

## Supporting Information

# Half-Sandwich Iridium Complexes with Hydrazone Ligands: Preparation, Structure and Catalytic Synthesis of Cyanosilylethers under Air

Song Gao,<sup>a</sup> Zhen-Jiang Liu,<sup>a</sup> Yu-Zhou Luo,<sup>\*b</sup> Zi-Jian Yao<sup>\*a</sup>

<sup>a</sup>School of Chemical and Environmental Engineering, Shanghai Institute of Technology, Shanghai, 201418, China.

<sup>b</sup>Scientific Research Office, Guangzhou College of Commerce, Guangzhou, 511363, China.

Corresponding author: Email: zjyao@sit.edu.cn; Tel: +86-21-60877231, Fax: +86-21-60873335.

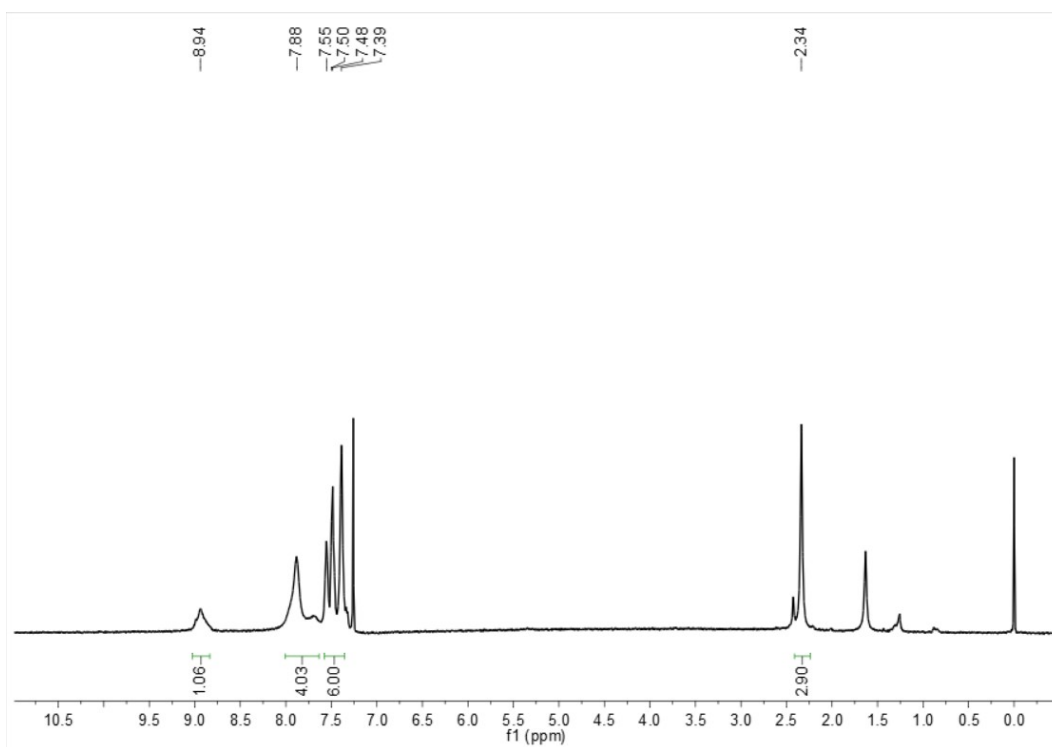


Figure S1.  $^1\text{H}$  NMR spectrum of **L1** in  $\text{CDCl}_3$ .

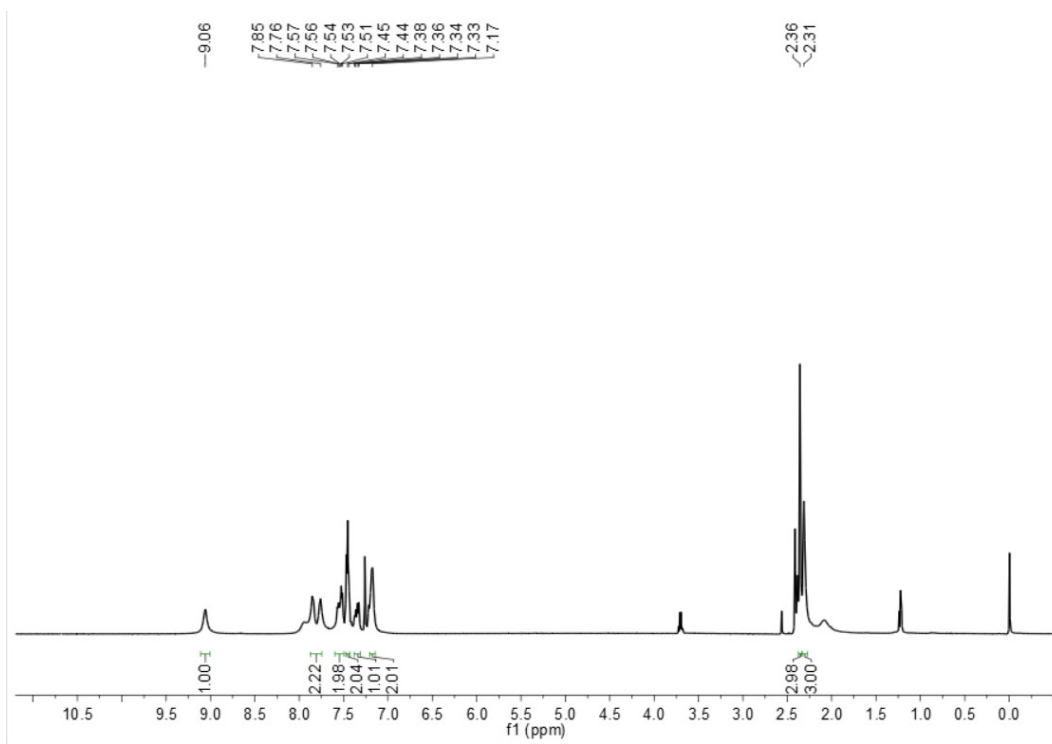


Figure S2.  $^1\text{H}$  NMR spectrum of **L2** in  $\text{CDCl}_3$ .

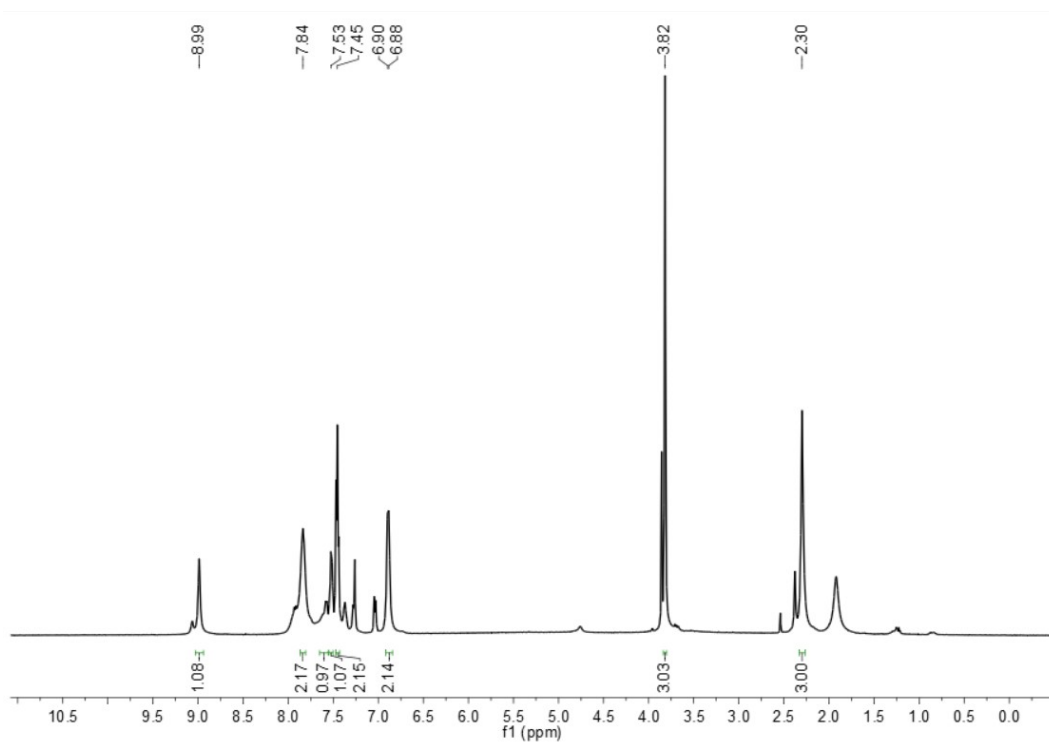


Figure S3.  $^1\text{H}$  NMR spectrum of L3 in  $\text{CDCl}_3$ .

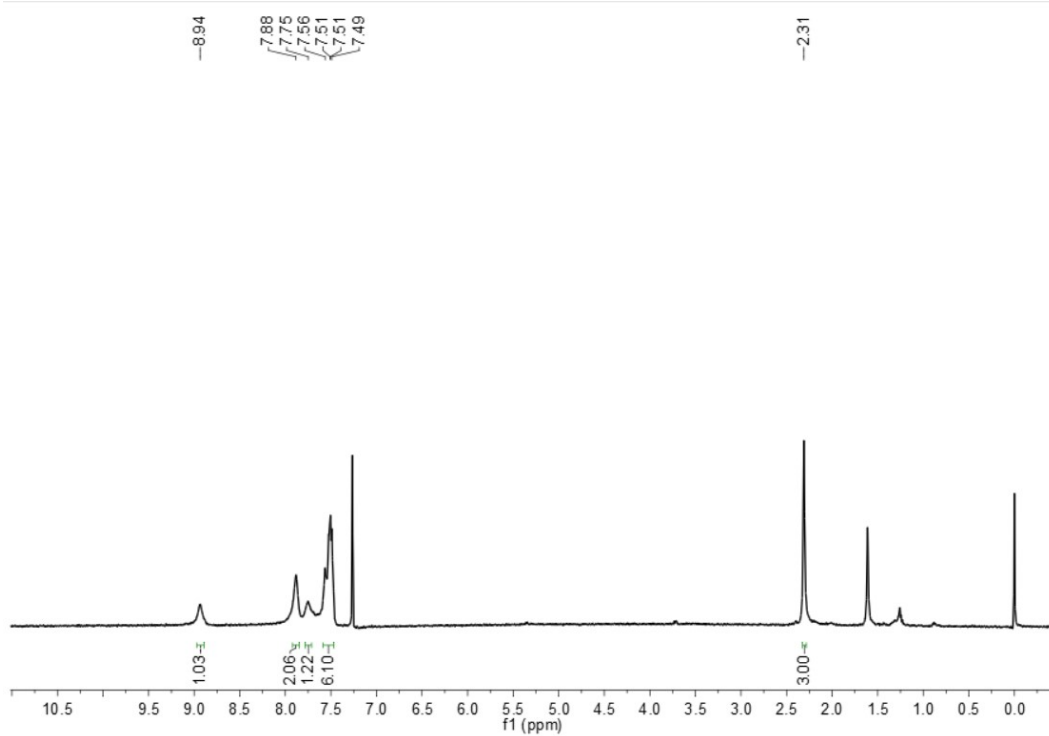


Figure S4.  $^1\text{H}$  NMR spectrum of L4 in  $\text{CDCl}_3$ .

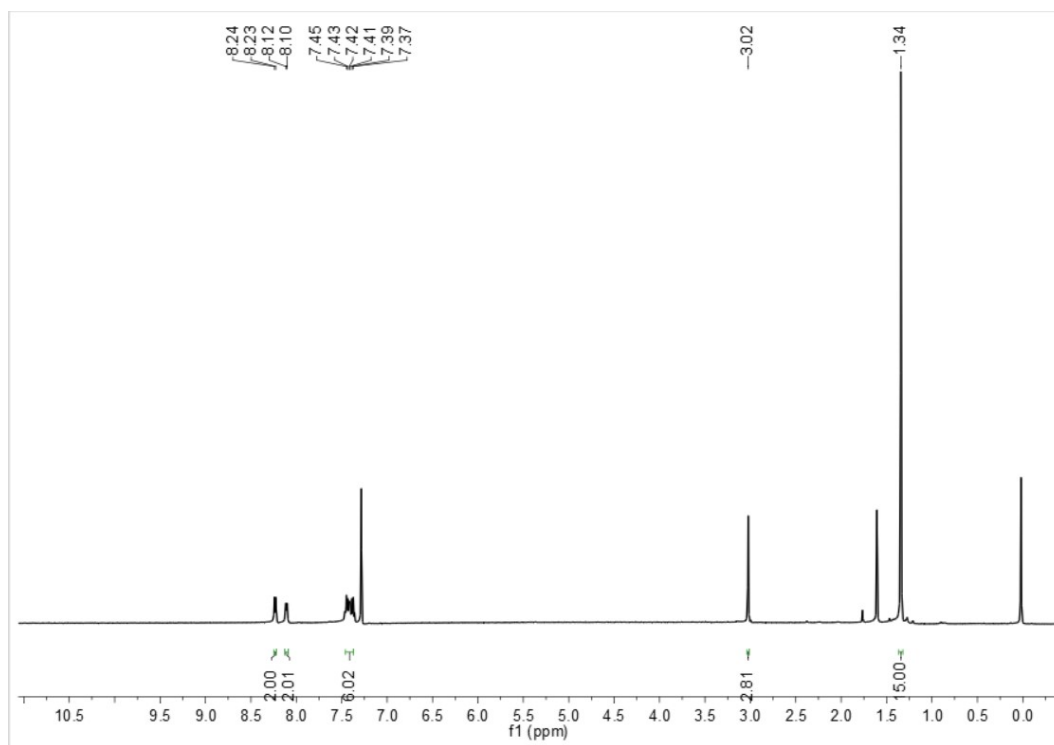


Figure S5.  $^1\text{H}$  NMR spectrum of **1** in  $\text{CDCl}_3$ .

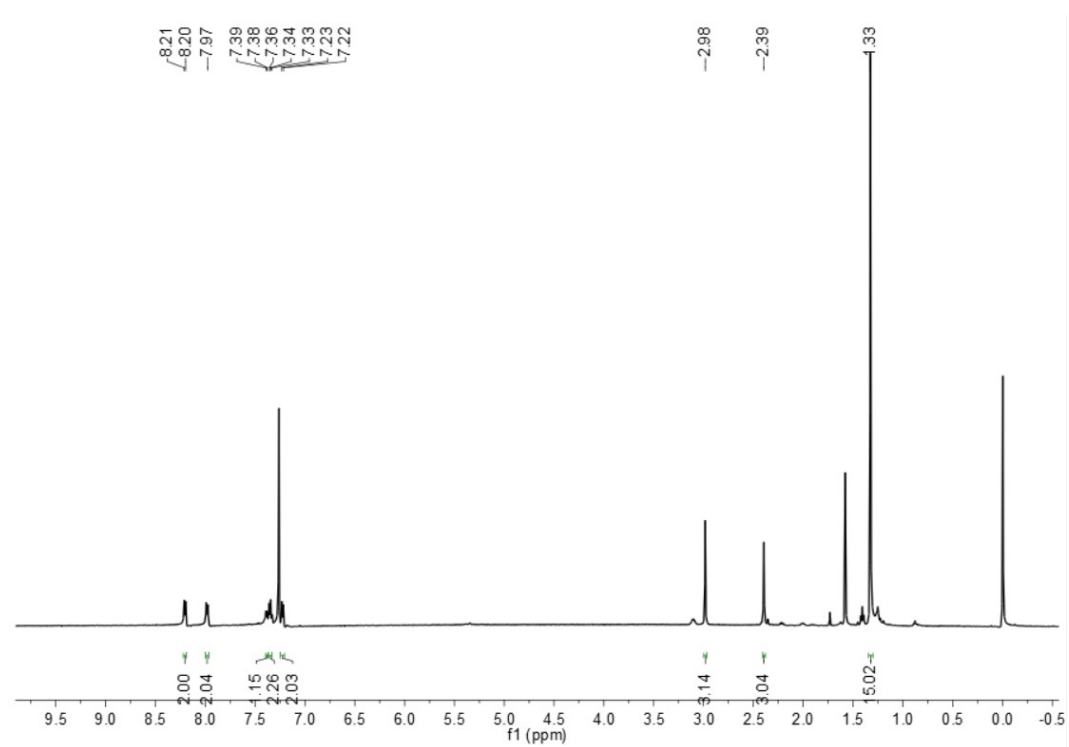


Figure S6.  $^1\text{H}$  NMR spectrum of **2** in  $\text{CDCl}_3$ .

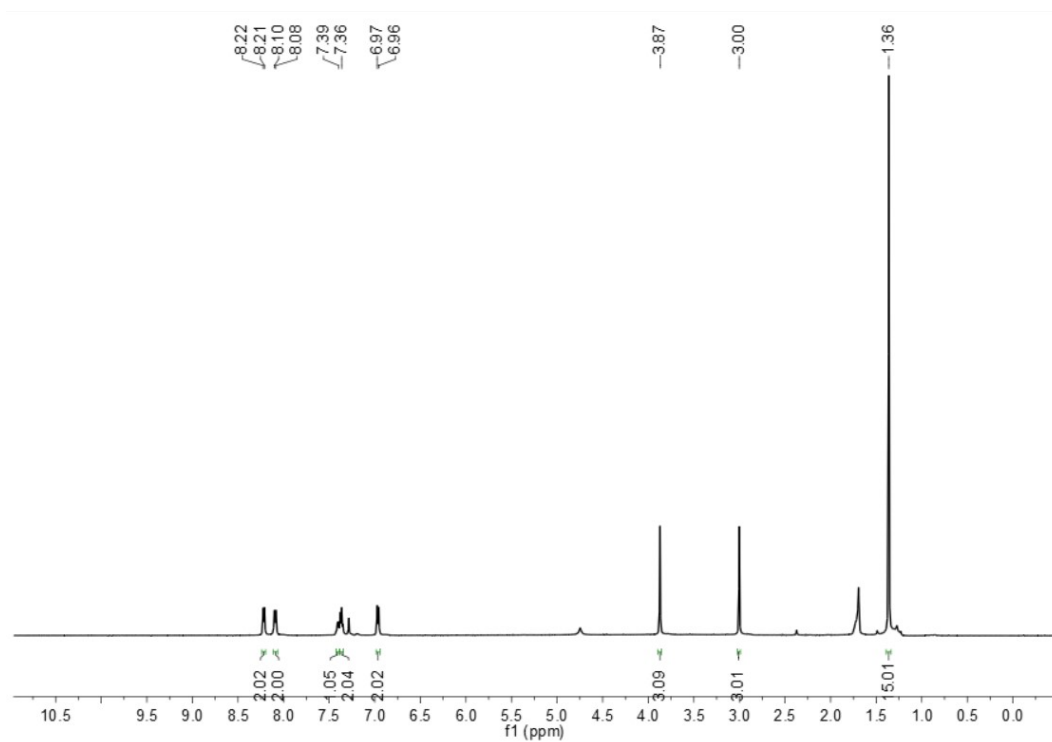


Figure S7.  $^1\text{H}$  NMR spectrum of **3** in  $\text{CDCl}_3$ .

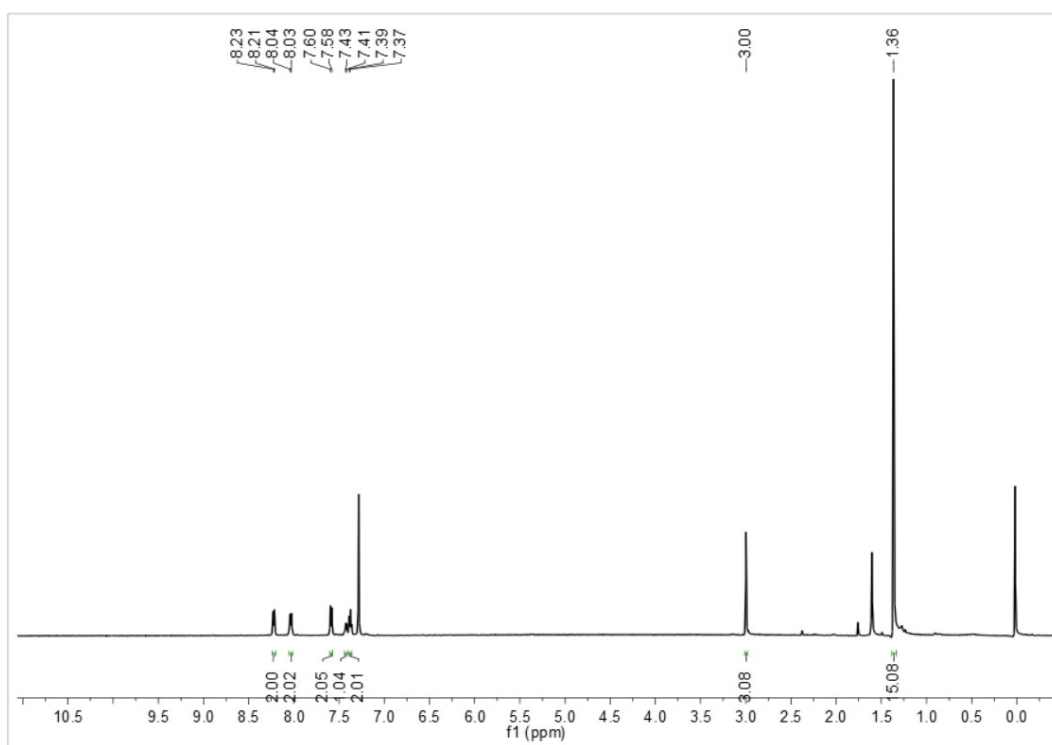


Figure S8.  $^1\text{H}$  NMR spectrum of **4** in  $\text{CDCl}_3$ .

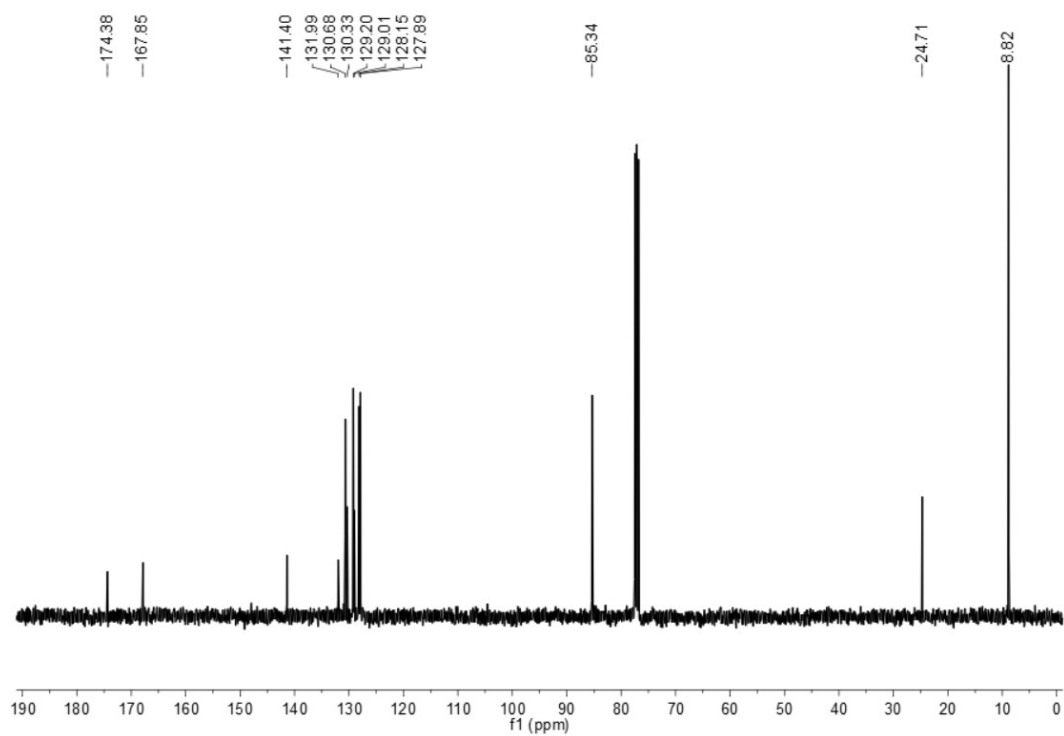


Figure S9.  $^{13}\text{C}$  NMR spectrum of **1** in  $\text{CDCl}_3$ .

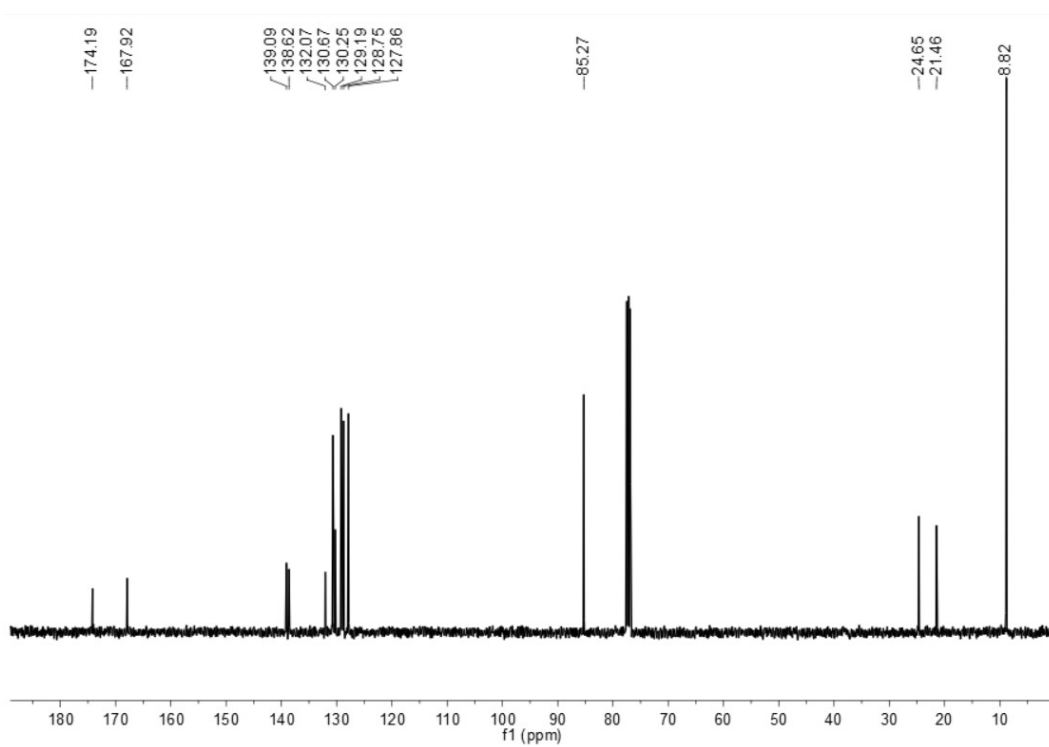


Figure S10.  $^{13}\text{C}$  NMR spectrum of **2** in  $\text{CDCl}_3$ .

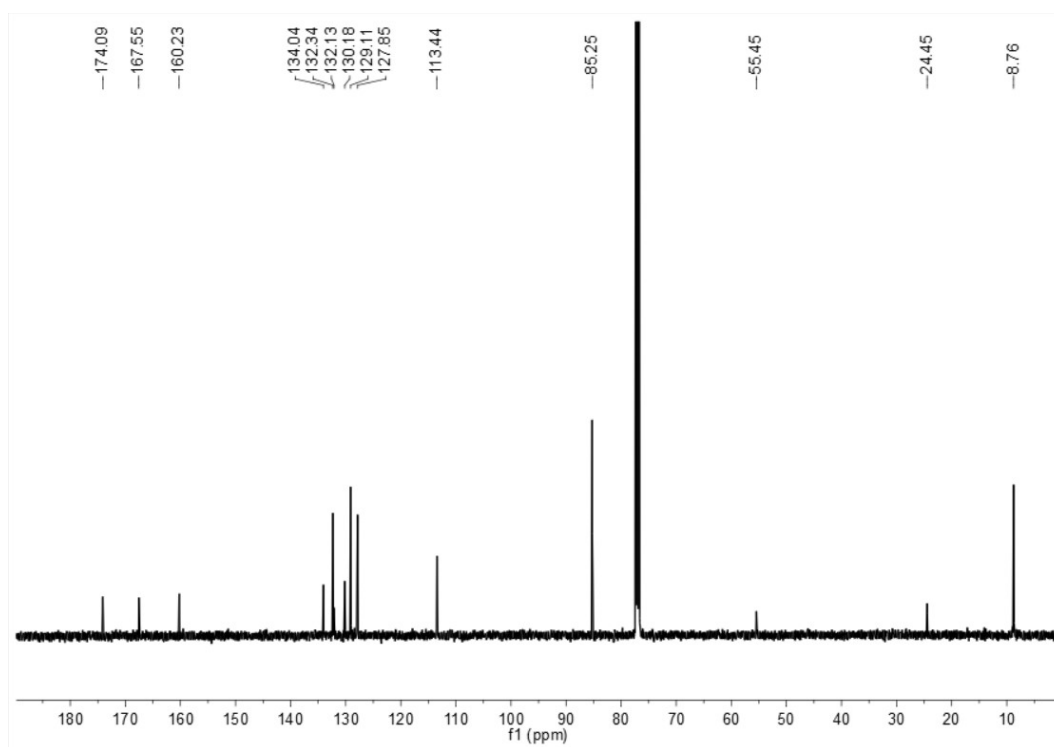


Figure S11.  $^{13}\text{C}$  NMR spectrum of **3** in  $\text{CDCl}_3$ .

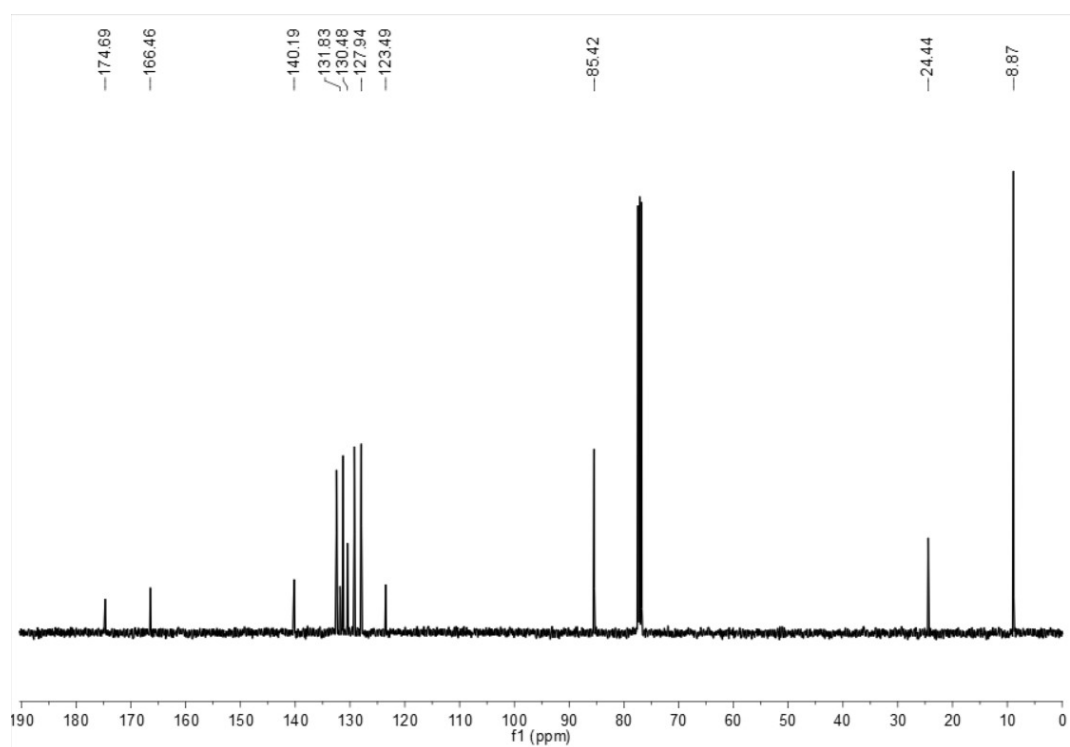


Figure S12.  $^{13}\text{C}$  NMR spectrum of **4** in  $\text{CDCl}_3$ .

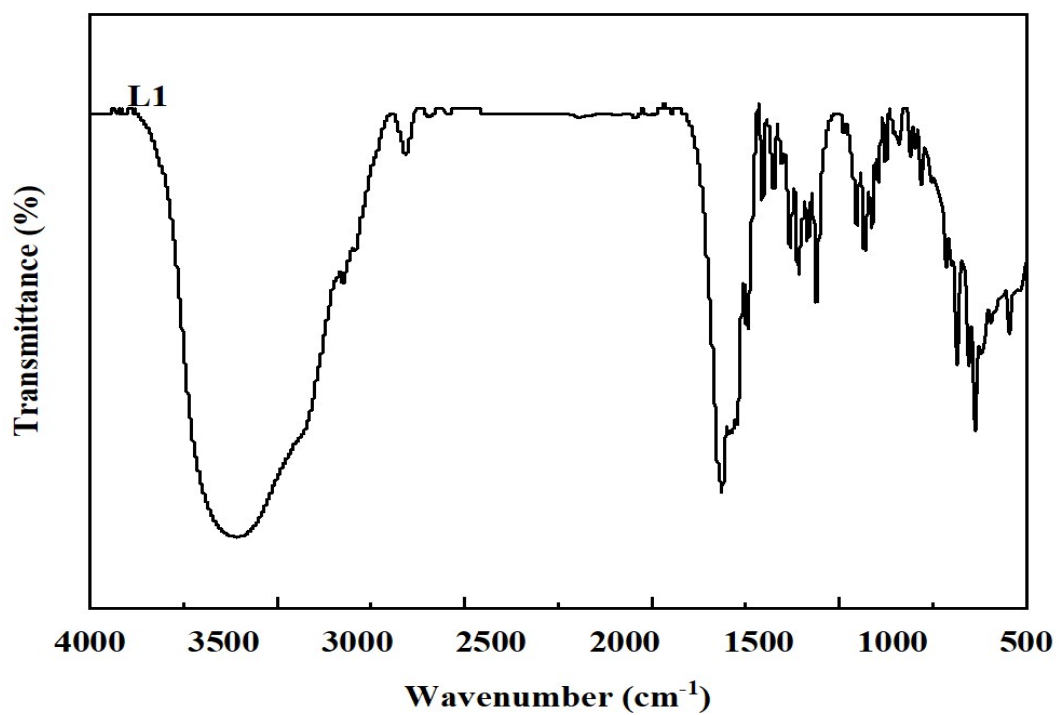


Figure S13. IR spectrum of the ligand L1.

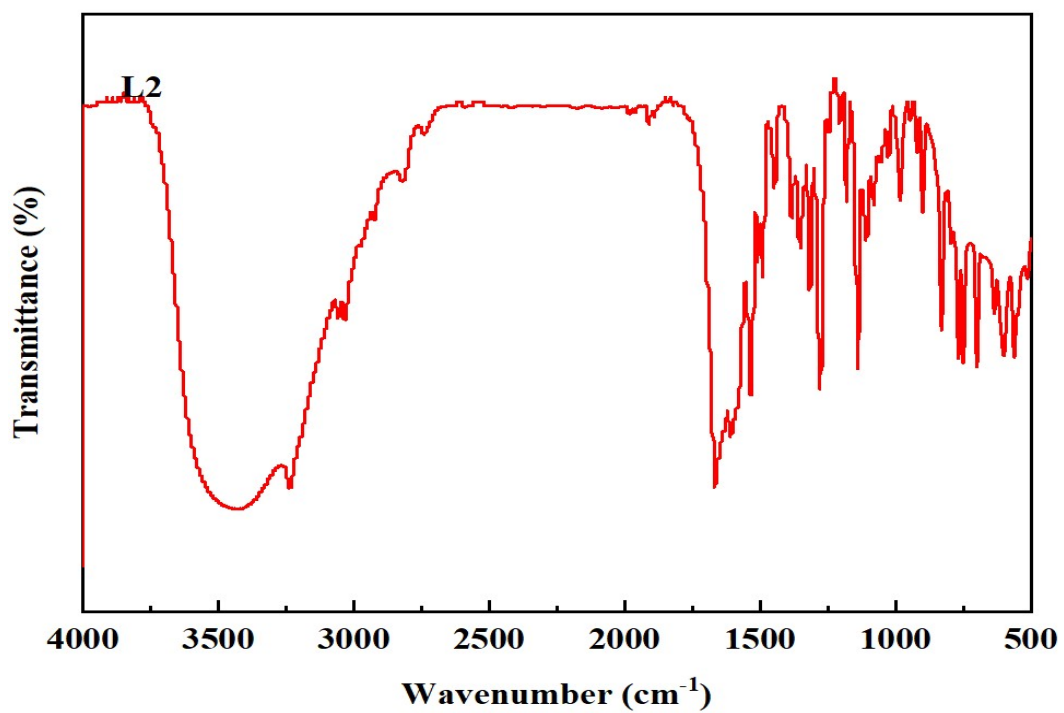


Figure S14. IR spectrum of the ligand L2.



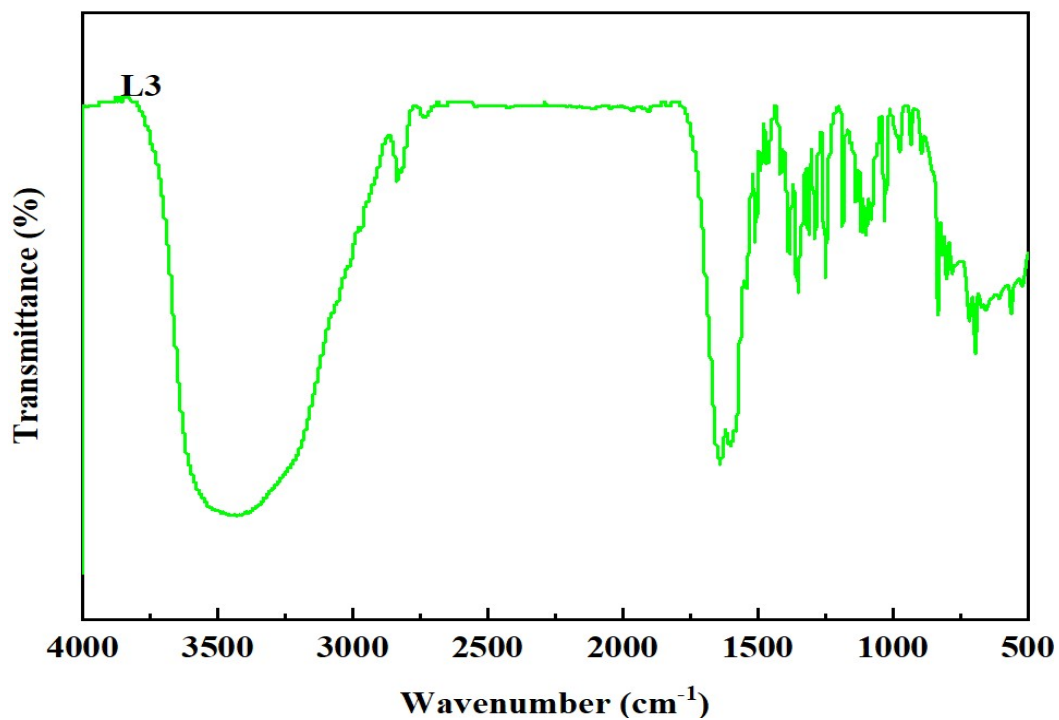


Figure S15. IR spectrum of the ligand L3.

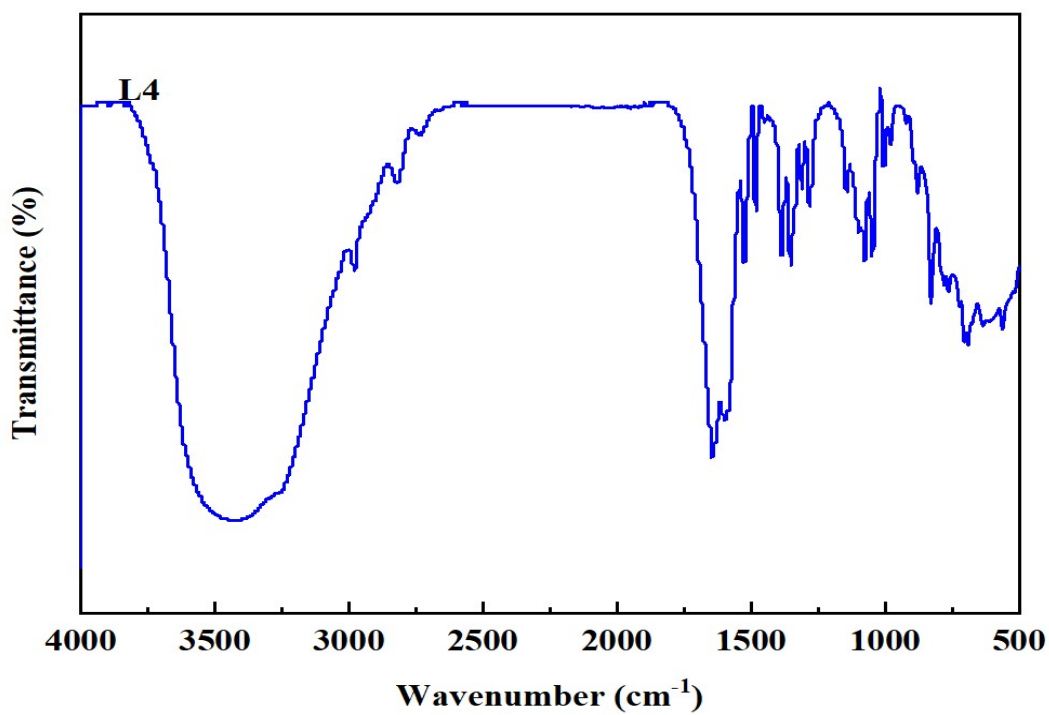


Figure S16. IR spectrum of the ligand L4.

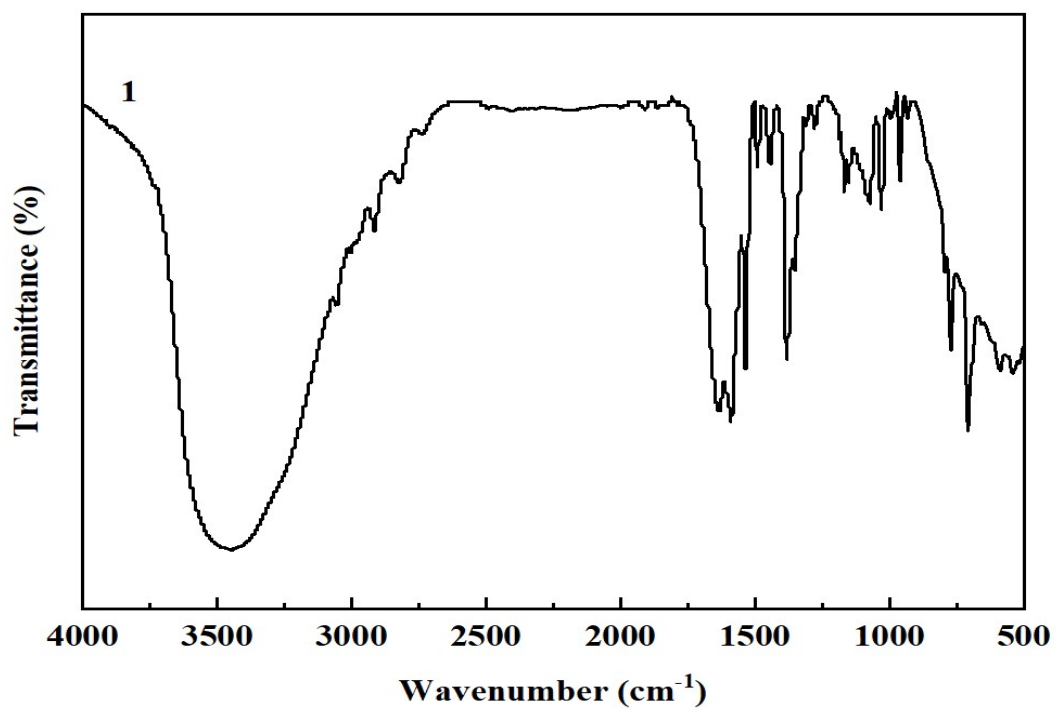


Figure S17. IR spectrum of the complex 1.

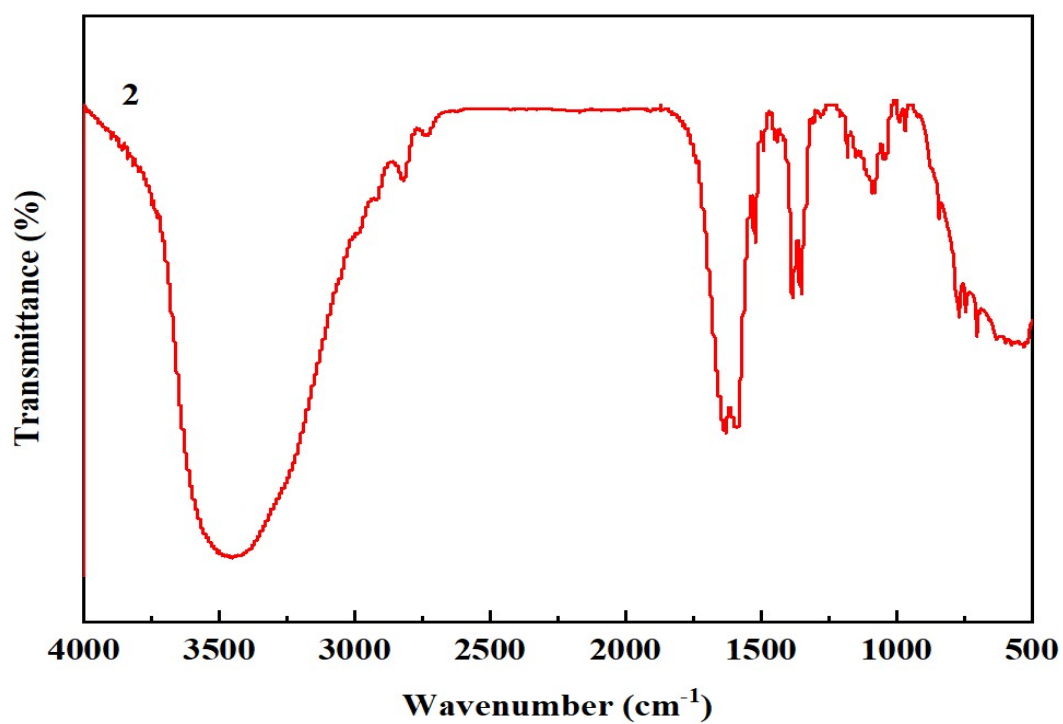


Figure S18. IR spectrum of the complex 2.

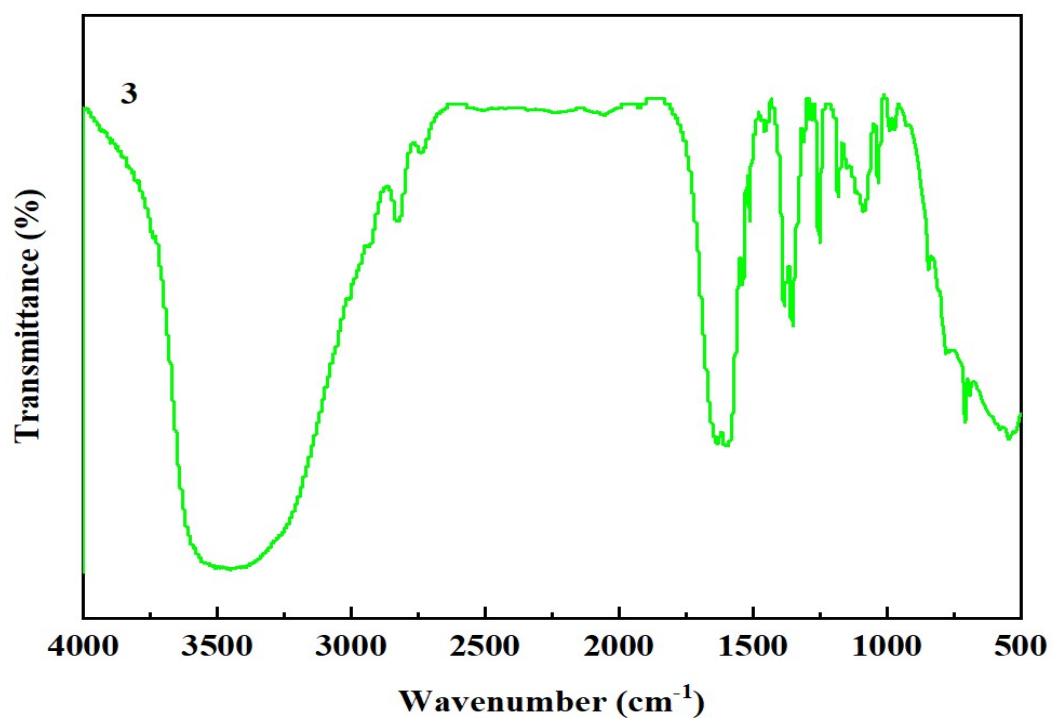


Figure S19. IR spectrum of the complex 3.

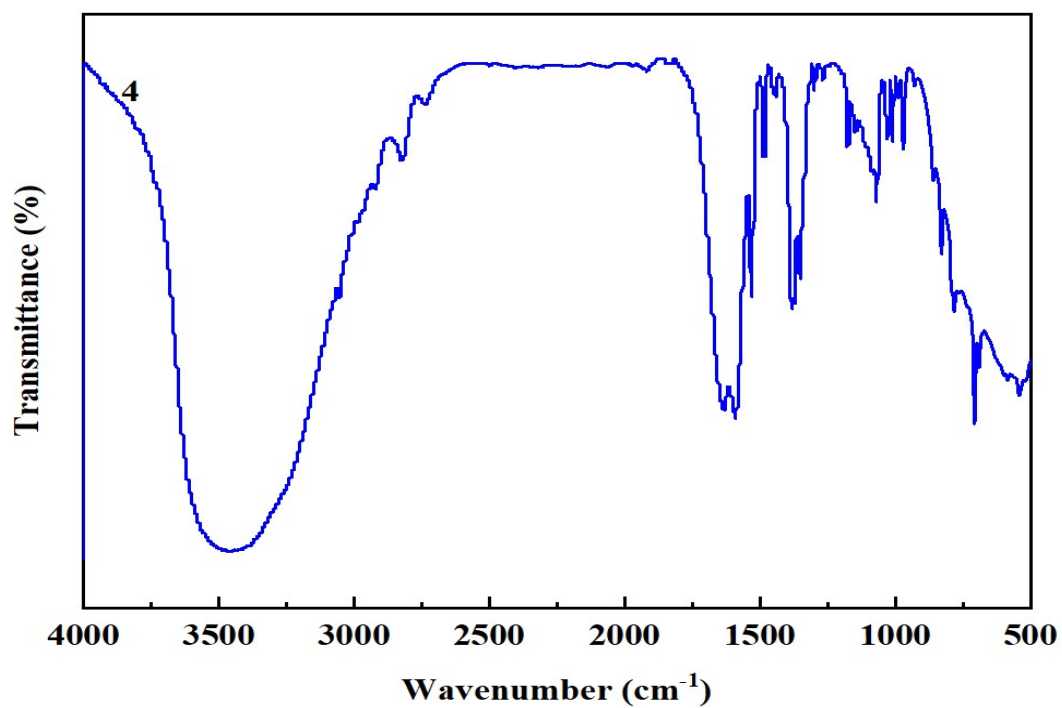


Figure S20. IR spectrum of the complex 4.

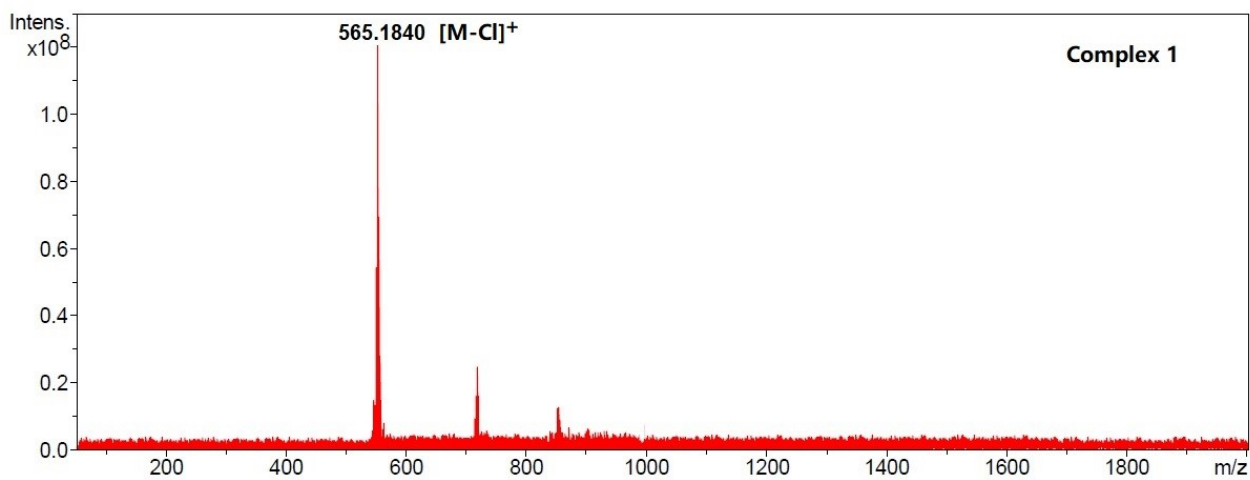


Figure S21. HRMS spectrum of complex 1.

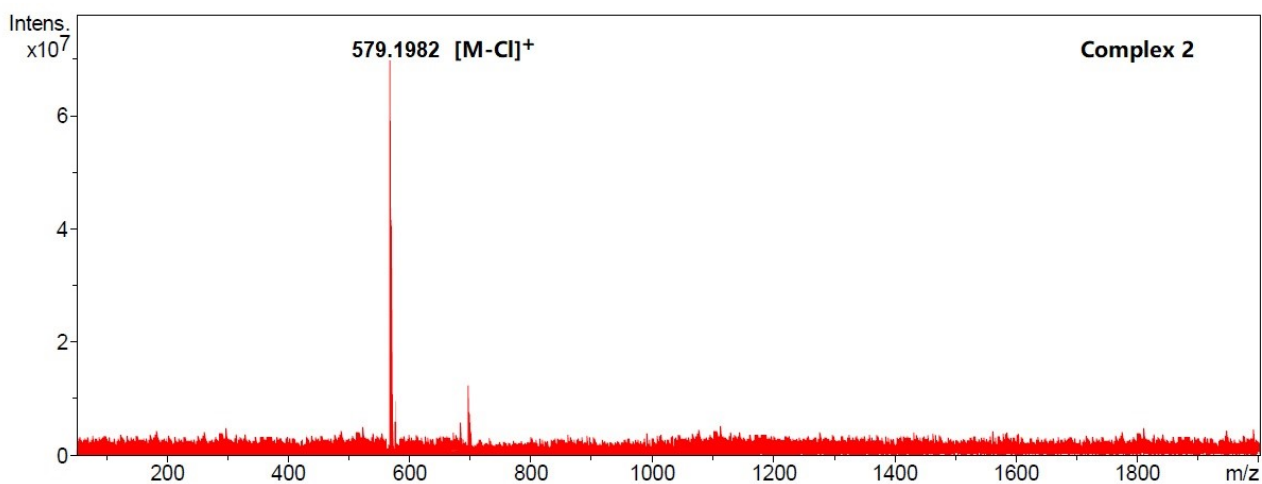


Figure S22. HRMS spectrum of complex 2.

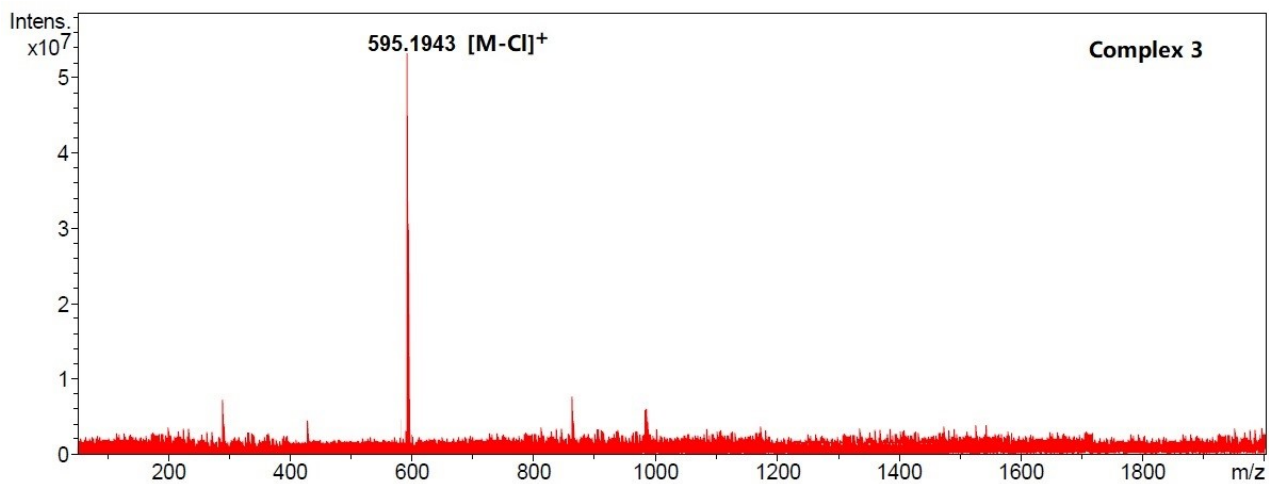


Figure S23. HRMS spectrum of complex 3.

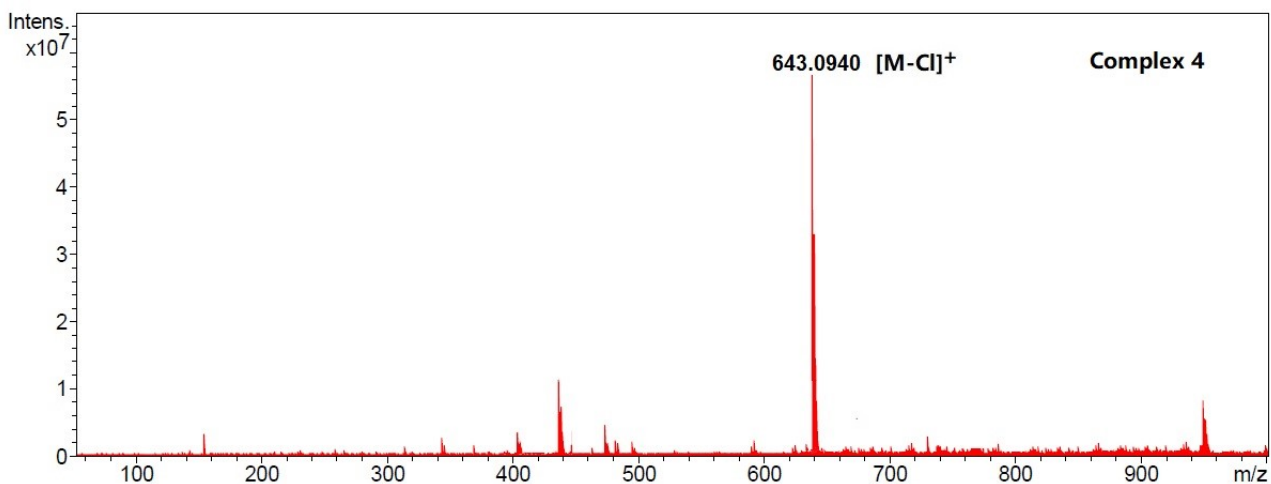


Figure S24. HRMS spectrum of complex 4.

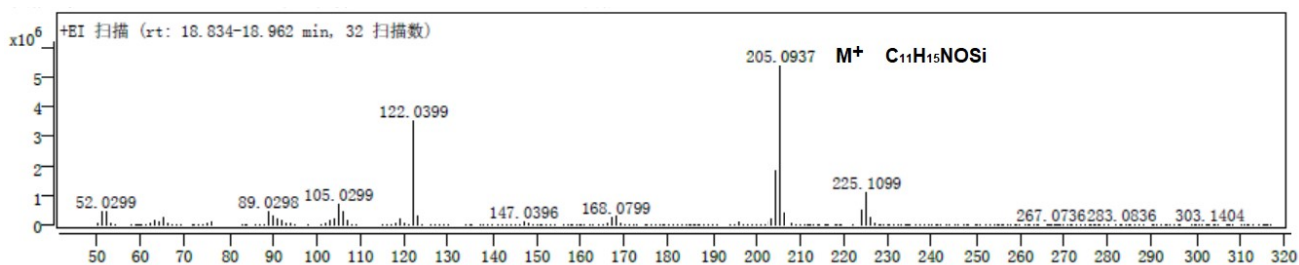


Figure S25. GC-MS spectrum of complex 5a.

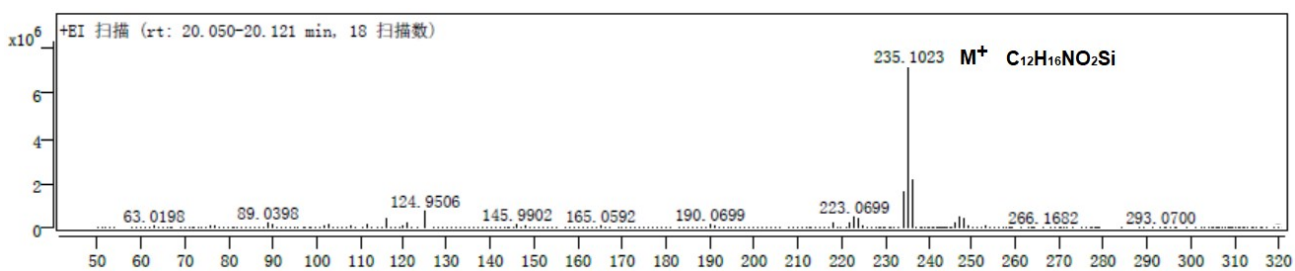


Figure S26. GC-MS spectrum of complex 5b.

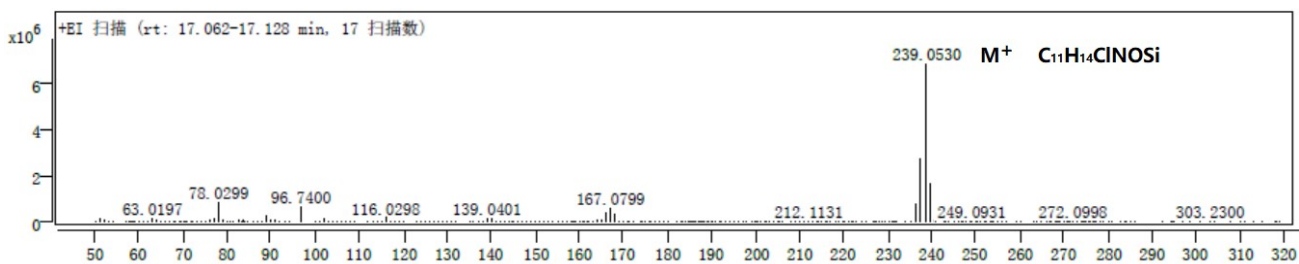


Figure S27. GC-MS spectrum of complex 5c.

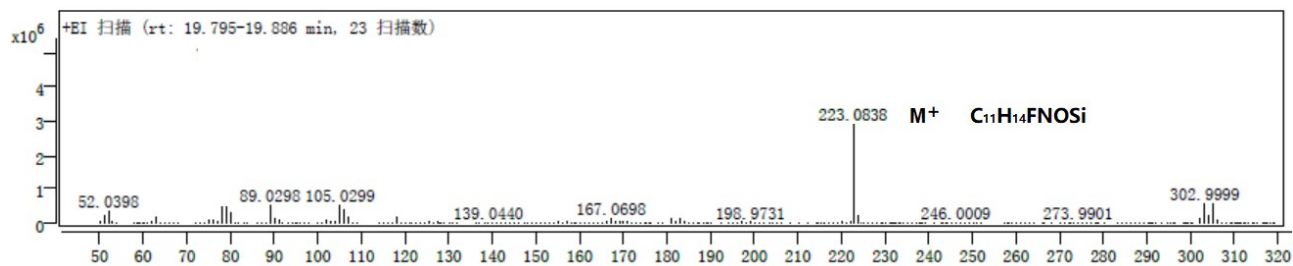


Figure S28. GC-MS spectrum of complex **5d**.

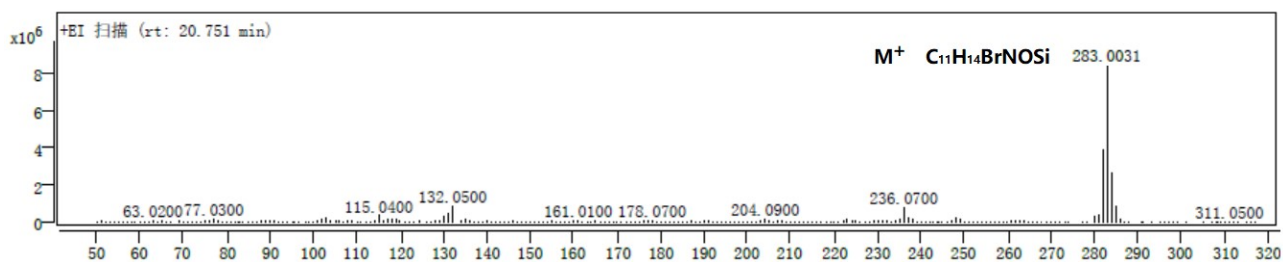


Figure S29. GC-MS spectrum of complex **5e**.

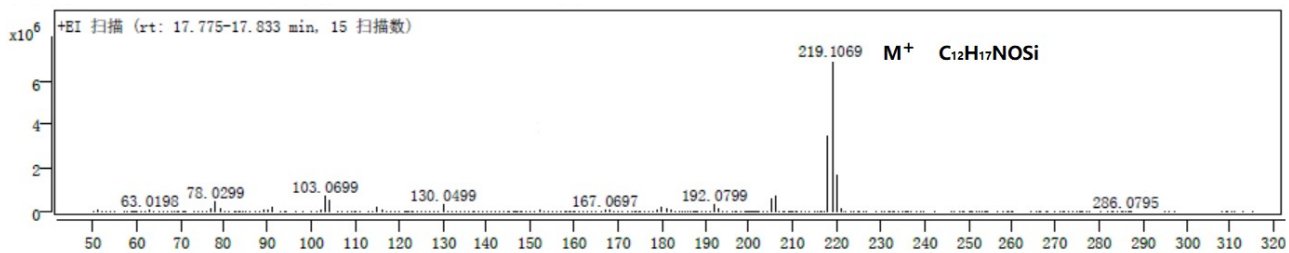


Figure S30. GC-MS spectrum of complex **5f**.

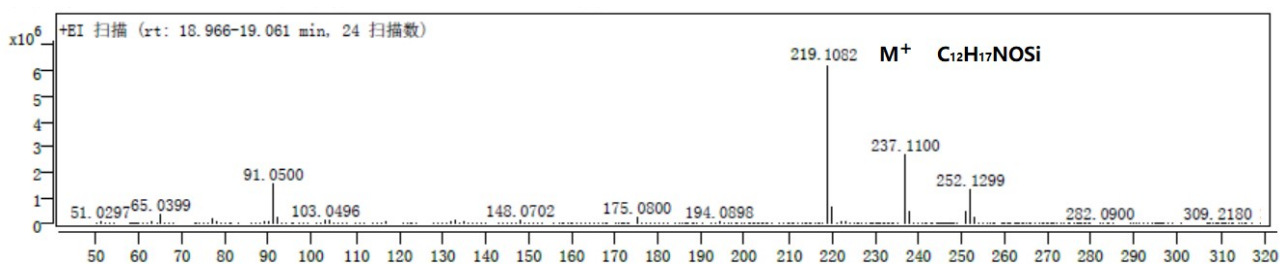


Figure S31. GC-MS spectrum of complex **5g**.

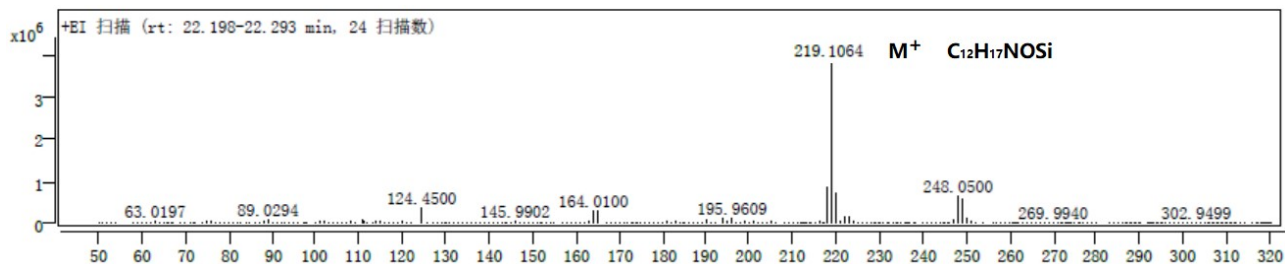


Figure S32. GC-MS spectrum of complex **5h**.

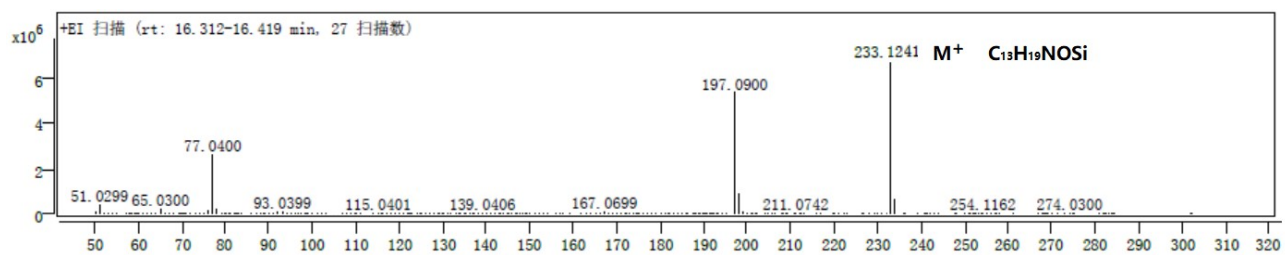


Figure S33. GC-MS spectrum of complex **5i**.

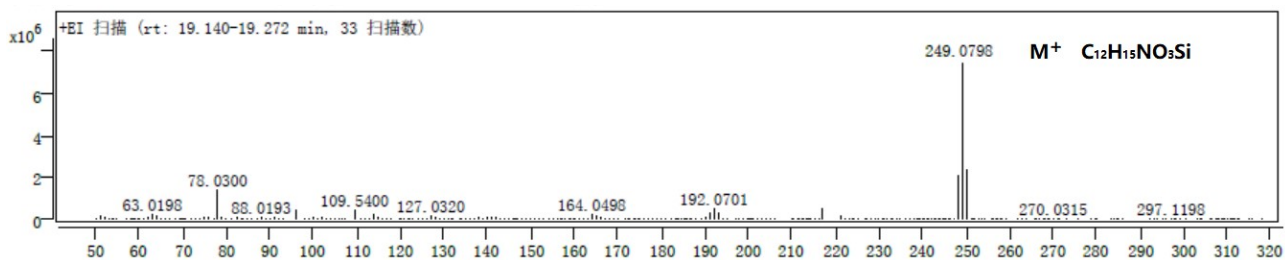


Figure S34. GC-MS spectrum of complex **5j**.

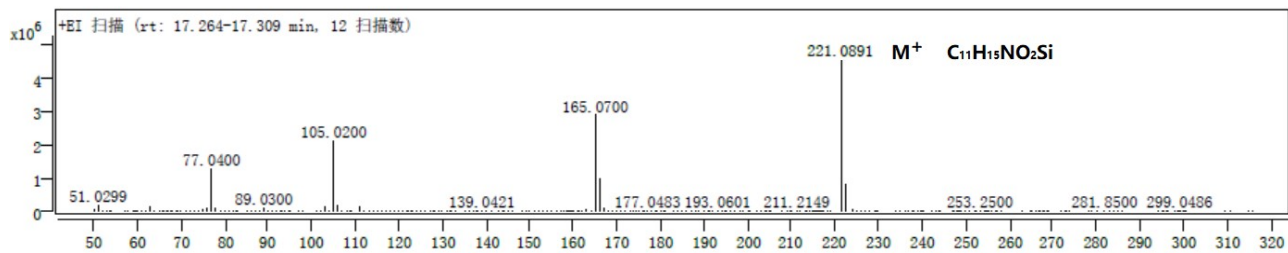


Figure S35. GC-MS spectrum of complex **5k**.

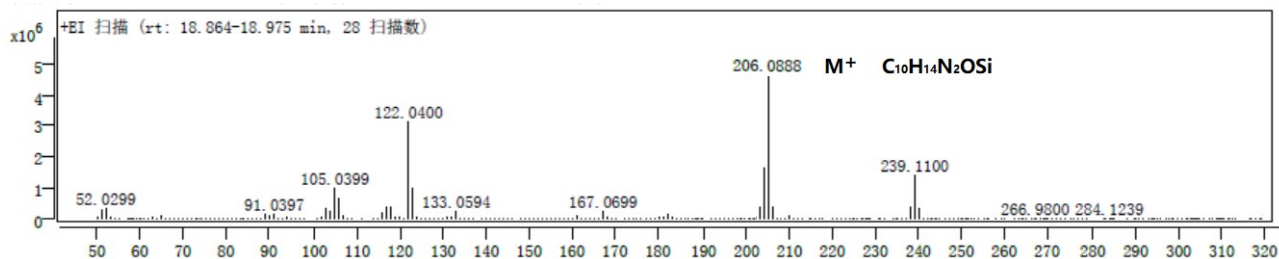


Figure S36. GC-MS spectrum of complex **5l**.

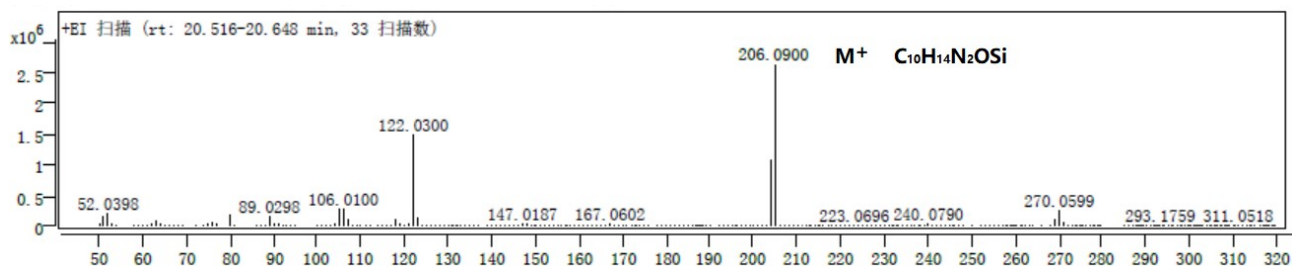


Figure S37. GC-MS spectrum of complex **5m**.

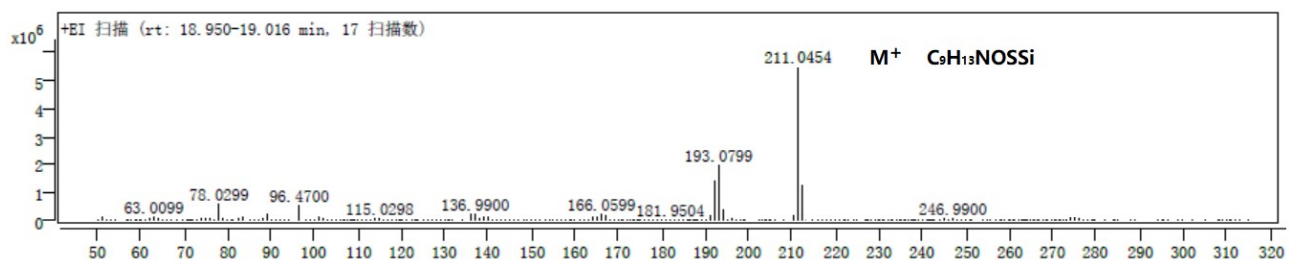


Figure S38. GC-MS spectrum of complex **5n**.

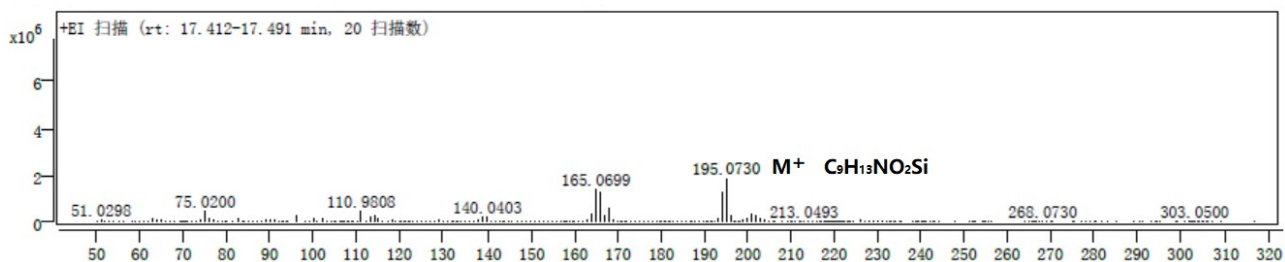


Figure S39. GC-MS spectrum of complex **5o**.



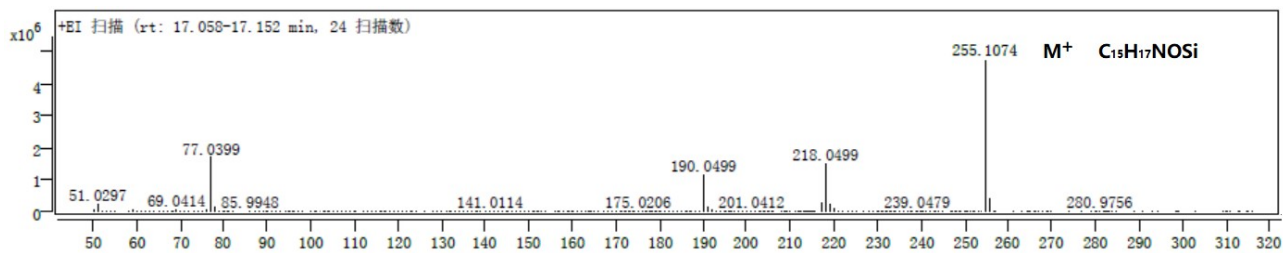


Figure S40. GC-MS spectrum of complex **5p**.

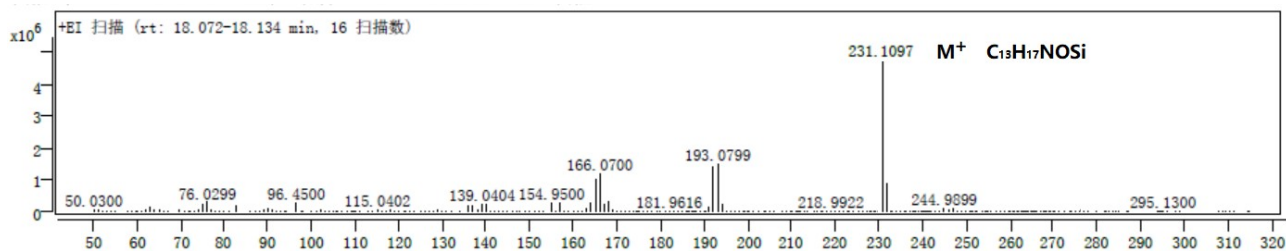


Figure S41. GC-MS spectrum of complex **5q**.

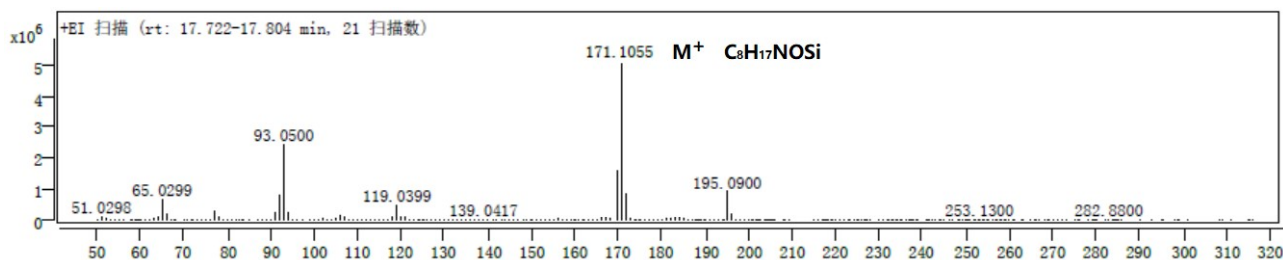


Figure S42. GC-MS spectrum of complex **5r**.

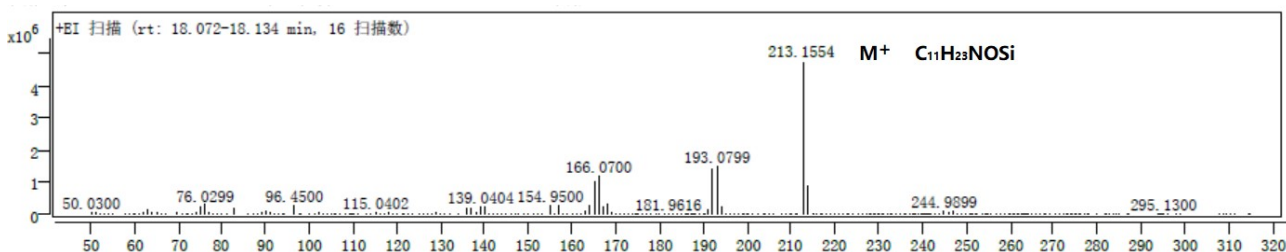


Figure S43. GC-MS spectrum of complex **5r**.

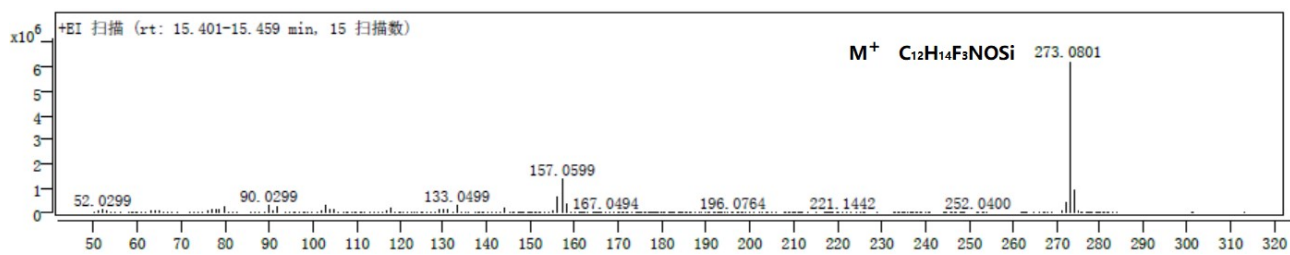


Figure S44. GC-MS spectrum of complex **5t**.