

The dataset contains data for this study:

Elemental microanalyses.

Electrospray mass spectra.

^1H and ^{13}C NMR spectra (raw and processed data).

X-ray Crystallographic data:

- Structure of L^1 (CCDC 2074276).
- Structure of L^2 (CCDC 2074277).
- Structure of L^3 (CCDC 2074278).
- Structure of *tert*butyl 2-[(2,6-di(pyrazol-1-yl)-pyridine)-4-carboxamido]acetate (CCDC 2074279).
- Structures of $[\text{Fe}(L^5)_2][\text{ClO}_4]_2 \cdot \text{MeCN}$ at 120 and 330 K (CCDC 2074280 and 2074281).
- Structures of $[\text{Fe}(L^6)_2][\text{ClO}_4]_2 \cdot 2\text{MeCN}$ at 120 and 290 K (CCDC 2074282 and 2074283).
- Preliminary structure solution of $[\text{Fe}(L^5)_2][\text{ClO}_4]_2 \cdot n\text{MeCN}$ ($n \approx 1.5$; not deposited with the CCDC)

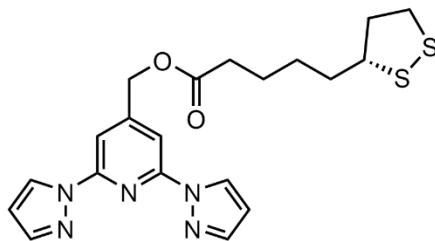
Hirshfeld surface analyses of $[\text{Fe}(L^6)_2][\text{ClO}_4]_2 \cdot 2\text{MeCN}$ at 120 and 290 K.

X-ray powder diffraction data (measured and simulated).

Solid state magnetic susceptibility measurements (raw and processed data).

Solution magnetic susceptibility measurements (Evans method; processed data).

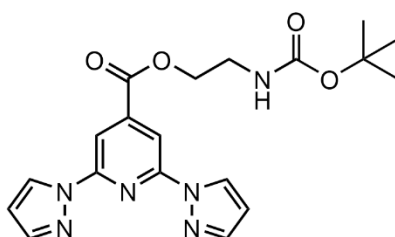
Organic compounds referred to in this dataset



[2,6-Di(pyrazol-1-yl)pyrid-4-yl]methyl (*R*)-lipoate

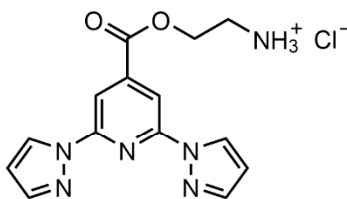
$C_{20}H_{23}N_5O_2S_2$

L^1



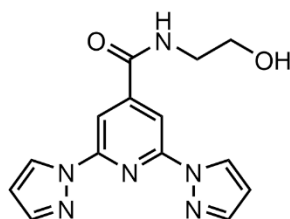
N-BOC-2-aminoethyl [2,6-di(pyrazol-1-yl)pyrid-4-yl]carboxylate

$C_{19}H_{22}N_6O_4$



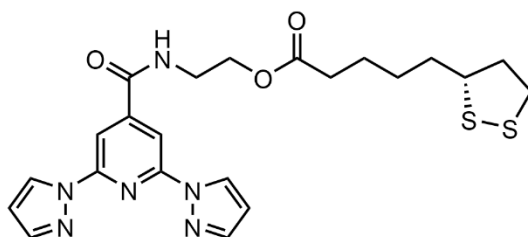
2-Aminoethyl [2,6-di(pyrazol-1-yl)pyrid-4-yl]carboxylate hydrochloride

$C_{14}H_{15}ClN_6O_2$



2-Hydroxyethyl [2,6-di(pyrazol-1-yl)pyrid-4-yl]carboxamide

$C_{14}H_{14}N_6O_2$

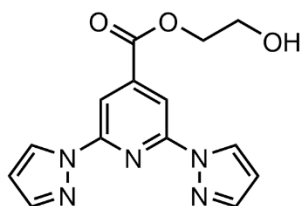


2-[(2,6-Di(pyrazol-1-yl)pyridine)-4-carboxamido]ethyl (*R*)-lipoate

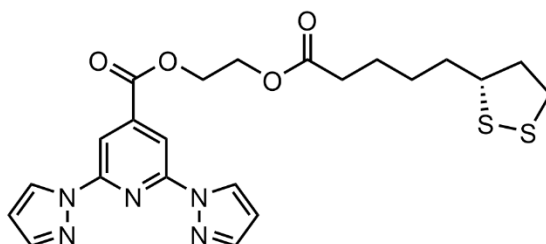
$C_{22}H_{26}N_6O_3S_2$

L^2

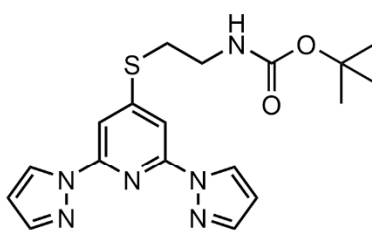
Organic compounds referred to in this dataset (continued)



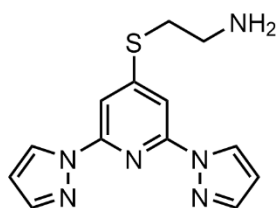
2-Hydroxyethyl [2,6-di(pyrazol-1-yl)pyrid-4-yl]carboxylate
 $C_{14}H_{13}N_5O_3$



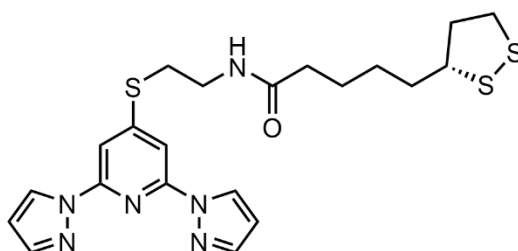
2-[(2,6-Di(pyrazol-1-yl)pyridine)-4-carboxy]ethyl (*R*)-lipoate
 $C_{22}H_{25}N_5O_4S_2$
 L^3



N-BOC-4-(2-aminoethylsulfanyl)-2,6-di(pyrazol-1-yl)pyridine
 $C_{18}H_{22}N_6O_2S$

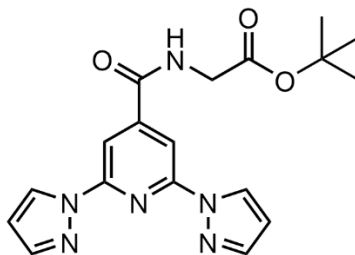


4-(2-Aminoethylsulfanyl)-2,6-di(pyrazol-1-yl)pyridine
 $C_{13}H_{14}N_6S$

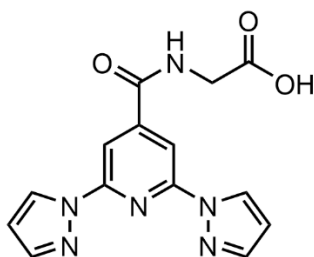


N-([2,6-Di(pyrazol-1-yl)pyrid-4-ylsulfanyl]-2-aminoethyl (*R*)-lipoamide
 $C_{21}H_{26}N_6OS_3$
 L^4

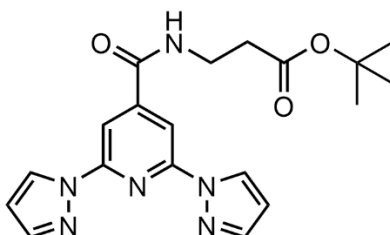
Organic compounds referred to in this dataset (continued)



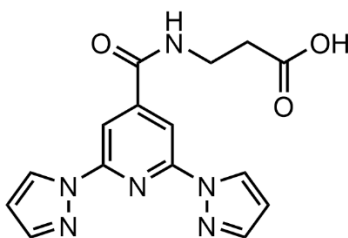
*Tert*butyl 2-[(2,6-di(pyrazol-1-yl)pyridine)-4-carboxamido]acetate
 $C_{18}H_{20}N_6O_3$



2-[(2,6-Di(pyrazol-1-yl)pyridine)-4-carboxamido]acetic acid
 $C_{14}H_{12}N_6O_3$
 L^5

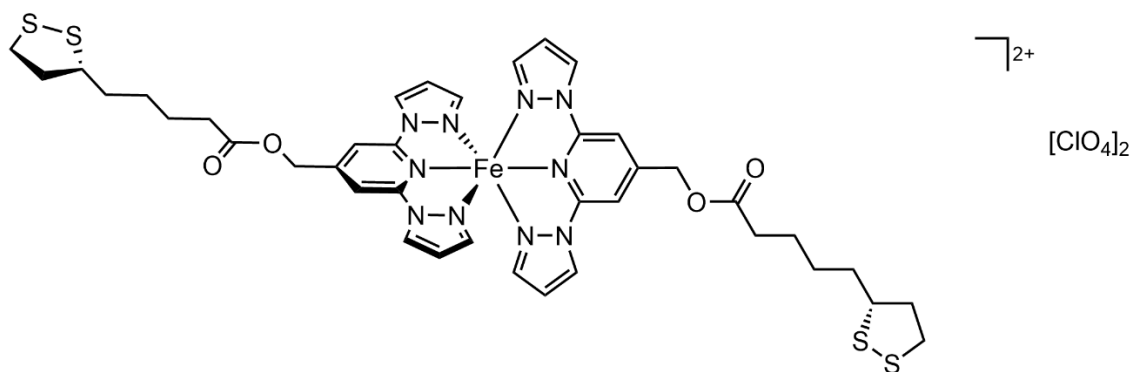


*Tert*butyl 2-[(2,6-di(pyrazol-1-yl)pyridine)-4-carboxamido]propionate
 $C_{19}H_{22}N_6O_3$

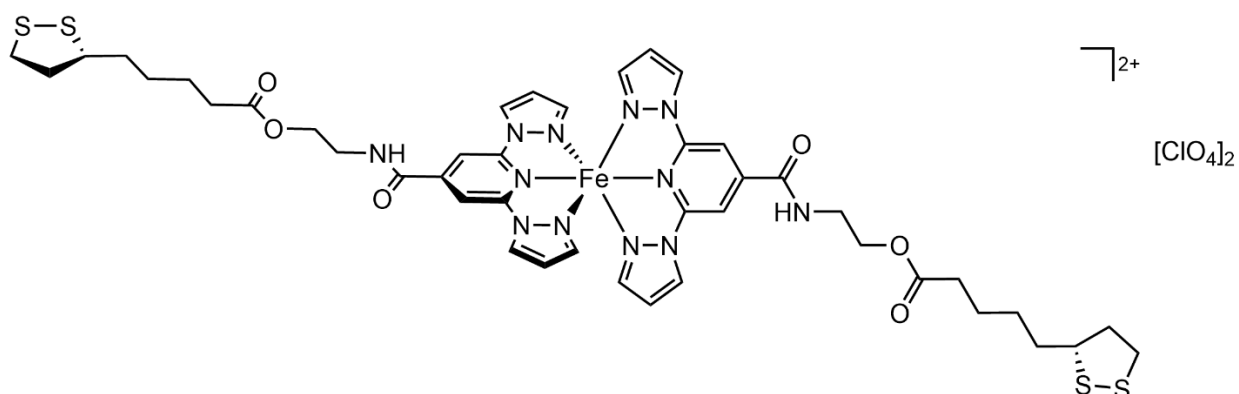


2-[(2,6-Di(pyrazol-1-yl)pyridine)-4-carboxamido]propionic acid
 $C_{15}H_{14}N_6O_3$
 L^6

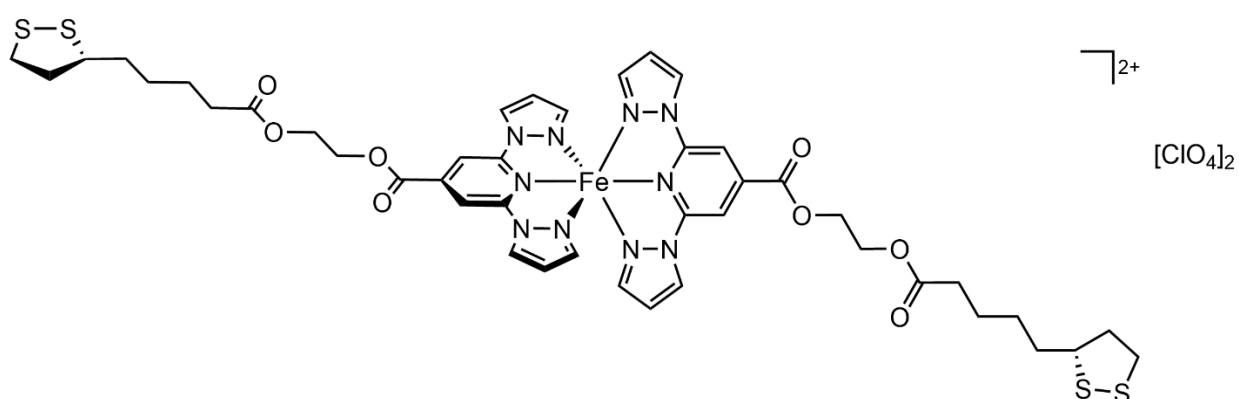
Metal complexes referred to in this dataset



Bis[2,6-di(pyrazol-1-yl)pyrid-4-yl]methyl (*R*)-lipoate]iron(II) diperchlorate
 $C_{40}H_{46}Cl_2FeN_{10}O_{12}S_4$
 $[Fe(L^1)_2][ClO_4]_2$

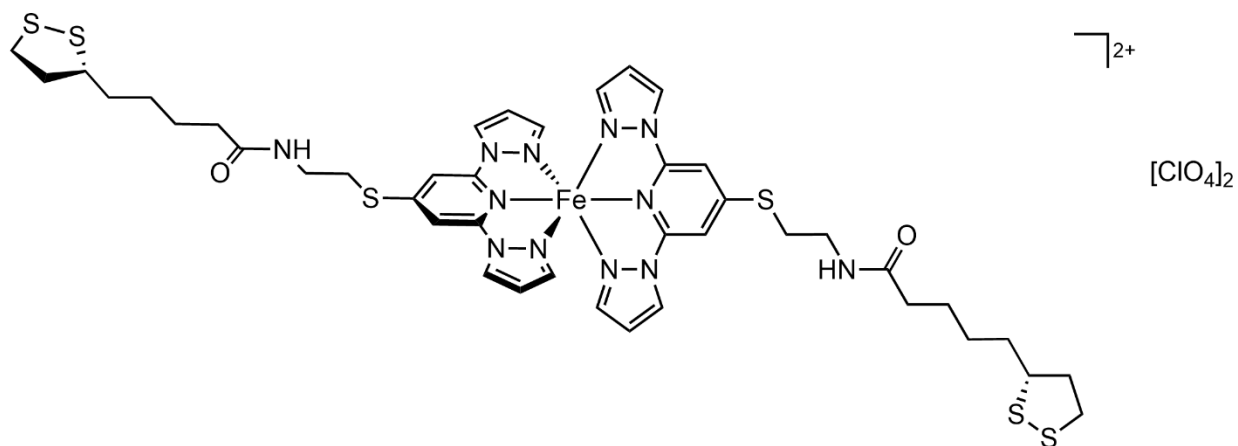


Bis[2-((2,6-di(pyrazol-1-yl)pyridine)-4-carboxamido)ethyl (*R*)-lipoate]iron(II) diperchlorate
 $C_{44}H_{52}Cl_2FeN_{12}O_{14}S_4$
 $[Fe(L^2)_2][ClO_4]_2$

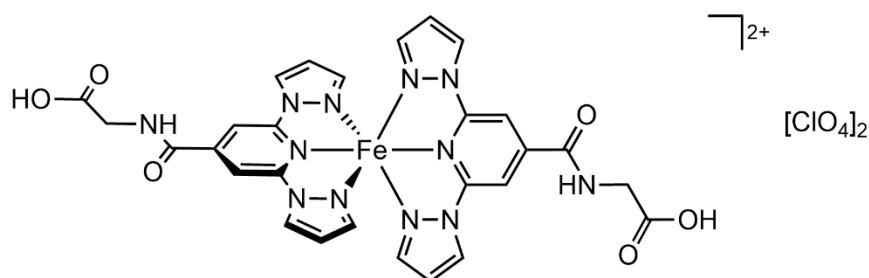


Bis[2-((2,6-Di(pyrazol-1-yl)pyridine)-4-carboxy)ethyl (*R*)-lipoate]iron(II) diperchlorate
 $C_{44}H_{50}Cl_2FeN_{10}O_{16}S_4$
 $[Fe(L^3)_2][ClO_4]_2$

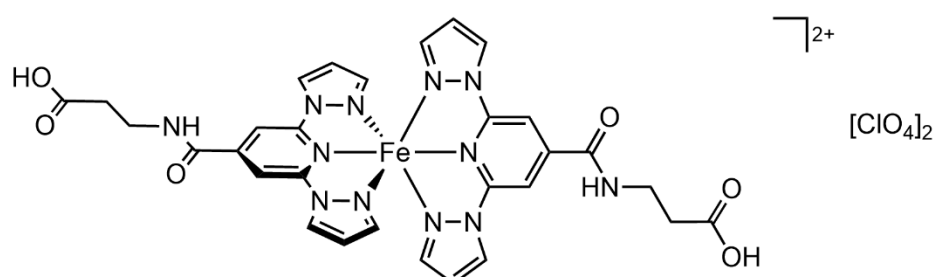
Metal complexes referred to in this dataset (continued)



Bis[*N*-((2,6-di(pyrazol-1-yl)pyrid-4-yl)sulfanyl)-2-aminoethyl (*R*)-lipoamide]iron(II) diperchlorate
 $C_{42}H_{52}Cl_2FeN_{12}O_{10}S_6$
 $[Fe(L^4)_2][ClO_4]_2$



Bis[2-((2,6-di(pyrazol-1-yl)pyridine)-4-carboxamido)acetic acid]iron(II) diperchlorate
 $C_{28}H_{24}Cl_2FeN_{12}O_{14}$
 $[Fe(L^5)_2][ClO_4]_2$



Bis[2-((2,6-di(pyrazol-1-yl)pyridine)-4-carboxamido)propionic acid]iron(II) diperchlorate
 $C_{30}H_{28}Cl_2FeN_{12}O_{14}$
 $[Fe(L^6)_2][ClO_4]_2$