

Supplementary Information

Design, synthesis, *in vitro* and computational analyses of anticancer nicotinamide derivatives

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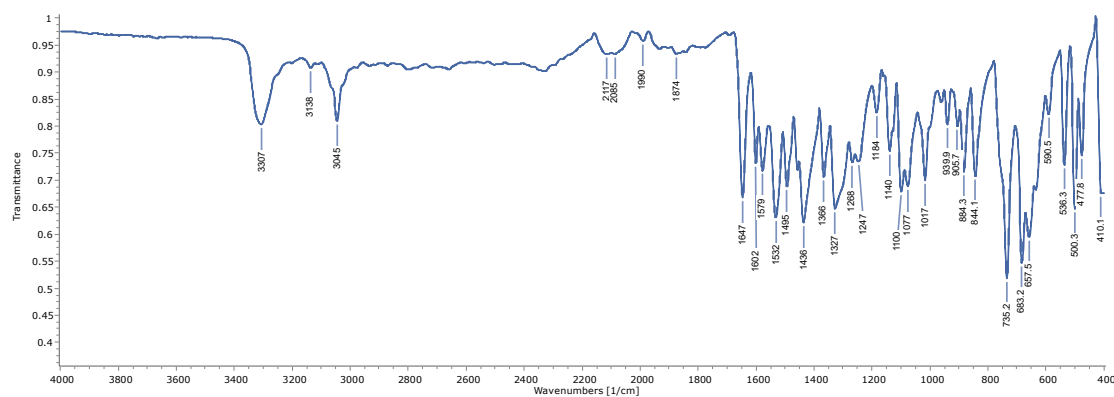
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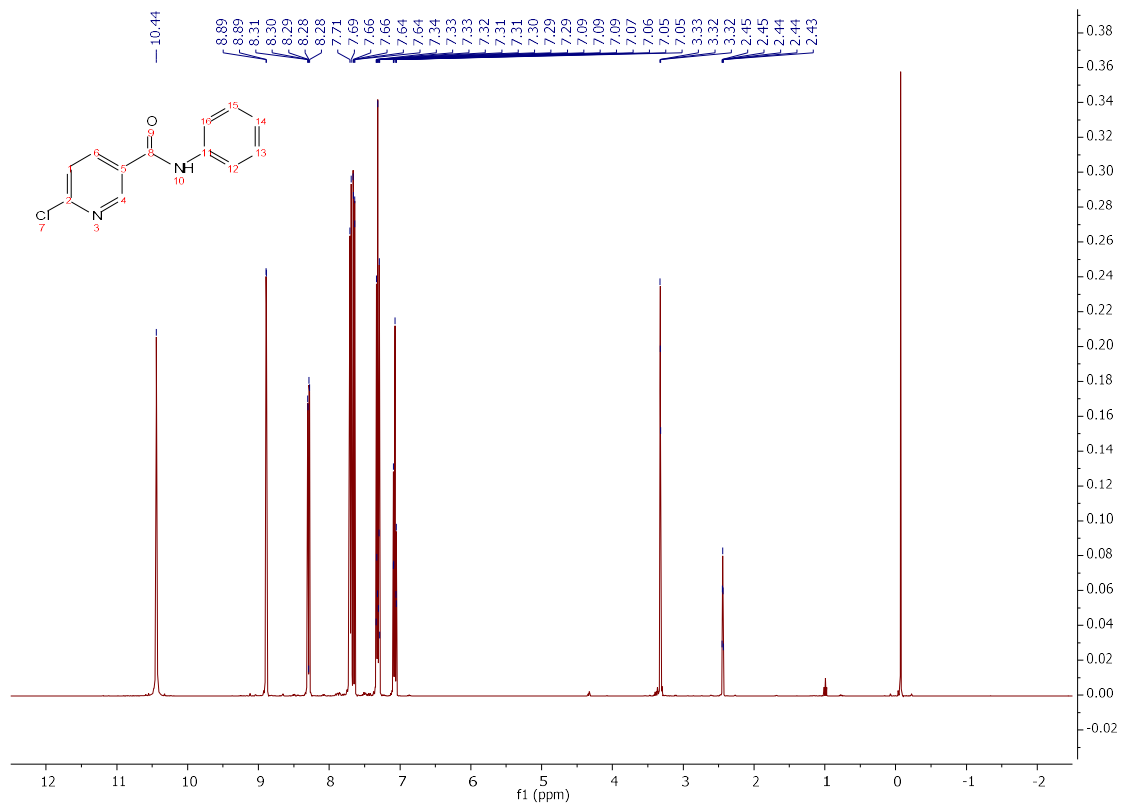
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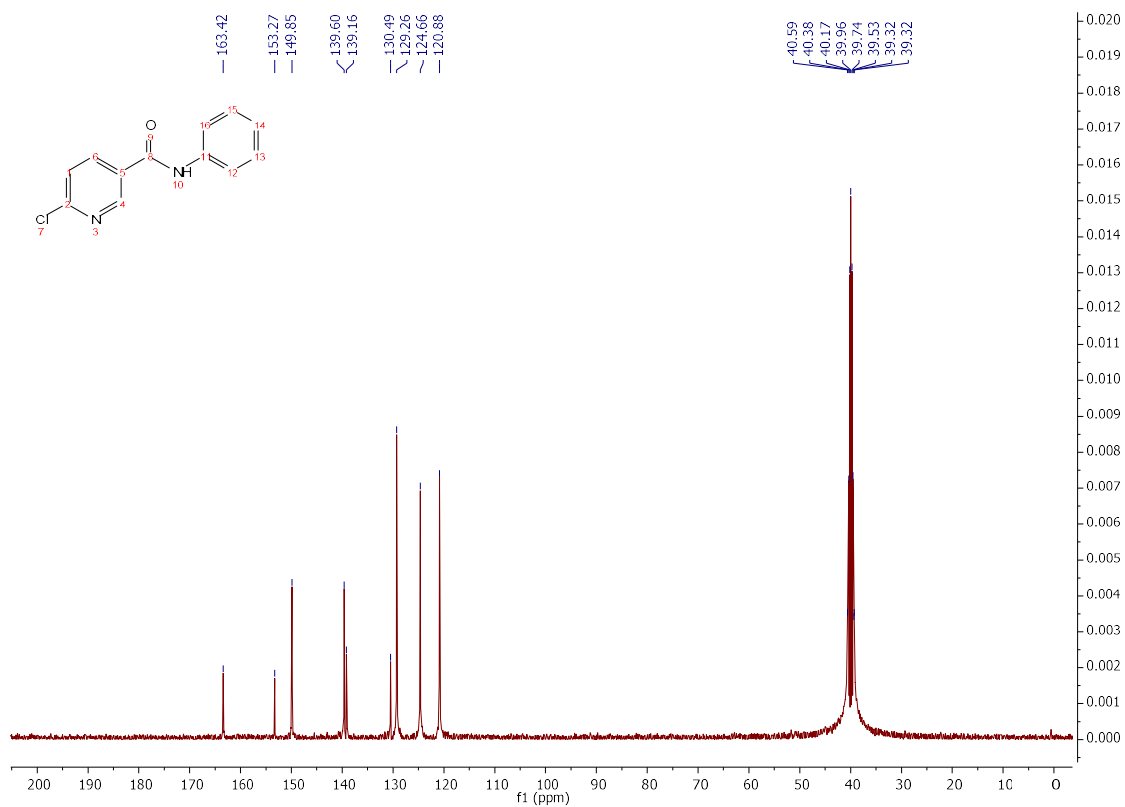
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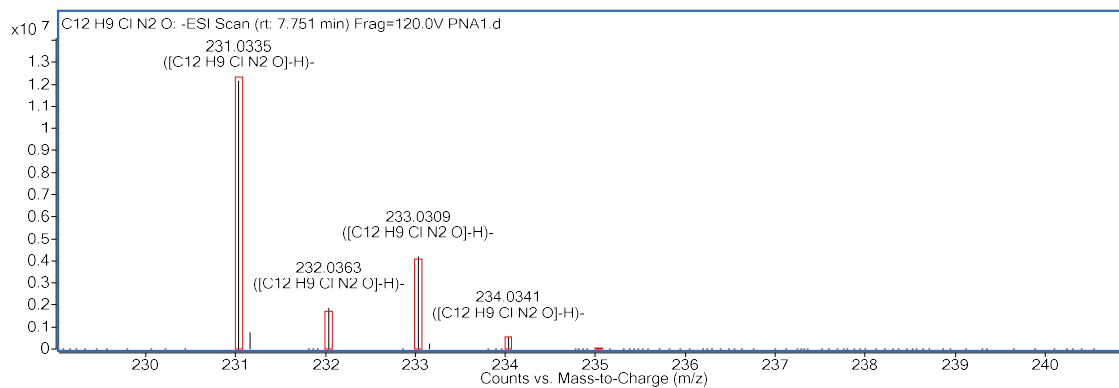
Supp. Fig. S1. The IR spectrum of N1.



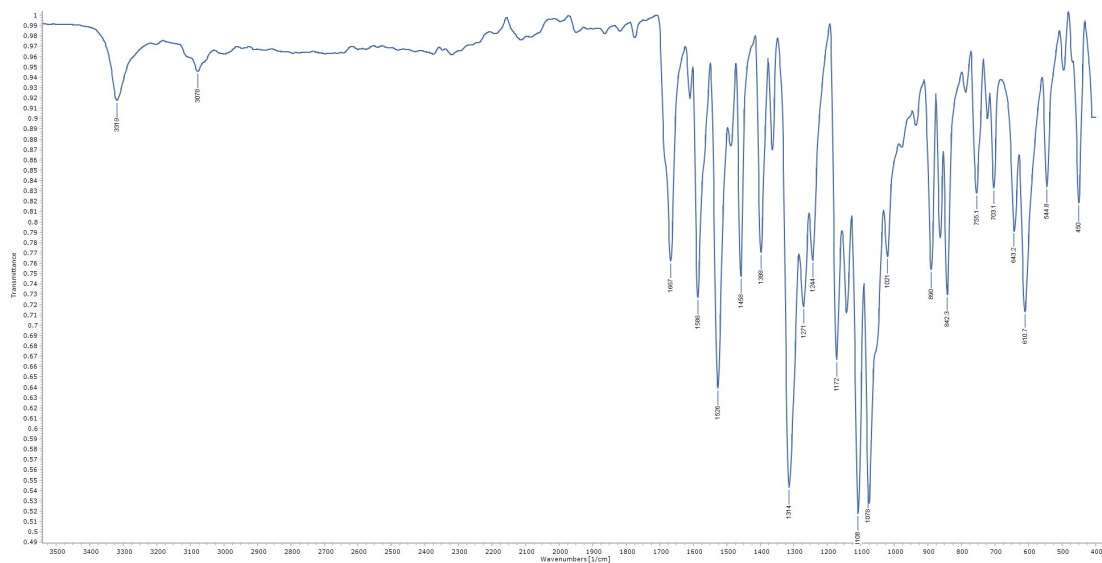
Supp. Fig. S2. ¹H-NMR (400 MHz) spectrum of N1.



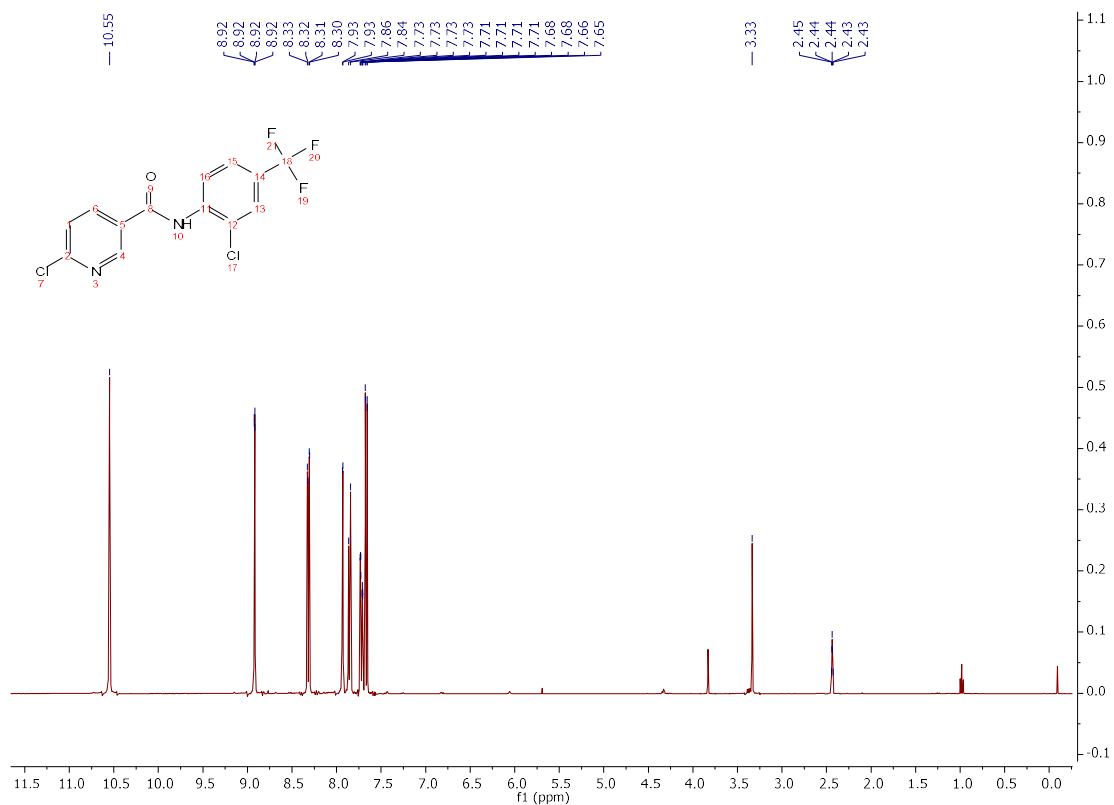
Supp. Fig. S3. $^{13}\text{C-NMR}$ (101 MHz) spectrum of N1.



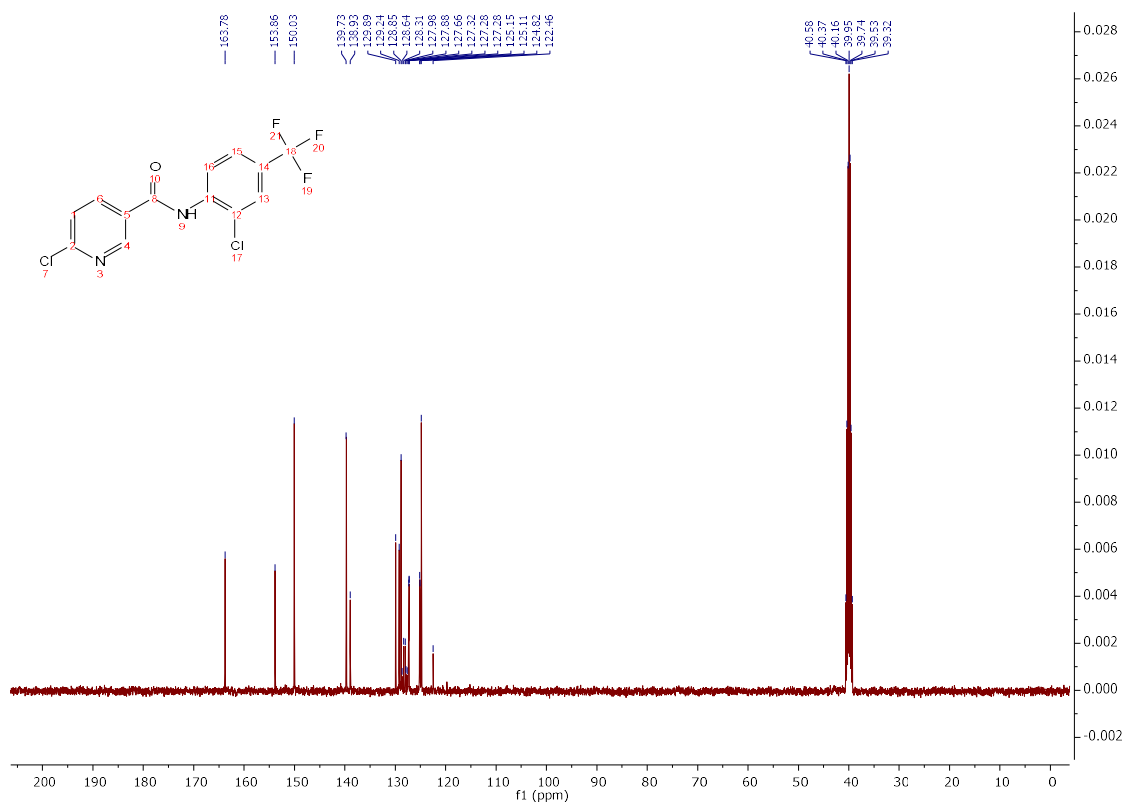
Supp. Fig. S4. HPLC-TOF/MS $[\text{M-H}]^-$ spectrum of N1.



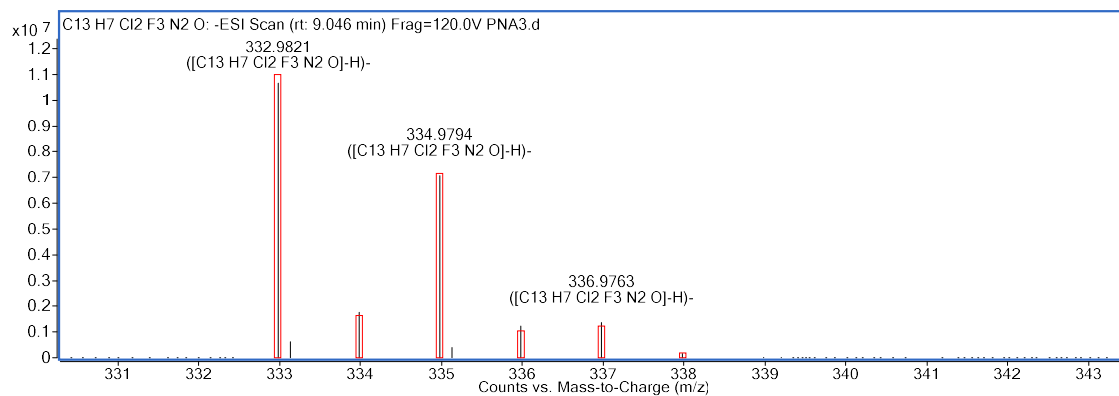
Supp. Fig. S5. The IR spectrum of N2.



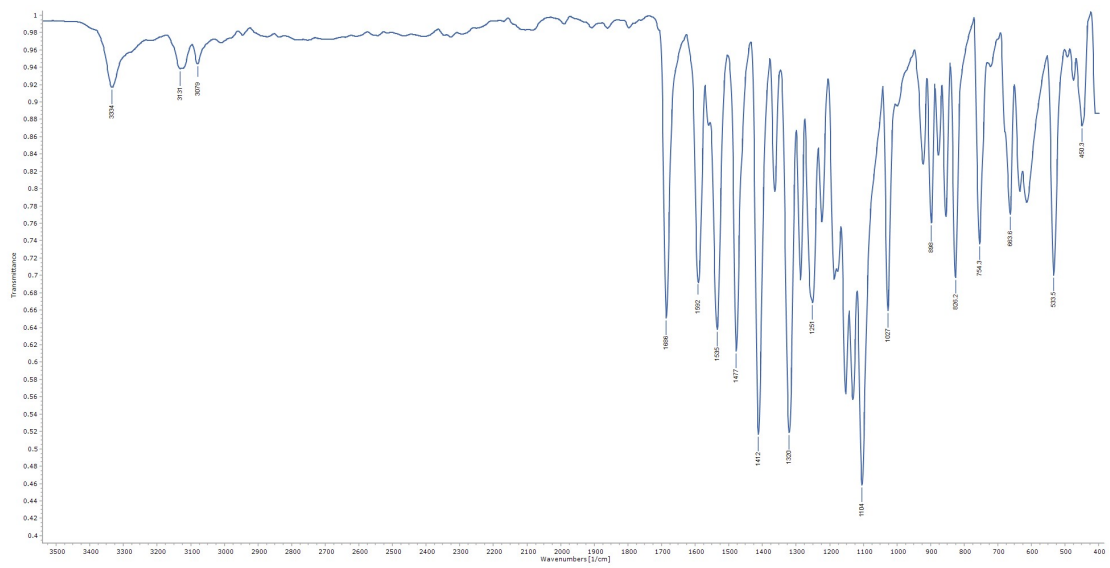
Supp. Fig. S6. $^1\text{H-NMR}$ (400 MHz) spectrum of N2.



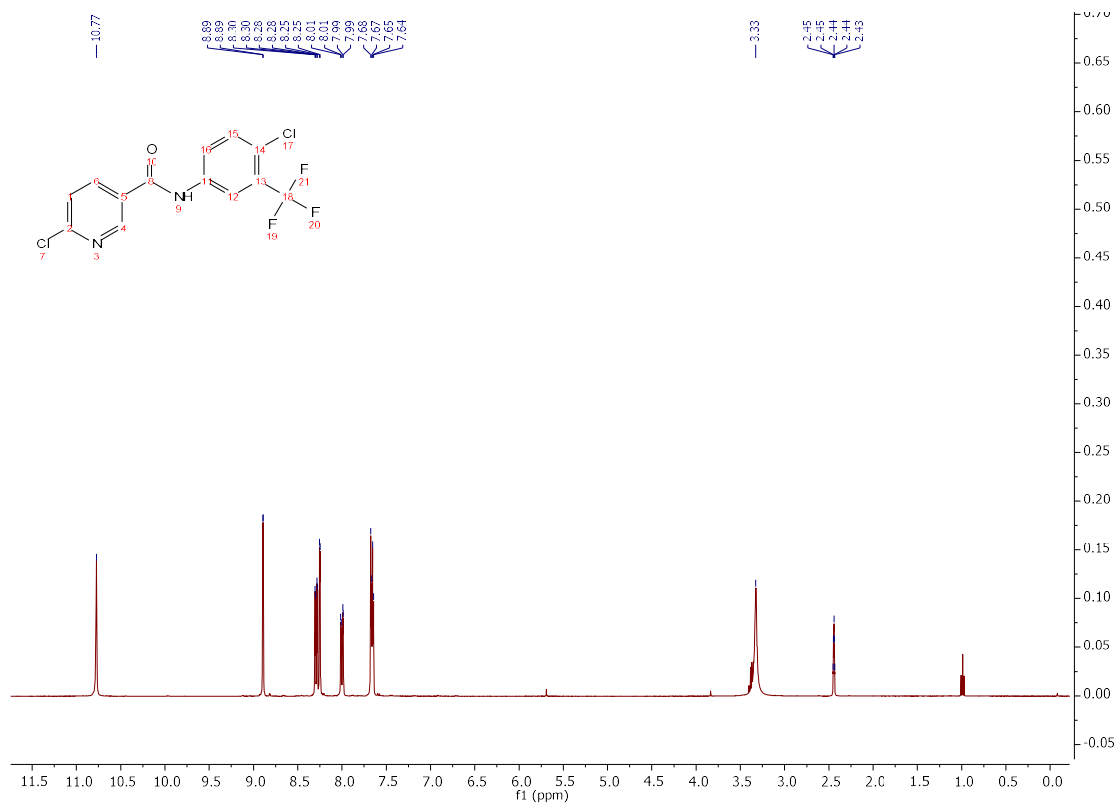
Supp. Fig. S7. ^{13}C -NMR (101 MHz) spectrum of N2.



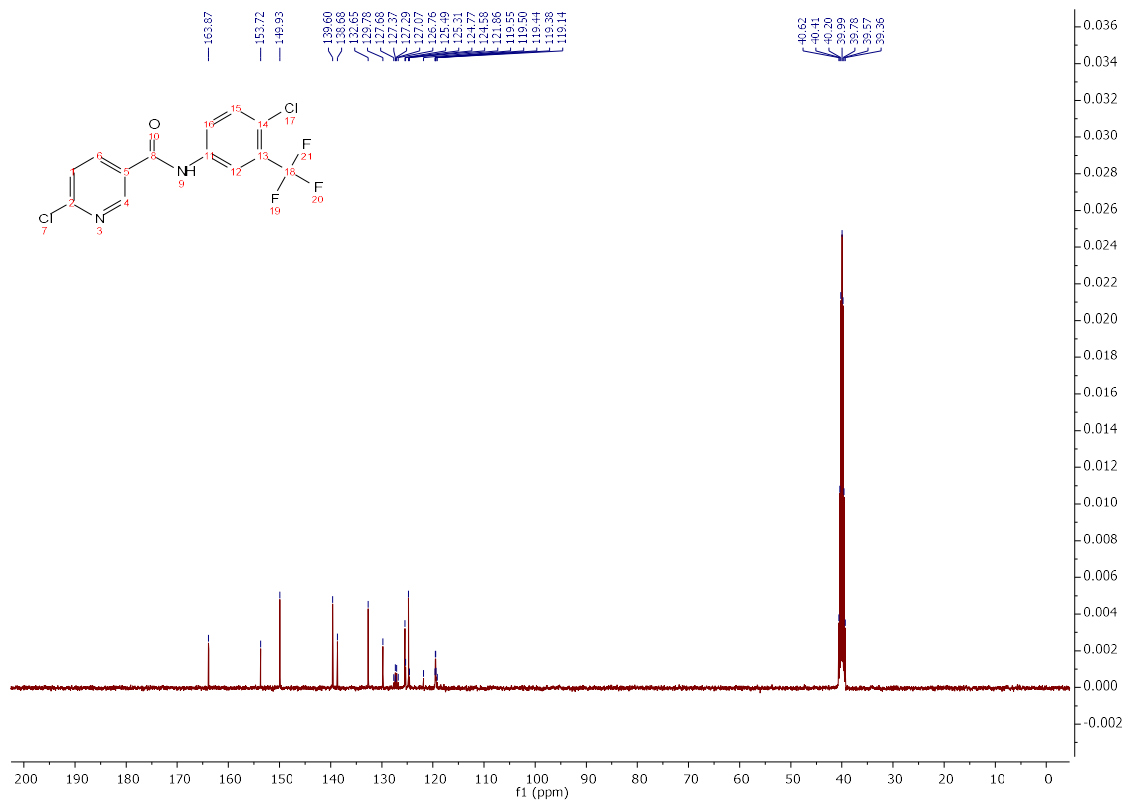
Supp. Fig. S8. HPLC-TOF/MS $[\text{M}-\text{H}]^-$ spectrum of N2.



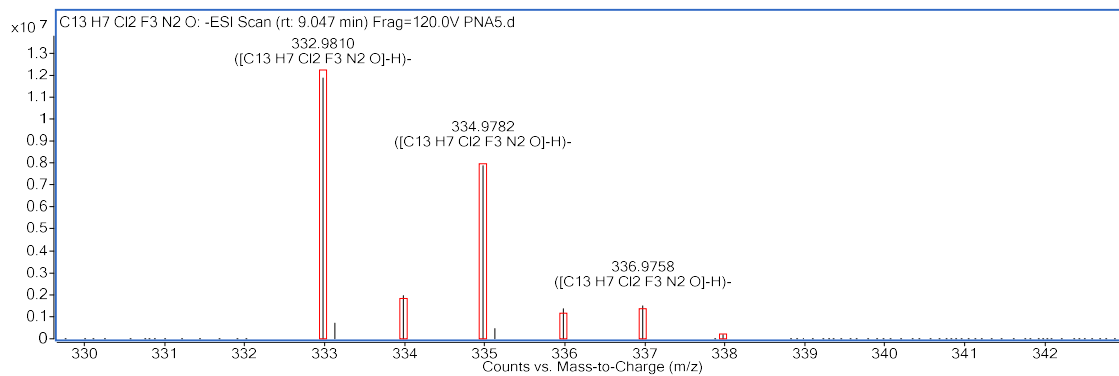
Supp. Fig. S9. The IR spectrum of N3.



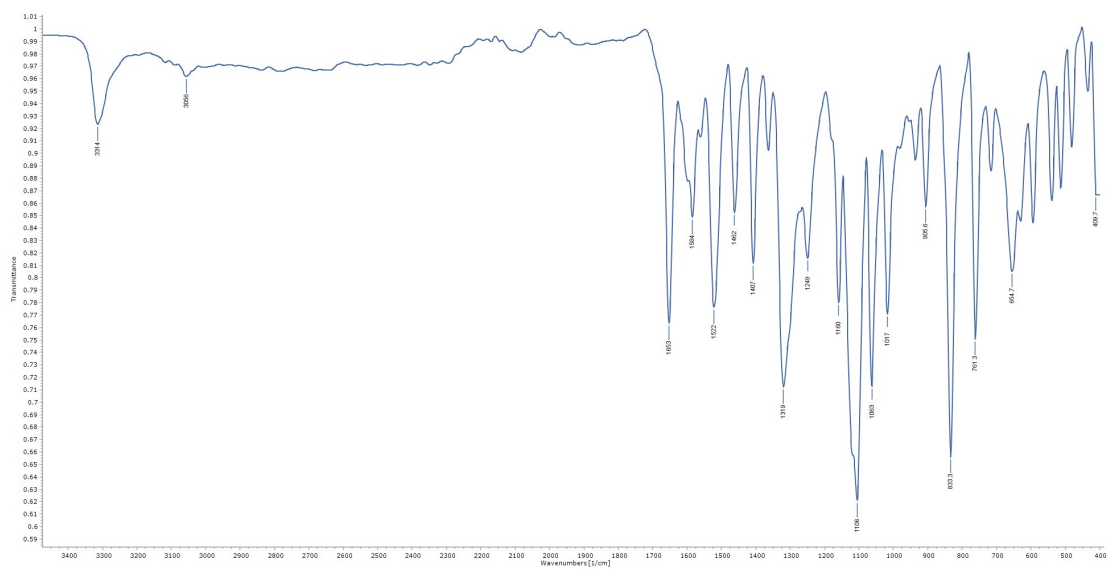
Supp. Fig. S10. ¹H-NMR (400 MHz) spectrum of N3.



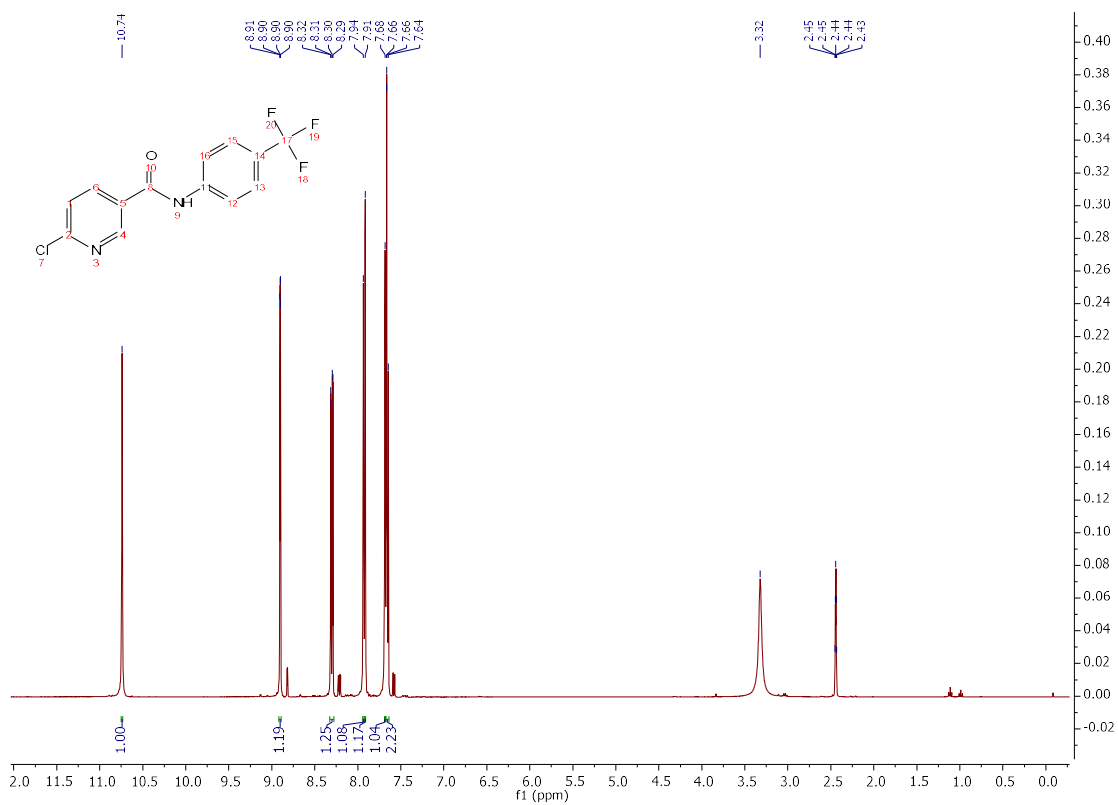
Supp. Fig. S11. ¹³C-NMR (101 MHz) spectrum of N3.



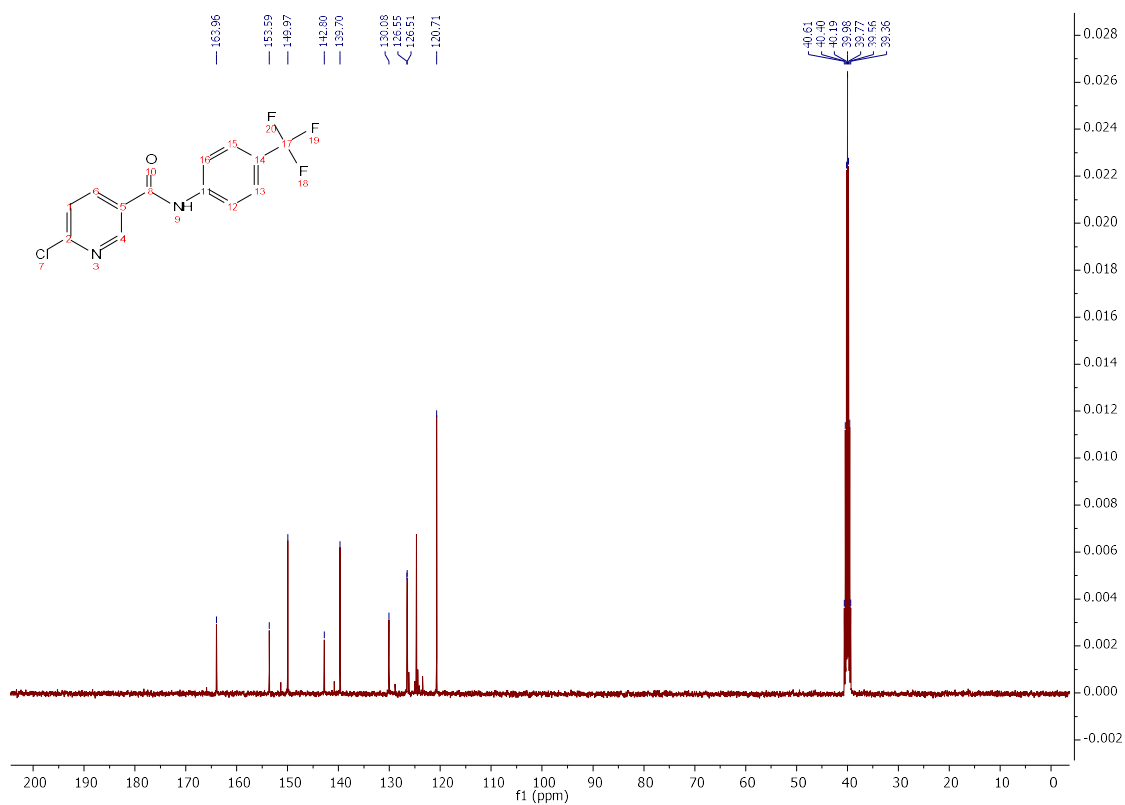
Supp. Fig. S12. HPLC-TOF/MS [M-H]⁻ spectrum of N3.



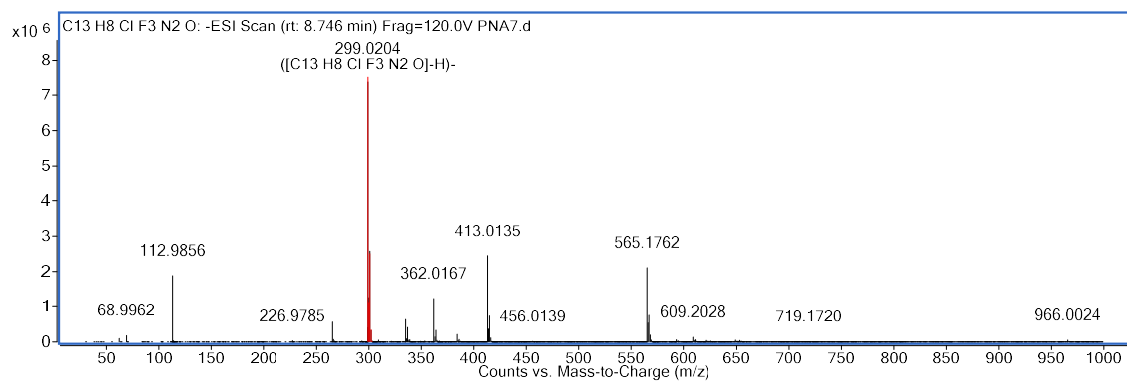
Supp. Fig. S13. The IR spectrum of N4.



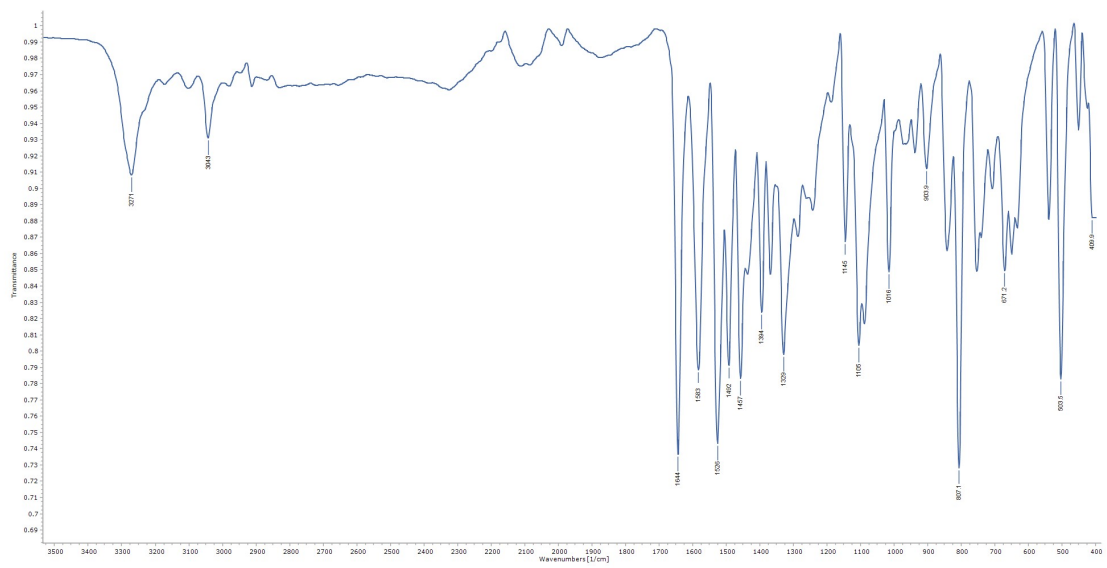
Supp. Fig. S14. ¹H-NMR (400 MHz) spectrum of N4.



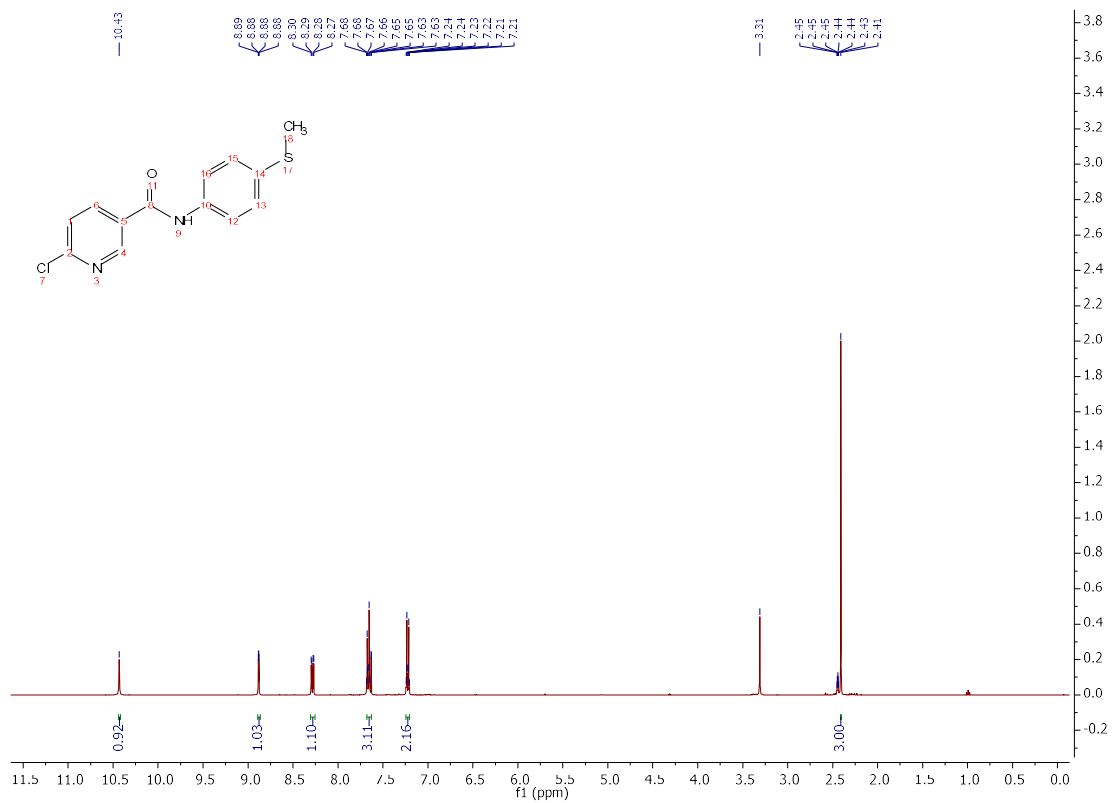
Supp. Fig. S15. ^{13}C -NMR (101 MHz) spectrum of N4.



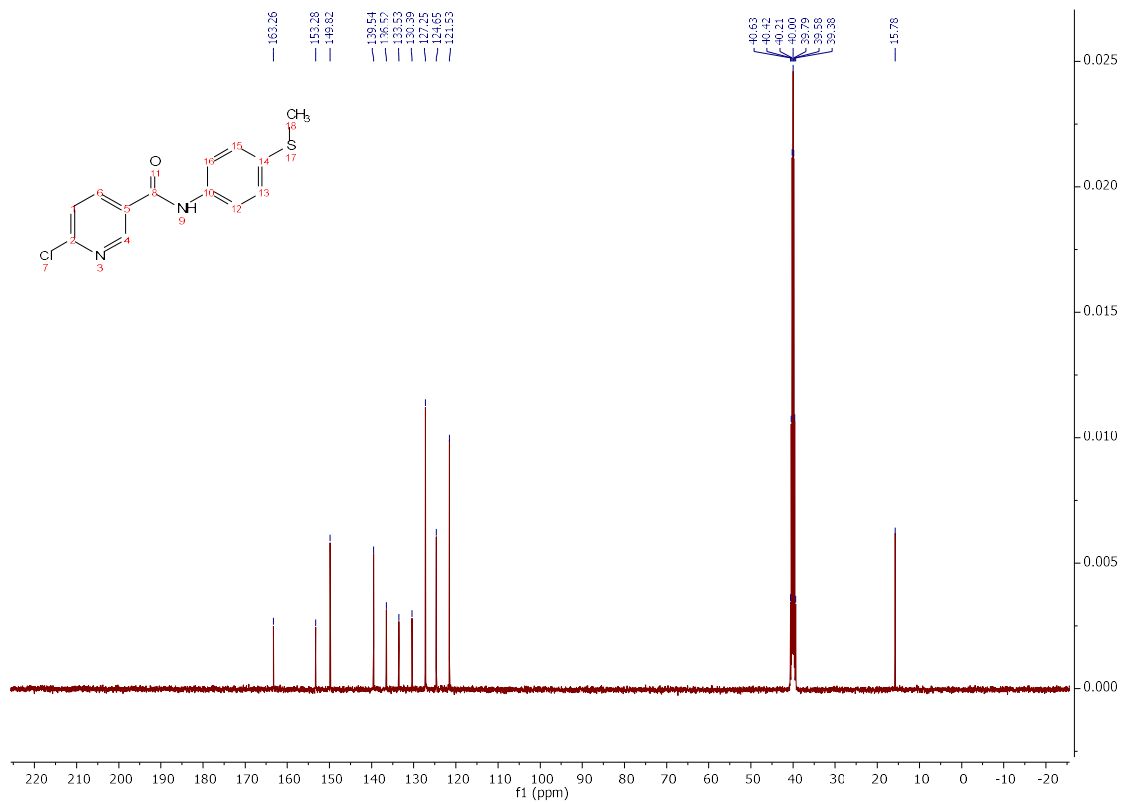
Supp. Fig. S16. HPLC-TOF/MS $[\text{M}-\text{H}]^-$ spectrum of N4.



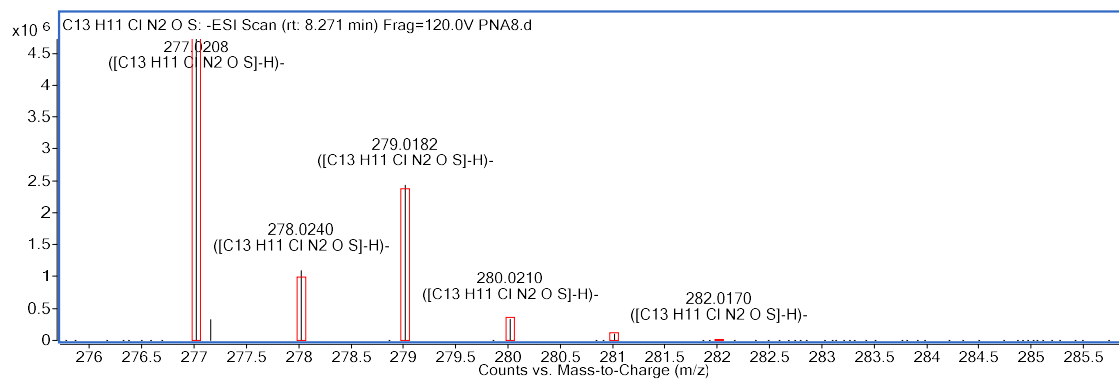
Supp. Fig. S17. The IR spectrum of N5.



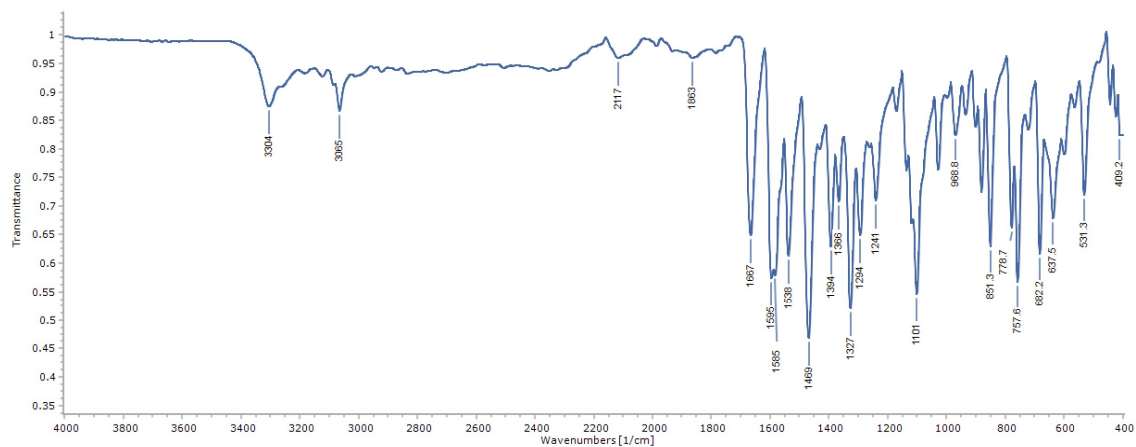
Supp. Fig. S18. ¹H-NMR (400 MHz) spectrum of N5.



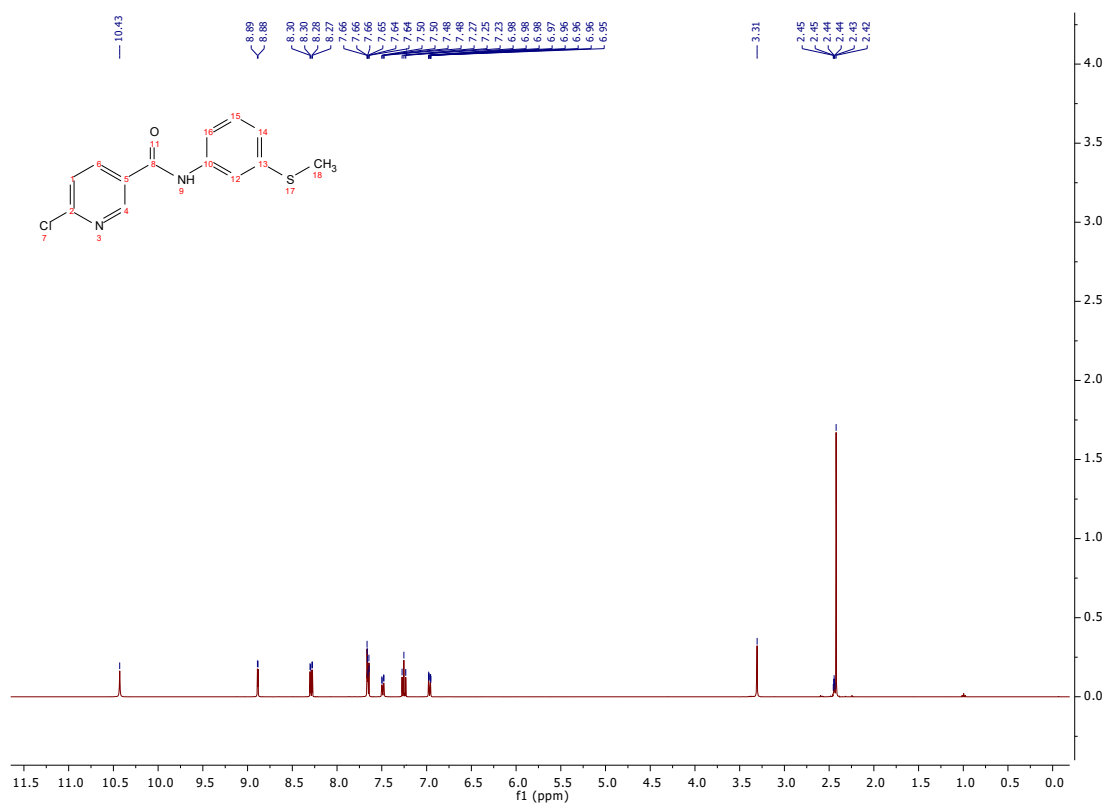
Supp. Fig. S19. ^{13}C -NMR (101 MHz) spectrum of N5.



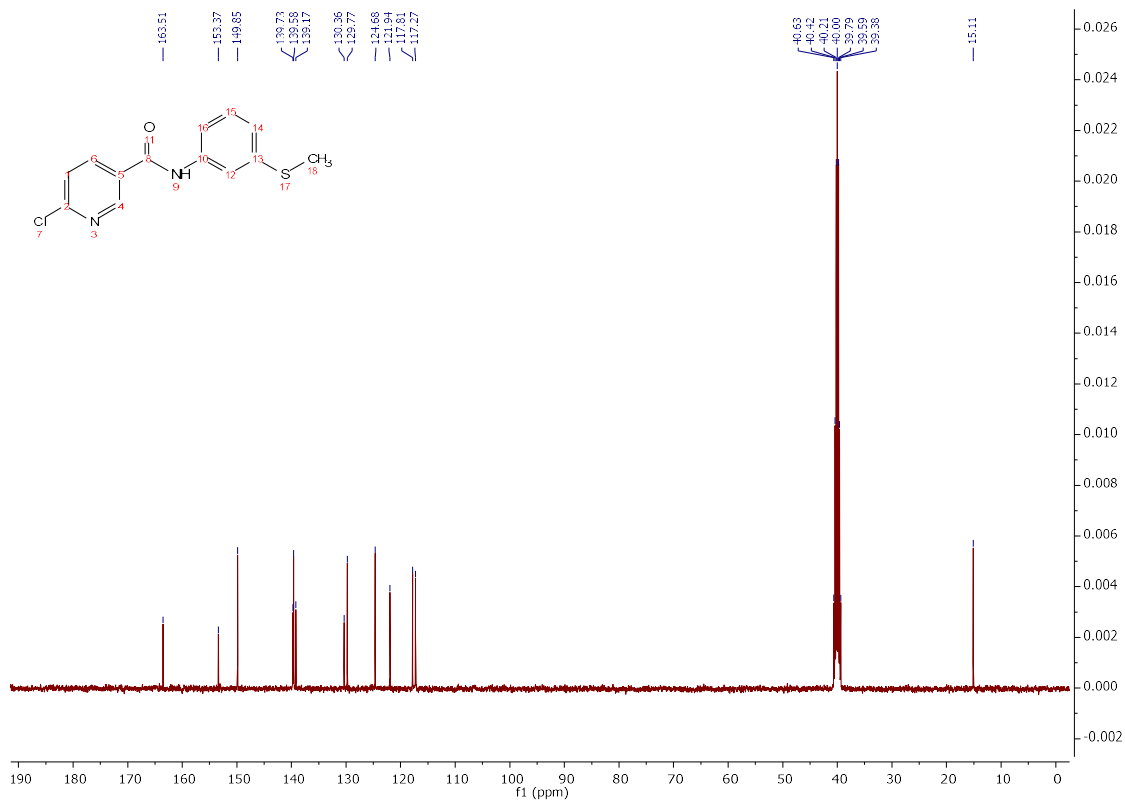
Supp. Fig. S20. HPLC-TOF/MS $[\text{M}-\text{H}]^-$ spectrum of N5.



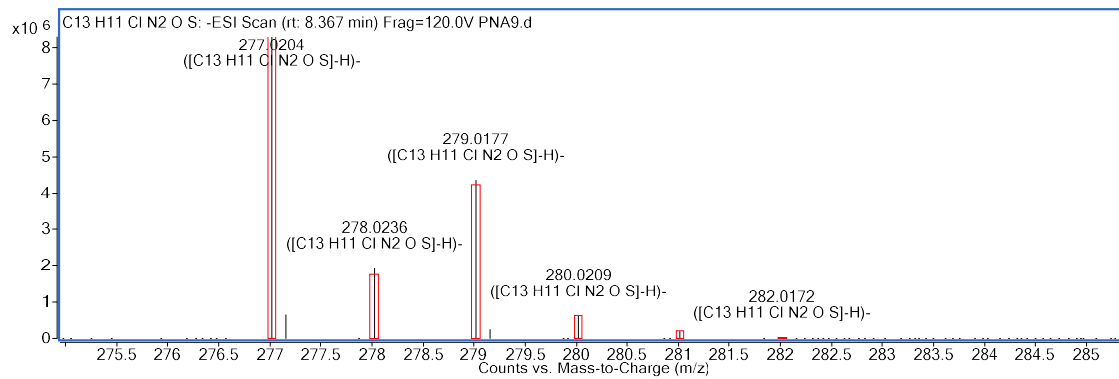
Supp. Fig. S21. The IR spectrum of N6.



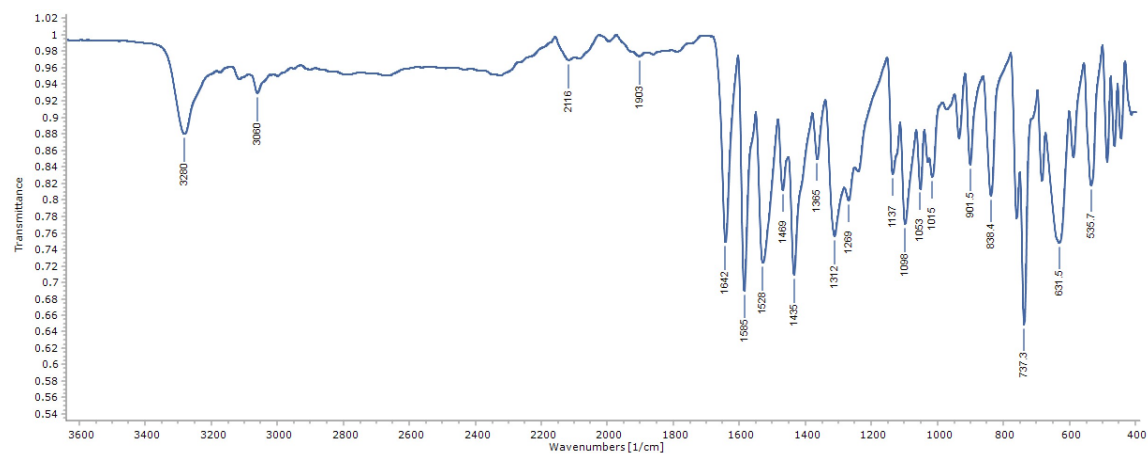
Supp. Fig. S22. ¹H-NMR (400 MHz) spectrum of N6.



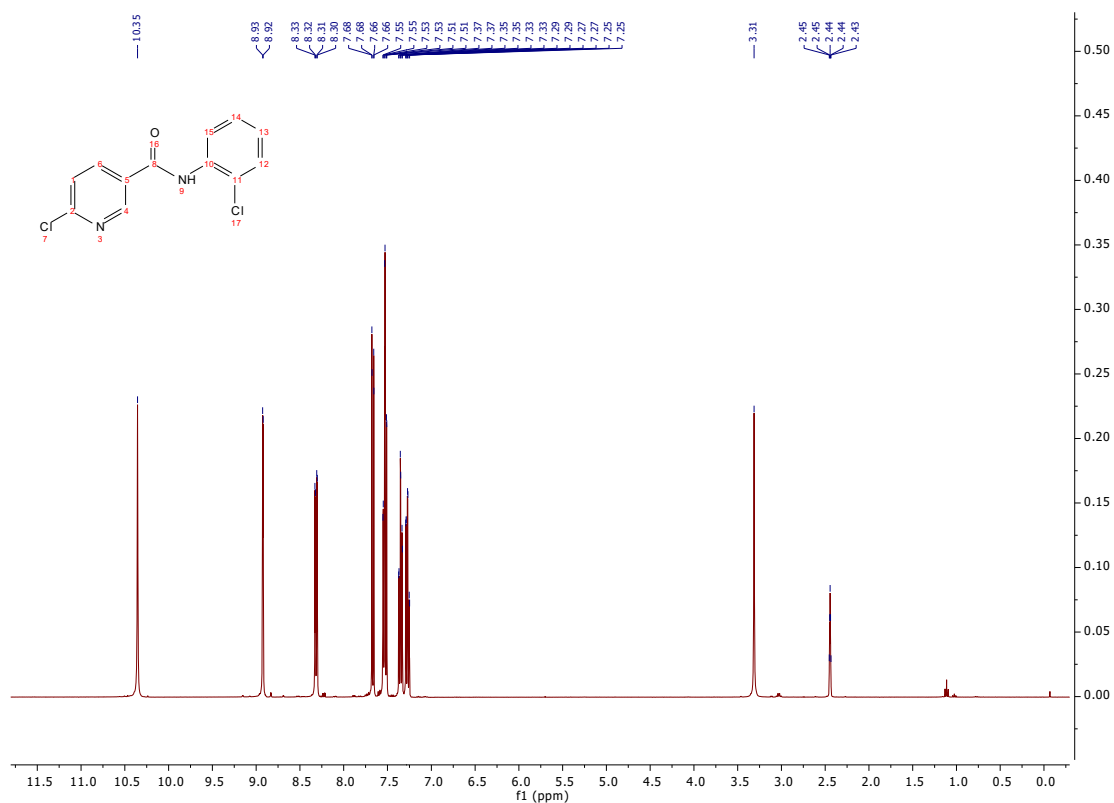
Supp. Fig. S23. ¹³C-NMR (101 MHz) spectrum of N6.



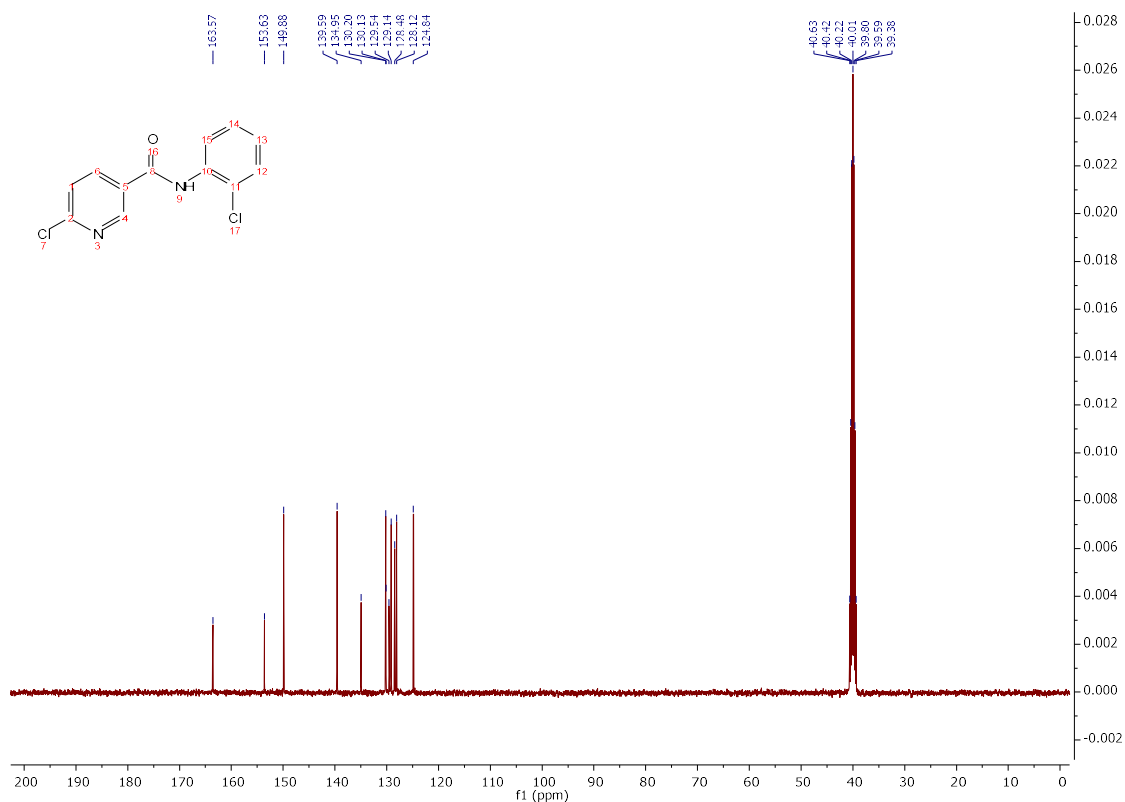
Supp. Fig. S24. HPLC-TOF/MS [M-H]⁻ spectrum of N6.



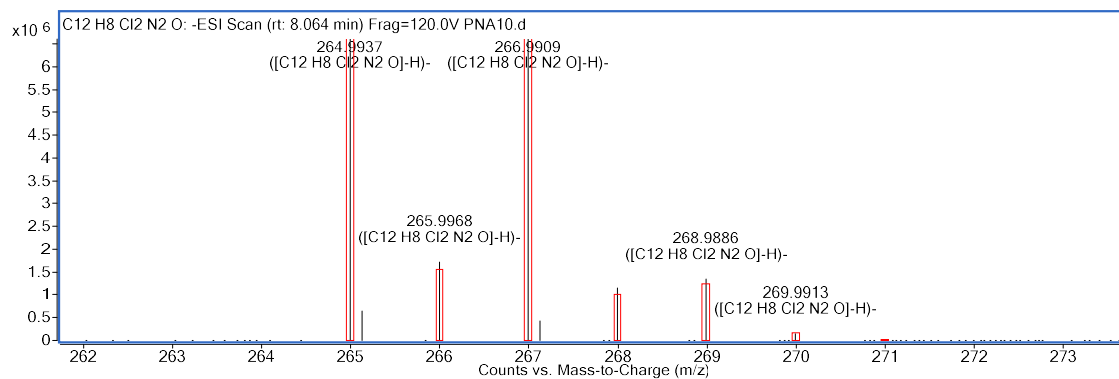
Supp. Fig. S25. The IR spectrum of N7.



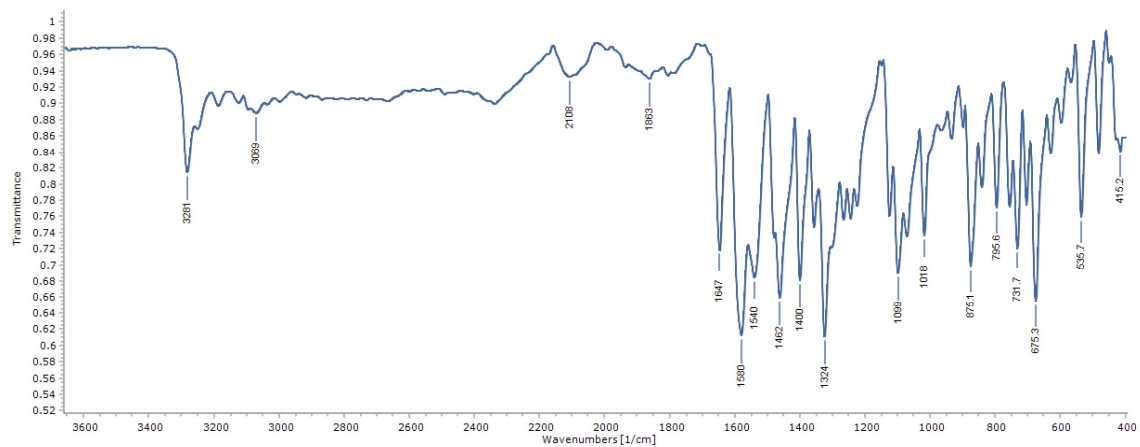
Supp. Fig. S26. ¹H-NMR (400 MHz) spectrum of N7.



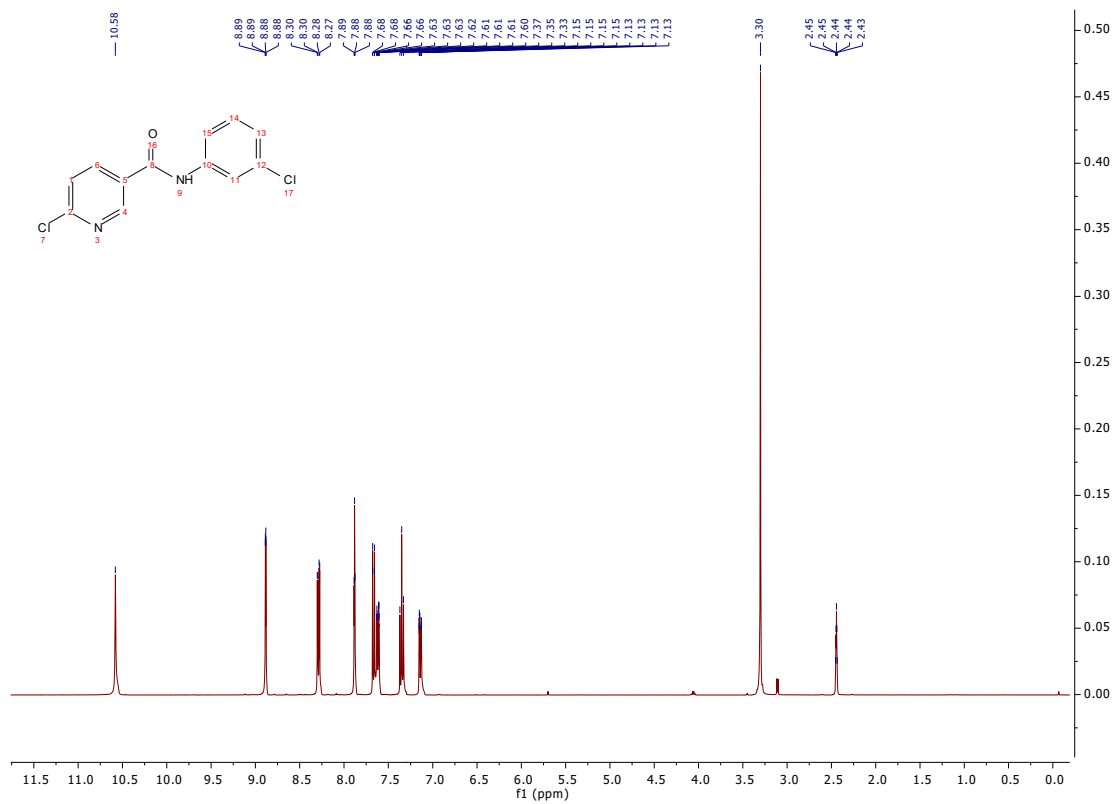
Supp. Fig. S27. ¹³C-NMR (101 MHz) spectrum of N7.



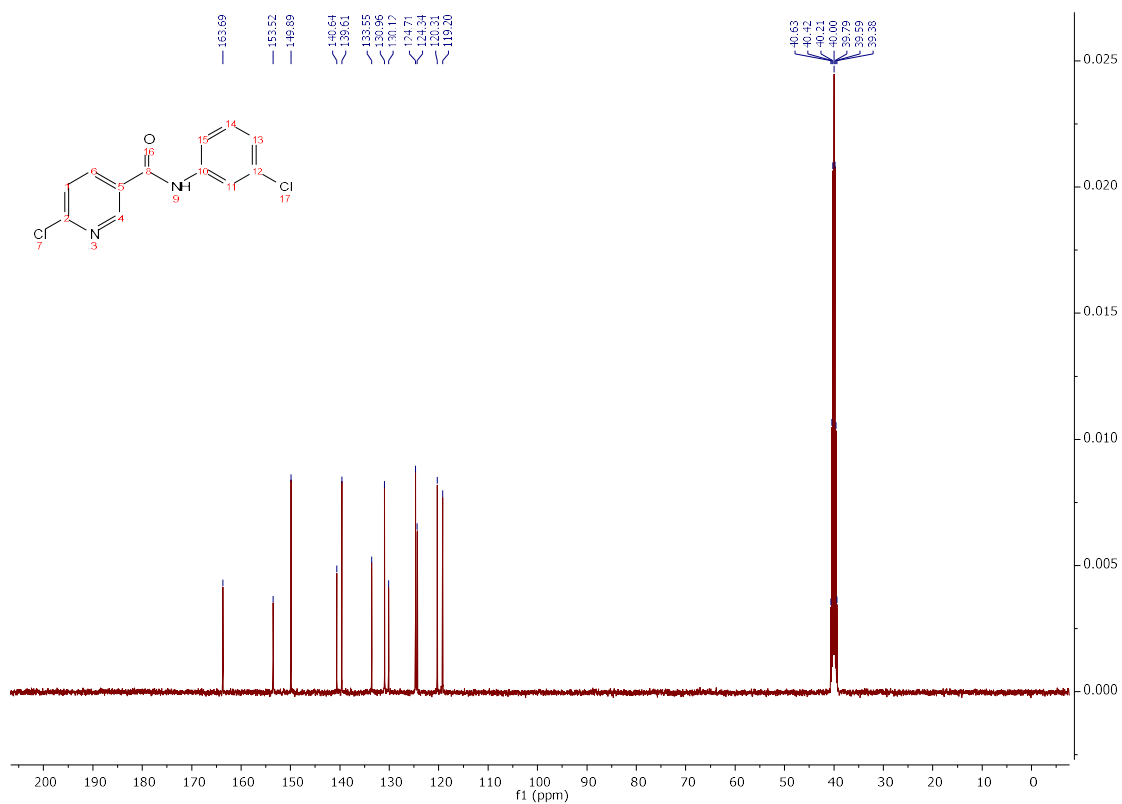
Supp. Fig. S28. HPLC-TOF/MS [M-H]⁻ spectrum of N7.



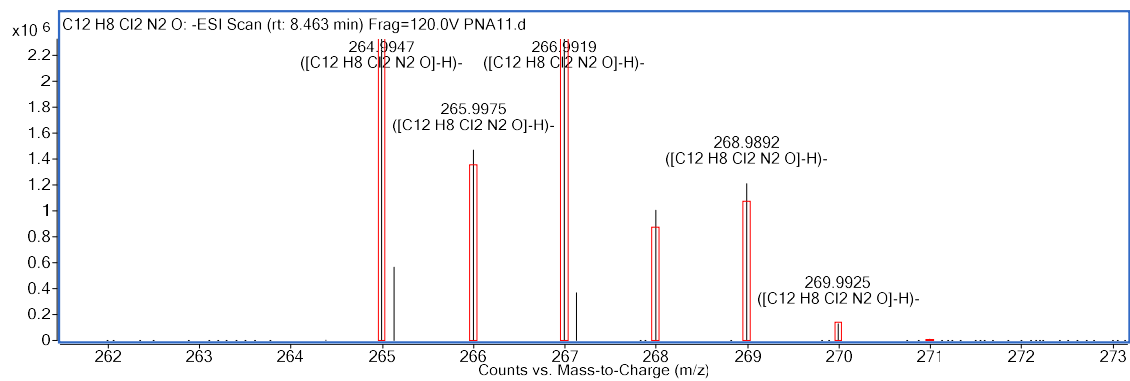
Supp. Fig. S29. The IR spectrum of N8.



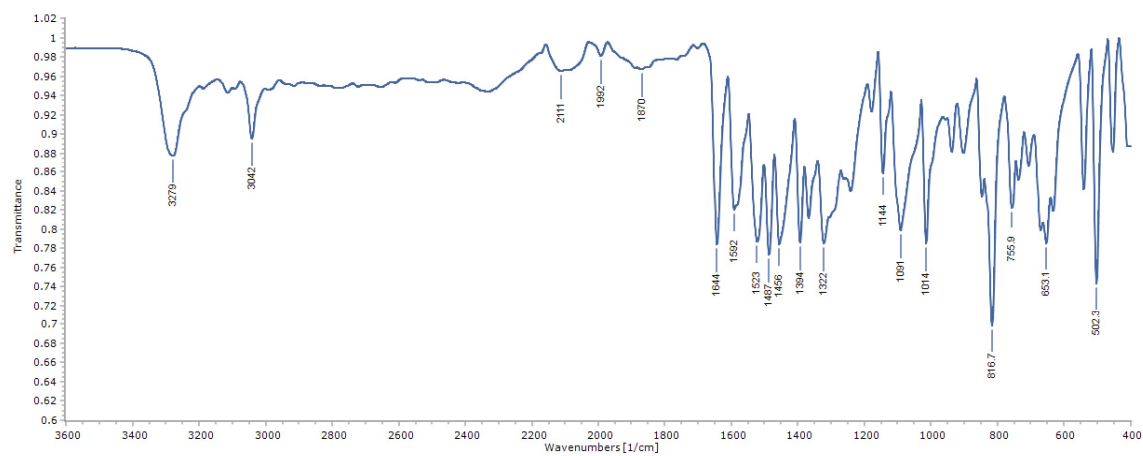
Supp. Fig. S30. ¹H-NMR (400 MHz) spectrum of N8.



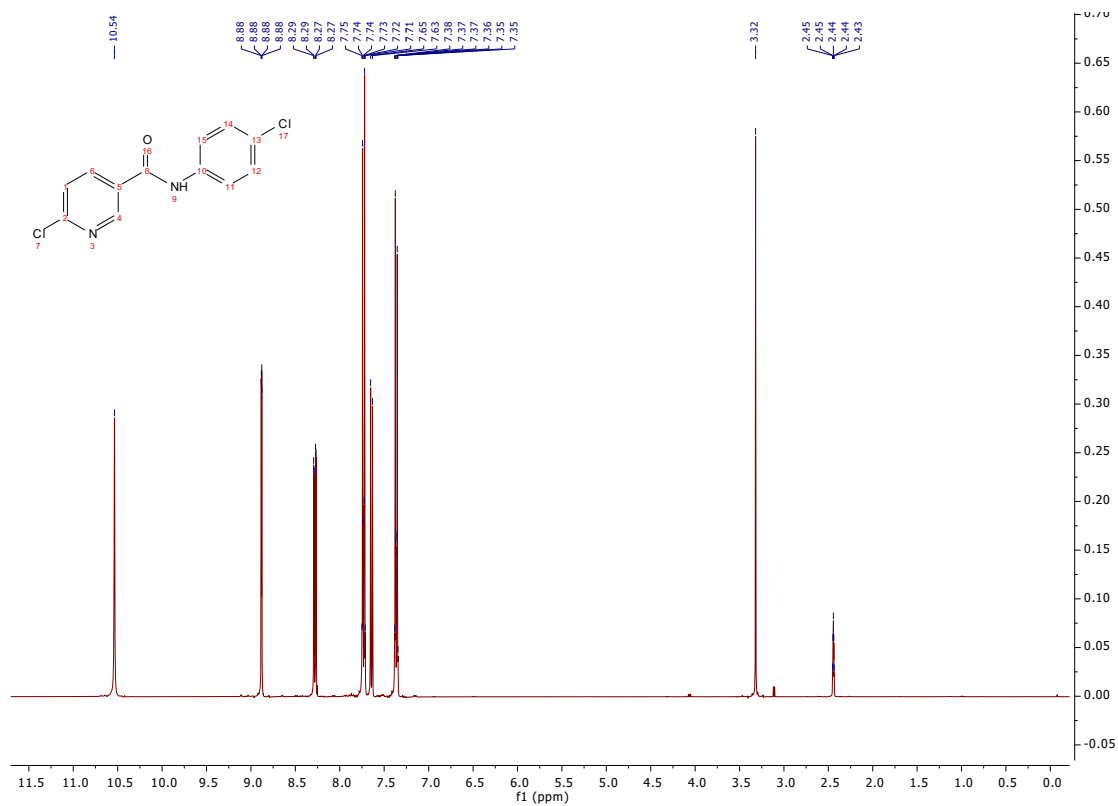
Supp. Fig. S31. ^{13}C -NMR (101 MHz) spectrum of N8.



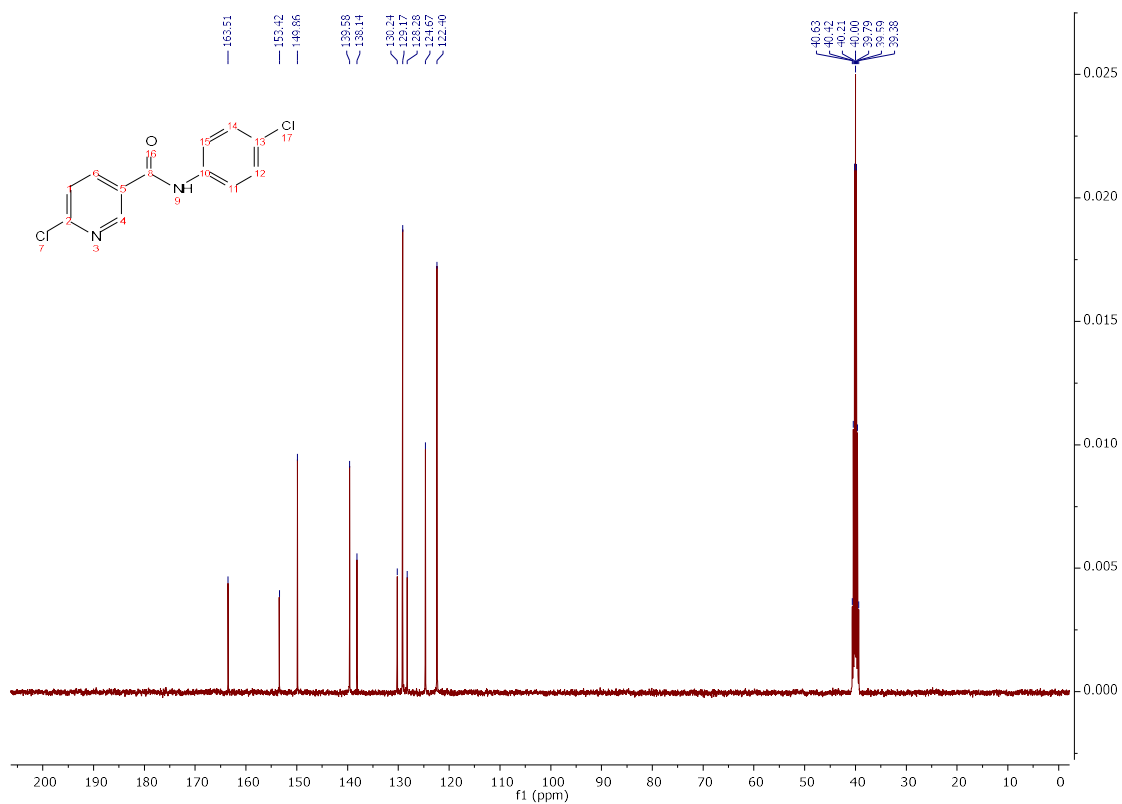
Supp. Fig. S32. HPLC-TOF/MS $[\text{M}-\text{H}]^-$ spectrum of N8.



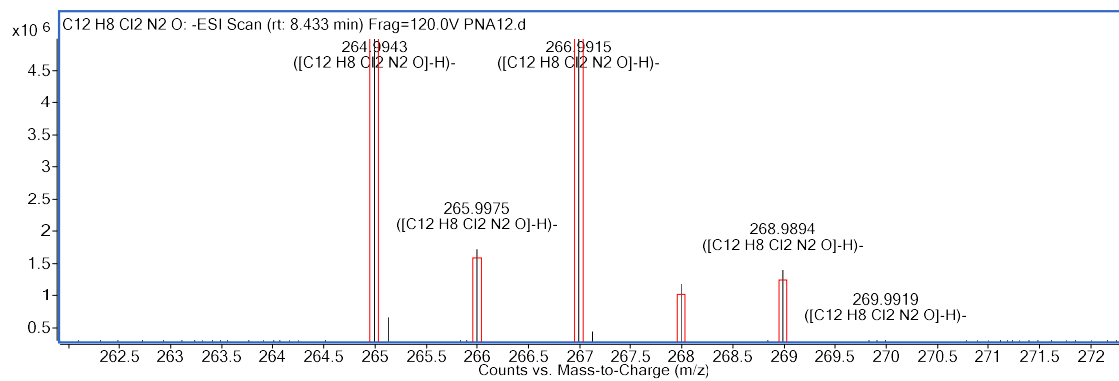
Supp. Fig. S33. The IR spectrum of N9.



Supp. Fig. S34. ¹H-NMR (400 MHz) spectrum of N9.



Supp. Fig. S35. ¹³C-NMR (101 MHz) spectrum of N9.



Supp. Fig. S36. HPLC-TOF/MS [M-H]⁻ spectrum of N9.