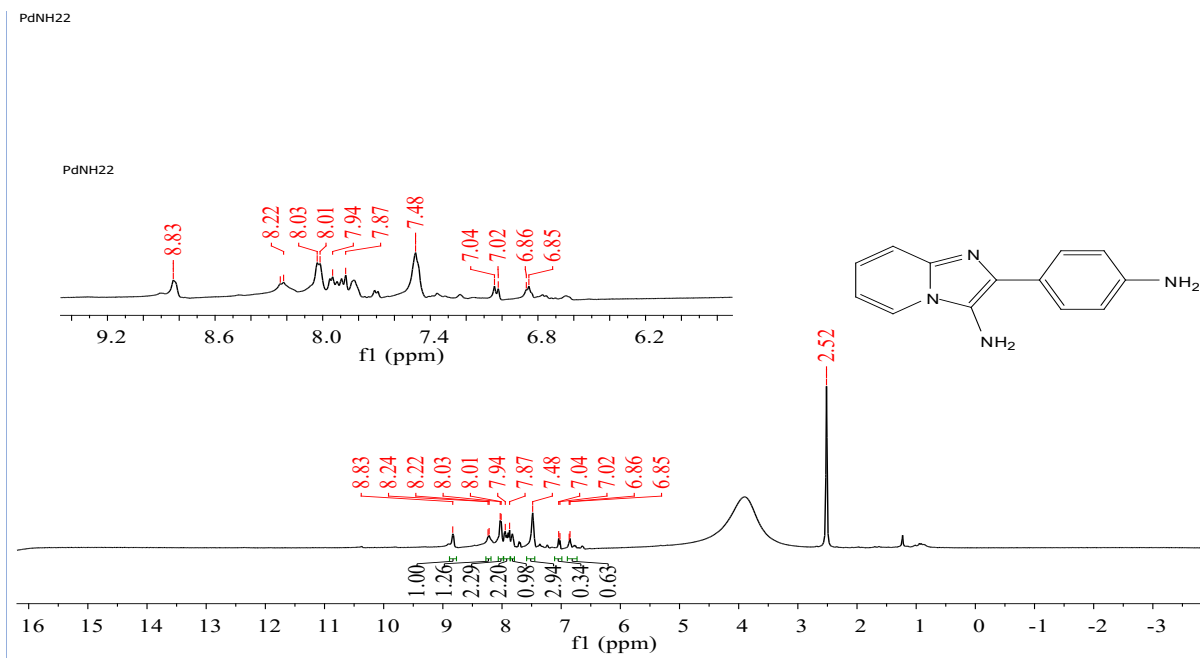
Supplementary Fig. 30 100 MHz (DMSO-d₆) ¹³C NMR spectrum of 2-(4-aminophenyl)-N-(tert-butyl)imidazo[1,2-a]pyridin-3-amine (12b).



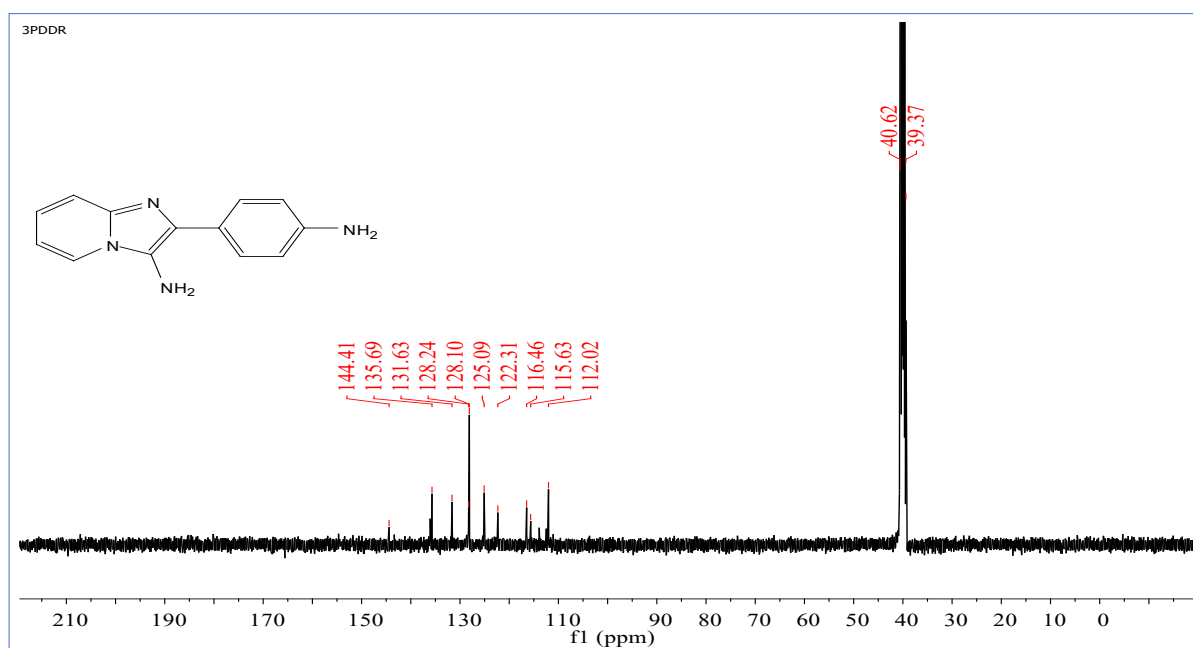
Supplementary Fig. 31 400 MHz (DMSO-d₆) ¹H NMR spectrum of 2-(4-nitrophenyl)imidazo[1,2-a]pyridin-3-amine (12c).



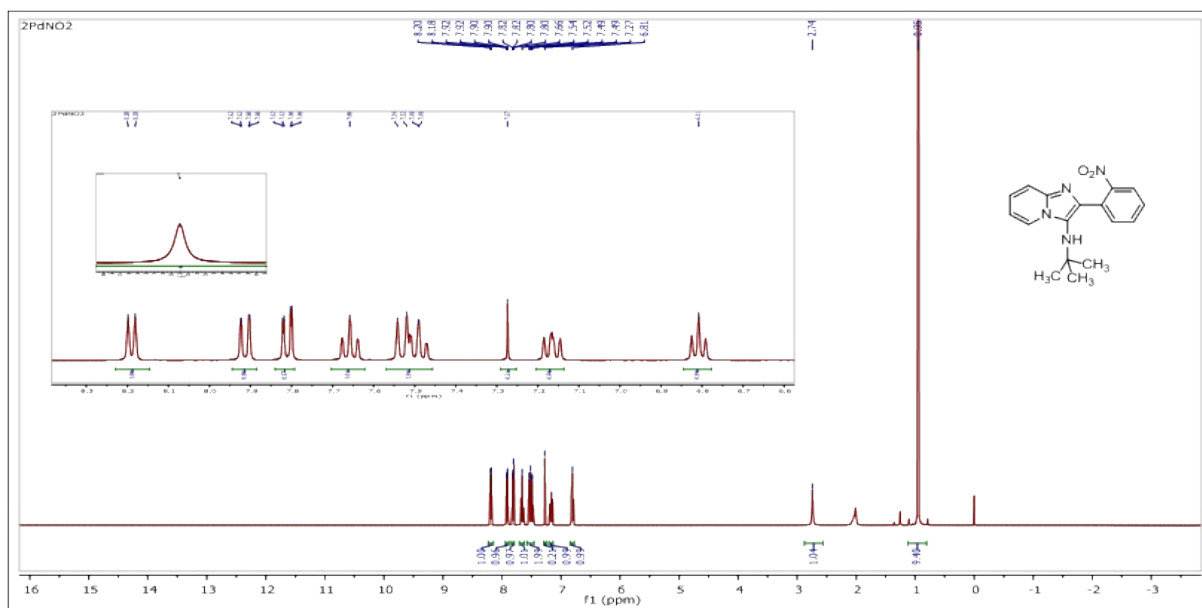
Supplementary Fig. 32 100 MHz (DMSO-d₆) ¹³C NMR spectrum of 2-(4-nitrophenyl)imidazo[1,2-a]pyridin-3-amine (12c).



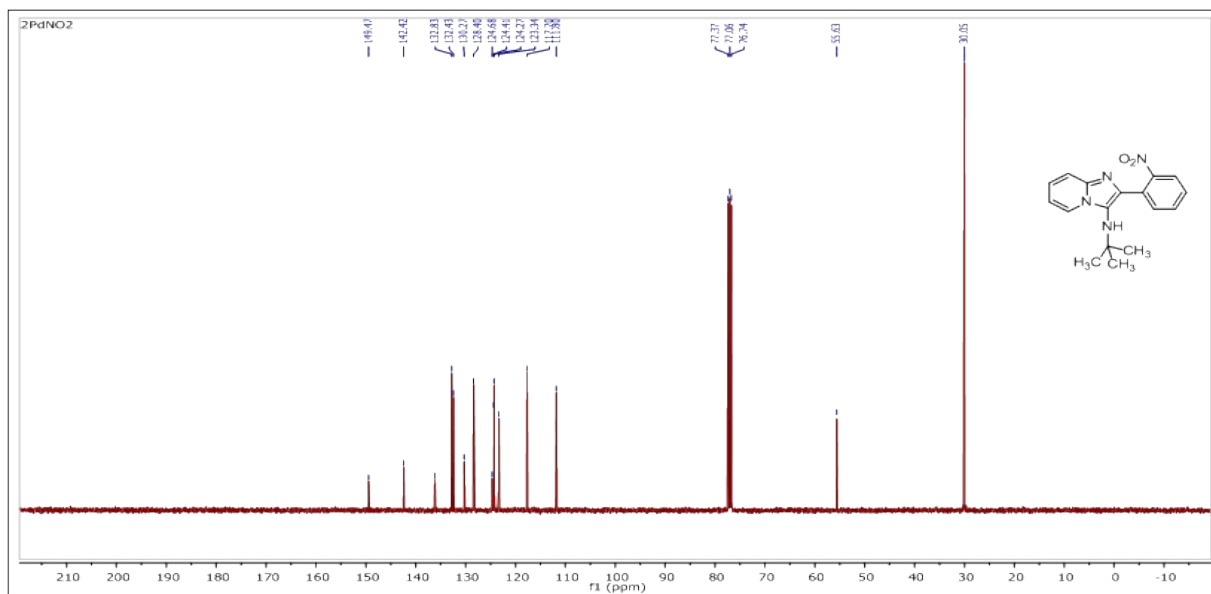
Supplementary Fig. 33 400 MHz (DMSO-d₆) ¹H NMR spectrum of 2-(4-aminophenyl)imidazo[1,2-a]pyridin-3-amine (12d).



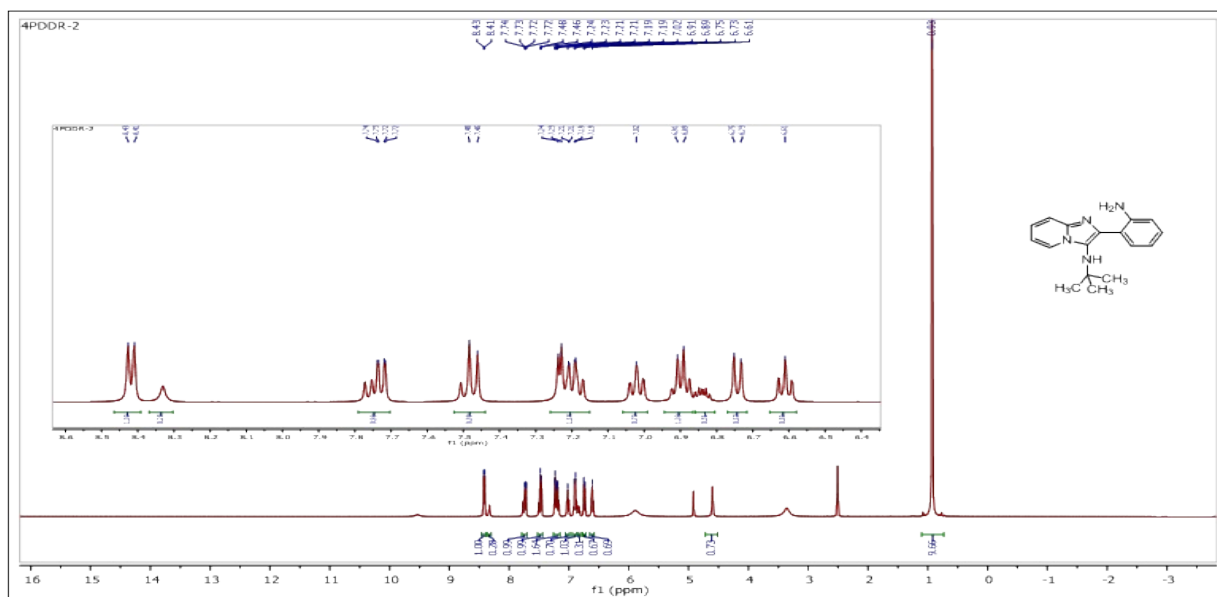
Supplementary Fig. 34 100 MHz (DMSO-d₆) ¹³C NMR spectrum of 2-(4-aminophenyl)imidazo[1,2-a]pyridin-3-amine (12d).



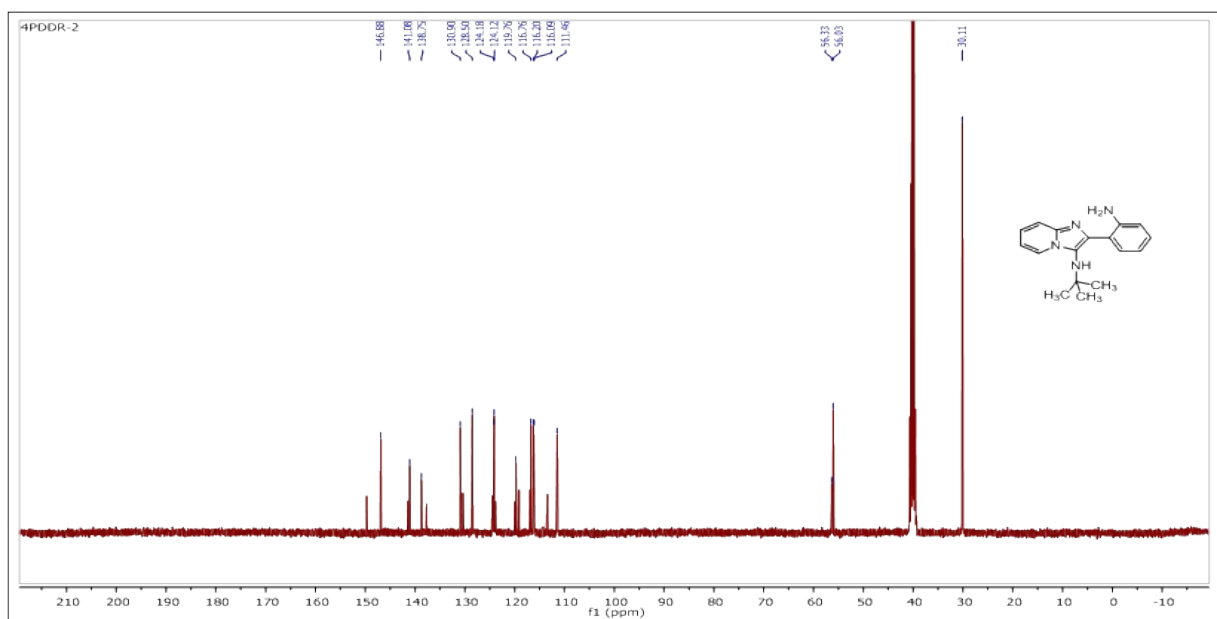
Supplementary Fig. 35 400 MHz (CDCl₃) ¹H NMR spectrum of N-(tert-butyl)-2-(2-nitrophenyl)imidazo[1,2-a]pyridin-3-amine (12e).



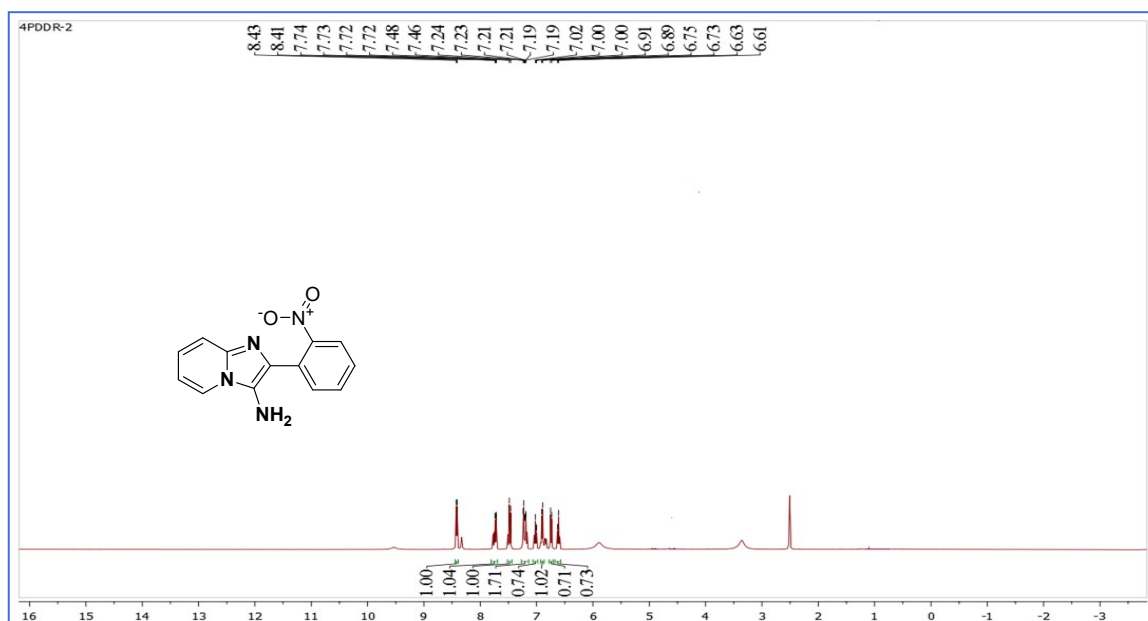
Supplementary Fig. 36 100 MHz (CDCl₃) ¹³C NMR spectrum of N-(tert-butyl)-2-(2-nitrophenyl)imidazo[1,2-a]pyridin-3-amine (12e).



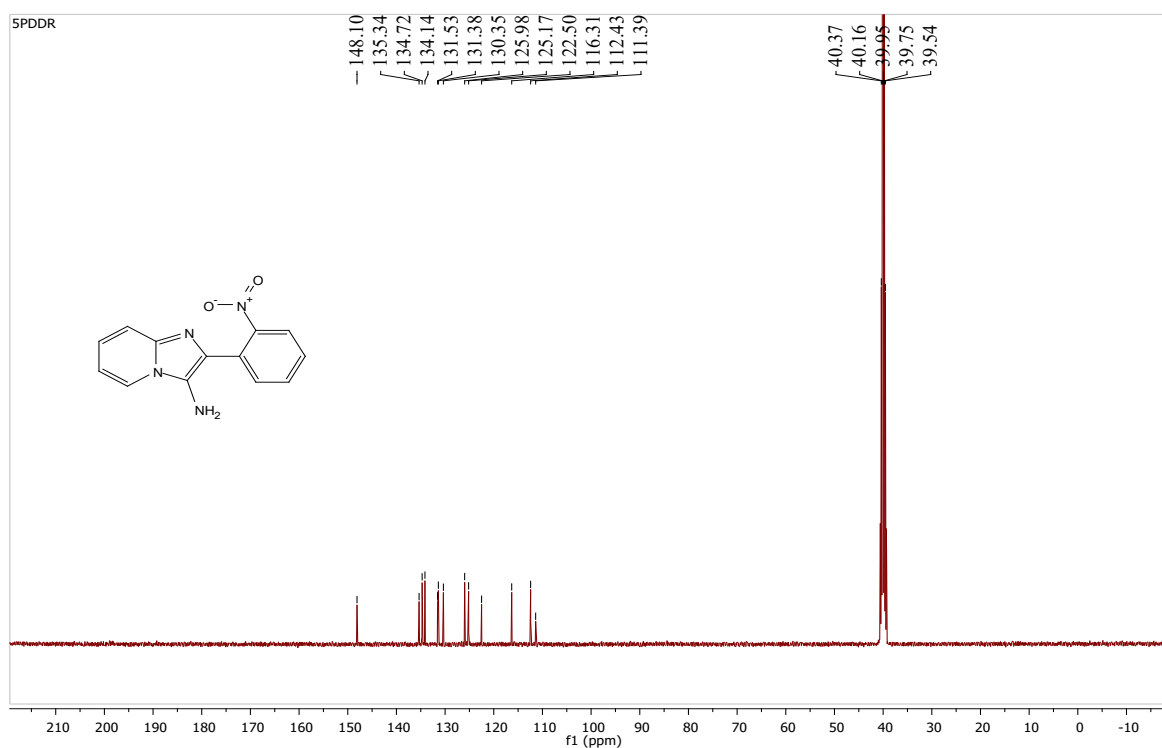
Supplementary Fig. 37 400 MHz (DMSO-d₆) ¹H NMR spectrum of 2-(2-aminophenyl)-N-(tert-butyl)imidazo[1,2-a]pyridin-3-amine (12f).



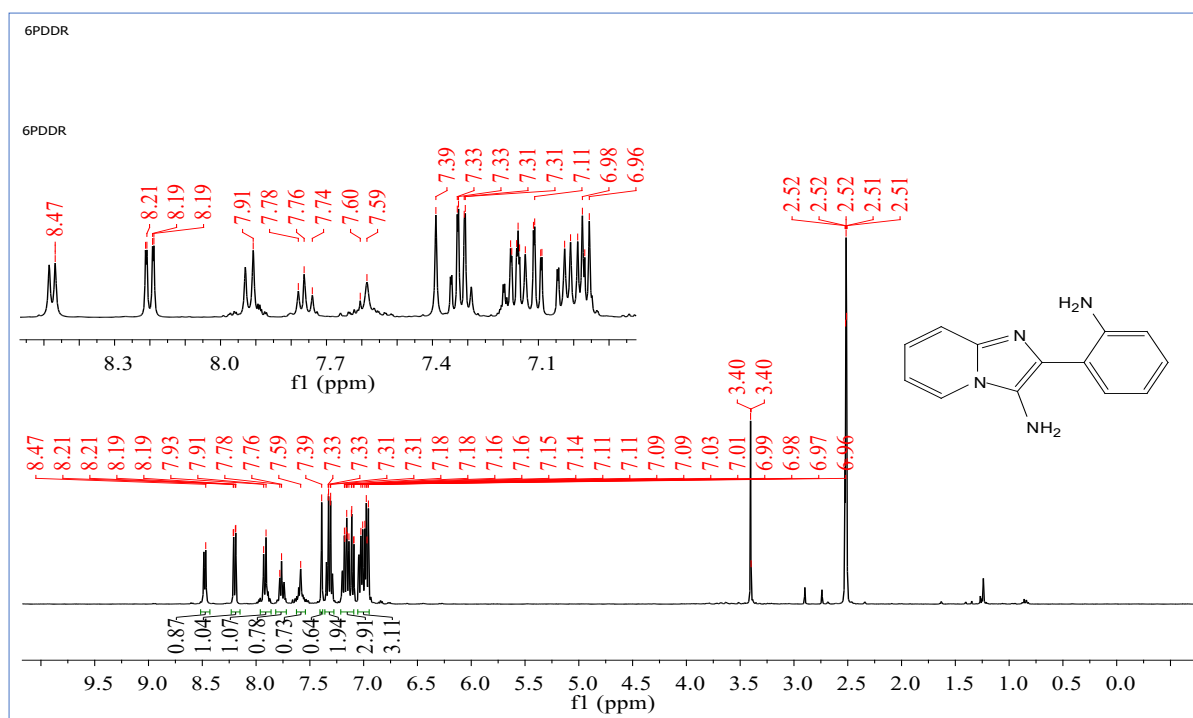
Supplementary Fig. 38 100 MHz (DMSO-d₆) ¹³C NMR spectrum of 2-(2-aminophenyl)-N-(tert-butyl)imidazo[1,2-a]pyridin-3-amine (12f).



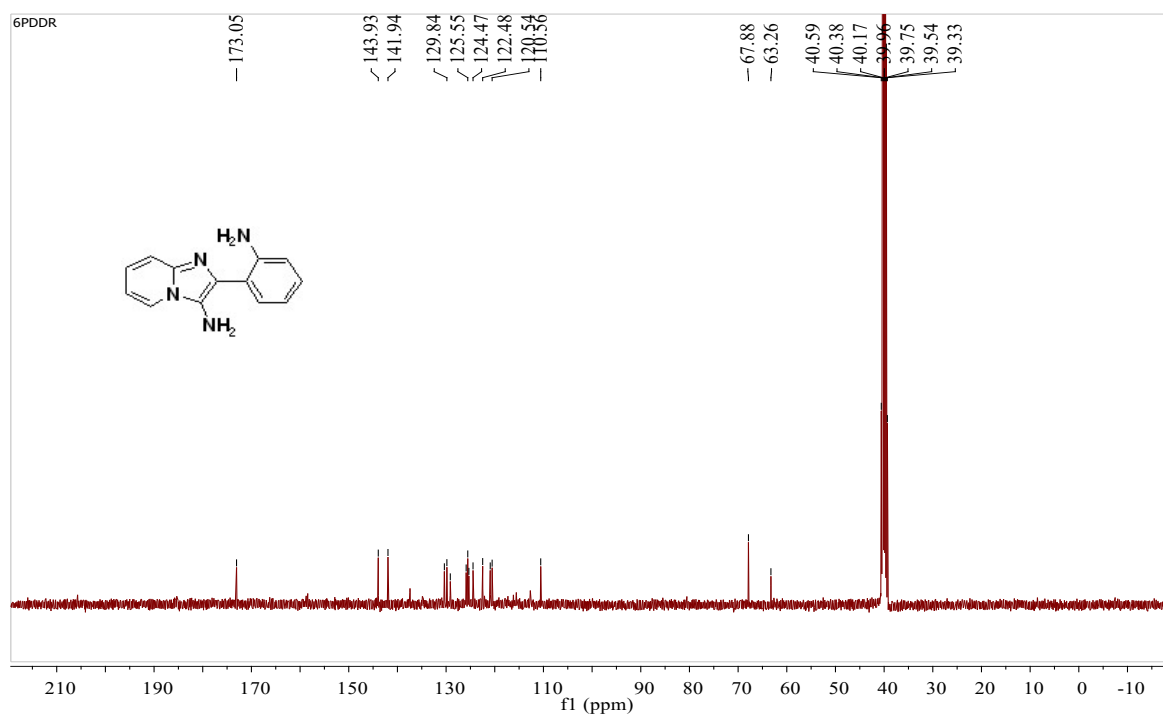
Supplementary Fig. 39 400 MHz (DMSO-d₆) ¹H NMR spectrum of 2-(2-nitrophenyl)imidazo[1,2-a]pyridin-3-amine (12g).



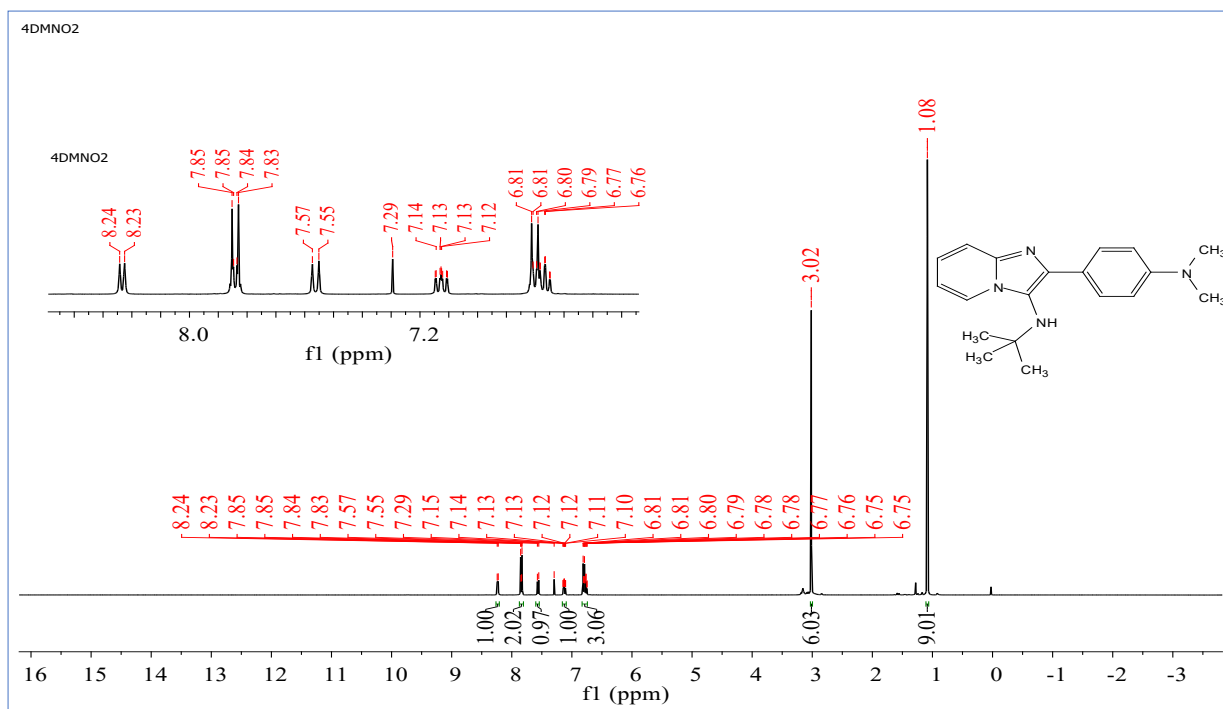
Supplementary Fig. 40 100 MHz (DMSO-d₆) ¹³C NMR spectrum of 2-(2-nitrophenyl)imidazo[1,2-a]pyridin-3-amine (12g).



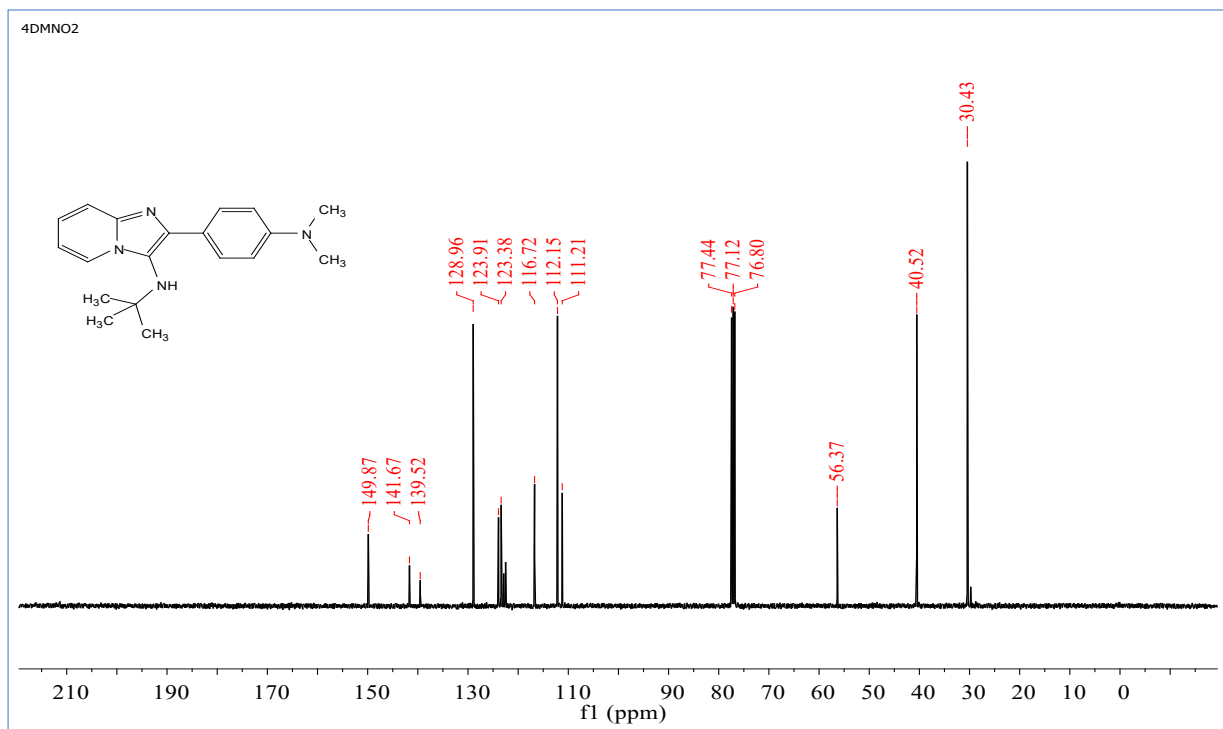
Supplementary Fig. 41 400 MHz (DMSO-d₆) ¹H NMR spectrum of 2-(2-aminophenyl)imidazo[1,2-a]pyridin-3-amine (12h).



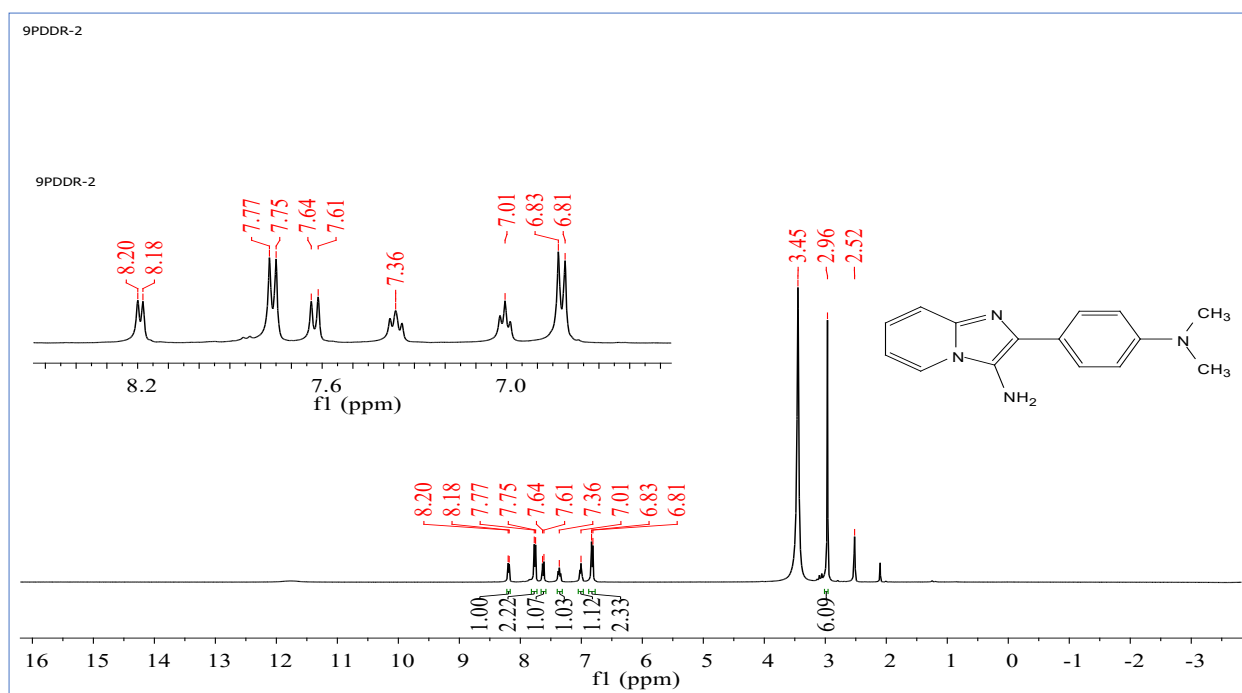
Supplementary Fig. 42 100 MHz (DMSO-d₆) ¹³C NMR spectrum of 2-(2-aminophenyl)imidazo[1,2-a]pyridin-3-amine (12h).



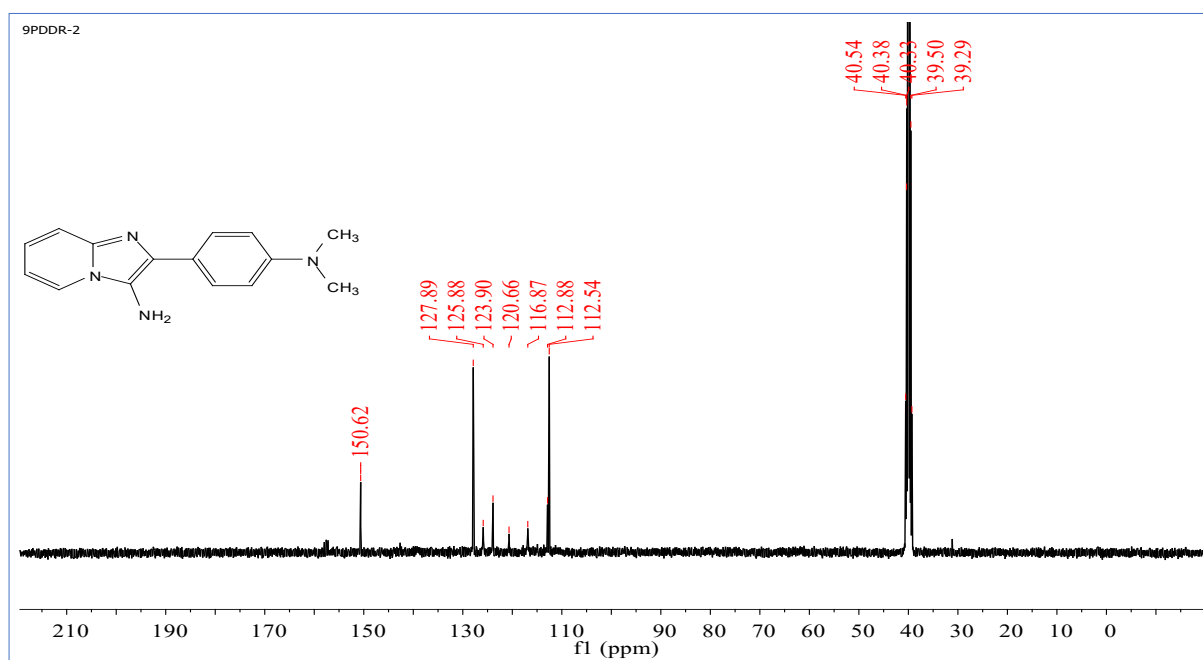
Supplementary Fig. 43 400 MHz (CDCl₃) ¹H NMR spectrum of N-(tert-butyl)-2-(4-(dimethylamino)phenyl)imidazo[1,2-a]pyridin-3-amine (12i)



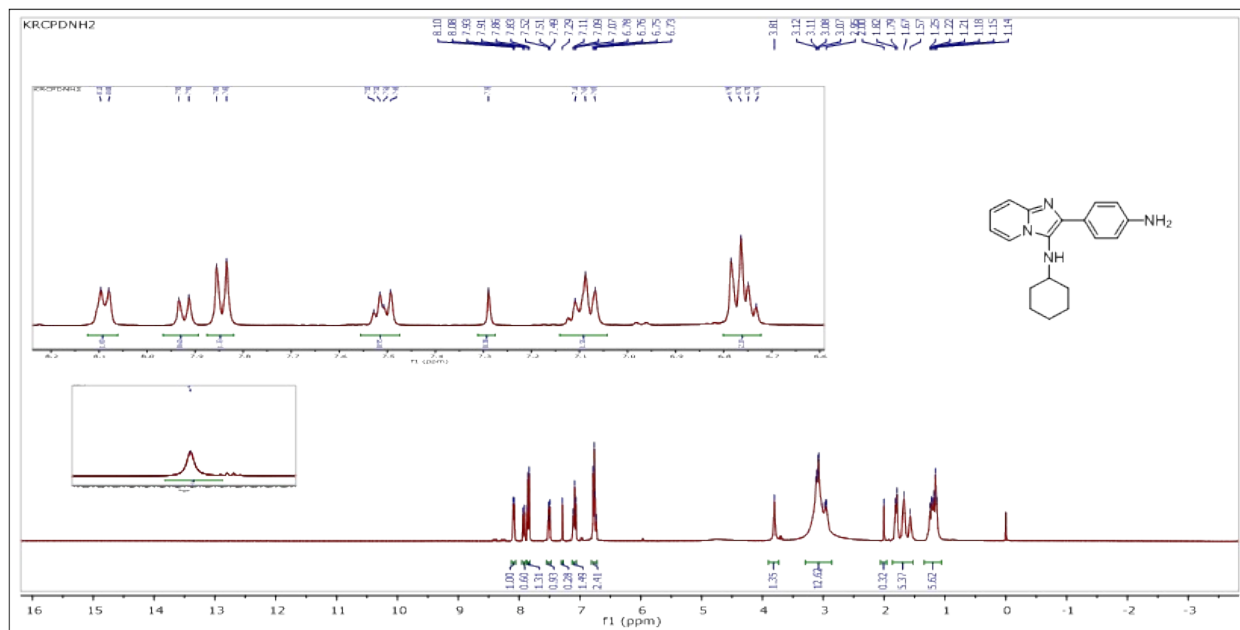
Supplementary Fig. 44 100 MHz (CDCl₃) ¹³C NMR spectrum of N-(tert-butyl)-2-(4-(dimethylamino)phenyl)imidazo[1,2-a]pyridin-3-amine (12i)



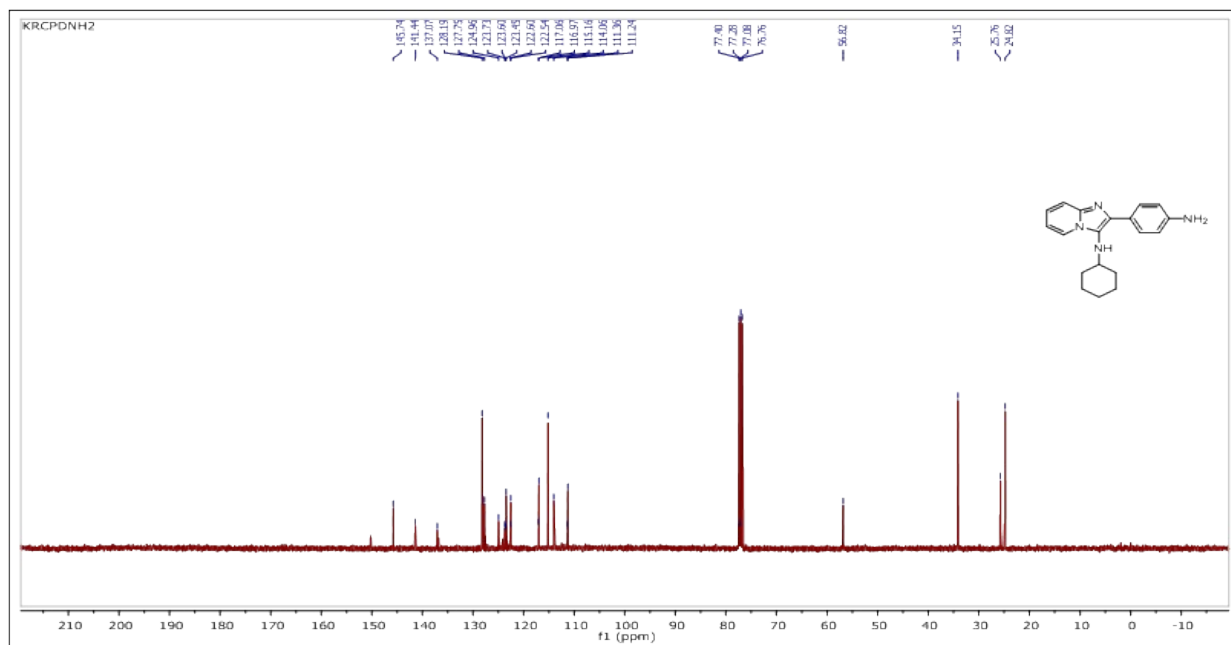
Supplementary Fig. 45 400 MHz (DMSO-d₆) ¹H NMR spectrum of 2-(4-(dimethylamino)phenyl)imidazo[1,2-a]pyridin-3-amine (12j).



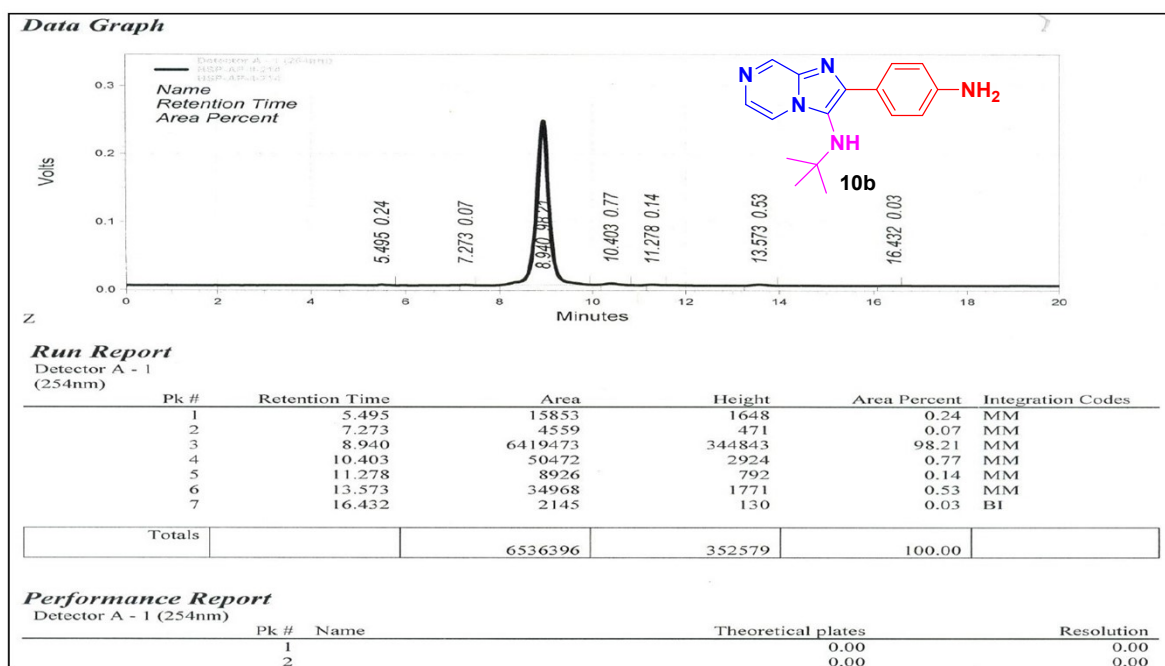
Supplementary Fig. 46 100 MHz (DMSO-d₆) ¹³C NMR spectrum of 2-(4-(dimethylamino)phenyl)imidazo[1,2-a]pyridin-3-amine (12j).



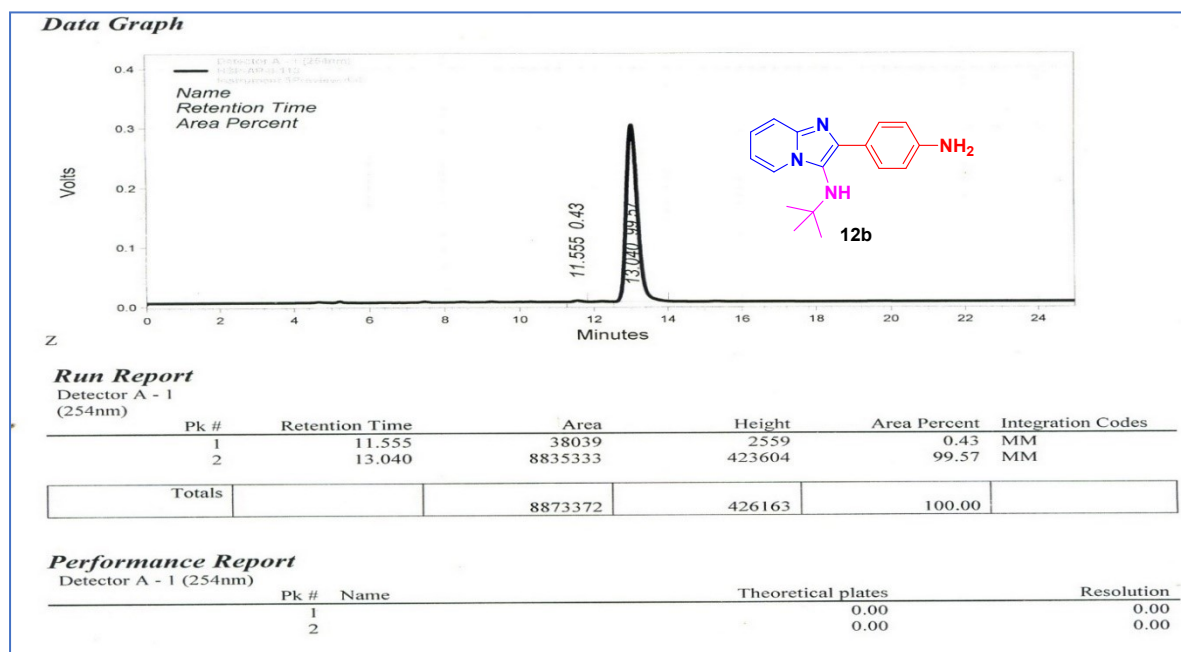
Supplementary Fig. 49 400 MHz (CDCl₃) ¹H NMR spectrum of 2-(4-aminophenyl)-N-cyclohexylimidazo[1,2-a]pyridin-3-amine (12).



Supplementary Fig. 50 100 MHz (CDCl₃) ¹³C NMR spectrum of 2-(4-aminophenyl)-N-cyclohexylimidazo[1,2-a]pyridin-3-amine (12).



Supplementary Fig. 51 HPLC profile of 2-(4-aminophenyl)-N-(tert-butyl)imidazo[1,2-a]pyrazin-3-amine (10b).



Supplementary Fig. 52 HPLC profile of 2-(4-aminophenyl)-N-(tert-butyl)imidazo[1,2-a]pyridin-3-amine (12b).