

APPENDICES

APPENDIX A

SUPPORTING INFORMATION

A.1 Mass spectrometry analysis data for $[\text{Fe}(\text{salRen-5-OMe})_2]\text{A}$ complexes

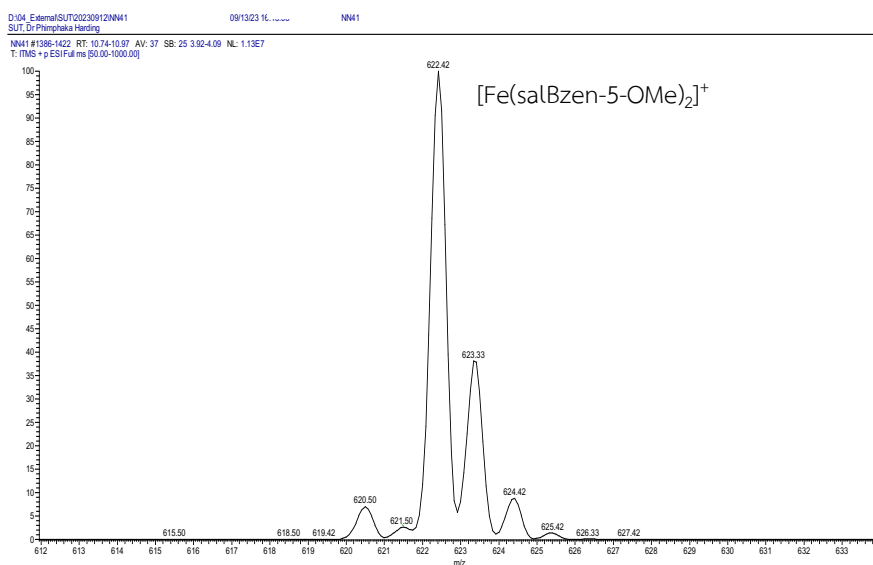


Figure S1. Mass spectra (LC-MS, positive) of **1**.

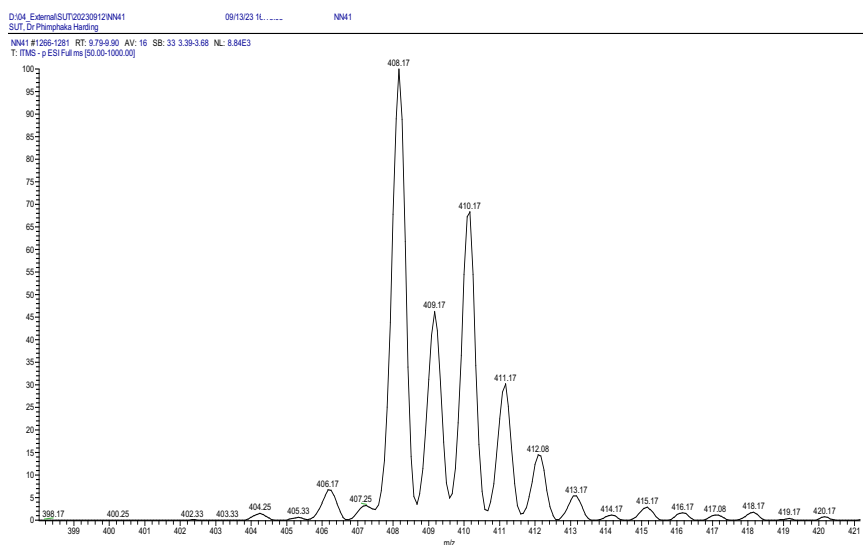


Figure S2. Mass spectra (LC-MS, negative) of **1**.

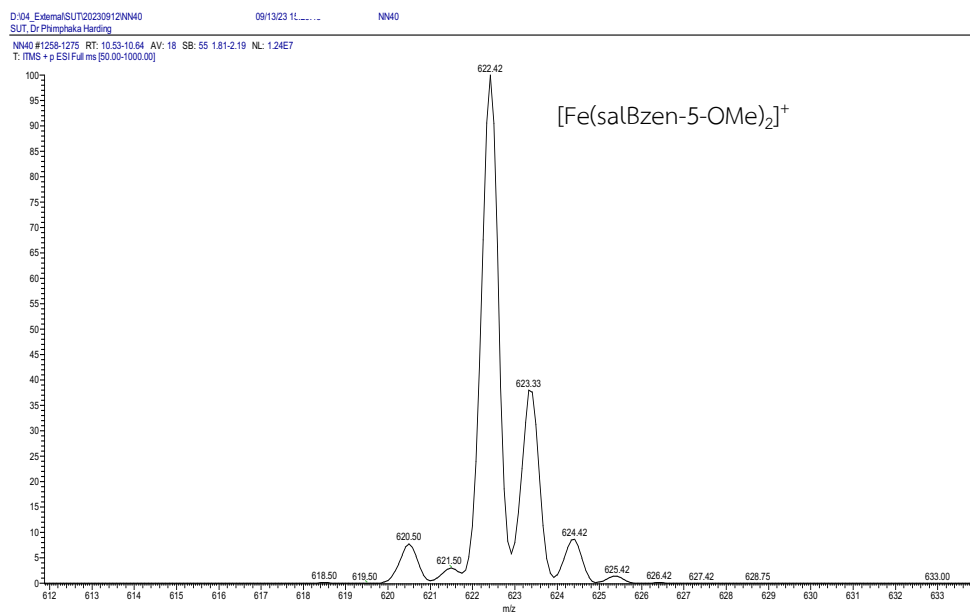


Figure S3. Mass spectra (LC-MS, positive) of 2.

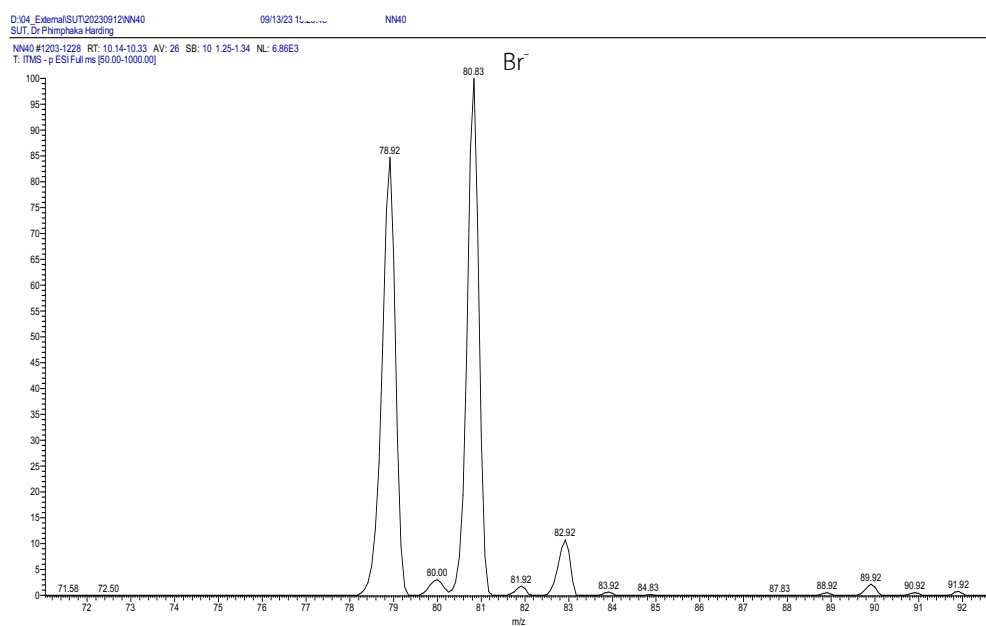
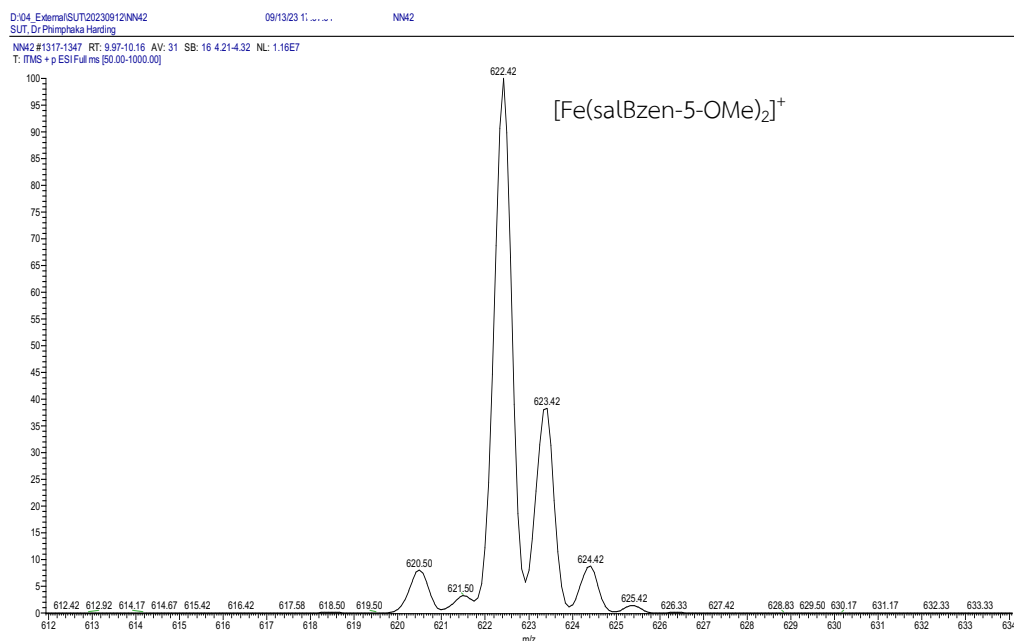
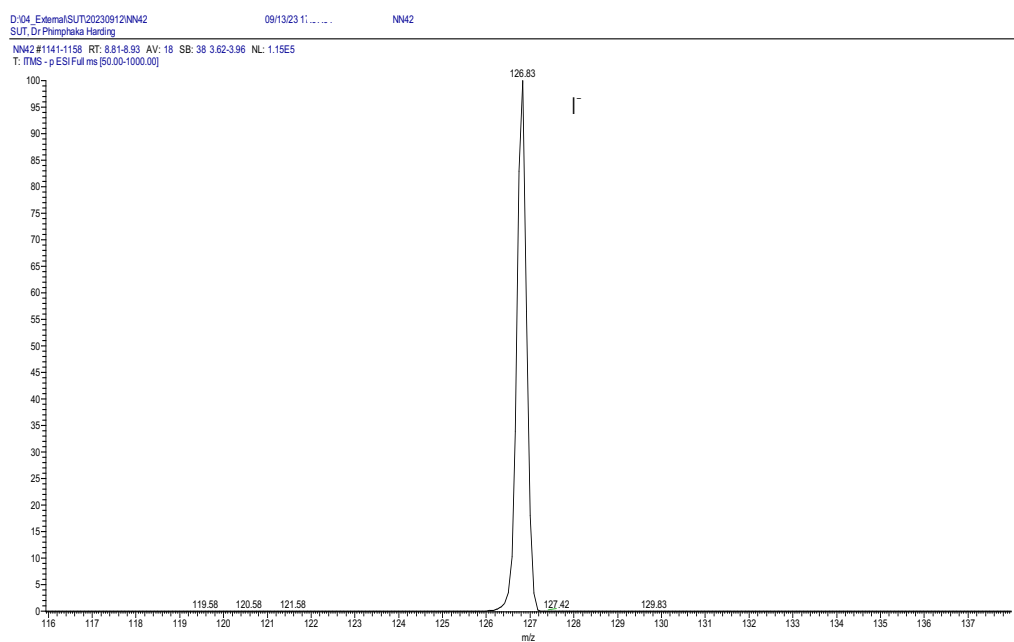
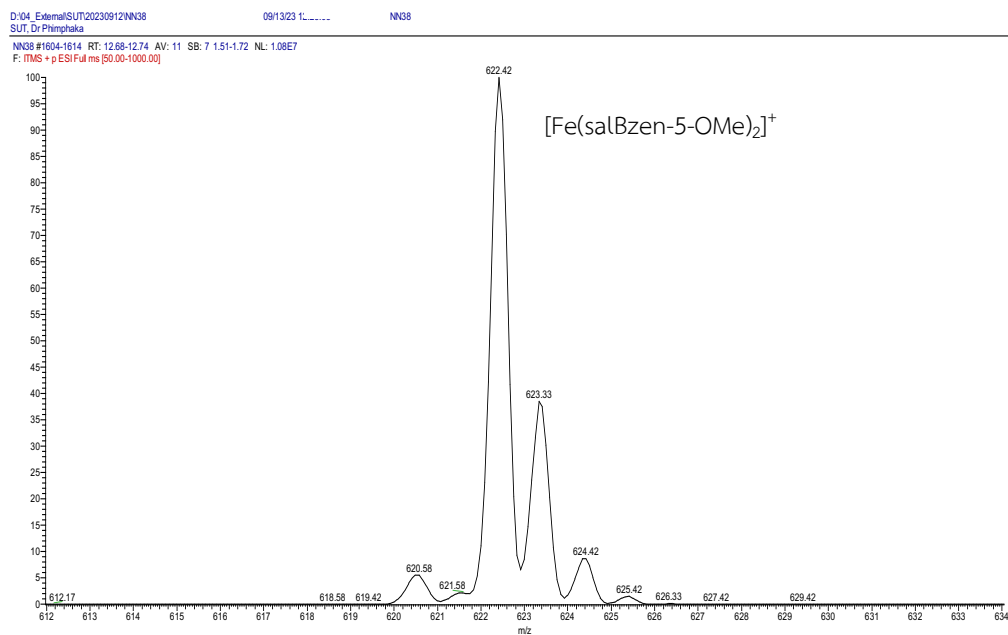
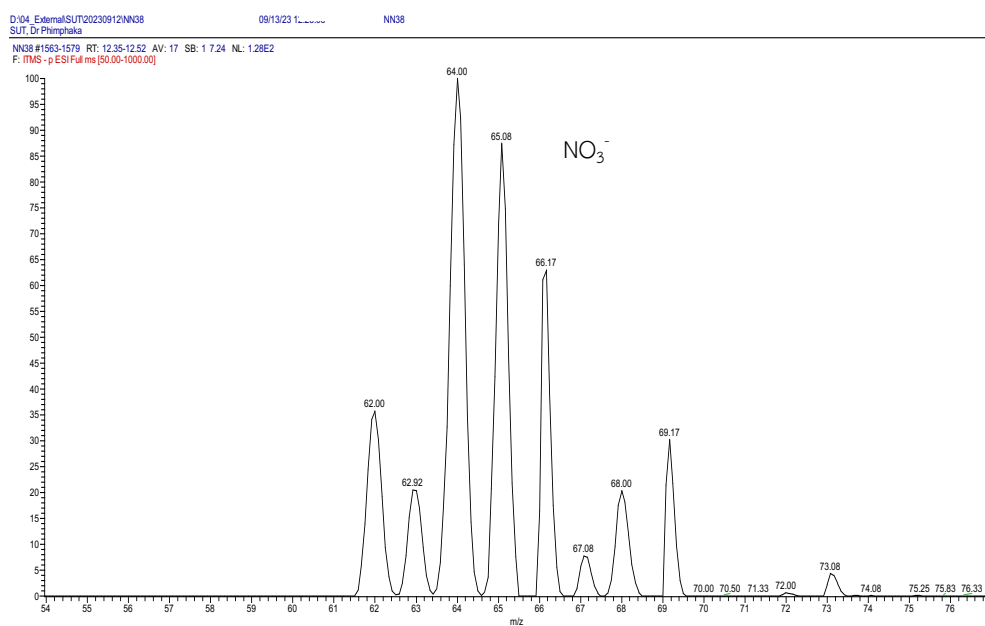


Figure S4. Mass spectra (LC-MS, negative) of 2.

Figure S5. Mass spectra (LC-MS, positive) of **3**.Figure S6. Mass spectra (LC-MS, negative) of **3**.

Figure S7. Mass spectra (LC-MS, positive) of **4**.Figure S8. Mass spectra (LC-MS, negative) of **4**.

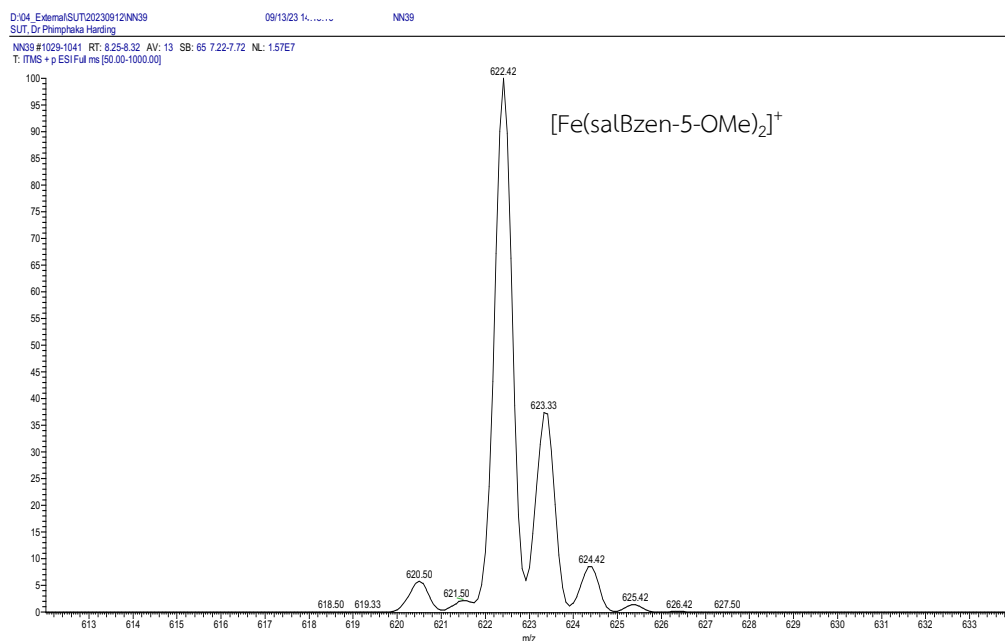


Figure S9. Mass spectra (LC-MS, positive) of 5.

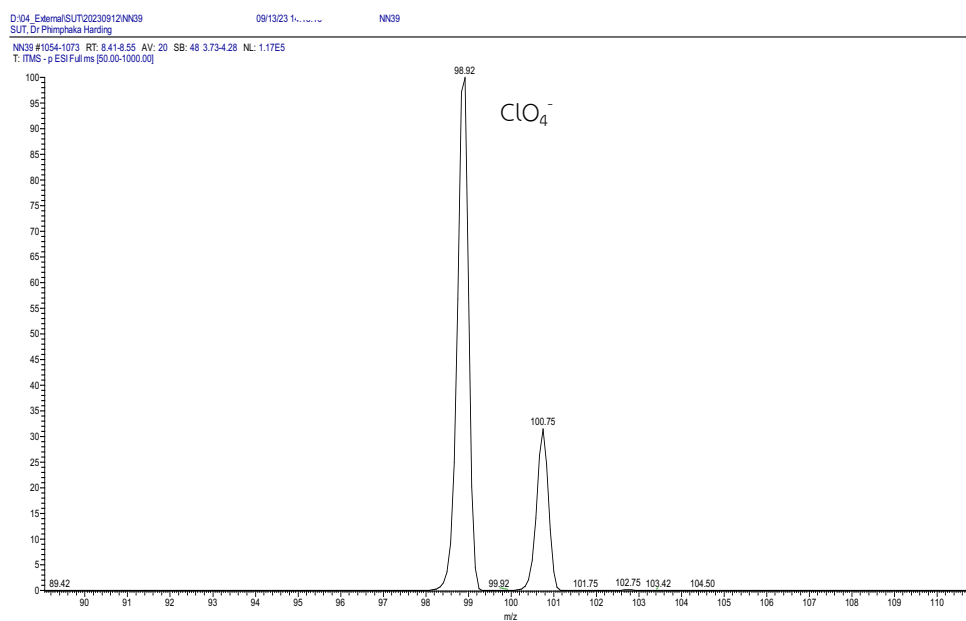


Figure S10. Mass spectra (LC-MS, negative) of 5.

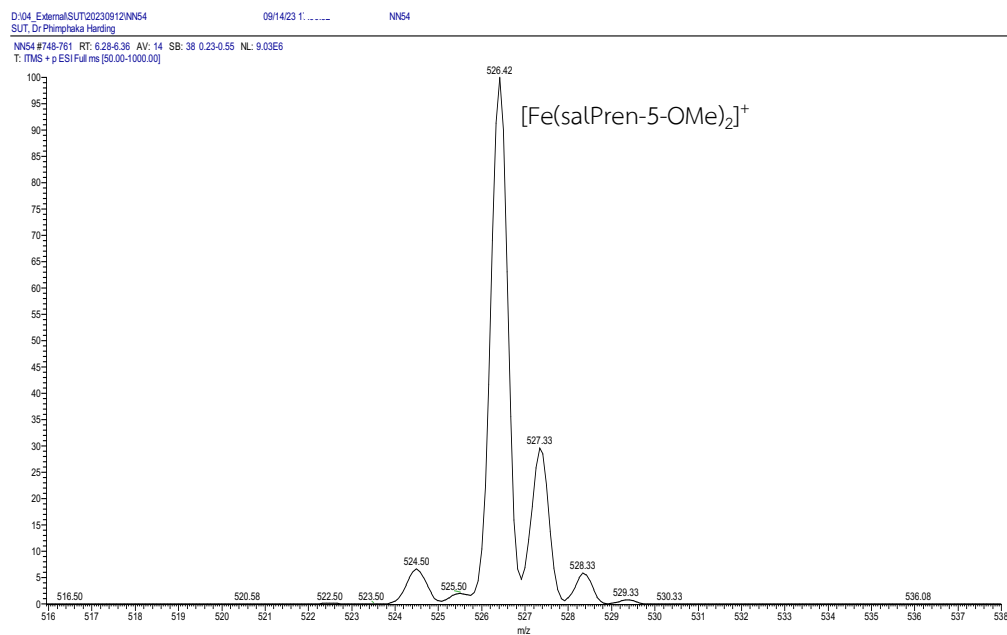


Figure S11. Mass spectra (LC-MS, positive) of 7.

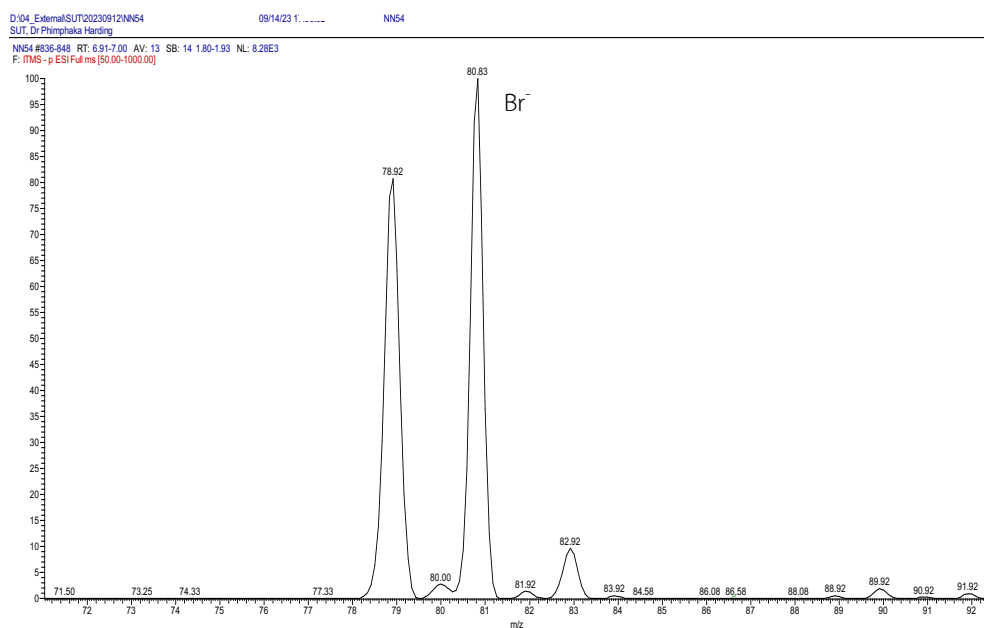
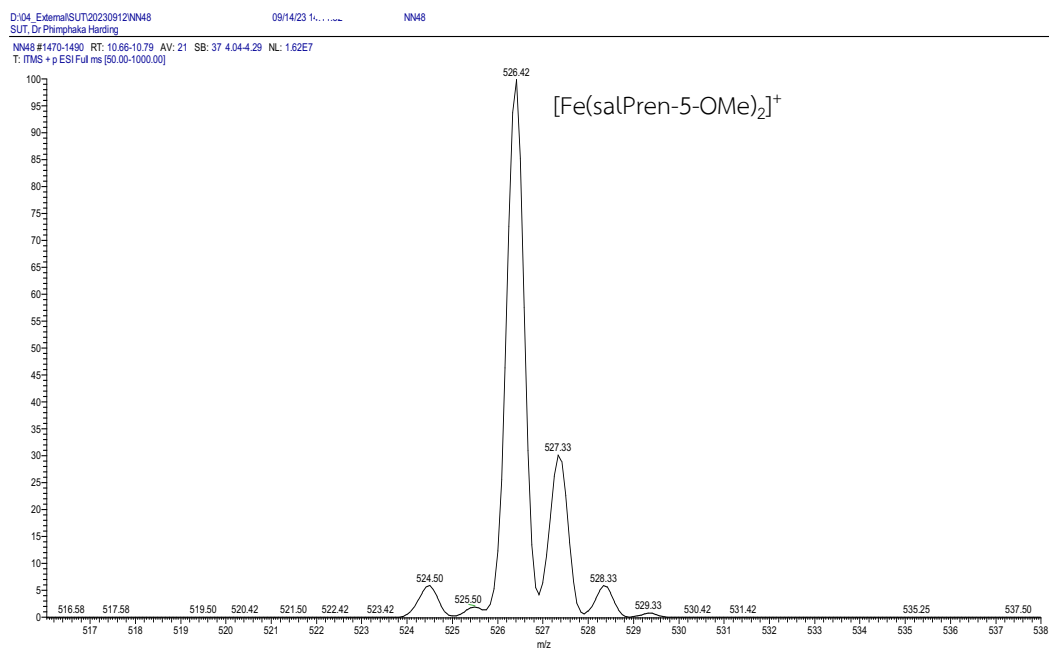
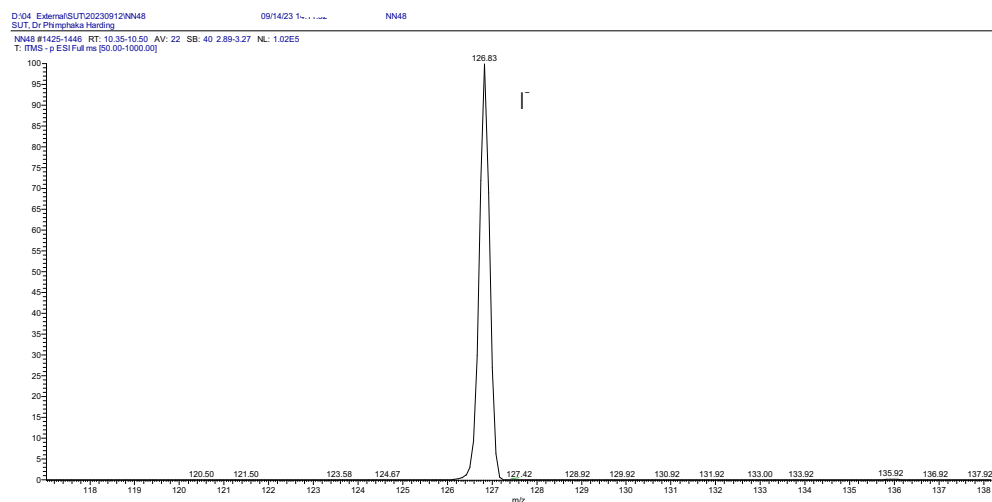


Figure S12. Mass spectra (LC-MS, negative) of 7.

Figure S13. Mass spectra (LC-MS, positive) of **8**.Figure S14. Mass spectra (LC-MS, negative) of **8**.

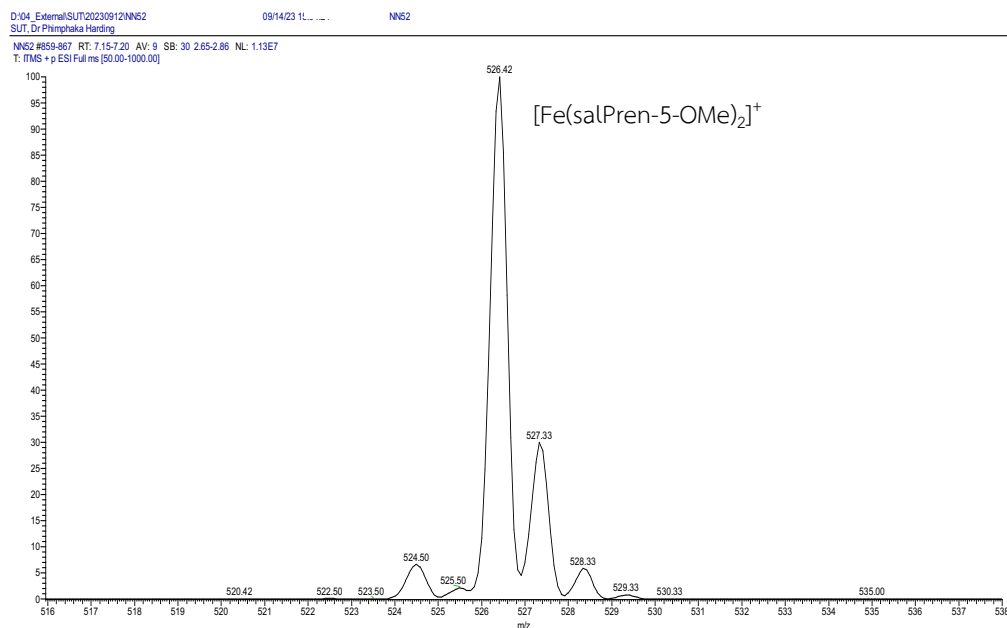


Figure S15. Mass spectra (LC-MS, positive) of 9.

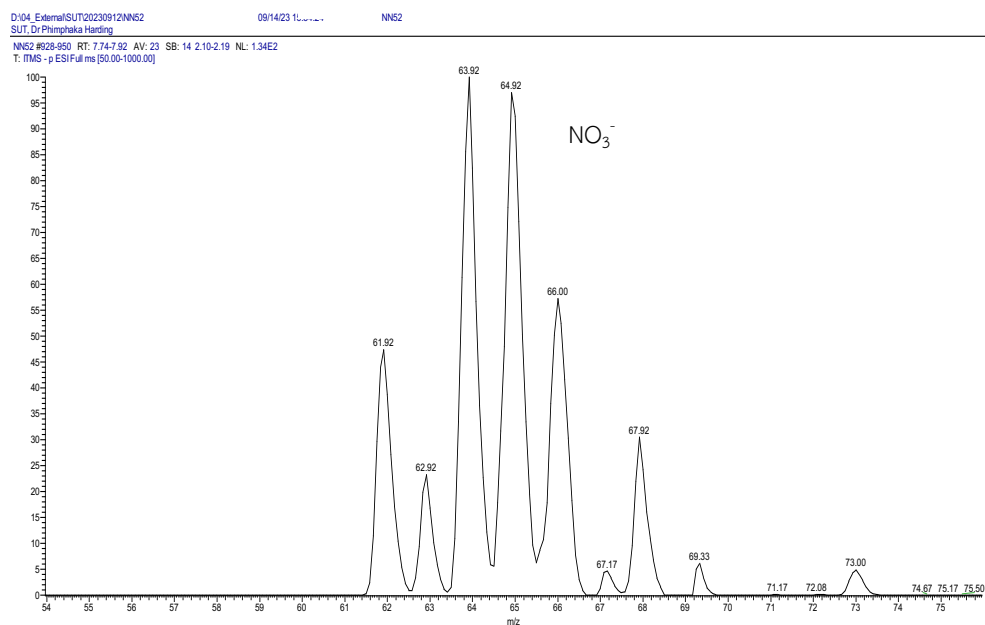


Figure S16. Mass spectra (LC-MS, negative) of 9.

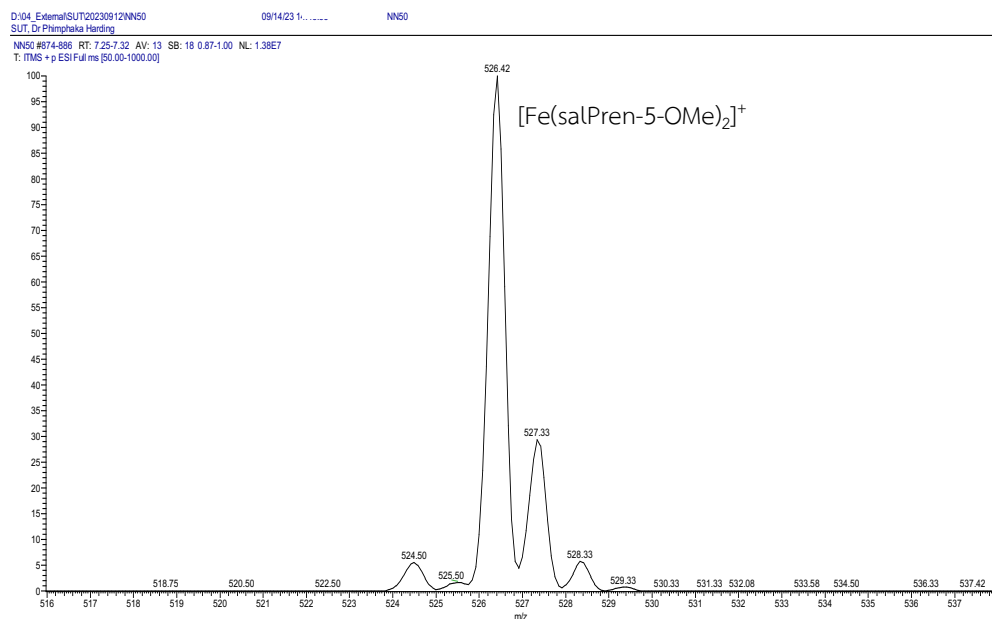


Figure S17. Mass spectra (LC-MS, positive) of 10.

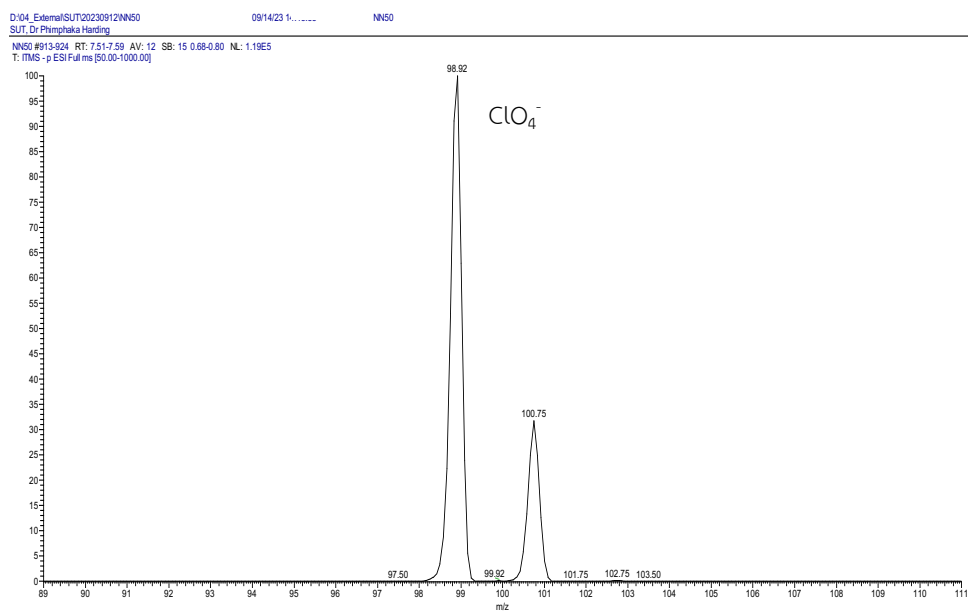


Figure S18. Mass spectra (LC-MS, negative) of 10.

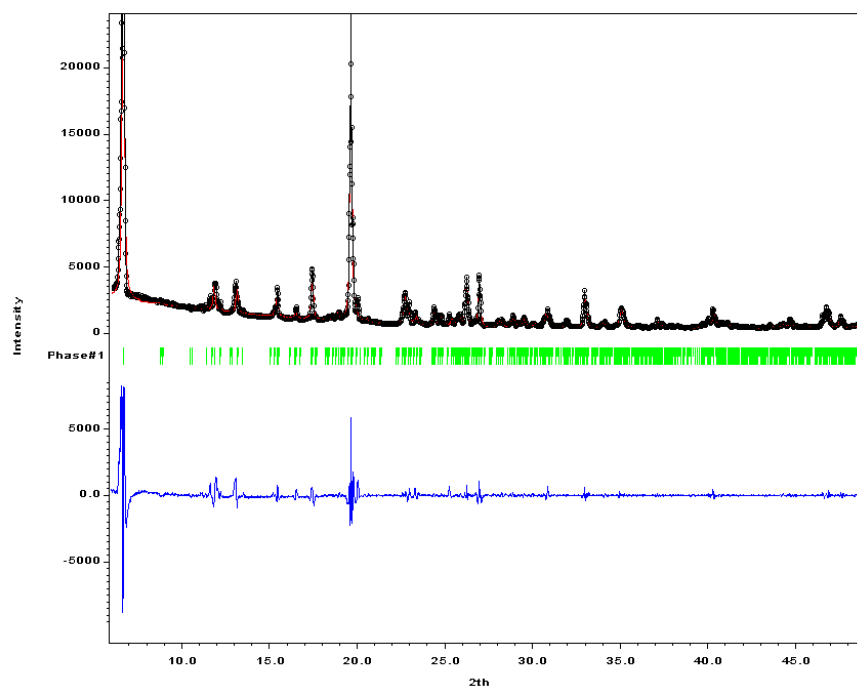
A.2 PXRD pattern data for $[\text{Fe}(\text{salRen-5-OMe})_2]\text{A}$ complexes

Figure S19. PXRD patterns of 1.

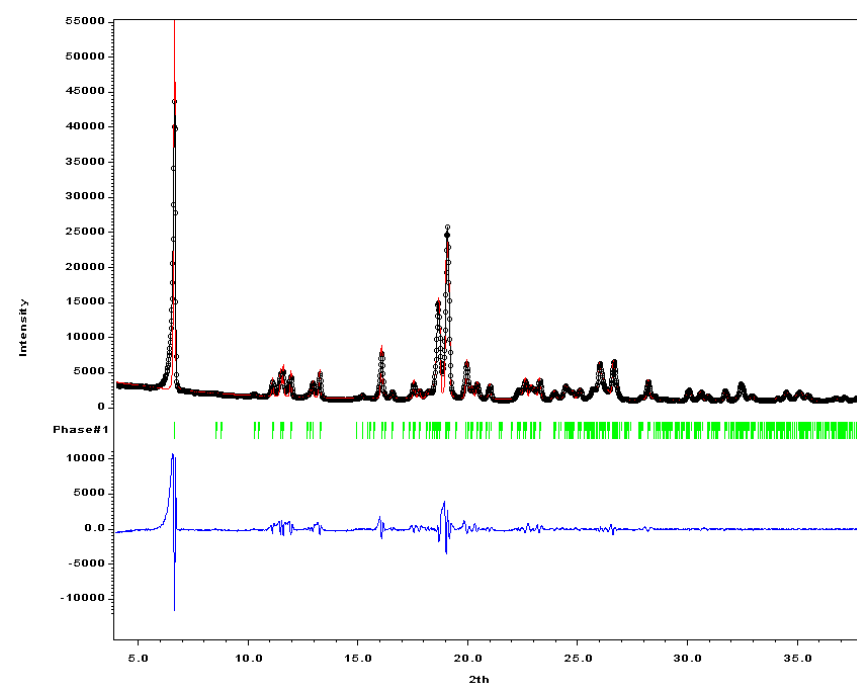


Figure S20. PXRD patterns of 2.

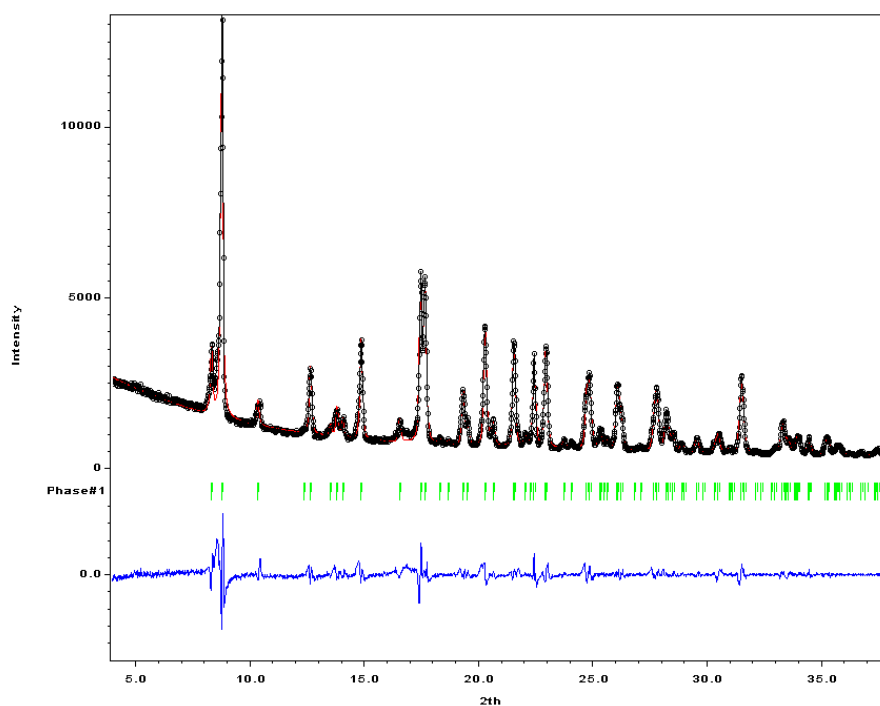


Figure S21. PXRD patterns of 3.

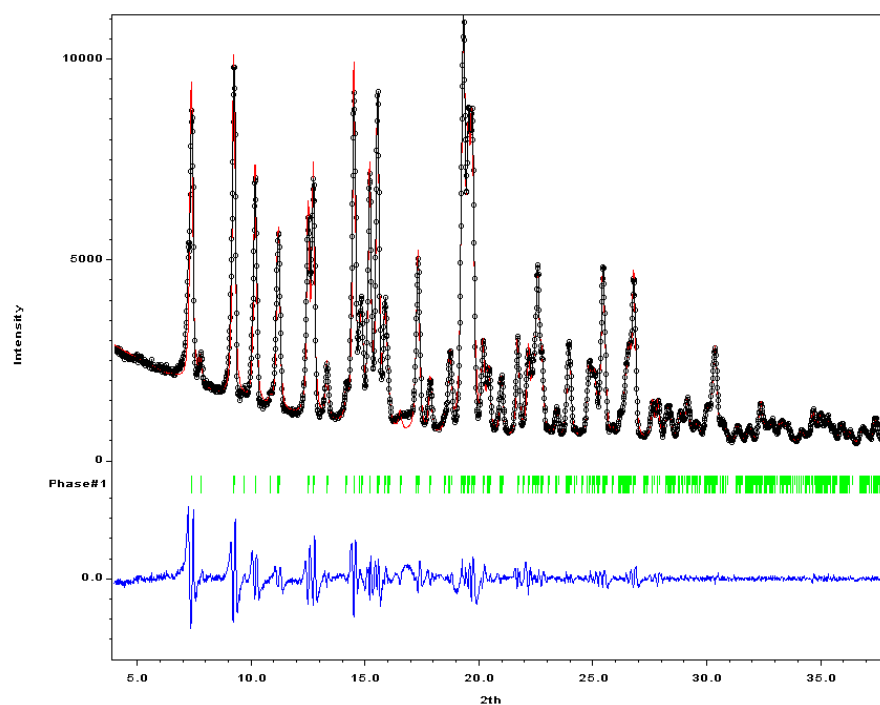


Figure S22. PXRD patterns of 4.

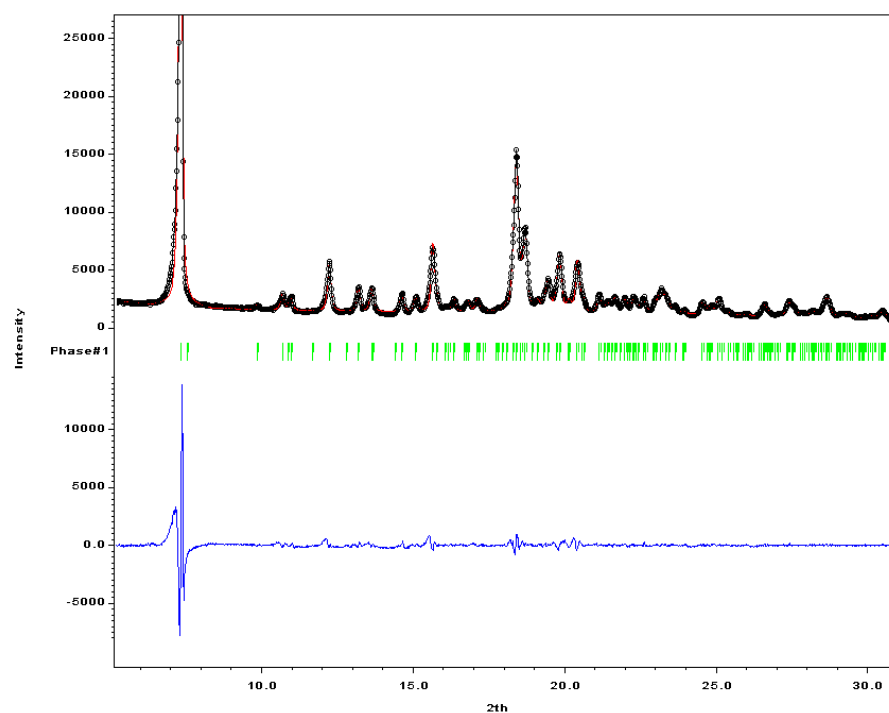


Figure S23. PXRD patterns of 5.

*Experimental PXRD diffractograms (black) and the corresponding simulated patterns (red) for each complex.

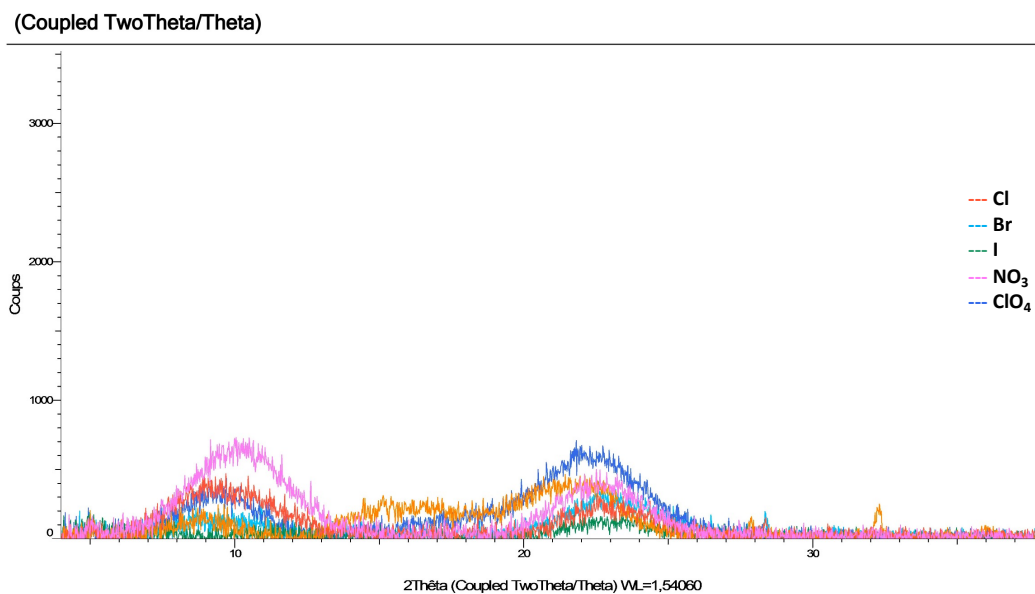


Figure S24. PXRD patterns of 6-10

*Experimental PXRD diffractograms of 6-10, on which all bulk measurements were done, are amorphous.

A.3 Hirshfeld surface data analysis for $[\text{Fe}(\text{salBzen-5-OMe})_2]\text{A}$ complexes

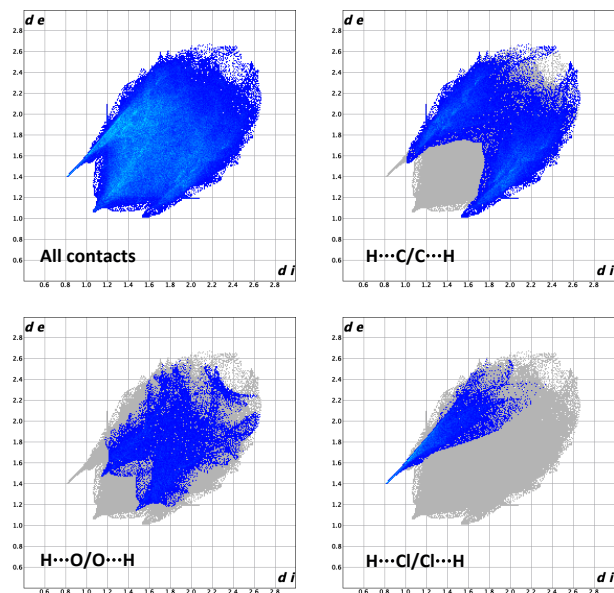


Figure S25. 2D fingerprint plots of all contacts: $\text{H}\cdots\text{C}$, $\text{H}\cdots\text{O}$ and $\text{H}\cdots\text{Cl}$ for **1** at 150 K.

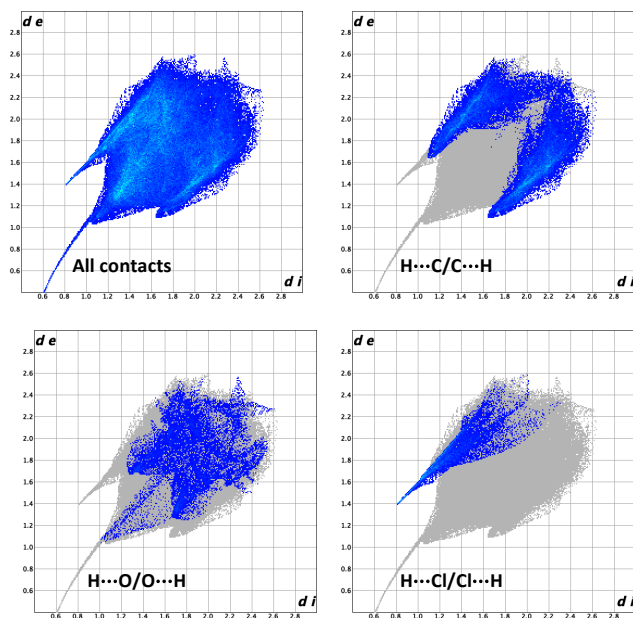


Figure S26. 2D fingerprint plots of all contacts: $\text{H}\cdots\text{C}$, $\text{H}\cdots\text{O}$ and $\text{H}\cdots\text{Cl}$ for **1** at 295 K.

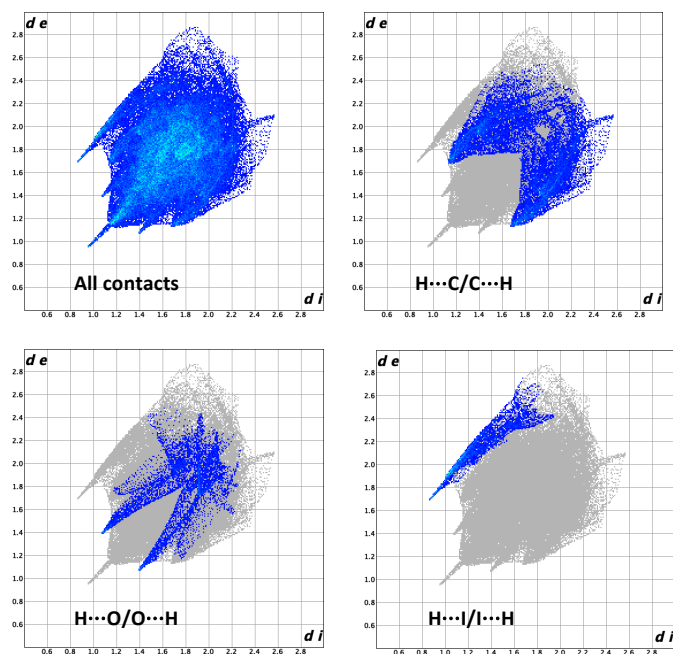


Figure S27. 2D fingerprint plots of all contacts: $\text{H}\cdots\text{C}$, $\text{H}\cdots\text{O}$ and $\text{H}\cdots\text{I}$ for **3** at 150 K.

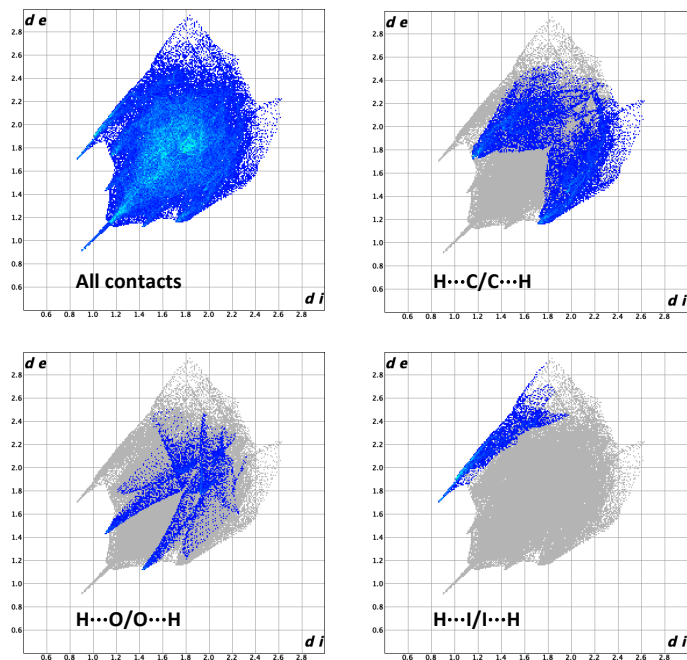


Figure S28. 2D fingerprint plots of all contacts: $\text{H}\cdots\text{C}$, $\text{H}\cdots\text{O}$ and $\text{H}\cdots\text{I}$ for **3** at 295 K.

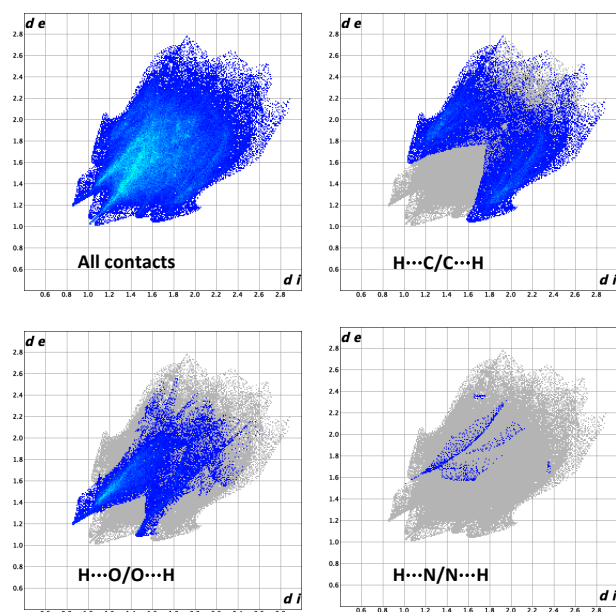


Figure S29. 2D fingerprint plots of all contacts: $\text{H}\cdots\text{C}$, $\text{H}\cdots\text{O}$ and $\text{H}\cdots\text{N}$ for **4** at 150 K.

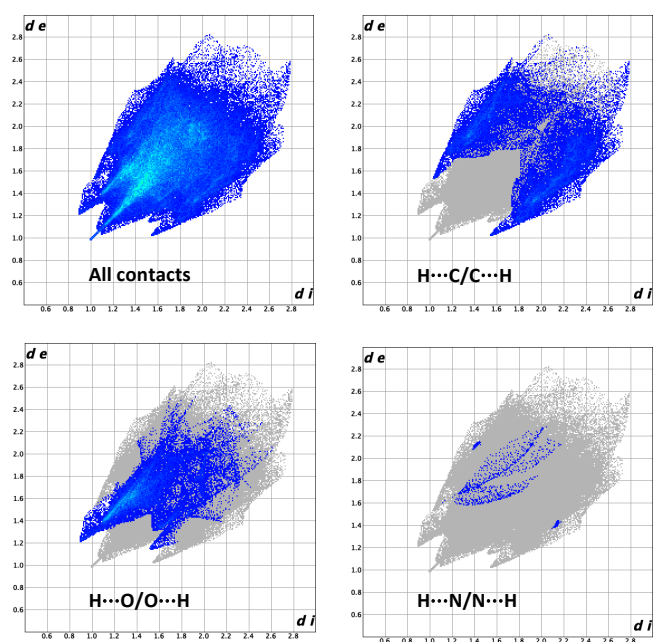


Figure S30. 2D fingerprint plots of all contacts: $\text{H}\cdots\text{C}$, $\text{H}\cdots\text{O}$ and $\text{H}\cdots\text{N}$ for **4** at 295 K.

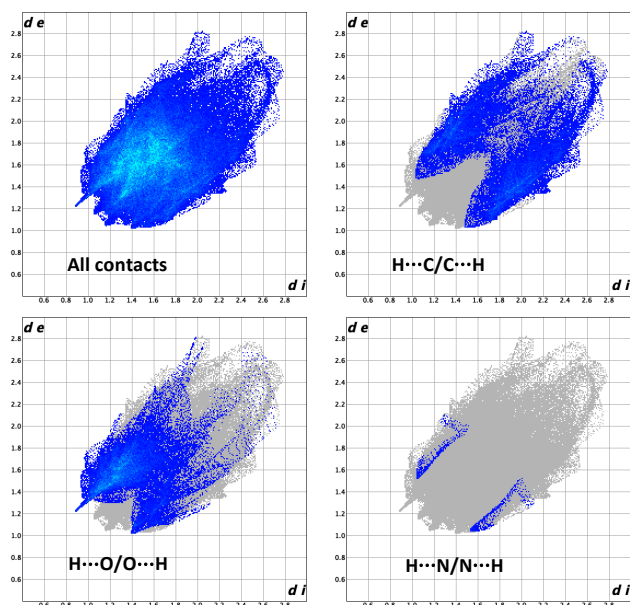


Figure S31. 2D fingerprint plots of all contacts: $\text{H}\cdots\text{C}$, $\text{H}\cdots\text{O}$ and $\text{H}\cdots\text{N}$ for **5** at 30 K.

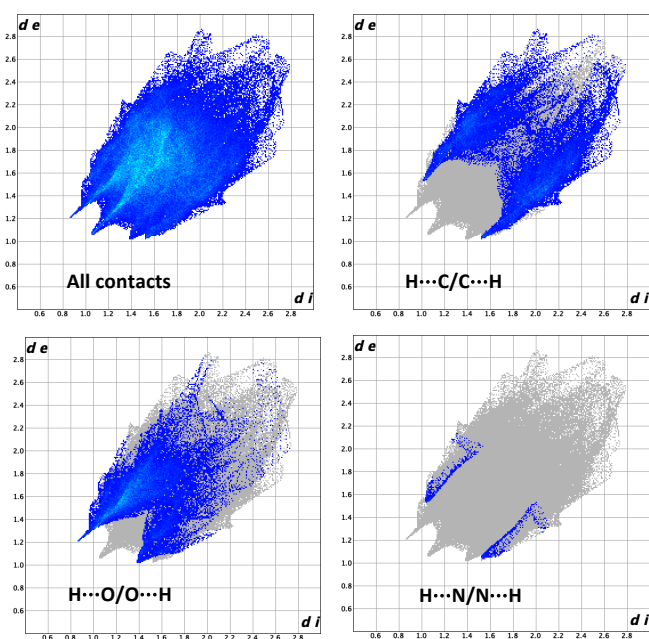


Figure S32. 2D fingerprint plots of all contacts: $\text{H}\cdots\text{C}$, $\text{H}\cdots\text{O}$ and $\text{H}\cdots\text{N}$ for **5** at 100 K.

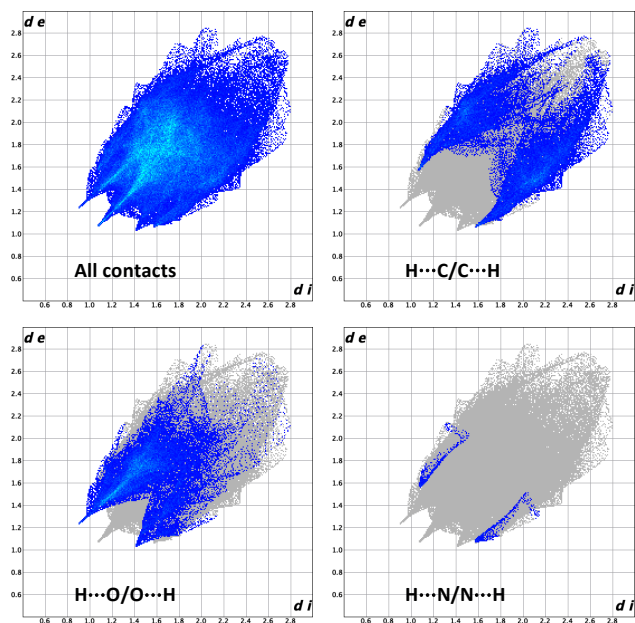


Figure S33. 2D fingerprint plots of all contacts: H...C, H...O and H...N for **5** at 295 K.

APPENDIX B

PUBLICATION AND PRESENTATIONS

B.1 List of publications

Natputree, N., Duverger-Nédellec, Songkerdthong, J., E., Chastanet, G., Harding, P., and Harding, D. J. (2025). Decoupling of symmetry breaking and spin crossover in iron(III) complexes bearing an N-benzylethylenediamine ligand. *Crystal Growth & Design*. 25, 1528-7483. doi: 10.1021/acs.cgd.5c00493

B.2 List of presentations

Natputree, N., Duverger-Nédellec, E., Chastanet, G., Harding, P., and Harding, D. (2024). Magnetic and Structural Studies $[\text{Fe}(\text{salBzen-5-OMe})]_2\text{Y}$ Complexes. **8th Bordeaux Olivier Kahn Discussions: Magnetism & Light**. 14-16 May 2024, Institute of Condensed Matter Chemistry of Bordeaux (ICMCB), Bordeaux, France. (Poster presentation)

Natputree, N., Duverger-Nédellec, E., Chastanet, G., Harding, P., and Harding, D. (2024). Magnetic and Structural Studies $[\text{Fe}(\text{salBzen-5-OMe})]_2\text{A}$ Complexes. **The Royal Australian Chemical Institute (RACI) Inorganic Division Meeting IC'24**. 8-12 December 2024, The Parramatta City Campus of Western Sydney University (WSU), New South Wales, Australia. (Oral presentation)

Natputree, N., Duverger-Nédellec, E., Chastanet, G., Harding, P., and Harding, D. (2025). Magnetic and Structural Studies $[\text{Fe}(\text{salBzen-5-OMe})]_2\text{A}$ Complexes. **The Pure and Applied Chemistry International Conference 2025**. 13-15 February 2025, Khao Yai Convention Center (KYCC) Greenery Resort Khao Yai, Nakhon Ratchasima, Thailand. (Oral presentation)