Electronic supporting information

"*Super hybrid tridentate ligands*": 4-substituted-2-(1-butyl-1h-1,2,3-triazol-4-yl)-6-(1H-pyrazol-1-yl)pyridine ligands coordinated to Fe(II) ions display above room temparature spin transitions†

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This supporting information contains:

PXRD Studies of I, II, III and IV:

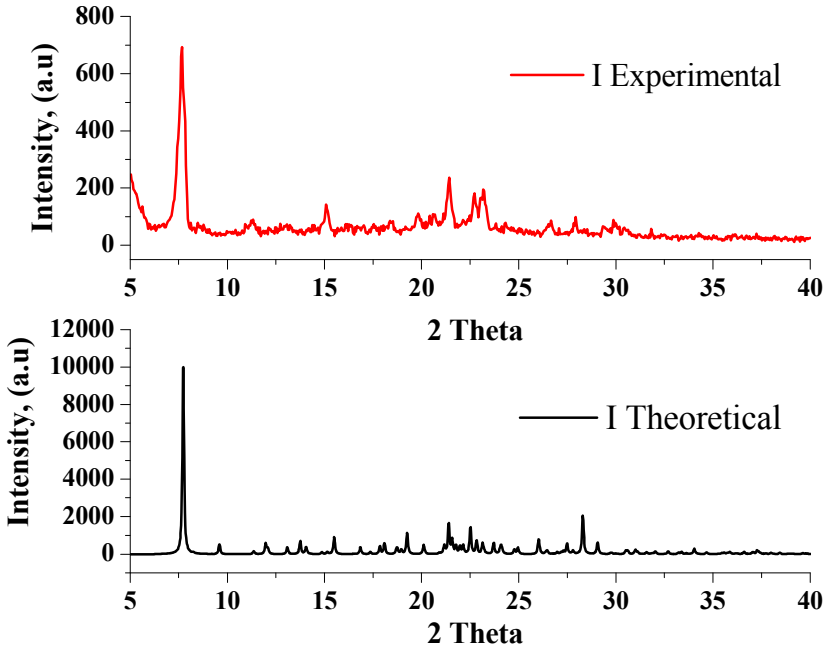

Fig. S1. Represents theoretical and experimental PXRD patterns of $[Fe^{II}(L_1)_2](ClO_4)_2 \cdot CH_3CN$ **(I).**

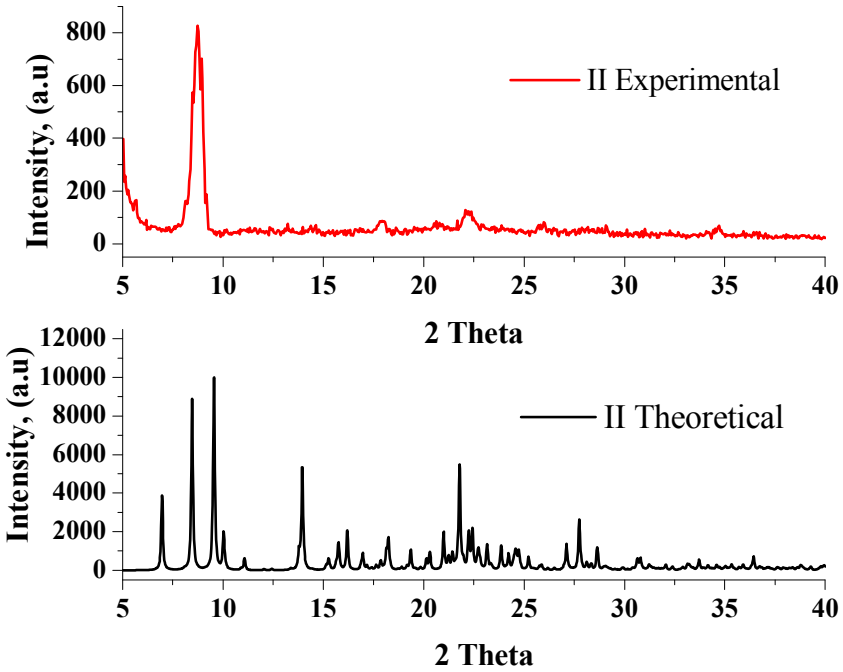

Fig. S2. Represents theoretical and experimental PXRD patterns of $[Fe^{II}(L_1)_2](BF_4)_2 \cdot CH_3CN$ **(II).**

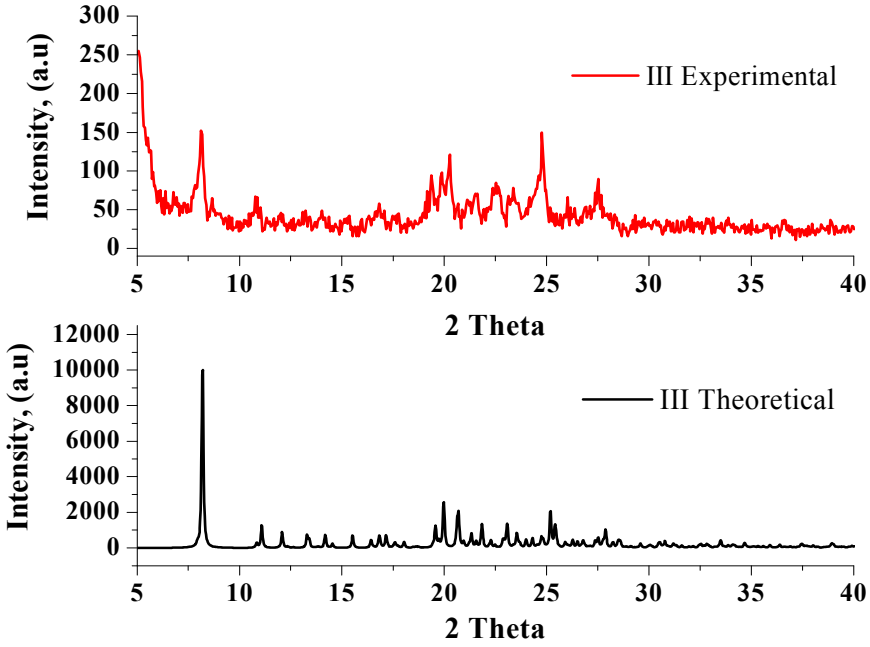

Fig. S3. Represents theoretical and experimental PXRD patterns of $[Fe^{II}(L_3)_2](ClO_4)_2.CH_3OH$ **(III).**

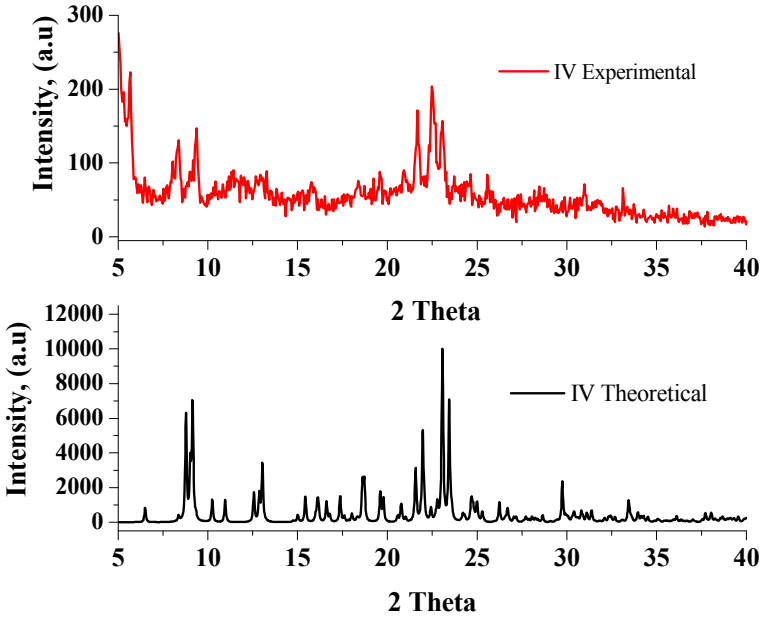

Fig. S4. Represents theoretical and experimental PXRD patterns of $[Fe^{II}(L_2)_2](ClO_4)_2 \cdot CH_3OH$ **(IV).**

^{1}H & ^{13}C NMR spectra of synthesized compounds:

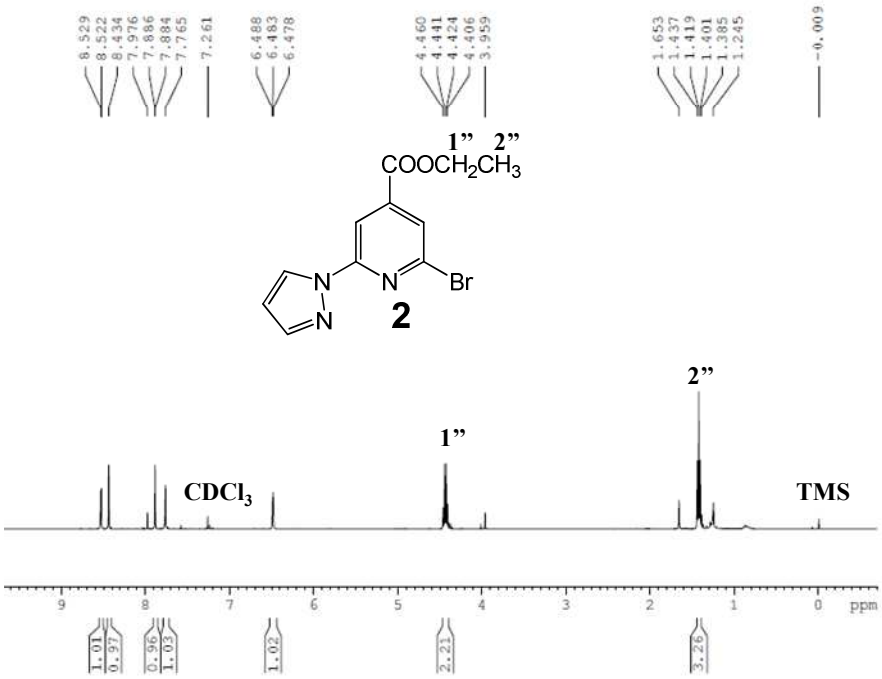

Figure S5: ^{1}H NMR (400 MHz, $CDCl_3$) of 2

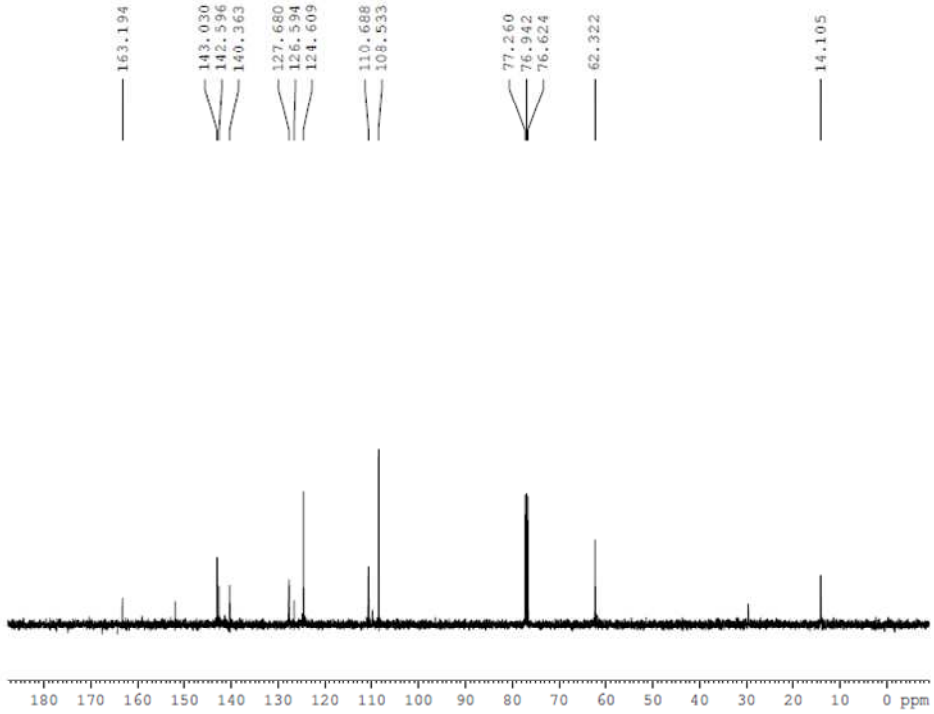

Figure S6: ^{13}C NMR (100 MHz, $CDCl_3$) of **3**

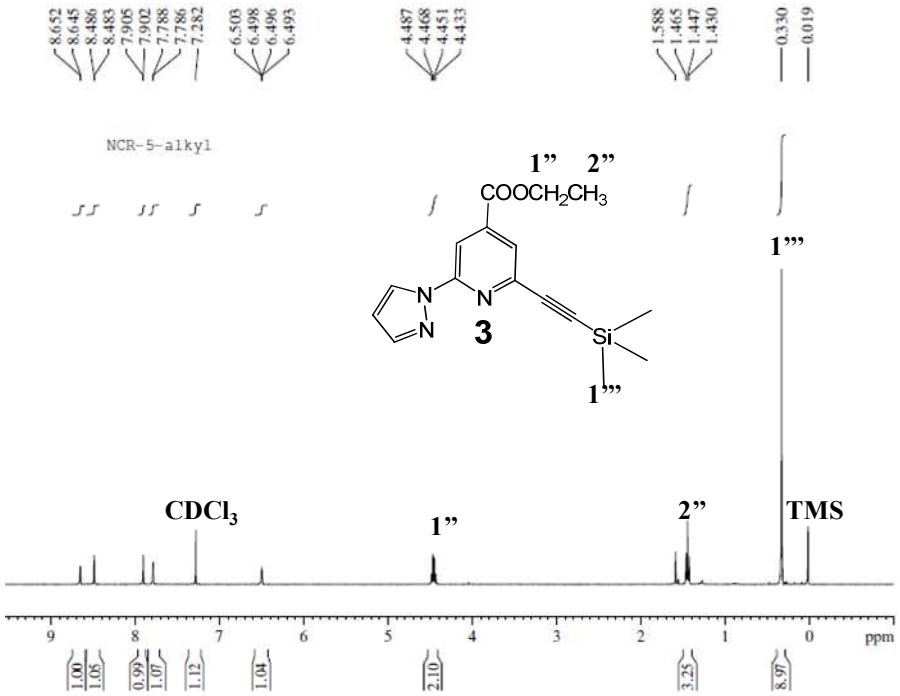

Figure S7: ^{1}**H** NMR (400 MHz, $CDCl_3$) of **3**

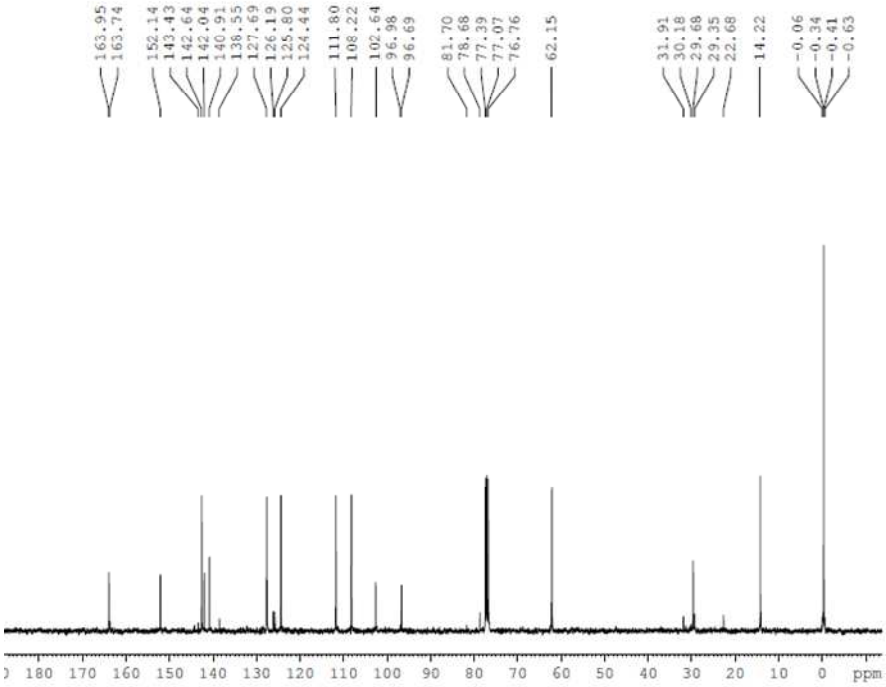

Figure S8: ^{13}**C** NMR (100 MHz, $CDCl_3$) of **3**

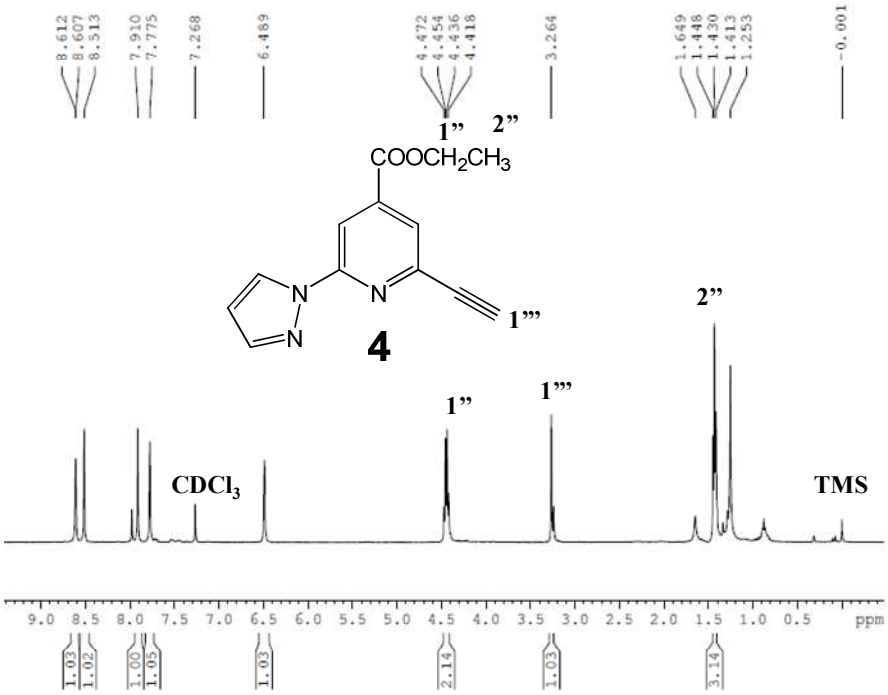

Figure S9: ^{1}**H** NMR (400 MHz, $CDCl_3$) of **4**

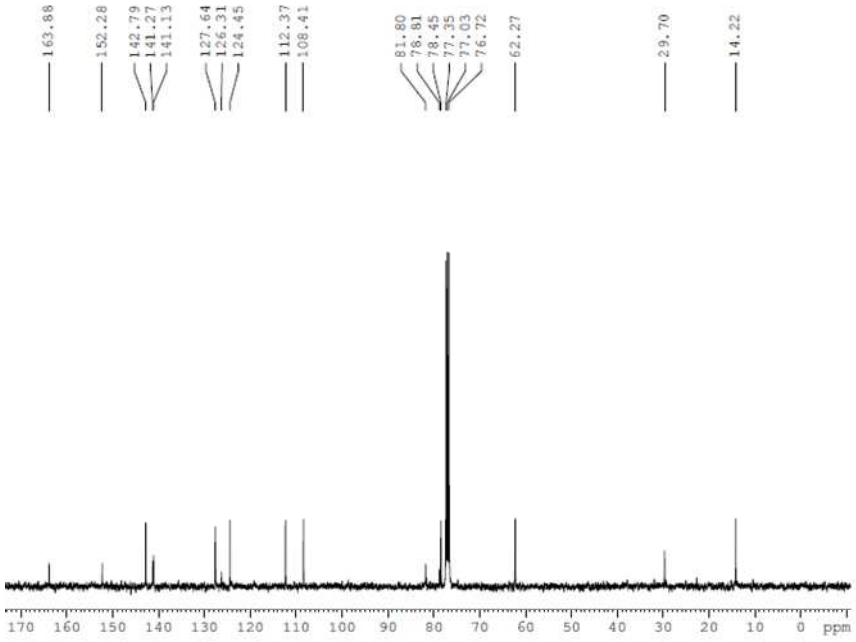

Figure S10: ^{13}**C** NMR (100 MHz, $CDCl_3$) of **4**

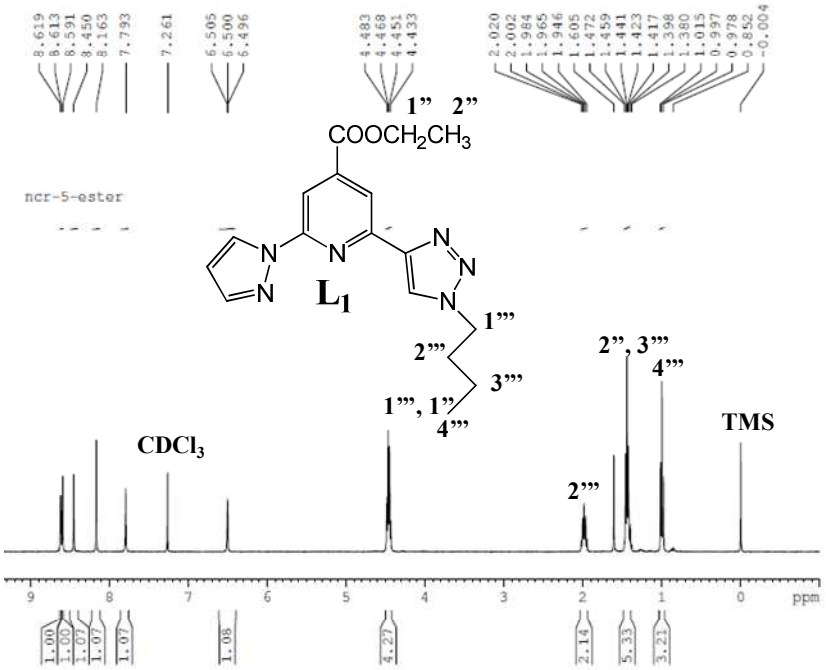

Figure S11: ^{1}**H** NMR (400 MHz, $CDCl_3$) of $\mathbf{L_1}$

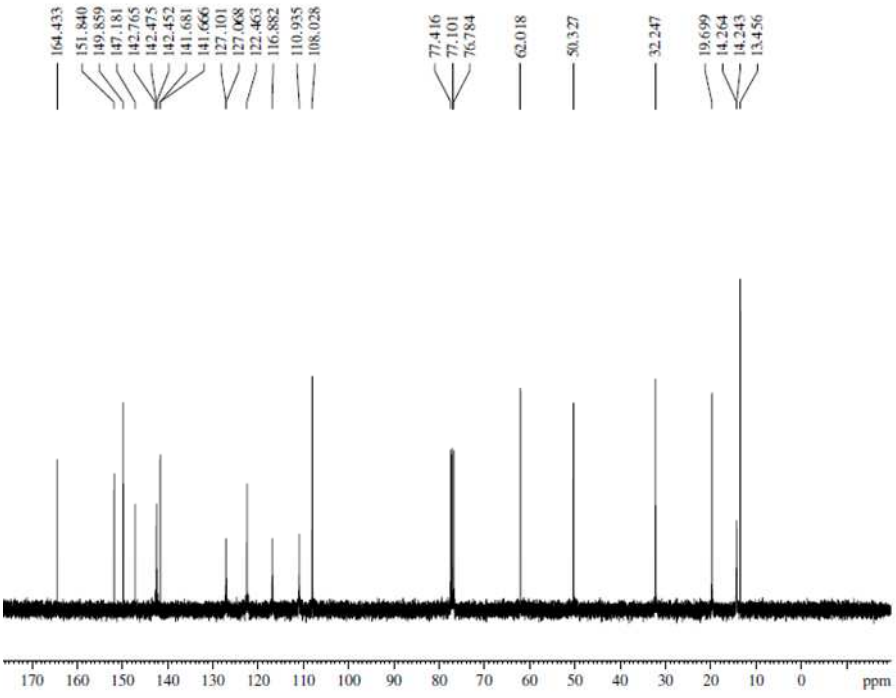

Figure S12: ^{13}**C** NMR (100 MHz, $CDCl_3$) of $\mathbf{L_1}$

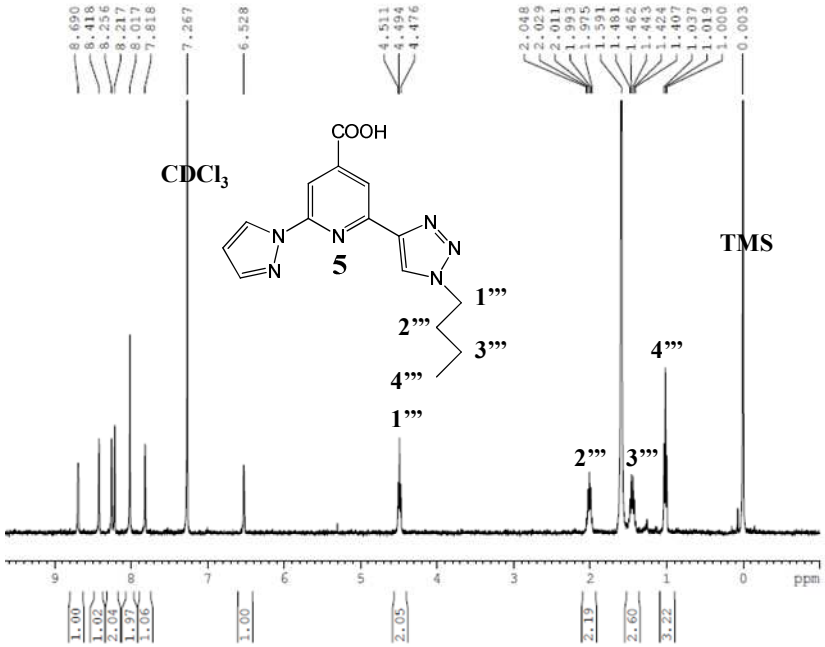

Figure S13: ^{1}**H** NMR (400 MHz, $CDCl_3$) of **5**

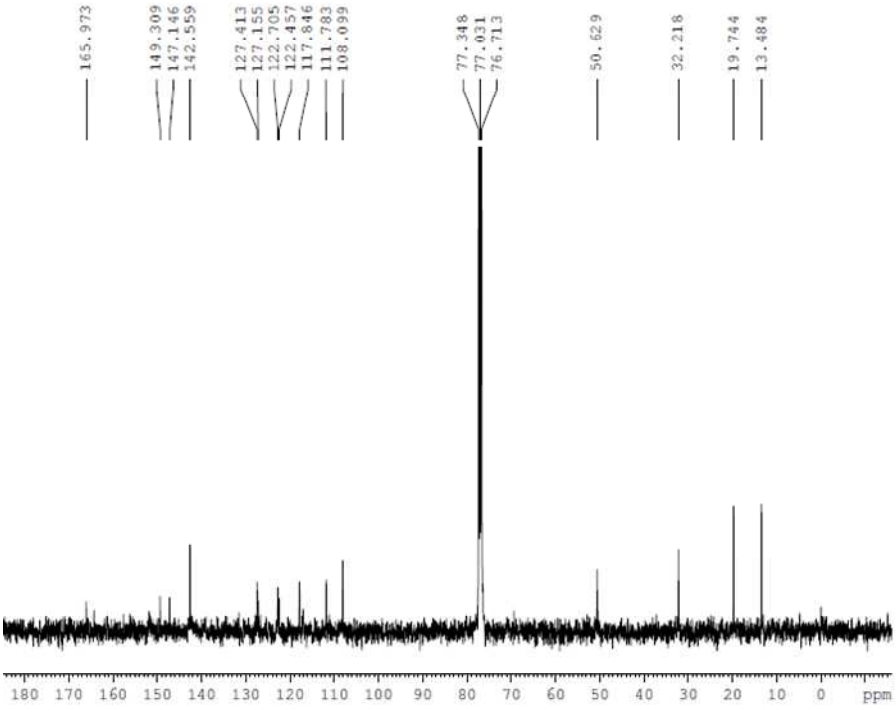

Figure S14: ^{13}**C** NMR (100 MHz, $CDCl_3$) of **5**

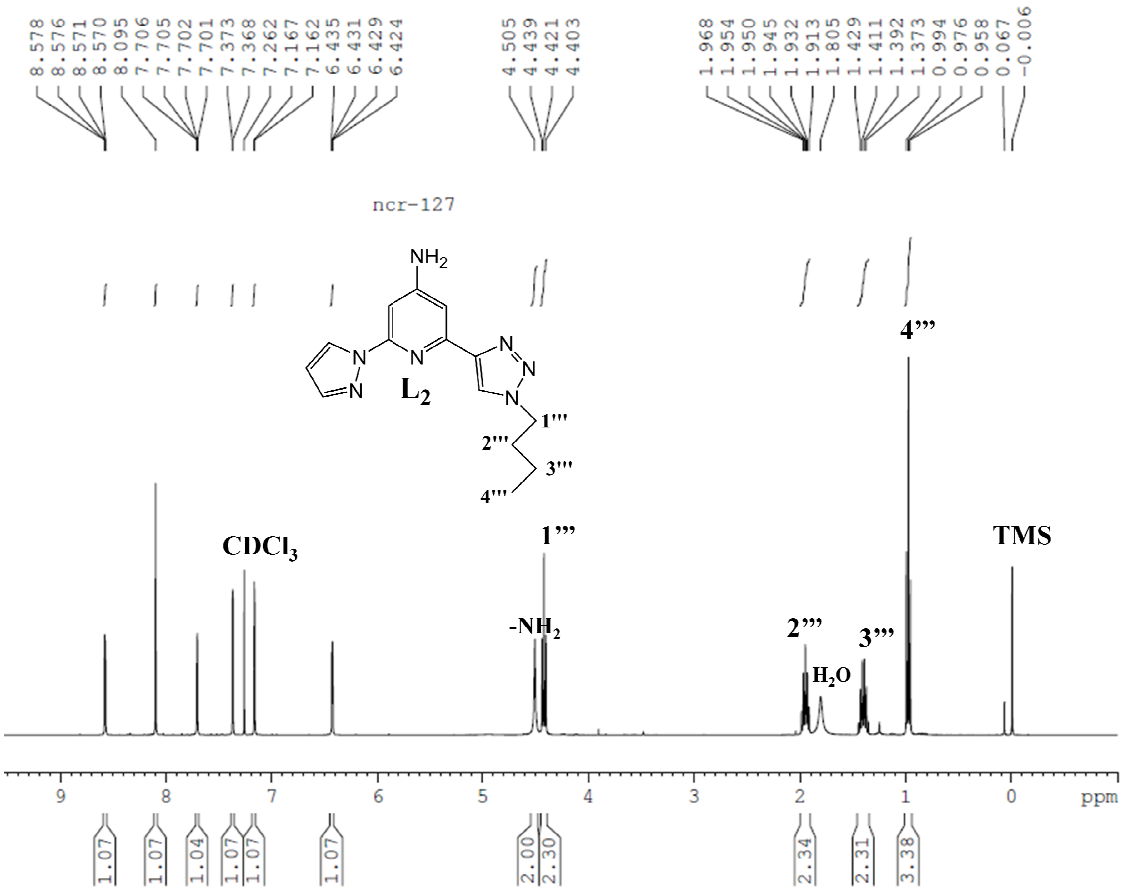

Figure S15: ^{1}**H** NMR (400 MHz, $CDCl_3$) of $\mathbf{L_2}$

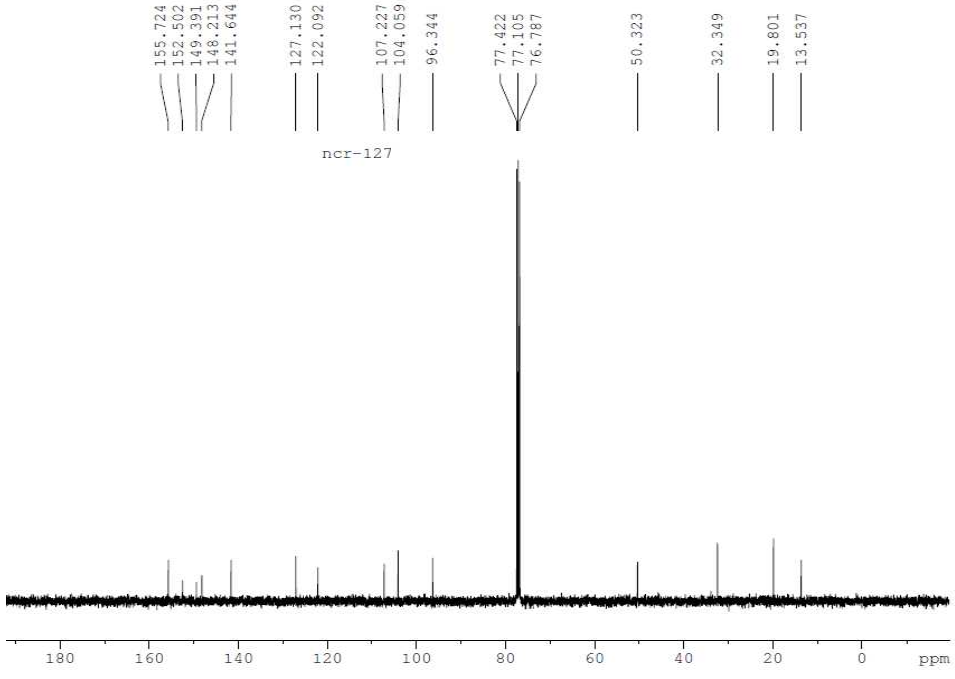

Figure S16: ^{13}**C** NMR (100 MHz, $CDCl_3$) of $\mathbf{L_2}$

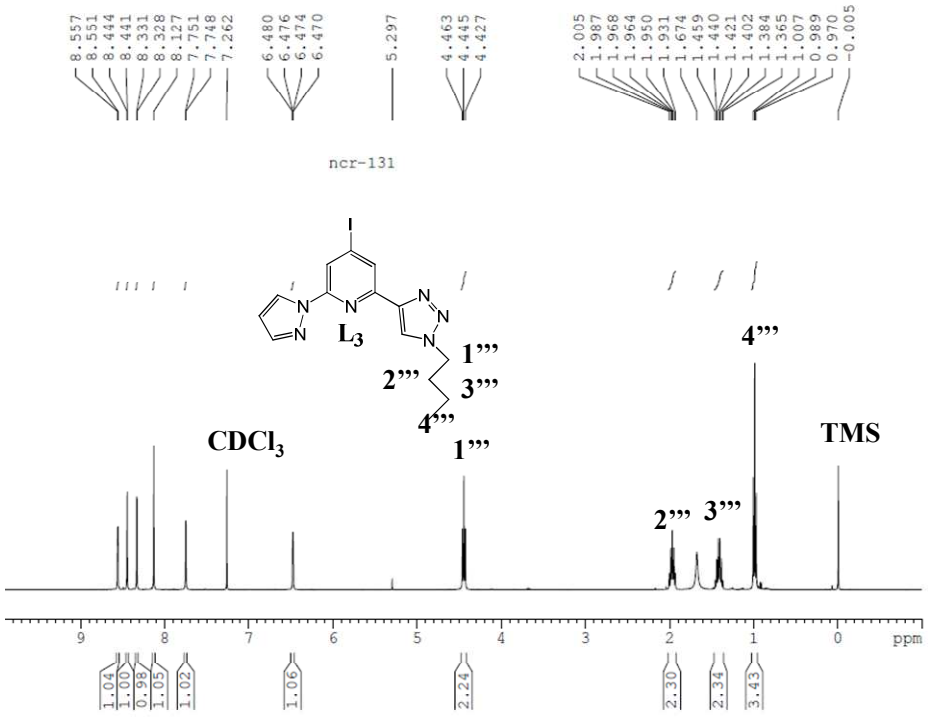

Figure S17: ^{1}**H** NMR (400 MHz, $CDCl_3$) of L_3

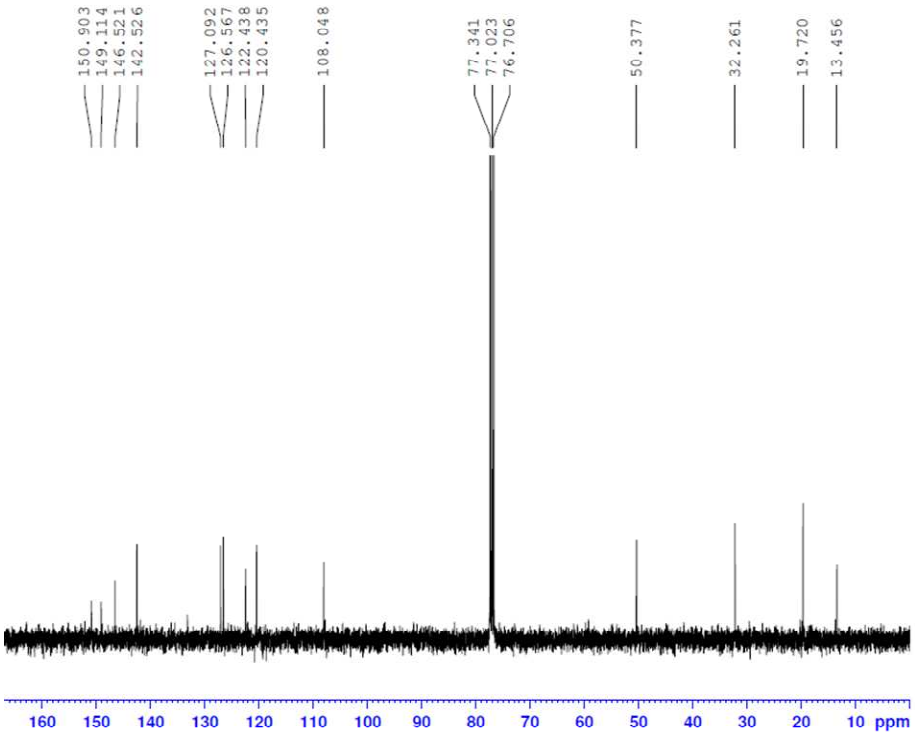

Figure S18: ^{13}**C** NMR (100 MHz, $CDCl_3$) of $\mathbf{L_3}$

FT- IR Spectra of I, II, III and IV

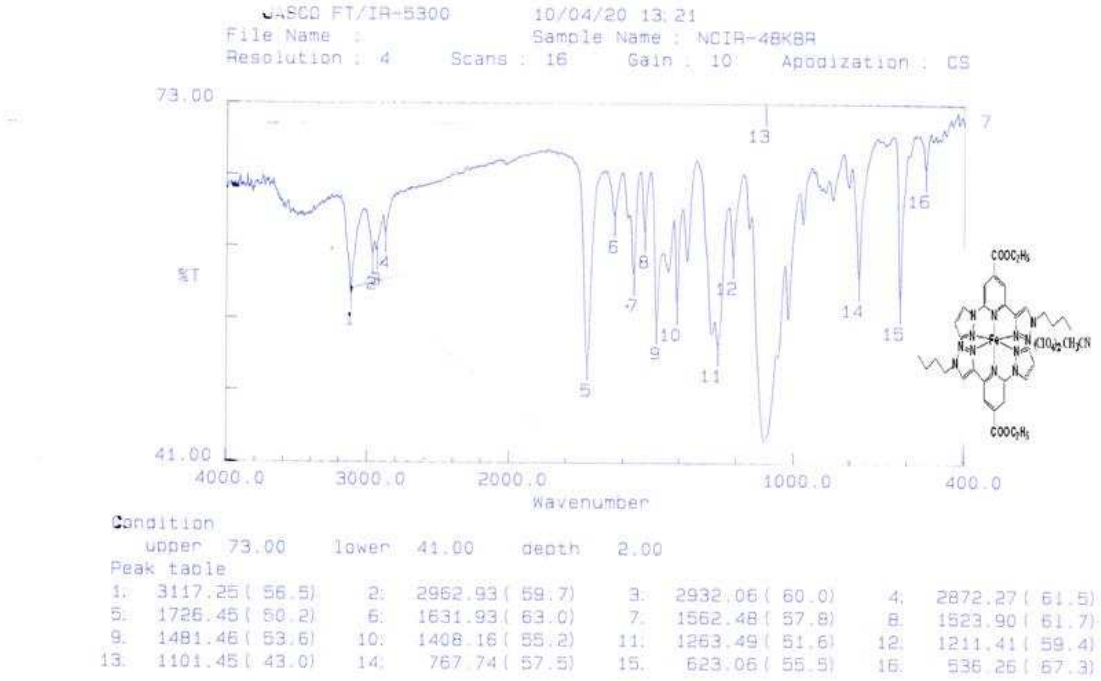

Figure S19: **FT- IR** spectra of $[Fe^{II}(L_1)_2](ClO_4)_2 \cdot CH_3CN$ **(I)**

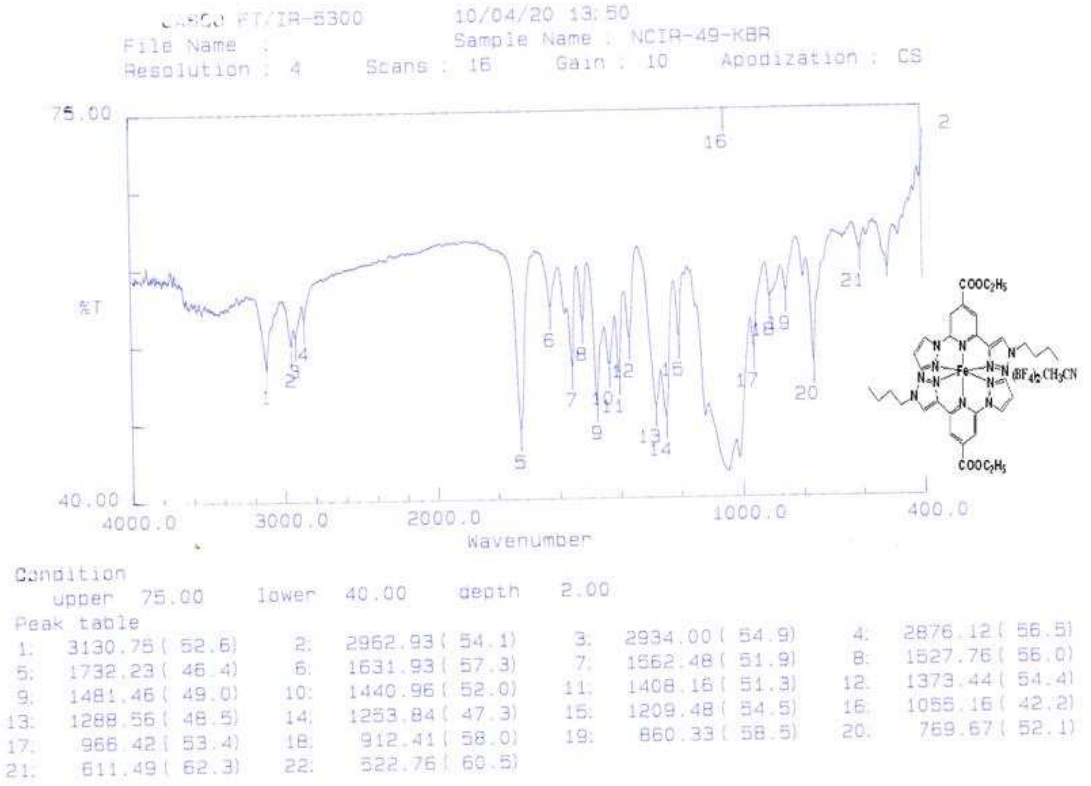

Figure S20: **FT- IR** spectra of $[Fe^{II}(L_1)_2](BF_4)_2 \cdot CH_3CN$ **(II)**

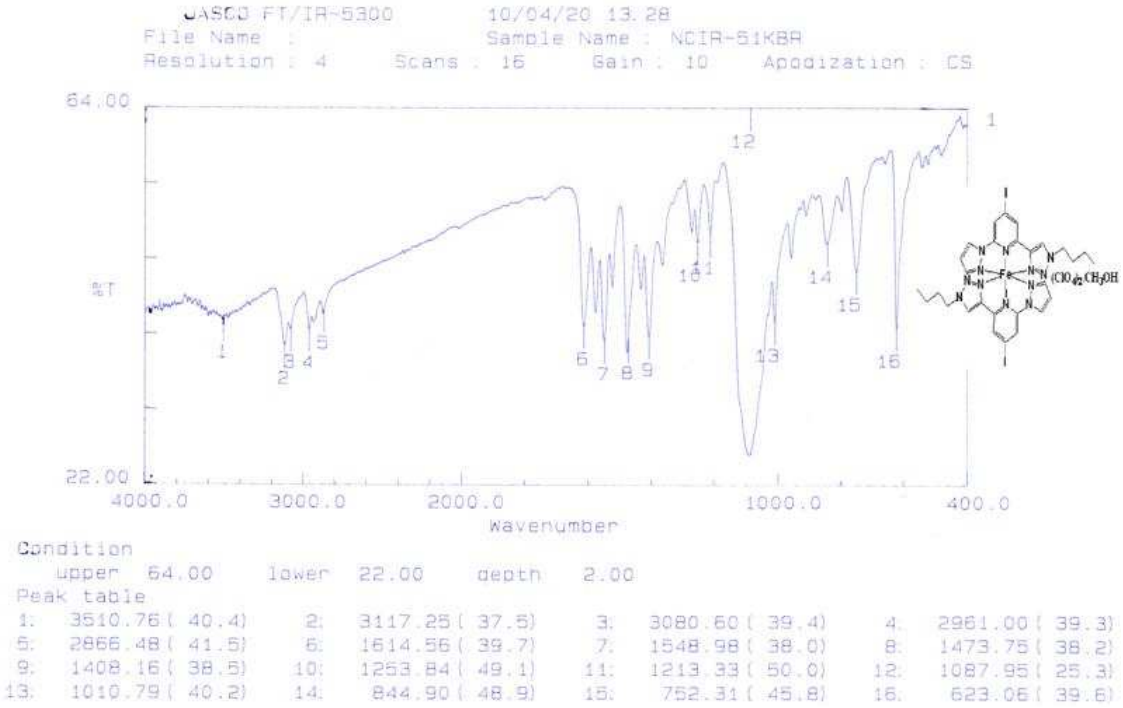

Figure S21: **FT- IR** spectra of $[Fe^{II}(L_3)_2](ClO_4)_2.\ CH_3OH$ **(III)**

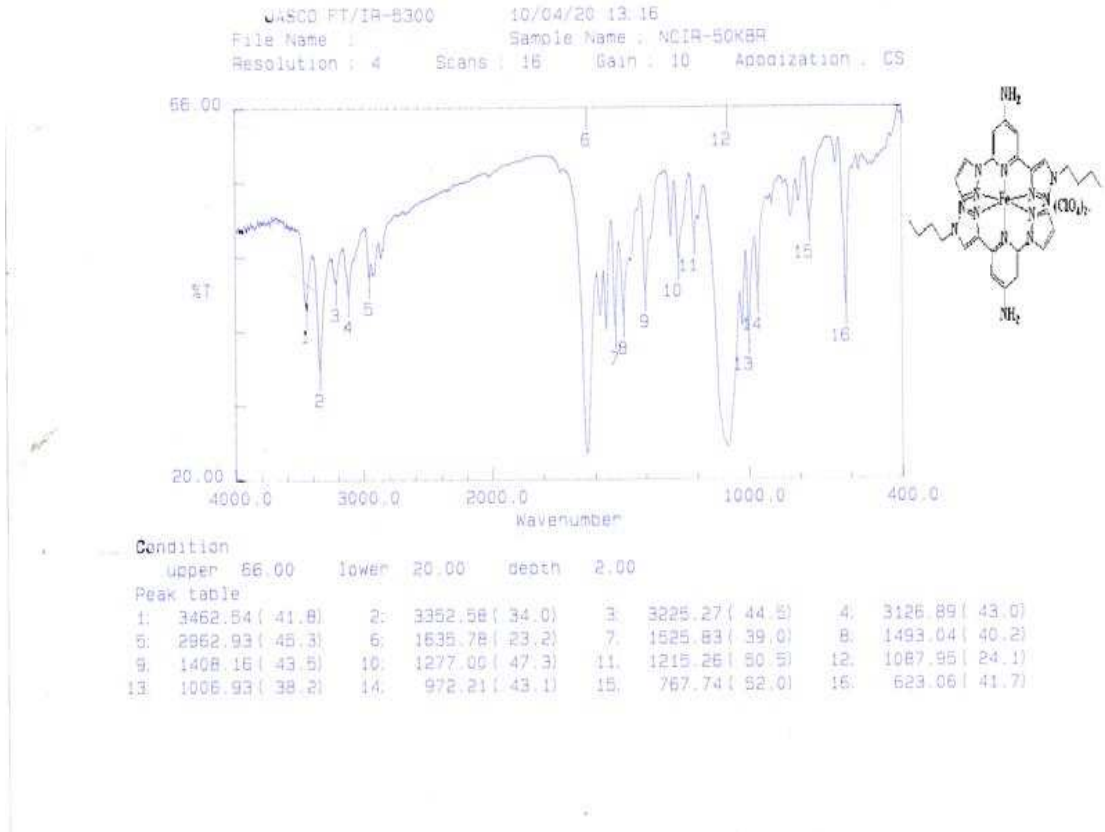

Figure S22: **FT- IR** spectra of of $[Fe^{II}(L_2)_2](ClO_4)_2$ **(IV)**

Elemental analysis of I, II and III:

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SCHOOL OF CHEMISTRY
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Method filename: I:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID: NCE-20 (# 198)
Analysis type: UnkNown
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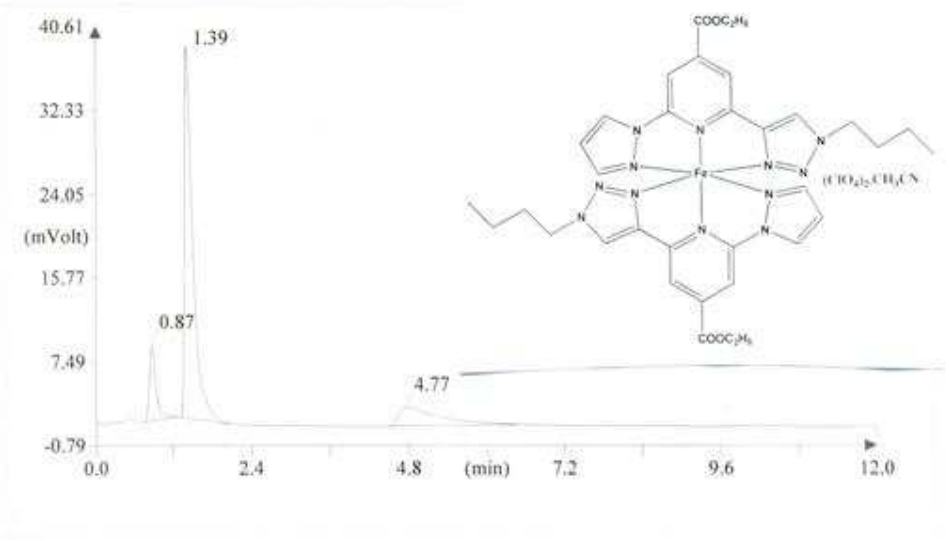
Sample weight: 1.188



Element Name	Element %	Ret. Time
Nitrogen	19. 12	0. 87
Carbon	44. 68	1. 39
Hydrogen	4. 61	4. 77

Figure S22: Elemental analysis spectra of $[Fe^{II}(L_1)_2](ClO_4)_2 \cdot CH_3CN$ **(I)**

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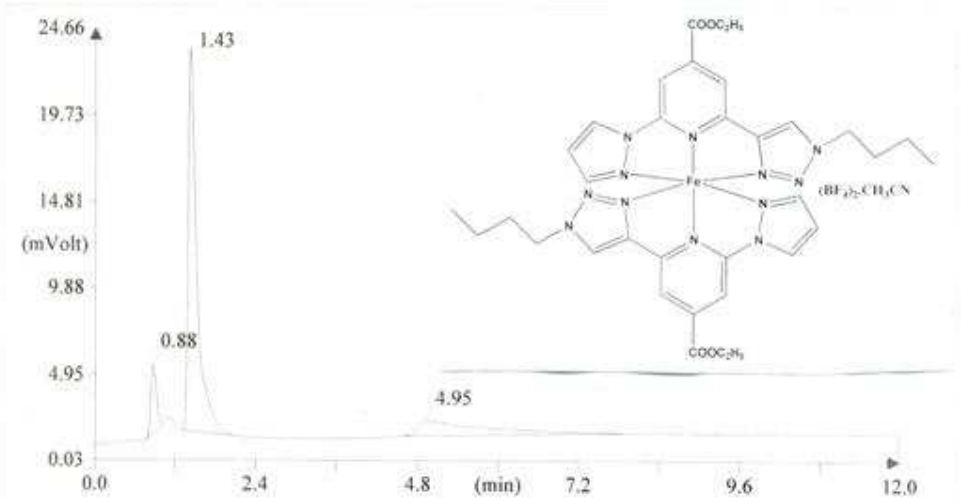

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Nitrogen	19. 88	0. 88
Carbon	45. 78	1. 43
Hydrogen	4. 58	4. 95

Figure S22: Elemental analysis spectra of $[Fe^{II}(L_1)_2](BF_4)_2 \cdot CH_3CN$ **(II)**

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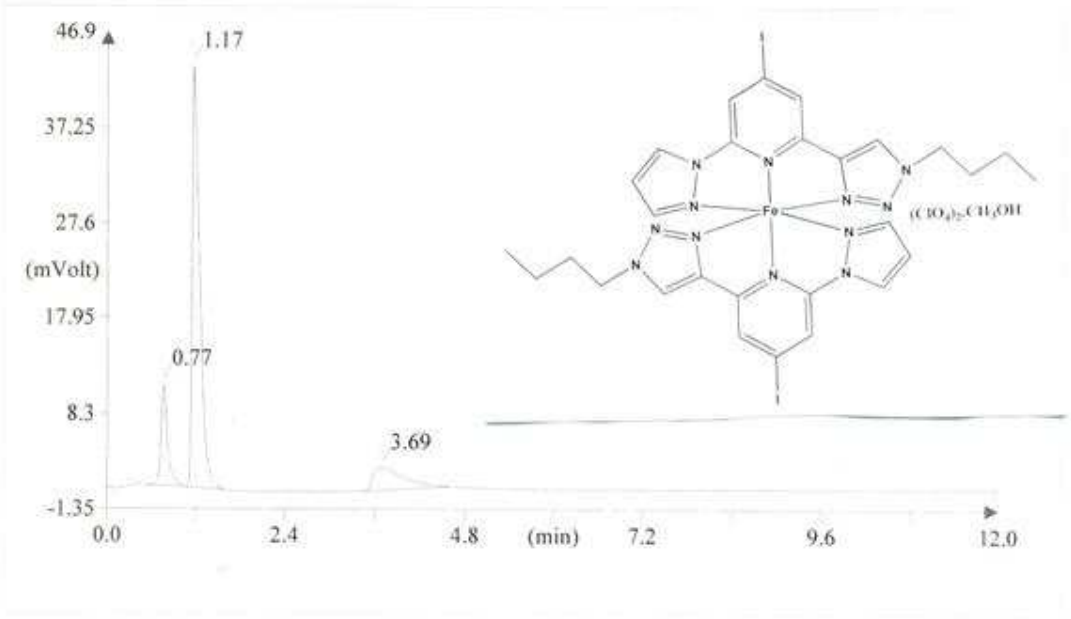

Element Name	Element %	Ret. Time
Nitrogen	17. 36	0. 77
Carbon	34. 25	1. 17
Hydrogen	3. 26	3. 69

Figure S22: Elemental analysis spectra of $[Fe^{II}(L_3)_2](ClO_4)_2.\ CH_3OH$ **(III)**