

Supporting Information

Synthesis and crystallographic characterization of heteroleptic Ir(III) complexes containing the *N*-oxide functional group and crystallographic characterization of Ir(III) *N*-oxide precursors.

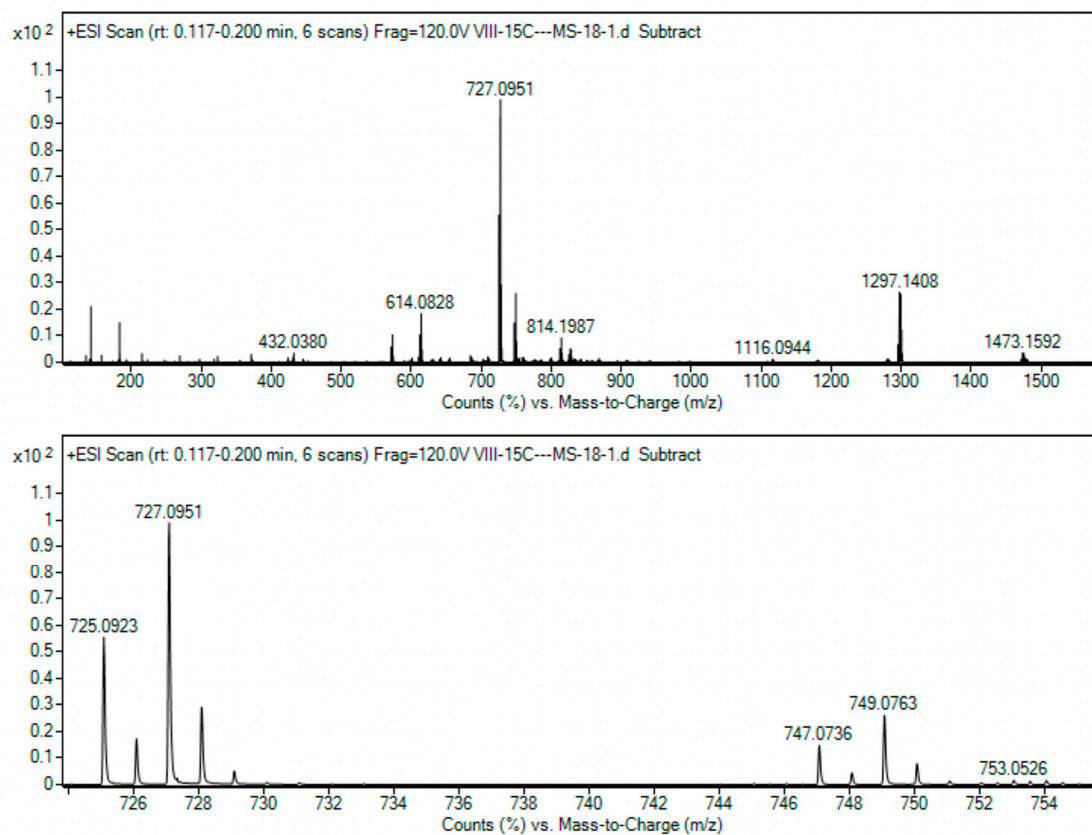


Figure S1: HRMS of compound 1.

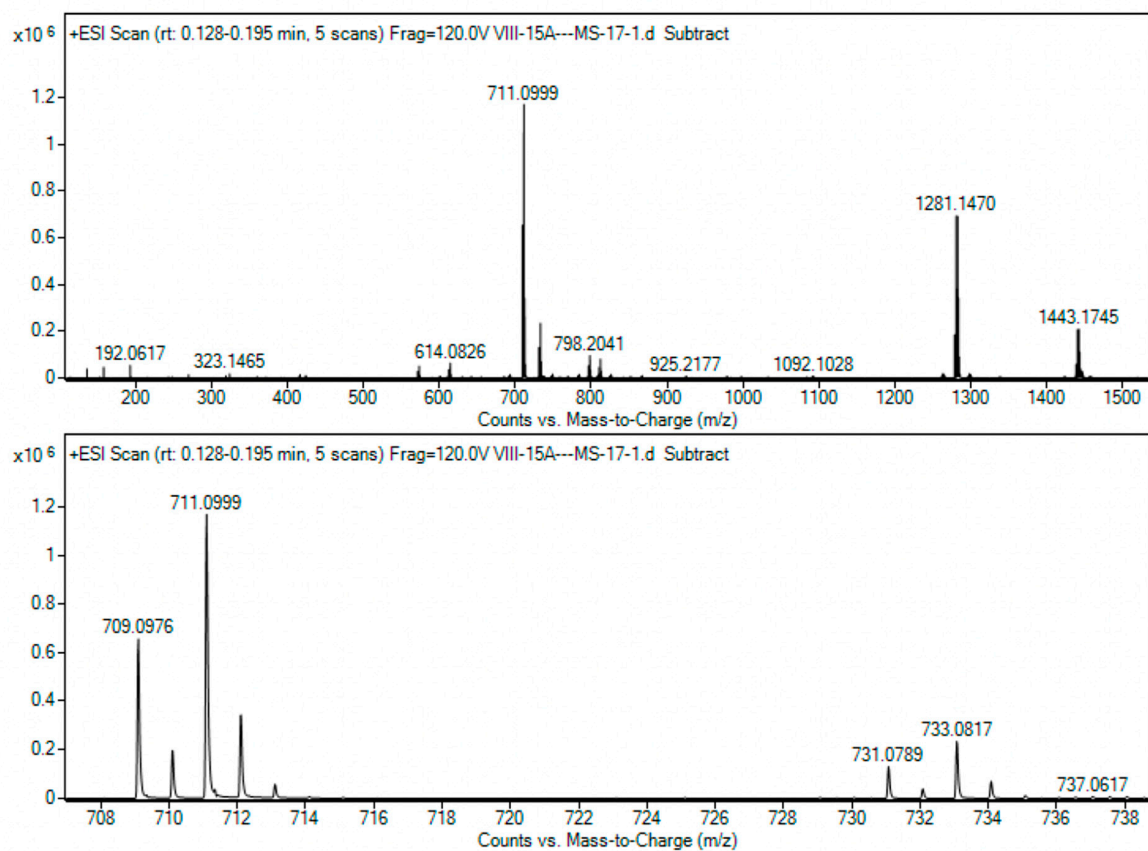


Figure S2: HRMS of compound 2.

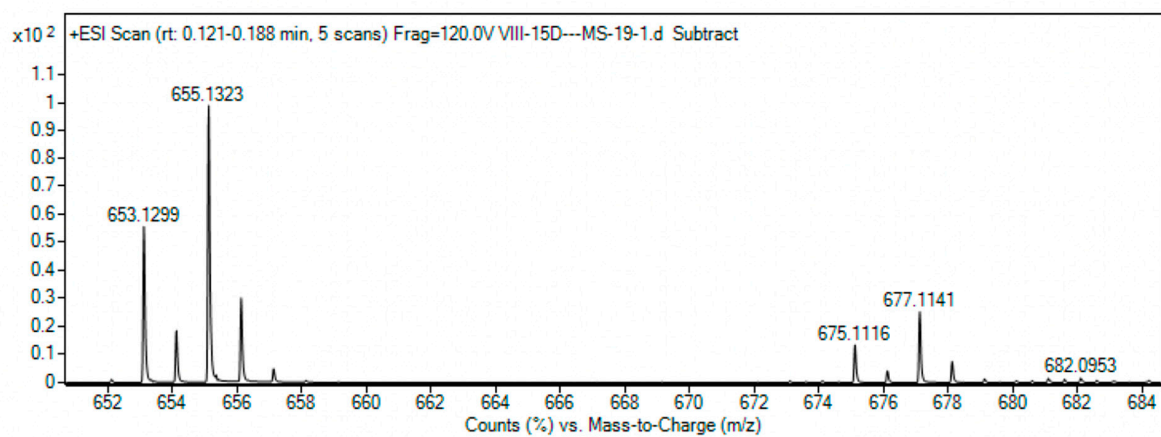
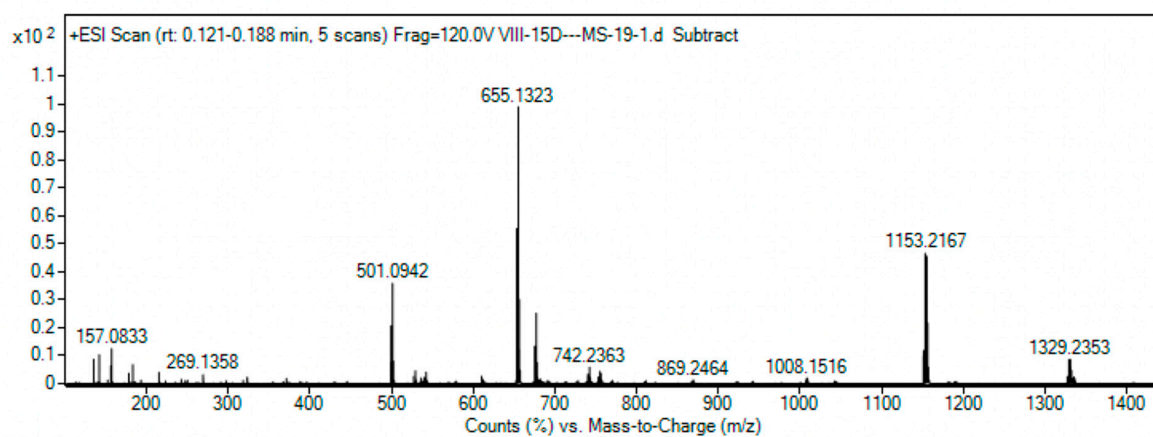


Figure S3: HRMS of compound 3.

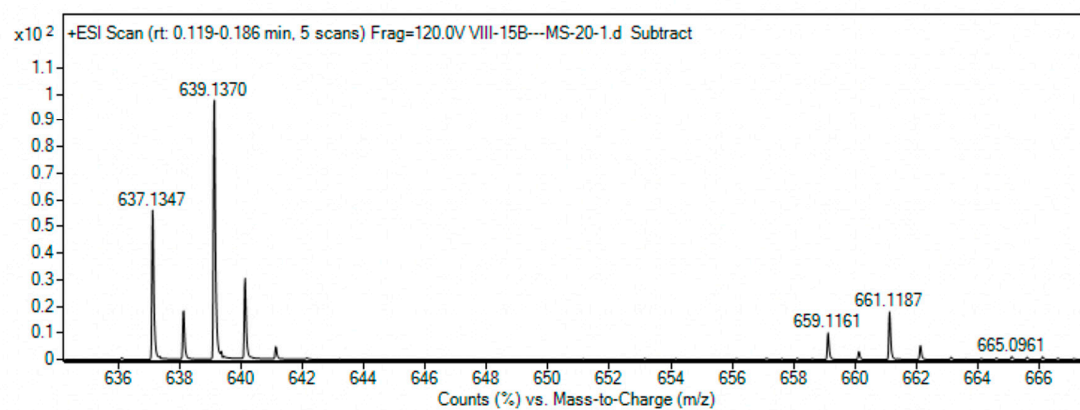
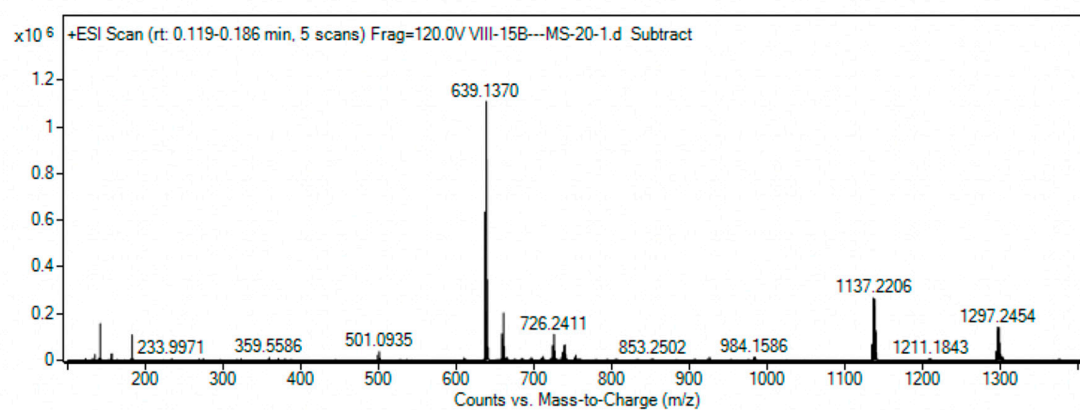


Figure S4: HRMS of compound 4.

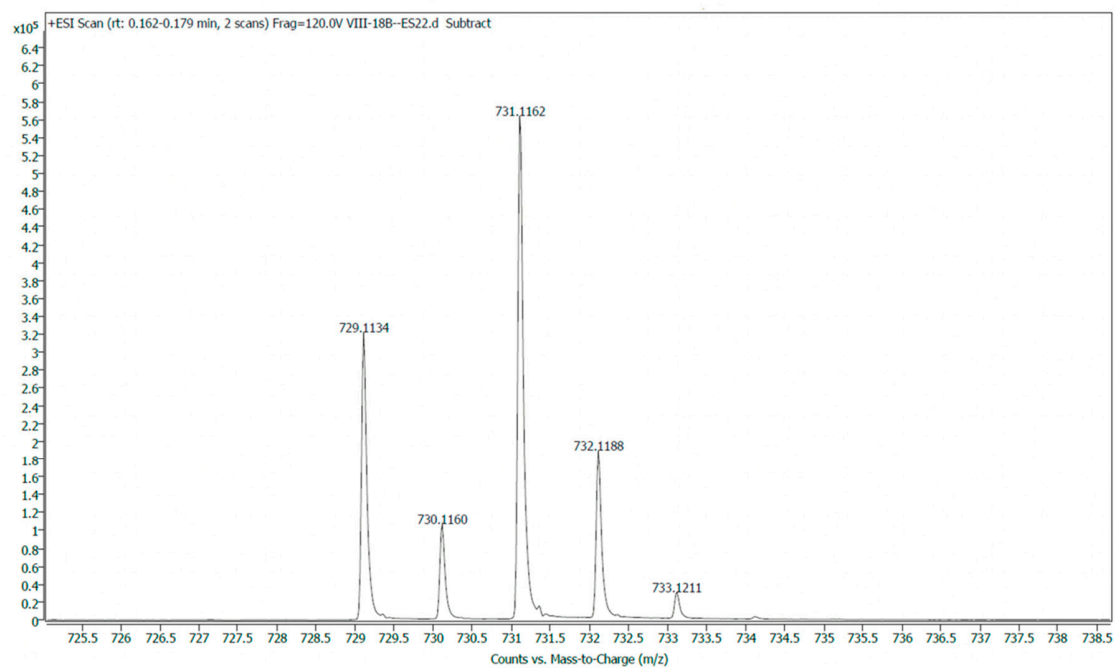


Figure S5: HRMS of compound 6.

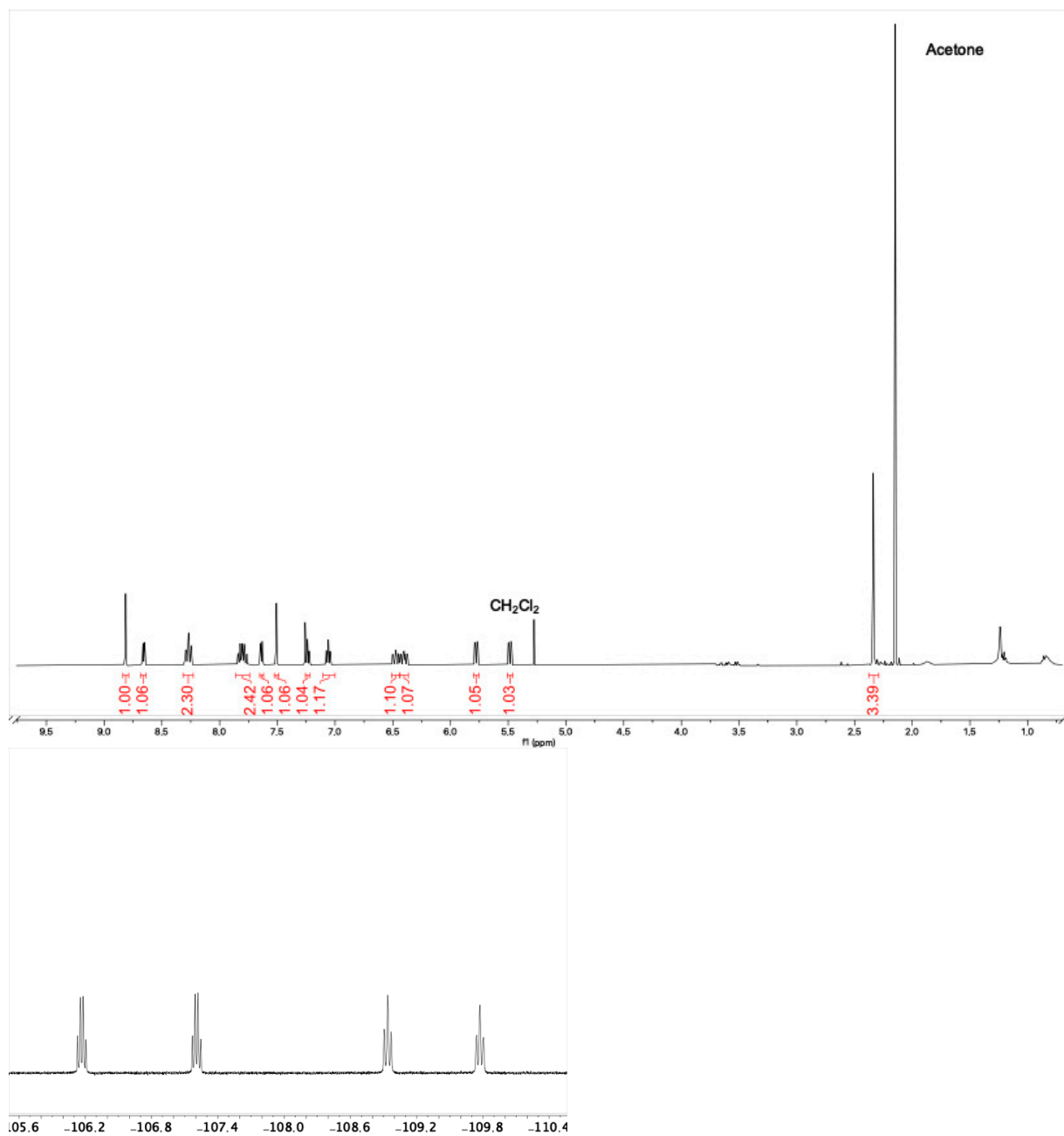


Figure S6: ¹H NMR (above) and ¹⁹F NMR (below) of compound **1** in CDCl₃.

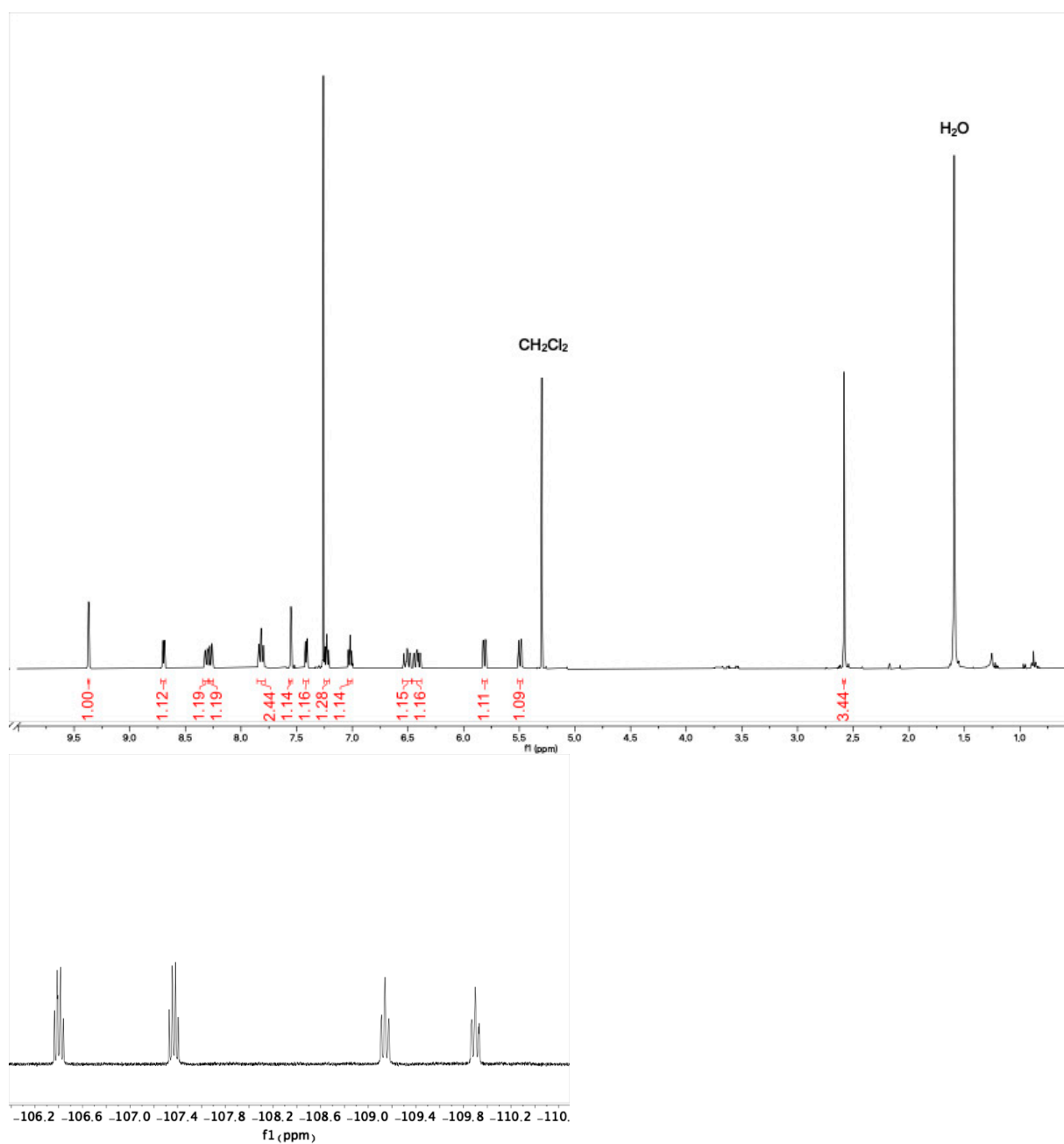


Figure S7: ¹H NMR (above) and ¹⁹F NMR (below) of compound **2** in CDCl₃.

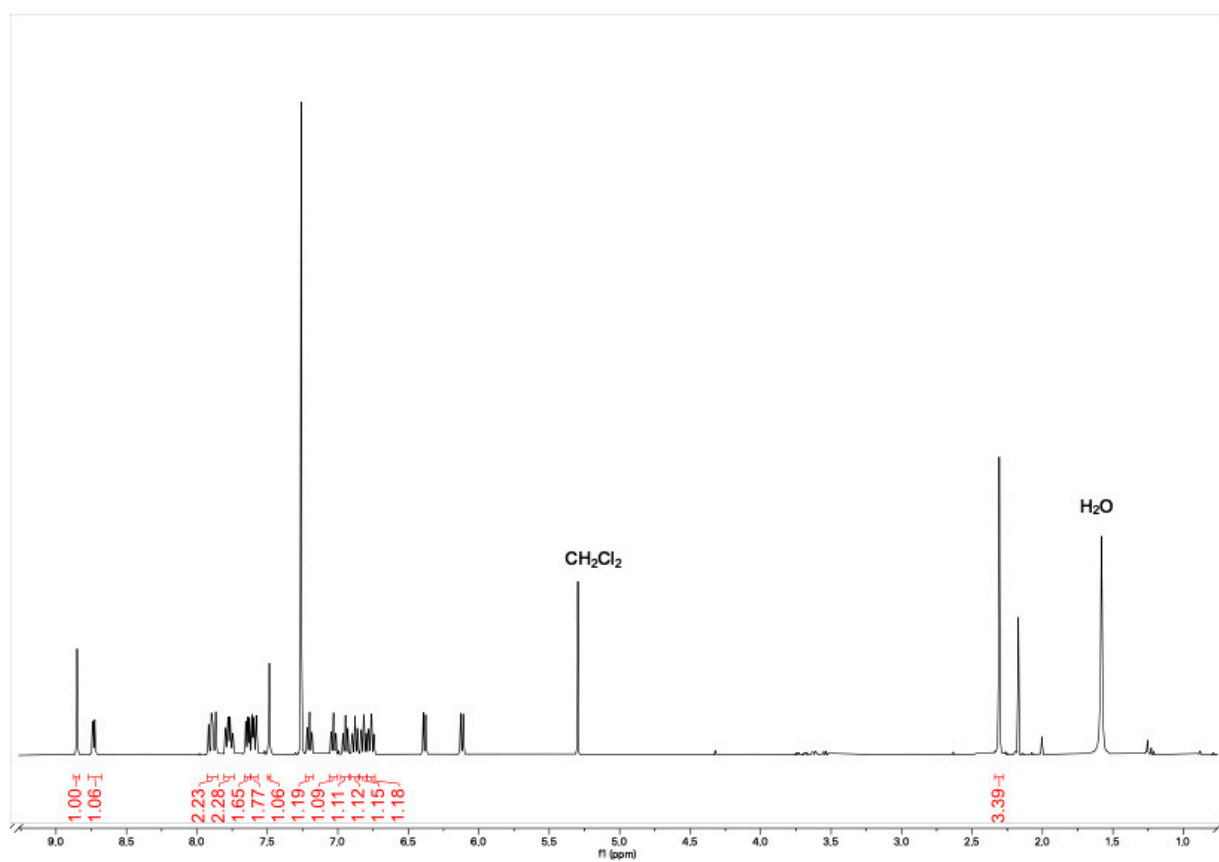


Figure S8: ¹H NMR of compound **3** in CDCl₃.

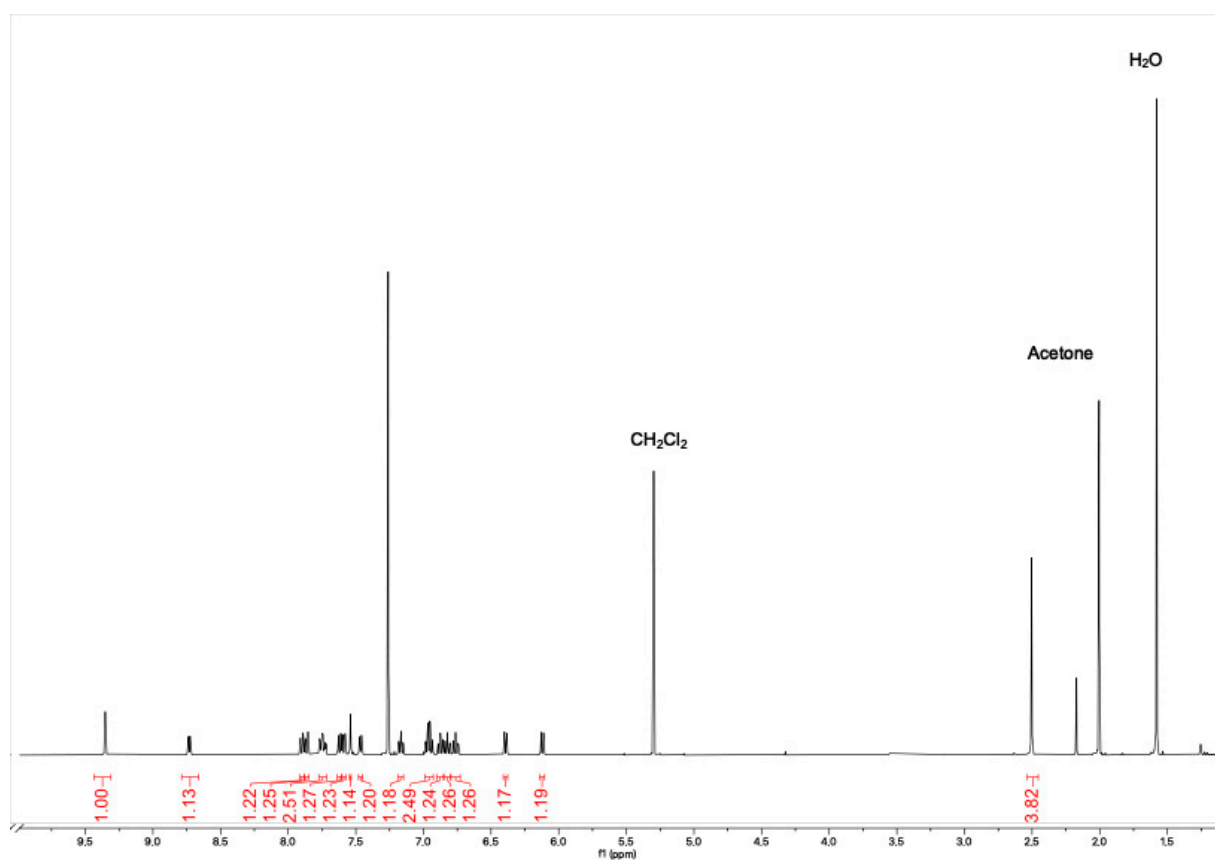


Figure S9: ¹H NMR of compound **4** in CDCl₃.

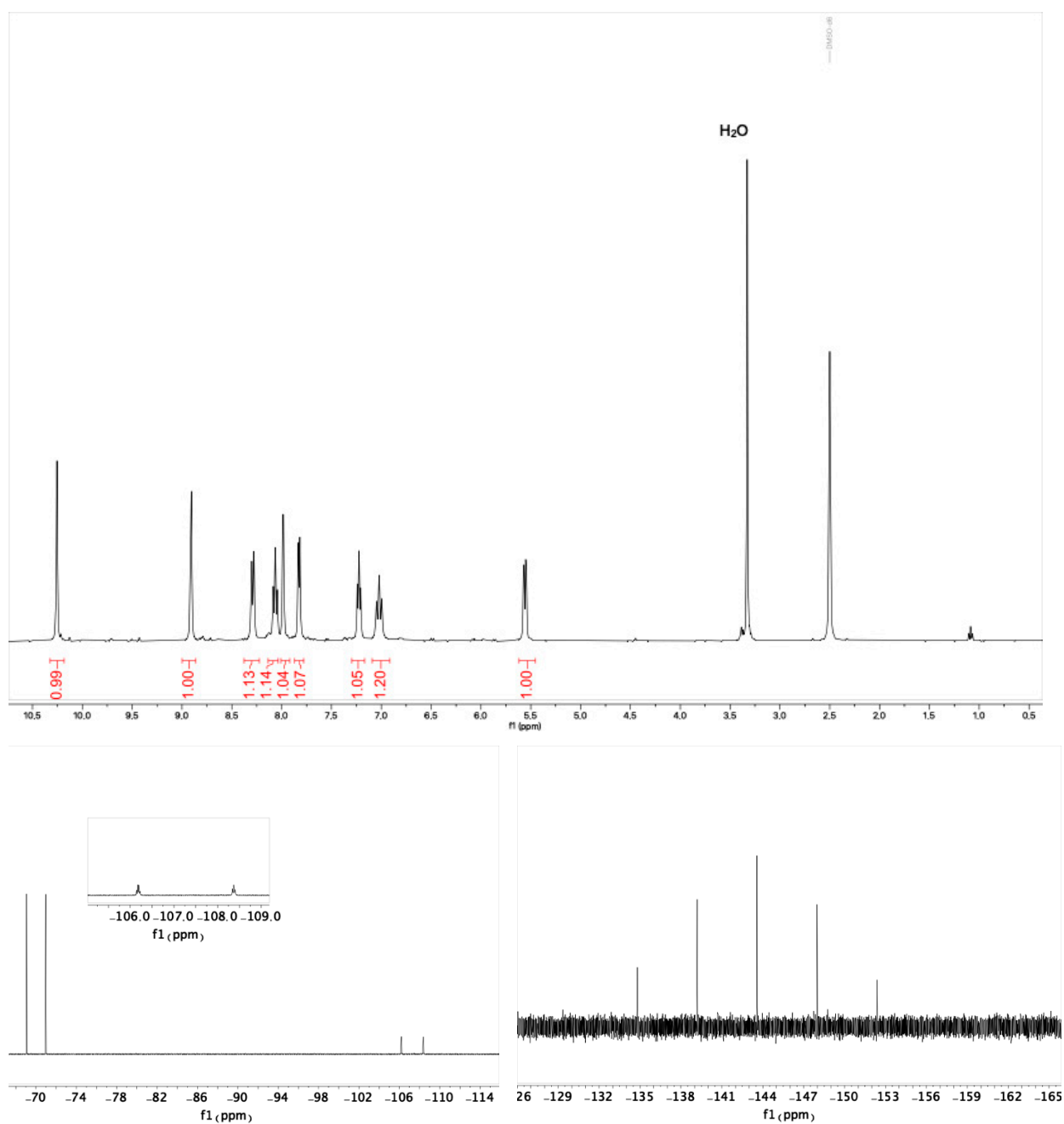


Figure S10: ¹H NMR (above), ¹⁹F NMR (below, left), and ³¹P NMR (below, right) of compound 6 in DMSO-d₆.

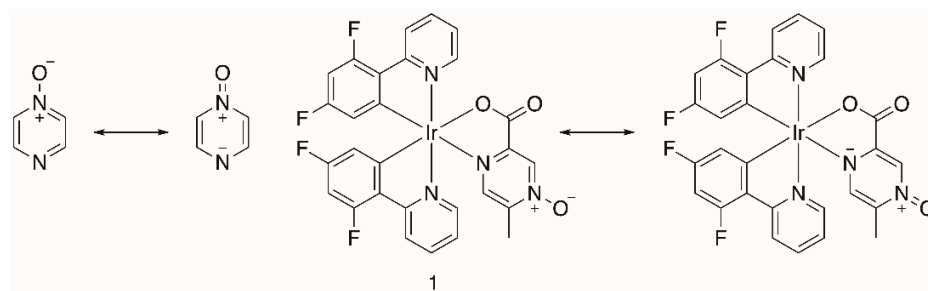


Figure S11: Resonance contributors of pyrazine *N*-oxide and compound **1**.

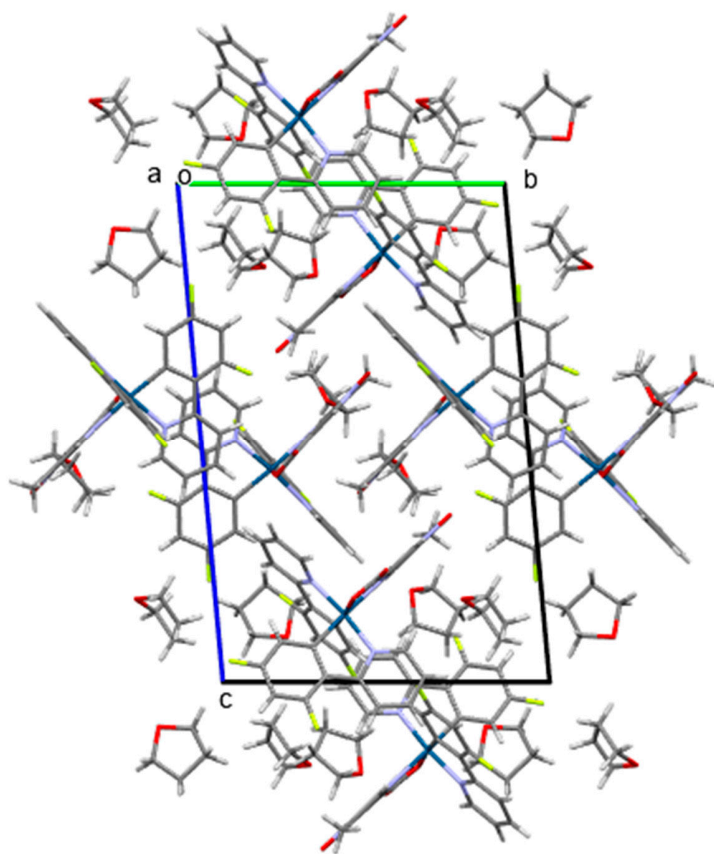


Figure S12: Packing diagram of $1 \cdot 1.25(\text{THF})$.

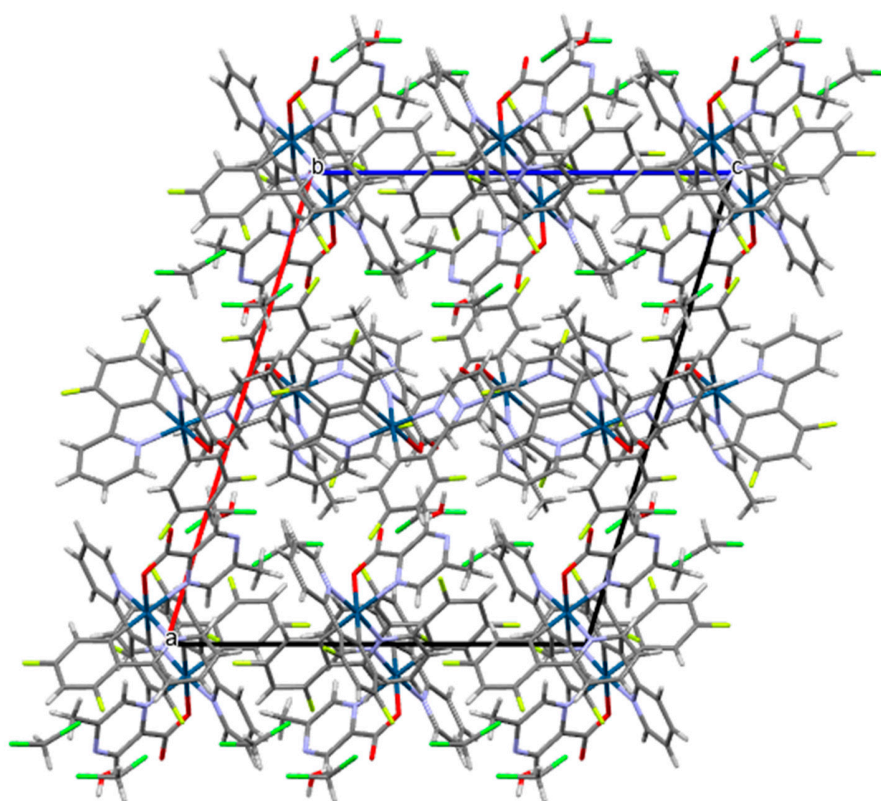


Figure S13: Packing diagram of $2 \cdot 0.5(\text{DCM}), 0.5(\text{H}_2\text{O})$.

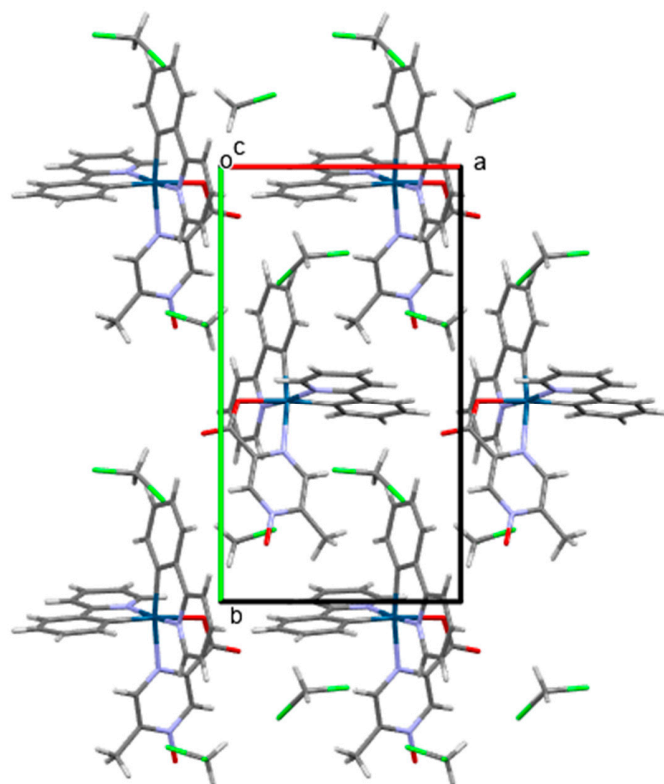


Figure S14: Packing diagram of $3 \cdot 2(\text{DCM})$.

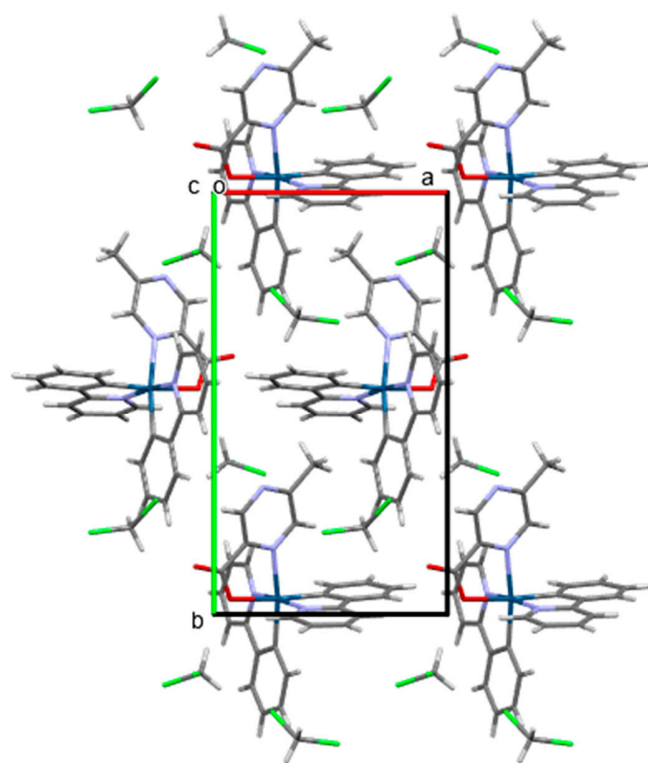


Figure S15: Packing diagram of $4 \cdot 2(\text{DCM})$.

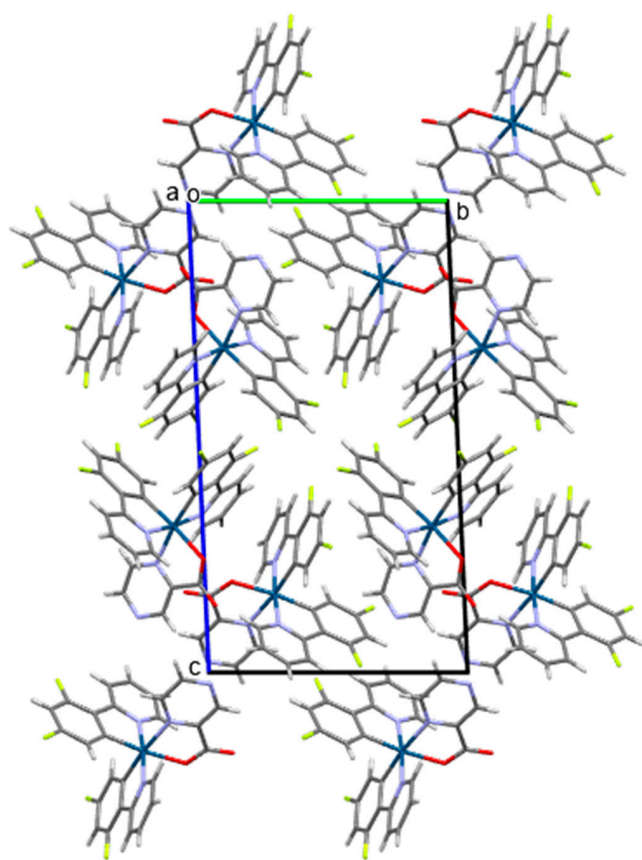


Figure S16: Packing diagram of 5.

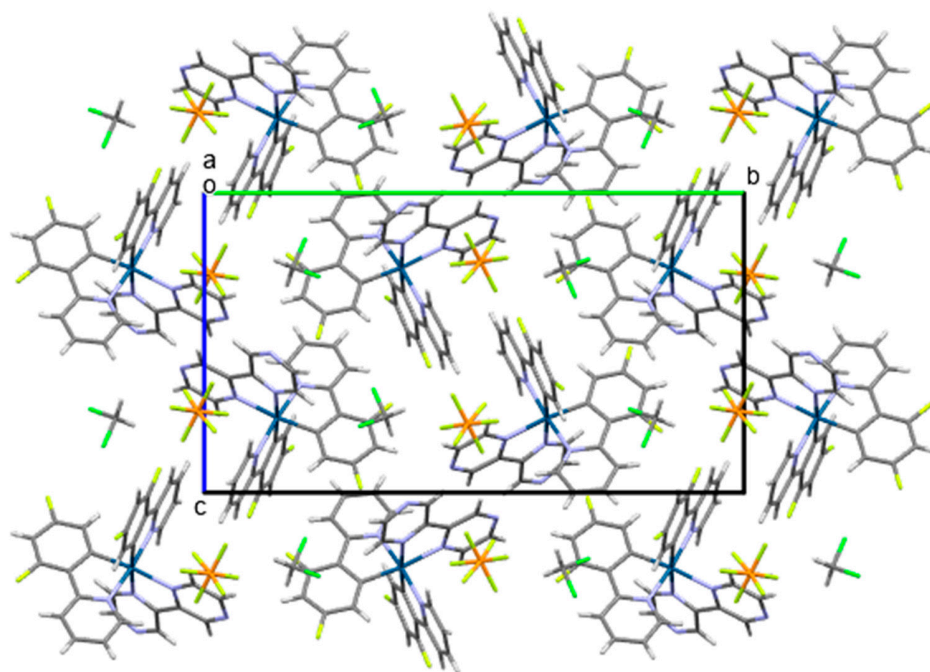


Figure S17: Packing diagram of **6 · (DCM)**.

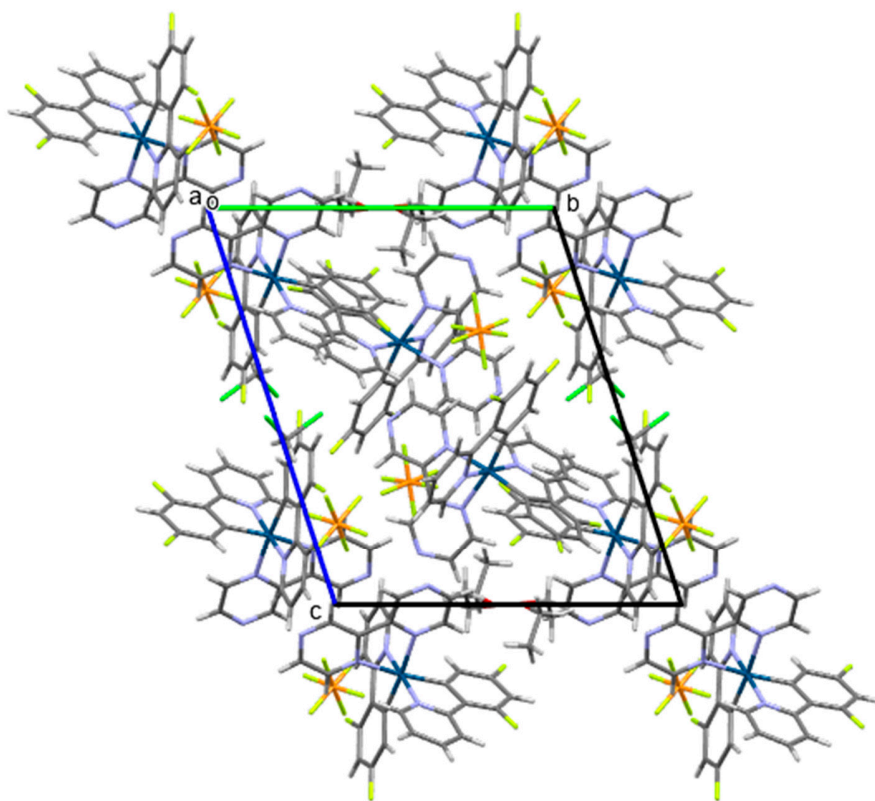


Figure S18: Packing diagram of $6 \cdot 0.5(\text{DCM}), 0.5(\text{Et}_2\text{O})$.

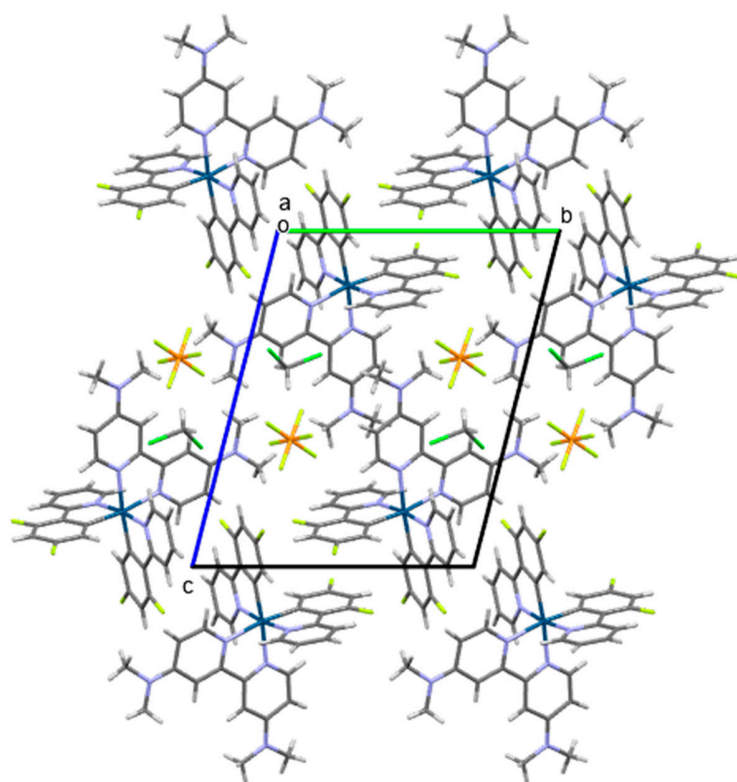


Figure S19: Packing diagram of 7 · (DCM).

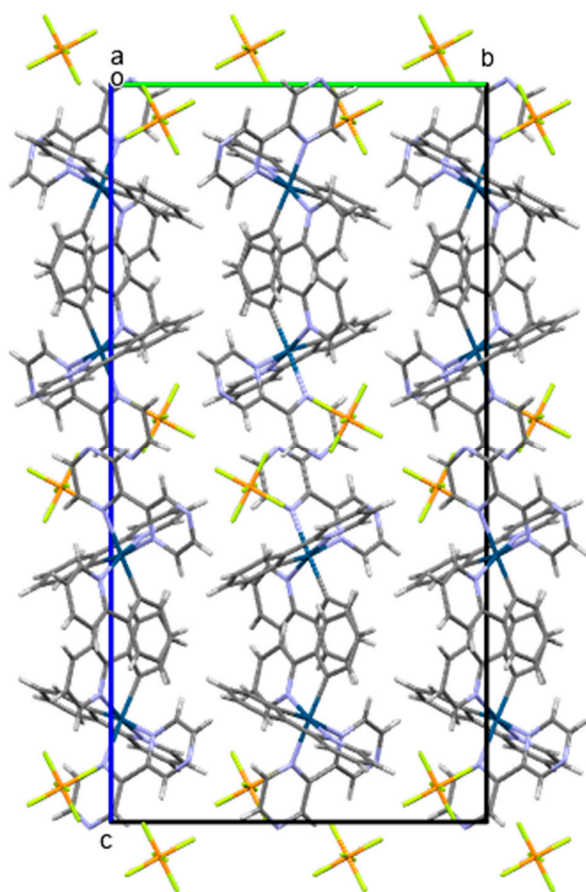


Figure S20: Packing diagram of **8**.