

## Supplementary Information

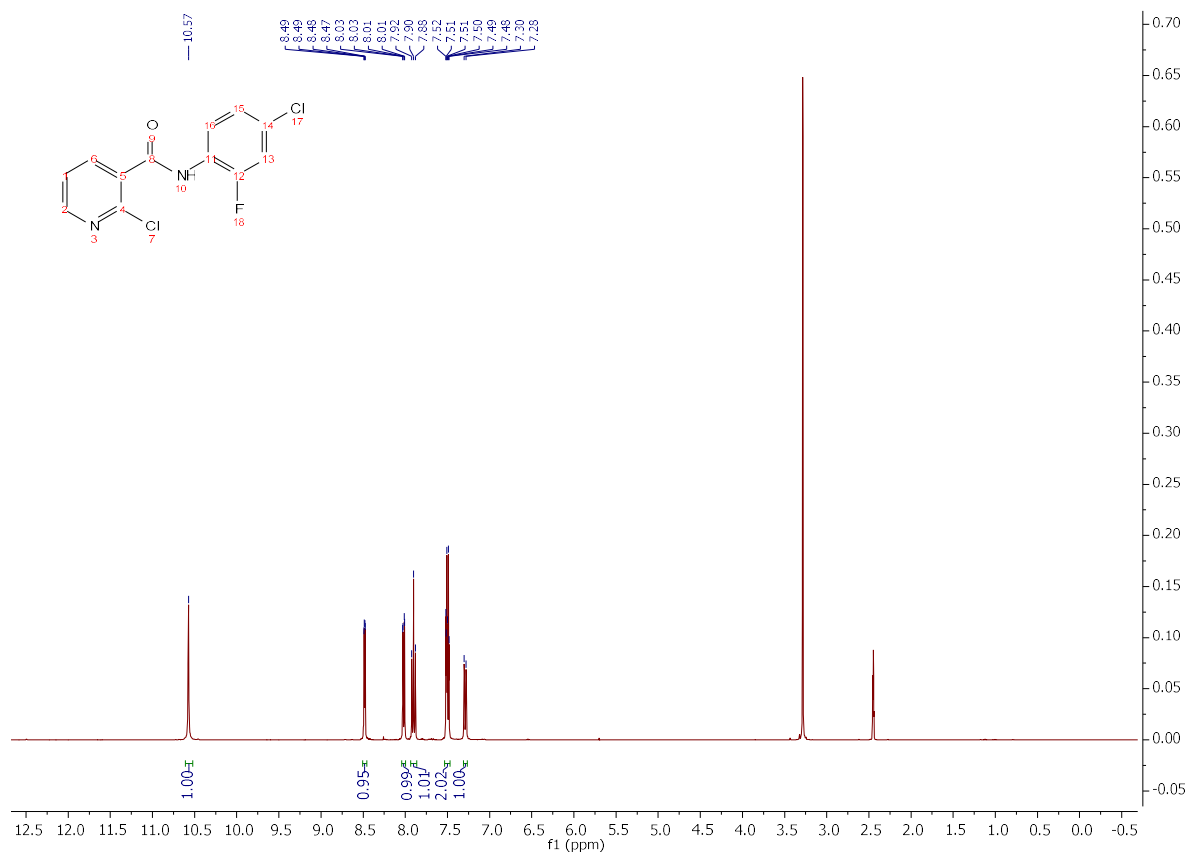
# Synthesis and characterization of new niacinamide compounds and computational and experimental investigation of their anticancer and antibacterial activity

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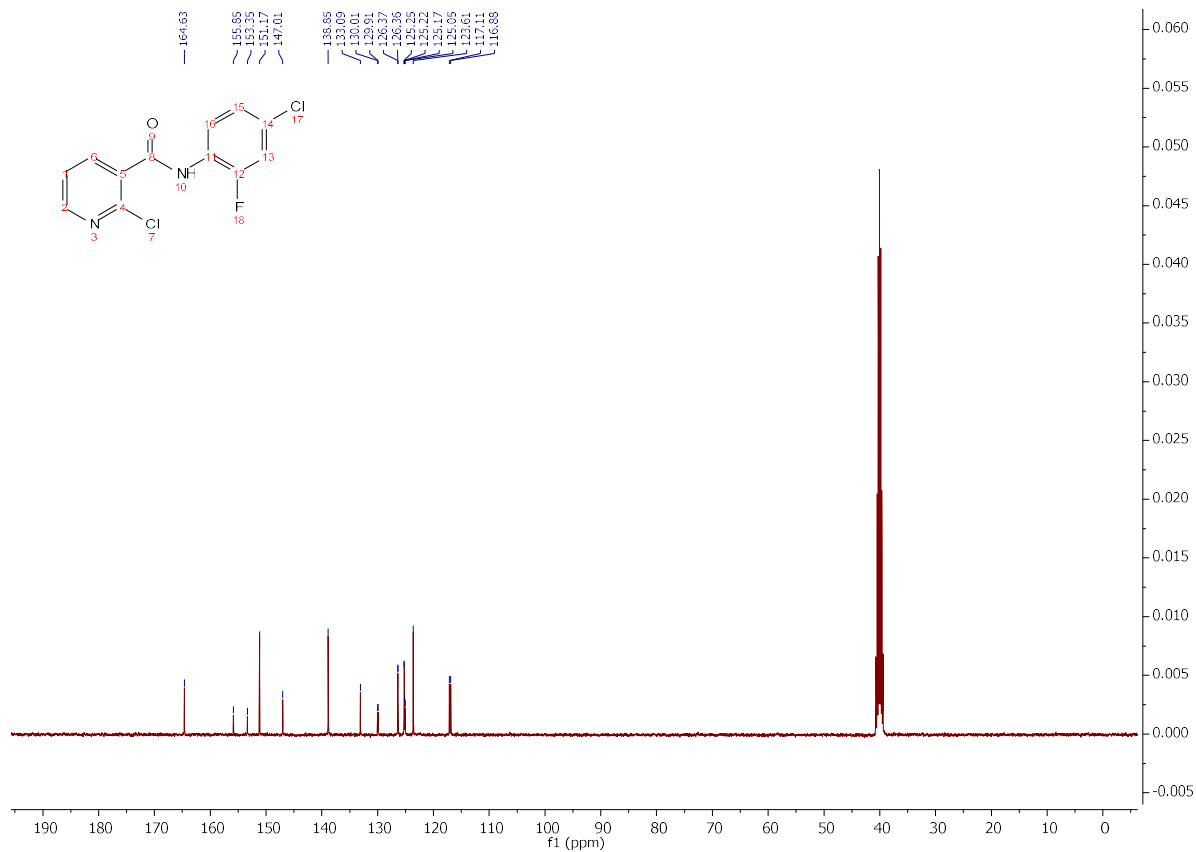
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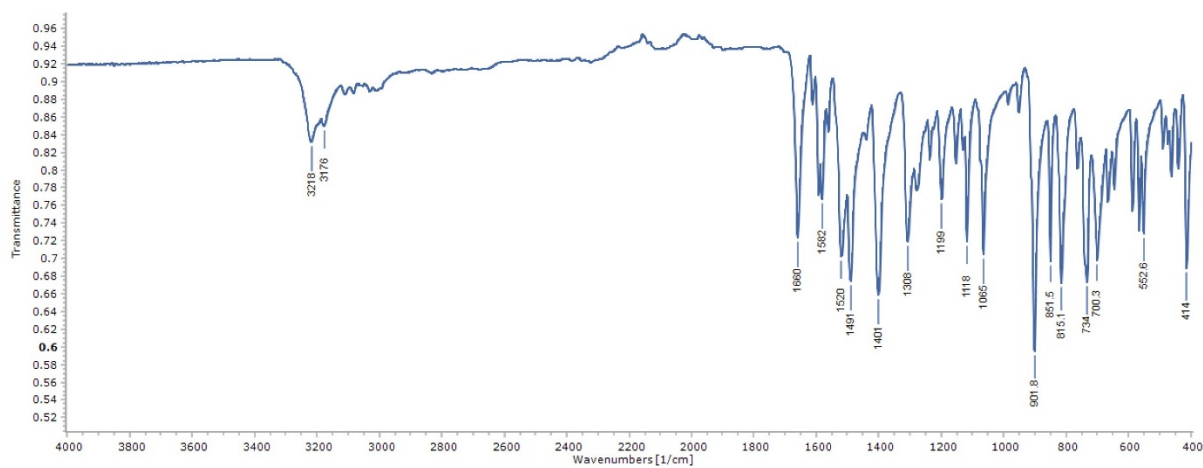
Received 27 January 2024; accepted (revised) 28 June 2024



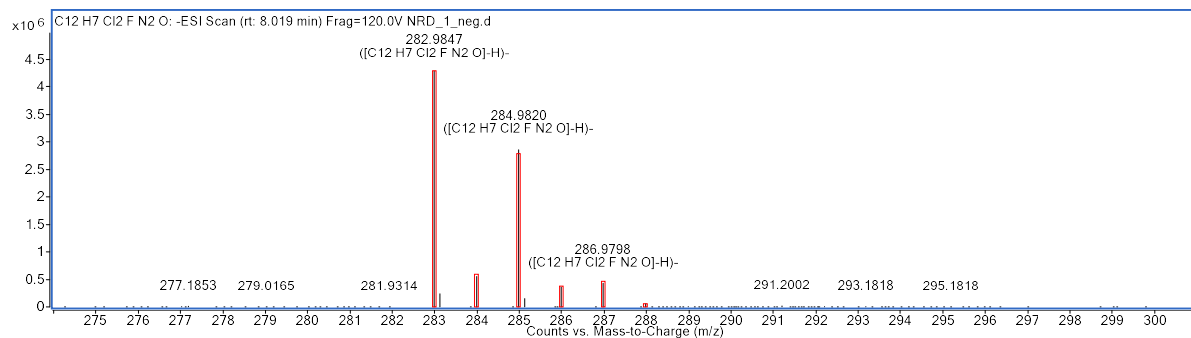
Supp. Fig. S1.  $^1\text{H-NMR}$  spectrum of NIA1.



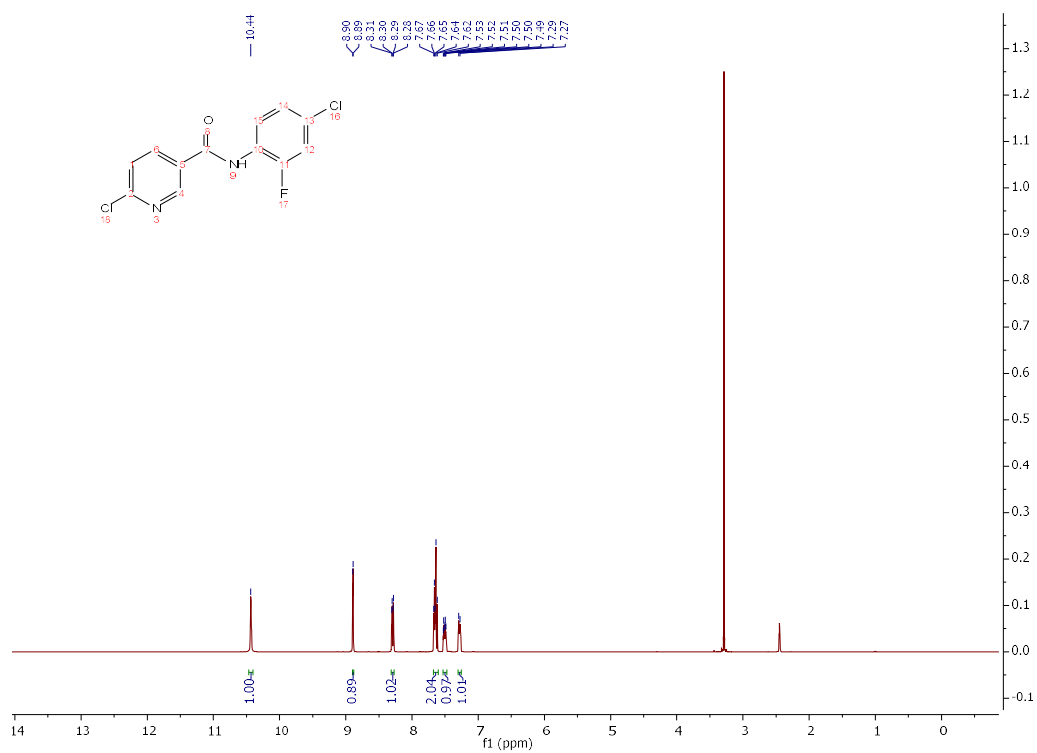
Supp. Fig. S2.  $^{13}\text{C}$ -NMR spectrum of NIA1.



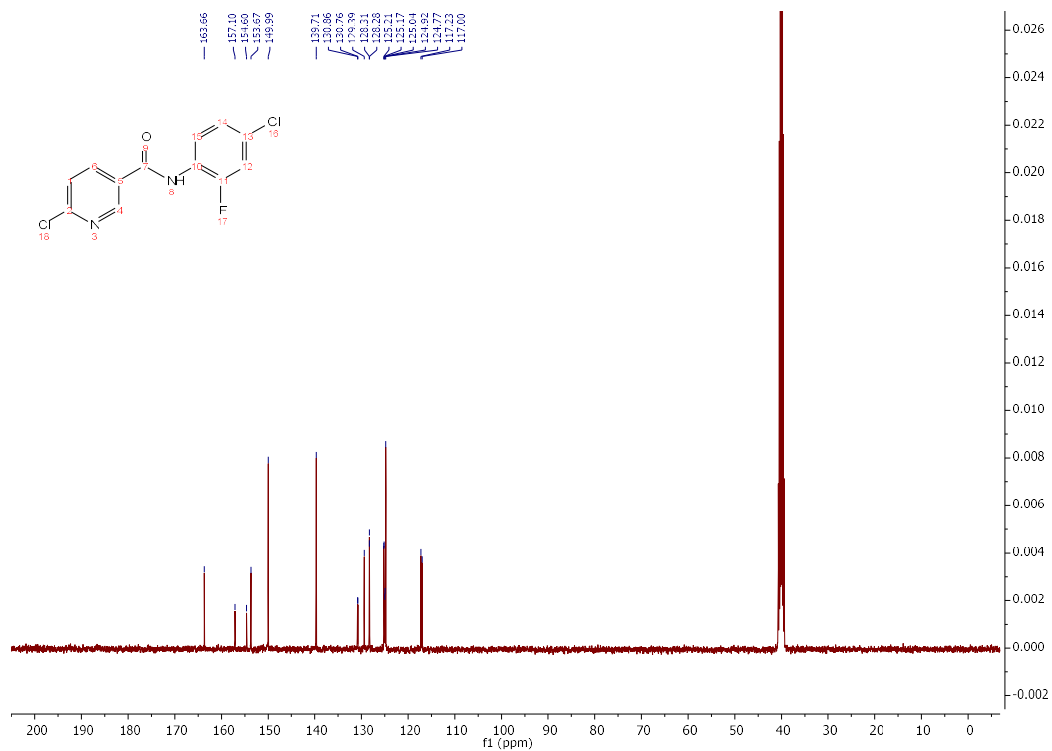
Supp. Fig. S3. ATR spectrum of NIA1.



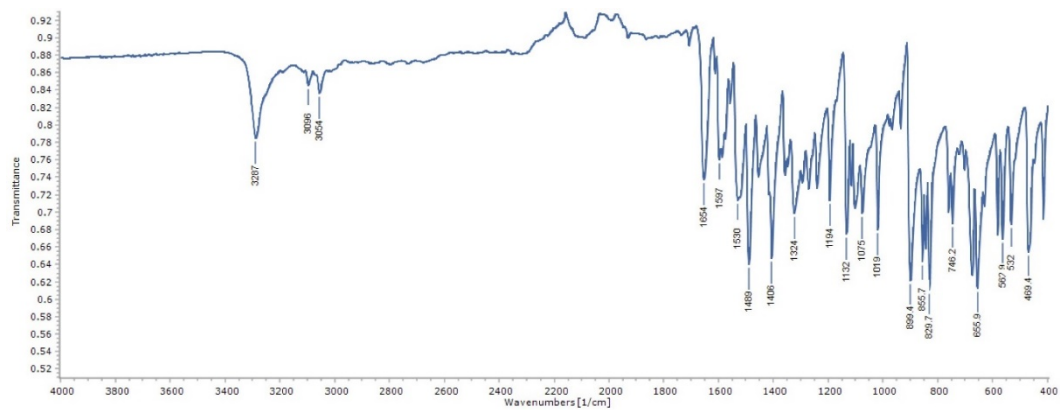
Supp. Fig. S4. LC-QTOF-MS spectrum of NIA1.



Supp. Fig. S5.  $^1\text{H}$ -NMR spectrum of NIA2.

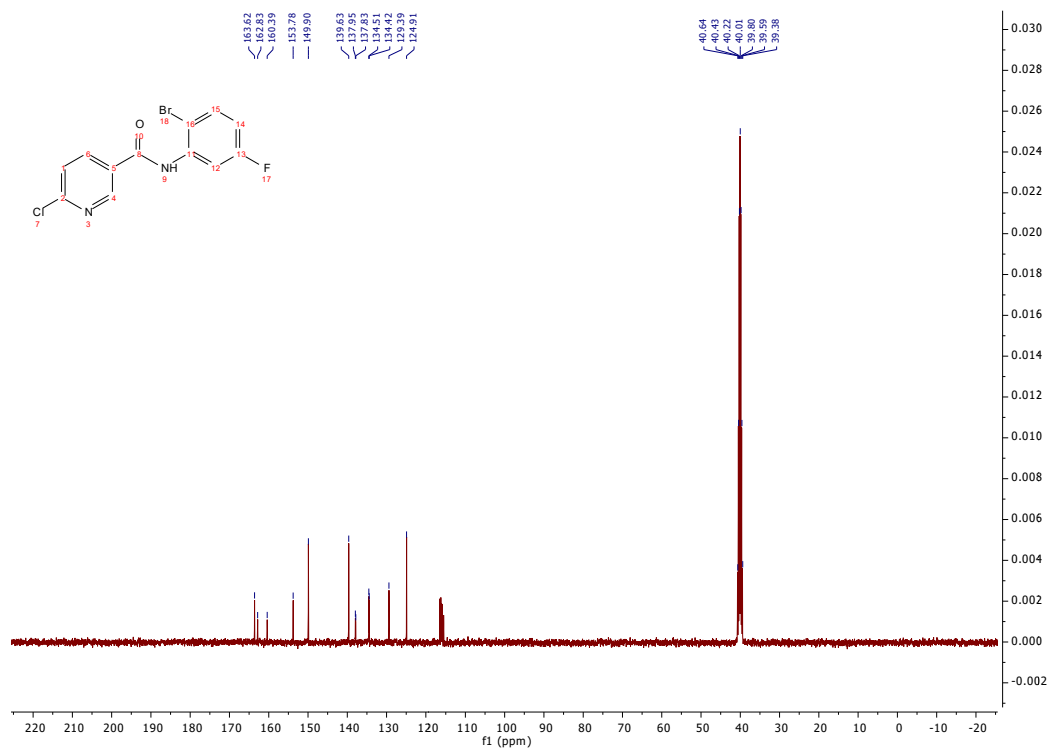


Supp. Fig. S6.  $^{13}\text{C}$ -NMR spectrum of NIA2.

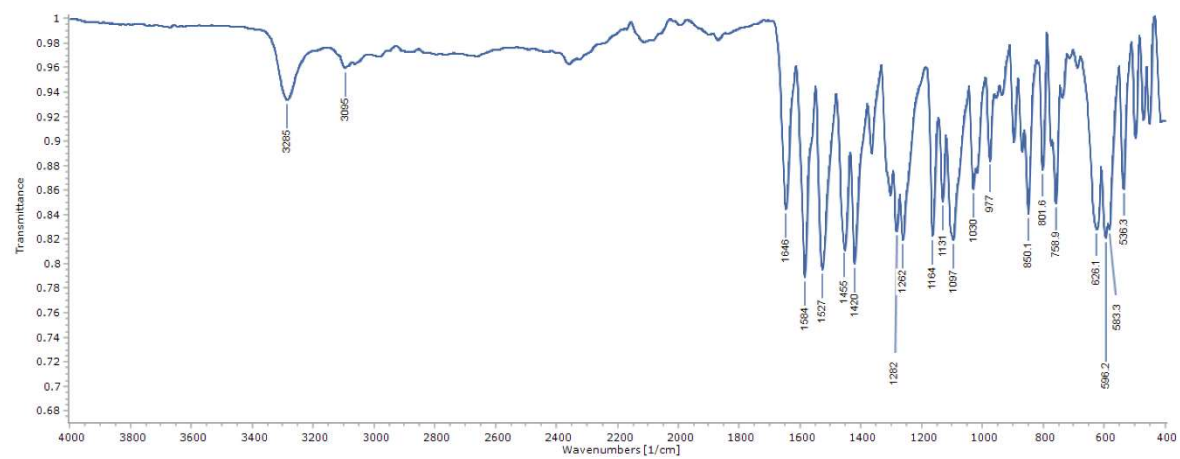


Supp. Fig. S7. ATR spectrum of NIA2.

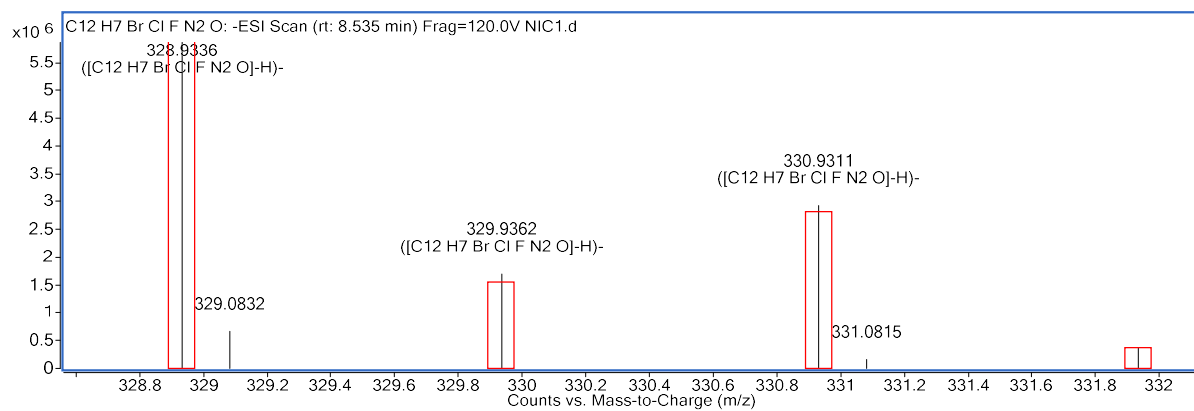




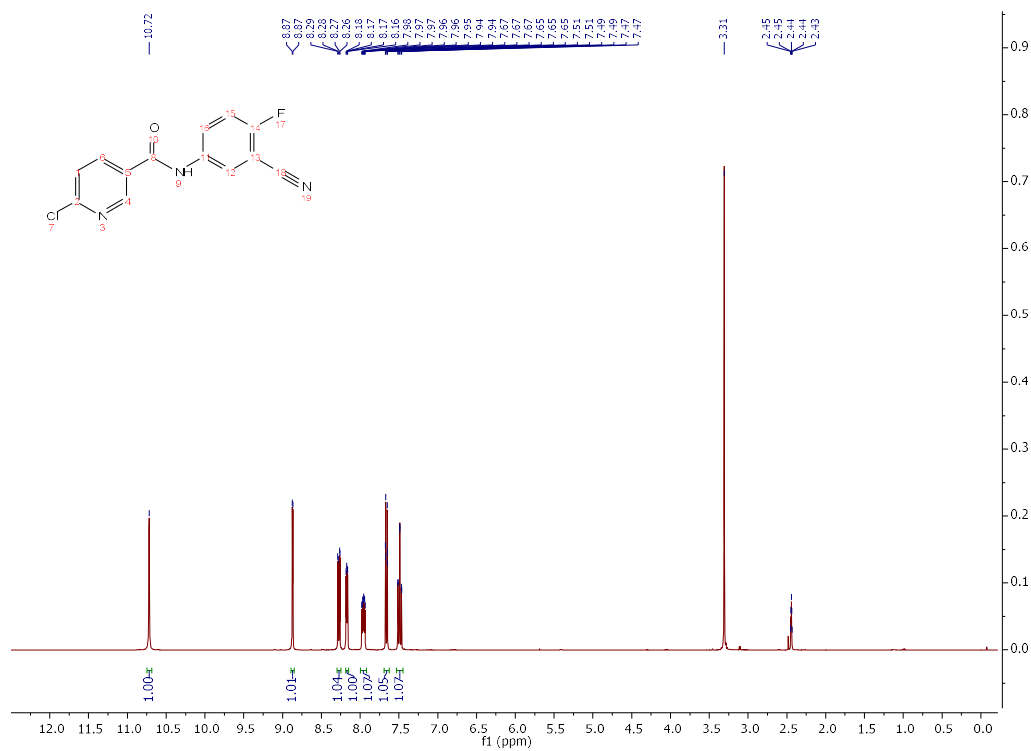
Supp. Fig. S10.  $^{13}\text{C}$ -NMR spectrum of NIA3.



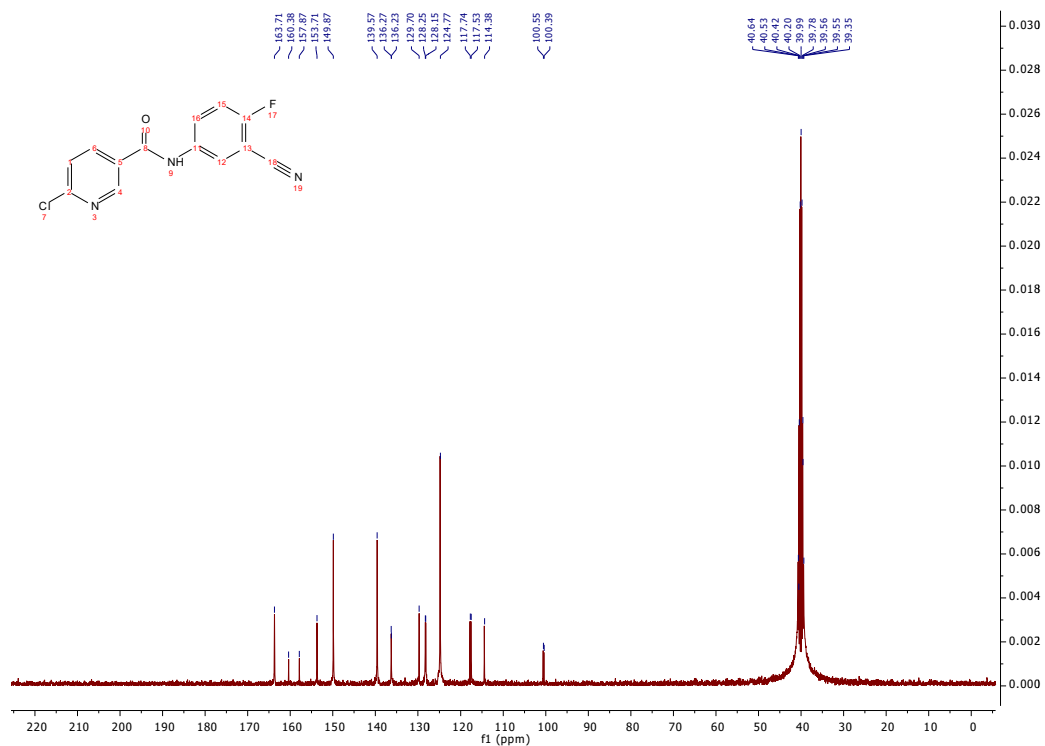
Supp. Fig. S11. ATR spectrum of NIA3.



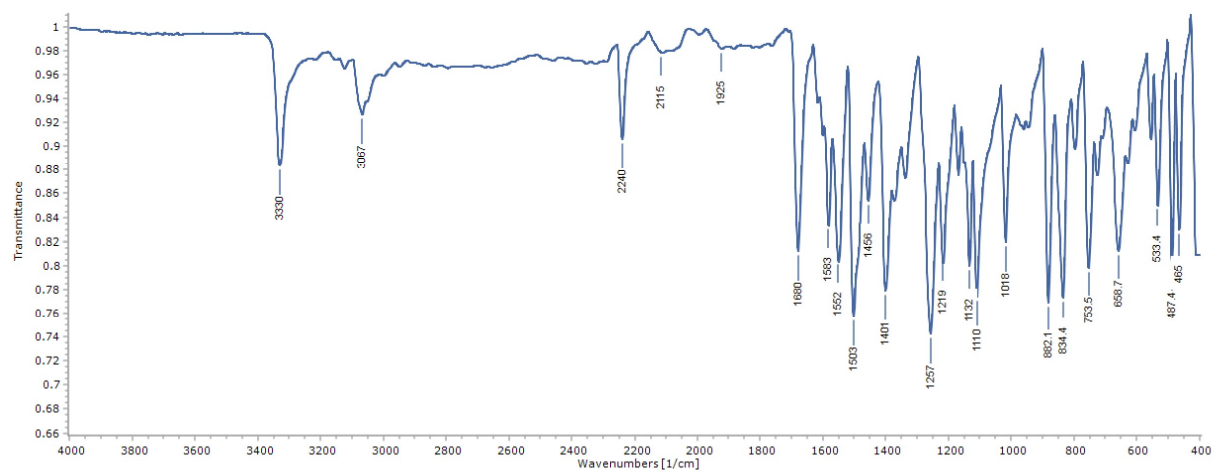
Supp. Fig. S12. LC-QTOF-MS spectrum of NIA3.



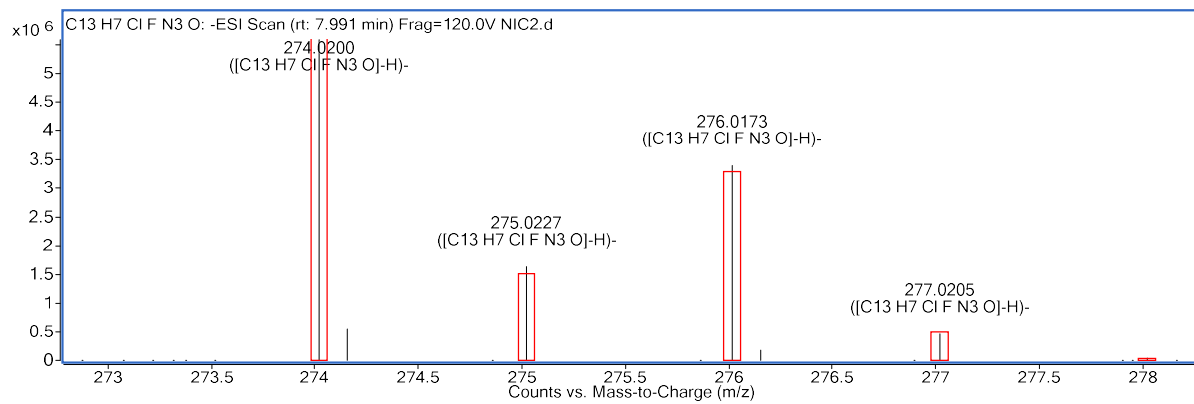
Supp. Fig. S13. <sup>1</sup>H-NMR spectrum of NIA4.



Supp. Fig. S14.  $^{13}\text{C}$ -NMR spectrum of NIA4.



Supp. Fig. S15. ATR spectrum of NIA4.



**Supp. Fig. S16.** LC-QTOF-MS spectrum of NIA4.