Electronic Supplementary Material (ESI) for Dalton Transactions.

Hysteretic thermal spin-crossover and in heteroleptic Fe(II) complexes using alkyl chain substituted 2,2'-dipyridylamine ligands.

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Supplementary Information

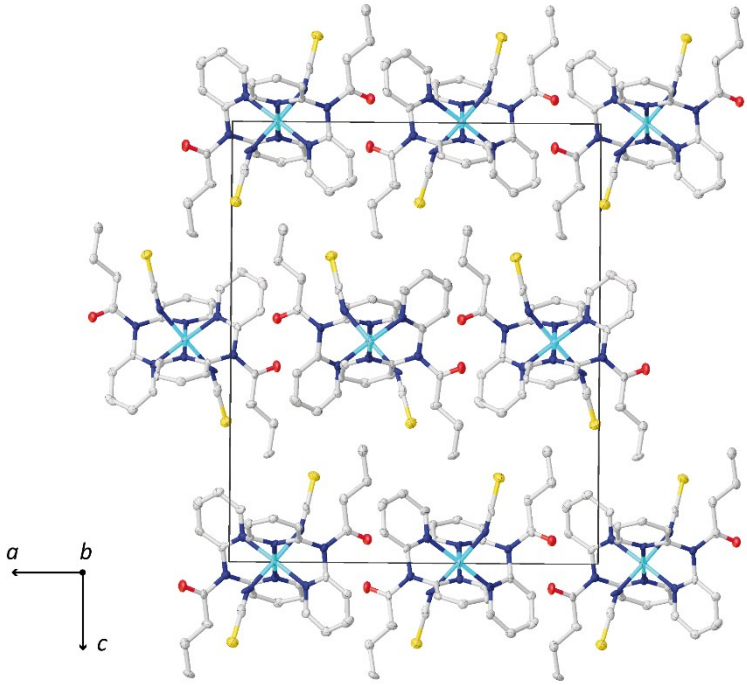

Fig. S1 Unit cell of **1C$_4$·85K** as viewed down the *b* axis. Legend: iron, turquoise; nitrogen, blue; carbon, grey; oxygen, red; sulfur, yellow. This is representative of the unit cell for **1C$_4$·120K** and **1C$_4$·200K**.

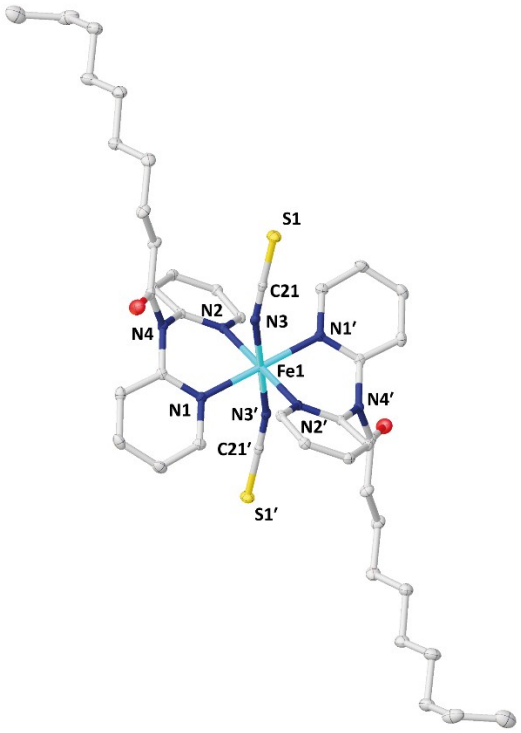

Fig. S2 Molecular structure of **1C$_{10}$.85K** with selected atom labels. Hydrogen atoms omitted for clarity. Legend: iron, turquoise; nitrogen, blue; carbon, grey; oxygen, red; sulfur, yellow. The second LC_{10} unit is symmetry generated through an inversion centre on the Fe atom. ′ labels denote atoms that are symmetry generated in this way. This is representative of the numbering in **1C$_{10}$.105K** and **1C$_{10}$.140K**.

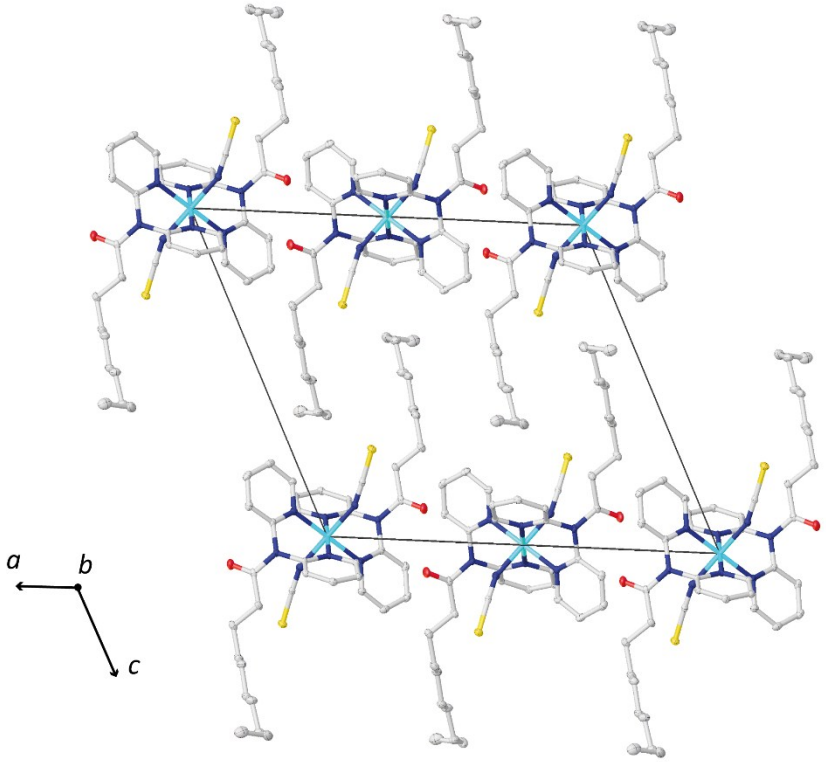

Fig. S3 Unit cell of **1C$_{10}$.85K** as viewed down the *b* axis. Legend: iron, turquoise; nitrogen, blue; carbon, grey; oxygen, red; sulfur, yellow.

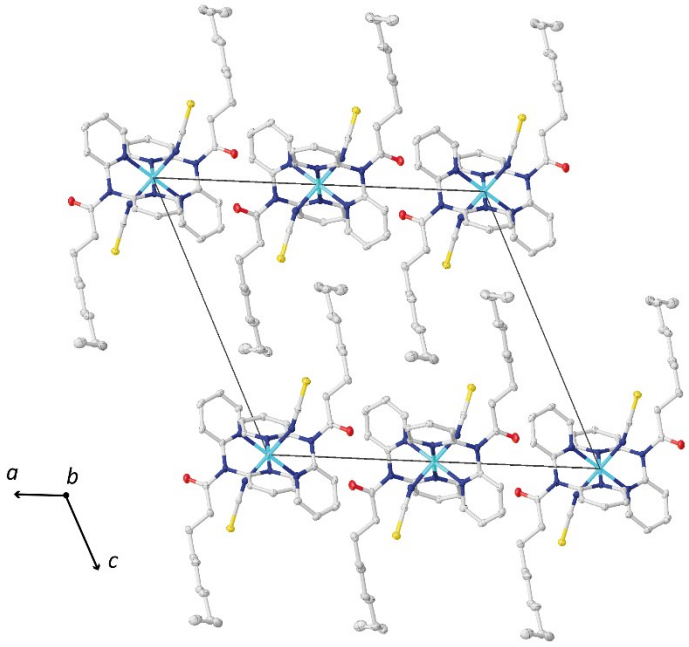

Fig. S4 Unit cell of **1C$_{10}$·105K** as viewed down the *b* axis. Legend: iron, turquoise; nitrogen, blue; carbon, grey; oxygen, red; sulfur, yellow.

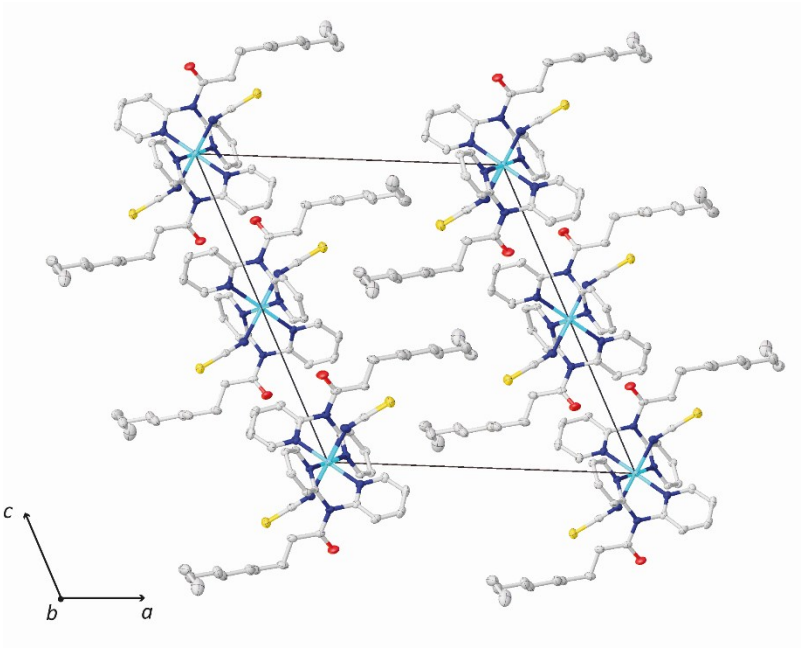

Fig. S5 Unit cell of **1C$_{10}$·140K** as viewed down the *b* axis. Legend: iron, turquoise; nitrogen, blue; carbon, grey; oxygen, red; sulfur, yellow.

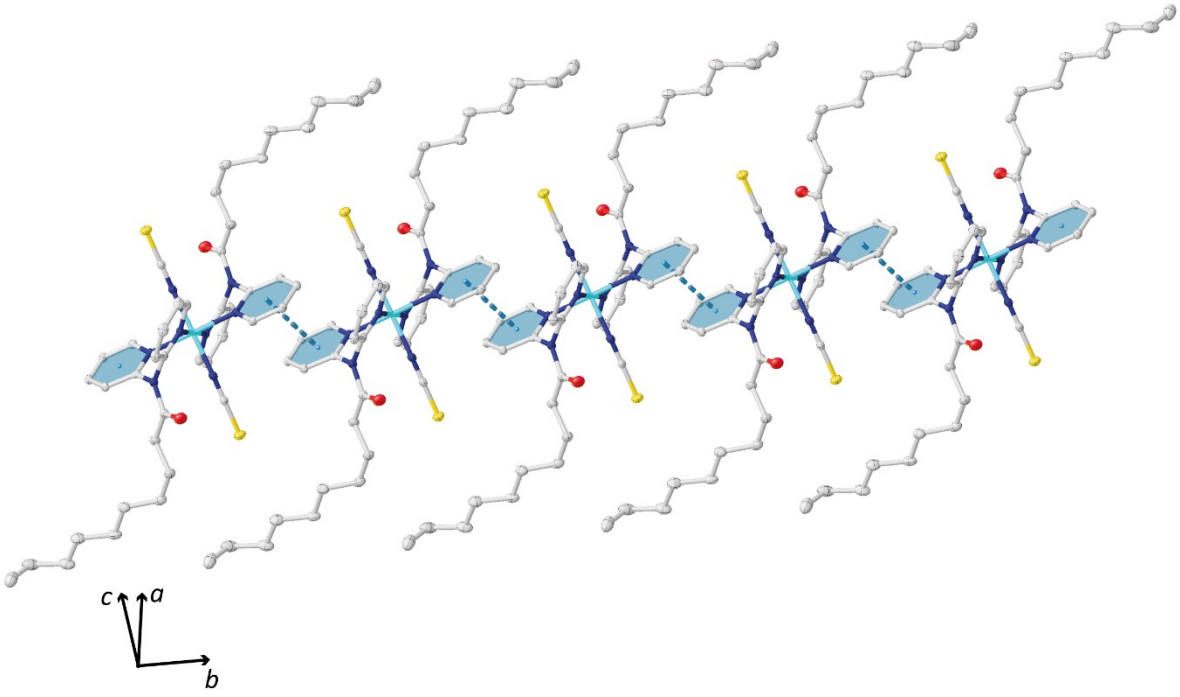

Fig. S6 Short $\pi\cdots\pi$ contacts in **1C$_{10}$·105K.** Hydrogen atoms omitted for clarity. Legend: iron, turquoise; nitrogen, blue; carbon, grey; oxygen, red; sulfur, yellow. This is representative of the interactions found in **1C$_{10}$·85K** and **1C$_{10}$·140K**.

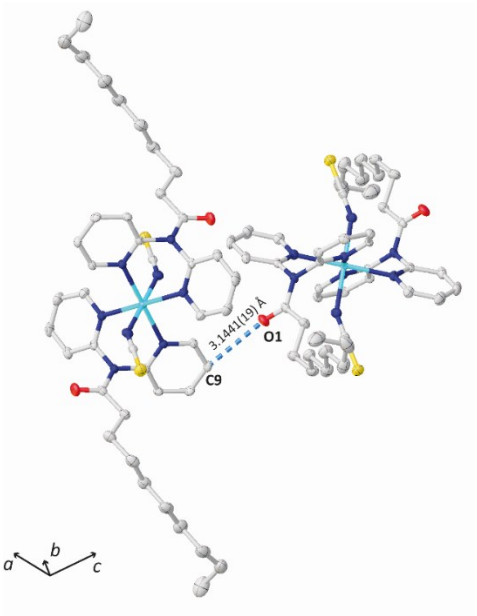

Fig. S7 Short C-H···O contact between **1C$_{10}$·140K** complexes. Hydrogen atoms omitted for clarity. Legend: iron, turquoise; nitrogen, blue; carbon, grey; oxygen, red; sulfur, yellow. This is representative of the interactions found in **1C$_{10}$·85K** and **1C$_{10}$·105K**.

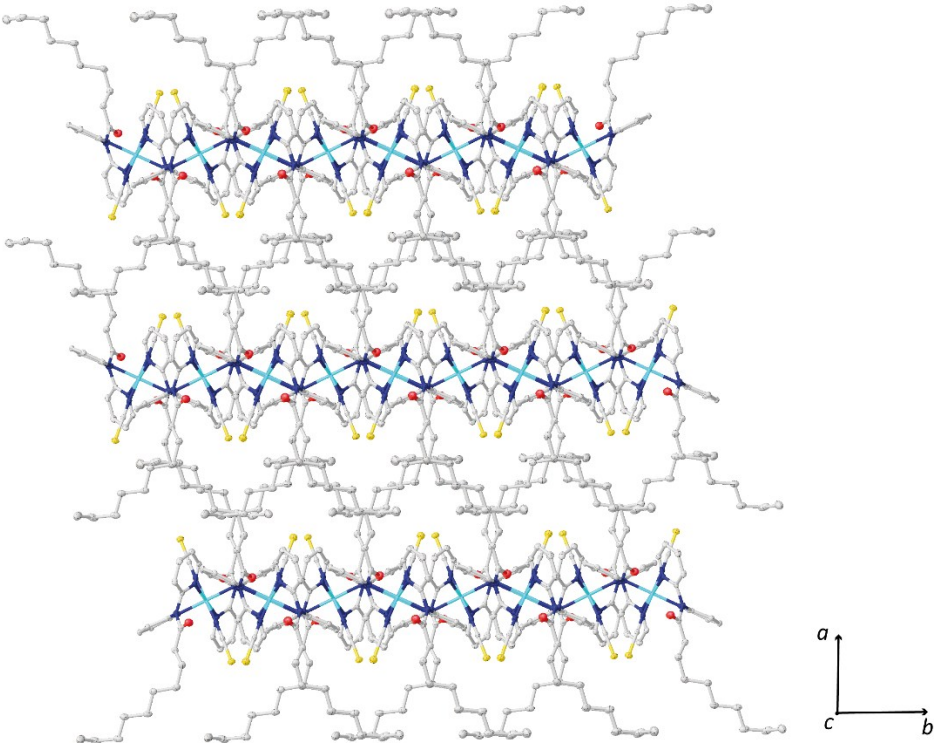

Fig. S8 Packing of **1C$_{10}$·105K** as viewed down the *c* axis. Legend: iron, turquoise; nitrogen, blue; carbon, grey; oxygen, red; sulfur, yellow. This is representative of the packing found in **1C$_{10}$·85K** and **1C$_{10}$·140K**.

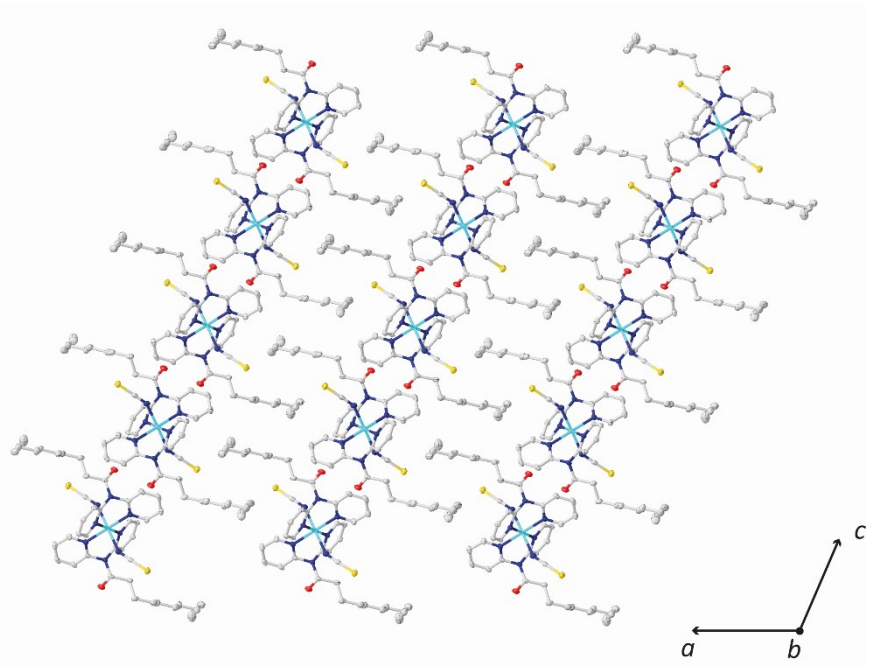

Fig. S9 Packing of **1C$_{10}$·140K** as viewed down the *b* axis. Legend: iron, turquoise; nitrogen, blue; carbon, grey; oxygen, red; sulfur, yellow. This is representative of the packing found in **1C$_{10}$·85K** and **1C$_{10}$·105K**.

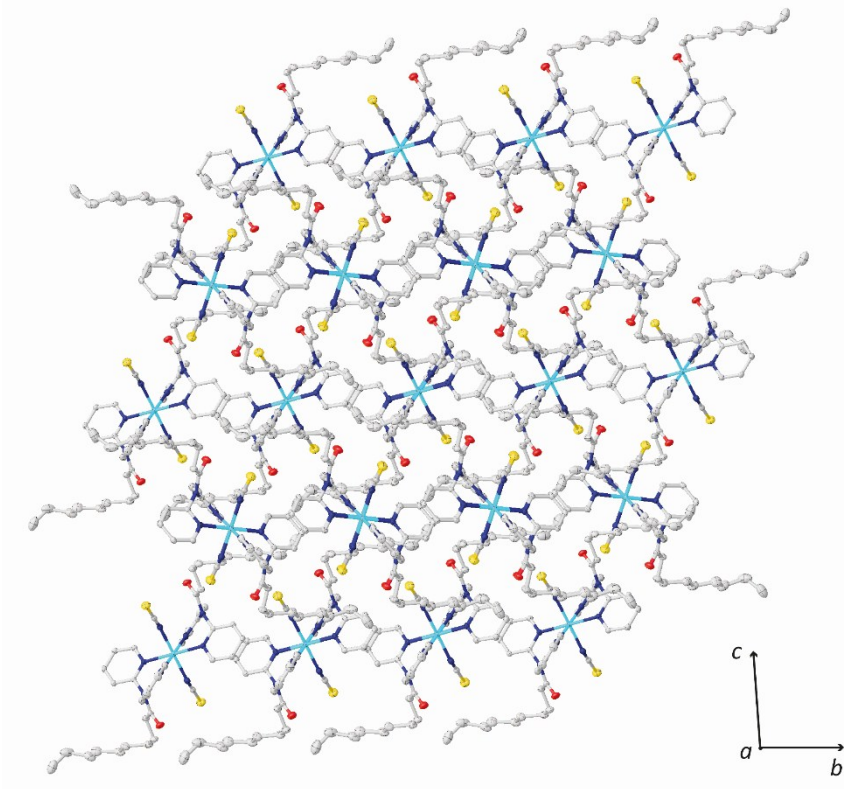

Fig. S10 Packing of **1C$_{10}$·140K** as viewed down the *a* axis. Legend: iron, turquoise; nitrogen, blue; carbon, grey; oxygen, red; sulfur, yellow. This is representative of the packing found in **1C$_{10}$·85K** and **1C$_{10}$·105K**.

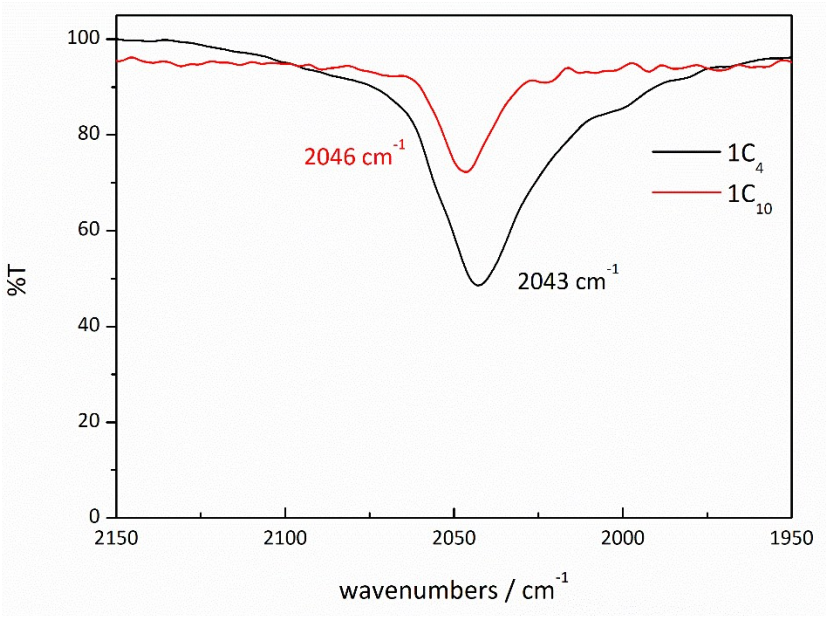

Fig. S11 Partial IR absorption spectra for single crystals of **1C$_4$** (black) and **1C$_{10}$** (red) at 293 K.

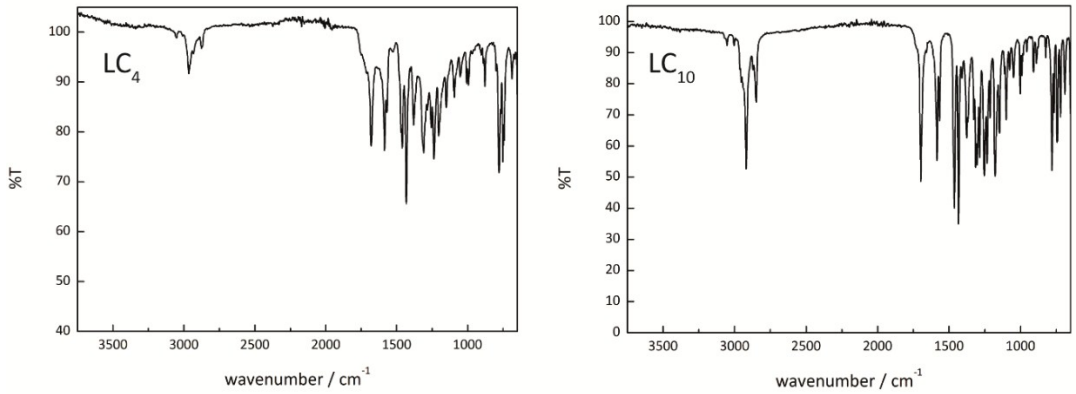

Fig. S12 IR absorption spectra for LC$_4$ (left) and LC$_{10}$ (right) at room temperature.

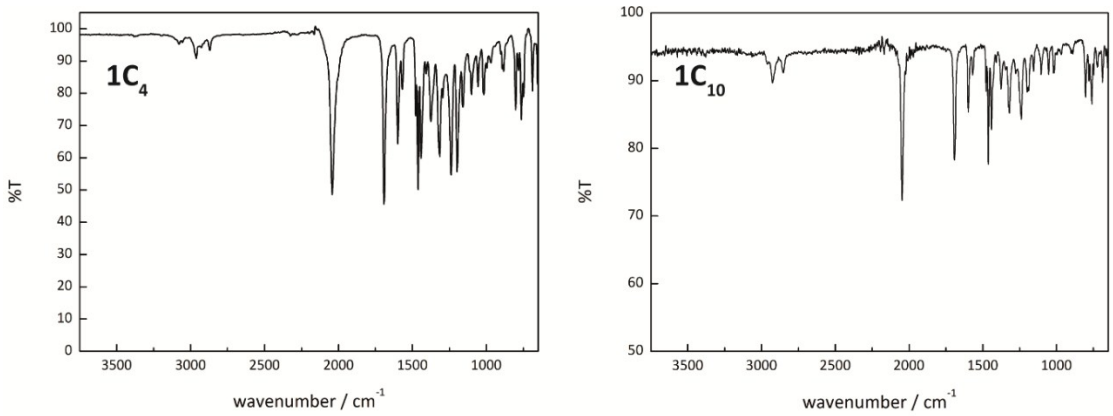

Fig. S13 IR absorption spectra for **1C$_4$** (left) and **1C$_{10}$** (right) at room temperature.

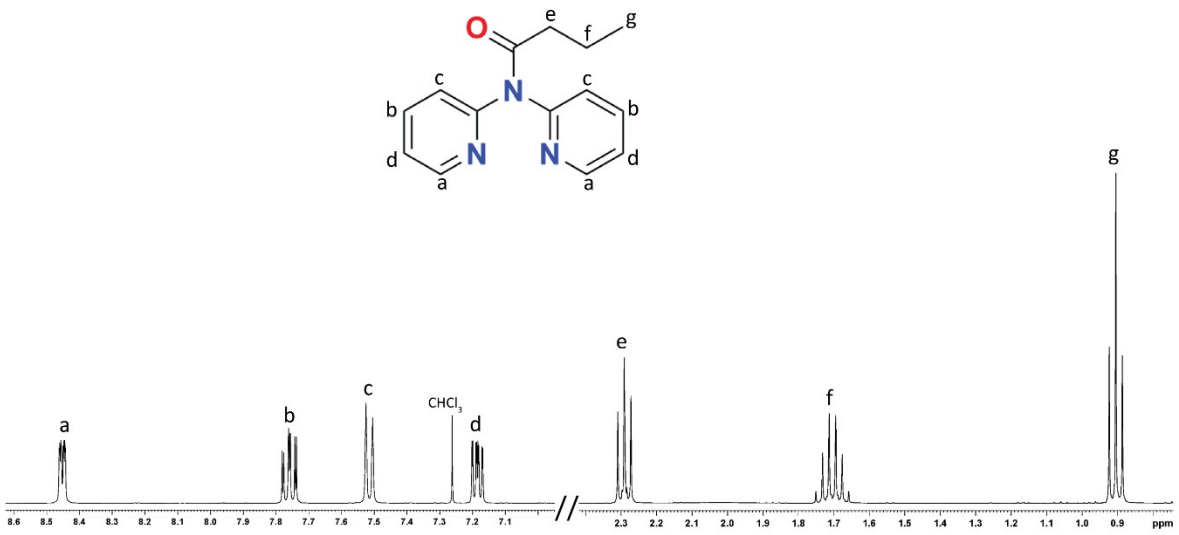

Fig. S14 Partial ^{1}H NMR spectrum of the ligand *N,N*-di(pyridin-2-yl)butanamide (LC_4) in $CDCl_3$. Shifts given in ppm (x axis).

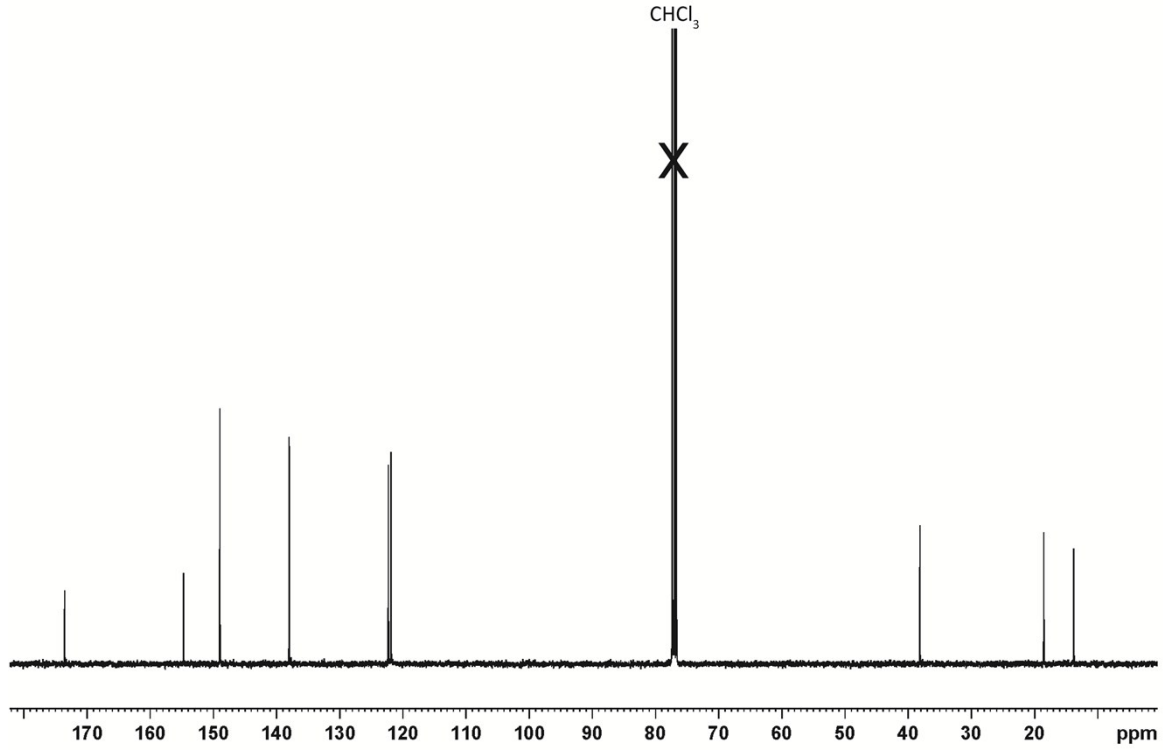

Fig. S15 ^{13}C NMR spectrum of the ligand *N,N*-di(pyridin-2-yl)butanamide (LC_4) in $CDCl_3$.

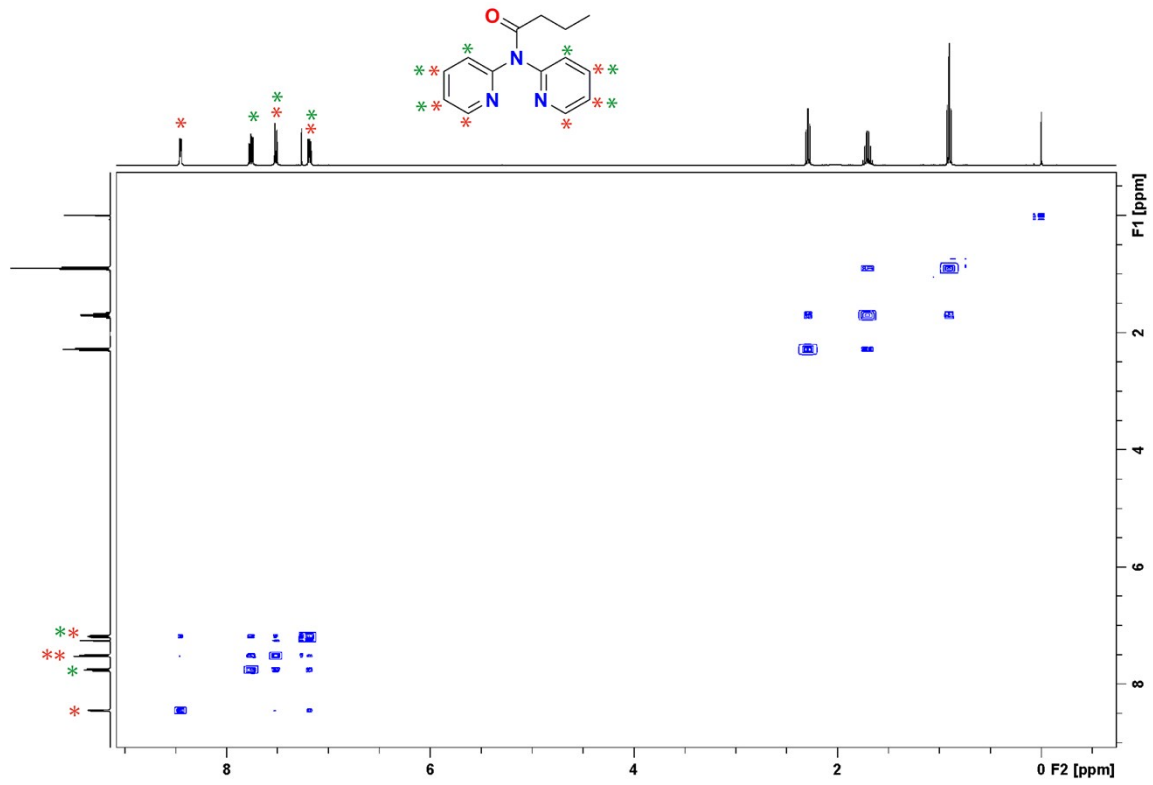

Fig. S16 COSY NMR spectrum of the ligand *N,N*-di(pyridin-2-yl)butanamide (LC_4) in $CDCl_3$.

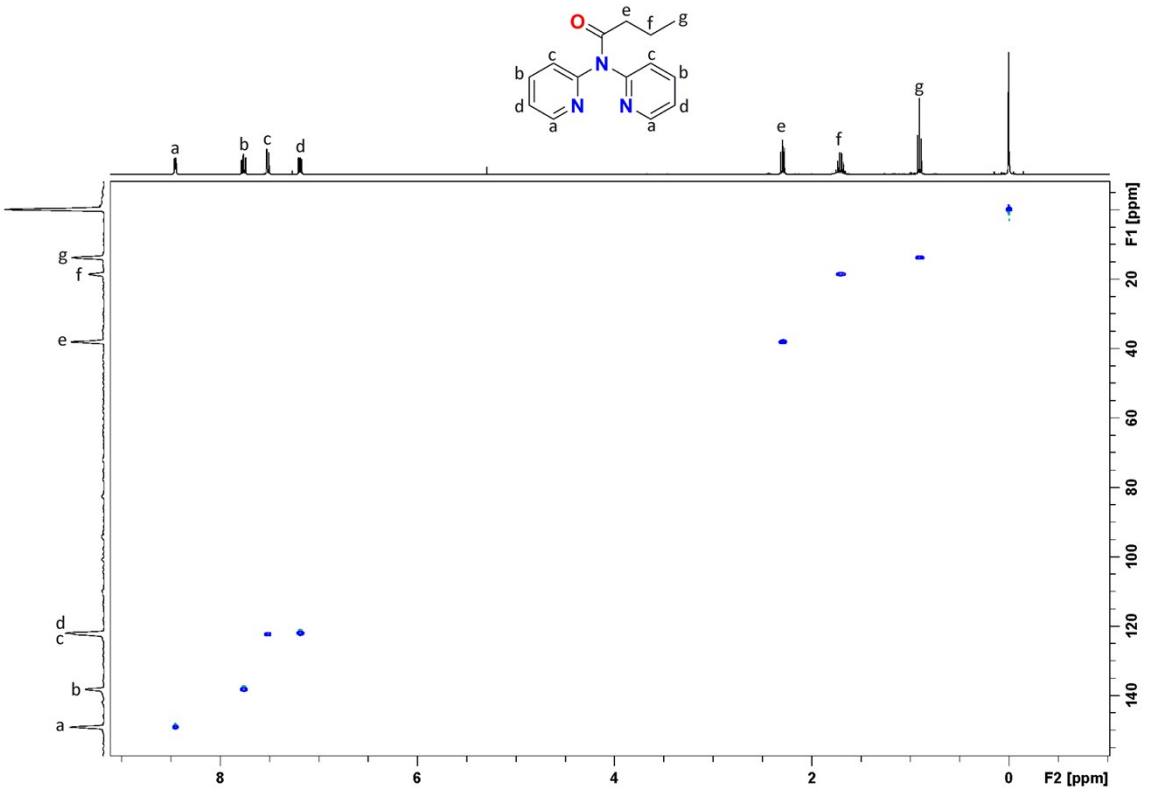

Fig. S17 HSQC NMR spectrum of the ligand *N,N*-di(pyridin-2-yl)butanamide (LC_4) in $CDCl_3$.

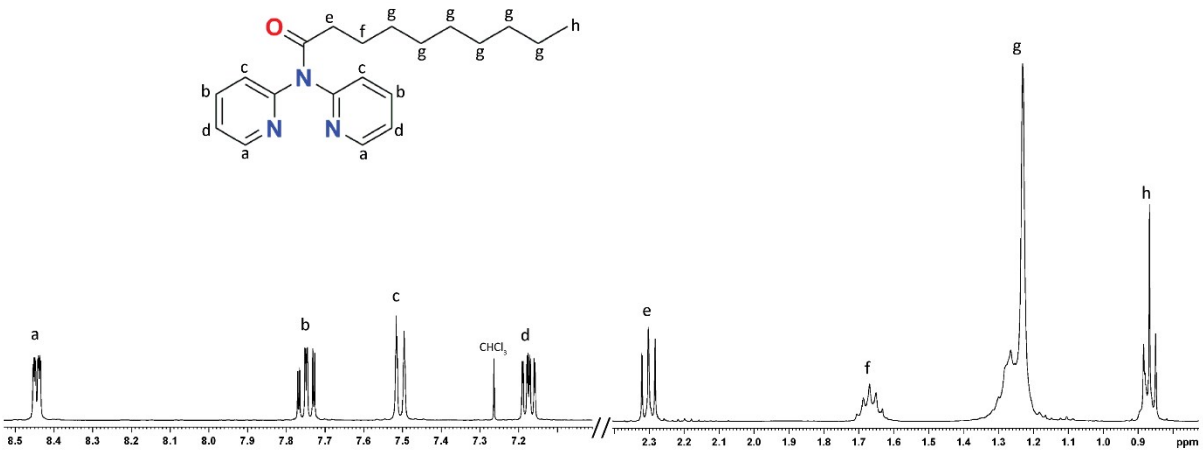

Fig. S18 Partial ^{1}H NMR spectrum of the ligand *N,N*-di(pyridin-2-yl)decanamide (LC_{10}) in $CDCl_3$. Shifts given in ppm (x axis).

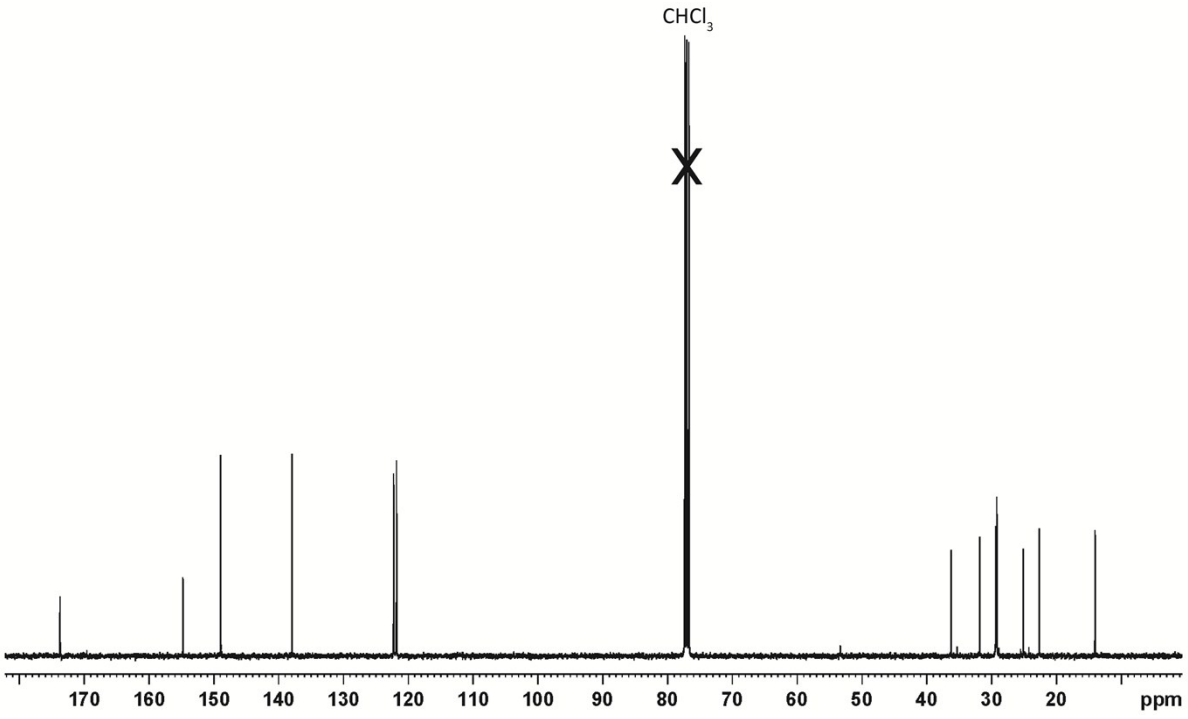

Fig. S19 ^{13}C NMR spectrum of the ligand *N,N*-di(pyridin-2-yl)decanamide (LC_{10}) in $CDCl_3$.

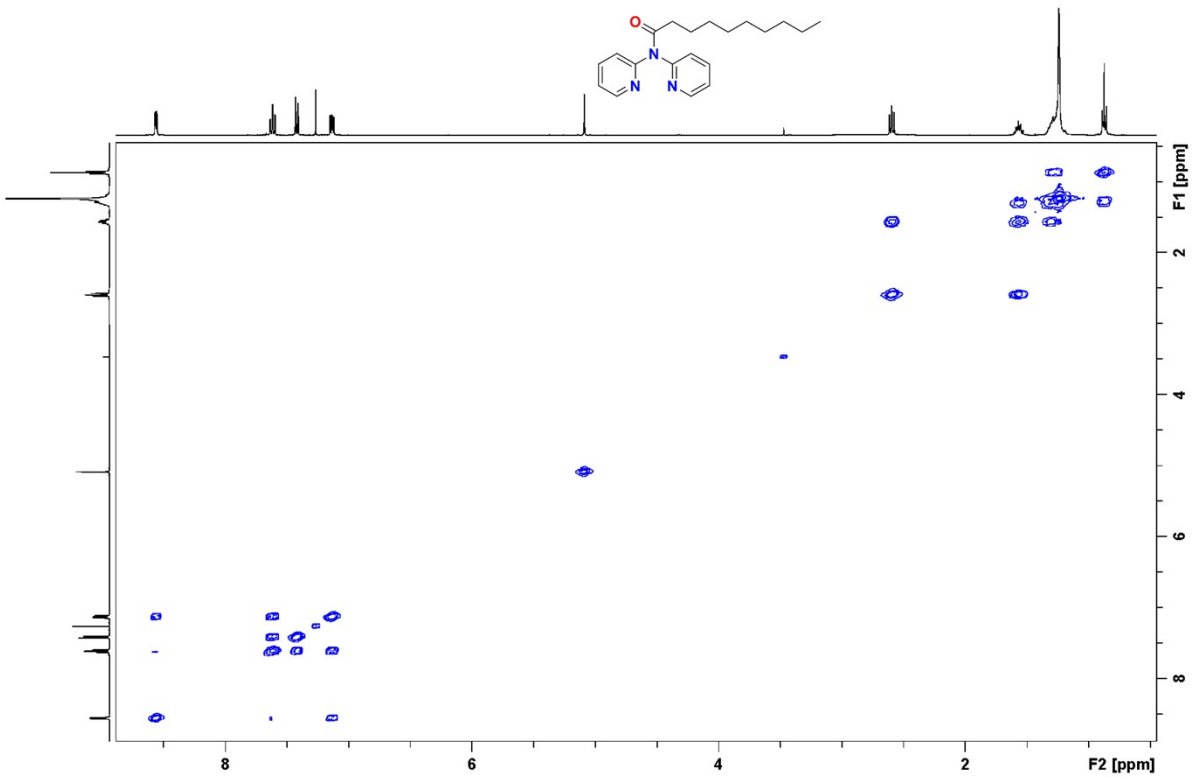

Fig. S20 COSY NMR spectrum of the ligand *N,N*-di(pyridin-2-yl)decanamide (LC_{10}) in $CDCl_3$. For ^{1}H and ^{13}C assignments see Fig S19.

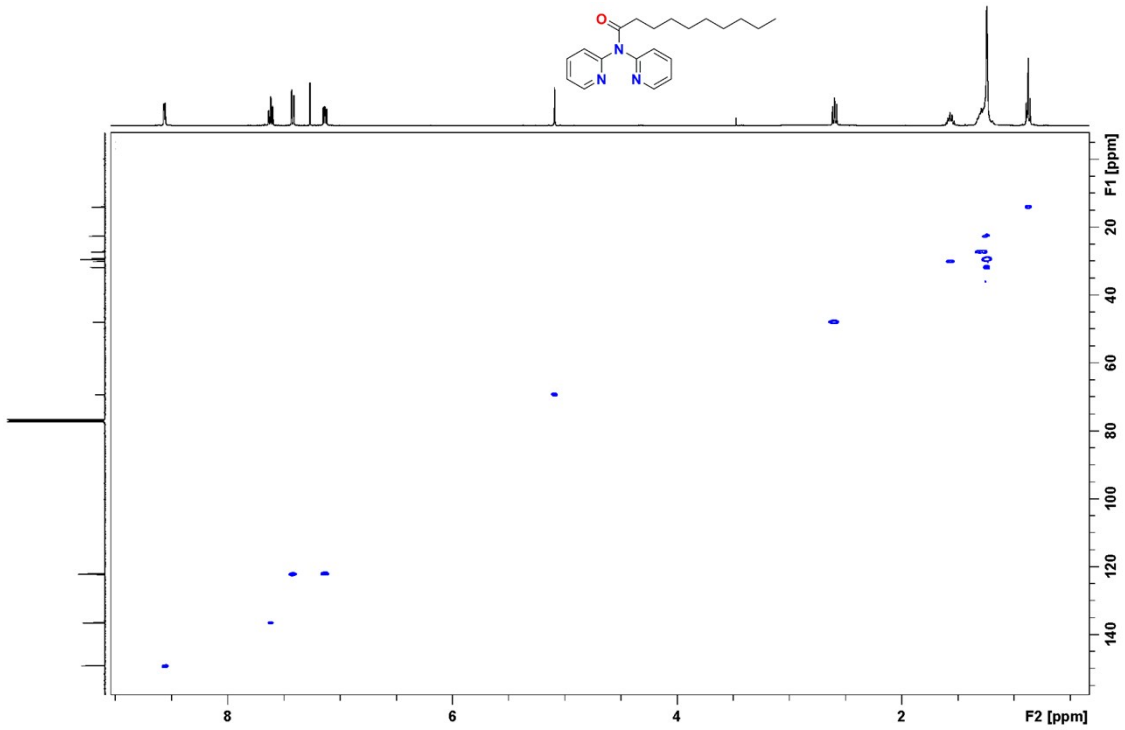

Fig. S21 HSQC NMR spectrum of the ligand *N,N*-di(pyridin-2-yl)decanamide (LC_{10}) in $CDCl_3$. For ^{1}H and ^{13}C assignments see Fig S20.

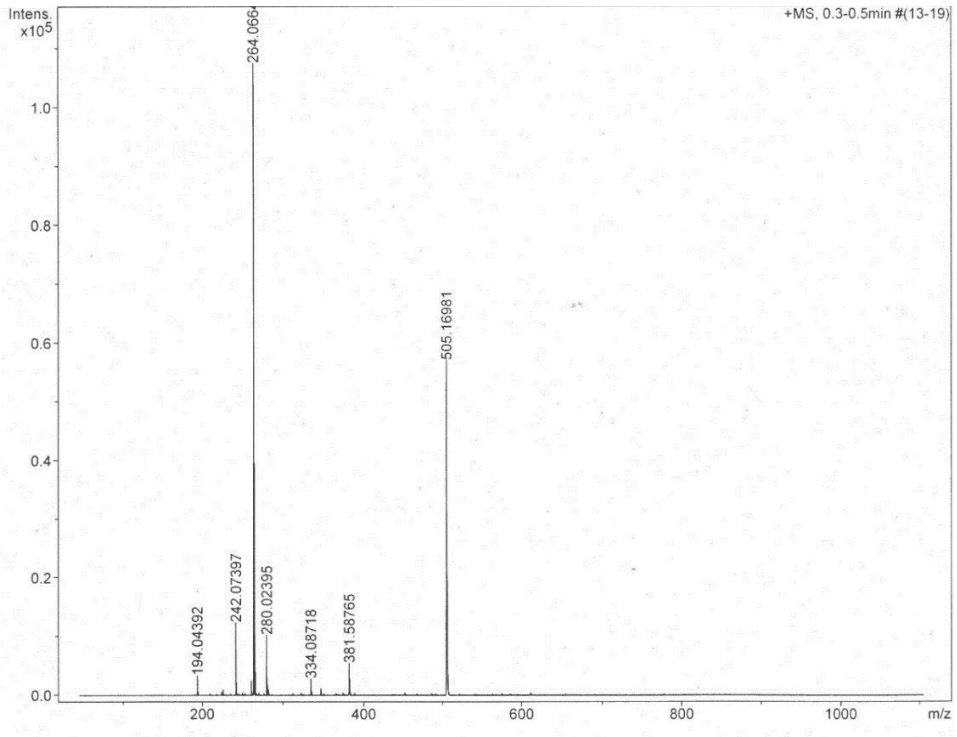

Fig. S22 Mass spectrum of LC_4. ESI^+ MS, methanol as eluent.

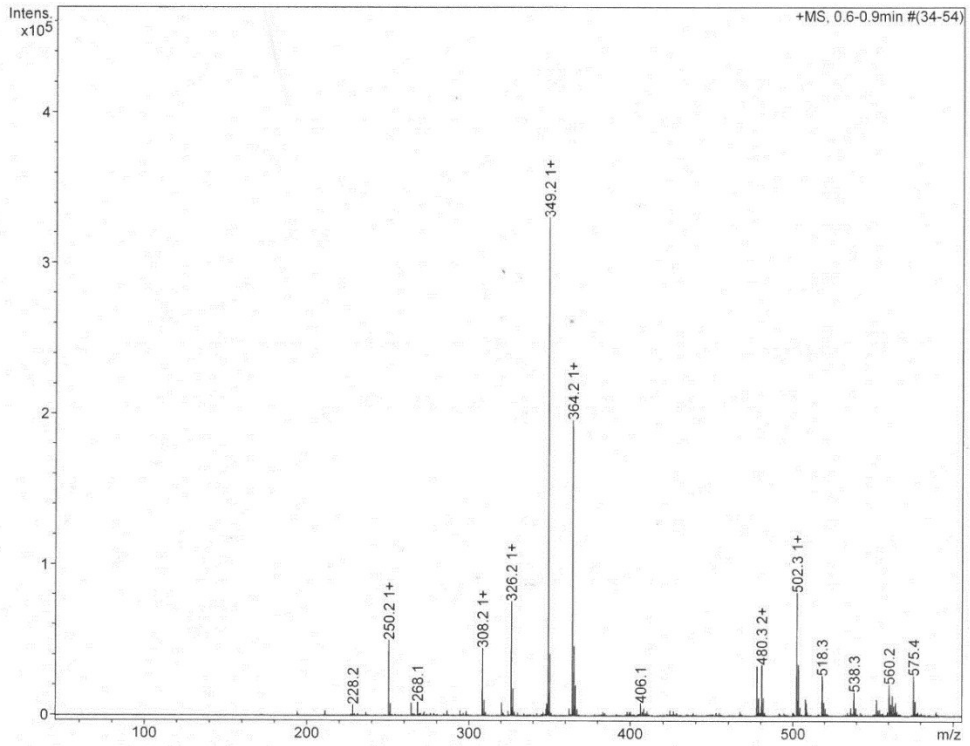

Fig. S23 Mass spectrum of LC_{10}. ESI^+ MS, methanol as eluent.