Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Probing the generality of spin crossover complex $T_{½}$ vs ligand ^{15}N NMR chemical shift correlations: towards predictable tuning

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ELECTRONIC SUPPORTING INFORMATION

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S1. Experimental Section

S1.1. Instruments and Measurements

Elemental analyses (C, H, N, S) were measured at the Campbell Microanalytical Laboratory, University of Otago.

Evans method NMR measurements were carried out on a Varian 500MHz NMR spectrometer, using a OneProbe with a variable temperature controller, between 243 to 313 K in intervals of 5 K, with expected error in T of ± 1 K. A diamagnetic correction for the sample ($-M \times 0.5 \times 10^{-6}$ cm^3mol^{-1}),[1] and a correction for the variation of the viscosity of the solvent with temperature,[2] were applied to each dataset (Table S9). The least squares fittings were obtained by modelling each dataset as a gradual and complete SCO using the regular solution model (equation S1),[3-5] with good fits obtained, providing the derived parameters ΔH and ΔS, and hence access to $T_{½}(\Delta H/\Delta S)$ (Table S1). This was carried out using OriginPro version 9.1.0 from OriginLab Corporation. For all fits, the maximum $\chi_M T$ value ($\chi_M T(max)$) was set to 3.5 $cm^3 \cdot K \cdot mol^{-1}$ in Equation S1, [3-5] the expected value for a *HS* iron(II) centre.[6-7]

Single-crystal X-ray diffraction data were collected on an Oxford Diffraction SuperNova diffractometer with Atlas CCD, equipped with a Cryostream N_2 open-flow cooling device,[8] using mirror monochromated micro-focus Cu-K_α radiation at 100 K. The series of scans was performed in such a way as to collect a complete set of unique reflections to a maximum resolution of 0.80 Å. Raw frame data (including data reduction, inter-frame scaling, unit cell refinement and absorption corrections)[9] for all structures were processed using CrysAlis Pro.[10] Structures were solved using SUPERFLIP[11] and refined using full-matrix least-squares on F^2 and refined against F^2 using all data by full-matrix least-squares techniques with SHELXS-2014[12] and refined using full-matrix least-squares on F2 within the X-Seed graphical user interface Olex2-1.2. All hydrogen atoms were inserted at calculated positions with U(H) = 1.2 U (attached atom), and rode on the atoms to which they were attached. Further details of the refinements, including modelling disordered solvent of crystallisation, and additional tables are provided in the ESI (Tables S1-S6). Crystallographic data for the structures has been deposited with the Cambridge Crystallographic Data Centre, CCDC 2098939-2098942.

All solid-state magnetic susceptibilities were measured under a magnetic field of 0.1 T on a Quantum Design Physical Property Measurement System (PPMS) equipped with a vibrating sample mount (VersaLab). Three 50–400–50 K cycles at 2 K min^{-1} (meas. each 10 K) were obtained for each $[Fe^{II}(L^{pytZ})_2(NCBH_3)_2]\cdot nH_2O$, to check for reproducibility. Measurements are obtained in settle mode (the instrument considers the temperature "settled" after 1 min of the temperature being within the smaller value of ±0.5 K or ±0.5% of the target value). Due to the observation of thermal hysteresis, a scan rate (at 20, 10, 5, 2 and 0.2 K min^{-1}) study of $\chi_M T$ vs T was carried out for $[Fe(L^{pytCF3})_2(NCBH_3)_2]\cdot 0.5H_2O$, from 150 to 250 K, in sweep mode (data collected continuously as T swept at specified rate). All of the data were corrected for the diamagnetism of the capsule and of the sample (estimated as $-M \times 0.5 \times 10^{-6}$ cm^3mol^{-1}).[1]

Solution UV-Vis spectra of a 1:6 ratio of $Fe(pyridine)_4(NCBH_3)_2$: $\boldsymbol{L^{pytZ}}$ (Section S1.14), in HPLC grade $CHCl_3$ that was first neutralized by filtering it through a pad of Al_2O_3, and were 0.5 mM in Fe(II), were recorded at room temperature on a PerkinElmer Lambda 950 UV-Vis/NIR.

S1.2. Multi-step Organic Synthesis of $\boldsymbol{L^{pytZ}}$ Ligands

The four pyridine carboxylic acids (AK Scientific) and 80% aqueous hydrazine hydrate (Sigma Aldrich) were used as supplied. The required N-(4-methylphenyl)benzenethioamide[13] and ethyl N-(4-methylphenyl)benzenethiocarboximidothioate[13] were synthesized as previously reported, as was $[Fe^{II}(pyridine)_4(NCBH_3)_2]$.[14] Ethanol and 1-butanol were reagent grade. Dry methanol was prepared by distilling absolute methanol with Mg/I_2.

5-Trifluoromethane-pyridine-2-methylcarboxylate. To a green suspension of 5-trifluoromethane-picolinic acid (1.70 g, 8.94 mmol) in dry methanol (30 mL), $SOCl_2$ (2.50 mL, 30.10 mmol) was added dropwise. The resulting green solution was stirred at RT for 24 h in air before being taken to dryness under reduced pressure. The green solid residue was taken up in, and neutralized with, sat. $NaHCO_3$ aqueous solution (10 mL), then extracted with dichloromethane (3 x 25 mL). The DCM phase was taken to dryness under reduced pressure, giving the ester as green powder that was used without further purification. (1.78 g, 8.68 mmol, 97%). $C_8H_6NOF_3$ (M=205.05 g mol^{-1}), calc. C 46.84% N 6.38% H 2.95%; found C 47.05% N 6.60% H 2.86%. ^1H NMR (400 MHz, $CDCl_3$) δ(ppm) = 9.00 (t, 1H); 8.26 (m, 1H); 8.10 (m, 1H); 4.00 (s, 3H). Similar synthesis was previously reported, by a different method in a lower yield, by Warren *et al.* in 2019.[15]

5-Bromo-pyridine-2-methylcarboxylate. To a colourless suspension of 5-bromo-picolinic acid (0.50 g, 2.48 mmol) in dry methanol (10 mL), $SOCl_2$ (0.40 mL, 4.81 mmol) was added dropwise. The resulting colourless solution was stirred at RT for 24 h in air before being taken to dryness under reduced pressure. The white solid residue was taken up in, and neutralized with, sat. $NaHCO_3$ aqueous solution (5 mL), then extracted with dichloromethane (3 x 10 mL). The combined DCM phase was taken to dryness under reduced pressure, giving the ester as a white powder that was used without further purification (0.46 g, 2.21 mmol, 89%). C_7H_6NOBr (M=215.94 g mol^{-1}): calc. C 38.92% N 6.48% H 2.80%; found C 39.25% N 6.26% H 2.65%. ^1H NMR (400 MHz, $CDCl_3$) δ(ppm) = 8.79 (m, 1H); 8.00 (m, 1H); 7.99 (m, 1H); 4.00 (s, 3H). Same synthetic procedure was previously reported by Krauss *et al.* in 2013, similar yield obtained.[16]

5-Fluoro-pyridine-2-methylcarboxylate. To a pale green coloured suspension of 5-fluoro-picolinic acid (1.70 g, 12.11 mmol) in dry methanol (30 mL), $SOCl_2$ (3.5 mL, 42.12 mmol) was added dropwise. The resulting pale green solution was stirred at RT for 24 h in air before being taken to dryness under reduced pressure. The pale green solid residue was taken up in, and neutralized with, sat. $NaHCO_3$ aqueous solution (10 mL), then extracted with dichloromethane (3 x 25 mL). The combined DCM phase was taken to dryness under reduced pressure, giving the ester as a pale green powder that was used without further purification (1.82 g, 11.7 mmol, 97%). C_7H_6NOF (M=155.03 g mol^{-1}): calc. C 54.20% N 9.03% H 3.90%; found C 53.95% N 8.71% H 3.90%. ^1H NMR (400 MHz, $CDCl_3$) δ(ppm) = 8.56 (t, 1H); 8.18 (m, 1H); 7.52 (m, 1H); 4.00 (s, 3H).

5-Methyl-pyridine-2-methylcarboxylate. To a green coloured suspension of 5-methyl-picolinic acid (1.00 g, 7.41 mmol) in dry methanol (10 mL), $SOCl_2$ (2.50 mL, 30.09 mmol) was added dropwise. The resulting pale green solution was stirred at 100°C for 24 h in air before being taken to dryness under

reduced pressure. The light green solid residue was taken up in, and neutralized, with sat. $NaHCO_3$ aqueous solution (5 mL), then extracted with dichloromethane (3 x 20 mL). The combined DCM phase was taken to dryness under reduced pressure, giving the ester as a pale green product that was used without further purification (0.75 g, 4.97 mmol, 67%). $C_8H_9NO_2$ (M=151.17 g mol^{-1}): calc. C 63.56% N 9.27% H 6.00%; found C 63.48% N 9.06% H 6.22%. ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm) = 8.56 (s, 1H); 8.03 (d, 1H); 7.63 (d, 1H); 4.00 (s, 3H); 2.38 (s, 3H).

5-Trifluoromethyl-pyridine-2-carbohydrazide. *Caution! Hydrazine hydrate is potentially explosive. Perform the reaction behind a blast screen in a fume hood. Dispose of hydrazine hydrate residues appropriately.* Behind a blast shield, to a green EtOH (10 mL) solution of 5-trifluoromethyl-pyridine-2-methylcarboxylate (0.53 g, 2.6 mmol) at room temperature was added dropwise 80% aqueous $N_2H_4{\cdot}H_2O$ (0.5 mL, 10 mmol). The resulting pale green mixture was refluxed in air for 30 min at 80°C, then allowed to cool down to RT, which caused a white precipitate to form. The precipitate was filtered off, washed with cold EtOH (5 mL), and air dried, giving the carbohydrazide as a white solid that was used without further purification (0.28 g, 1.37 mmol, 53%). $C_7H_6N_3OF_3$ (M=205.05 g mol^{-1}), calc. C 40.99% N 20.48% H 2.95%; found C 41.11% N 20.09% 3.03%. ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm) = 8.94 (m, 1H); 8.81 (m, 1H); 8.29 (m, 1H); 8.10 (m, 1H); 4.07 (m, 2H).

5-Bromo-pyridine-2-carbohydrazide. *Caution! Hydrazine hydrate is potentially explosive. Perform the reaction behind a blast screen in a fume hood. Dispose of hydrazine hydrate residues appropriately.* Behind a blast shield, to a colourless EtOH (10 mL) solution of 5-bromo-pyridine-2-methylcarboxylate (0.46 g, 2.14 mmol) at room temperature was added dropwise 80% aqueous $N_2H_4{\cdot}H_2O$ (0.2 mL, 4 mmol). The resulting colourless solution was stirred in air at RT until a white precipitate was formed (approx. 5 min), then kept stirring for 15 min longer. The white precipitate was filtered off, washed with cold EtOH (5 mL) and air dried, giving the carbohydrazide as a white solid that was used without further purification (0.41 g, 1.90 mmol, 89%). $C_6H_6N_3OBr$ (M=216.04 g mol^{-1}), calc. C 33.33% N 19.44% H 2.78%; found C 33.08% N 19.21% 2.88%. ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm) = 8.84 (s, 1H); 8.60 (m, 1H); 8.01 (m, 1H); 7.98 (m, 1H); 3.96 (s, 2H). Same synthetic procedure was previously reported by Noel *et al.* in 2015 with similar yield.[17]

5-Fluoro-pyridine-2-carbohydrazide. *Caution! Hydrazine hydrate is potentially explosive. Perform the reaction behind a blast screen in a fume hood. Dispose of hydrazine hydrate residues appropriately.* Behind a blast shield, to a pale green EtOH (10 mL) solution of 5-fluoro-pyridine-2-methylcarboxylate (0.96 g, 6.19 mmol) at room temperature was added dropwise 80% aqueous $N_2H_4{\cdot}H_2O$ (1 mL, 20 mmol). The resulting colourless solution was stirred in air at RT until a white precipitate was formed (approx. 5 min), then kept stirring for 15 min longer. The precipitate was filtered off, washed with cold EtOH (5 mL), and air dried, giving the carbohydrazide as a white solid that was used without further purification (0.67g, 4.32 mmol,70%). $C_6H_6N_3OF$ (M=155.05 g mol^{-1}), calc. C 46.45% N 27.09% H 3.90%; found C 46.42% N 27.33% 3.82%. ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm) = 8.79 (s, 1H); 8.38 (m, 1H); 8.19 (m, 1H); 7.53 (m, 1H); 3.91 (s, 2H).

5-Methyl-pyridine-2-carbohydrazide. *Caution! Hydrazine hydrate is potentially explosive. Perform the reaction behind a blast screen in a fume hood. Dispose of hydrazine hydrate residues appropriately.* Behind a blast shield, to a pale green EtOH (2 mL) solution of 5-methyl-pyridine-2-methylcarboxylate (0.50 g, 2.14 mmol) at room temperature was added dropwise 80% aqueous $N_2H_4{\cdot}H_2O$ (4 mL, 80 mmol). The resulting green mixture was refluxed for 30 min at 80°C, then the resulting solution was

carefully taken to dryness using a gentle air flow, then dried under vacuum for 48 h. The resulting white solid was used without further purification (0.5g, 2.14 mmol, 99%). $C_7H_9N_3O$ (M=151.17g mol^{-1}), calc. C 55.62% N 27.80% H 6.00%; found C 55.40% N 27.55% H 5.82%. ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm) = 8.91 (s, 1H); 8.36 (s, 1H); 8.04 (d, 1H); 7.64 (d, 1H). Same synthetic procedure was previously reported by Noel *et al.* in 2015 with similar yield.[17]

4-(4-Methylphenyl)-3-(5-trifluoromethyl-pyridyl)-5-phenyl-1,2,4-triazole (L^{pytCF3}). Crude ethyl N-(4-methylphenyl)-benzenecarboximidothioate (1 g, 4.5 mmol) and 5-trifluoromethyl-pyridine-2-carbohydrazide (0.61 g, 3.0 mmol) were dissolved in 1-butanol (15 mL) and refluxed for 3 d at 145 °C under argon. After cooling down to RT no precipitate was observed, so the reaction mixture was taken to dryness. The resulting white solid was suspended in water (20 mL) filtered off, and then washed with cold diethyl ether (3 x 5 mL) to remove unreacted reagents, (as L^{pytCF3} ligand shows low solubility in diethyl ether. The resulting white powder was air dried (0.47g, 1.24 mmol, 42%). $C_{21}H_{15}N_4F_3$ (M=380.37 g mol^{-1}), calc. C 66.31.% N 17.73% H 3.98%; found C 66.35% N 17.50% 4.08%. ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm) = 8.58 (s, 1H, H_1); 8.34 (d, 2H, H_3); 7.99 (d, 1H, H_2); 7.46 (m, 2H, H_9); 7. 36 (m, 1H, H_7); 7.29 (m, 2H, H_8); 7.19 (d, 2H, H_4); 7.09 (d, 2H, H_5); 2.41 (s, 3H, H_6). ^{13}C NMR (400 MHz, $CDCl_3$) δ(ppm) = 156.3 (C_6); 152.6 (C_{12}); 150.3 (C_5); 145.7 (C_1); 139.4 (C_{16}); 133.8 (q, C_{17}); 133.0 (C_{10}); 129.9 (C_9); 129.8 (C_7); 128.8 (C_{14}); 128.38 (C_{15}); 127.6 (C_8); 126.6 (C_2); 124.6 (C_3); 123.7 (C_4); 121.9 (C_{13}); 21.2(C_{11});. ^{15}N NMR (500 MHz, $CDCl_3$) δ(ppm) = 320.9 (N_2); 313.8 (N_1); 315.1 (N_3); 177.2 (N_4). HR-ESI-MS (acetone) m/z: $[H(C_{21}H_{15}N_4F_3)]^+$, calc. 381.13, exp. 381.13; $[Na(C_{21}H_{15}N_4F_3)]^+$, calc. 403.11, exp. 403.11; $[K(C_{21}H_{15}N_4F_3)]^+$, calc. 419.08, exp. 419.08; $[Na(C_{21}H_{15}N_4F_3)_2]^+$, calc. 783.23, exp. 783.23.

4-(4-Methylphenyl)-3-(5-bromo-pyridyl)-5-phenyl-1,2,4-triazole (L^{pytBr}). Crude ethyl N-(4-methylphenyl)-benzenecarboximidothioate (0.70 g, 3.3 mmol) and 5-bromo-pyridine-2-carbohydrazide (0.90 g, 4.0 mmol) were dissolved in 1-butanol (20 mL) and refluxed for 5 d at 145 °C under argon. After cooling down to RT no precipitate was observed, so the reaction mixture was taken to dryness. The resulting white solid was suspended in water (20 mL) filtered off, and then washed with cold diethyl ether (3 x 5 mL) to remove unreacted reagents, (like for the L^{pytCF3} ligand, L^{pytBr} has low solubility in diethyl ether). The resulting white powder was recrystallised from EtOH and air dried, to give L^{pytBr} as an analytically pure white powder (0.47g, 1.24 mmol, 42%). (0.13 g, 0.34 mmol 11%). $C_{20}H_{15}N_4Br$ (M=391.27 g mol^{-1}), calc. C 61.39% N 14.32% H 3.86%; found C 60.91% N 14.28% 3.86%. ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm) = 8.40 (s, 1H, H_1); 8.07 (d, 2H, H_3); 7.88 (d, 1H, H_2); 7.45 (m, 2H, H_9); 7. 35 (m, 1H, H_7);7.18 (d, 2H, H_4); 7.18 (m, 2H, H_8);7.07 (d, 2H, H_5); 2.40 (s, 3H, H_6);. ^{13}C NMR (400 MHz, $CDCl_3$) δ(ppm) = 155.85 (C_{12}); 152.98 (C_6); 150.0 (C_1); 145.5 (C_5); 139.3 (C_7); 139.2 (C_3); 133.0 (C_{10}); 129.8 (C_{16}); 129.7 (C_9); 128.8 (C_{14}); 128.4 (C_{15}); 127.6 (C_8); 126.7 (C_{13}); 125.3 (C_4); 121.4 (C_2); 21.2(C_{11});. ^{15}N NMR (500 MHz, $CDCl_3$) δ(ppm) = 318.1 (N_2); 317.8 (d), 317.0 (i) (N_1); 313.8 (N_3); 176.8 (d), 176.0 (i) (N_4). HR-ESI-MS (acetone) m/z: $[H(C_{20}H_{15}N_4Br)]^+$, calc. 391.05, exp. 391.06; $[Na(C_{20}H_{15}N_4Br)]^+$, calc. 413.04, exp. 413.04; $[K(C_{20}H_{15}N_4Br)]^+$, calc. 431.00, exp. 431.00; $[Na(C_{20}H_{15}N_4Br)_2]^+$, calc. 805.08, exp. 805.08.

4-(4-Methylphenyl)-3-(5-fluoro-pyridyl)-5-phenyl-1,2,4-triazole (L^{pytF}). Crude ethyl N-(4-methylphenyl)-benzenecarboximidothioate (0.55 g, 2.2 mmol) and 4-methoxyl-pyridazine-2-carbohydrazide (0.33 g, 1.96 mmol) were dissolved in 1-butanol (20 mL) and refluxed for 3 d at 145 °C under argon. After cooling down to RT the desired product only partially precipitated, so the reaction mixture was taken to dryness, the solid suspended in water (25 mL), filtered off, and then washed with cold diethyl ether (3 x 5 mL) to remove unreacted reagents as the L^{pytF} ligand shows low solubility in

diethyl ether. The resulting white powder was recrystallized from MeOH, and air dried, to give L^{pytF} as analytically pure white fluffy crystals (0.4 g, 1.2 mmol, 61%). $C_{20}H_{15}N_4F$ (M=330.36 g mol^{-1}), calc. C 72.71% N 16.96% H 4.58%; found C 72.68% N 16.72% 4.69%. ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm) = 8.19 (m, 1H, H_1); 8.11 (m, 2H, H_3); 7.46 (m, 1H, H_2); 7.44 (m, 2H, H_9); 7. 32 (m, 1H, H_7); 7.27 (m, 2H, H_8); 7.15 (d, 2H, H_4); 7.06 (d, 2H, H_5); 2.38 (s, 3H, H_6). ^{13}C NMR (400 MHz, $CDCl_3$) δ(ppm) = 159.3 (d, C_2); 155.7 (C_{12}); 153.1 (C_6); 143.5 (d, C_5); 139.2 (C_7); 137.4 (d, C_1); 133.0 (C_{10}); 129.8 (C_9); 129.7 (C_{16}); 128.8 (C_{14}); 128.4 (C_{15}); 127.7 (C_8); 126.8 (d, C_4); 125.7 (C_{13}); 123.5 (d, C_3); 21.3 (C_{11});. HR-^{15}N NMR (500 MHz, $CDCl_3$) δ(ppm) = 319.9 (N_1); 176.0 (N_4). ESI-MS (acetone) m/z: $[H(C_{20}H_{15}N_4F)]^+$, calc. 331.13, exp. 331.13; $[Na(C_{20}H_{15}N_4F)]^+$, calc. 353.12, exp. 353.12; $[K(C_{20}H_{15}N_4F)]^+$, calc. 369.09, exp. 369.09; $[Na(C_{20}H_{15}N_4F)_2]^+$, calc. 683.24, exp. 683.24.

4-(4-Methylphenyl)-3-(5-methyl-pyridyl)-5-phenyl-1,2,4-triazole (L^{pytMe}). Crude ethyl N-(4-methylphenyl)-benzenecarboximidothioate (0.58 g, 2.57 mmol) and 4-methyl-pyridine-2-carbohydrazide (0.5 g, 2.14 mmol,) were dissolved in 1-butanol (10 mL) and refluxed for 4 d at 145 ˚C under argon. After cooling down to RT the resulting precipitate was filtered off and washed with a copious volume of water (approx. 100 mL), then with a copious volume of diethyl ether (approx. 100 mL) to remove the unreacted reagents as the L^{pytMe} does not show any solubility in either solvent. The powder was then crystallised from MeOH, and air dried, to give L^{pytMe} as an analytically pure white powder (0.62g, 1.9 mmol, 58%). $C_{21}H_{18}N_4$ (M=326.4 g mol^{-1}), calc. C 77.28% N 17.17% H 5.56%; found C 77.58% N 16.91% 5.49%. ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm) = 8.20 (s, 1H, H_1); 7.90 (d, 2H, H_3); 7.52 (d, 1H, H_2); 7.44 (m, 2H, H_9); 7.33 (m, 2H, H_8); 7. 28 (m, 1H, H_7); 7.12 (d, 2H, H_4); 7.06 (d, 2H, H_5); 2.37 (s, 3H, H_6); 2.29 (s, 3H, H_{10}). ^{13}C NMR (400 MHz, $CDCl_3$) δ(ppm) = 155.4 (C_{12}); 154.0 (C_6); 149.5 (C_1); 144.4 (C_5); 139.0 (C_7); 136.9 (C_4); 133.2 (C_3); 130.5 (C_{10}); 129.7 (C_9); 129.5 (C_{16}); 128.8 (C_{14}); 128.3 (C_{15}); 127.7 (C_8); 127.1 (C_{13}); 123.9 (C_2); 21.3 (C_{11}); 18.4 (C_{17}). ^{15}N NMR (500 MHz, $CDCl_3$) δ(ppm) = 313.7 (N_2); 312.2 (N_1); 311.6 (N_3); 175.8 (N_4). HR-ESI-MS (acetone) m/z: $[H(C_{21}H_{18}N_4)]^+$, calc. 327.16, exp. 327.16; $[Na(C_{21}H_{18}N_4)]^+$, calc. 349.14, exp. 349.14; $[K(C_{21}H_{18}N_4)]^+$, calc. 365.11, exp. 365.12; $[Na(C_{21}H_{18}N_4)_2]^+$, calc. 675.30, exp. 675.29.

S1.3. NMR and MS Figures for L^{pytCF3} Ligand

^{1}H-NMR Spectrum

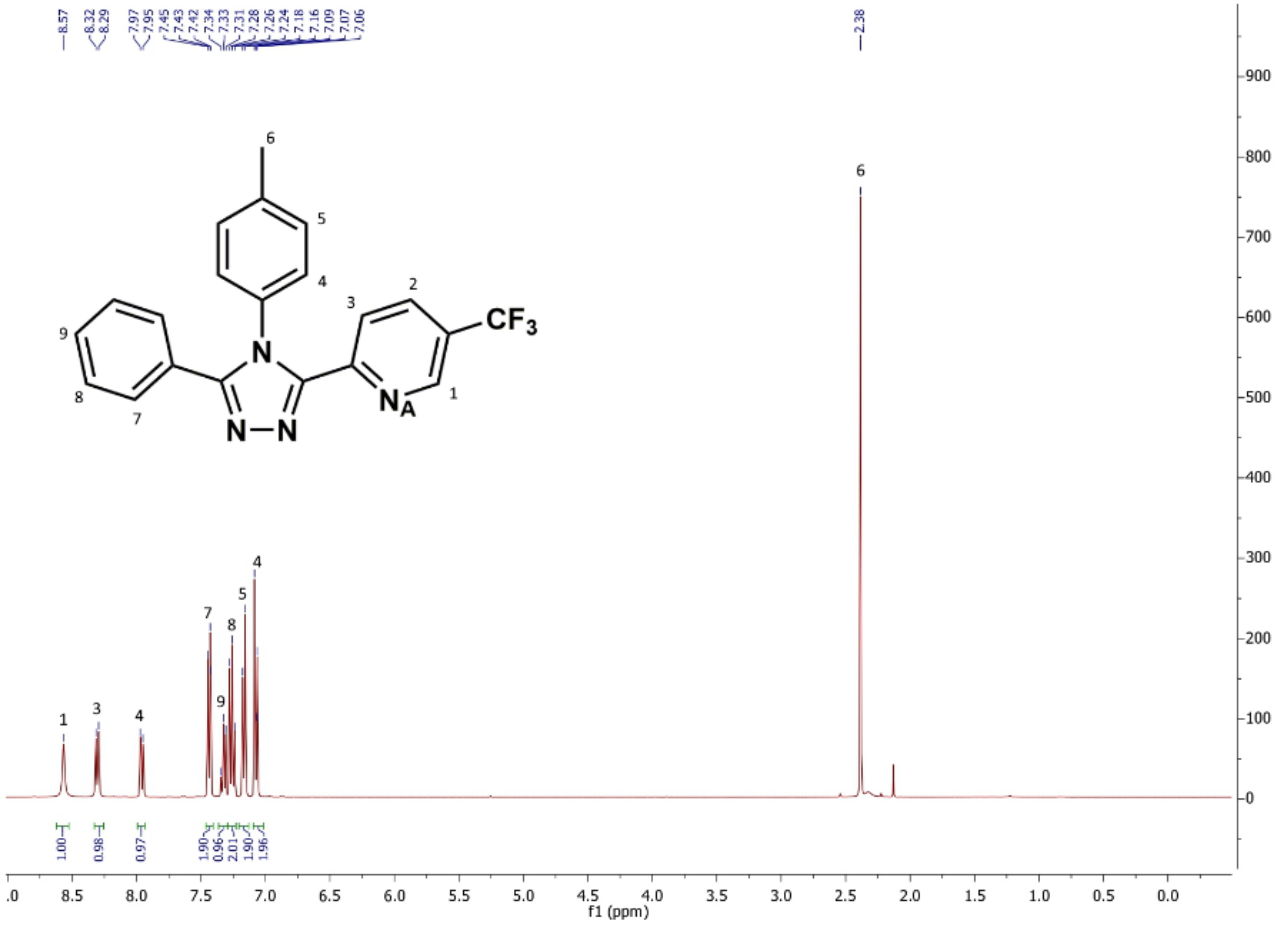

Figure S11. The full range ^{1}H NMR spectrum of ligand L^{pytCF3} in $CDCl_3$ at 298 K.

^{13}C-NMR Spectrum

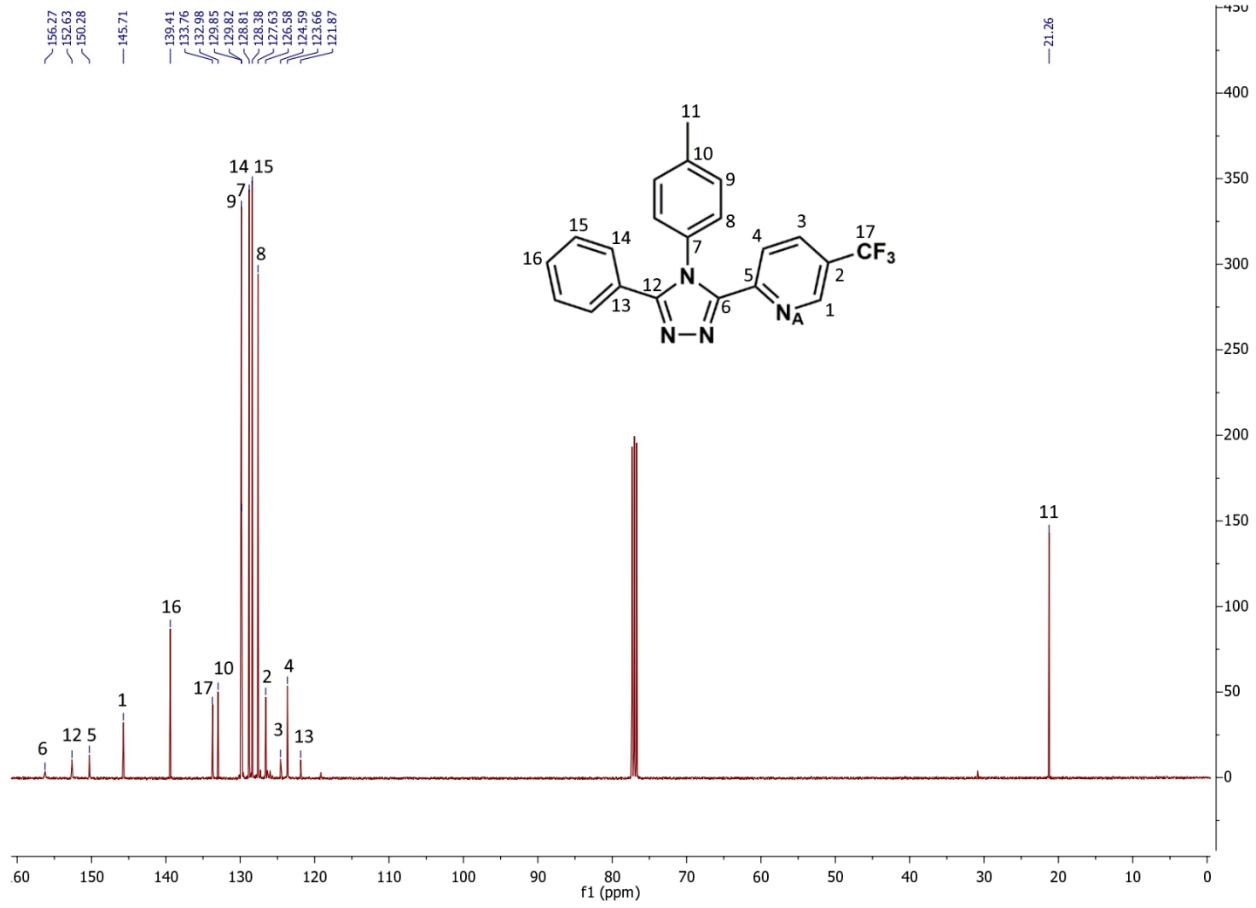

Figure S22. The full range ^{13}C NMR spectrum of ligand ***L^{pytCF3}*** in $CDCl_3$ at 298 K.

HSQCAD Spectrum

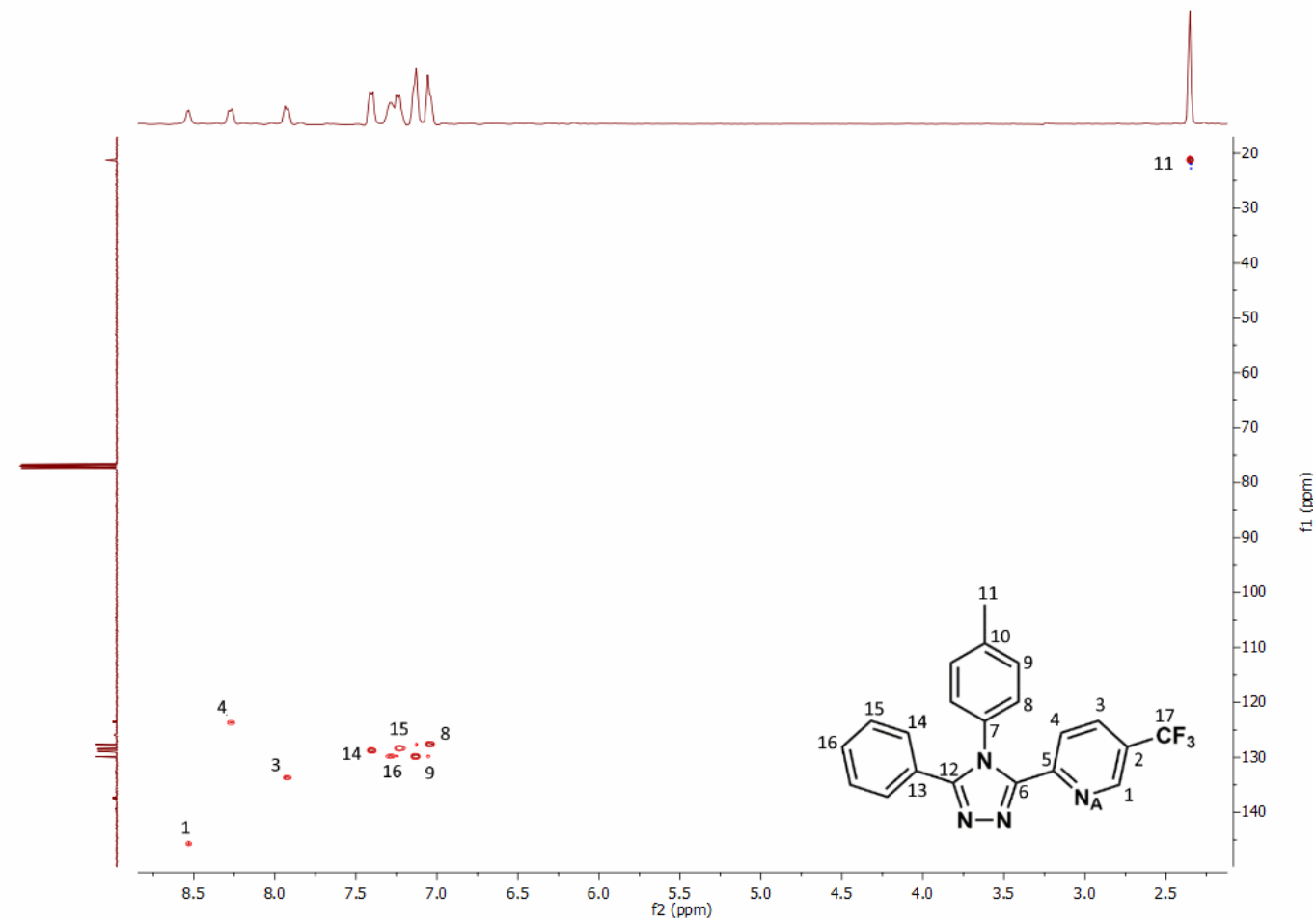

Figure S3. Heteronuclear ^{1}H-^{13}C NMR spectrum of ligand ***L*^{pytCF3}** in $CDCl_3$ at 298 K.

^{15}N-NMR Spectrum

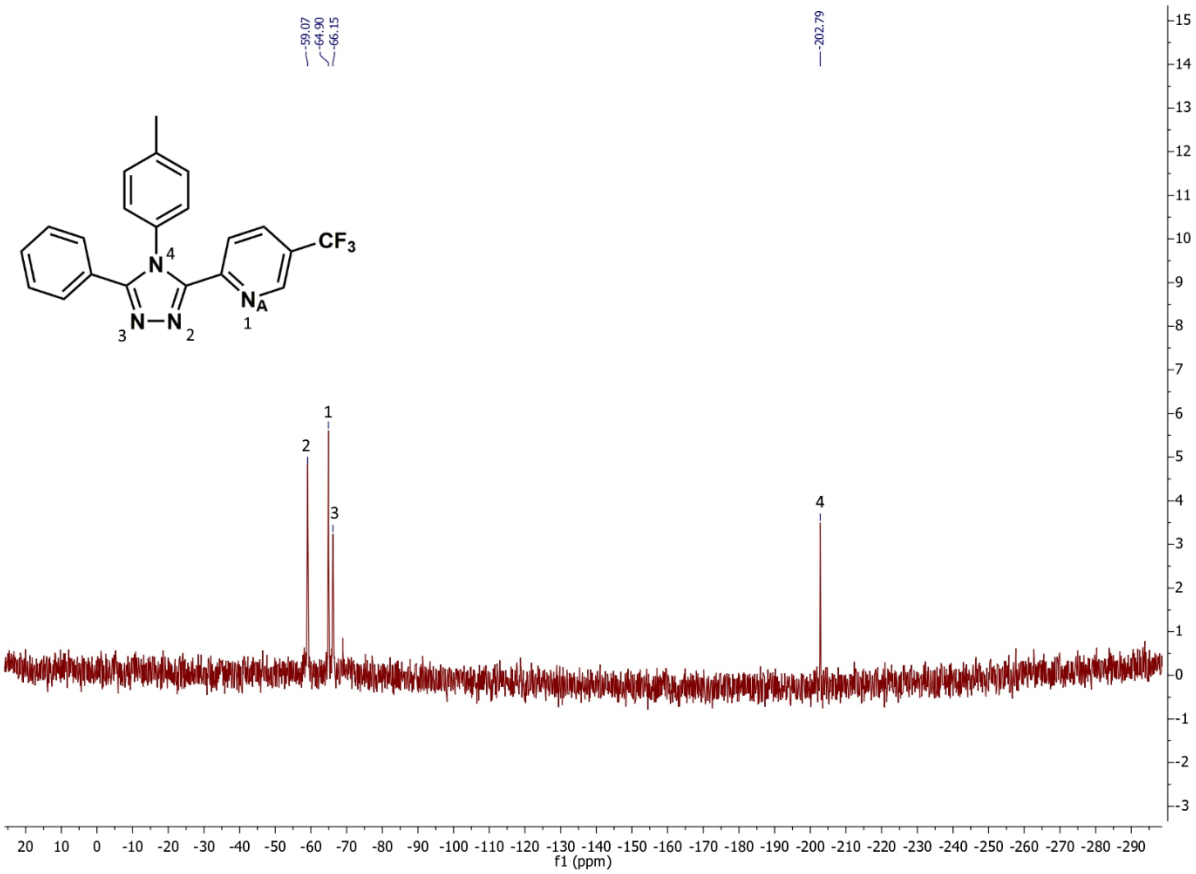

Figure S4. The full range ^{15}N NMR spectrum (direct measurement) of ligand ***L^{pytCF3}*** in $CDCl_3$ at 298 K.

Mass Spectrum

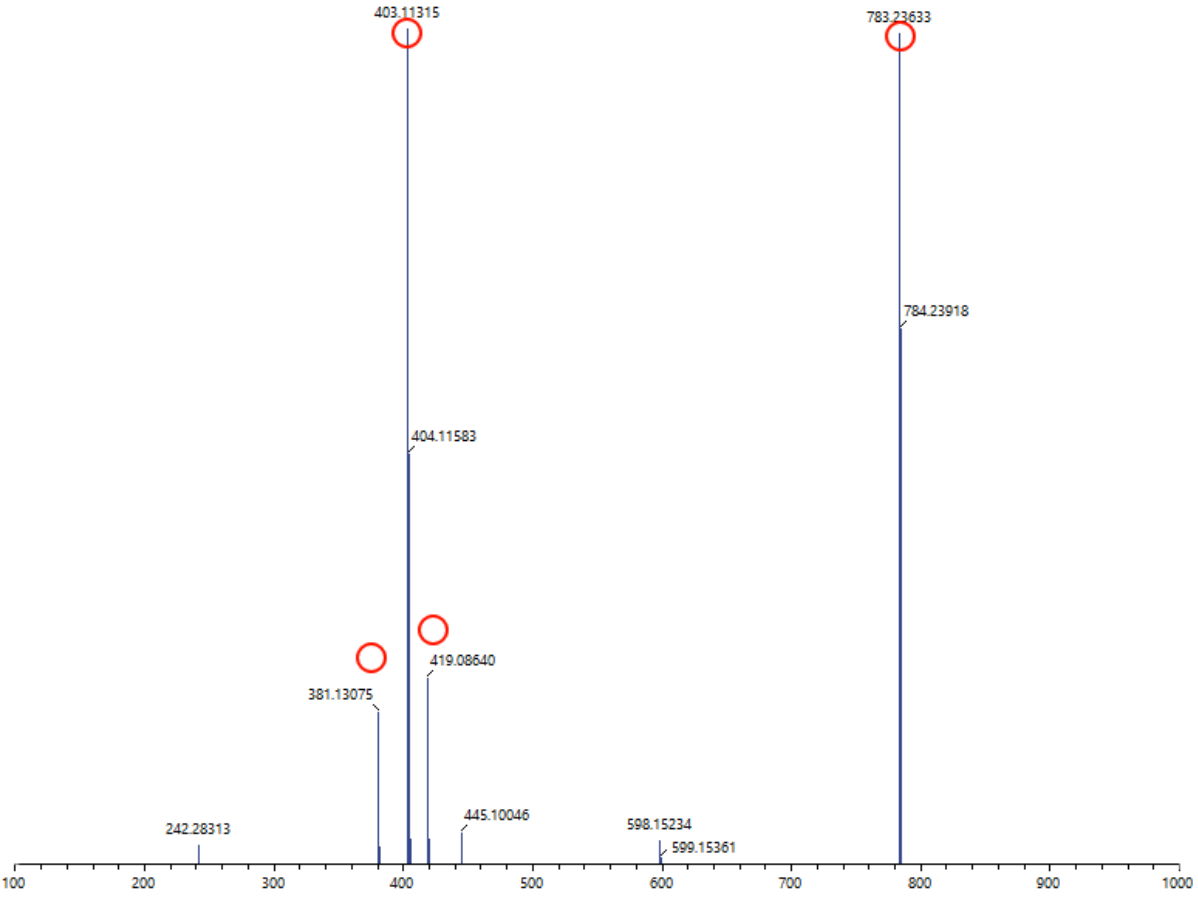

Figure S5. Complete mass spectrum of L^{pytCF3}. Reported circles refer to zoomed regions reported below.

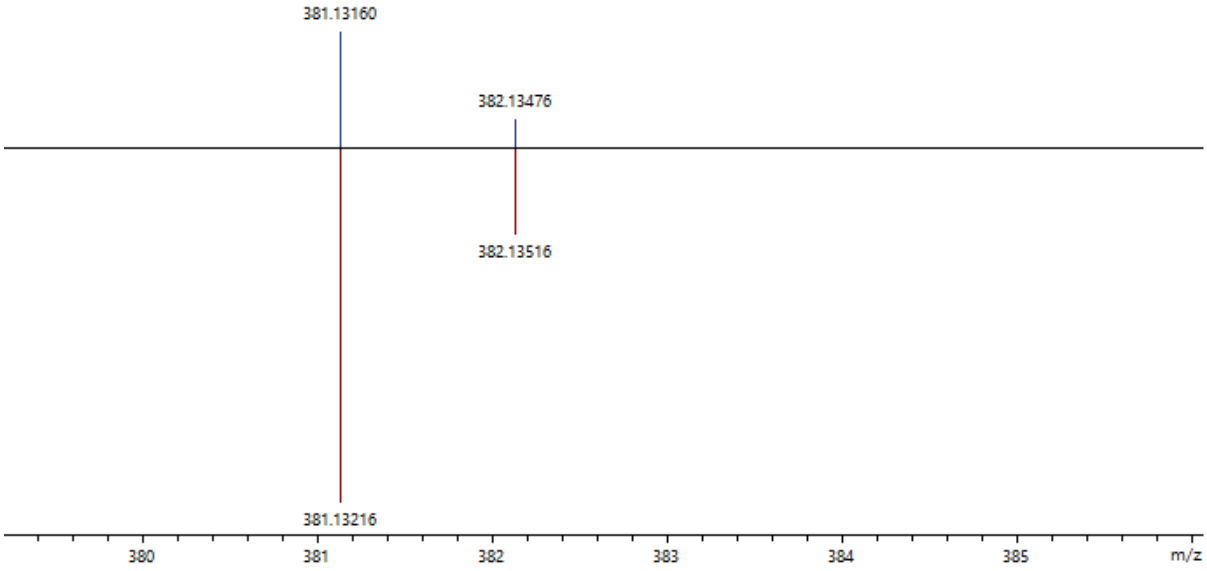

Figure S6. Fit of a peak in the mass spectrum of $[L^{pytCF3}+H]^+$ experimental (blue) and simulated pattern (red).

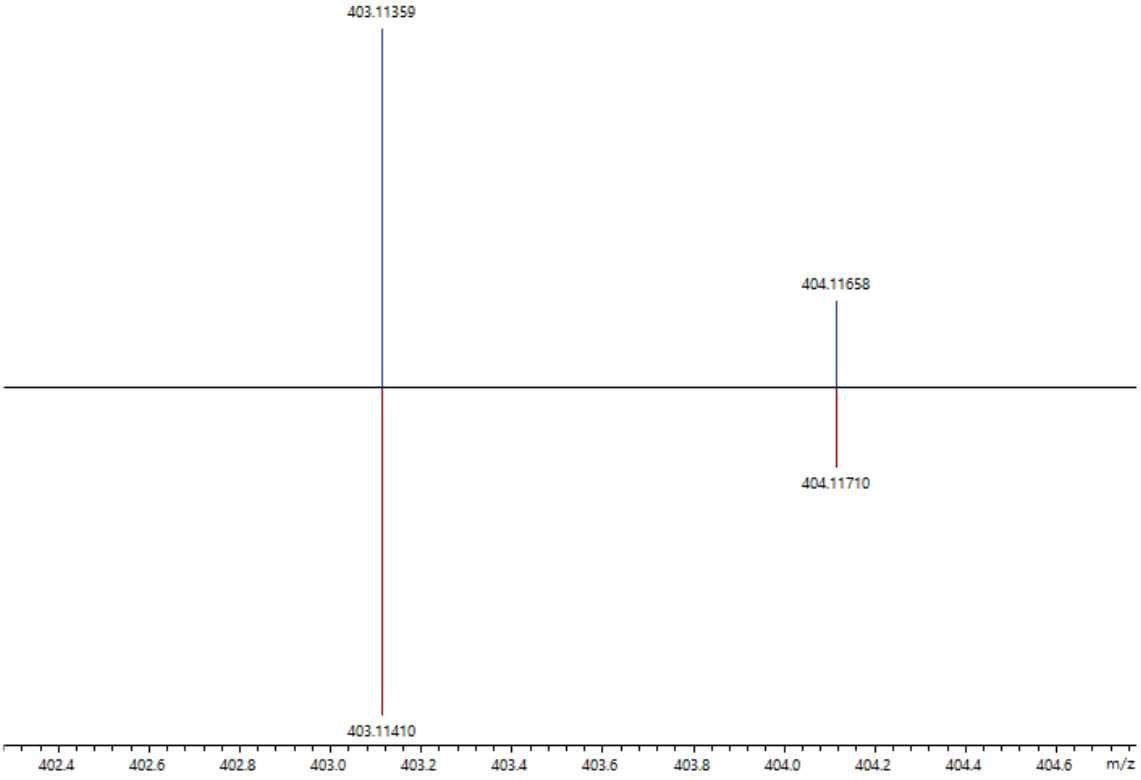

Figure S7. Fit of a peak in the mass spectrum of $[L^{pytCF3}+Na]^+$ experimental (blue) and simulated pattern (red).

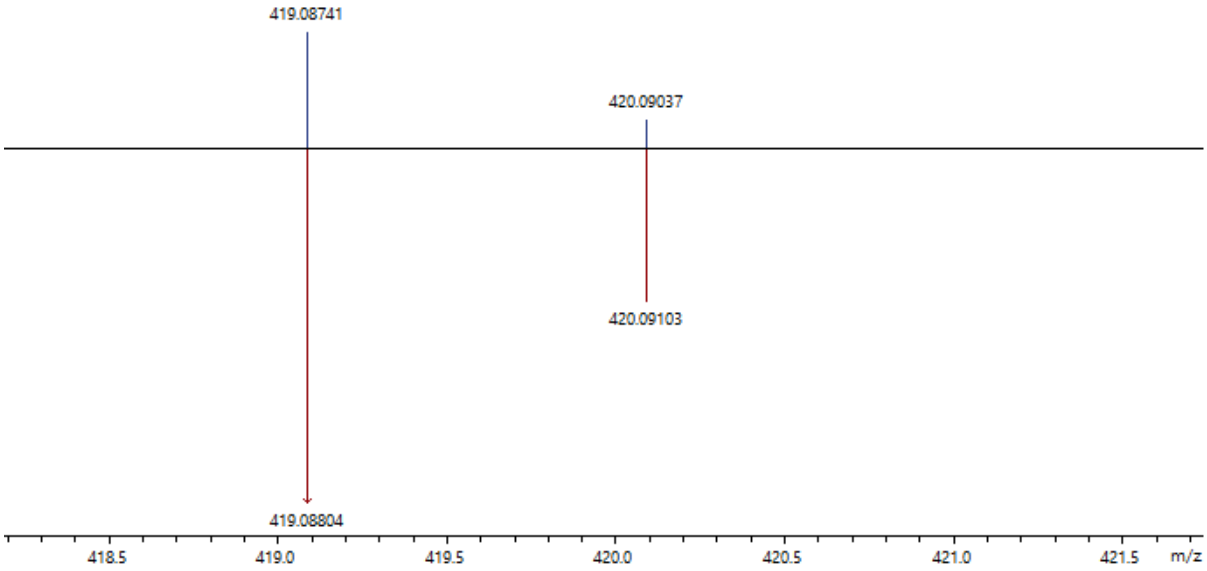

Figure S8. Fit of a peak in the mass spectrum of ***[L^{pytCF3}+K]$^{+}$*** experimental (blue) and simulated pattern (red).

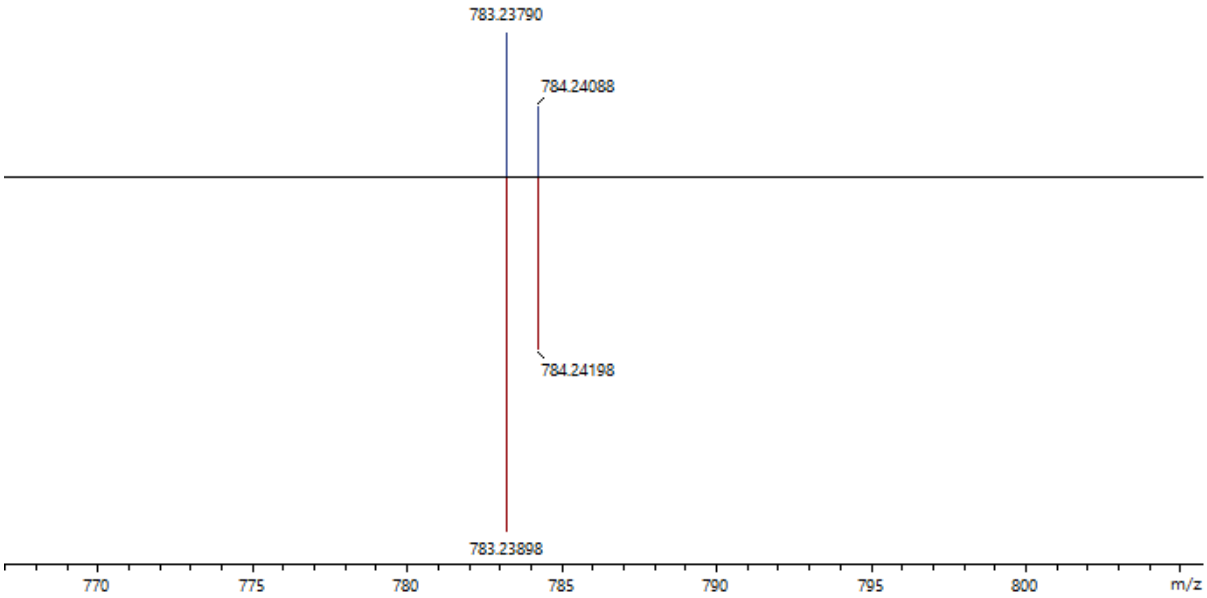

Figure S9. Fit of a peak in the mass spectrum of ***[2L^{pytCF3}+Na]$^{+}$*** experimental (blue) and simulated pattern (red).

S1.4. MS Figures for [Fe(L^{pytCF3})$_2$(NCBH$_3$)$_2$] Complex

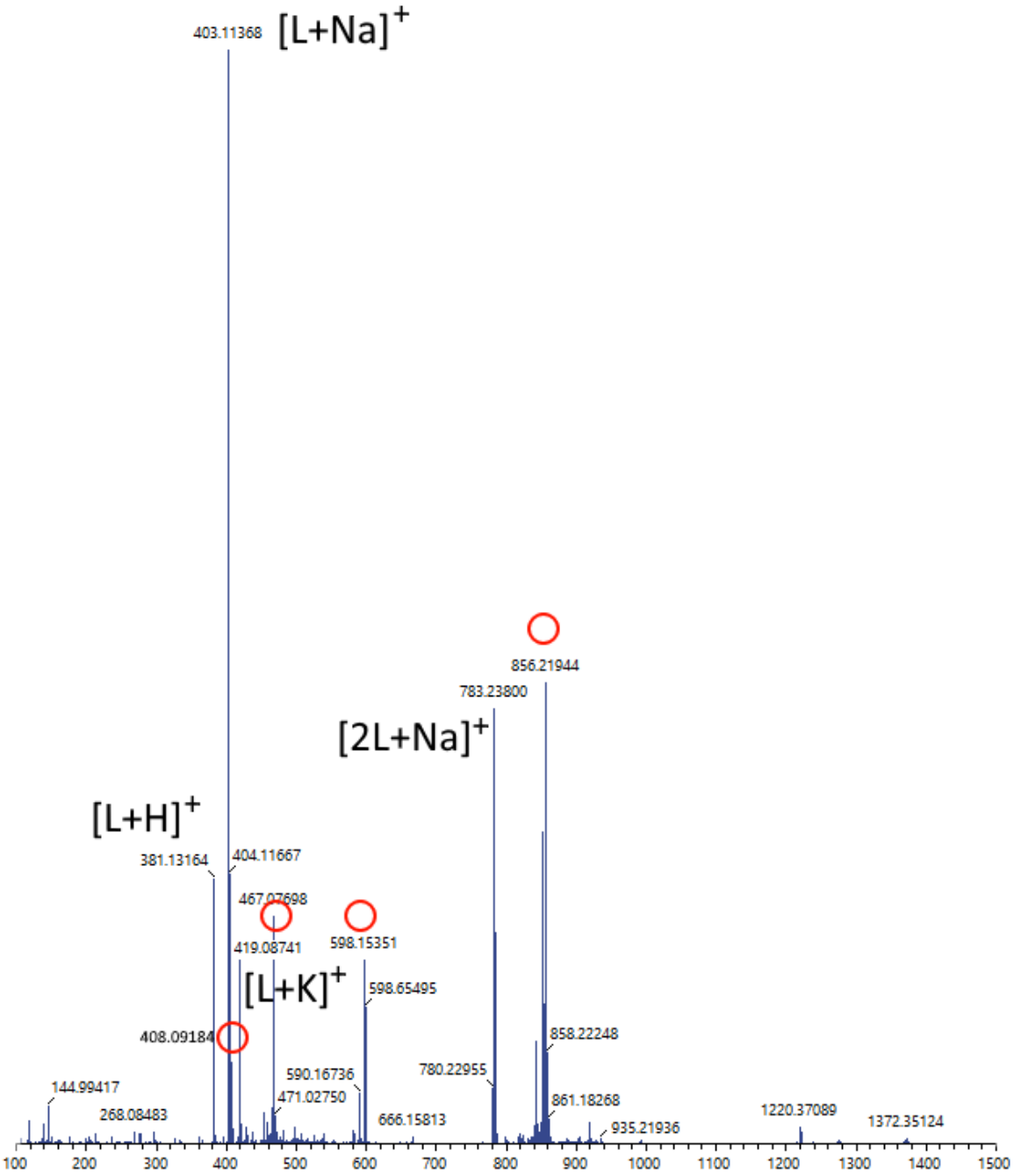

Figure S10. Complete mass spectrum of Fe(L^{pytCF3})$_2$(NCBH$_3$)$_2$ Reported circles refer to zoomed regions reported below.

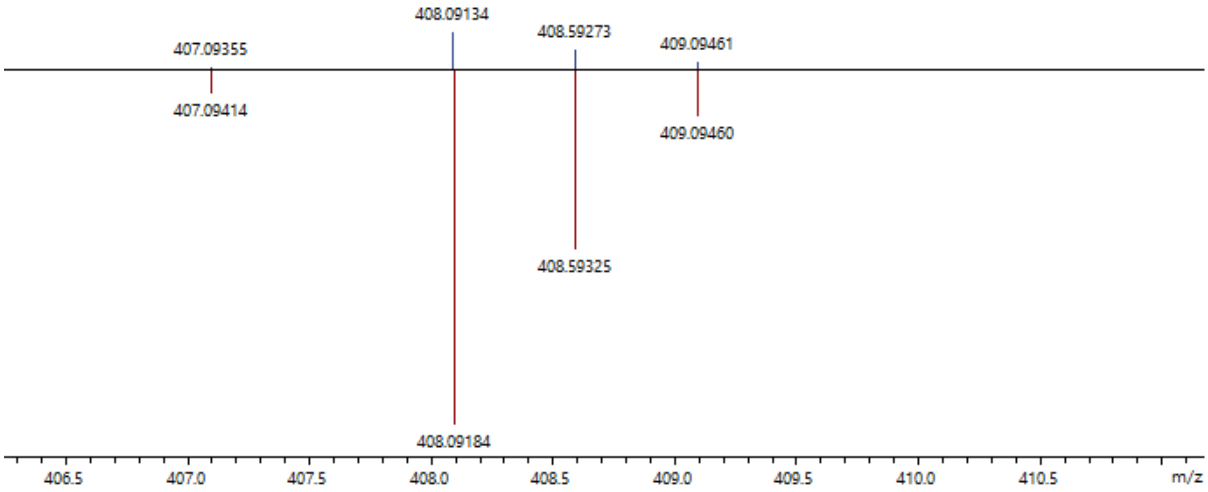

Figure S11. Fit of a peak in the mass spectrum of ***[Fe(L^{pytCF3})$_2$]$^{2+}$*** experimental (blue) and simulated pattern (red).

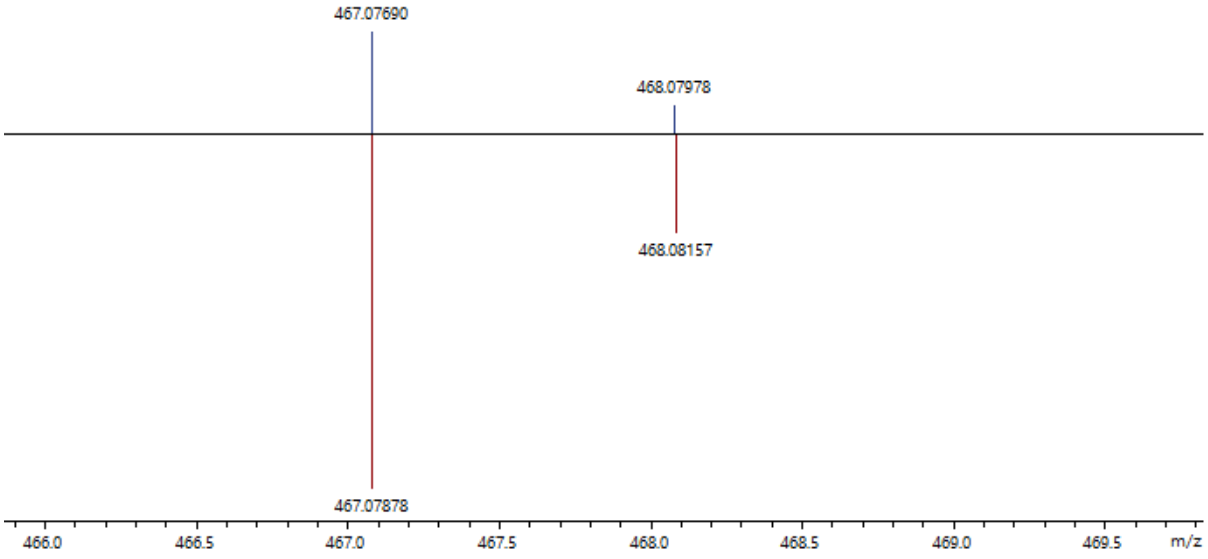

Figure S12. Fit of a peak in the mass spectrum of ***[Fe(L^{pytCF3})(MeOH)-H]$^{+}$*** experimental (blue) and simulated pattern (red).

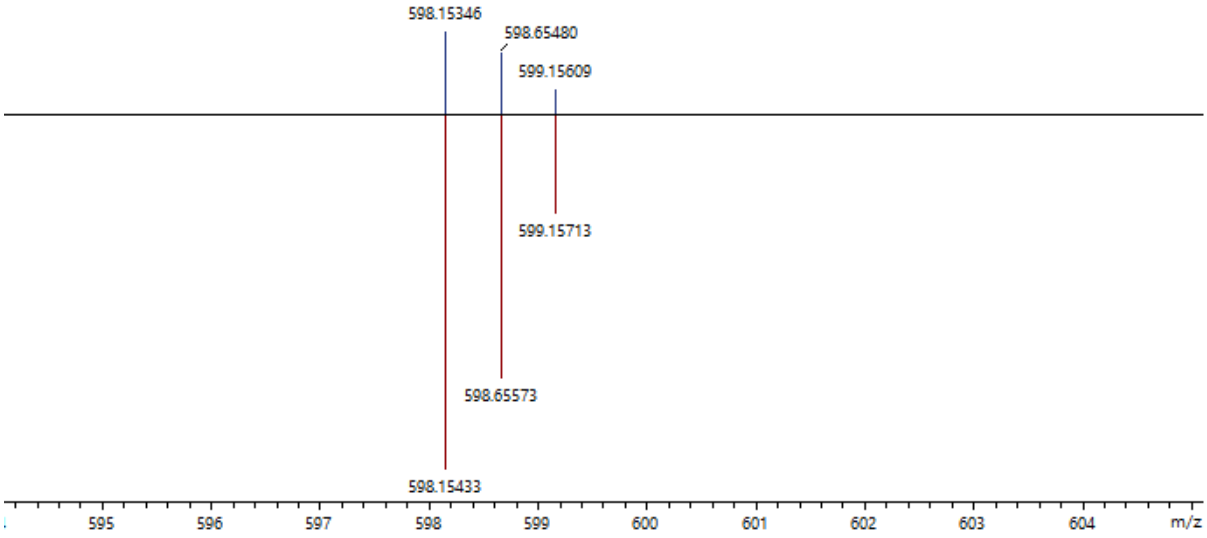

Figure S13. Fit of a peak in the mass spectrum of ***[Fe(L^{pytCF3})$_3$]$^{2+}$*** experimental (blue) and simulated pattern (red).

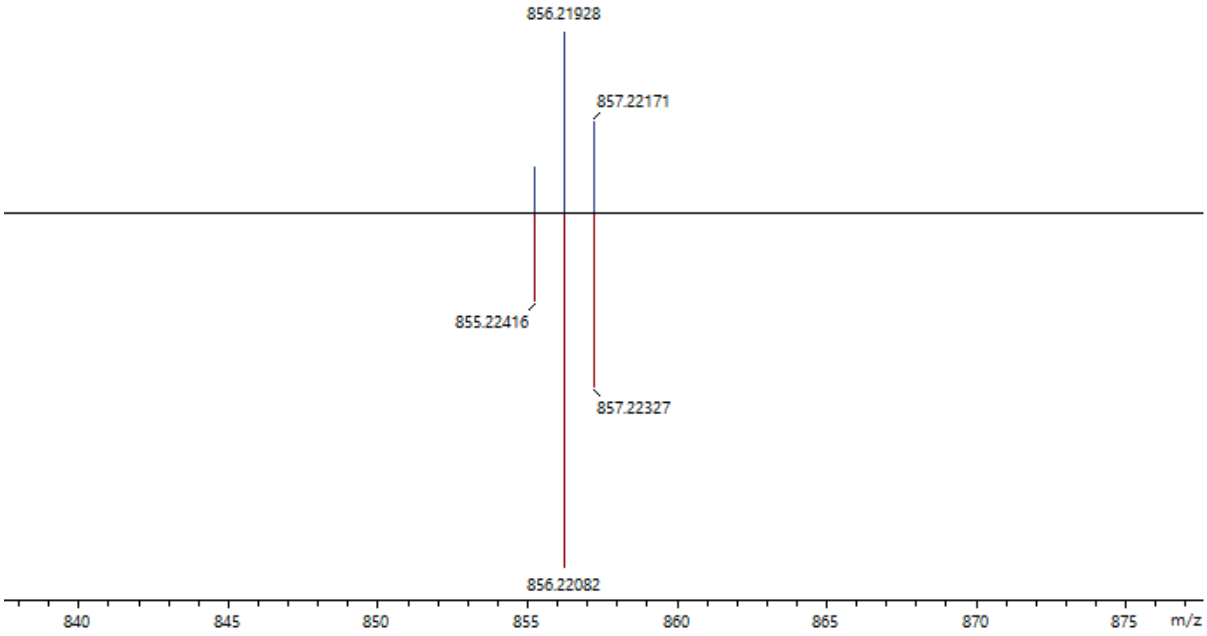

Figure S14. Fit of a peak in the mass spectrum of ***[Fe(L^{pytCF3})$_2$(NCBH$_3$)]$^+$*** experimental (blue) and simulated pattern (red).

S1.5. NMR and MS Figures for L^{pytBr} Ligand

^{1}H-NMR Spectrum

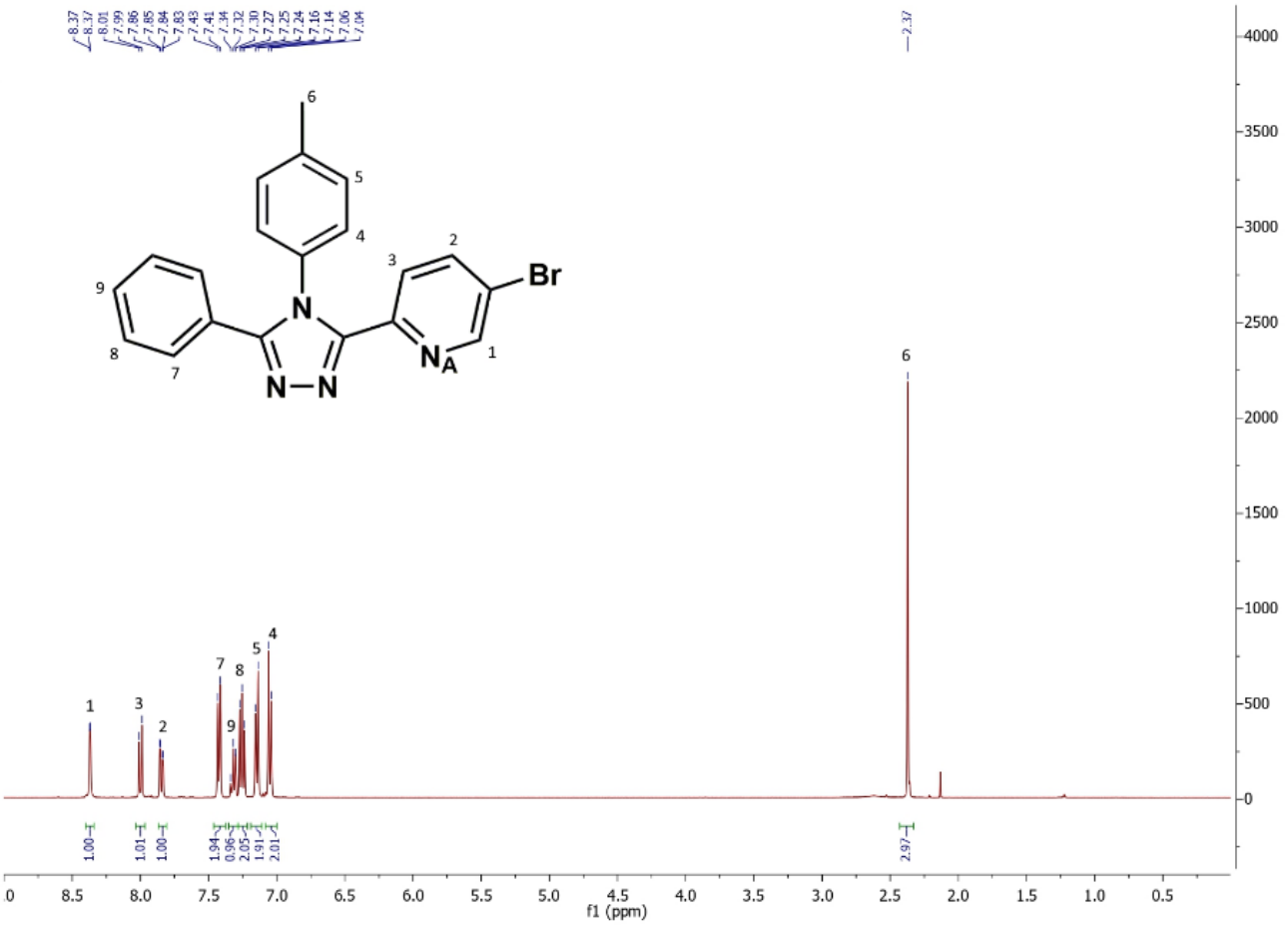

Figure S15. The full range ^{1}H NMR spectrum of ligand L^{pytBr} in $CDCl_3$ at 298 K.

^{13}C-NMR Spectrum

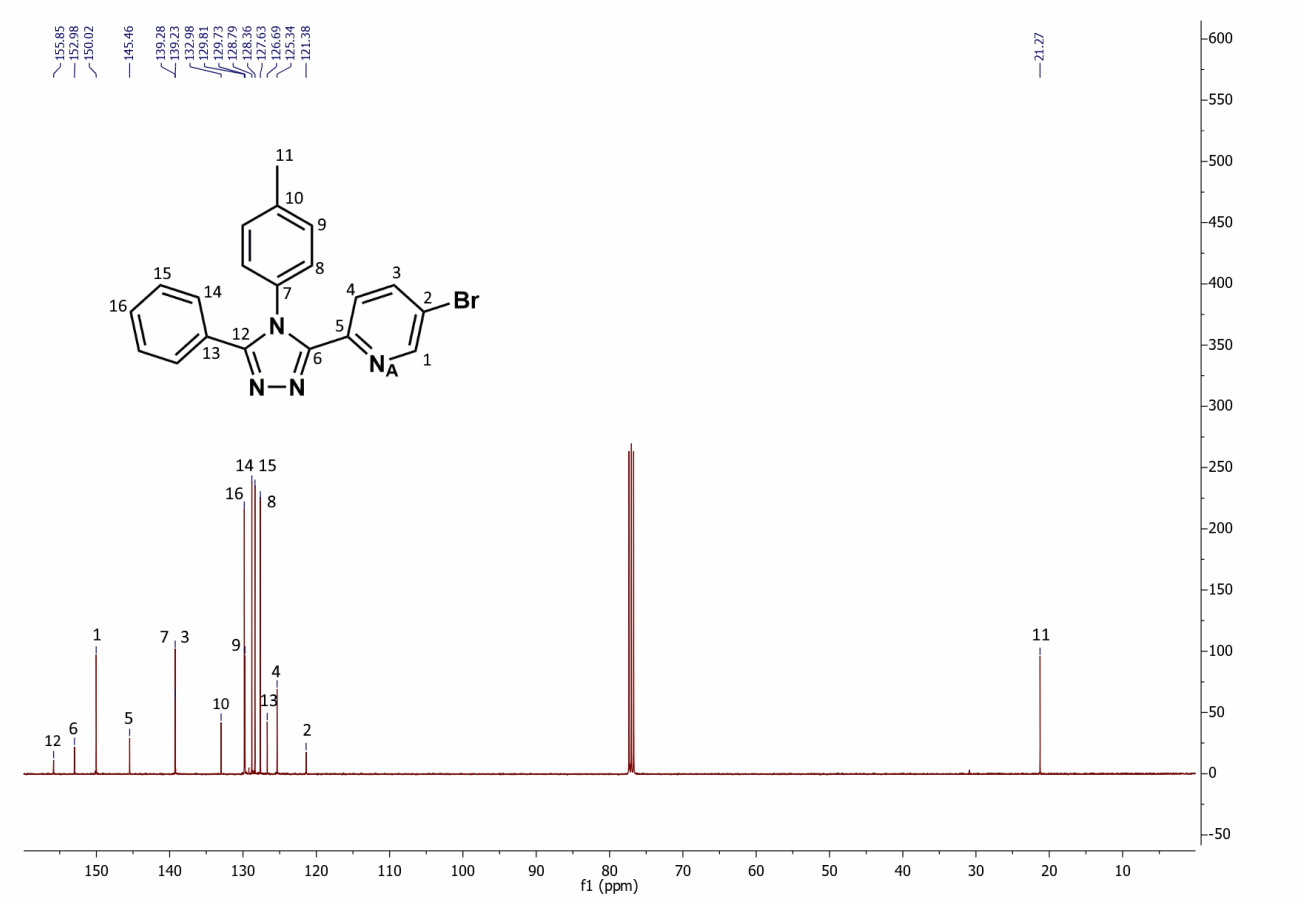

Figure S16. The full range ^{13}C NMR spectrum of ligand ***L^{pytBr}*** in $CDCl_3$ at 298 K.

HSQCAD Spectrum

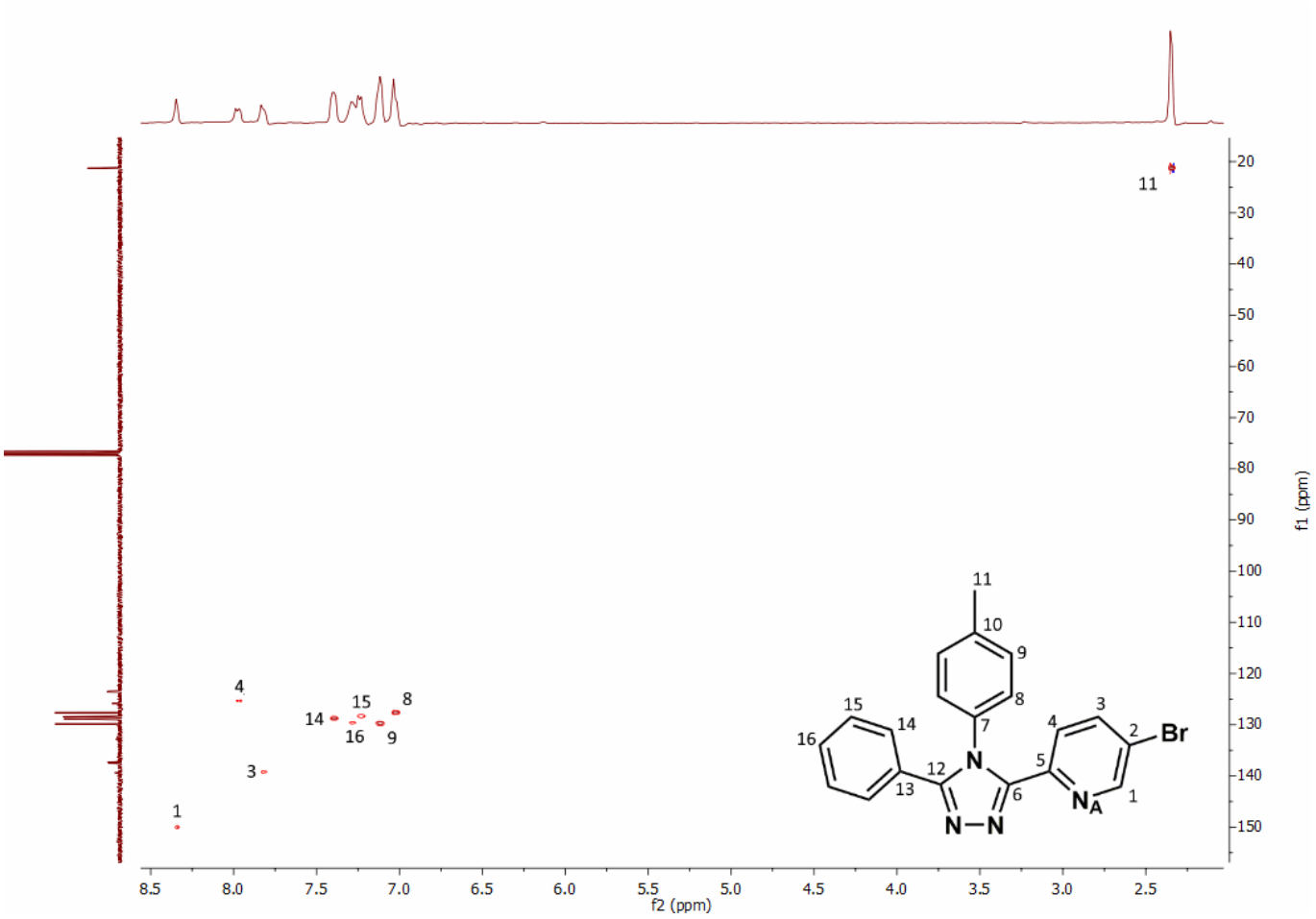

Figure S17. Heteronuclear ^{1}H-^{13}C NMR spectrum of ligand ***L*^{pytBr}** in $CDCl_3$ at 298 K.

^{15}N-NMR Spectrum

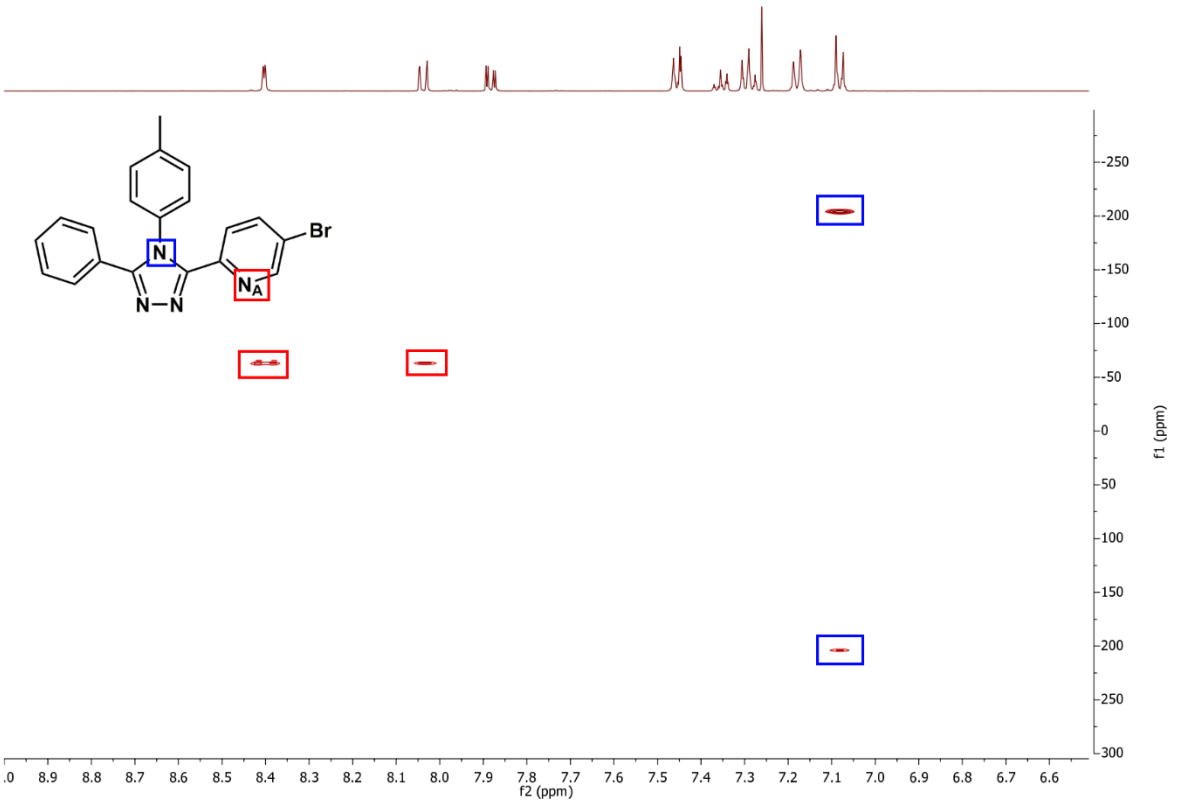

Figure S184. The full range CIGARD ^{1}H-^{15}N NMR spectrum (indirect measurement) of ligand ***L^{pytBr}*** in $CDCl_3$ at 298 K.

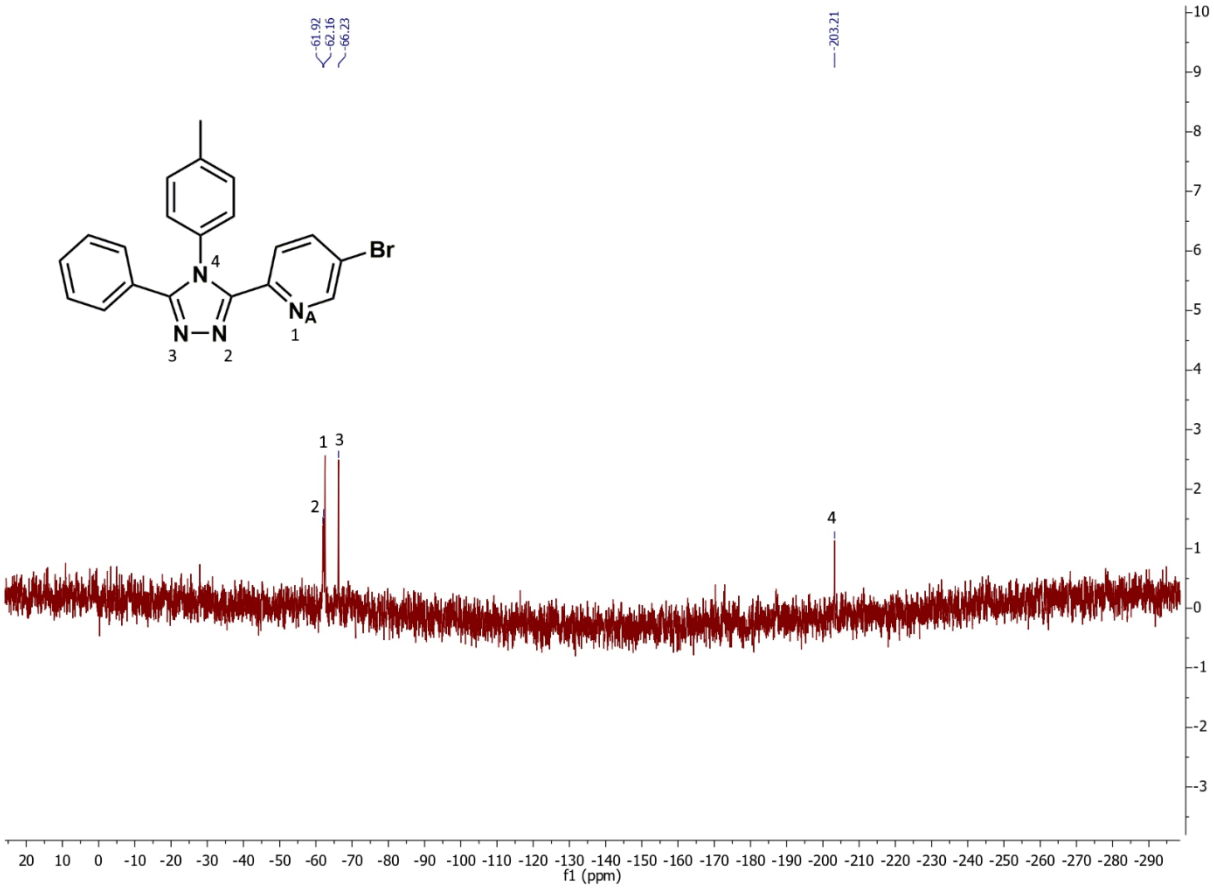

Figure S19. The full range ^{15}N NMR spectrum (direct measurement) of ligand ***L*^{pytBr}** in $CDCl_3$ at 298 K.

Mass Spectrum

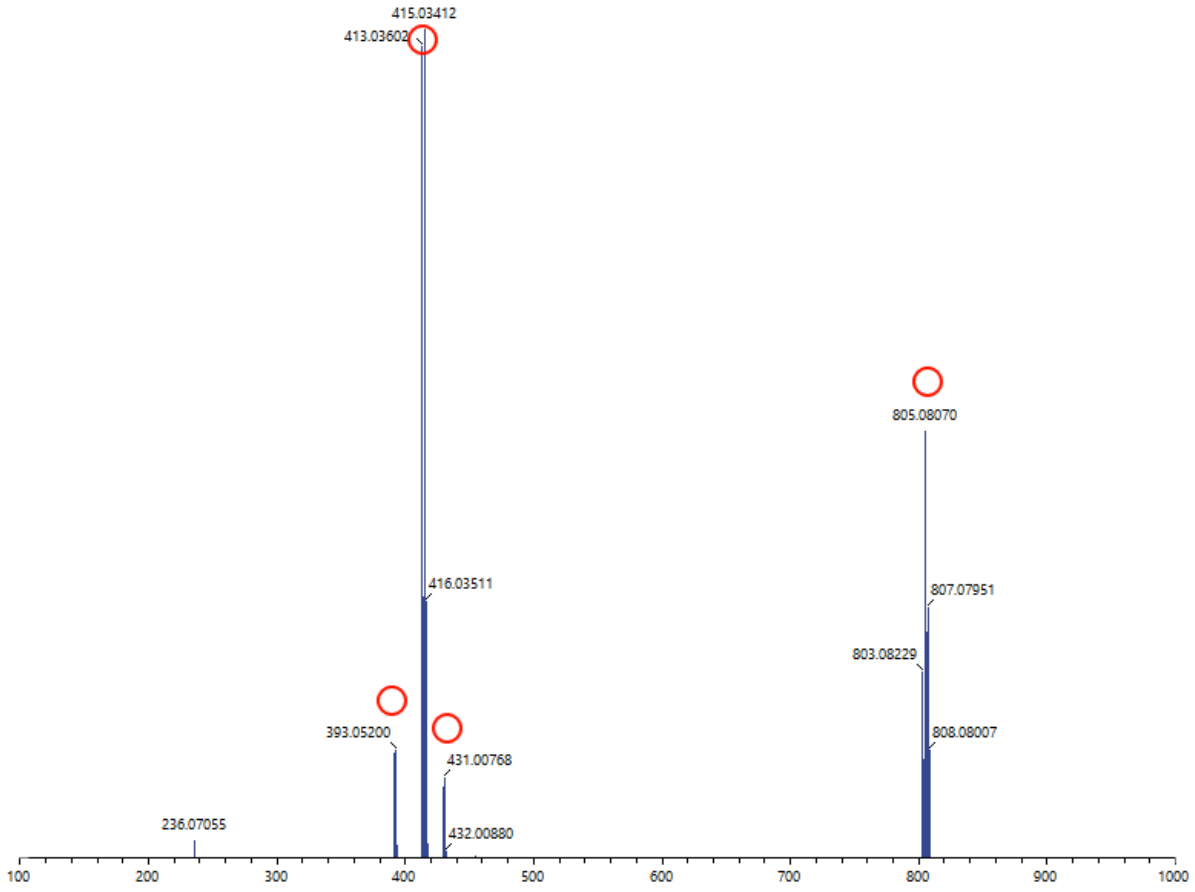

Figure S20. Complete mass spectrum of L^{pytBr}. Reported circles refer to zoomed regions reported below.

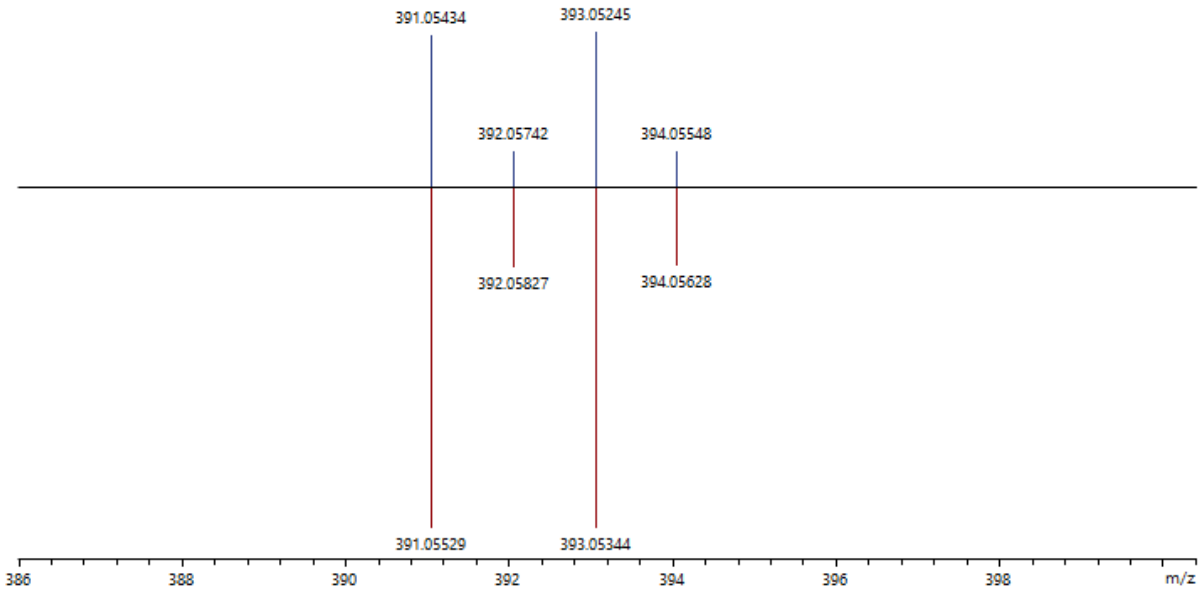

Figure S21. Fit of a peak in the mass spectrum of $[L^{pytBr}+H]^+$ experimental (blue) and simulated pattern (red).

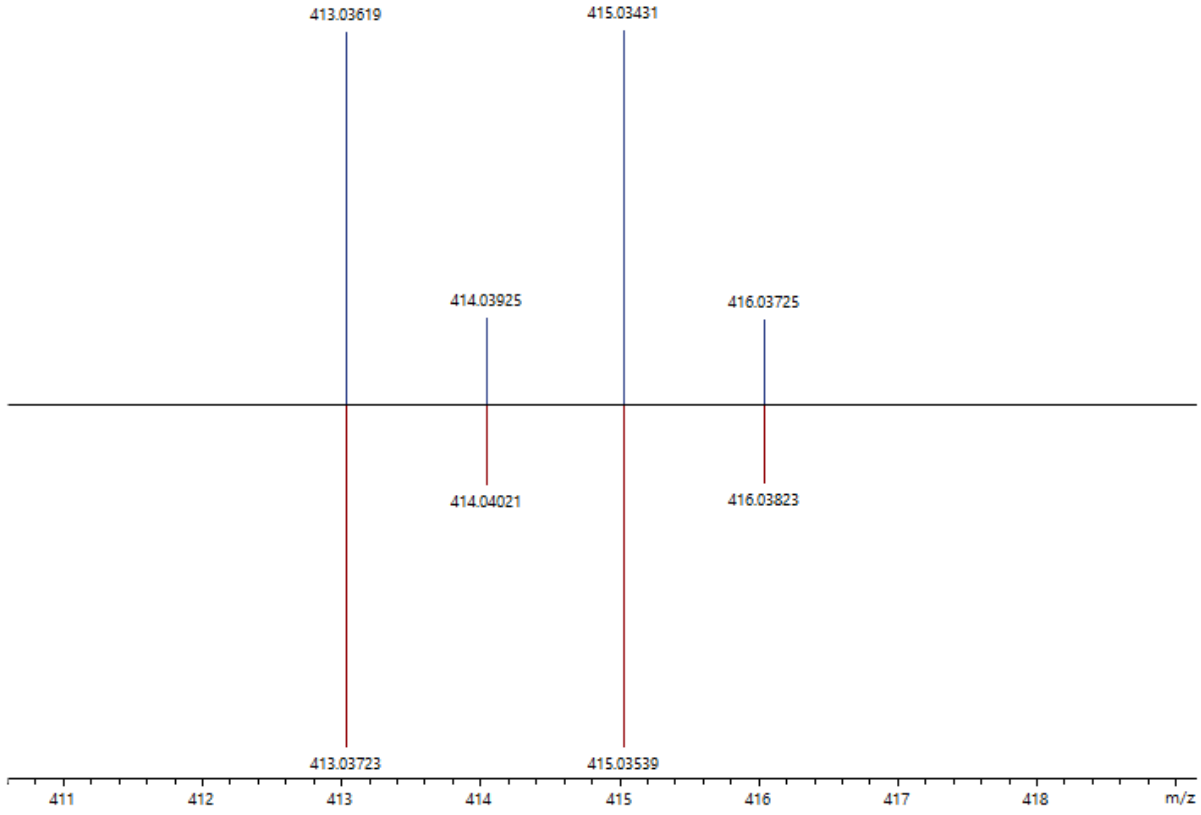

Figure S22. Fit of a peak in the mass spectrum of $[L^{pytBr}+Na]^+$ experimental (blue) and simulated pattern (red).

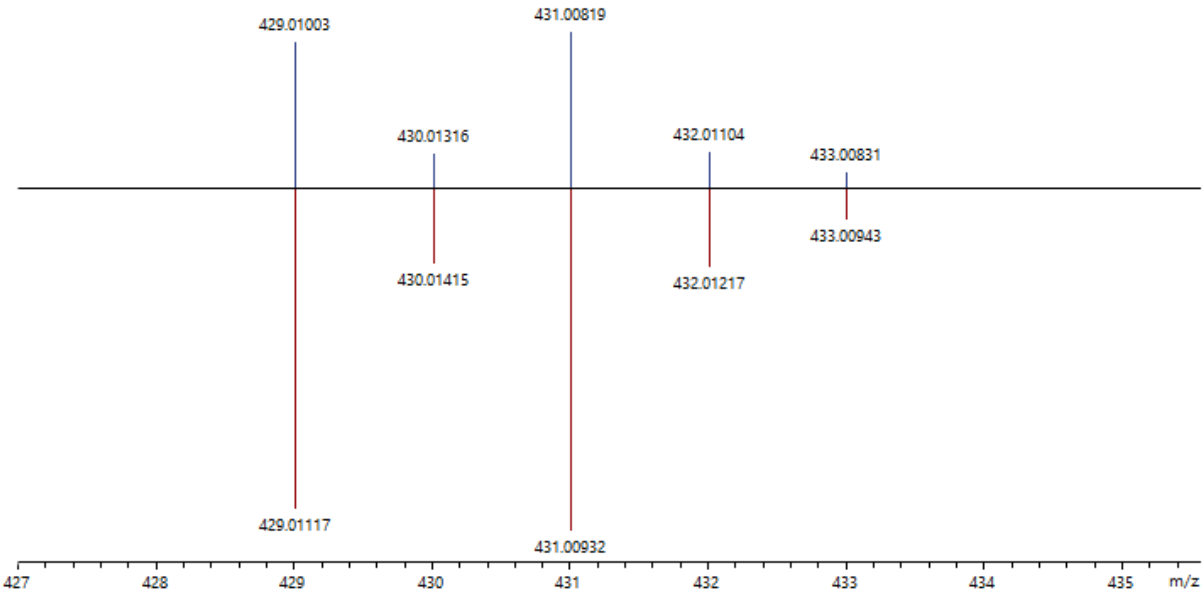

Figure S23. Fit of a peak in the mass spectrum of $[L^{pytBr}+K]^+$ experimental (blue) and simulated pattern (red).

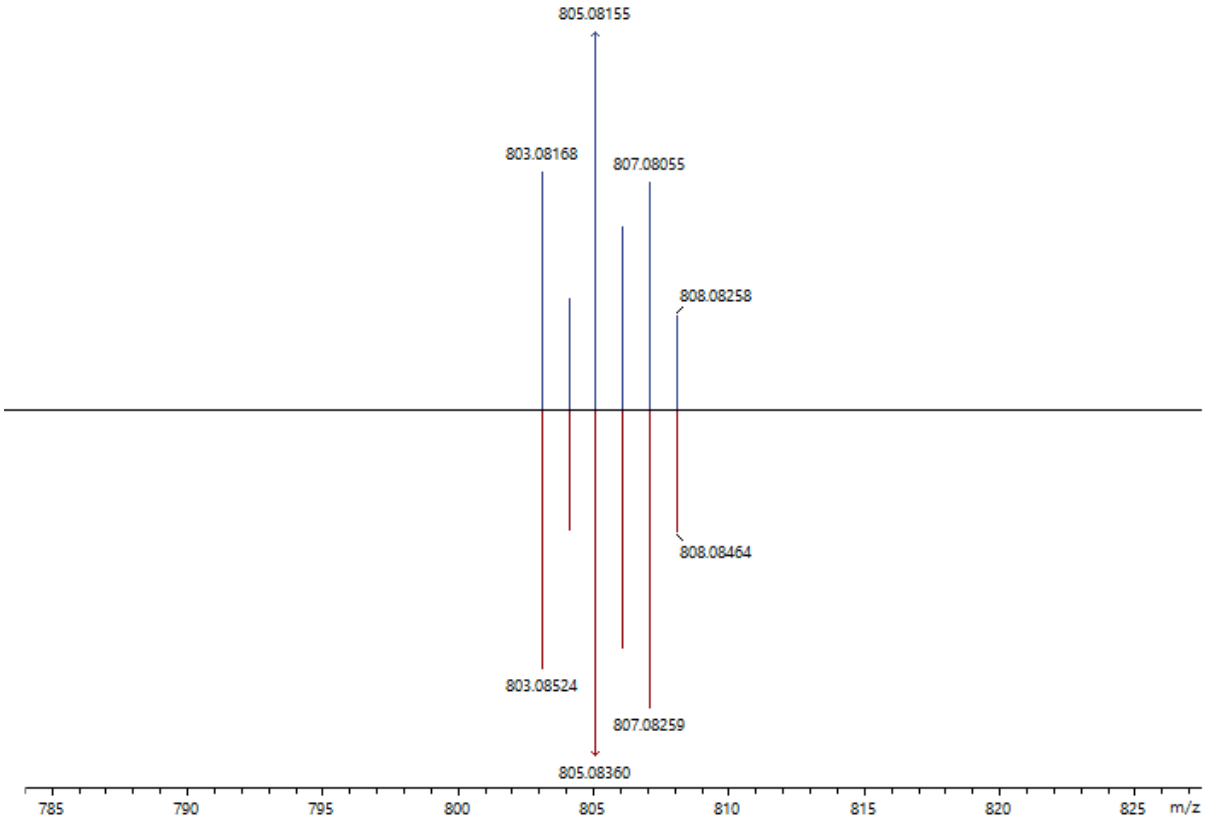

Figure S24 Fit of a peak in the mass spectrum of $[(L^{pytMe})_2+Na]^+$ experimental (blue) and simulated pattern (red).

S1.6. MS Figures for [Fe(L^{pytBr})$_2$(NCBH$_3$)$_2$] Complex

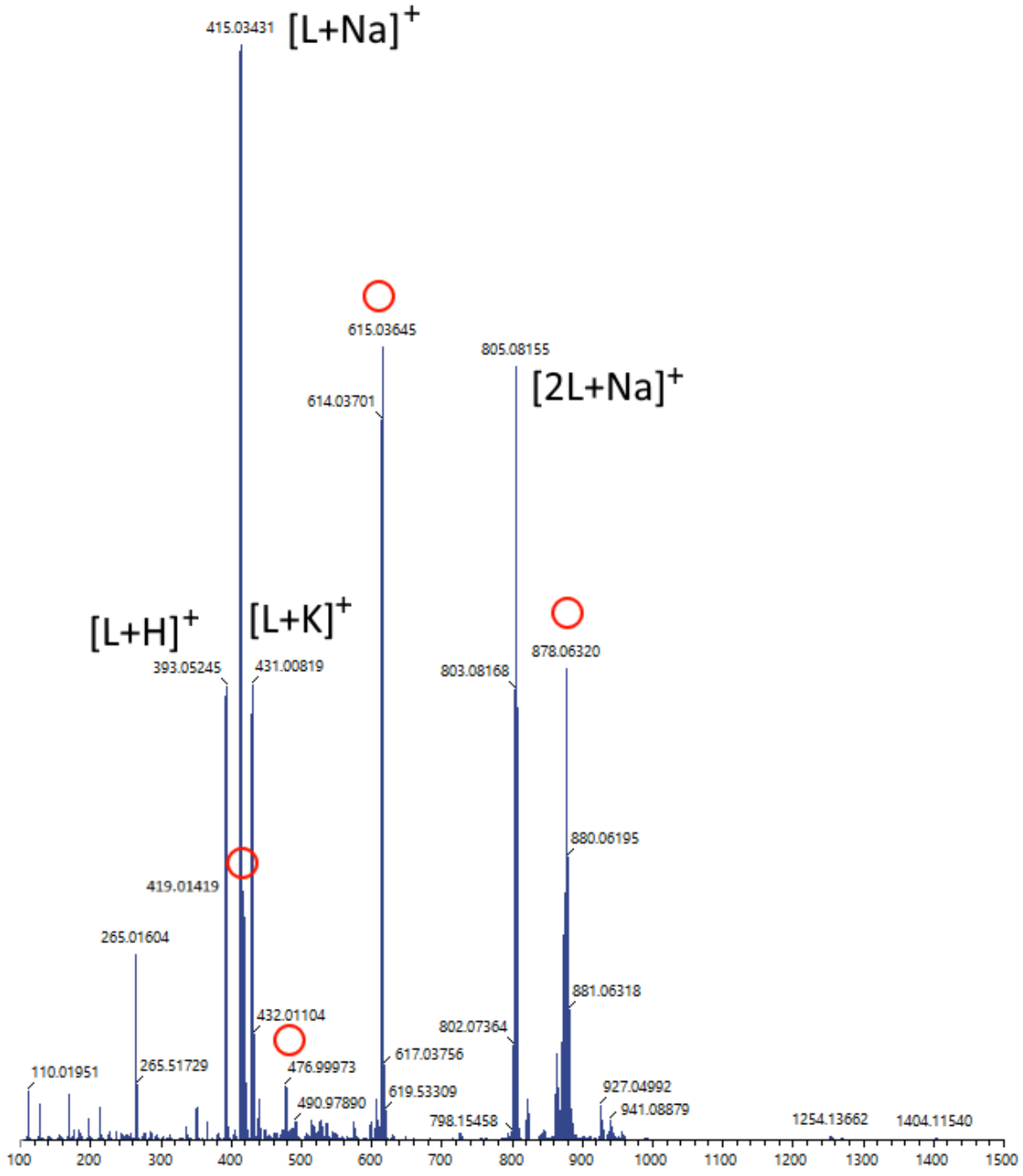

Figure S25. Complete mass spectrum of Fe(L^{pytBr})$_2$(NCBH$_3$)$_2$ Reported circles refer to zoomed regions reported below.

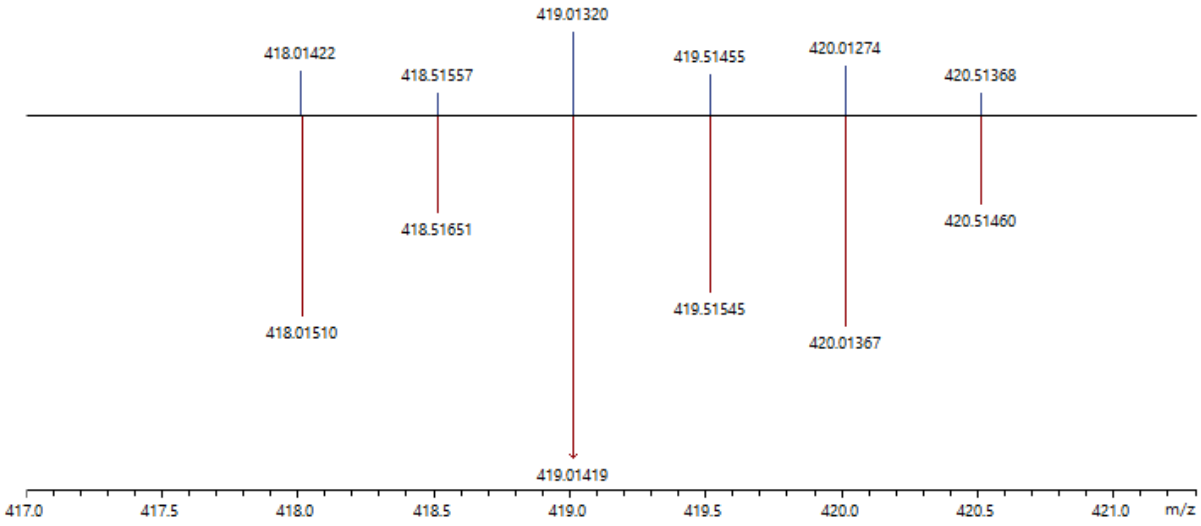

Figure S26. Fit of a peak in the mass spectrum of ***[Fe(L^{pytBr})$_2$]$^{2+}$*** experimental (blue) and simulated pattern (red).

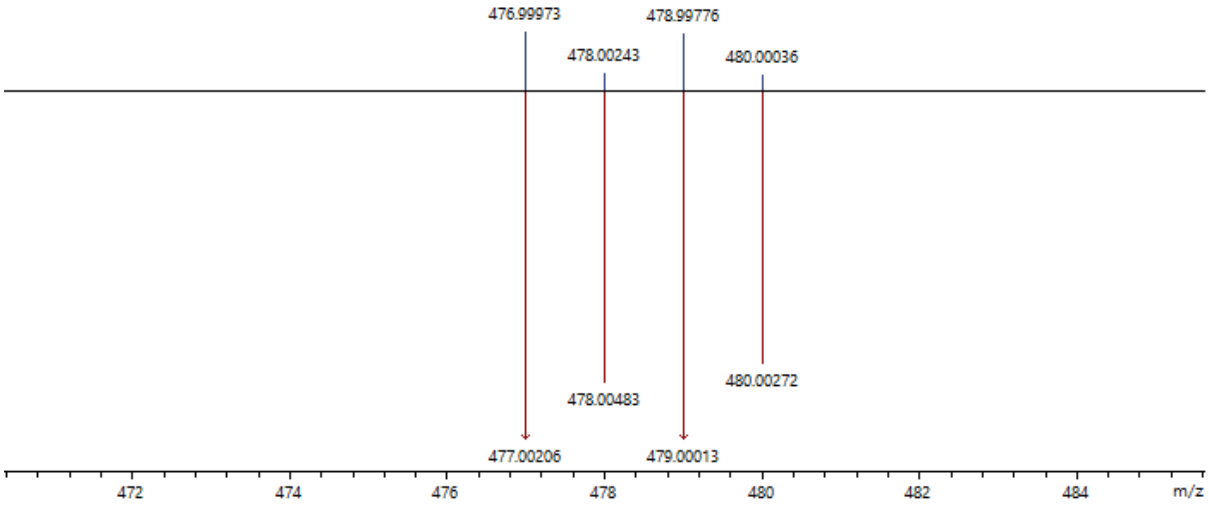

Figure S27. Fit of a peak in the mass spectrum of ***[Fe(L^{pytBr})(MeOH)-H]$^{+}$*** experimental (blue) and simulated pattern (red).

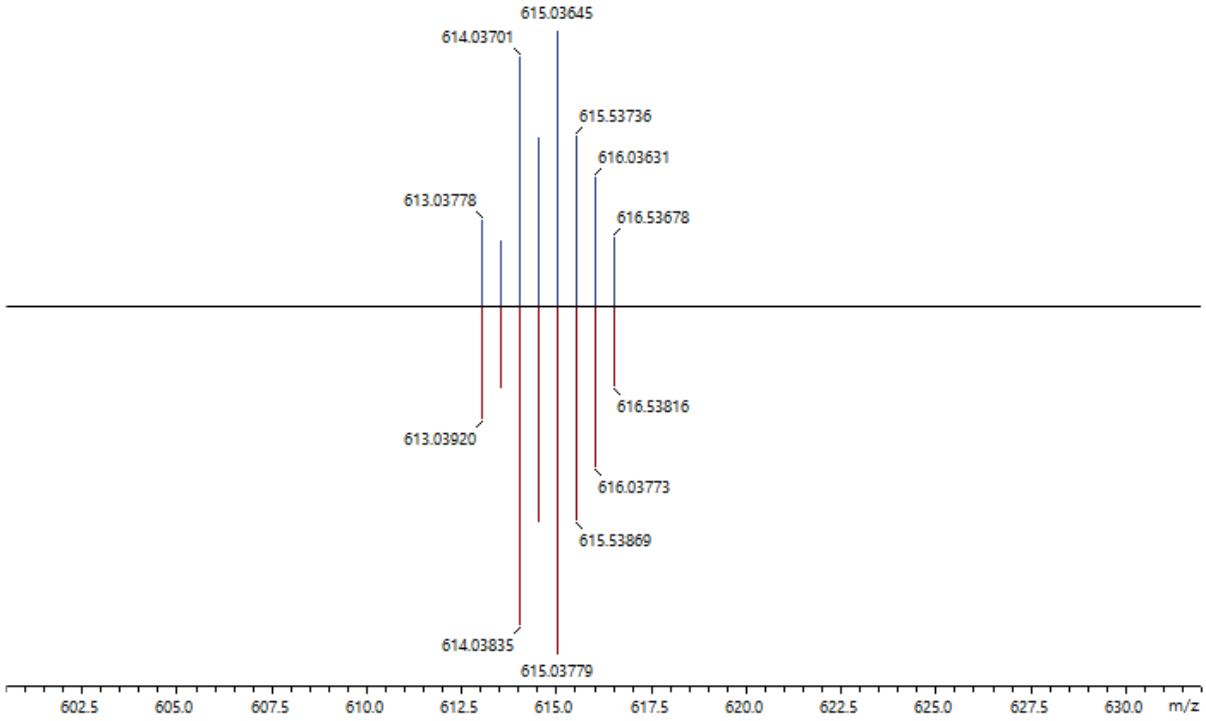

Figure S28. Fit of a peak in the mass spectrum of ***[Fe(L^{pytBr})$_3$]$^{2+}$*** experimental (blue) and simulated pattern (red).

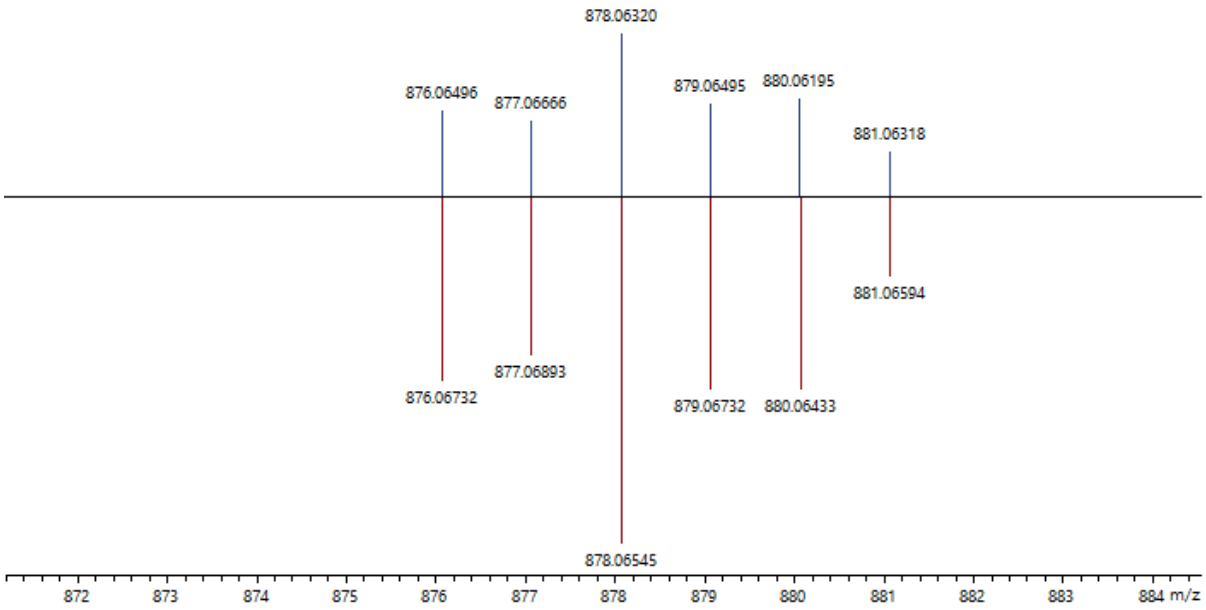

Figure S29. Fit of a peak in the mass spectrum of ***[Fe(L^{pytBr})$_2$(NCBH$_3$)]$^{+}$*** experimental (blue) and simulated pattern (red).

S1.7. NMR and MS Figures for L^{pytF} Ligand

^{1}H-NMR Spectrum

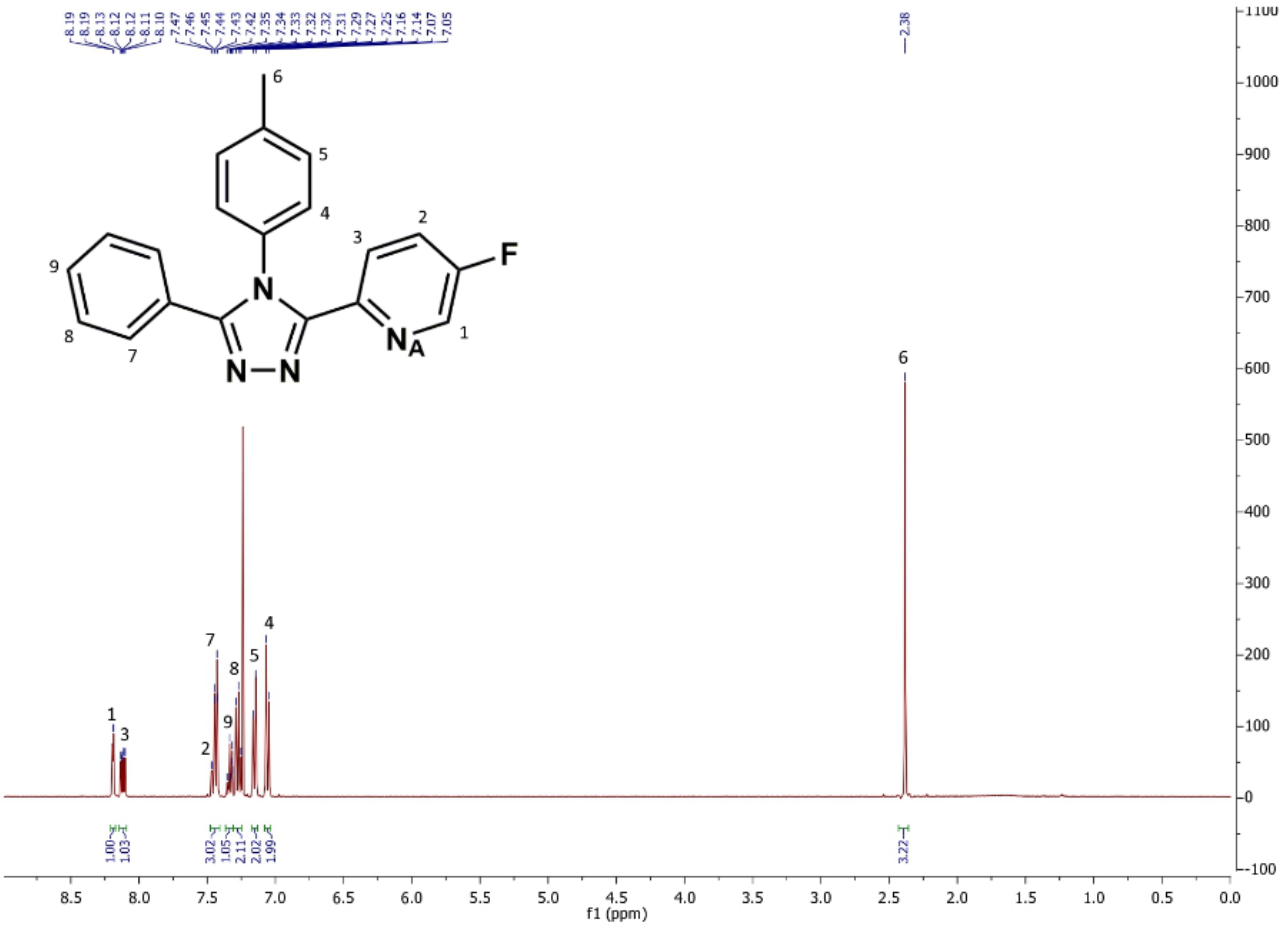

Figure S30. The full range ^{1}H NMR spectrum of ligand L^{pytF} in $CDCl_3$ at 298 K.

^{13}C-NMR Spectrum

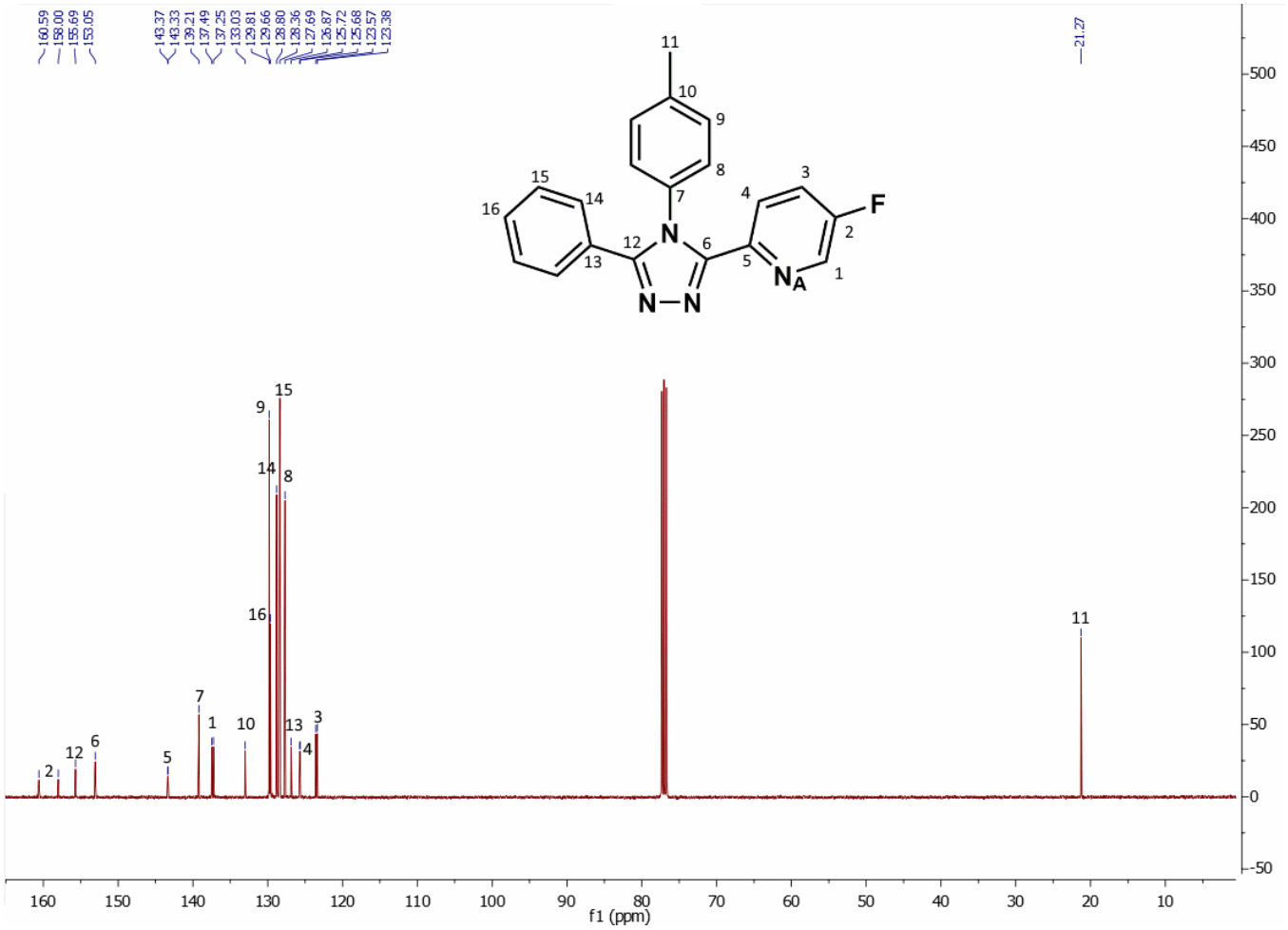

Figure S31. The full range ^{13}C NMR spectrum of ligand ***L^{pytF}*** in $CDCl_3$ at 298 K.

HSQCAD Spectrum

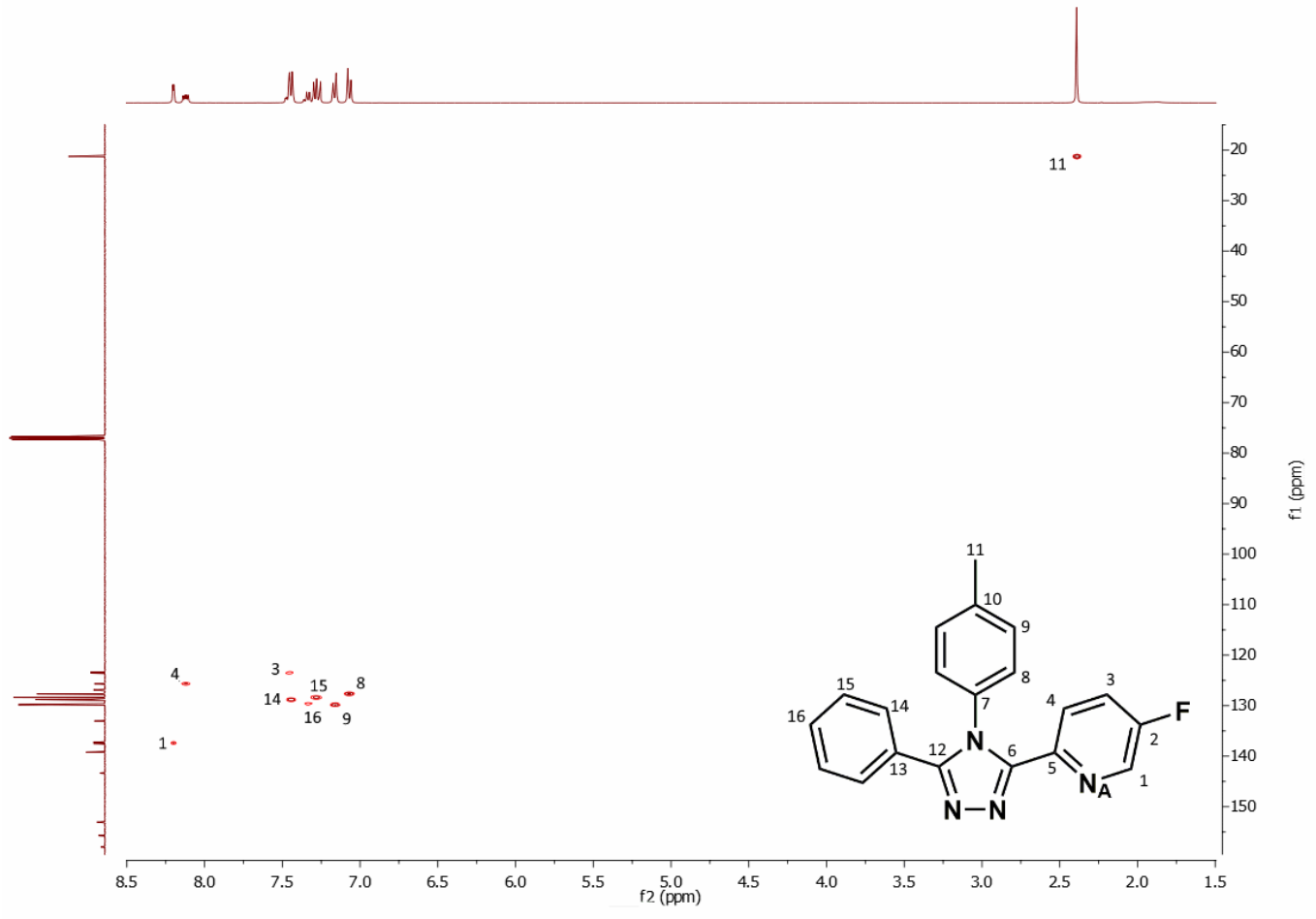

Figure S32. Heteronuclear ^{1}H-^{13}C NMR spectrum of ligand ***L^{pytF}*** in $CDCl_3$ at 298 K.

^{15}N-NMR Spectrum

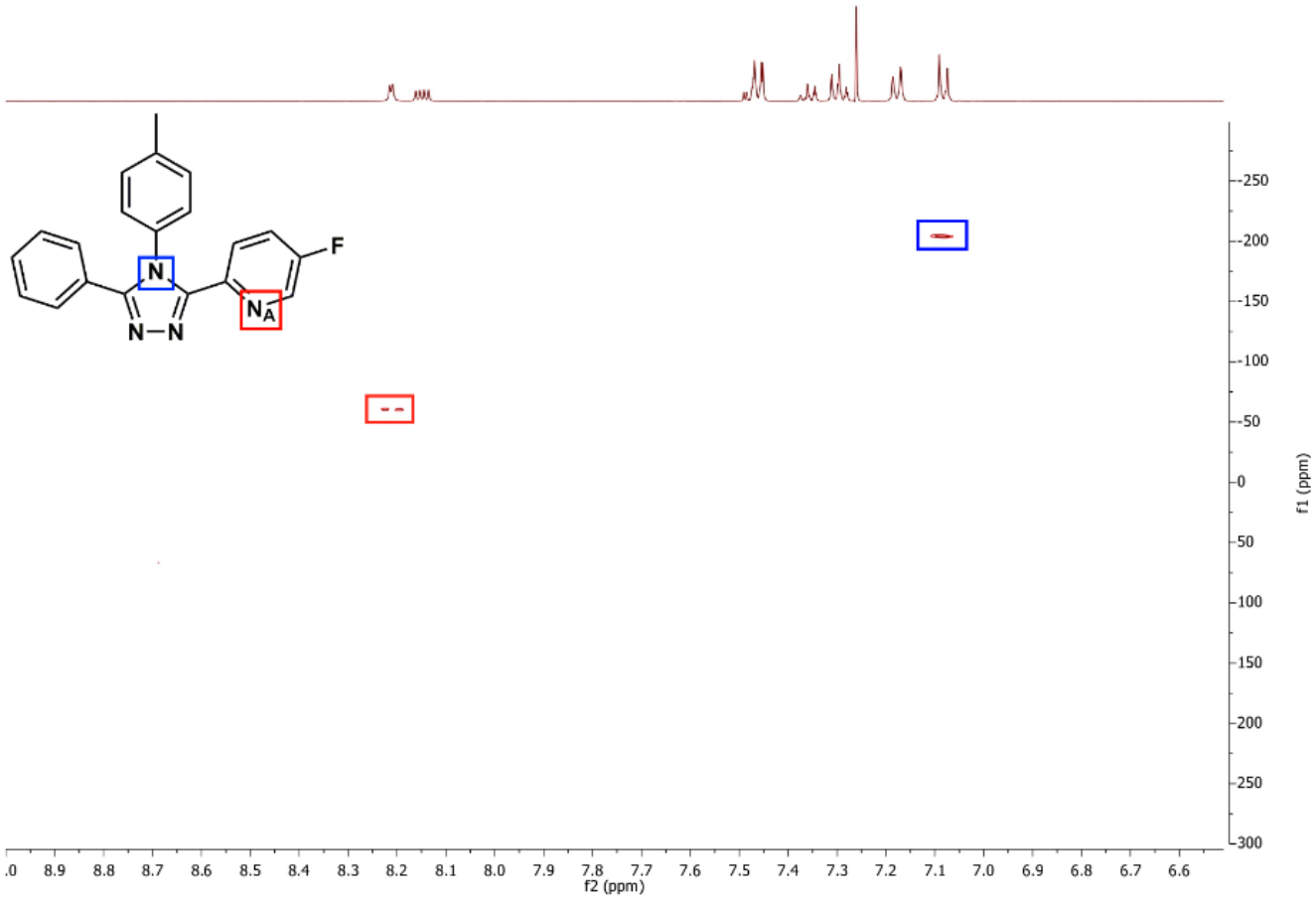

Figure S5. The full range CIGARD ^{1}H-^{15}N NMR spectrum (indirect measurement) of ligand ***L^{pytF}*** in $CDCl_3$ at 298 K.

Mass Spectrum

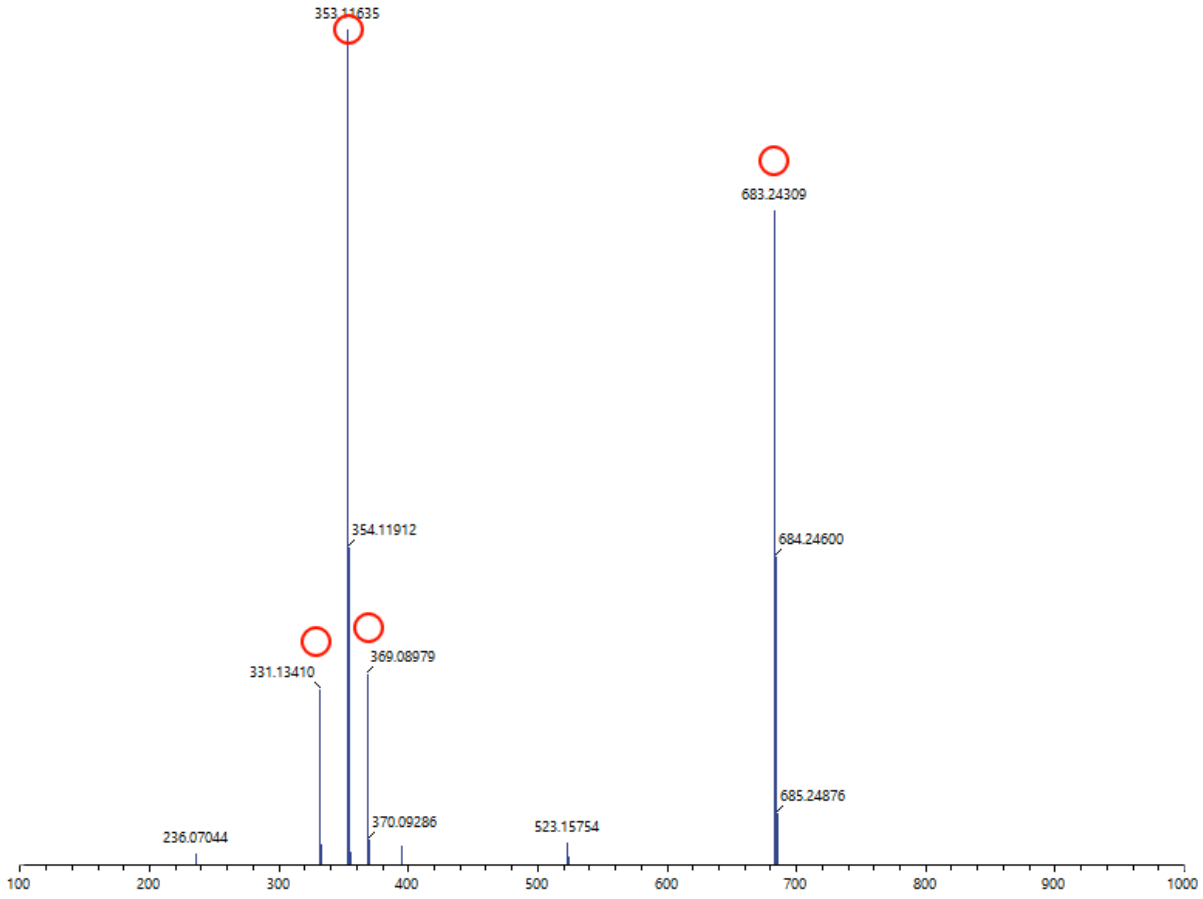

Figure S6. Complete mass spectrum of L^{pytF}. Reported circles refer to zoomed regions reported below.

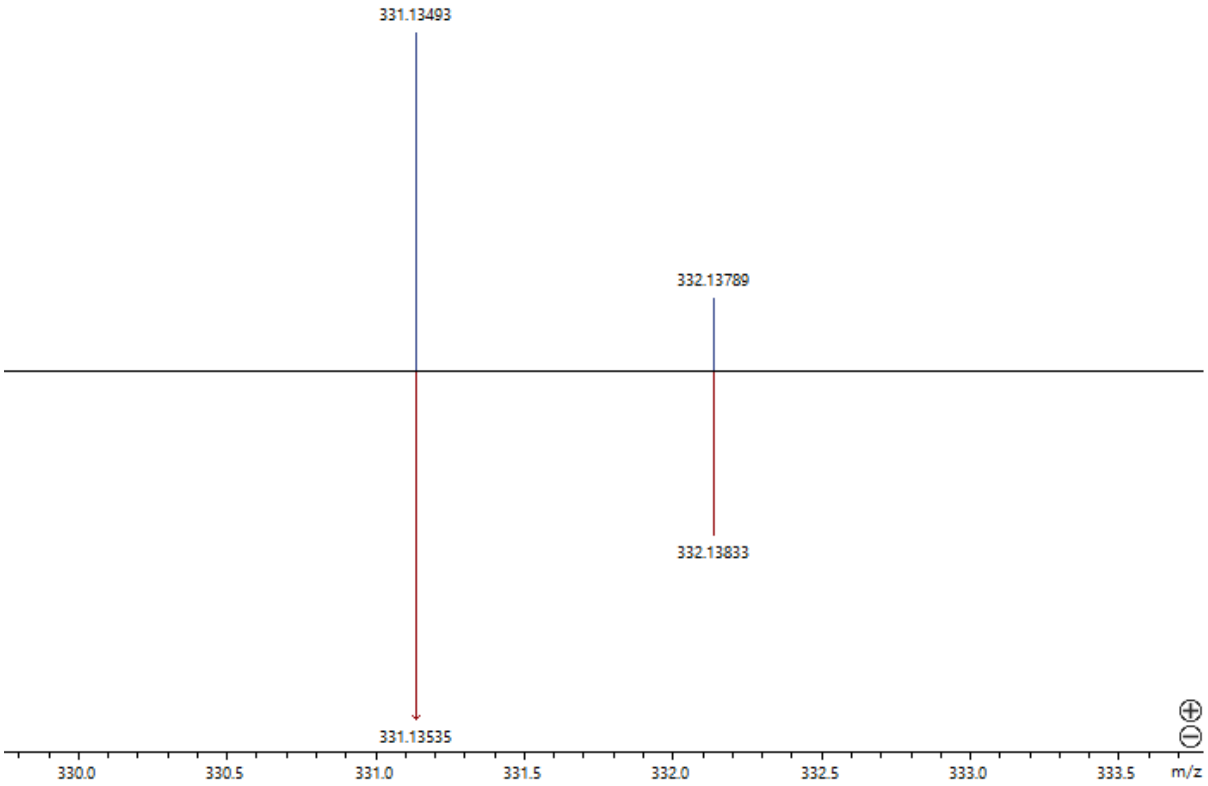

Figure S35. Fit of a peak in the mass spectrum of $[L^{pytF}+H]^+$ experimental (blue) and simulated pattern (red).

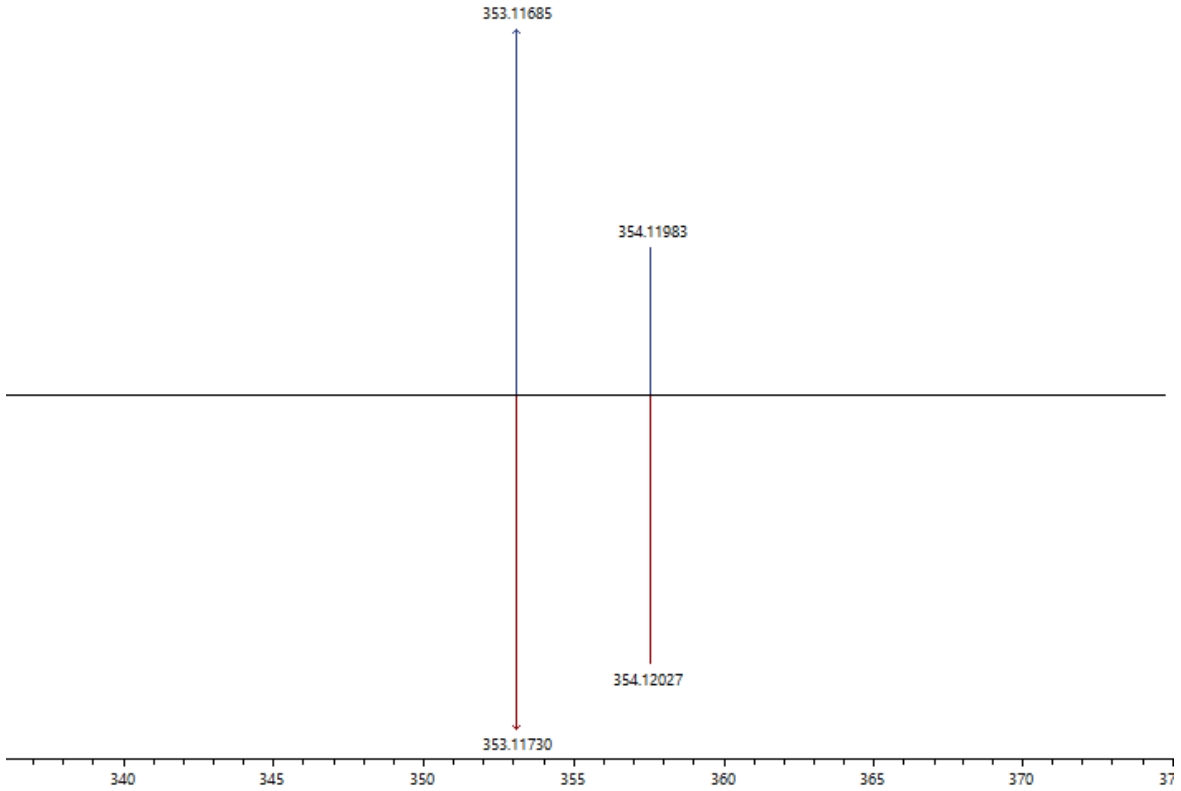

Figure S7. Fit of a peak in the mass spectrum of $[L^{pytF}+Na]^+$ experimental (blue) and simulated pattern (red).

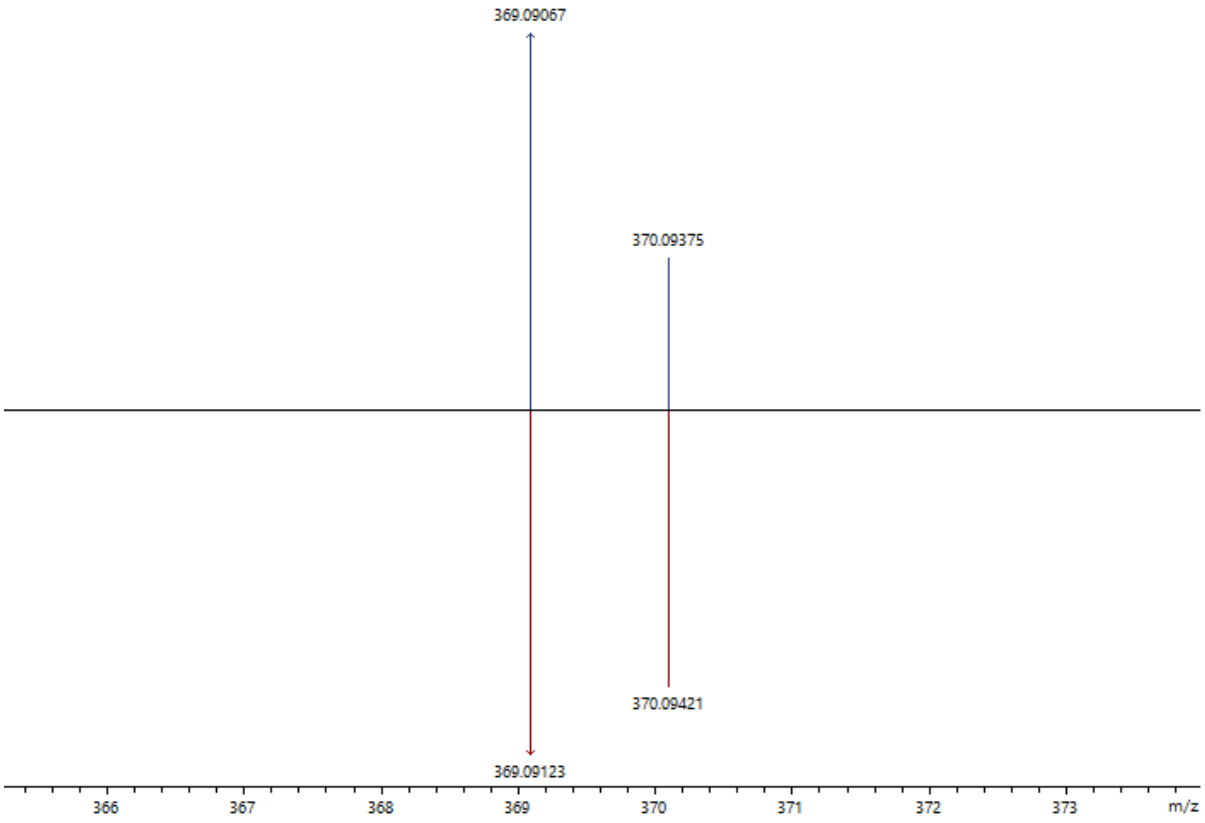

Figure S8. Fit of a peak in the mass spectrum of $[L^{pytF}+K]^+$ experimental (blue) and simulated pattern (red).

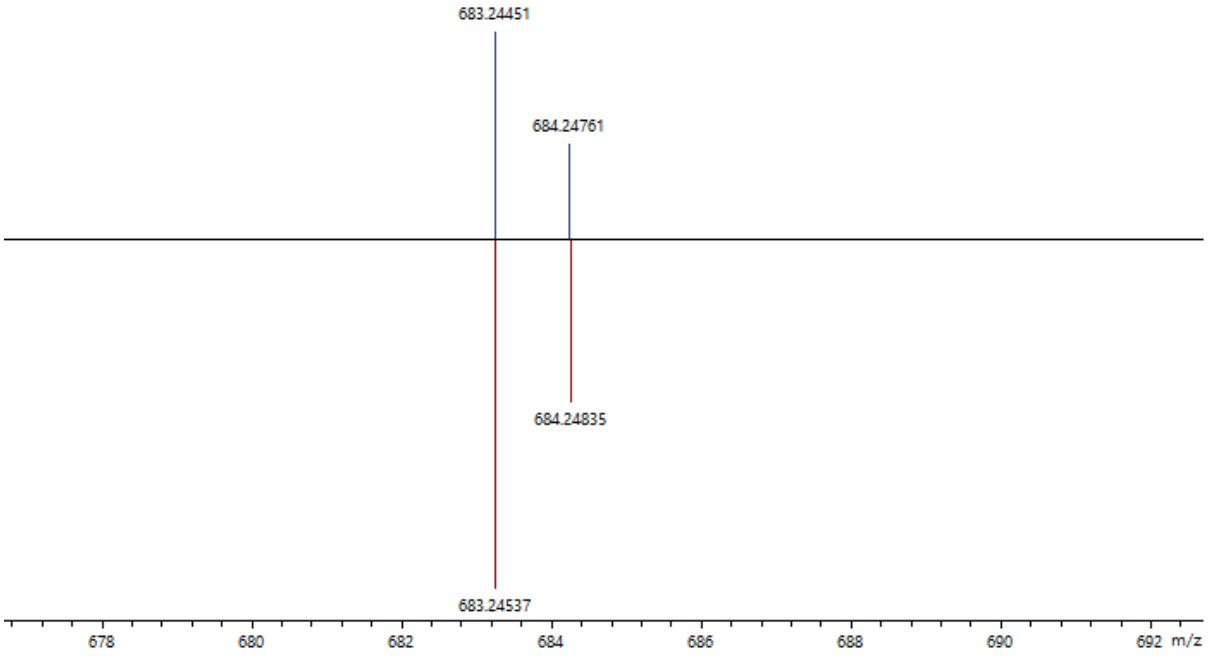

Figure S9. Fit of a peak in the mass spectrum of $[(L^{pytF})_2+Na]^+$ experimental (blue) and simulated pattern (red).

S1.8. MS Figures for [Fe($\boldsymbol{L}^{pytF}$)$_2$(NCBH$_3$)$_2$] Complex

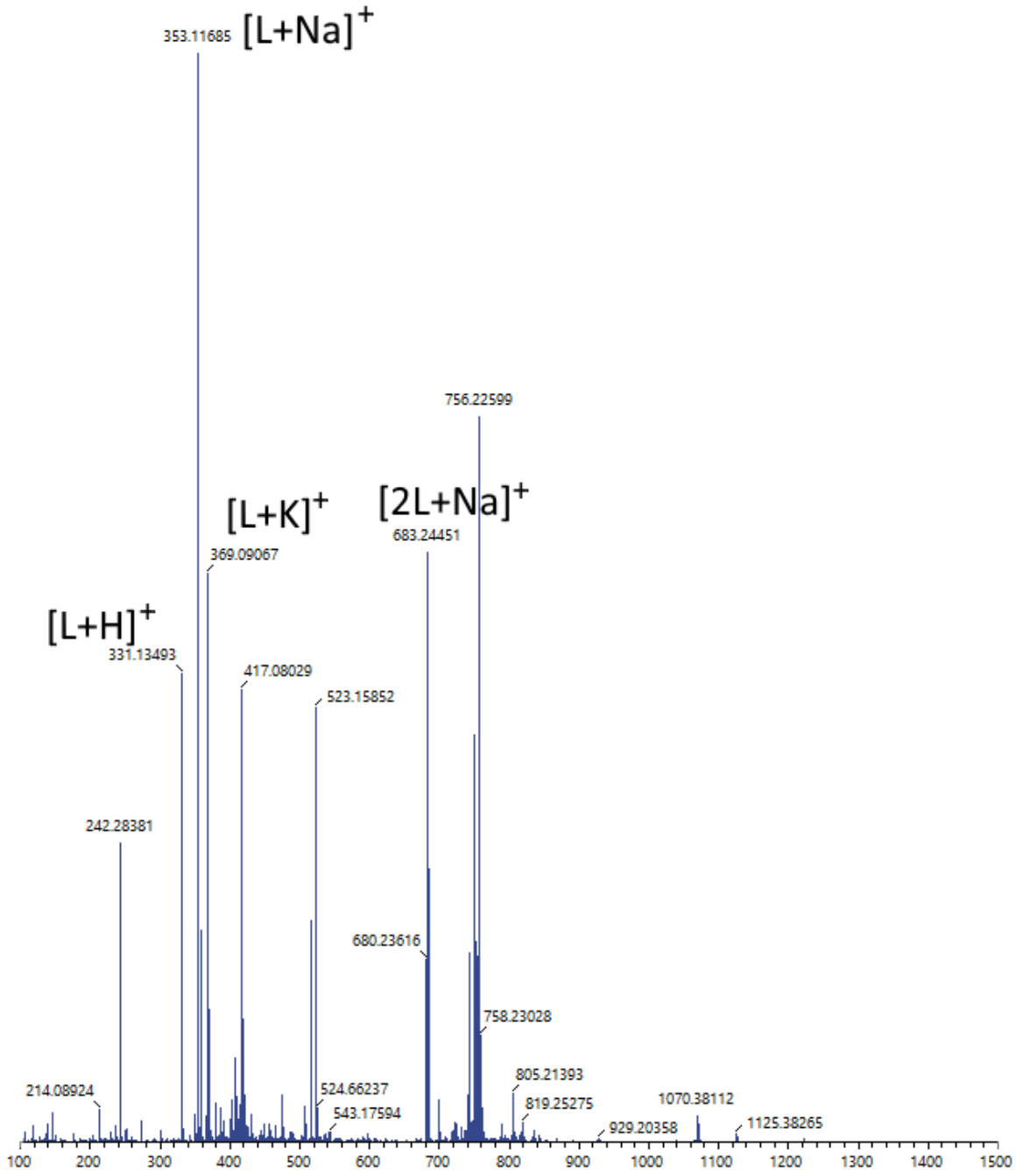

Figure S39. Complete mass spectrum of Fe($\boldsymbol{L}^{pytF}$)$_2$(NCBH$_3$)$_2$ Reported circles refer to zoomed regions reported below.

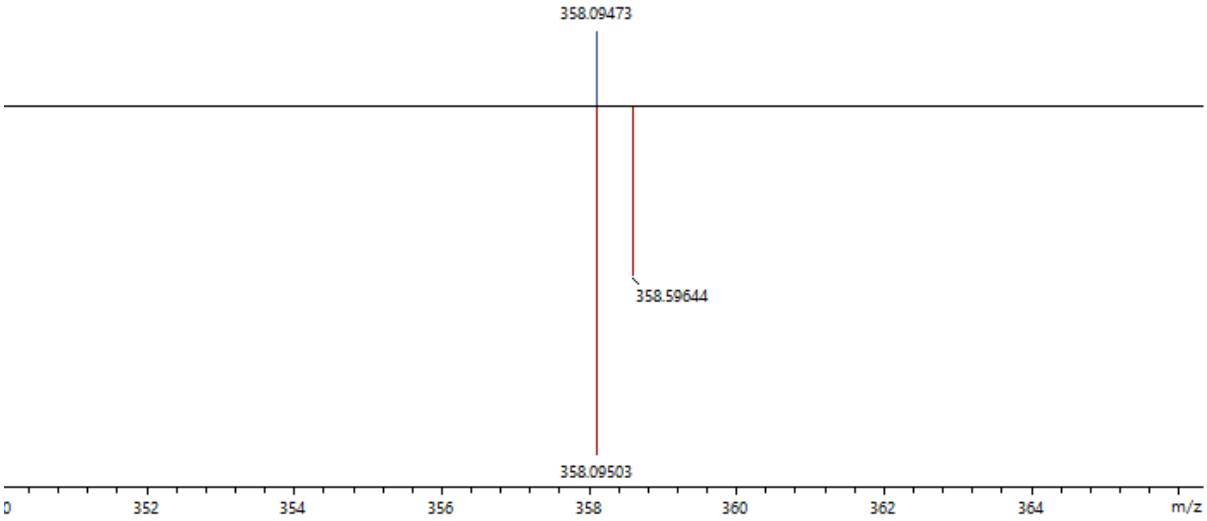

Figure S40. Fit of a peak in the mass spectrum of ***[Fe(L^{pytF})$_2$]$^{2+}$*** experimental (blue) and simulated pattern (red).

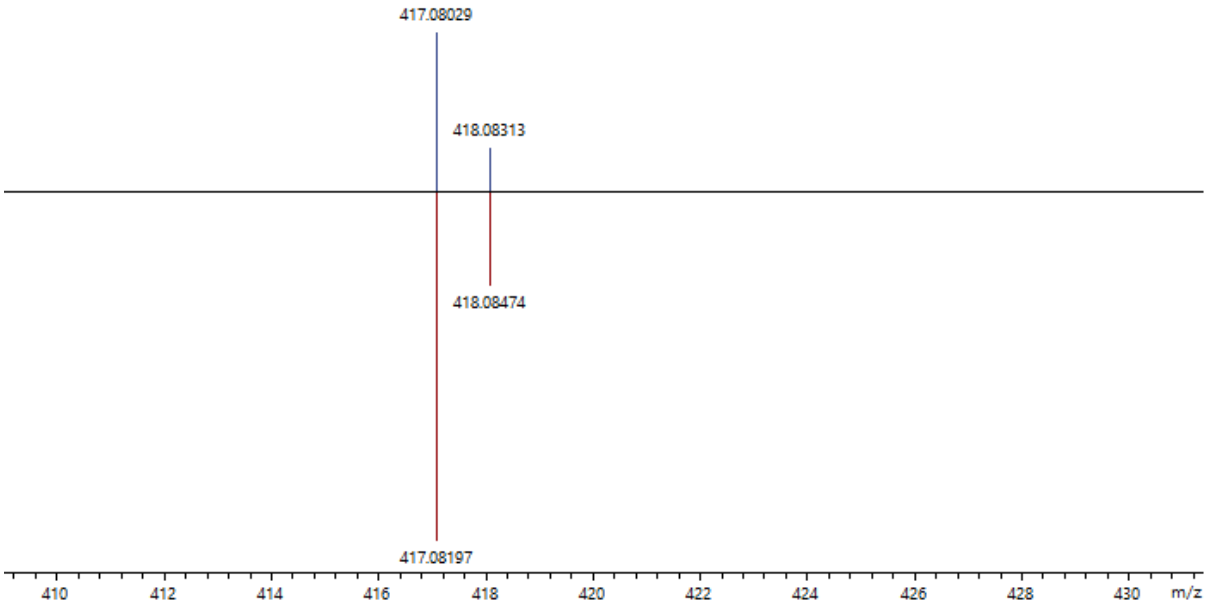

Figure S41. Fit of a peak in the mass spectrum of ***[Fe(L^{pytF})(MeOH)-H]$^{+}$*** experimental (blue) and simulated pattern (red).

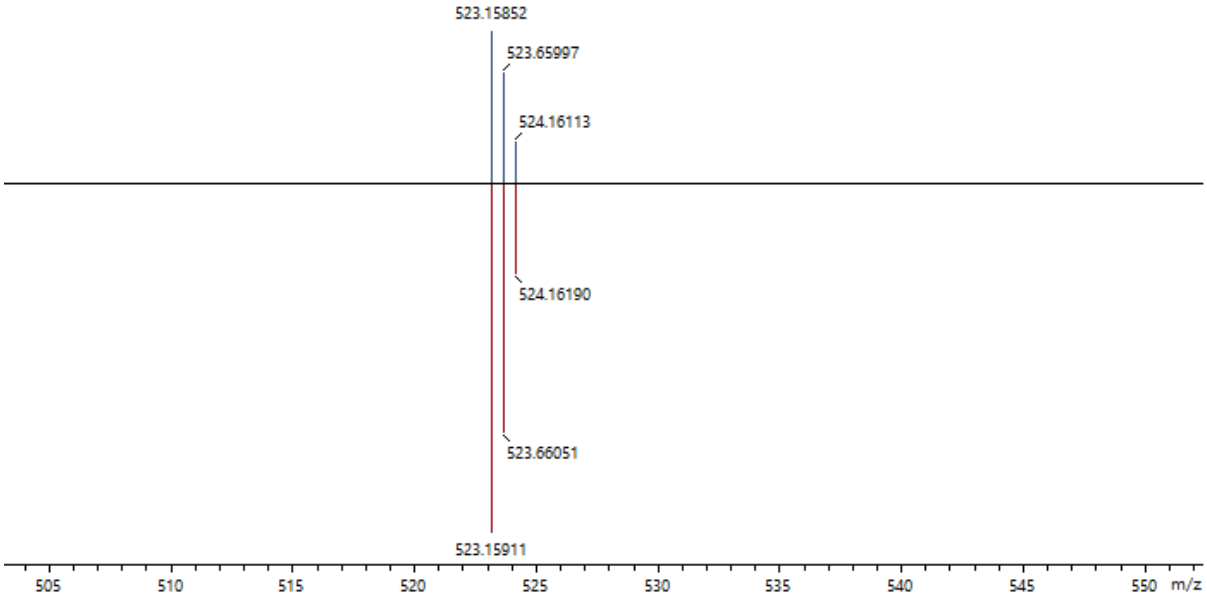

Figure S42. Fit of a peak in the mass spectrum of ***[Fe(L^{pytF})$_3$]$^{2+}$*** experimental (blue) and simulated pattern (red).

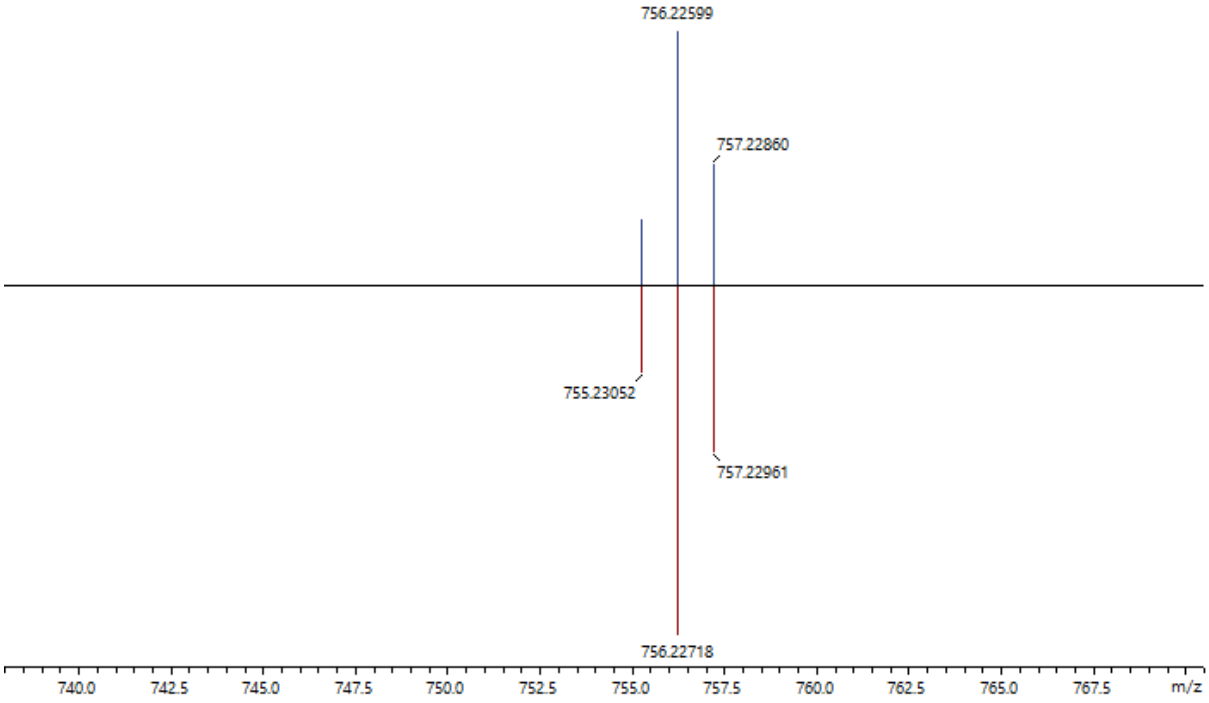

Figure S43. Fit of a peak in the mass spectrum of ***[Fe(L^{pytF})$_2$(NCBH$_3$)]$^{+}$*** experimental (blue) and simulated pattern (red).

S1.9. NMR and MS Figures for L^{pytMe} Ligand

^{1}H-NMR Spectrum

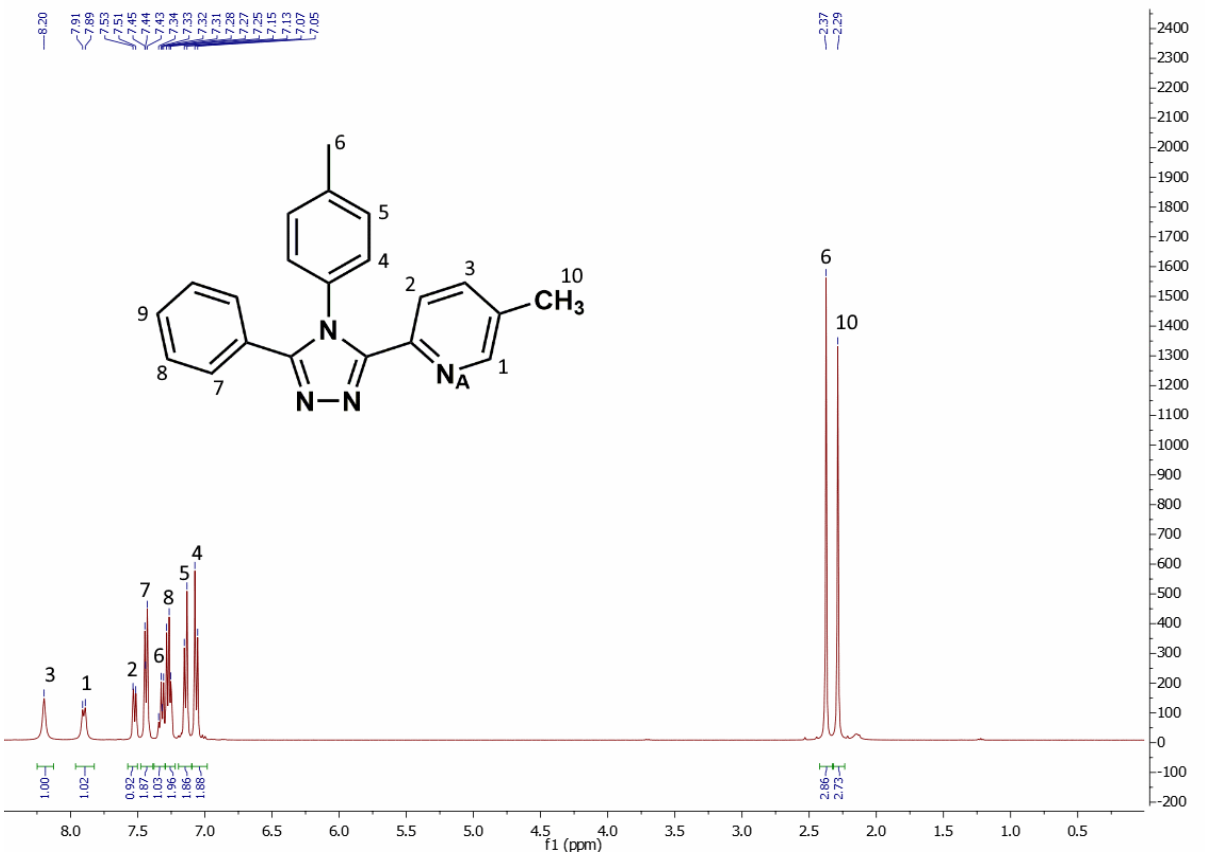

Figure S44. The full range ^{1}H NMR spectrum of ligand L^{pytMe} in $CDCl_3$ at 298 K.

^{13}C-NMR Spectrum

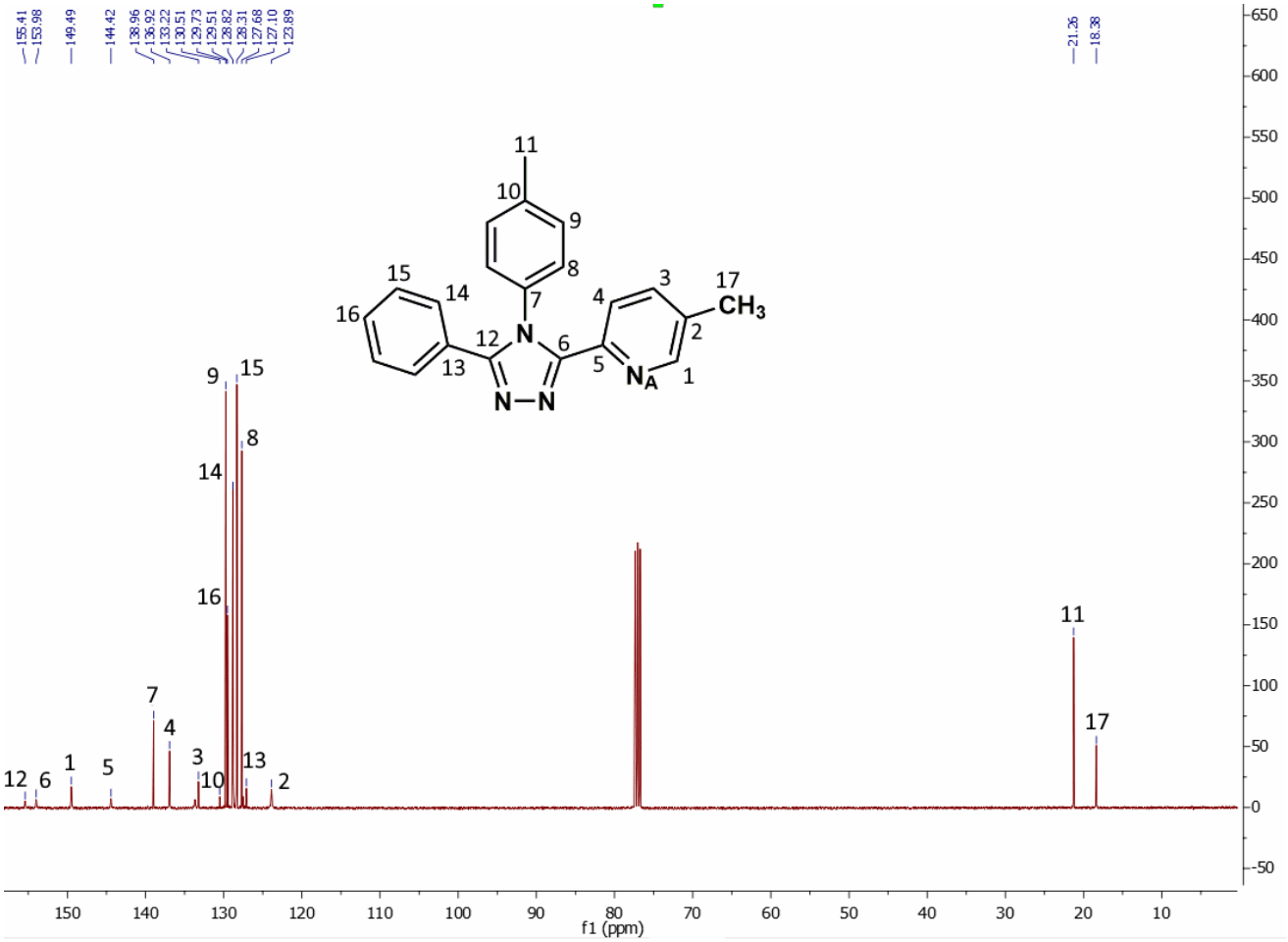

Figure S45. The full range ^{13}C NMR spectrum of ligand ***L^{pytMe}*** in $CDCl_3$ at 298 K.

HSQCAD Spectrum

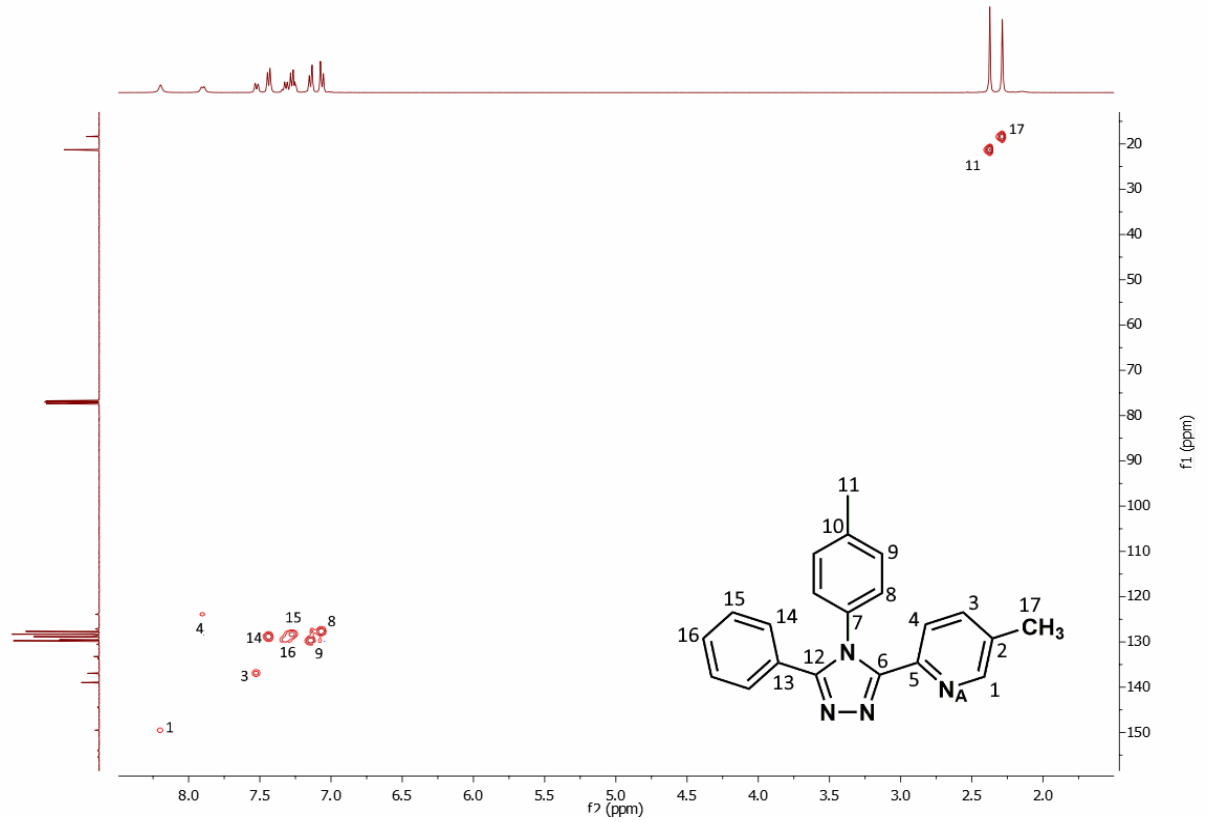

Figure S46. Heteronuclear ^{1}H-^{13}C NMR spectrum of ligand ***L*^{pytMe}** in $CDCl_3$ at 298 K.

^{15}N-NMR Spectrum

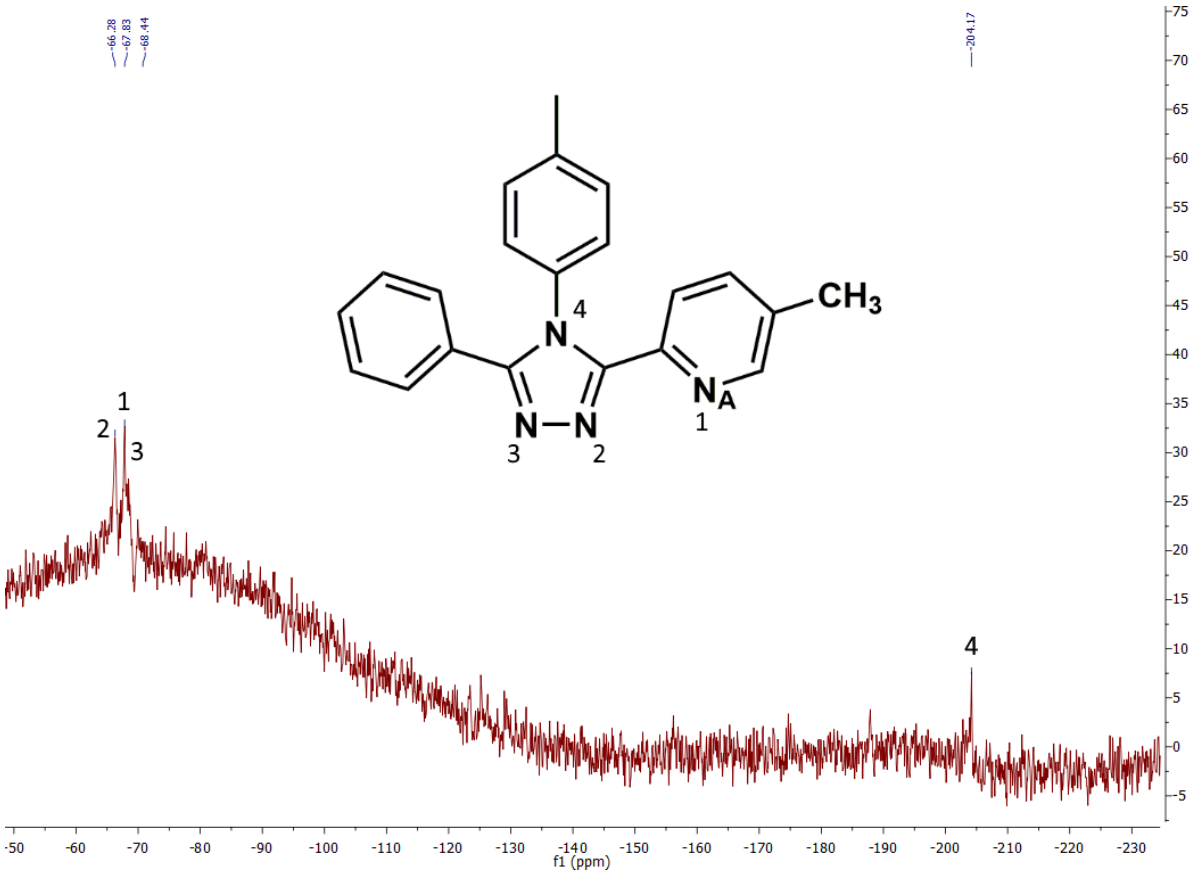

Figure S47. The full range ^{15}N NMR spectrum (direct measurement) of ligand ***L^{pytMe}*** in $CDCl_3$ at 298 K.

Mass Spectrum

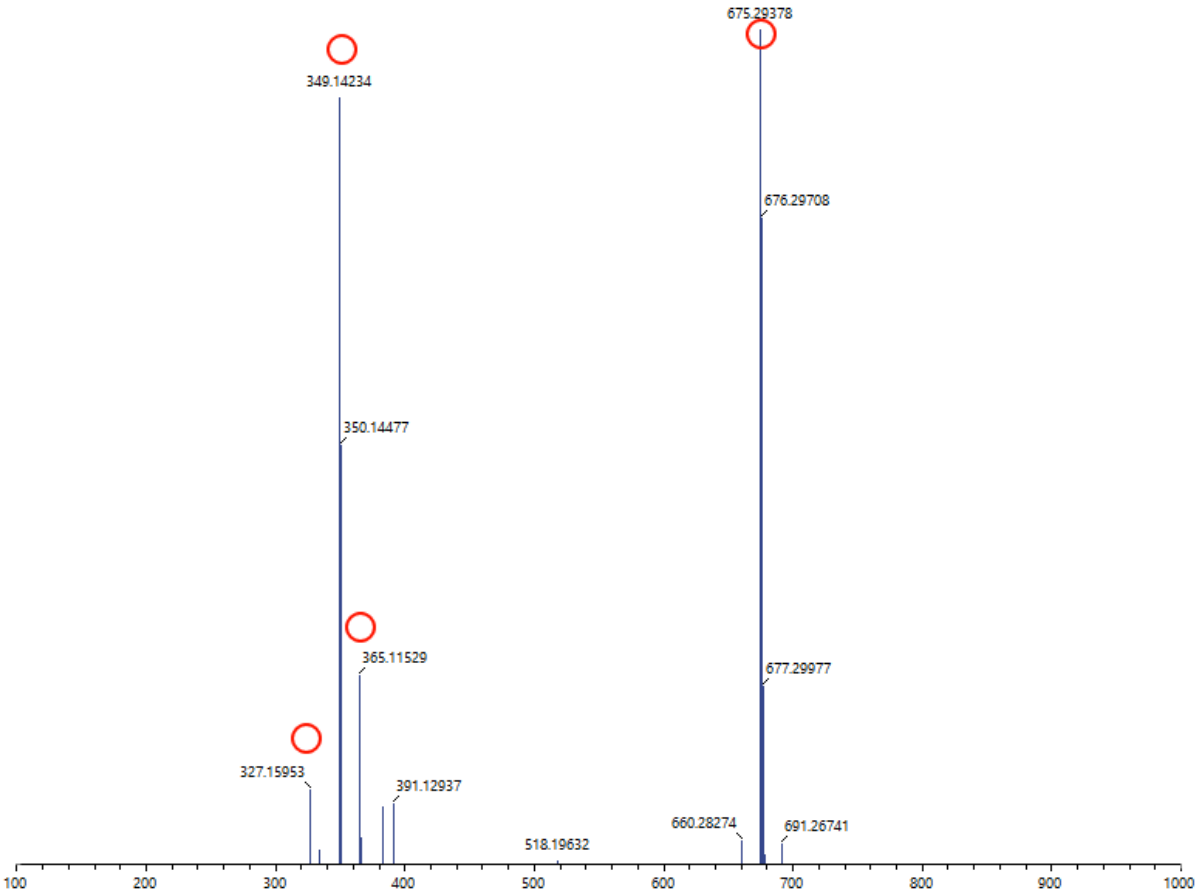

Figure S48. Complete mass spectrum of L^{pytMe}. Circled peaks are those reported and fitted in the following figures.

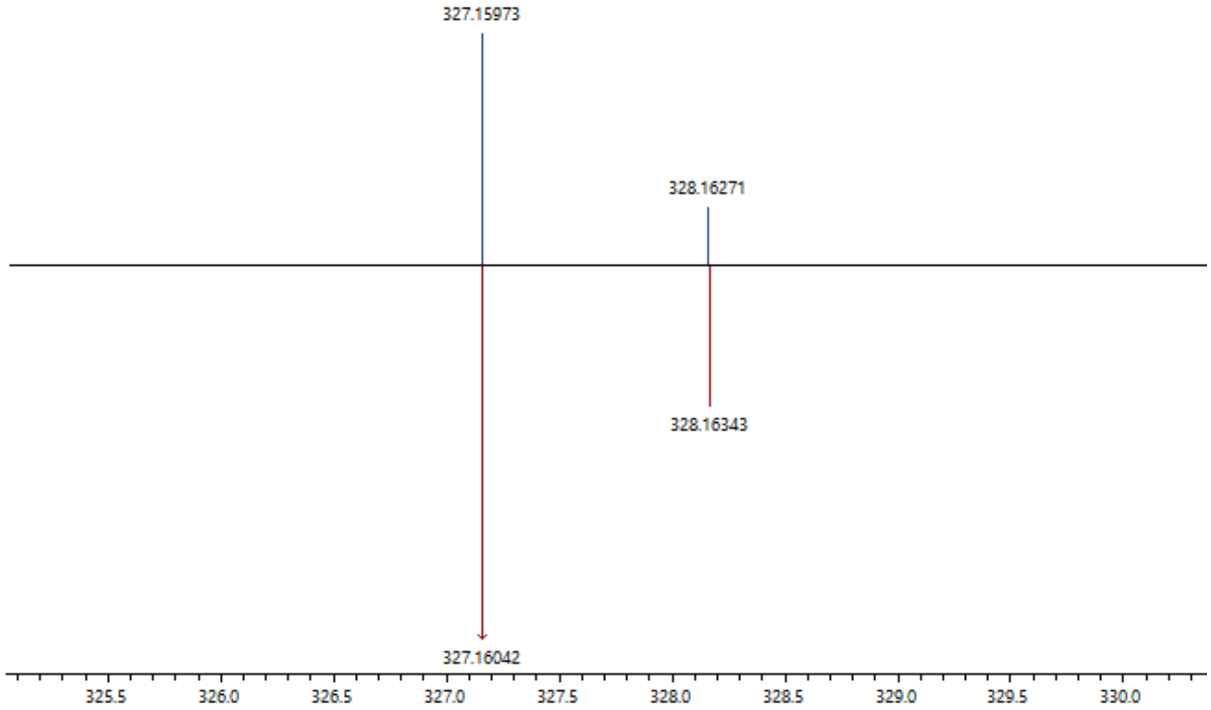

Figure S49. Fit of a peak in the mass spectrum of $[L^{pytMe}+H]^+$ experimental (blue) and simulated pattern (red).

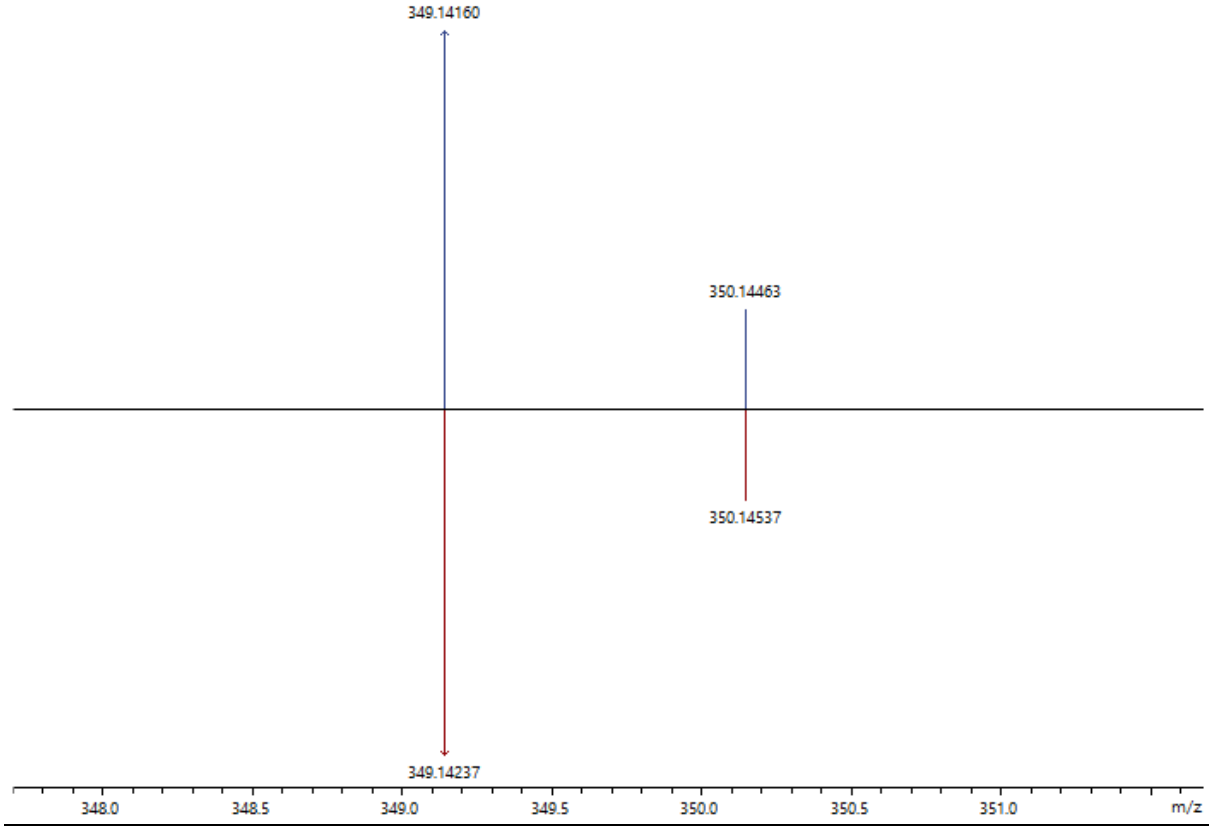

Figure S50. Fit of a peak in the mass spectrum of $[L^{pytMe}+Na]^+$ experimental (blue) and simulated pattern (red).

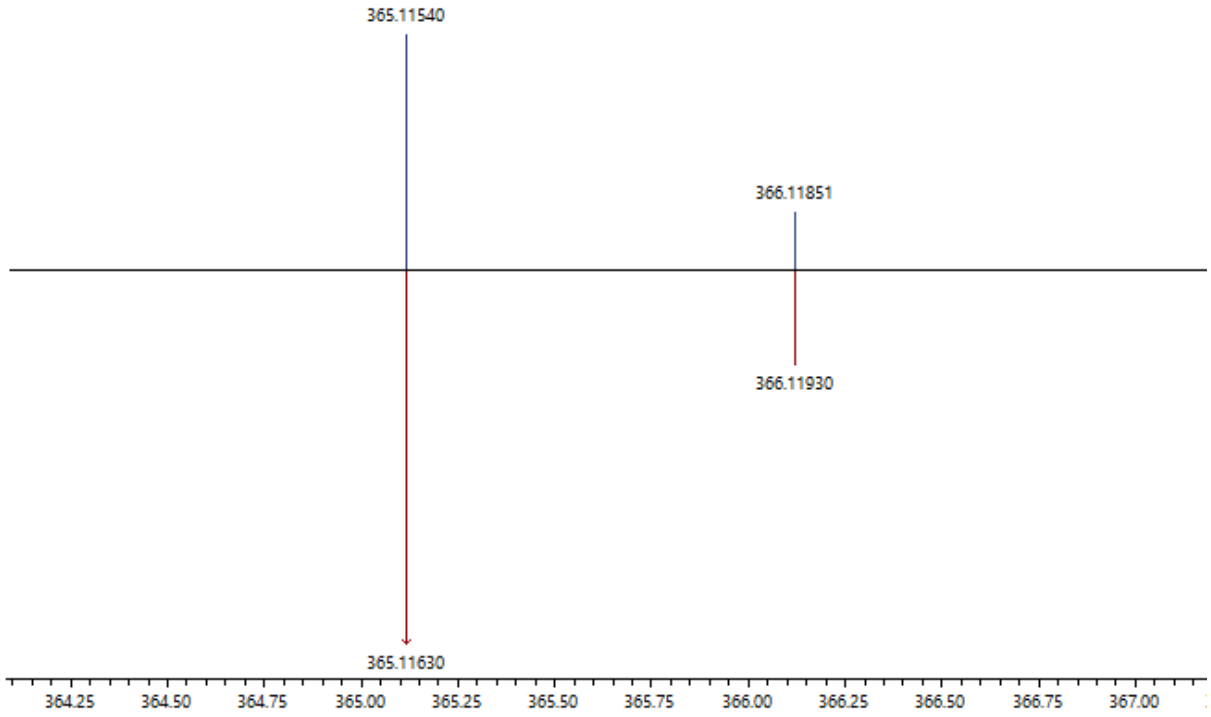

Figure S51. Fit of a peak in the mass spectrum of $[L^{pytMe}+K]^+$ experimental (blue) and simulated pattern (red).

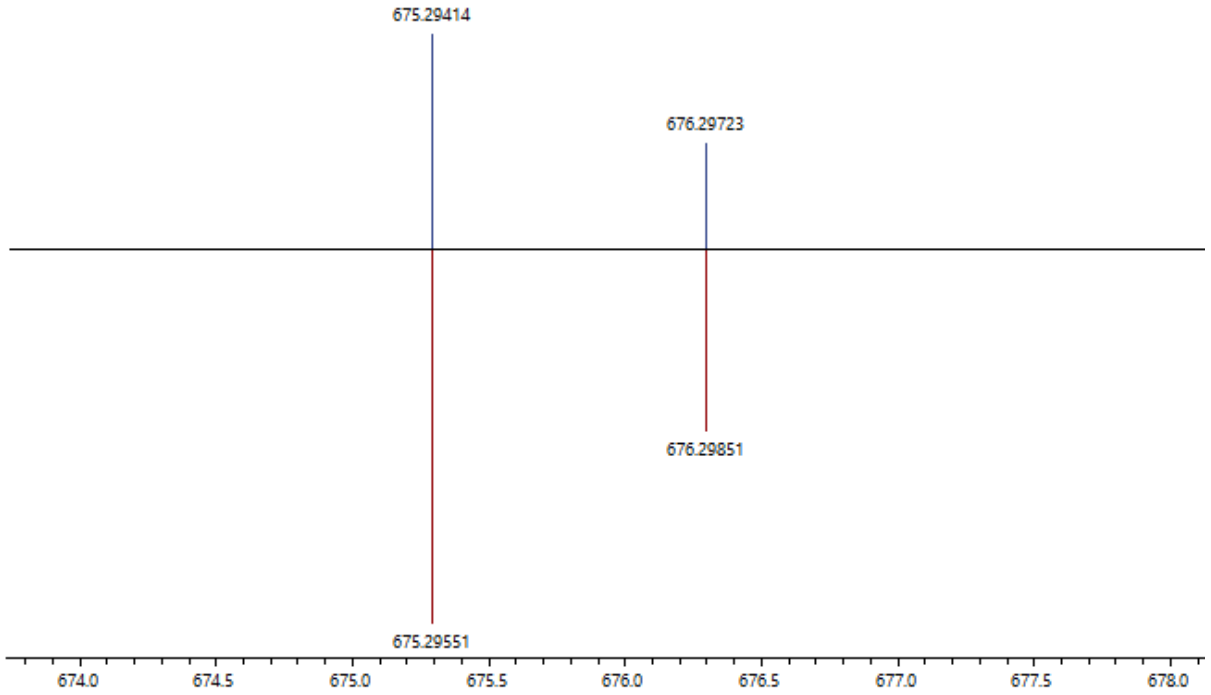

Figure S52. Fit of a peak in the mass spectrum of $[(L^{pytMe})_2+Na]^+$ experimental (blue) and simulated pattern (red).

S1.10. MS Figures for [Fe($\boldsymbol{L}^{pytMe}$)$_2$(NCBH$_3$)$_2$] Complex

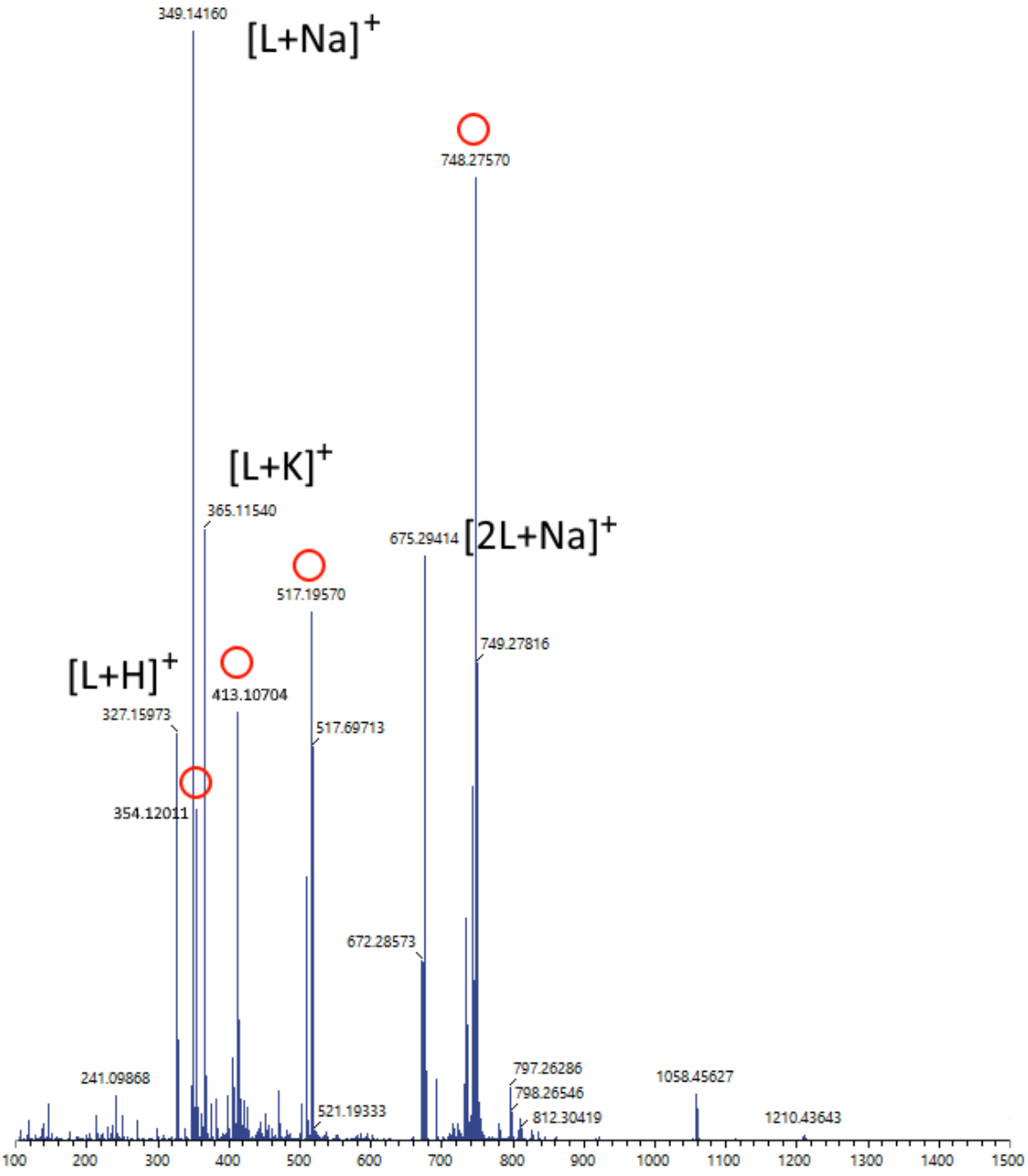

Figure S53. Complete mass spectrum of Fe($\boldsymbol{L}^{pytMe}$)$_2$(NCBH$_3$)$_2$ Reported circles refer to zoomed regions reported below.

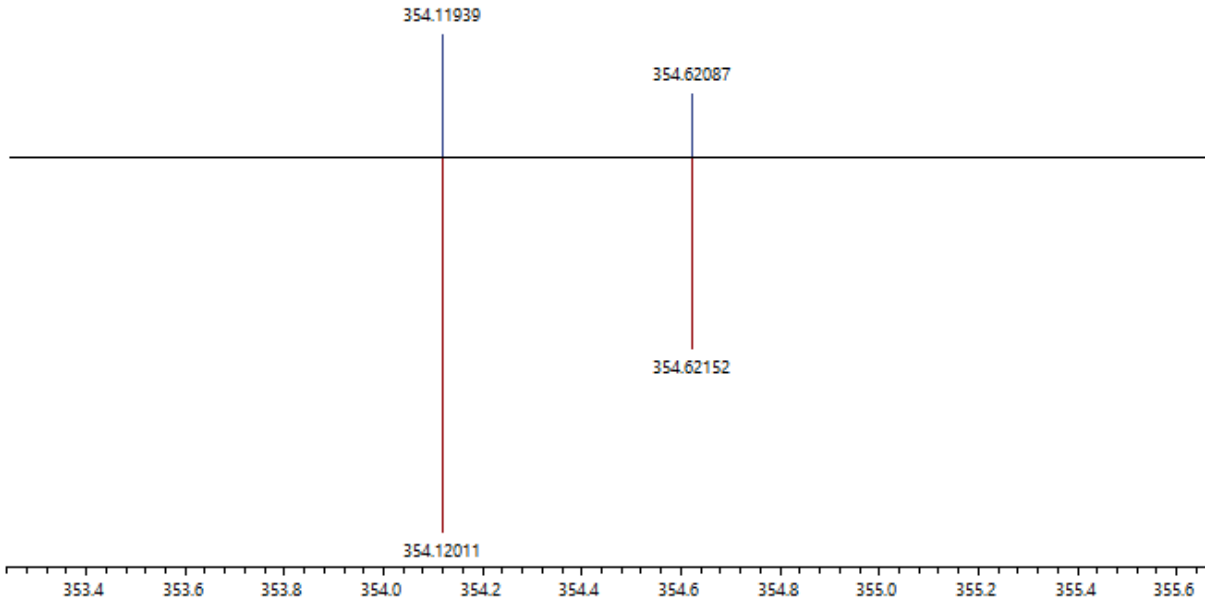

Figure S54. Fit of a peak in the mass spectrum of ***[Fe(L^{pytMe})$_2$]$^{2+}$*** experimental (blue) and simulated pattern (red).

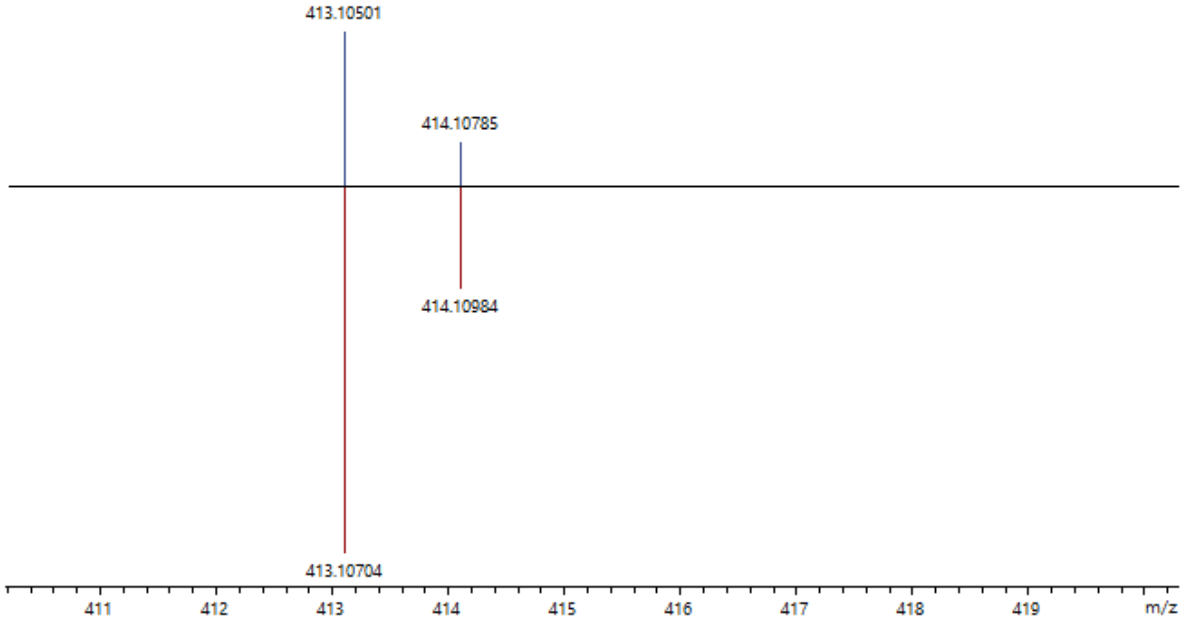

Figure S55. Fit of a peak in the mass spectrum of ***[Fe(L^{pytMe})(MeOH)-H]$^{+}$*** experimental (blue) and simulated pattern (red).

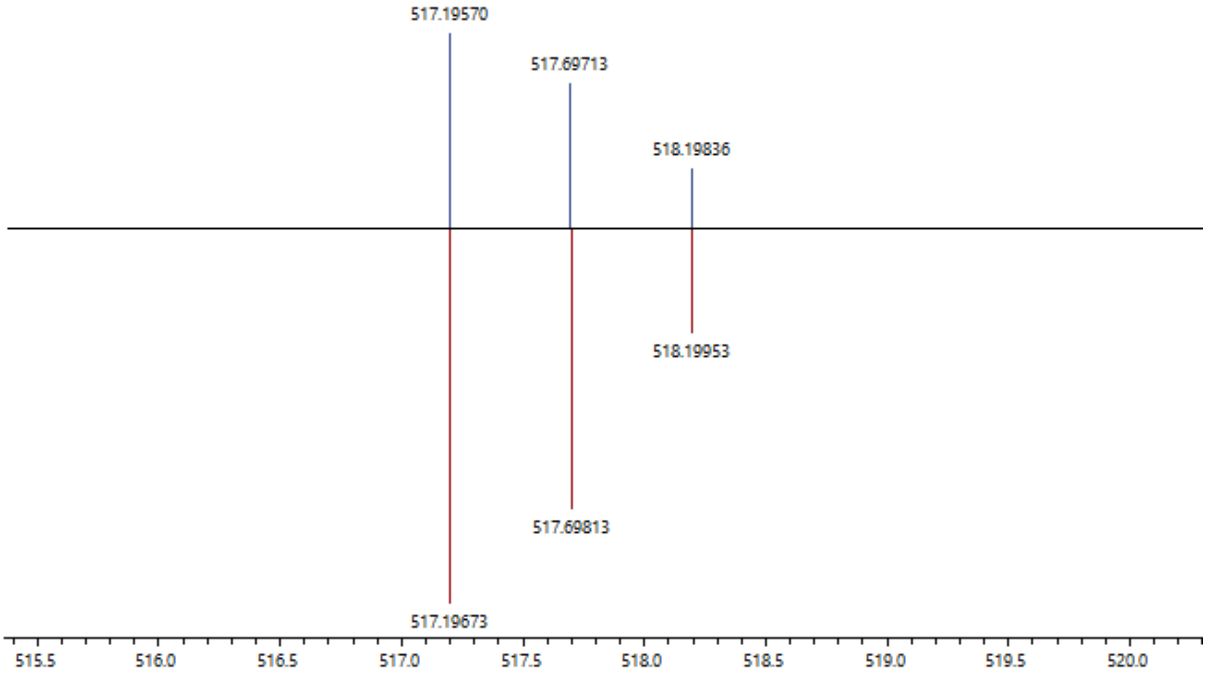

Figure S56. Fit of a peak in the mass spectrum of ***[Fe(L^{pytMe})$_3$]$^{2+}$*** experimental (blue) and simulated pattern (red).

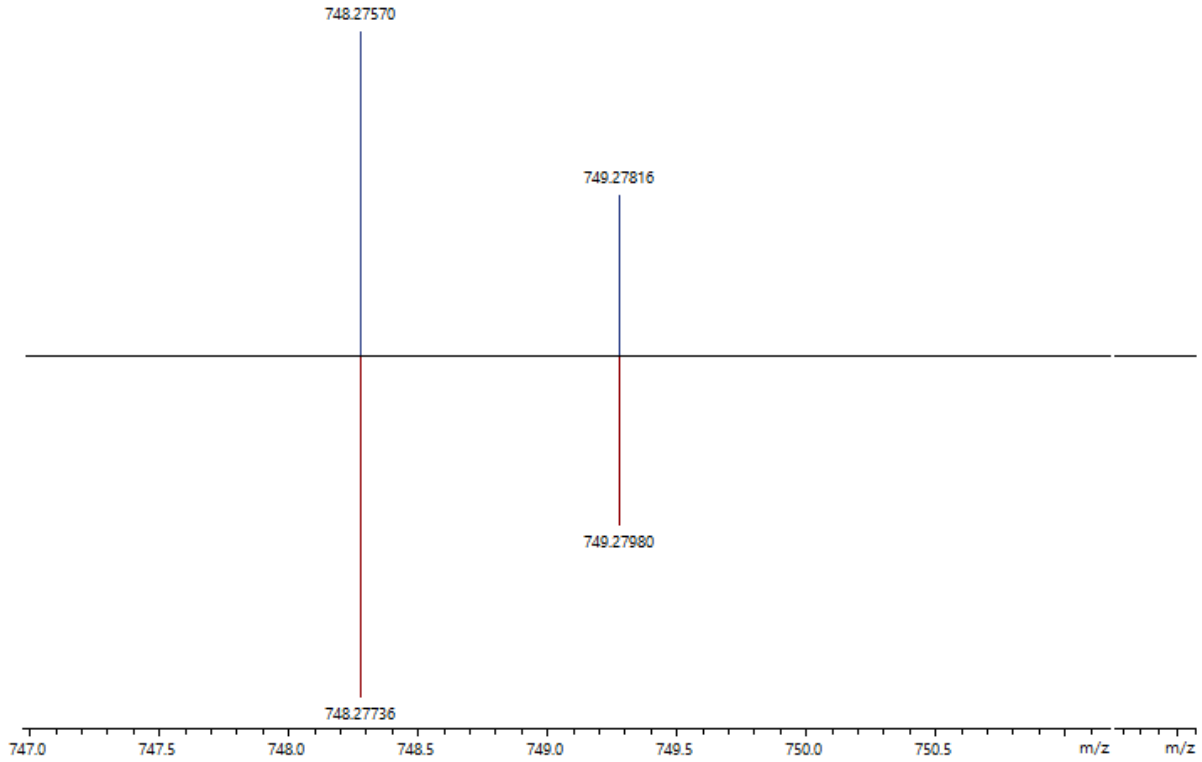

Figure S57. Fit of a peak in the mass spectrum of ***[Fe(L^{pytMe})$_2$NCBH$_3$]$^{+}$*** experimental (blue) and simulated pattern (red).

S1.11. Single Crystal X-Ray Data

The four $[Fe^{II}(\boldsymbol{L}^{pytZ})_2(NCBH_3)_2]$ complexes are isomorphous, all having crystallised in the triclinic space group P-1 (Table S1), with half of the complex in the asymmetric unit and the other half generated by an inversion centre located at the iron(II) centre. One solvent molecule of crystallisation was present in the asymmetric unit in three cases: in both $[Fe(\boldsymbol{L}^{pytCF3})_2(NCBH_3)_2]\cdot 2CHCl_3$ and $[Fe(\boldsymbol{L}^{pytMe})_2(NCBH_3)_2]\cdot 2CHCl_3$ the $CHCl_3$ molecule was disordered over two sites (Fig. S59 and S65); in $[Fe(\boldsymbol{L}^{pytF})_2(NCBH_3)_2]\cdot 2CH_3NO_2$ whereas the nitromethane molecule was ordered (Fig. S62-S63). The average Fe−N length for the iron(II) centers at 100 K is 1.98 Å (Table 1) as expected for related *LS* complexes of **Rat/Rdpt** complexes (1.93-2.02 Å). for the three ($[Fe(\boldsymbol{L}^{pytZ})_2(NCBH_3)_2]\cdot$solvents first (**Z** = **CF_3**, **Br**, **Me**) and then ($[Fe(\boldsymbol{L}^{pytF})_2(NCBH_3)_2]\cdot 2CH_3NO_2$. These three iron(II) have a quite homogeneous structure: firstly, octahedral distortion parameter Σ (the sum of the deviations of the 12 *cis* N−Fe−N angles from 90°) for three of the complexes lies in the range 43-45°, which is at the bottom end of the range usually seen for related *LS* complexes of **Rat/Rdpt** complexes (42.5−65.7°);[18-19] then, the azine ring is expected to be close to being coplanar with the triazole ring due to the restrictions imposed by coordination of both of them to the iron(II) centre, as seen in related **Rat/Rdpt** -based complexes,[18-19] and this is also seen here (0.2-3.1°). Whilst the dihedral angle between the phenyl and triazole ring is not constrained in this way it too is usually not far from being co-planar (0°-25°),[18-19] whereas the tolyl ring is usually closer to perpendicular to the triazole ring due to steric factors. Finally, the Fe-NC(BH_3) bond is extremely close to being linear (174.7-178.6°). $[Fe(\boldsymbol{L}^{pytF})_2(NCBH_3)_2]\cdot 2CH_3NO_2$ reveal a very intense distortion (Σ=70.8° vs 43.0-45.0° for the other three members of the family); this value is beyond reported range for *LS* complexes of **Rdpt** complexes (42.5−65.7°)[18-19] but not yet in the range seen for related complexes in the *HS* state (92.9°-112.2°).[18-21] Moreover, the azine-triazole dihedral angles shows an important deviation from plane (6.1°); along with phenyl-triazole dihedral angles (41.5°). Last but not least, $[Fe(\boldsymbol{L}^{pytF})_2(NCBH_3)_2]\cdot 2CH_3NO_2$ reports an Fe-$NCBH_3$ angle which is very far from linearity (166.4°).

All the four structures $[Fe(\boldsymbol{L}^{pytZ})_2(NCBH_3)_2]\cdot$solvents (**Z** = **$CF_3$**, **Br**, **F**, **Me**) show one crystallographically independent non-classical[22-24] *intramolecular* N···HC H-bond occurring between the pair of equatorial $\boldsymbol{L}^{pytZ}$ ligands, and involves the non-coordinated triazole nitrogen atom and the pyridine CH of the opposite $\boldsymbol{L}^{pytZ}$ ligand (C–H···N 3.07-3.12 Å; Figures S58, S60, S62, S64 and Table S3-S6). When solvent is present (**Z** = **CF_3** and **Me**), H-bonds between CH in the tolyl ring and the Cl of in the $CHCl_3$ molecule are observed (for **Z** = **CF_3**: C8–H8···Cl1 3.57 Å, Figures S58-S59 and Table S3; for **Z** = **Me**: C13–H13···Cl1 3.48 Å, Figures S64-S65 and Table S6). When **Z** = **CF_3** a long interaction occurs between the adjacent one of the F on the *meta*-**CF_3** substituent, and one of the of the phenyl ring of the opposite $\boldsymbol{L}^{pytCF3}$ ligand (C20S–H20S···F1 3.78 Å, Figures S58 and Table S3), of the opposite $\boldsymbol{L}^{pytCF3}$ ligand. When **Z** = **Me** a second, longer interaction occurs between the CH in the pyridyl ring with the same non-coordinated triazole nitrogen atom of the opposite $\boldsymbol{L}^{pytMe}$ ligand (C19–H19···N2S 3.61 Å, Figures S64 and Table S6). When **Z** = **F**, three H-bonds are directly engaged by the fluorine substituents with three different CH (C10–H10···F1T 3.42 Å, C13–H13···F1R 3.31 Å, C6–H6···F1 3.61 Å, Figures S62 and Table S5). Three more are engaged by the CH_3NO_2 solvent molecule: from CH_3 ending in nitromethane is H-bonded by non-coordinating triazole nitrogen (C22–H22B···N2S 3.46 Å) and $NCBH_3$ nitrogen atom (C22–H22C···N5T 3.60 Å); also, a H-bond between is observed between the oxygen atom from the NO_2 ending and the substituted pyridyl ring (C17–H17···O1R 3.31 Å, Figures S62-S63 and Table S5).

Table S1. Crystal data and structure refinement details for the four $[Fe(L^{pytZ})_2(NCBH_3)_2]\cdot 2CHCl_3$,.

Empirical formula	**$[Fe(L^{pytCF3})_2(NCBH_3)_2]$ $\cdot$ $2CHCl_3$**	**$[Fe(L^{pytBr})_2(NCBH_3)_2]$**	**$[Fe(L^{pytF})_2(NCBH_3)_2]$ $\cdot 2CH_3NO_2$**	**$[Fe(L^{pytMe})_2(NCBH_3)_2]$ $\cdot 2CHCl_3$**
Formula weight	1135.03	918.10	918.36	1027.08
Temperature/K	100(2)	100(2)	100(2)	100(2)
Crystal system	triclinic	triclinic	triclinic	triclinic
Space group	P-1	P-1	P-1	P-1
a [Å]	9.5845(3)	8.9066(4)	8.3350(6)	9.3639(4)
b [Å]	11.4336(8)	9.4038(3)	11.0887(8)	11.3127(4)
c [Å]	11.7405(7)	13.0691(6)	12.5957(6)	11.9801(4)
α [°]	91.135(5)	70.425(4)	90.610(5)	91.075(3)
β [°]	94.601(4)	75.239(4)	92.312(5)	95.484(3)
γ [°]	100.639(4)	82.491(3)	106.356(7)	102.546(3)
Volume [$Å^3$]	1259.61(12)	996.08(8)	1115.83(13)	1232.07(8)
Z	1	1	1	1
ρ_{calc} [g/cm^3]	1.496	1.531	1.367	1.384
μ [mm^{-1}]	5.907	5.744	3.258	5.797
F(000)	576.0	464.0	476.0	528.0
Crystal size [mm^3]	0.19 × 0.07 × 0.07	0.009 × 0.05 × 0.08	0.004 × 0.007 × 0.012	0.008 × 0.01 × 0.013
Radiation	CuK_α (λ = 1.54184)	CuK_α (λ = 1.54184)	CuK_α (λ = 1.54184)	CuK_α (λ = 1.54184)
2Θ range for data collection [°]	7.558-145.322	10.210-152.546	8.312-154.182	10.608 -152.186
Reflections collected	8656	6308	7840	9638
Independent reflections	4834	4026	4482	4993
Data/restraints/parameters	4834/ 0/ 362	4026/ 0/ 272	4482/ 0/ 317	4993/ 0/ 340
Goof [F^2]	1.046	1.010	1.068	1.203
R_1 [I>=2σ (I)]	0.0547	0.0351	0.0886	0.0398
wR_2 [all data]	0.1479	0.1114	0.2610	0.1329
Largest diff. peak/hole [$eÅ^{-3}$]	1.35 to -0.89	0.8 to -0.85	2.1 to -0.86	0.49 to -0.68

Table S2. Summary of key structural parameters for the four [Fe(L^{pytZ})$_2$(NCBH$_3$)$_2$]·solvent complexes.

	[Fe(L^{pytCF3})$_2$(NCBH$_3$)$_2$]·2CHCl$_3$	**[Fe(L^{pyBr})$_2$(NCBH$_3$)$_2$]**	**[Fe(L^{pyF})$_2$(NCBH$_3$)$_2$]·2CH$_3$NO$_2$**	**[Fe(L^{pyMe})$_2$(NCBH$_3$)$_2$]·2CHCl$_3$**
av. Fe-N$_{triazole}$ (Å)	1.957 Å	1.959 Å	1.982 Å	1.974 Å
av. Fe-N$_{pyridine}$(Å)	1.999 Å	1.987 Å	2.005 Å	2.010 Å
av. Fe-N$_{NCBH3}$(Å)	1.933 Å	1.945 Å	1.945 Å	1.938 Å
av. Fe-N(Å)	1.963 Å	1.964 Å	1.977 Å	1.974 Å
Distortion angle (Σ°)	44.9°	44.9°	70.8°	43.0°
Temperature	100 K	100 K	100 K	100 K
Spin State	*LS*	*LS*	*LS*	*LS*
N$_{triazole}$–Fe–N$_{azine}$ angle (°)	80.2°	80.1°	79.9°	80.3°
N$_{triazole}$–Fe–N$_{azine}$ dihedral angle (°)	3.06°	0.24°	6.21°	0.91°
Fe–NCBH$_3$ angle (°)	178.3°	174.7°	166.37°	178.6°
triazole-tolyl ring dihedral angle (°)	78.7°	76.0°	75.2°	73.0°
triazole-phenyl ring dihedral angle (°)	24.2°	3.6°	41.5°	21.6°

Table S3. Non-classical H-bonds observed in [Fe(L^{pytCF3})$_2$(NCBH$_3$)$_2$]·2CHCl$_3$. Symmetry Operation: S = -x, -y, -z.

D–H···A	D–A (Å)	H···A (Å)	D–H···A (°)
C1-H1···N2S	3.070	2.266	144.4
C20S-H20S···F1	3.775	2.980	144.3
C8-H8···Cl1	3.569	2.825	137.8

Table S4. Non-classical H-bonds observed in [Fe(L^{pytBr})$_2$(NCBH$_3$)$_2$]. Symmetry Operation: S = -x, 1-y, -z.

D–H···A	D–A (Å)	H···A (Å)	D–H···A (°)
C1-H1··· N2S	3.065	2.277	142.1
C20-H20··· Br1S	4.690	3.864	149.7

Table S5. Non-classical H-bonds observed in [Fe(L^{pytF})$_2$(NCBH$_3$)$_2$]·2CH$_3$NO$_2$. Symmetry Operation: R = -x, -y, -z. S = -x, 1-y, -z. T = 1-x, -y, -z.

D–H···A	D–A (Å)	H···A (Å)	D–H···A (°)
C20-H20···N2S	3.117	2.331	141.9
C6-H6···F1	3.607	2.736	156.4
C3S-H3···F1	5.590 (provided for comparison)	5.207	109.4
C17-H17···O1R	3.305	2.533	140.7
C13-H13···F1R	3.314	2.592	134.8
C10-H10···F1T	3.423	2.812	124.3
C22-H22B···N2S	3.461	2.533	162.6
C22-H22C···N5T	3.604	2.953	126.3

Table S6. Non-classical H-bonds observed in [Fe(L^{pytMe})$_2$(NCBH$_3$)$_2$]·2CHCl$_3$. Symmetry Operation: S = -x, -y, -z.

D–H···A	D–A (Å)	H···A (Å)	D–H···A (°)
C1-H1···N2S	3.107	2.276	145.6
C19-H19···N2S	3.612	2.998	123.7
C13-H13···Cl1	3.480	2.741	144.5

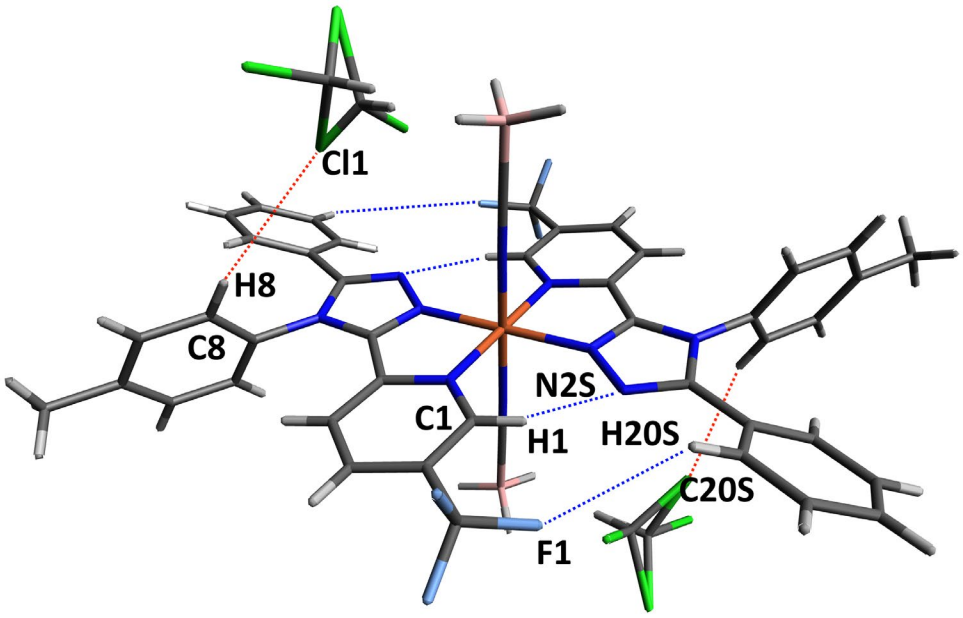

Figure S58. Crystal structure of [Fe(L^{pytCF3})$_2$(NCBH$_3$)$_2$·2CHCl$_3$]. Blue dotted lines report the non-classical C-H···X H-bond interactions (*intramolecular H-bonds:* C1–H1 ··· N2S and C20S–H20S ··· F1); red dotted lines report complex-solvent H-bond interactions (*intermolecular H-bonds:* C8–H8 ··· Cl1). See Table S3. Symmetry Operation: S = -x, -y, -z. Colour code: Fe orange, N blue, C black, Cl green, F light blue, B pink, H white.

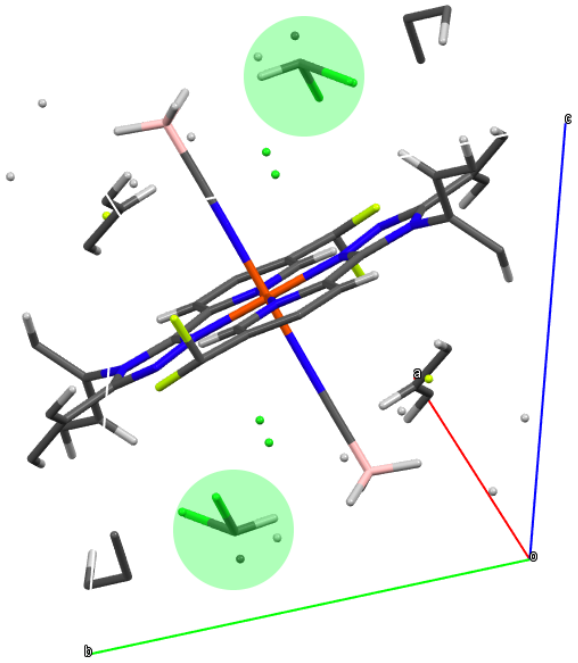

Figure S59. Unit cell crystal packing of [Fe(L^{pytCF3})$_2$(NCBH$_3$)$_2$]·2CHCl$_3$, one mononuclear complex per unit cell. Two disordered half molecules of CHCl$_3$ are highlighted in green. Colour code: Fe orange, N blue, C black, Cl green, F light blue, B pink, H white.

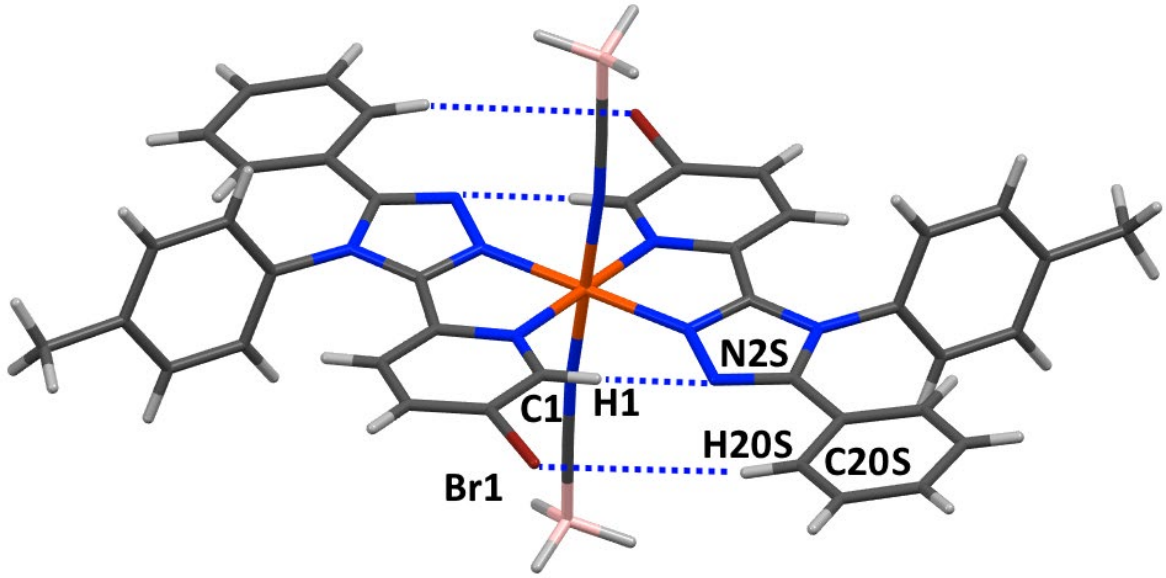

Figure S60. Crystal structure of [Fe(L^{pytBr})$_2$(NCBH$_3$)$_2$]. Blue dotted lines report the non-classical C-H···X H-bond interactions (*intramolecular H-bond:* C1–H1···N2S). Details in Table S4 (S = -x, 1-y, -z). Note: C20S-H20S···Br1 3.864 Å, C20S···Br1 4.690 Å, C20S-H20S···Br1 149.67°, so is at best a weak intramolecular interaction in this case (*cf* the **Z** = **CF$_3$** case, Figure S58). Symmetry Operation: S = -x, 1-y, -z. Colour code: Fe orange, N blue, C black, Br crimson, B pink, H white.

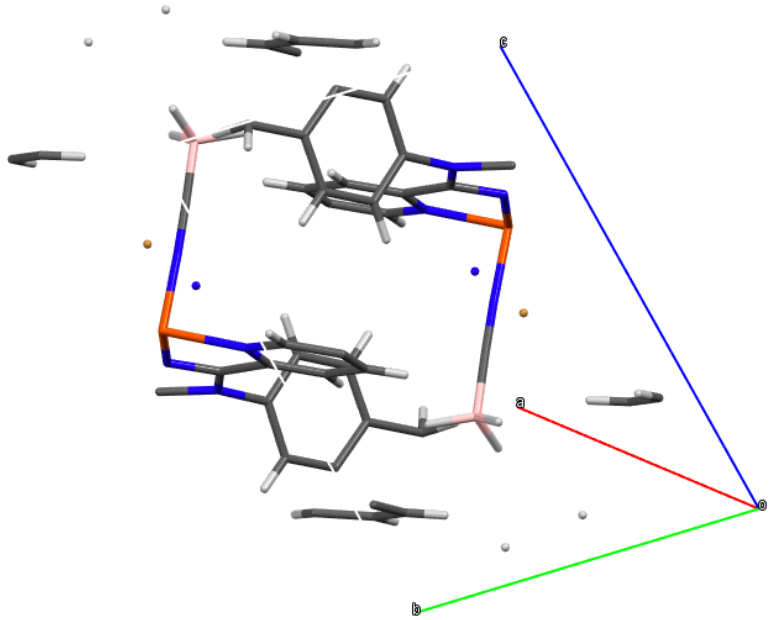

Figure S61. Unit cell crystal packing of [Fe(L^{pytBr})$_2$(NCBH$_3$)$_2$], one mononuclear complex per unit cell. Colour code: Fe orange, N blue, C black, Br crimson, B pink, H white.

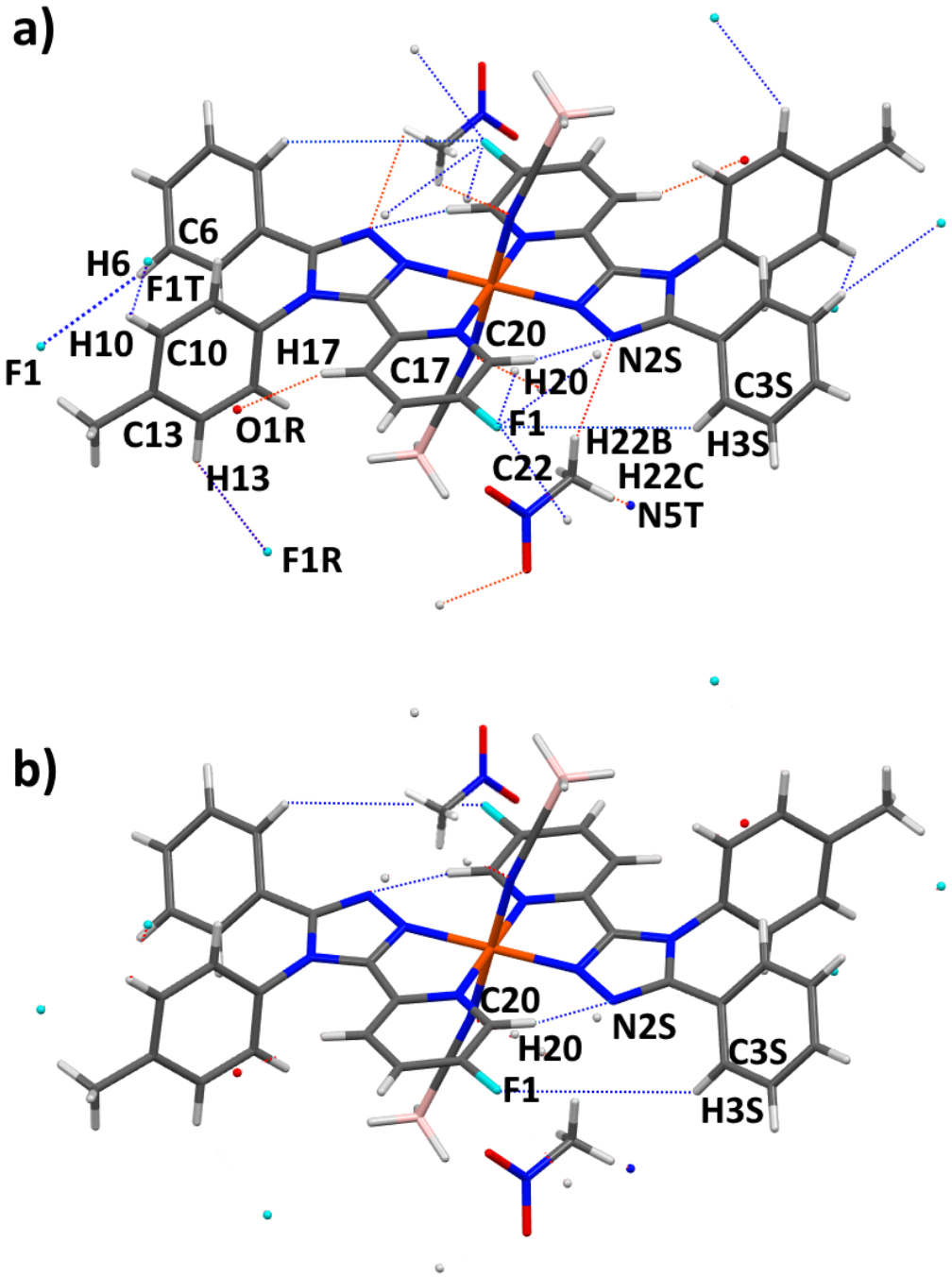

Figure S62. Crystal structure of [Fe(L^{pytF})$_2$(NCBH$_3$)$_2$]·2CH$_3$NO$_2$. (a) Blue dotted lines report the non-classical C-H···X interactions (*intramolecular H-bonds:* C20–H20···N2S; *intermolecular H-bonds:* C10–H10···F1S, C13–H13···F1R, C6–H6···F1); red dotted lines report complex-solvent H-bond interactions (*H-bonds:* C22–H22B···N2S, C22–H22C···N5T, C17–H17···O1R). See Table S5. (b) Blue dotted lines highlight the *intermolecular* non classical H-bonds made by the **Z** = **F** substituents (C3S-H3S···F1 5.207 Å, C3S···F1 5.590 Å, C3S···F1 109.4°; S = -x, 1-y, -z), which contrast with the intramolecular non classical H-bonds made by the **Z** = **CF$_3$** substituents (Figure S58, Table S3) and **Z** = **Br** substituents (Figure S60, Table S4). Symmetry Operation: R = -x, -y, -z. S = -x, 1-y, -z. T = 1-x, -y, -z. Colour code: Fe orange, N blue, C black, F light blue, B pink, H white, O red.

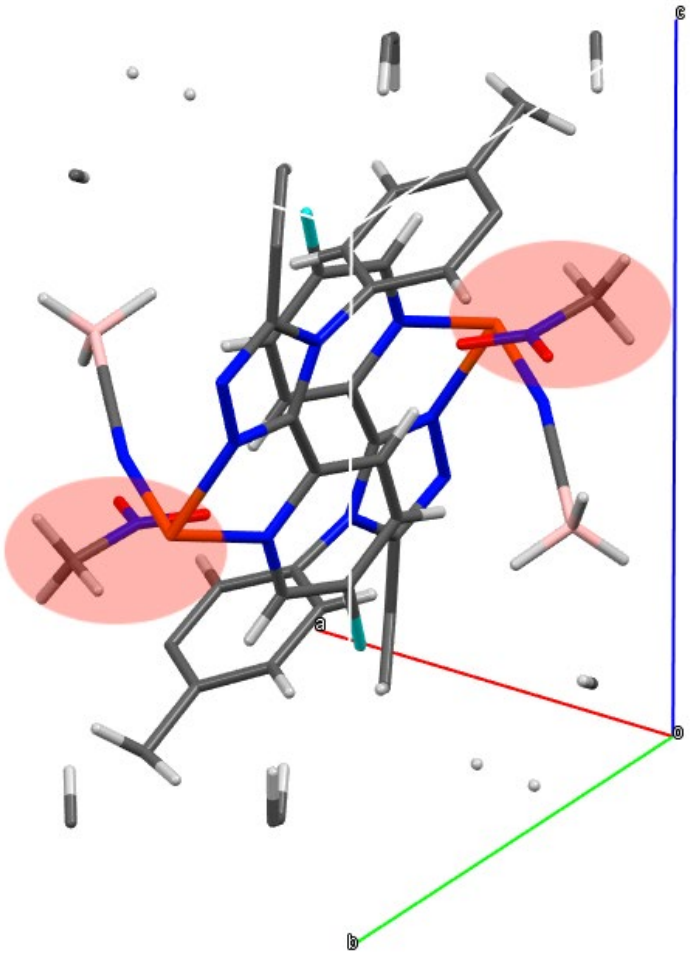

Figure S63. Unit cell crystal packing of [Fe($\boldsymbol{L}^{pytF}$)$_2$(NCBH$_3$)$_2$], two mononuclear complex per unit cell. Two disordered half molecules of CH_3NO_2 are highlighted in red. Colour code: Fe orange, N blue, C black, F light blue, B pink, H white, O red.

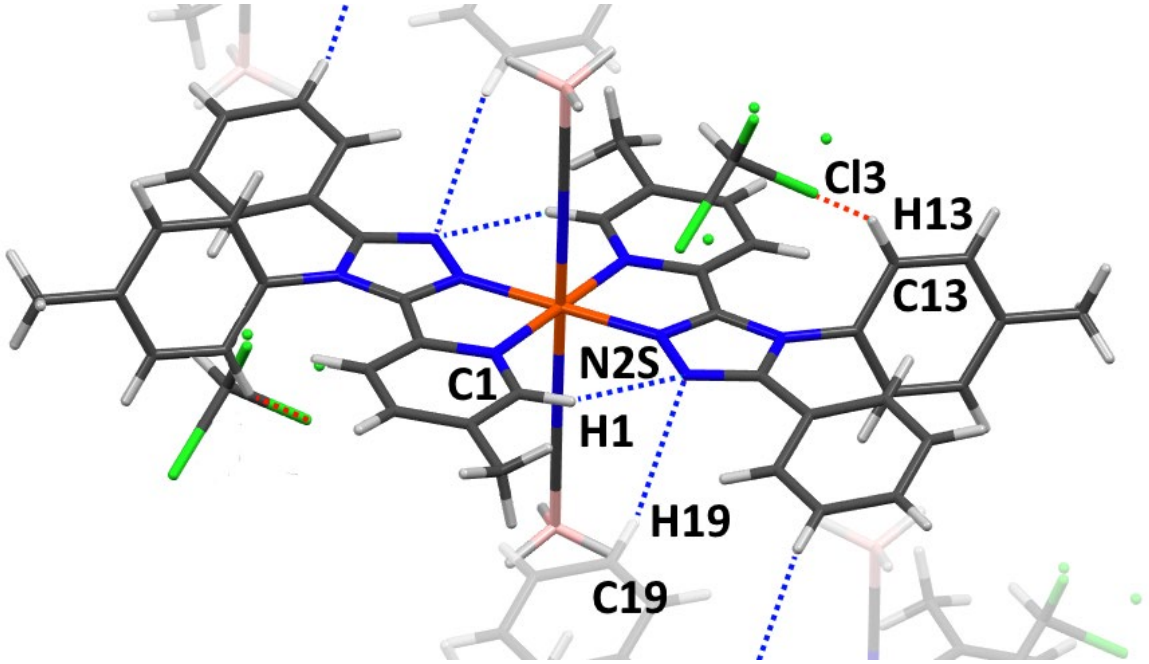

Figure S64. Crystal structure of [Fe($\boldsymbol{L}^{pytMe}$)$_2$(NCBH$_3$)$_2$·2CHCl$_3$. Blue dotted lines report the non-classical C-H···X interactions (*intramolecular H-bonds:* C1–H1···N2S; *intermolecular H-bonds:* C19–H19··· N2S); red dotted lines report complex-solvent H-bond interactions (*H-bonds:* C13–H13···Cl3). See Table S6. Symmetry Operation: S = -x, -y, -z. Colour code: Fe orange, N blue, C black, Cl green, B pink, H white

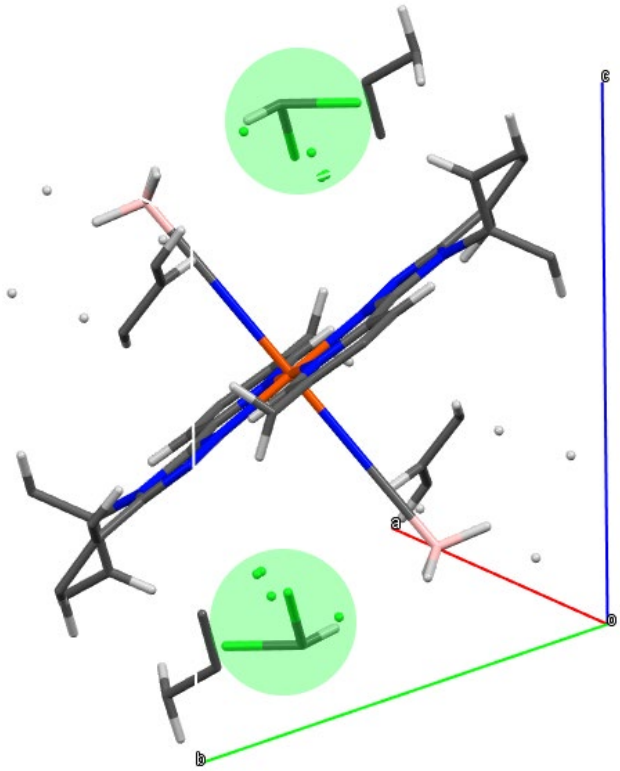

Figure S65. Unit cell crystal packing of [Fe($\boldsymbol{L}^{pytMe}$)$_2$(NCBH$_3$)$_2$]·2CHCl$_3$, one mononuclear complex per unit cell. Two disordered molecules of CHCl$_3$ are highlighted in green. Colour code: Fe orange, N blue, C black, Cl green, B pink, H white.

S1.12. Solid State Magnetic Measurements

The solid-state magnetic susceptibilities were measured from 50–400–50 K for each $[Fe^{II}(\boldsymbol{L}^{pytZ})_2(NCBH_3)_2]\cdot nH_2O$ (measuring in 10 K steps, ramping between steps at 2 K min^{-1}). These measurements are obtained in settle mode (the instrument considers the temperature "settled" after 1 min of the temperature being within the smaller value of ±0.5 K or ±0.5% of the target value). Scan rate study of $\chi_M T$ vs T for $[Fe(\boldsymbol{L}^{pytCF3})_2(NCBH_3)_2]\cdot 0.5H_2O$ from 150 to 250 K was obtained in sweep mode. In this instrumental set up, $\chi_M T$ measurements are collected continuously as the temperature was swept at different rates (20, 10, 5, 2 and 0.2 K min^{-1}). Measurements were obtained by applying a magnetic field of 0.1 T with a Quantum Design Physical Property Measurement System equipped with a vibrating sample mount (VersaLab). The data were corrected for the diamagnetism of the capsule and of the sample ((−M × 0.5) $\times 10^{-6}$ $cm^3 mol^{-1}$).[1]

Table S7. Reported obtained $T_{1/2}$ from solid state measurements on $[Fe(\boldsymbol{L}^{pytZ})_2(NCBH)_3]\cdot xH_2O$ family.

$[Fe(\boldsymbol{L}^{pytZ})_2(NCBH_3)_2]\cdot xH_2O$	$T_{1/2}$ (K)
$[Fe(\boldsymbol{L}^{pytCF3})_2(NCBH_3)_2]\cdot 0.5H_2O$	$T_{1/2}\downarrow$ = 203 K, $T_{1/2}\uparrow$ = 213 K; $\Delta T_{1/2}$ = 10 K
$[Fe(\boldsymbol{L}^{pytBr})_2(NCBH_3)_2]\cdot 0.5H_2O$	**LS**
$[Fe(\boldsymbol{L}^{pytF})_2(NCBH_3)_2]\cdot 1H_2O$	290
$[Fe(\boldsymbol{L}^{pytMe})_2(NCBH_3)_2]\cdot 0.5H_2O$	300

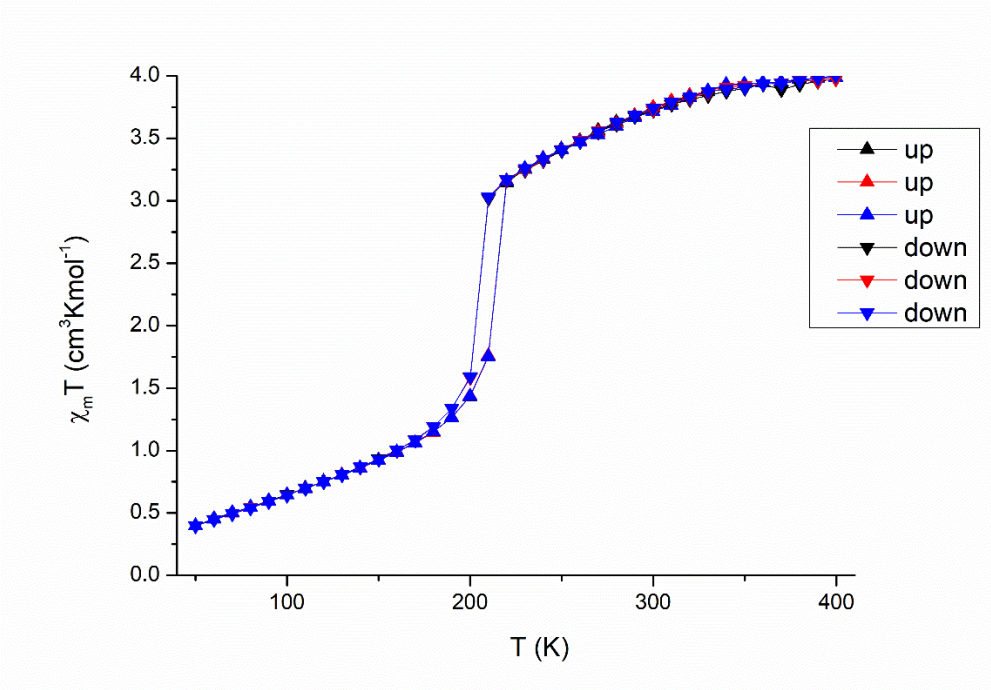

Figure S66. $\chi_M T$ versus T plot for a solid sample of Fe(L^{pytCF3})$_2$(NCBH$_3$)$_2$·0.5H$_2$O from 50 to 400 K. Cycle was performed by cooling first (down triangles), then heating (up triangles) for three cycles, in 10 K steps, changing temperatures at 2 K min^{-1} , in settle mode.

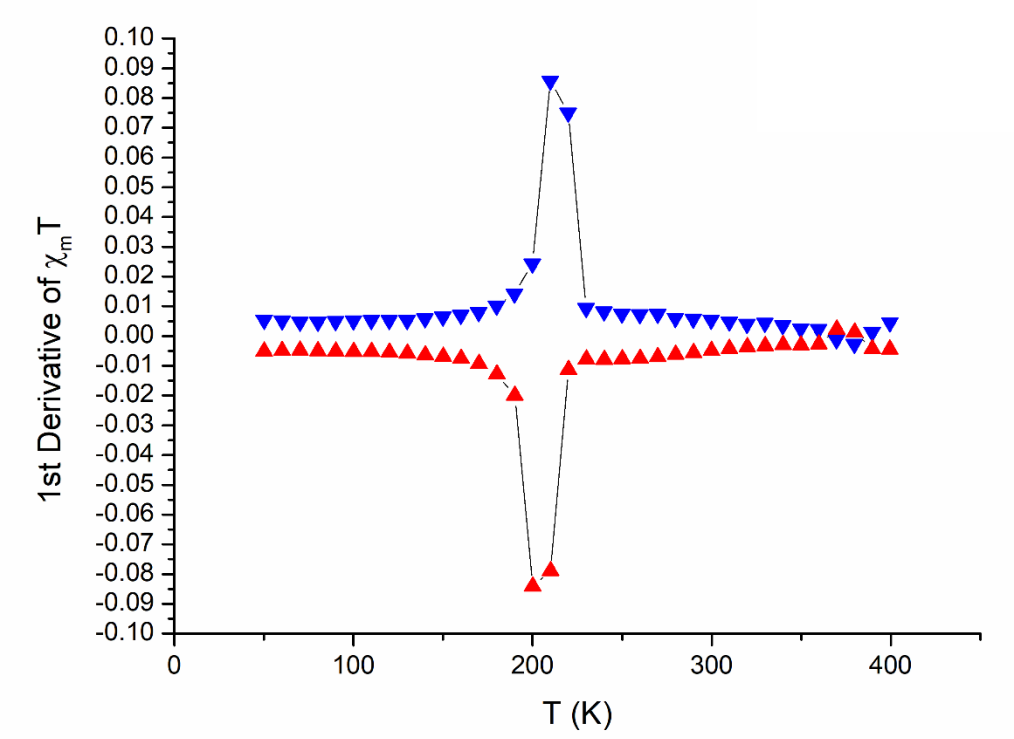

Figure S67. First derivative of $\chi_M T$ versus T plot for a solid sample of Fe(L^{pytCF3})$_2$(NCBH$_3$)$_2$·0.5H$_2$O from 50 to 400 K. Cycle was performed by cooling first (down triangles), then heating (up triangles) in 10 K steps, changing temperatures at 2 K min^{-1} , in settle.

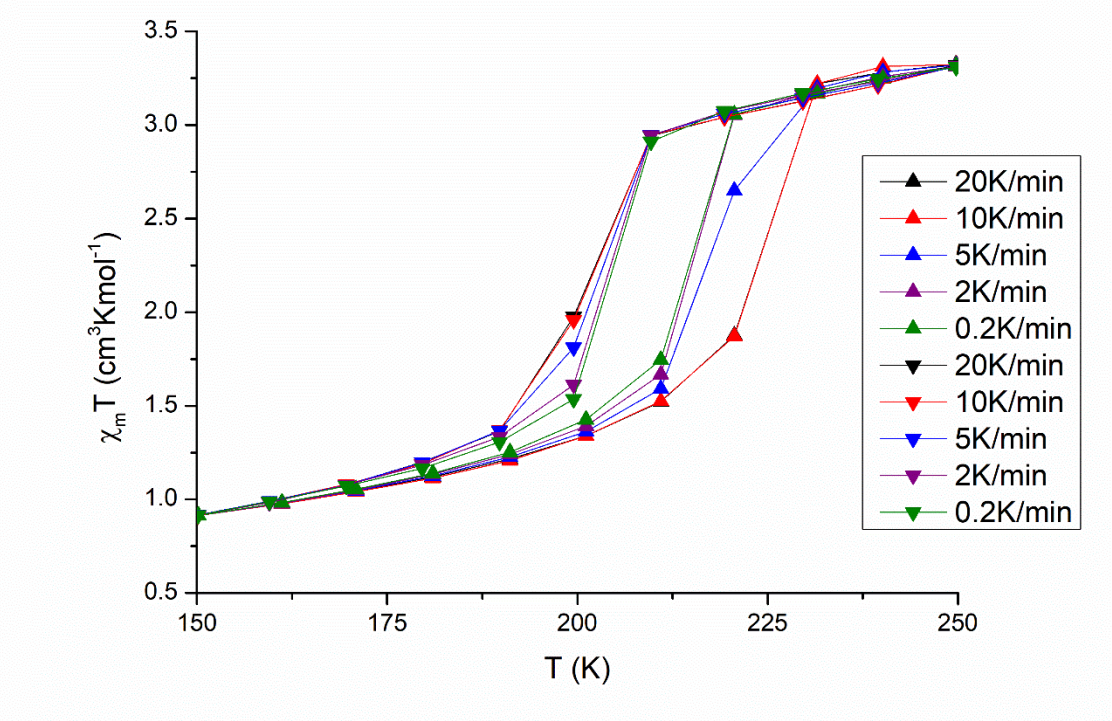

Figure S68. Scan rate study (20 to 0.2 K min^{-1}) of $\chi_M T$ vs T for [Fe(L^{pytCF3})$_2$(NCBH$_3$)$_2$]·0.5H$_2$O from 150 to 250 K in sweep mode.

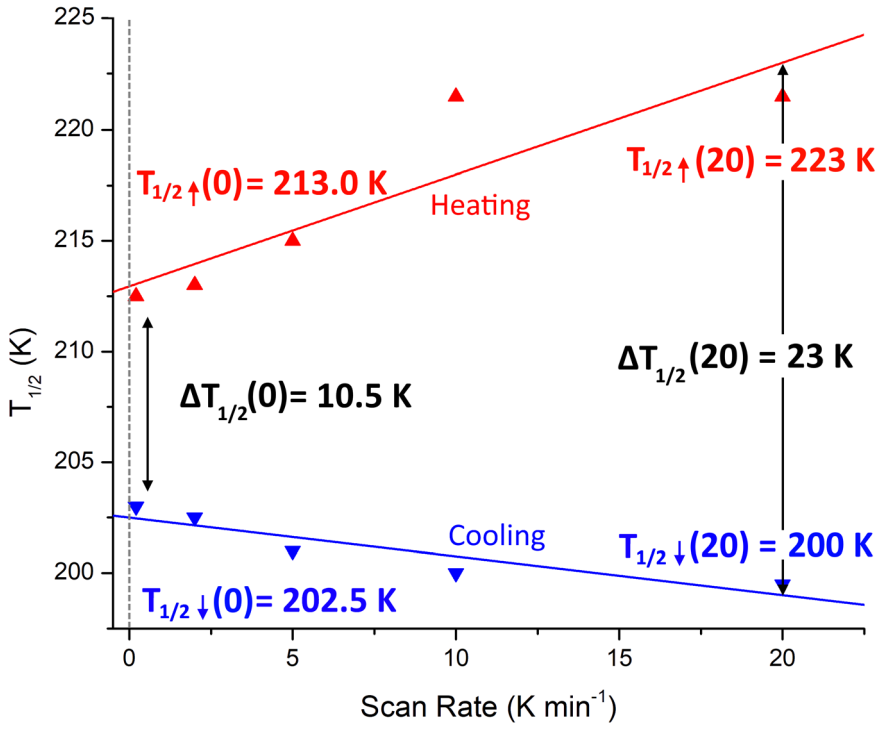

Figure S69. Plots of $T_{½}$ values obtained from the cooling (blue, at 20 K·min^{-1} ($T_{½}\downarrow(20)$) and extrapolated at limit speed of 0 K·min^{-1} ($T_{½}\downarrow(0)$) and heating (red, at 20 K·min^{-1} ($T_{½}\downarrow(20)$) and extrapolated at limit speed of 0 K·min^{-1} ($T_{½}\downarrow(0)$) modes from magnetic experiments run at different scan rates (in sweep mode) for [Fe^{II}(L^{pytCF3})$_2$(NCBH$_3$)$_2$]·0.5H$_2$O. The lines shown were obtained by linear fitting of the magnetic data, as reported by Brooker *et al.*[25-26]

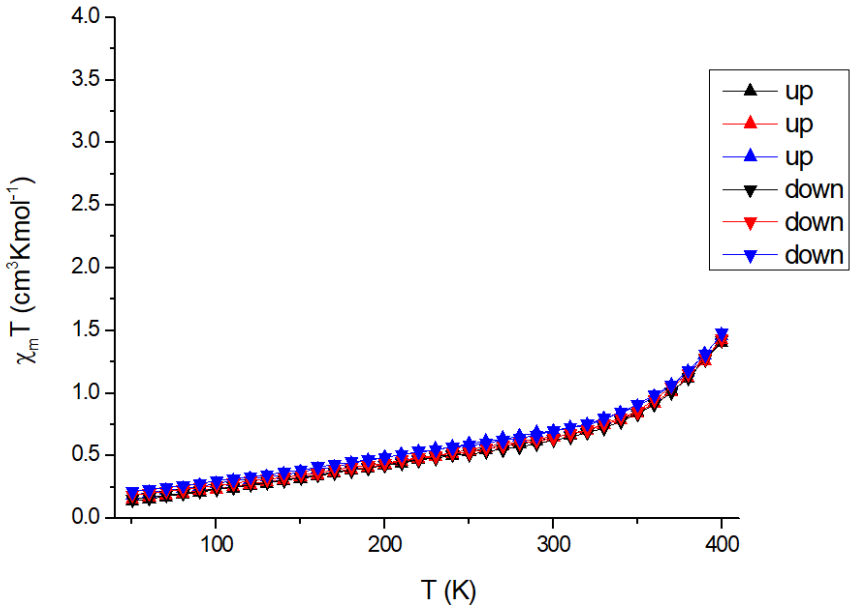

Figure S70. $\chi_M T$ versus T plot for a solid sample of Fe(***L***^{pytBr})$_2$(NCBH$_3$)$_2$·0.5H$_2$O from 50 to 400 K. Cycle was performed by cooling first (down triangles), then heating (up triangles) for three cycles, in 10 K steps, changing temperatures at 2 K min^{-1} , in settle.

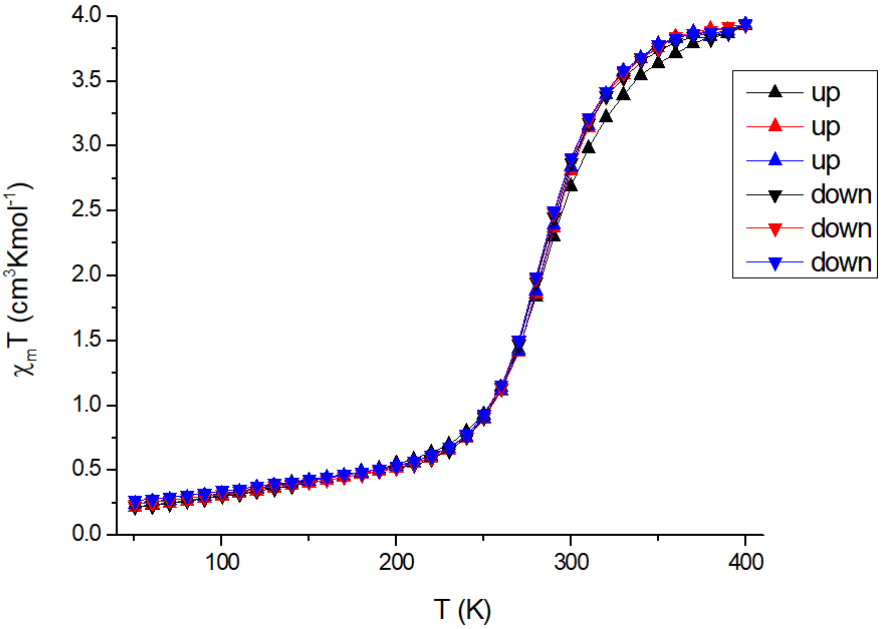

Figure S71. $\chi_M T$ versus T plot for a solid sample of Fe($\boldsymbol{L}^{pytF}$)$_2$(NCBH$_3$)$_2$·1H$_2$O from 50 to 400 K. Cycle was performed by cooling first (down triangles), then heating (up triangles) for three cycles, in 10 K steps, changing temperatures at 2 K min^{-1} , in settle mode.

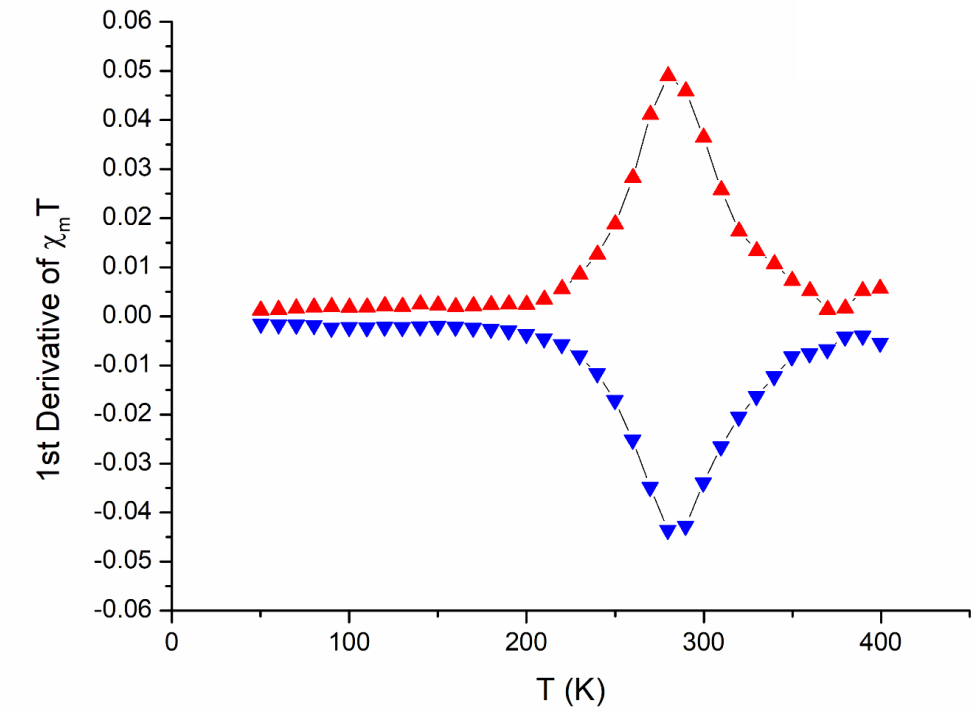

Figure S72. First derivative of $\chi_M T$ versus T plot for a solid sample of Fe($\boldsymbol{L}^{pytF}$)$_2$(NCBH$_3$)$_2$·1H$_2$O from 50 to 400 K. Cycle was performed by cooling first (down triangles), then heating (up triangles) in 10 K steps, changing temperatures at 2 K min^{-1} , in settle mode.

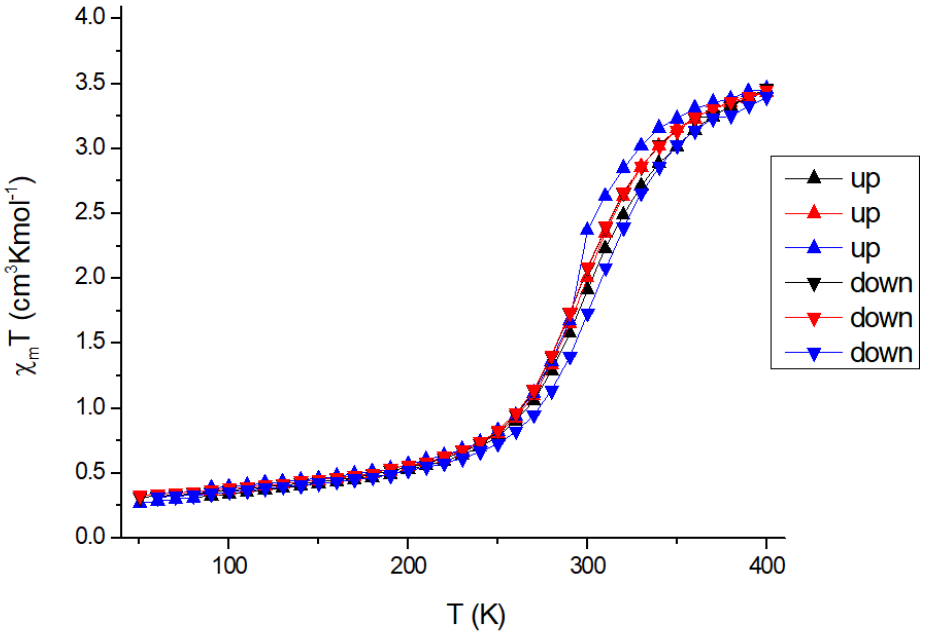

Figure S73. $\chi_M T$ versus T plot for a solid sample of Fe($\boldsymbol{L}^{\boldsymbol{pytMe}}$)$_2$(NCBH$_3$)$_2$·0.5H$_2$O from 50 to 400 K. Cycle was performed by cooling first (down triangles), then heating (up triangles) for three cycles, in 10 K steps, changing temperatures at 2 K min^{-1} , in settle mode.

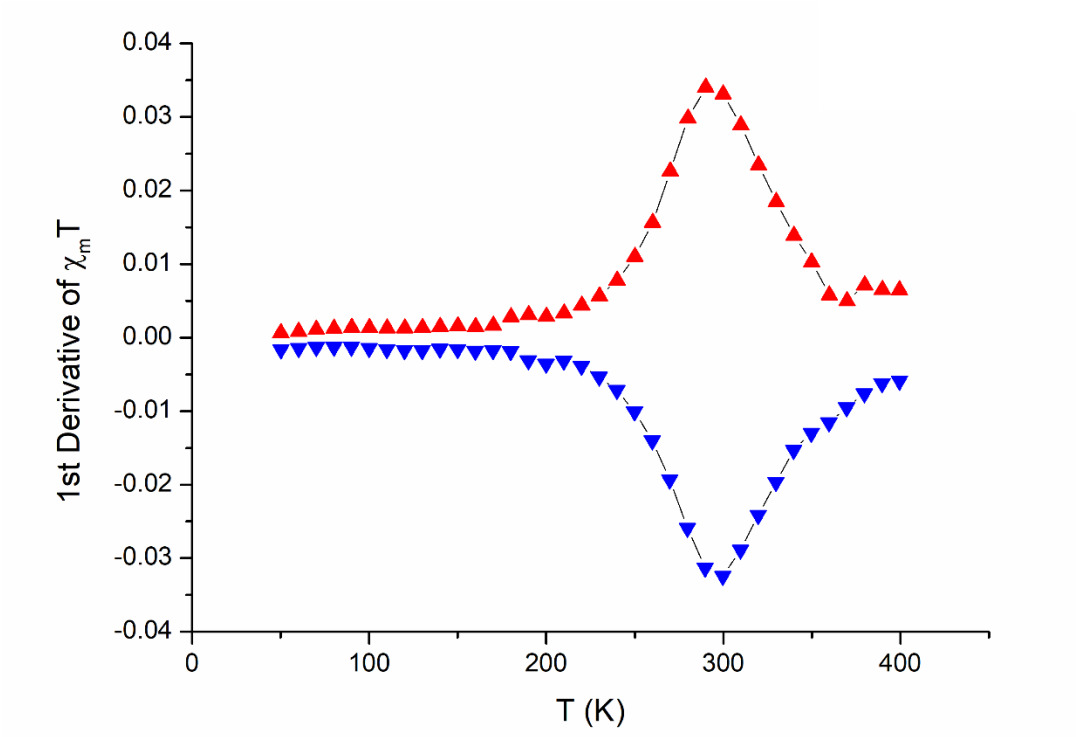

Figure S74. First derivative of $\chi_M T$ versus T plot for a solid sample of Fe($\boldsymbol{L}^{\boldsymbol{pytMe}}$)$_2$(NCBH$_3$)$_2$·0.5H$_2$O from 50 to 400 K. Cycle was performed by cooling first (down triangles), then heating (up triangles) in 10 K steps, changing temperatures at 2 K min^{-1} , in settle mode.

S1.13 Solution Phase Magnetic Measurements

The complex solutions for this study were prepared by reacting a precisely known mass of $[Fe^{II}(pyridine)_4(NCBH_3)_2]$ in 0.500 mL of $CDCl_3$ with the corresponding $\boldsymbol{L^{pytZ}}$ ligand in a 6:1 $\boldsymbol{L^{pytZ}}$ / iron(II) ratio.[27] Solution magnetic susceptibility data were obtained from these $CDCl_3$ solutions using the Evans ^{1}H-NMR method[28] on a Varian500 AR with a 5 mm OneProbe with a variable temperature controller between 243 to 313 K in intervals of 5 K. A diamagnetic correction for the sample (-0.5×10^{-6}),[1] and a correction for the variation of the density of the solvent with temperature,[2] were applied to each dataset (Table S9). The derived parameters, i.e. ΔH, ΔS, and the least squares fittings were obtained by modelling each dataset as a gradual and complete SCO using the regular solution model (equation S1)[1, 4-5] with good fits obtained. These were carried out using OriginPro version 9.1.0 from OriginLab Corporation. For all data, a maximum $\chi_m T$ value ($\chi_m T(max)$) of 3.5 $cm^3 \cdot K \cdot mol^{-1}$ was used in Equation S1.[1, 4-5] Note that the expected error in temperature in an VT-NMR instrument is ±1 K, and error associated with the Evan's method determination of $\chi_M T(T)$ is 5%, so significant errors are expected in the derived parameters (Table S8).[7]

Excel was also employed, to determine 95% confidence intervals and help assign appropriate errors to the parameters obtained from the fit (Figures S79-S82). This error analysis in the gradual SCO fitting was evaluated using the non-linear regression of the experimental data as reported by Brown and co-workers.[29]

$$\chi_M T(T) = \frac{\chi_M T(MAX)}{1 + \exp\left(\frac{\Delta H}{RT} - \frac{\Delta S}{R}\right)} \qquad \text{eq. } \mathbf{S1}$$

$$T_{1/2} = \frac{\Delta H}{\Delta S} \qquad \text{eq. } \mathbf{S2}$$

S1.13.1. Evans method VT ^{1}H-NMR spectra

Table S8. Reported results obtained by fitting points obtained by Evan's method measurement on regular solution SCO phenomenon. First line report values of change in enthalpy (ΔH); in the second line the change in entropy (ΔS) is reported. In the bottom line the correlation factor R^2 for the fitting curves is reported.

	$Fe(\boldsymbol{L}^{pytCF3})_2(NCBH_3)_2$	$Fe(\boldsymbol{L}^{pytBr})_2(NCBH_3)_2$	$Fe(\boldsymbol{L}^{pytF})_2(NCBH_3)_2$	$Fe(\boldsymbol{L}^{pytMe})_2(NCBH_3)_2$
ΔH / J mol^{-1}	-35806.0±3353.7	-9645.8±292.4	-22095.1±201.6	-20526.4±807.1
ΔS / J mol^{-1}	-95.7±10.44	-32.8±1.1	-78.7±0.7	-73.7±2.9
$T_{1/2}$	374.1±23.3	293.9±0.2	280.6±3.5	278.5±1.0
R^2	0.96	0.99	0.99	0.99

Table S9. Molar magnetic susceptibility ($\chi_M T$ in $cm_3 \cdot K \cdot mol^{-1}$) values calculated from ^{1}H NMR data by Evans method at different temperatures in $CDCl_3$ solution. Note that all concentrations are based on moles of $[Fe(pyridine)_4(NCBH_3)_2]$, and each solution has a $\boldsymbol{L}^{pytZ}$/iron(II) ratio of 6:1 equivalents. Evans method has a relative error of 5%,[7] therefore significant errors associated with the data fitting discussed (Figures S83-S86). Second column from the left reports the viscosity of $CDCl_3$ solvent at in the range of temperatures employed for the ^{1}H NMR measurements.

T	***η***	***$\chi_m T$ ($cm^3 \cdot K \cdot mol^{-1}$)***				
		CF_3	***Br***	***F***	***H^{21}***	***Me***
313	1451.73	0.41658		2.89185	2.574	2.82624
308	1461.09	0.29182	2.34856	2.77622	2.458	2.75084
303	1470.35	0.2342	2.29631	2.66389	2.328	2.66911
298	1479.52	0.19241	2.24484	2.55476	2.173	2.59229
293	1488.6	0.14416	2.23836	2.38442	1.956	2.46143
288	1497.6	0.12363	2.14607	2.23578	1.768	2.36266
283	1506.51	0.08985	2.0756	2.09228	1.529	2.20489
278	1515.35	0.06519	1.99741	1.93878	1.331	1.99378
273	1524.1	0.06402	1.90116	1.76164	1.165	1.85119
268	1532.78	0.06285	1.8043	1.5628	0.931	1.65362
263	1541.39	0.06167	1.70355	1.44317	0.737	1.4549
258	1549.93	0.0605	1.59594	1.24642	0.573	1.25553
253	1558.4		1.49046	1.08198	0.435	
248	1566.8		1.40171		0.357	
243	1575.14		1.34283		0.311	

VT ^{1}H-NMR of $Fe^{II}(L^{pytCF3})_2(NCBH_3)_2$

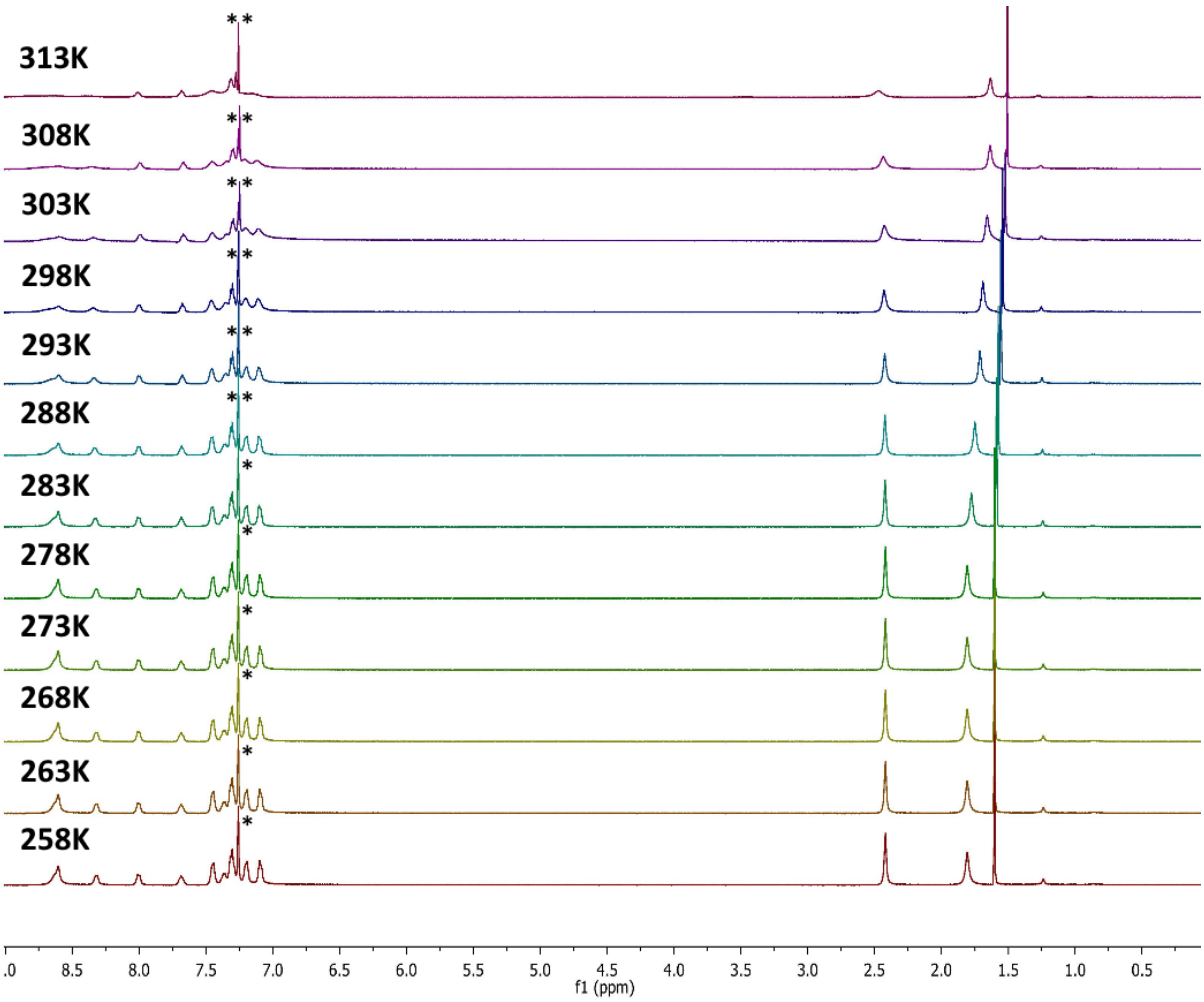

Figure S75. Stacked spectra, obtained by the Evans ^{1}H NMR method, from 258 to 313 K for complex $[Fe^{II}(\boldsymbol{L^{pytCF3}})_2(NCBH_3)_2]$. Note that the solution was prepared using 6 eq. of $\boldsymbol{L^{pytCF3}}$ ligand per eq. of Fe(II).

VT ^{1}H-NMR of $Fe^{II}(L^{pytBr})_2(NCBH_3)_2$

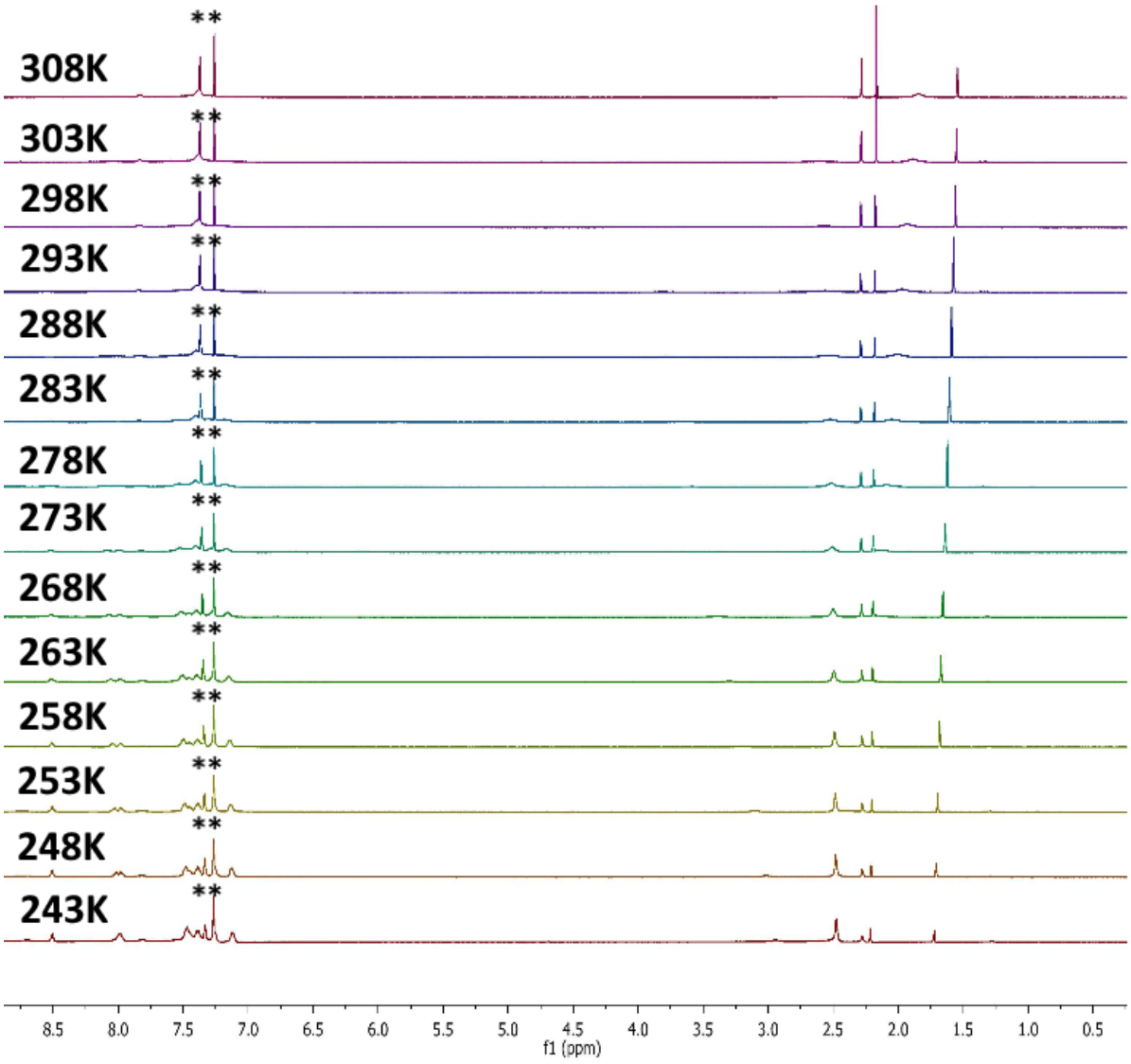

Figure S76. Stacked spectra, obtained by the Evans ^{1}H NMR method, from 243 K to 308 K for complex $[Fe^{II}(\boldsymbol{L}^{pytBr})_2(NCBH_3)_2]$. Note that the solution was prepared using 6 eq. of $\boldsymbol{L}^{pytBr}$ ligand per eq. of Fe(II).

VT ^{1}H-NMR of $Fe^{II}(L^{pytF})_2(NCBH_3)_2$

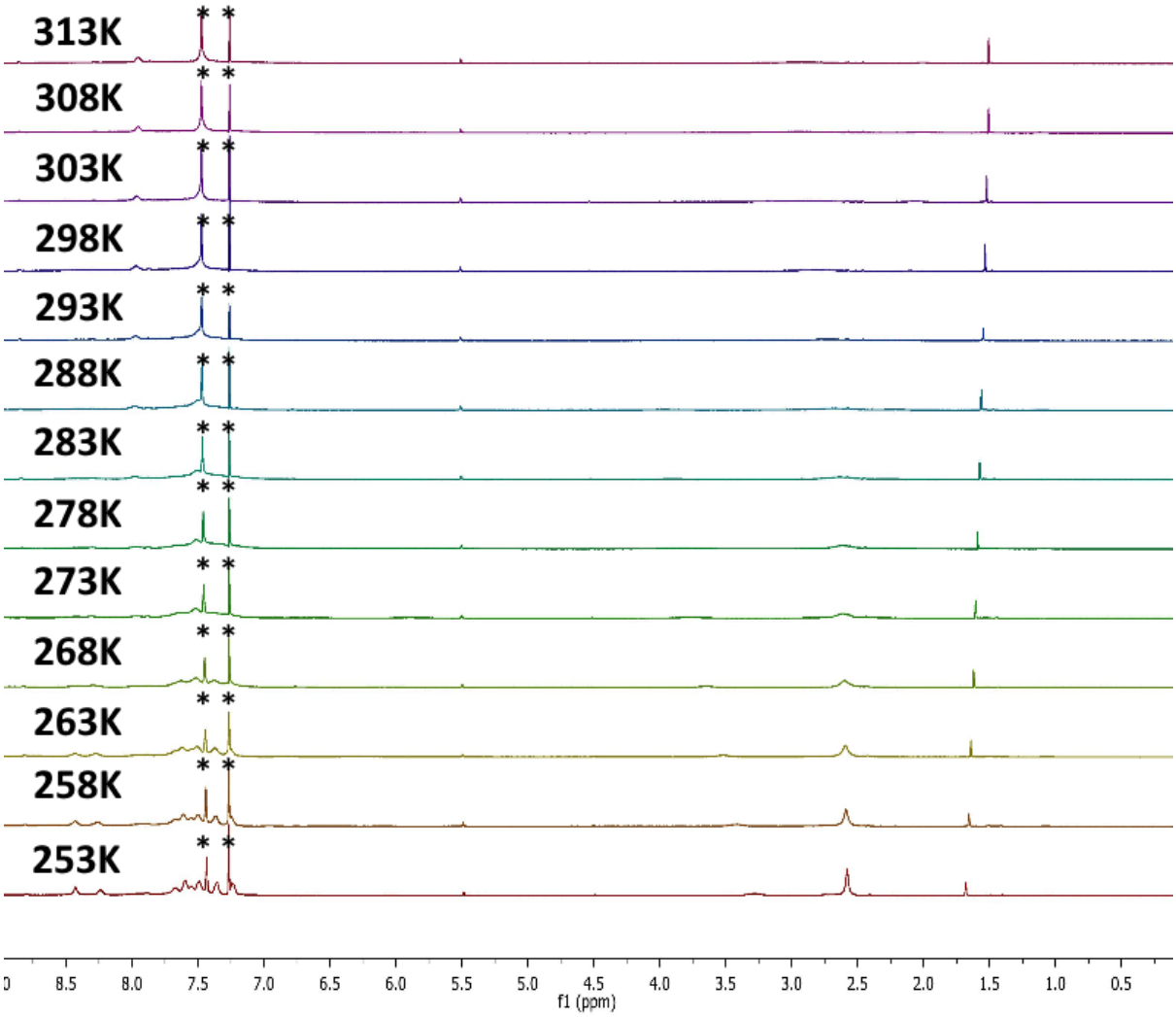

Figure S77. Stacked spectra, obtained by the Evans ^{1}H NMR method, from 253 K to 313 K for complex $[Fe^{II}(\boldsymbol{L^{pytF}})_2(NCBH_3)_2]$. Note that the solution was prepared using 6 eq. of $\boldsymbol{L^{pytF}}$ ligand per eq. of Fe(II).

VT ^{1}H-NMR of $Fe^{II}(L^{pytMe})_2(NCBH_3)_2$

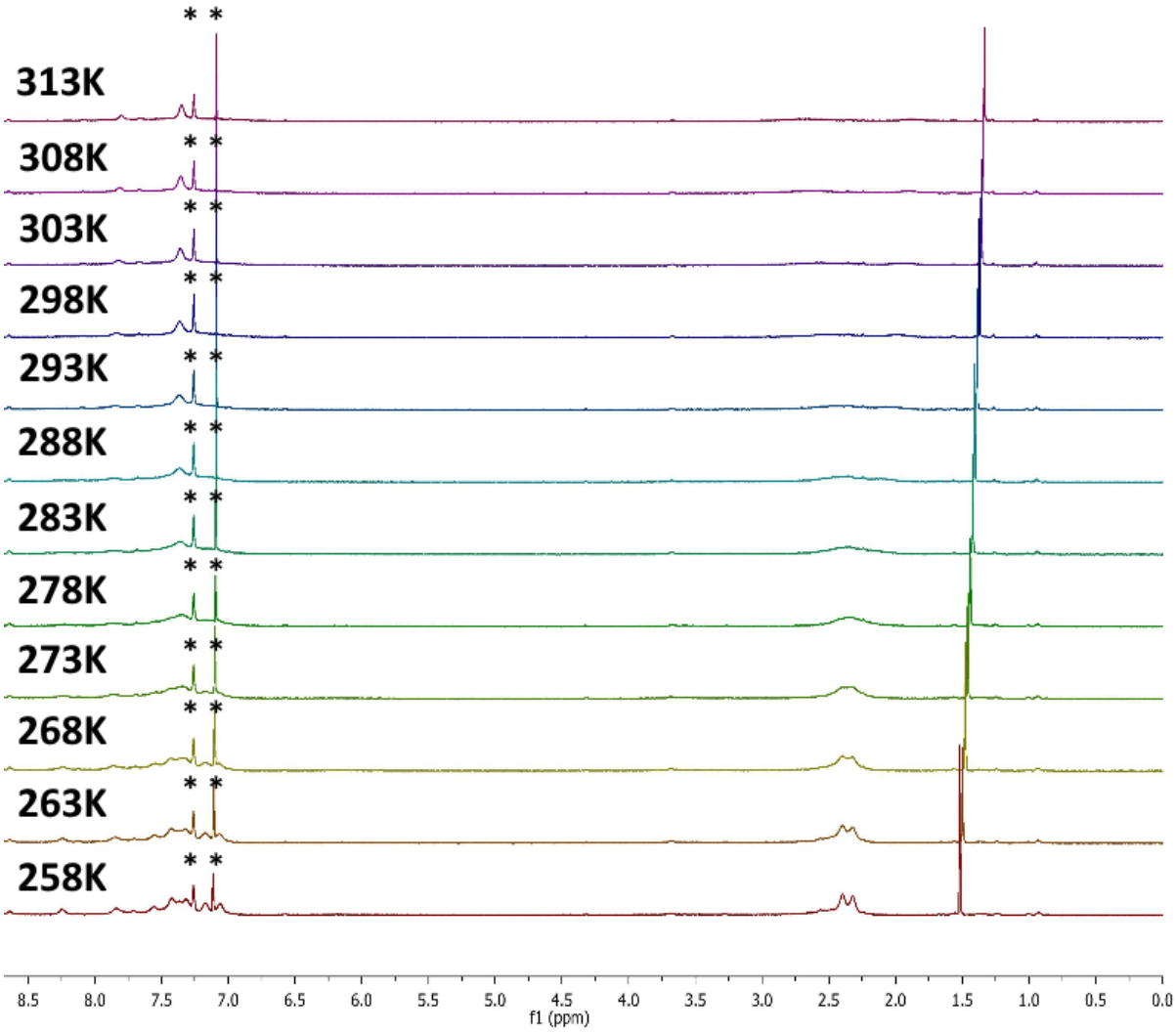

Figure S78. Stacked spectra, obtained by the Evans ^{1}H NMR method, from 258 K to 313 K for complex $[Fe^{II}(\boldsymbol{L^{pytMe}})_2(NCBH_3)_2]$. Note that the solution was prepared using 6 eq. of $\boldsymbol{L^{pytMe}}$ ligand per eq. of Fe(II).

S1.13.2. Evans Method: Error Analysis

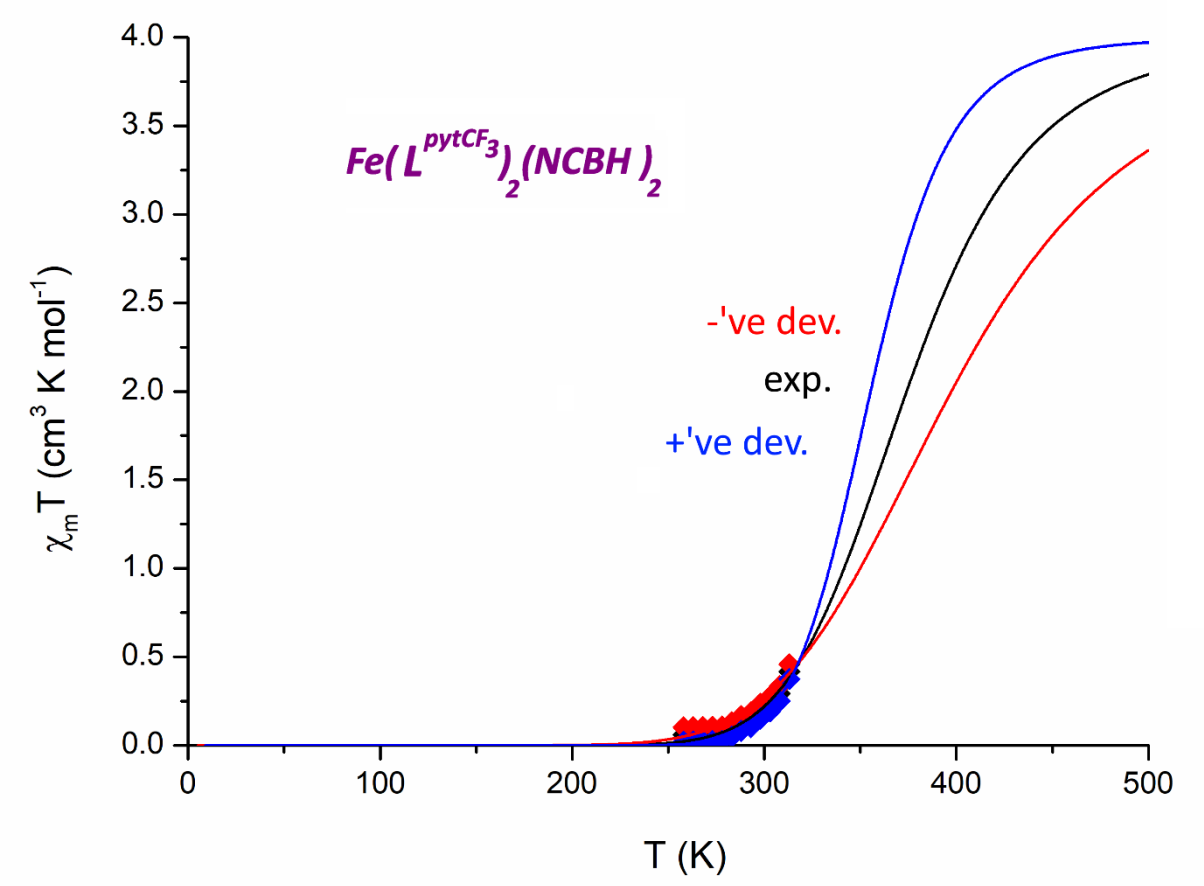

Figure S79. X_mT vs T for $[Fe^{II}(\boldsymbol{L}^{pytCF3})_2(NCBH_3)_2]$ in **$CDCl_3$** solution from Evans NMR method studies (500 MHz); this graph displays the experimental data points (black squares), and the 95% confidence intervals (red and blue) around the fit.

Table S10. Derived parameters obtained by fitting of regular SCO transition (eq. S1) in X_mT vs T for $[Fe^{II}(\boldsymbol{L}^{pytCF3})_2(NCBH_3)_2]$ in **$CDCl_3$** solution from Evans NMR method studies (500 MHz) reported in Fig. S79. Energies are reported in J mol^{-1}.

	+'ve deviation	**experimental**	**-'ve deviation**
ΔH	-26729.9±3019.4	-35806.0±3353.6	-50453.9±2938.4
ΔS	-67.3±9.6	-95.7±10.4	-142.0±8.8
T	397.4	374.1	355.3
R^2	0.92	0.96	0.99

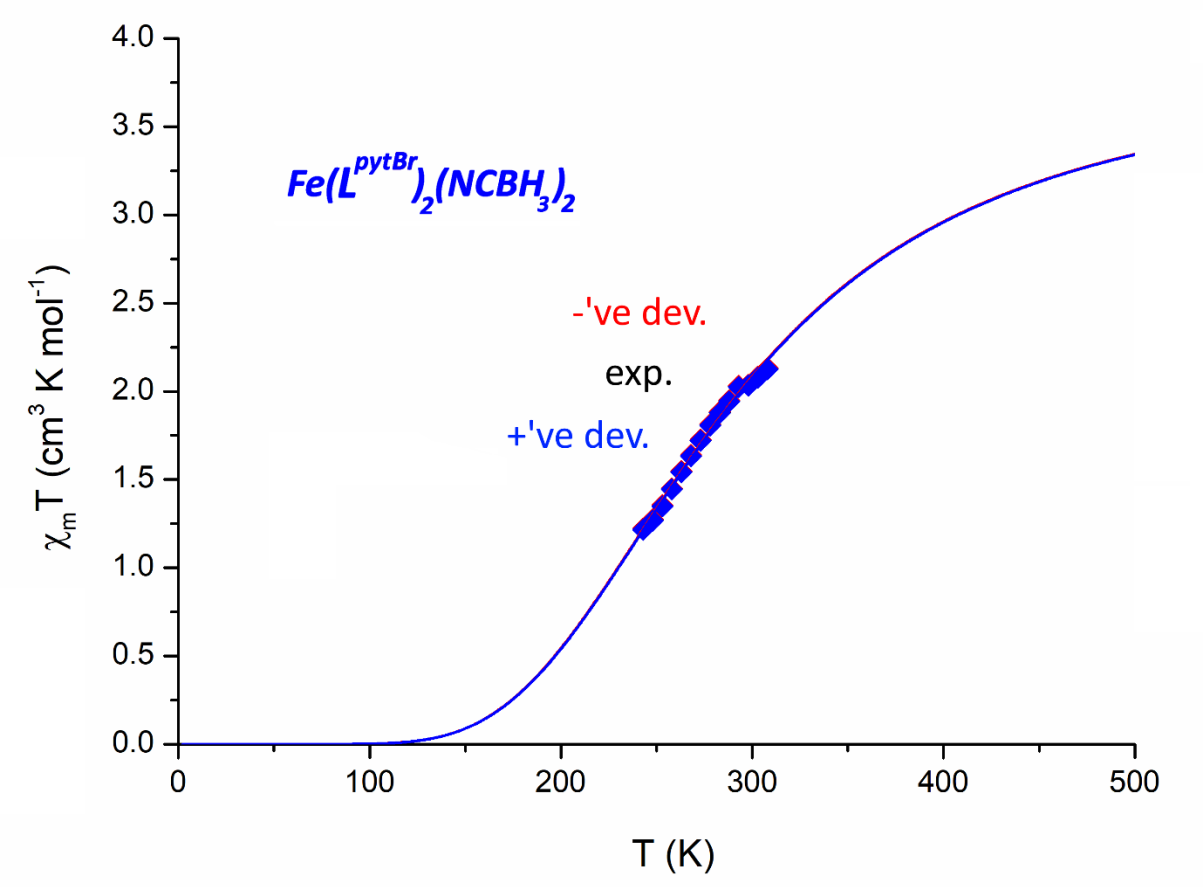

Figure S80. X_mT vs T for $[Fe^{II}(L^{pytBr})_2(NCBH_3)_2]$ in **$CDCl_3$** solution from Evans NMR method studies (500 MHz); this graph displays the experimental data points (black squares), and the 95% confidence intervals (red and blue) around the fit.

Table S11. Derived parameters obtained by fitting of regular SCO transition (eq. S1) in X_mT vs T for $[Fe^{II}(L^{pytBr})_2(NCBH_3)_2]$ in **$CDCl_3$** solution from Evans NMR method studies (500 MHz) reported in Fig. S80. Energies are reported in J mol^{-1}.

	+'ve deviation	**experimental**	**-'ve deviation**
ΔH	-9641.2±291.7	-9645.8±292.4	-9650.4±293.1
ΔS	-32.8±1.1	-32.8±1.1	-32.8±1.1
T	293.7	293.9	294.1
R^2	0.99	0.99	0.99

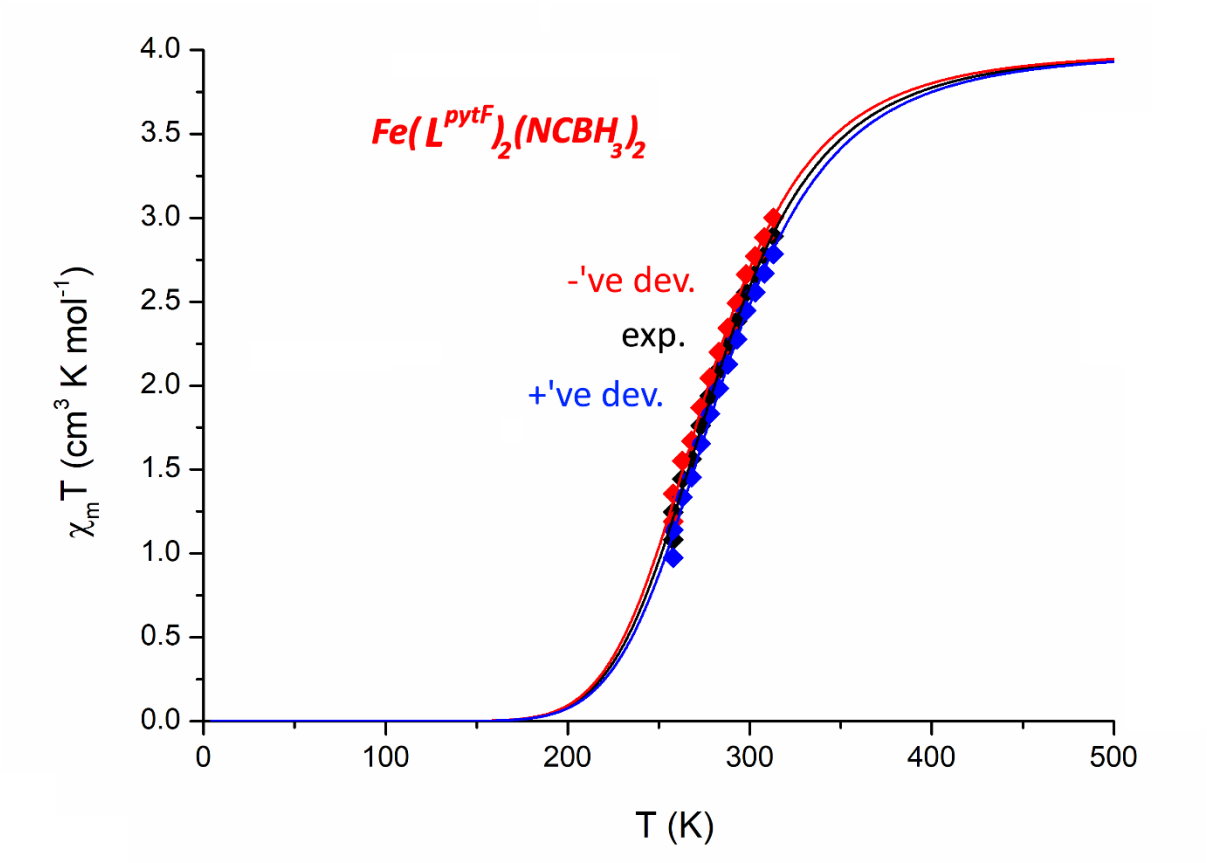

Figure S81. X_mT vs T for $[Fe^{II}(L^{pytF})_2(NCBH_3)_2]$ in **$CDCl_3$** solution from Evans NMR method studies (500 MHz); this graph displays the experimental data points (black squares), and the 95% confidence intervals (red and blue) around the fit.

Table S12. Derived parameters obtained by fitting of regular SCO transition (eq. S1) in X_mT vs T for $[Fe^{II}(L^{pytF})_2(NCBH_3)_2]$ in **$CDCl_3$** solution from Evans NMR method studies (500 MHz) reported in Fig. S81. Energies are reported in J mol^{-1}.

	+'ve deviation	**experimental**	**-'ve deviation**
ΔH	-22221.9±671.8	-22095.1±705.9	-22089.0±764.8
ΔS	-80.2±2.4	-78.7±2.5	-77.7±2.7
T	277.3	280.6	284.1
R^2	0.99	0.99	0.99

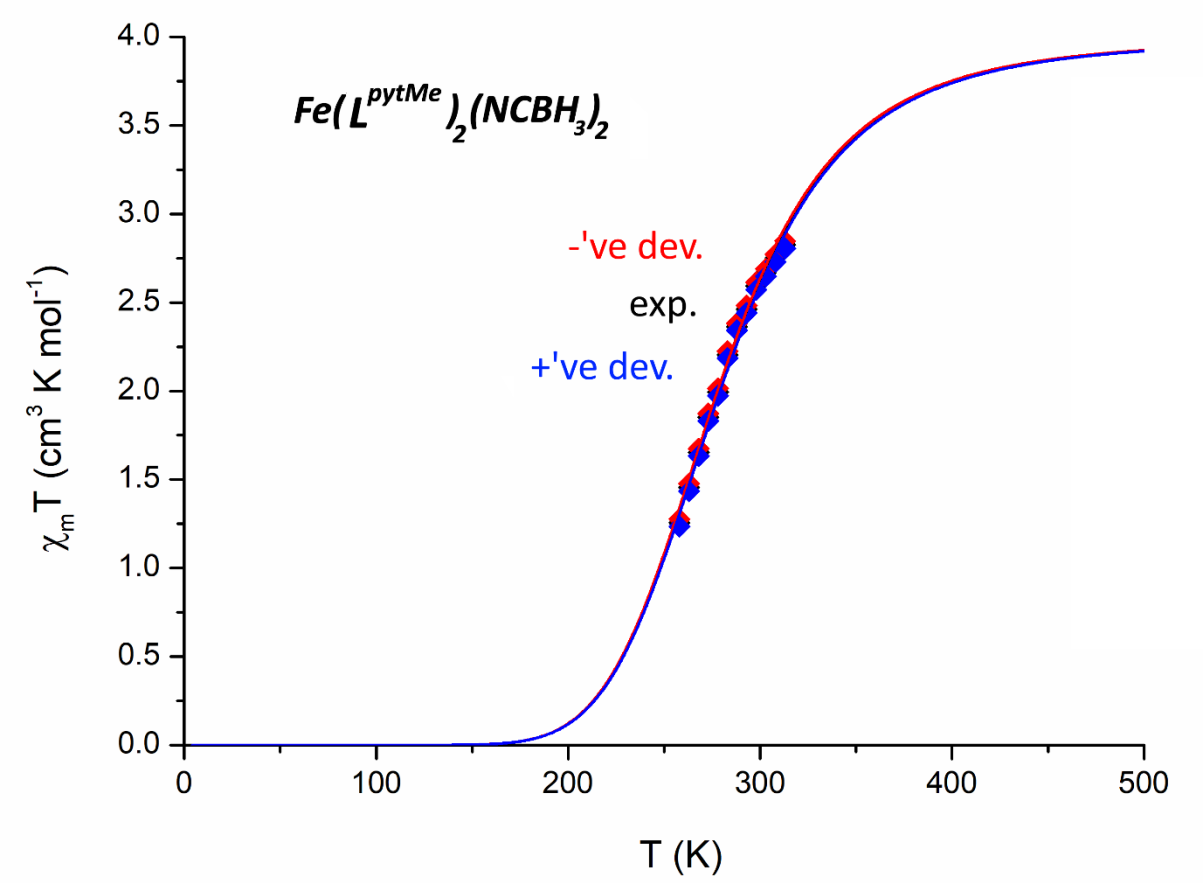

Figure S82. X_mT vs T for $[Fe^{II}(L^{pytMe})_2(NCBH_3)_2]$ in **$CDCl_3$** solution from Evans NMR method studies (500 MHz); this graph displays the experimental data points (black squares), and the 95% confidence intervals (red and blue) around the fit.

Table S13. Derived parameters obtained by fitting of regular SCO transition (eq. S1) in X_mT vs T for $[Fe^{II}(L^{pytMe})_2(NCBH_3)_2]$ in **$CDCl_3$** solution from Evans NMR method studies (500 MHz) reported in Fig. S82. Energies are reported in J mol^{-1}.

	+'ve deviation	experimental	-'ve deviation
ΔH	-20571.0±789.4	-20526.4±807.2	-20488.6±825.2
ΔS	-74.1±2.9	-73.7±2.9	-73.4±2.9
T	277.8	278.5	279.2
R^2	0.99	0.99	0.99

S1.14. UV-Vis spectra of [Fe(L^{pytZ})$_2$(NCBH$_3$)$_2$]

UV-Vis studies for all the complexes were carried out in chloroform (Figure S83). The concentration of samples was 0.04 mM. Fe(***L***^{pytF})$_2$(NCBH$_3$)$_2$ shows λ_{max} at 411 and 506 nm; Fe(***L***^{pytCF3})$_2$(NCBH$_3$)$_2$ shows λ_{max} at 520 and 566 nm; Fe(***L***^{pytBr})$_2$(NCBH$_3$)$_2$ shows λ_{max} at 495 and 531 nm; Fe(***L***^{pytMe})$_2$(NCBH$_3$)$_2$ shows λ_{max} at 450 and 500 nm. The all four other Fe(***L***^{pytZ})$_2$(NCBH$_3$)$_2$ shows an extinction coefficient between 1500 and 2500 $M^{-1}cm^{-1}$ for the higher energy transition and between 2000 and 6000 $M^{-1}cm^{-1}$ for the lower energy transition. For all complexes, bands observed in the visible region, originate from charge transfer (CT), with large value of molar extinction coefficient.

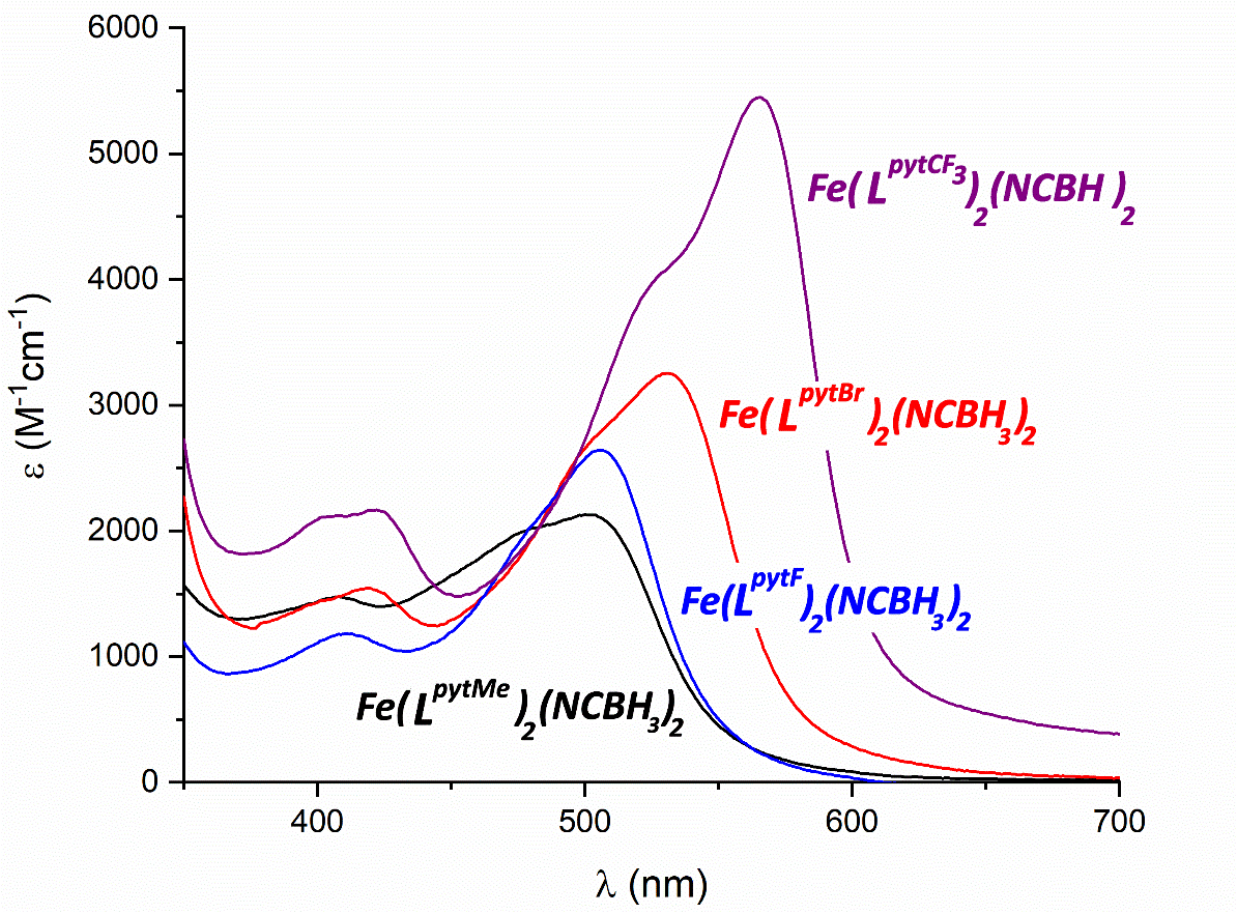

Figure S83. UV-visible spectra (700nm to 350 nm) collected using a 1:6 ratio of Fe(pyridine)$_4$(NCBH$_3$)$_2$: ***L***^{pytZ}, with [Fe] = 0.5 mM.

S2. Computational Details

S2.1. Protocol

Calculations were performed using ORCA4.1.[30] The computational protocol used to optimise the structures of the ligands was RIJCOSX-TPSS-D3(BJ)/*pcSseg-2*+CPCM.[31-36] i.e. use of the TPSS functional[49] together with the resolution of identity (RIJCOSX) approximation,[35-36] Grimme's D3 dispersion correction (including BJ damping),[33-34] a *pcSseg-2* basis set[50] and implicit CPCM-solvent model. Finally, ^{15}N NMR calculations were performed on the DFT optimised structures through a single point calculation. Different CPCM models were applied, based on the solvent used experimentally to measure the SCO phenomenon: $CDCl_3$ for $\boldsymbol{L^{azine}}$ and $\boldsymbol{L^{pytZ}}$; acetone for **pybox**^{X} and **bpp**^{X,Y}, acetonitrile for **pytacn**^{X}.

S2.2. Ligand Structures

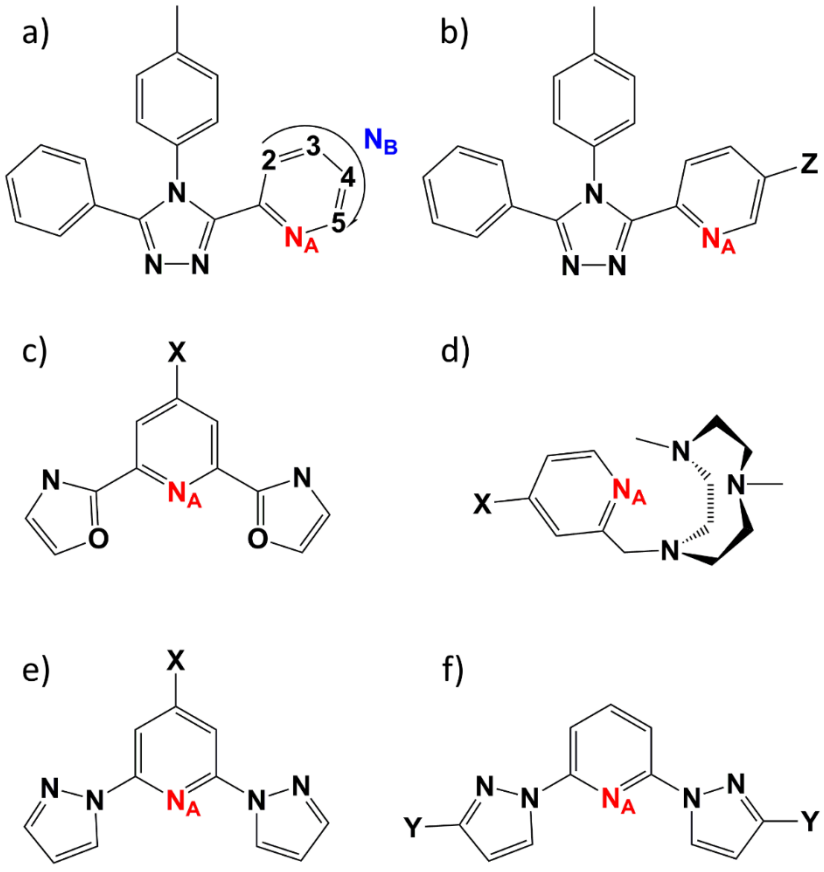

Figure S84. Five families of ligands focussed on in this study. (a) five of $\boldsymbol{L^{azine}}$; (b) five of $\boldsymbol{L^{pytZ}}$; (c) twelve of **pybox**^{X}; (d) seven of **pytacn**^{X}; (e) eleven of **bpp**^{X}; (e) four of **bpp**^{Y}.

S2.3. Calculated N_A-NMR

Table S14. Summary of the $T_{1/2}$ (K) for the family of five $[Fe^{II}(\mathbf{L^{azine}})_2(NCBH_3)_2]$ complexes (right column) and of the comparison between found and calculated ^{15}N NMR chemical shift values (ppm) for N_A (coordinated azine N) of the $\mathbf{L^{azine}}$ ligand previously reported by Brooker and co-workers[27] and those calculated in this study. Deviation to experimental ^{15}N NMR chemical shift is also reported as a % for both the computational protocols.

	Measured ^{15}N-NMR from ref[27]	Lit. study:[27] **B3LYP/ 6-31G(d) CPCM($CHCl_3$)**		This study: **TPSS/pcSseg-2 aug-cc-pVTZ/ RIJCOSX/D3BJ/CPCM(CH_3Cl)**		**$T_{1/2}$** from ref[27]
		^{15}N NMR	**Err%**	**^{15}N NMR**	**Err%**	
***L*^{4pyrimidine}**	288	269	6.6%	286	0.7%	232
***L*^{2pyrimidine}**	290	282	2.8%	291	0.3%	242
***L*^{pytH}**	311	300	3.9%	308	1.0%	288
***L*^{pyrazine}**	334	315	5.7%	321	3.9%	315
***L*^{pyridazine}**	398	402	1.0%	401	0.8%	455

Table S15. Values of σ_m^+ and σ_m from the literature,[37] along with the $\mathbf{N_A}$ (N of pyridine ring) ^{15}N chemical shift (ppm) for the new four ***L*^{pytZ}** ligands obtained herein by calculation using the improved protocol (TPSS/pcSseg-2/aug-cc-pVTZ/ RIJCOSX/D3BJ/CPCM($CHCl_3$)) and by experimental measurement (d = direct method, i = indirect method), along with the experimentally determined solution $T_{1/2}$ (K) of the respective new $[Fe(\boldsymbol{L^{pytZ}})_2(NCBH_3)_2]$ complex also determined herein (right column).

	σ_m^+ ref[37]	σ_m ref[37]	**Solvent**	**δN_A (ppm) Measured**	**δN_A (ppm) Calculated**	**Err%**	**$T_{1/2}$**
***L*^{pytMe}**	-0.31	-0.17	$CDCl_3$	312 (d)	310	0.6%	279
***L*^{pytF}**	0.35	0.34	$CDCl_3$	319 (i)	315	1.3%	281
***L*^{pytBr}**	0.15	0.23	$CDCl_3$	318 (d/i)	312	1.6%	294
***L*^{pytCF3}**	0.52	0.43	$CDCl_3$	314 (d)	307	2.2%	374

Table S16. Results calculated **δN_A** (ppm) for the twelve **pybox^X** family calculated using the TPSS/pcSseg-2/aug-cc-pVTZ/ RIJCOSX/D3BJ/CPCM(Acetone) computational protocol, along with the literature values of σ_p^+ and/or σ_p for the substituents for which they are available,[37] and the literature $T_{1/2}$ values in K.[38]

	σ_p^+ ref[37]	σ_p ref[37]	Solvent	δN_A (ppm)	$T_{1/2}$ ref[38]
pybox-X-4Py	-	0.44	$CO(CD_3)_2$	277	310
pybox-X-3Py	-	0.25	$CO(CD_3)_2$	273	270
pybox-X-2Th	-0.43	0.05	$CO(CD_3)_2$	269	260
pybox-X-3Th	-0.38	-0.02	$CO(CD_3)_2$	269	240
pybox-X-Cl	0.11	0.23	$CO(CD_3)_2$	274	270
pybox-X-Br	0.15	0.23	$CO(CD_3)_2$	272	280
pybox-X-H	0	0	$CO(CD_3)_2$	279	260
pybox-X-OMe	-0.78	-0.27	$CO(CD_3)_2$	258	170
pybox-X-Ph	-0.18	-0.01	$CO(CD_3)_2$	272	240
pybox-X-SMe	-0.60	0.00	$CO(CD_3)_2$	261	210
pybox-X-N$_3$	-	0.08	$CO(CD_3)_2$	268	215
pybox-X-Me	-0.31	-0.17	$CO(CD_3)_2$	271	220

Table S17. Results calculated **δN_A** (ppm) for the seven **pytacn^X** family calculated using the TPSS/pcSseg-2/aug-cc-pVTZ/ RIJCOSX/D3BJ/CPCM(Acetonitrile) computational protocol, along with the literature values of σ_p^+ and/or σ_p for all of the substituents employed,[37] and the literature μ_{eff} values at 298 K in acetonitrile in BM.[39]

Name	σ_p^+ ref[37]	σ_p ref[37]	Solvent	δN_A (ppm)	μ_{eff} ref[39]
Pytacn-X-NO$_2$	0.79	0.78	CD_3CN	320	0.00
Pytacn-X-CO$_2$Et	0.48	0.45	CD_3CN	303	0.78
Pytacn-X-Me	-0.31	-0.17	CD_3CN	281	1.24
Pytacn-X-H	0	0	CD_3CN	291	1.26
Pytacn-X-Cl	0.11	0.23	CD_3CN	284	1.71
Pytacn-X-OMe	-0.78	-0.27	CD_3CN	267	2.09
Pytacn-X-NMe$_2$	-1.70	-0.83	CD_3CN	249	2.62

Table S18. Results calculated **δN$_A$** (ppm) for the eleven *para*-substituted **bpp^X** family calculated using the TPSS/pcSseg-2/aug-cc-pVTZ/ RIJCOSX/D3BJ/CPCM(Acetone) computational protocol, along with the literature values of σ_p^+ and/or σ_p for the substituents for which they are available,[37] and the literature $T_{1/2}$ values in K.[6]

	σ_p^+ ref[37]	σ_p ref[37]	Solvent	δN$_A$ (ppm)	$T_{1/2}$
bpp-X-H	0	0	$CO(CD_3)_2$	235	248[40]
bpp-X-Br	0.15	0.23	$CO(CD_3)_2$	231	234[6]
bpp-X-CCPh-CN	--	--	$CO(CD_3)_2$	231	259[41]
bpp-X-CCPh	--	--	$CO(CD_3)_2$	230	245[41]
bpp-X-CCPh-NO2	--	--	$CO(CD_3)_2$	232	261[41]
bpp-X-Cl	0.11	0.23	$CO(CD_3)_2$	230	226[6]
bpp-X-CO2H	0.42	0.45	$CO(CD_3)_2$	244	281[6]
bpp-X-OH	-0.92	-0.37	$CO(CD_3)_2$	217	164[6]
bpp-X-OMe	-0.78	-0.27	$CO(CD_3)_2$	216	158[6]
bpp-X-SMe	-0.60	0.00	$CO(CD_3)_2$	222	194[42]
bpp-X-SOMe	--	0.49	$CO(CD_3)_2$	235	284[42]

Table S19. Results calculated **δN$_A$** (ppm) for the four *meta*-substituted **bpp^Y** family calculated using the TPSS/pcSseg-2/aug-cc-pVTZ/ RIJCOSX/D3BJ/CPCM(Acetone) computational protocol, along with the literature values of σ_p^+ and/or σ_p for the substituents for which they are available,[37] and the literature $T_{1/2}$ values in K.[6]

	σ_m^+ ref[37]	σ_m ref[37]	Solvent	δN$_A$ (ppm)	$T_{1/2}$
bpp-Y-H	0	0	$CO(CD_3)_2$	235	248[40]
bpp-Y-CO2Et	0.37	0.45	$CO(CD_3)_2$	240	246[43]
bpp-Y-tBu	-0.06	-0.10	$CO(CD_3)_2$	239	251[6]
bpp-Y-CH2OH	--	0.00	$CO(CD_3)_2$	236	259[43]

S3. Correlations

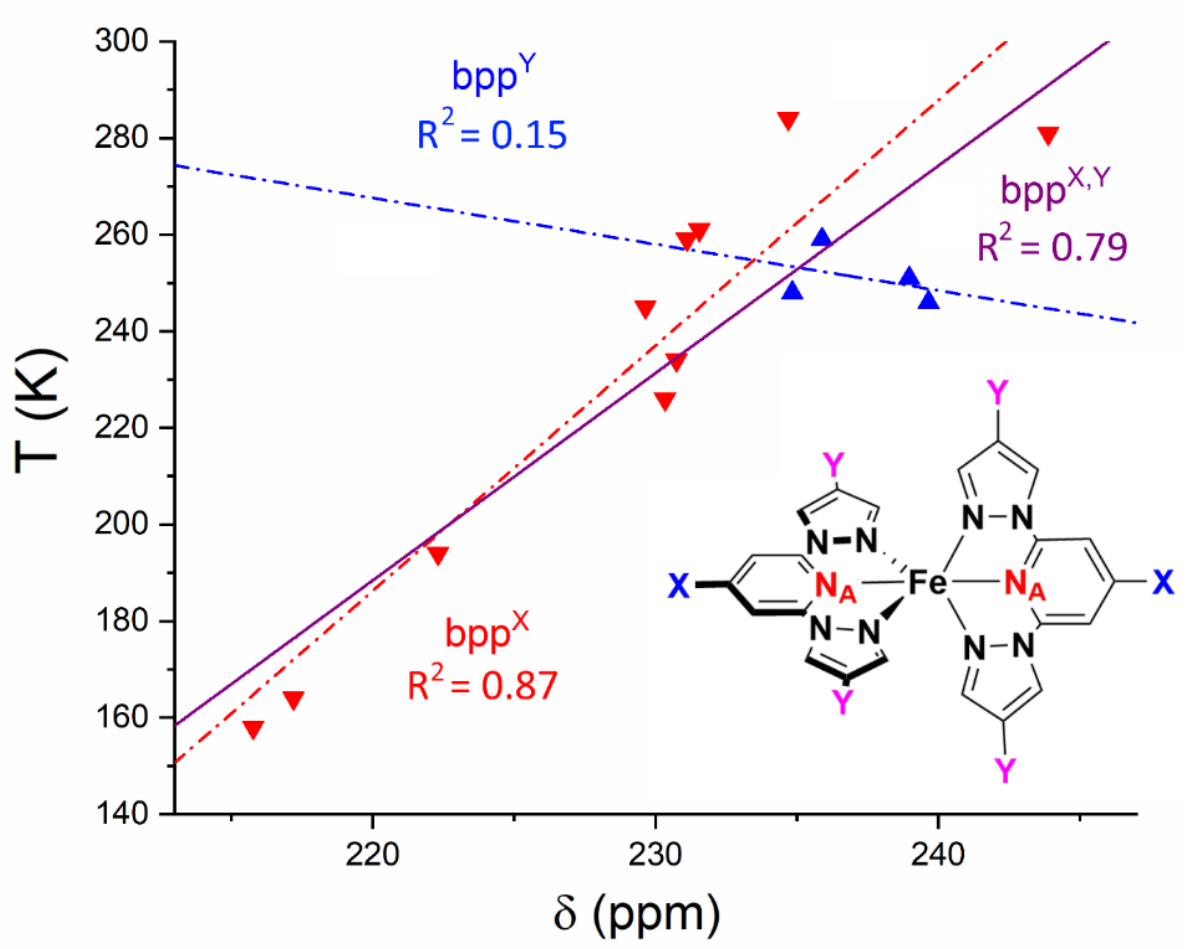

Figure S85. Correlations between the $T_{1/2}$ of the $[Fe^{II}(\mathbf{bpp^{X,Y}})_2]^{2+}$ complexes and the measured $\delta\mathbf{N_A}$ chemical shift for the corresponding tridentate ligand $\mathbf{bpp^{X,Y}}$. Correlation lines are shown for: (purple) for all fourteen compounds with no distinction made between **X** and **Y** substituents (R^2 = 0.80; $\mathbf{T_{1/2}}$ = 4.29·$\boldsymbol{\delta N_A}$ – 756.29); and then taking in account only the (blue; $\mathbf{T_{1/2}}$ = -0.96·$\boldsymbol{\delta N_A}$ – 478.37) four **Y**-substituted (R^2 = 0.15) and the (red; $\mathbf{T_{1/2}}$ = 5.23·$\boldsymbol{\delta N_A}$ – 1169.24) eleven **X**-substituted (R^2 = 0.87) compounds.

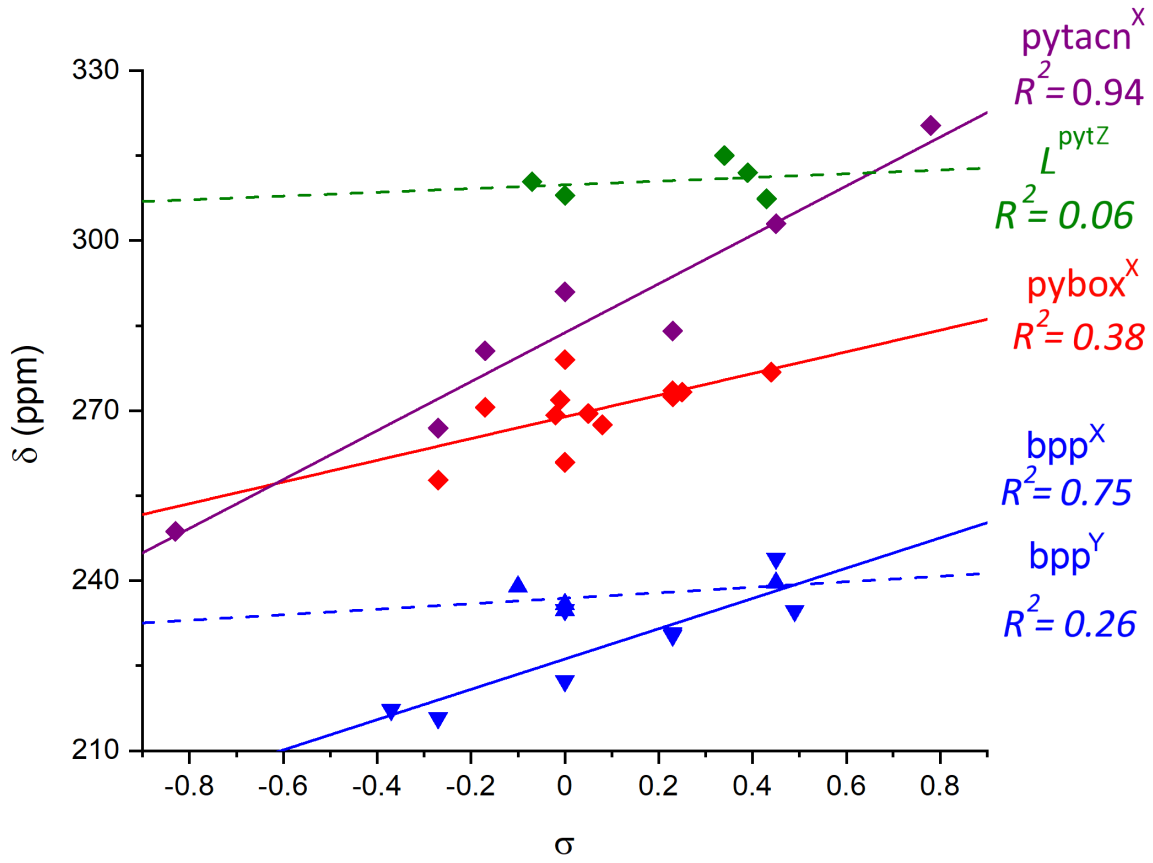

Figure S86. Correlation between the calculated ^{15}N chemical shift $\delta\mathbf{N_A}$ of the free ligand for each of the families reported in this study against the relative value of the Hammett parameter σ (rather than σ^+; see Tables S15-S19 for the values of σ and σ^+, where they are available in the literature[37]) of the substituent on the pyridine ring (note: a substituent with a positive Hammett parameter is **EWG**, whilst one with a negative value is **EDG**; H is by definition 0).[37] Solid lines for ligands with *para* substituents (σ_p is used in this case); dashed lines for ligands with *meta* substituents (σ_m is used in this case). Good correlation found for a family of eight **bpp^X** ligands (blue, down-faced triangles; $\mathbf{\delta N_A} = 26.73\cdot\boldsymbol{\sigma} - 226.18$) and seven **pytacn^X** ligands (purple, diamonds; $\mathbf{\delta N_A} = 44.13\cdot\boldsymbol{\sigma} - 283.46$); poor correlation found for four **bpp^Y** ligands (blue, up-faced triangles; $\mathbf{\delta N_A} = 4.85\cdot\boldsymbol{\sigma} - 236.91$); twelve **pybox^X** (red, diamonds; $\mathbf{\delta N_A} = 19.13\cdot\boldsymbol{\sigma} - 268.90$) and five ***L^{pytZ}*** (green, diamonds; $\mathbf{\delta N_A} = 3.28\cdot\boldsymbol{\sigma} - 309.84$). Note: The difference between σ and σ^+ is due to the use of a different reference reaction in which the effect of the **EDG**/**EWG** substituent is assessed: for σ it is acid/base dissociation of a *para/meta* substituted benzoic acid and whereas for σ^+ it is nucleophilic substitution at the carbonyl carbon in a *para/meta* substituted benzoic acid derivative.[44]

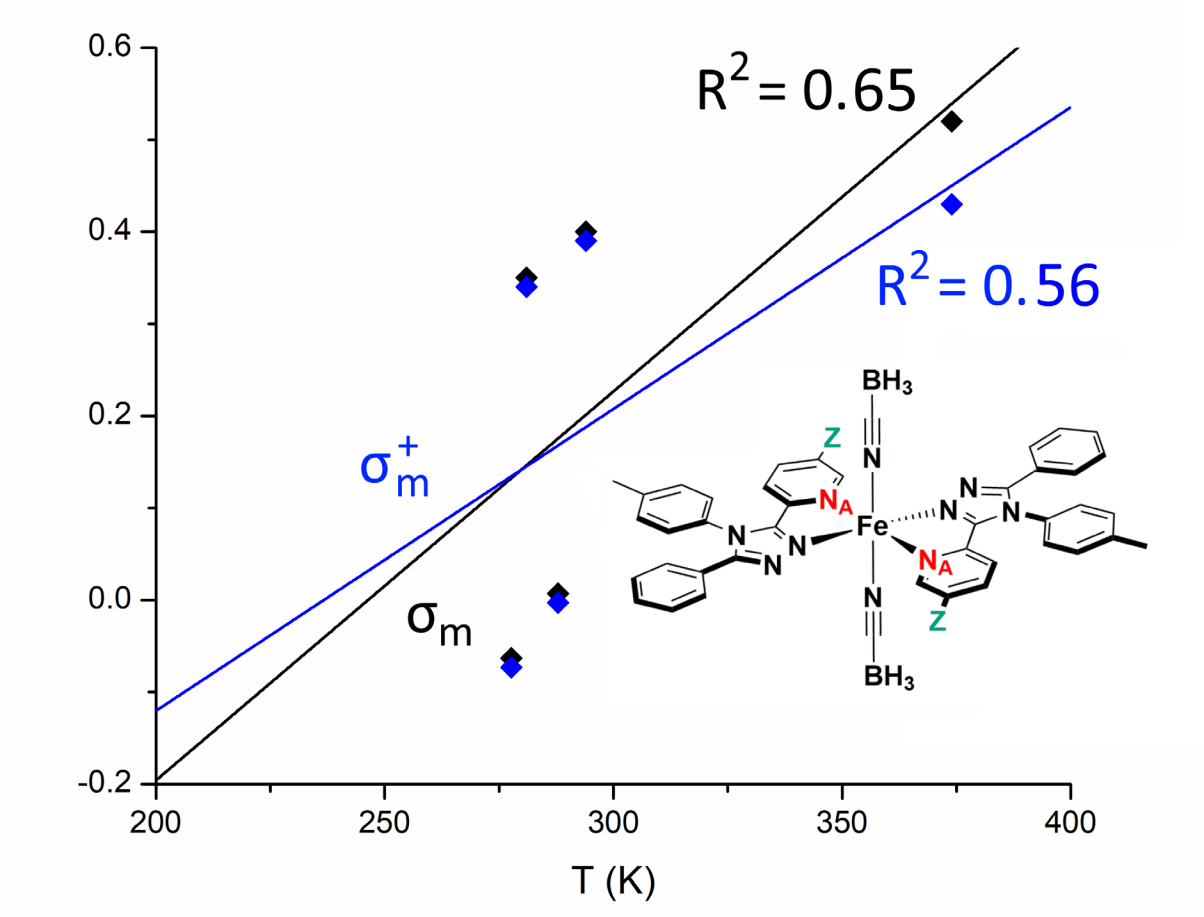

Figure S87. Reported correlation between the measured $T_{1/2}$ for the new family of L^{pytZ} versus the relative value of Hammett parameter[37] σ_m (blue dots, R^2 = 0.22, $\boldsymbol{\sigma_m}$ = 0.003·$\mathbf{T_{1/2}}$ -0.78) and the Hammett parameter[37] σ^+_m (black dots, R^2 = 0.32, $\boldsymbol{\sigma^+_m}$ = 0.004·$\mathbf{T_{1/2}}$ -1.04).

S4. Atomic Coordinates

Pybox-H

N	0.007624	0.001767	1.590152
O	2.351818	0.062627	0.157968
C	1.159722	0.022291	2.289069
C	1.211062	0.014276	3.702619
H	2.183214	0.032022	4.214007
C	0.001481	-0.016500	4.408657
C	2.411271	0.054378	1.524907
N	3.643141	0.077562	1.991561
C	4.451789	0.102706	0.866578
H	5.546495	0.125696	0.929133
C	3.656569	0.093537	-0.256003
C	-1.205014	-0.038184	3.696998
C	-1.147487	-0.027894	2.283689
C	-2.395372	-0.050538	1.513266
O	-2.329019	-0.040411	0.146611
C	-3.631695	-0.067059	-0.274286
C	-4.432507	-0.091853	0.844078
H	-5.527472	-0.116684	0.901101
N	-3.629522	-0.081107	1.973357
H	-2.179268	-0.062686	4.204052
H	-0.000885	-0.023641	5.508574
H	3.834335	0.104972	-1.335583
H	-3.803930	-0.064196	-1.354825

Pybox-X-F

N	0.007708	0.001921	1.573997
O	2.356889	0.062699	0.147561
C	1.159252	0.022573	2.273568
C	1.219737	0.014830	3.685362
H	2.179792	0.032316	4.217520
C	0.001548	-0.016222	4.368349
C	2.412991	0.054622	1.513718
N	3.642561	0.077749	1.985080
C	4.454637	0.102766	0.863146
H	5.549091	0.125715	0.929061
C	3.662476	0.093467	-0.262137
C	-1.213613	-0.038400	3.679629
C	-1.146888	-0.027847	2.268135
C	-2.396986	-0.050606	1.502023

O	-2.334042	-0.040477	0.136131
C	-3.637603	-0.066715	-0.280440
C	-4.435308	-0.092215	0.840671
H	-5.530026	-0.117289	0.901086
N	-3.628844	-0.081030	1.966884
H	-2.175901	-0.062945	4.207420
F	-0.001424	-0.024971	5.710535
H	3.843577	0.104707	-1.341164
H	-3.813244	-0.063595	-1.360427

Pybox-X-Me

N	0.005256	0.001526	1.571842
O	2.356877	0.062604	0.155617
C	1.152969	0.022093	2.280219
C	1.199167	0.014132	3.690184
H	2.174125	0.032110	4.198253
C	-0.005529	-0.016733	4.420110
C	2.409710	0.054342	1.522961
N	3.639465	0.077655	1.995027
C	4.453546	0.102957	0.873545
H	5.547952	0.126102	0.941374
C	3.663833	0.093668	-0.252569
C	-1.202245	-0.038086	3.682295
C	-1.145895	-0.028009	2.270064
C	-2.397682	-0.050781	1.504994
O	-2.336614	-0.040945	0.137906
C	-3.641024	-0.067136	-0.278376
C	-4.437568	-0.091980	0.842808
H	-5.532328	-0.116711	0.903910
N	-3.630329	-0.080930	1.969301
H	-2.180400	-0.062434	4.183522
C	-0.000353	-0.026269	5.925401
H	3.846452	0.105065	-1.331324
H	-3.817175	-0.064263	-1.358273
H	-1.026743	-0.050459	6.337188
H	0.516665	0.872792	6.319845
H	0.553919	-0.907929	6.308395

Pybox-X-N3

N	0.086906	-0.164540	1.922790
O	2.369139	0.218264	0.444200
C	1.266292	-0.239463	2.572642
C	1.386610	-0.499520	3.952856

H	2.372311	-0.549804	4.433274
C	0.206643	-0.692029	4.694338
C	2.485754	-0.036075	1.782814
N	3.734452	-0.064958	2.200387
C	4.495411	0.185460	1.070105
H	5.591066	0.225826	1.095092
C	3.654358	0.358788	-0.005175
C	-1.035540	-0.617345	4.034318
C	-1.032641	-0.351183	2.649636
C	-2.317637	-0.269822	1.946508
O	-2.321354	-0.013634	0.603517
C	-3.643003	0.000435	0.247409
C	-4.384947	-0.245949	1.379884
H	-5.474846	-0.309528	1.483703
N	-3.524691	-0.415612	2.452482
H	-1.989158	-0.758680	4.562050
N	0.346034	-0.951152	6.069685
H	3.786526	0.569986	-1.070625
H	-3.870411	0.192168	-0.805559
N	-0.657991	-1.127839	6.772010
N	-1.486034	-1.311776	7.546480

Pybox-X-NH2

N	0.007128	0.000398	1.580377
O	2.356672	0.062757	0.175274
C	1.151335	0.020850	2.299499
C	1.210740	0.013377	3.702823
H	2.186394	0.031903	4.208476
C	-0.000064	-0.017742	4.446508
C	2.411201	0.053604	1.542876
N	3.642104	0.076862	2.011854
C	4.454552	0.102819	0.888351
H	5.549133	0.125979	0.954439
C	3.663331	0.094307	-0.235954
C	-1.207086	-0.039945	3.696424
C	-1.140611	-0.029481	2.293413
C	-2.396363	-0.051726	1.529669
O	-2.334102	-0.040982	0.162363
C	-3.638487	-0.066504	-0.256587
C	-4.435991	-0.091577	0.863028
H	-5.530905	-0.115836	0.922885
N	-3.629863	-0.081654	1.991336
H	-2.185307	-0.064450	4.197047
N	-0.003383	-0.025927	5.802963

H	3.843560	0.106471	-1.315081
H	-3.812583	-0.062886	-1.336787
H	-0.877935	-0.044679	6.325676
H	0.868779	-0.006887	6.329607

Pybox-X-NMe2

N	0.024204	0.000613	1.528556
O	2.373580	0.050336	0.122288
C	1.168497	0.010891	2.246963
C	1.233933	-0.001047	3.650110
H	2.219804	0.010318	4.129389
C	0.024754	-0.027901	4.404251
C	2.428252	0.037071	1.489740
N	3.659492	0.050188	1.958395
C	4.471944	0.073601	0.834849
H	5.566665	0.088811	0.900819
C	3.680488	0.073668	-0.289294
C	-1.184644	-0.036497	3.650061
C	-1.119809	-0.022342	2.246965
C	-2.379822	-0.032173	1.489837
O	-2.325526	-0.017340	0.122365
C	-3.632653	-0.031262	-0.289159
C	-4.423745	-0.053693	0.835022
H	-5.518435	-0.069550	0.901322
N	-3.610913	-0.054098	1.958525
H	-2.170243	-0.053773	4.129502
N	0.024666	-0.043553	5.769807
H	3.860443	0.087383	-1.368440
H	-3.812924	-0.022826	-1.368308
C	-1.238575	-0.057027	6.497106
C	1.287133	-0.014950	6.497977
H	1.867757	0.907398	6.278212
H	1.925195	-0.888823	6.244317
H	1.079043	-0.042947	7.581653
H	-1.030288	-0.085011	7.580622
H	-1.849317	-0.948534	6.237886
H	-1.847144	0.848339	6.282202

Pybox-X-OH

N	0.005893	0.001618	1.567080
O	2.358508	0.062585	0.150510
C	1.153422	0.022425	2.274190
C	1.212199	0.014873	3.682762

H	2.184376	0.033244	4.196220
C	0.001015	-0.016705	4.400858
C	2.410769	0.054646	1.517267
N	3.639815	0.077889	1.990505
C	4.454776	0.102993	0.869716
H	5.549123	0.126093	0.938278
C	3.665633	0.093335	-0.256897
C	-1.209009	-0.038876	3.678677
C	-1.144990	-0.028299	2.271949
C	-2.397892	-0.050952	1.506692
O	-2.334135	-0.040697	0.140070
C	-3.637709	-0.066817	-0.278779
C	-4.436236	-0.091592	0.840921
H	-5.531103	-0.116122	0.900158
N	-3.630853	-0.081184	1.968922
H	-2.176013	-0.063647	4.198478
O	-0.056967	-0.026676	5.747656
H	0.851204	-0.008381	6.115184
H	3.848879	0.104372	-1.335541
H	-3.811666	-0.063728	-1.359026

Pybox-X-OMe

N	-0.027413	0.001131	1.553551
O	2.344581	0.061844	0.170753
C	1.107504	0.021504	2.276845
C	1.154298	0.013733	3.688453
H	2.129005	0.031927	4.190619
C	-0.067770	-0.017582	4.389548
C	2.375887	0.053696	1.538130
N	3.597739	0.076912	2.029878
C	4.429718	0.101972	0.921768
H	5.522884	0.124925	1.007022
C	3.657759	0.092718	-0.216709
C	-1.268552	-0.039072	3.647309
C	-1.189072	-0.028572	2.243809
C	-2.432027	-0.051117	1.462560
O	-2.350323	-0.042401	0.096869
C	-3.648525	-0.067930	-0.339023
C	-4.461487	-0.091303	0.770151
H	-5.557063	-0.114931	0.815277
N	-3.670890	-0.079925	1.908677
H	-2.240501	-0.063684	4.157779
O	-0.180745	-0.029103	5.732577
C	1.019573	-0.008235	6.515786

H	3.857373	0.103975	-1.292441
H	-3.808235	-0.065805	-1.421456
H	0.695176	-0.023067	7.571090
H	1.607711	0.912625	6.320604
H	1.648025	-0.899106	6.307473

Pybox-X-Ph

N	0.008289	0.074633	1.300416
O	2.380629	0.393495	-0.049044
C	1.141712	0.067689	2.029993
C	1.169105	-0.086020	3.431970
H	2.137016	-0.059948	3.950434
C	-0.044101	-0.244891	4.133680
C	2.408775	0.237514	1.309834
N	3.626885	0.263025	1.810472
C	4.459567	0.447489	0.718298
H	5.550225	0.511397	0.814018
C	3.691906	0.526706	-0.420444
C	-1.230058	-0.239513	3.370202
C	-1.151005	-0.076805	1.971225
C	-2.390140	-0.074798	1.185432
O	-2.311486	0.080659	-0.171615
C	-3.607891	0.042268	-0.611079
C	-4.417150	-0.134069	0.487241
H	-5.510423	-0.211607	0.526393
N	-3.625736	-0.206476	1.622418
H	-2.215731	-0.376825	3.834669
C	-0.071996	-0.409257	5.608698
H	3.893179	0.663838	-1.487180
H	-3.769319	0.150461	-1.687837
C	-1.196268	0.005797	6.361331
C	1.025089	-0.983841	6.293346
C	0.997229	-1.140629	7.687131
C	-1.220592	-0.146607	7.755693
C	-0.124850	-0.721480	8.424125
H	-0.145326	-0.842585	9.517989
H	-2.052401	0.474746	5.853776
H	-2.099824	0.191811	8.324893
H	1.900962	-1.334145	5.727322
H	1.856310	-1.598827	8.200523

Pybox-X-SMe

N	0.320182	0.020971	1.495251

O	2.467307	0.277557	-0.195841
C	1.539460	0.159785	2.059241
C	1.764411	0.181266	3.448686
H	2.787844	0.298144	3.832773
C	0.656882	0.050760	4.316516
C	2.687381	0.294840	1.154224
N	3.957664	0.436670	1.471819
C	4.623334	0.518678	0.258961
H	5.711096	0.641324	0.191837
C	3.706164	0.420745	-0.761563
C	-0.620975	-0.095114	3.741466
C	-0.726421	-0.102780	2.333587
C	-2.057234	-0.254808	1.732999
O	-2.169527	-0.265991	0.369952
C	-3.507559	-0.419692	0.122885
C	-4.151192	-0.495509	1.336379
H	-5.222460	-0.618538	1.536377
N	-3.212980	-0.388674	2.350528
H	-1.532487	-0.202570	4.341949
S	0.972859	0.082376	6.049883
C	-0.683009	-0.108236	6.779220
H	3.753455	0.432163	-1.854598
H	-3.817166	-0.453708	-0.926027
H	-0.520088	-0.089581	7.873240
H	-1.137097	-1.076491	6.493553
H	-1.345245	0.731544	6.493610

Pybox-X-2Th

N	0.047174	0.082839	1.213764
O	2.420001	0.277255	-0.155912
C	1.185343	0.026666	1.935858
C	1.221447	-0.123425	3.336126
H	2.195544	-0.157826	3.841309
C	0.005914	-0.224481	4.050363
C	2.453050	0.129966	1.203417
N	3.675371	0.099754	1.693251
C	4.506093	0.235243	0.592339
H	5.599386	0.246520	0.677909
C	3.732608	0.343911	-0.540097
C	-1.186216	-0.165990	3.294681
C	-1.111504	-0.012875	1.896072
C	-2.357765	0.048362	1.123909
O	-2.287404	0.200352	-0.233476
C	-3.589062	0.223866	-0.658000

C	-4.393200	0.086215	0.449743
H	-5.488374	0.060774	0.501692
N	-3.592894	-0.024201	1.575660
H	-2.175850	-0.236753	3.768623
C	-0.005315	-0.381619	5.504040
H	3.930480	0.463605	-1.609550
H	-3.757693	0.339672	-1.732851
S	-1.517031	-0.498929	6.392287
C	1.077137	-0.460711	6.379528
C	0.689278	-0.612898	7.742526
C	-0.686629	-0.649585	7.903896
H	2.122691	-0.410582	6.046645
H	-1.264094	-0.756638	8.831086
H	1.396645	-0.693095	8.579431

Pybox-X-3Py

N	0.001164	0.070293	1.307005
O	2.383758	0.387987	-0.026950
C	1.130893	0.049423	2.041452
C	1.149261	-0.117415	3.442725
H	2.112228	-0.099196	3.970598
C	-0.071431	-0.277230	4.129672
C	2.402477	0.218667	1.330189
N	3.617397	0.232234	1.839341
C	4.458013	0.422072	0.754427
H	5.548387	0.478530	0.857611
C	3.698015	0.517174	-0.388558
C	-1.254290	-0.257460	3.363312
C	-1.164610	-0.079955	1.966436
C	-2.397615	-0.058718	1.172221
O	-2.309085	0.112592	-0.181980
C	-3.602872	0.090013	-0.629741
C	-4.420477	-0.093255	0.461566
H	-5.514540	-0.162537	0.492950
N	-3.636899	-0.185710	1.600526
H	-2.242307	-0.392930	3.823687
C	-0.112325	-0.458848	5.599755
H	3.907672	0.663545	-1.452442
H	-3.757423	0.212441	-1.705974
C	-1.206222	-0.013493	6.373928
C	0.947211	-1.100068	6.285634
N	0.974787	-1.293330	7.613999
C	-1.187594	-0.212136	7.760019
C	-0.074410	-0.850107	8.334102

H	-0.027640	-1.009350	9.425834
H	-2.053307	0.502861	5.897526
H	-2.019652	0.131550	8.391931
H	1.806377	-1.494915	5.715269

Pybox-X-3Th

N	0.015295	0.115540	1.201546
O	2.405162	0.298906	-0.142484
C	1.143925	0.067216	1.935856
C	1.161756	-0.069757	3.339638
H	2.131715	-0.099203	3.852520
C	-0.058216	-0.164234	4.042910
C	2.420562	0.164418	1.218591
N	3.636615	0.139856	1.724328
C	4.481423	0.265683	0.633064
H	5.573509	0.278711	0.732674
C	3.722558	0.363012	-0.510241
C	-1.240767	-0.113449	3.272520
C	-1.150936	0.025593	1.873583
C	-2.387905	0.078169	1.085363
O	-2.299926	0.215883	-0.272692
C	-3.595910	0.234052	-0.714749
C	-4.414443	0.107581	0.383553
H	-5.510200	0.081919	0.421300
N	-3.628984	0.009581	1.521169
H	-2.235888	-0.178874	3.731846
C	-0.090500	-0.308256	5.510125
H	3.934168	0.472835	-1.578129
H	-3.750209	0.338374	-1.792919
C	-1.261756	-0.404620	6.261122
C	1.080608	-0.367533	6.352308
C	0.777911	-0.504042	7.689899
S	-0.941134	-0.562442	7.949805
H	1.465557	-0.574102	8.541930
H	2.113249	-0.311925	5.983492
H	-2.300409	-0.391331	5.909721

Pybox-X-4Py

N	-0.002165	0.070501	1.295201
O	2.390454	0.320719	-0.037258
C	1.125867	0.031197	2.031346
C	1.137755	-0.125356	3.433949
H	2.100674	-0.131495	3.962069

C	-0.087046	-0.245266	4.119670
C	2.402221	0.164515	1.321429
N	3.615846	0.155824	1.833722
C	4.463083	0.315845	0.749291
H	5.554183	0.348934	0.854766
C	3.708100	0.416757	-0.396599
C	-1.268065	-0.204513	3.352707
C	-1.172083	-0.046972	1.953450
C	-2.403056	-0.008408	1.157189
O	-2.309391	0.148126	-0.198365
C	-3.602813	0.147946	-0.647479
C	-4.425293	-0.008316	0.444466
H	-5.520564	-0.054965	0.475083
N	-3.645103	-0.105759	1.585177
H	-2.260327	-0.309089	3.811539
C	-0.132043	-0.406677	5.595139
H	3.923544	0.548107	-1.461284
H	-3.753611	0.263393	-1.725018
C	-1.245176	0.024187	6.349437
C	0.936440	-0.996446	6.304970
C	0.842652	-1.126138	7.698898
C	-1.236457	-0.149840	7.741722
N	-0.218354	-0.714370	8.420293
H	-2.105622	0.510204	5.867038
H	-2.100688	0.190496	8.339050
H	1.827745	-1.372116	5.781995
H	1.671736	-1.592198	8.260057

Pybox-X-Br

N	0.007694	0.001856	1.545532
O	2.361352	0.062671	0.122417
C	1.158133	0.022658	2.245323
C	1.217669	0.015069	3.658603
H	2.188046	0.033147	4.171454
C	0.001609	-0.016141	4.351513
C	2.413647	0.054802	1.488713
N	3.641888	0.078187	1.963686
C	4.457137	0.103145	0.844311
H	5.551369	0.126261	0.913412
C	3.668127	0.093572	-0.283362
C	-1.211465	-0.038494	3.652993
C	-1.145757	-0.027967	2.239983
C	-2.397633	-0.050704	1.477069
O	-2.338378	-0.040434	0.111020

C	-3.643109	-0.066631	-0.301756
C	-4.437787	-0.091866	0.821691
H	-5.532314	-0.116691	0.885183
N	-3.628227	-0.081092	1.945434
H	-2.183929	-0.063234	4.161599
Br	-0.002300	-0.028269	6.254012
H	3.852330	0.104648	-1.361869
H	-3.821752	-0.063434	-1.381251

Pybox-X-Cl

N	0.015295	0.115540	1.201546
O	2.405162	0.298906	-0.142484
C	1.143925	0.067216	1.935856
C	1.161756	-0.069757	3.339638
H	2.131715	-0.099203	3.852520
C	-0.058216	-0.164234	4.042910
C	2.420562	0.164418	1.218591
N	3.636615	0.139856	1.724328
C	4.481423	0.265683	0.633064
H	5.573509	0.278711	0.732674
C	3.722558	0.363012	-0.510241
C	-1.240767	-0.113449	3.272520
C	-1.150936	0.025593	1.873583
C	-2.387905	0.078169	1.085363
O	-2.299926	0.215883	-0.272692
C	-3.595910	0.234052	-0.714749
C	-4.414443	0.107581	0.383553
H	-5.510200	0.081919	0.421300
N	-3.628984	0.009581	1.521169
H	-2.235888	-0.178874	3.731846
C	-0.090500	-0.308256	5.510125
H	3.934168	0.472835	-1.578129
H	-3.750209	0.338374	-1.792919
C	-1.261756	-0.404620	6.261122
C	1.080608	-0.367533	6.352308
C	0.777911	-0.504042	7.689899
S	-0.941134	-0.562442	7.949805
H	1.465557	-0.574102	8.541930
H	2.113249	-0.311925	5.983492
H	-2.300409	-0.391331	5.909721

Pytacn-X-NO2

N	-2.285719	1.174006	-1.589278

N	-2.763172	0.447309	1.145136
N	-0.353373	-0.652128	-0.215244
C	-0.300848	2.612185	-1.208740
C	-0.177092	2.195380	0.127710
C	1.046051	2.436054	0.735479
C	2.106449	3.036951	0.057758
C	1.869544	3.410466	-1.257046
C	-1.609684	2.394715	-1.952223
C	-3.640135	1.239880	-1.067241
C	-3.730405	1.313850	0.473653
C	-2.720323	-0.936735	0.663759
C	-1.288719	-1.482680	0.551466
C	1.029527	-0.974418	0.135357
H	-0.995925	1.676565	0.624050
N	1.242041	2.028694	2.136927
H	3.062674	3.203188	0.535783
H	-1.385496	2.430141	-3.031031
H	-2.272302	3.240945	-1.732373
H	-4.186063	0.361277	-1.424512
H	-4.165896	2.117173	-1.470204
H	-4.778432	1.092621	0.761598
H	-3.520100	2.338199	0.806904
H	-3.221115	-1.000543	-0.299292
H	-3.276555	-1.611429	1.337165
H	-1.344954	-2.512384	0.147125
H	-0.869473	-1.560156	1.559575
H	1.703851	-0.270274	-0.360879
H	1.321993	-1.998046	-0.165210
H	1.160280	-0.886766	1.217437
C	-1.827006	-0.049318	-2.221296
C	-0.506575	-0.630601	-1.670486
C	-2.871339	0.530013	2.596934
H	-1.656896	0.110750	-3.301459
H	-2.623374	-0.791058	-2.139849
H	0.324050	-0.025056	-2.049856
H	-0.387105	-1.641163	-2.110172
H	-2.759693	1.571370	2.913492
H	-2.070763	-0.054172	3.058131
H	-3.842141	0.151325	2.971462
O	0.257161	1.633773	2.772249
O	2.388566	2.095612	2.609777
N	0.694006	3.205879	-1.886224
H	2.651588	3.889435	-1.839170

Pytacn-X-CO2Et

N	-2.498739	0.457307	-1.791962
N	-2.733650	0.921603	1.040022
N	-0.190923	-0.187124	0.028888
C	-0.902015	2.285902	-2.346479
C	-0.640407	2.563902	-0.999604
C	0.508482	3.289258	-0.683797
C	1.354332	3.714026	-1.717398
C	0.996420	3.408934	-3.024379
C	-2.129555	1.477466	-2.743540
C	-3.815542	0.495275	-1.181037
C	-3.875169	1.221884	0.181837
C	-2.416537	-0.497747	1.202325
C	-0.903660	-0.774245	1.165048
C	1.231608	-0.036694	0.324256
H	-1.289664	2.158175	-0.226641
H	2.260512	4.270412	-1.509601
H	-1.929955	1.044765	-3.738412
H	-2.974448	2.168461	-2.858234
H	-4.167489	-0.534652	-1.061297
H	-4.534000	0.992456	-1.848481
H	-4.849275	0.974477	0.653469
H	-3.869806	2.307453	0.019090
H	-2.919707	-1.070299	0.426225
H	-2.799939	-0.888839	2.161434
H	-0.752294	-1.870547	1.230507
H	-0.453600	-0.340194	2.063827
H	1.713695	0.514108	-0.489194
H	1.757480	-1.004302	0.442070
H	1.352704	0.531664	1.251104
C	-1.791022	-0.807082	-1.870482
C	-0.365832	-0.819145	-1.277436
C	-2.786332	1.637641	2.306542
H	-1.678687	-1.122505	-2.924351
H	-2.403242	-1.569075	-1.384023
H	0.297299	-0.279326	-1.962814
H	-0.025150	-1.875760	-1.275591
H	-2.880579	2.710580	2.115986
H	-1.857420	1.474429	2.859431
H	-3.634732	1.316387	2.943005
N	-0.104849	2.703240	-3.346816
H	1.619977	3.730674	-3.854972
C	0.805153	3.580163	0.747862
O	-0.024893	3.551930	1.645106
O	2.108578	3.874423	0.943842
C	2.494000	4.181173	2.325683

C	3.982108	4.460881	2.323125
H	2.234049	3.319675	2.945658
H	1.908275	5.043256	2.653962
H	4.542954	3.588886	1.975153
H	4.302723	4.694067	3.342975
H	4.218597	5.314988	1.682406

Pytacn-X-Me

N	-2.028360	1.114342	-1.767341
N	-2.707630	0.549341	1.010227
N	0.433629	3.900757	-1.746940
N	-0.502240	-0.941383	-0.098132
C	-0.235577	2.817584	-1.299342
C	-0.031727	2.264574	-0.036101
C	0.914749	2.834536	0.821152
C	1.608542	3.960383	0.360776
C	1.335435	4.449614	-0.913948
C	-1.243017	2.214632	-2.273164
C	-3.360503	1.387720	-1.259381
C	-3.468961	1.549013	0.274078
C	-2.919846	-0.842501	0.625610
C	-1.599403	-1.638565	0.573387
C	0.799162	-1.398801	0.381982
H	-0.609387	1.385964	0.251148
C	1.190187	2.236371	2.176514
H	2.349246	4.454878	0.983156
H	1.861646	5.325851	-1.288074
H	-0.686592	1.881878	-3.162225
H	-1.906050	3.027042	-2.609257
H	-4.029746	0.583773	-1.587680
H	-3.745585	2.314852	-1.708458
H	-4.549195	1.553598	0.533572
H	-3.067636	2.527198	0.566738
H	-3.411322	-0.872265	-0.344848
H	-3.599001	-1.362392	1.325002
H	-1.806173	-2.632027	0.128433
H	-1.264921	-1.818460	1.600098
H	1.582780	-0.761200	-0.039851
H	1.025268	-2.447473	0.104295
H	0.833718	-1.318205	1.472284
C	-1.714632	-0.223422	-2.236846
C	-0.516563	-0.917712	-1.559966
C	-2.720278	0.763771	2.446928
H	-1.474105	-0.205538	-3.314907

H	-2.610545	-0.839740	-2.132491
H	0.397369	-0.393490	-1.863500
H	-0.453034	-1.940611	-1.989134
H	-2.405924	1.789603	2.665693
H	-2.015652	0.079196	2.929555
H	-3.719140	0.604292	2.900579
H	0.312659	1.707594	2.555709
H	1.490097	3.002239	2.897284
H	2.008277	1.508832	2.107523

Pytacn-X-H

N	-2.046193	1.137724	-1.507675
N	-2.466754	0.002132	1.129479
N	-0.537810	-1.326400	-0.558032
C	-0.167717	2.649670	-0.806254
C	0.160247	1.786563	0.242464
C	1.143034	2.183747	1.146528
C	1.764035	3.422140	0.978119
C	1.369873	4.214913	-0.098133
C	-1.220790	2.273136	-1.842665
C	-3.287291	1.378473	-0.793601
C	-3.218376	1.185824	0.739341
C	-2.841913	-1.248851	0.479833
C	-1.611325	-2.089702	0.081802
C	0.759212	-1.973806	-0.371346
H	-0.362398	0.833839	0.323619
H	2.531659	3.771107	1.661395
H	-0.699451	2.065802	-2.788042
H	-1.841849	3.166156	-2.020592
H	-4.059915	0.720246	-1.207547
H	-3.627133	2.408750	-0.975668
H	-4.260593	1.189641	1.124070
H	-2.709206	2.044937	1.192841
H	-3.441206	-1.025239	-0.400683
H	-3.480127	-1.874640	1.129595
H	-1.953953	-2.939686	-0.540688
H	-1.180241	-2.520939	0.990939
H	1.548159	-1.315365	-0.748666
H	0.843231	-2.944886	-0.898211
H	0.929293	-2.147155	0.695266
C	-1.917189	-0.067254	-2.307898
C	-0.719041	-0.973607	-1.966351
C	-2.279688	-0.116040	2.564756
H	-1.803598	0.185392	-3.377173

H	-2.848433	-0.631883	-2.224475
H	0.198599	-0.455751	-2.269876
H	-0.801650	-1.875733	-2.609237
H	-1.842676	0.810019	2.952889
H	-1.588610	-0.936822	2.780941
H	-3.224338	-0.309613	3.111837
N	0.422624	3.849986	-0.980315
H	1.827352	5.188397	-0.262844
H	1.421447	1.536589	1.973962

Pytacn-X-Cl

N	-2.113451	1.121306	-1.504800
N	-2.495160	0.041776	1.165323
N	-0.516203	-1.259676	-0.479883
C	-0.186950	2.624546	-0.930174
C	0.087038	1.821438	0.179583
C	1.147377	2.204702	0.986244
C	1.900490	3.339568	0.703451
C	1.534942	4.067406	-0.427815
C	-1.328275	2.271359	-1.877478
C	-3.364892	1.333685	-0.797446
C	-3.291611	1.185394	0.740004
C	-2.823697	-1.238995	0.544688
C	-1.561693	-2.044909	0.178771
C	0.805383	-1.845364	-0.265164
H	-0.513836	0.929728	0.365808
H	2.730180	3.648768	1.327709
H	-0.890141	2.108226	-2.872885
H	-1.970781	3.161178	-1.961925
H	-4.110747	0.635704	-1.194654
H	-3.742514	2.344774	-1.007032
H	-4.333318	1.158349	1.123486
H	-2.817810	2.075996	1.171212
H	-3.423230	-1.058953	-0.345332
H	-3.445786	-1.867302	1.206760
H	-1.868105	-2.926132	-0.418474
H	-1.119120	-2.430402	1.102727
H	1.569120	-1.165244	-0.655498
H	0.934358	-2.826969	-0.762358
H	0.973405	-1.978705	0.807144
C	-1.933612	-0.101878	-2.268899
C	-0.704247	-0.954049	-1.897773
C	-2.335673	-0.039572	2.608178
H	-1.822137	0.128866	-3.342977

H	-2.843859	-0.697959	-2.175478
H	0.195538	-0.412727	-2.213275
H	-0.752369	-1.875961	-2.515288
H	-1.944259	0.909936	2.986788
H	-1.616926	-0.826588	2.855749
H	-3.285066	-0.260458	3.135333
N	0.517068	3.732281	-1.237203
H	2.090318	4.964189	-0.692281
Cl	1.549549	1.234475	2.398848

Pytacn-X-OMe

N	-1.952945	1.184883	-1.865796
N	-2.884546	0.875231	0.875970
N	0.951938	3.398317	-2.322017
N	-0.439120	-0.580004	0.145521
C	-0.021487	2.756153	-1.647035
C	-0.001982	2.538355	-0.269651
C	1.101877	2.996887	0.451696
C	2.130653	3.665068	-0.228532
C	2.000842	3.839915	-1.598176
C	-1.203673	2.261864	-2.471510
C	-3.354705	1.395117	-1.542139
C	-3.642253	1.708639	-0.057646
C	-2.930271	-0.565725	0.610207
C	-1.565382	-1.250718	0.800030
C	0.830518	-0.998445	0.741040
H	-0.808309	1.960163	0.175536
O	1.260908	2.826675	1.794030
H	3.002596	4.028924	0.304566
H	2.782201	4.355642	-2.152332
H	-0.815721	1.964429	-3.460101
H	-1.878256	3.111862	-2.638860
H	-3.921276	0.506360	-1.843551
H	-3.756037	2.230902	-2.131467
H	-4.739027	1.628537	0.093347
H	-3.367099	2.749080	0.156376
H	-3.293001	-0.732593	-0.401170
H	-3.650770	-1.073108	1.274873
H	-1.664686	-2.308929	0.485307
H	-1.330920	-1.262531	1.869937
H	1.639271	-0.381963	0.335767
H	1.073582	-2.060039	0.539197
H	0.792364	-0.859298	1.825328
C	-1.505624	-0.166263	-2.161300

C	-0.338387	-0.704645	-1.311464
C	-3.206675	1.191970	2.261828
H	-1.157352	-0.228182	-3.208166
H	-2.363393	-0.837914	-2.084031
H	0.572206	-0.165025	-1.595427
H	-0.187751	-1.762029	-1.615435
H	-3.054588	2.261009	2.439569
H	-2.547973	0.633051	2.933389
H	-4.254575	0.944408	2.522052
C	0.145801	2.236573	2.505227
H	0.497925	2.093607	3.525676
H	-0.139288	1.285570	2.050515
H	-0.705418	2.922818	2.487793

Pytacn-X-NMe2

N	-1.812939	1.137311	-1.985416
N	-3.048713	1.073738	0.676576
N	0.860706	3.677911	-2.409648
N	-0.524828	-0.357714	0.385151
C	-0.033257	2.896493	-1.755959
C	-0.081769	2.745940	-0.381114
C	0.870242	3.406403	0.430909
C	1.796783	4.239638	-0.244076
C	1.742041	4.330109	-1.627492
C	-1.034783	2.163620	-2.642023
C	-3.242964	1.337206	-1.821611
C	-3.690887	1.798457	-0.418621
C	-3.048597	-0.386008	0.560481
C	-1.699998	-1.009330	0.966943
C	0.676434	-0.637310	1.171742
H	-0.827777	2.068292	0.024112
N	0.911633	3.230507	1.790618
H	2.547411	4.807864	0.291395
H	2.456060	4.970024	-2.143907
H	-0.471775	1.731849	-3.486306
H	-1.716068	2.910979	-3.071877
H	-3.760171	0.405595	-2.081517
H	-3.597234	2.095164	-2.534000
H	-4.798544	1.726035	-0.384644
H	-3.436437	2.857283	-0.285080
H	-3.295123	-0.665325	-0.461250
H	-3.830100	-0.841062	1.193437
H	-1.736898	-2.093886	0.741485
H	-1.591747	-0.917337	2.052849

H	1.497819	-0.011575	0.808365
H	0.996316	-1.696157	1.111818
H	0.491590	-0.395100	2.221789
C	-1.309589	-0.223590	-2.062501
C	-0.240226	-0.623079	-1.027320
C	-3.521436	1.531080	1.976033
H	-0.838866	-0.395853	-3.047135
H	-2.157821	-0.909821	-2.005035
H	0.679871	-0.073365	-1.255968
H	-0.019734	-1.698098	-1.198754
H	-3.379482	2.613077	2.057959
H	-2.946505	1.047890	2.771821
H	-4.594196	1.308453	2.141754
C	-0.216097	2.618663	2.491748
H	0.142222	2.220242	3.443388
H	-0.632844	1.804765	1.898504
H	-1.008823	3.353355	2.693750
C	1.805945	4.050599	2.603343
H	2.829026	3.994519	2.223130
H	1.794453	3.660826	3.622088
H	1.495267	5.105388	2.624966

L4pym

C	-6.694879	1.015276	-0.825076
C	-5.298161	1.130417	-0.759019
C	-4.528060	0.101831	-0.165303
C	-5.187185	-1.045153	0.342157
C	-6.582119	-1.152424	0.271238
C	-7.342472	-0.120021	-0.307969
C	-3.061718	0.134920	-0.077447
N	-2.251486	1.258761	-0.028169
C	-0.959081	0.763115	0.065088
N	-2.293537	-0.962304	-0.016142
N	-0.996338	-0.571369	0.068845
C	-2.683995	2.628207	-0.039855
C	-3.316056	3.159602	1.091713
C	-3.789795	4.480191	1.056682
C	-3.638219	5.281917	-0.093842
C	-2.993039	4.718142	-1.219759
C	-2.519121	3.401815	-1.200682
C	-4.145864	6.702578	-0.133911
C	0.276081	1.544191	0.180387
C	1.525939	0.889251	0.101699
C	2.662094	1.693522	0.231450

N	2.590562	3.028512	0.420929
N	0.191796	2.877140	0.379542
C	1.350757	3.543123	0.485325
H	-4.810144	2.015471	-1.186159
H	-7.080576	-2.046776	0.675096
H	-8.438900	-0.202431	-0.359482
H	-3.439278	2.538582	1.990649
H	-4.288858	4.896817	1.945425
H	-2.862804	5.324268	-2.130100
H	-2.024606	2.965015	-2.080204
H	-4.641078	6.985763	0.814680
H	-4.874780	6.843383	-0.959285
H	-3.315861	7.417360	-0.315480
H	1.586476	-0.196089	-0.054761
H	3.671668	1.250047	0.178947
H	-7.281274	1.821158	-1.291950
H	-4.583868	-1.845115	0.794386
H	1.273180	4.634075	0.644804

L2pym

C	-6.672765	0.995897	-0.833411
C	-5.276268	1.110519	-0.760120
C	-4.511654	0.094716	-0.138309
C	-5.175607	-1.040209	0.388856
C	-6.570308	-1.147500	0.310478
C	-7.325503	-0.127025	-0.296032
C	-3.045355	0.128902	-0.045100
N	-2.238079	1.254386	0.001031
C	-0.942454	0.761149	0.079816
N	-2.274371	-0.964676	0.012354
N	-0.973218	-0.571882	0.084323
C	-2.669281	2.622412	-0.029521
C	-3.348131	3.158045	1.073177
C	-3.814562	4.479815	1.016732
C	-3.607027	5.281923	-0.125354
C	-2.914547	4.715652	-1.220804
C	-2.450001	3.395746	-1.181566
C	-4.105929	6.705100	-0.186792
C	0.278243	1.578452	0.198493
N	1.442119	0.967109	-0.114601
C	2.552746	1.709205	0.012694
C	2.521474	3.049862	0.433937
N	0.134727	2.848794	0.628474
C	1.256829	3.577516	0.735946

H	-4.783389	1.984755	-1.204177
H	-7.072669	-2.032539	0.729834
H	-8.421663	-0.209372	-0.353419
H	-3.511177	2.538434	1.966640
H	-4.351284	4.898831	1.882170
H	-2.741682	5.320871	-2.124689
H	-1.921920	2.955477	-2.039869
H	-4.645707	6.988260	0.737223
H	-4.793268	6.851375	-1.046181
H	-3.265264	7.417089	-0.325554
H	-7.254763	1.791877	-1.322377
H	-4.575970	-1.830983	0.861817
H	1.140962	4.619507	1.082739
H	3.438022	3.649746	0.525631
H	3.509564	1.216782	-0.236269

Lpyrazt

C	-6.690187	0.998065	-0.831843
C	-5.294188	1.119311	-0.759864
C	-4.522635	0.098577	-0.154674
C	-5.179616	-1.047306	0.357891
C	-6.573729	-1.161136	0.280511
C	-7.335670	-0.136156	-0.309803
C	-3.056868	0.139839	-0.060709
N	-2.254685	1.270957	-0.008358
C	-0.959044	0.785127	0.089271
N	-2.281589	-0.950191	0.002903
N	-0.985345	-0.549257	0.092576
C	-2.692226	2.637883	-0.029932
C	-3.344810	3.171334	1.089257
C	-3.819164	4.491195	1.043275
C	-3.646897	5.291617	-0.105450
C	-2.980713	4.726763	-1.218285
C	-2.507149	3.410249	-1.188744
C	-4.155329	6.711689	-0.157023
C	0.265903	1.581314	0.201397
C	1.526557	0.948469	0.040941
N	2.674695	1.627844	0.150844
C	2.576697	2.945757	0.416831
N	0.175937	2.898639	0.475825
C	1.329372	3.574886	0.576615
H	-4.807503	2.002956	-1.191635
H	-7.070409	-2.054719	0.688315
H	-8.431476	-0.223597	-0.366138

H	-3.483215	2.551916	1.987099
H	-4.335001	4.908771	1.921964
H	-2.834950	5.331381	-2.127291
H	-1.997856	2.971976	-2.059180
H	-4.666476	6.996383	0.782629
H	-4.870904	6.849770	-0.994466
H	-3.323441	7.427219	-0.326636
H	1.576580	-0.130374	-0.180494
H	-7.277556	1.798082	-1.307562
H	-4.575132	-1.841224	0.819201
H	1.264707	4.654198	0.798077
H	3.514725	3.519642	0.507944

Lpyrdt

C	-6.681133	1.018552	-0.827751
C	-5.284223	1.130766	-0.758657
C	-4.518055	0.104419	-0.156176
C	-5.181476	-1.037605	0.356708
C	-6.576463	-1.142339	0.282324
C	-7.332934	-0.111893	-0.305443
C	-3.051475	0.134304	-0.065692
N	-2.239697	1.258908	-0.012321
C	-0.948876	0.761599	0.080554
N	-2.285707	-0.962493	-0.006670
N	-0.985975	-0.572083	0.080662
C	-2.671401	2.628305	-0.030485
C	-3.318473	3.161656	1.091701
C	-3.794386	4.480980	1.047205
C	-3.630042	5.280207	-0.103363
C	-2.970384	4.714686	-1.219808
C	-2.495064	3.398904	-1.191741
C	-4.138908	6.700140	-0.152965
C	0.290820	1.536683	0.191882
C	1.536484	0.877553	0.041780
C	2.680158	1.656294	0.171277
C	2.499912	3.029521	0.433717
N	0.189848	2.856496	0.462440
N	1.291119	3.600098	0.575432
H	-4.792870	2.011814	-1.190295
H	-7.078050	-2.033024	0.690468
H	-8.429412	-0.192105	-0.359494
H	-3.450996	2.543023	1.990916
H	-4.304931	4.899086	1.928709
H	-2.830272	5.318625	-2.130133

H	-1.990487	2.960339	-2.064735
H	-4.646143	6.984755	0.788843
H	-4.857740	6.838459	-0.987591
H	-3.307377	7.415369	-0.325499
H	1.566533	-0.200839	-0.167321
H	3.687390	1.226572	0.069296
H	3.359541	3.711293	0.539625
H	-7.264221	1.822954	-1.301319
H	-4.581257	-1.835942	0.815947

LpytH

C	-6.682799	1.020904	-0.831745
C	-5.285643	1.131289	-0.763363
C	-4.519992	0.106191	-0.157688
C	-5.185594	-1.032974	0.358940
C	-6.580759	-1.136474	0.284588
C	-7.336349	-0.107000	-0.306066
C	-3.053326	0.134721	-0.067907
N	-2.240433	1.259622	-0.015109
C	-0.948000	0.763715	0.079360
N	-2.288281	-0.961082	-0.009723
N	-0.986887	-0.570114	0.078705
C	-2.674871	2.627333	-0.031562
C	-3.326715	3.157087	1.089629
C	-3.807806	4.474857	1.046841
C	-3.644540	5.276703	-0.101867
C	-2.979937	4.715510	-1.217741
C	-2.499150	3.401813	-1.190519
C	-4.161111	6.694064	-0.151011
C	0.286031	1.553865	0.193157
C	1.533159	0.899098	0.053646
C	2.701103	1.659445	0.178663
C	2.592007	3.038021	0.433600
N	0.175984	2.874953	0.448409
C	1.305829	3.590944	0.559654
H	-4.792955	2.010241	-1.197854
H	-7.083325	-2.025421	0.695408
H	-8.432953	-0.185872	-0.359508
H	-3.459443	2.536110	1.987227
H	-4.322561	4.889069	1.927811
H	-2.840745	5.321443	-2.126970
H	-1.990001	2.966829	-2.062564
H	-4.666611	6.976854	0.792313
H	-4.884140	6.827731	-0.982818

H	-3.334824	7.414374	-0.327705
H	1.558571	-0.180701	-0.147703
H	3.687694	1.182938	0.074864
H	3.483881	3.673727	0.535569
H	1.181579	4.668929	0.765884
H	-7.264872	1.824726	-1.307654
H	-4.586236	-1.830507	0.820716

LpytF

C	-6.692118	1.013501	-0.832283
C	-5.295070	1.124883	-0.762075
C	-4.529324	0.099489	-0.157344
C	-5.194452	-1.041064	0.356695
C	-6.589413	-1.145657	0.280580
C	-7.345233	-0.115854	-0.309309
C	-3.062578	0.129305	-0.066197
N	-2.250808	1.255582	-0.013710
C	-0.958469	0.761075	0.082790
N	-2.296336	-0.965070	-0.006153
N	-0.995257	-0.572617	0.083728
C	-2.683709	2.623744	-0.031618
C	-3.332442	3.157023	1.089806
C	-3.807106	4.477030	1.046920
C	-3.639642	5.278177	-0.101797
C	-2.977940	4.713738	-1.217638
C	-2.503947	3.397474	-1.190468
C	-4.148627	6.698273	-0.150646
C	0.274713	1.551259	0.194389
C	1.522211	0.896479	0.050621
C	2.694995	1.647197	0.171854
C	2.564033	3.018544	0.428132
N	0.170632	2.871706	0.452207
C	1.291059	3.595757	0.563313
H	-4.802860	2.005146	-1.194501
H	-7.091674	-2.035692	0.689450
H	-8.441706	-0.195687	-0.364352
H	-3.467874	2.536858	1.987604
H	-4.319724	4.893883	1.927895
H	-2.835966	5.318926	-2.126915
H	-1.997405	2.959905	-2.062821
H	-4.653906	6.983121	0.792184
H	-4.869733	6.836224	-0.983411
H	-3.318135	7.414165	-0.325633
H	1.550431	-0.182953	-0.152142

H	3.691342	1.193652	0.067819
F	3.659424	3.790985	0.548498
H	1.196827	4.675683	0.772073
H	-7.274304	1.817640	-1.307544
H	-4.594928	-1.838848	0.817888

LpytBr

C	-6.707041	1.024051	-0.826820
C	-5.309603	1.131072	-0.758444
C	-4.545897	0.099690	-0.161326
C	-5.213307	-1.042119	0.347161
C	-6.608649	-1.142017	0.273128
C	-7.362427	-0.106504	-0.309339
C	-3.079218	0.124719	-0.071334
N	-2.263310	1.247081	-0.020394
C	-0.972963	0.747132	0.077016
N	-2.316797	-0.973446	-0.009720
N	-1.015224	-0.586788	0.079408
C	-2.689079	2.617779	-0.039727
C	-3.323448	3.158868	1.087640
C	-3.785050	4.482099	1.047502
C	-3.621131	5.280332	-0.105592
C	-2.971564	4.709969	-1.223777
C	-2.509970	3.387804	-1.199511
C	-4.151235	6.692614	-0.153143
C	0.263040	1.530359	0.190447
C	1.508682	0.870348	0.063564
C	2.682291	1.619572	0.185852
C	2.564097	2.999265	0.428188
N	0.165256	2.854185	0.434201
C	1.285364	3.576581	0.547190
H	-4.815641	2.012461	-1.186429
H	-7.112814	-2.032934	0.677655
H	-8.459217	-0.182817	-0.362851
H	-3.453003	2.541862	1.988506
H	-4.282026	4.905810	1.934241
H	-2.826224	5.314807	-2.132610
H	-2.010097	2.946725	-2.073886
H	-4.141882	7.164821	0.849063
H	-5.203788	6.705541	-0.511043
H	-3.562522	7.325364	-0.846230
H	1.537518	-0.211180	-0.128025
H	3.668793	1.143895	0.090909
Br	4.115485	4.090501	0.598596

H	1.175401	4.656868	0.744307
H	-7.287748	1.832647	-1.296252
H	-4.615313	-1.844387	0.802460

LpytCF3

C	-6.739769	1.014861	-0.824543
C	-5.342330	1.121088	-0.756413
C	-4.578985	0.086240	-0.164882
C	-5.246341	-1.057960	0.338329
C	-6.641762	-1.156671	0.264963
C	-7.395243	-0.117921	-0.312025
C	-3.112415	0.109708	-0.075124
N	-2.294927	1.229530	-0.021734
C	-1.005351	0.726516	0.072190
N	-2.351375	-0.991058	-0.017093
N	-1.050401	-0.607494	0.070810
C	-2.718385	2.601362	-0.038194
C	-3.352253	3.140858	1.088544
C	-3.814971	4.465128	1.048121
C	-3.650456	5.263315	-0.103151
C	-3.004596	4.691515	-1.224510
C	-2.542182	3.371109	-1.200027
C	-4.145424	6.688357	-0.148625
C	0.233052	1.505230	0.187465
C	1.475510	0.840235	0.060985
C	2.648650	1.588157	0.185195
C	2.547090	2.969370	0.428335
N	0.135482	2.830506	0.432022
C	1.262947	3.539289	0.544555
H	-4.848549	2.004539	-1.180285
H	-7.146117	-2.049258	0.665473
H	-8.492096	-0.193415	-0.365179
H	-3.484838	2.523054	1.988364
H	-4.315429	4.887832	1.933244
H	-2.865197	5.294311	-2.135738
H	-2.047403	2.927911	-2.076270
H	-4.644949	6.977063	0.796056
H	-4.867162	6.834703	-0.979330
H	-3.308004	7.395825	-0.324916
H	1.496972	-0.240821	-0.131394
H	3.632999	1.108676	0.091045
C	3.766031	3.845402	0.568906
H	1.148261	4.619491	0.742166
H	-7.320394	1.825973	-1.289644

H	-4.648459	-1.862816	0.789125
F	4.919352	3.149088	0.429957
F	3.804030	4.454457	1.783921
F	3.776319	4.836684	-0.361928

LpytMe

C	-6.73161	1.02066	-0.83247
C	-5.33365	1.12113	-0.76291
C	-4.57515	0.08879	-0.16074
C	-5.24911	-1.04749	0.35146
C	-6.64486	-1.14134	0.27584
C	-7.39325	-0.10464	-0.31151
C	-3.10810	0.10688	-0.07038
N	-2.28695	1.22638	-0.01723
C	-0.99783	0.72171	0.07784
N	-2.35094	-0.99362	-0.01239
N	-1.04609	-0.61185	0.07711
C	-2.70965	2.59748	-0.03411
C	-3.35697	3.13415	1.08649
C	-3.82439	4.45678	1.04370
C	-3.65168	5.25731	-0.10459
C	-2.99234	4.68933	-1.22009
C	-2.52533	3.37067	-1.19266
C	-4.15286	6.68027	-0.15349
C	0.24000	1.50535	0.19013
C	1.48541	0.85442	0.04215
C	2.65365	1.61367	0.16711
C	2.57169	2.99670	0.43187
N	0.14155	2.82577	0.45450
C	1.27083	3.53562	0.56485
H	-4.83497	1.99862	-1.19361
H	-7.15364	-2.02837	0.68326
H	-8.49035	-0.17592	-0.36603
H	-3.49663	2.51444	1.98395
H	-4.33556	4.87616	1.92436
H	-2.84641	5.29400	-2.12916
H	-2.02007	2.93052	-2.06443
H	-4.65774	6.96743	0.78889
H	-4.87228	6.82279	-0.98698
H	-3.31835	7.39189	-0.32698
H	1.51442	-0.22404	-0.16637
H	3.63816	1.13261	0.05479
C	3.79178	3.86872	0.57150
H	1.14824	4.61362	0.77939

H	-7.30779	1.83035	-1.30568
H	-4.65535	-1.85070	0.81070
H	4.69352	3.63374	-0.02578
H	4.10339	4.00526	1.62823
H	3.39361	4.84578	0.22623

Bpp-H

C	-3.795930	0.165902	-0.002031
N	-2.778089	1.029060	-0.002237
C	-3.351725	-1.177562	0.000429
C	-1.976546	-1.097916	0.002139
N	-1.662573	0.236159	0.000396
C	-0.370878	0.811167	0.000678
C	-0.205088	2.197120	-0.000008
C	1.101731	2.677326	0.000303
C	2.176698	1.792560	0.001082
C	1.875600	0.429547	0.001492
N	0.635788	-0.065766	0.001505
N	2.904924	-0.539785	0.001317
N	4.219692	-0.159713	0.000688
C	4.895452	-1.310479	-0.000836
C	2.760821	-1.902753	0.000106
C	4.032597	-2.431959	-0.001211
H	-4.810196	0.541901	-0.003901
H	-3.950977	-2.075561	0.001089
H	-1.201674	-1.847065	0.004401
H	-1.062988	2.855057	-0.001045
H	1.283469	3.746773	-0.000358
H	3.203700	2.130456	0.001079
H	5.977010	-1.290524	-0.002119
H	1.782138	-2.354279	-0.000032
H	4.301923	-3.477431	-0.002922

Bpp-X-Br

C	-3.800662	0.169401	-0.002152
N	-2.775858	1.022491	-0.003263
C	-3.369278	-1.179291	0.002507
C	-1.994314	-1.114401	0.002540
N	-1.667681	0.217694	-0.000584
C	-0.374897	0.780177	-0.001565
C	-0.216564	2.168015	-0.004586
C	1.094186	2.627840	-0.005070
C	2.179213	1.760532	-0.002769

C	1.869943	0.398346	-0.000370
N	0.630637	-0.097858	0.000445
N	2.904156	-0.559822	0.000692
N	4.216009	-0.166337	-0.000799
C	4.901459	-1.310023	-0.000905
C	2.772413	-1.925077	0.001406
C	4.048769	-2.440508	0.000366
H	-4.811275	0.555010	-0.003949
H	-3.977890	-2.070837	0.004957
H	-1.226636	-1.870938	0.004923
H	-1.071027	2.828620	-0.006460
Br	1.413535	4.504414	-0.009639
H	3.204022	2.101542	-0.003188
H	5.982751	-1.280032	-0.002512
H	1.798027	-2.385852	0.002173
H	4.328822	-3.483046	-0.000110

Bpp-X-CCPh

C	-3.807123	-0.319767	-0.078621
N	-2.840351	0.599385	-0.036537
C	-3.286946	-1.635537	-0.096428
C	-1.918582	-1.477580	-0.062193
N	-1.681856	-0.128500	-0.027073
C	-0.423791	0.517725	0.015471
C	-0.342366	1.908200	0.042869
C	0.930140	2.493504	0.107383
C	2.051119	1.650246	0.094040
C	1.834358	0.278151	0.056274
N	0.629633	-0.302350	0.025810
N	2.928550	-0.619136	0.048461
N	4.213536	-0.150025	0.065359
C	4.966813	-1.251825	0.057531
C	2.877656	-1.988157	0.030053
C	4.183081	-2.429757	0.035599
H	-4.840903	-0.001689	-0.094388
H	-3.833370	-2.566021	-0.129112
H	-1.102282	-2.181352	-0.059322
H	-1.241226	2.510077	0.028400
C	1.048067	3.957600	0.121989
H	3.058431	2.039322	0.109308
H	6.044423	-1.157335	0.066574
H	1.932210	-2.505532	0.015816
H	4.522888	-3.454424	0.024962
C	1.981697	4.715743	0.733855

C	3.040631	4.299550	1.664774
H	0.280474	4.477632	-0.447443
H	1.944949	5.785140	0.531575
C	4.278580	4.965274	1.640505
C	2.843671	3.286282	2.620058
C	5.305716	4.594513	2.507328
C	3.865116	2.924570	3.493156
C	5.104272	3.569278	3.433785
H	4.436146	5.767854	0.925107
H	1.880590	2.790974	2.683155
H	6.260267	5.110188	2.464009
H	3.693481	2.142608	4.226756
H	5.900742	3.283908	4.114166

Bpp-X-CCPh-CN

C	-3.784278	-0.320658	-0.004249
N	-2.820968	0.602471	0.016642
C	-3.258984	-1.634757	-0.015521
C	-1.891193	-1.471382	-0.000708
N	-1.659450	-0.120849	0.018337
C	-0.404525	0.530408	0.036900
C	-0.328649	1.921840	0.052280
C	0.943212	2.509358	0.088230
C	2.067503	1.672761	0.059088
C	1.855883	0.298781	0.041832
N	0.653021	-0.284375	0.037428
N	2.953717	-0.591917	0.029501
N	4.235735	-0.113839	0.034167
C	4.996176	-1.210235	0.029607
C	2.911878	-1.961576	0.023439
C	4.220110	-2.393814	0.023155
H	-4.819442	-0.006969	-0.010015
H	-3.801976	-2.567626	-0.031729
H	-1.072507	-2.172322	-0.001505
H	-1.229520	2.520665	0.050370
C	1.060271	3.973750	0.098464
H	3.073263	2.065981	0.044267
H	6.073071	-1.108413	0.030529
H	1.970128	-2.485814	0.020506
H	4.566901	-3.416106	0.018609
C	1.998871	4.729773	0.703853
C	3.061225	4.306717	1.625850
H	0.293689	4.495404	-0.470362
H	1.970719	5.798795	0.501571

C	4.302385	4.967550	1.589892
C	2.862982	3.298497	2.587847
C	5.333156	4.604726	2.445812
C	3.878072	2.932302	3.457280
C	5.126477	3.577963	3.383243
H	4.461155	5.764990	0.870717
H	1.899065	2.808444	2.661802
H	6.291246	5.109804	2.399876
H	3.714550	2.157469	4.197611
C	6.176863	3.202913	4.272456
N	7.034442	2.896719	4.997518

Bpp-X-CCPh-NO2

C	-3.749477	-0.300881	0.085702
N	-2.785958	0.622141	0.081854
C	-3.224594	-1.615099	0.065285
C	-1.856972	-1.452168	0.046018
N	-1.624854	-0.101472	0.056465
C	-0.370526	0.550042	0.044772
C	-0.296406	1.941913	0.047283
C	0.975189	2.529095	0.057527
C	2.100272	1.694457	0.014553
C	1.890333	0.319839	0.011821
N	0.687861	-0.263579	0.033208
N	2.988658	-0.569431	-0.010694
N	4.270243	-0.089736	-0.019670
C	5.031773	-1.185280	-0.029310
C	2.948392	-1.939350	-0.014100
C	4.257000	-2.369813	-0.026626
H	-4.784494	0.012739	0.104775
H	-3.768160	-2.547760	0.064416
H	-1.038104	-2.152658	0.026872
H	-1.198249	2.538999	0.058969
C	1.097508	3.993598	0.066750
H	3.105057	2.089220	-0.020515
H	6.108575	-1.082666	-0.038639
H	2.007034	-2.464263	-0.007133
H	4.605086	-3.391675	-0.033320
C	2.032289	4.734463	0.695847
C	3.062803	4.275768	1.634578
H	0.348812	4.522796	-0.518388
H	2.030676	5.804814	0.500176
C	4.327156	4.894257	1.623346
C	2.809481	3.266160	2.584255

C	5.330950	4.483843	2.489429
C	3.796504	2.852097	3.463569
C	5.051818	3.459879	3.394368
H	4.525687	5.691137	0.914104
H	1.826180	2.814413	2.639029
H	6.311367	4.942055	2.472622
H	3.607131	2.078926	4.196947
N	6.102412	3.019605	4.311627
O	7.208471	3.580490	4.254314
O	5.842865	2.102713	5.107356

Bpp-X-Cl

C	-3.800872	0.179373	-0.001562
N	-2.774140	1.030101	-0.002632
C	-3.372434	-1.170213	0.001990
C	-1.997264	-1.108353	0.002551
N	-1.667780	0.222829	-0.000156
C	-0.374260	0.783496	-0.001150
C	-0.216064	2.170322	-0.004550
C	1.094536	2.630077	-0.005296
C	2.179514	1.762968	-0.002759
C	1.870509	0.401754	0.000029
N	0.631150	-0.095133	0.001097
N	2.906030	-0.554944	0.001122
N	4.217003	-0.158580	-0.000005
C	4.905002	-1.300709	-0.000055
C	2.777224	-1.920280	0.001293
C	4.054751	-2.432974	-0.000478
H	-4.810551	0.567421	-0.003151
H	-3.983070	-2.060342	0.003735
H	-1.231154	-1.866480	0.004678
H	-1.066922	2.835586	-0.007048
Cl	1.387075	4.350586	-0.010352
H	3.202448	2.109613	-0.003606
H	5.986223	-1.268177	-0.001285
H	1.803773	-2.383030	0.001656
H	4.337137	-3.474854	-0.001971

Bpp-X-CO2H

C	-3.864918	-0.001715	0.100569
N	-2.858553	0.864888	-0.018558
C	-3.405863	-1.336274	0.216448
C	-2.033187	-1.247570	0.161779

N	-1.734681	0.083536	0.020785
C	-0.455131	0.666993	-0.078802
C	-0.314383	2.047288	-0.216762
C	0.984815	2.545506	-0.308064
C	2.077669	1.679091	-0.261019
C	1.797988	0.318529	-0.120800
N	0.567682	-0.189924	-0.030381
N	2.844900	-0.624727	-0.065889
N	4.150251	-0.219502	-0.151855
C	4.851290	-1.350658	-0.067431
C	2.732347	-1.984874	0.069669
C	4.014988	-2.484791	0.072113
H	-4.882754	0.364157	0.098614
H	-3.995283	-2.234069	0.324891
H	-1.250515	-1.987064	0.208664
H	-1.174270	2.700475	-0.251108
C	1.160433	4.021959	-0.454997
H	3.096744	2.028974	-0.328713
H	5.931323	-1.310079	-0.110617
H	1.765273	-2.453960	0.149512
H	4.309163	-3.519588	0.161360
O	0.238179	4.820044	-0.497056
O	2.459076	4.382216	-0.536455
H	2.497356	5.354168	-0.627296

Bpp-X-OH

C	-3.737568	0.249632	-0.028155
N	-2.691398	1.078129	-0.045305
C	-3.338360	-1.107478	0.000130
C	-1.961162	-1.073505	-0.001364
N	-1.603302	0.248946	-0.028667
C	-0.292026	0.779091	-0.038373
C	-0.097094	2.154888	-0.059811
C	1.226548	2.600916	-0.065176
C	2.280203	1.683287	-0.051796
C	1.935032	0.335297	-0.031439
N	0.684403	-0.135114	-0.024031
N	2.944495	-0.655175	-0.016494
N	4.266960	-0.304496	-0.025950
C	4.917237	-1.469826	-0.007286
C	2.769987	-2.014274	0.007649
C	4.029695	-2.571617	0.014431
H	-4.738560	0.659639	-0.036495
H	-3.967165	-1.984801	0.018928

H	-1.210916	-1.847128	0.014612
H	-0.928985	2.844986	-0.070180
O	1.432280	3.943846	-0.082972
H	3.316556	1.995932	-0.055518
H	5.998985	-1.473766	-0.010566
H	1.781173	-2.443009	0.017602
H	4.275684	-3.622678	0.031984
H	2.387069	4.129364	-0.076158

Bpp-X-OMe

C	-3.768347	0.206015	-0.002126
N	-2.736919	1.053419	-0.008803
C	-3.344764	-1.143795	-0.004003
C	-1.968076	-1.084426	-0.012643
N	-1.634450	0.244413	-0.015296
C	-0.331326	0.797002	-0.023797
C	-0.154848	2.172651	-0.024025
C	1.164519	2.646090	-0.032715
C	2.230096	1.740190	-0.041357
C	1.899294	0.386392	-0.039793
N	0.659317	-0.104842	-0.031125
N	2.926689	-0.586947	-0.047914
N	4.242552	-0.213398	-0.059313
C	4.913431	-1.366998	-0.065141
C	2.776058	-1.948953	-0.046526
C	4.045369	-2.484465	-0.057406
H	-4.776555	0.597872	0.003860
H	-3.957188	-2.032784	0.000349
H	-1.203960	-1.844419	-0.016977
H	-0.996212	2.851353	-0.017901
O	1.317591	3.990911	-0.032119
H	3.265671	2.044569	-0.048624
H	5.994980	-1.351530	-0.075129
H	1.794923	-2.394926	-0.038197
H	4.309648	-3.531151	-0.060045
C	2.671216	4.506836	-0.040186
H	3.206694	4.175188	0.853555
H	2.560789	5.589434	-0.037385
H	3.194503	4.178649	-0.942330

Bpp-X-SMe

C	-3.754372	0.178408	-0.048614
N	-2.706423	1.003134	-0.074988

C	-3.359398	-1.178521	0.014440
C	-1.982846	-1.147917	0.025064
N	-1.621001	0.171876	-0.029542
C	-0.308960	0.700244	-0.036775
C	-0.121734	2.080926	-0.055450
C	1.196202	2.546892	-0.061453
C	2.250842	1.623214	-0.048204
C	1.917904	0.274089	-0.029177
N	0.668461	-0.206687	-0.023484
N	2.936085	-0.704854	-0.016158
N	4.251612	-0.335131	-0.012162
C	4.916806	-1.489031	-0.001221
C	2.778676	-2.066089	-0.008177
C	4.045507	-2.605103	0.001614
H	-4.753399	0.590738	-0.076627
H	-3.990110	-2.053157	0.048436
H	-1.234950	-1.921728	0.071125
H	-0.981605	2.733032	-0.063333
S	1.627052	4.253546	-0.083975
H	3.289414	1.926133	-0.052671
H	5.997952	-1.475435	0.005019
H	1.795216	-2.505687	-0.010627
H	4.305539	-3.652583	0.008910
C	0.009164	5.086269	-0.098543
H	0.238612	6.152733	-0.116148
H	-0.557887	4.850383	0.803549
H	-0.556754	4.820245	-0.992943

Bpp-X-SOMe

C	-3.854275	0.020303	-0.274111
N	-2.842861	0.880529	-0.398218
C	-3.402160	-1.298198	-0.025317
C	-2.028723	-1.206066	-0.001229
N	-1.723176	0.111387	-0.227925
C	-0.440213	0.693256	-0.293779
C	-0.297505	2.059393	-0.539861
C	1.007592	2.539146	-0.571075
C	2.099886	1.704634	-0.394580
C	1.811892	0.356690	-0.163584
N	0.579061	-0.150386	-0.109550
N	2.855079	-0.571036	0.031965
N	4.162105	-0.164621	-0.011876
C	4.859879	-1.279042	0.208233
C	2.738263	-1.915980	0.275163

C	4.019738	-2.404076	0.393963
H	-4.870249	0.379197	-0.368116
H	-3.996316	-2.188118	0.116818
H	-1.249928	-1.935024	0.152473
H	-1.163246	2.689259	-0.694575
S	1.326462	4.295111	-0.936761
H	3.113685	2.078837	-0.432943
H	5.940427	-1.233664	0.224404
H	1.769386	-2.383860	0.338100
H	4.310973	-3.425322	0.587440
C	0.672621	4.945574	0.644648
H	0.806759	6.027069	0.601583
H	1.242448	4.499137	1.460492
H	-0.387021	4.690524	0.703044
O	2.839625	4.479367	-0.903236

Bpp-Y-CO2Et

C	-3.538618	0.051546	-0.097058
N	-2.629105	0.978418	0.162853
C	-2.949580	-1.206788	-0.419620
C	-1.581529	-0.977651	-0.328307
N	-1.429030	0.325609	0.022149
C	-0.202630	1.003697	0.239633
C	-0.182234	2.336640	0.648242
C	1.069310	2.916672	0.841071
C	2.229141	2.175580	0.627009
C	2.065047	0.852841	0.218028
N	0.885101	0.264849	0.024526
N	3.186675	0.021401	-0.031590
N	4.464496	0.484559	0.165271
C	5.237821	-0.535712	-0.172551
C	3.158471	-1.260921	-0.477443
C	4.482407	-1.673215	-0.586767
H	-4.590979	0.293878	-0.058756
C	-3.759535	-2.399973	-0.702618
H	-0.713779	-1.599949	-0.450682
H	-1.102249	2.882094	0.806437
H	1.141170	3.950751	1.159515
H	3.216072	2.594754	0.765696
H	6.313126	-0.448246	-0.112719
H	2.212409	-1.729135	-0.677802
C	5.132930	-2.914144	-1.031338
O	-3.223066	-3.525110	-1.228969
O	-4.966289	-2.412248	-0.471639

O	6.354973	-2.976759	-1.146115
O	4.432525	-4.032864	-1.329266
C	2.977958	-4.136185	-1.190403
C	-1.825178	-3.627750	-1.657005
C	-1.704755	-4.899166	-2.471920
H	-1.198928	-3.670358	-0.761772
H	-1.575229	-2.745628	-2.251019
C	2.610888	-5.581000	-1.460094
H	2.516281	-3.466514	-1.920899
H	2.703640	-3.838235	-0.175523
H	2.895538	-5.872711	-2.474386
H	1.528073	-5.698969	-1.354993
H	3.101293	-6.245671	-0.744069
H	-1.962703	-5.774264	-1.869678
H	-0.671116	-5.005387	-2.815164
H	-2.357406	-4.861070	-3.348010

Bpp-Y-tBu

C	-3.865855	-0.200566	-0.314844
N	-2.899623	0.715779	-0.184073
C	-3.354614	-1.527165	-0.362269
C	-1.983313	-1.361066	-0.248209
N	-1.746892	-0.013741	-0.144315
C	-0.491910	0.619403	-0.008672
C	-0.394679	2.011399	0.087905
C	0.885235	2.548824	0.219531
C	2.001492	1.714567	0.250961
C	1.770624	0.338433	0.145259
N	0.557347	-0.207091	0.018036
N	2.839029	-0.582137	0.167416
N	4.130720	-0.157714	0.297285
C	4.852530	-1.281186	0.277752
C	2.753025	-1.950283	0.068465
C	4.042424	-2.445728	0.136463
H	-4.899948	0.125689	-0.371547
C	-4.108651	-2.832952	-0.504973
H	-1.162406	-2.066071	-0.231233
H	-1.285034	2.631709	0.059641
H	1.013689	3.627543	0.298132
H	3.011205	2.100034	0.352299
H	5.933574	-1.217229	0.366775
H	1.791690	-2.433879	-0.039903
C	4.502351	-3.884713	0.076264
C	-5.621648	-2.571590	-0.578459

C	-3.807252	-3.735145	0.710525
C	-3.653594	-3.549152	-1.794426
C	3.300745	-4.828541	-0.086194
C	5.252944	-4.232003	1.379784
C	5.457297	-4.062361	-1.123552
H	-3.857667	-2.928478	-2.677931
H	-4.190287	-4.502039	-1.908661
H	-2.576351	-3.762868	-1.767058
H	-5.985071	-2.072837	0.331007
H	-6.159738	-3.523740	-0.682154
H	-5.876580	-1.941673	-1.442235
H	-4.118278	-3.247442	1.644784
H	-2.733574	-3.956861	0.780468
H	-4.348863	-4.687706	0.619427
H	2.604215	-4.734476	0.758745
H	3.646029	-5.870636	-0.128584
H	2.749908	-4.614222	-1.012813
H	4.594276	-4.115603	2.251530
H	6.125787	-3.579671	1.519642
H	5.605518	-5.272924	1.347679
H	4.946879	-3.822366	-2.066538
H	5.811024	-5.102092	-1.175021
H	6.334588	-3.407435	-1.032015

Bpp-Y-CH2OH

C	-3.899521	-0.196932	-0.211945
N	-2.919919	0.697644	-0.074593
C	-3.404311	-1.517862	-0.367791
C	-2.031813	-1.380913	-0.309188
N	-1.774226	-0.046031	-0.131953
C	-0.509490	0.573890	-0.015982
C	-0.400698	1.964162	0.054832
C	0.882560	2.493528	0.158287
C	1.990858	1.651344	0.189954
C	1.745999	0.279006	0.115352
N	0.530209	-0.263492	0.012526
N	2.811932	-0.648720	0.155535
N	4.108947	-0.216240	0.245797
C	4.827905	-1.335832	0.293450
C	2.725748	-2.015049	0.145586
C	4.015454	-2.500389	0.236685
H	-4.929630	0.134338	-0.194260
C	-4.197623	-2.774836	-0.576559
H	-1.229119	-2.097158	-0.369961

H	-1.283026	2.588221	0.025316
H	1.019989	3.568118	0.213827
H	3.000903	2.027975	0.271638
H	5.905945	-1.274105	0.365800
H	1.770074	-2.510853	0.083509
C	4.449215	-3.931773	0.251997
H	-5.177987	-2.679107	-0.093791
O	-3.514025	-3.954582	-0.108525
H	-4.366465	-2.953494	-1.642811
H	3.583226	-4.585484	0.404724
H	5.167219	-4.112205	1.055189
O	5.153885	-4.312928	-0.959218
H	-3.363784	-3.845934	0.844615
H	4.557106	-4.139578	-1.705315

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