

Supplementary file

Synthesis, crystal structure, and antiviral evaluation of new imidazopyridine-schiff base derivatives: *in vitro* and *in silico* anti-HIV studies

Mohamed Azzouzi^{1*}, Abderrahim Ait Ouchoui², Omar Azougagh¹, Salah Eddine El Hadad², Mohamed Abou-salama¹, Adyl Oussaid¹, Christophe Pannecouque³, Taoufik Rohand^{1*}

¹ *Laboratory of Molecular Chemistry, Materials and Environment (LCM2E), Department of Chemistry, Multidisciplinary Faculty of Nador, University Mohamed I, 60700 Nador, Morocco.*

² *Chemical and Biochemical Sciences-Green Process Engineering, University Mohammed VI Polytechnic, Ben Guerir, Morocco.*

³ *Rega Institute for Medical Research, Laboratory of Virology and Chemotherapy, K.U. Leuven, Leuven, B-3000, Belgium.*

*Corresponding authors: M. Azzouzi (azzouzi.mohamed@ump.ac.ma) and T. Rohand (t.rohand@ump.ac.ma)

**¹H-NMR , ¹³C-NMR and LC-MS(ESI⁺) of
(E)-6-chloro-N-(4-nitrobenzylidene)-2-phenylimidazo[1,2-a]pyridin-3-amine (4a)**

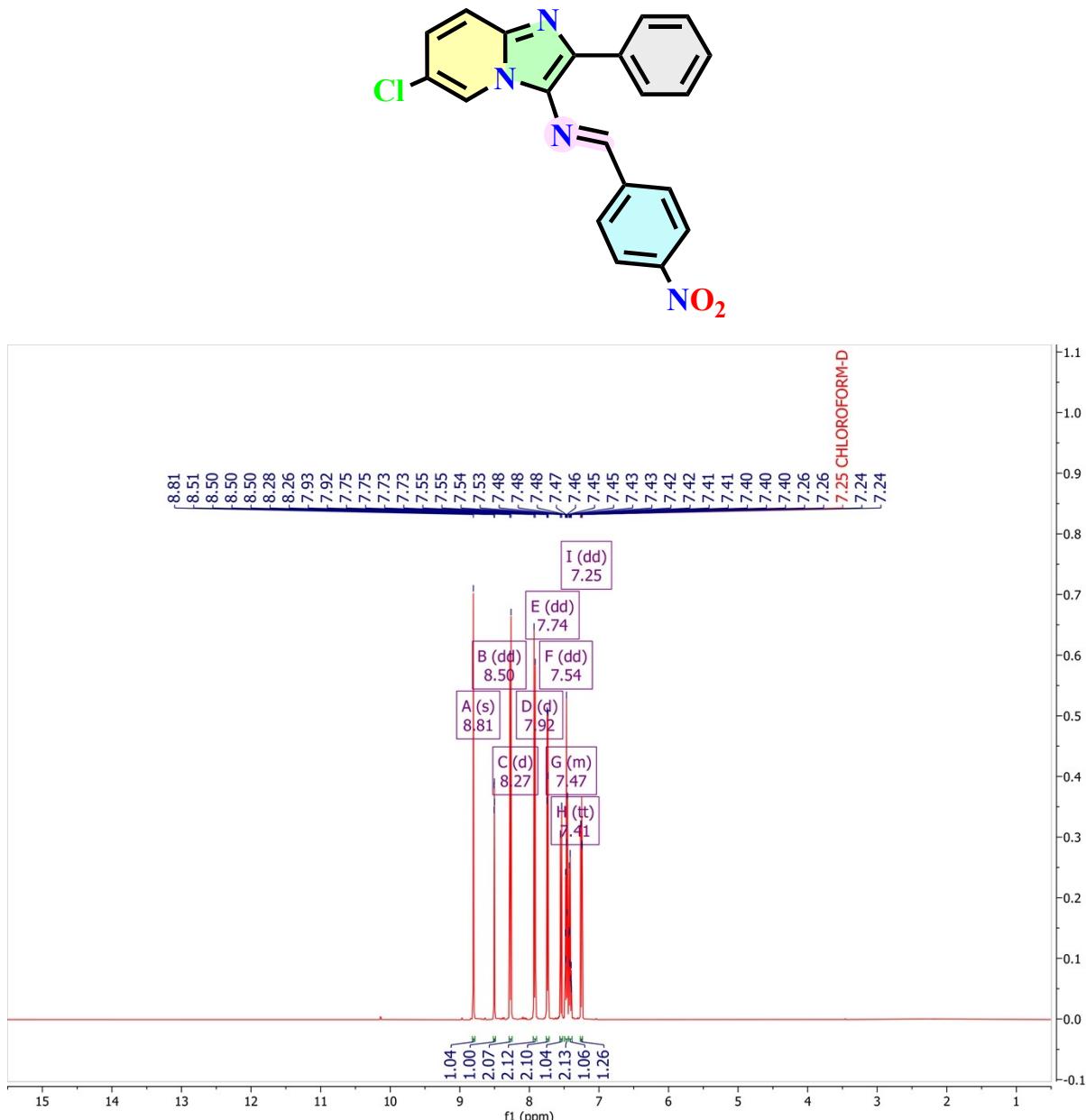


Figure S1. ¹H NMR spectra of (4a)

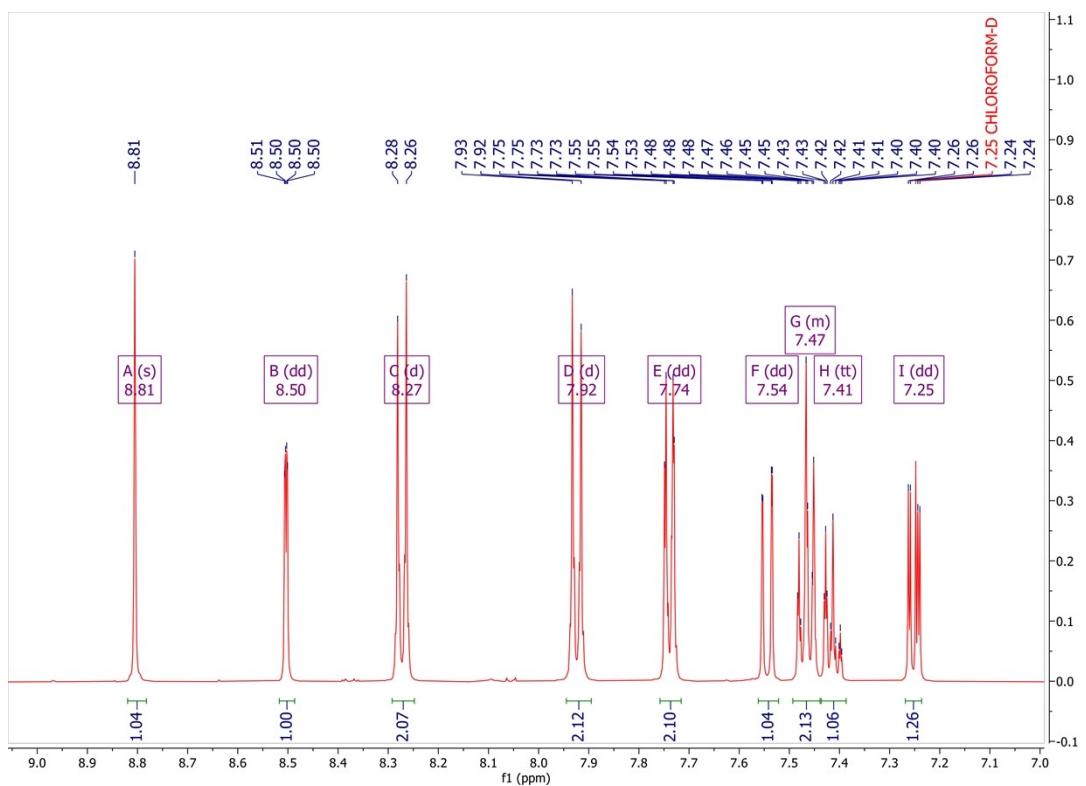


Figure S2. ^1H NMR spectra (9-7 ppm) of (4a)

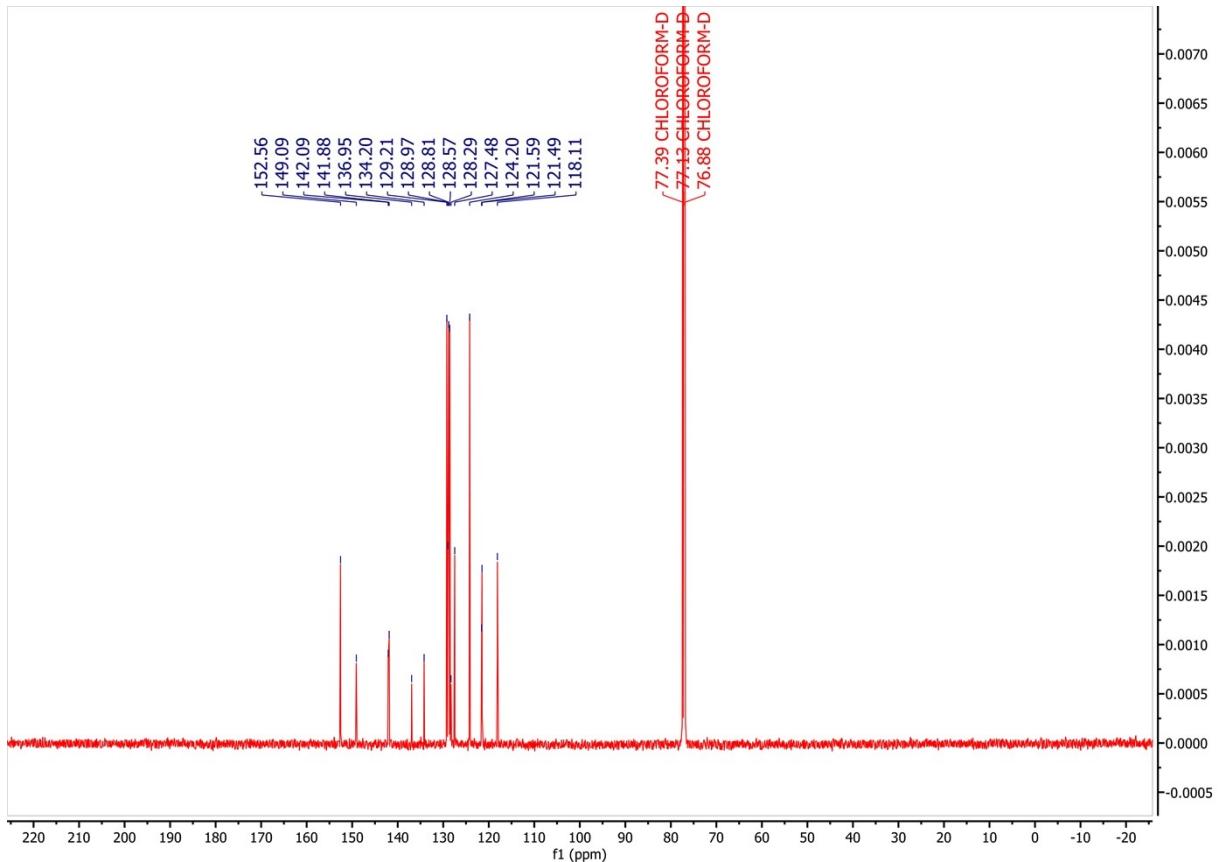


Figure S3. ^{13}C NMR spectra of (4a)

21P #17 RT: 0.15 AV: 1 NL: 1.16E6
T: FTMS + p ESI Full ms [300.0000-450.0000]

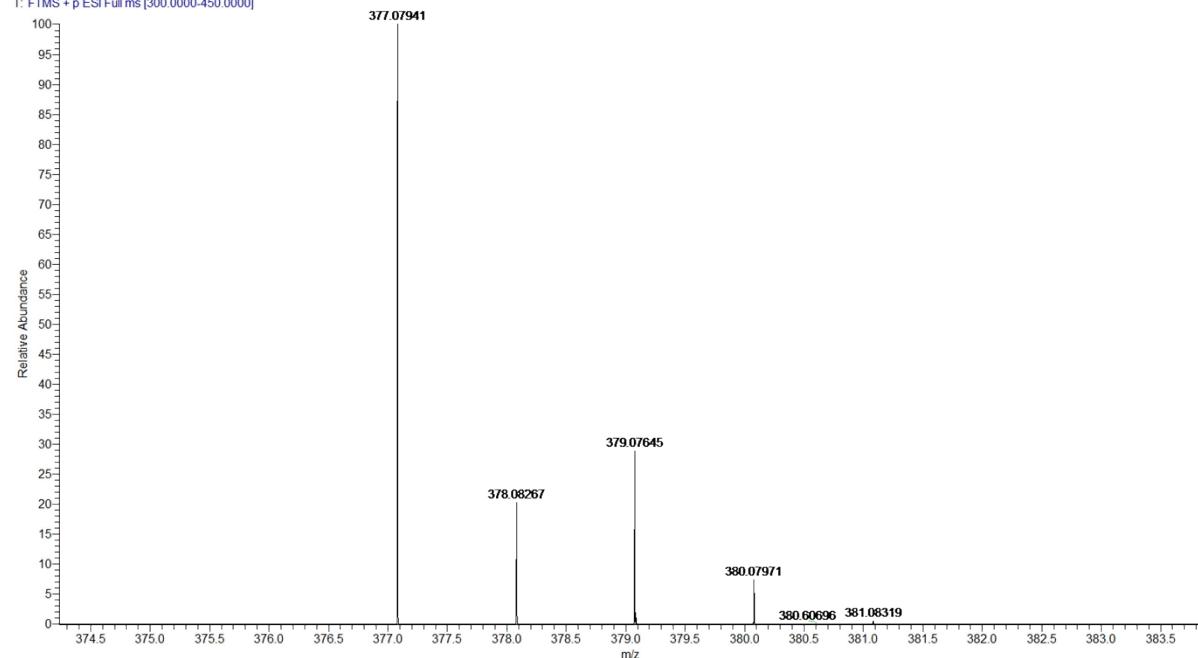
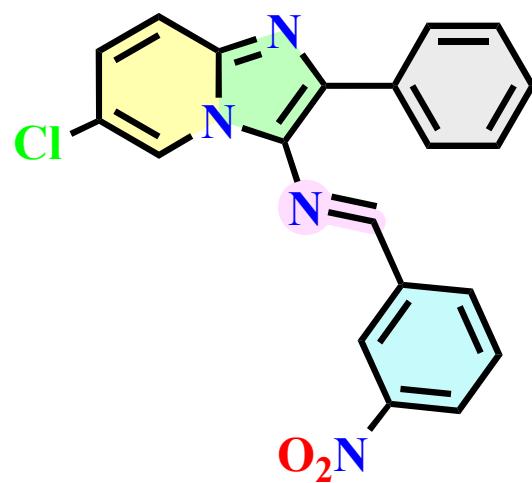


Figure S4. ESI⁺-MS spectra of (**4a**)

**¹H-NMR , ¹³C-NMR and LC-MS(ESI⁺) of
(E)-6-chloro-N-(3-nitrobenzylidene)-2-phenylimidazo[1,2-a]pyridin-3-amine (4b)**



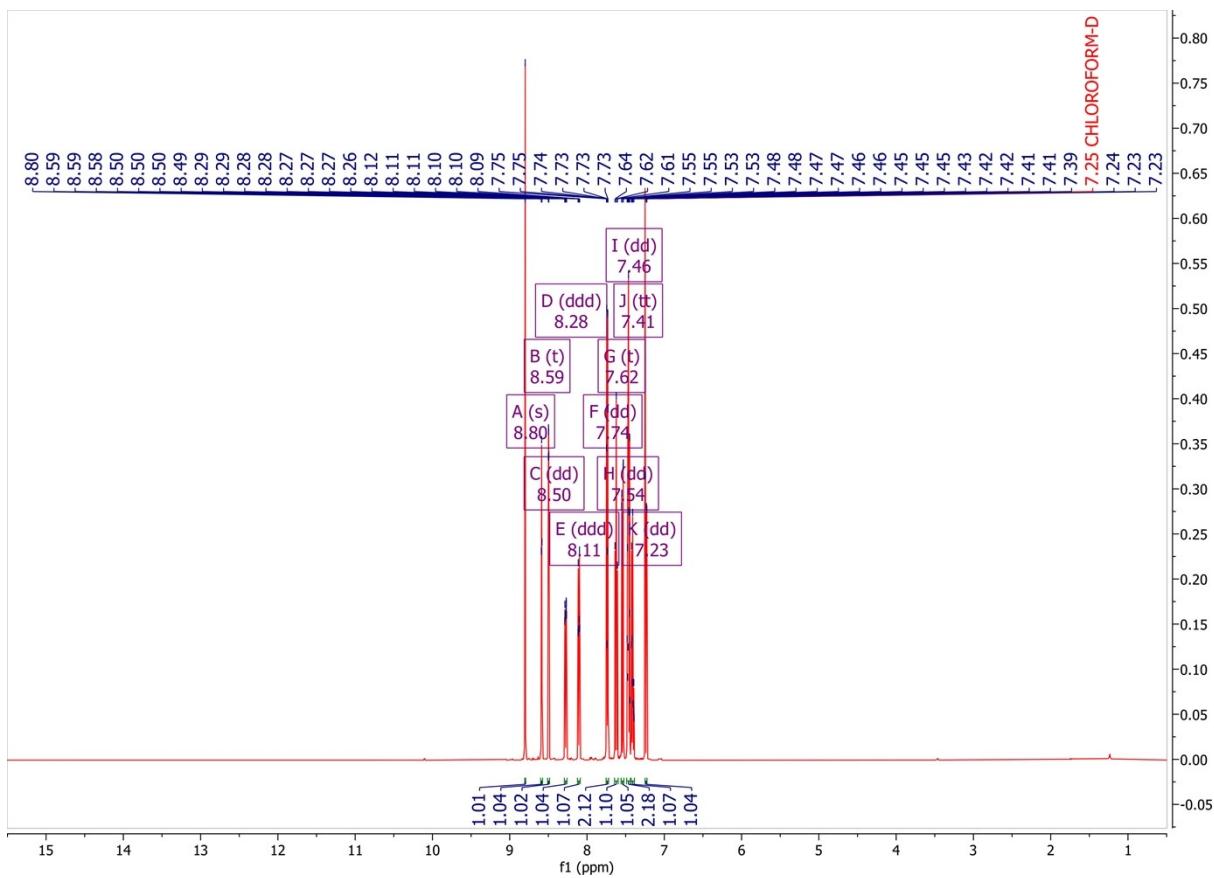


Figure S5. ^1H NMR spectra of (**4b**)

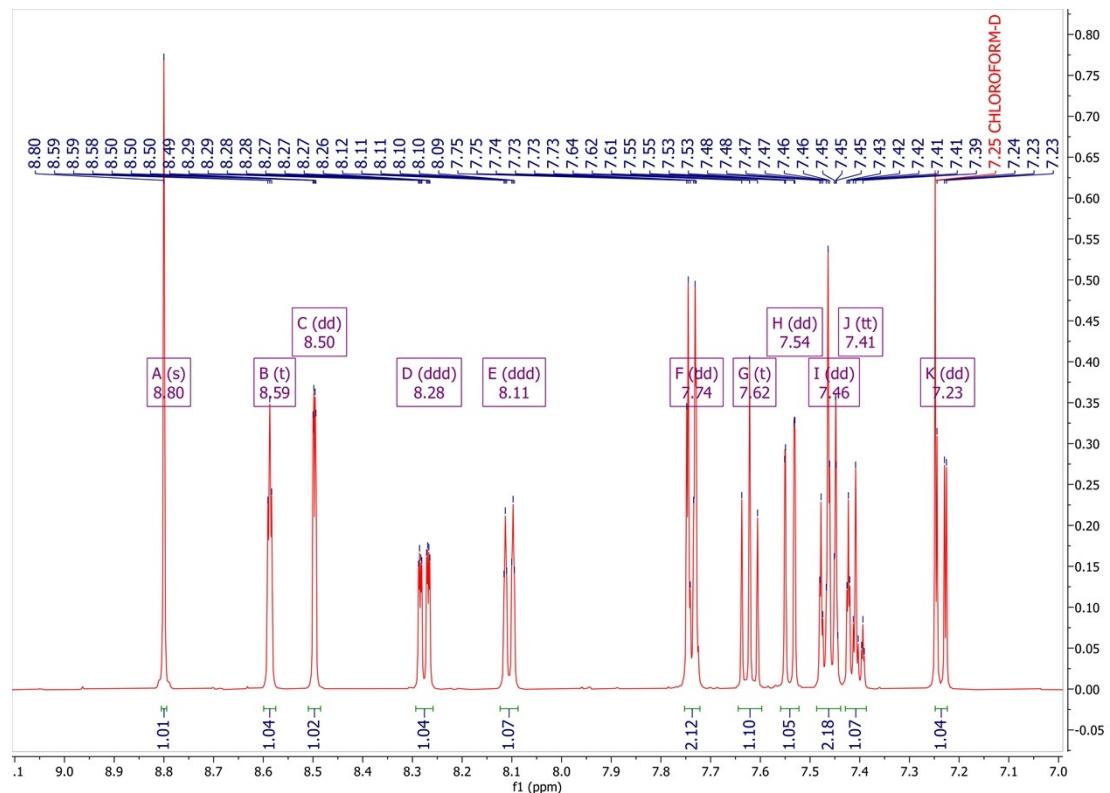


Figure S6. ^1H NMR spectra (9-7 ppm) of (**4b**)

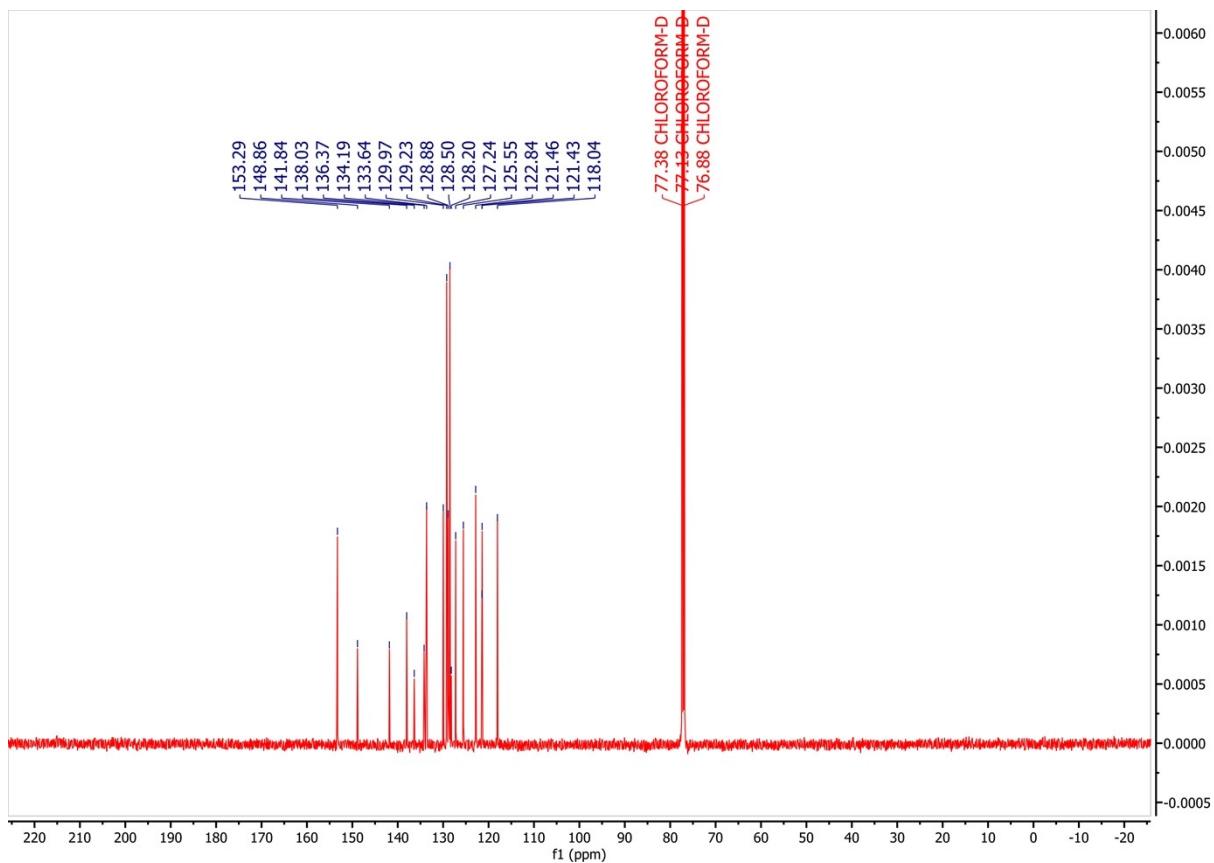


Figure S7. ^{13}C NMR spectra of (**4b**)

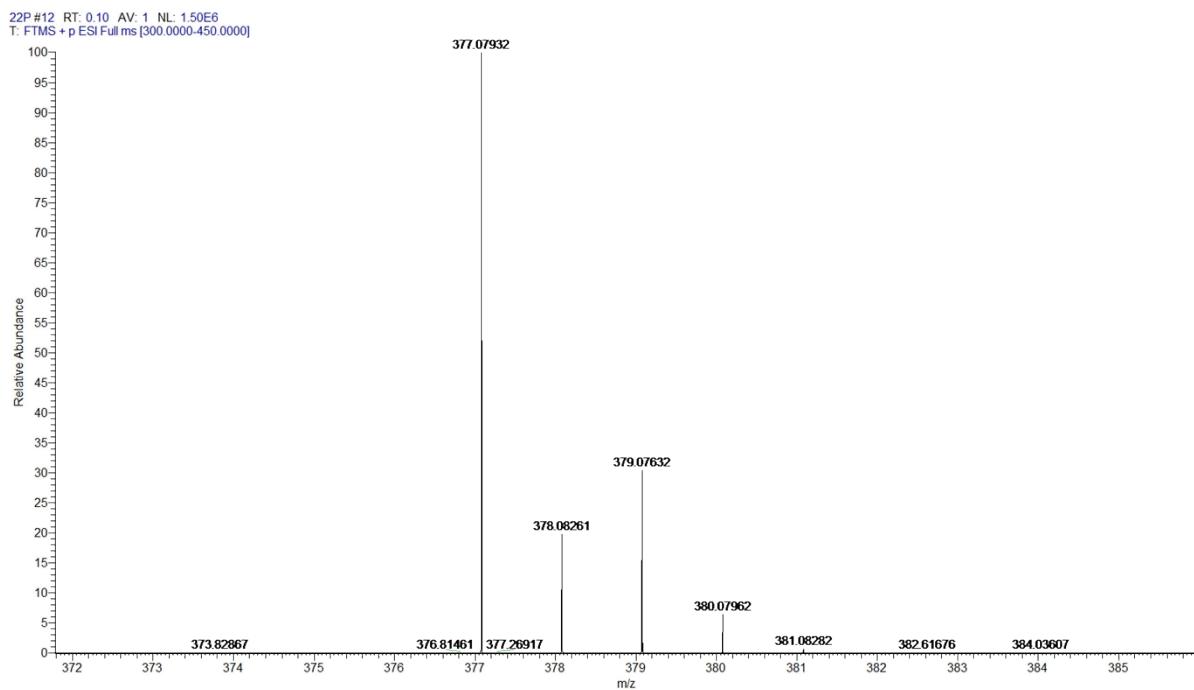


Figure S8. ESI $^+$ -MS spectra of (**4b**)

**¹H-NMR , ¹³C-NMR and LC-MS(ESI⁺) of
(E)-6-chloro-N-(2-nitrobenzylidene)-2-phenylimidazo[1,2-a]pyridin-3-amine (4c)**

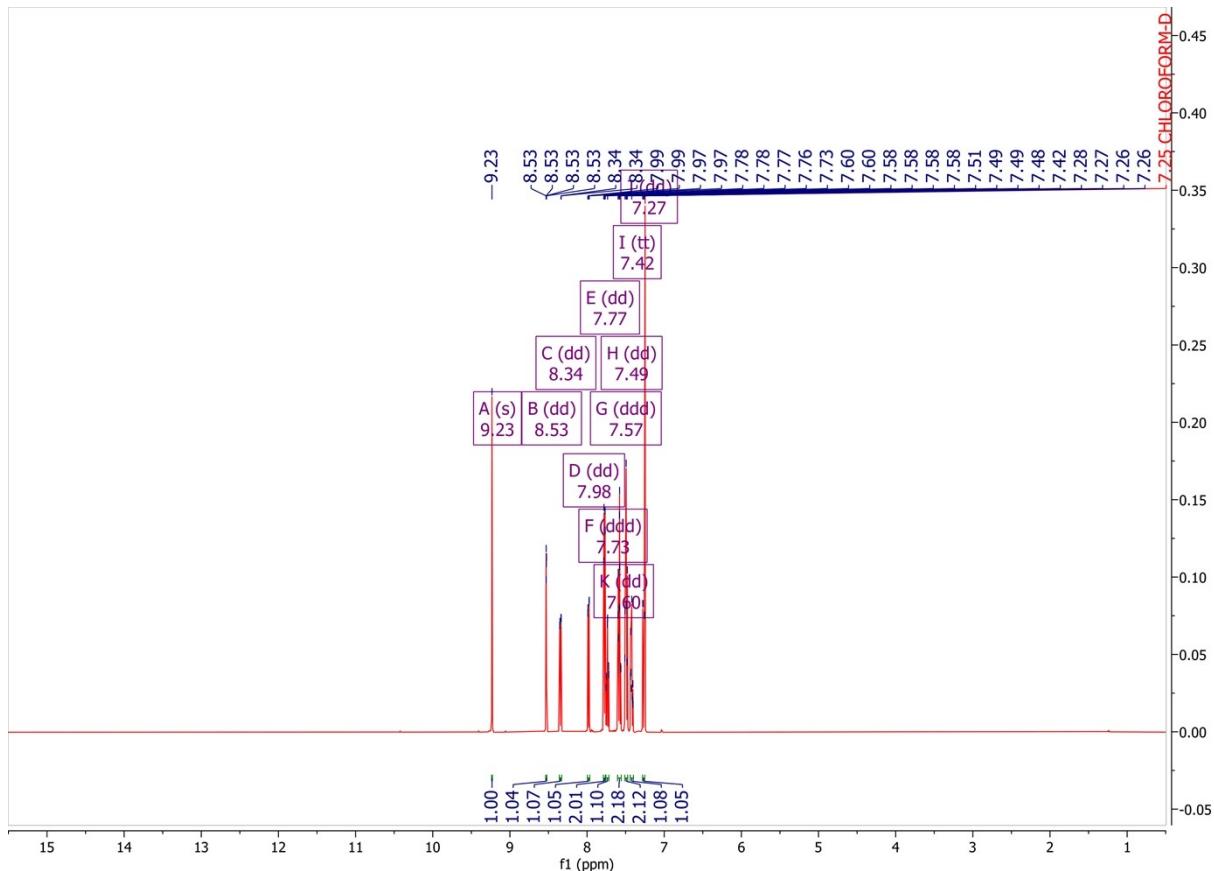
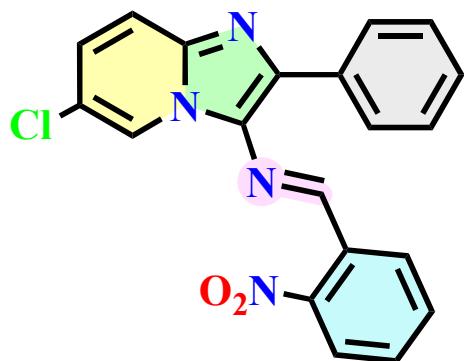


Figure S9. ¹H NMR spectra of (4c)



Figure S10. ^1H NMR spectra (9-7 ppm) of (**4c**)

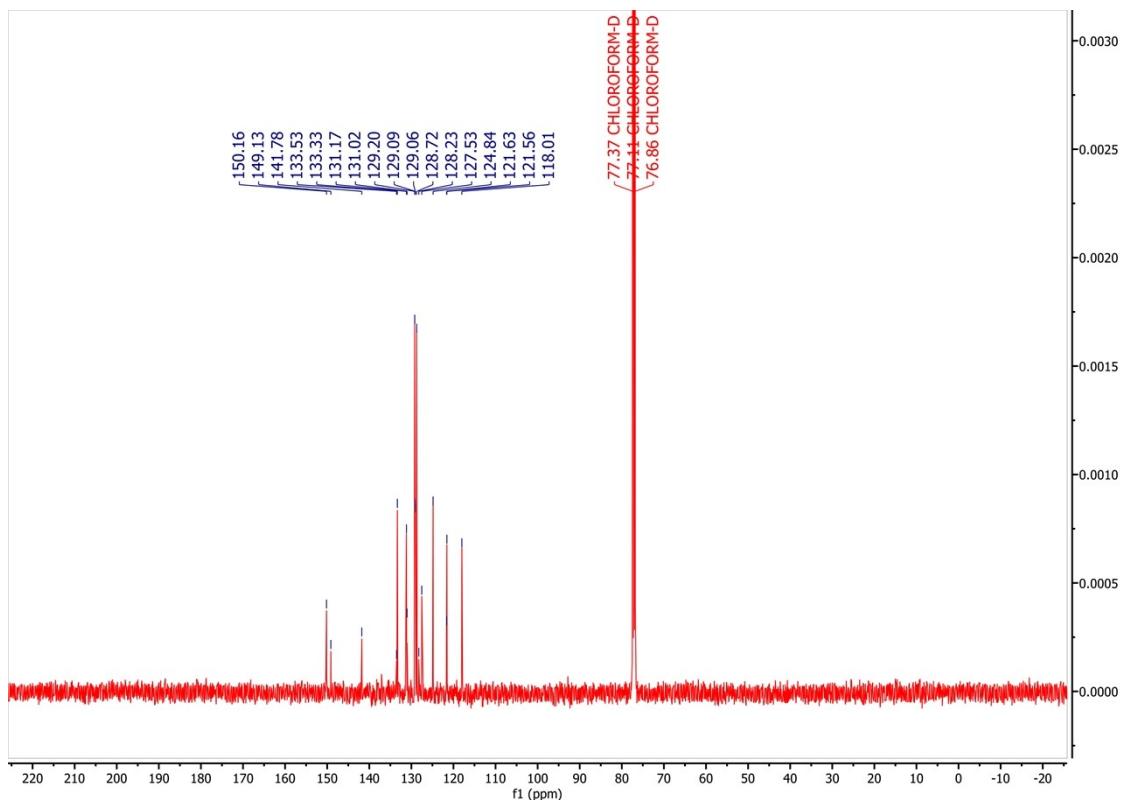


Figure S11. ^{13}C NMR spectra of (**4c**)

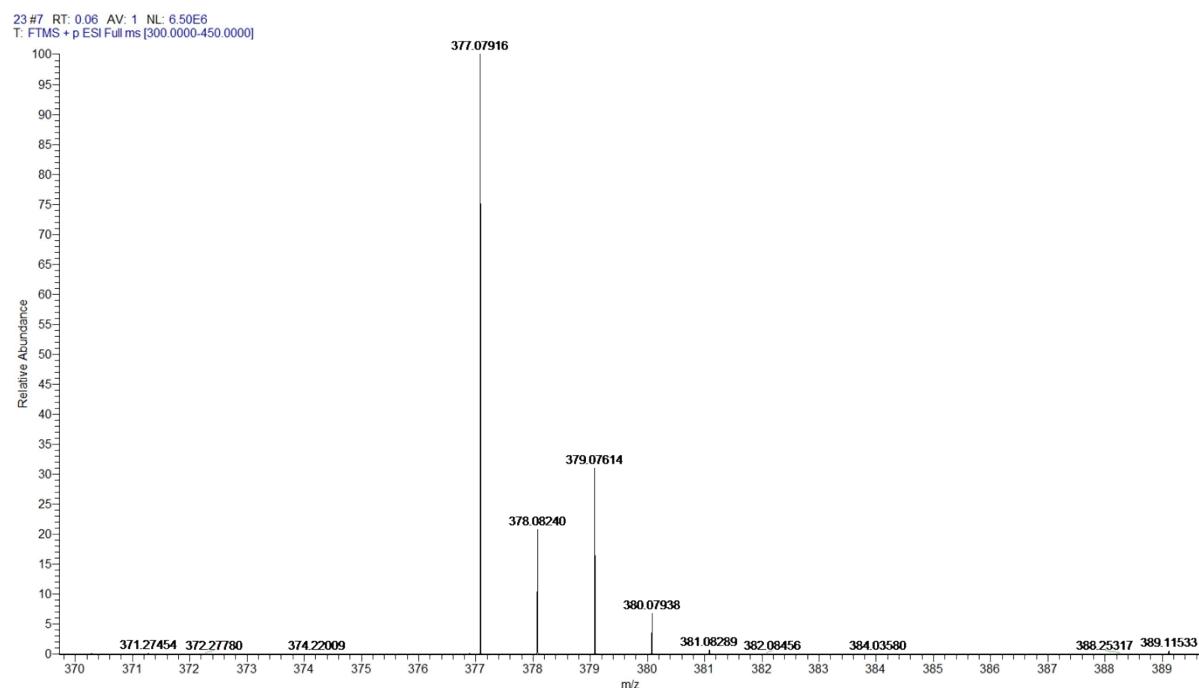
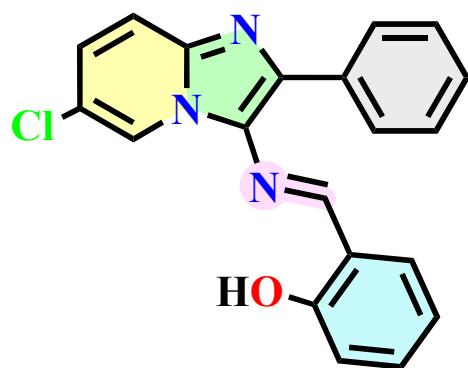


Figure S12. ESI⁺-MS spectra of (**4c**)

**¹H-NMR , ¹³C-NMR and LC-MS(ESI⁺) of
(E)-2-(((6-chloro-2-phenylimidazo[1,2-a]pyridin-3-yl)imino)methyl)phenol (4d)**



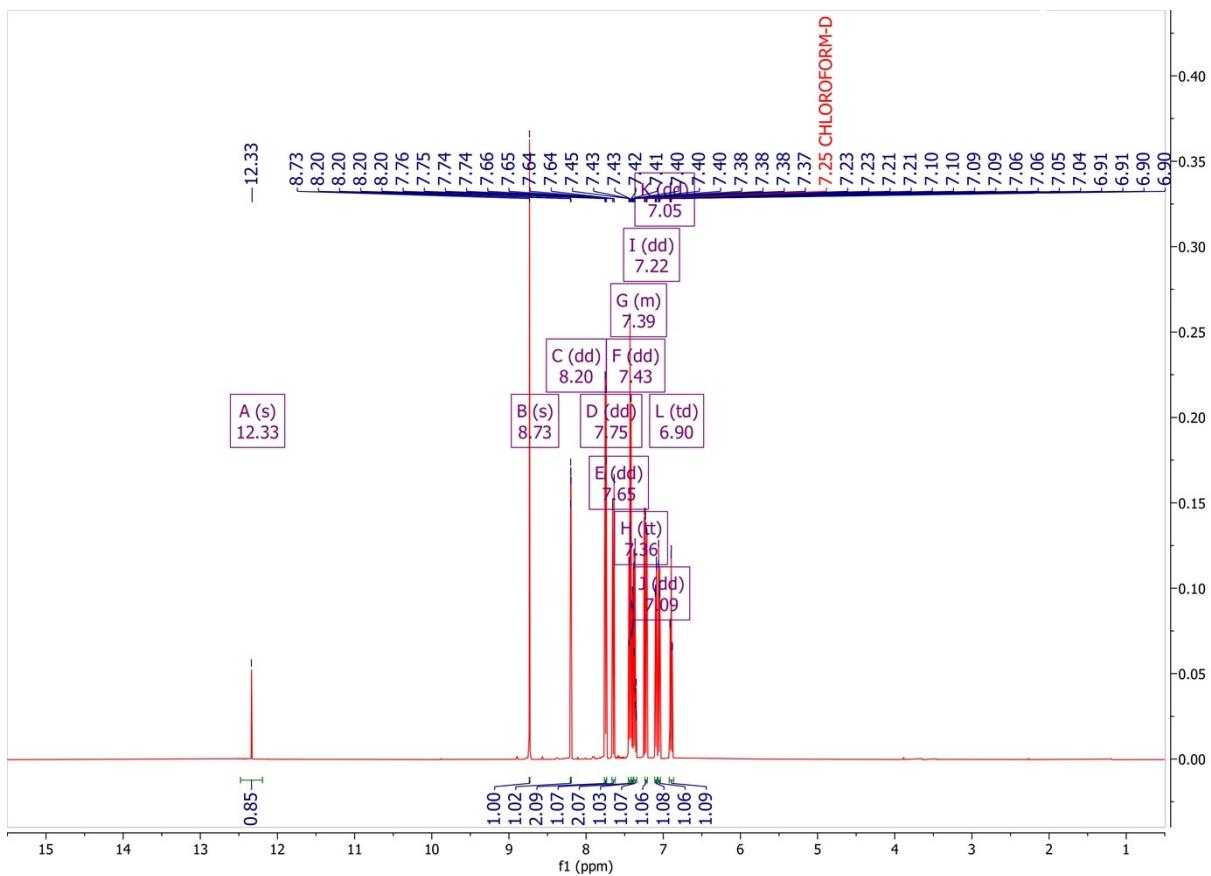


Figure S13. ^1H NMR spectra of (**4d**)

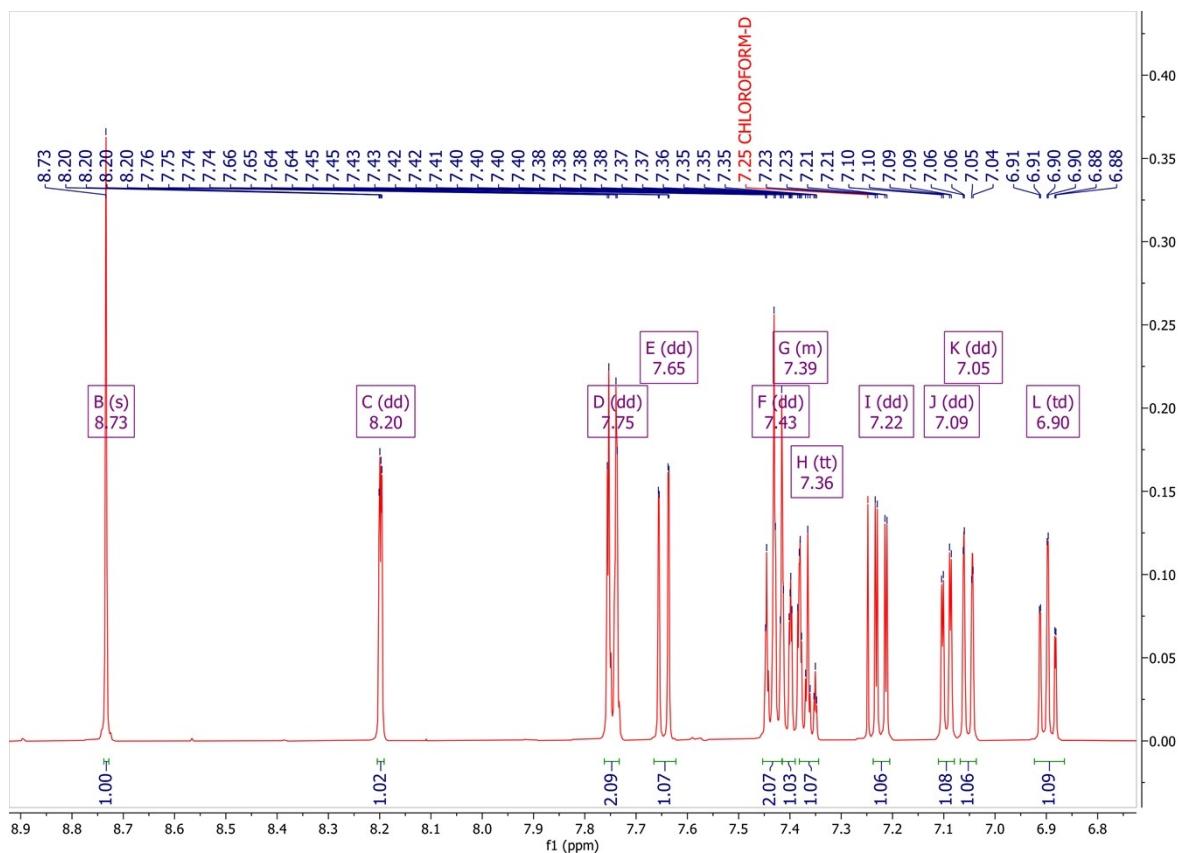


Figure S14. ^1H NMR spectra (9-7 ppm) of (**4d**)

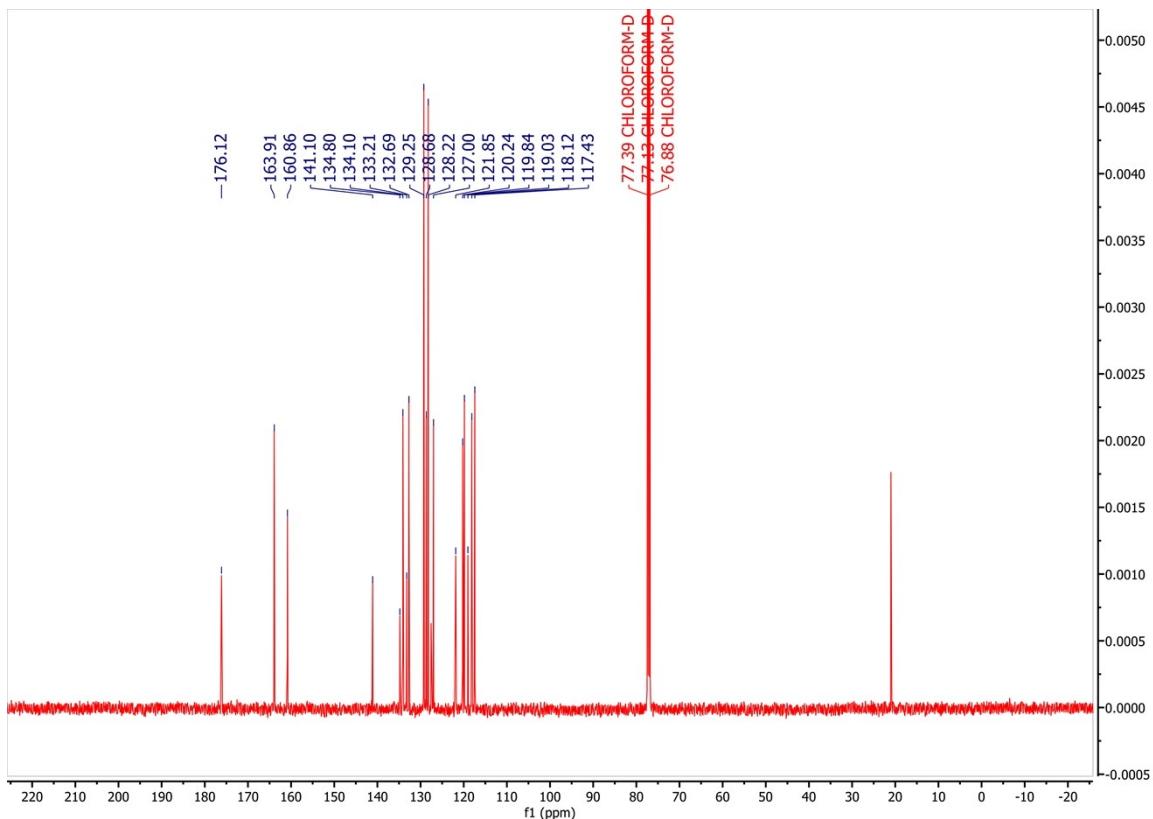


Figure S15. ^{13}C NMR spectra of (**4d**)

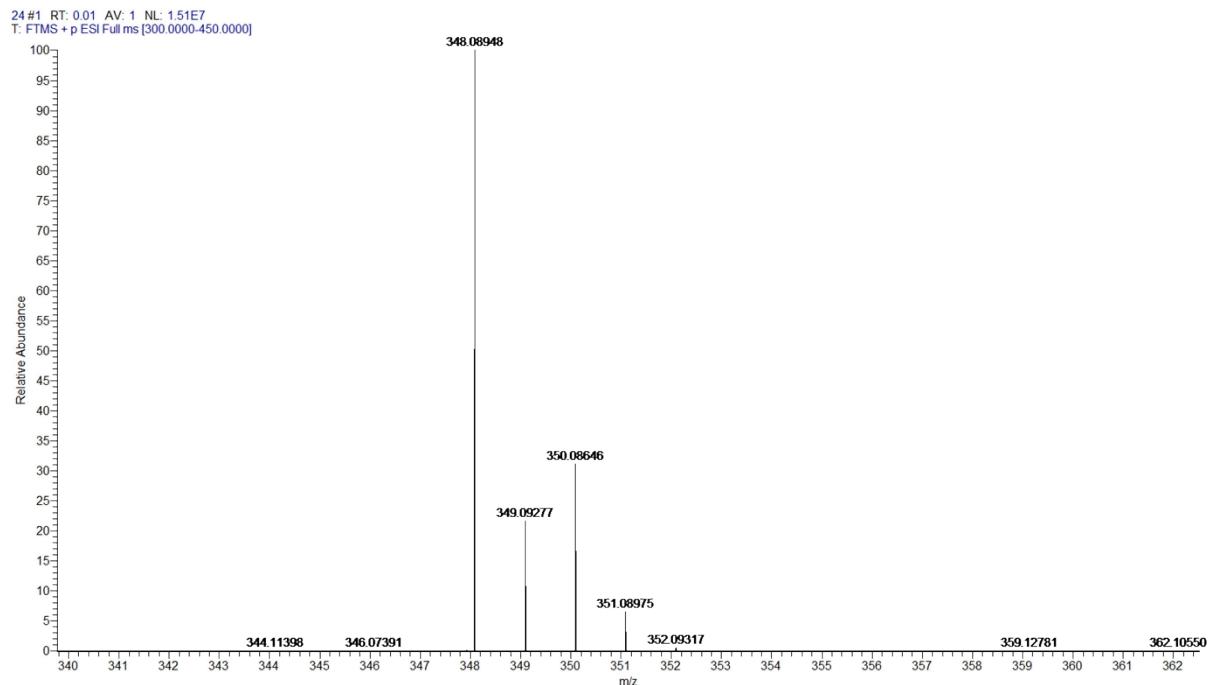


Figure S16. ESI $^+$ -MS spectra of (**4d**)