

Supplementary Information

A comparison of the structural motifs and packing arrangements of six novel derivatives and one polymorph of 2-(1-Phenyl-1H-1,2,3-triazol-4-yl)pyridine

Kinaan M. Tawfiq,^{a,b} Gary J. Miller,^c Mohamad J. Al-Jeboori,^d Paul S. Fennell,^d Simon J. Coles,^e Graham J. Tizzard,^e Claire Wilson^f and Herman Potgeiter.^g

a Division of Chemistry and Environmental Sciences, School of Science and the Environment, Manchester Metropolitan University, Chester Street, Manchester, M1 5GD, UK.

b Department of Chemistry, College of Education for Pure Sciences – Ibn Al-Haitham, University of Baghdad, Republic of Iraq

c Analytical Sciences, Manchester Metropolitan University, Chester Street, Manchester, M1 5GD, UK.

d Department of Chemical Engineering and Chemical Technology, Imperial College London, London, SW7 2AZ, UK.

e EPSRC National Crystallography Service, School of Chemistry, University of Southampton, Southampton, SO17 1BJ, UK.

f Diamond Light Source Ltd, Diamond House, Harwell Science and Innovation Campus, Didcot, Oxfordshire, OX11 0DE, UK.

g School of Research, Enterprise and Innovation, Manchester Metropolitan University, Chester Street, Manchester, M1 5GD, UK.

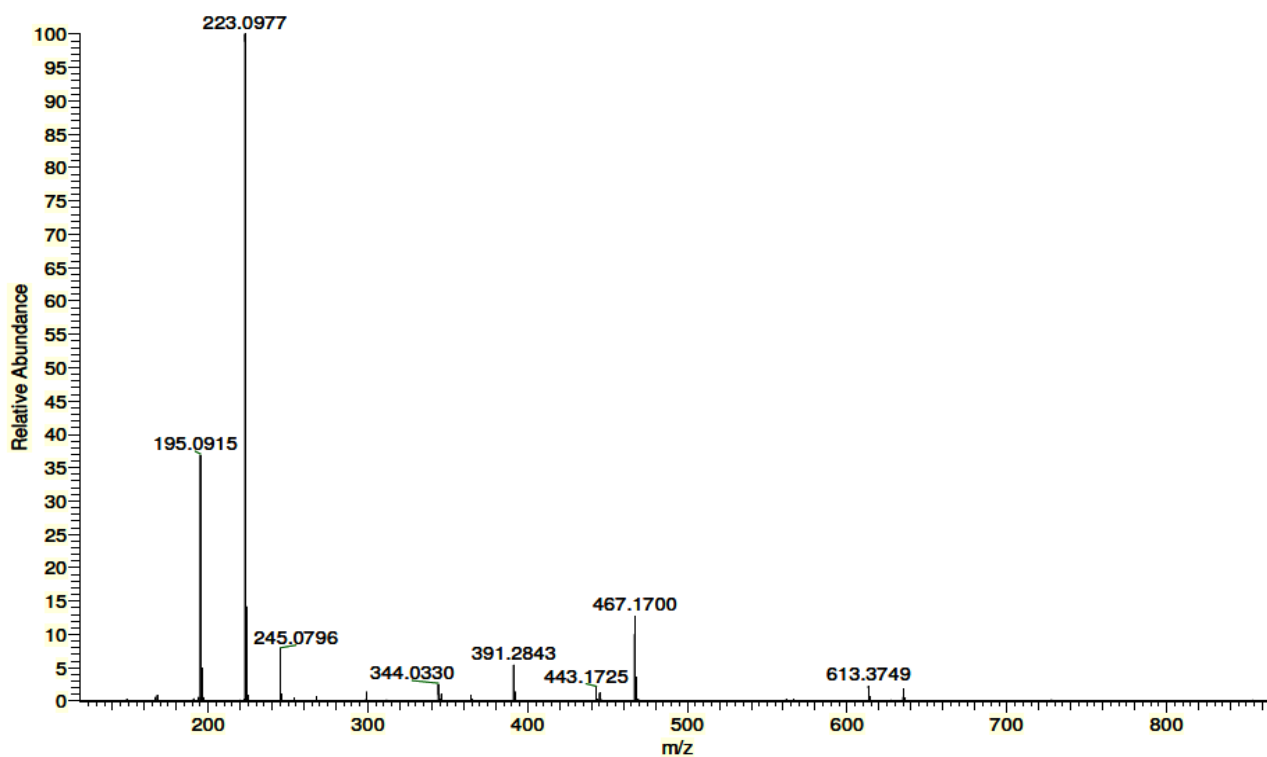


Figure SI 1. The accurate mass spectrum for ligand, 2-(1-phenyl-1H-1, 2, 3-triazol-4-yl) pyridine (L1)

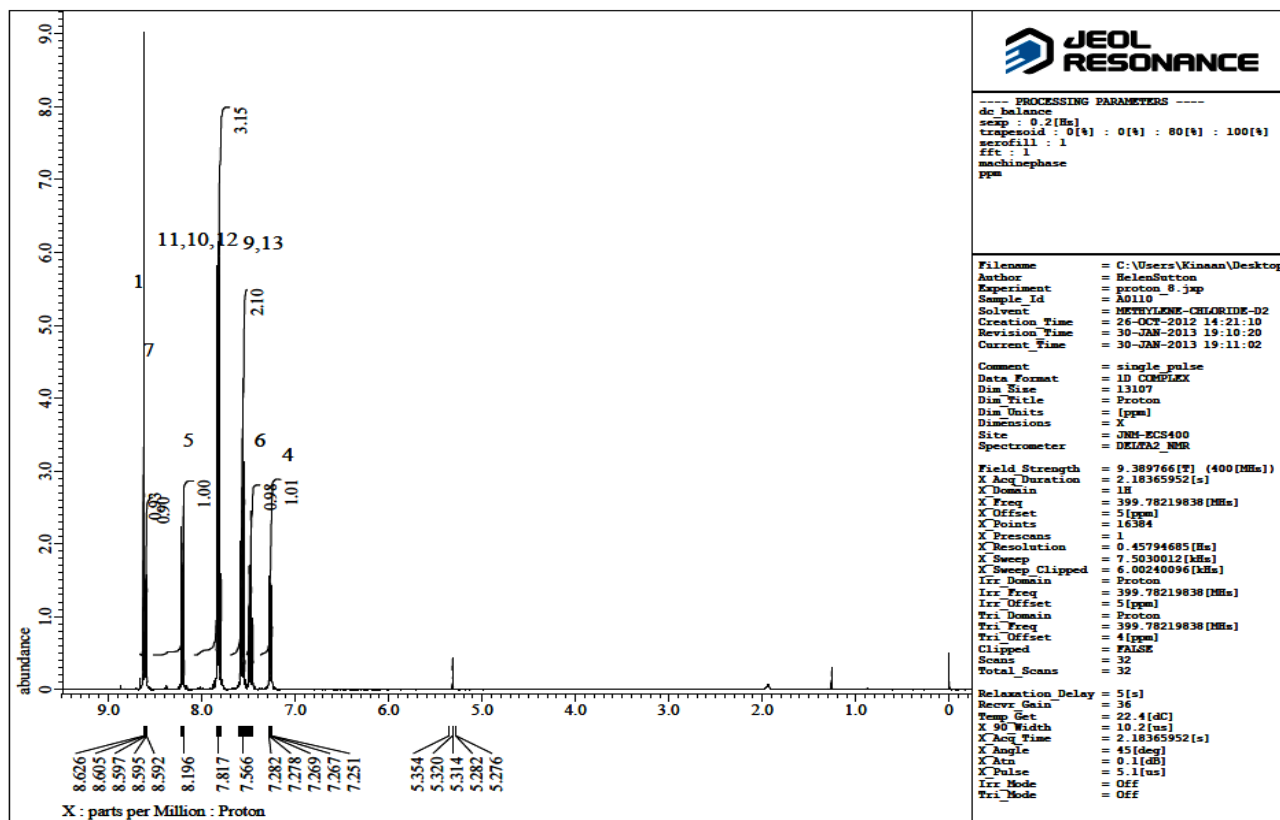


Figure SI 2. ¹H NMR spectrum for L1 in CDCl₃

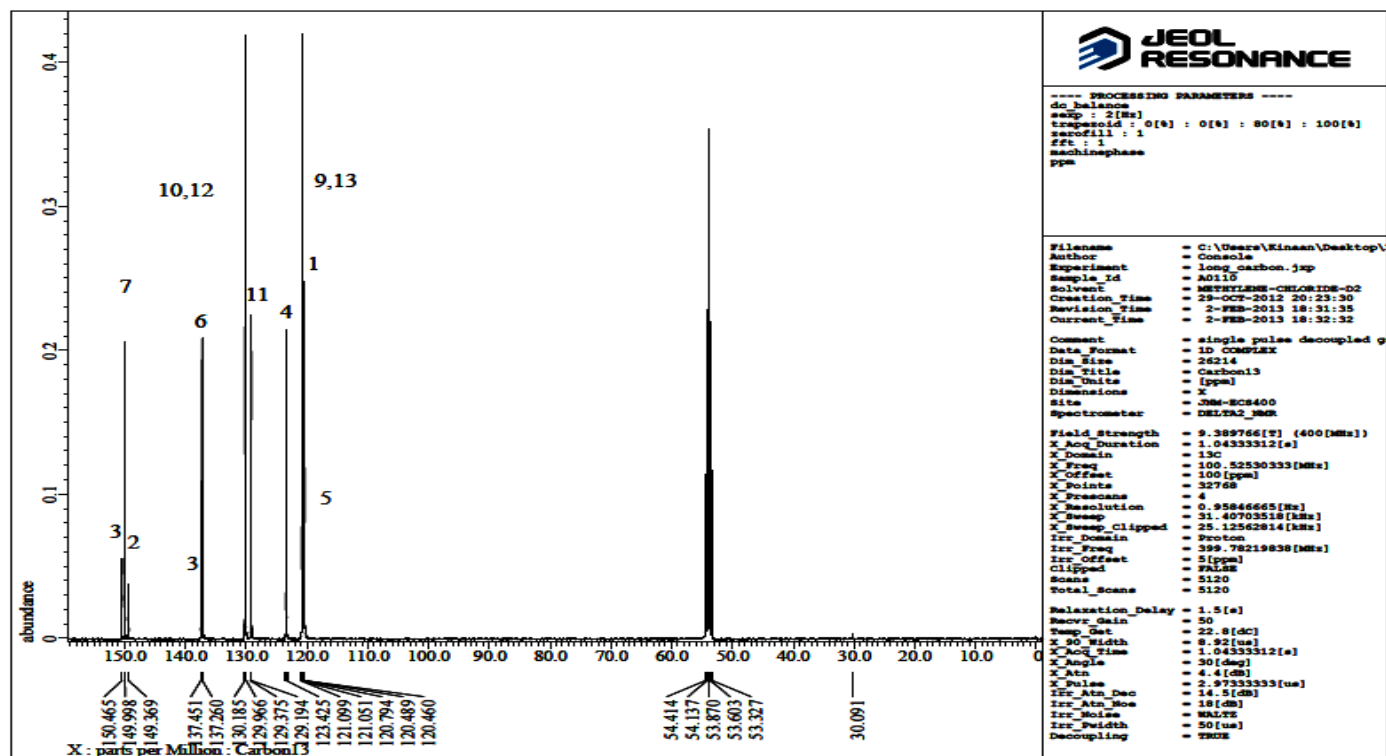


Figure SI 3. ^{13}C NMR spectrum for L1 in CDCl_3

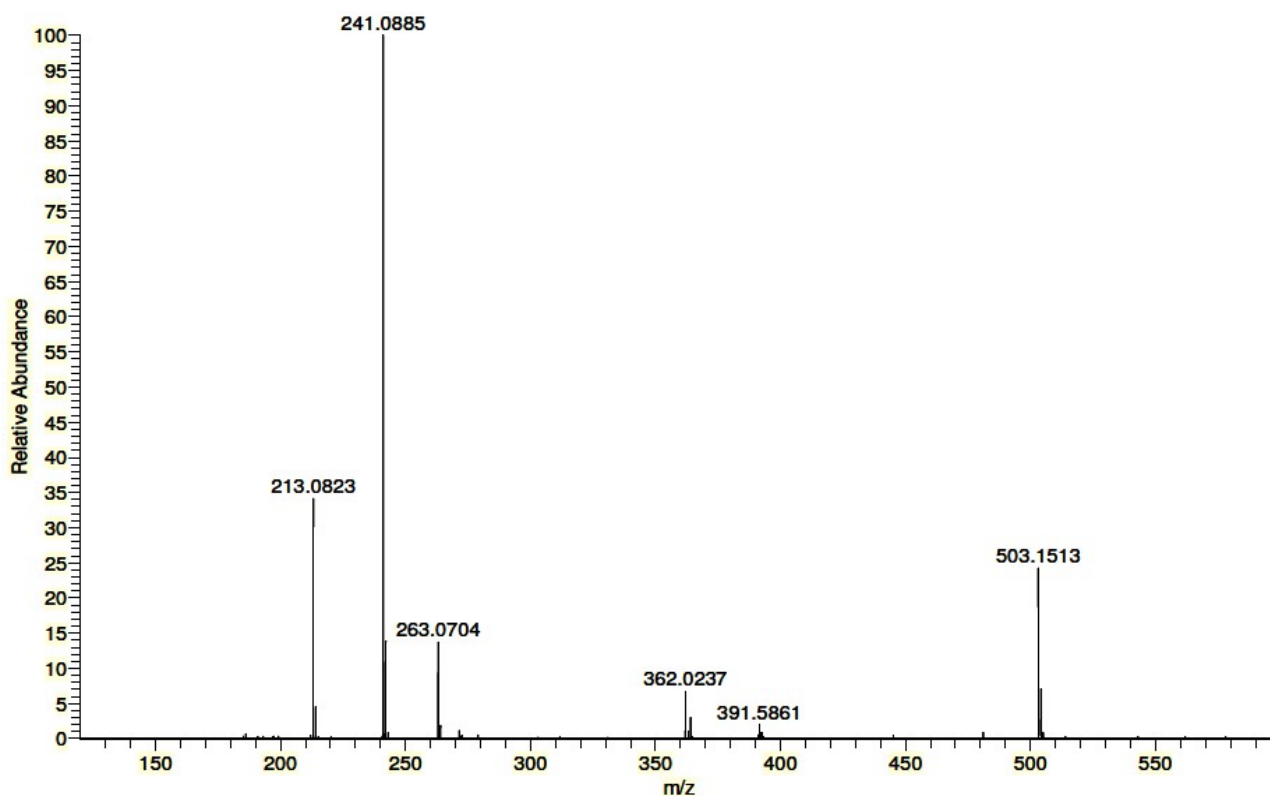


Figure SI 4. The accurate mass spectrum for ligand, 2-(1-(4-fluorophenyl)-1H-1, 2, 3-triazol-4-yl)-pyridine (L3)

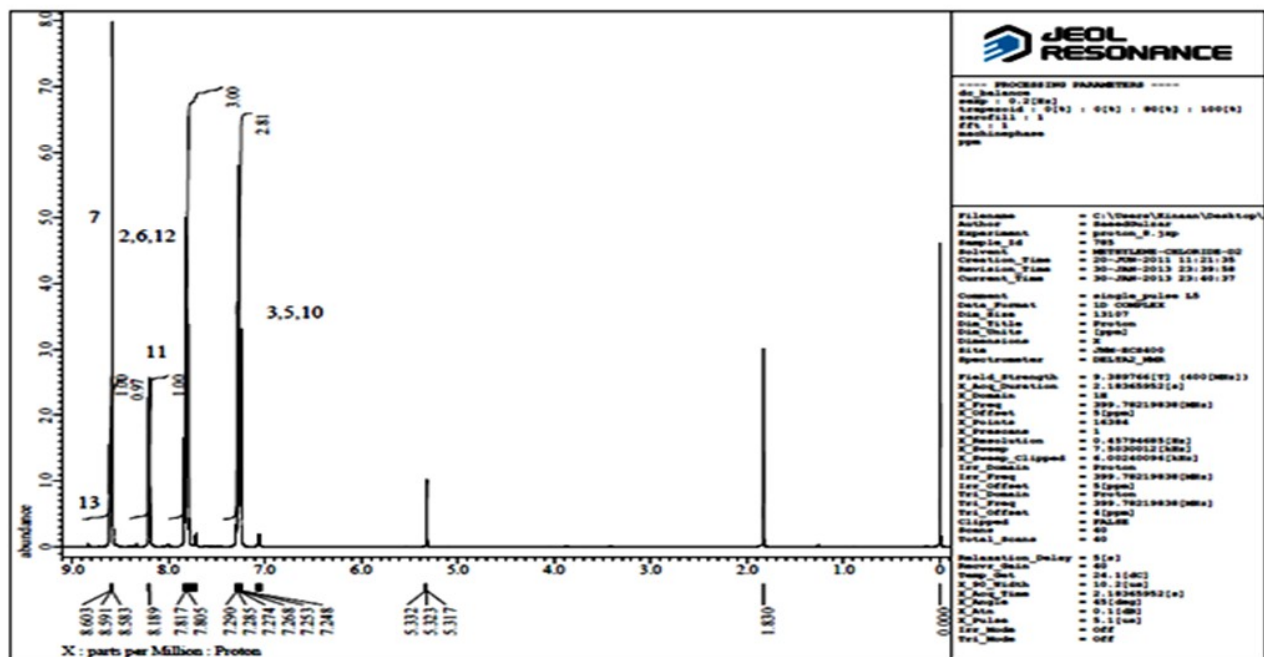


Figure SI 5. ^1H NMR spectrum for L3 in CD_2Cl_2

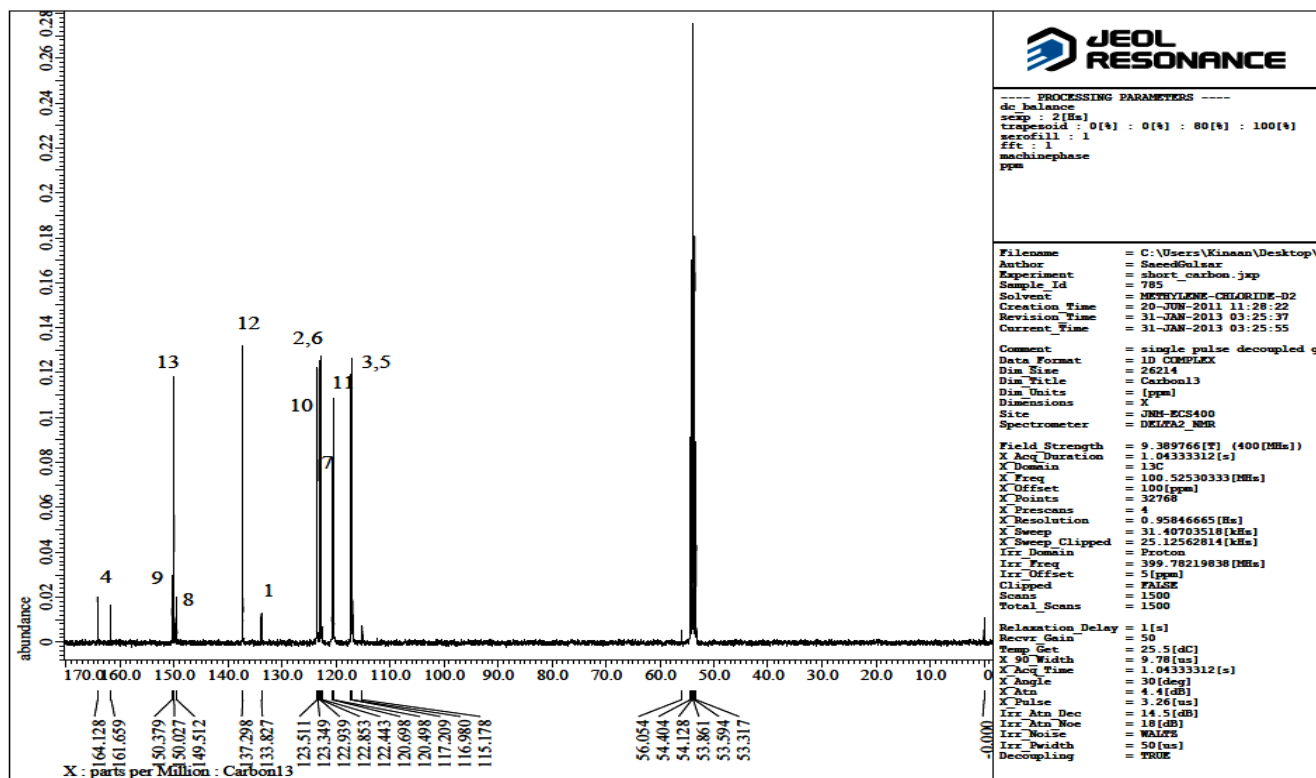


Figure SI 6. ^{13}C NMR spectrum for L3 in CD_2Cl_2

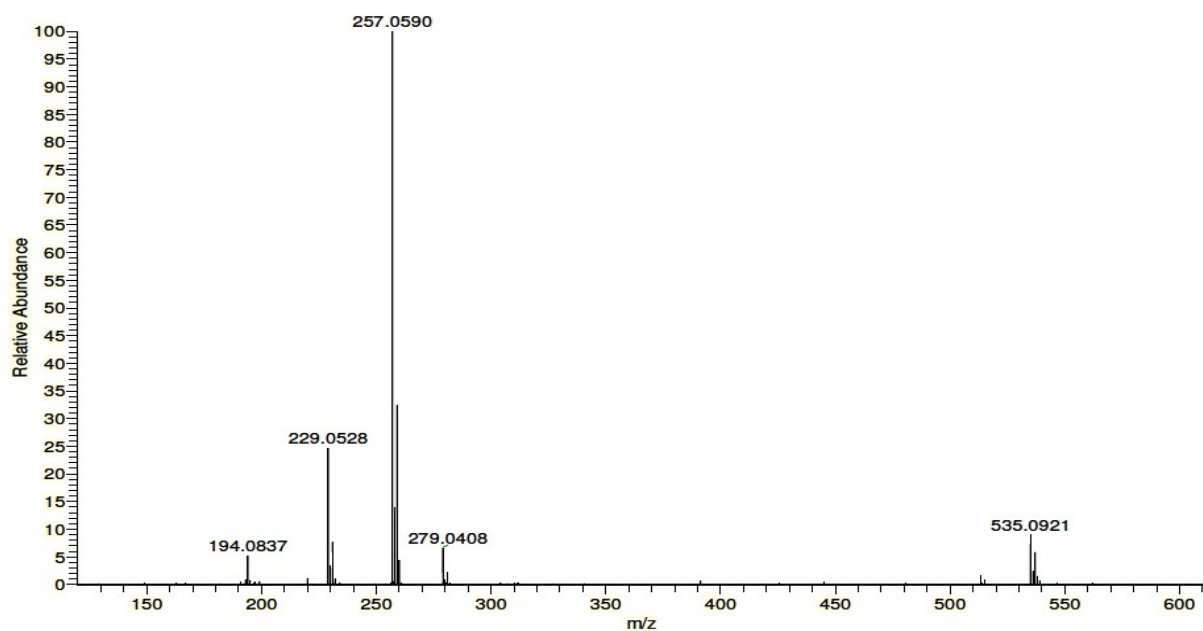


Figure SI 7. The accurate mass spectrum for ligand, 2-(1-(4-chlororophenyl)-1H-1,2,3-triazol-4-yl)pyridine (L4)

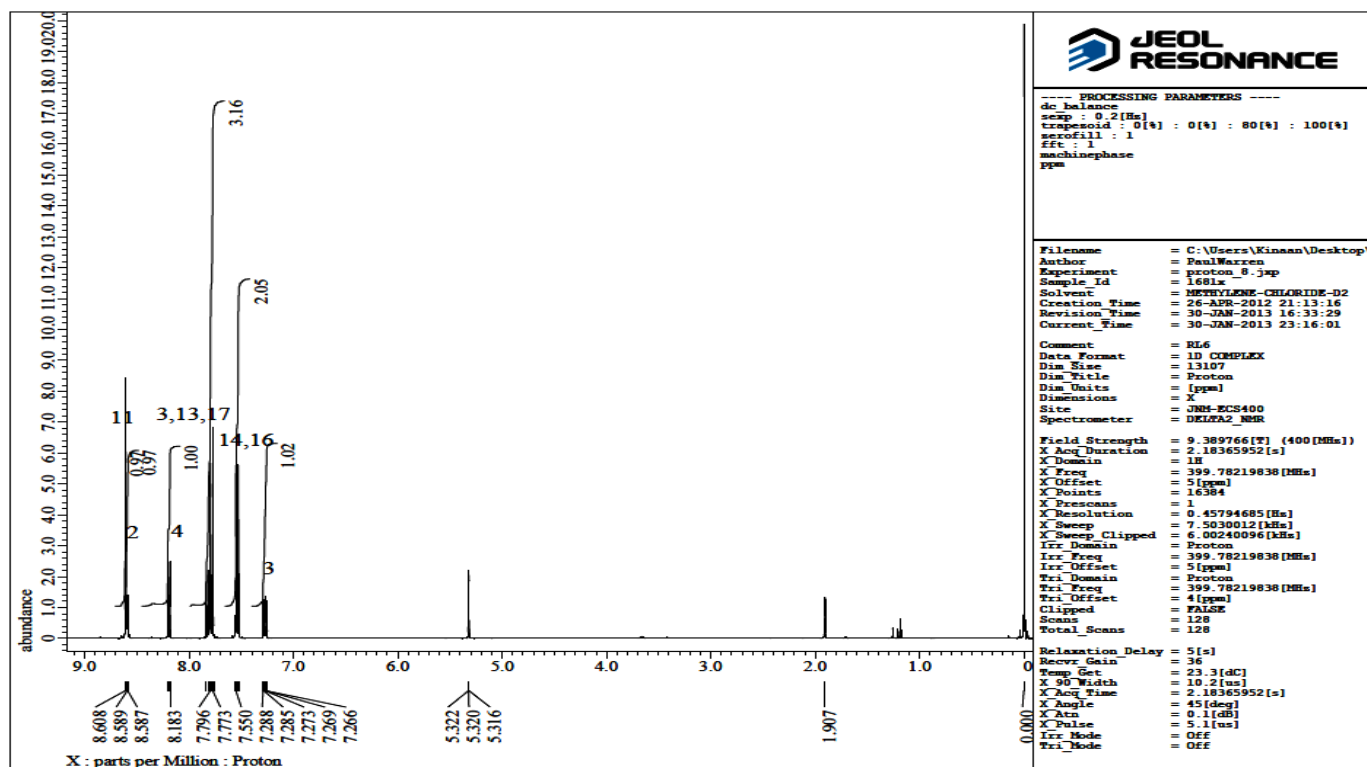


Figure SI 8. ¹H NMR spectrum for L4 in CD₂Cl₂

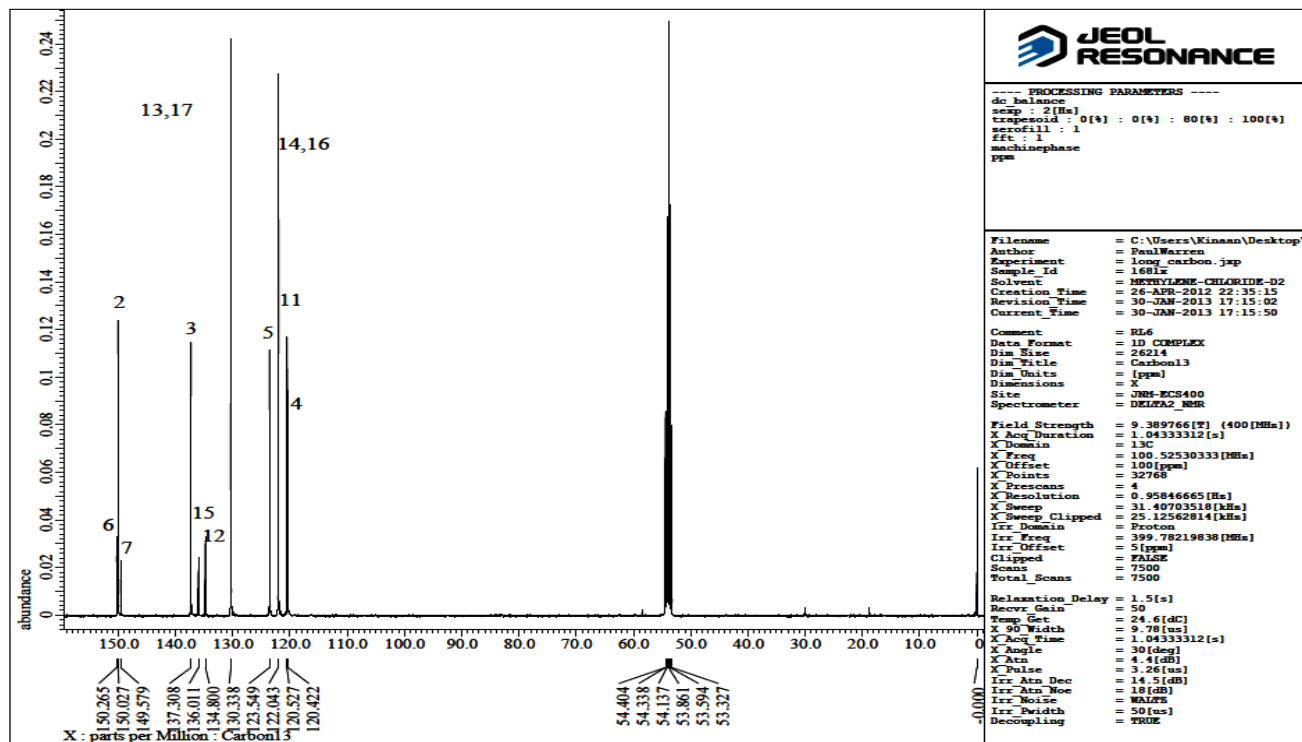


Figure SI 9. ¹³CNMR spectrum for L4 in CD₂Cl₂

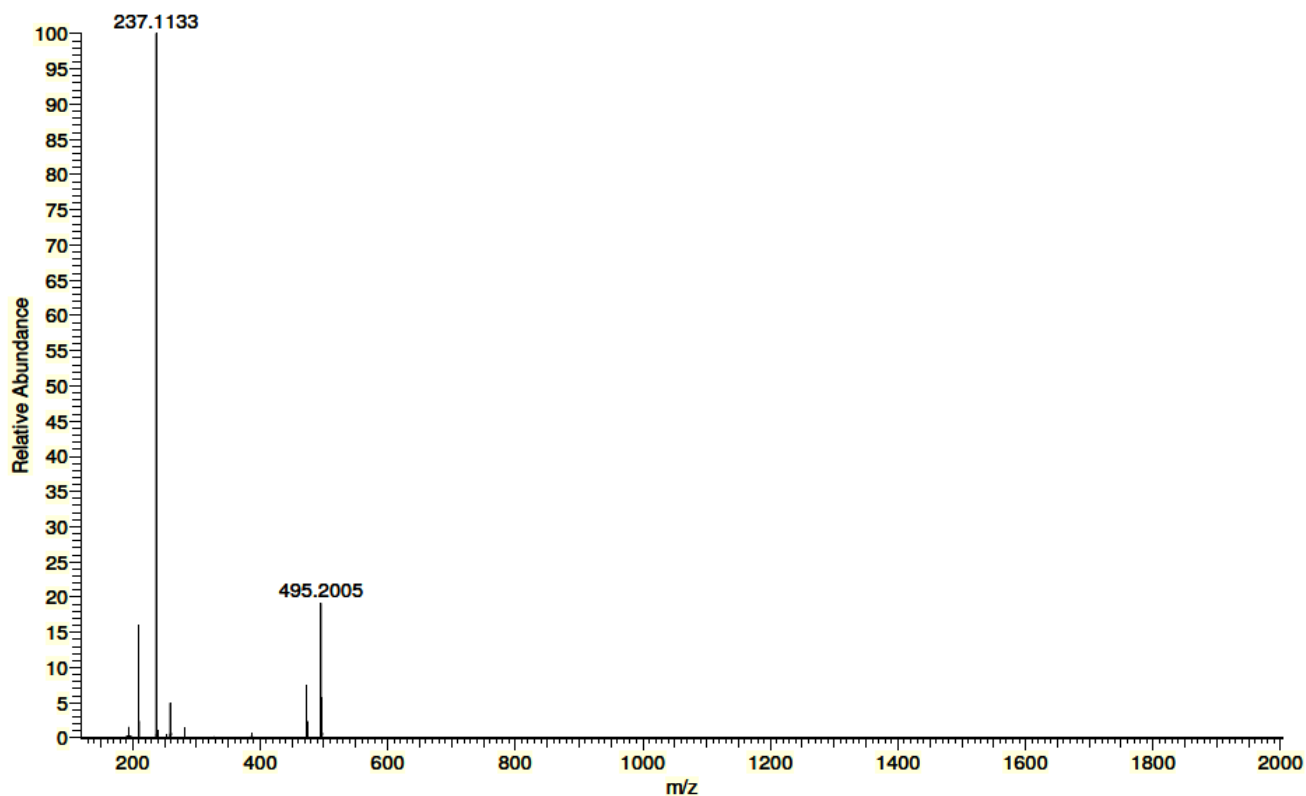


Figure SI 10. The accurate mass spectrum for ligand, 2-(1-(*p*-tolyl)-1H-1,2,3-triazol-4-yl) pyridine, (L5)

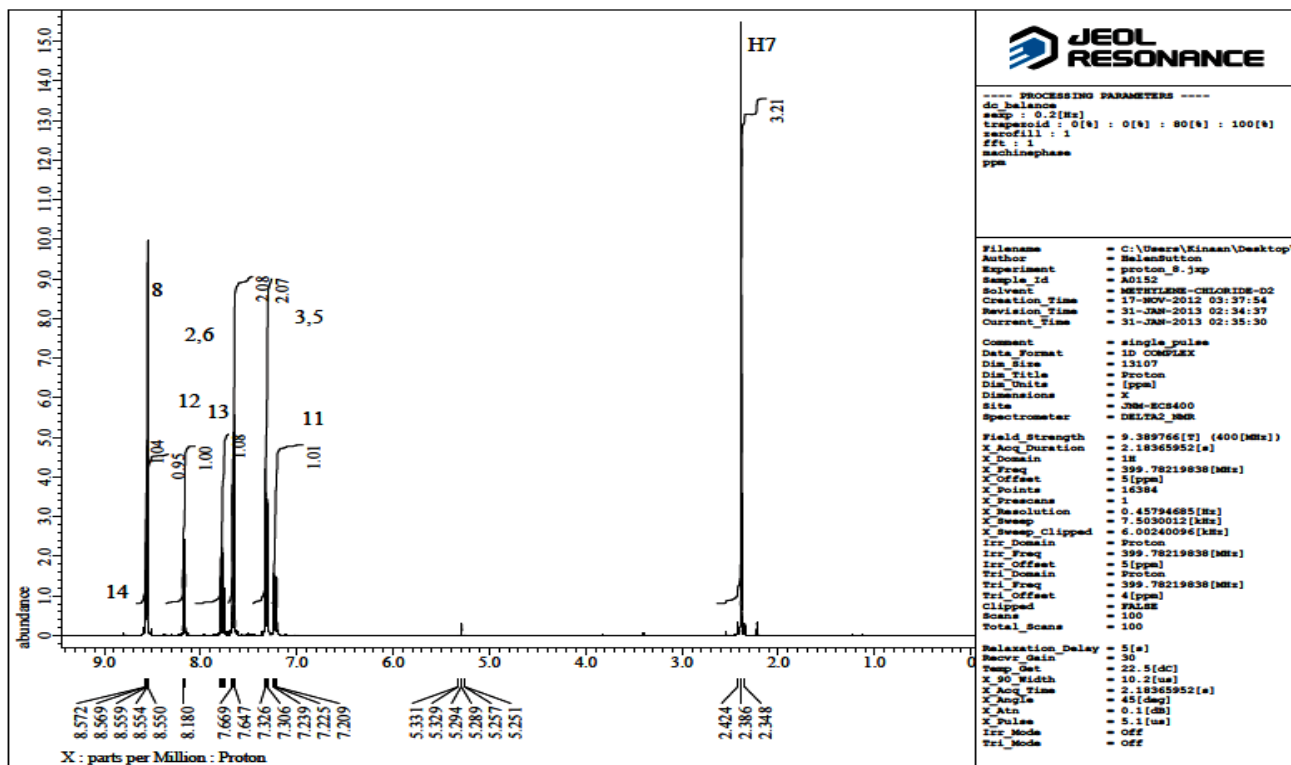


Figure SI 11. ^1H NMR spectrum for L5 in CDCl_3

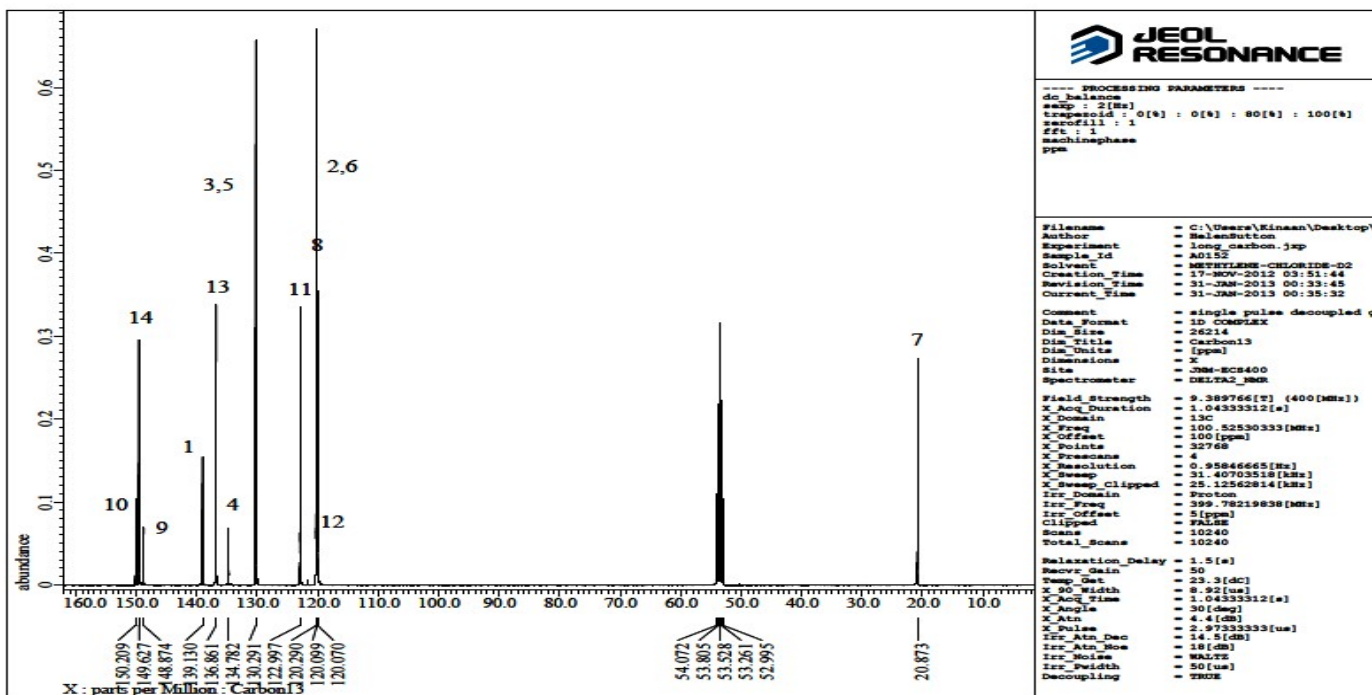


Figure SI 12. ^{13}C NMR spectrum for L5 in CDCl_3

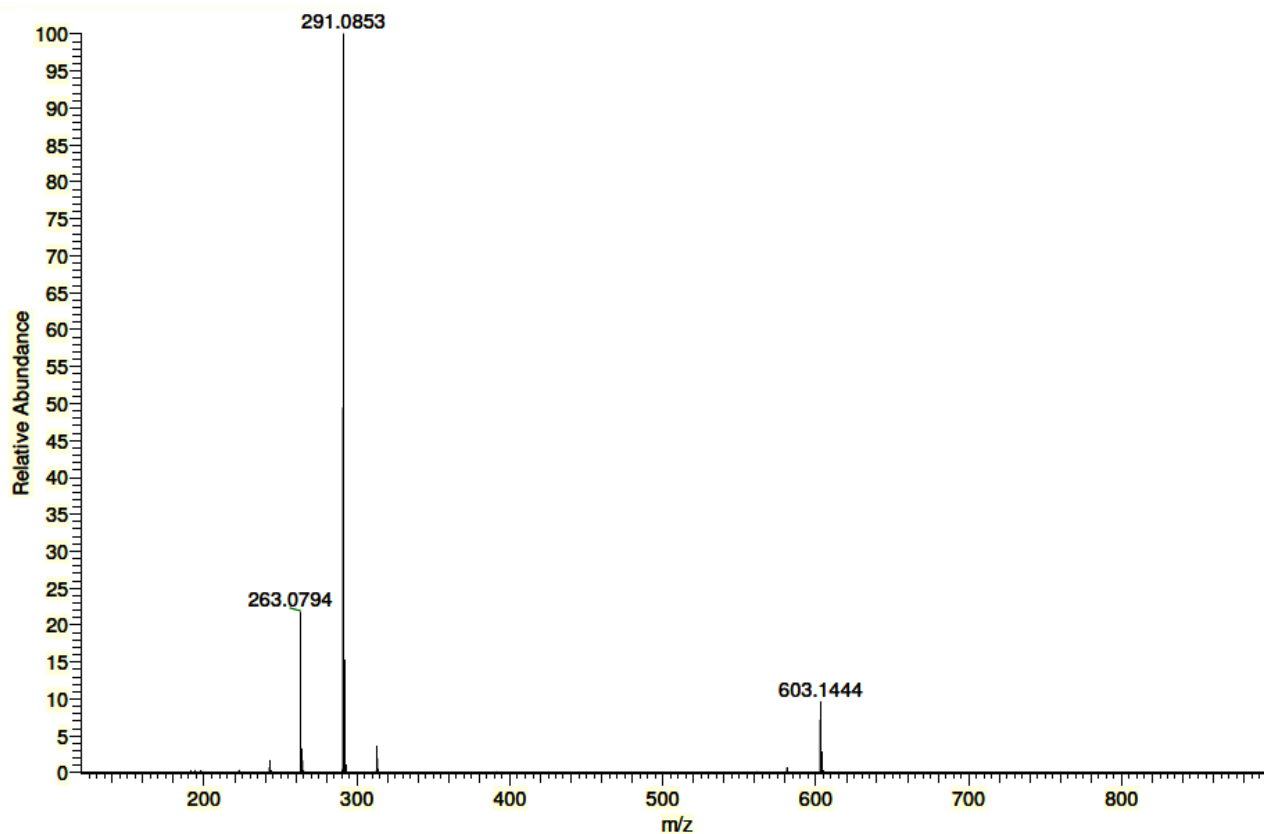


Figure SI 13. The accurate mass spectrum for ligand, 2-(1-(4-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-4-yl)pyridine (L6)

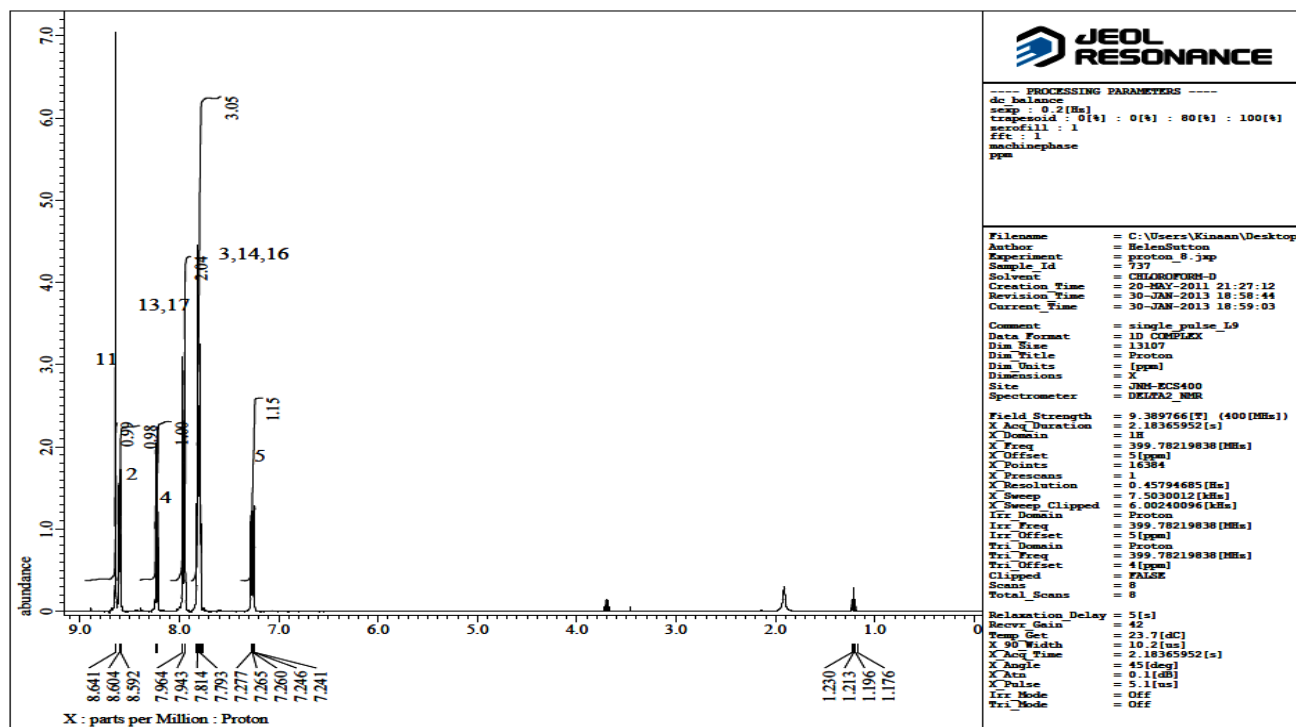


Figure SI 14. ^1H NMR spectrum for L6 in CD_2Cl_2

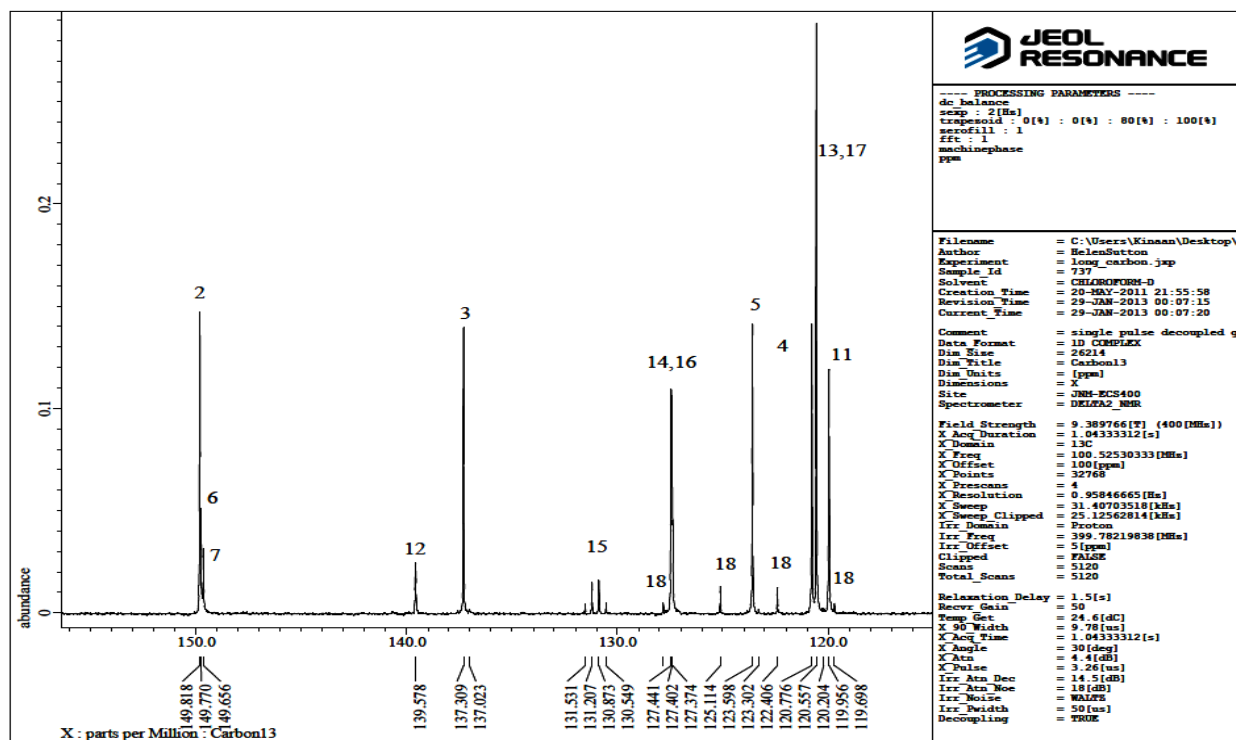


Figure SI 15. ^{13}C NMR spectrum for L6 in CD_2Cl_2

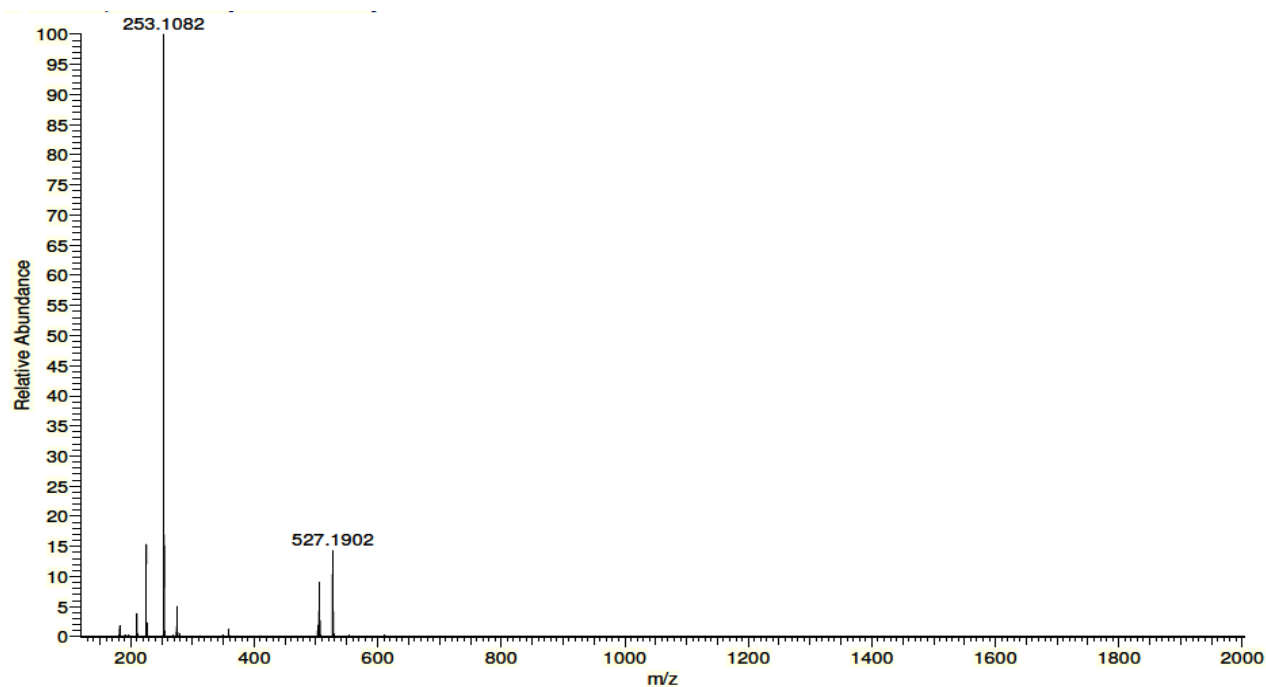


Figure SI 16. The accurate mass spectrum for ligand, 2-(1-(4-Methoxy-phenyl)-1*H*-1, 2, 3-triazol-4-yl)pyridine L8

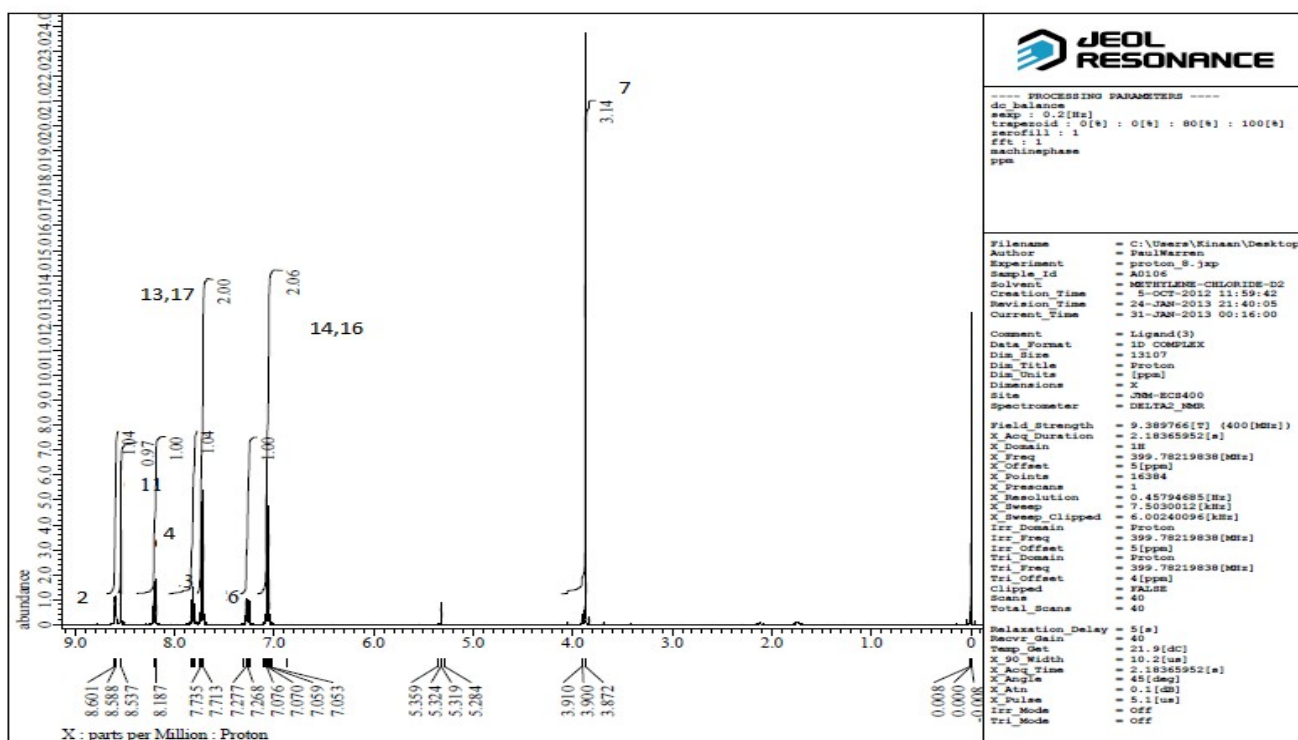


Figure SI 17. ¹H NMR spectrum for L8 in CD₂Cl₂

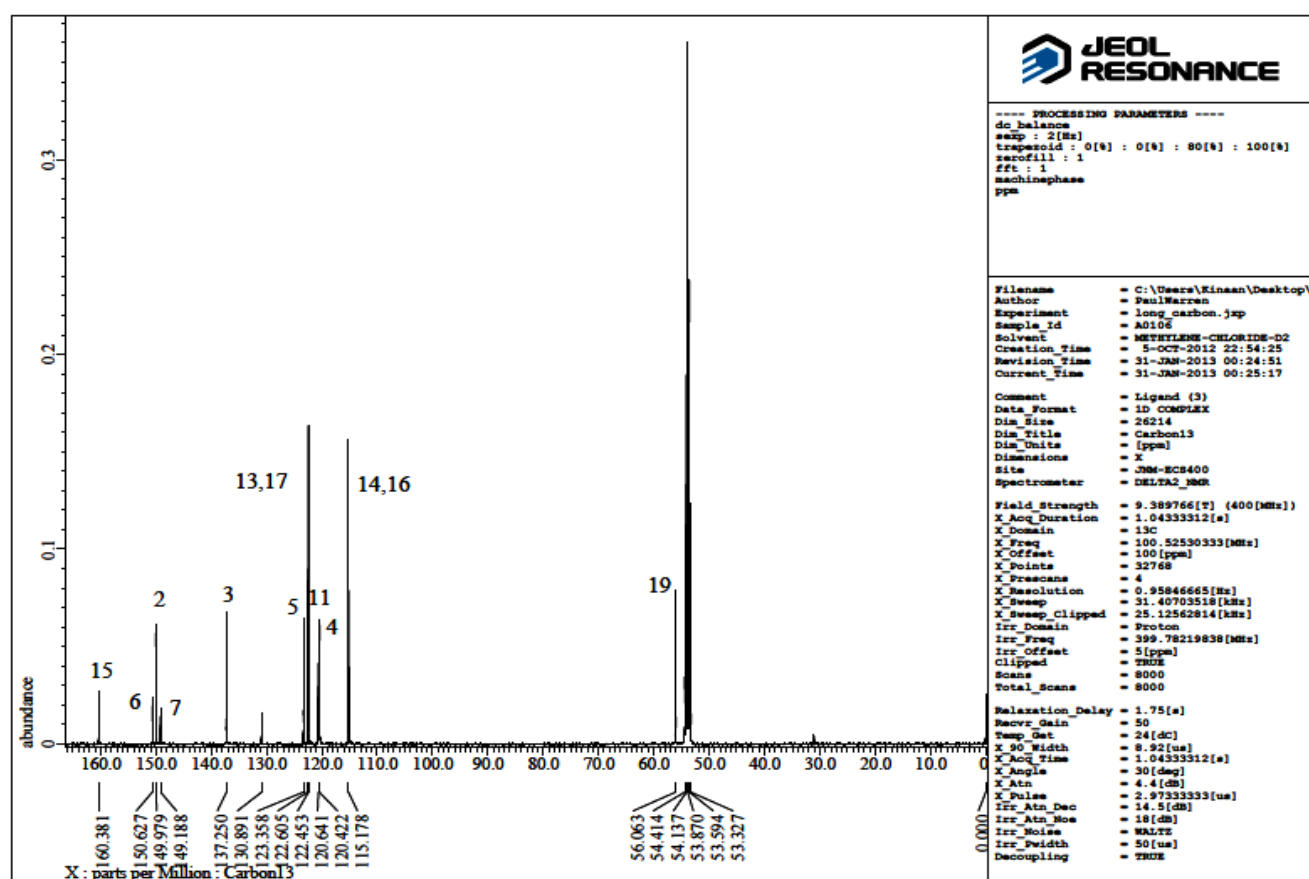


Figure SI 18. ^{13}C NMR spectrum for L8 in CD_2Cl_2

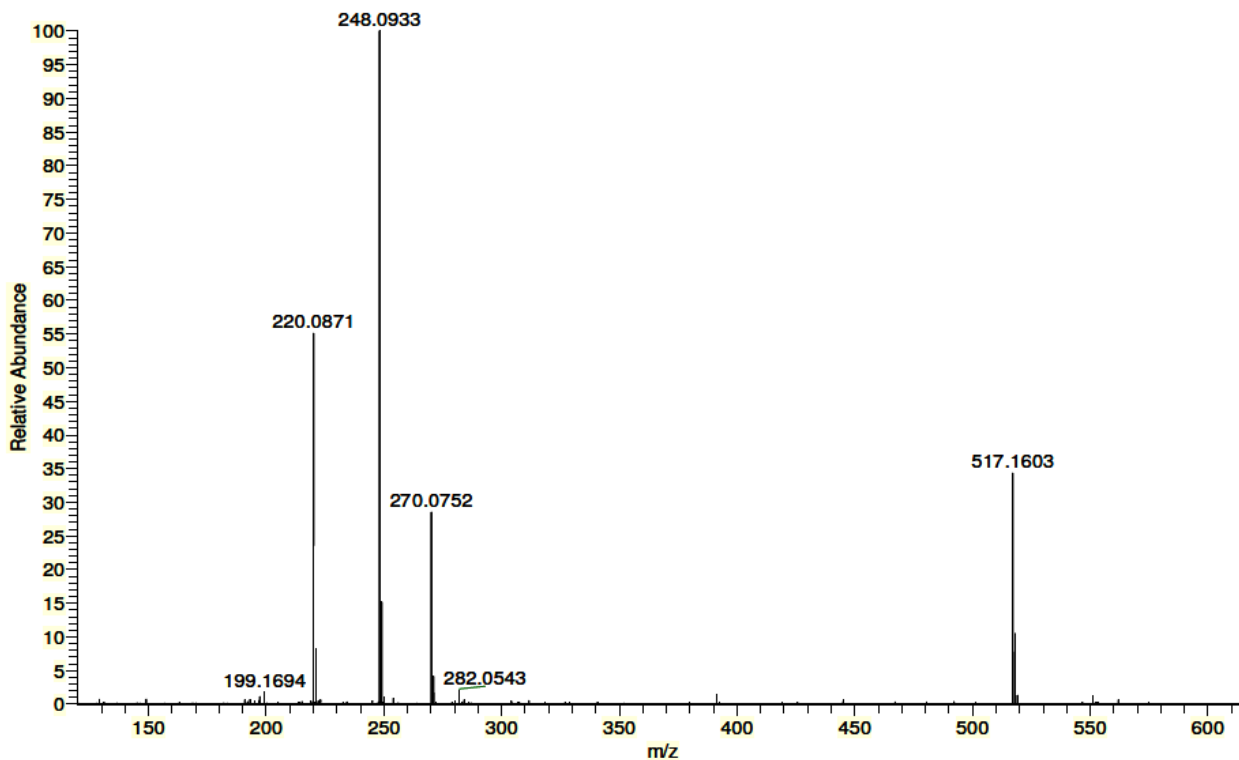


Figure SI 19. The accurate mass spectrum for ligand, 4-(4-(pyridin-2-yl)-1H-1,2,3-triazol-1-yl) benzonitrile (L7)

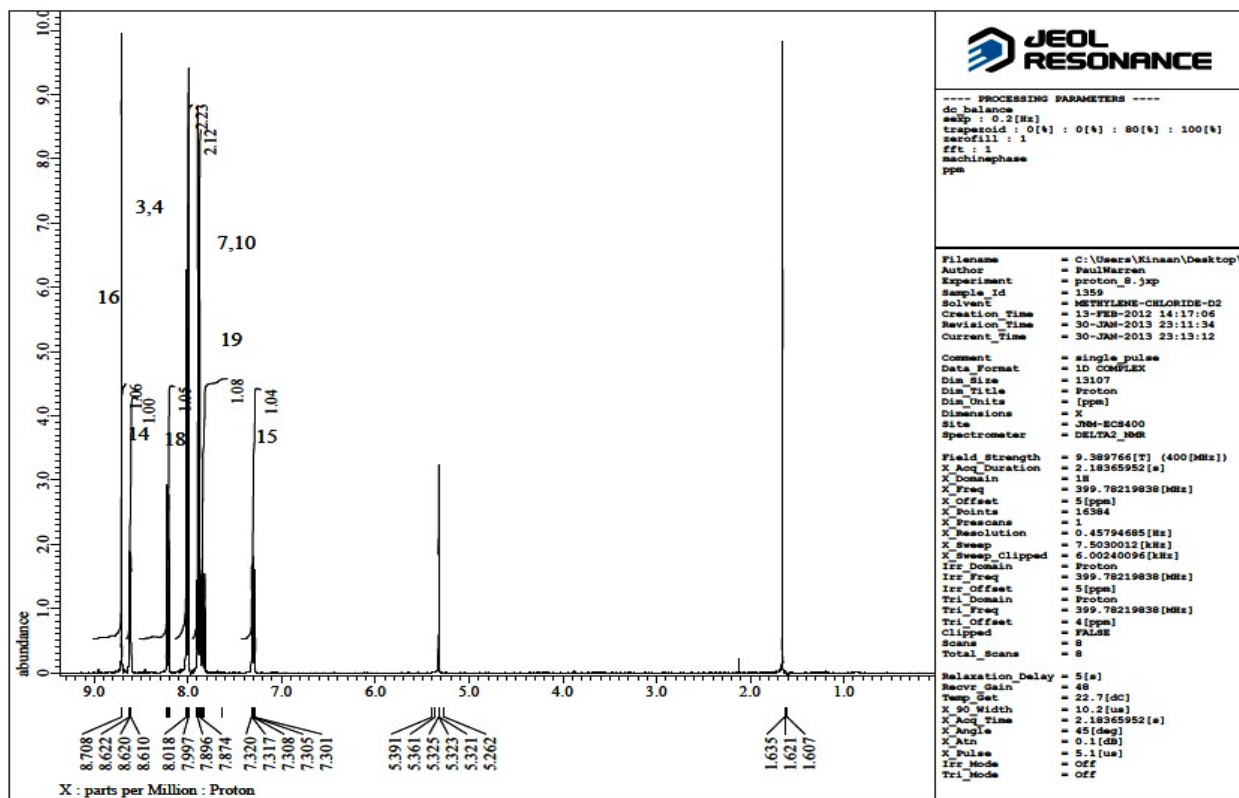


Figure SI 20. ^1H NMR spectrum for L7 in CD_2Cl_2

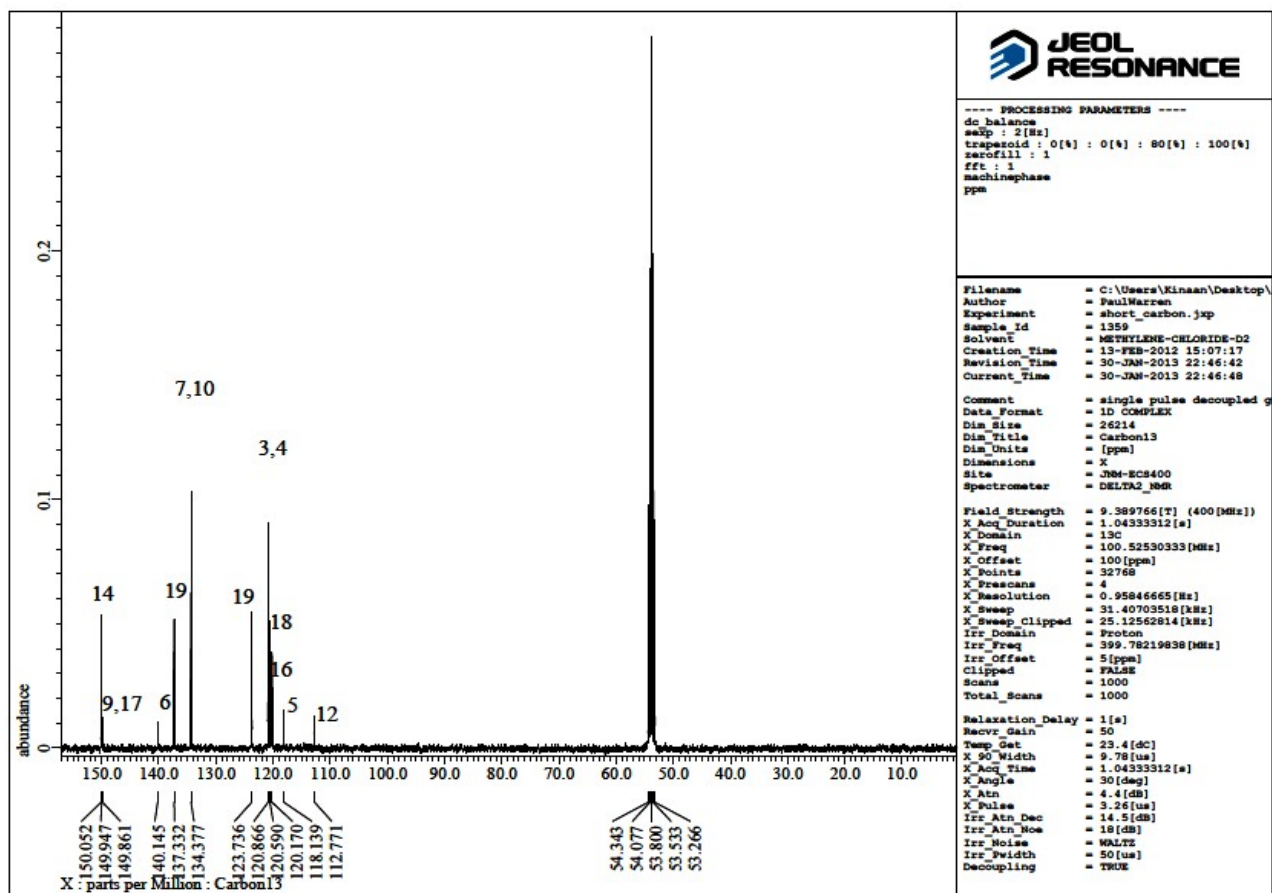


Figure SI 21. ^{13}C NMR spectrum for L7 in CD_2Cl_2

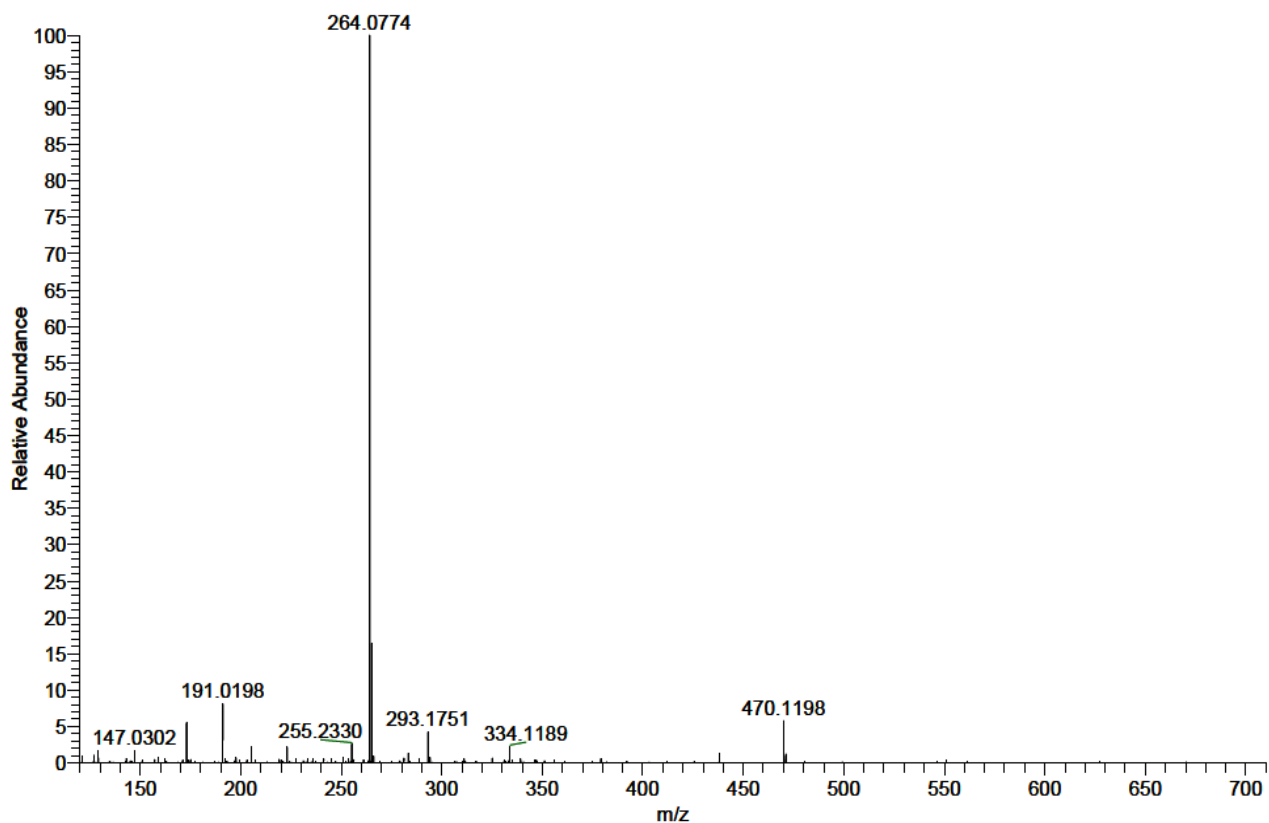


Figure SI 22. The accurate mass spectrum for ligand, 4-(4-(pyridin-2-yl)-1H-1,2,3-triazol-1-yl) benzoic acid (L11)

