

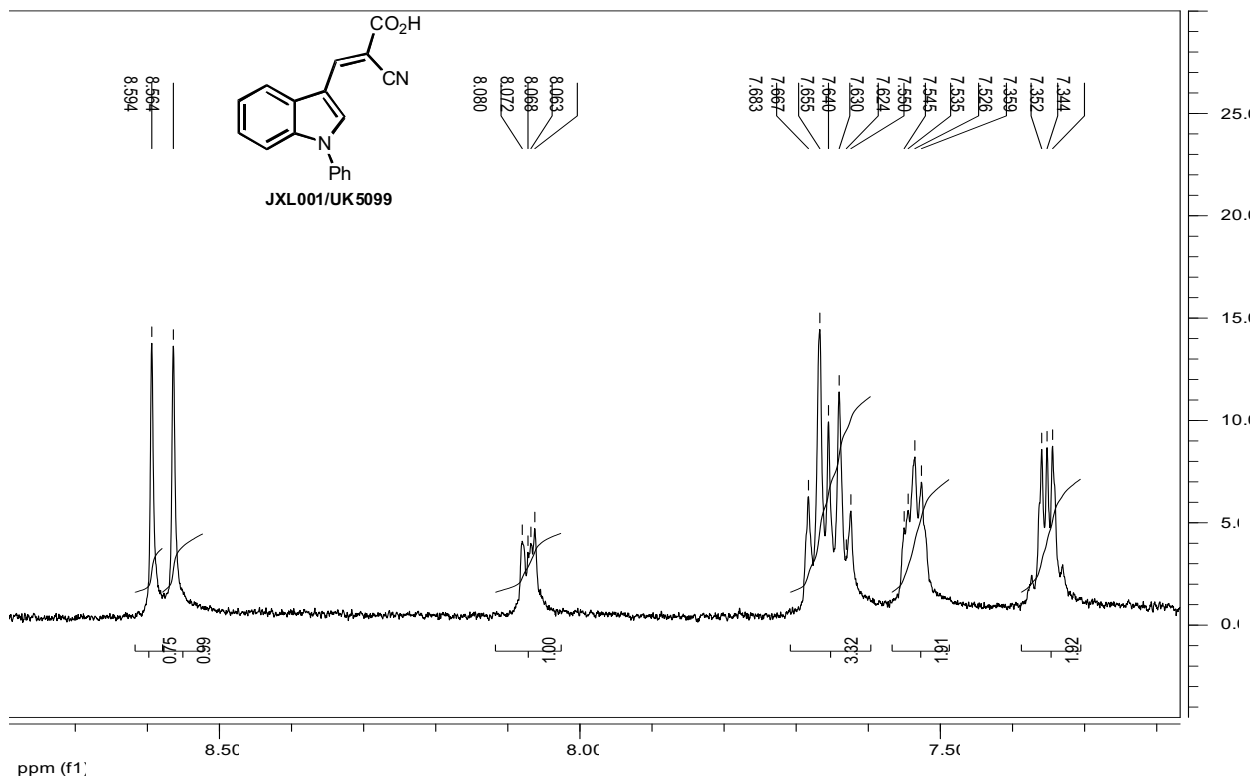
Supporting Information for

Development of Novel Mitochondrial Pyruvate Carrier Inhibitors to Treat Hair Loss

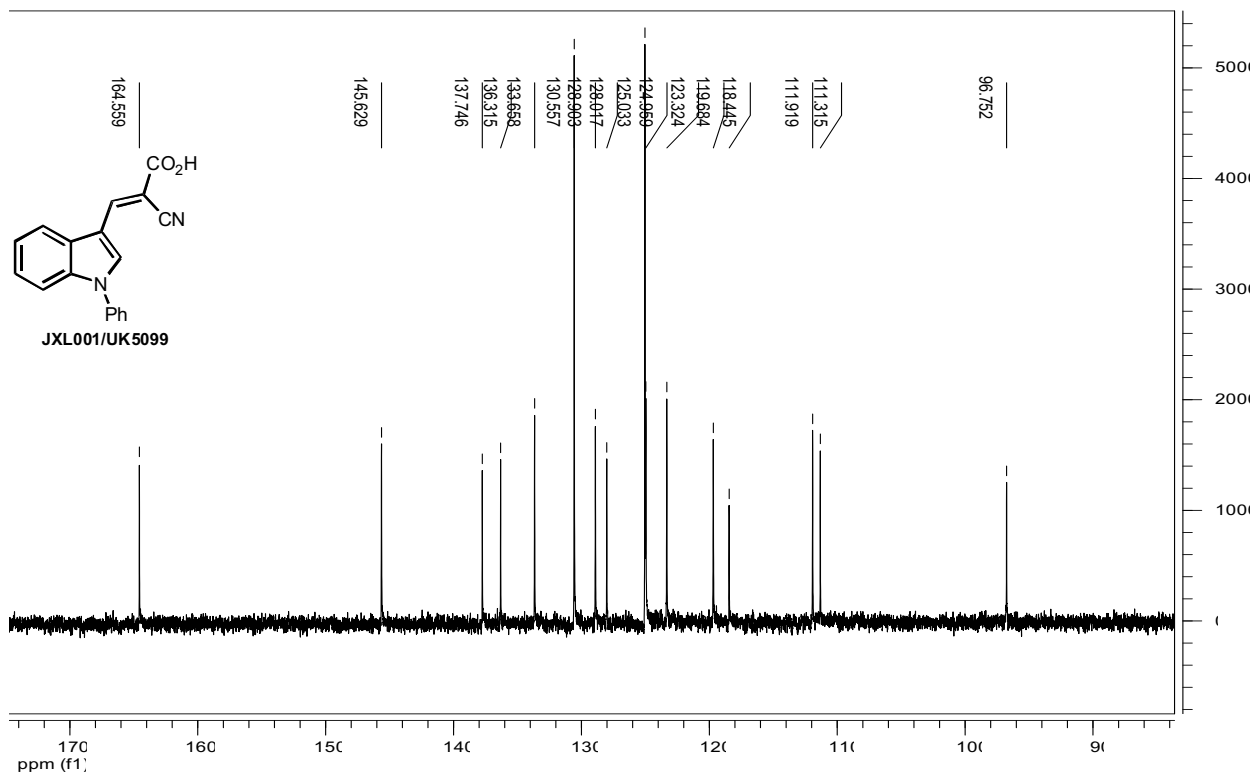
Xiaoguang Liu[†], Aimee A. Flores^{‡, ⊥, #}, Lisa Situ^{‡, ¶}, Wen Gu[§], Pete Mullen[‡], Hui Ding,[†] Heather R. Christofk^{§, ¶, ⊥, ¶}, William E. Lowry^{‡, ¶, ⊥, #}, Michael E. Jung^{*, †, §}

[†]Department of Chemistry and Biochemistry, UCLA; [‡] Department of Molecular Cell and Developmental Biology, UCLA; [§]Department of Molecular and Medical Pharmacology, UCLA; [¶] Jonsson Comprehensive Cancer Center, UCLA; [⊥] Eli and Edythe Broad Center for Regenerative Medicine, UCLA; [#] Molecular Biology Institute, UCLA; ^{*} Department of Biological Chemistry, UCLA

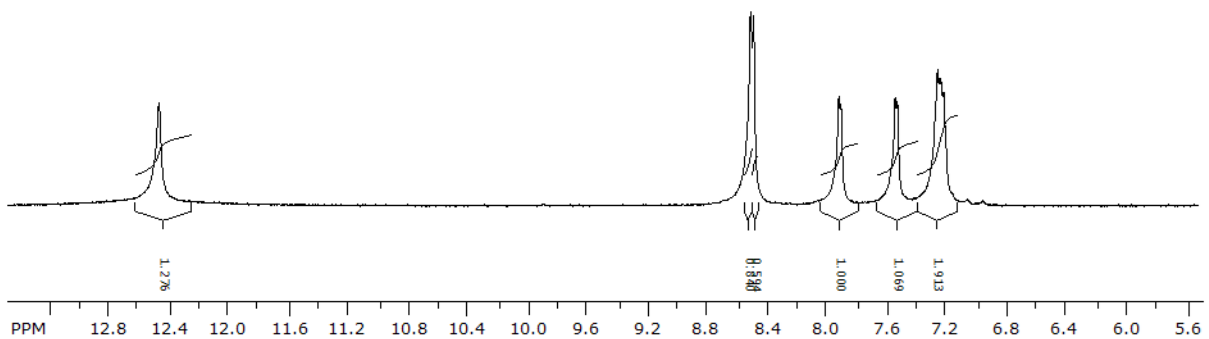
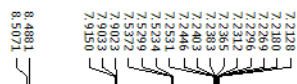
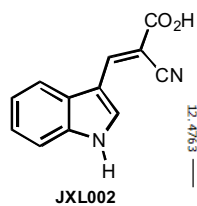
¹H NMR and ¹³C NMR of JXL001–JXL096



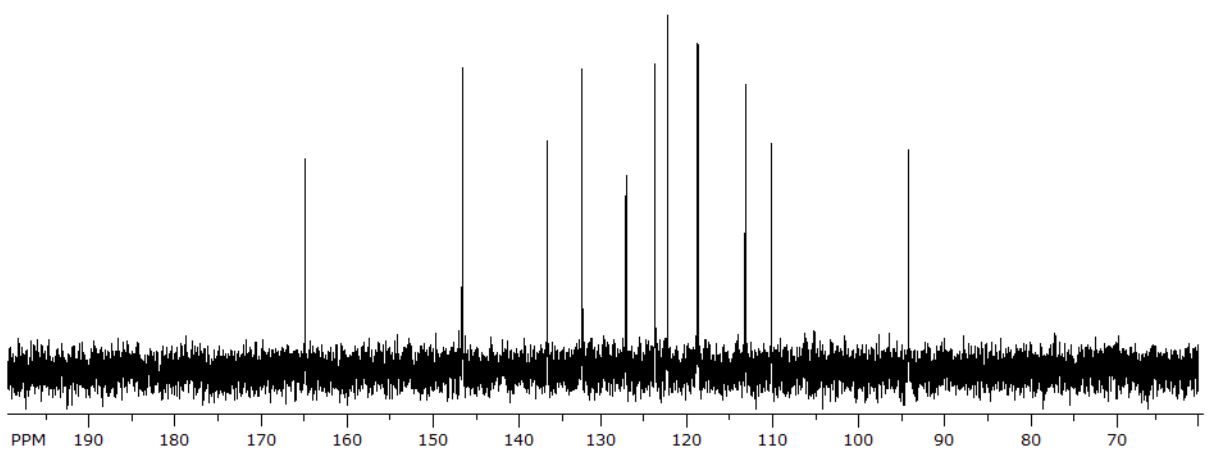
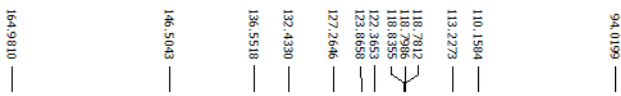
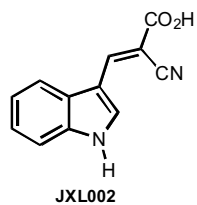
¹H NMR (500 MHz, DMSO-d₆)



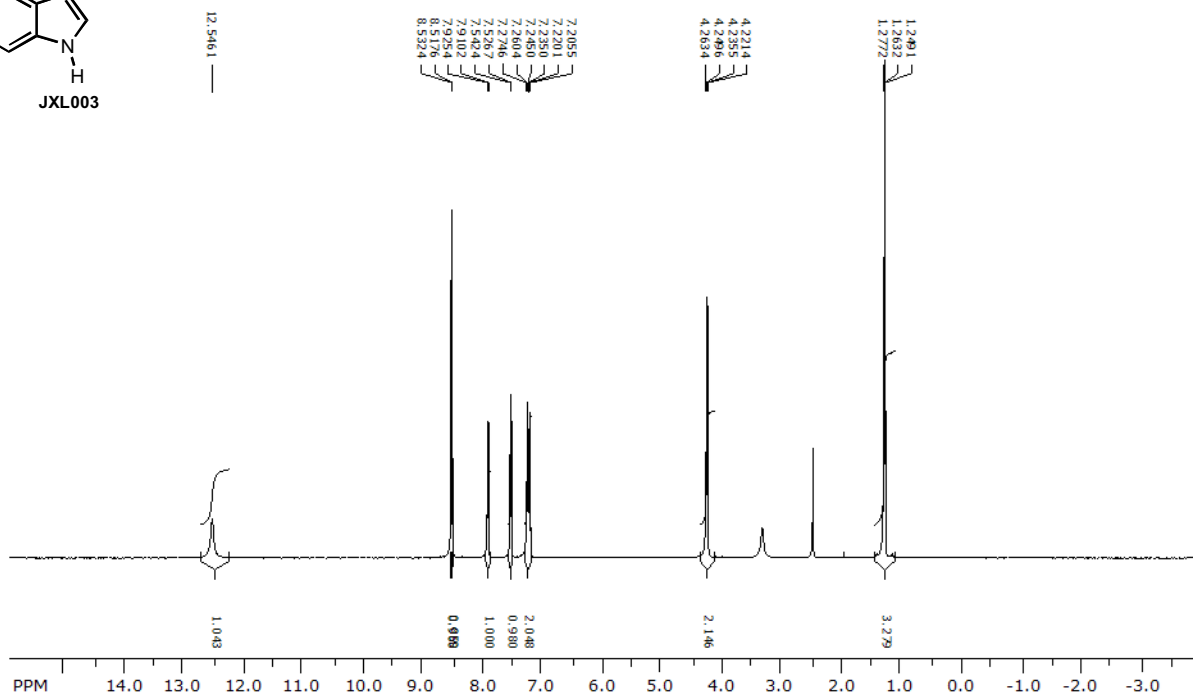
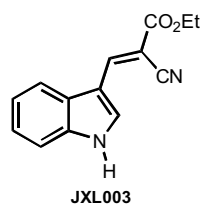
¹³C NMR (126 MHz, DMSO-d₆)



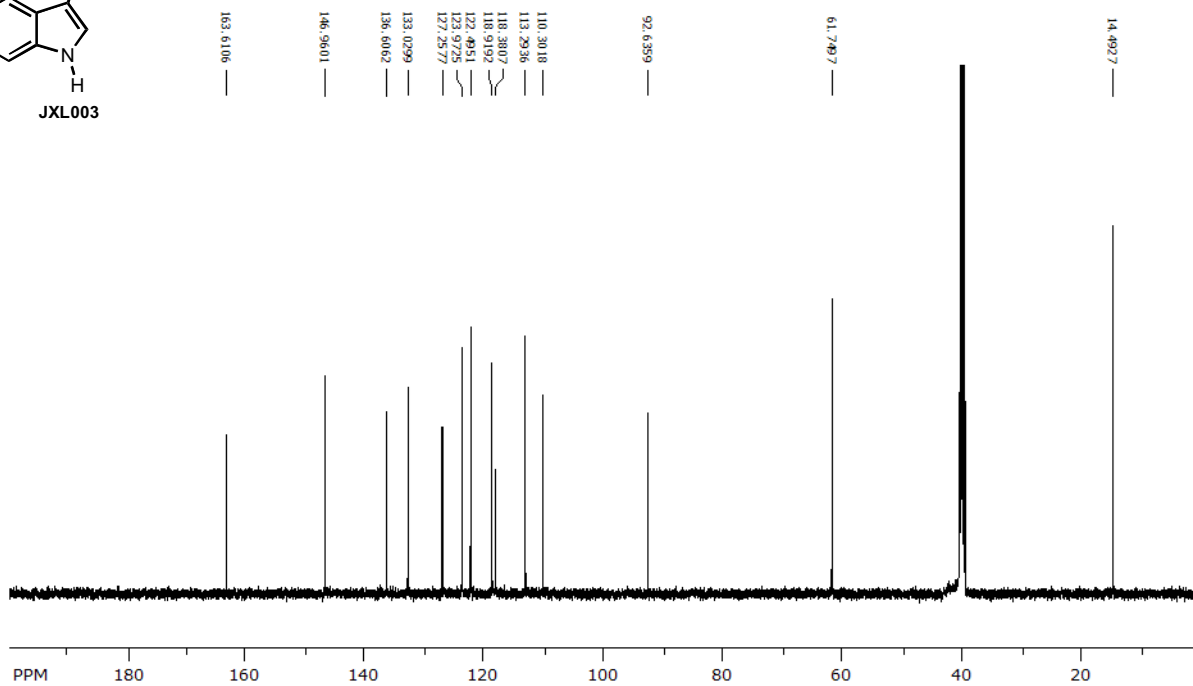
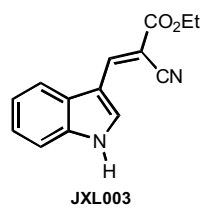
¹H NMR (500 MHz, DMSO-d₆)



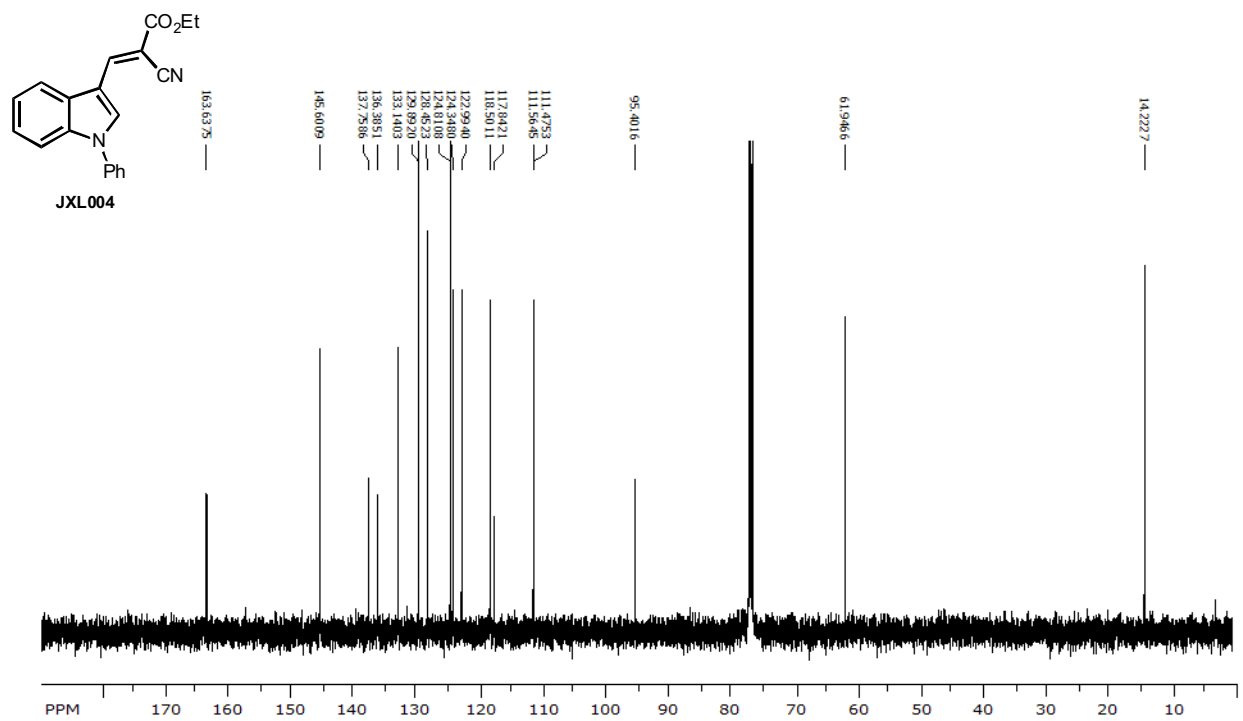
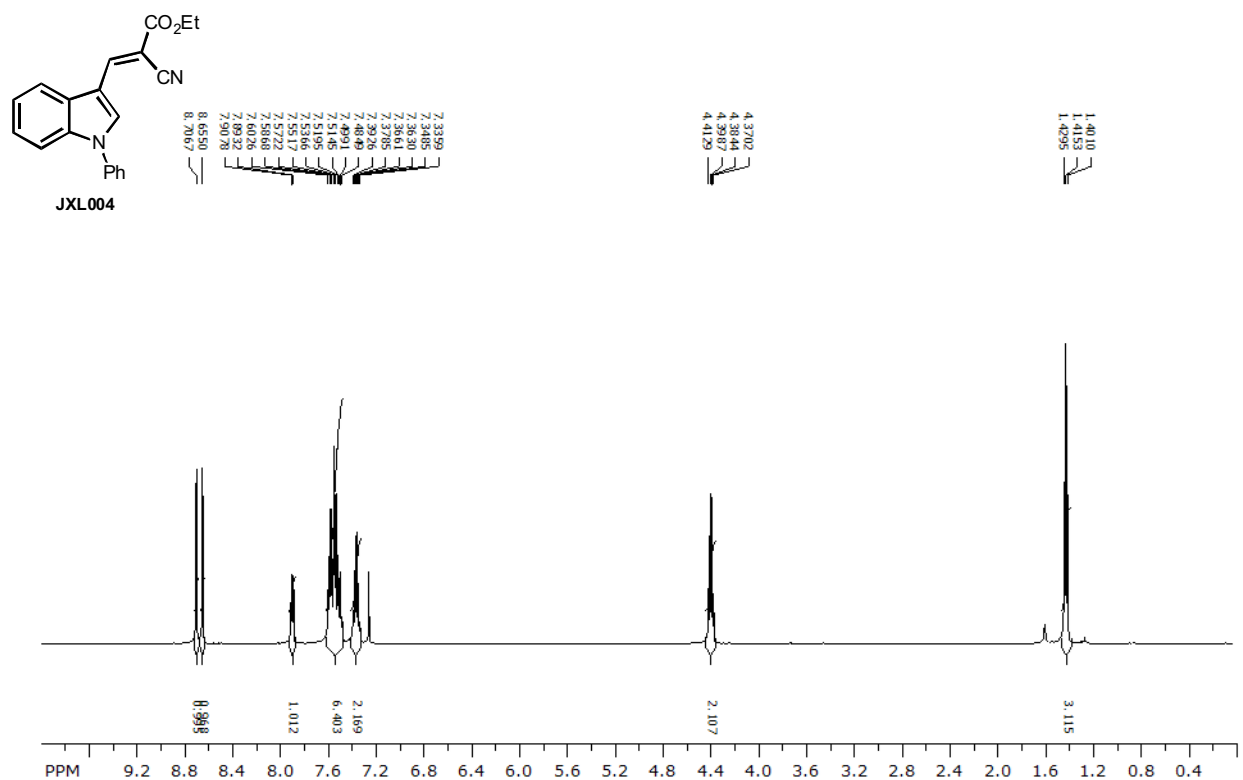
¹³C NMR (126 MHz, DMSO-d₆)

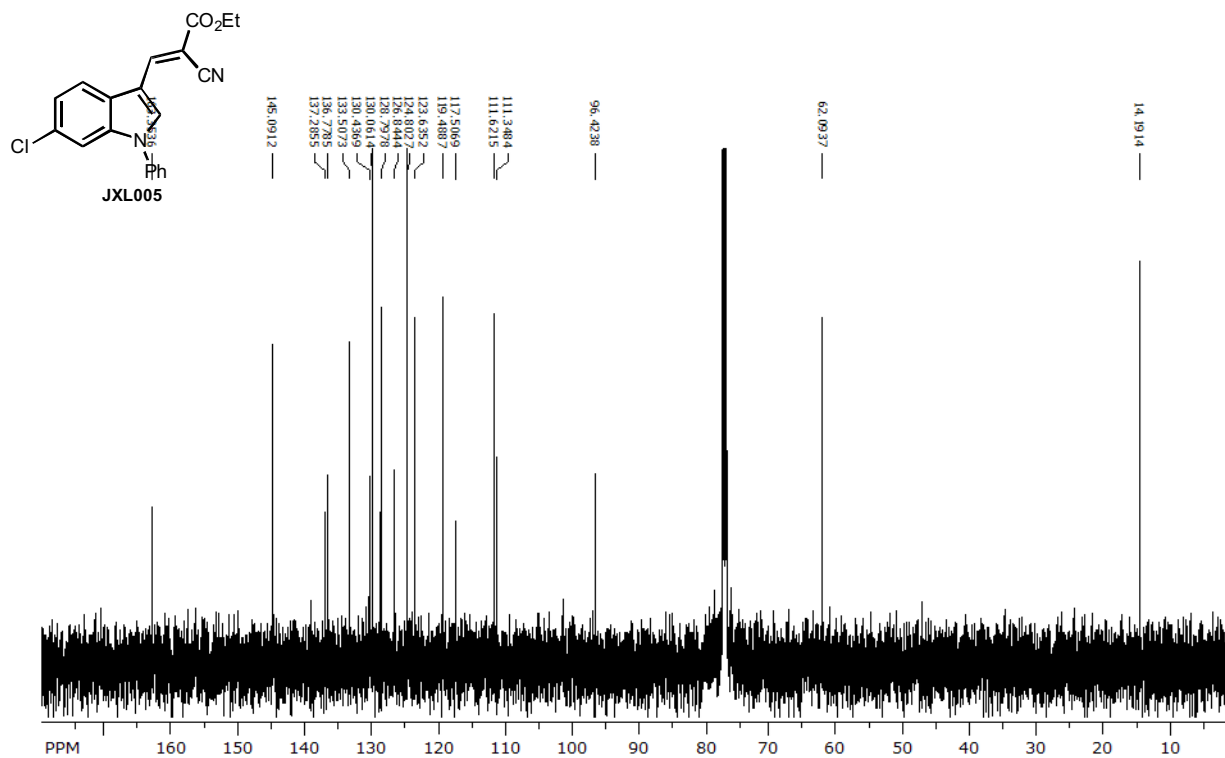
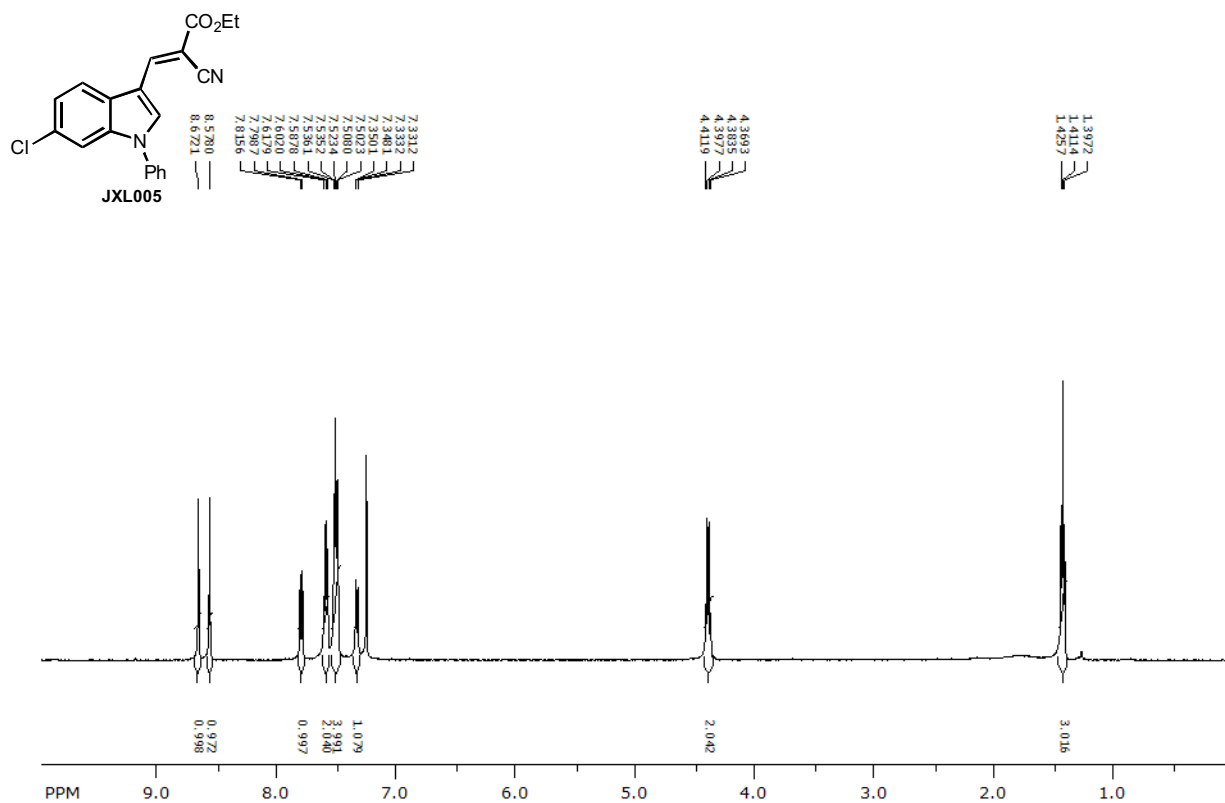


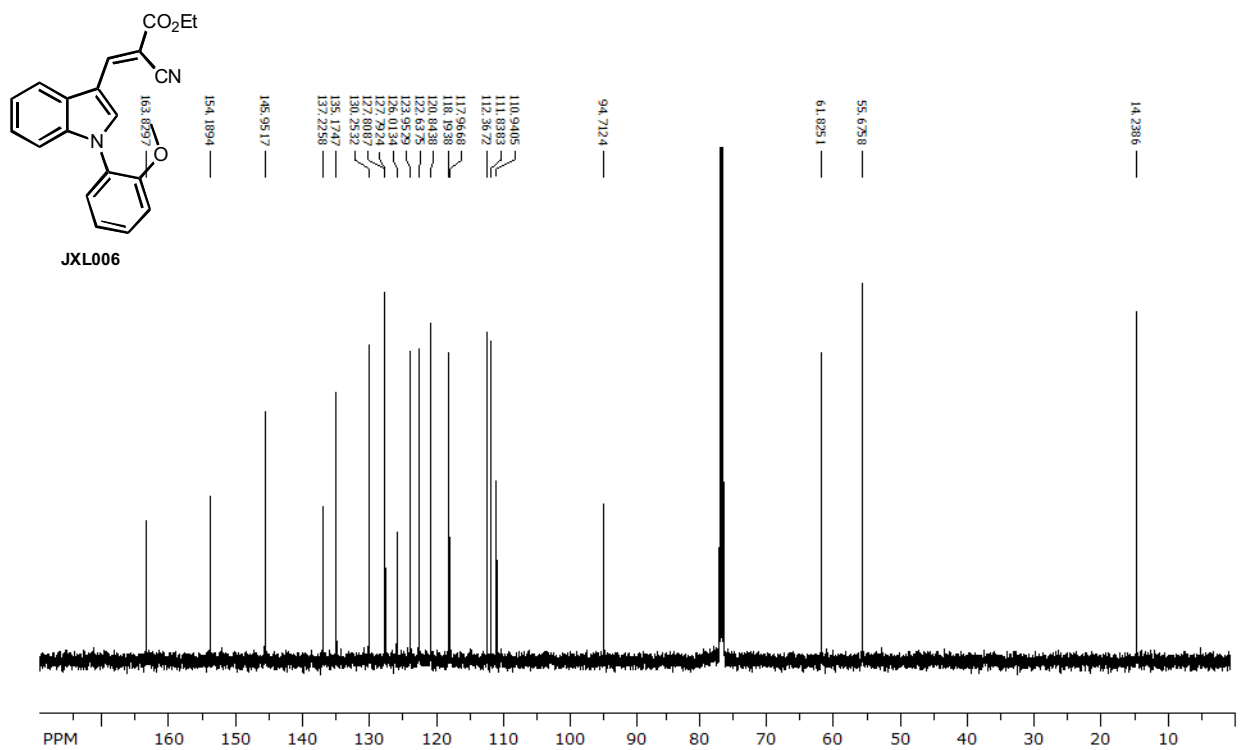
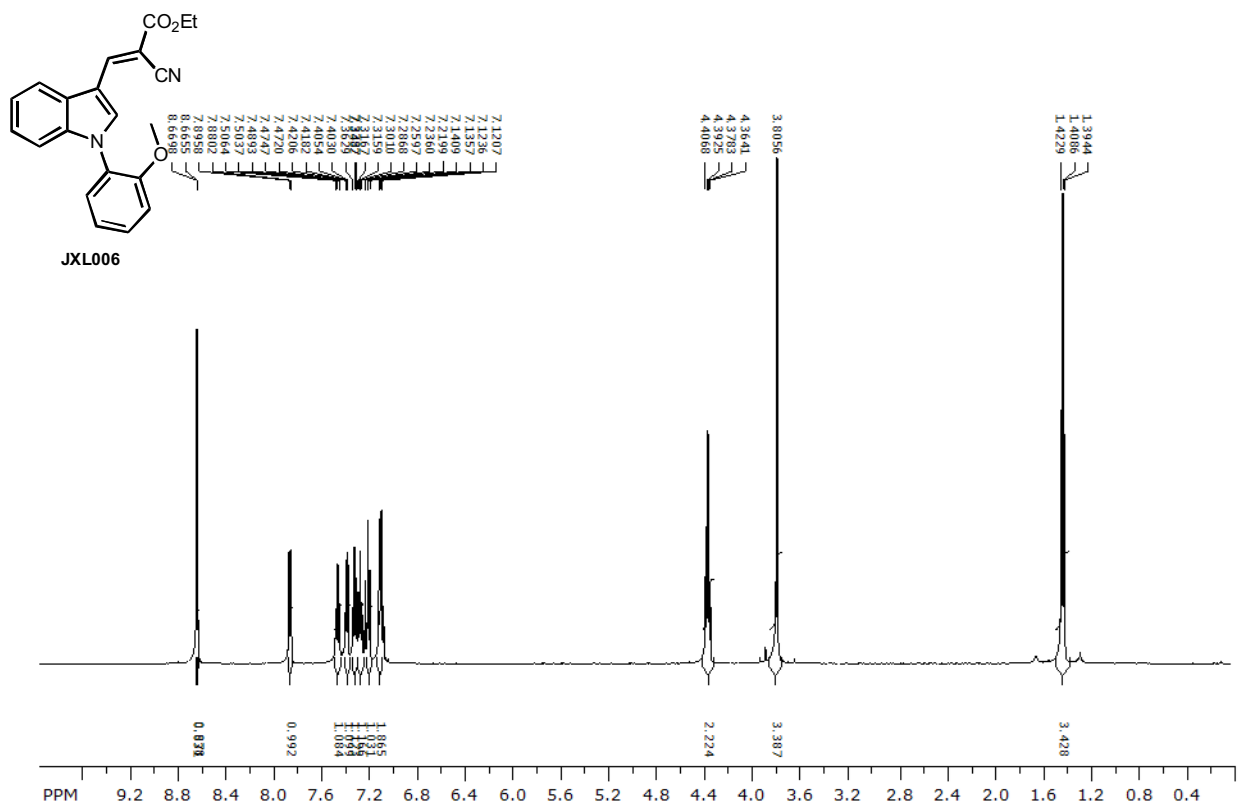
¹H NMR (500 MHz, CDCl₃)

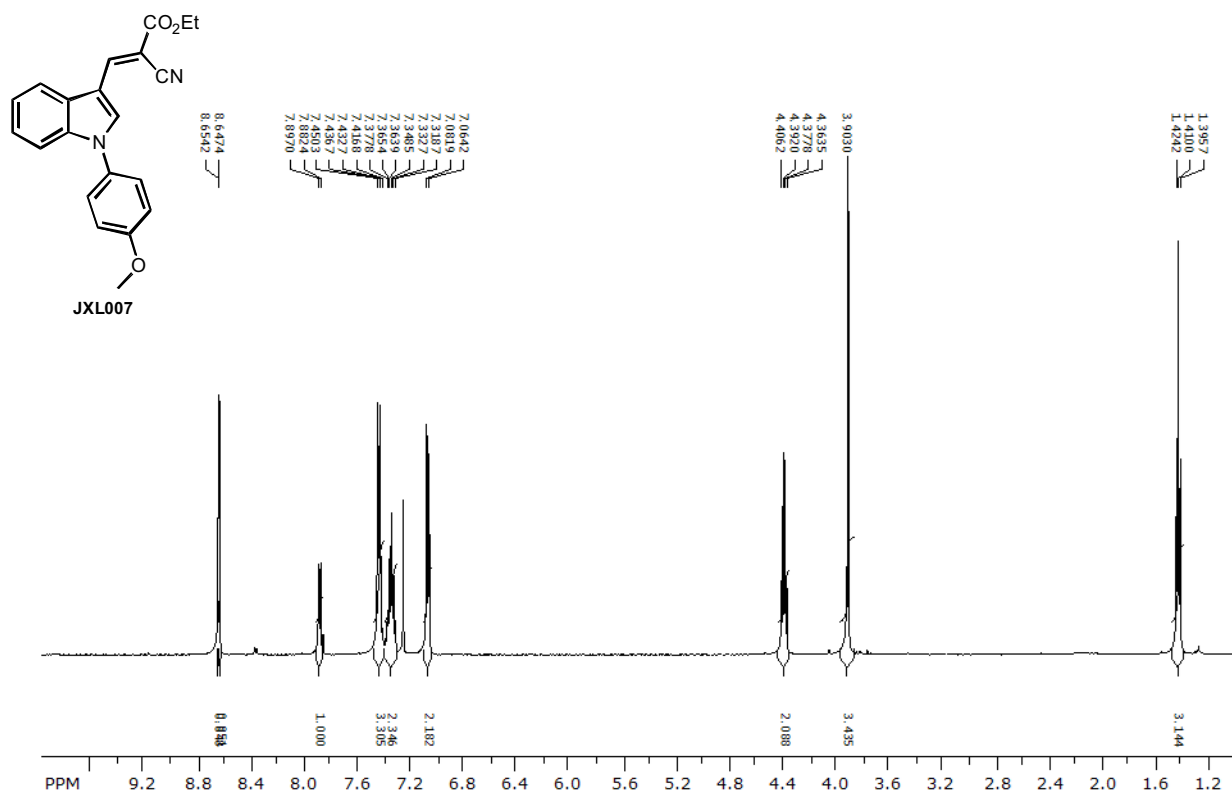


¹³C NMR (126 MHz, CDCl₃)

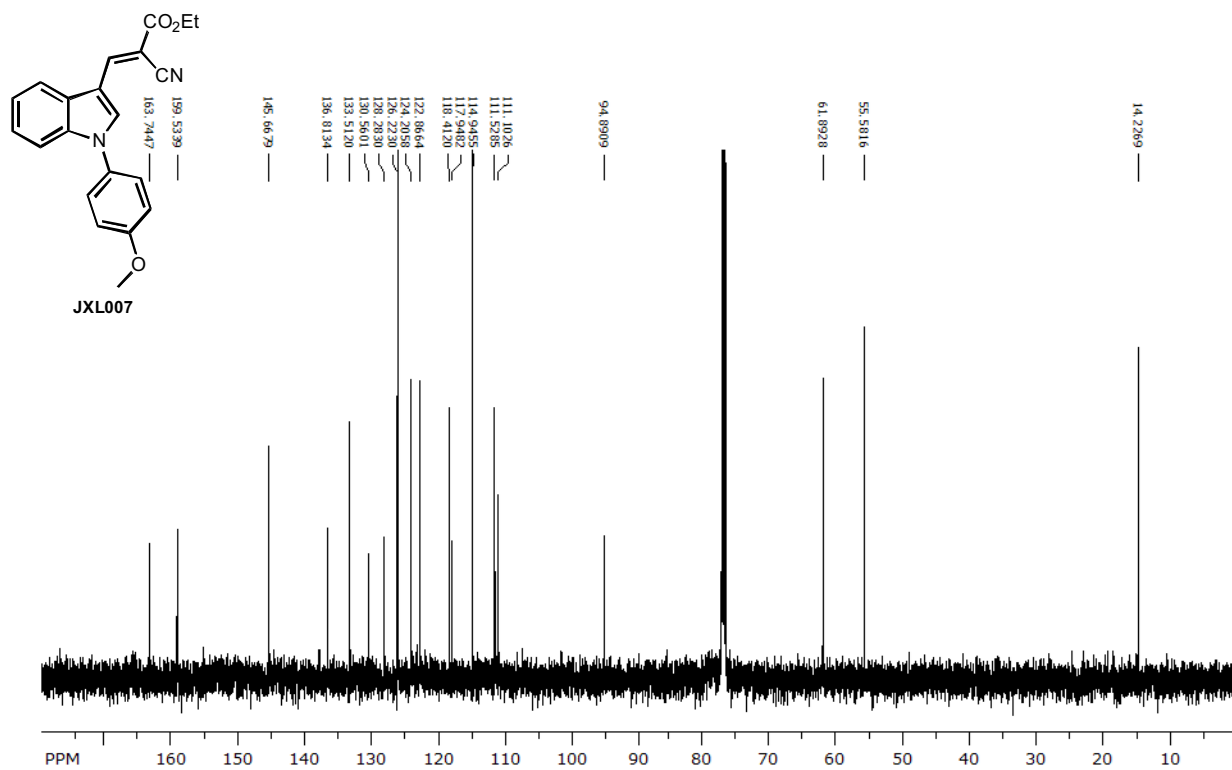




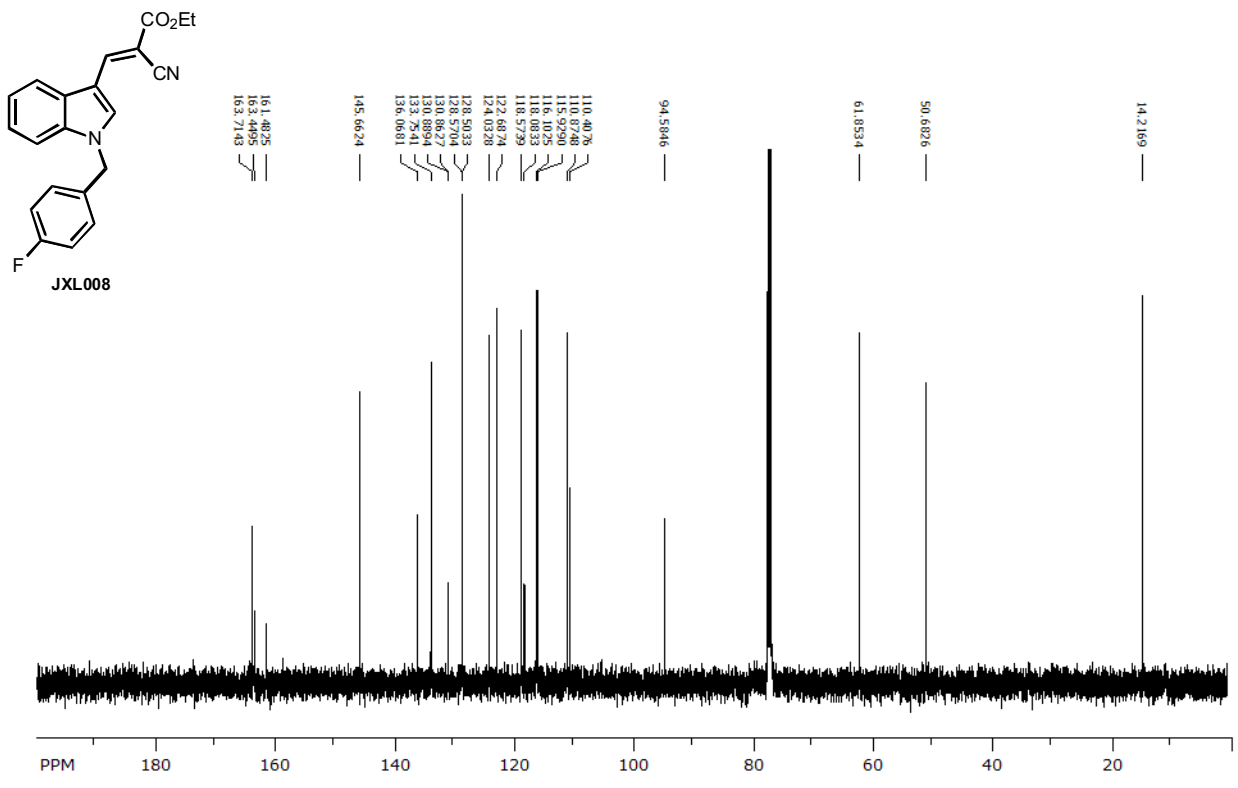
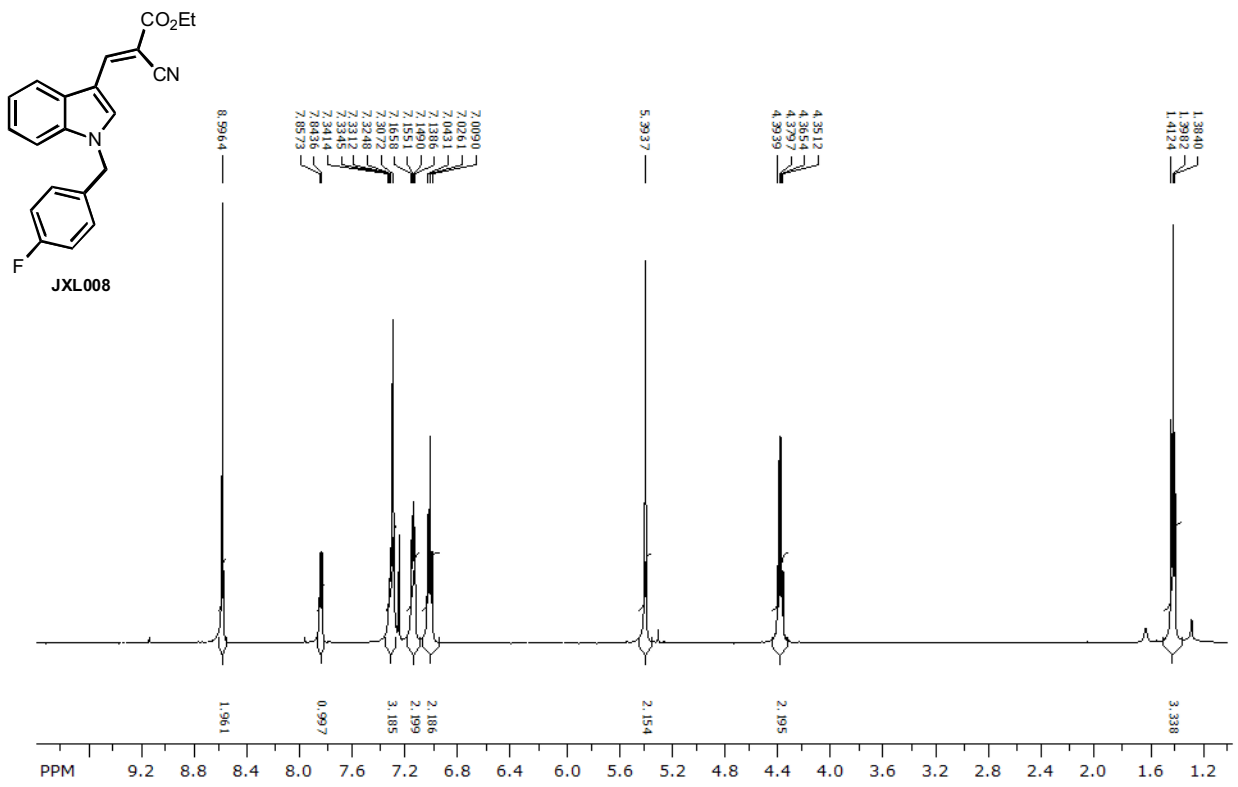


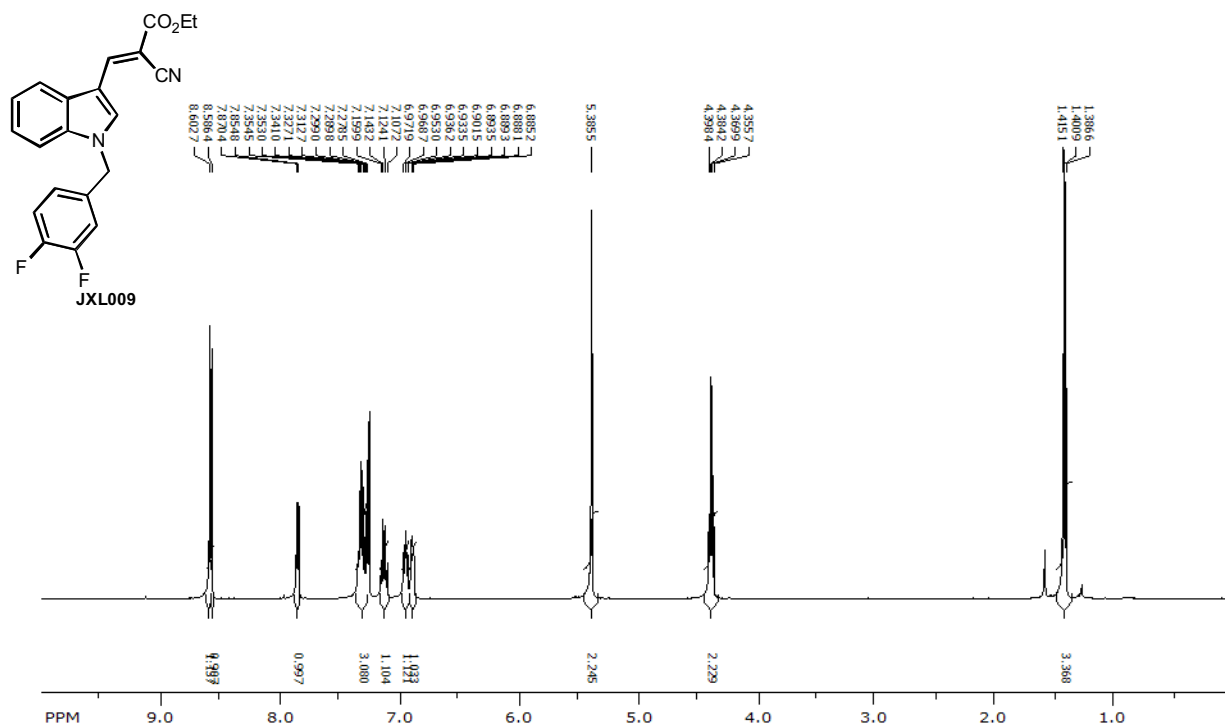


^1H NMR (500 MHz, CDCl_3)

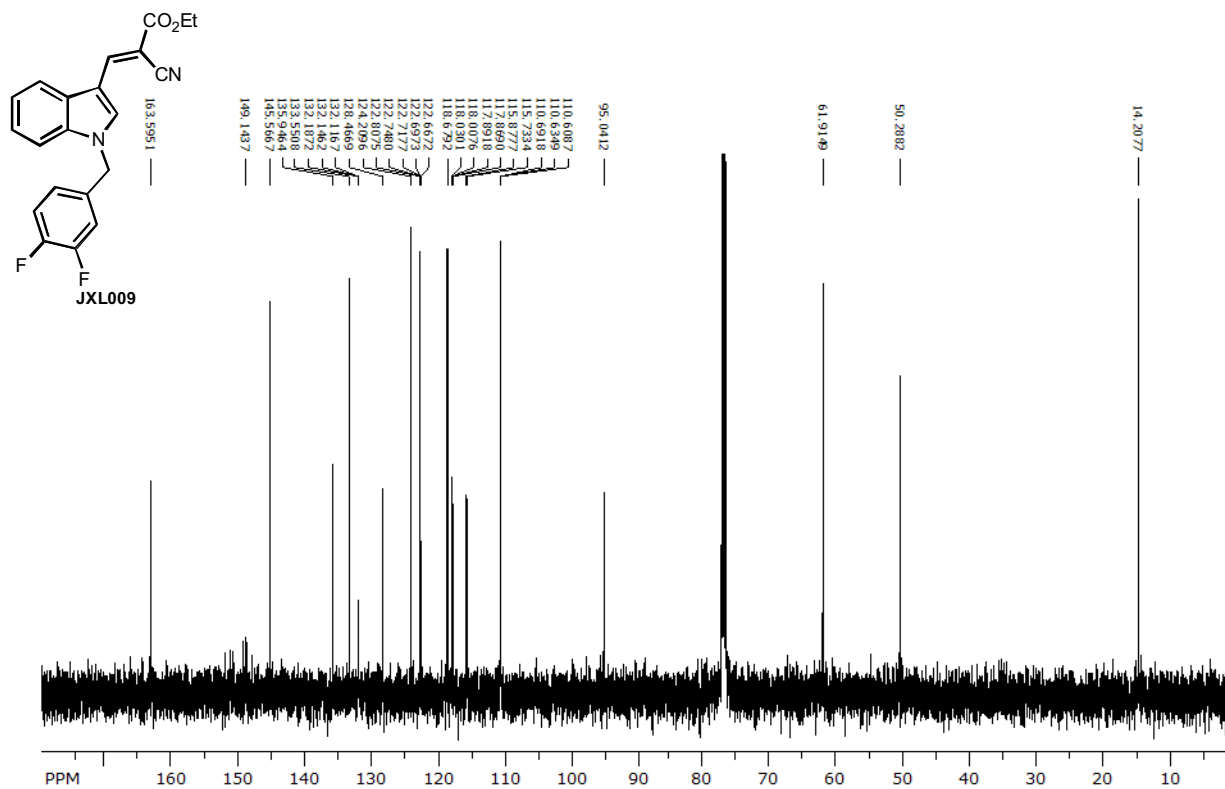


^{13}C NMR (126 MHz, CDCl_3)

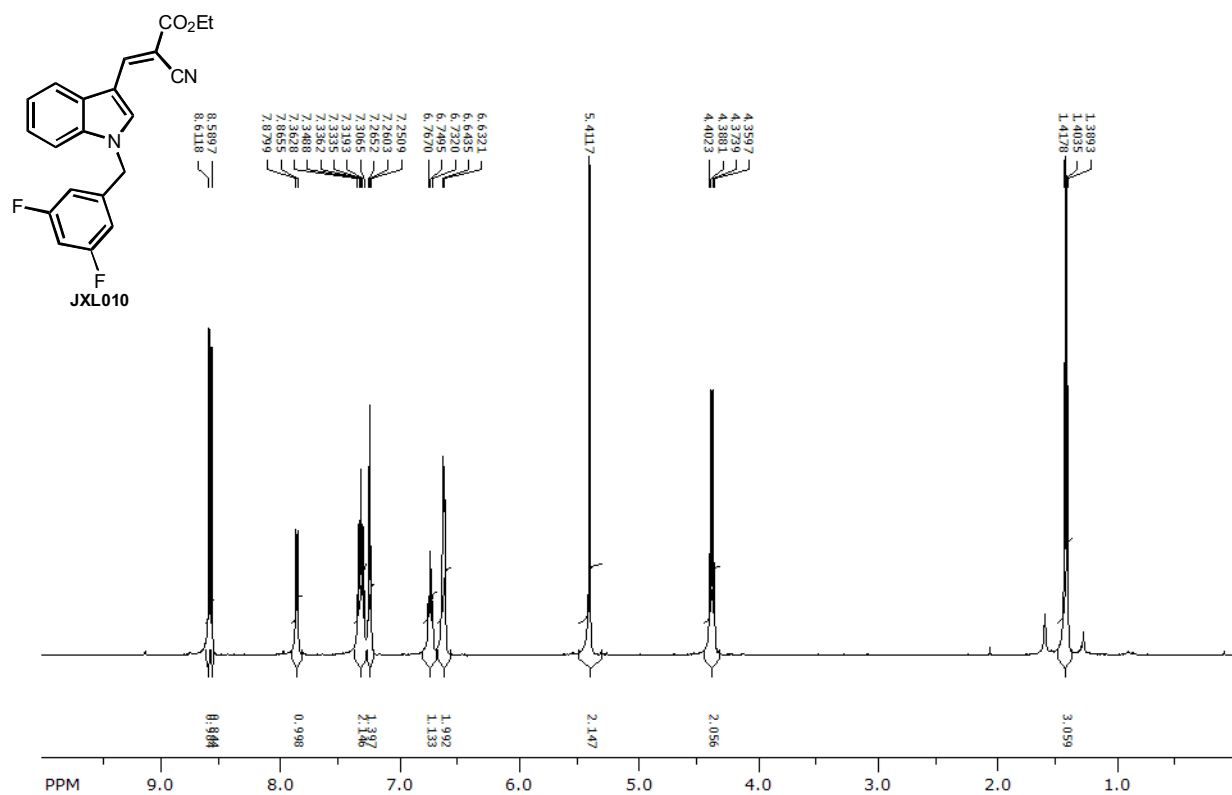




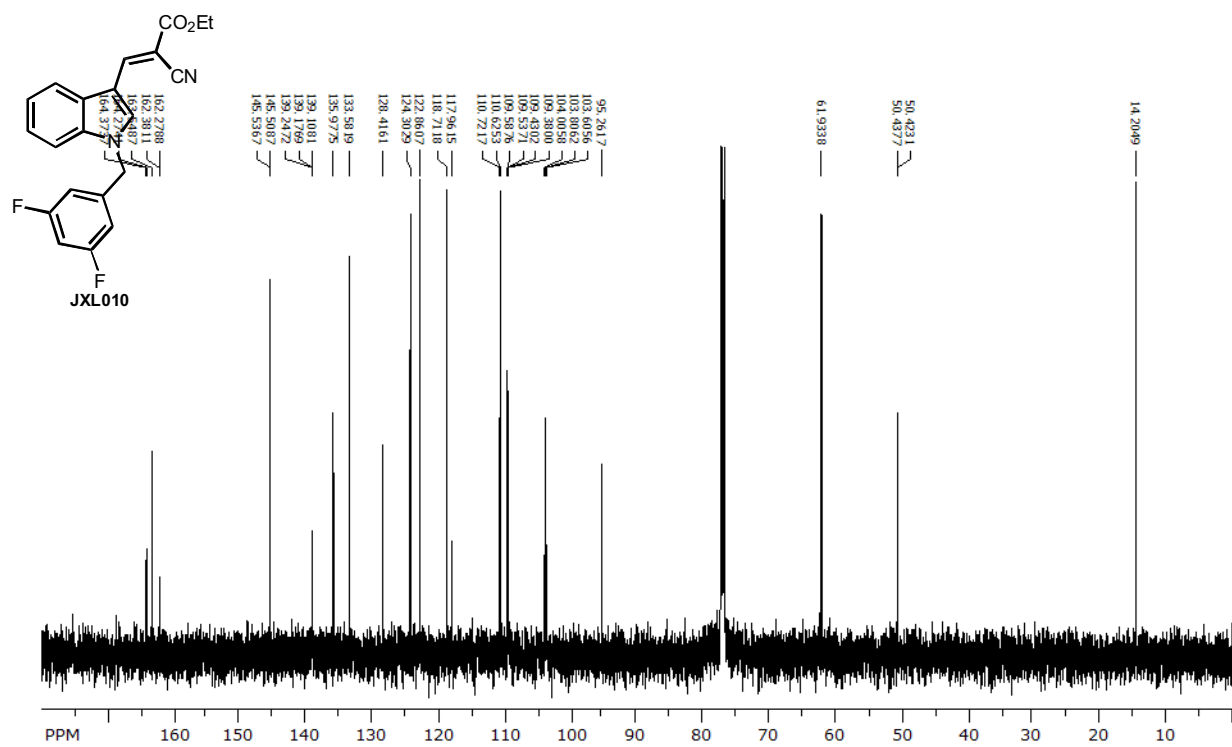
^1H NMR (500 MHz, CDCl_3)



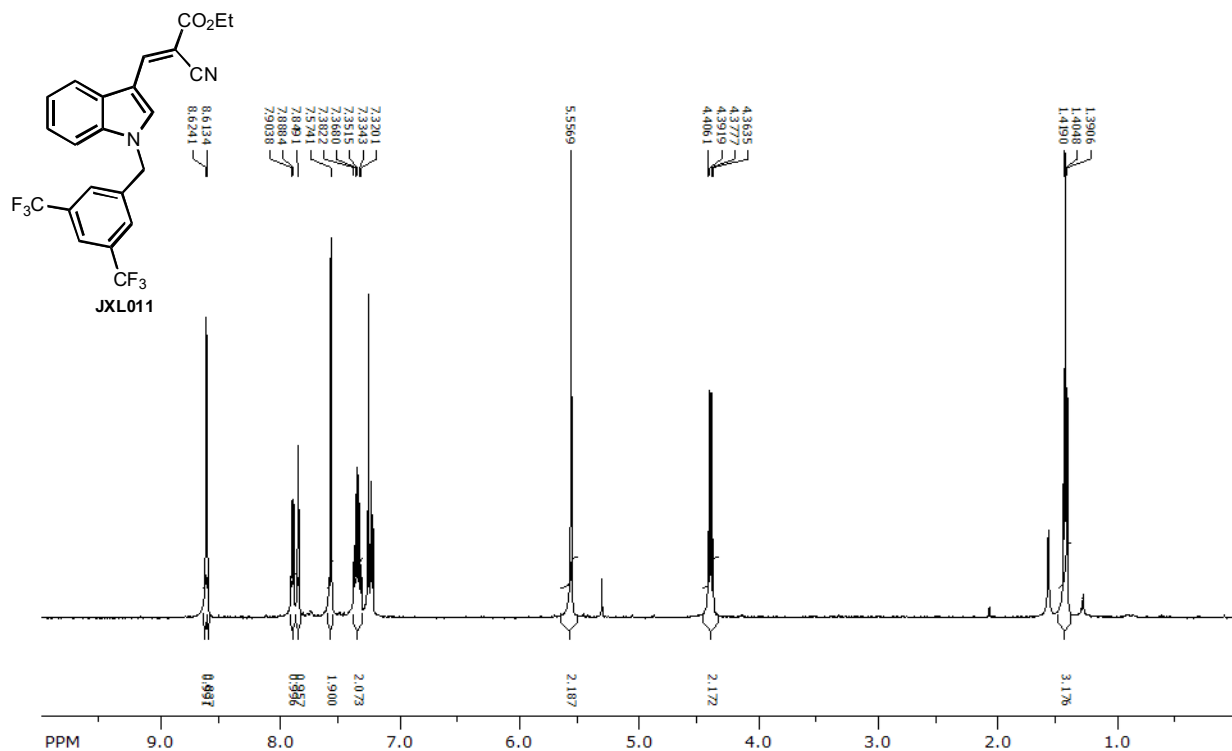
^{13}C NMR (126 MHz, CDCl_3)



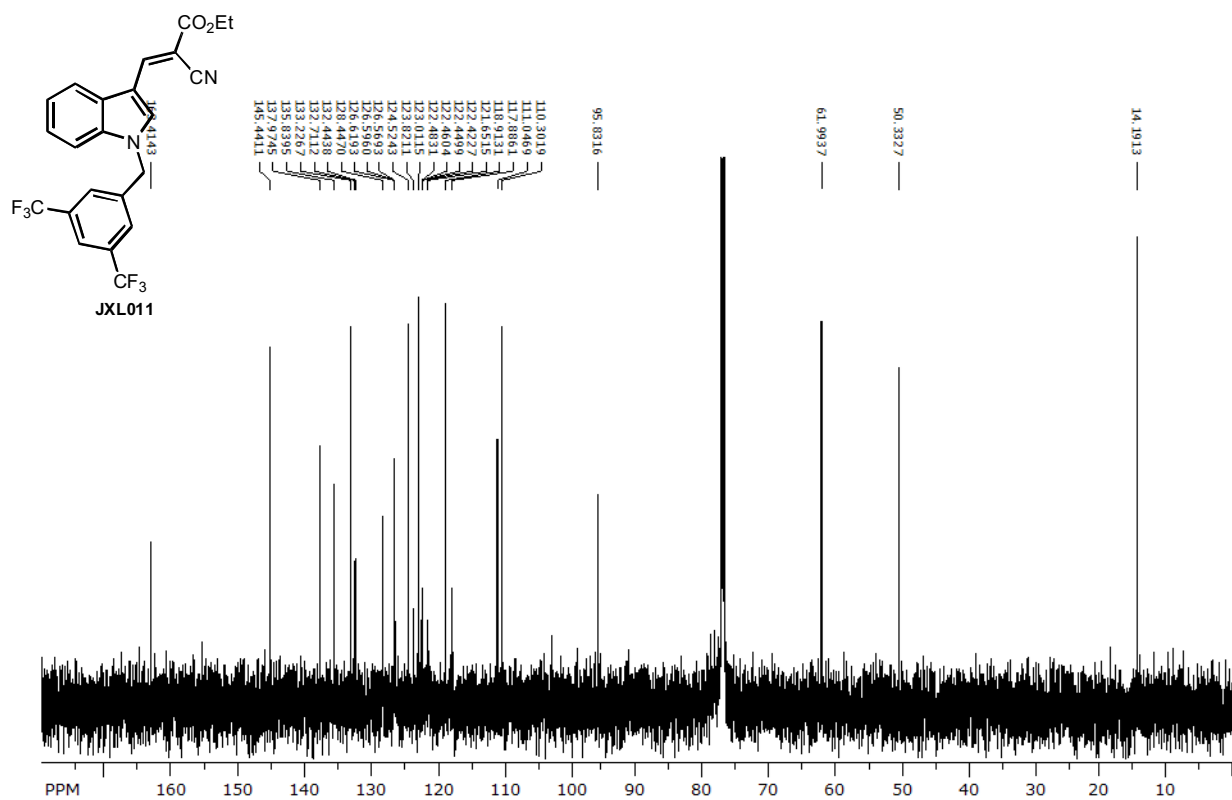
^1H NMR (500 MHz, CDCl_3)



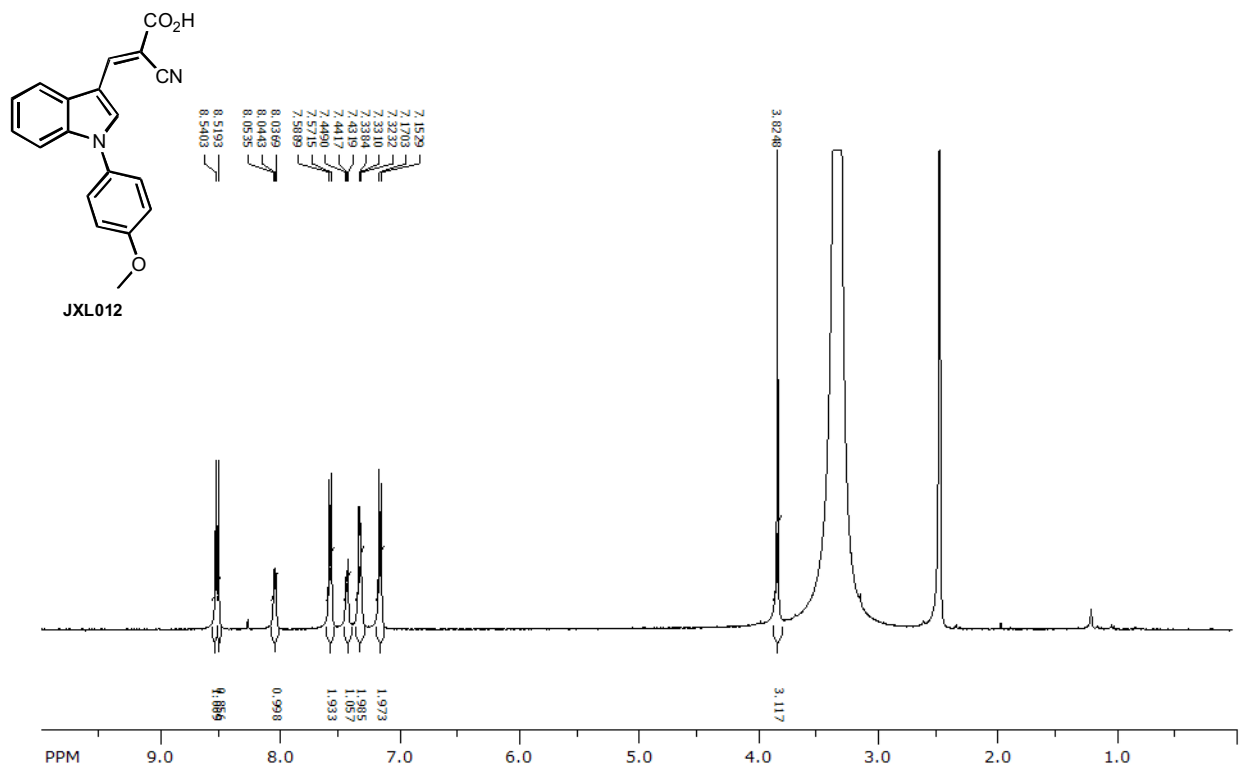
^{13}C NMR (126 MHz, CDCl_3)



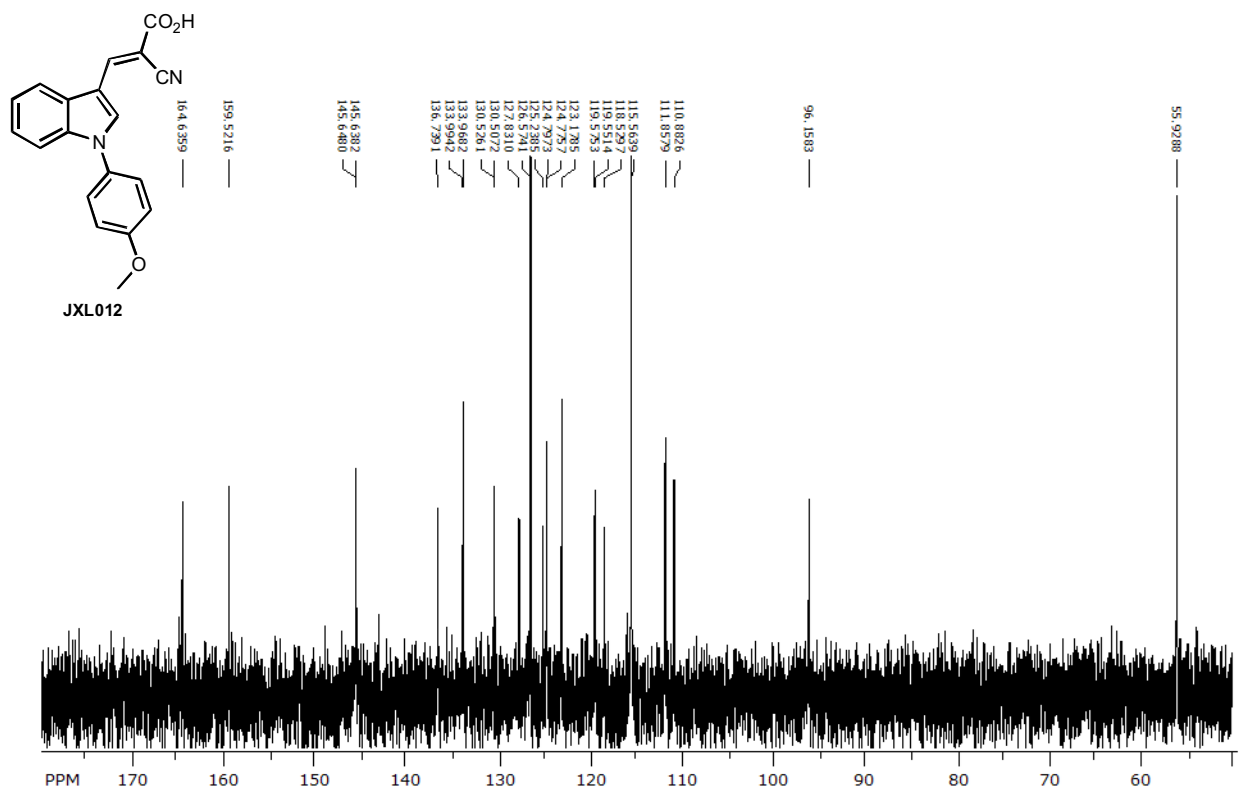
^1H NMR (500 MHz, CDCl_3)



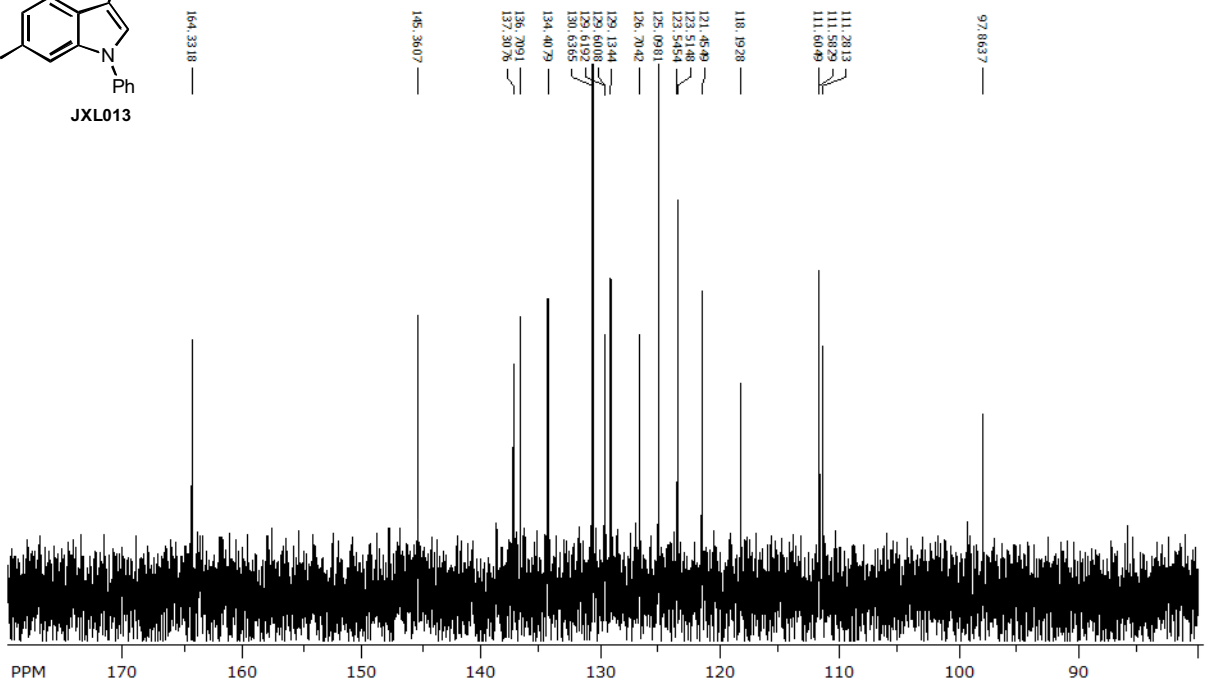
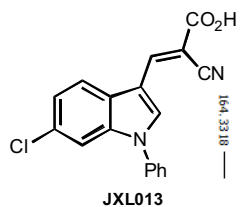
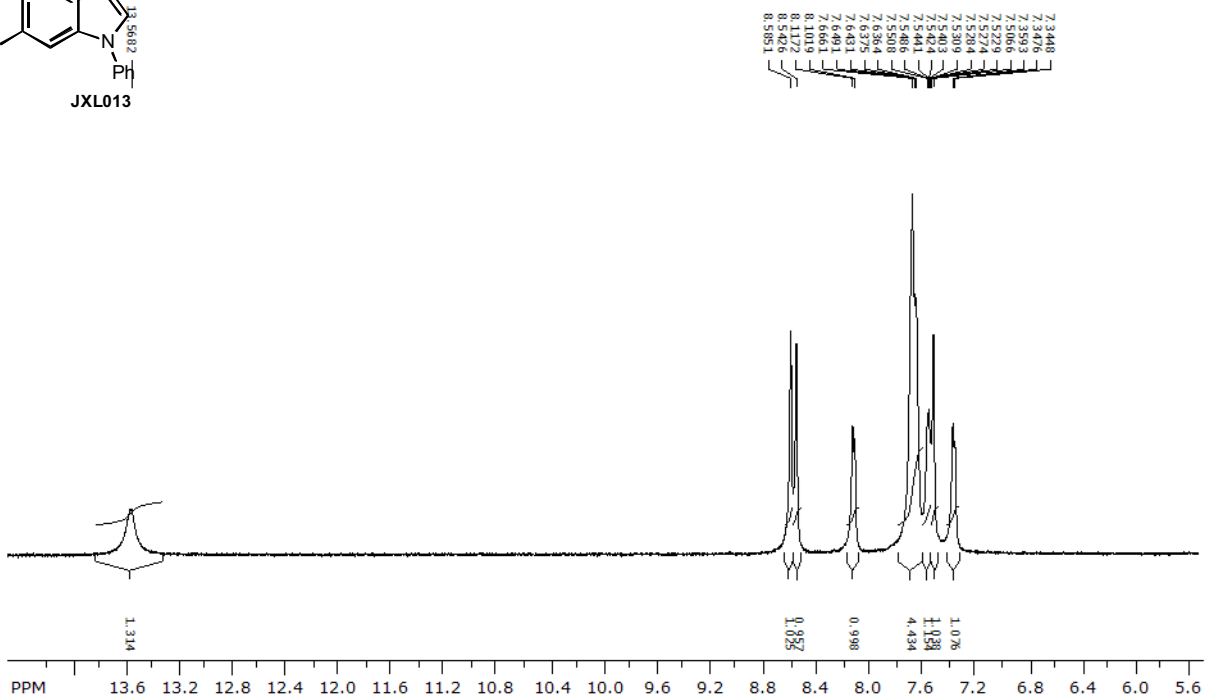
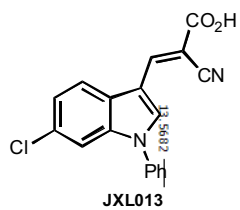
^{13}C NMR (126 MHz, CDCl_3)

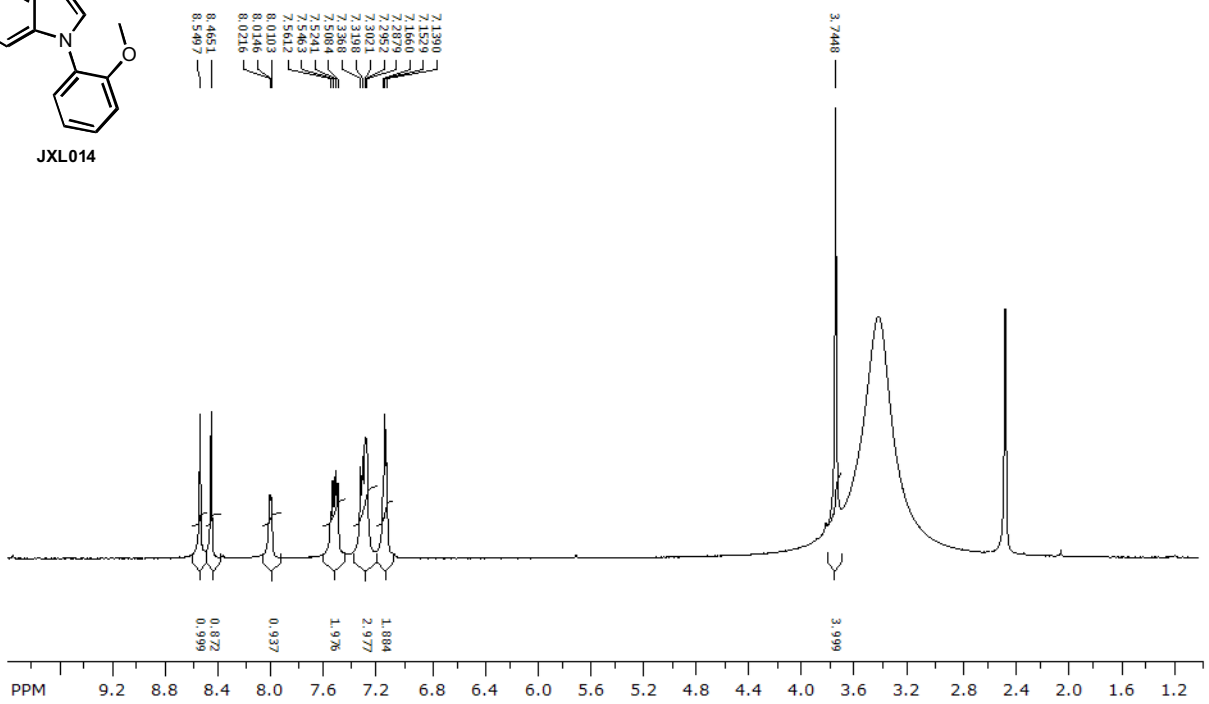
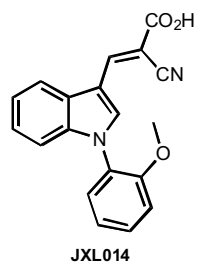


¹H NMR (500 MHz, DMSO-d₆)

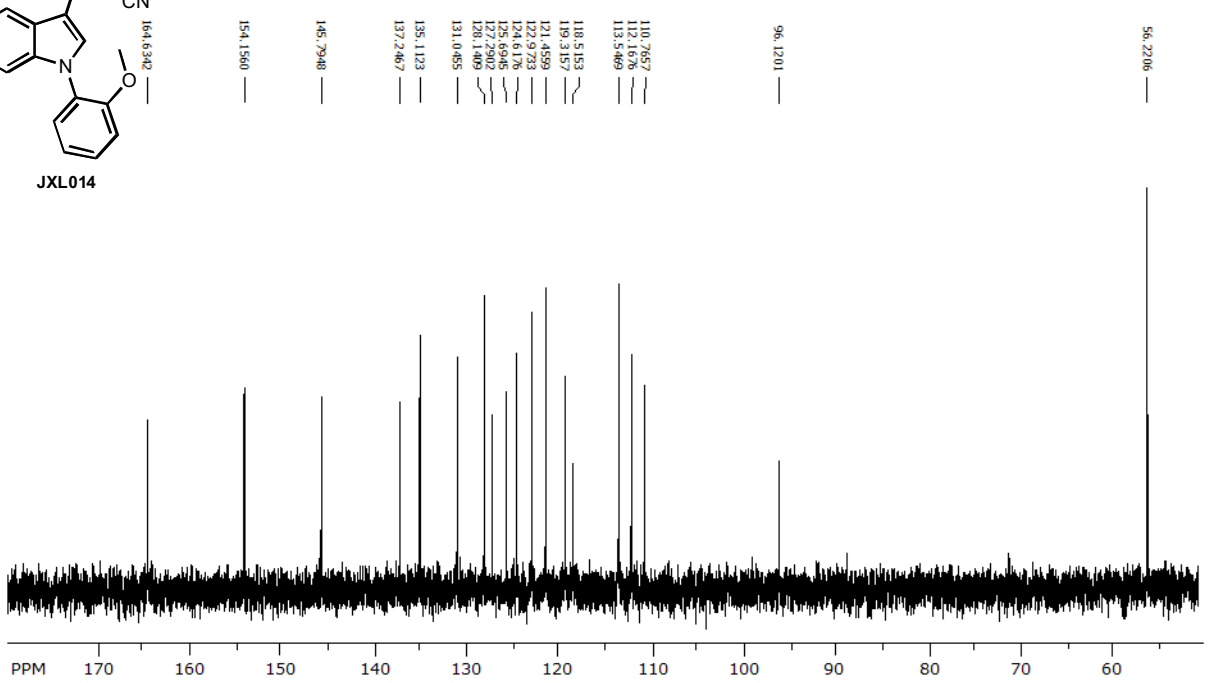
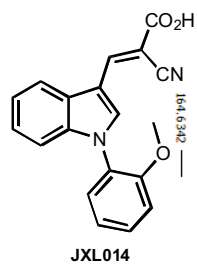


¹³C NMR (126 MHz, DMSO-d₆)

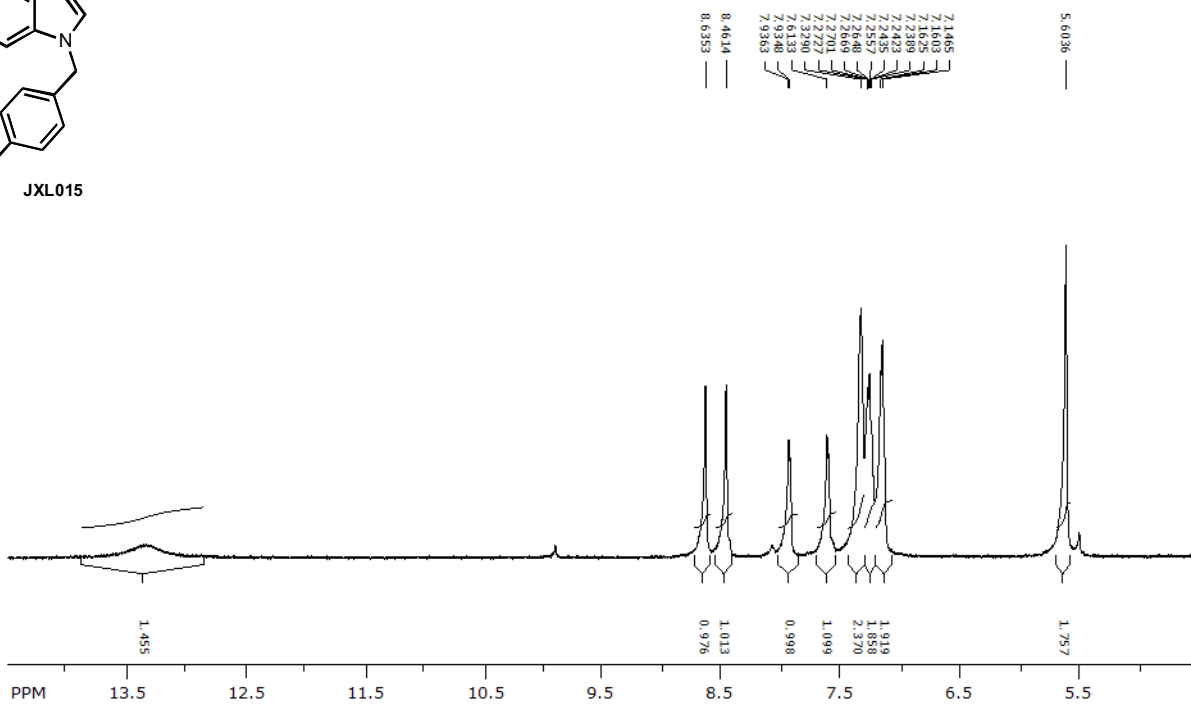
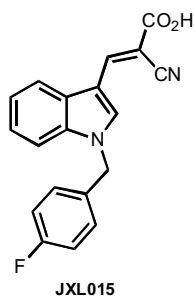




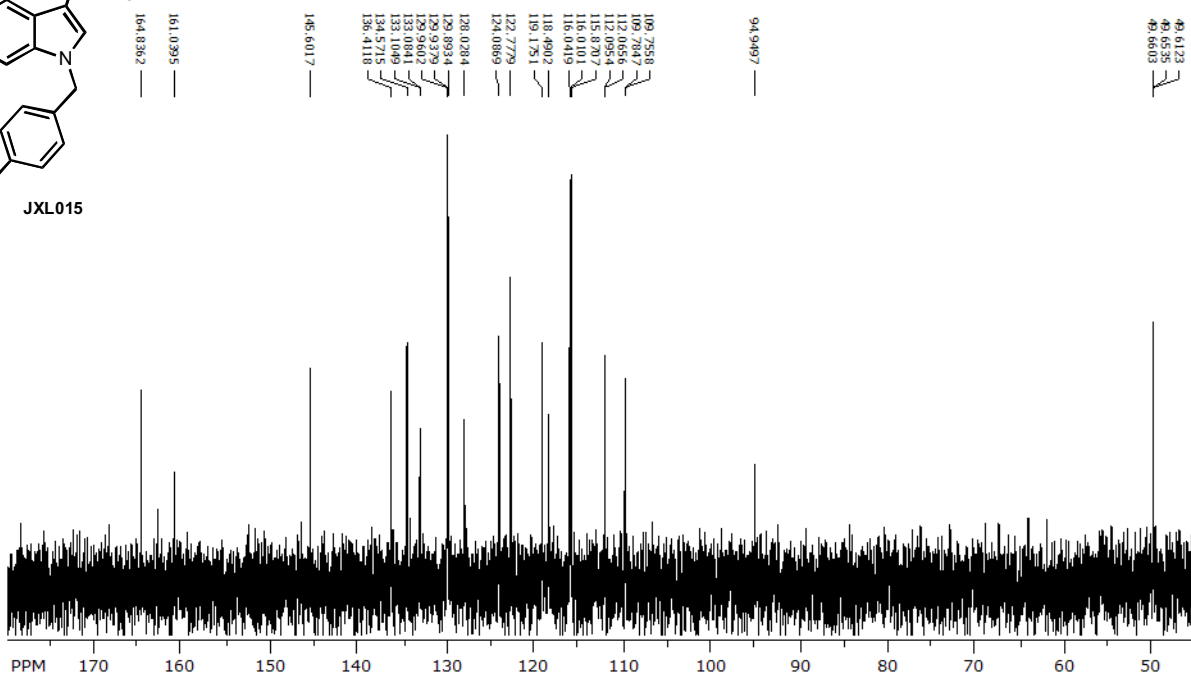
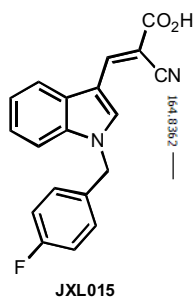
¹H NMR (500 MHz, DMSO-d₆)



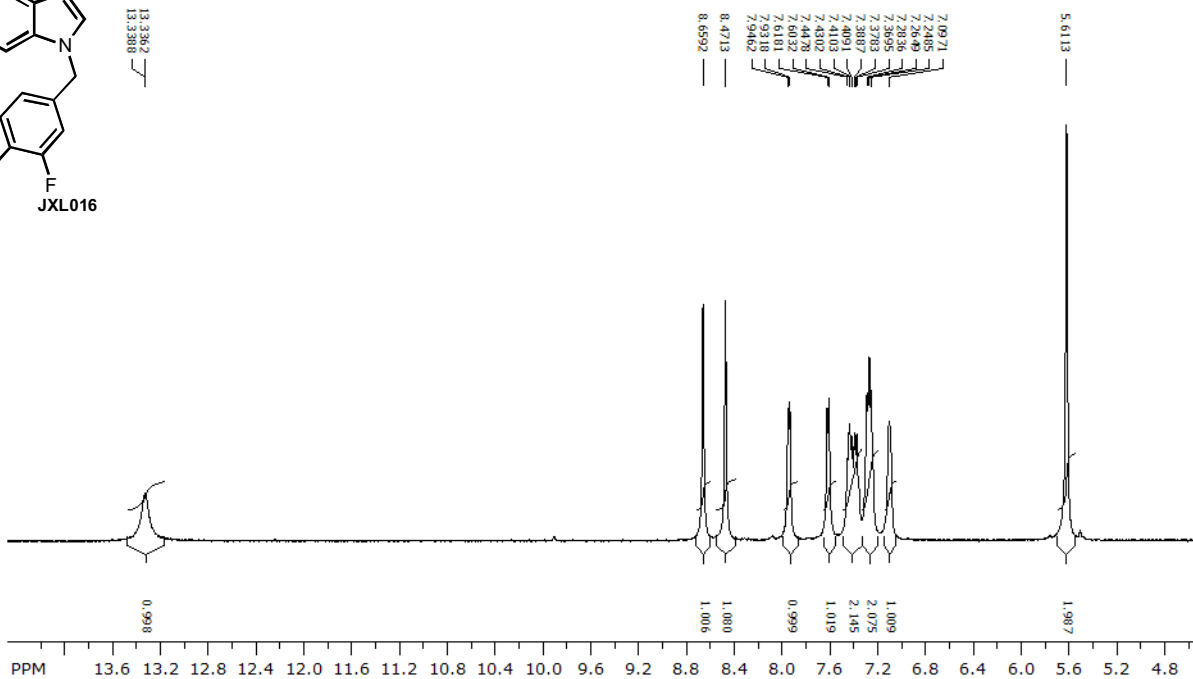
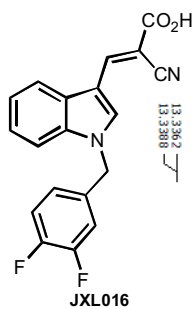
¹³C NMR (126 MHz, DMSO-d₆)



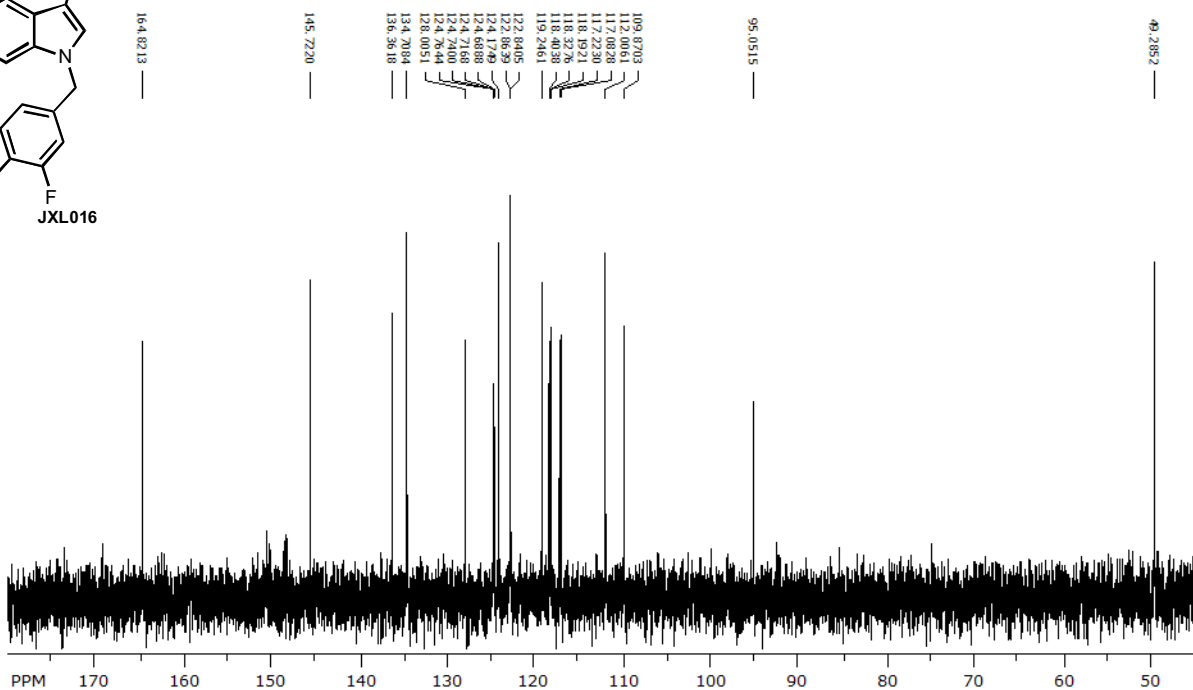
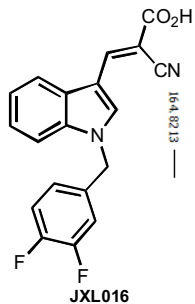
¹H NMR (500 MHz, DMSO-d₆)



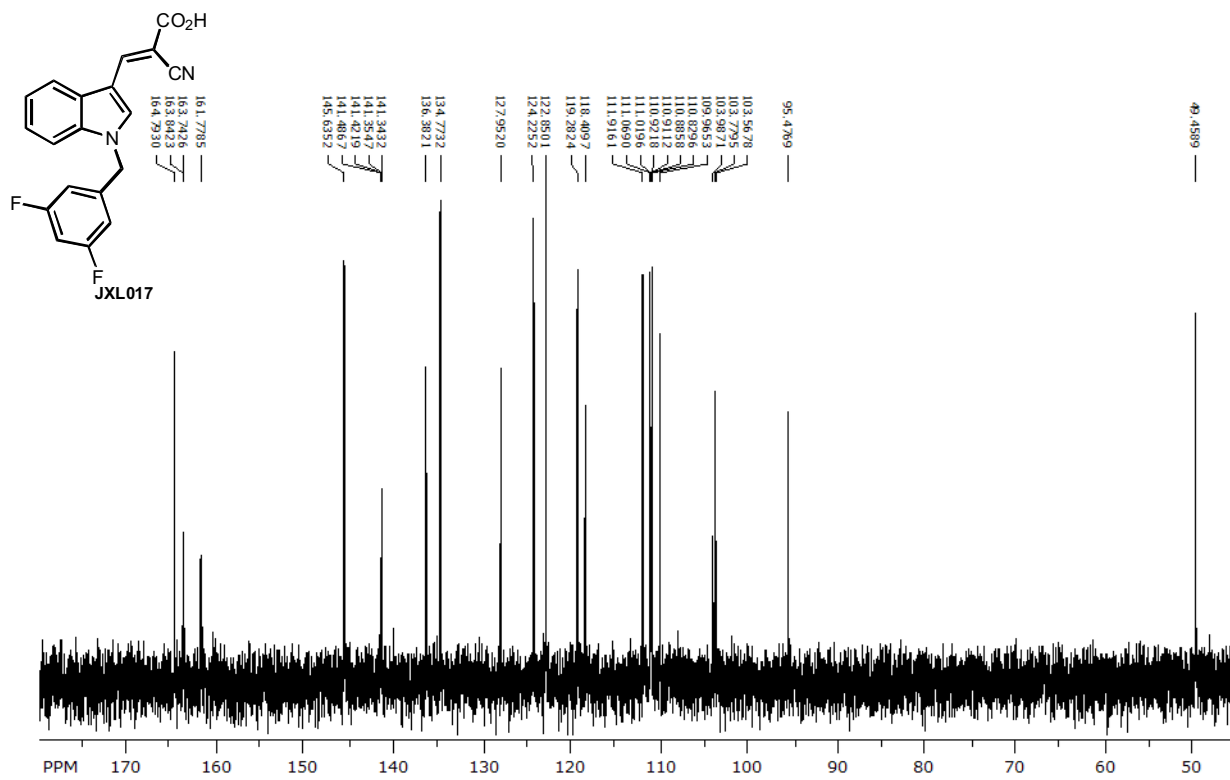
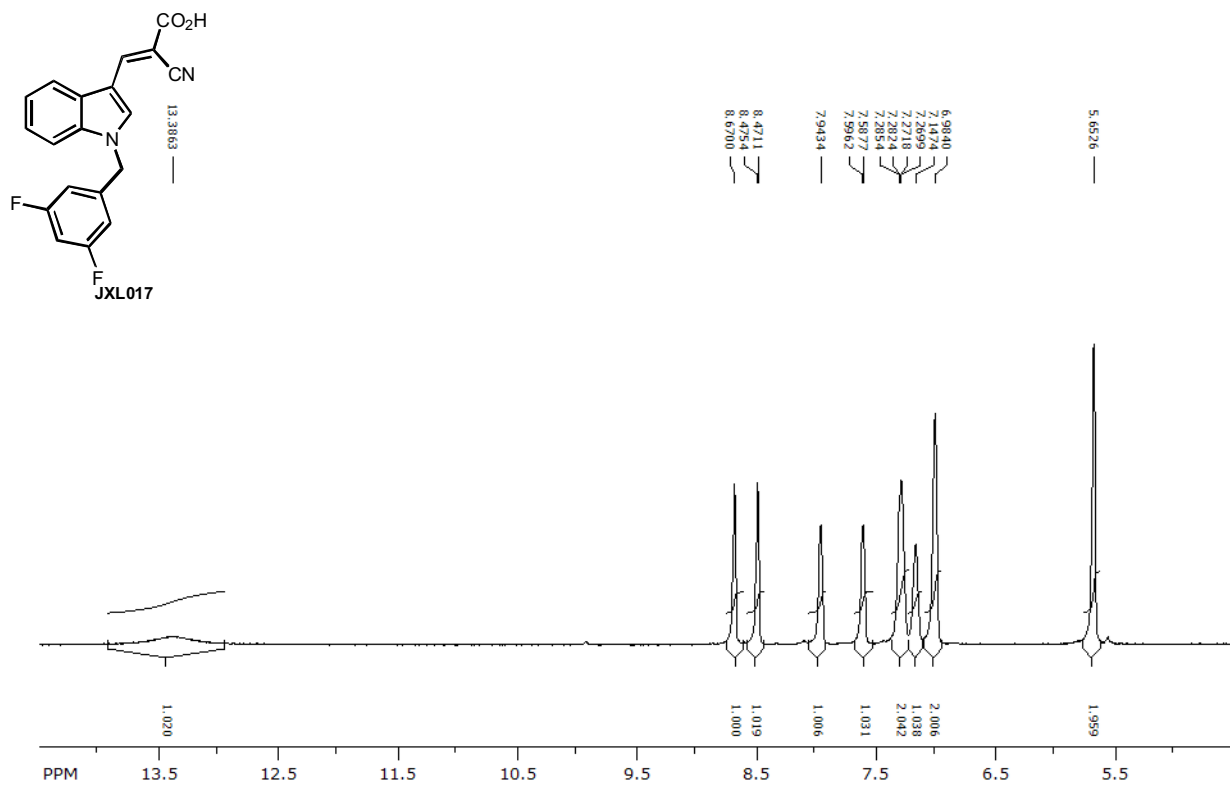
¹³C NMR (126 MHz, DMSO-d₆)



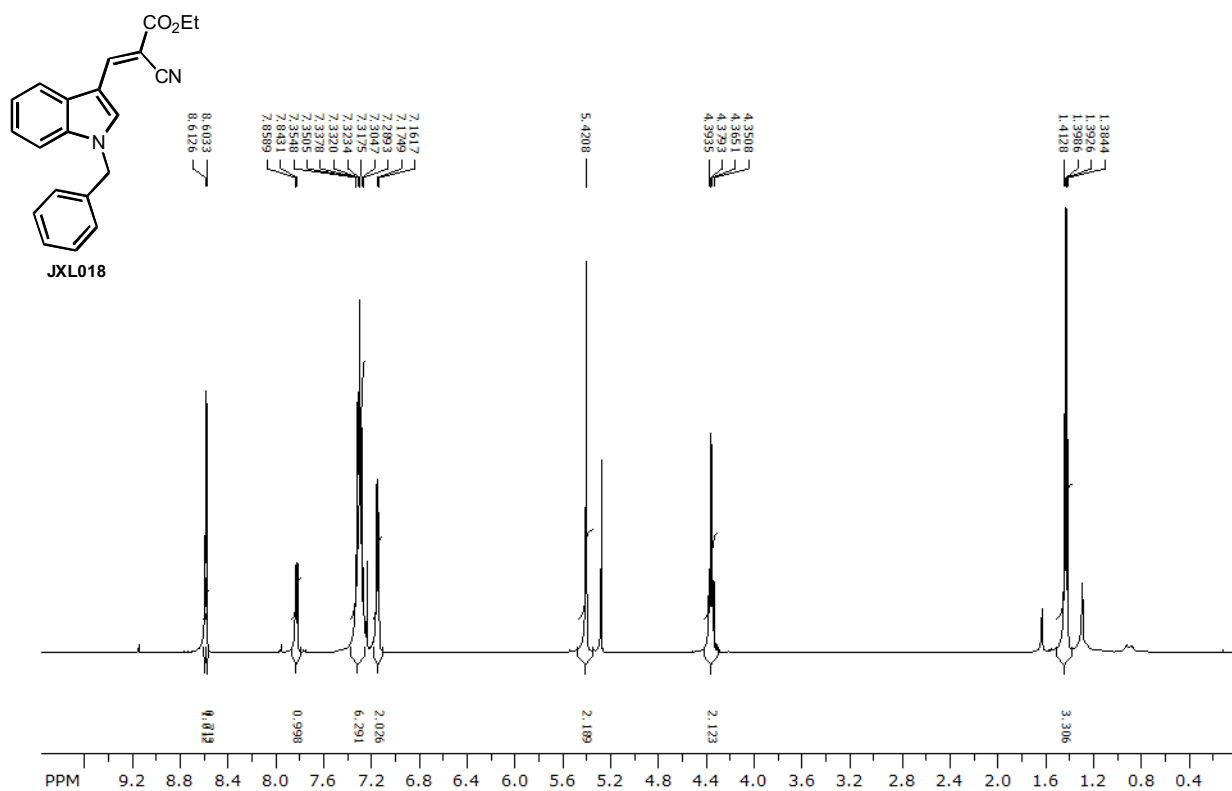
¹H NMR (500 MHz, DMSO-d₆)



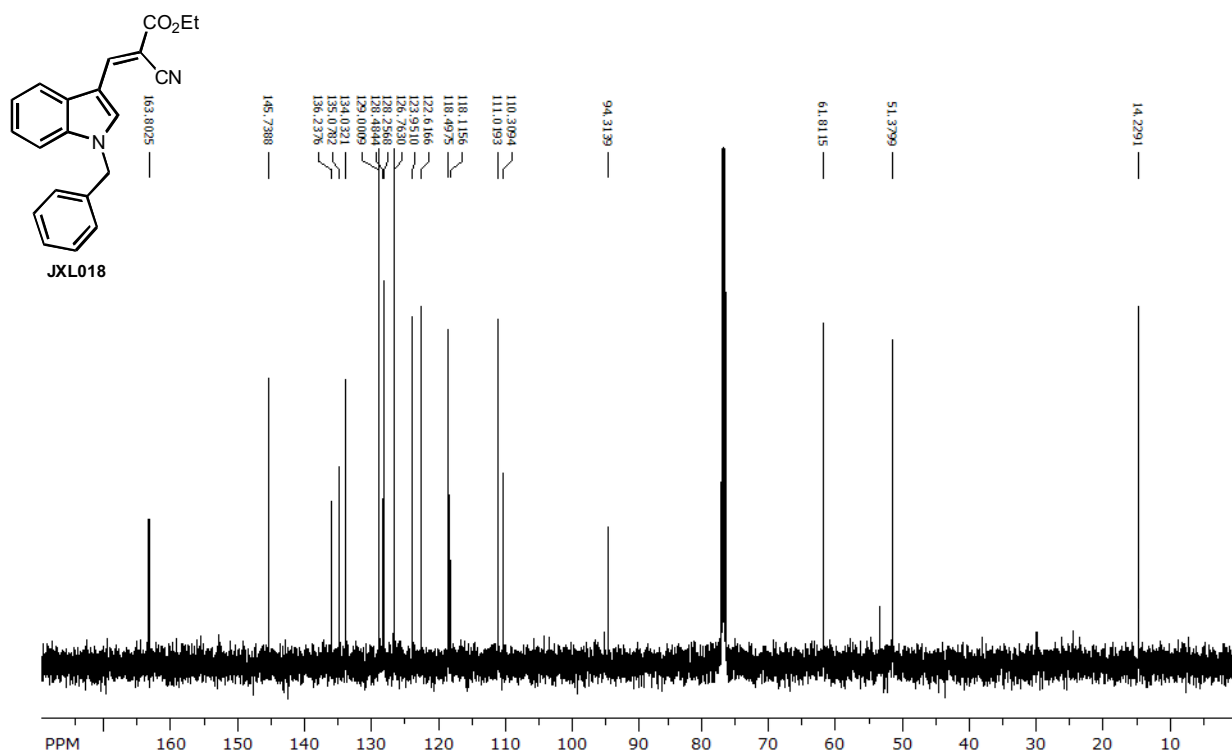
¹³C NMR (126 MHz, DMSO-d₆)



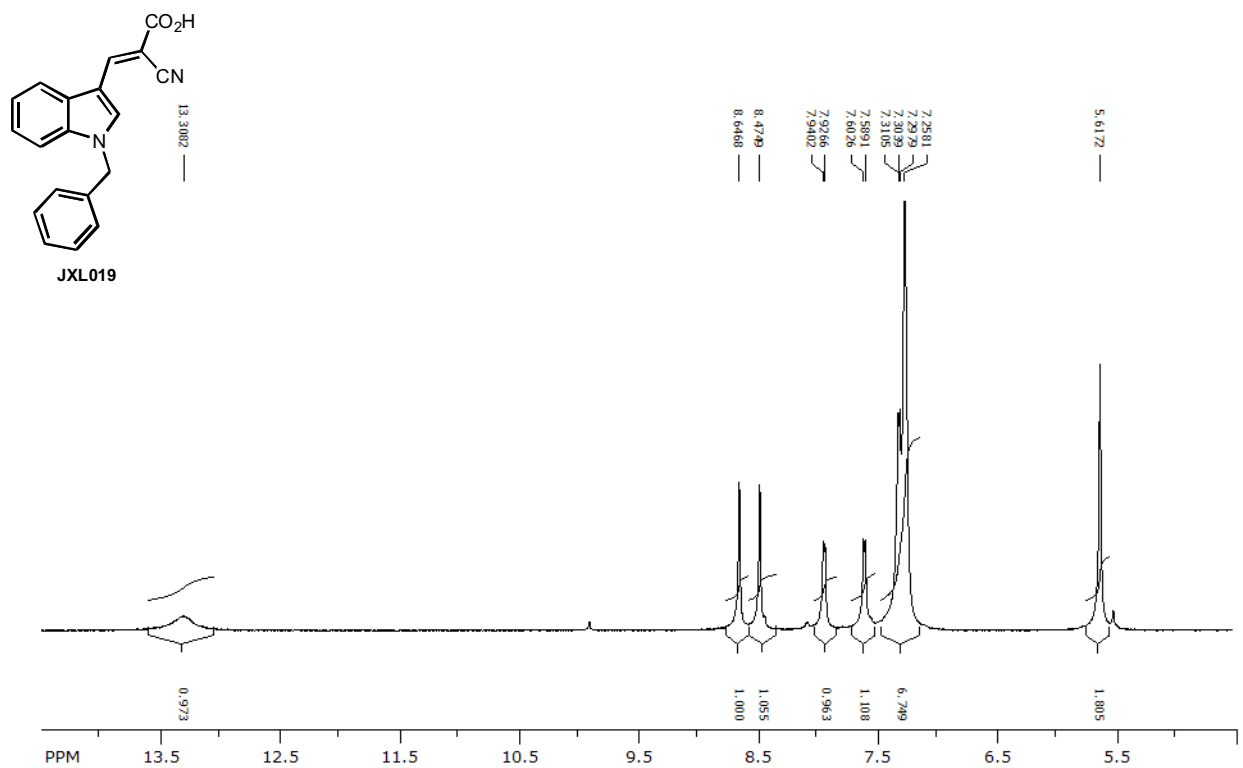
¹³C NMR (126 MHz, DMSO-d₆)



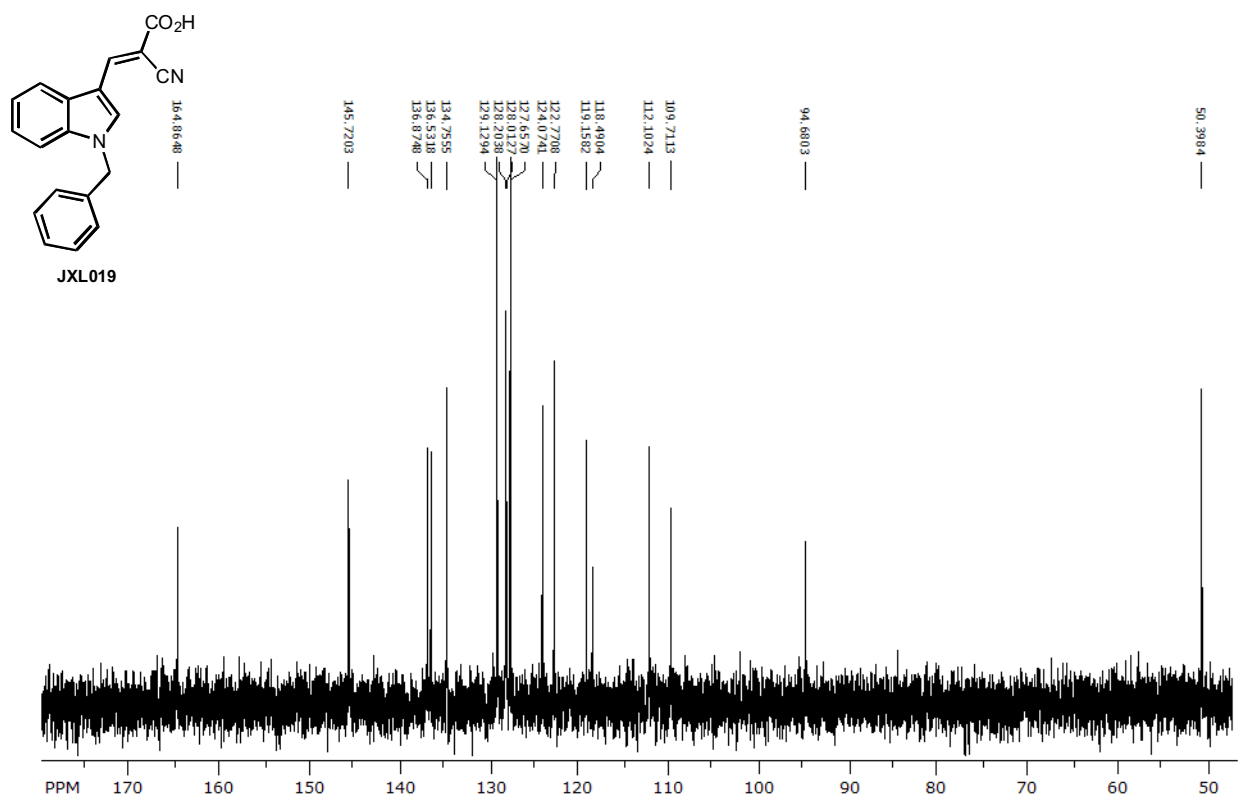
¹H NMR (500 MHz, CDCl₃)



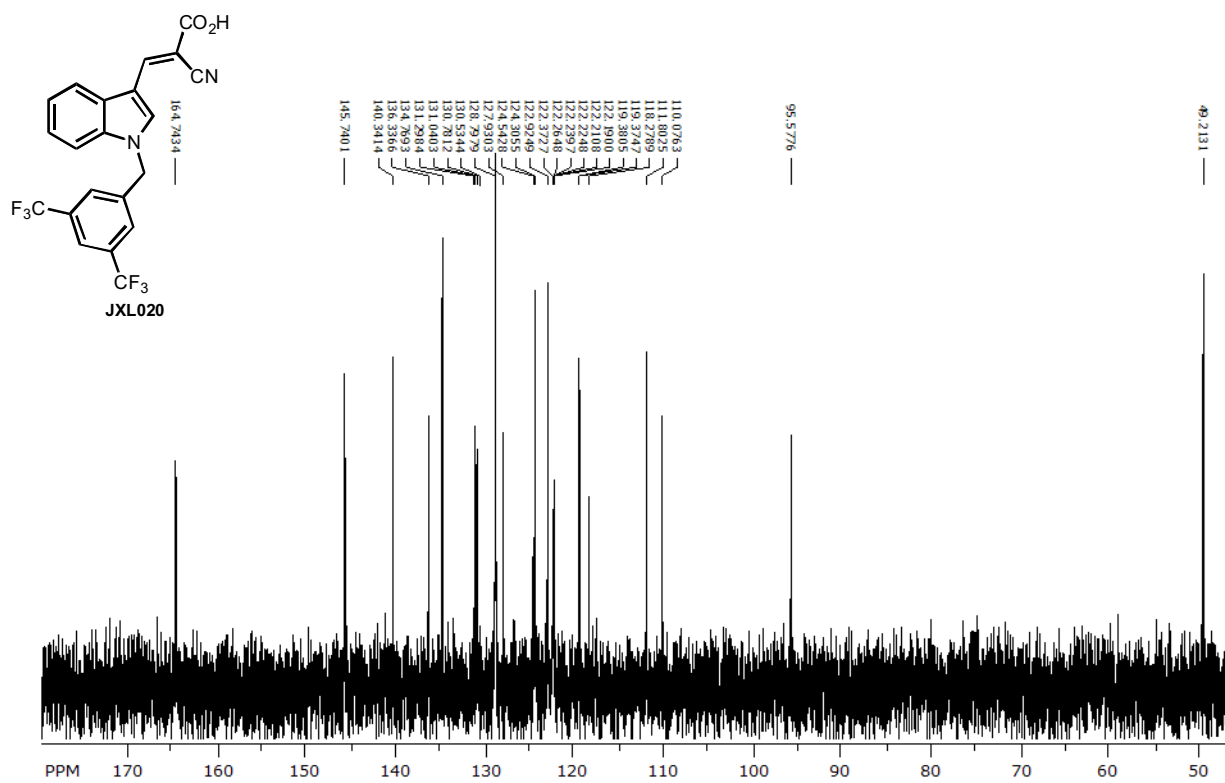
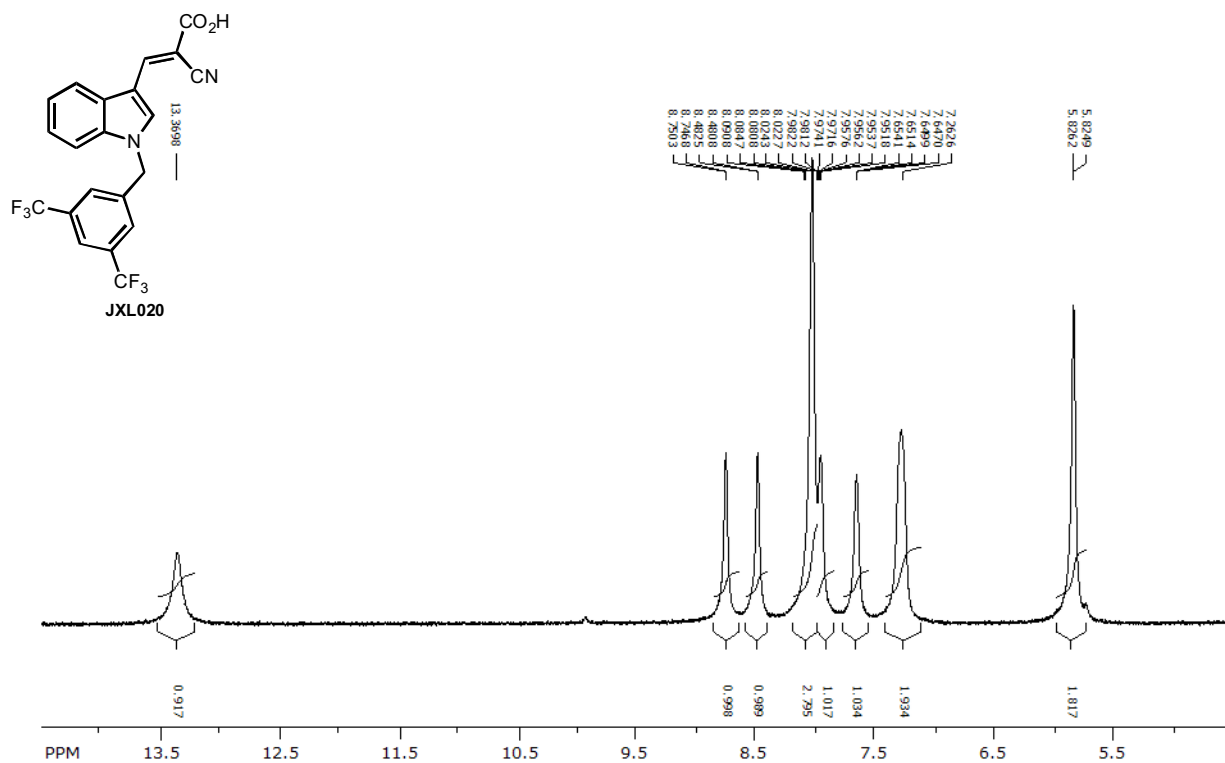
¹³C NMR (126 MHz, CDCl₃)

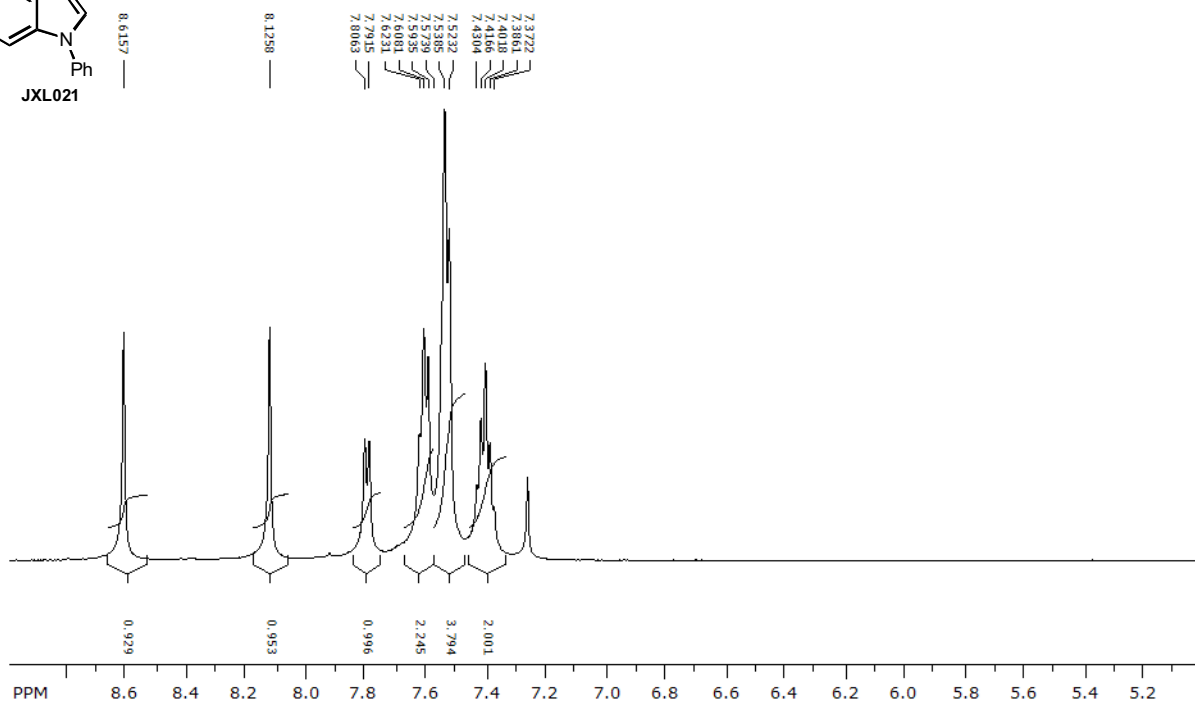
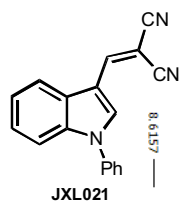


^1H NMR (500 MHz, DMSO- d_6)

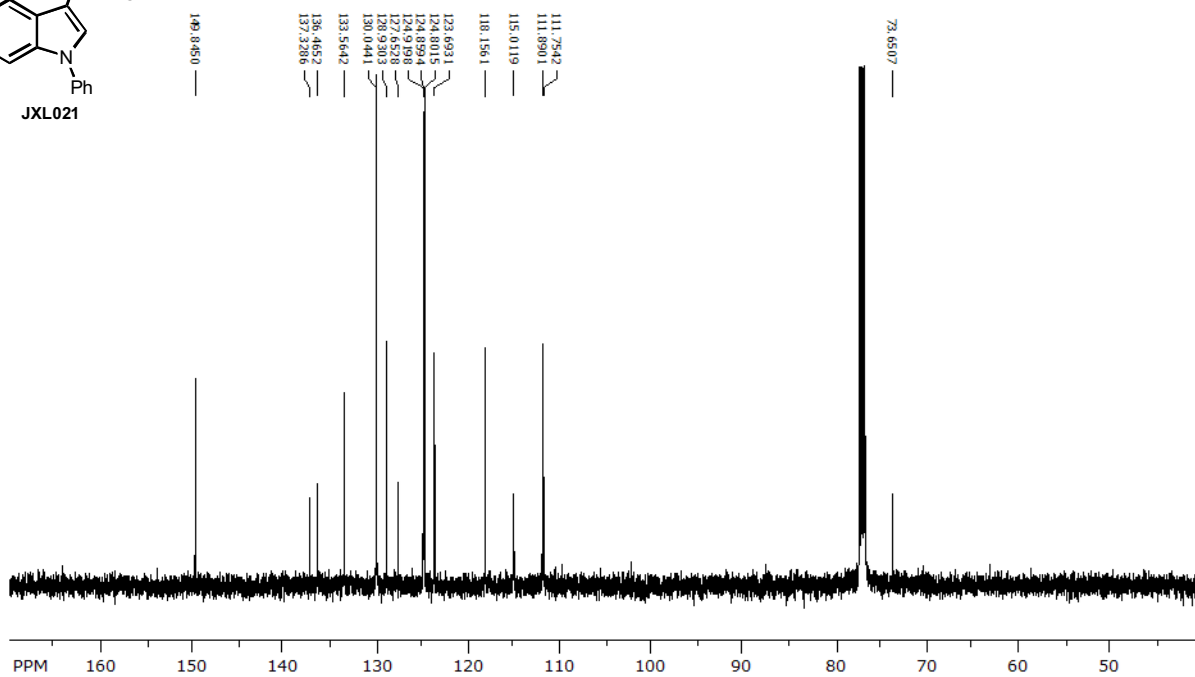
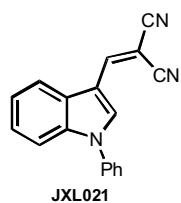


^{13}C NMR (126 MHz, DMSO- d_6)

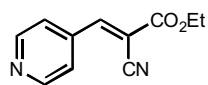




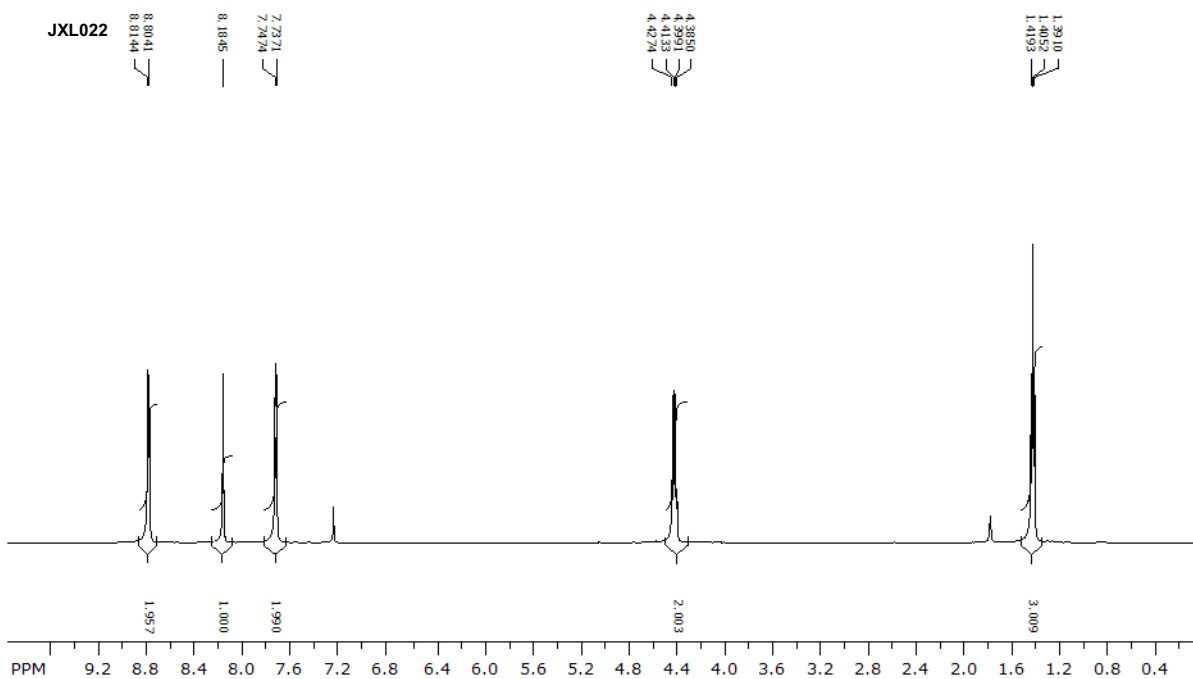
¹H NMR (500 MHz, CDCl₃)



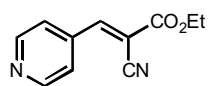
¹³C NMR (126 MHz, CDCl₃)



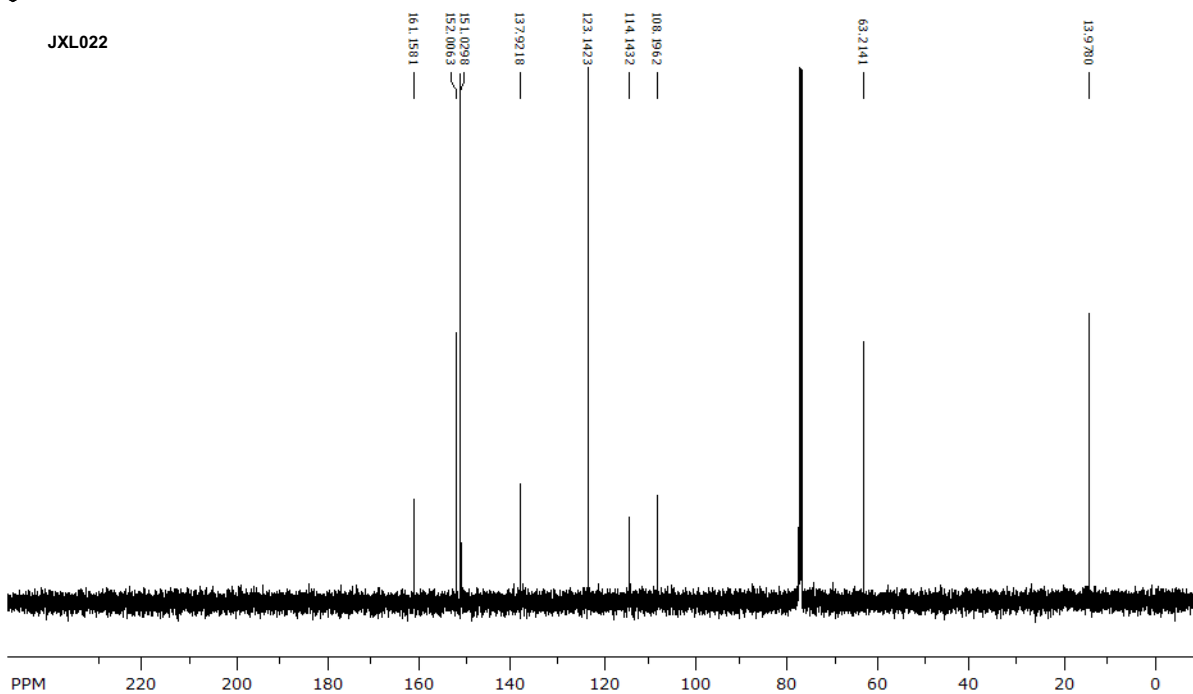
JXL022



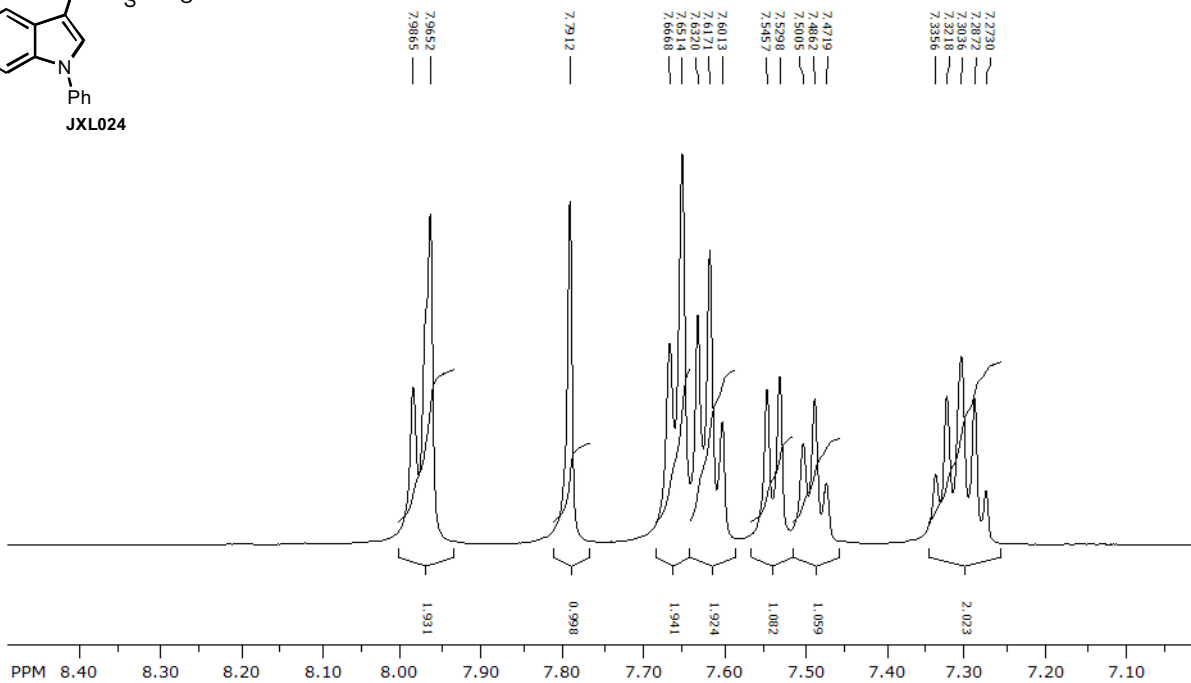
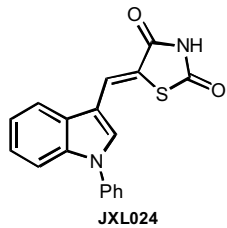
¹H NMR (500 MHz, CDCl₃)



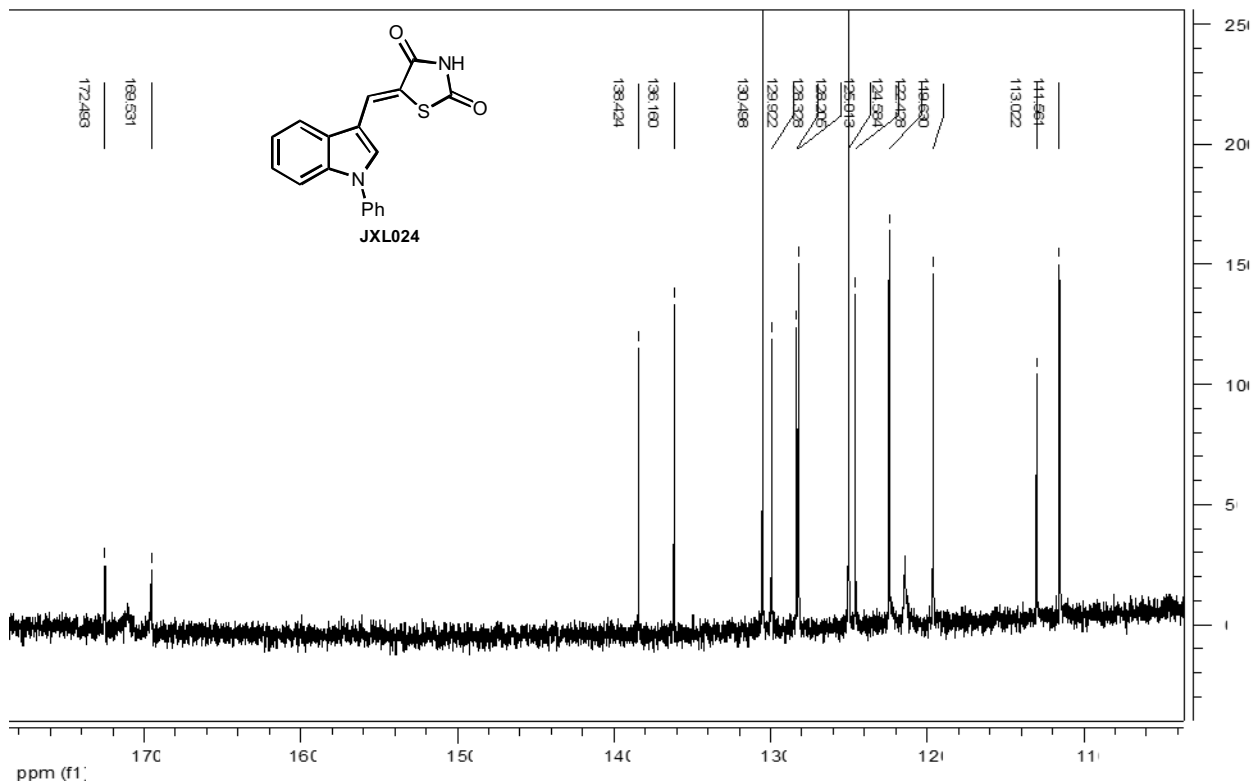
JXL022



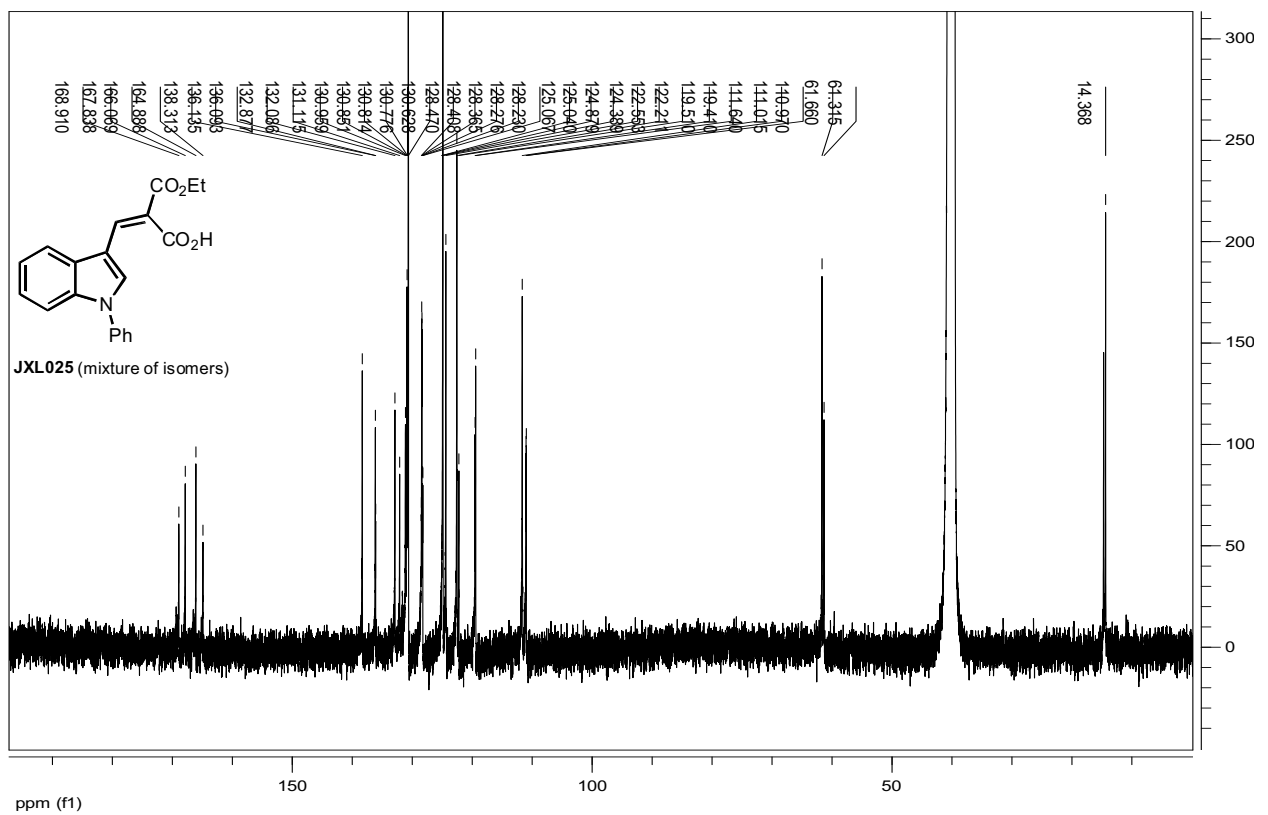
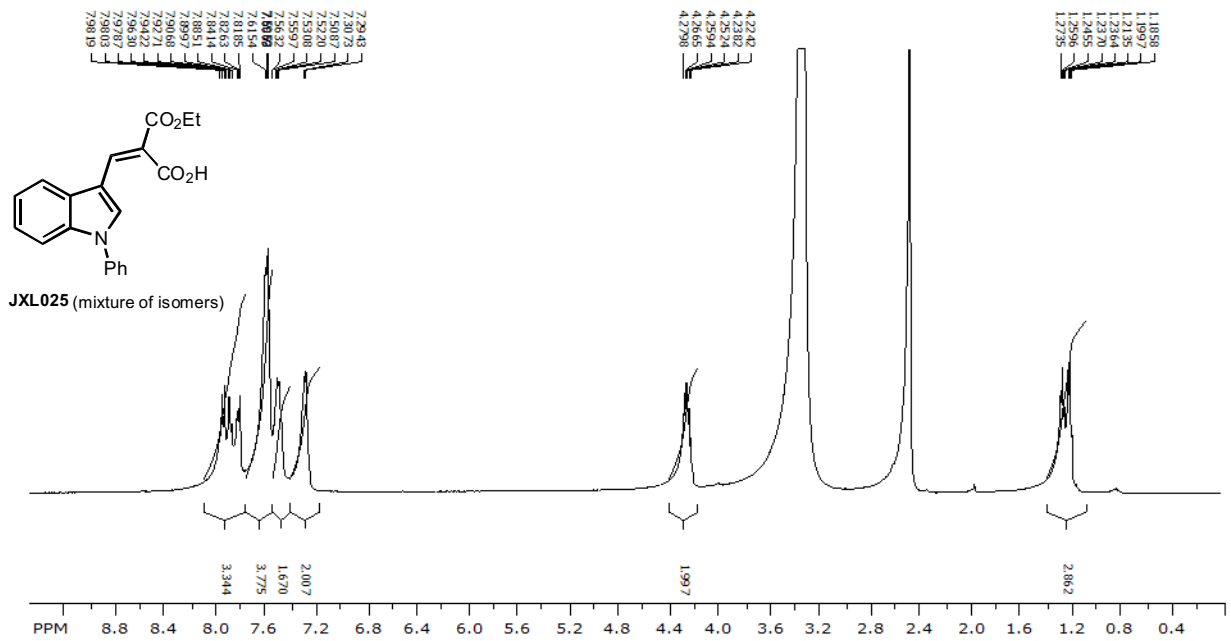
¹³C NMR (126 MHz, CDCl₃)



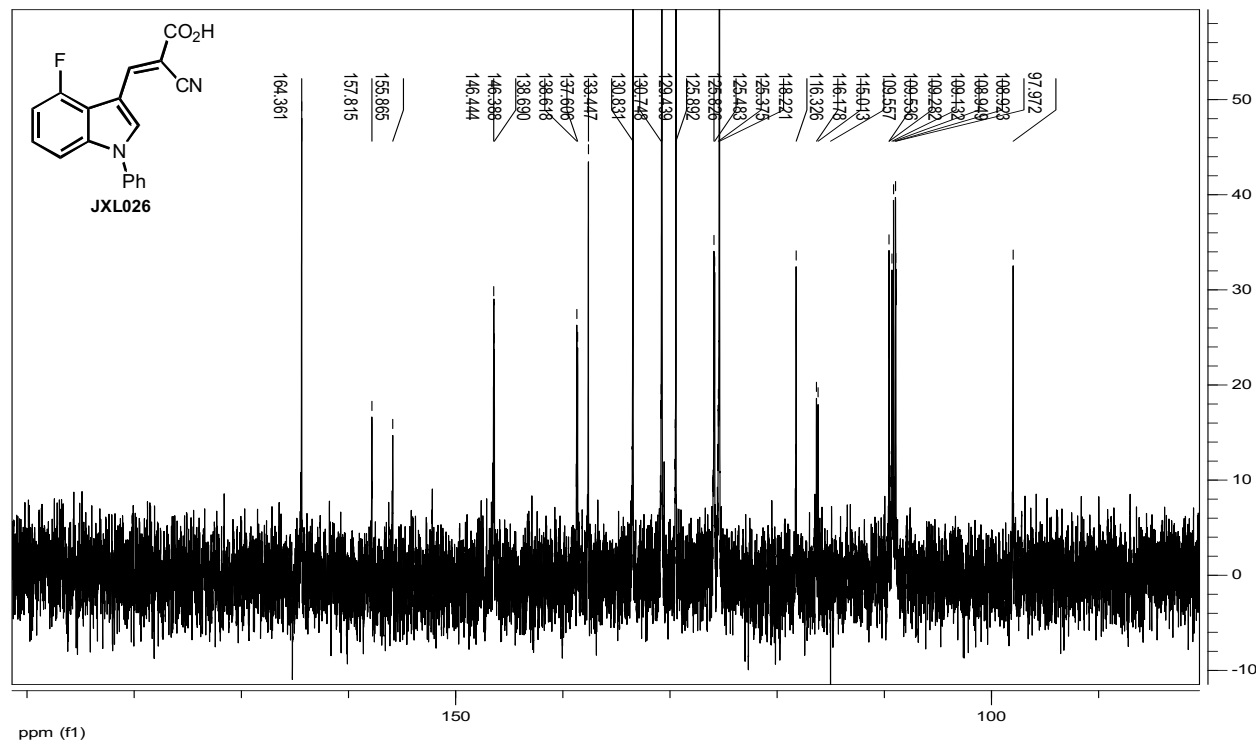
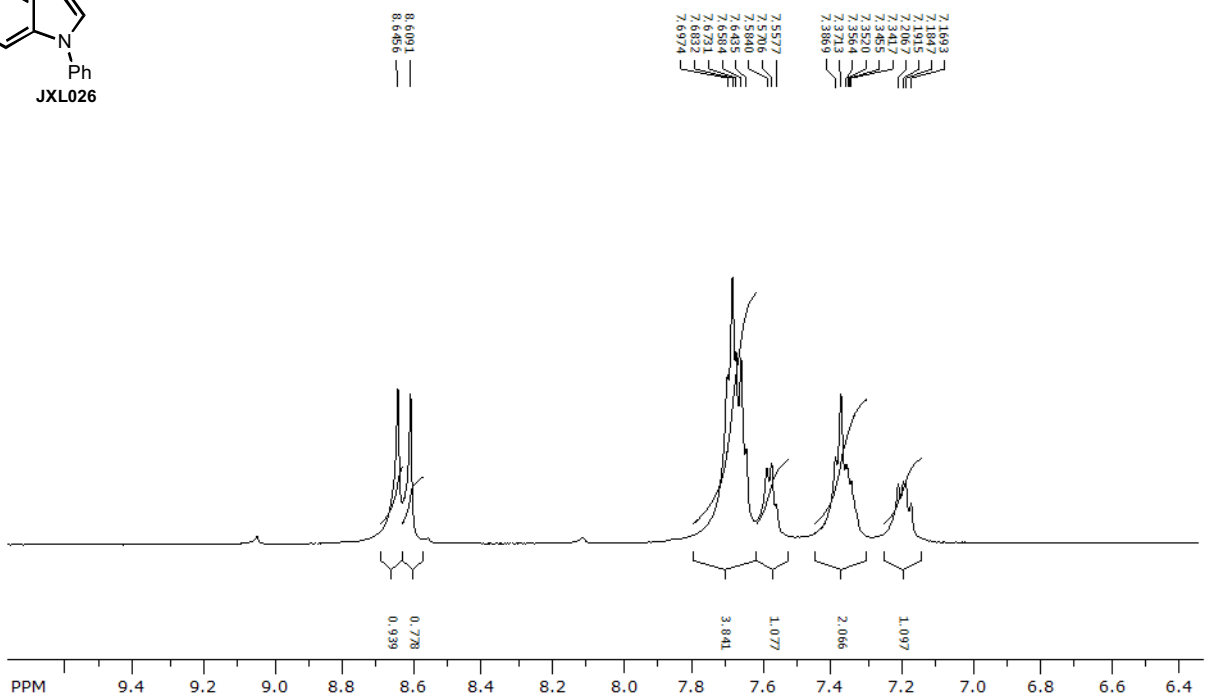
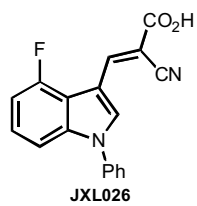
¹H NMR (500 MHz, DMSO-d₆)

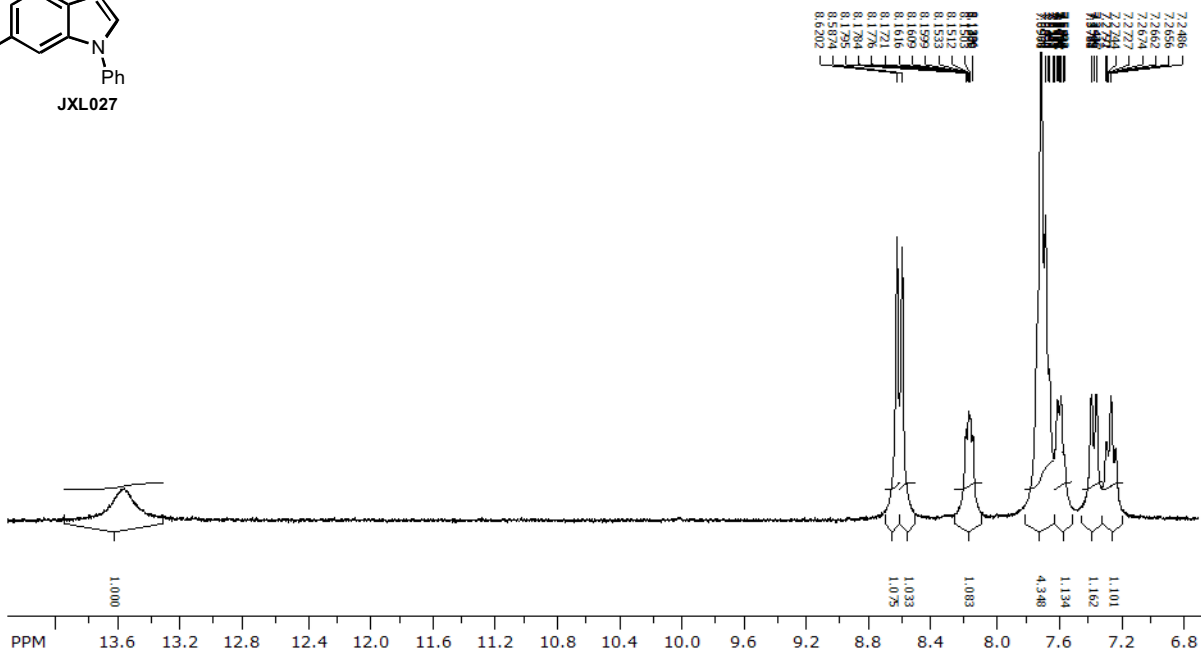
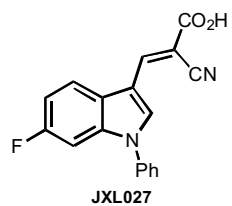


¹³C NMR (126 MHz, DMSO-d₆)

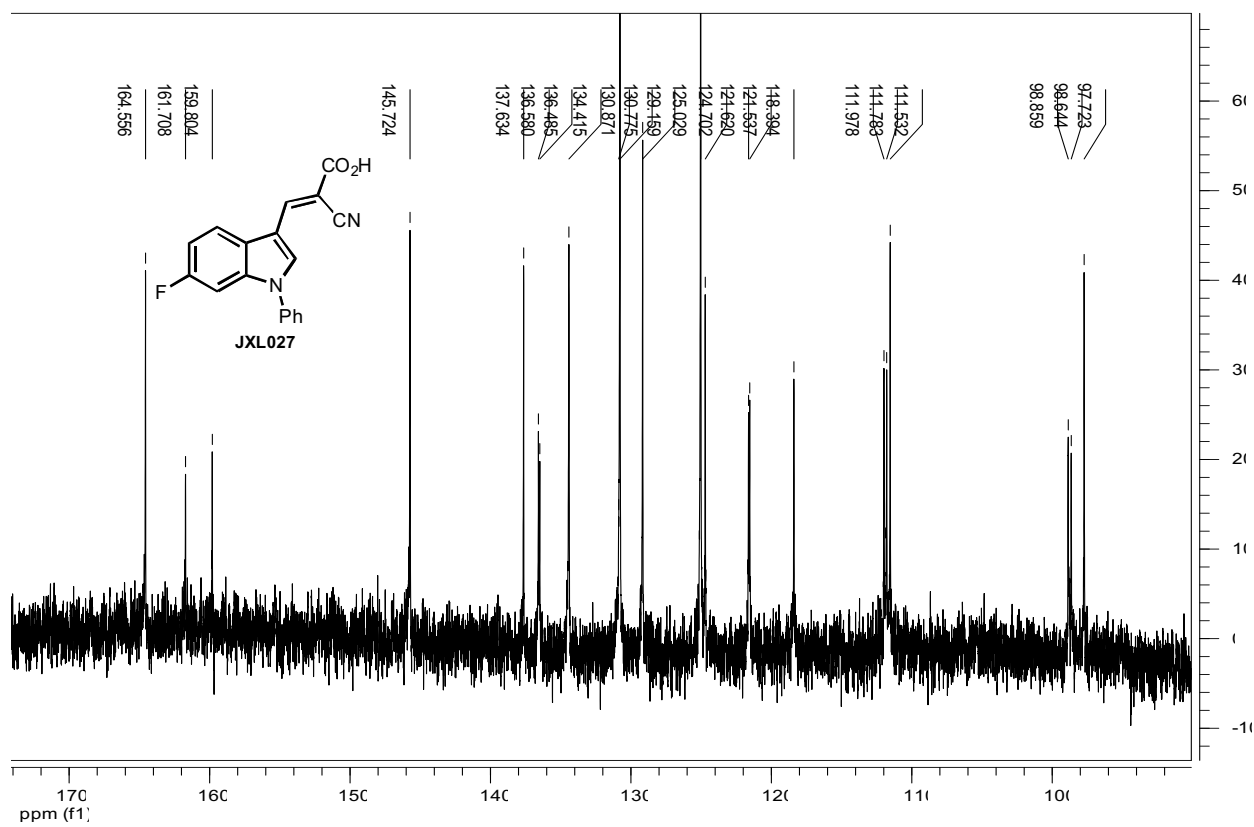


¹³C NMR (126 MHz, DMSO-d₆)

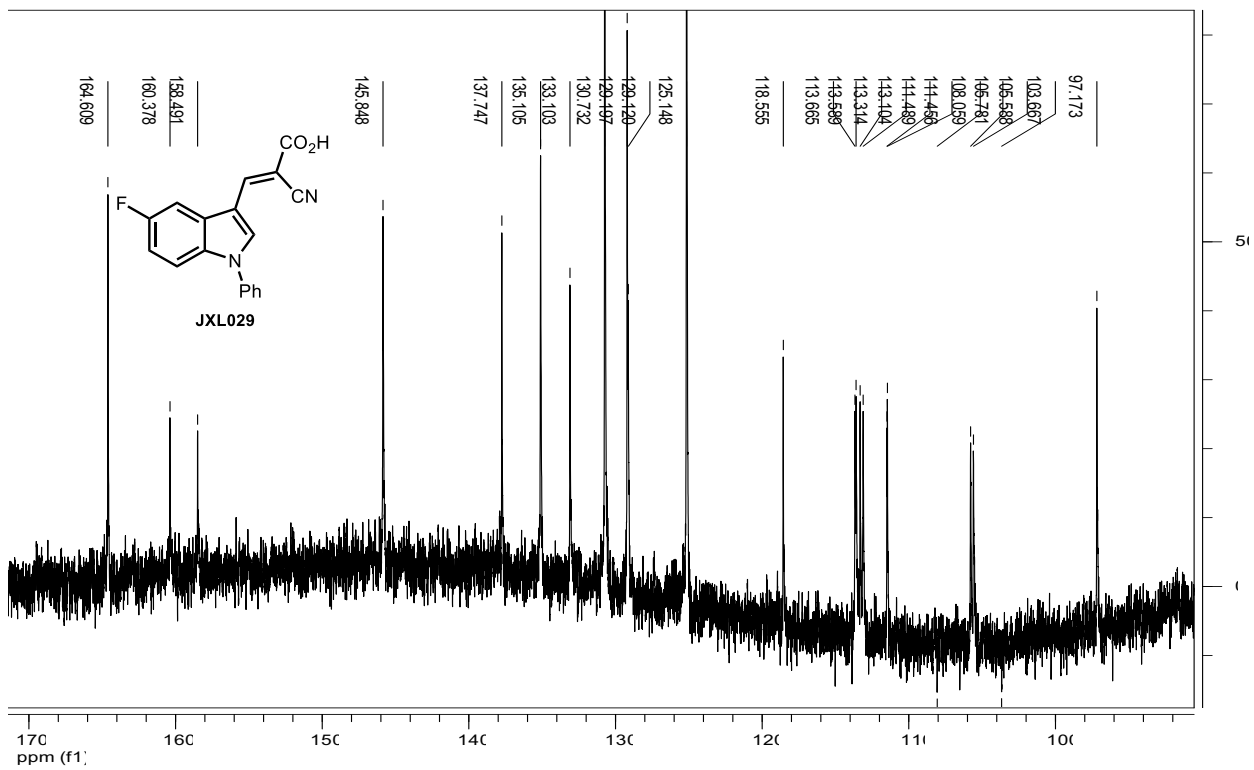
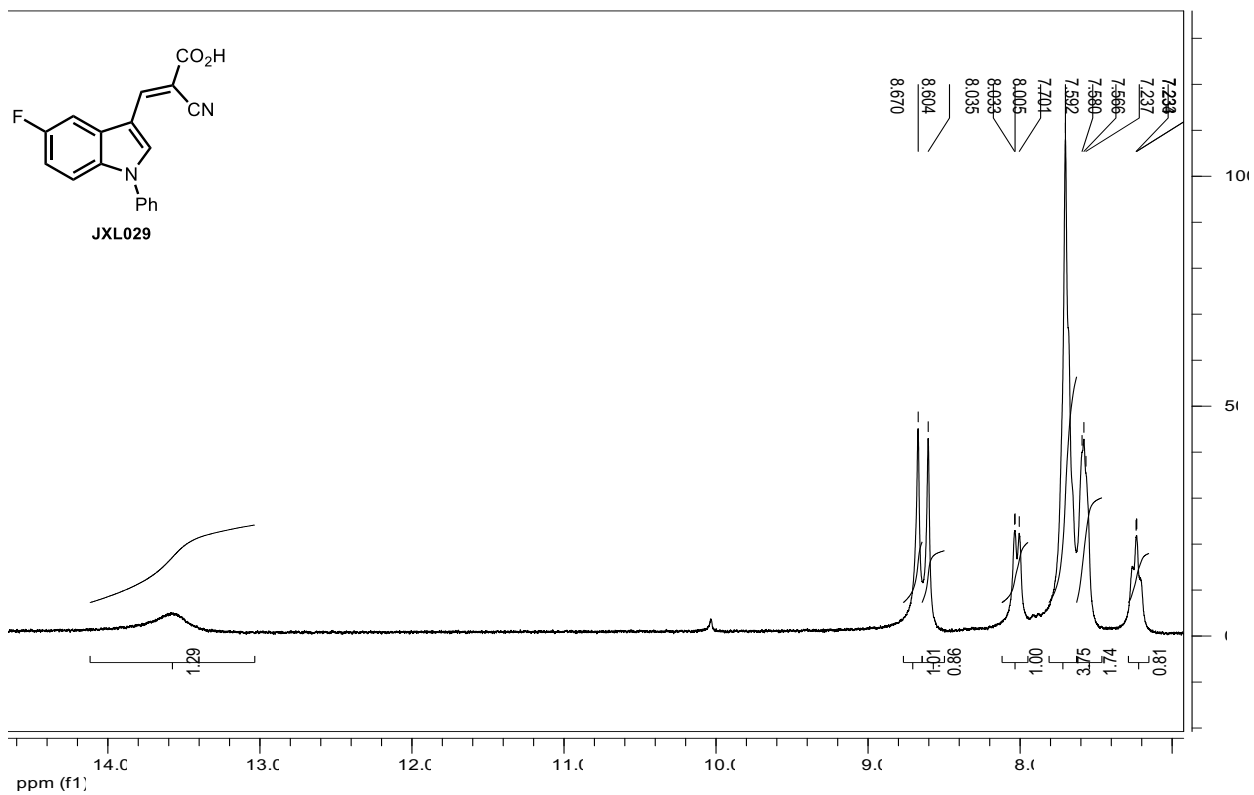




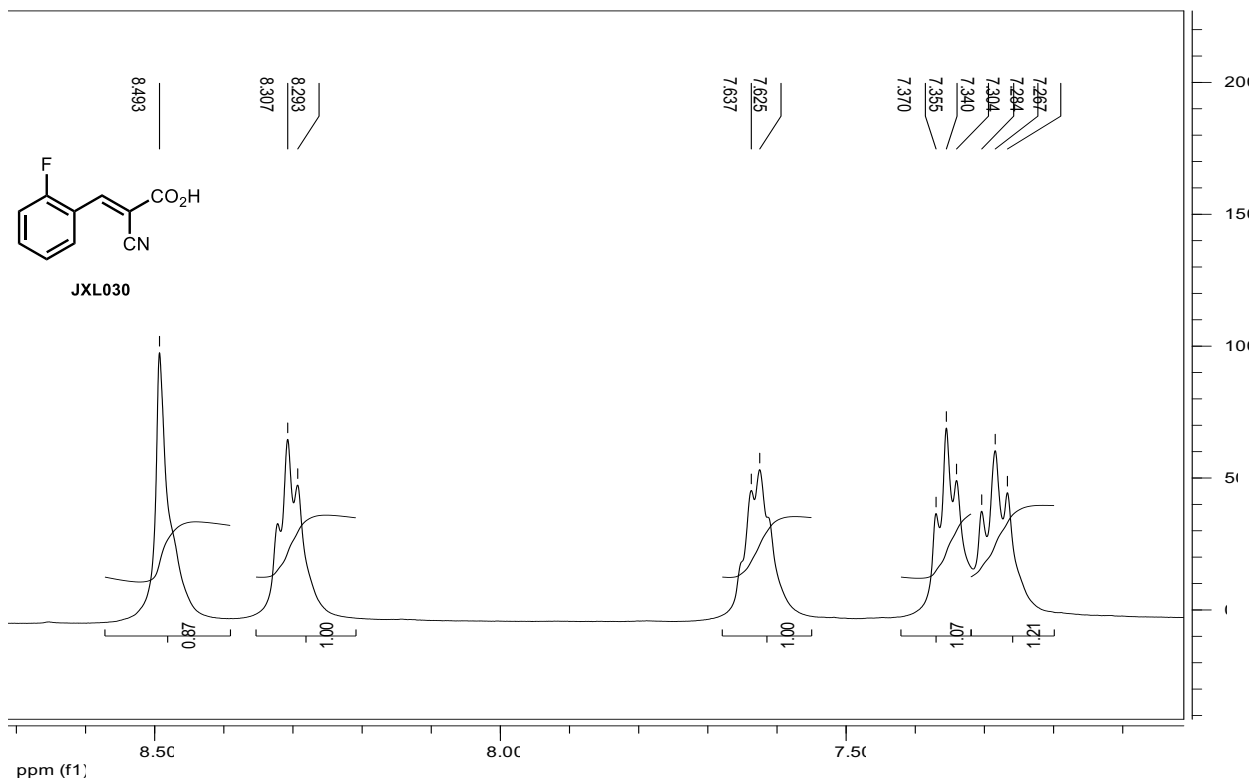
¹H NMR (500 MHz, DMSO-d₆)



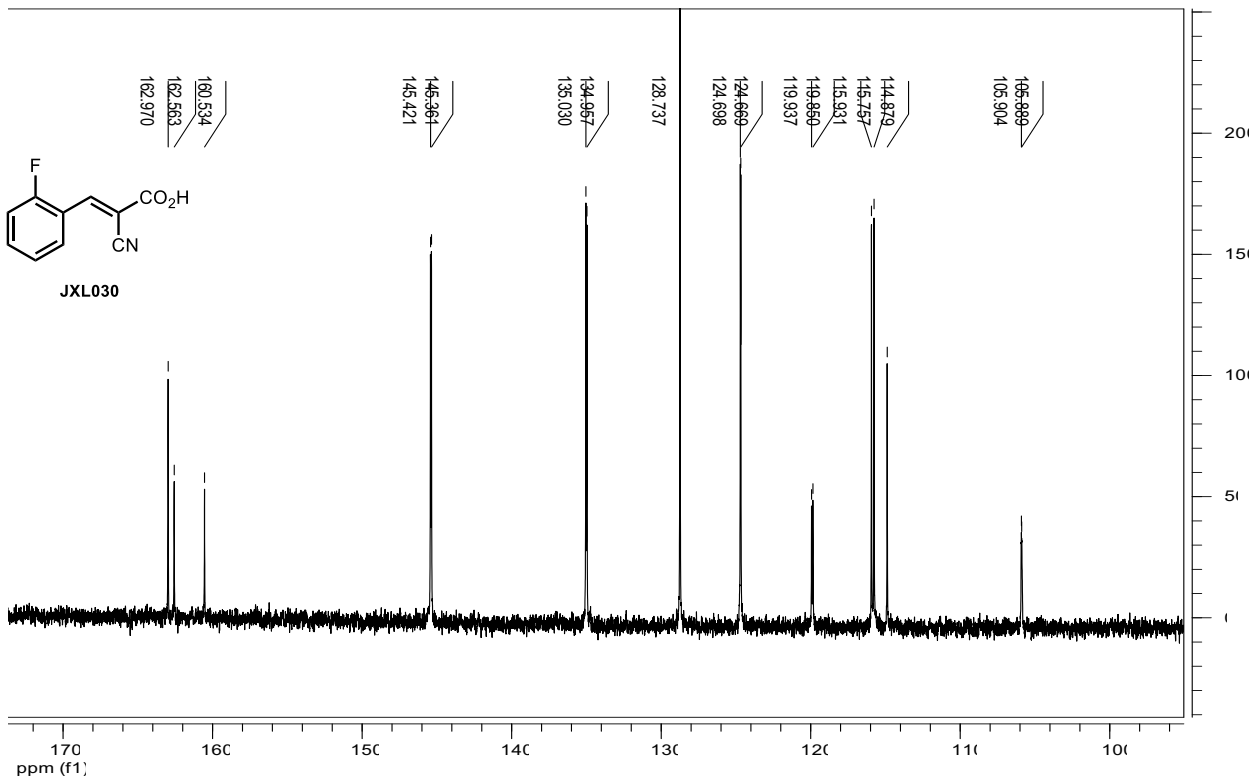
¹³C NMR (126 MHz, DMSO-d₆)



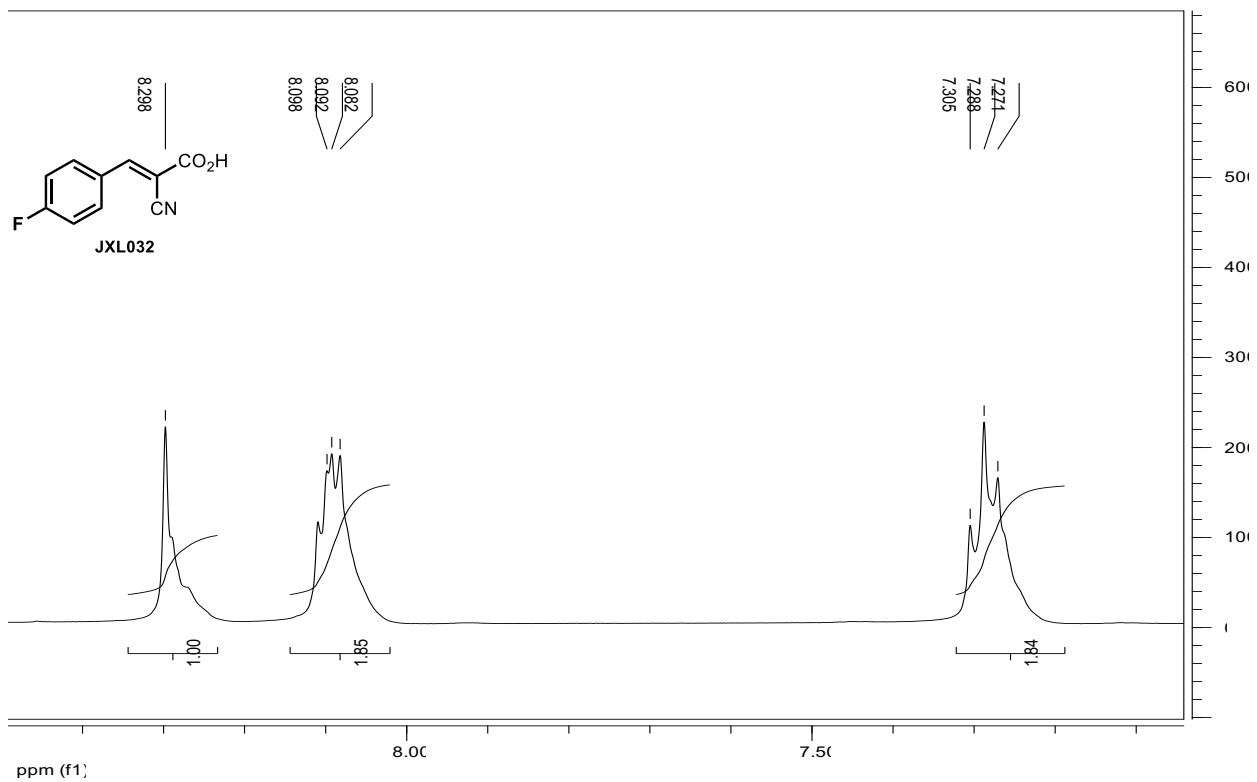
¹³C NMR (126 MHz, DMSO-d₆)



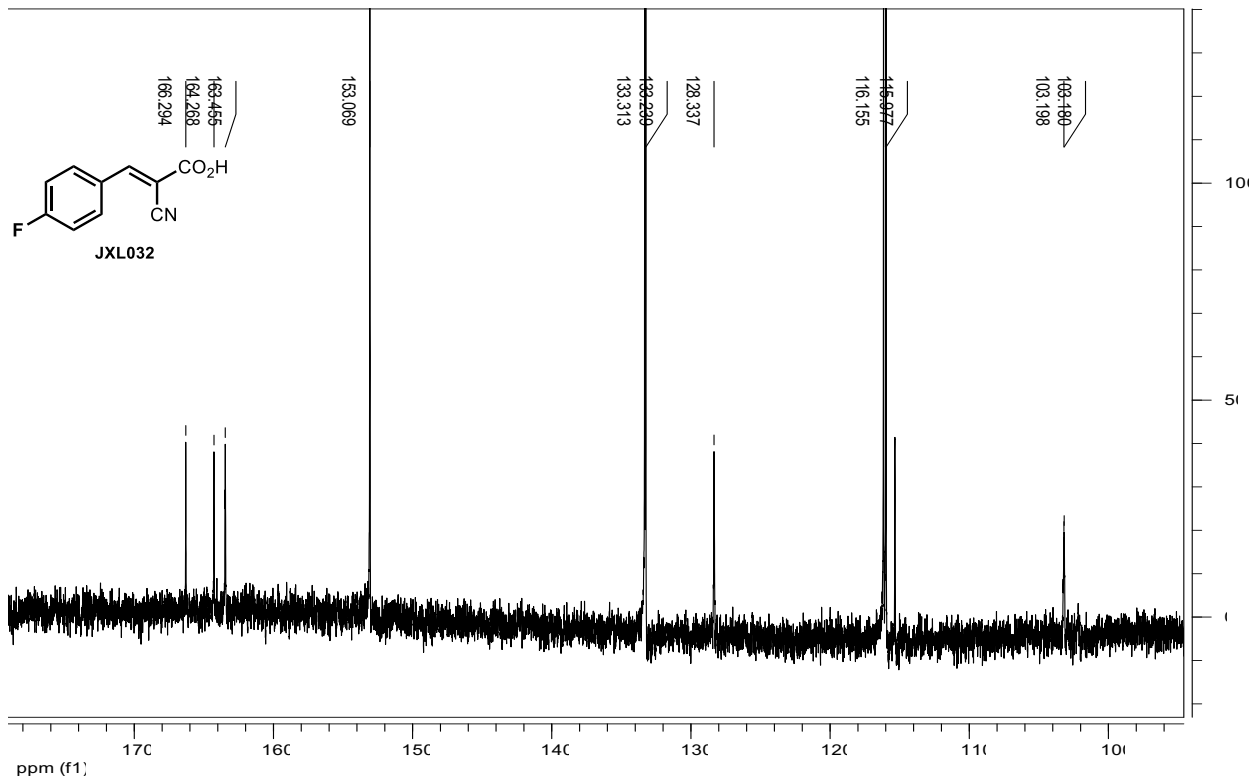
¹H NMR (500 MHz, DMSO-d₆)



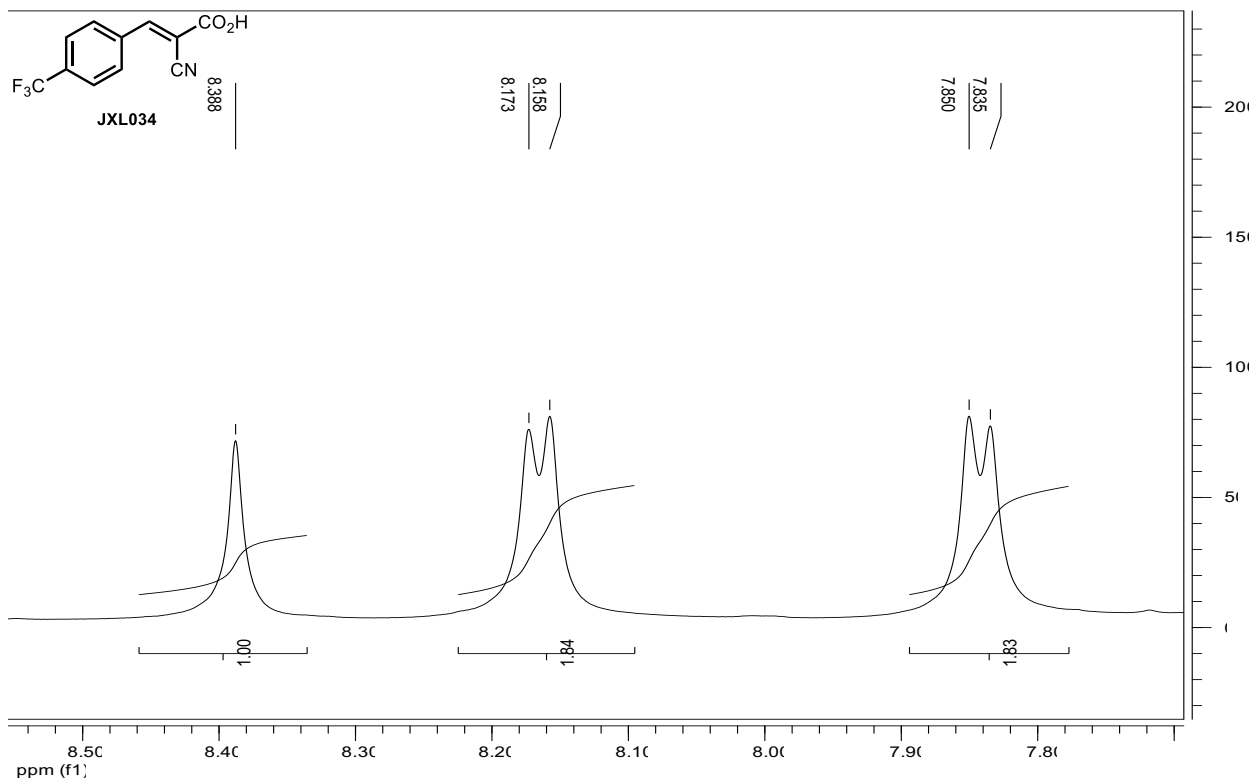
¹³C NMR (126 MHz, DMSO-d₆)



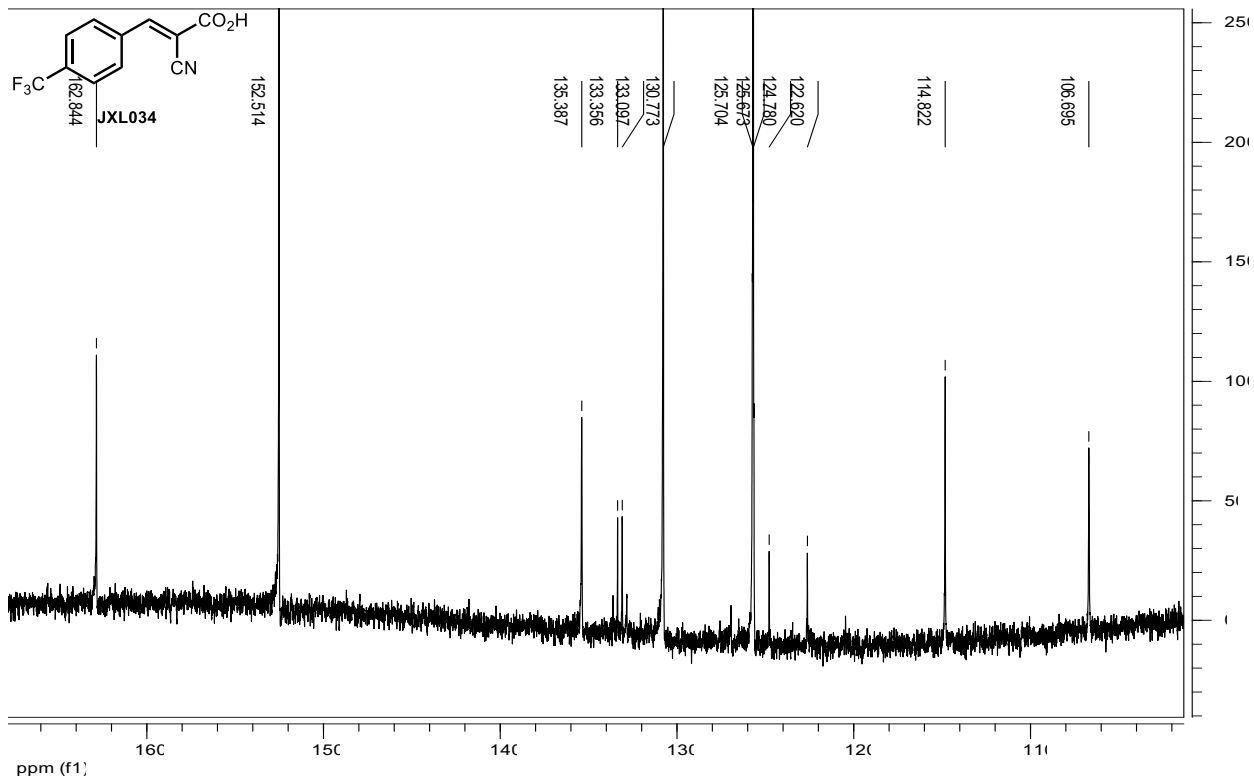
¹H NMR (500 MHz, DMSO-d₆)



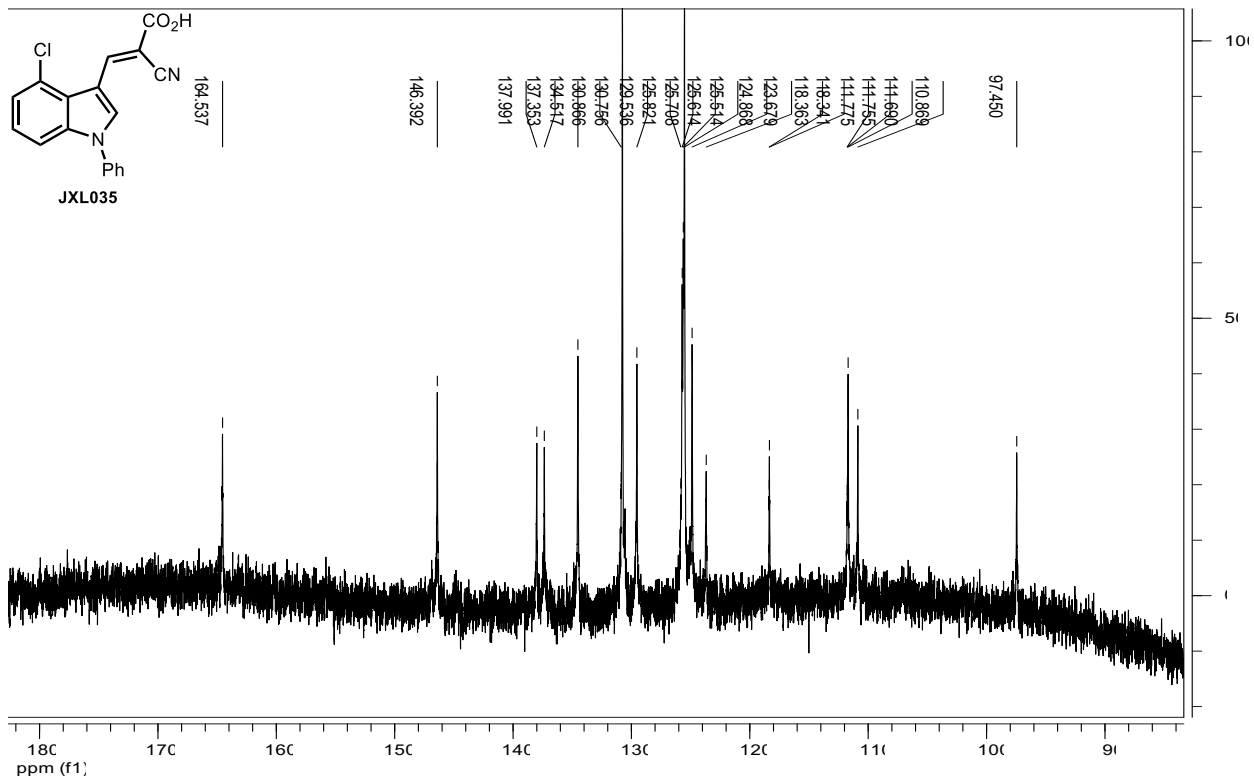
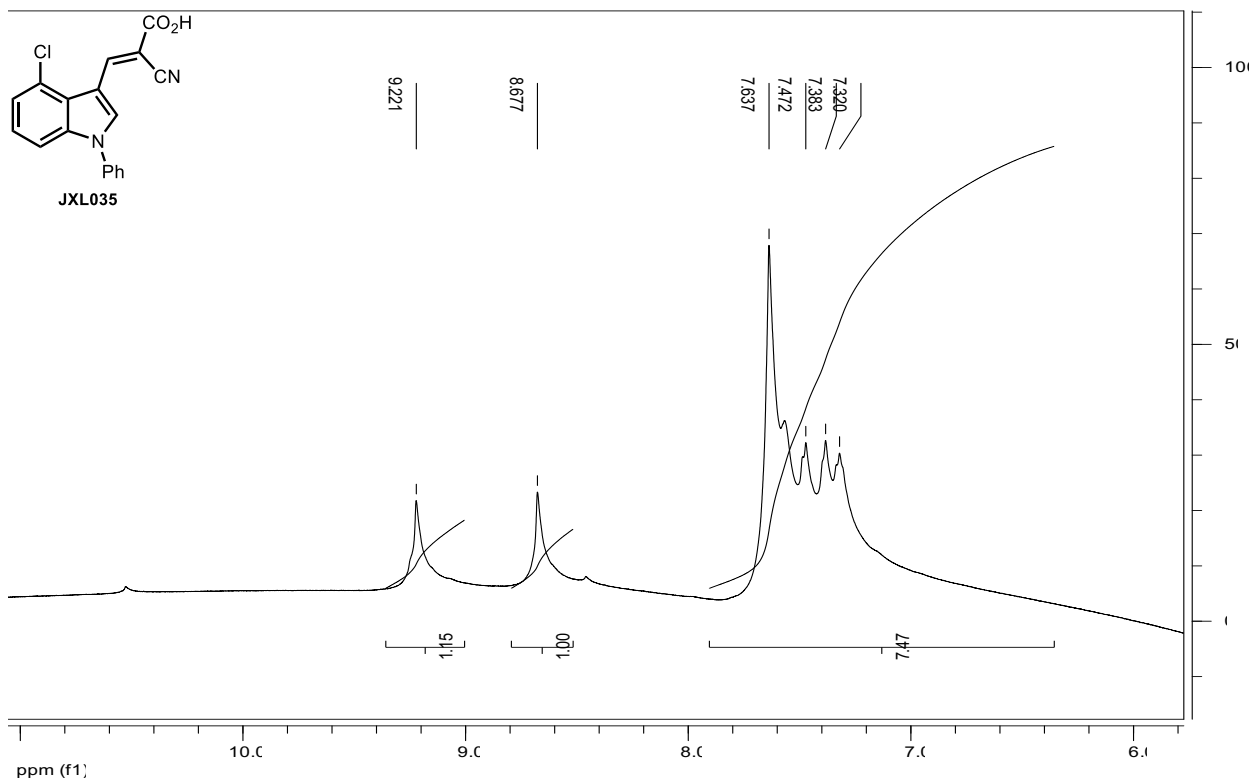
¹³C NMR (126 MHz, DMSO-d₆)



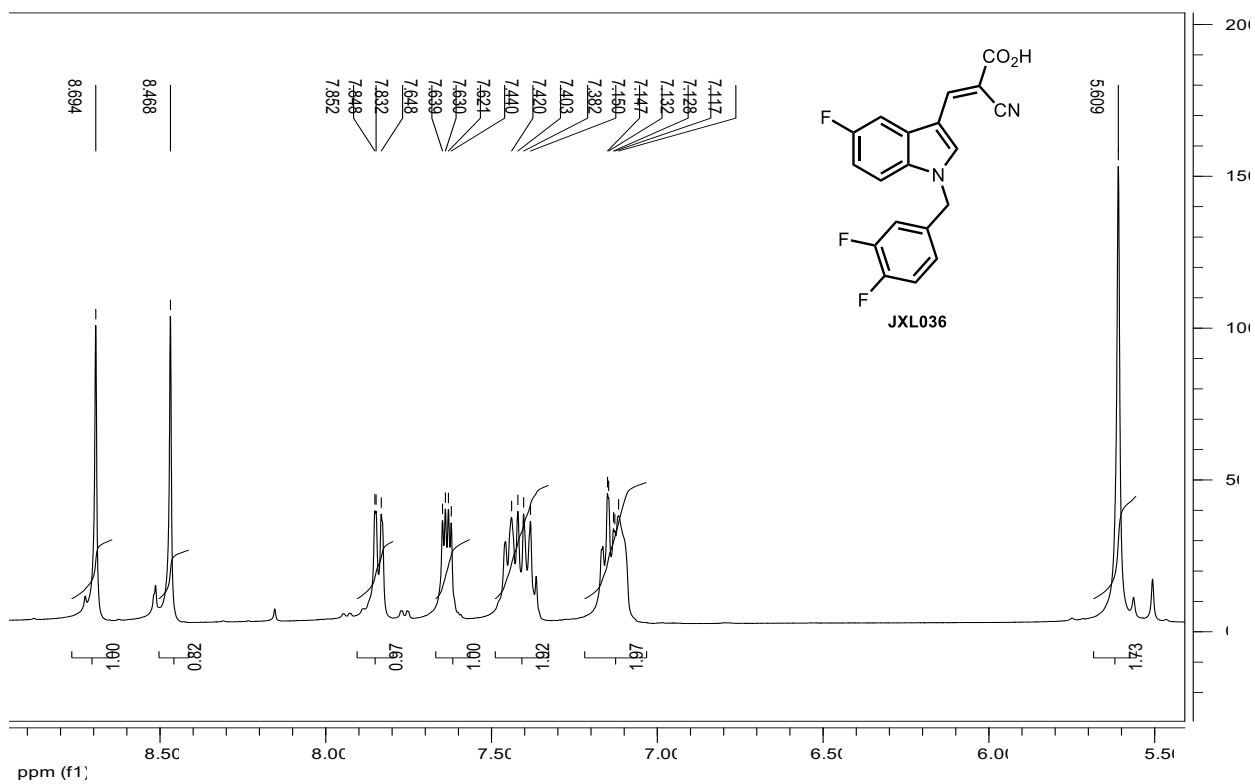
¹H NMR (500 MHz, DMSO-d₆)



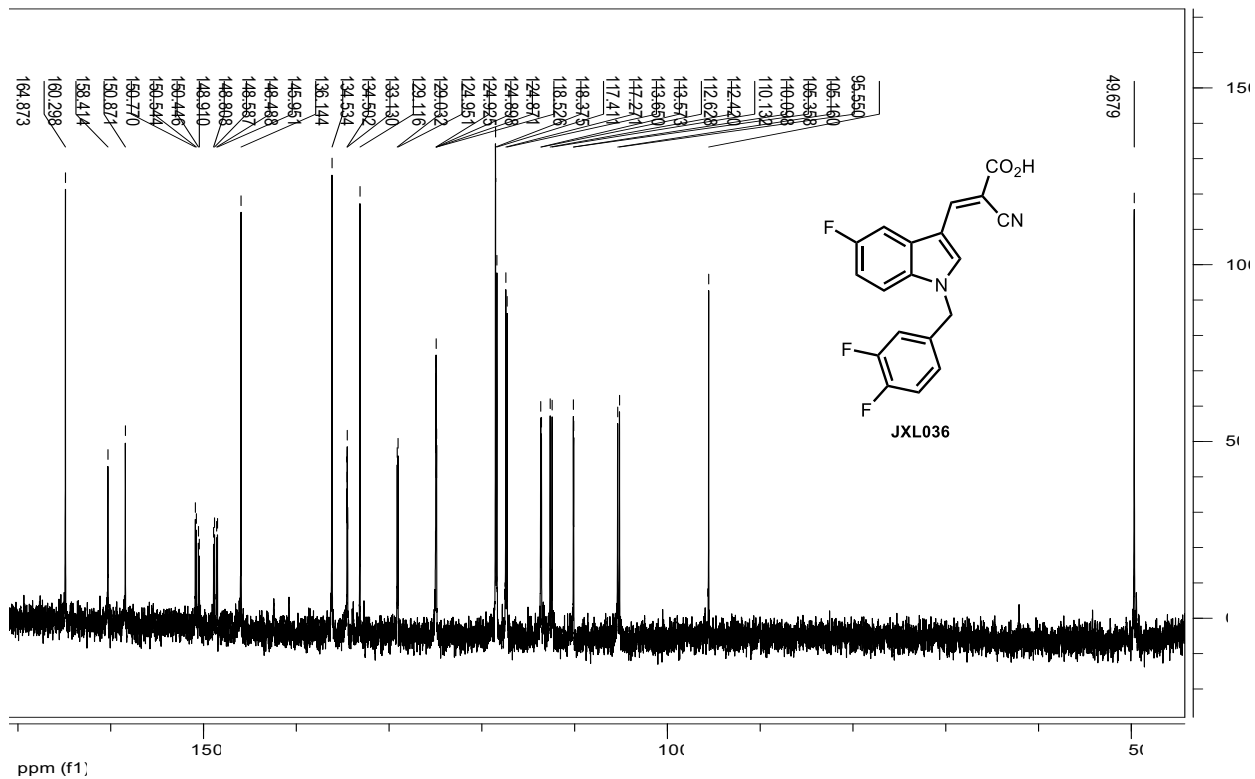
¹³C NMR (126 MHz, DMSO-d₆)



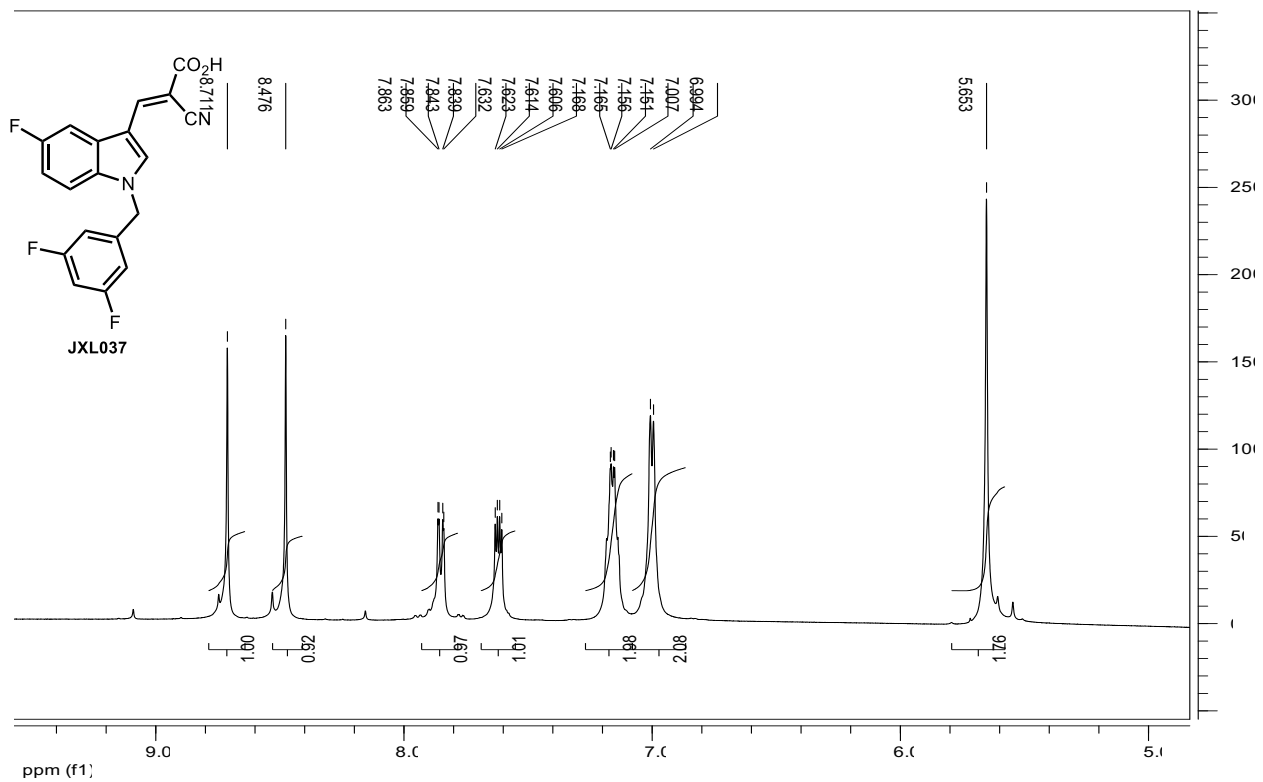
¹³C NMR (126 MHz, DMSO-d₆)



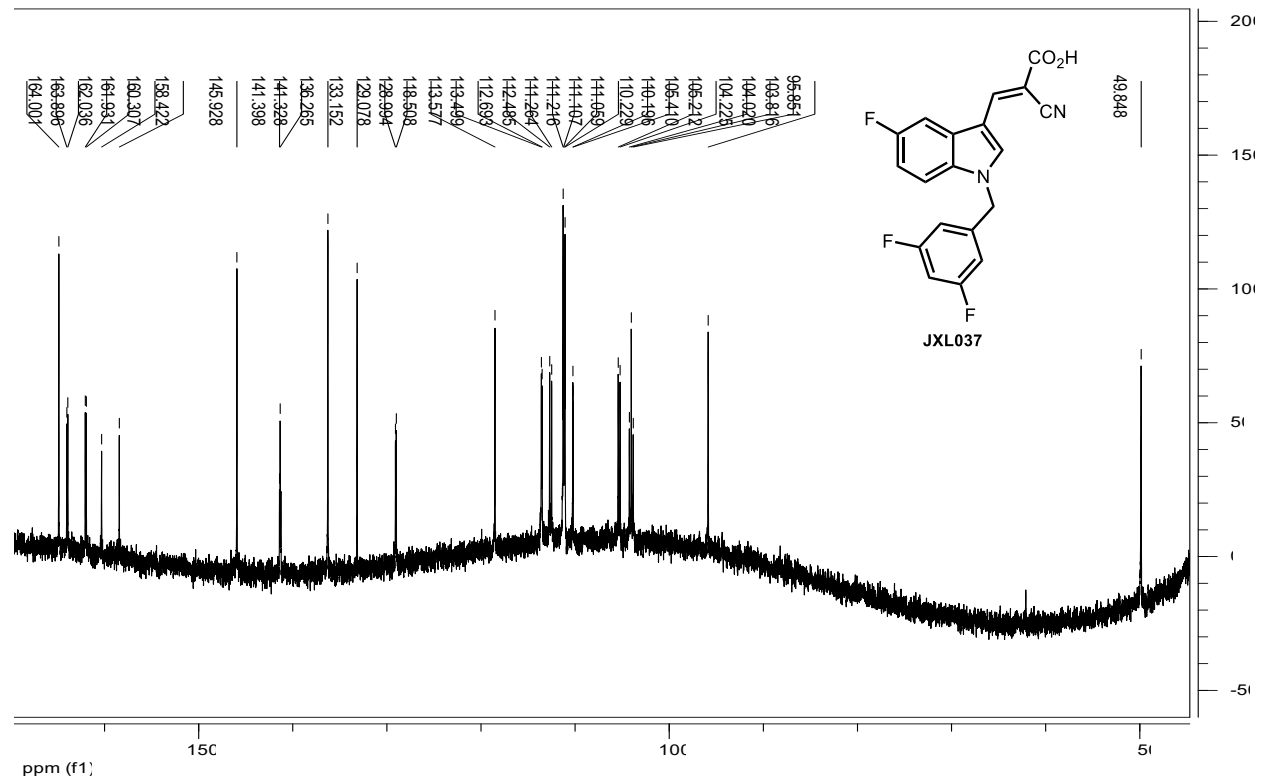
¹H NMR (500 MHz, DMSO-d₆)



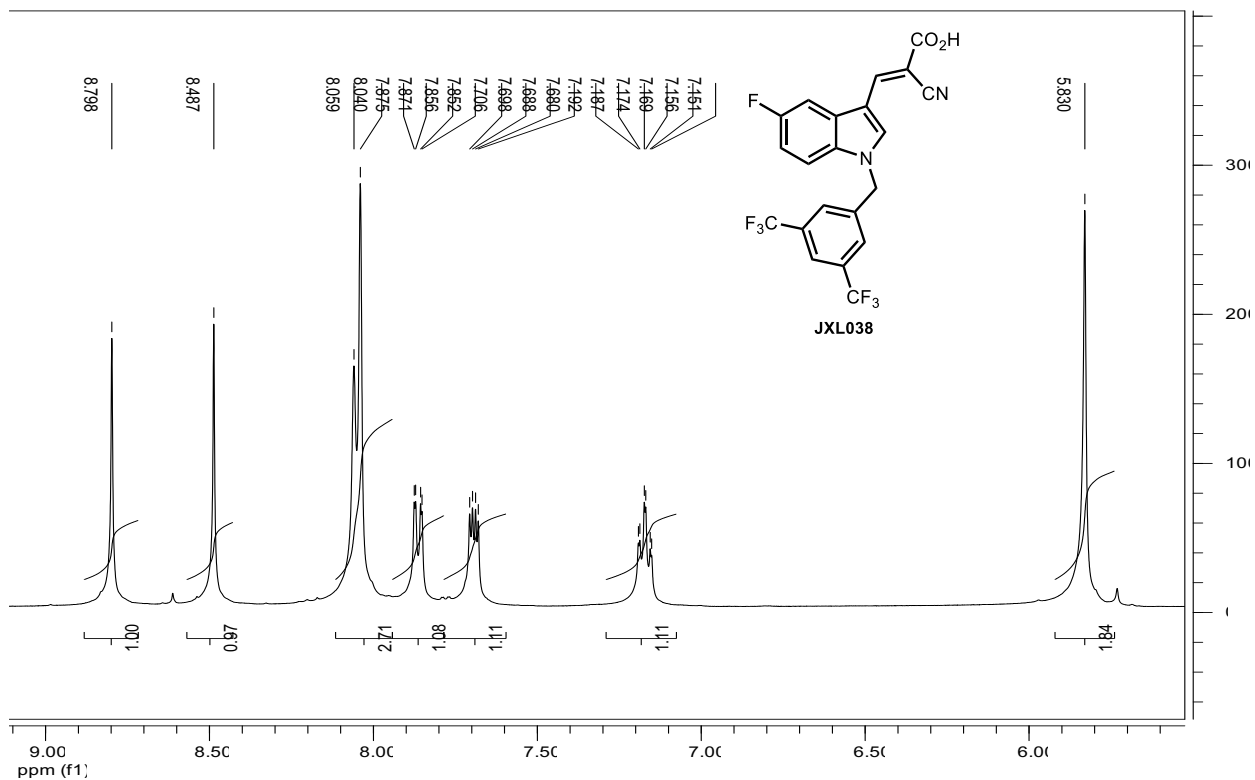
¹³C NMR (126 MHz, DMSO-d₆)



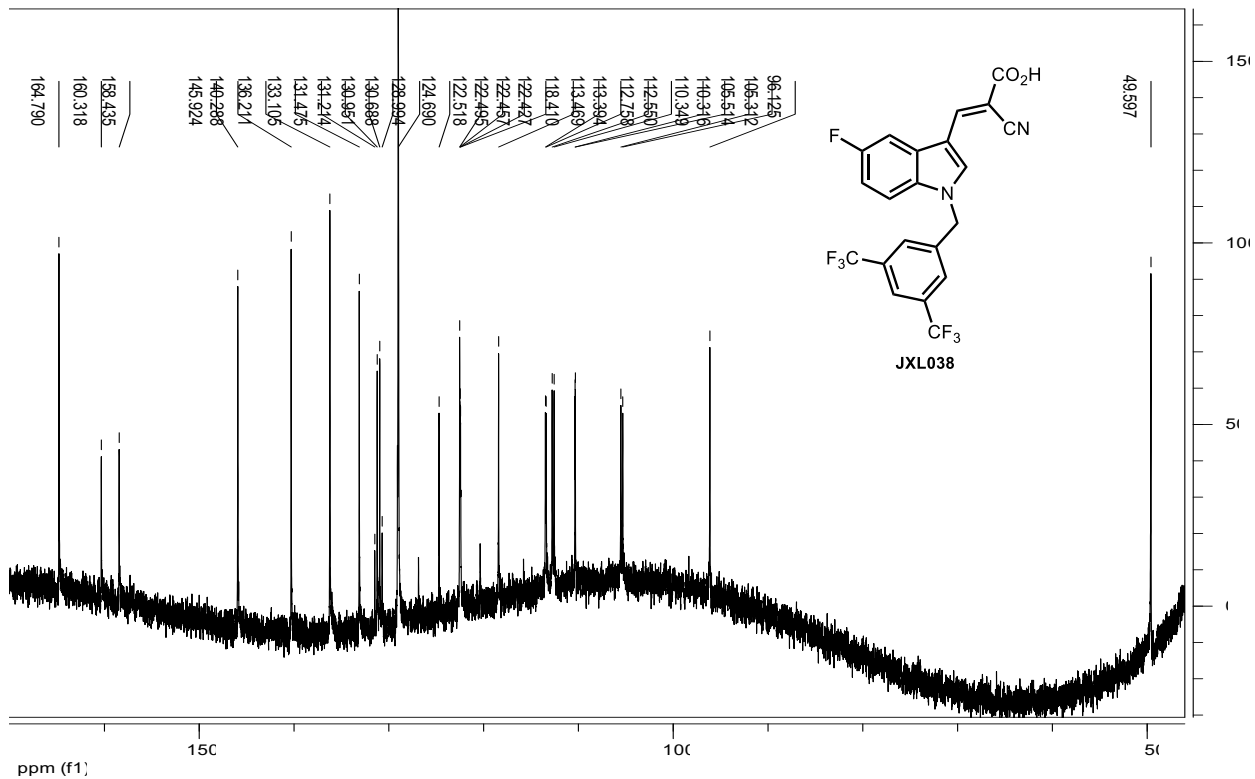
¹H NMR (500 MHz, DMSO-d₆)



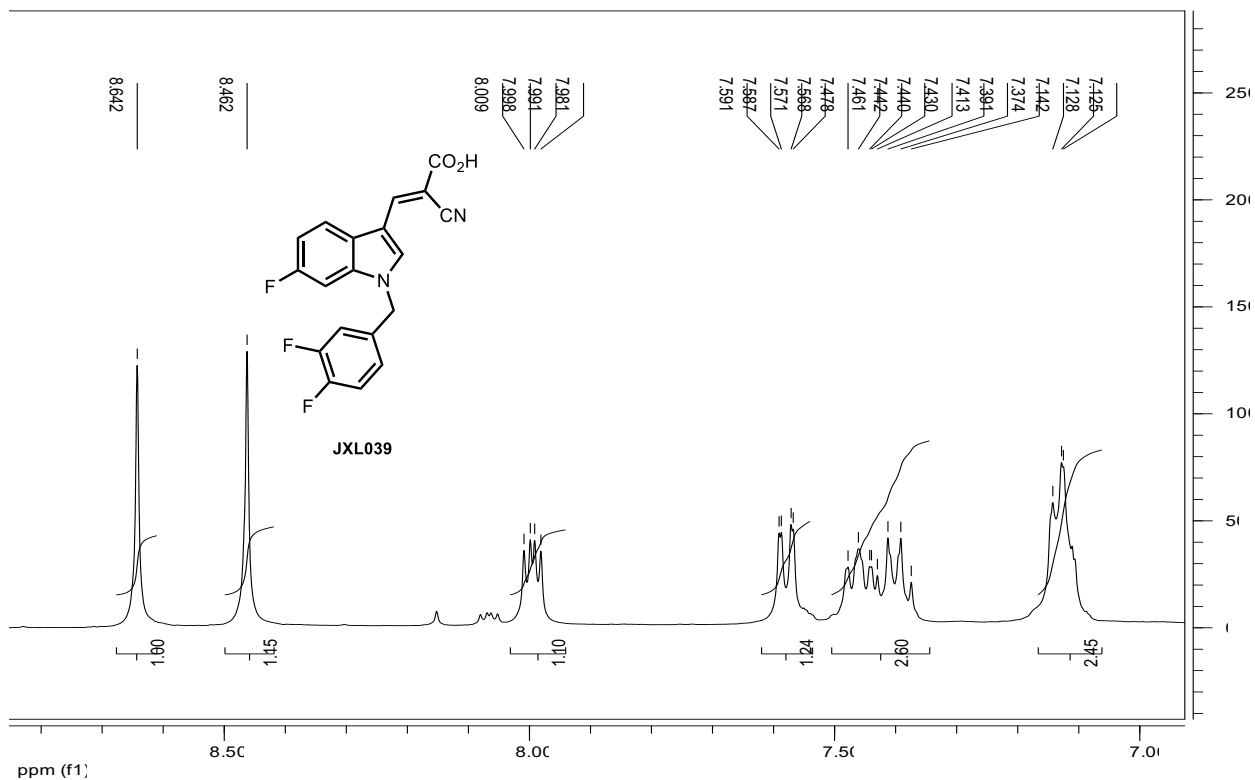
¹³C NMR (126 MHz, DMSO-d₆)



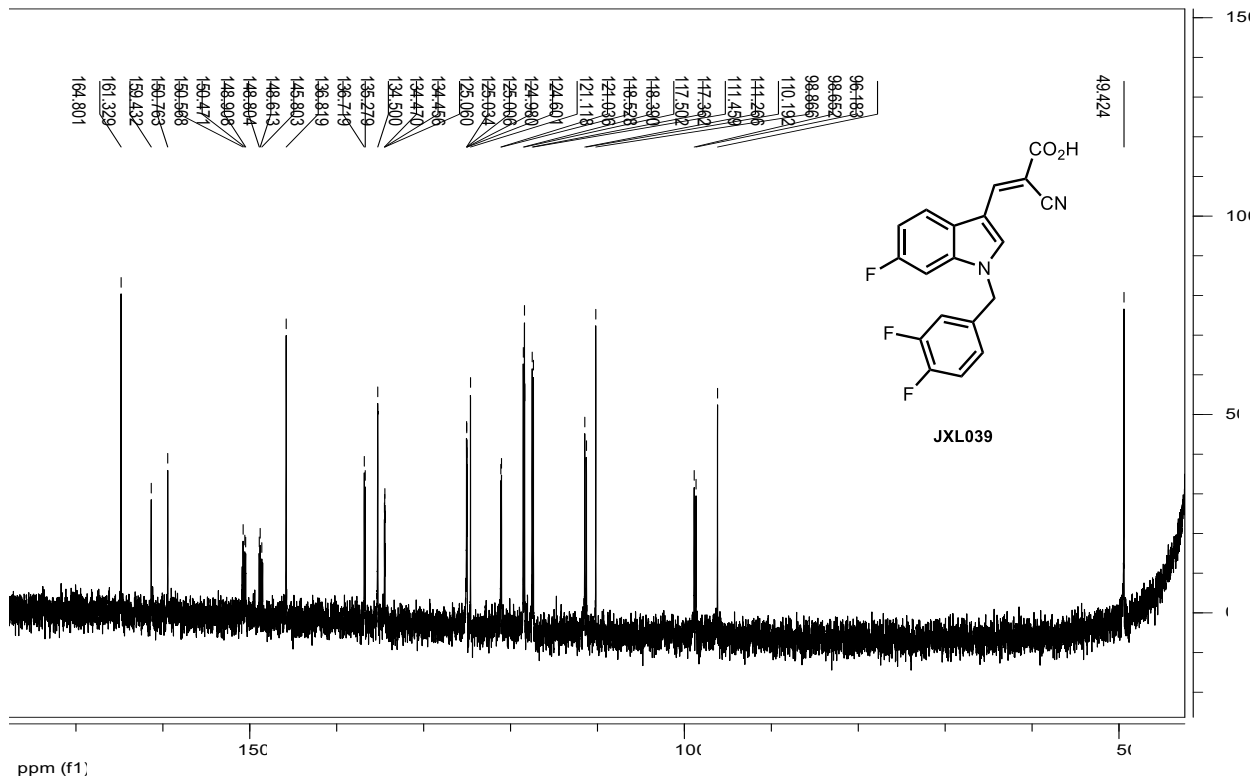
¹H NMR (500 MHz, DMSO-d₆)



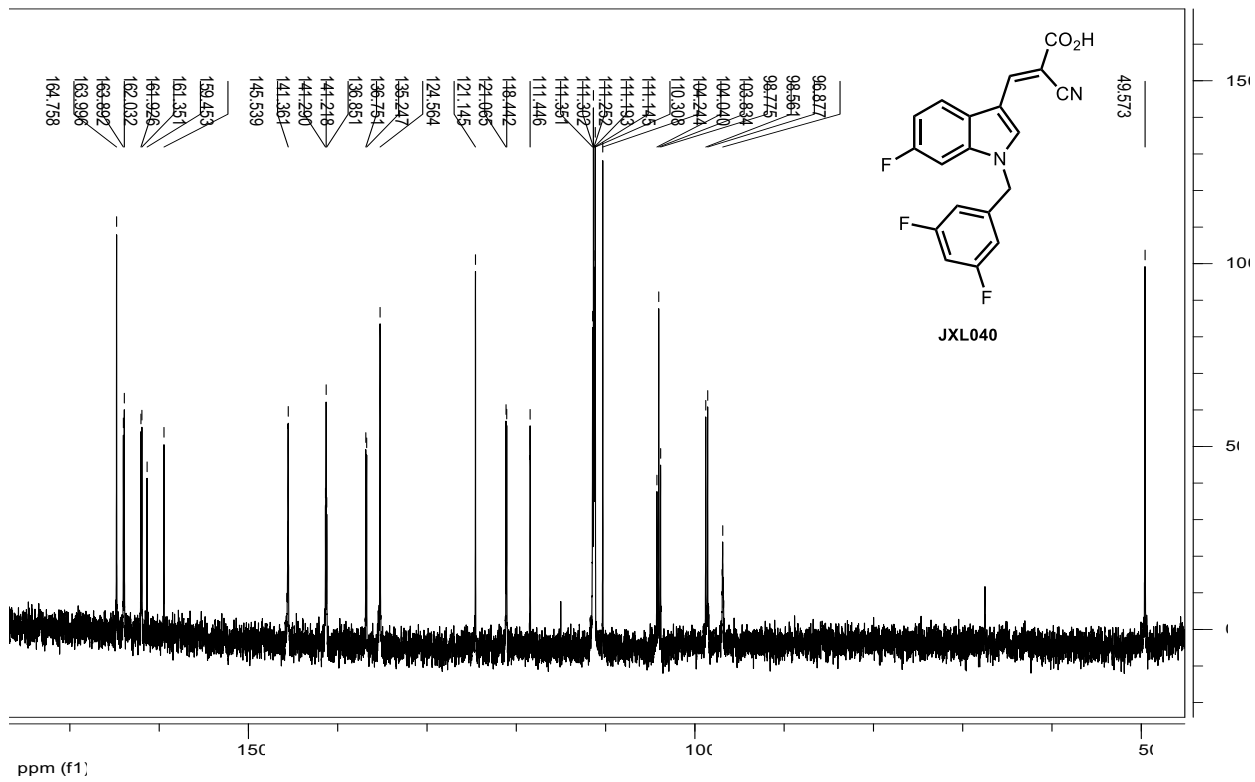
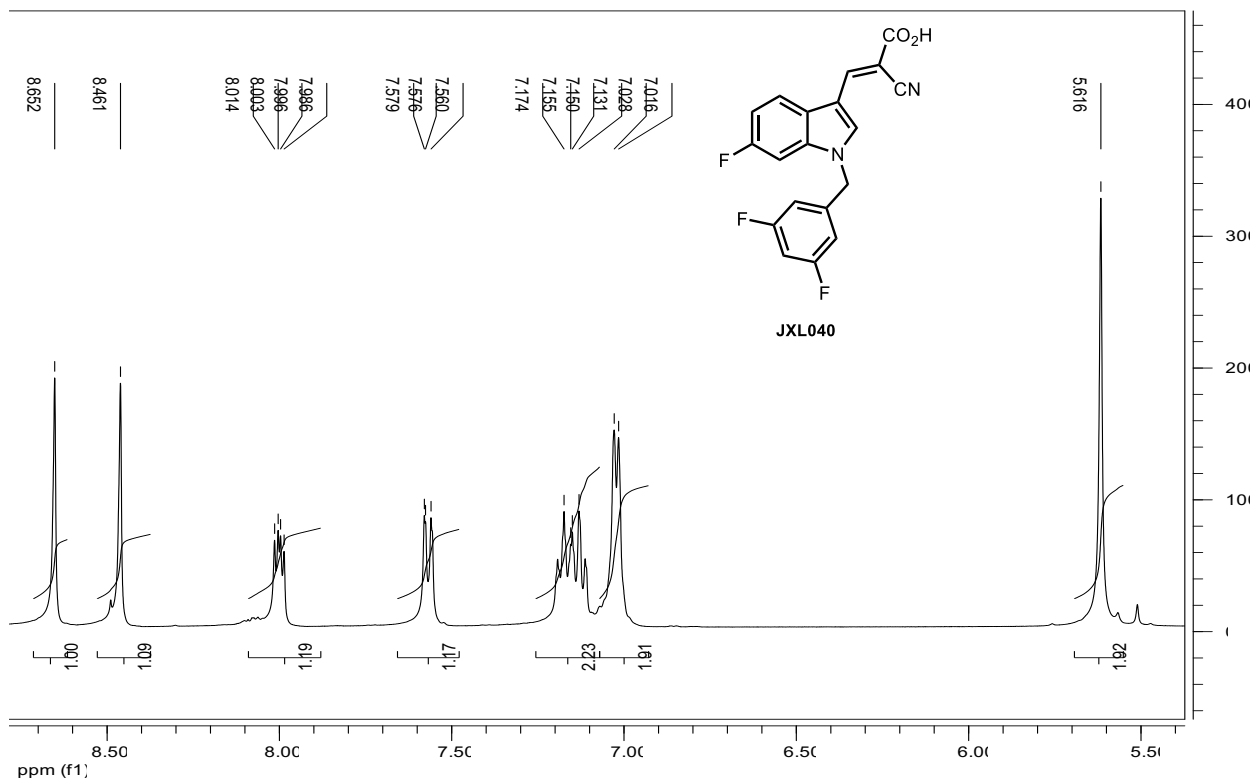
¹³C NMR (126 MHz, DMSO-d₆)



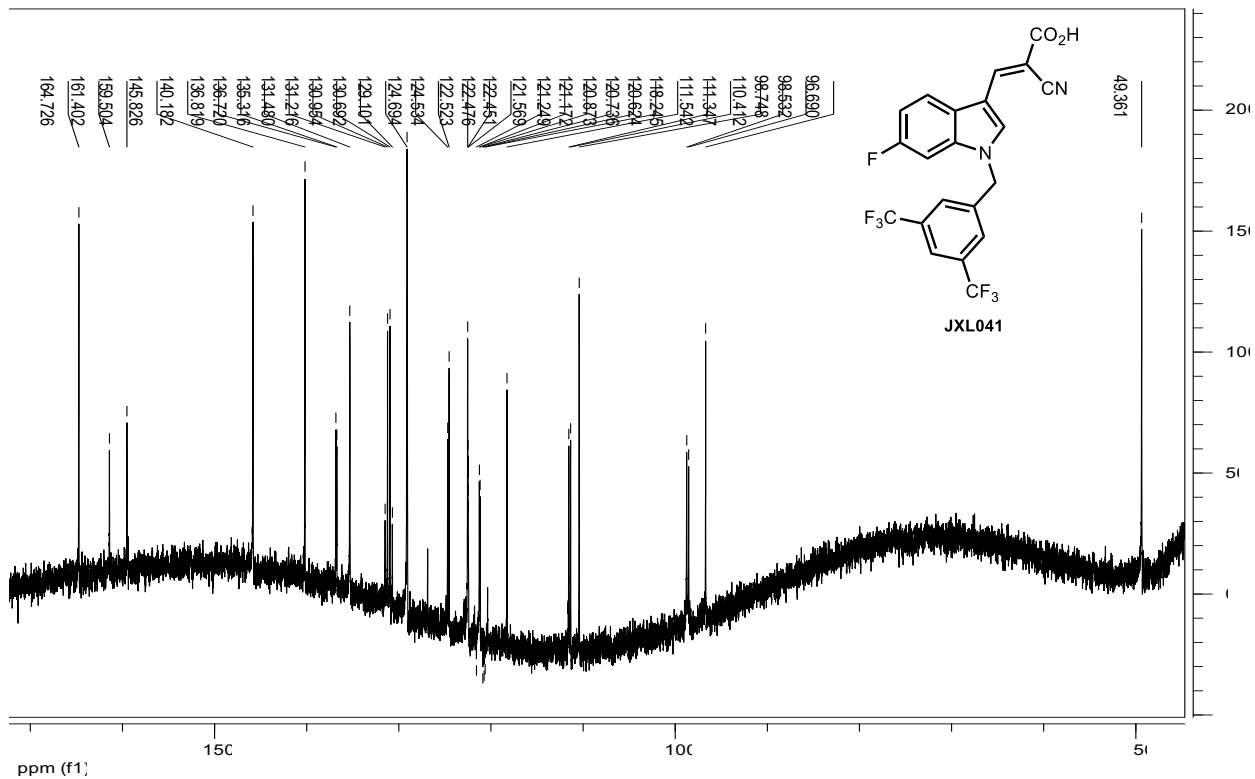
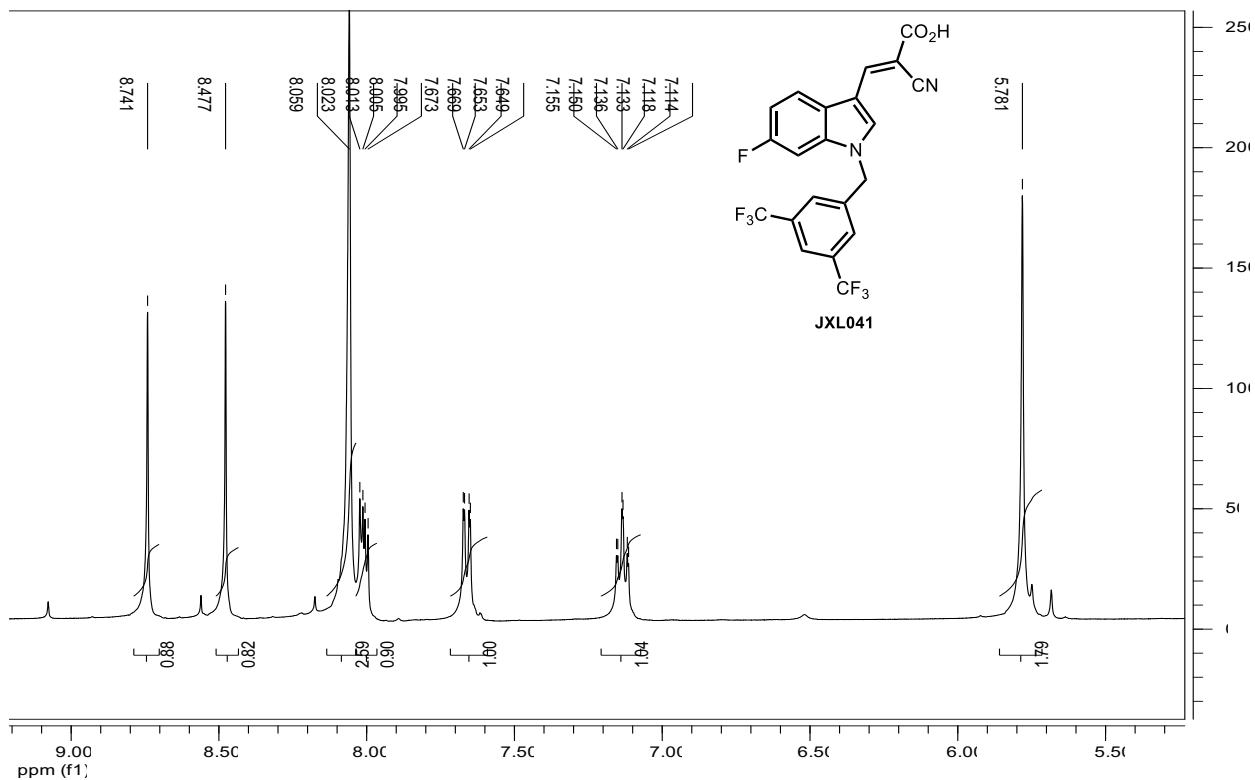
¹H NMR (500 MHz, DMSO-d₆)



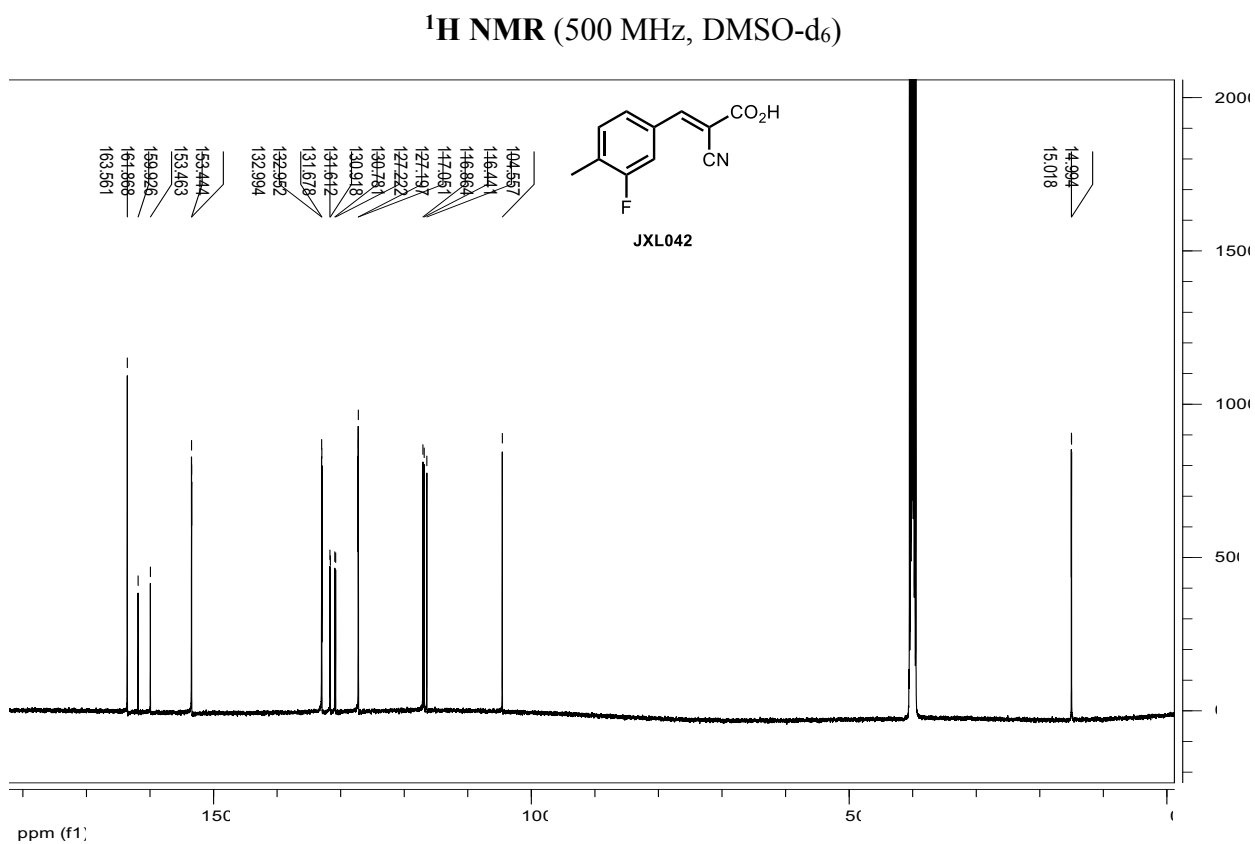
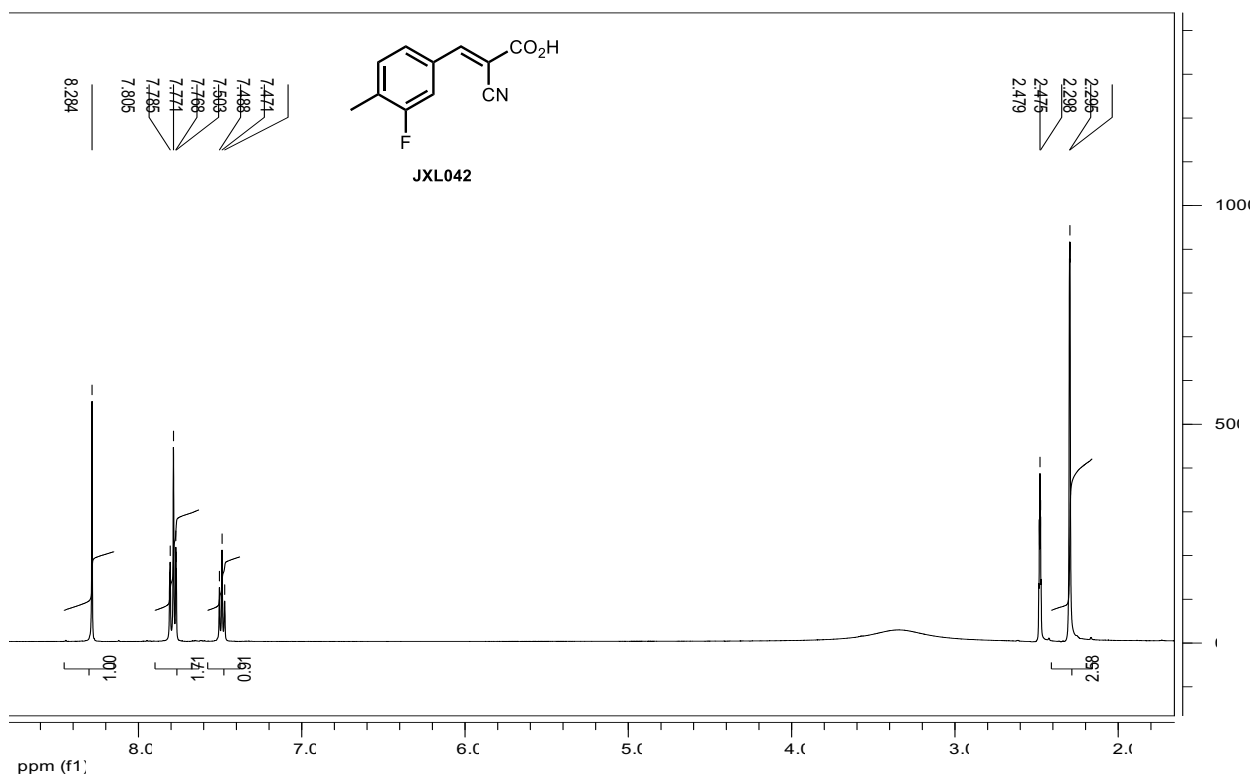
¹³C NMR (126 MHz, DMSO-d₆)



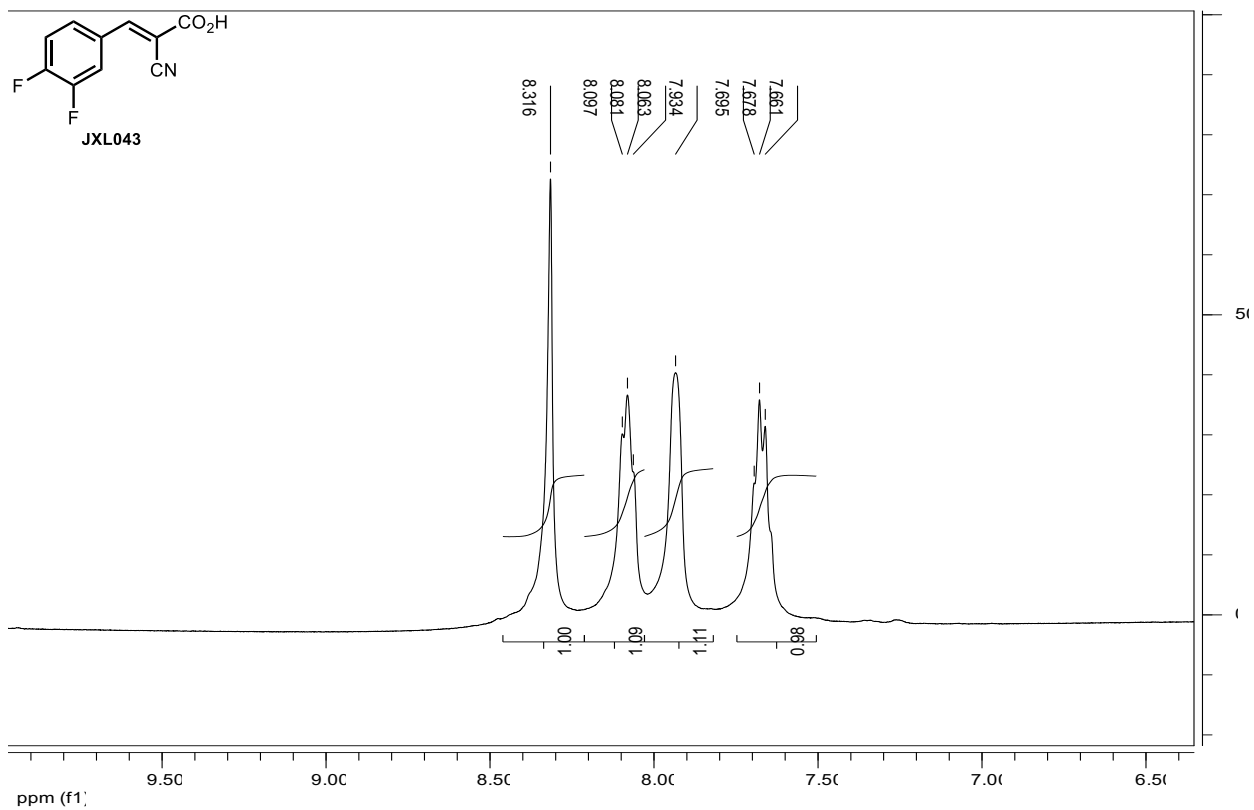
¹³C NMR (126 MHz, DMSO-d₆)



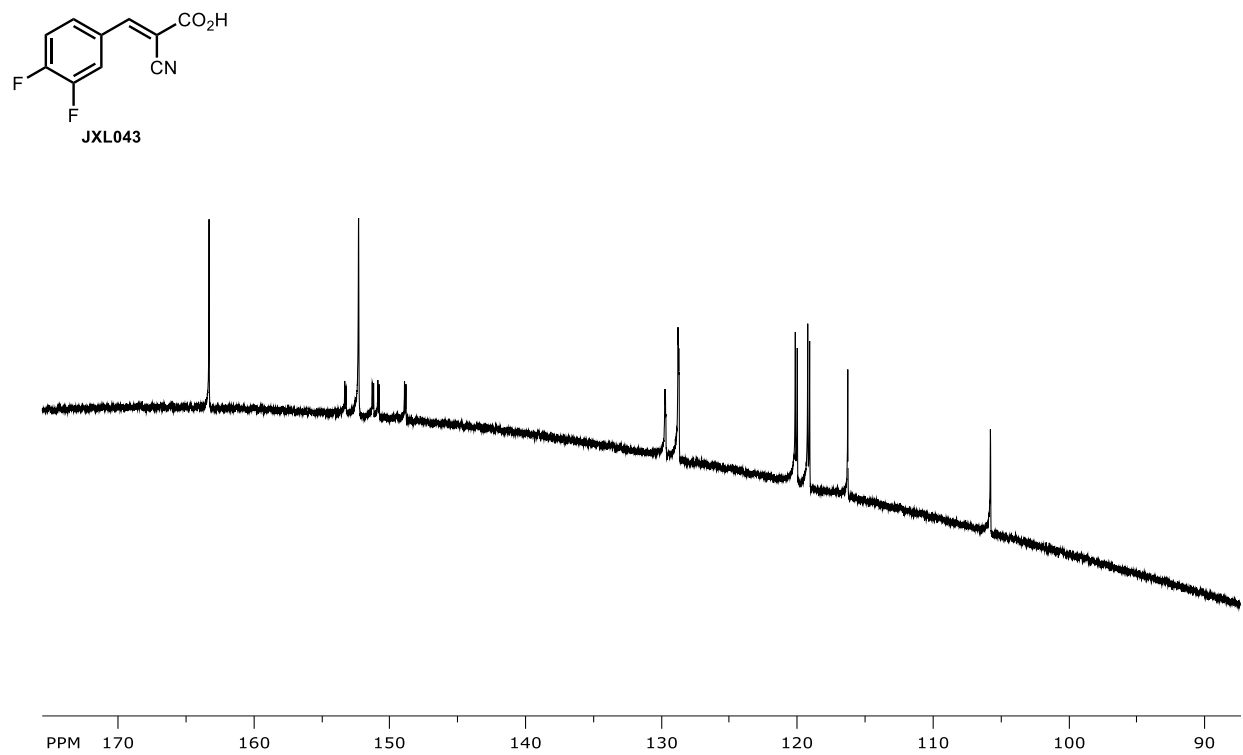
¹³C NMR (126 MHz, DMSO-d₆)



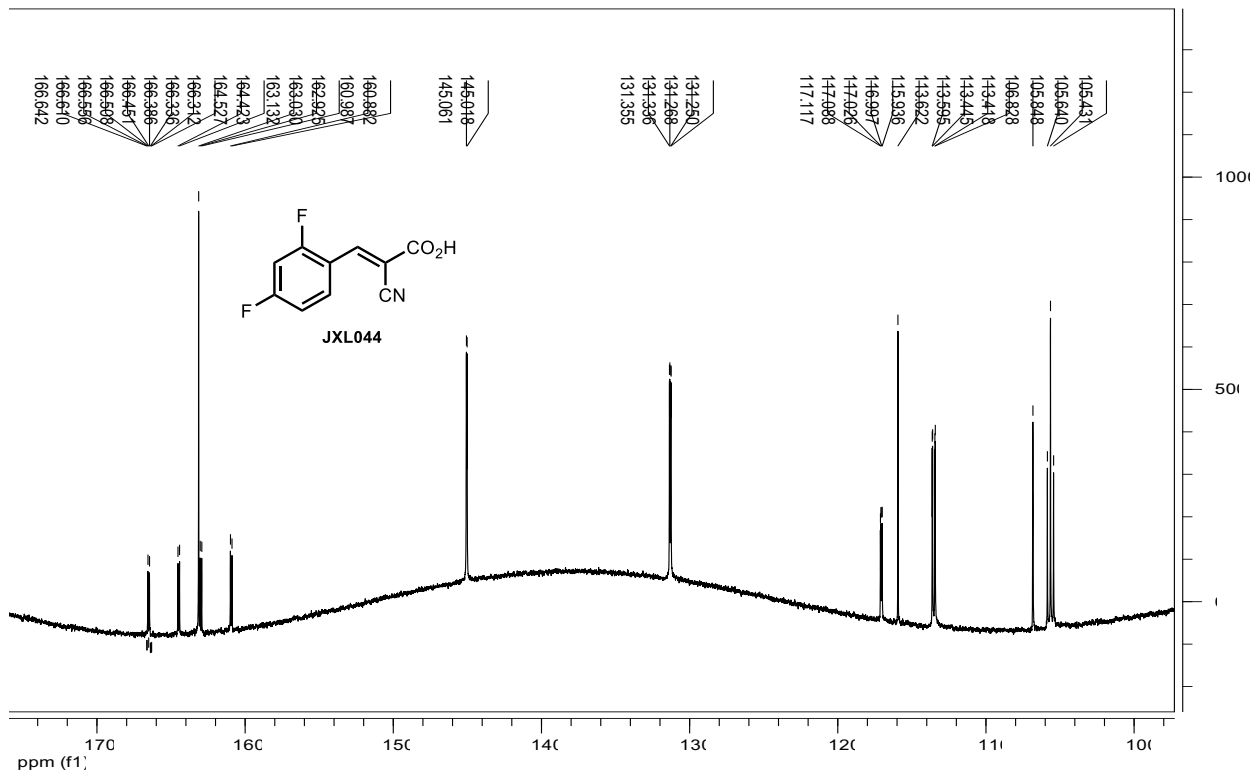
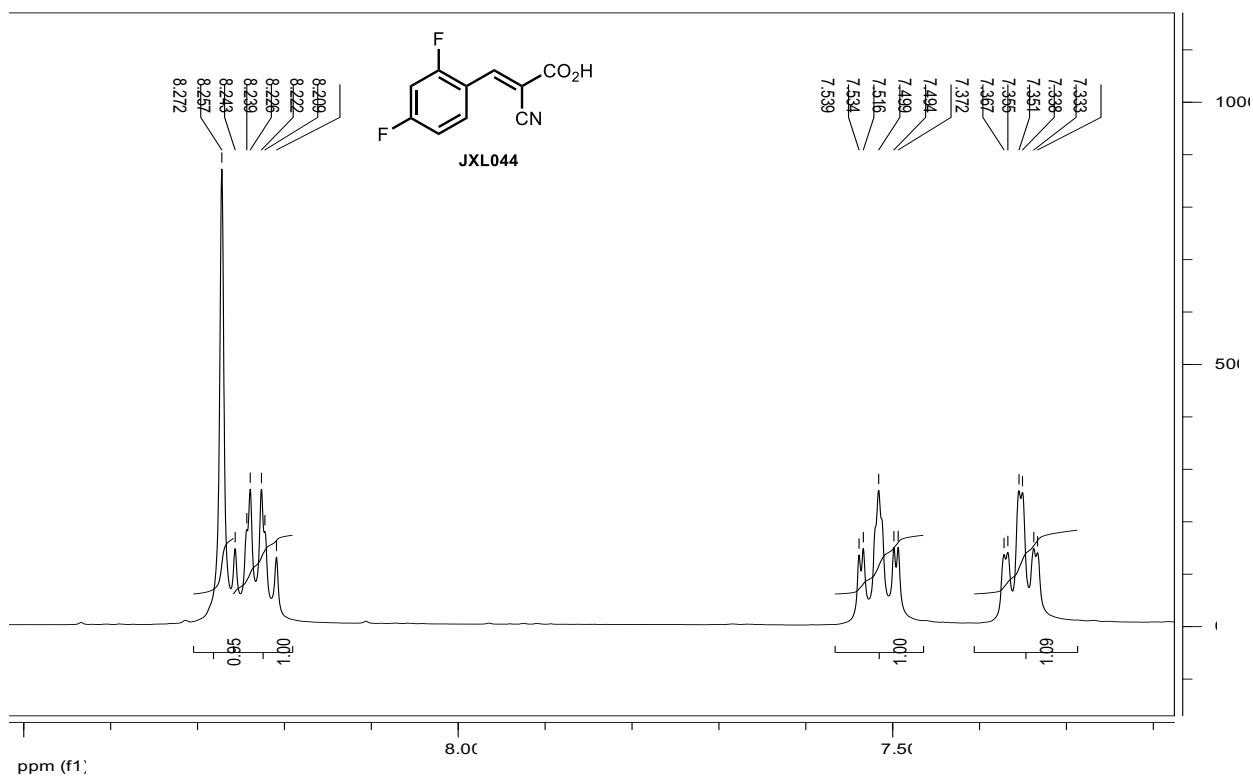
¹³C NMR (126 MHz, DMSO-d₆)



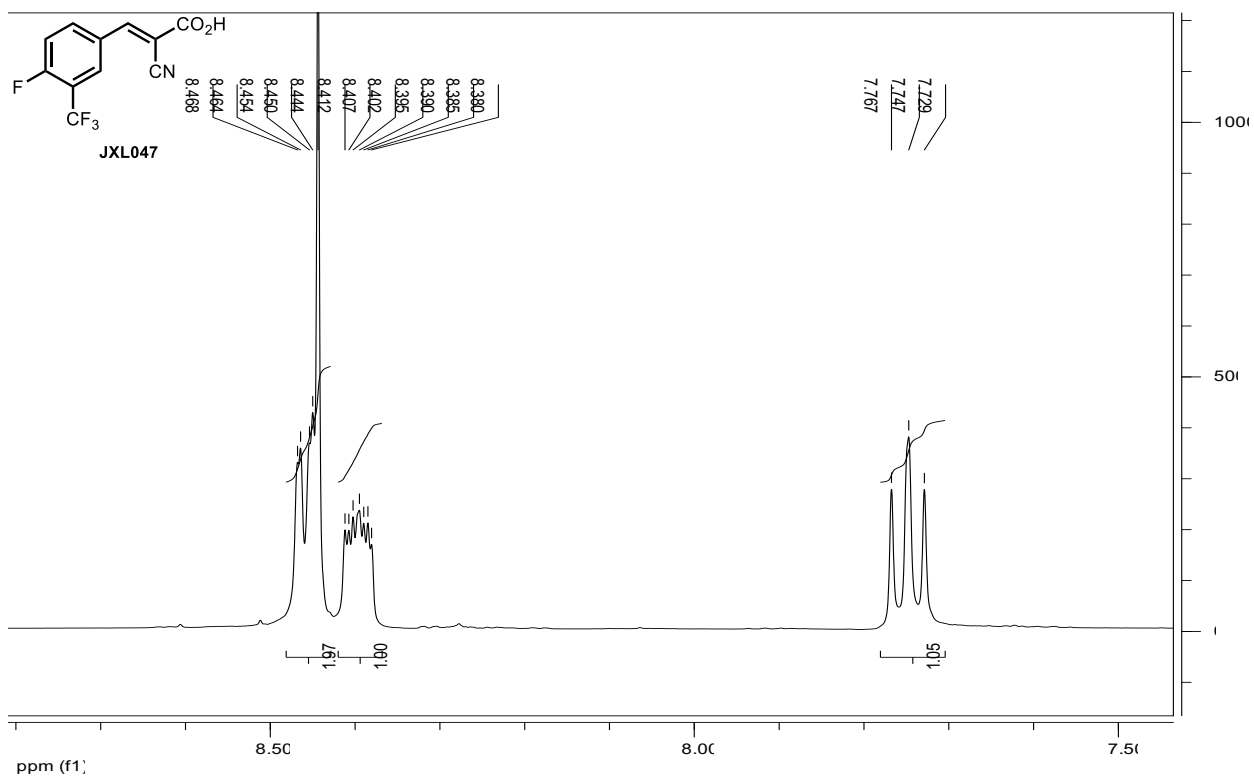
¹H NMR (500 MHz, DMSO-d₆)



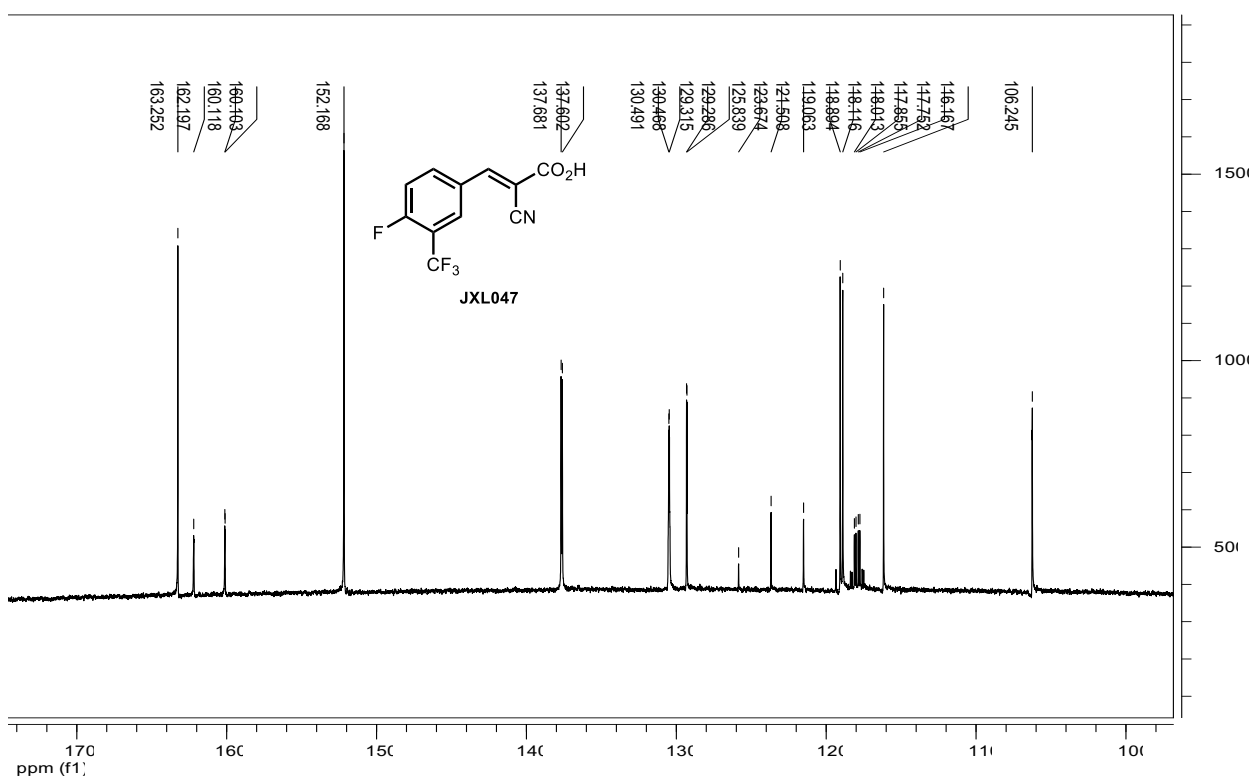
¹³C NMR (126 MHz, DMSO-d₆)



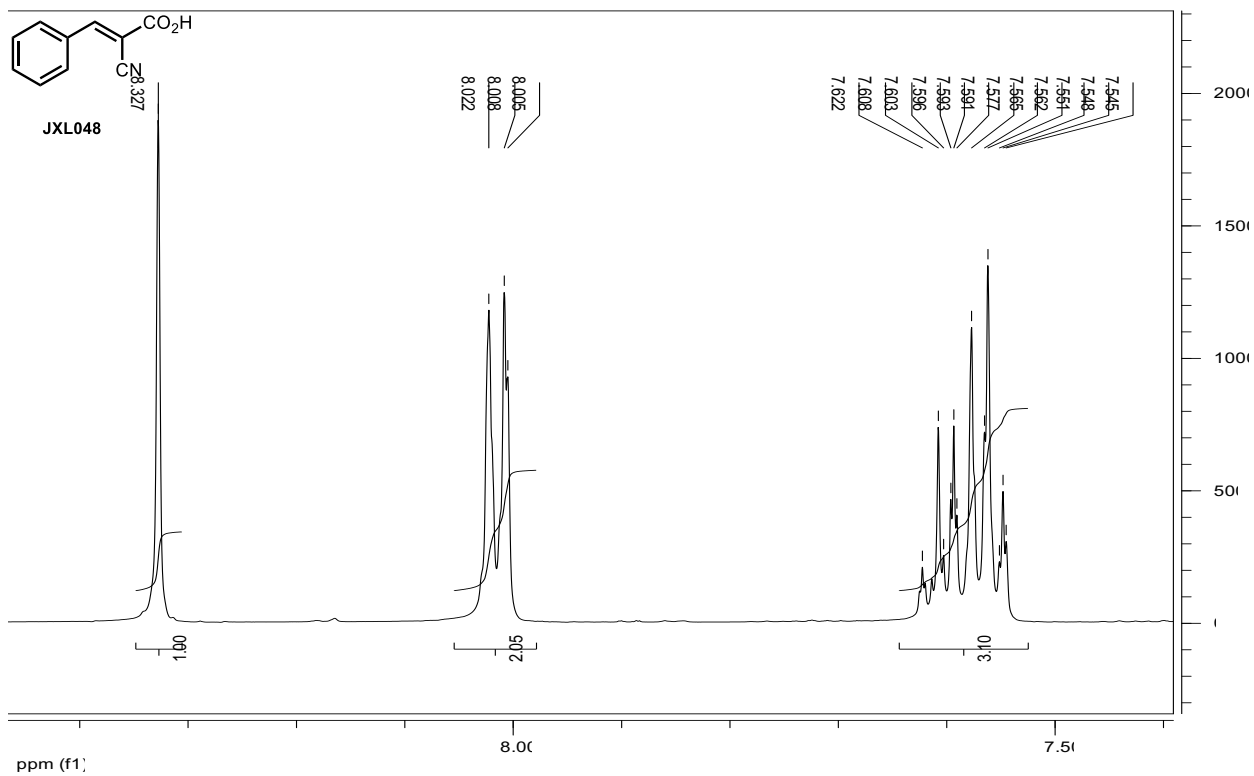
¹³C NMR (126 MHz, DMSO-d₆)



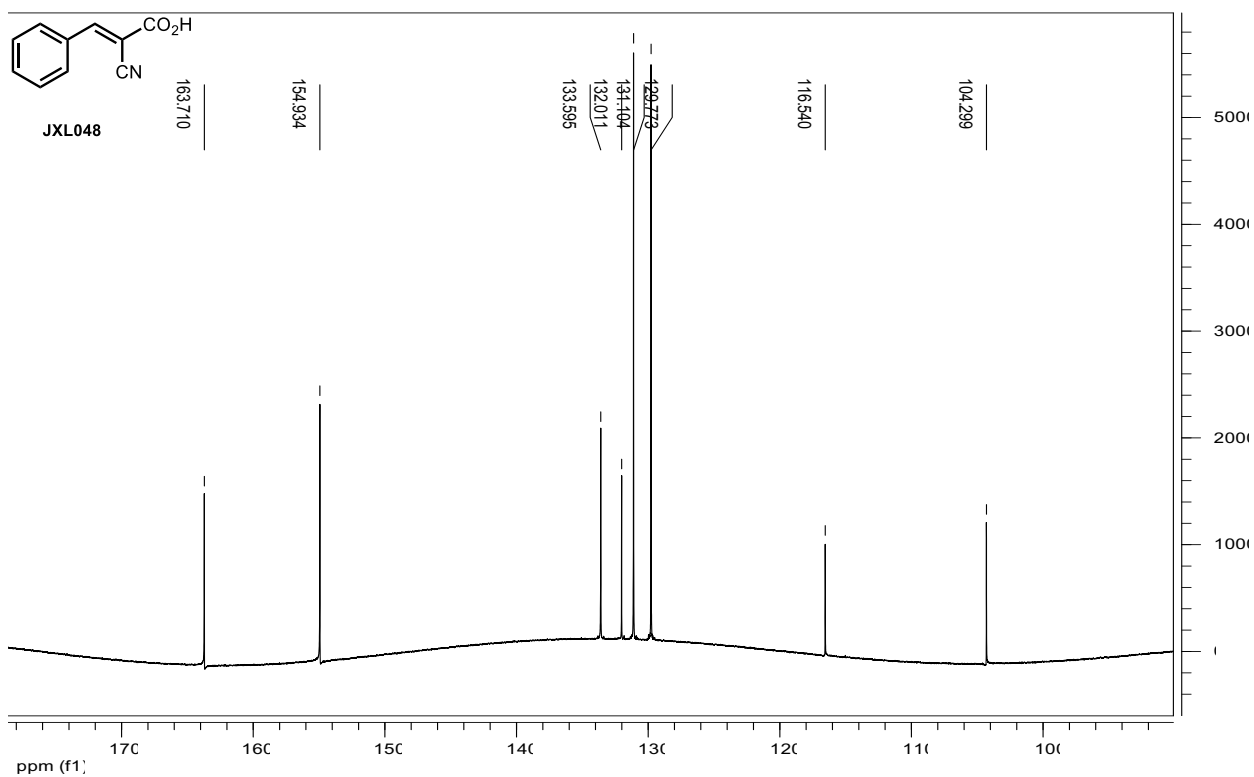
¹H NMR (500 MHz, DMSO-d₆)



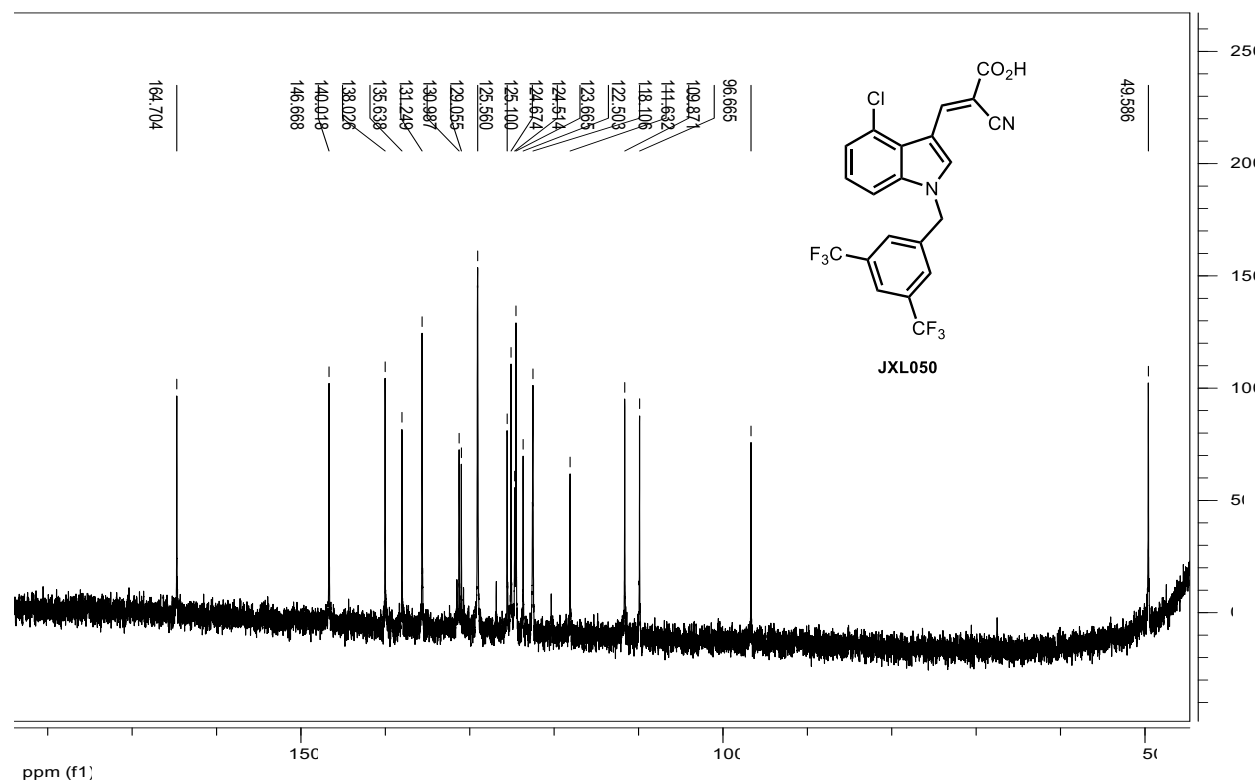
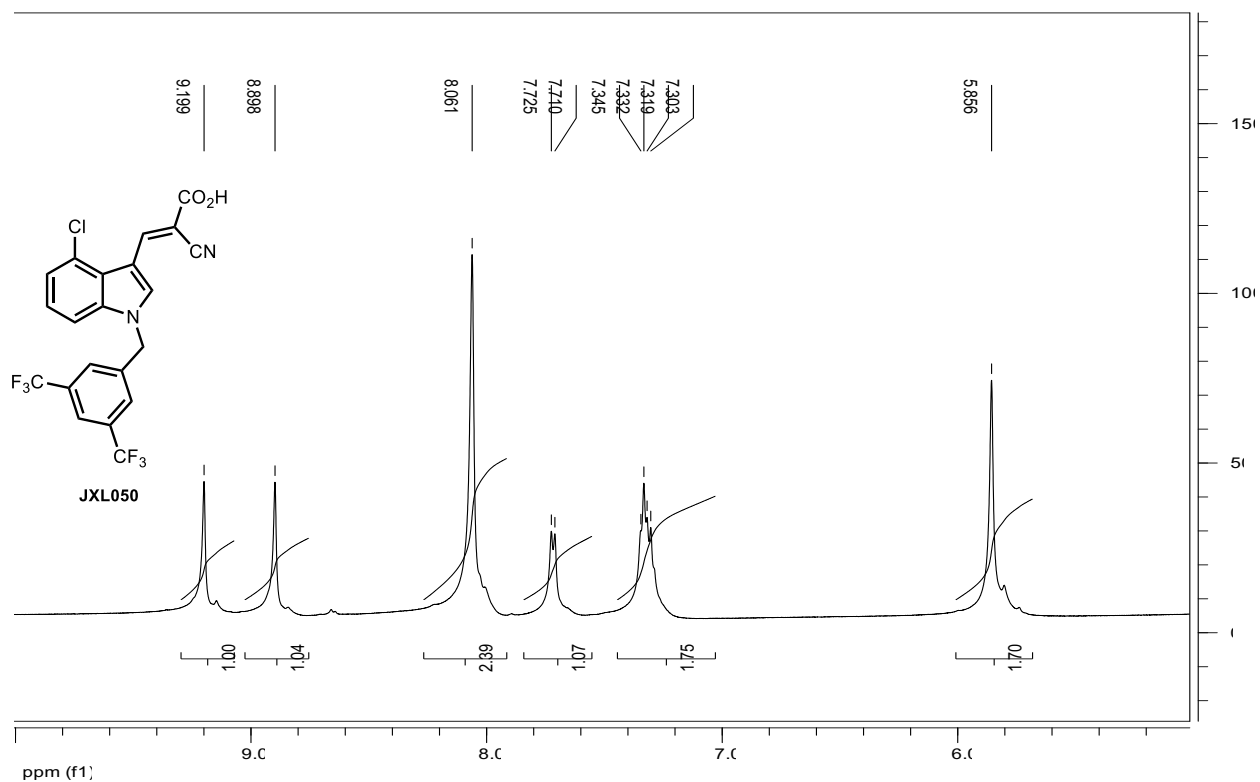
¹³C NMR (126 MHz, DMSO-d₆)



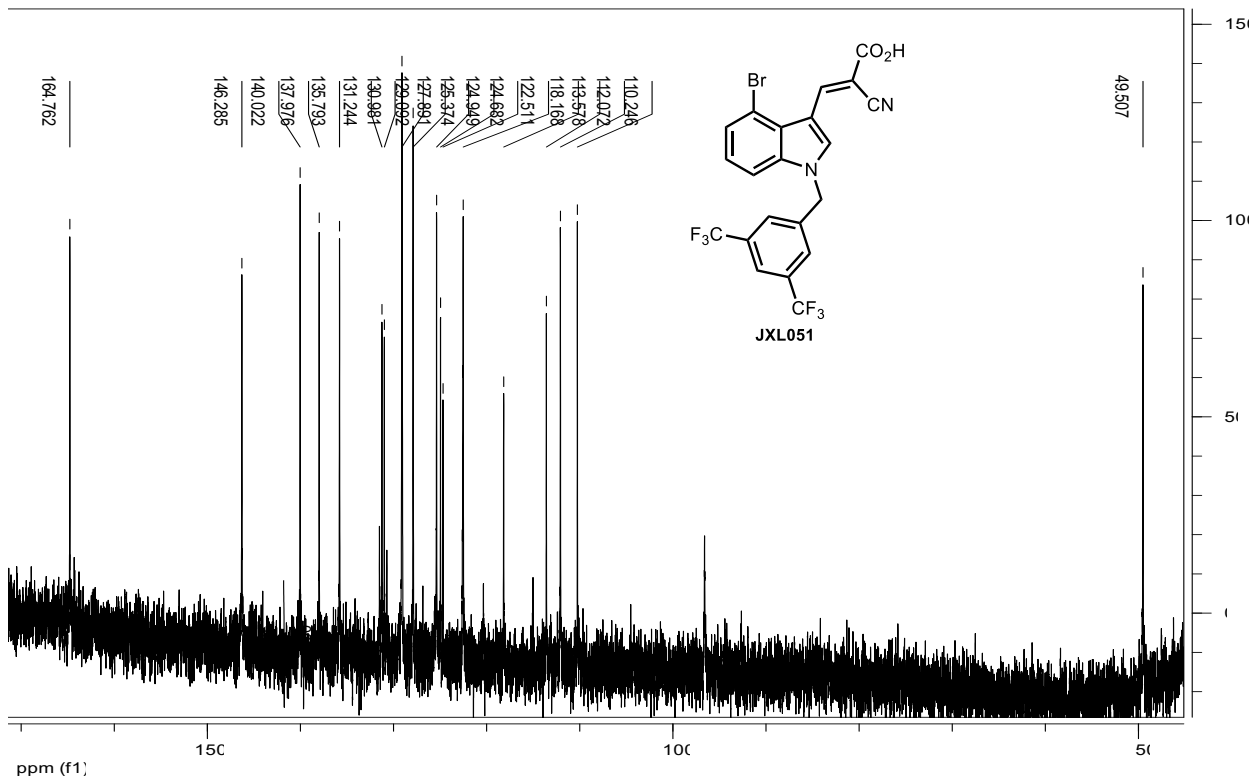
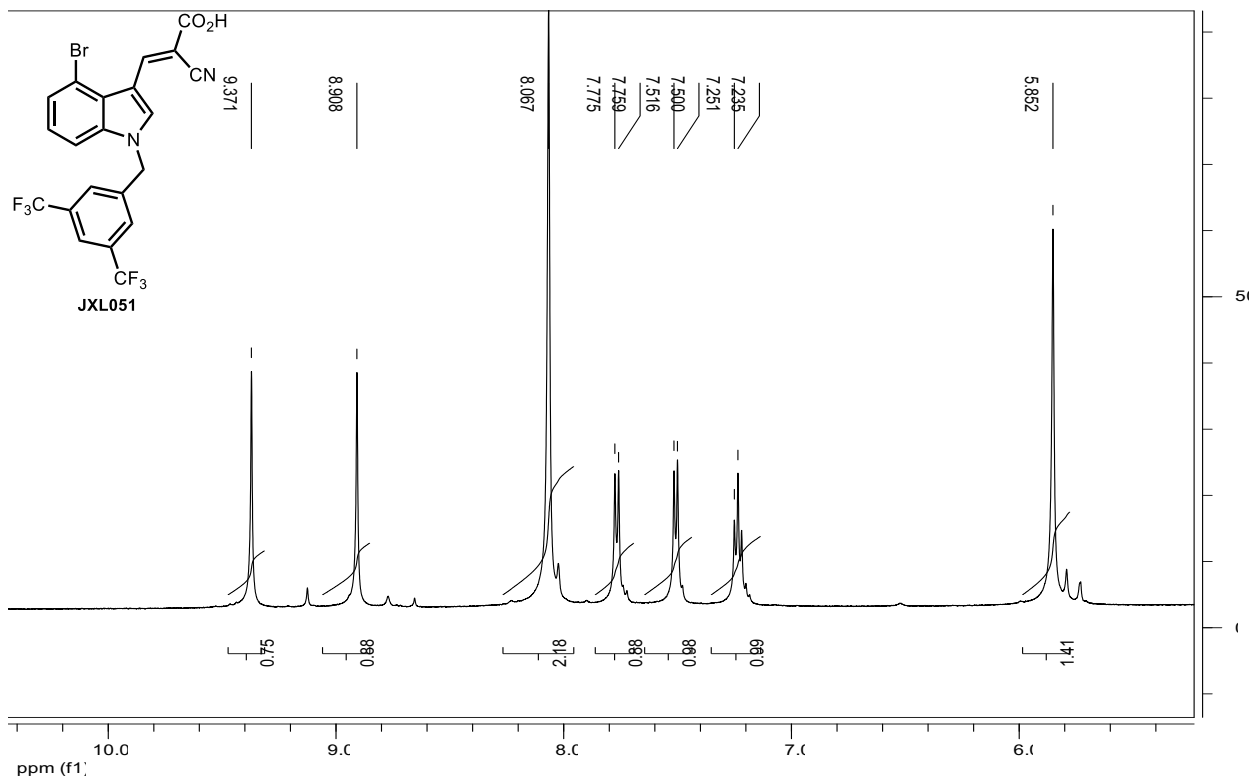
¹H NMR (500 MHz, DMSO-d₆)



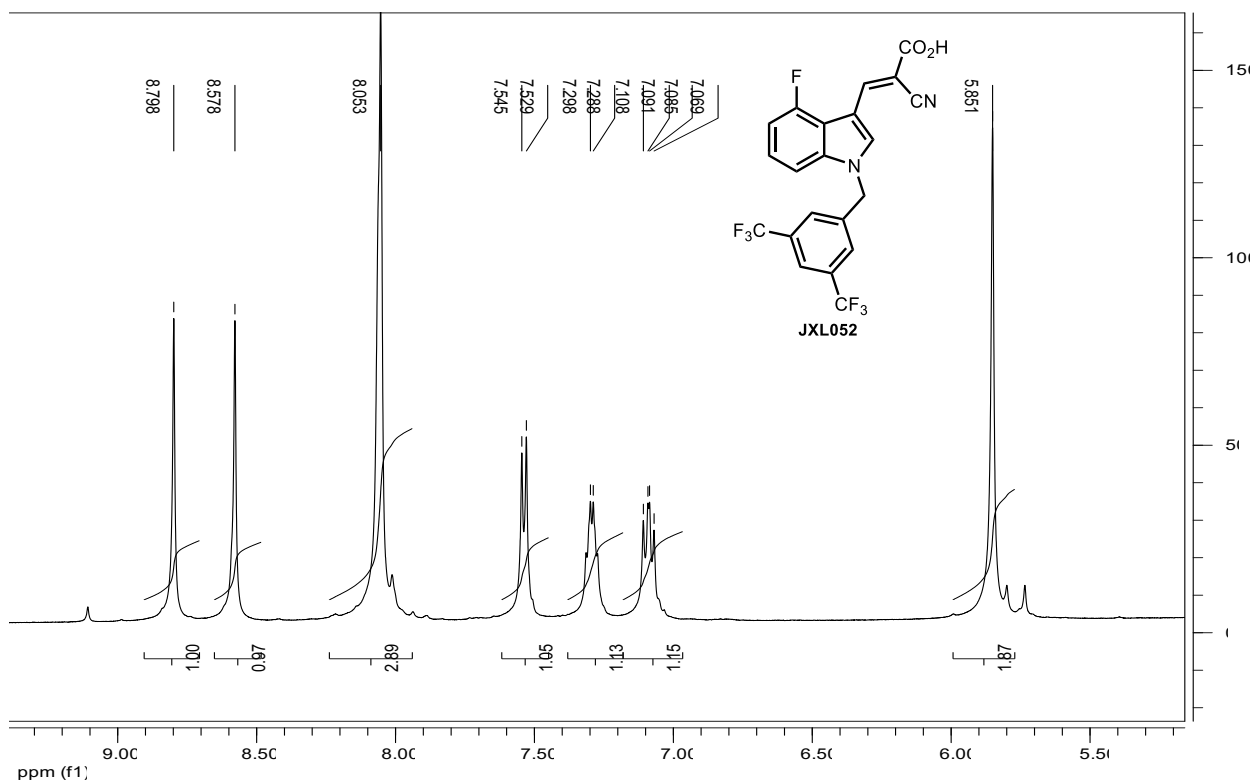
¹³C NMR (126 MHz, DMSO-d₆)



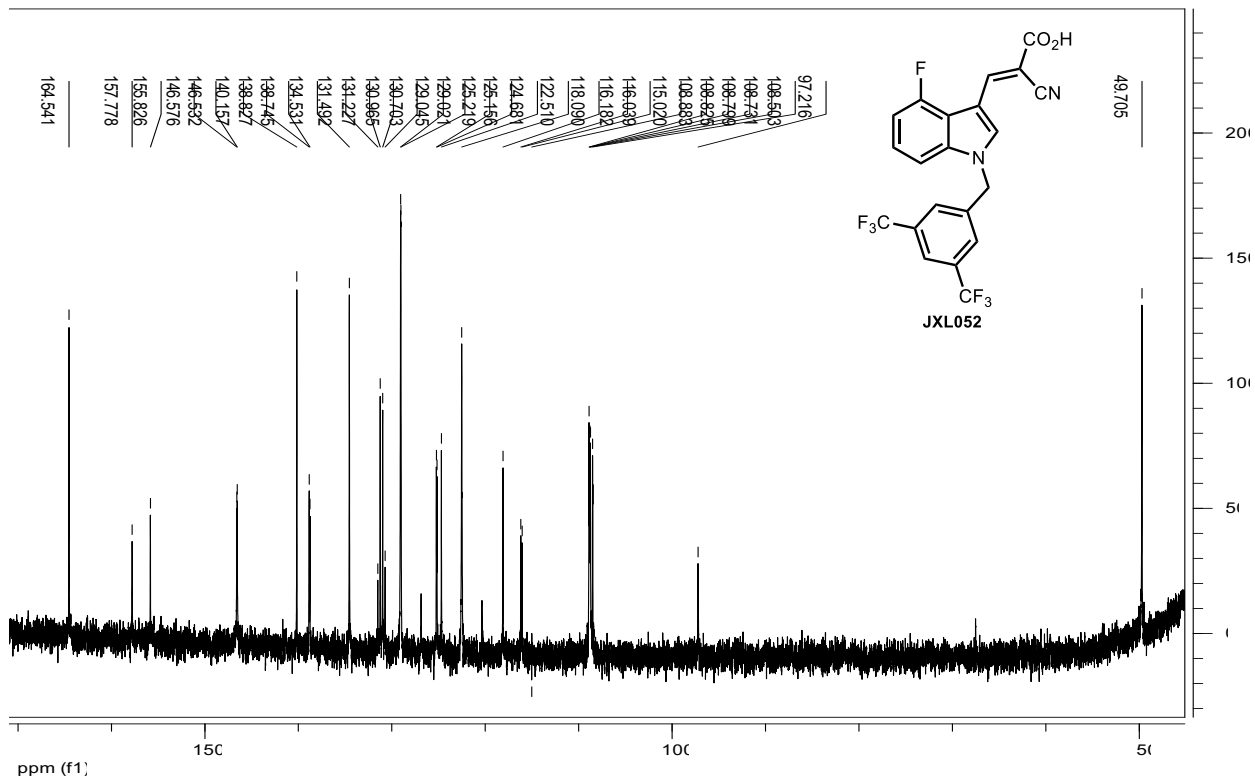
¹³C NMR (126 MHz, DMSO-d₆)



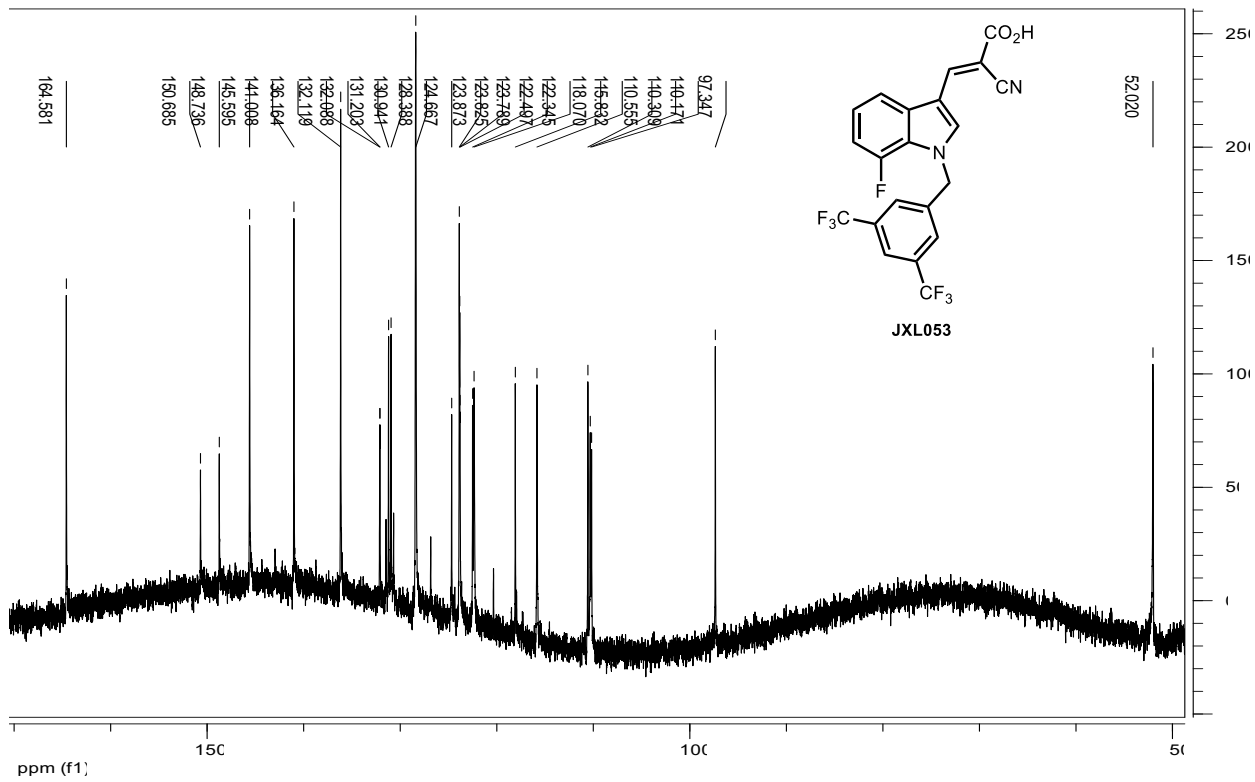
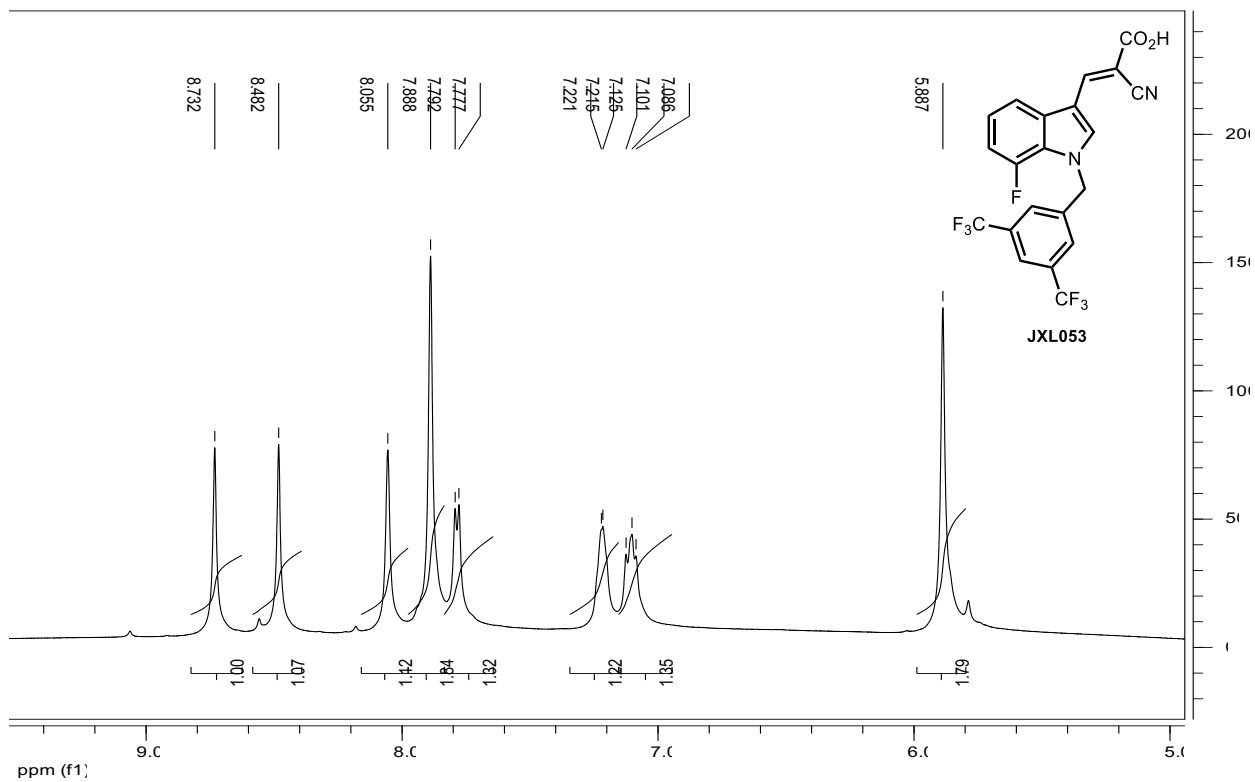
¹³C NMR (126 MHz, DMSO-d₆)

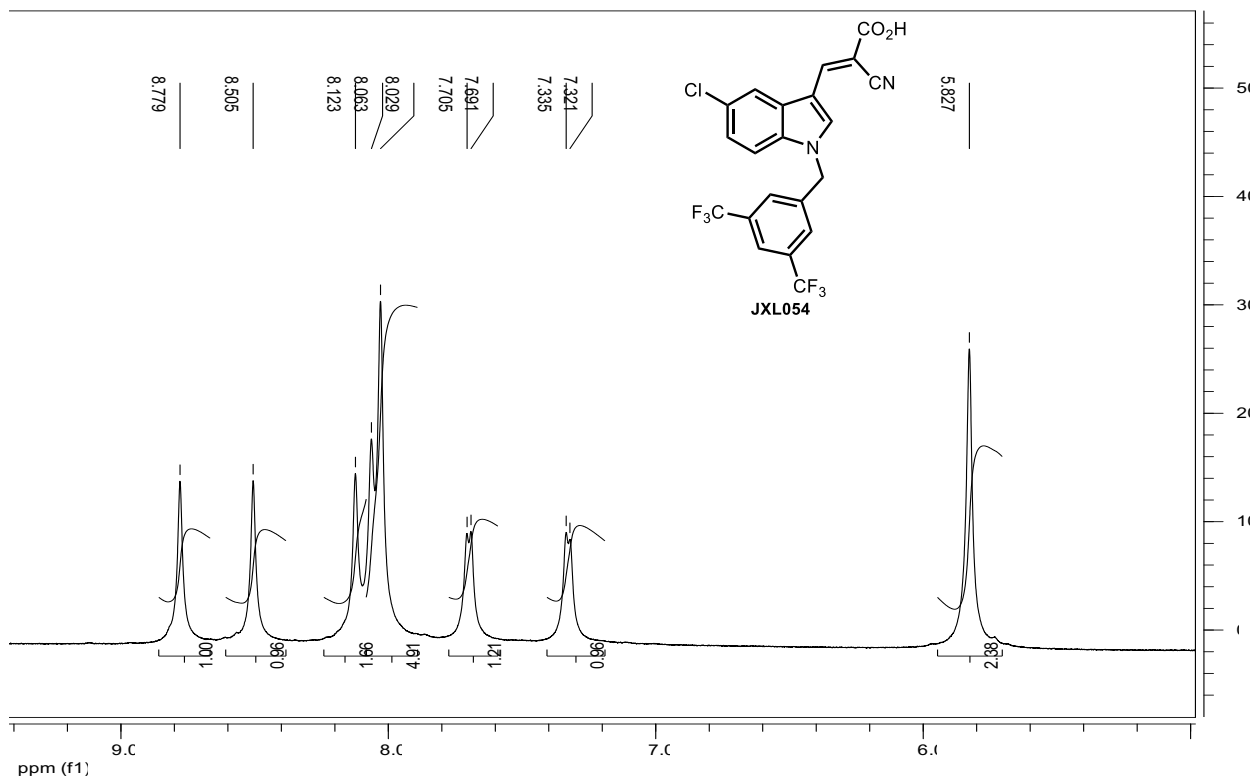


¹H NMR (500 MHz, DMSO-d₆)

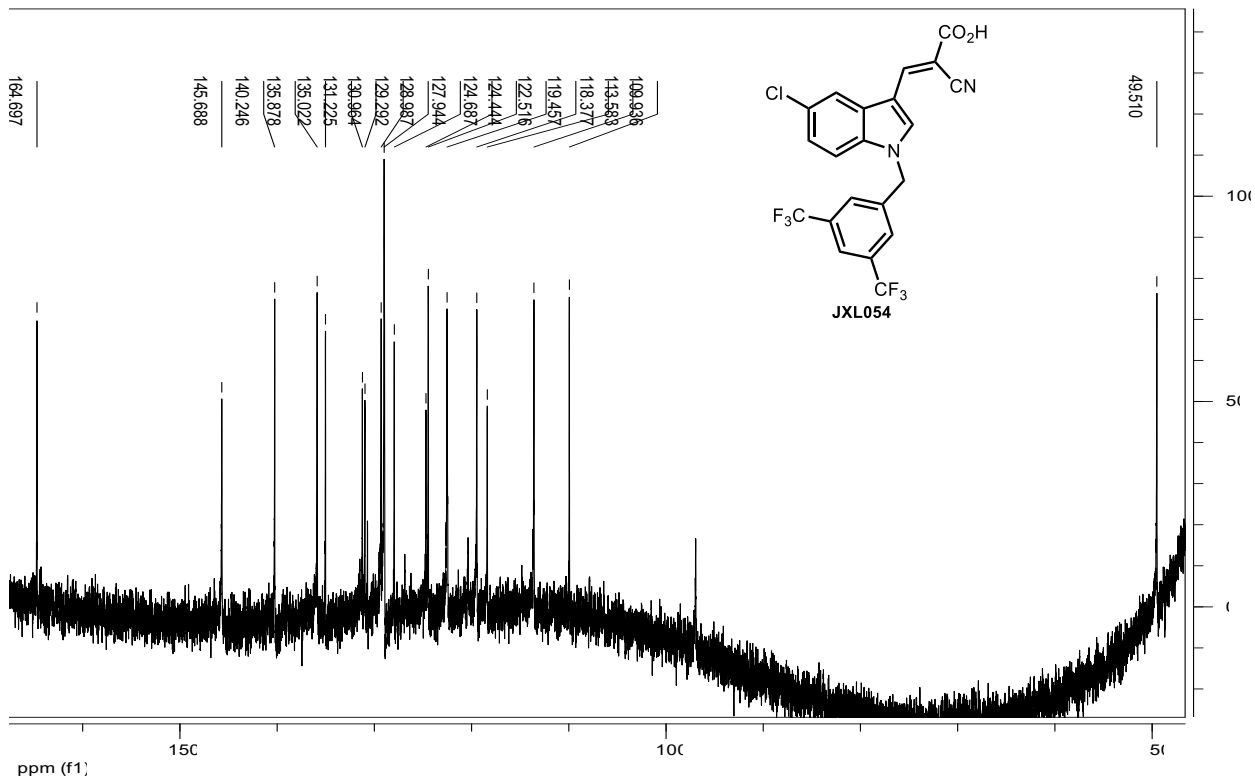


¹³C NMR (126 MHz, DMSO-d₆)

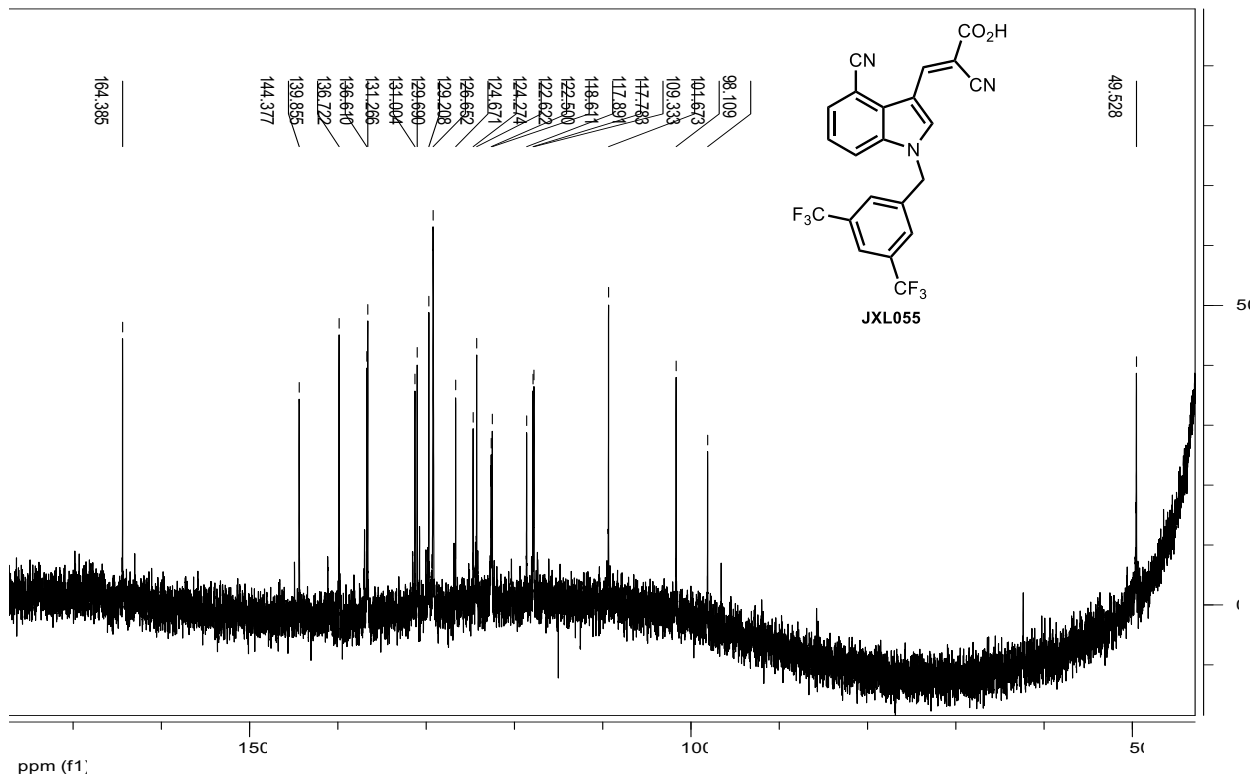
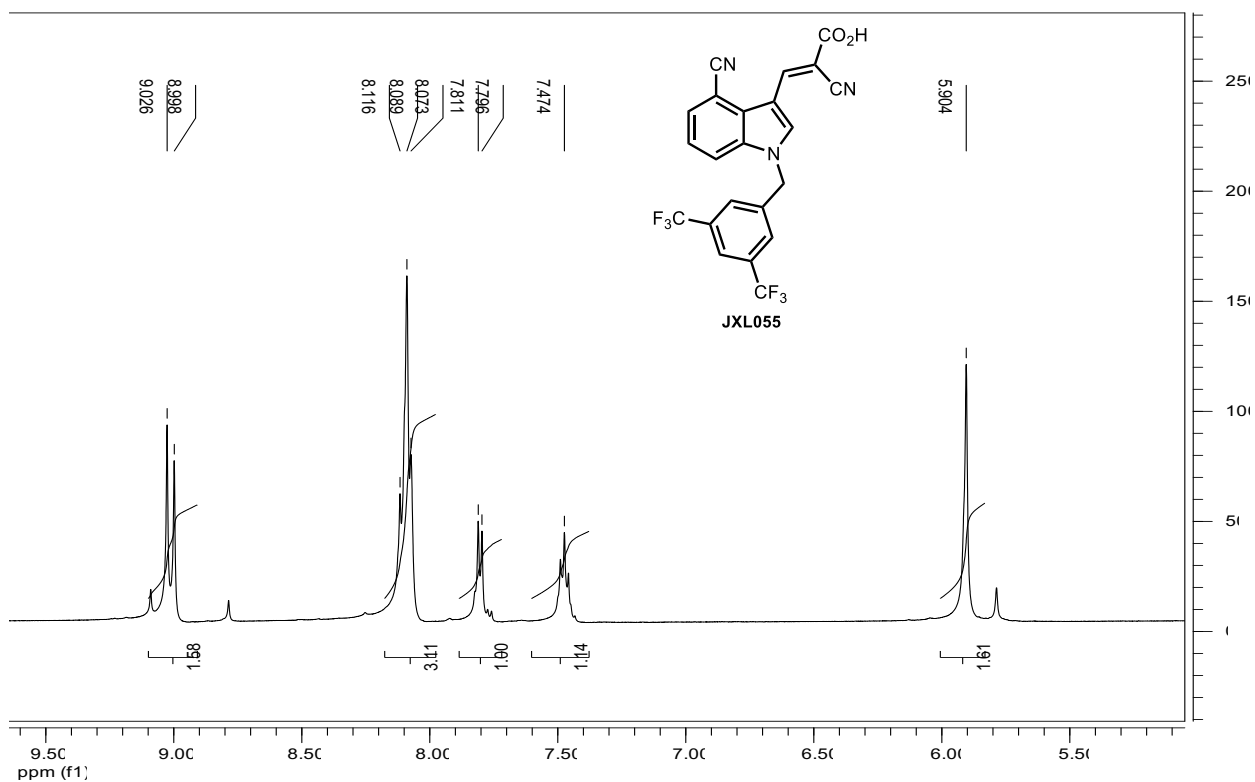




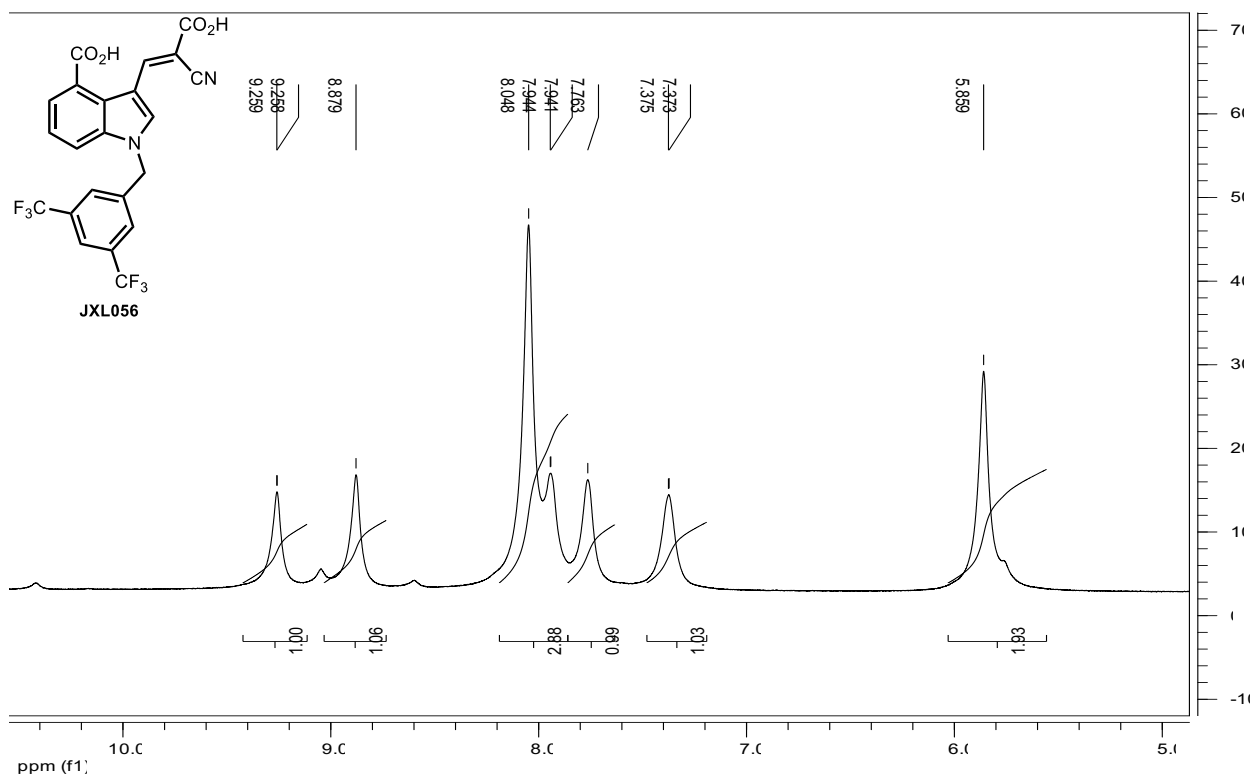
¹H NMR (500 MHz, DMSO-d₆)



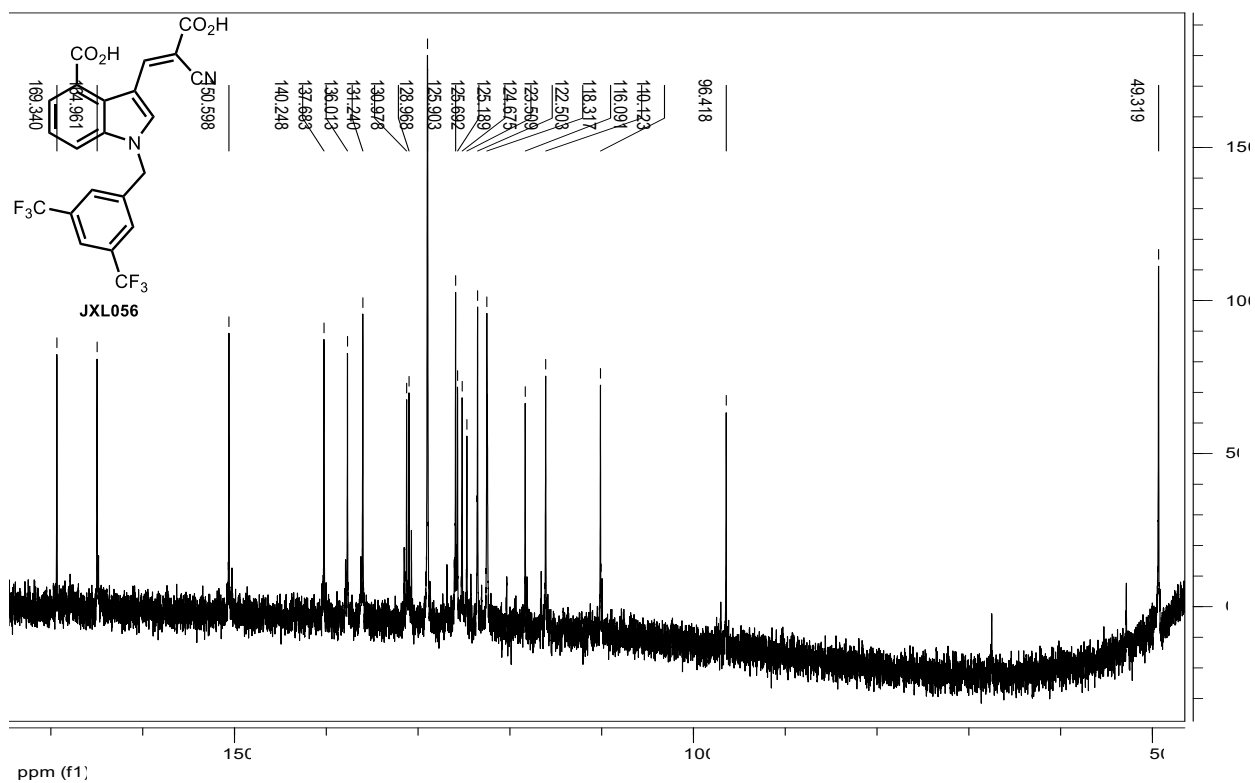
¹³C NMR (126 MHz, DMSO-d₆)



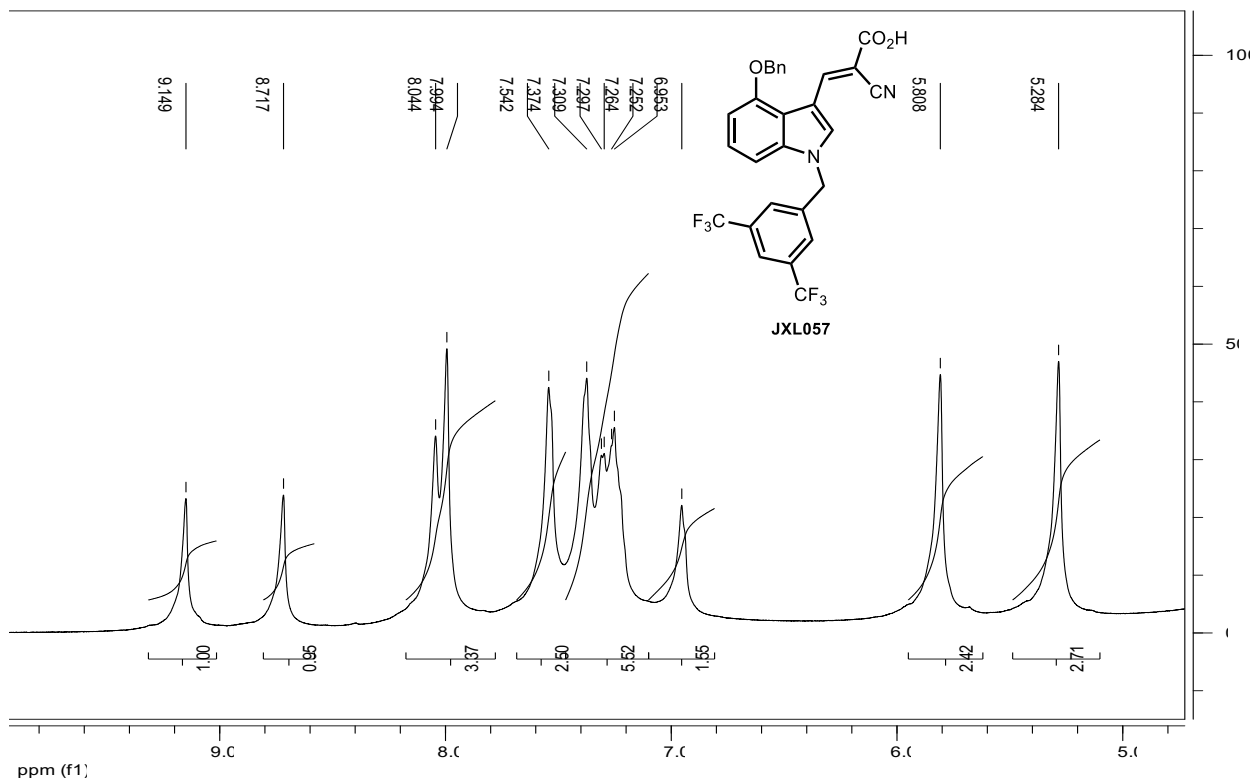
¹³C NMR (126 MHz, DMSO-d₆)



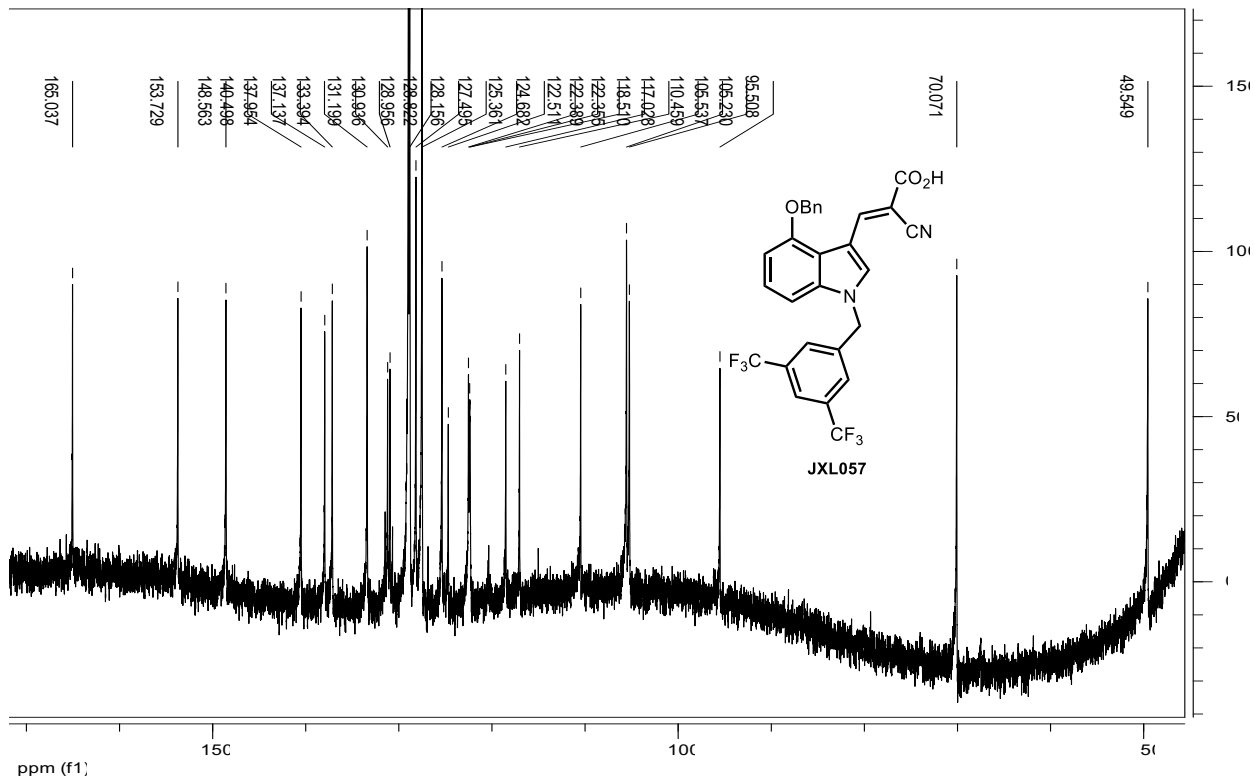
¹H NMR (500 MHz, DMSO-d₆)



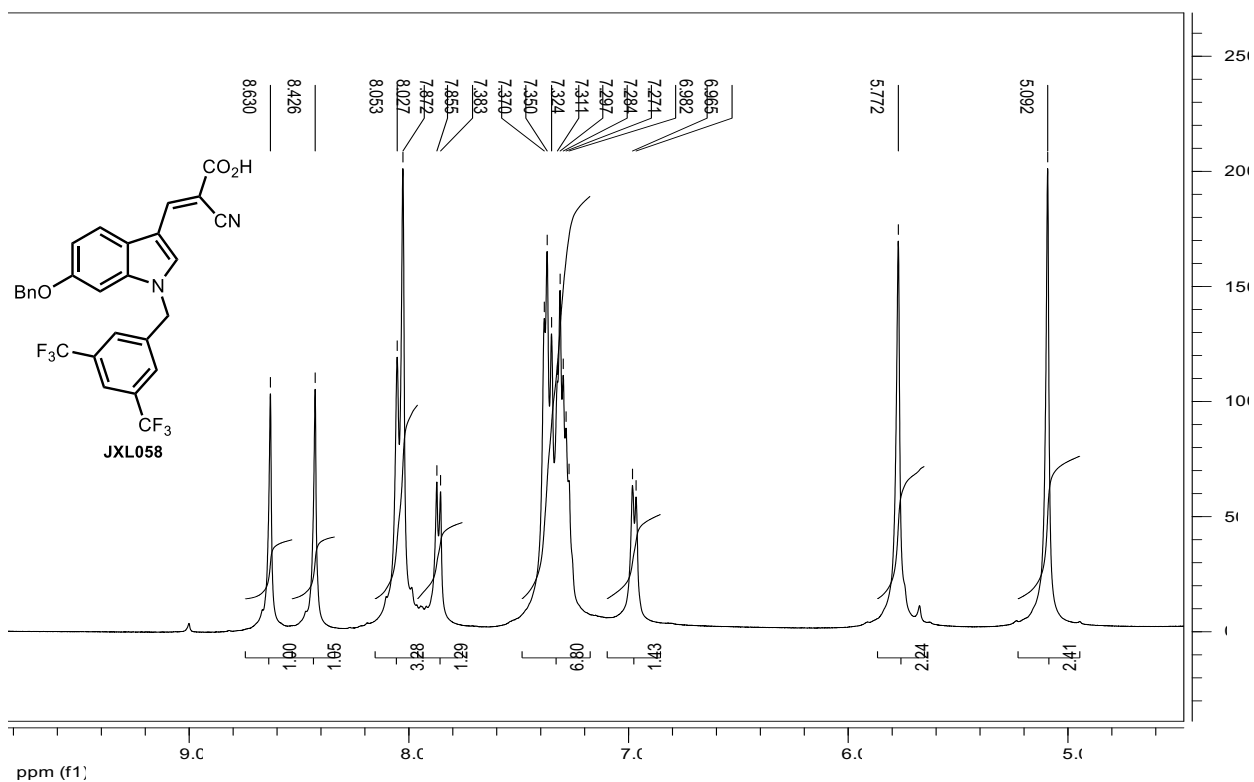
¹³C NMR (126 MHz, DMSO-d₆)



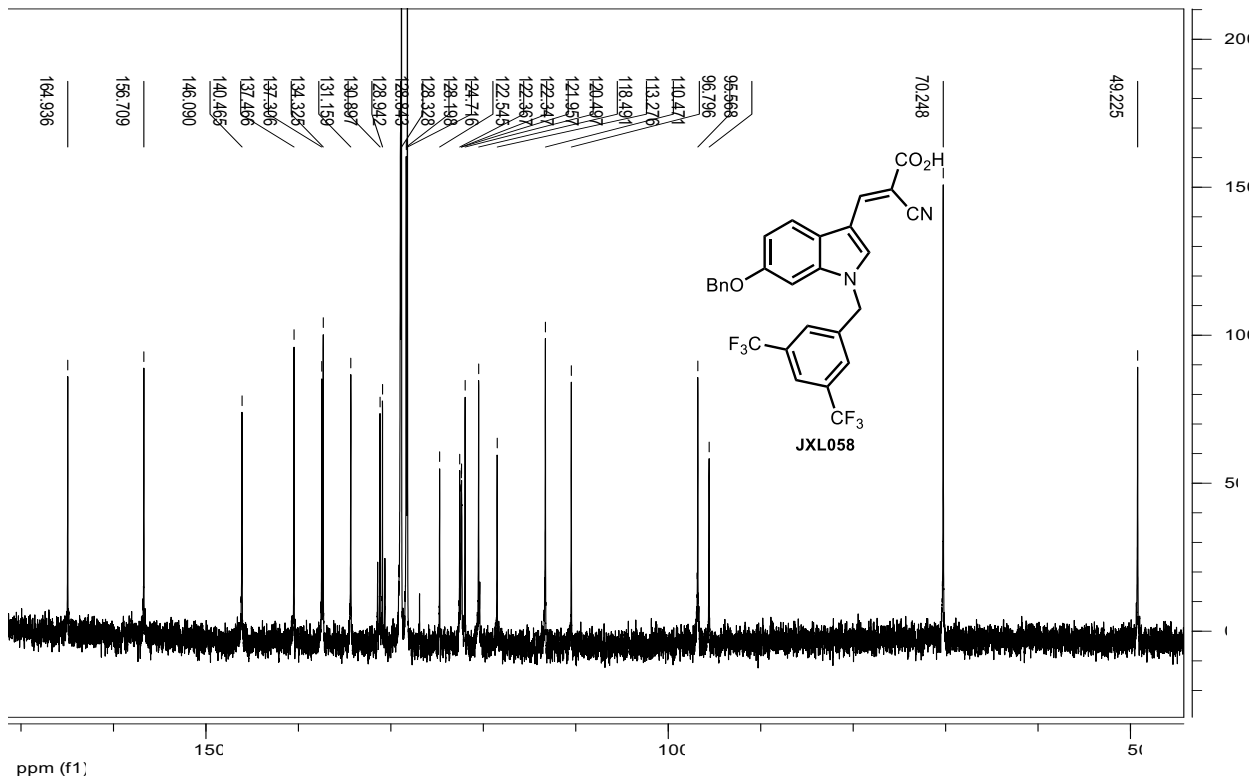
¹H NMR (500 MHz, DMSO-d₆)



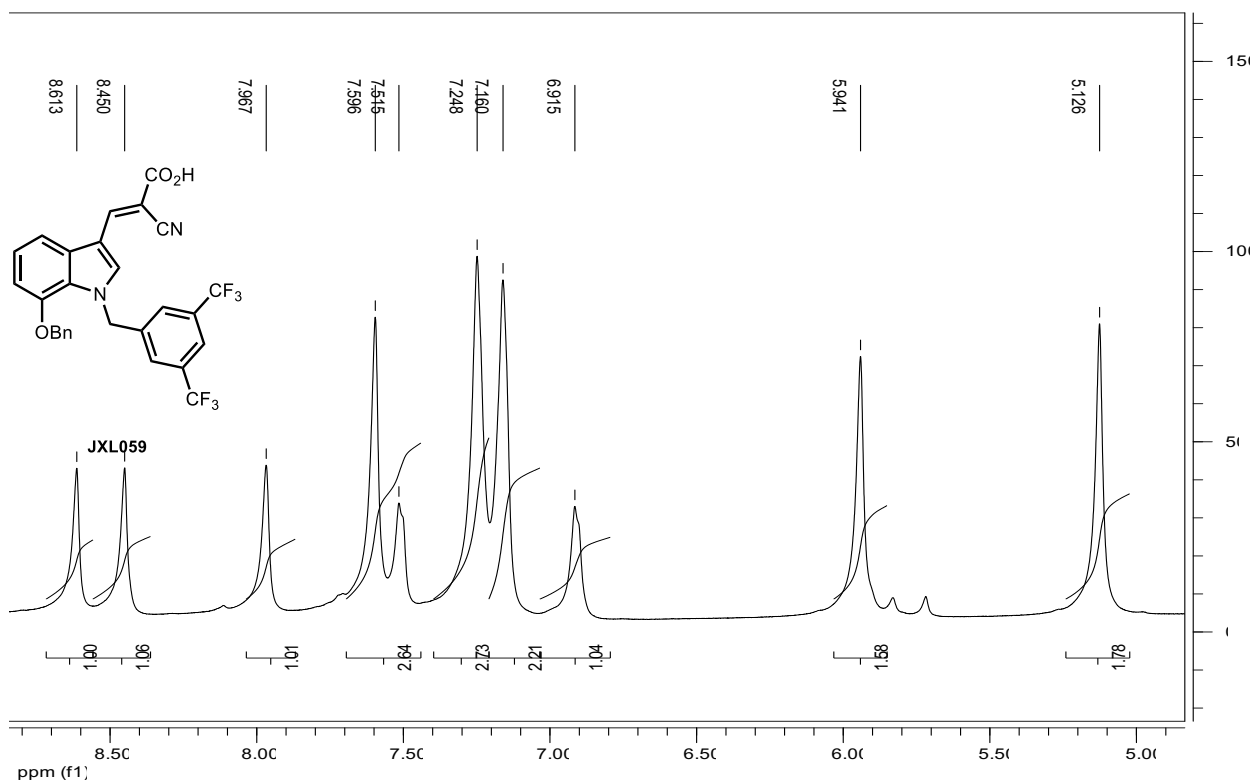
¹³C NMR (126 MHz, DMSO-d₆)



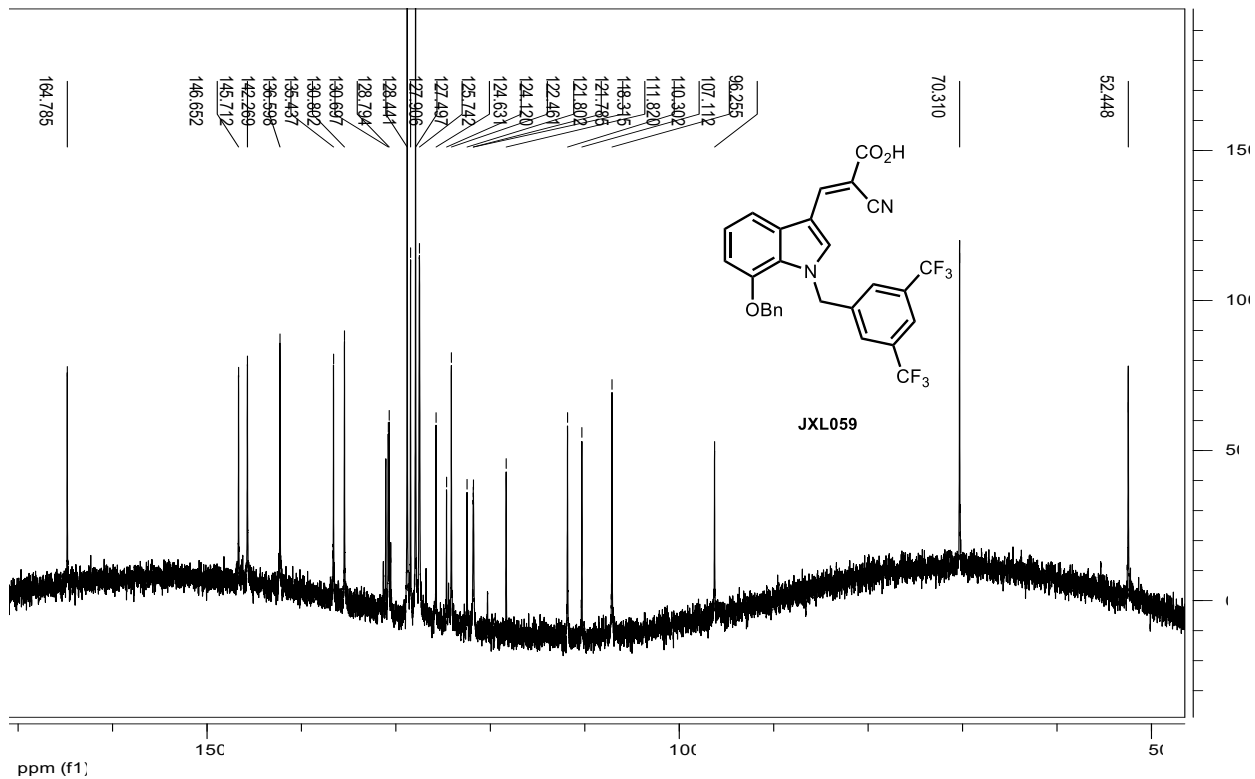
¹H NMR (500 MHz, DMSO-d₆)



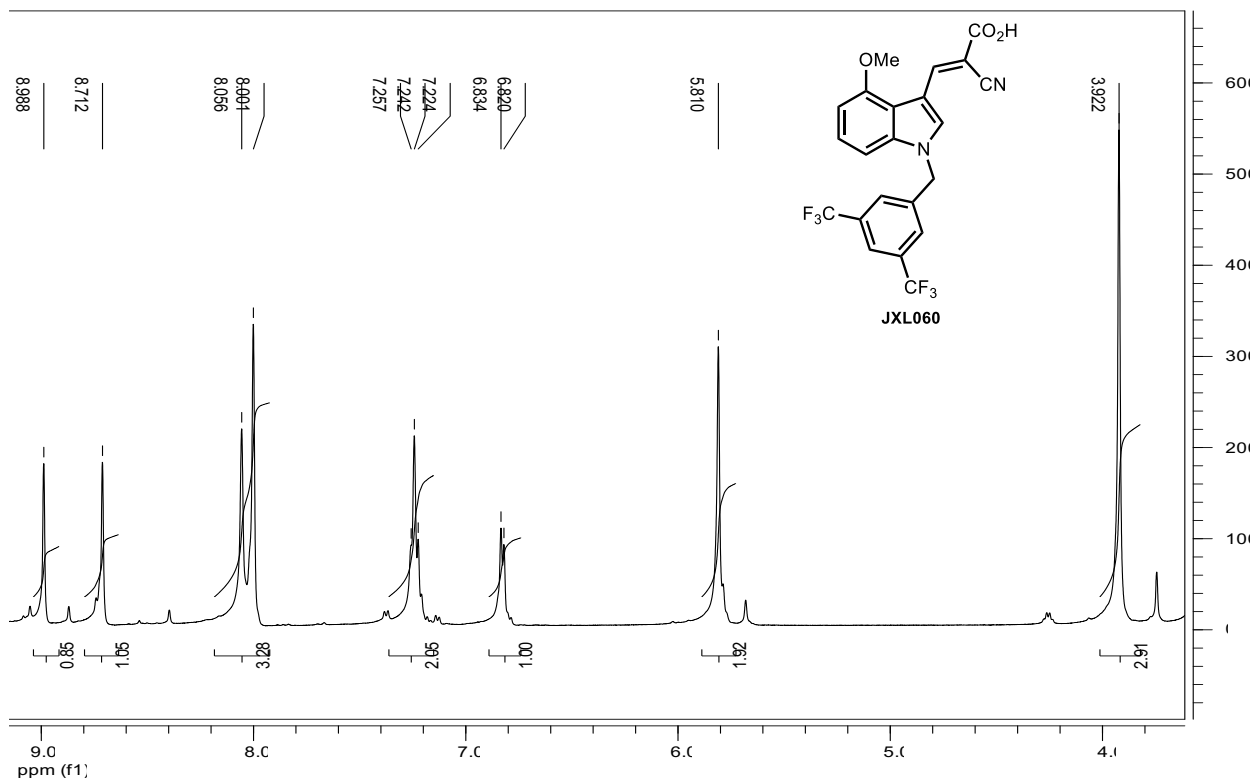
¹³C NMR (126 MHz, DMSO-d₆)



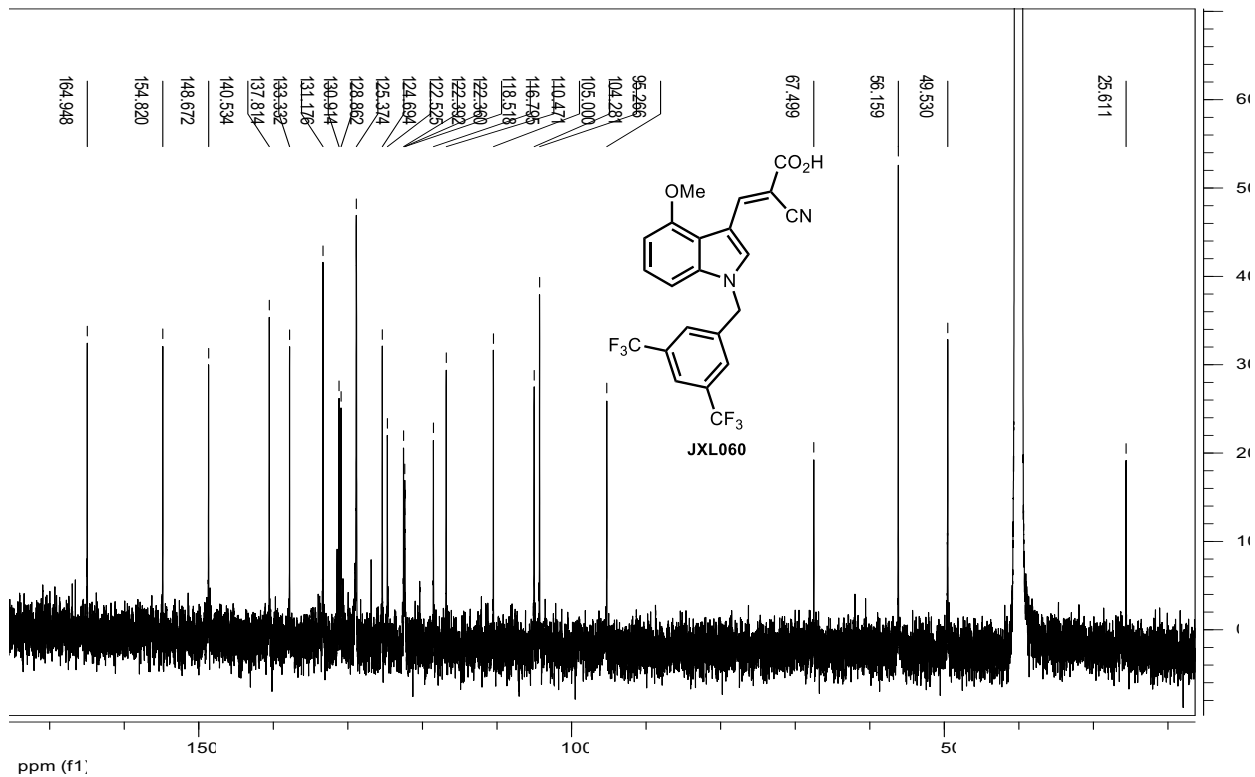
¹H NMR (500 MHz, DMSO-d₆)



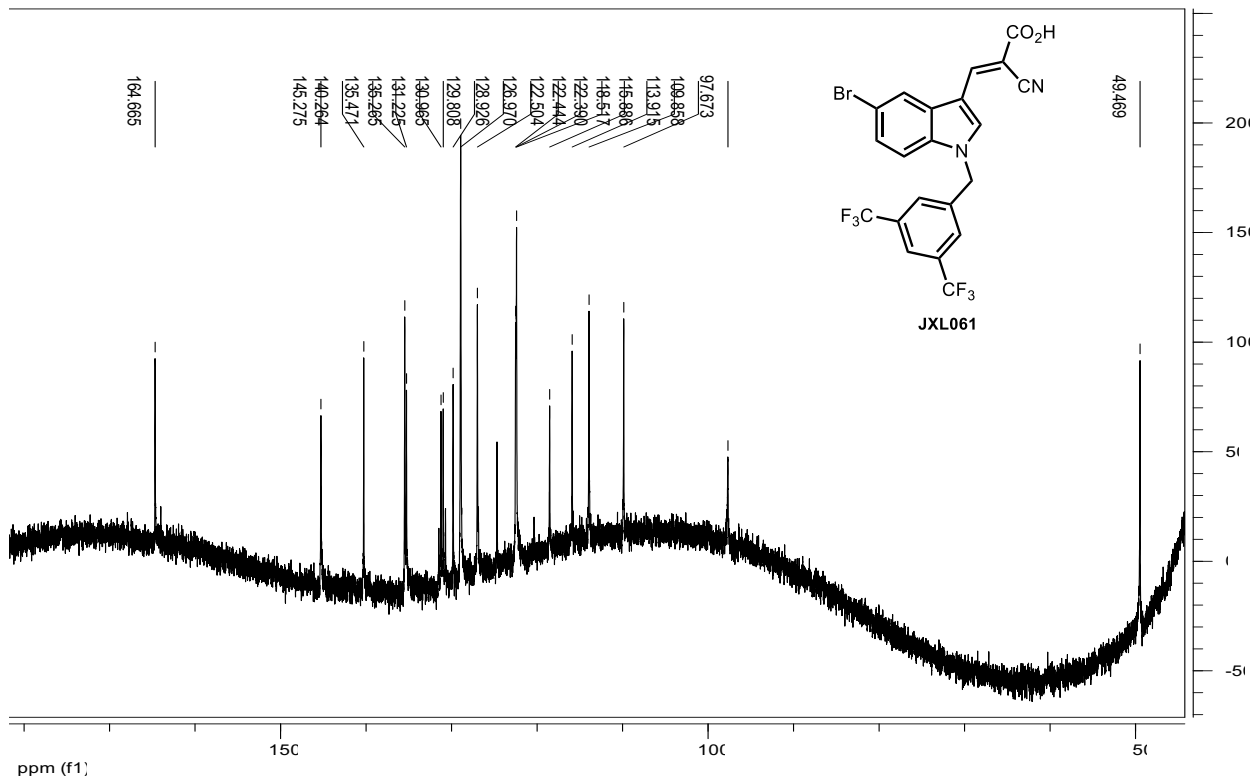
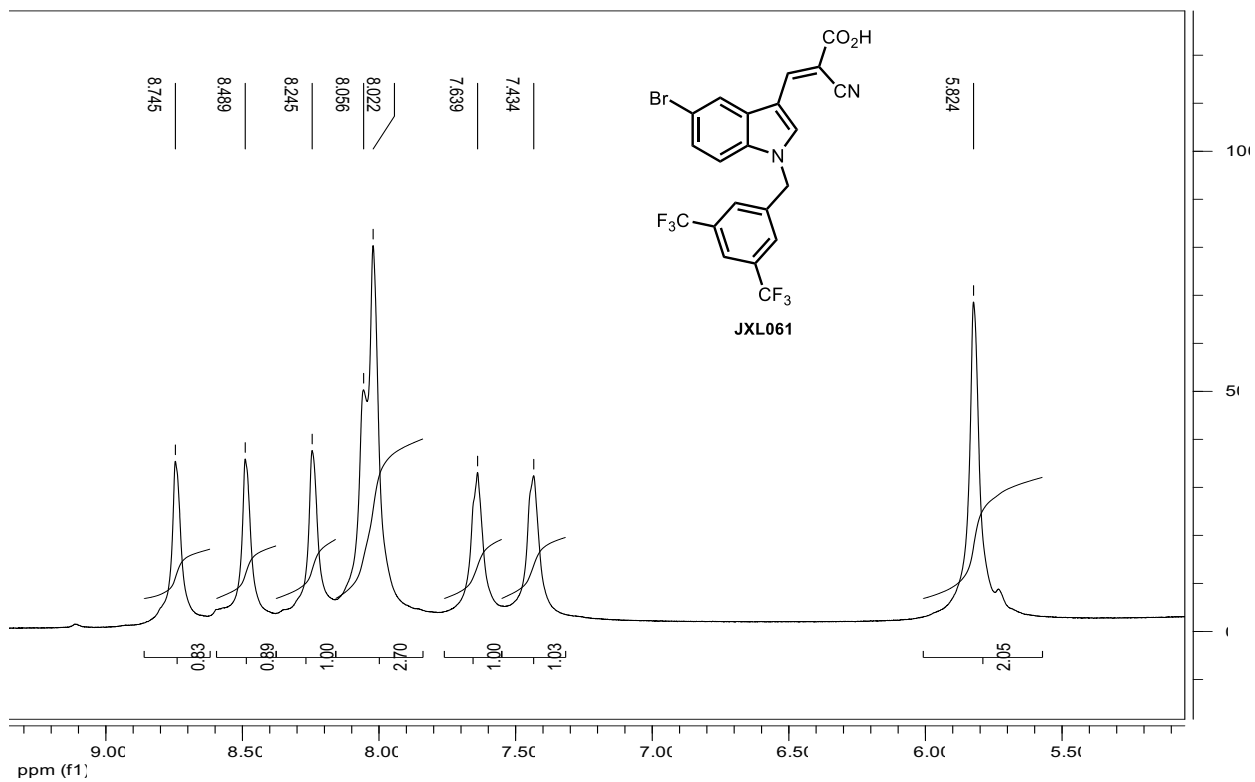
¹³C NMR (126 MHz, DMSO-d₆)



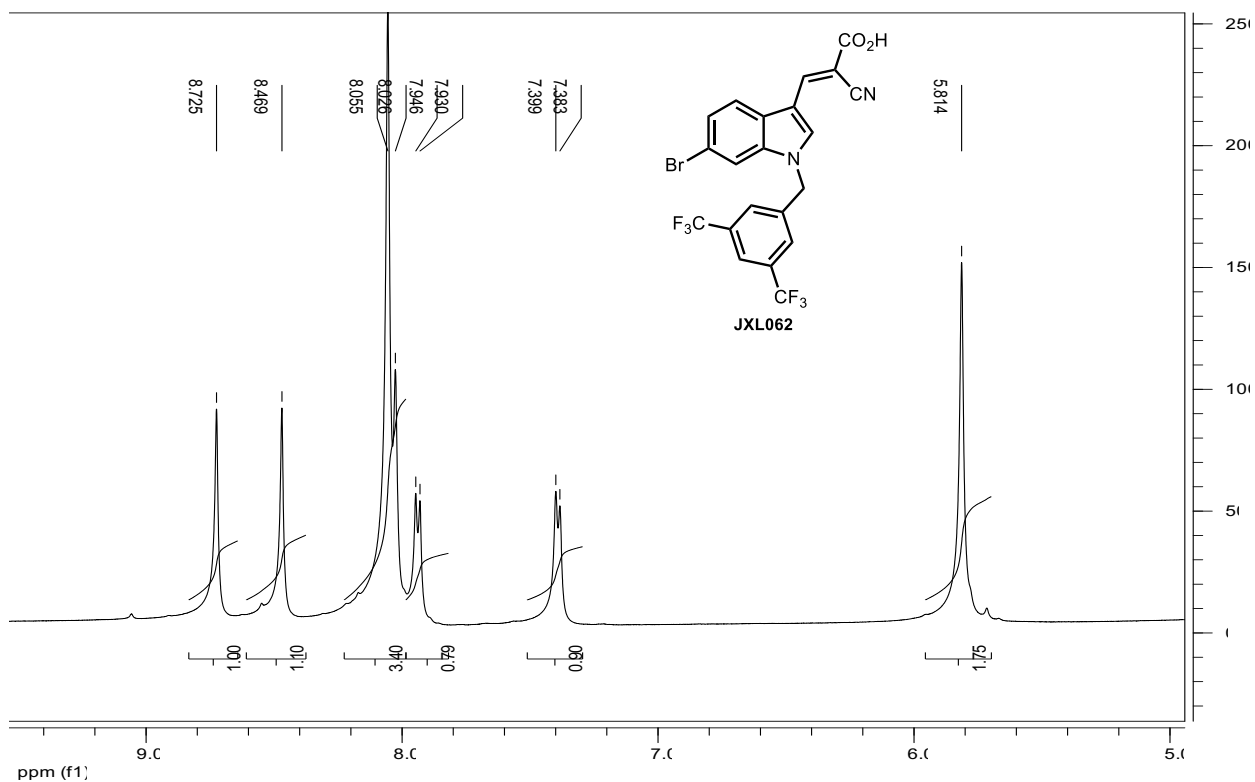
¹H NMR (500 MHz, DMSO-d₆)



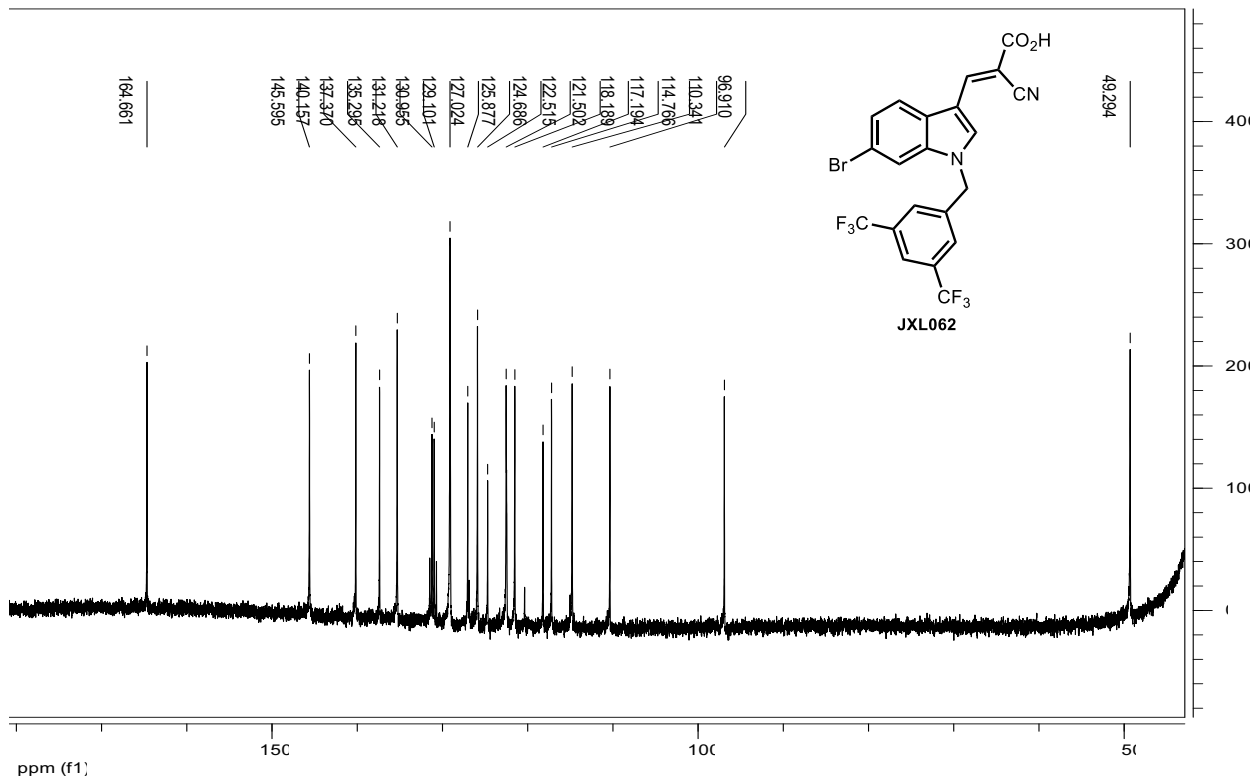
¹³C NMR (126 MHz, DMSO-d₆)



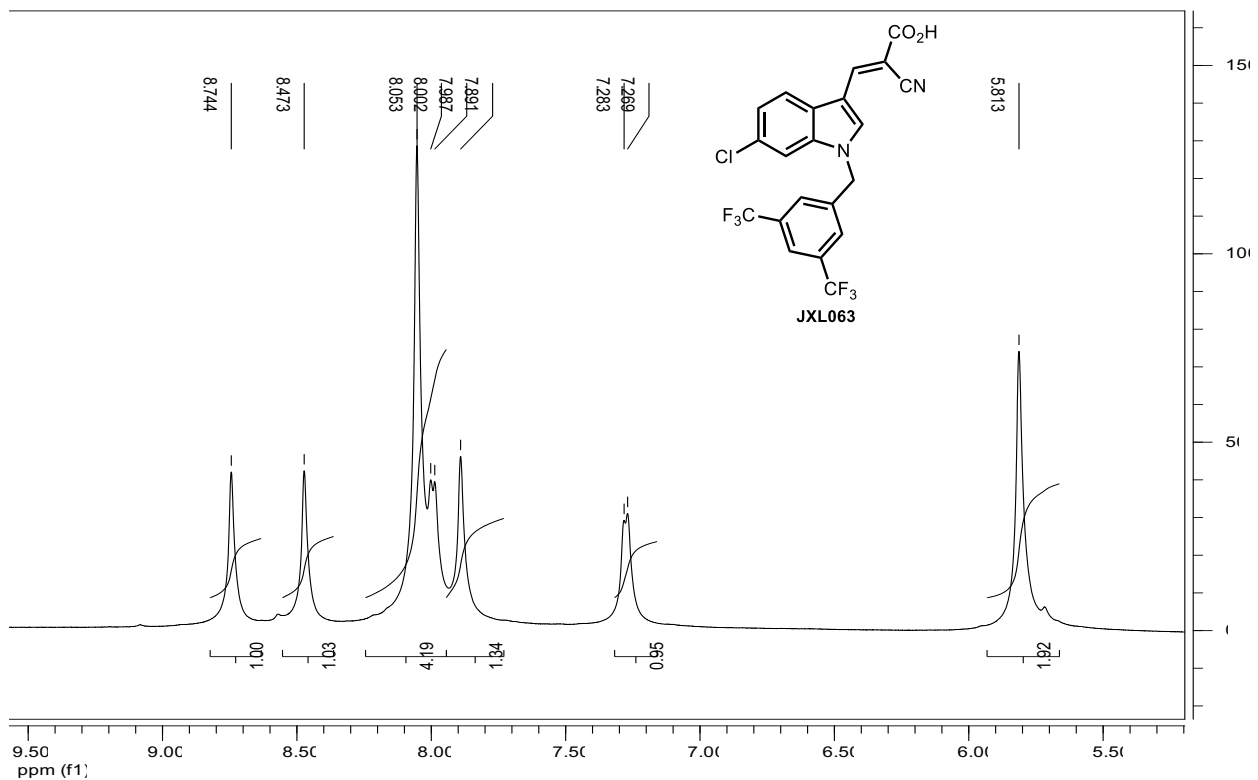
¹³C NMR (126 MHz, DMSO-d₆)



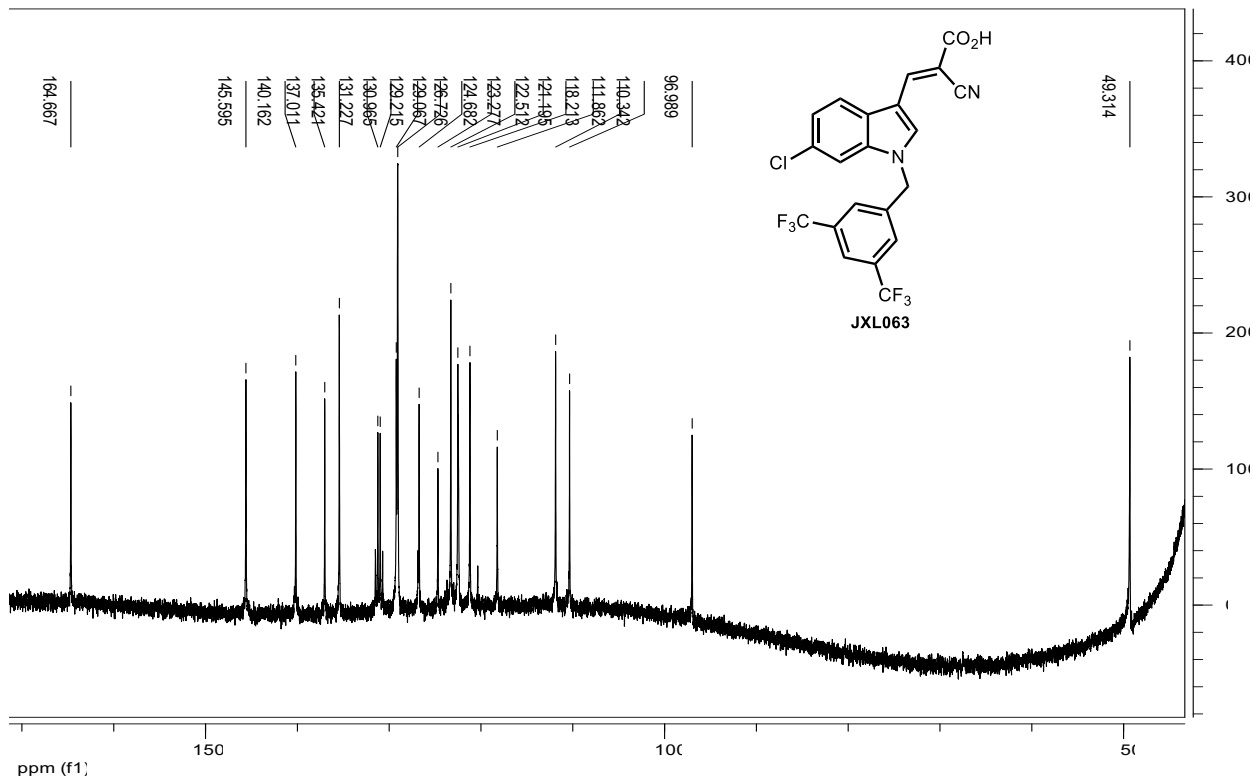
¹H NMR (500 MHz, DMSO-d₆)



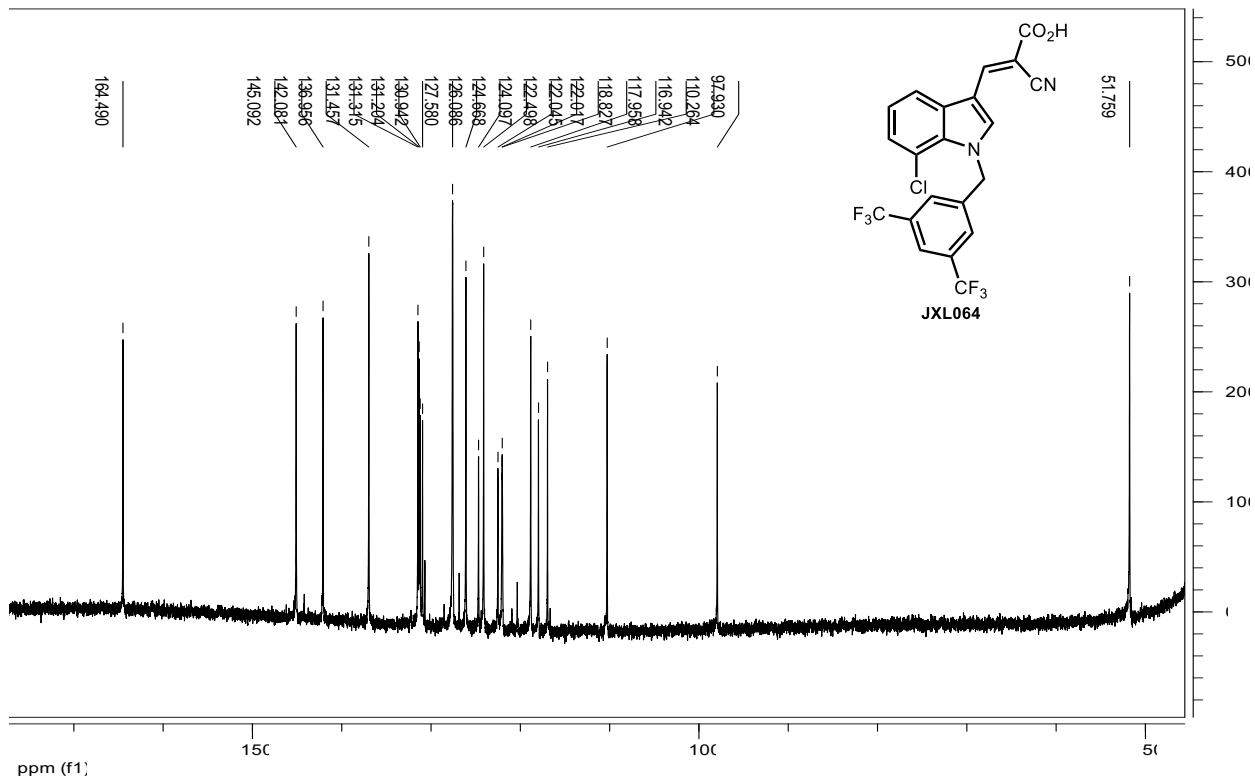
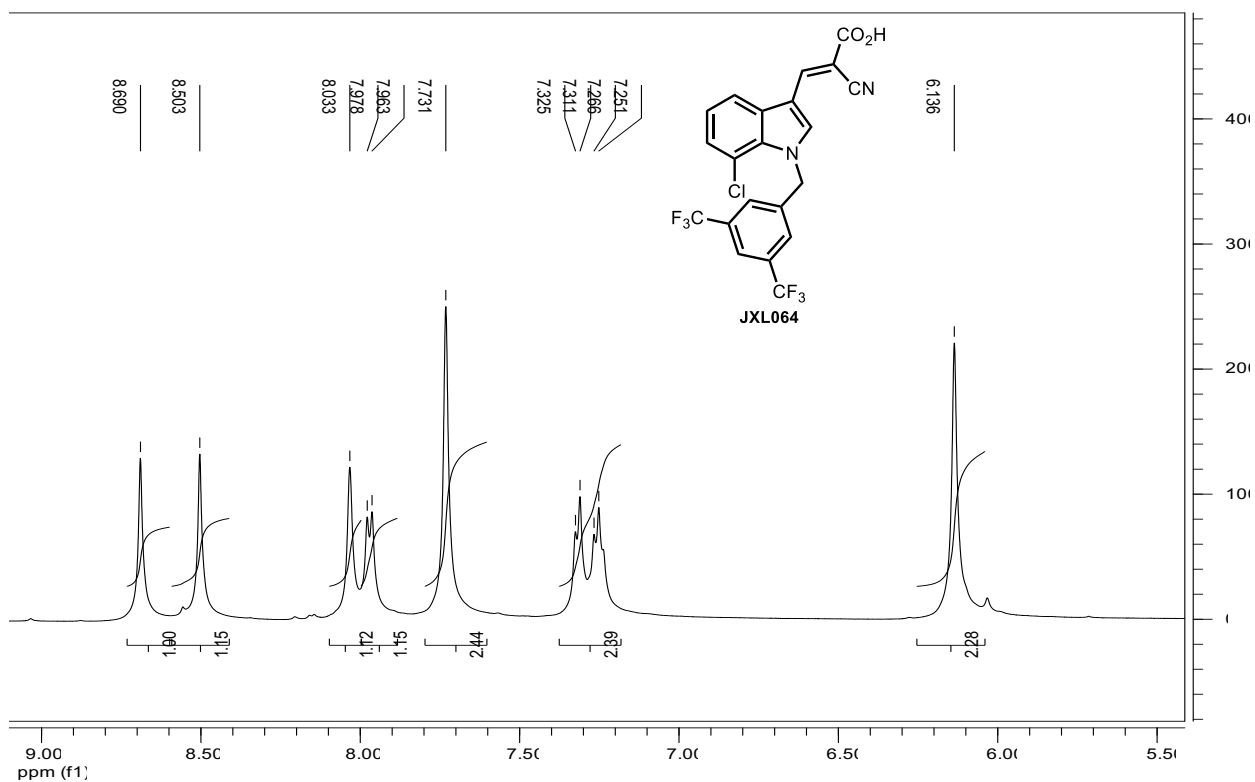
¹³C NMR (126 MHz, DMSO-d₆)



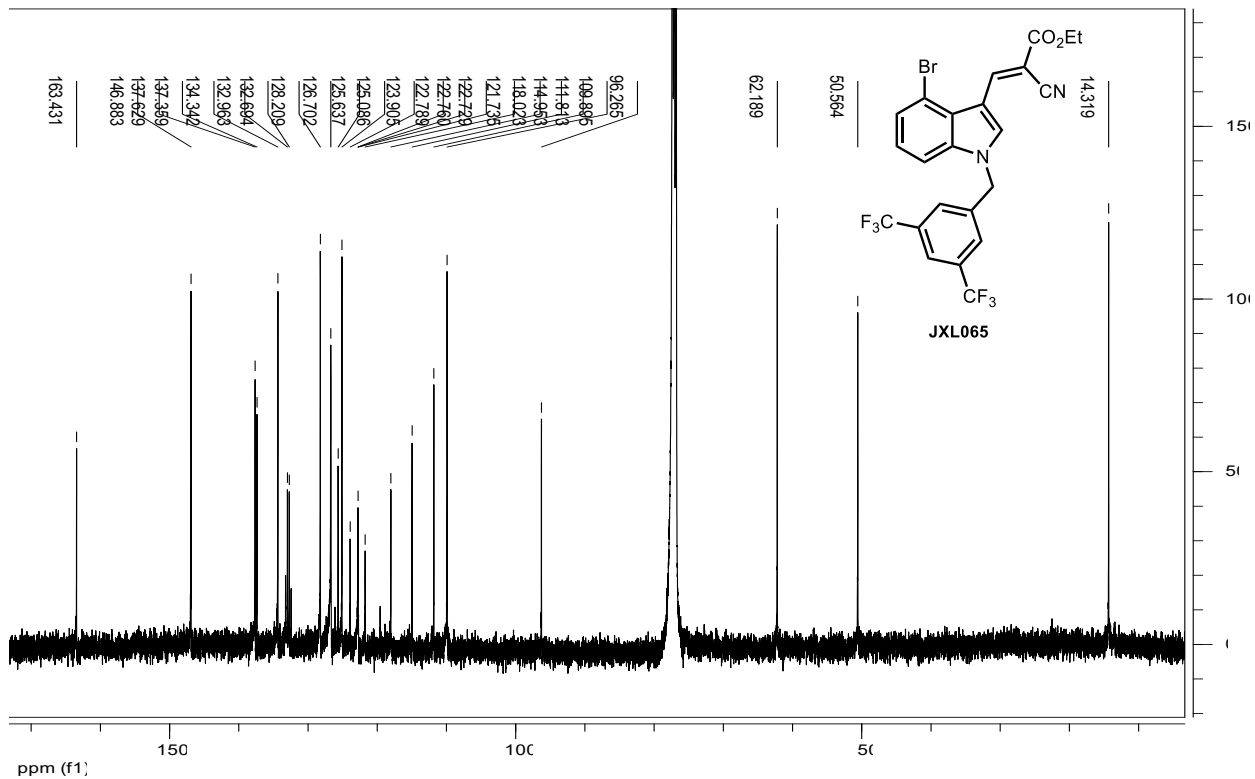
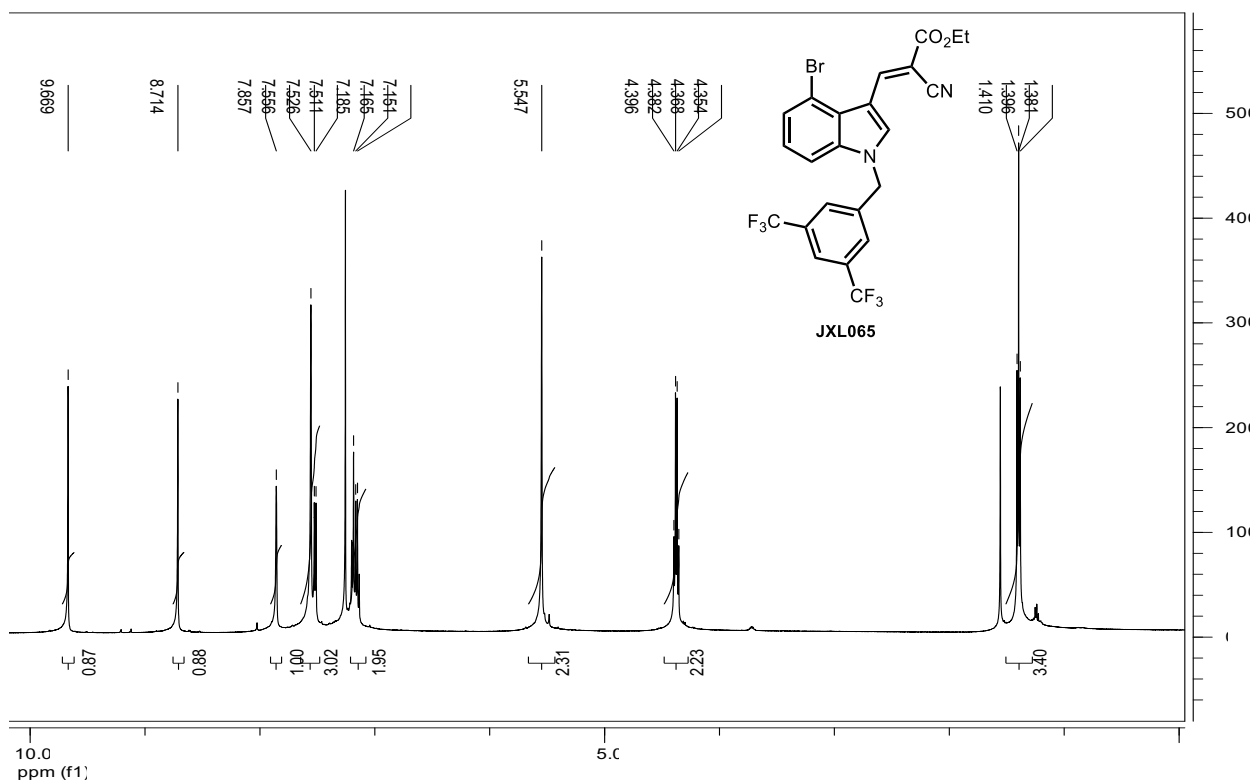
¹H NMR (500 MHz, DMSO-d₆)

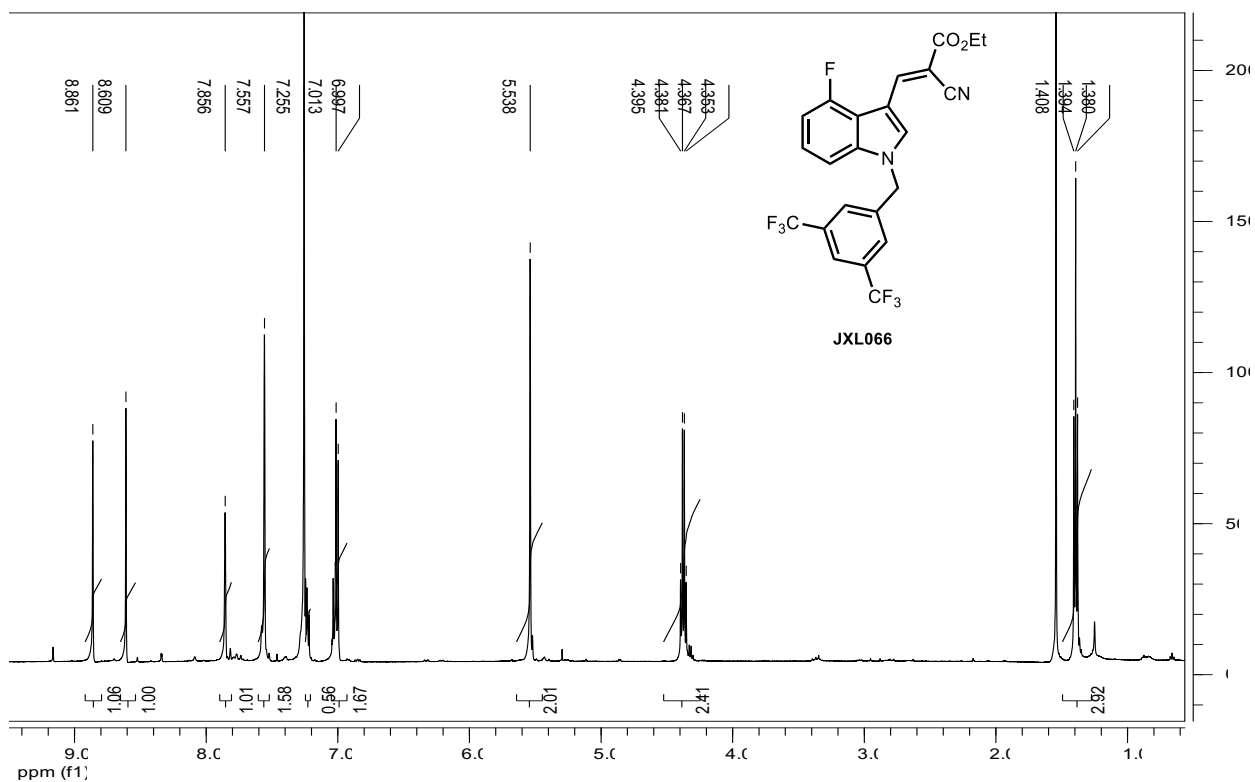


¹³C NMR (126 MHz, DMSO-d₆)

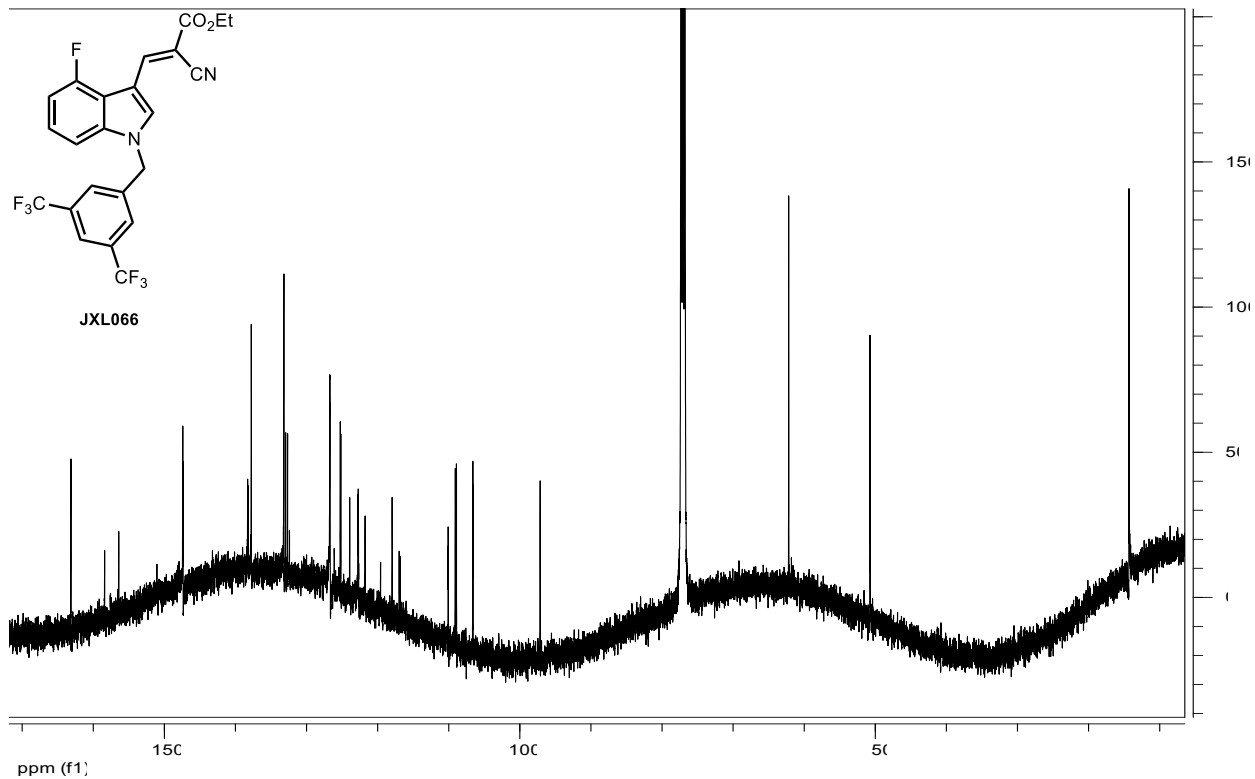


¹³C NMR (126 MHz, DMSO-d₆)

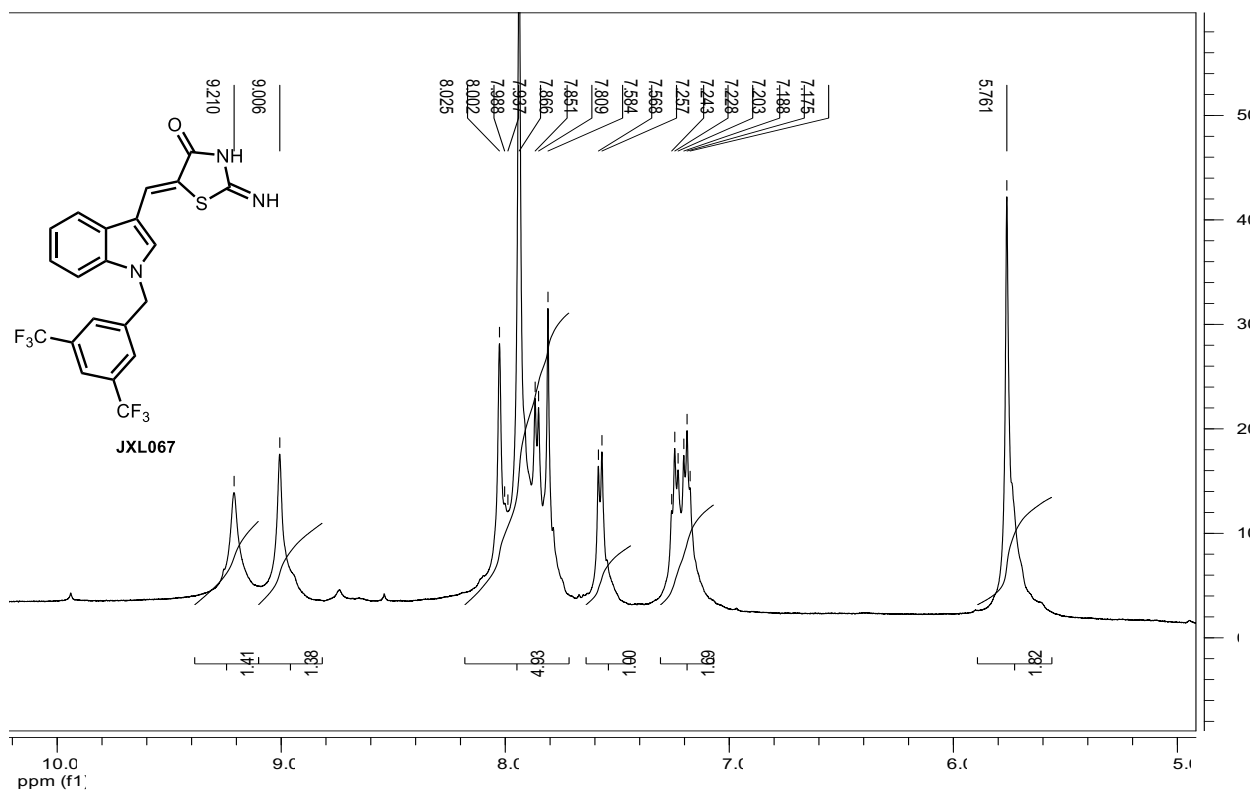




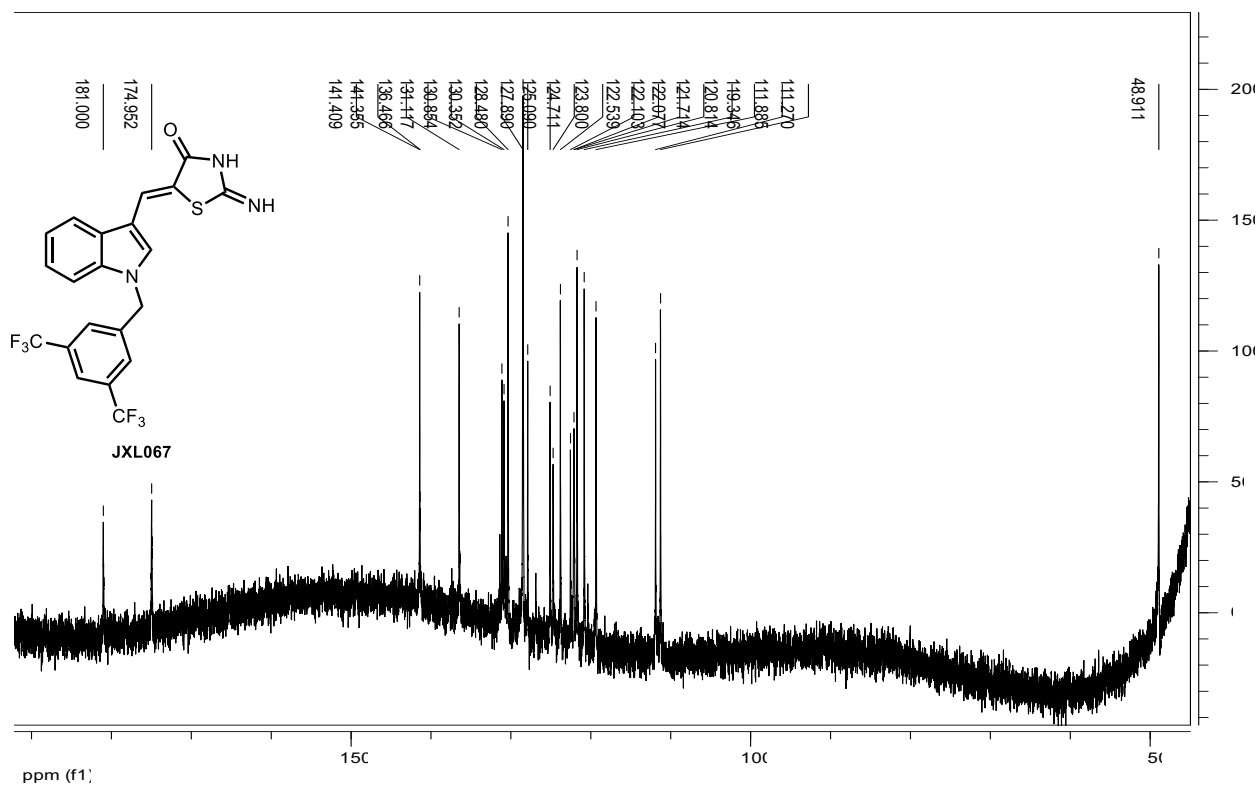
¹H NMR (500 MHz, DMSO-d₆)



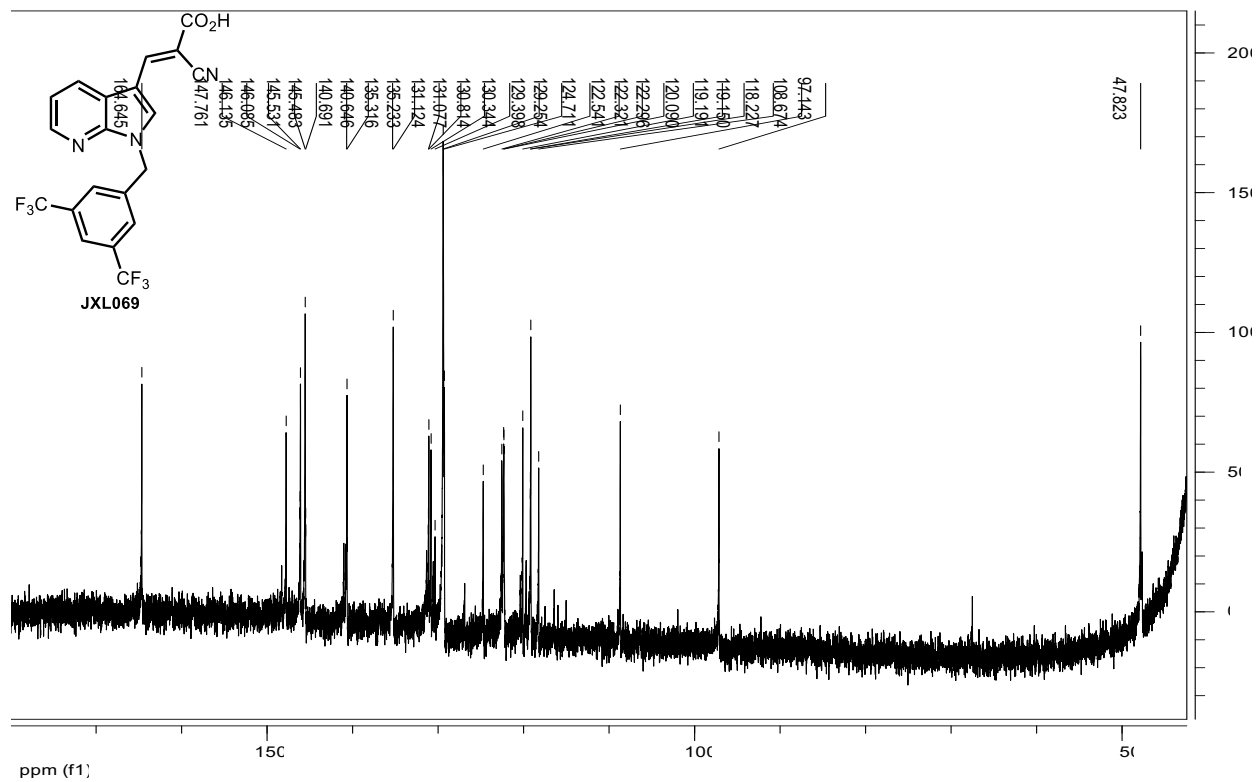
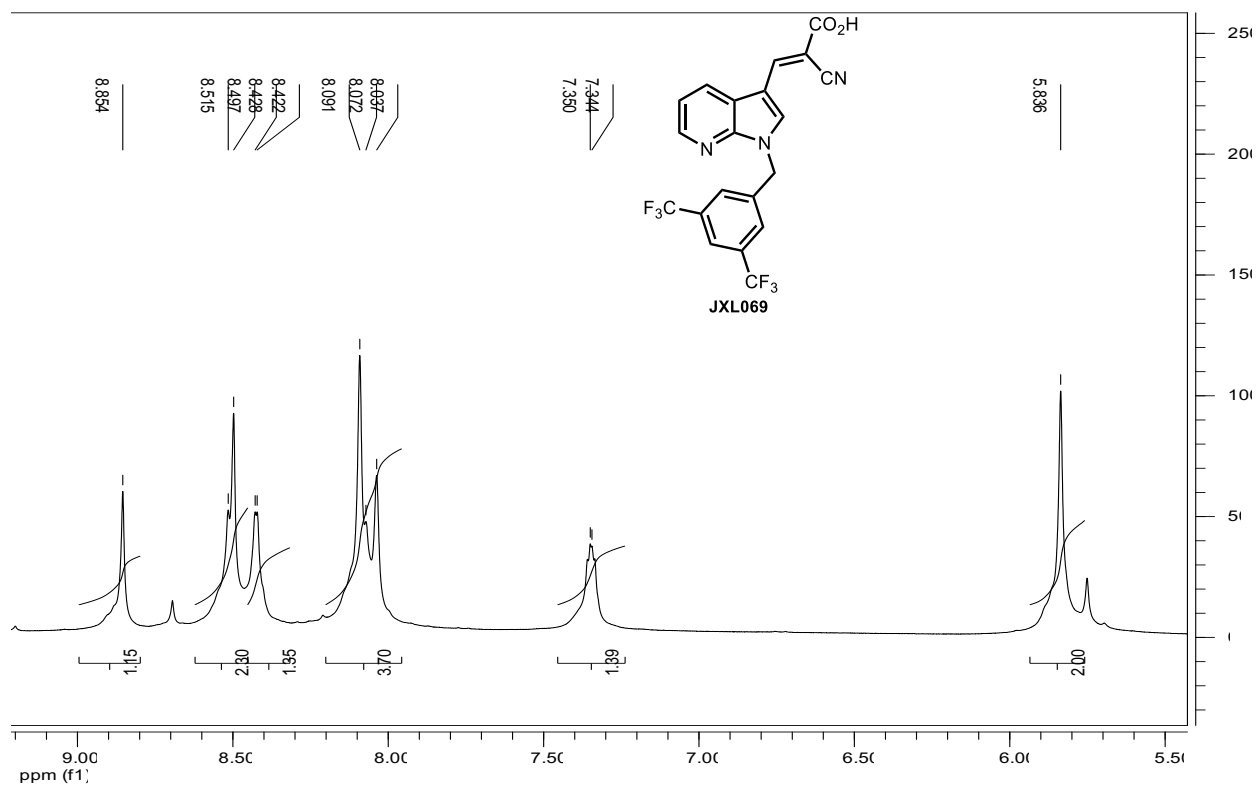
¹³C NMR (126 MHz, DMSO-d₆)



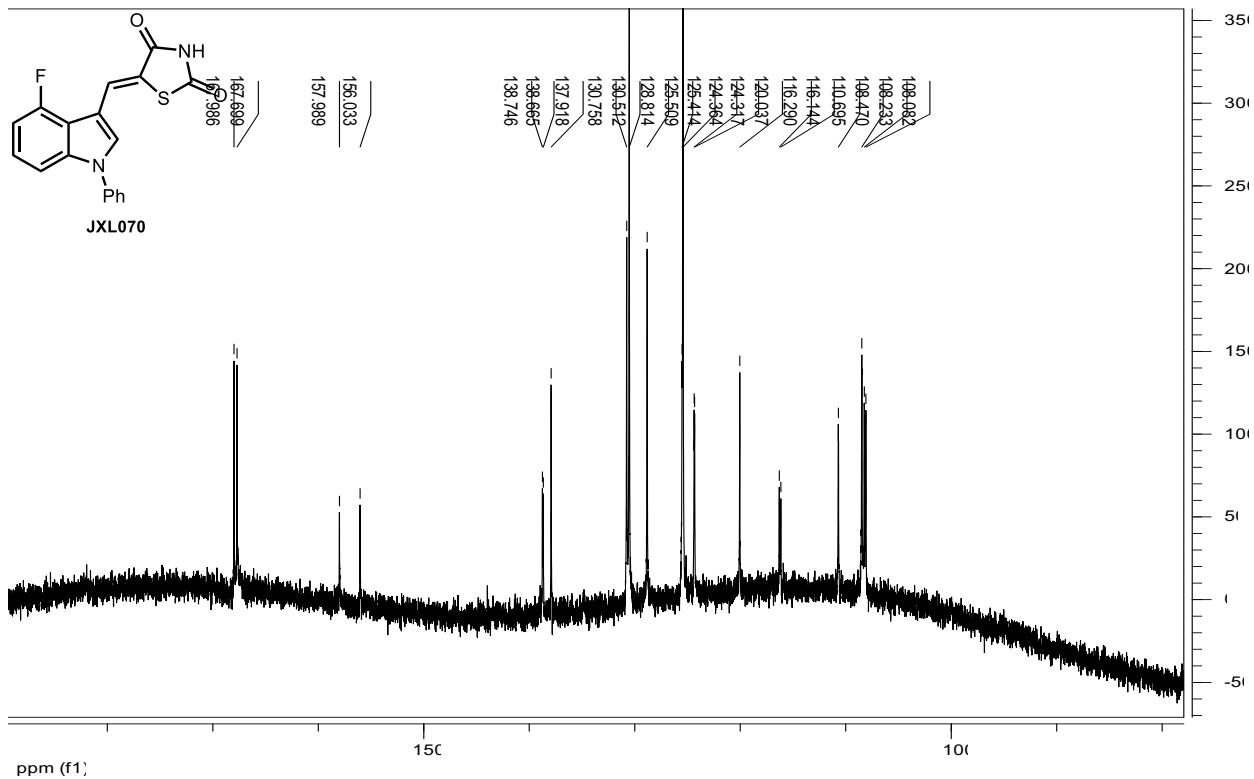
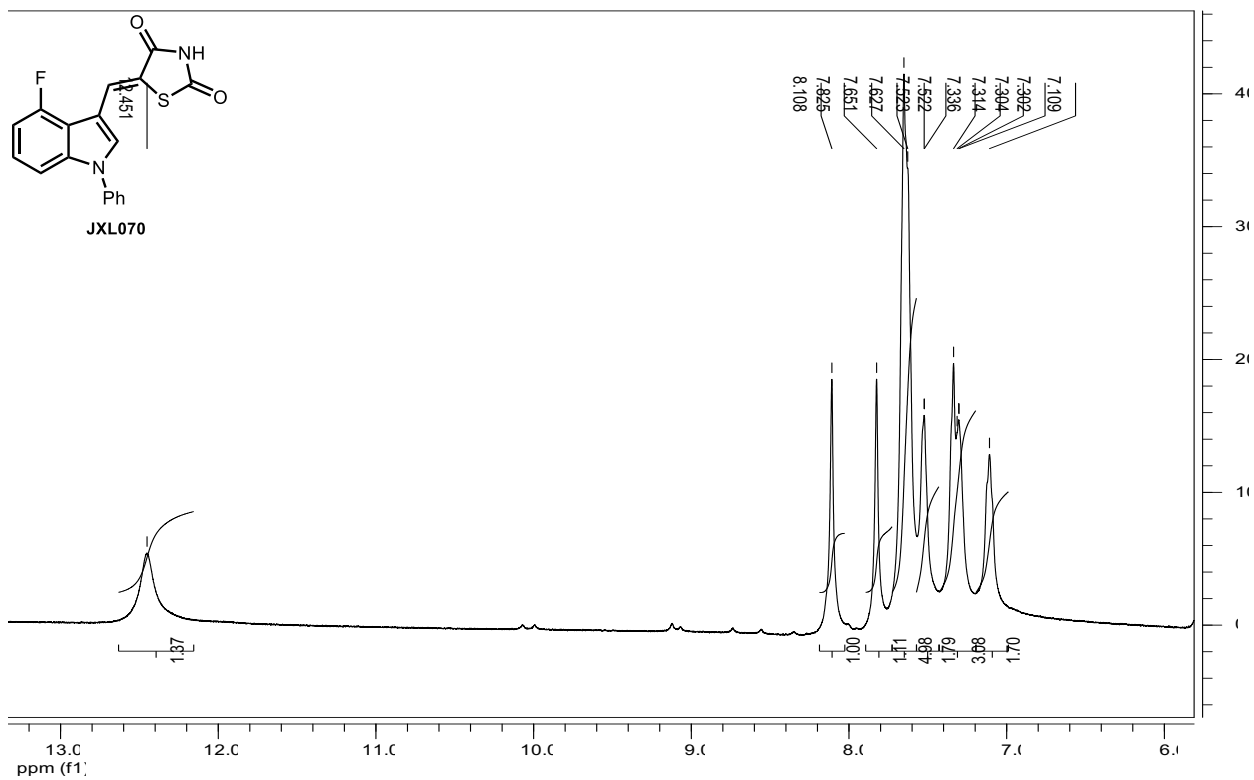
¹H NMR (500 MHz, DMSO-d₆)



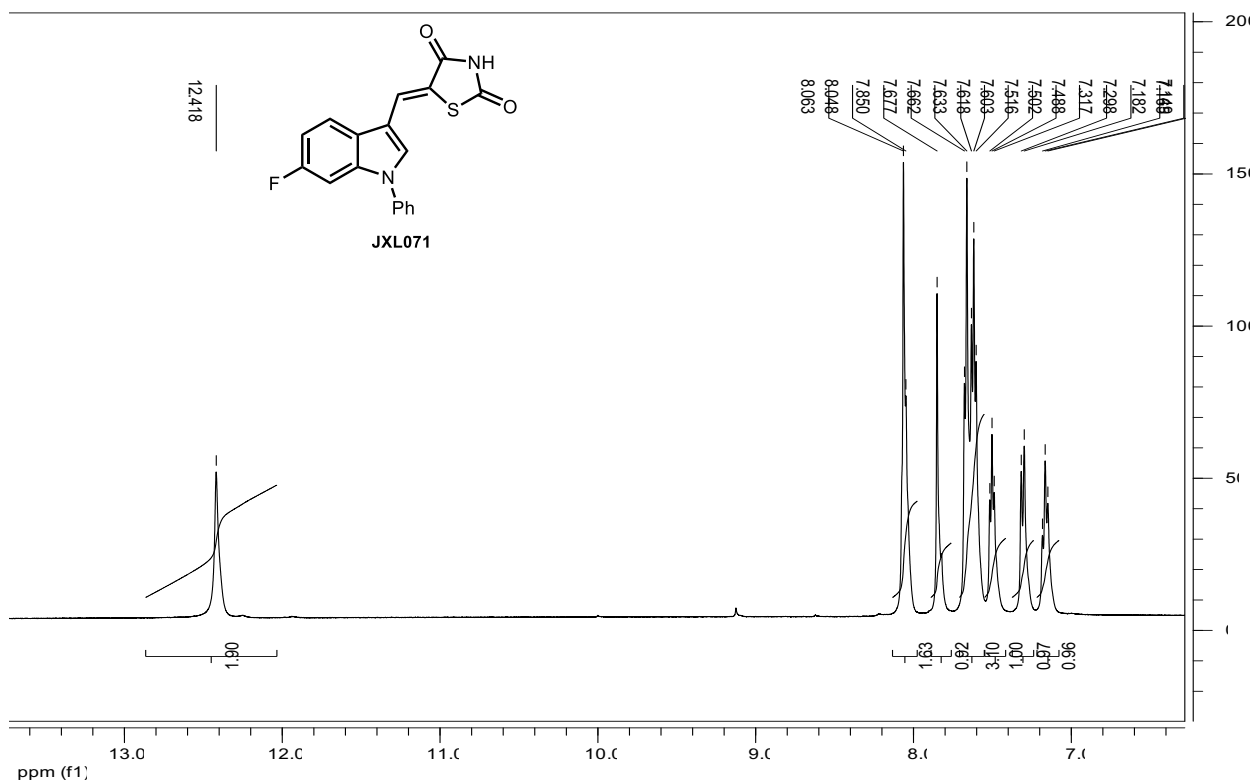
¹³C NMR (126 MHz, DMSO-d₆)



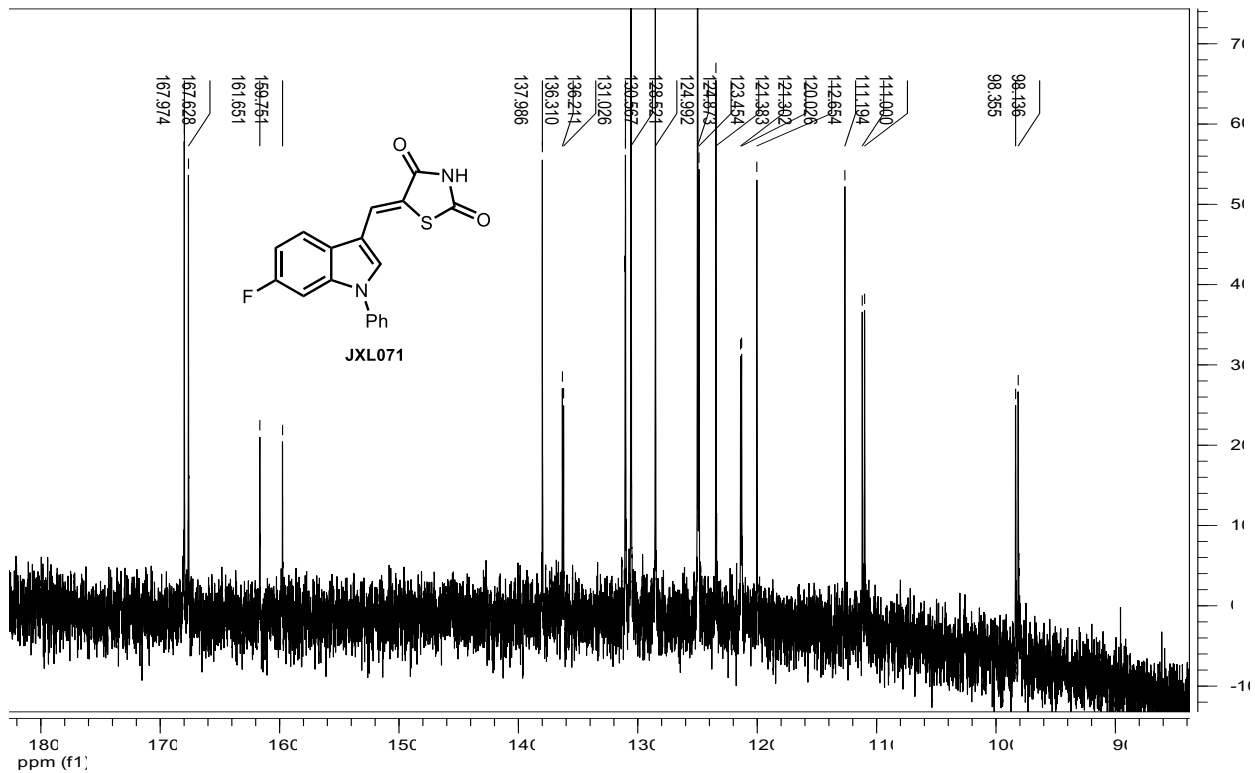
¹³C NMR (126 MHz, DMSO-d₆)



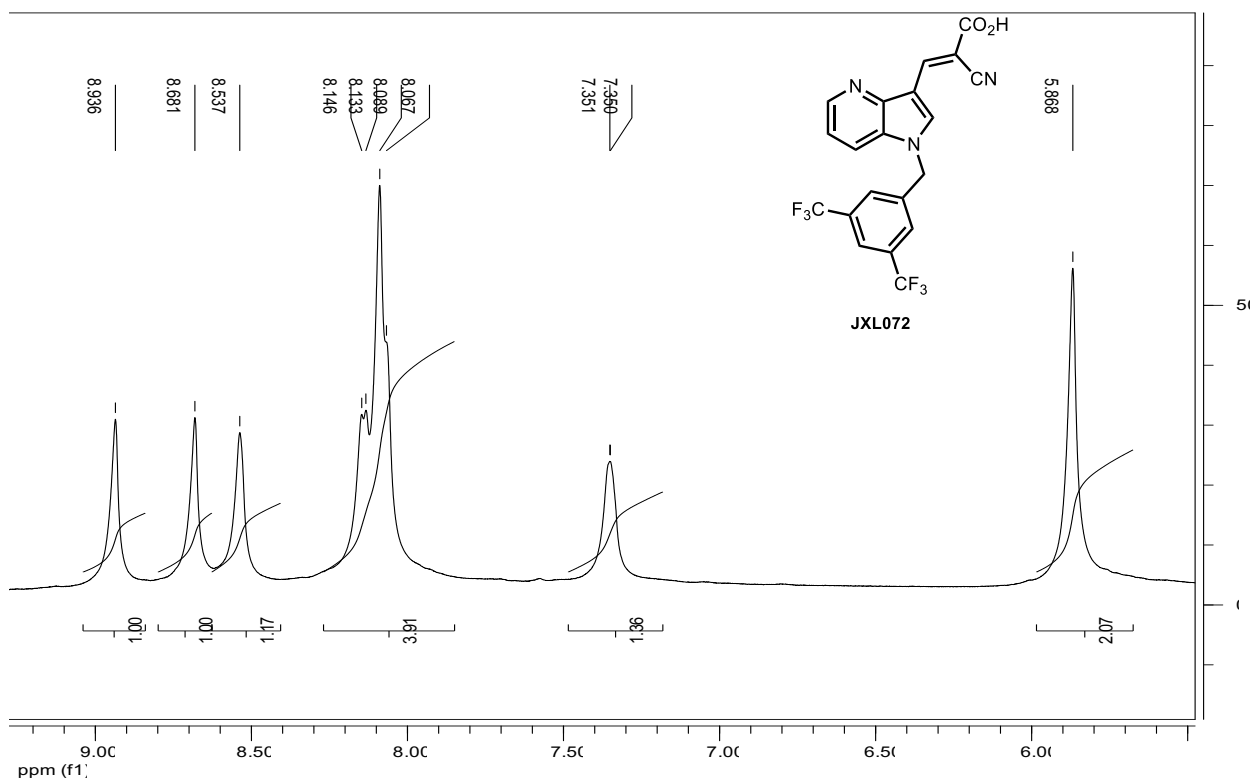
¹³C NMR (126 MHz, DMSO-d₆)



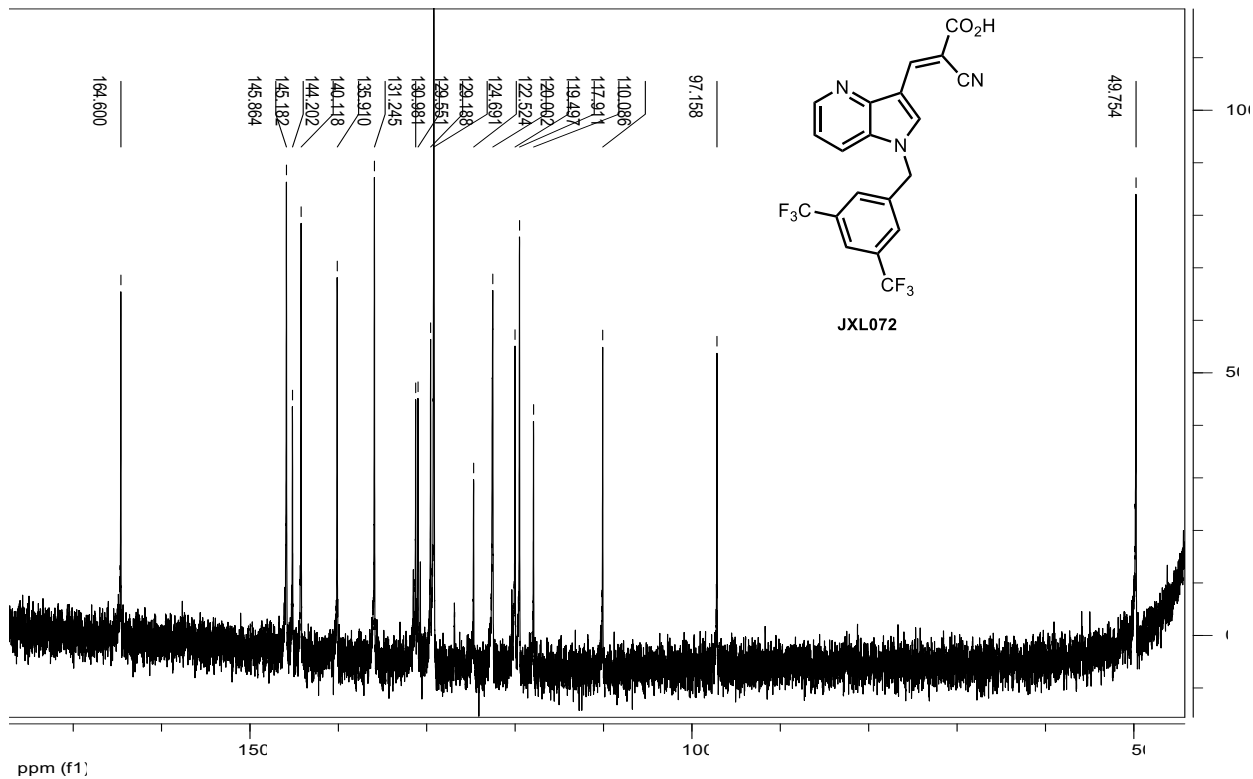
¹H NMR (500 MHz, DMSO-d₆)



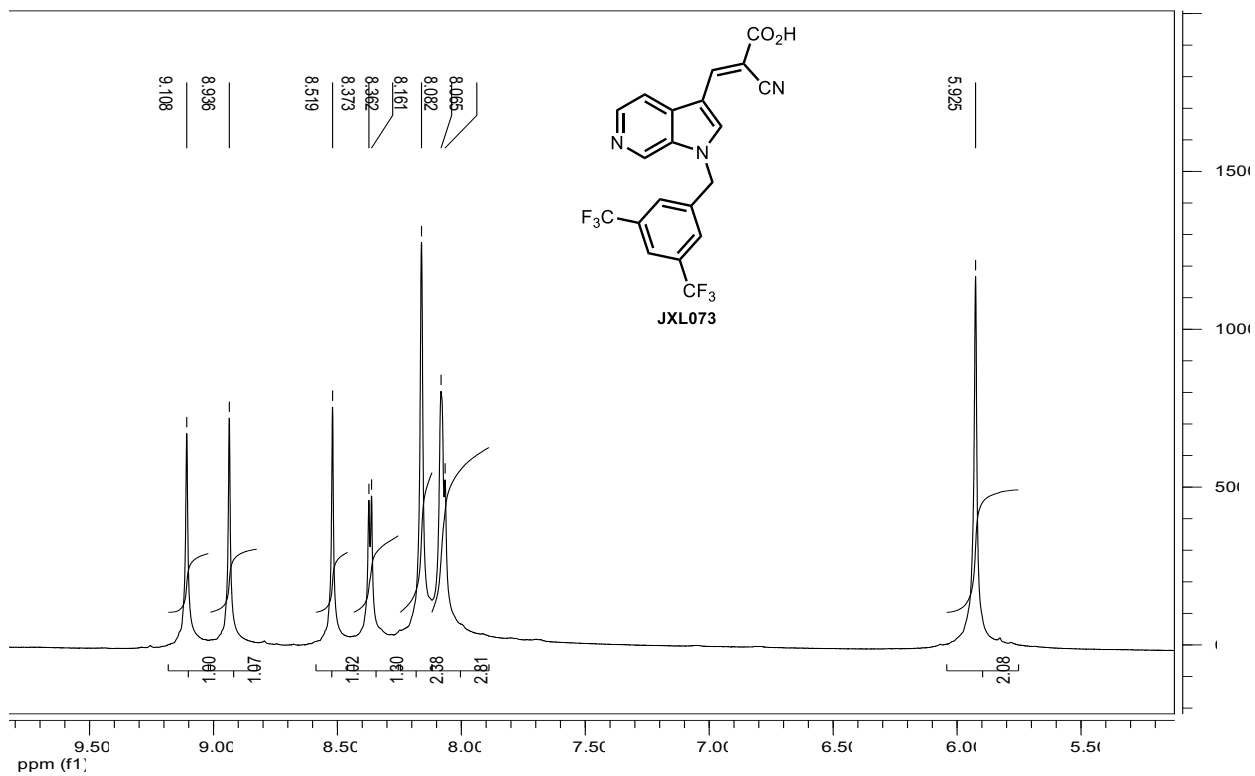
¹³C NMR (126 MHz, DMSO-d₆)



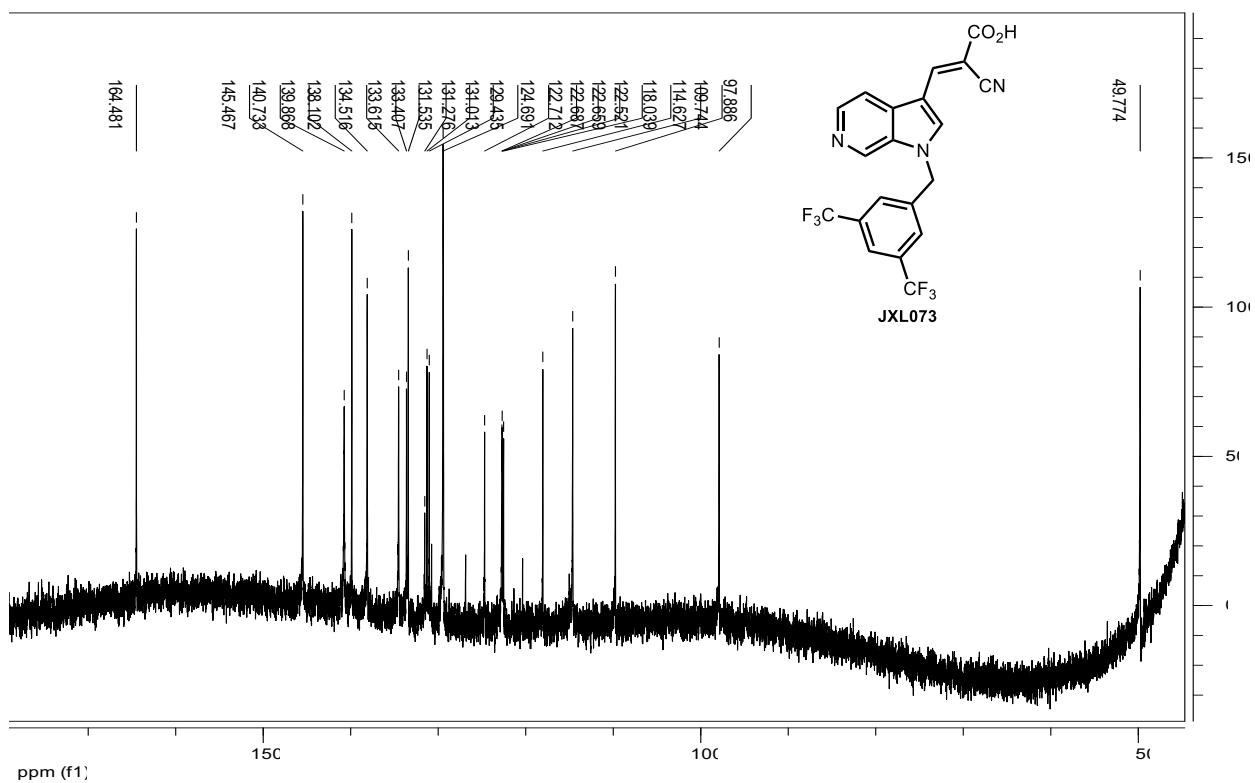
¹H NMR (500 MHz, DMSO-d₆)



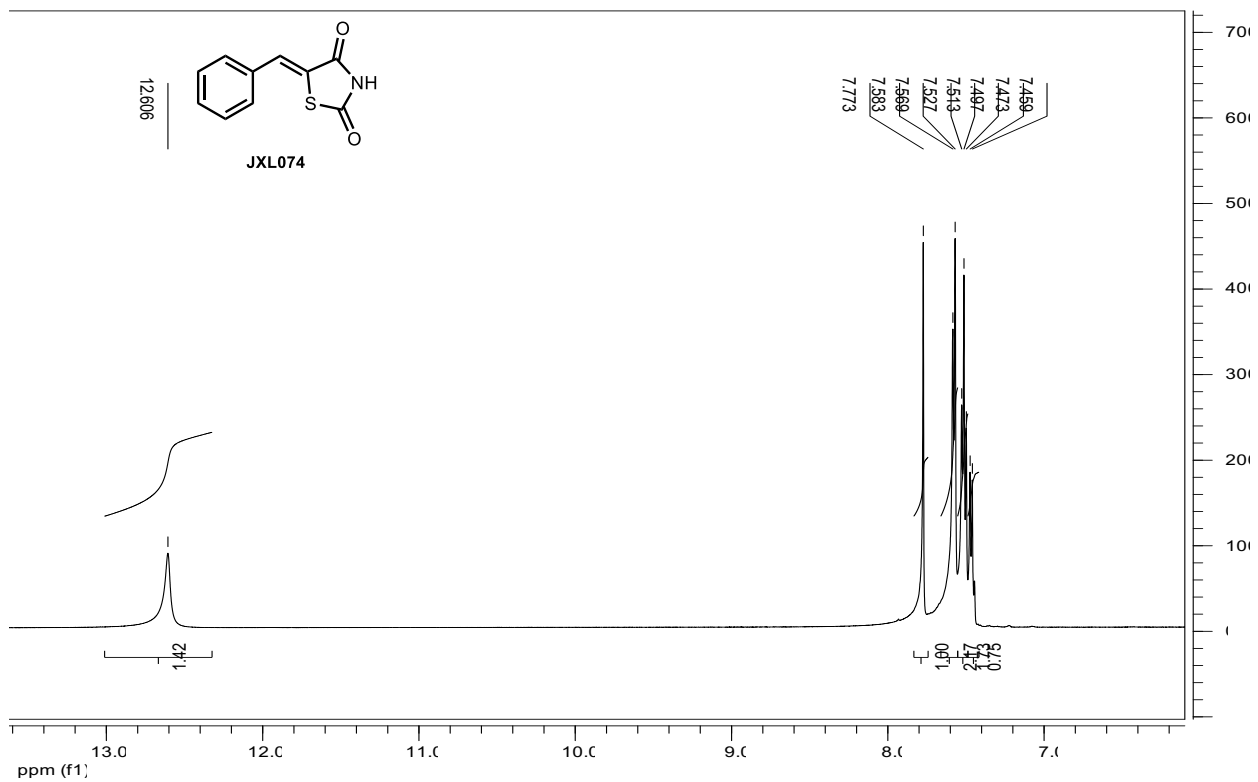
¹³C NMR (126 MHz, DMSO-d₆)



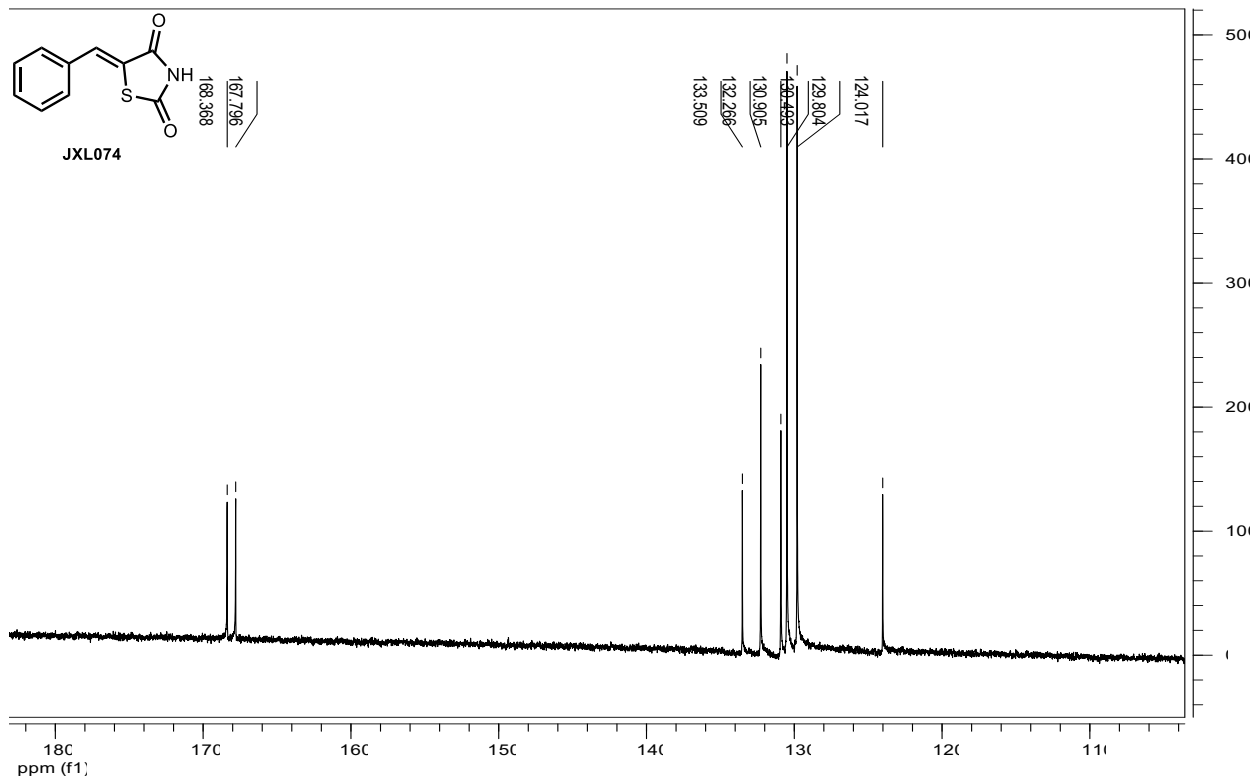
¹H NMR (500 MHz, DMSO-d₆)



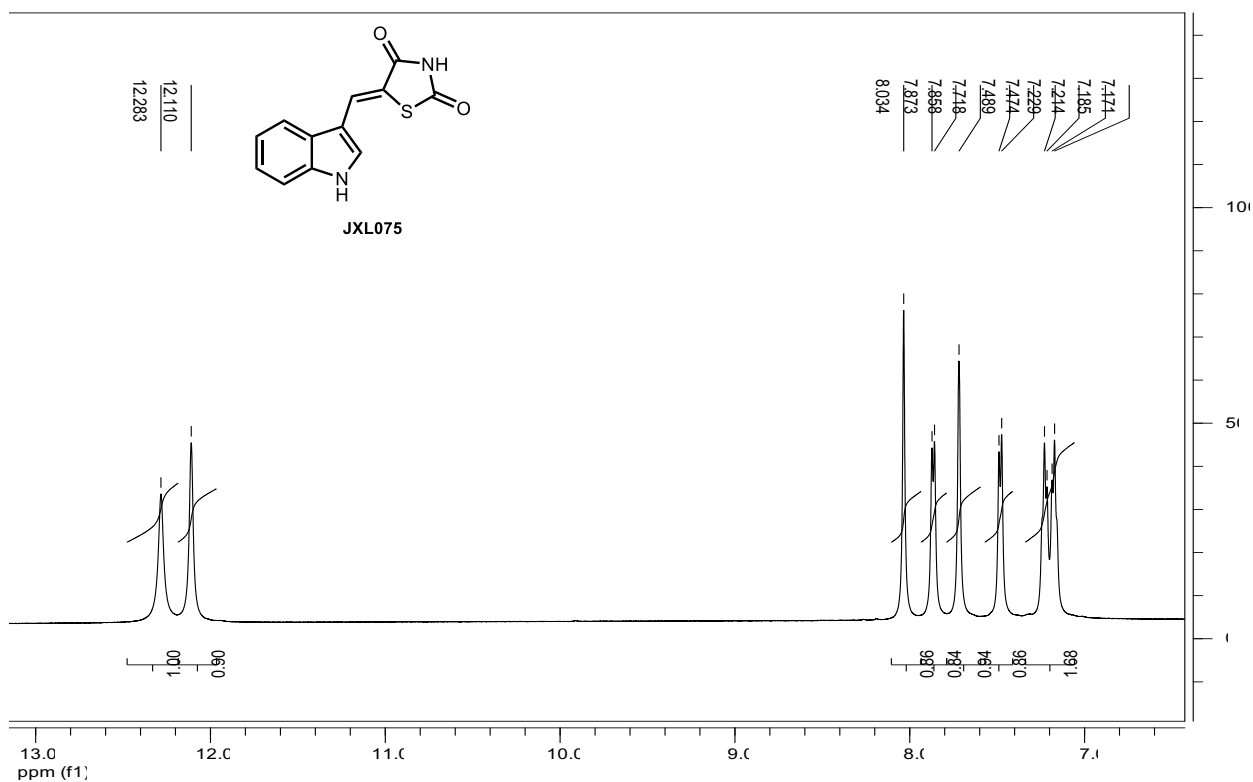
¹³C NMR (126 MHz, DMSO-d₆)



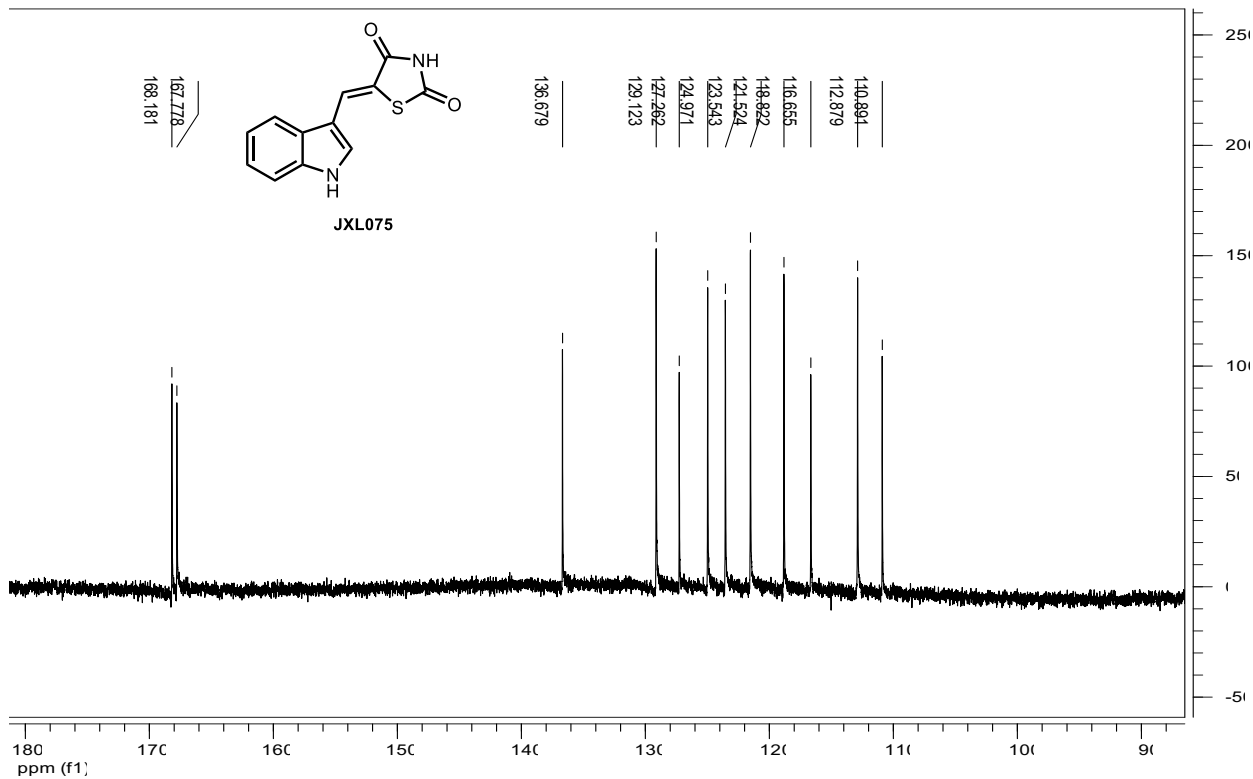
¹H NMR (500 MHz, DMSO-d₆)



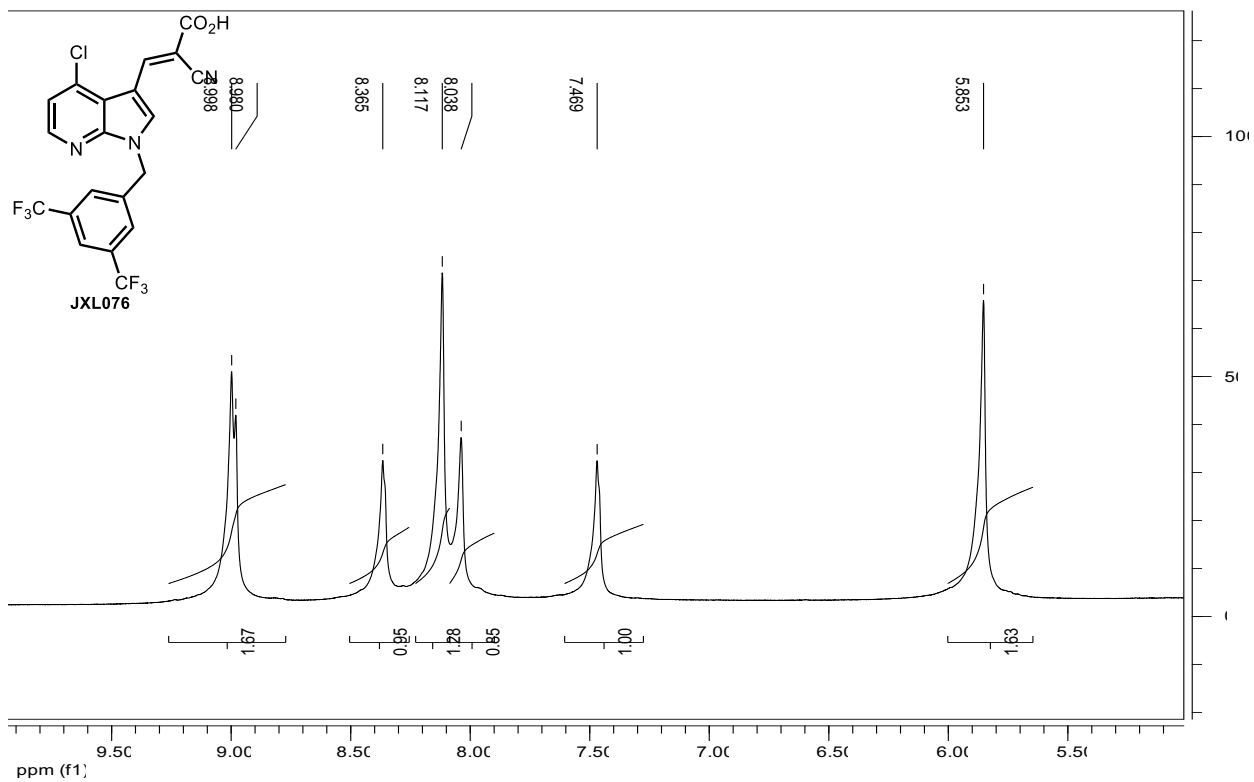
¹³C NMR (126 MHz, DMSO-d₆)



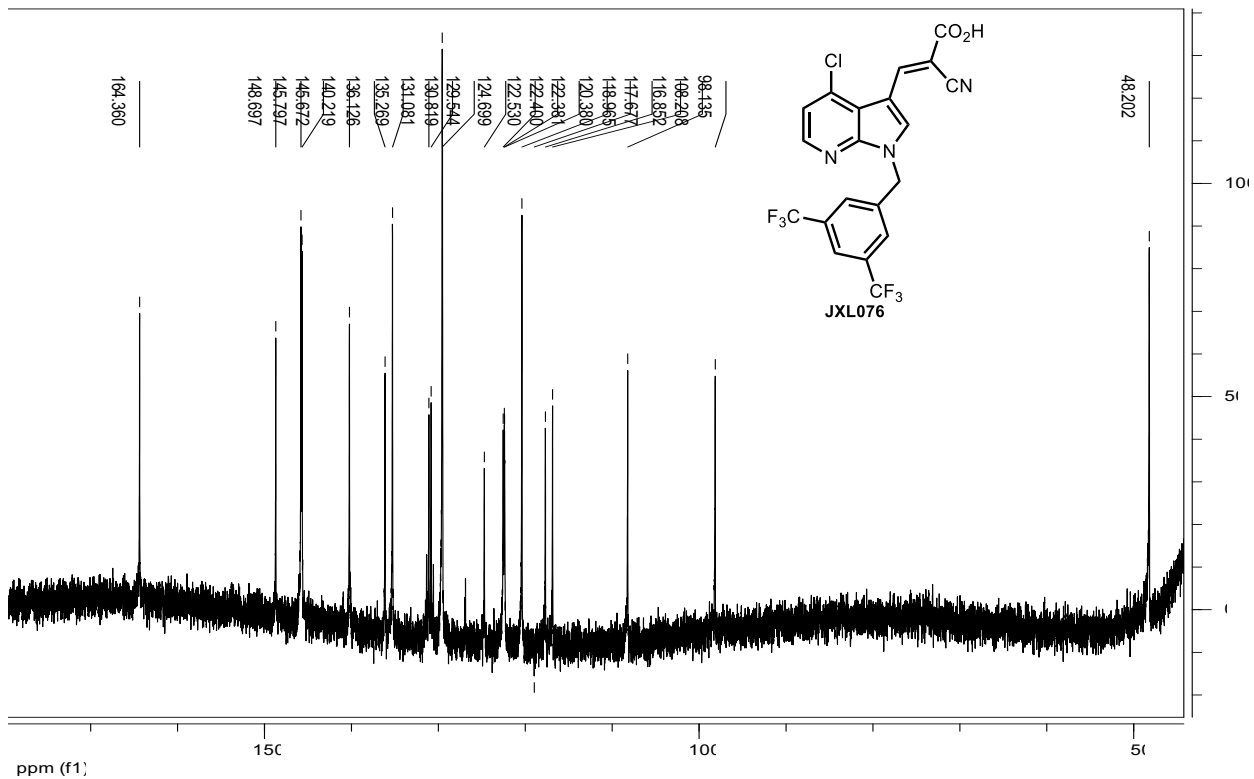
¹H NMR (500 MHz, DMSO-d₆)



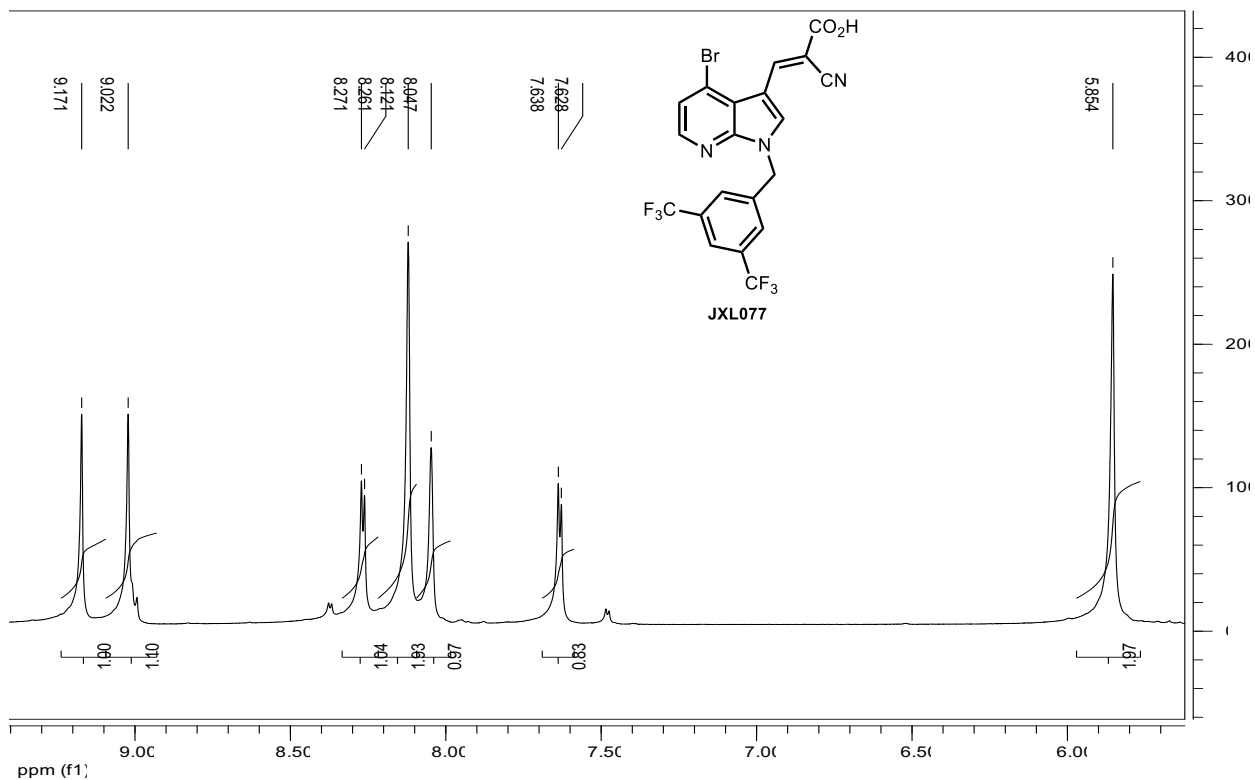
¹³C NMR (126 MHz, DMSO-d₆)



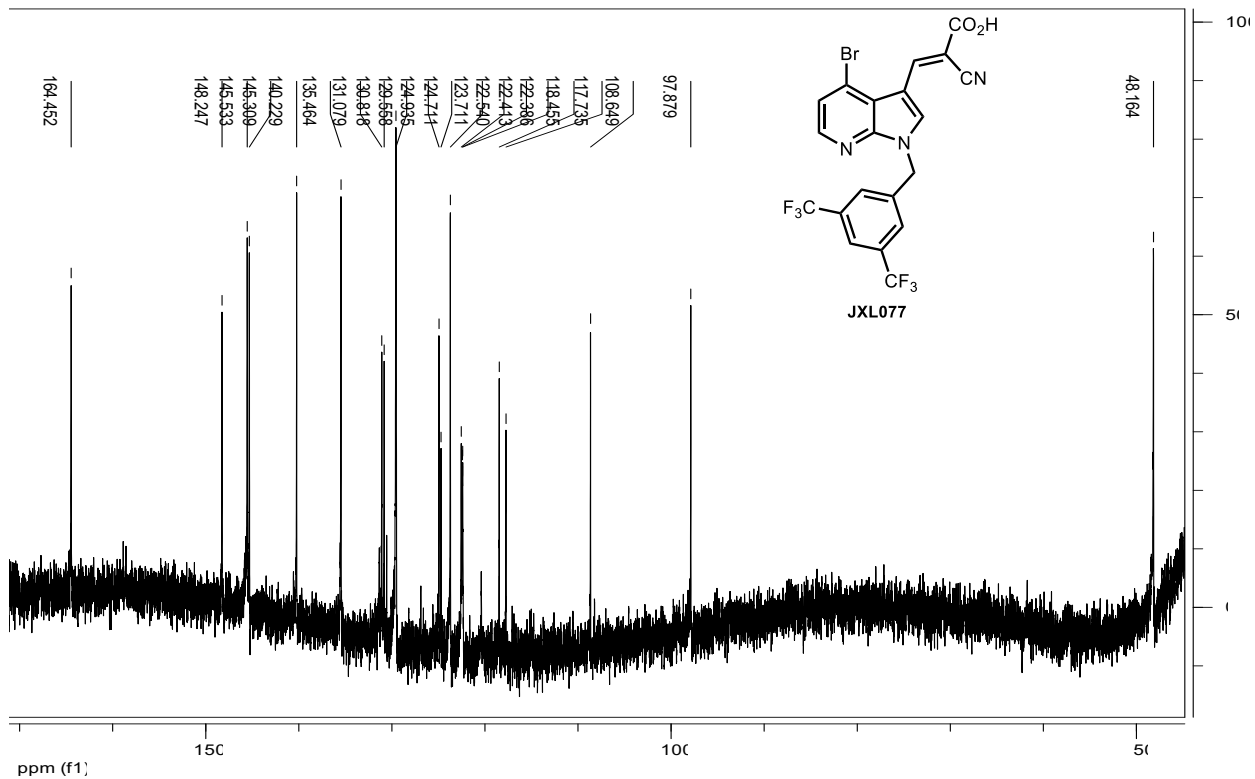
¹H NMR (500 MHz, DMSO-d₆)



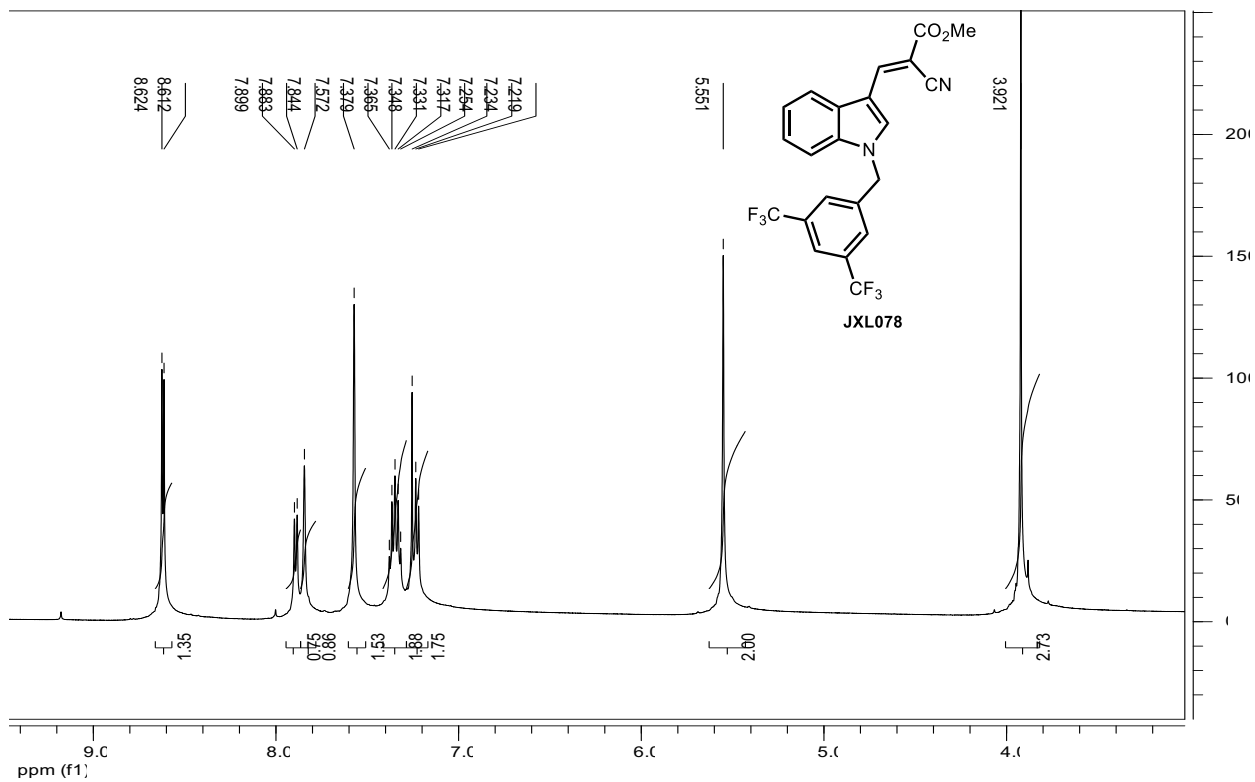
¹³C NMR (126 MHz, DMSO-d₆)



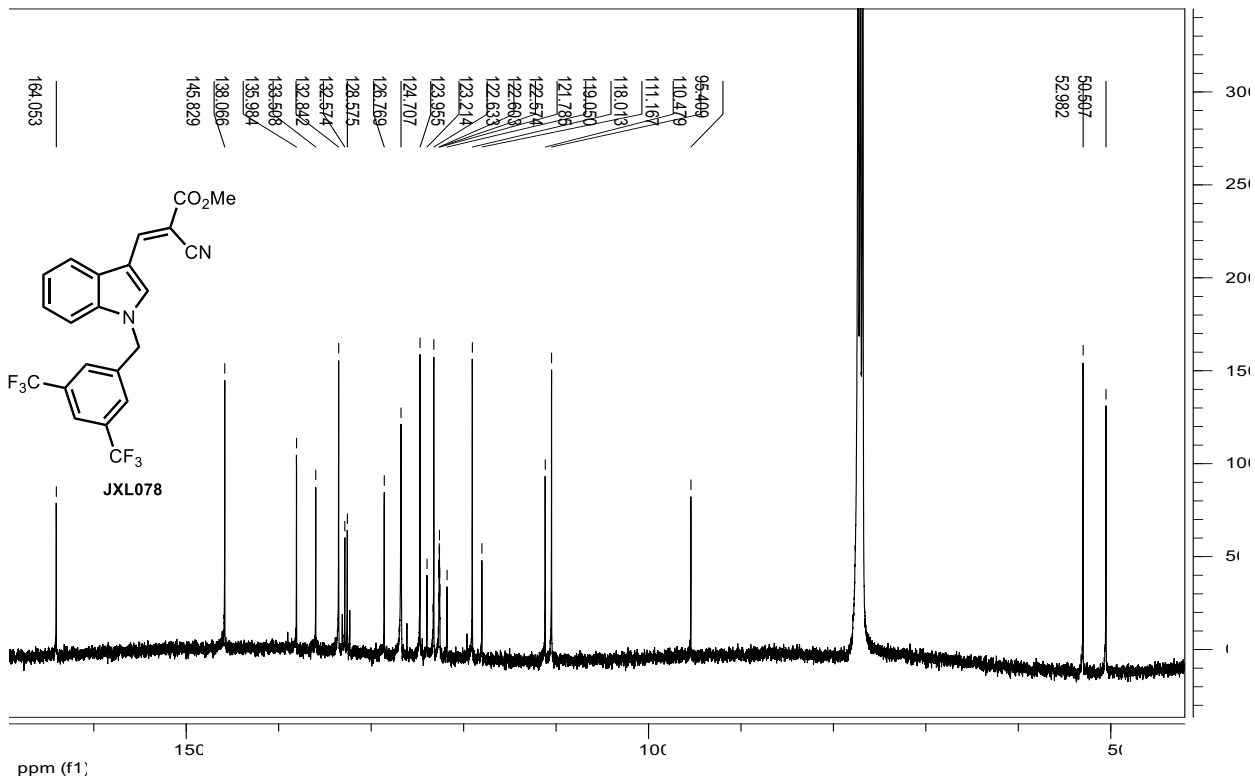
¹H NMR (500 MHz, DMSO-d₆)



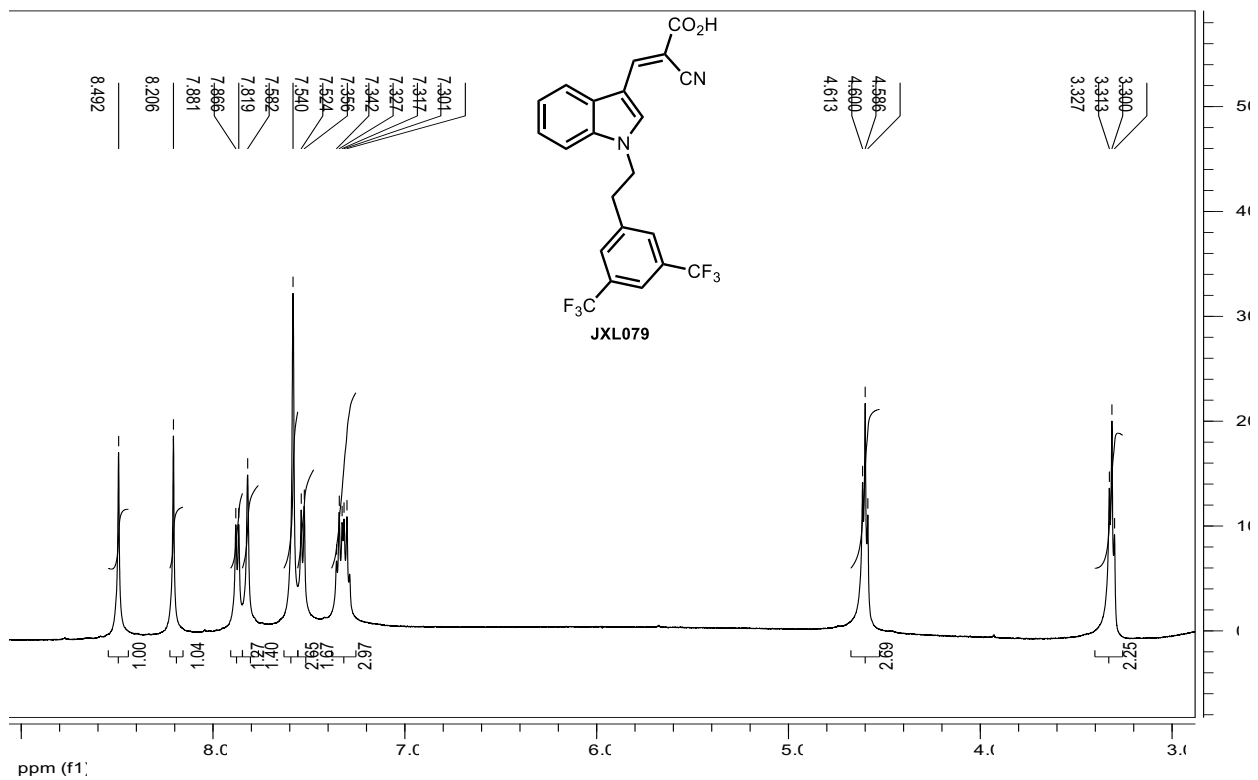
¹³C NMR (126 MHz, DMSO-d₆)



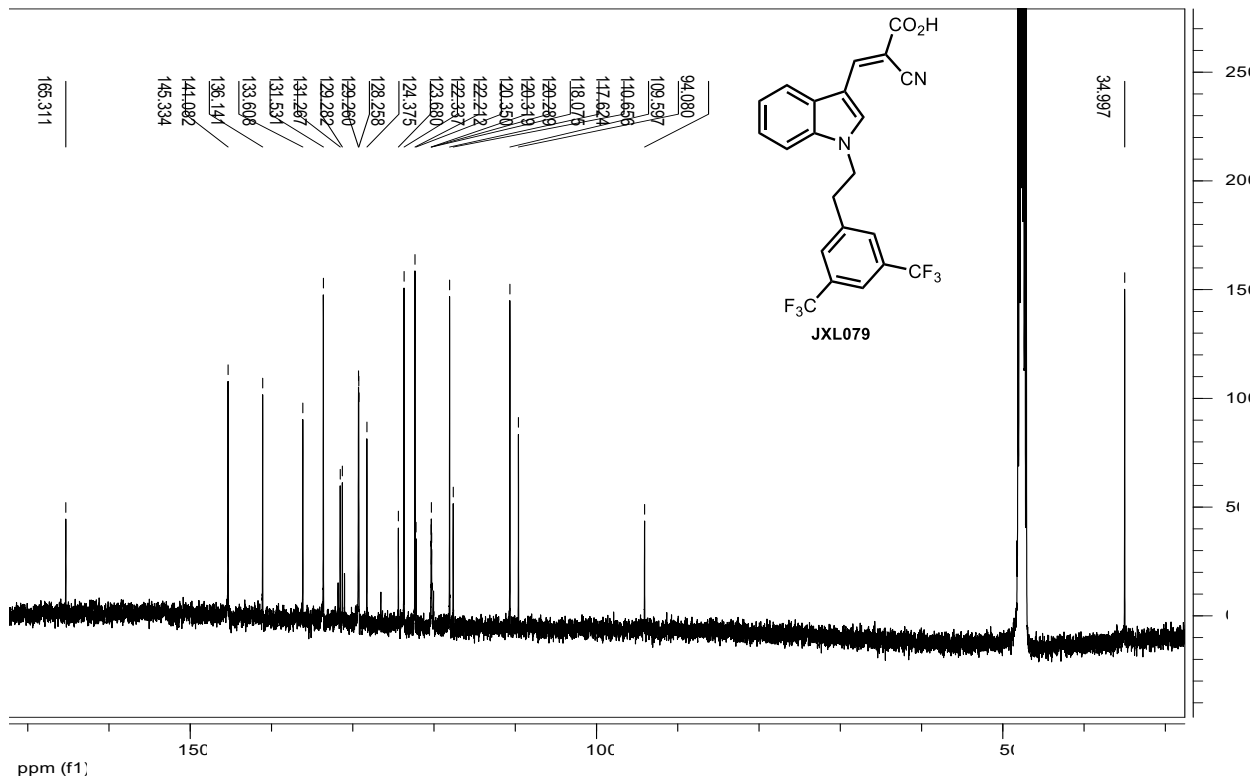
¹H NMR (500 MHz, CDCl₃)



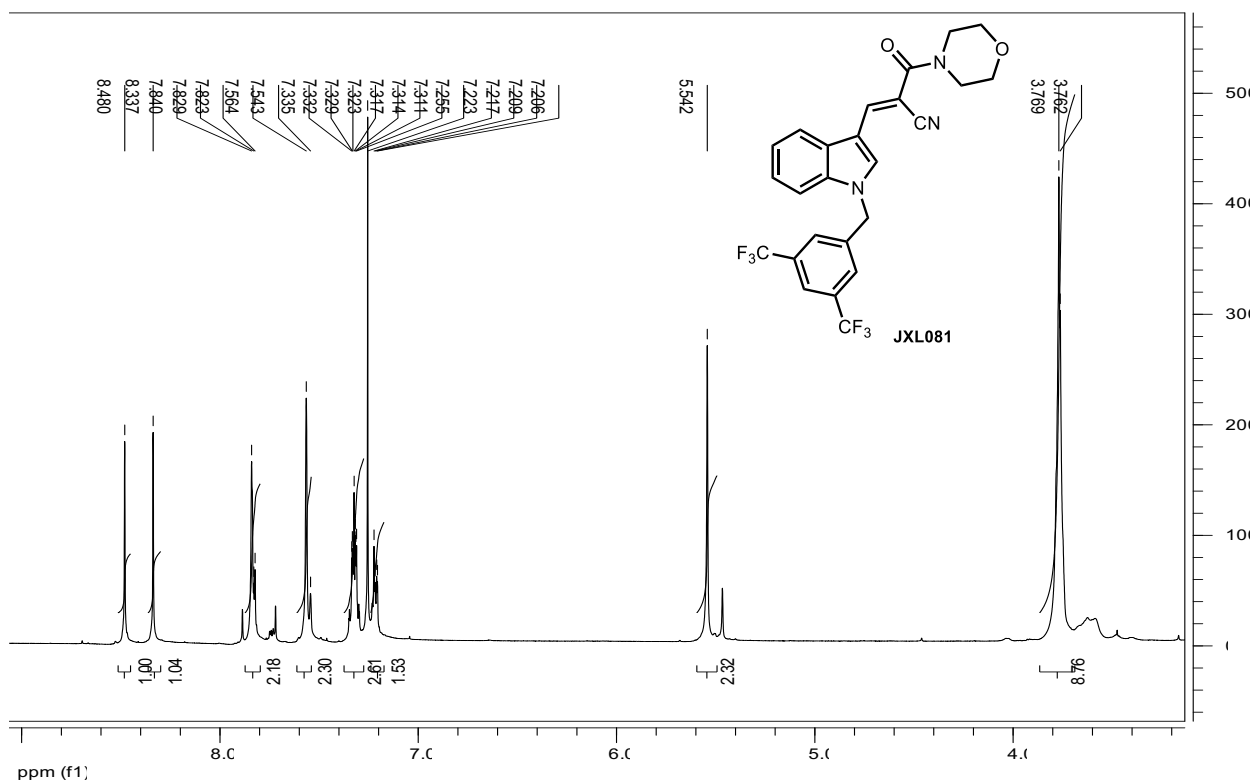
¹³C NMR (126 MHz, CDCl₃)



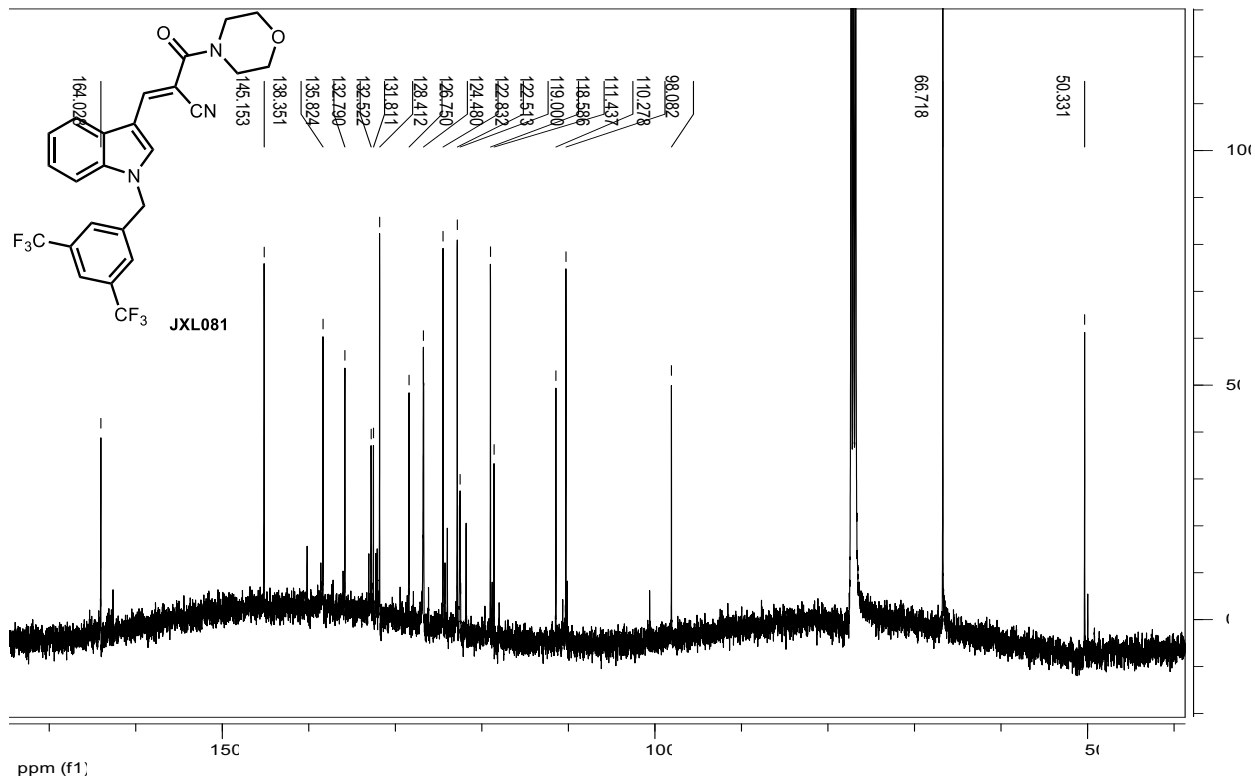
¹H NMR (500 MHz, DMSO-d₆)



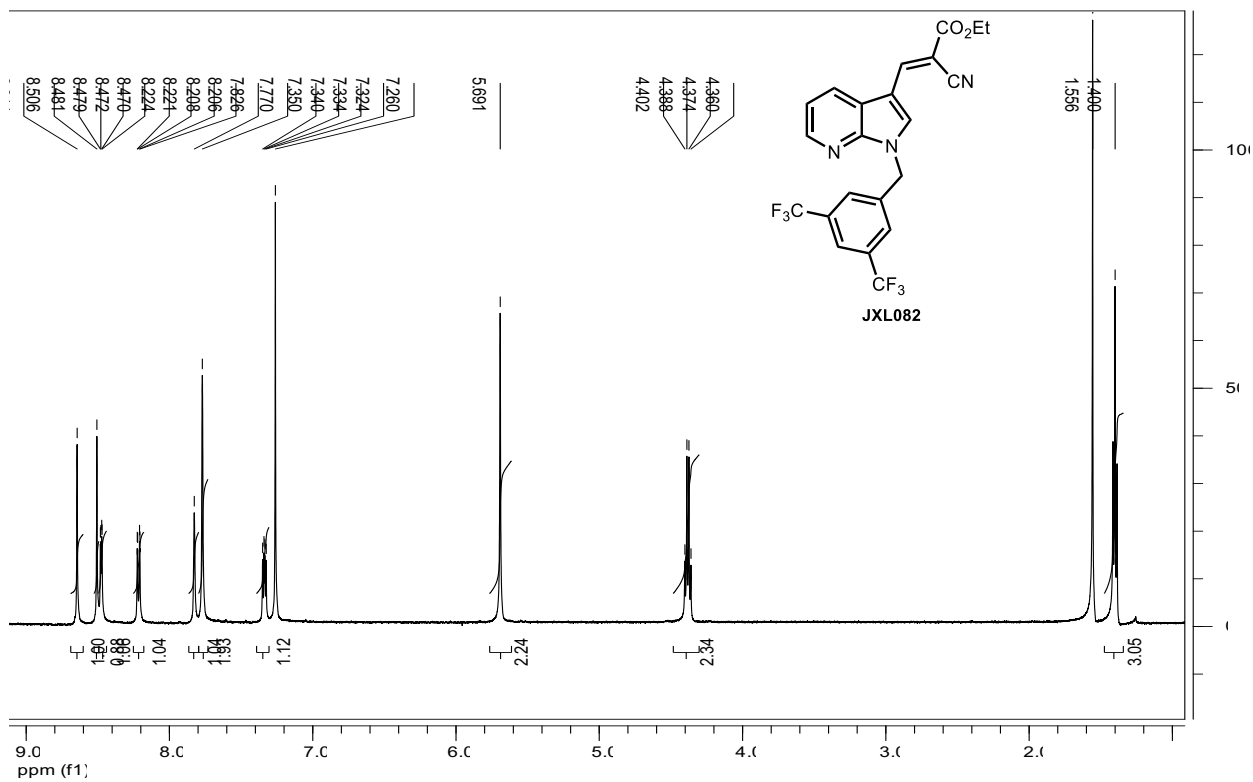
¹³C NMR (126 MHz, DMSO-d₆)



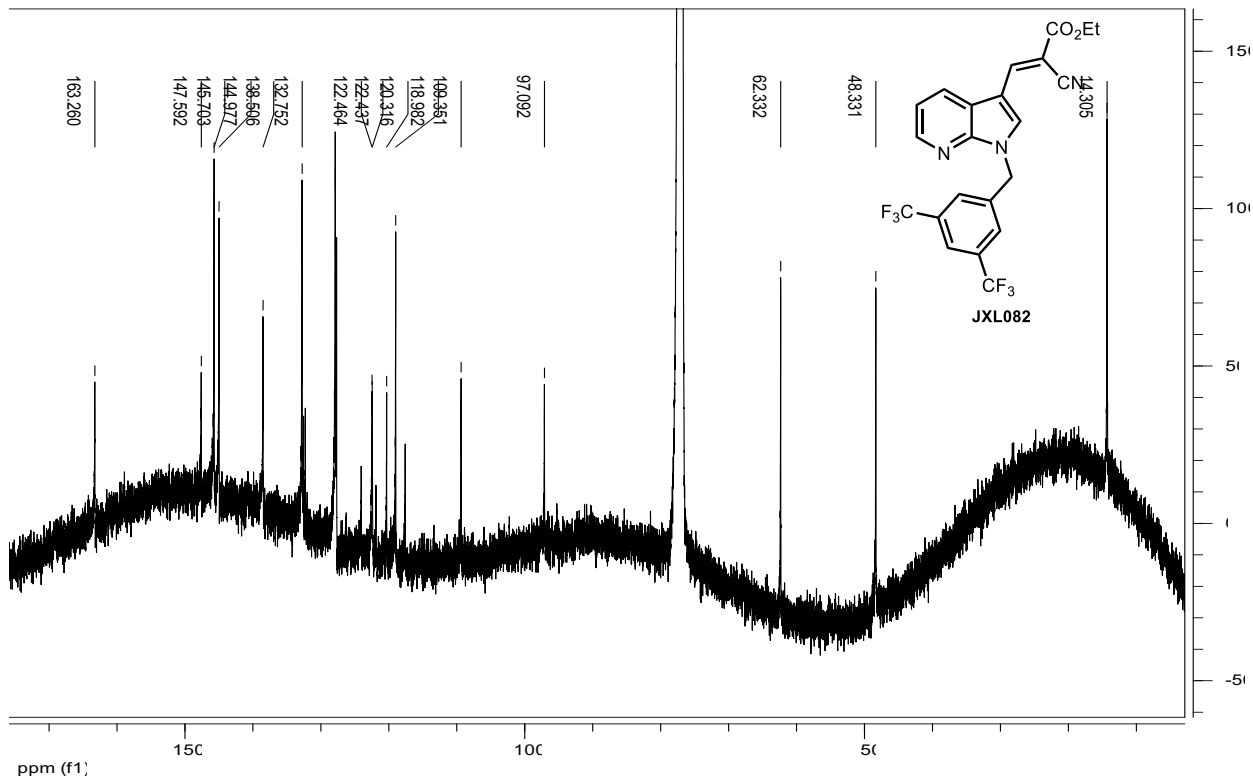
¹H NMR (500 MHz, CDCl₃)



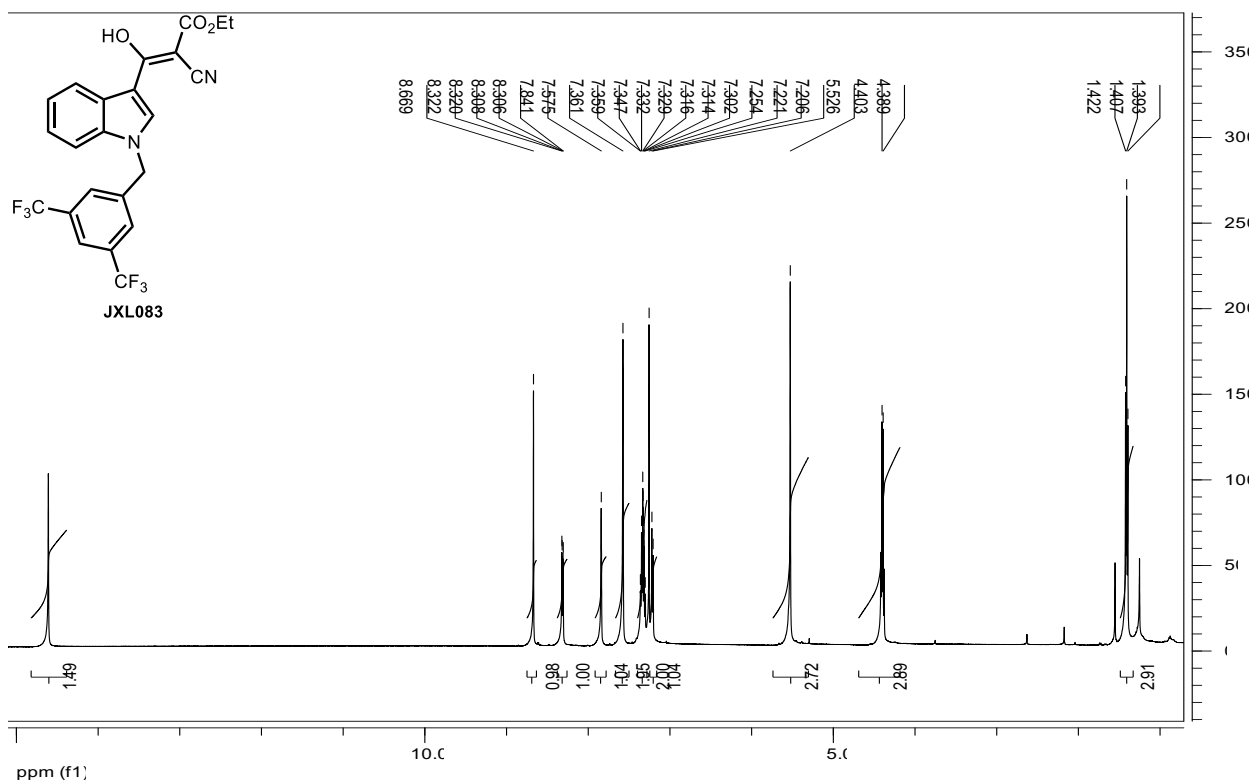
¹³C NMR (126 MHz, CDCl₃)



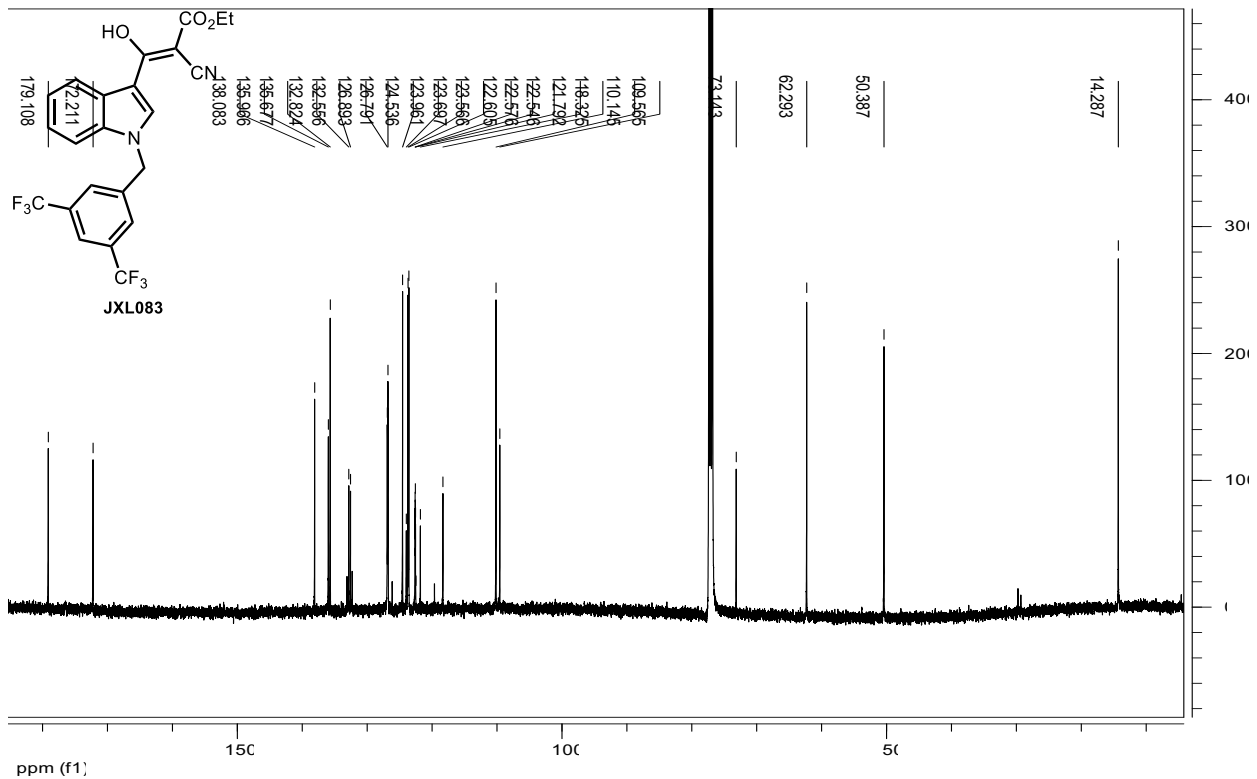
¹H NMR (500 MHz, CDCl₃)



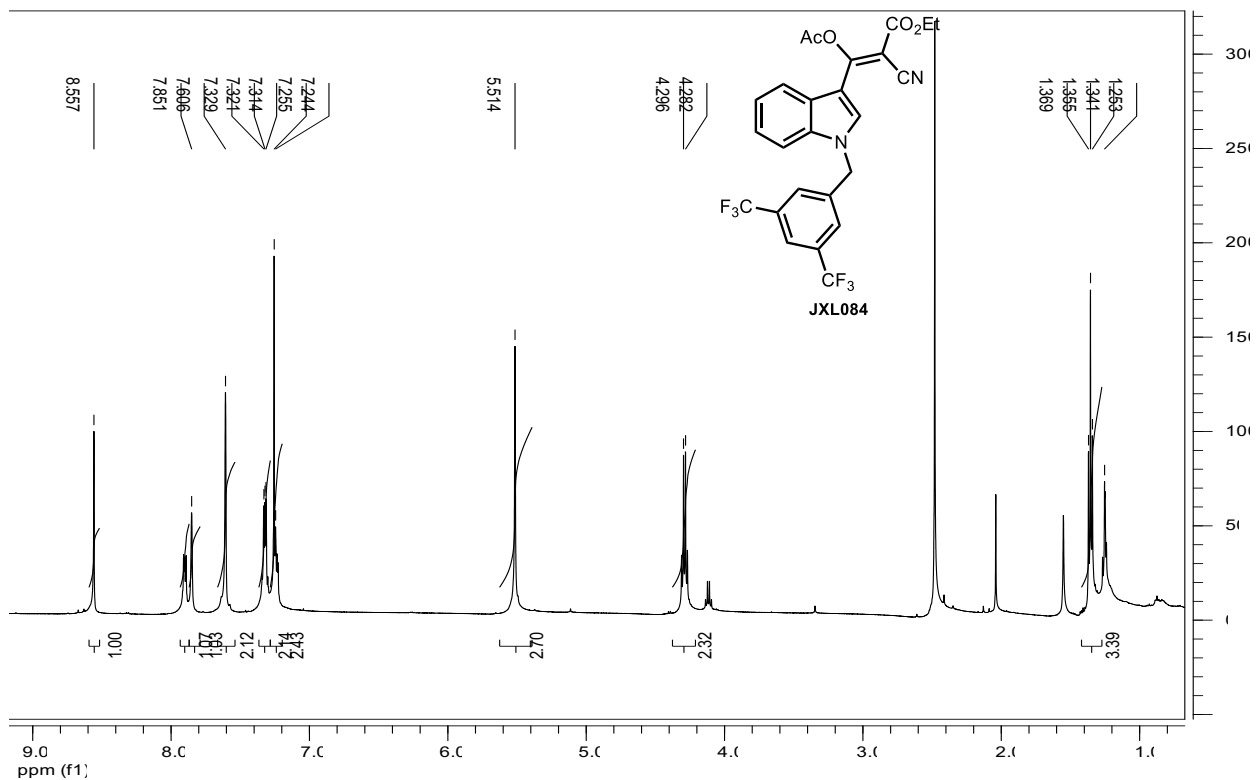
¹³C NMR (126 MHz, CDCl₃)



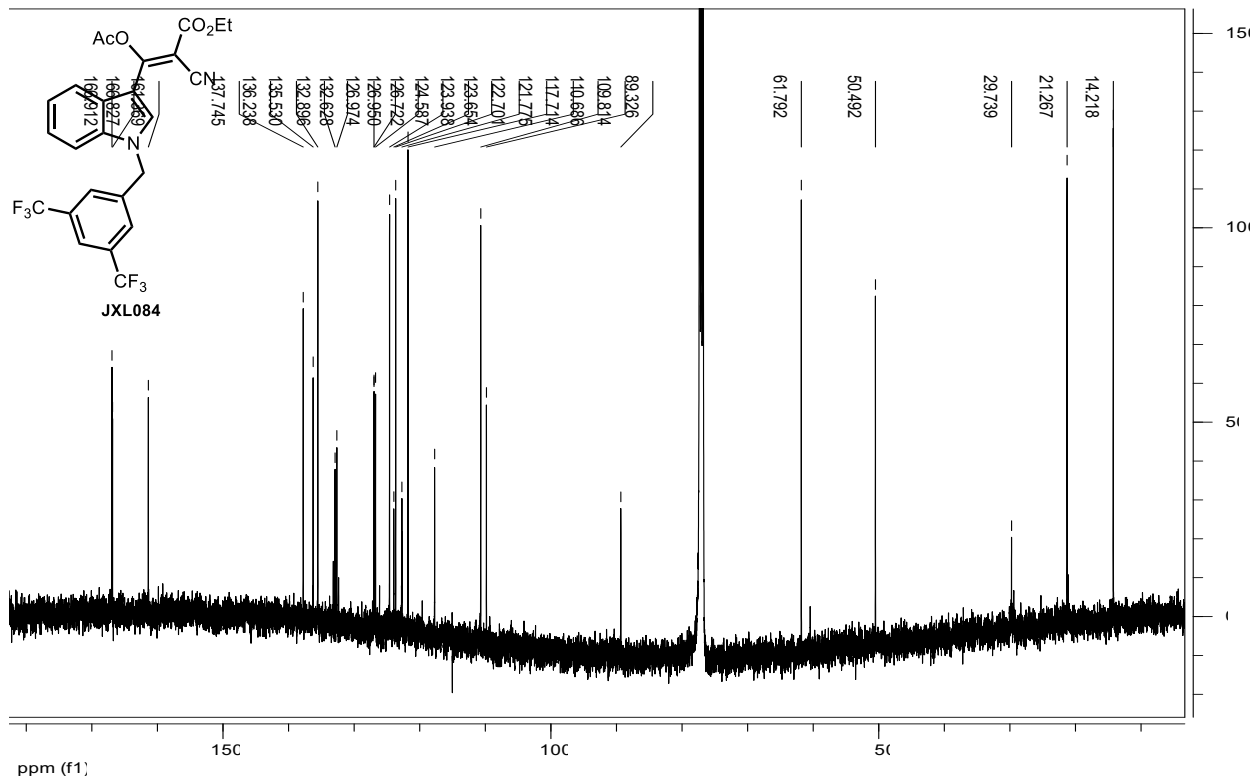
¹H NMR (500 MHz, CDCl₃)



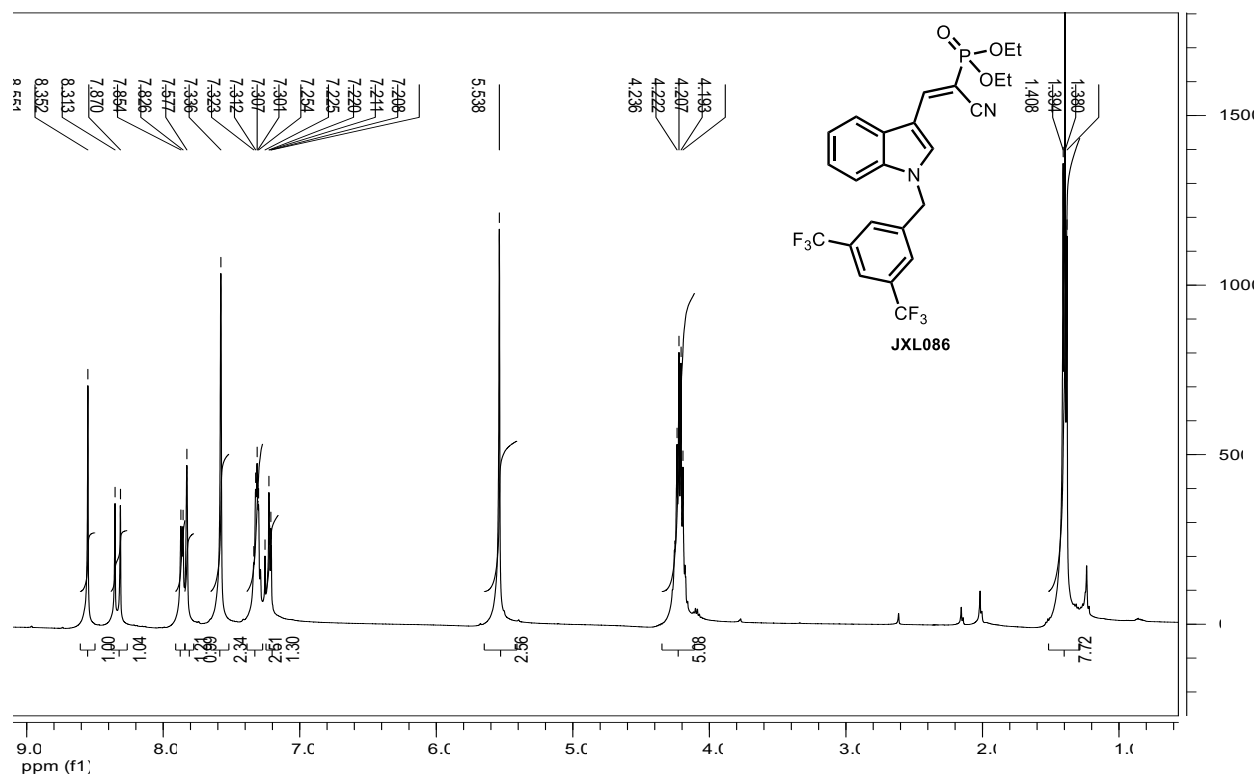
¹³C NMR (126 MHz, CDCl₃)



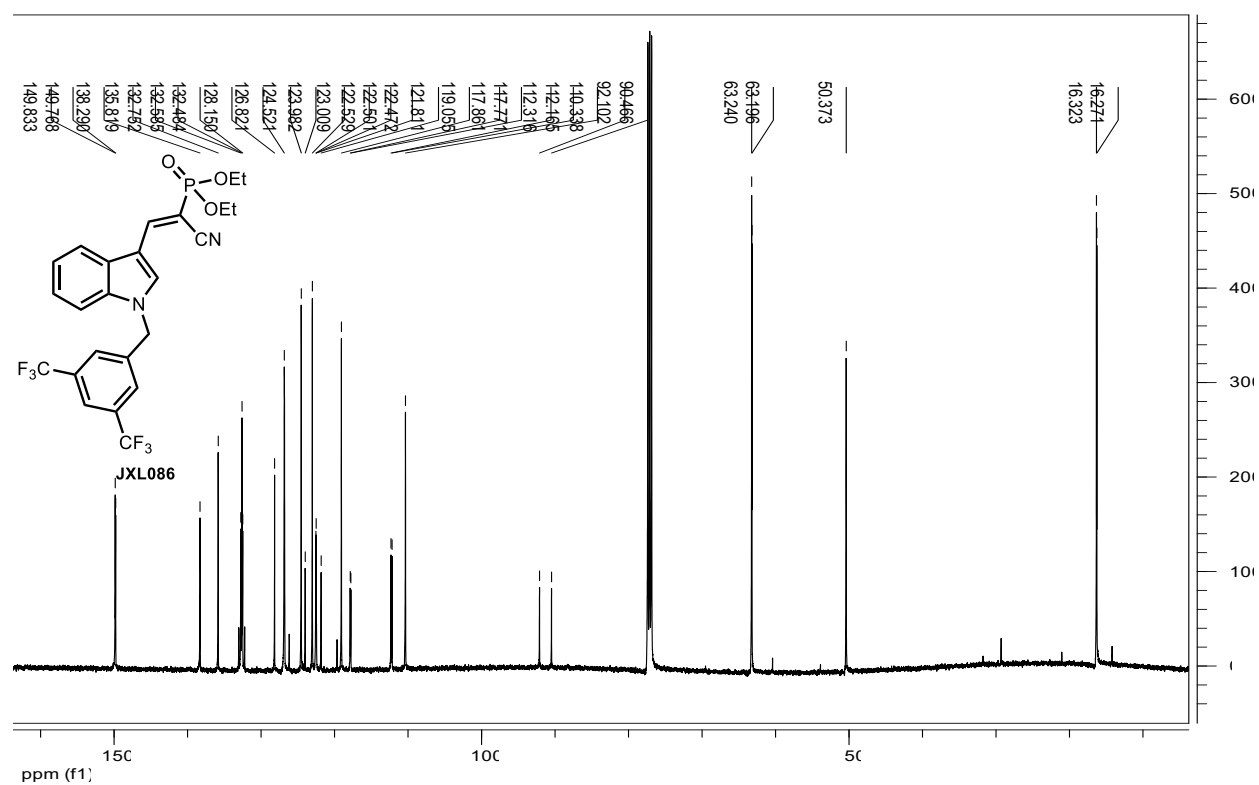
¹H NMR (500 MHz, CDCl₃)



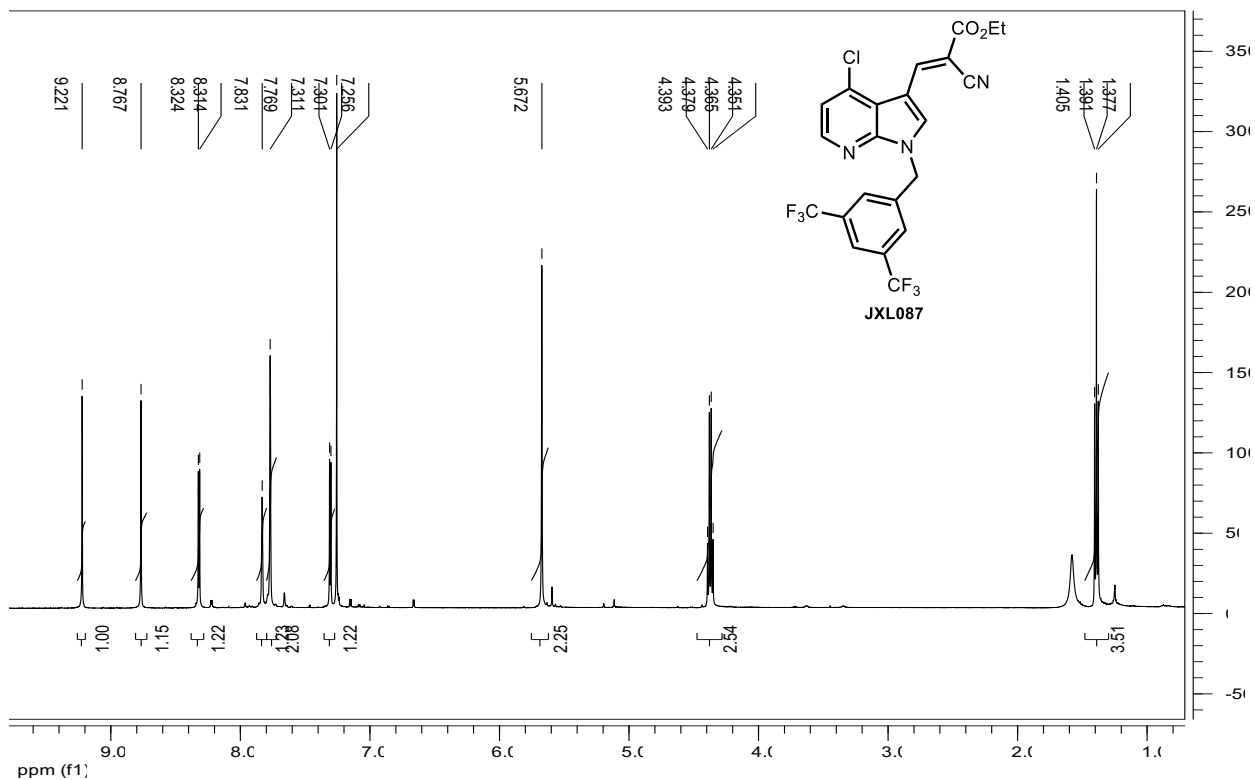
¹³C NMR (126 MHz, CDCl₃)



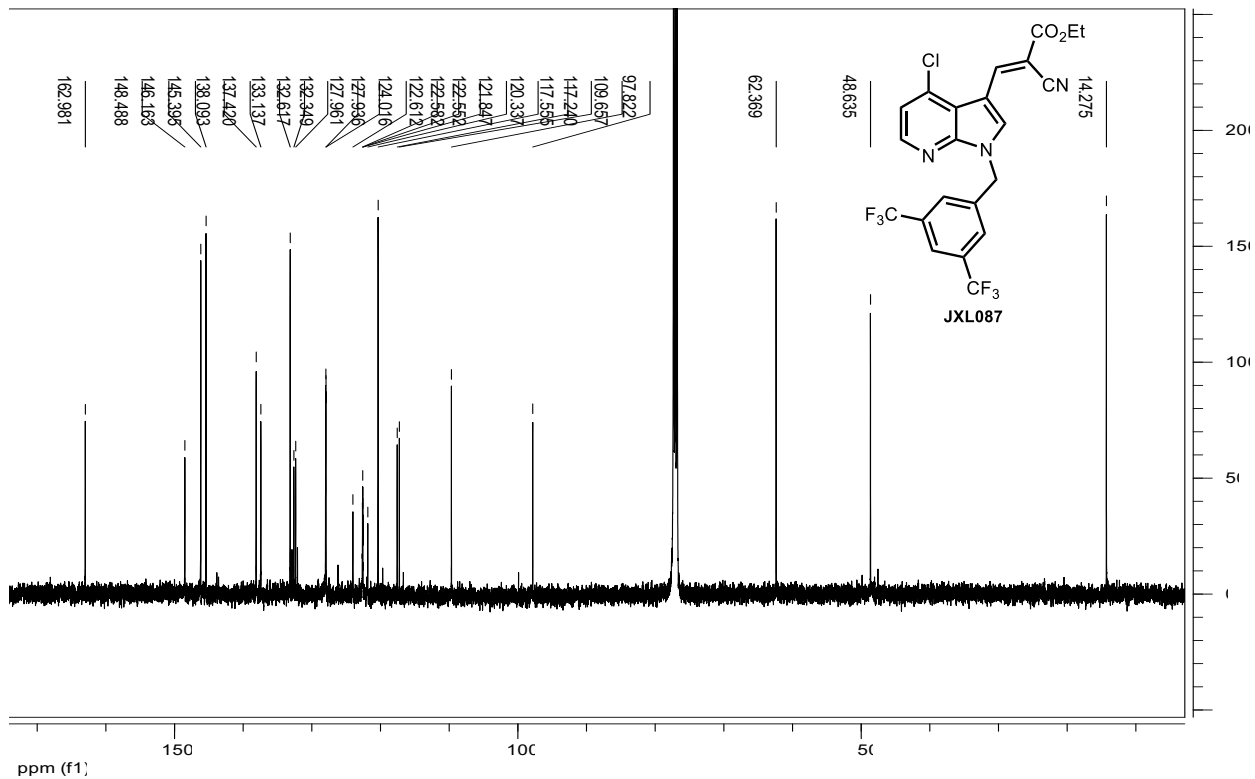
¹H NMR (500 MHz, CDCl₃)



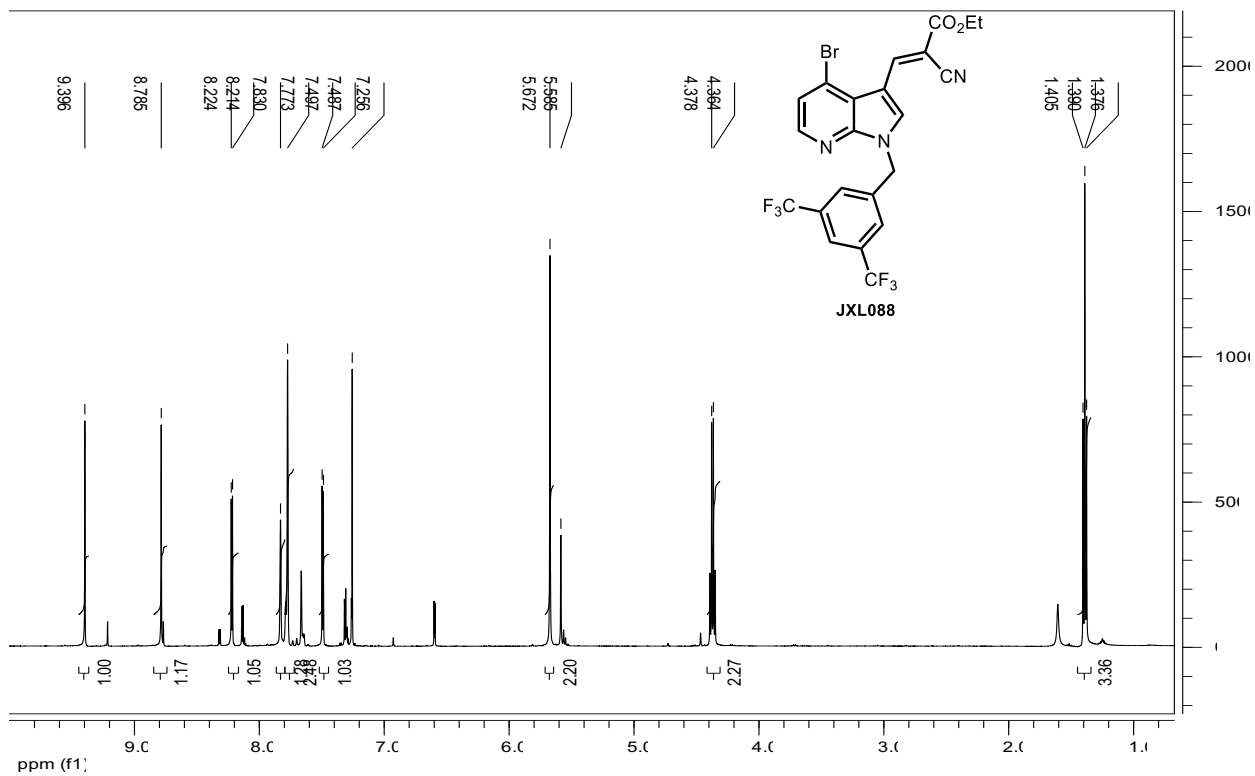
¹³C NMR (126 MHz, CDCl₃)



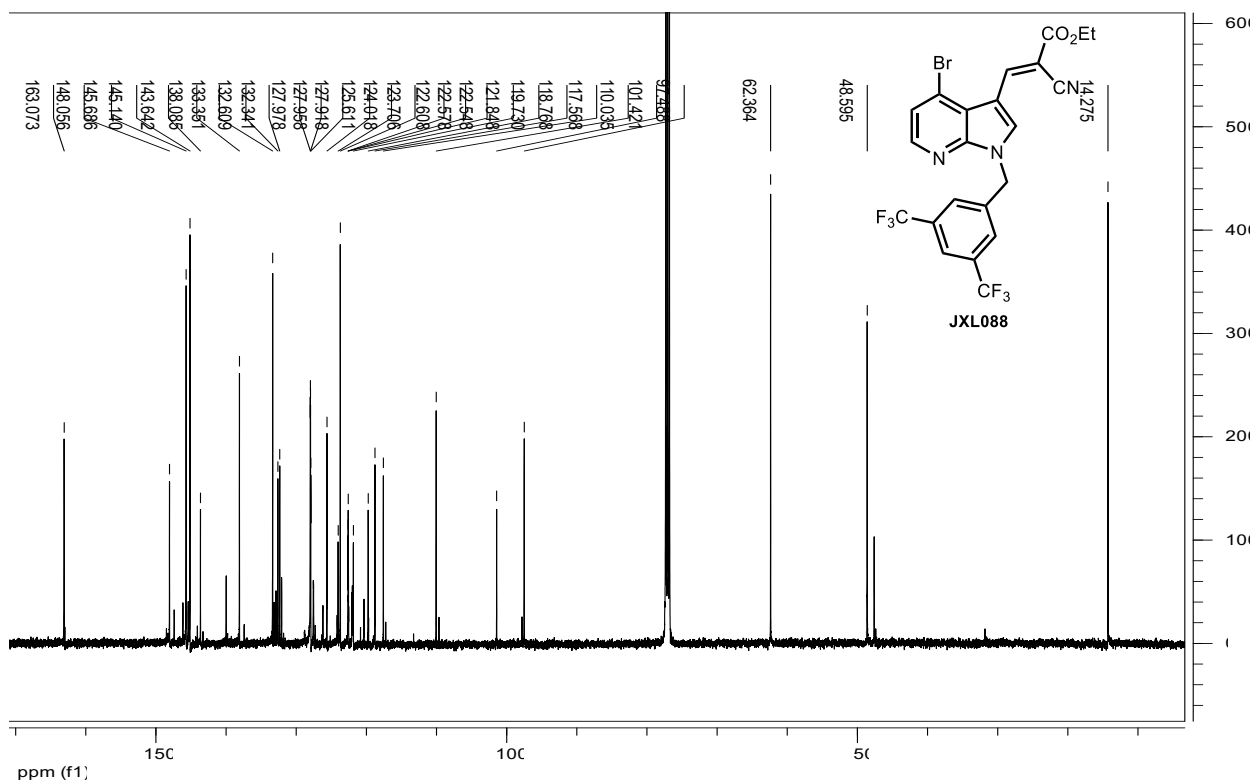
¹H NMR (500 MHz, CDCl₃)



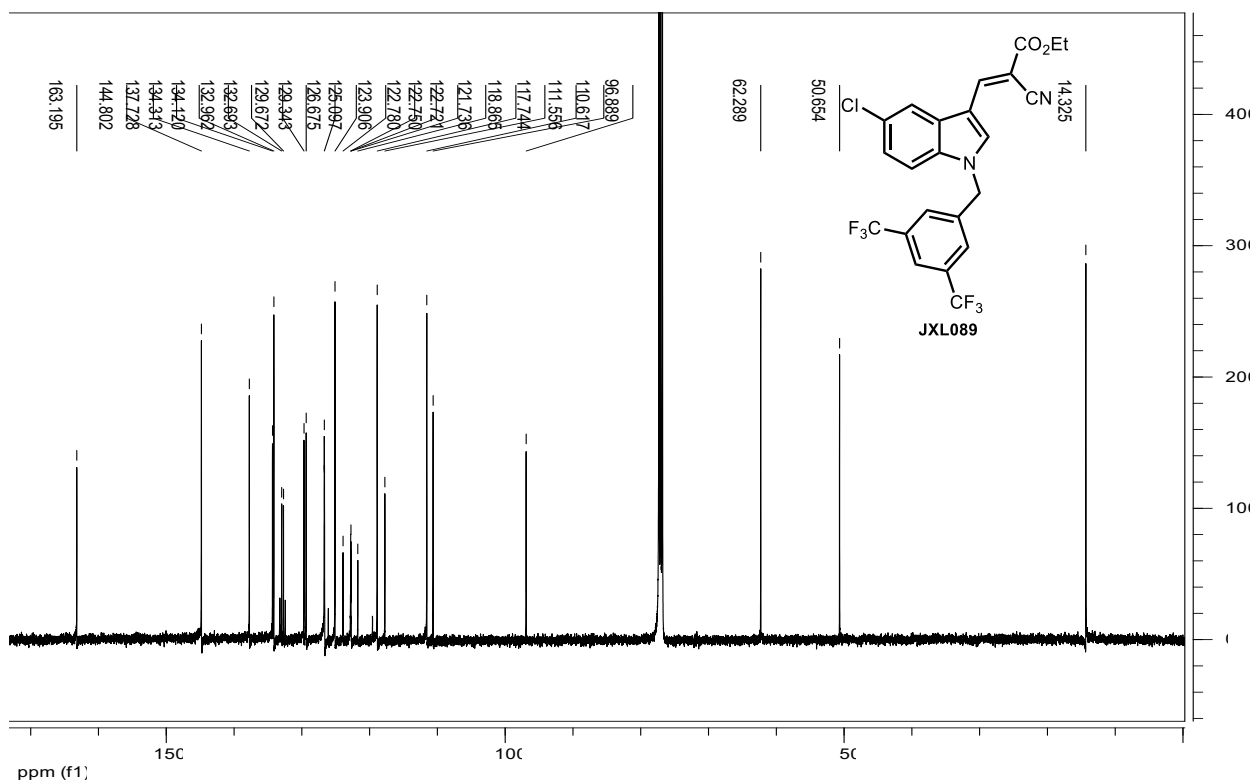
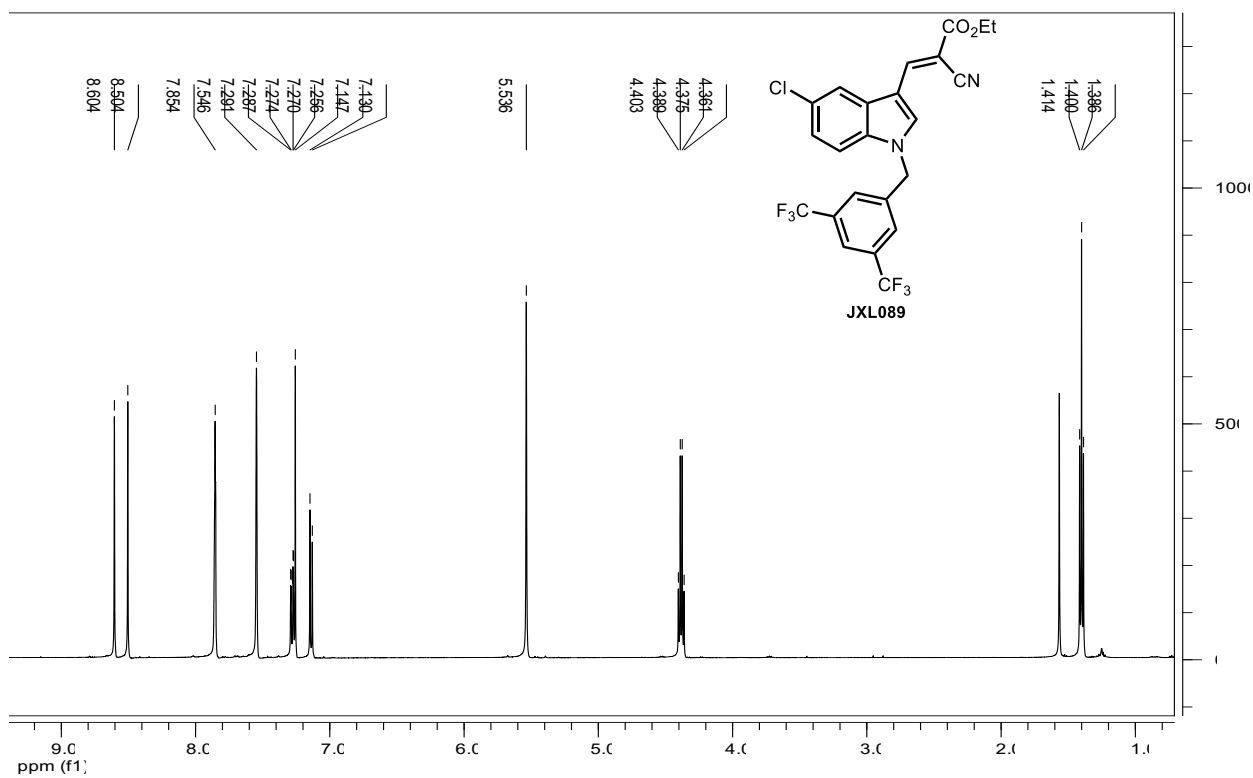
¹³C NMR (126 MHz, CDCl₃)



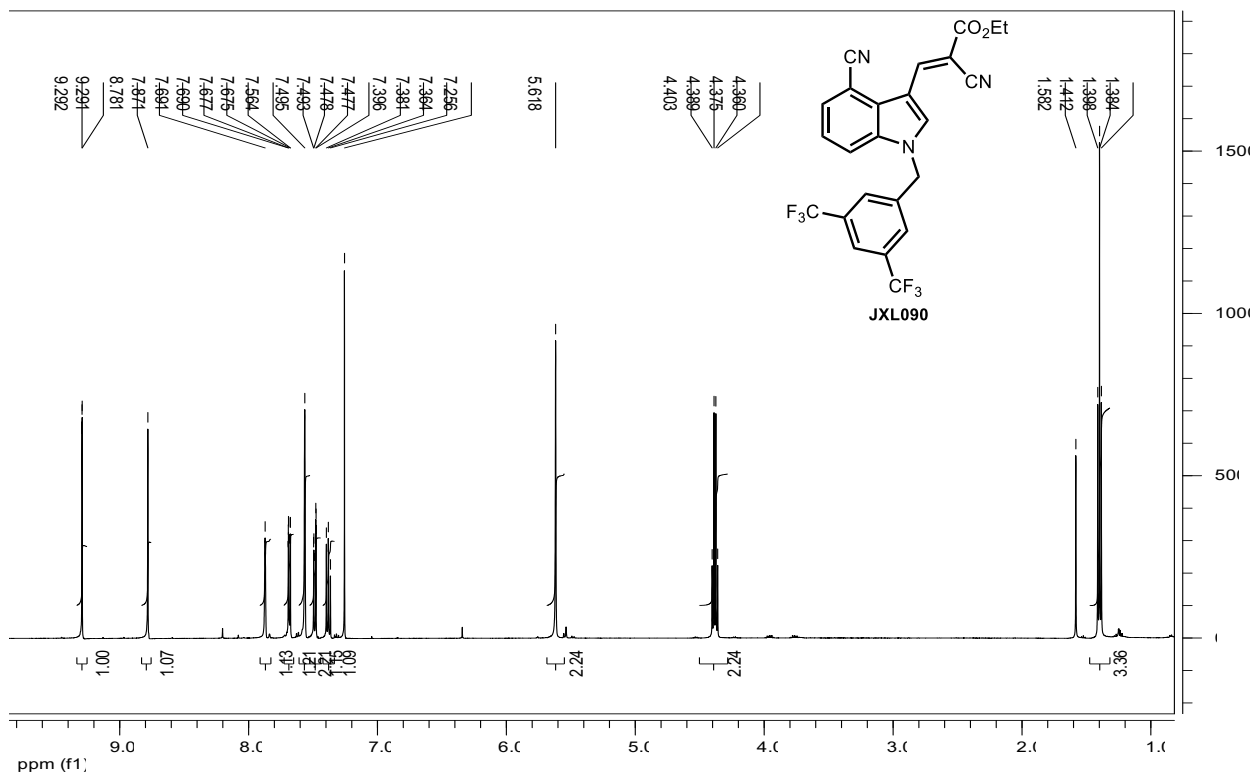
¹H NMR (500 MHz, CDCl₃)



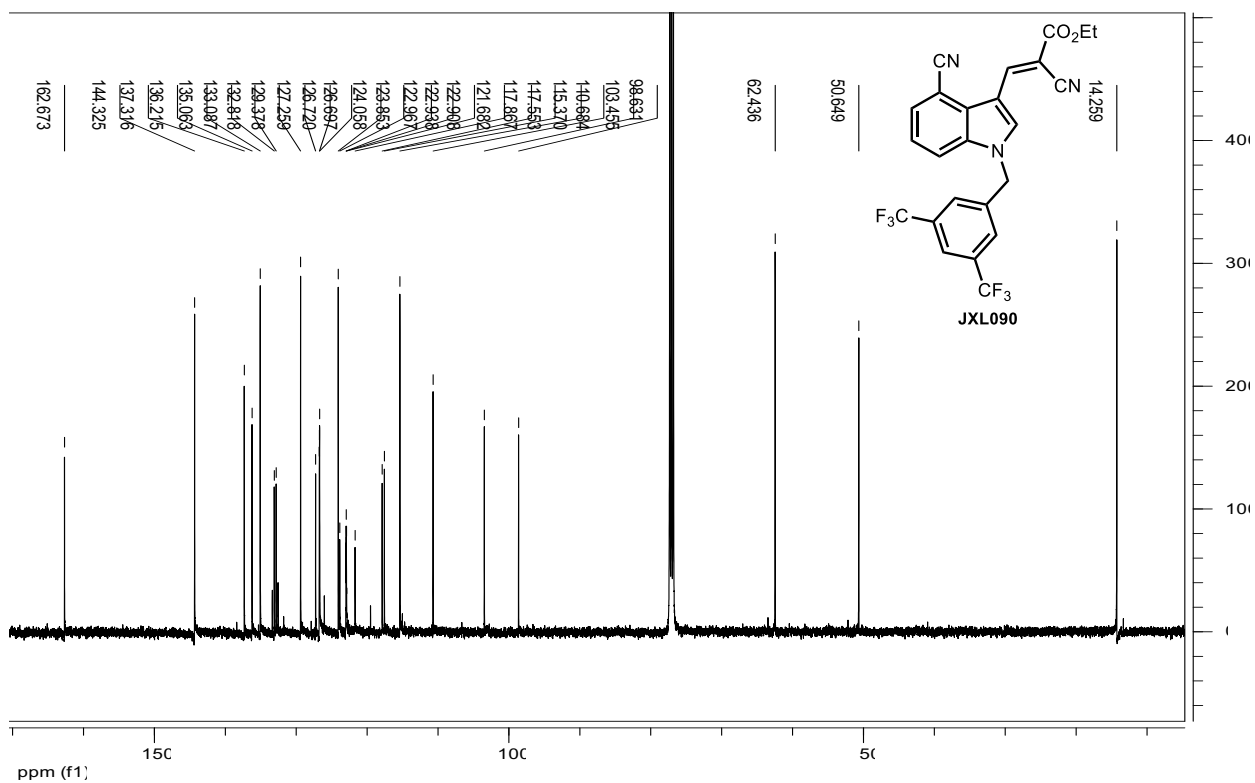
¹³C NMR (126 MHz, CDCl₃)



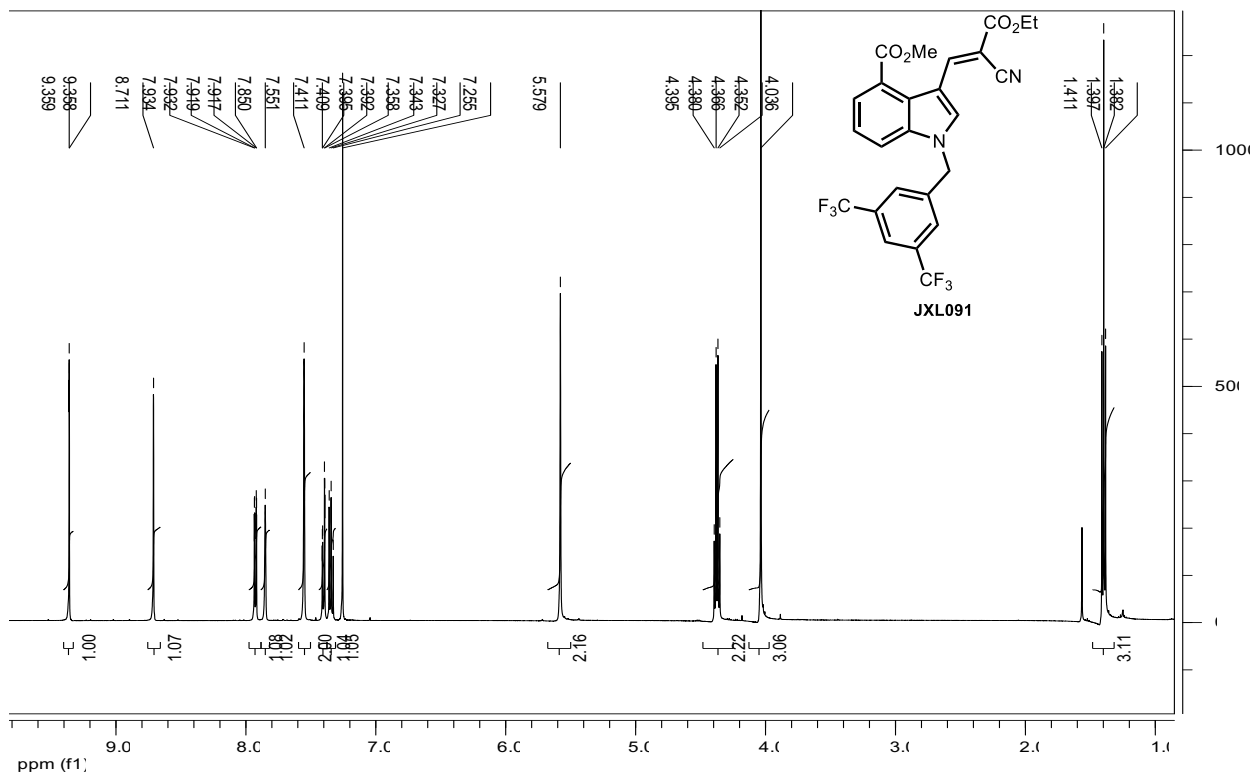
¹³C NMR (126 MHz, CDCl₃)



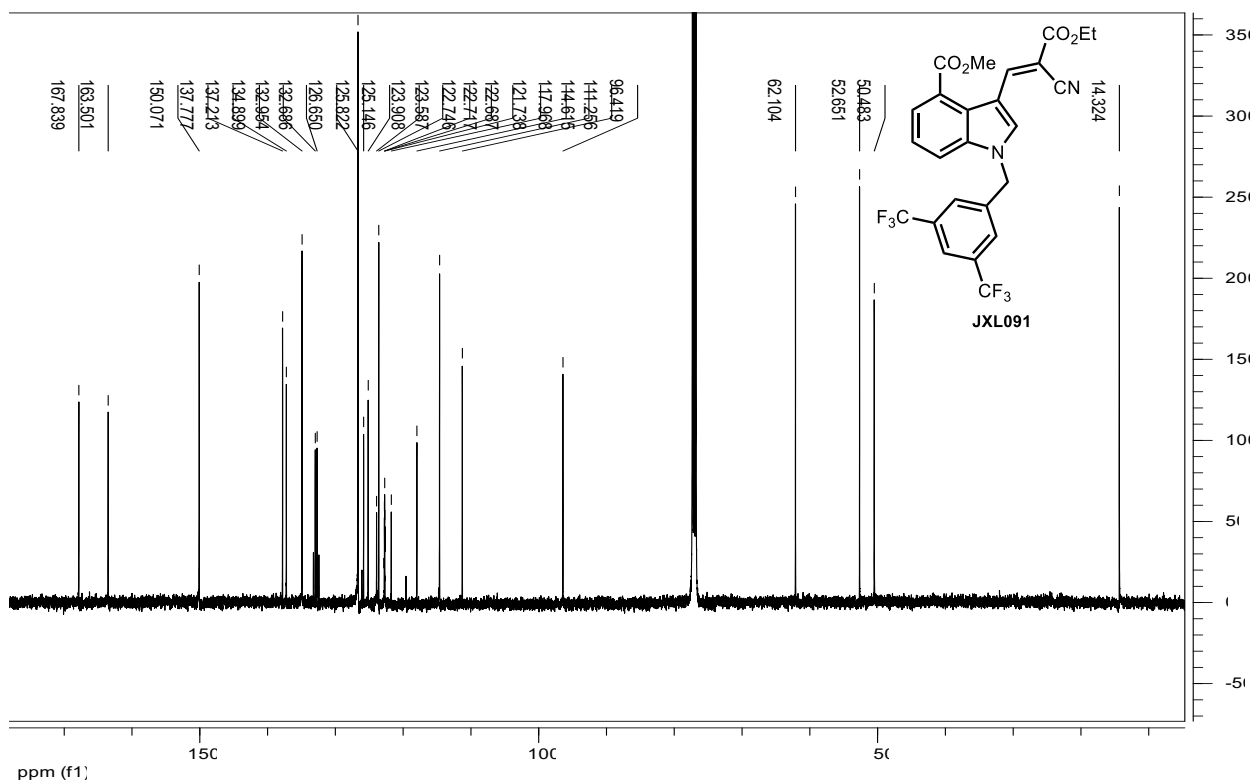
¹H NMR (500 MHz, CDCl₃)



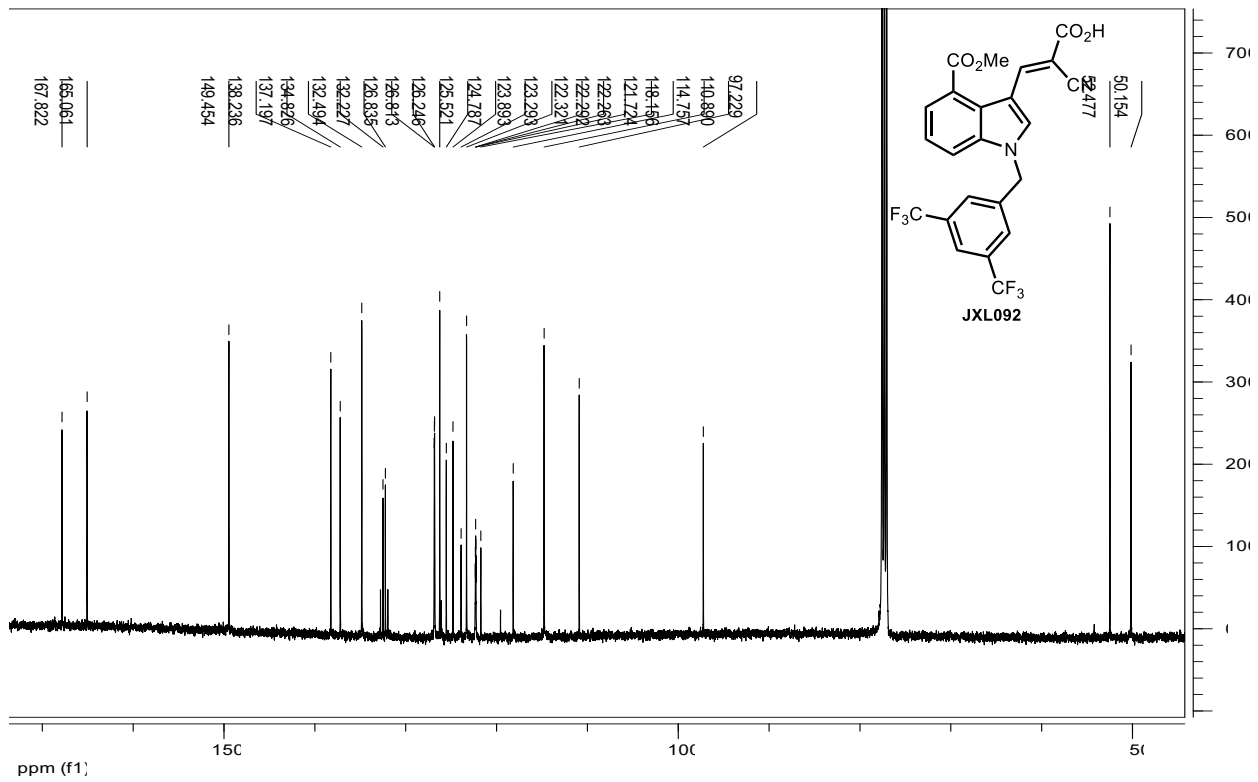
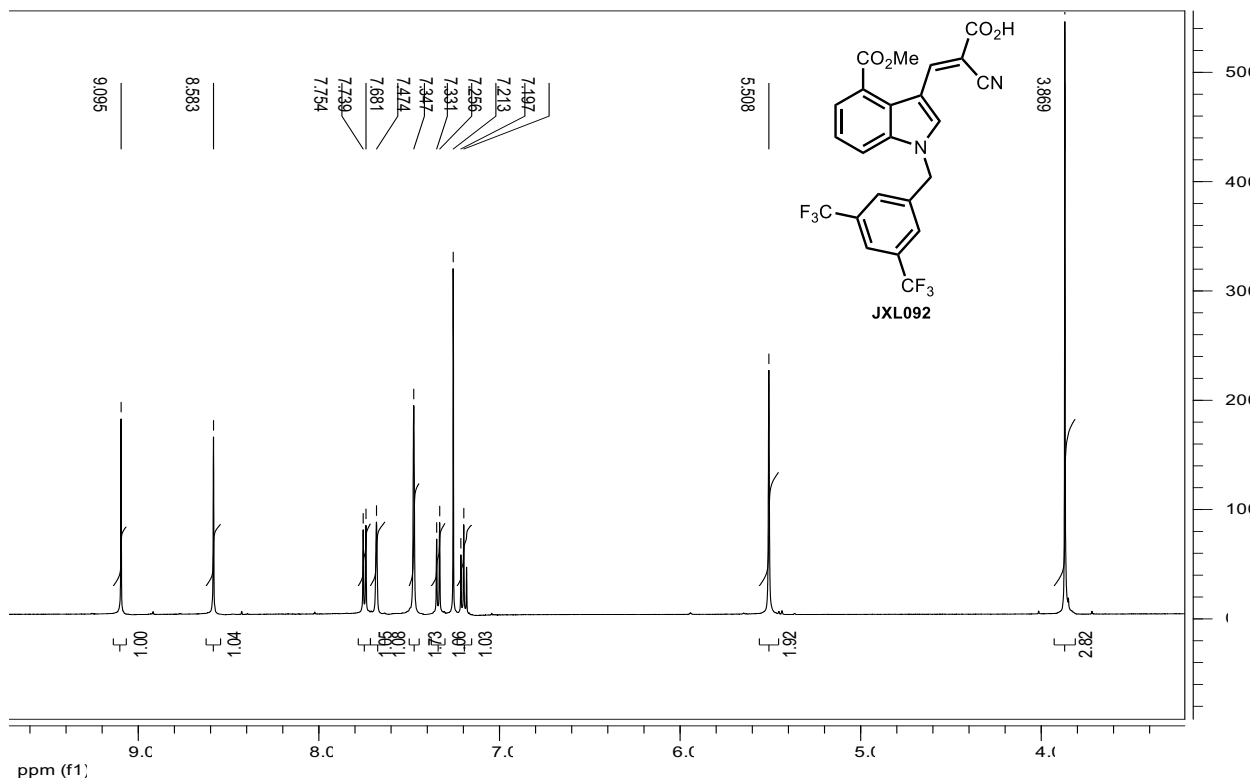
¹³C NMR (126 MHz, CDCl₃)

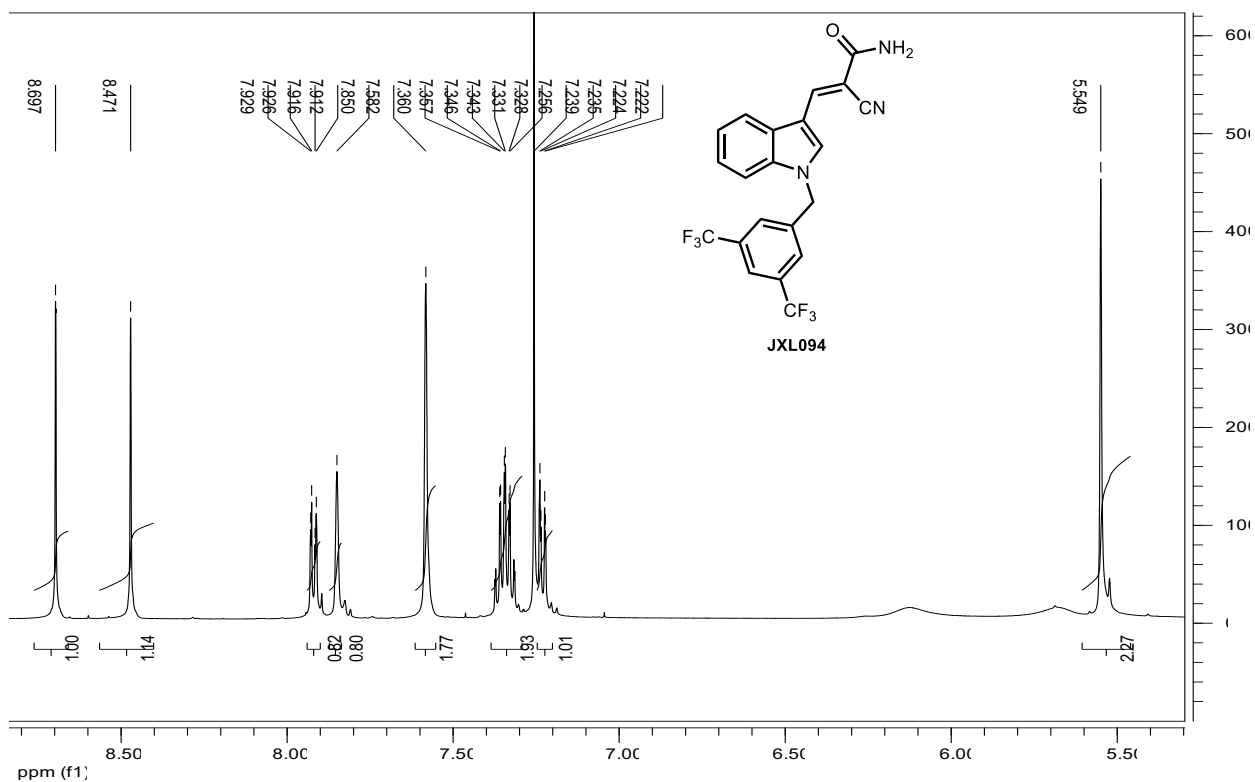


¹H NMR (500 MHz, CDCl₃)

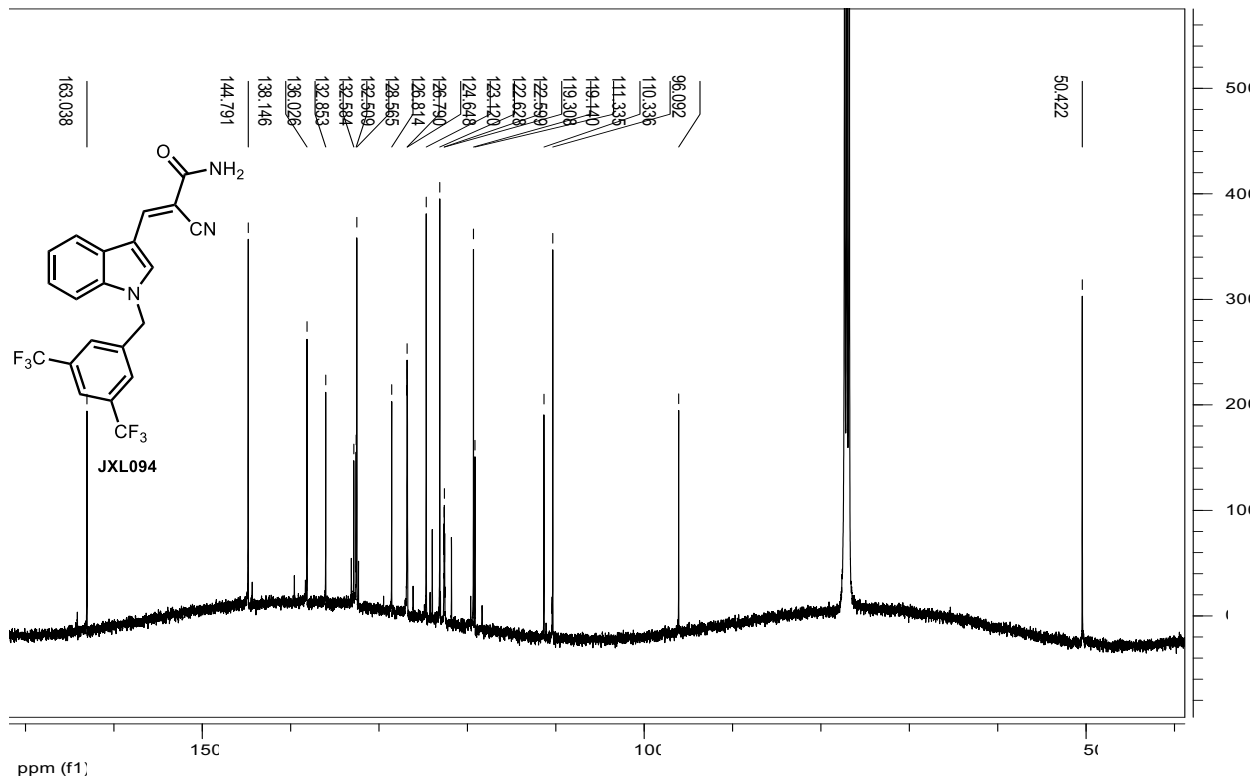


¹³C NMR (126 MHz, CDCl₃)

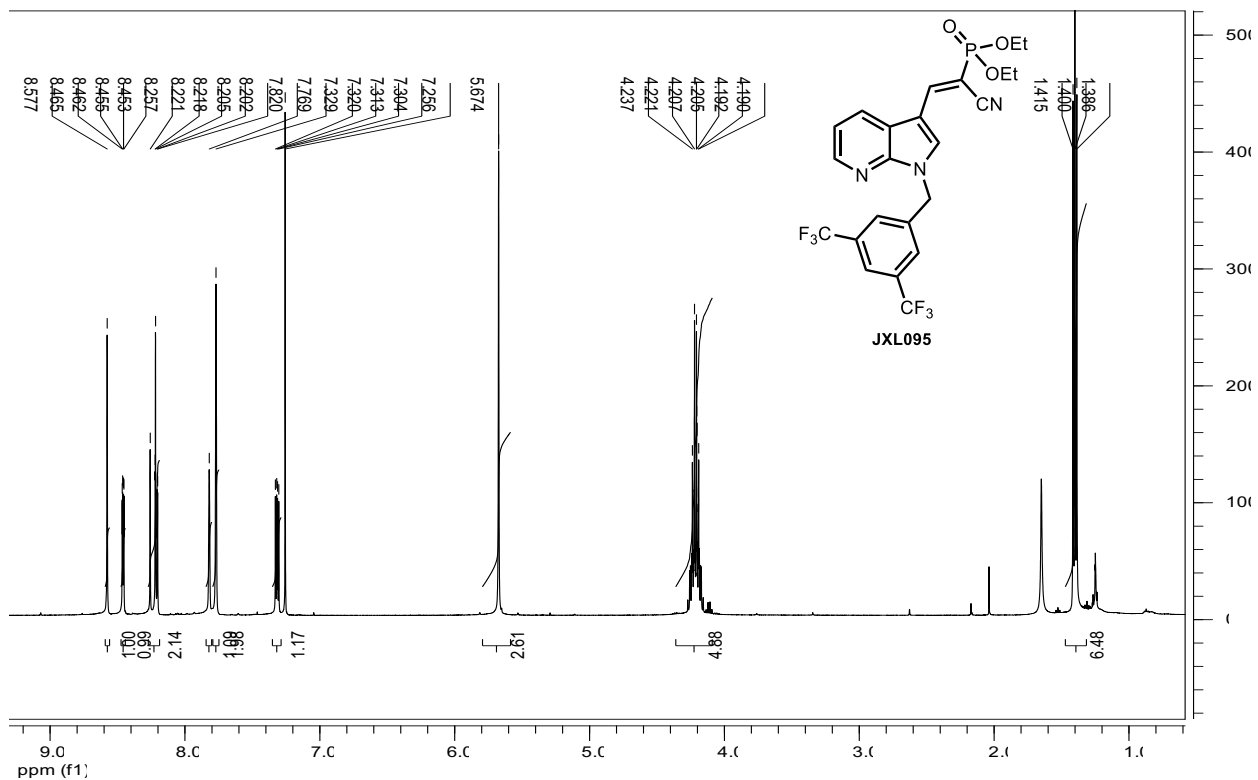




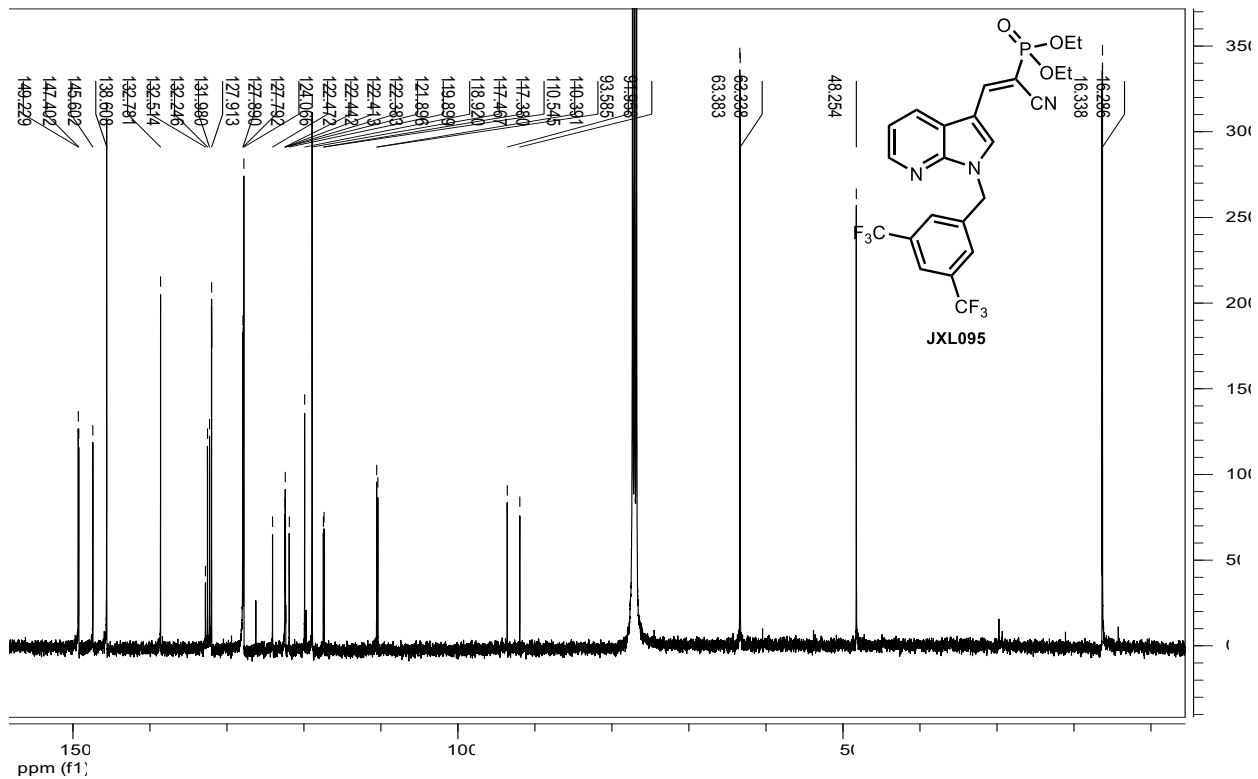
¹H NMR (500 MHz, CDCl₃)



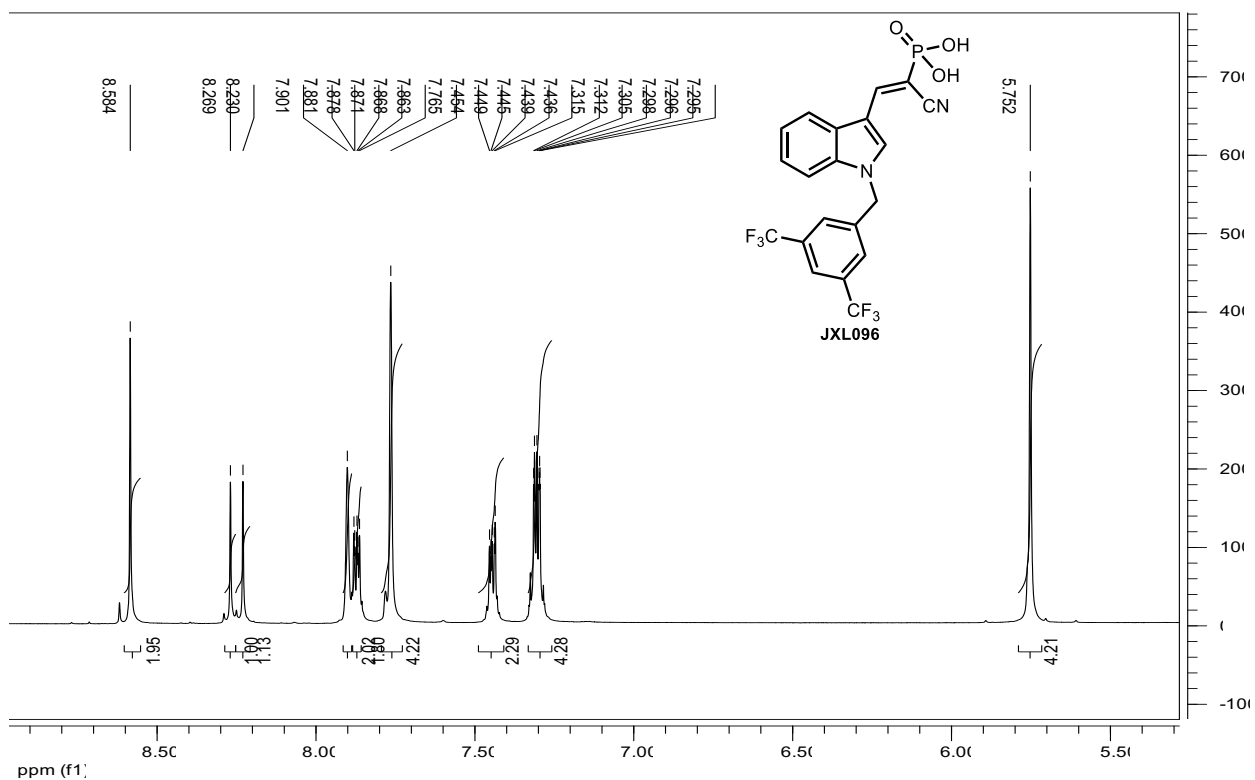
¹³C NMR (126 MHz, CDCl₃)



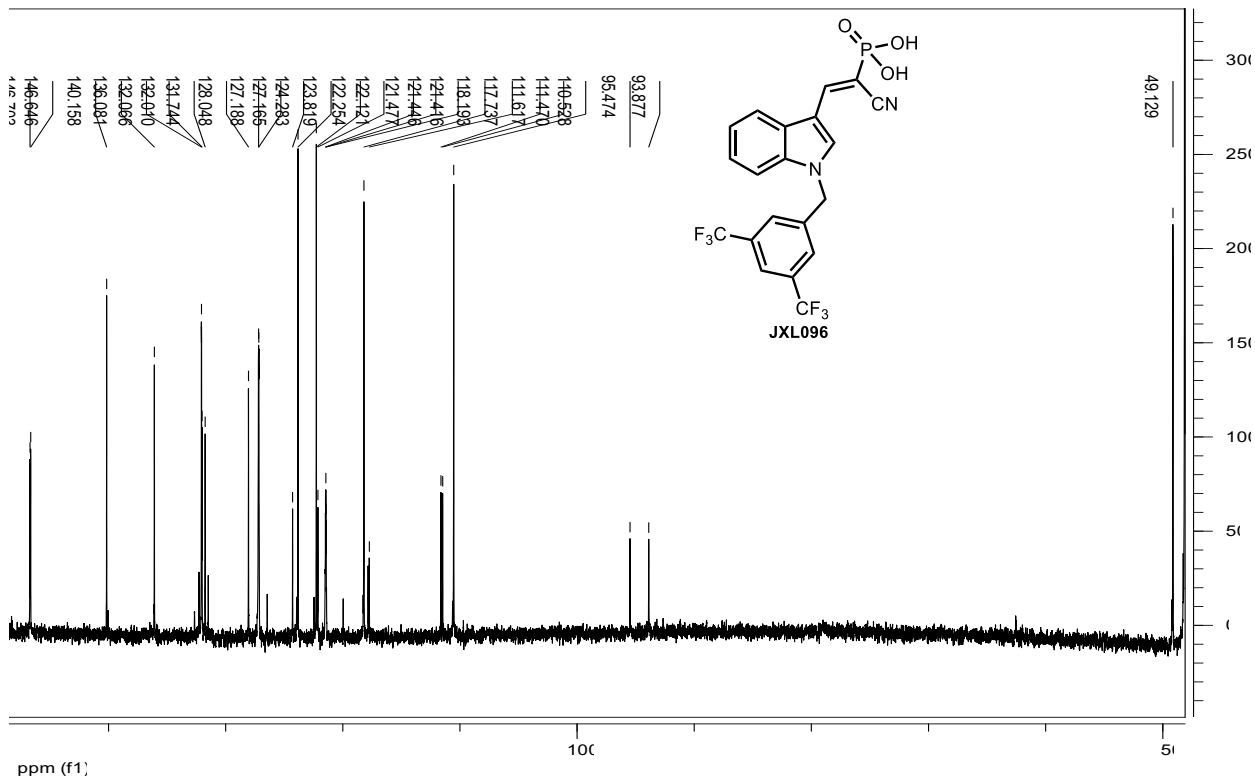
¹H NMR (500 MHz, CDCl₃)



¹³C NMR (126 MHz, CDCl₃)



¹H NMR (500 MHz, DMSO-d₆)



¹³C NMR (126 MHz, DMSO-d₆)