

Supplementary material to:

**[(7-CHLOROQUINOLIN-4-YL)AMINO]ACETOPHENONES AND
THEIR COPPER(II) DERIVATIVES:
SYNTHESIS, CHARACTERIZATION, COMPUTATIONAL STUDIES
AND ANTIMALARIAL ACTIVITY**

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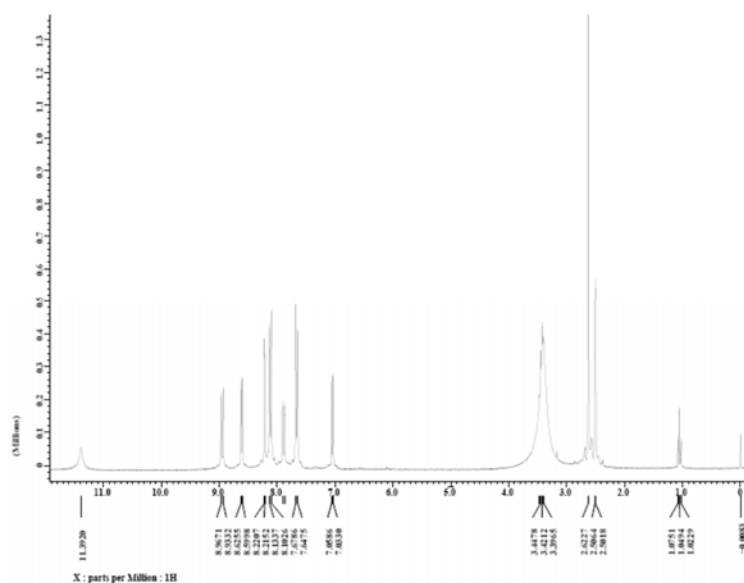
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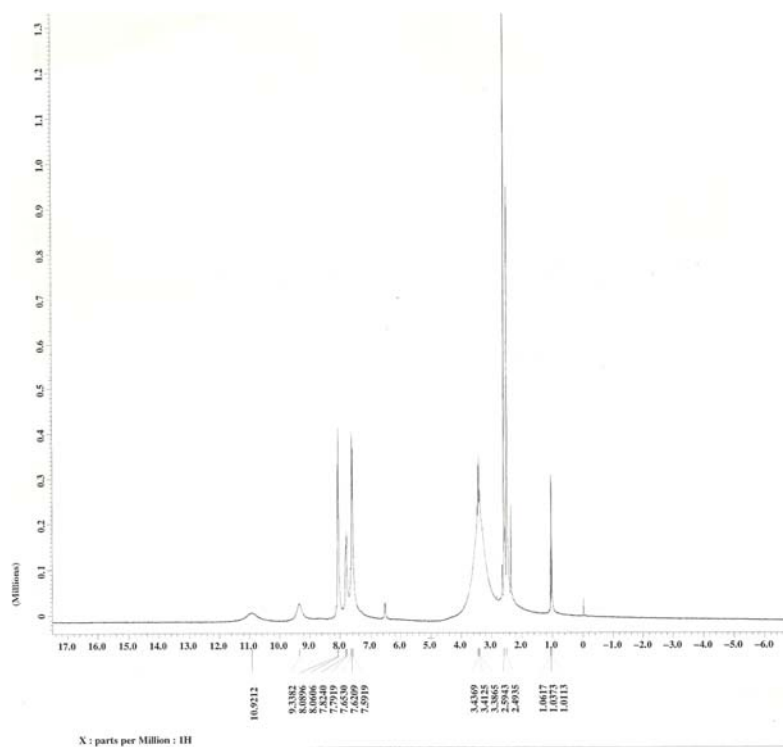
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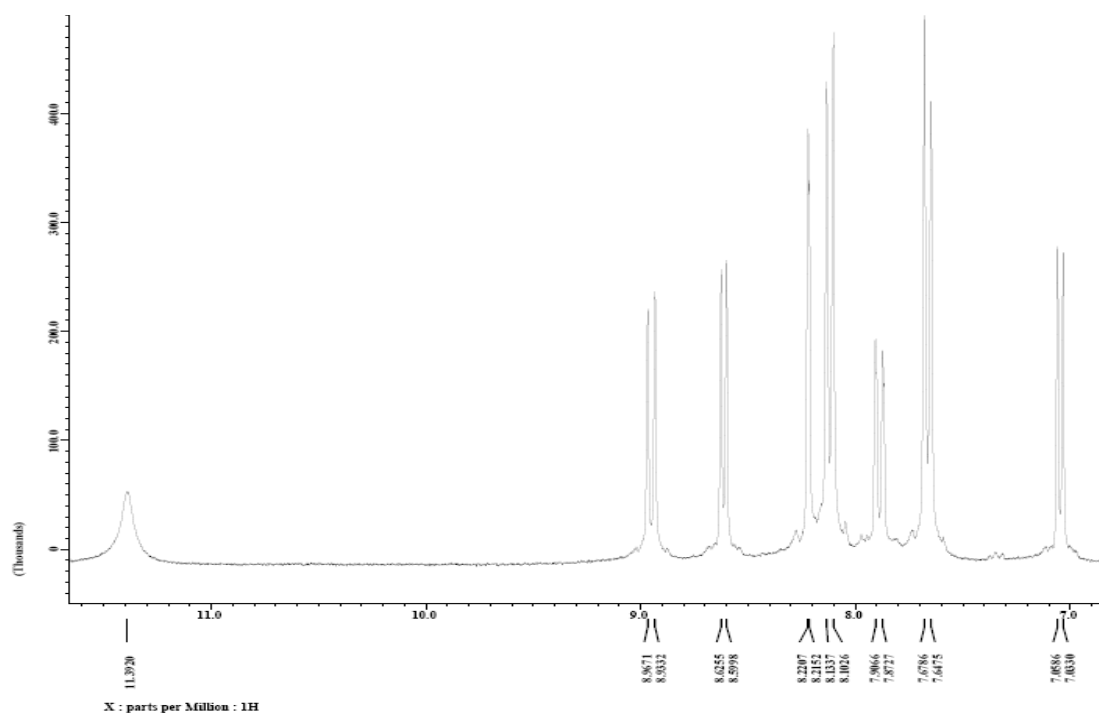
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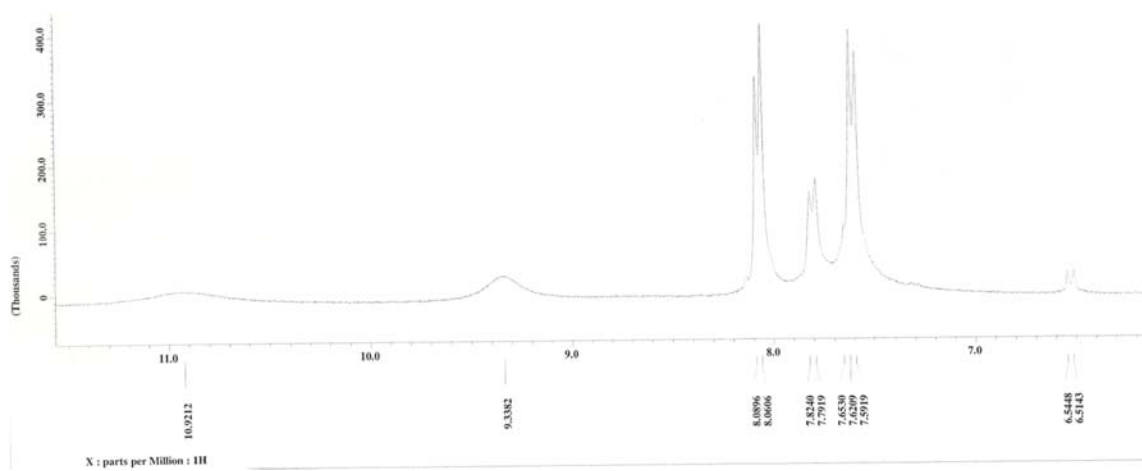
Supplementary Figure 1: ^1H NMR spectrum of 4-[(7-chloroquinolin-4-yl)amino]acetophenone (**4**)



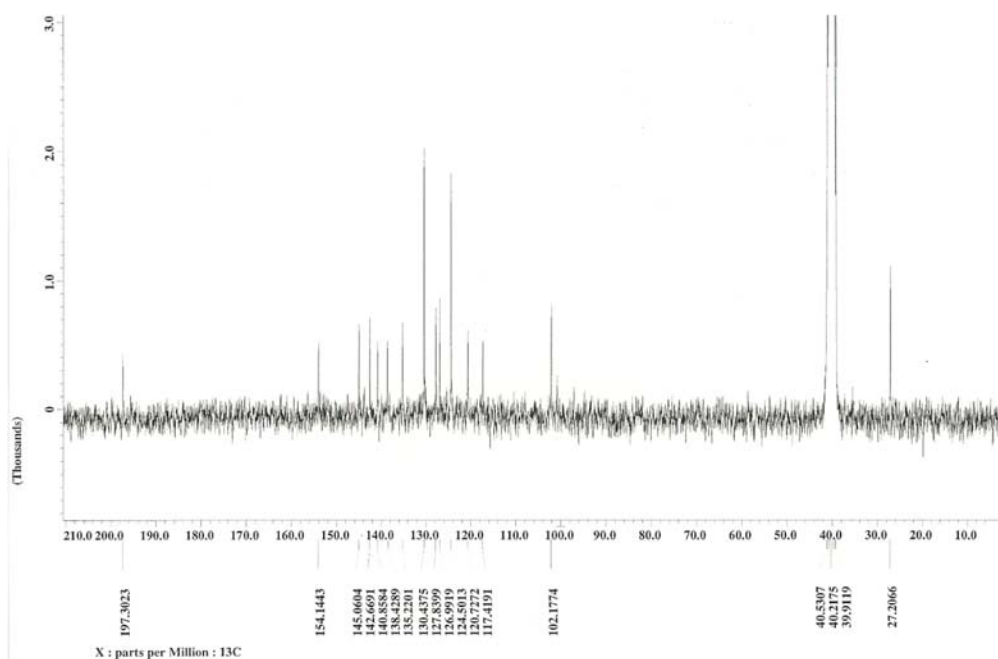
Supplementary Figure 2: ^1H NMR spectrum of {4-[(7-chloroquinolin-4-yl)amino]acetophenone} copper (II) chloride (**4a**)



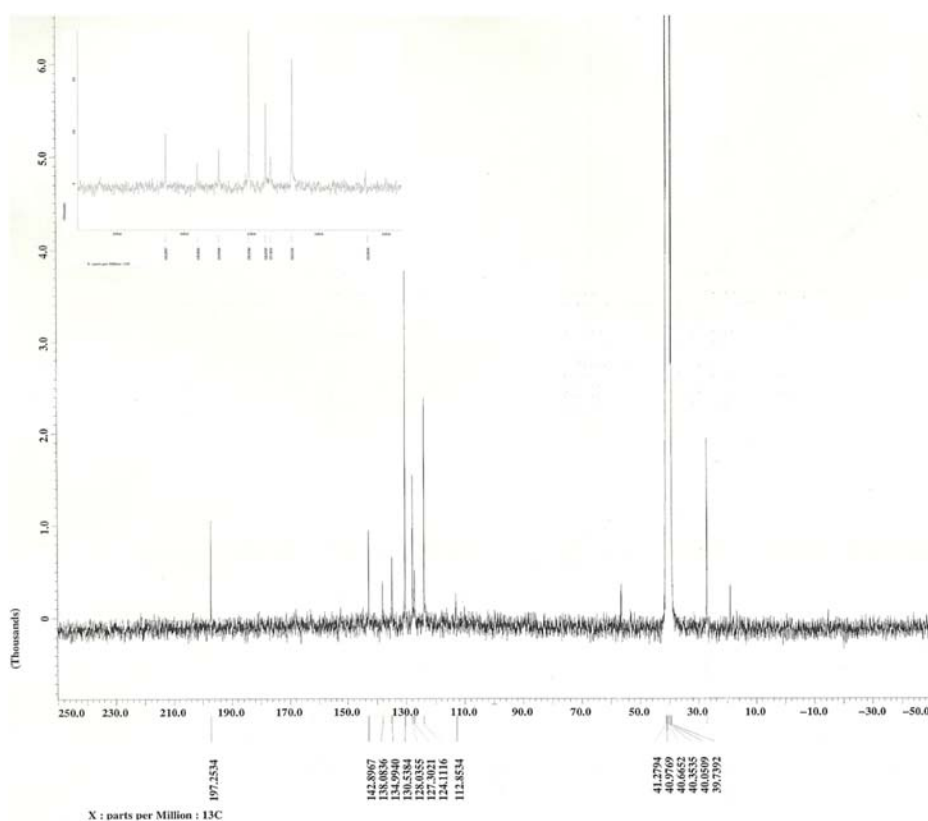
Supplementary Figure 3: Amplified ^1H NMR spectrum of 4-[(7-chloroquinolin-4-yl)amino]acetophenone (**4**)



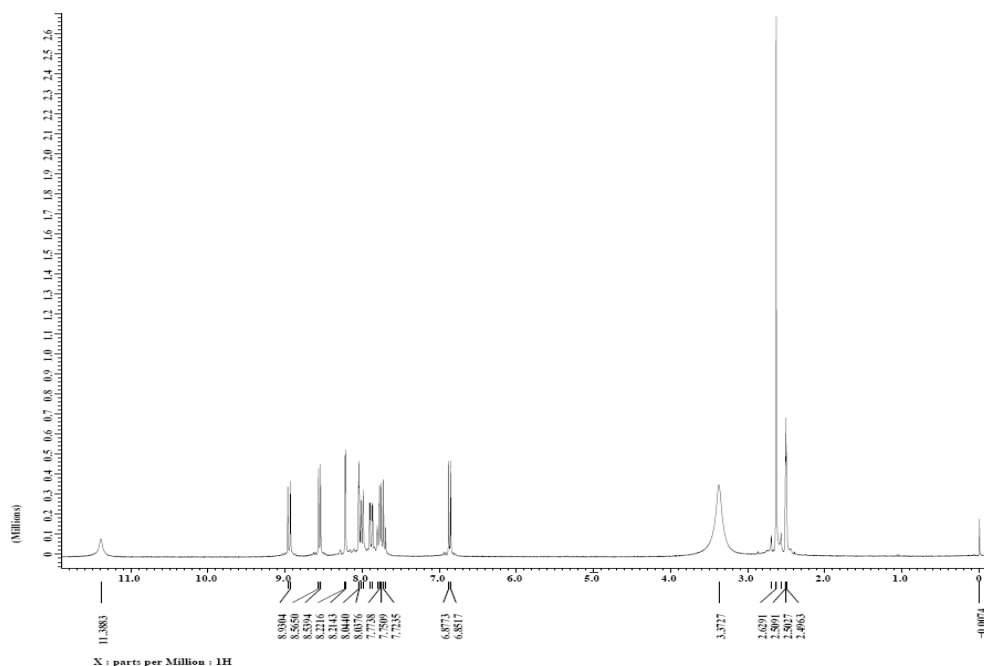
Supplementary Figure 4: Amplified ^1H NMR spectrum of {4-[(7-chloroquinolin-4-yl)amino]acetophenone}copper(II) chloride (**4a**)



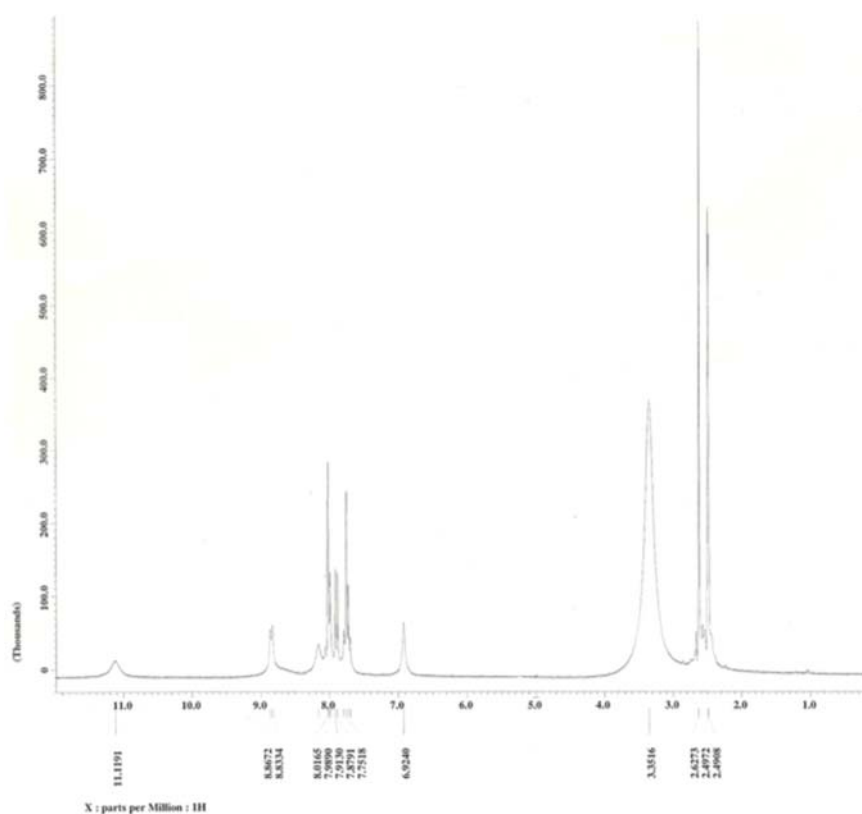
Supplementary Figure 5: ^{13}C NMR spectrum of 4-[(7-chloroquinolin-4-yl)amino]acetophenone (4)



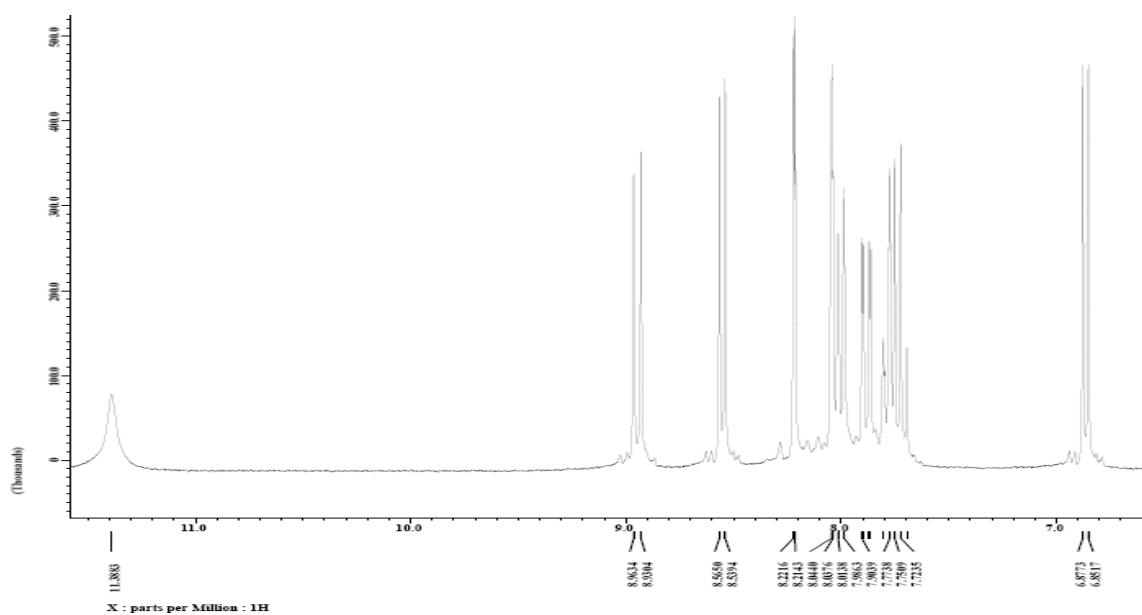
Supplementary Figure 6: ^{13}C NMR spectrum of {4-[(7-chloroquinolin-4-yl)amino]acetophenone}copper(II) chloride (4a)



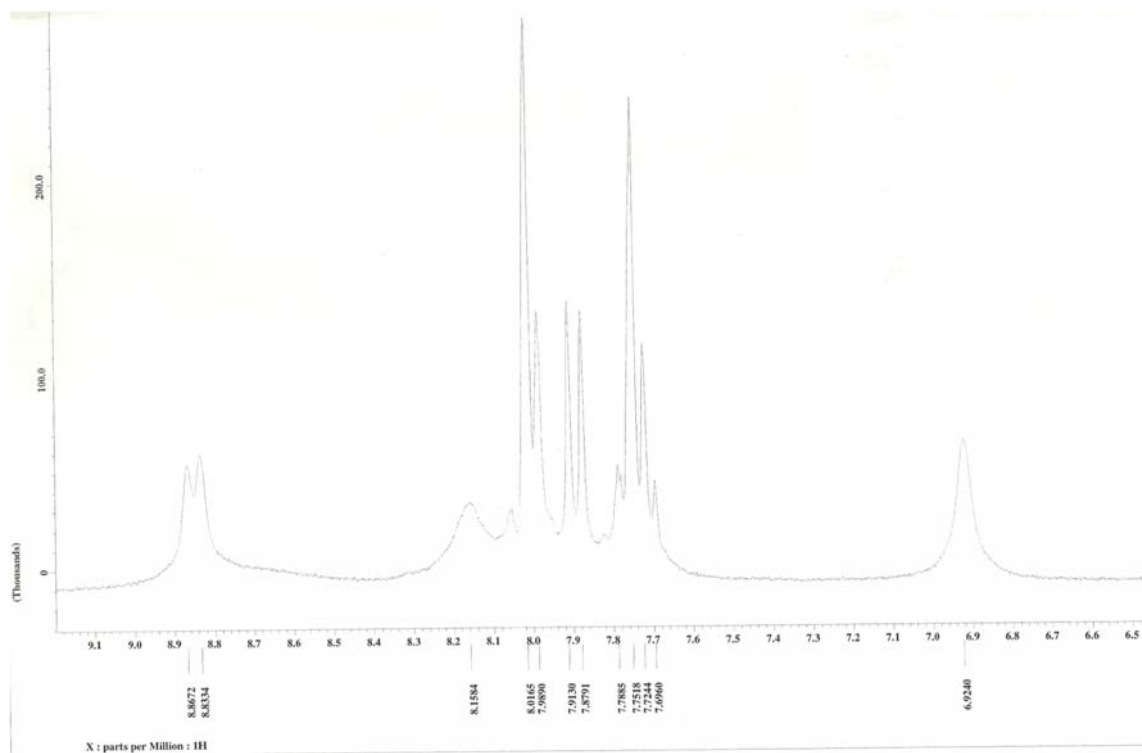
Supplementary Figure 7: ¹H NMR spectrum of 3-[(7-chloroquinolin-4-yl)amino]acetophenone (5)



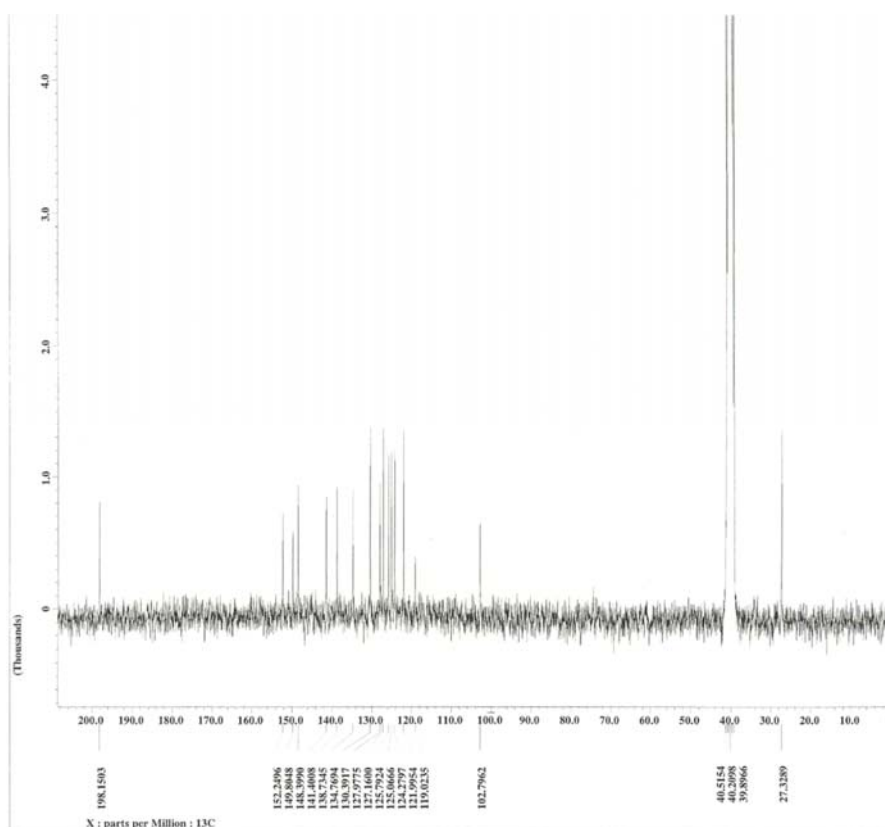
Supplementary Figure 8: ¹H NMR spectrum of {3-[(7-chloroquinolin-4-yl)amino]acetophenone} copper(II) chloride (5a)



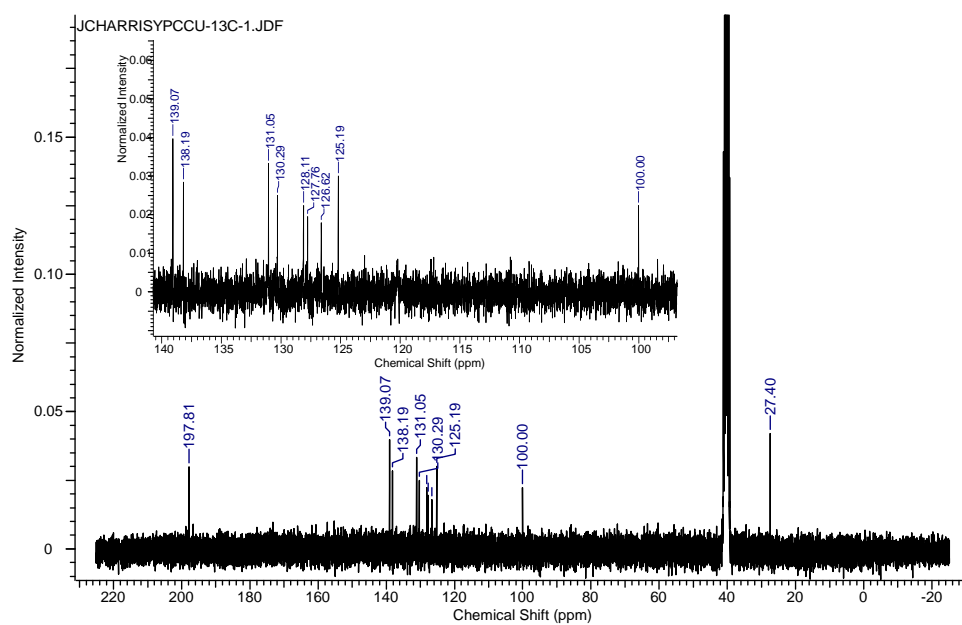
Supplementary Figure 9: Amplified ^1H NMR spectrum of 3-[(7-chloroquinolin-4-yl)amino]acetophenone (5)



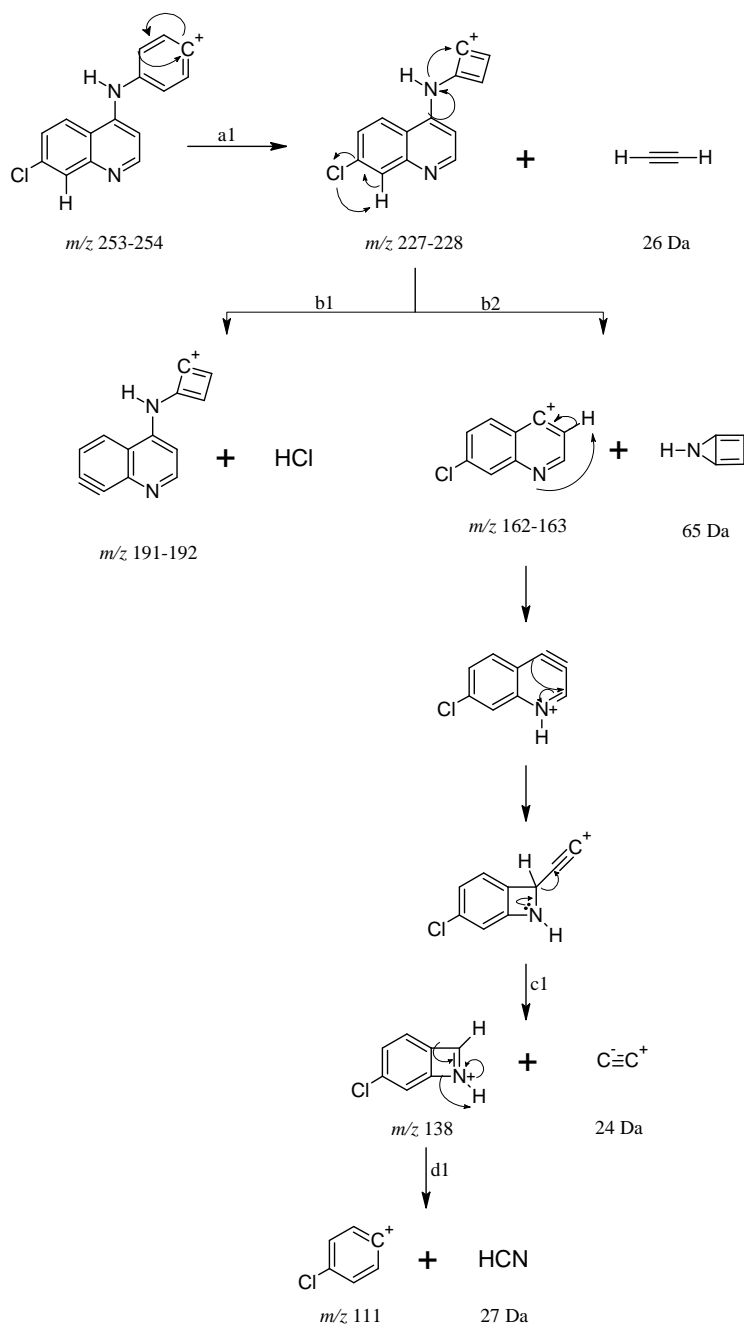
Supplementary Figure 10: Amplified ^1H NMR spectrum of {3-[(7-chloroquinolin-4-yl)amino]acetophenone}copper(II) chloride (5a)



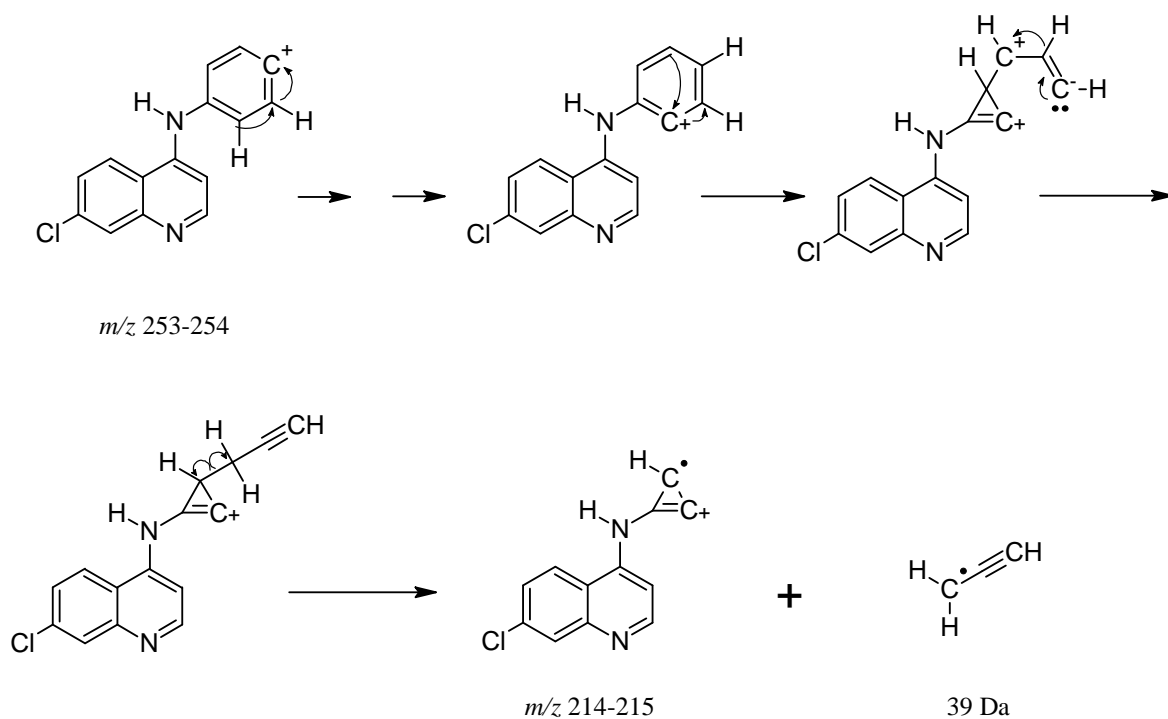
Supplementary Figure 11: ^{13}C NMR spectrum of 3-[(7-chloroquinolin-4-yl)amino]acetophenone (5)



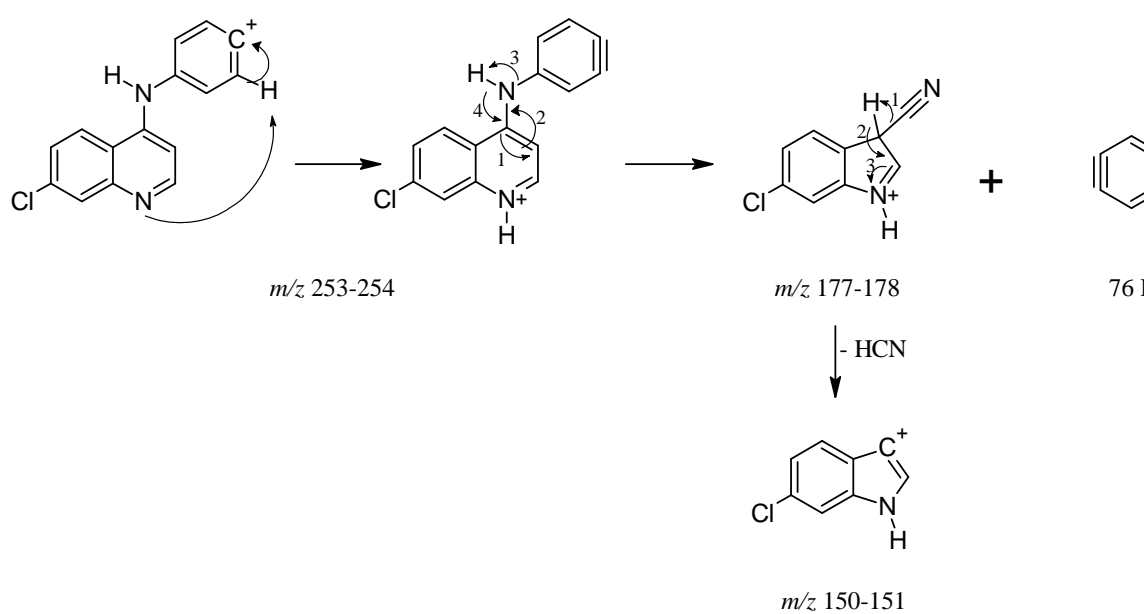
Supplementary Figure 12: ^{13}C NMR spectrum of {3-[(7-chloroquinolin-4-yl)amino]acetophenone}copper(II) chloride (5a)



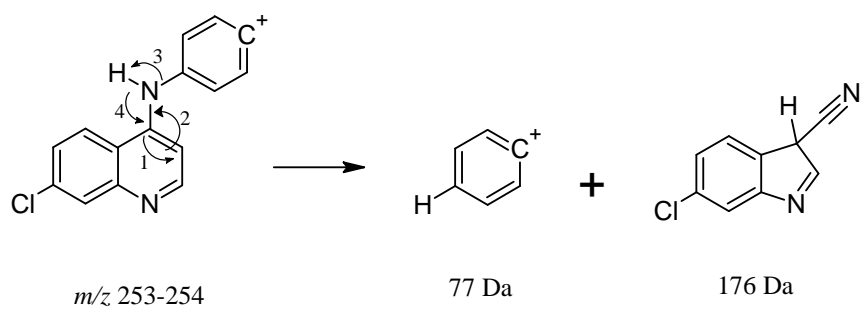
Supplementary Figure 13: Dissociative heterolytic mechanism for the a1, b1, b2, c1, d1 pathways; from the fragment at m/z 253-254 generated by the precursor molecular ion at m/z 297 for compound **4**. (Analogue mechanism for compound **5**)



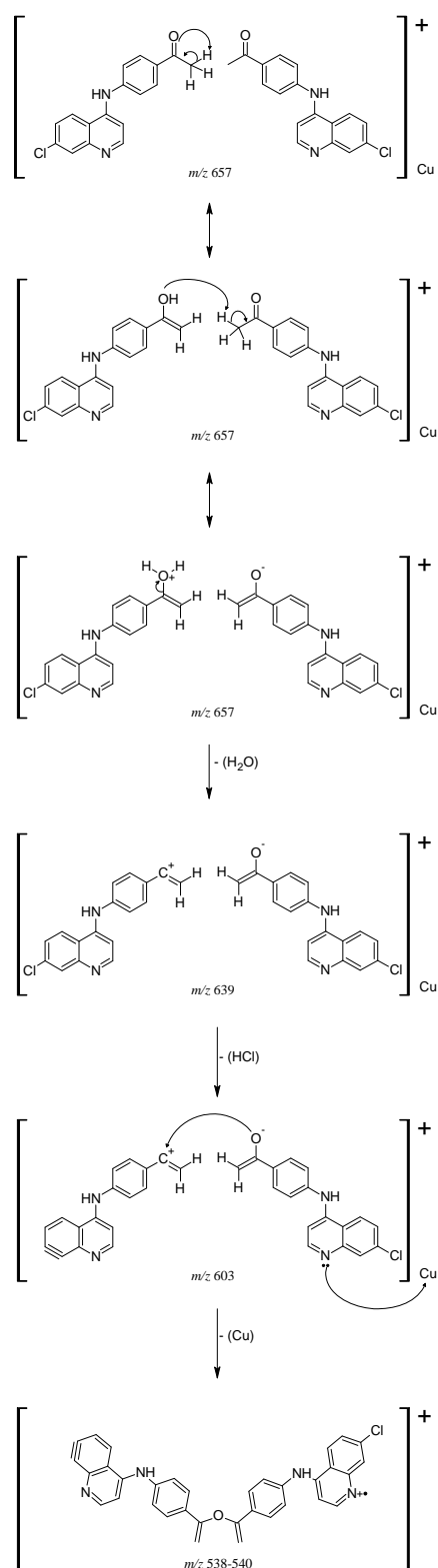
Supplementary Figure 14: Dissociative homolytic mechanism for a2 pathway



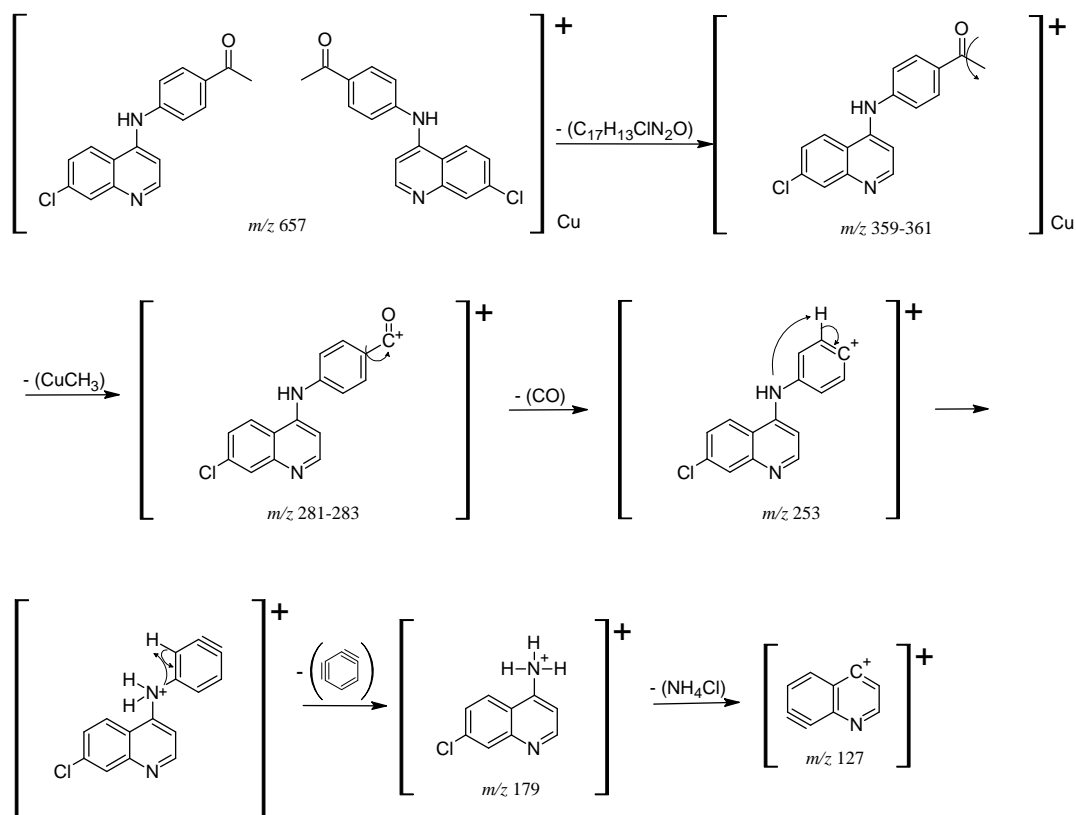
Supplementary Figure 15: Dissociative heterolytic mechanism for the a4 and b3 pathways



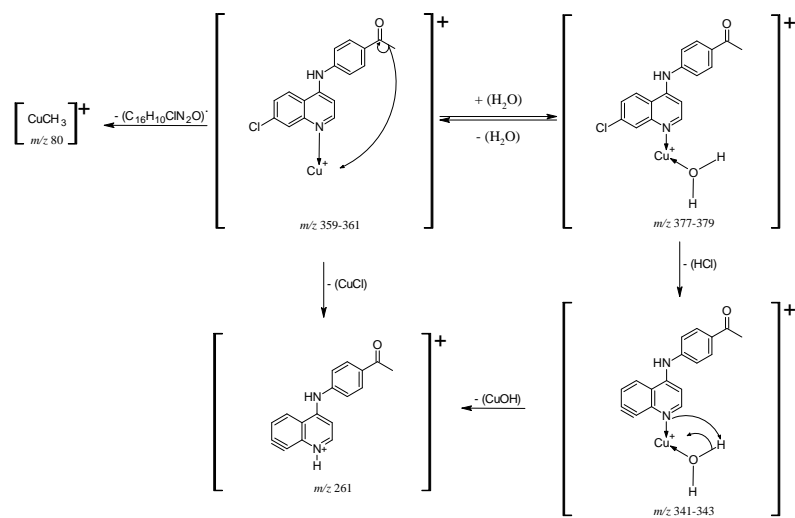
Supplementary Figure 16: Dissociative heterolytic mechanism for the α_5 pathway



Supplementary Figure 17: Minor fragmentation channel of the cationic fragment [4a]⁺ at m/z 657



Supplementary Figure 18: Extensive dissociation of the cationic fragment **[4a]⁺** at *m/z* 657



Supplementary Figure 19: Homolytic dissociation and reversible re-coordination/de-coordination of a water molecule for the fragment at *m/z* 359-361, derived from the ion **[4a]⁺** at *m/z* 657