Synthesis, physical and antimicrobial studies of ferrocenyl-*N*-(pyridinylmethylene)anilines and ferrocenyl-*N*-(pyridinylmethyl)anilines

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Supplementary information

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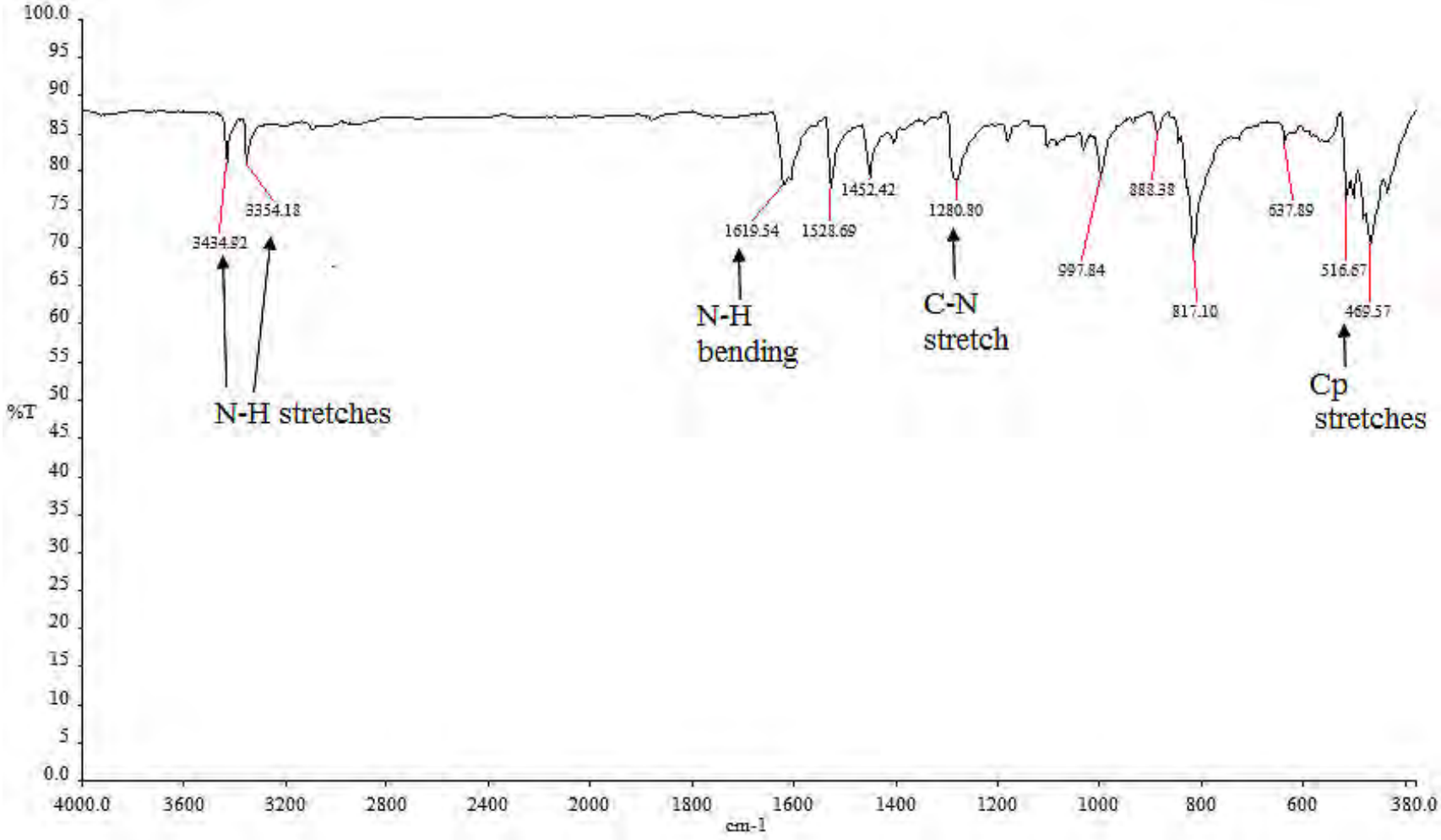


Figure S1: IR spectrum of compound **1**

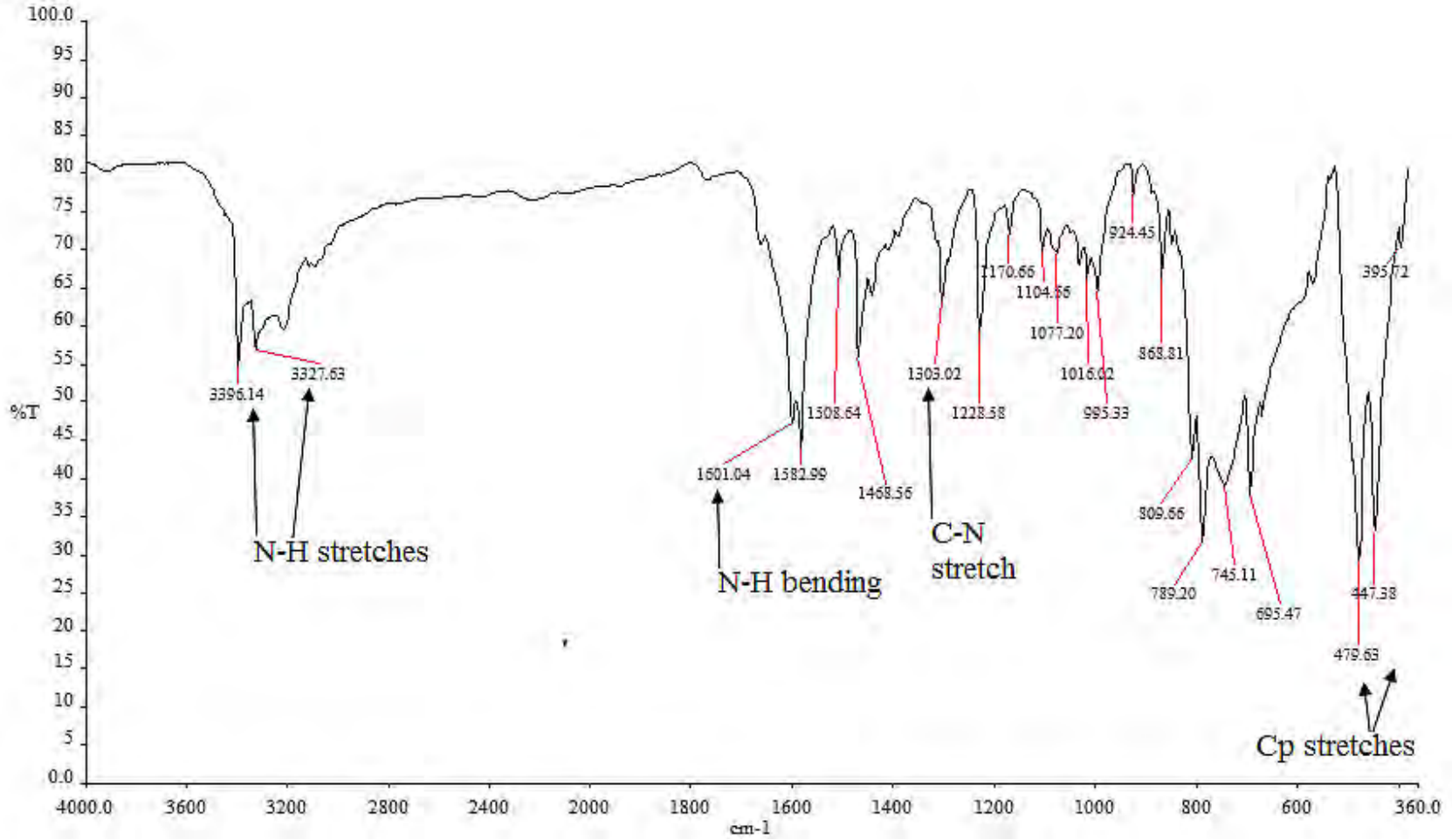


Figure S2: IR spectrum of compound **2**

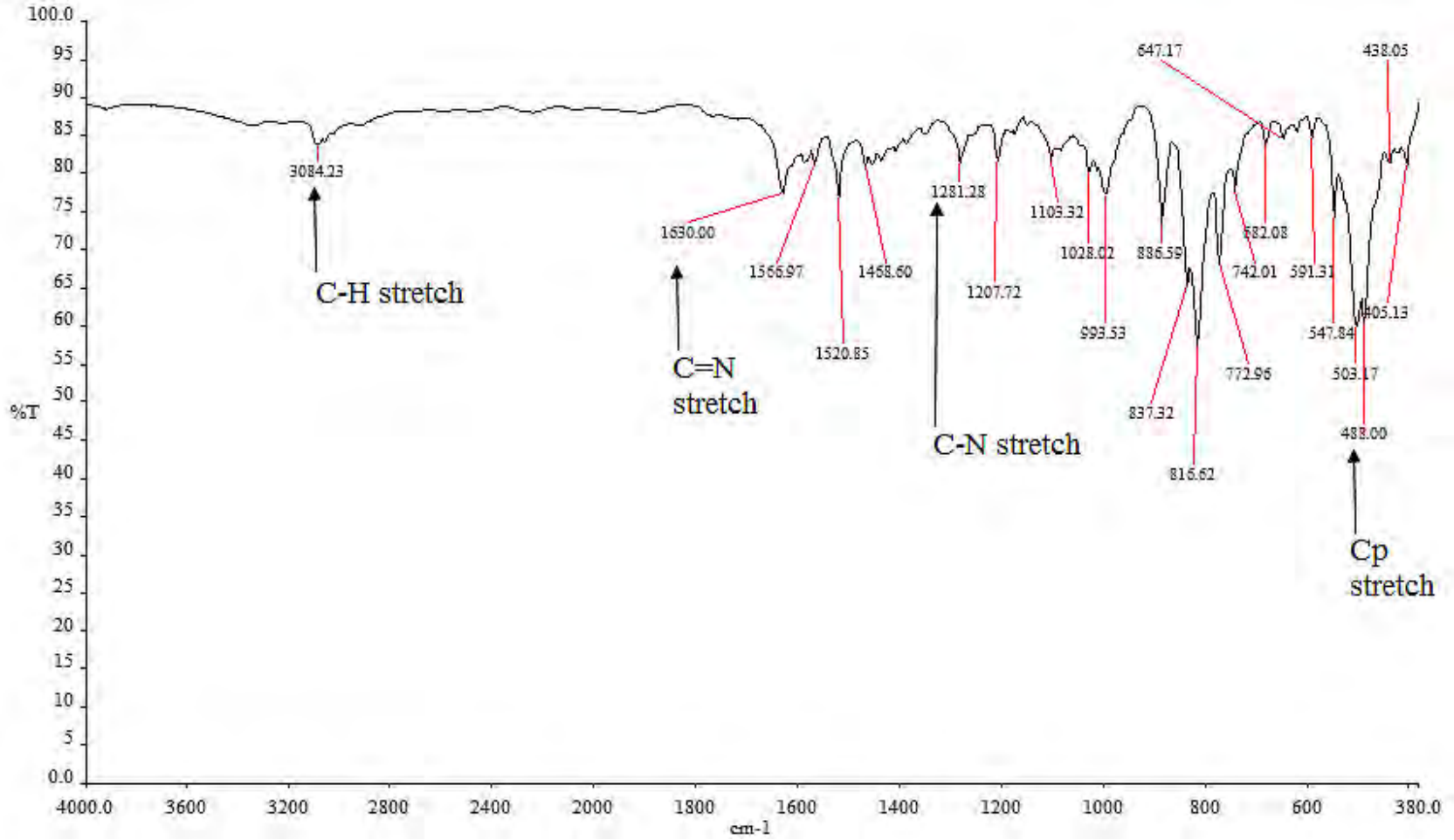


Figure S3: IR spectrum for compound **3**

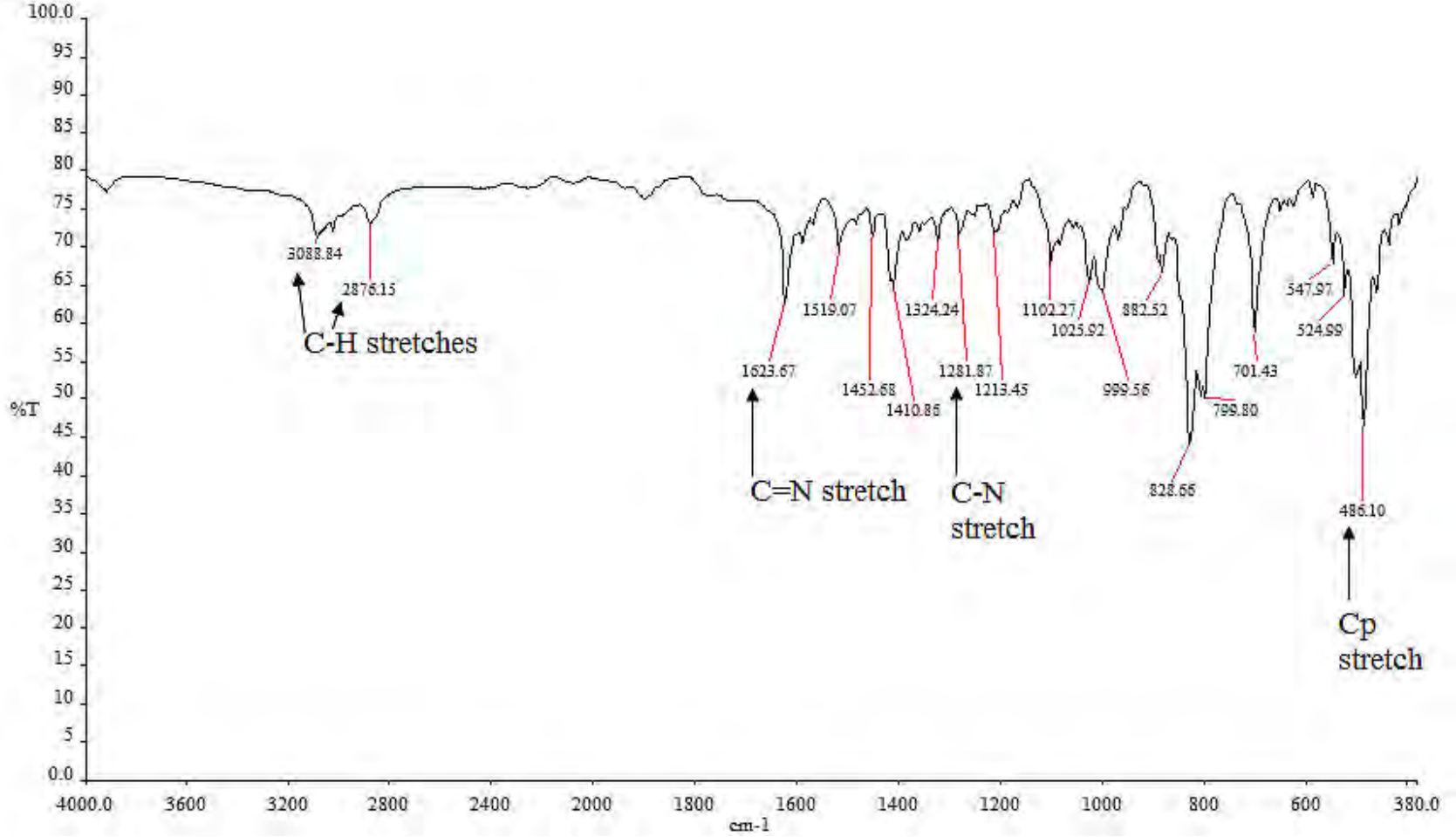


Figure S4: IR spectrum for compound **4**

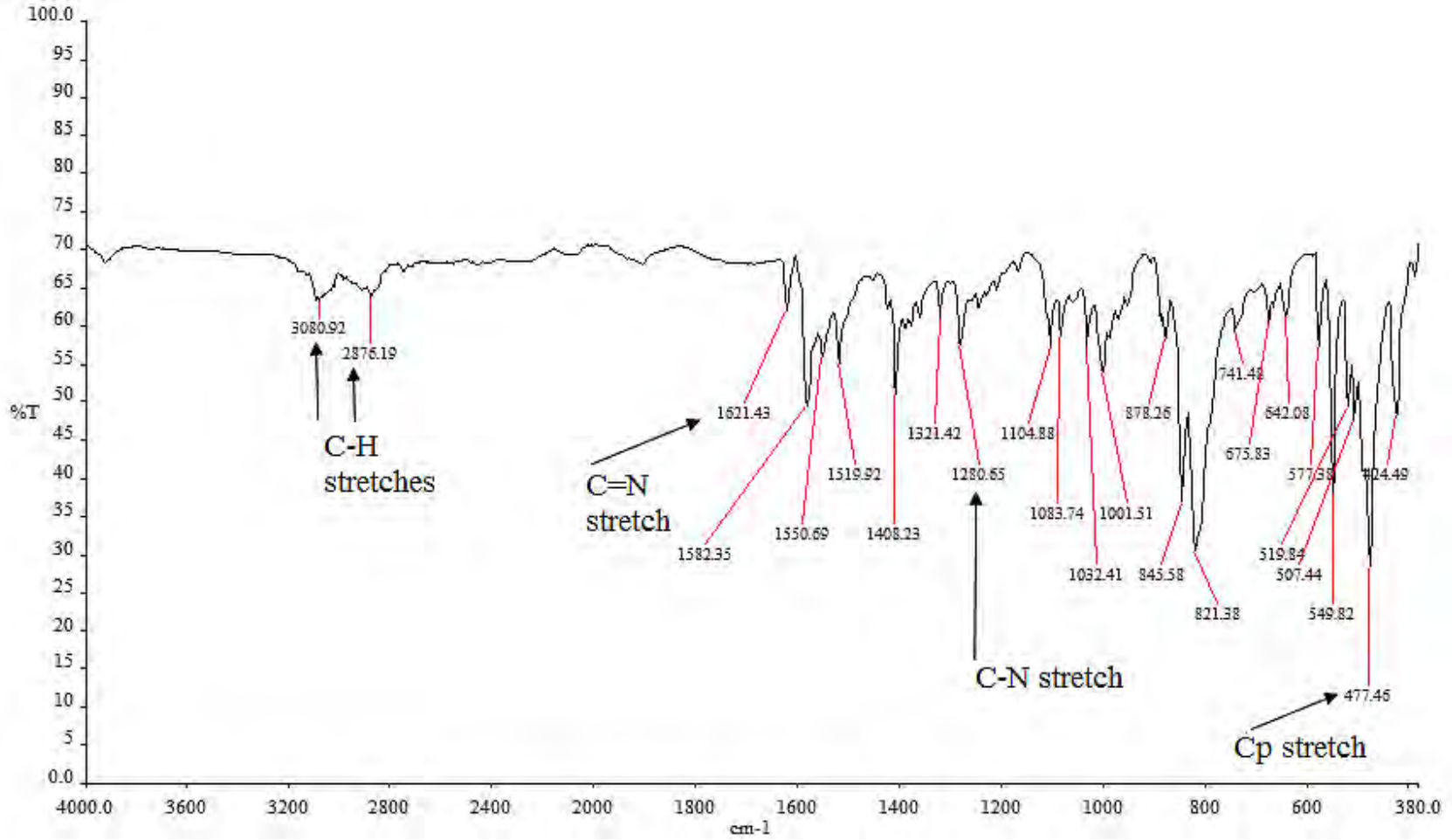


Figure S5: IR spectrum for compound **5**

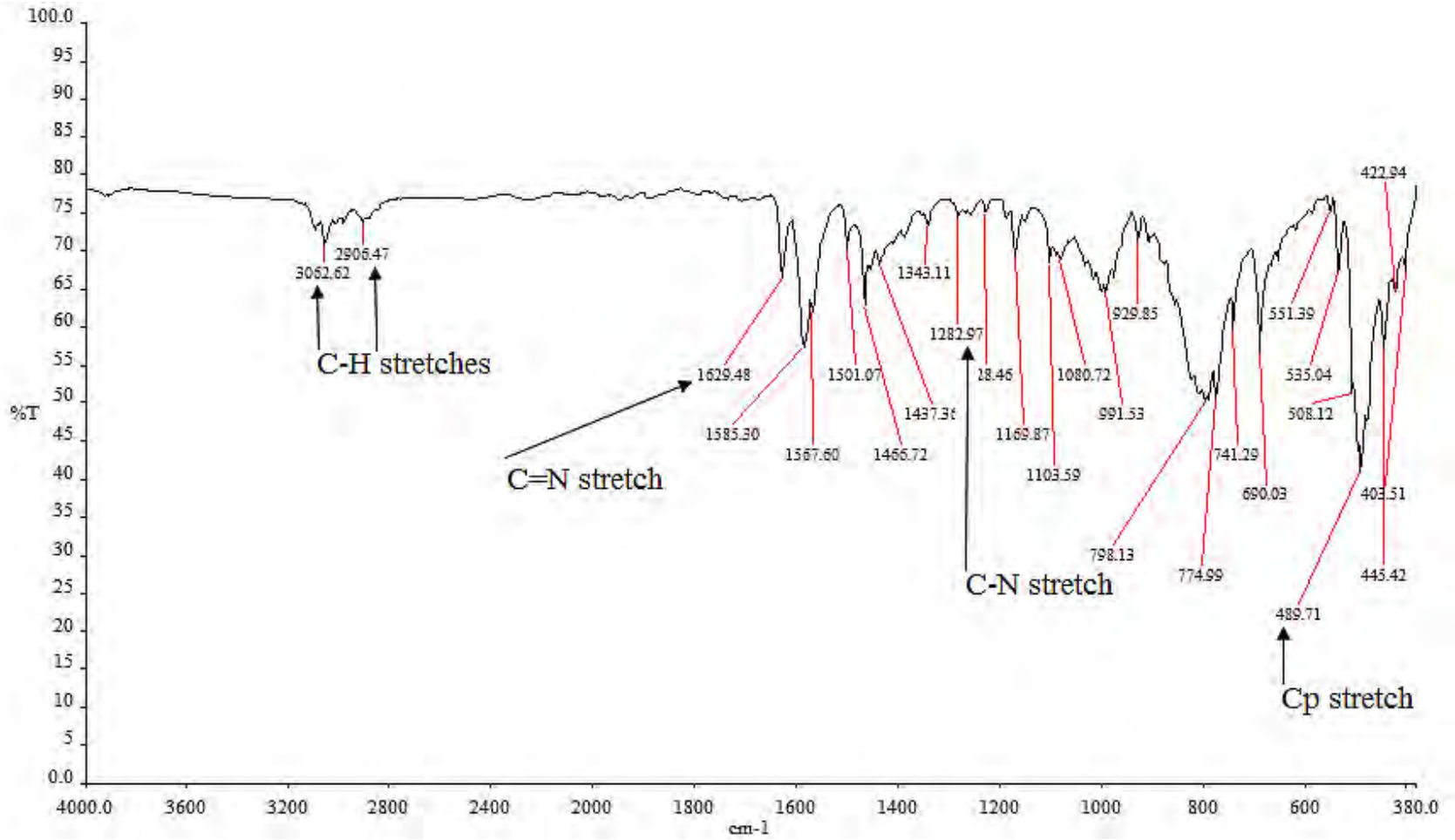


Figure S6: IR spectrum for compound **6**

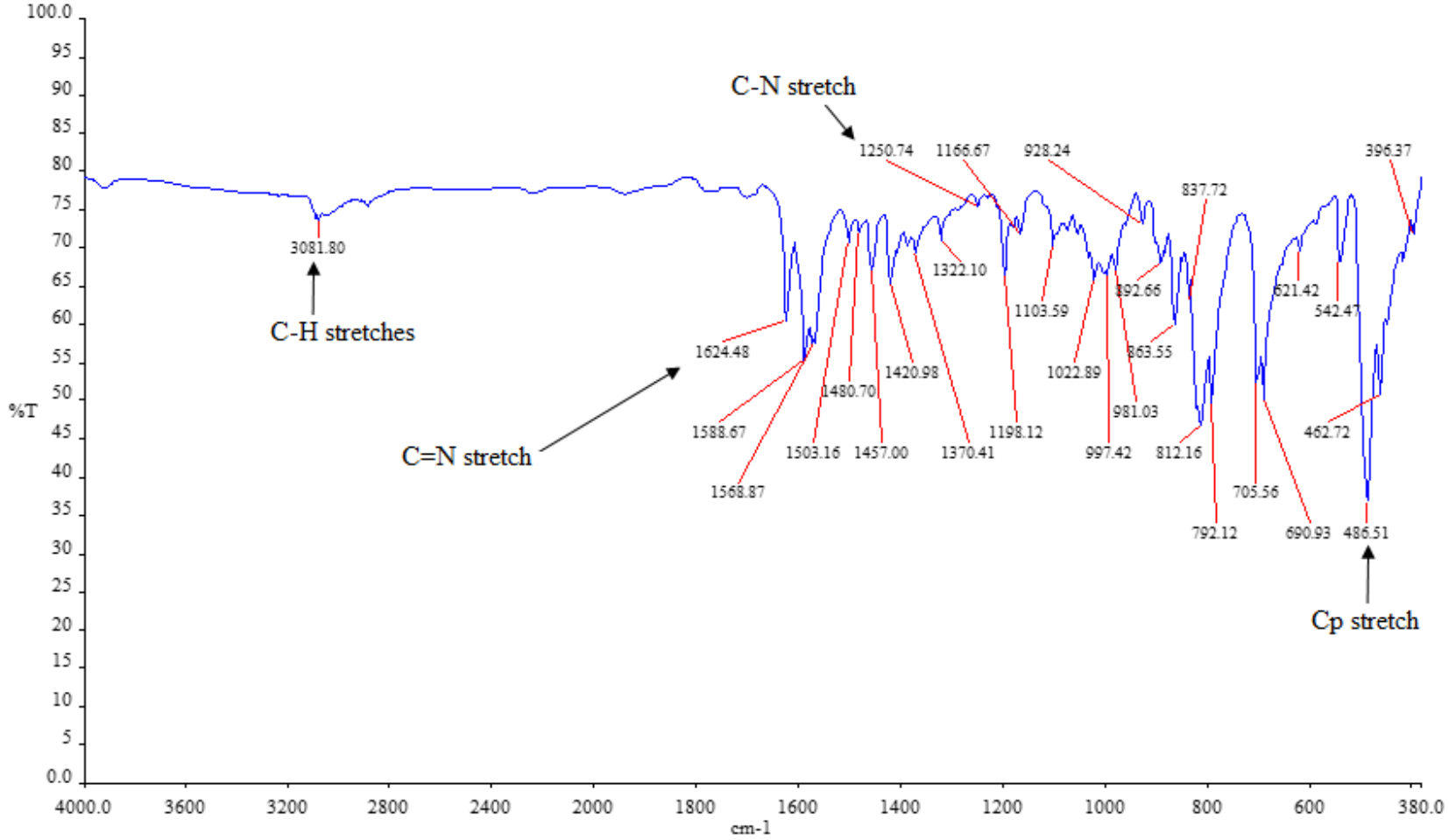


Figure S7: IR spectrum for compound **7**

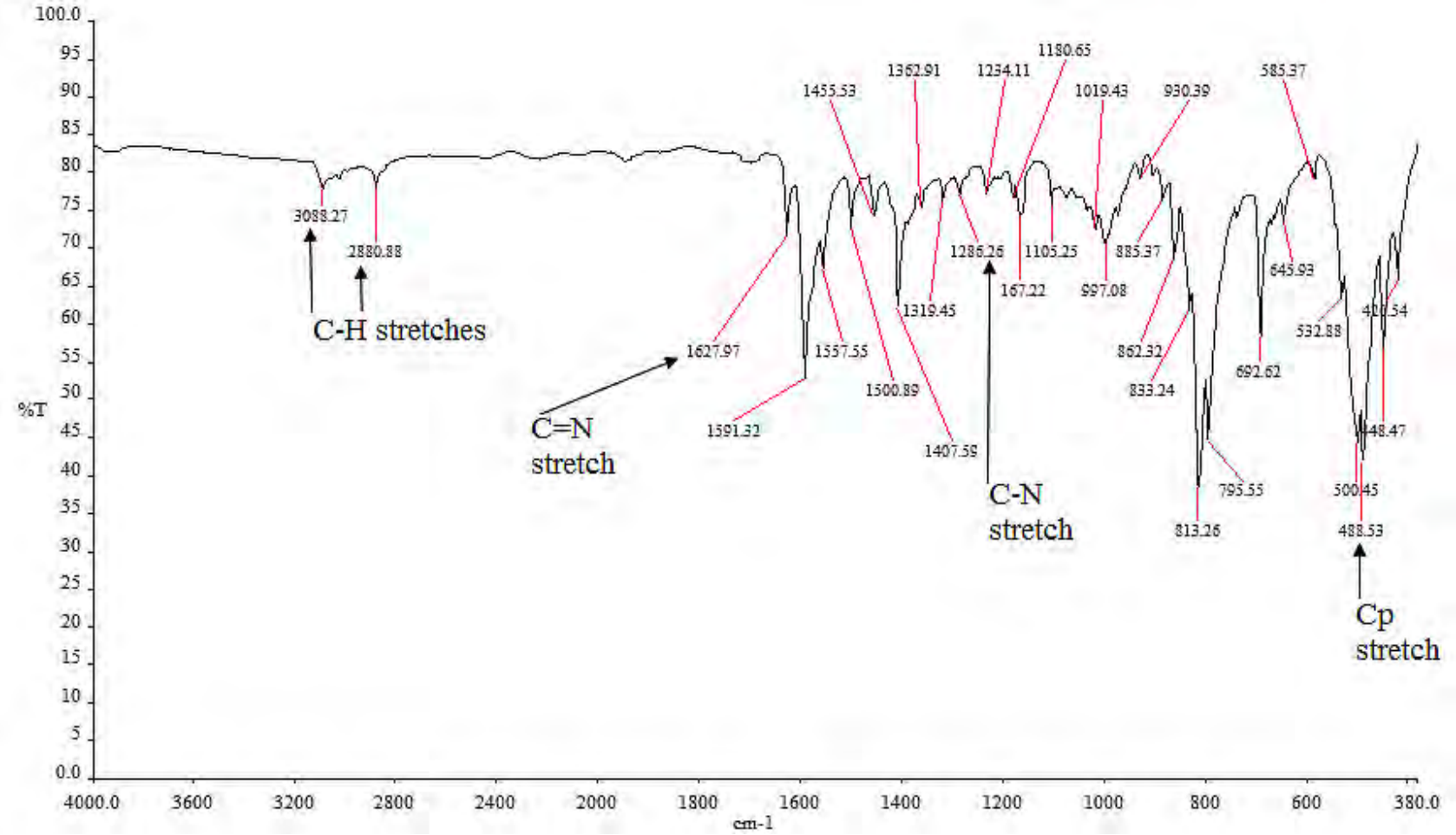


Figure S8: IR spectrum for compound **8**

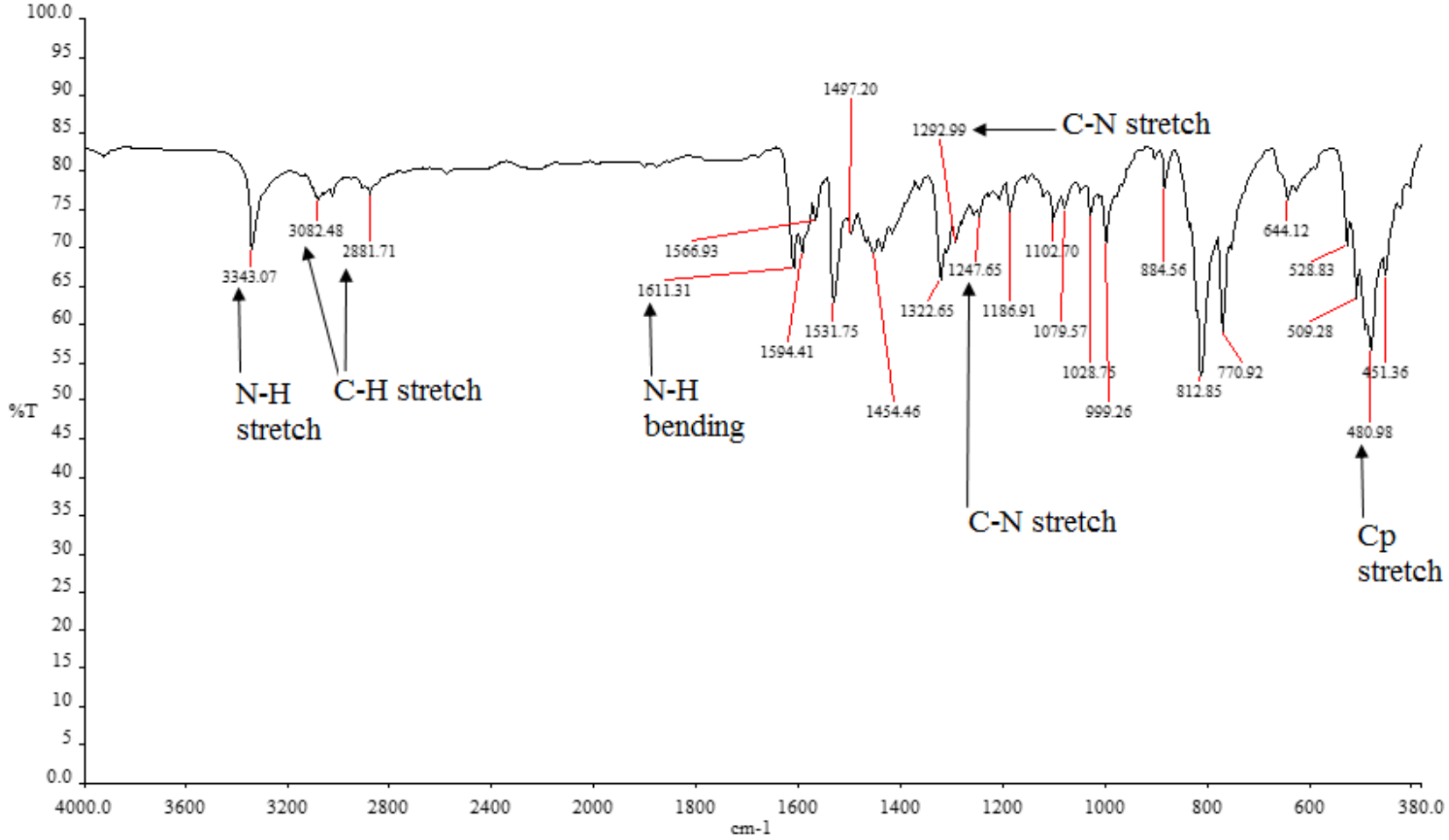


Figure S9: IR spectrum for compound **9**

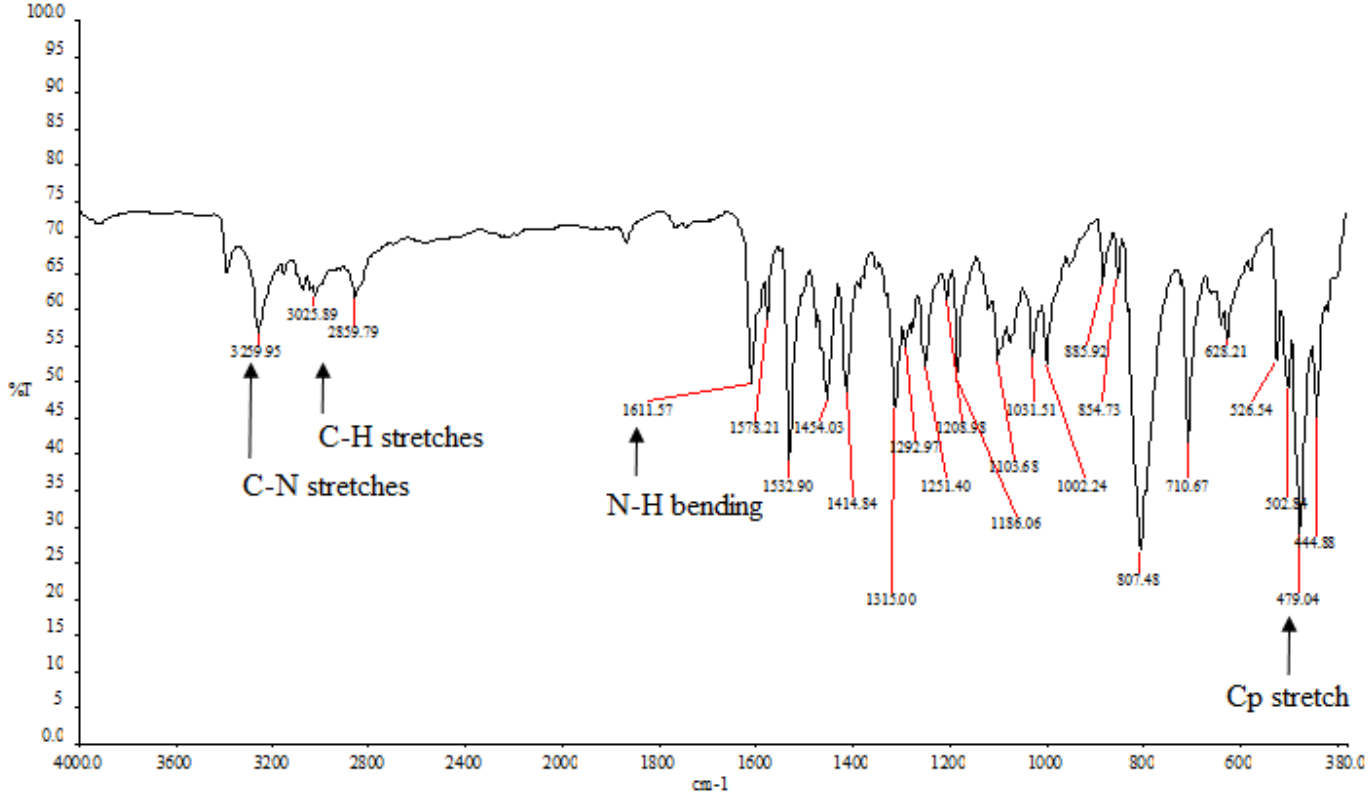


Figure S10: IR spectrum for compound **10**

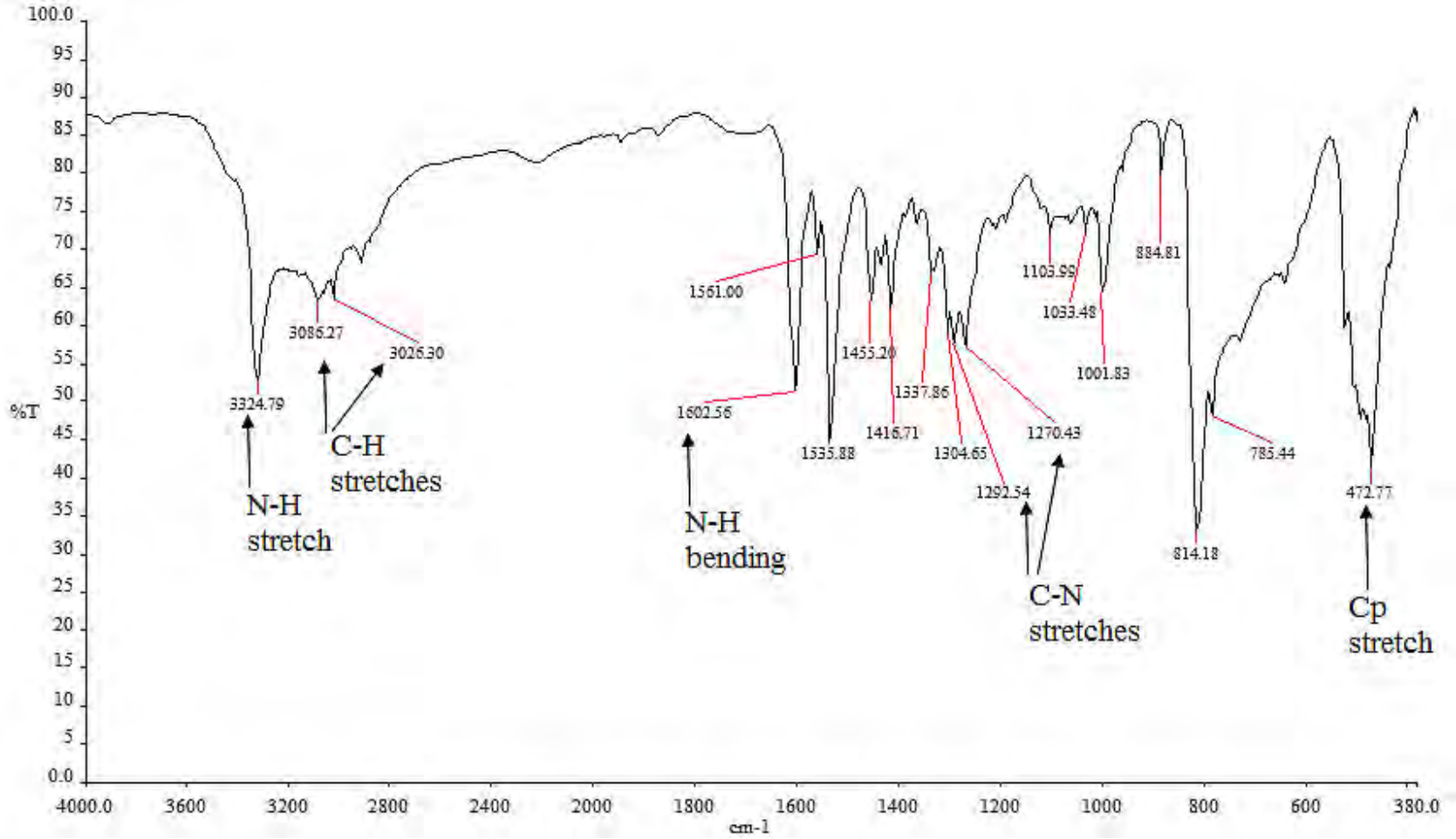


Figure S11: IR spectrum for compound **11**

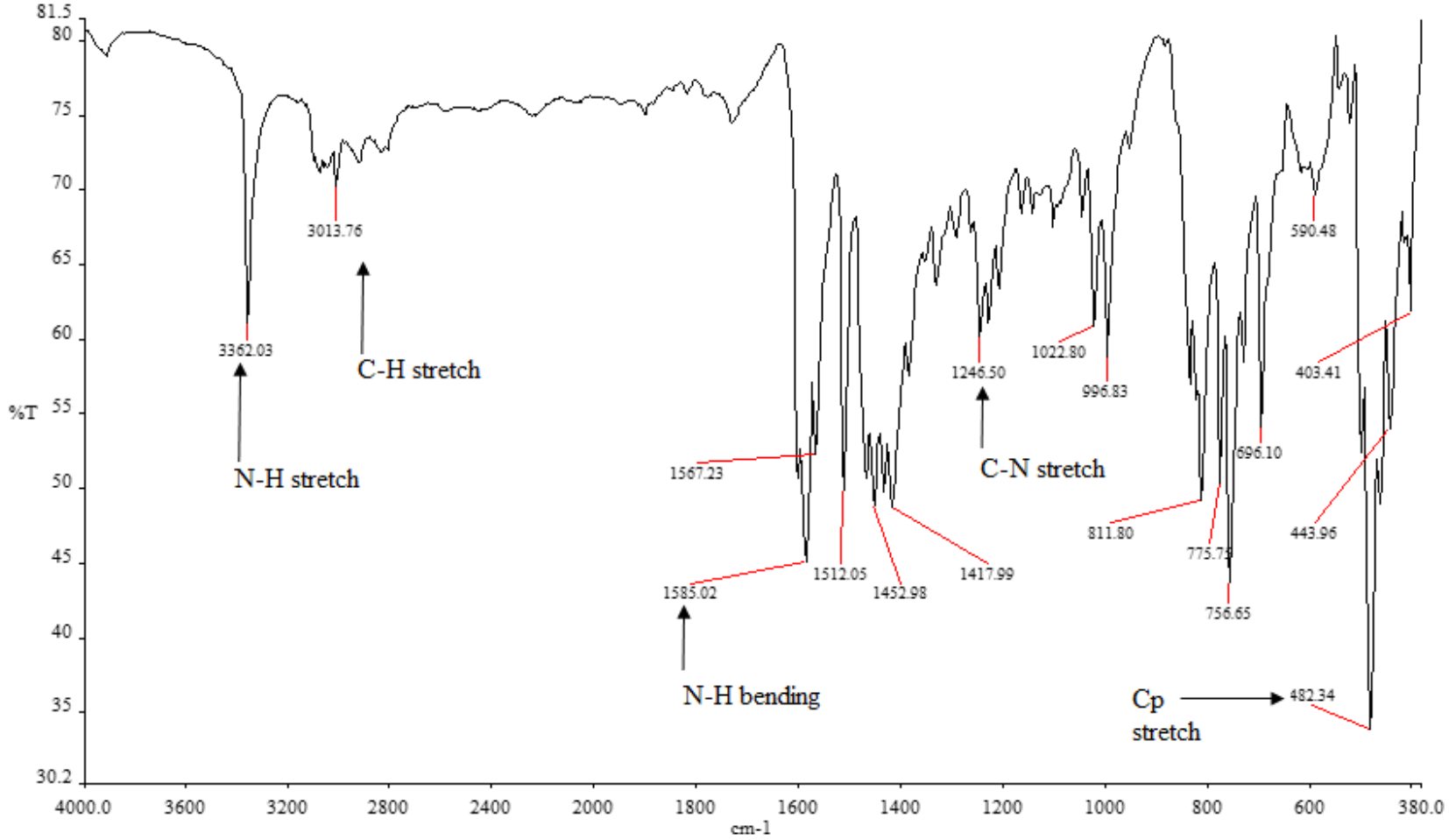


Figure S12: IR spectrum for compound **12**

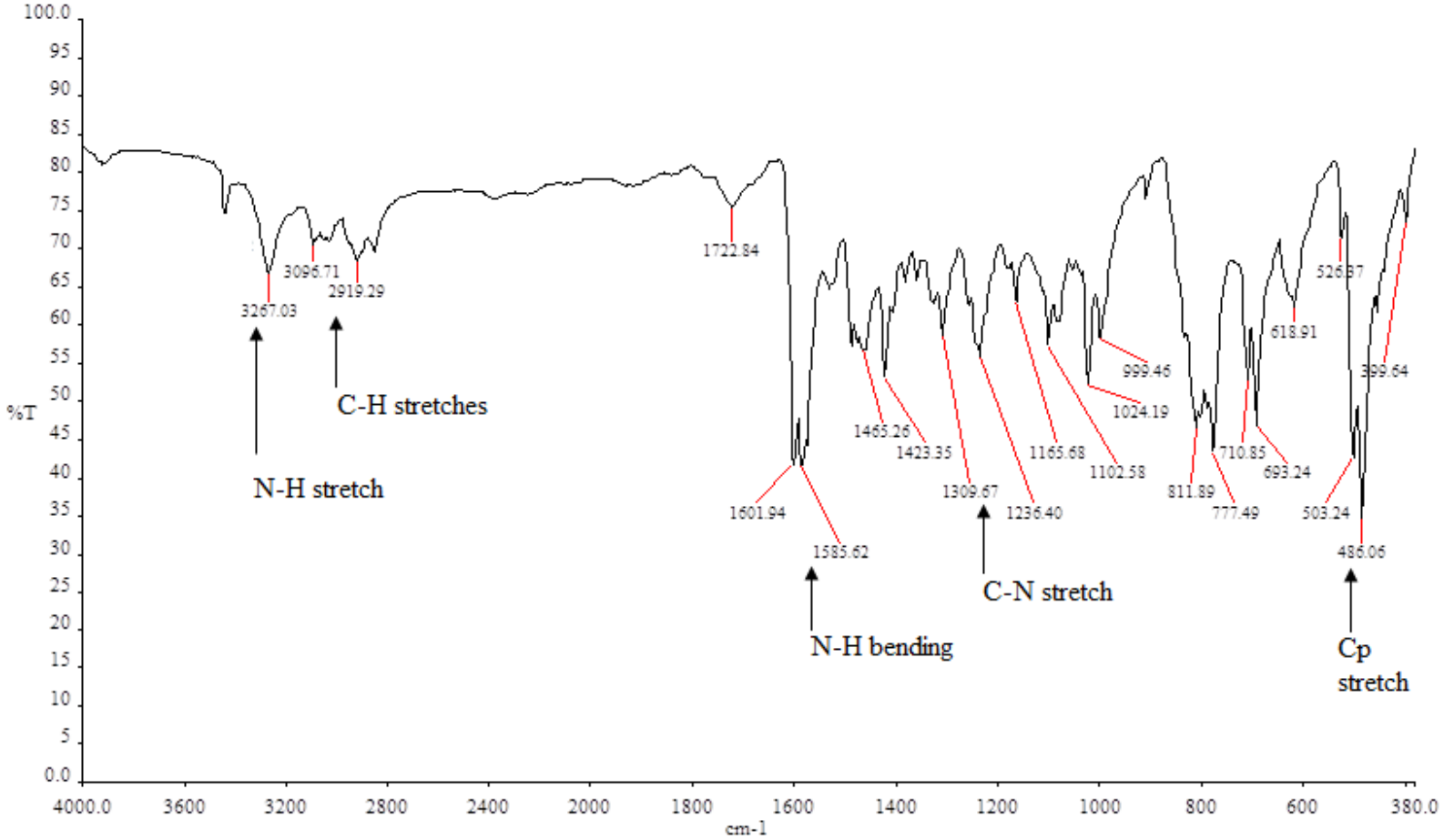


Figure S13: IR spectrum for compound **13**

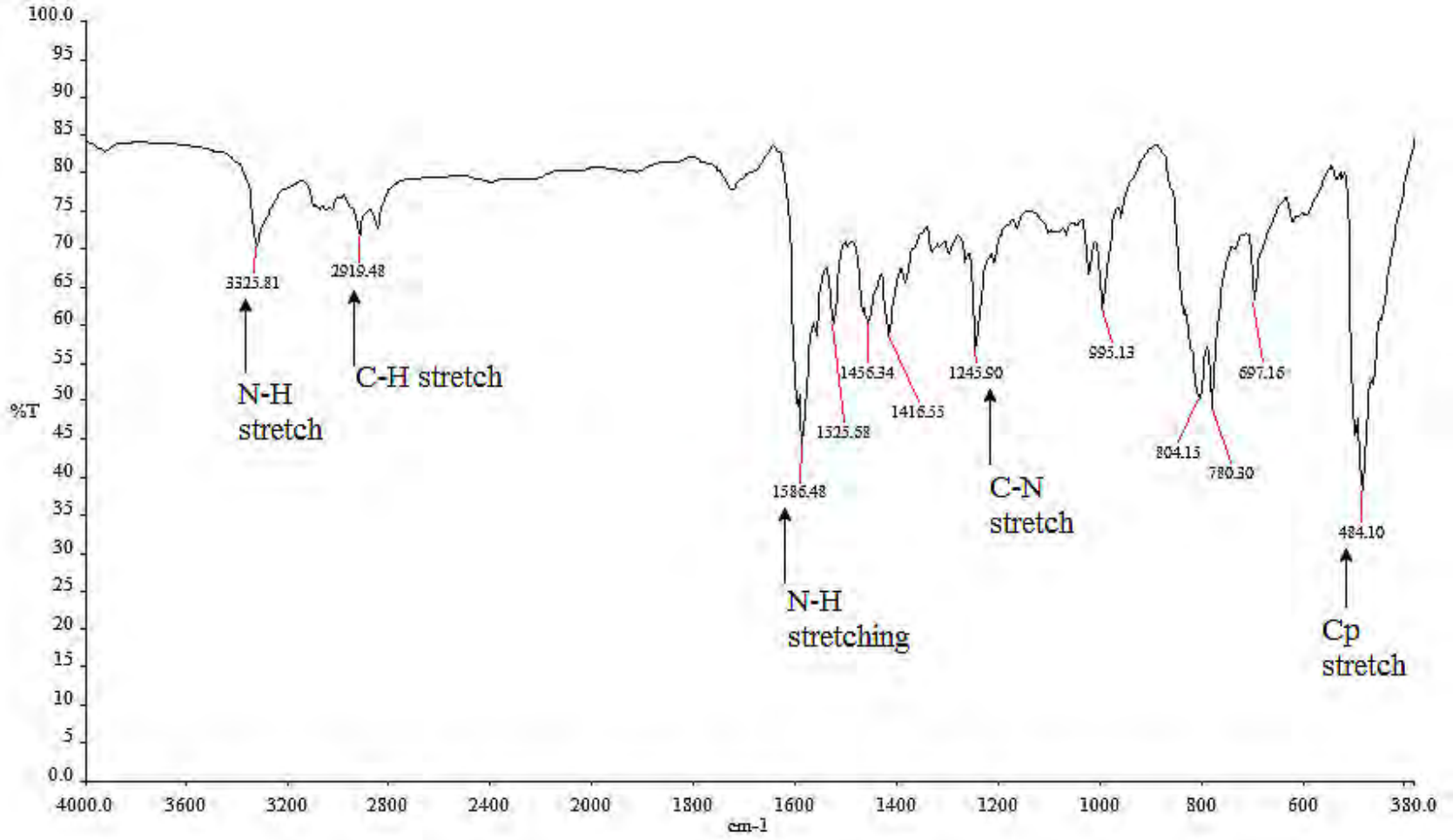
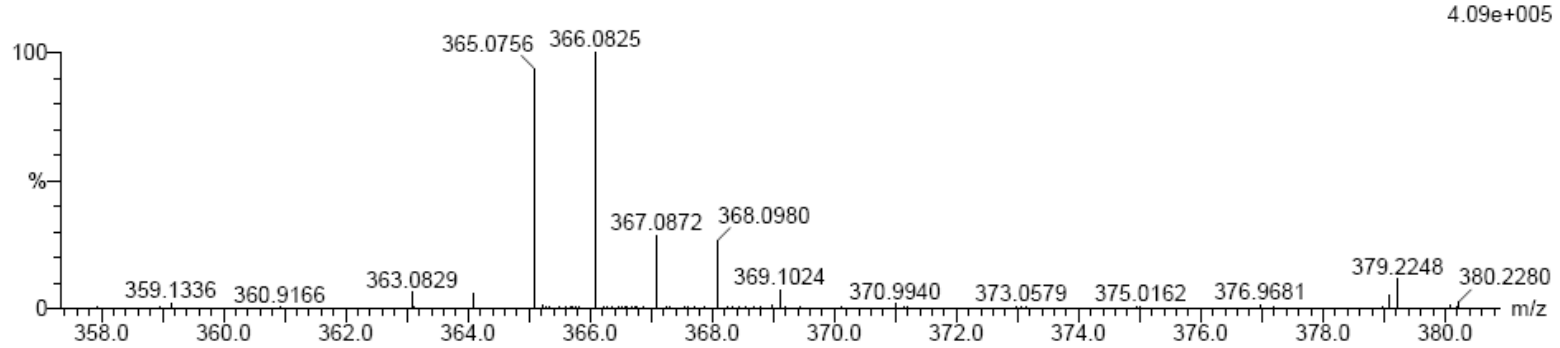


Figure S14: IR spectrum for compound **14**

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
4 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 20-25 H: 15-20 N: 0-5 Fe: 0-1
1 PhPy21mFe 29 (0.944) Cm (1:61)
TOF MS ES+



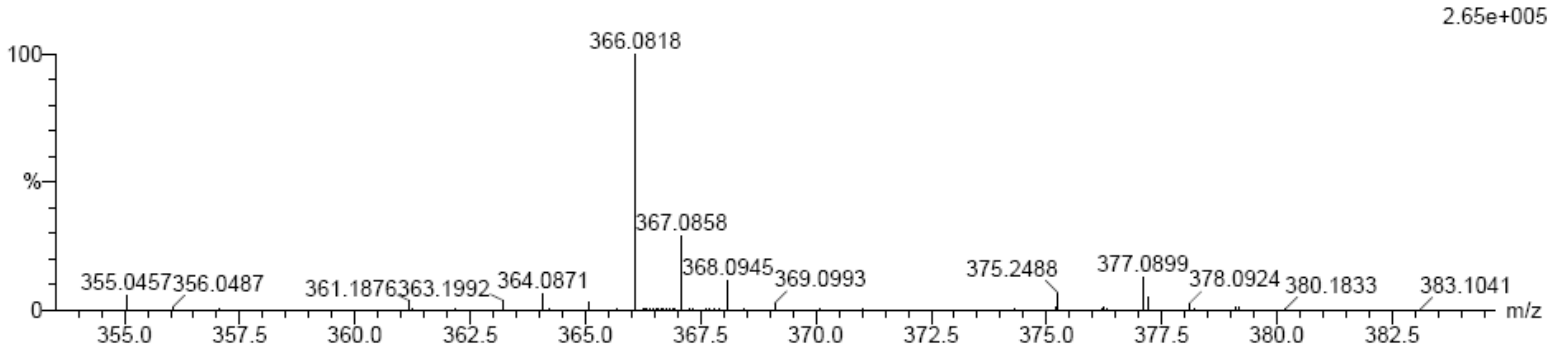
Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
366.0825	366.0819	0.6	1.6	15.0	697.9	0.0	C22 H18 N2 Fe

Figure S15: Mass spectrum for compound **3**

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 20-25 H: 15-25 N: 0-5 Fe: 0-1
3 PhPy31mFe 50 (1.653) Cm (1:61)
TOF MS ES+



Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
366.0818	366.0819	-0.1	-0.3	15.0	622.4	0.0	C22 H18 N2 Fe

Figure S16: Mass spectrum for compound **4**

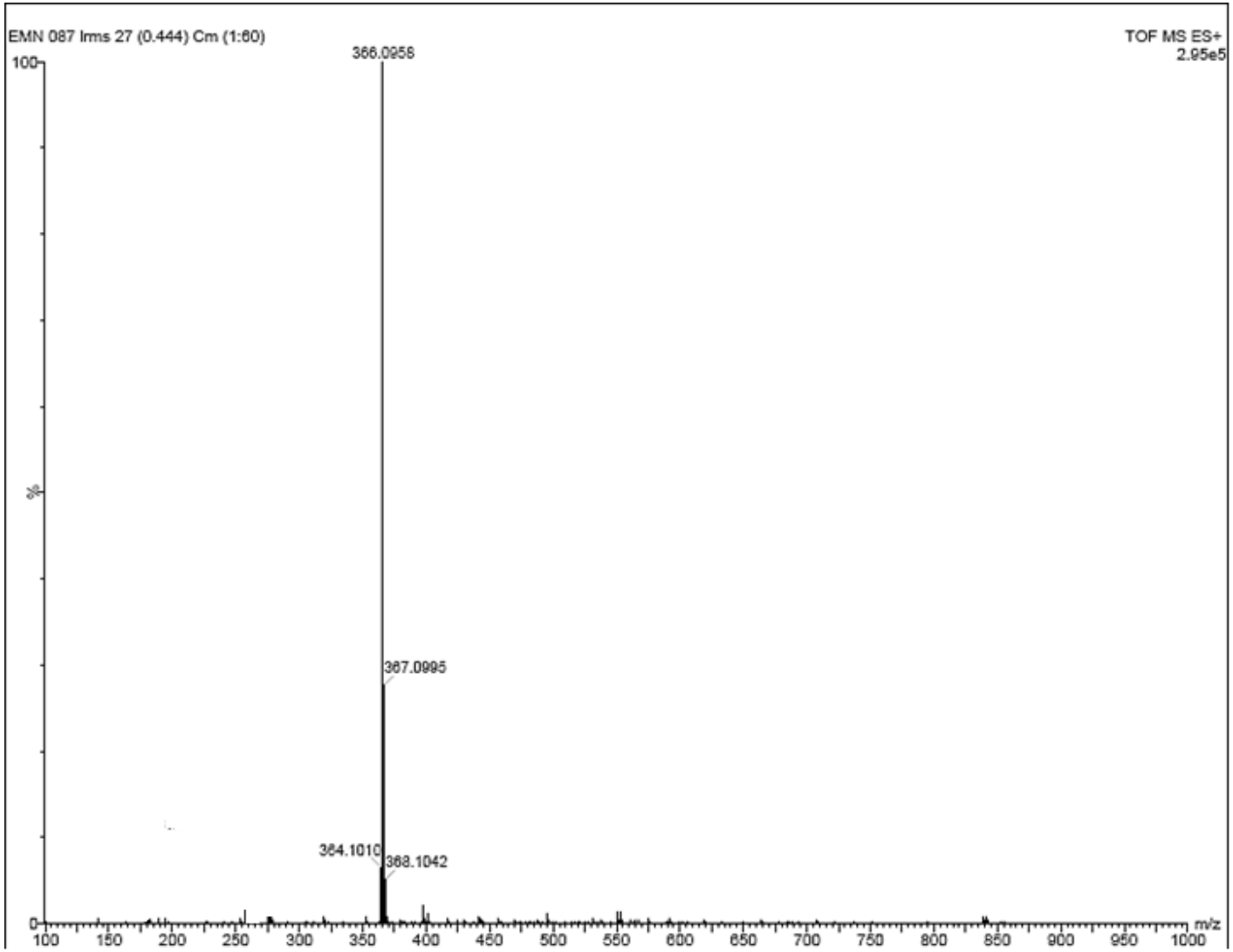
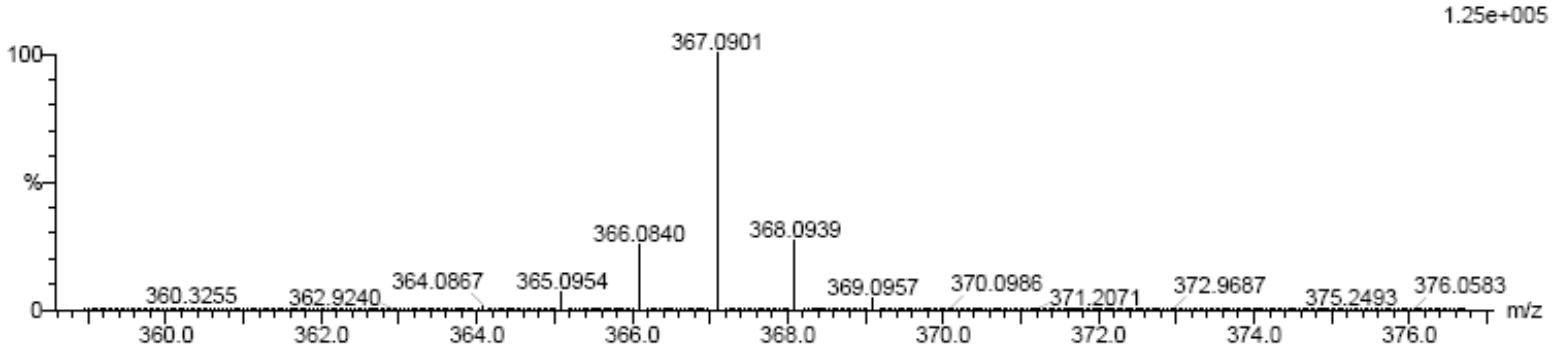


Figure S17: Mass spectrum for compound **5**

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
3 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 20-25 H: 15-20 N: 0-5 Fe: 0-1
1 26 (0.844) Cm (1:61)
TOF MS ES+



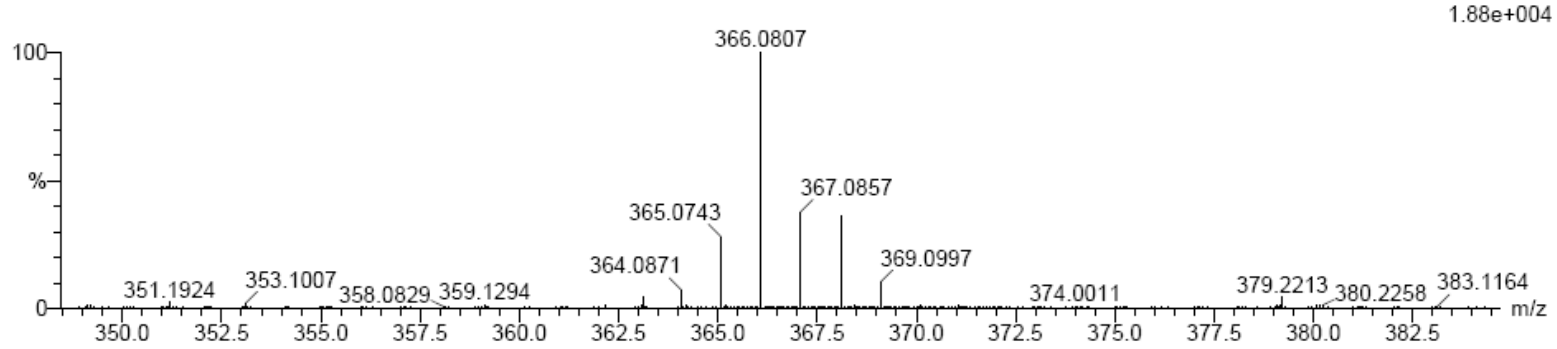
Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
367.0901	367.0898	0.3	0.8	14.5	599.1	0.0	C22 H19 N2 Fe

Figure S18: Mass spectrum for compound **6**

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 20-25 H: 15-25 N: 0-5 Fe: 0-1
7 3Pylm3PhFe 52 (1.721) Cm (1:61)
TOF MS ES+



Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
366.0807	366.0819	-1.2	-3.3	15.0	462.0	0.0	C22 H18 N2 Fe

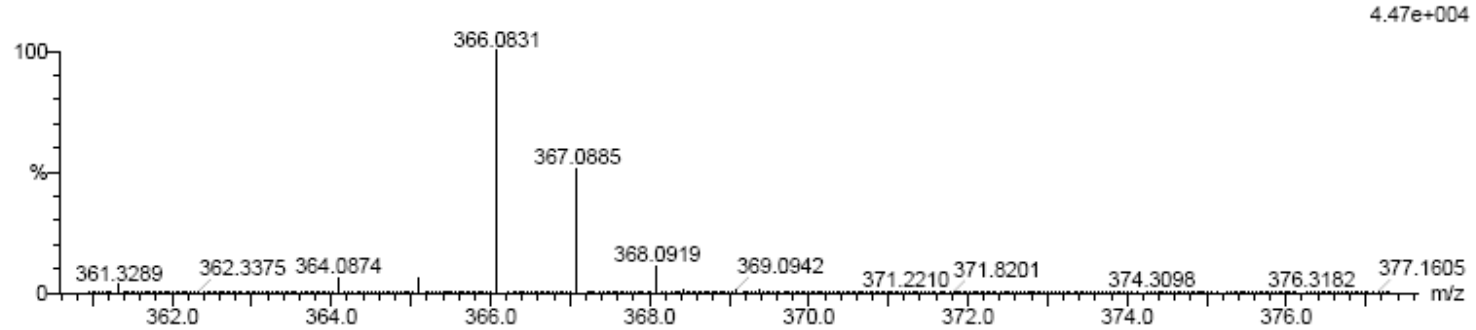
Figure S19: Mass spectrum for compound **7**

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
3 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 20-25 H: 15-20 N: 0-5 Fe: 0-1

2 15 (0.473) Cm (1:24)
TOF MS ES+



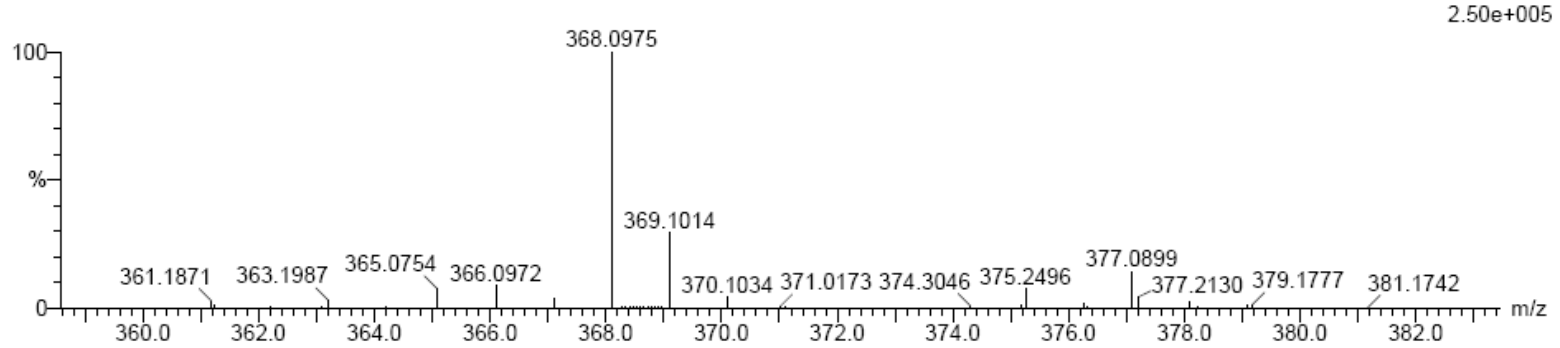
Minimum:				-1.5			
Maximum:		5.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
367.0885	367.0898	-1.3	-3.5	14.5	475.4	0.0	C22 H19 N2 Fe

Figure S20: Mass spectrum for compound **8**

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 20-25 H: 15-25 N: 0-5 Fe: 0-1
2 PhPy2AmFe 10 (0.304) Cm (1:61)
TOF MS ES+



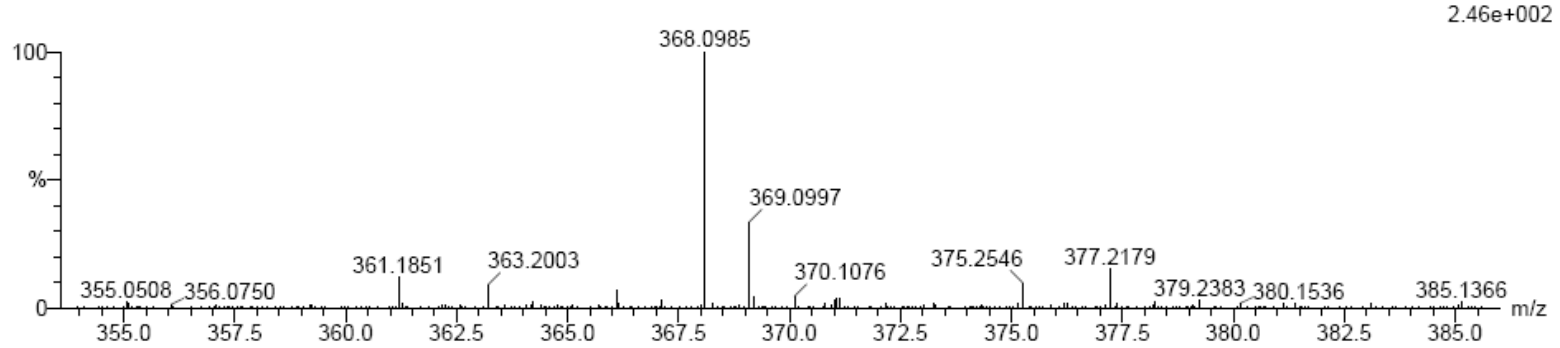
Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
368.0975	368.0976	-0.1	-0.3	14.0	670.3	0.0	C22 H20 N2 Fe

Figure S21: Mass spectrum for compound **9**

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 20-25 H: 15-25 N: 0-5 Fe: 0-1
4 PhPy3AmFe 6 (0.169)
TOF MS ES+



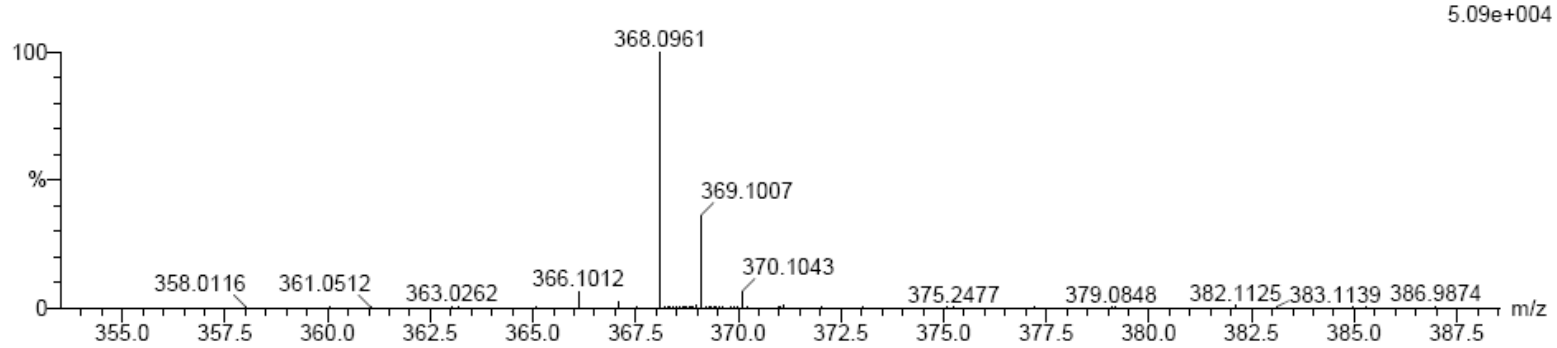
Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
368.0985	368.0976	0.9	2.4	14.0	65.6	0.0	C22 H20 N2 Fe

Figure S22: Mass spectrum for compound **10**

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 20-25 H: 15-25 N: 0-5 Fe: 0-1
5 PhPy4AmFe 13 (0.405) Cm (1:61)
TOF MS ES+



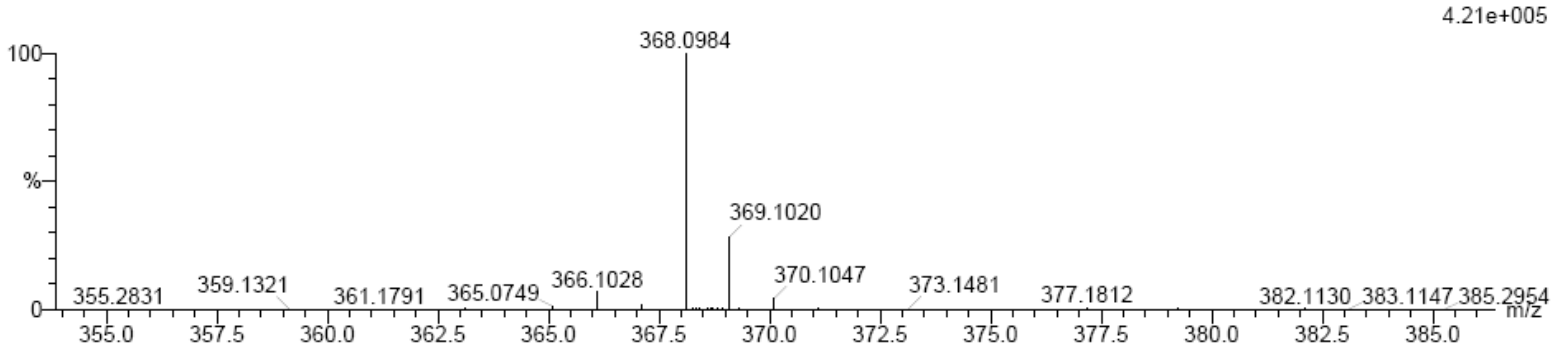
Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
368.0961	368.0976	-1.5	-4.1	14.0	532.8	0.0	C22 H20 N2 Fe

Figure S23: Mass spectrum for compound **11**

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
3 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 20-25 H: 15-20 N: 0-5 Fe: 0-1
EMN 084 34 (1.114) Cm (1:61)
TOF MS ES+



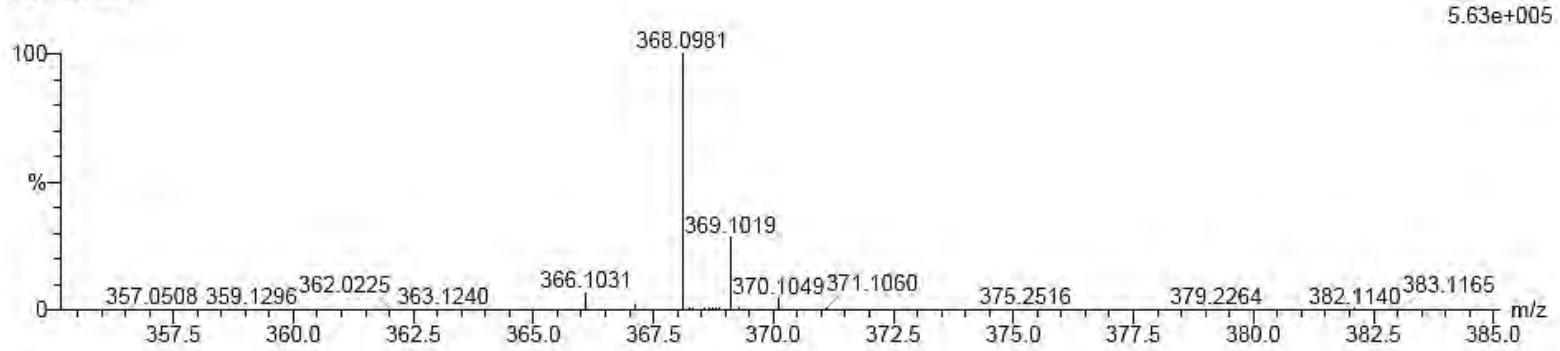
Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
368.0984	368.0976	0.8	2.2	14.0	673.9	0.0	C22 H20 N2 Fe

Figure S24: Mass spectrum for compound **12**

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
3 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 20-25 H: 15-20 N: 0-5 Fe: 0-1
EMN 085 53 (1.754) Cm (1:61)
TOF MS ES+



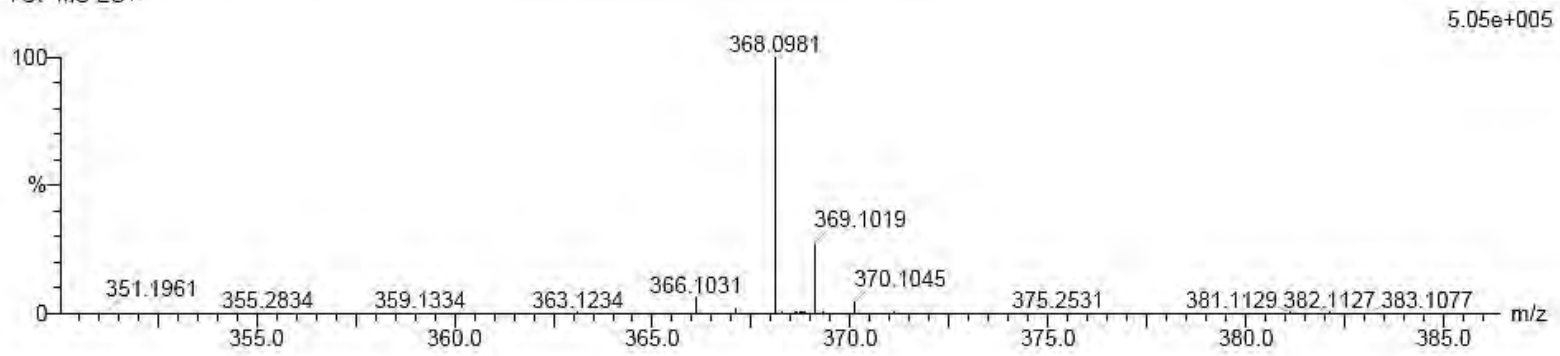
Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
368.0981	368.0976	0.5	1.4	14.0	692.0	0.0	C22 H20 N2 Fe

Figure S25: Mass spectrum for compound **13**

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
3 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 20-25 H: 15-20 N: 0-5 Fe: 0-1
EMN 086 58 (1.923) Cm (1:61)
TOF MS ES+



Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
368.0981	368.0976	0.5	1.4	14.0	694.5	0.0	C22 H20 N2 Fe

Figure S26: Mass spectrum for compound **14**

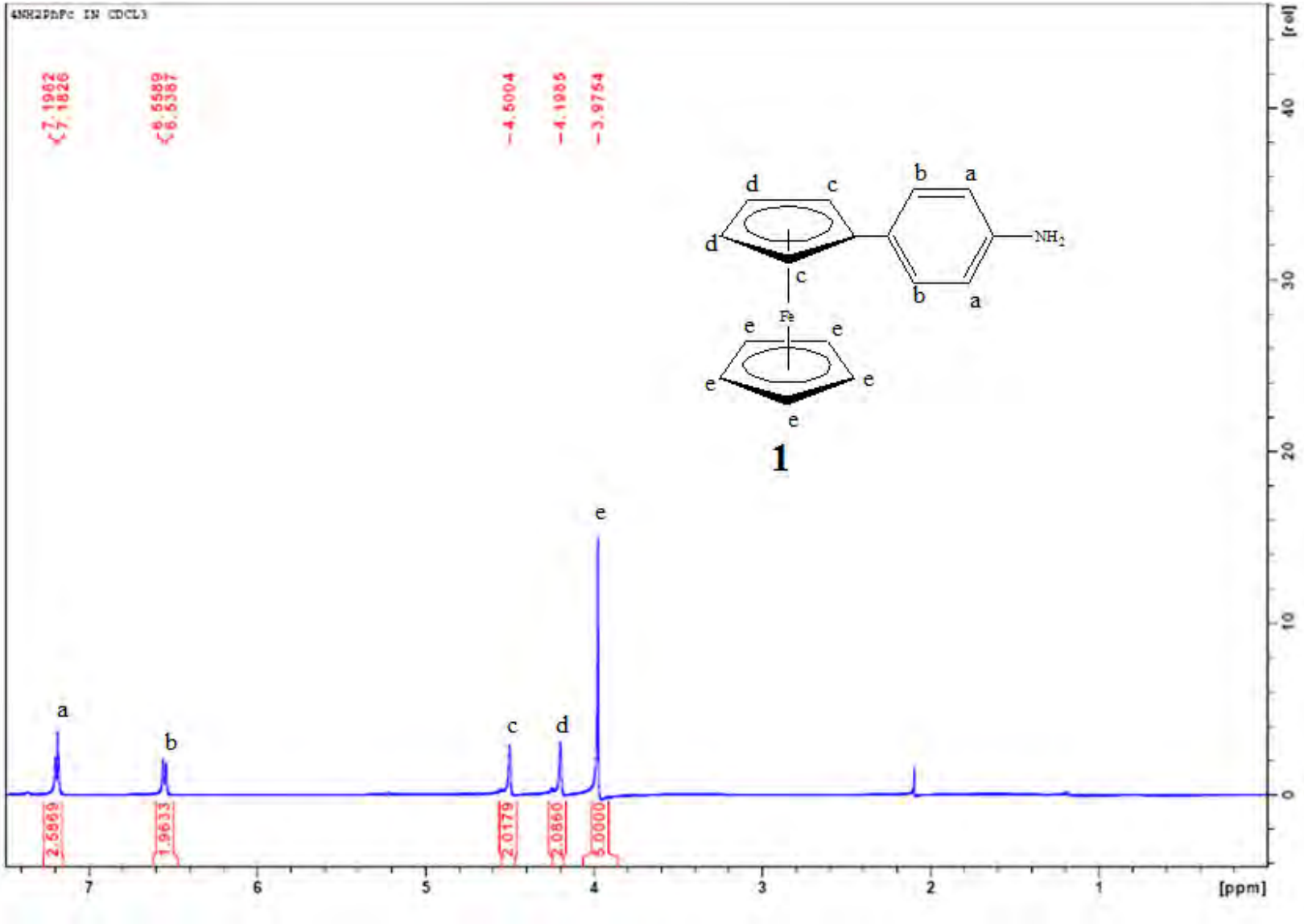


Figure S27: ^{1}H-NMR spectrum for compound **1**

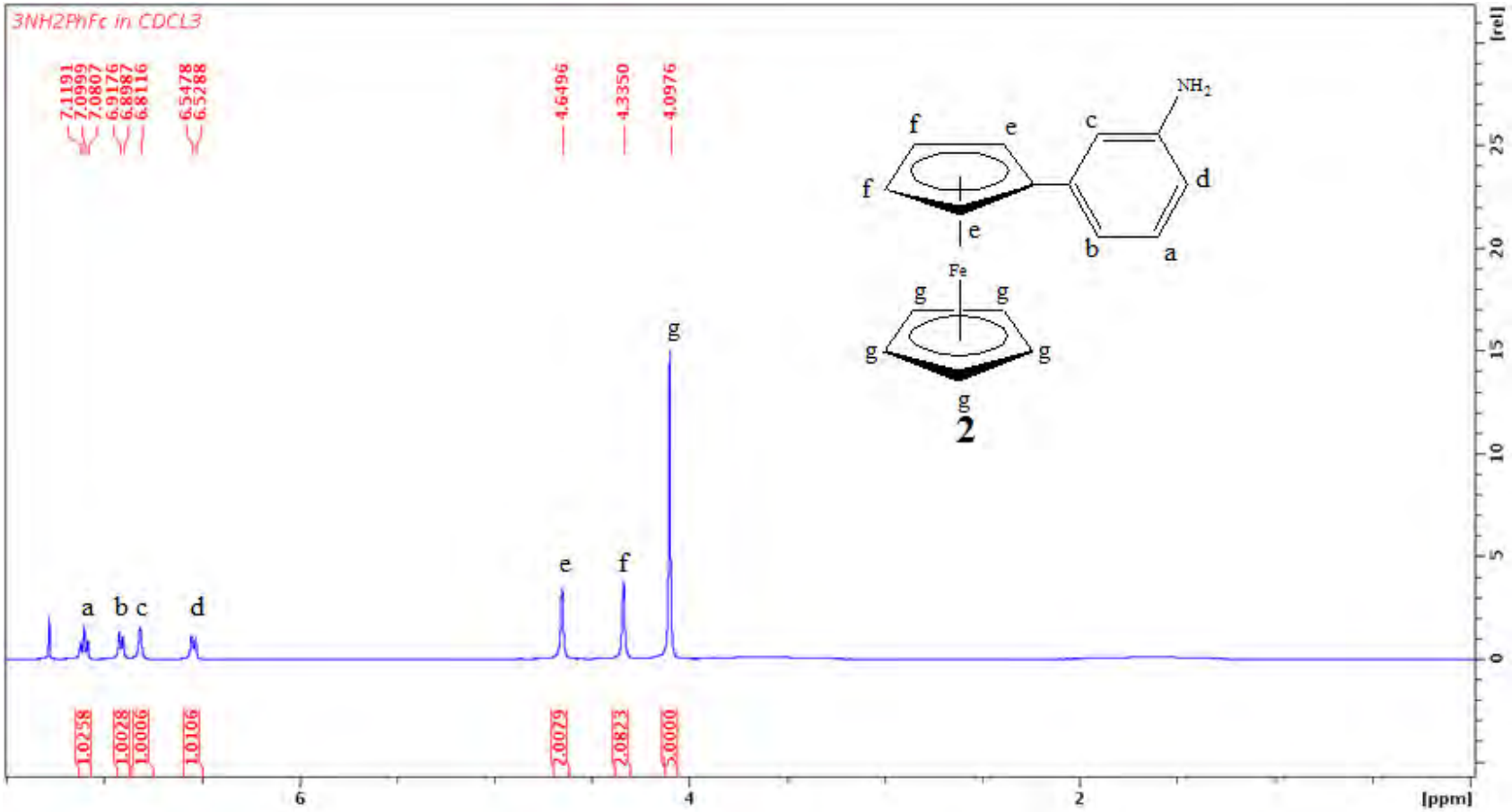


Figure S28: ^{1}H-NMR spectrum for compound **2**

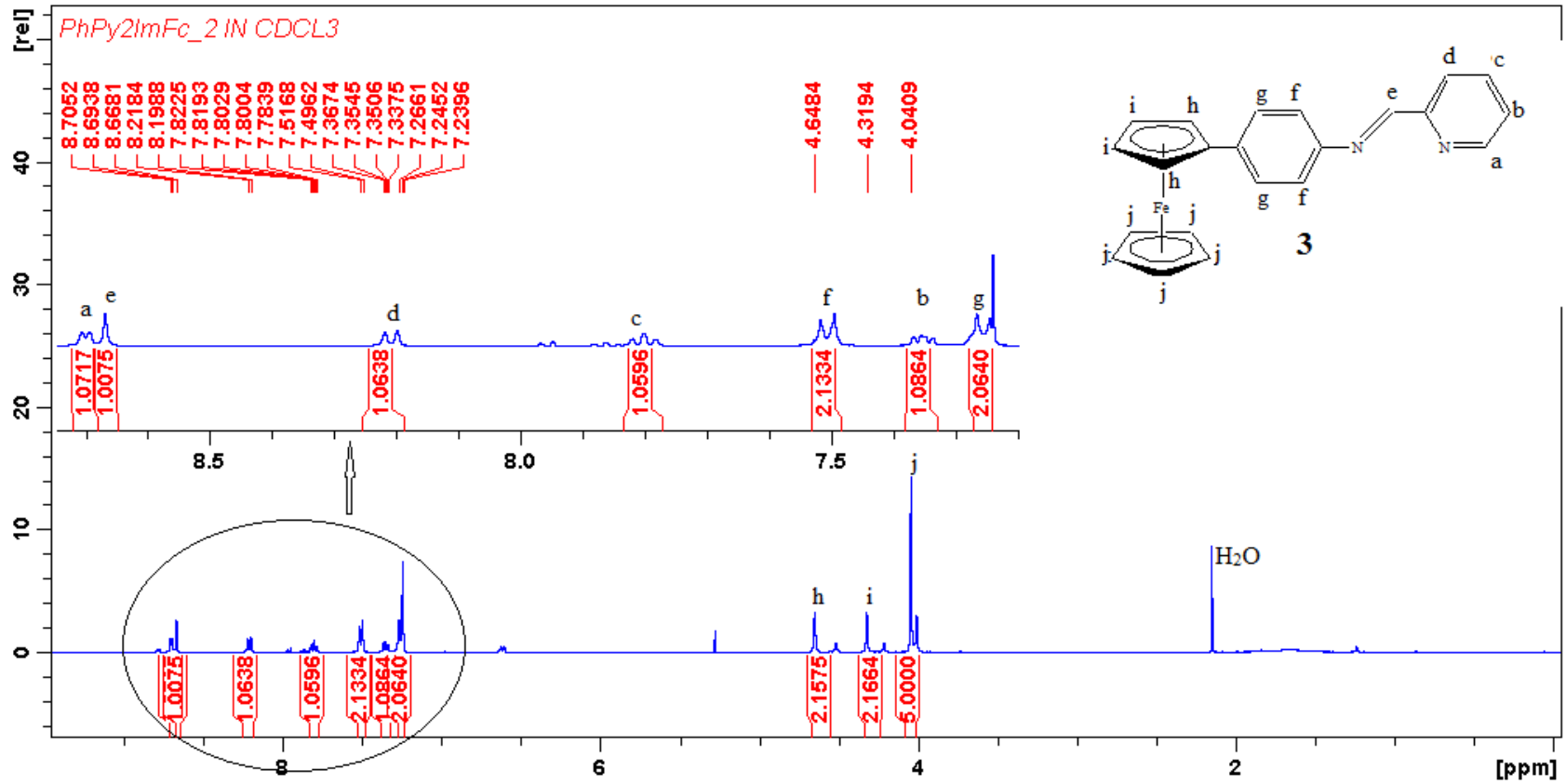


Figure S29: ^{1}H-NMR spectrum for compound **3**

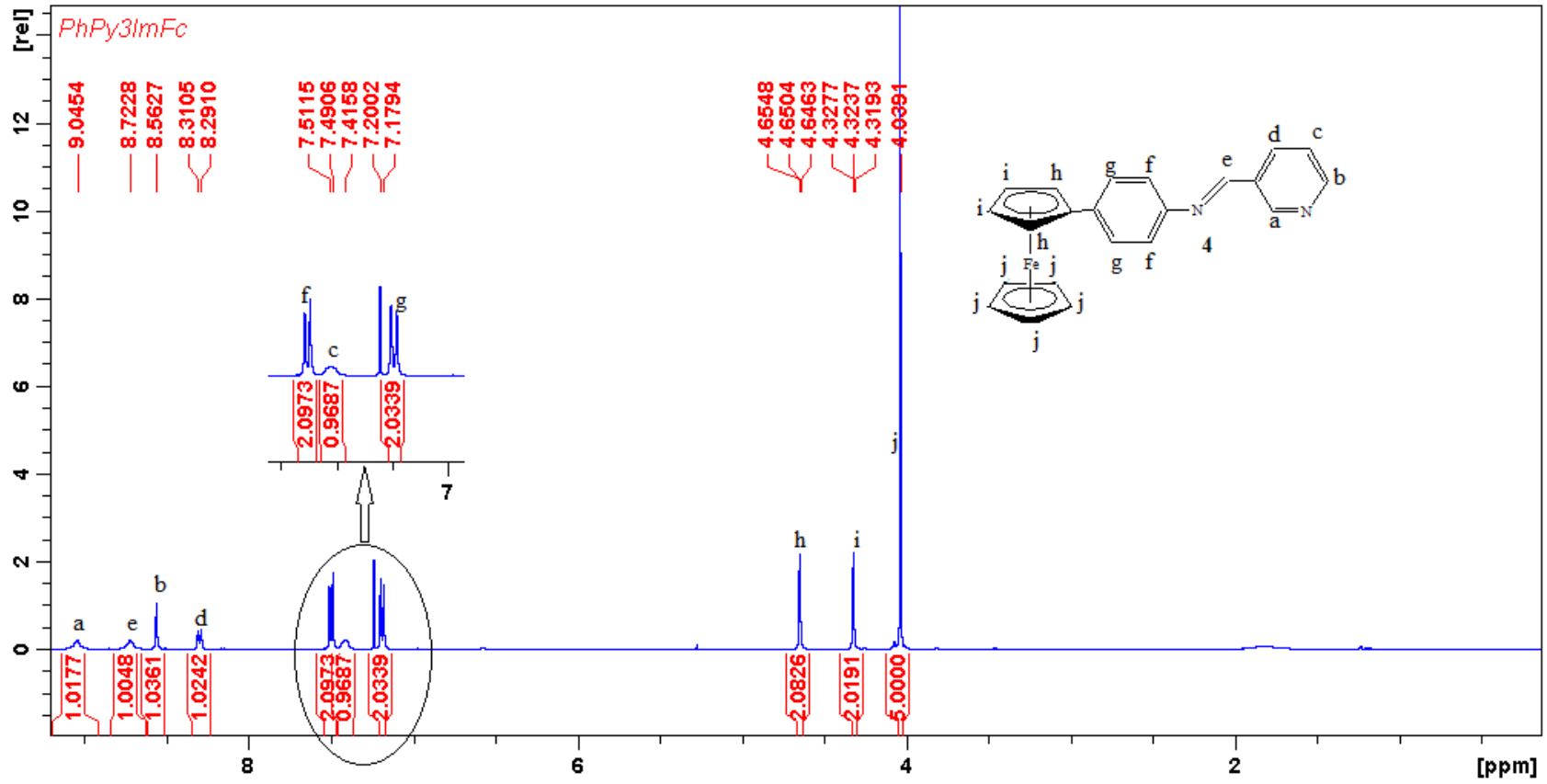


Figure S30: ^{1}H-NMR spectrum for compound **4**

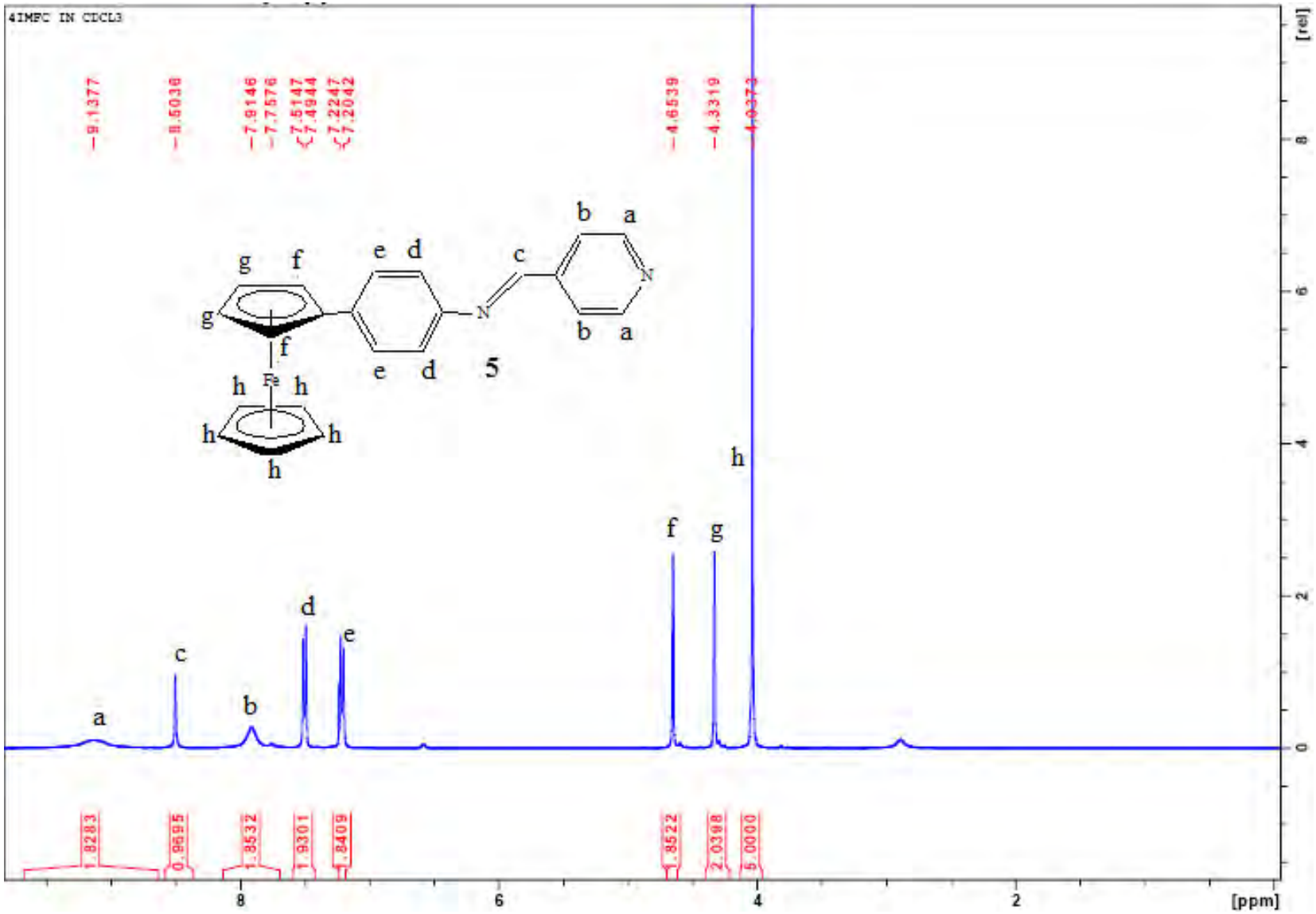


Figure S31: ^{1}H-NMR spectrum for compound **5**

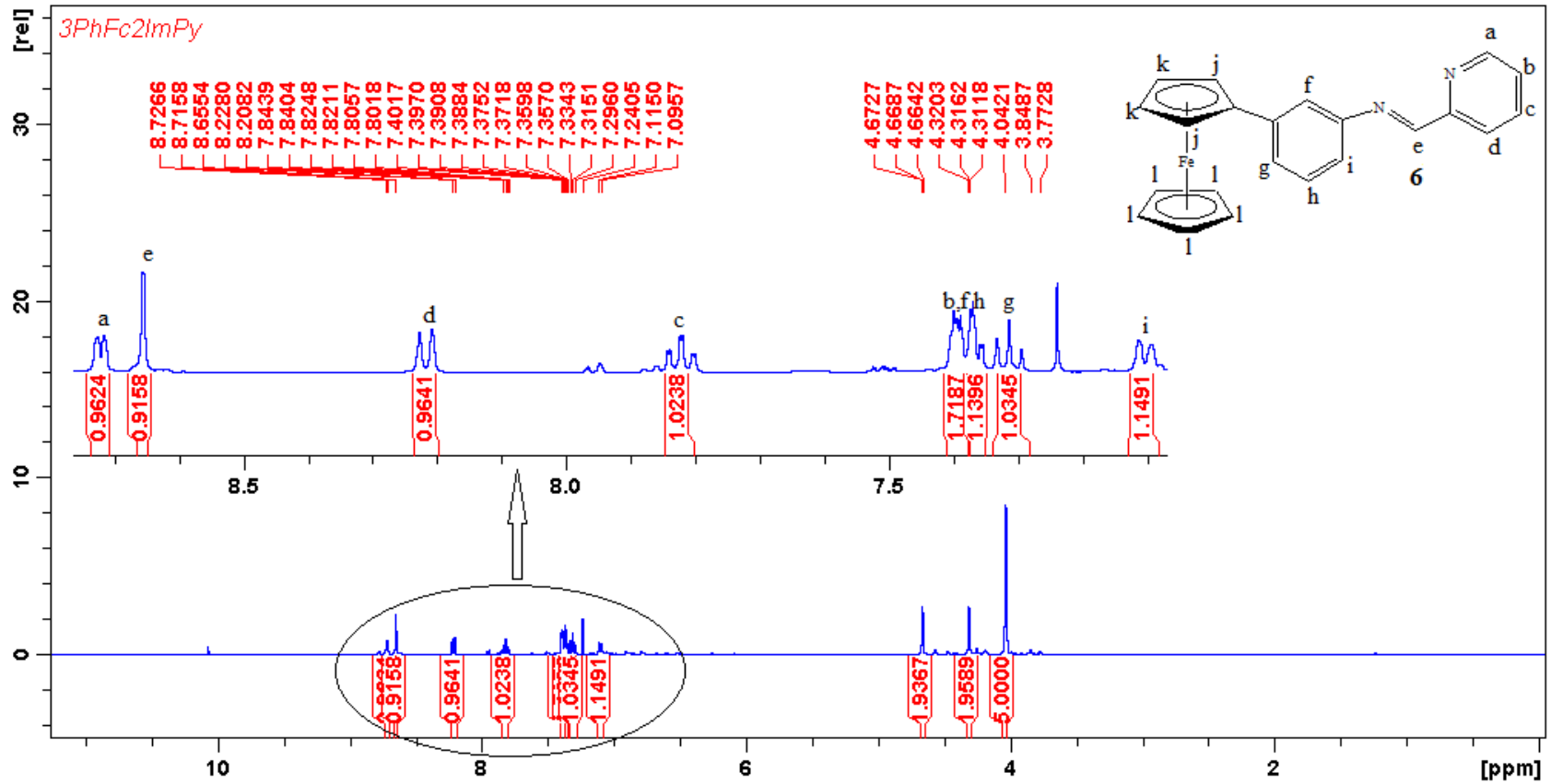


Figure S32: ^{1}H-NMR spectrum for compound **6**

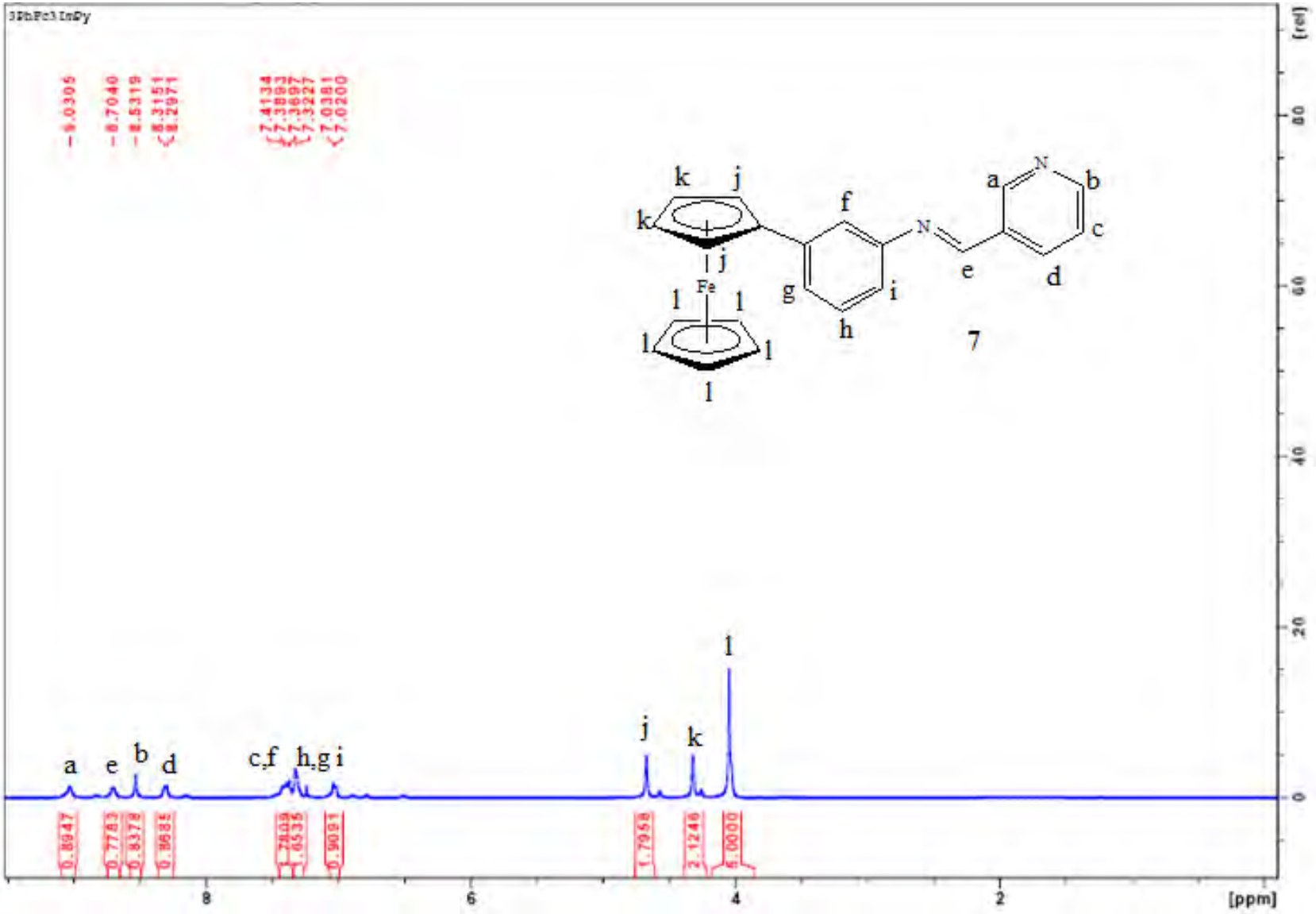


Figure S33: ^{1}H-NMR spectrum for compound **7**

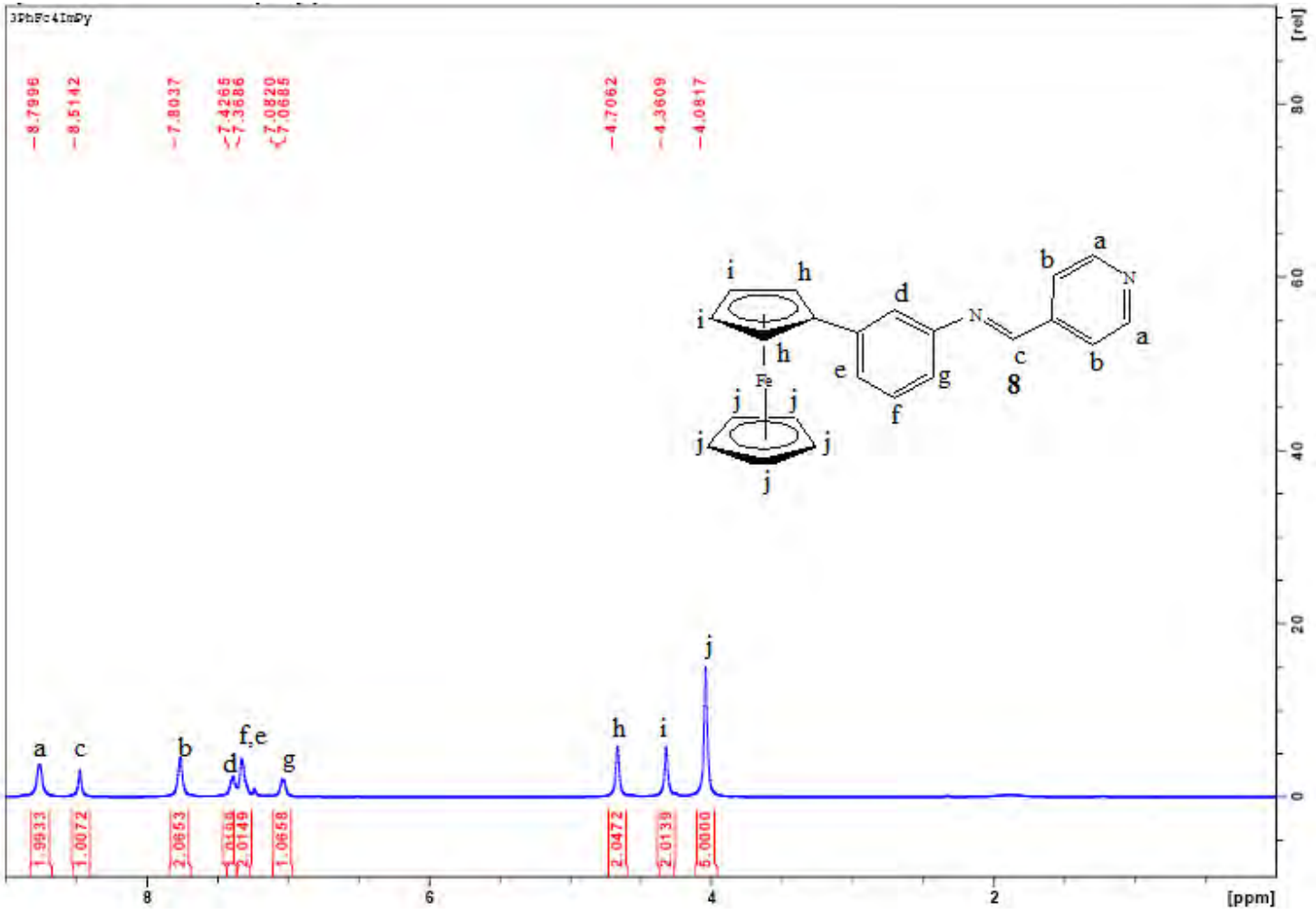


Figure S34: ^{1}H-NMR spectrum for compound **8**

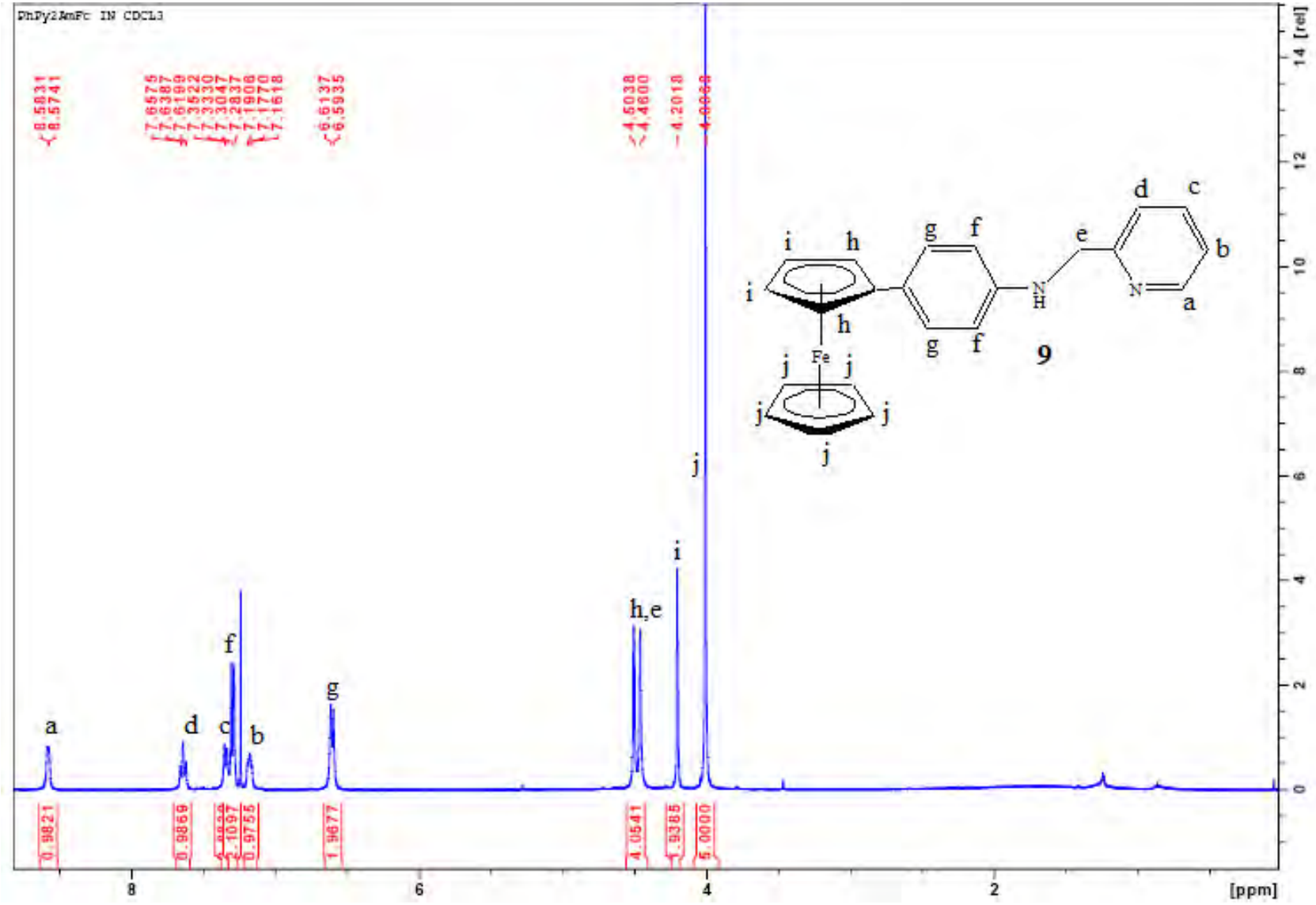


Figure S35: ^{1}H-NMR spectrum for compound **9**

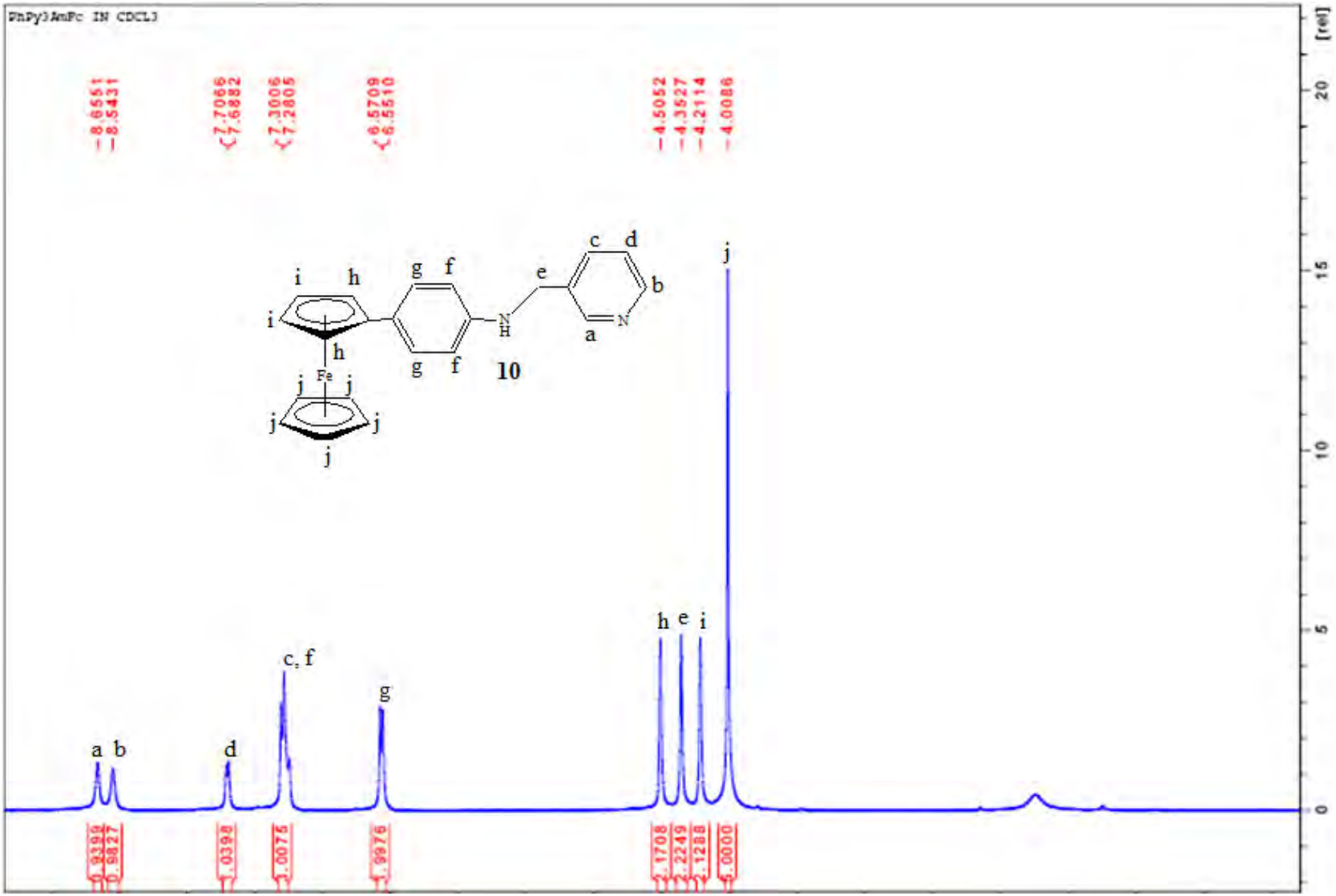


Figure S36: ^{1}H-NMR spectrum for compound **10**

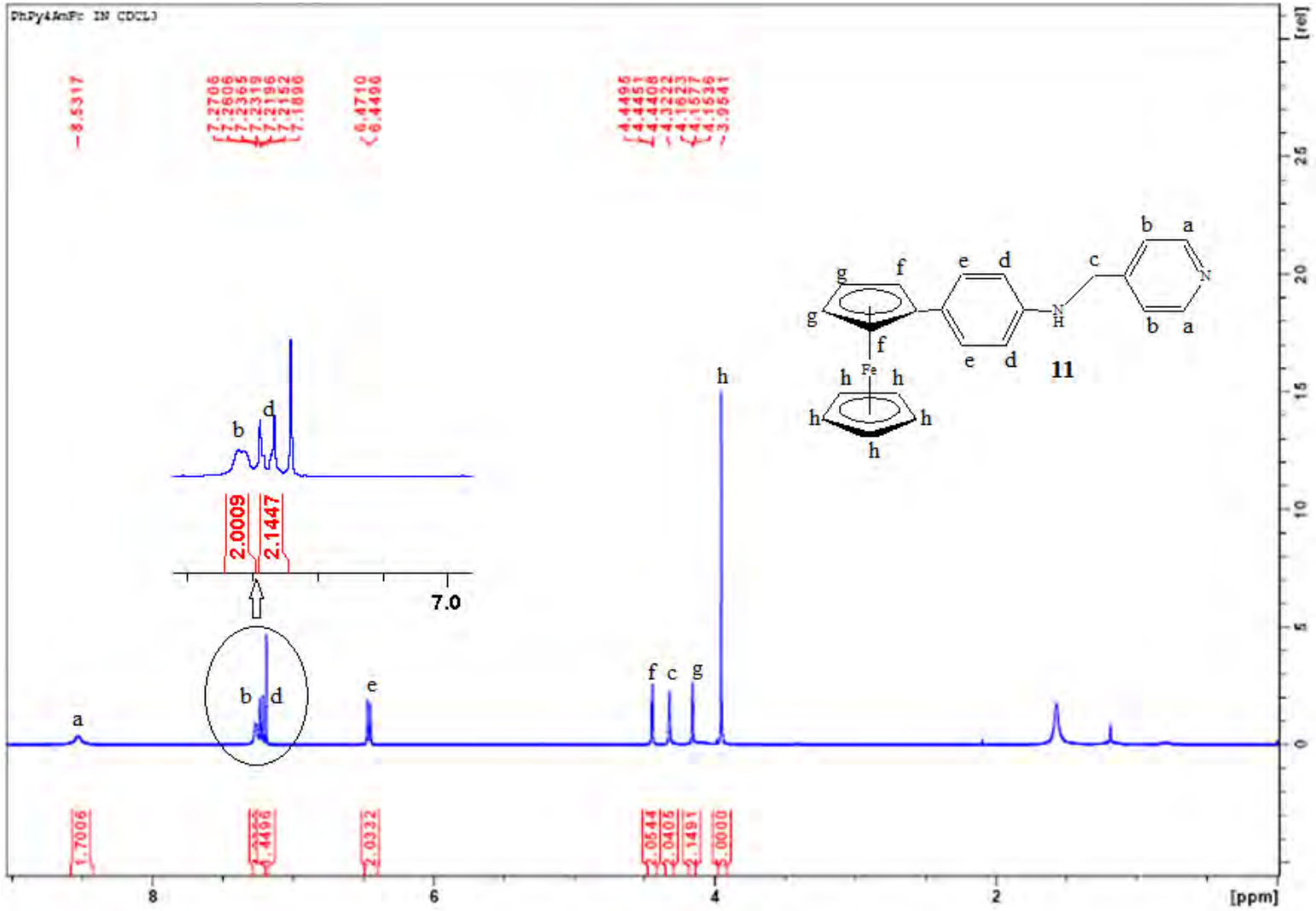


Figure S37: ^{1}H-NMR spectrum for compound **11**

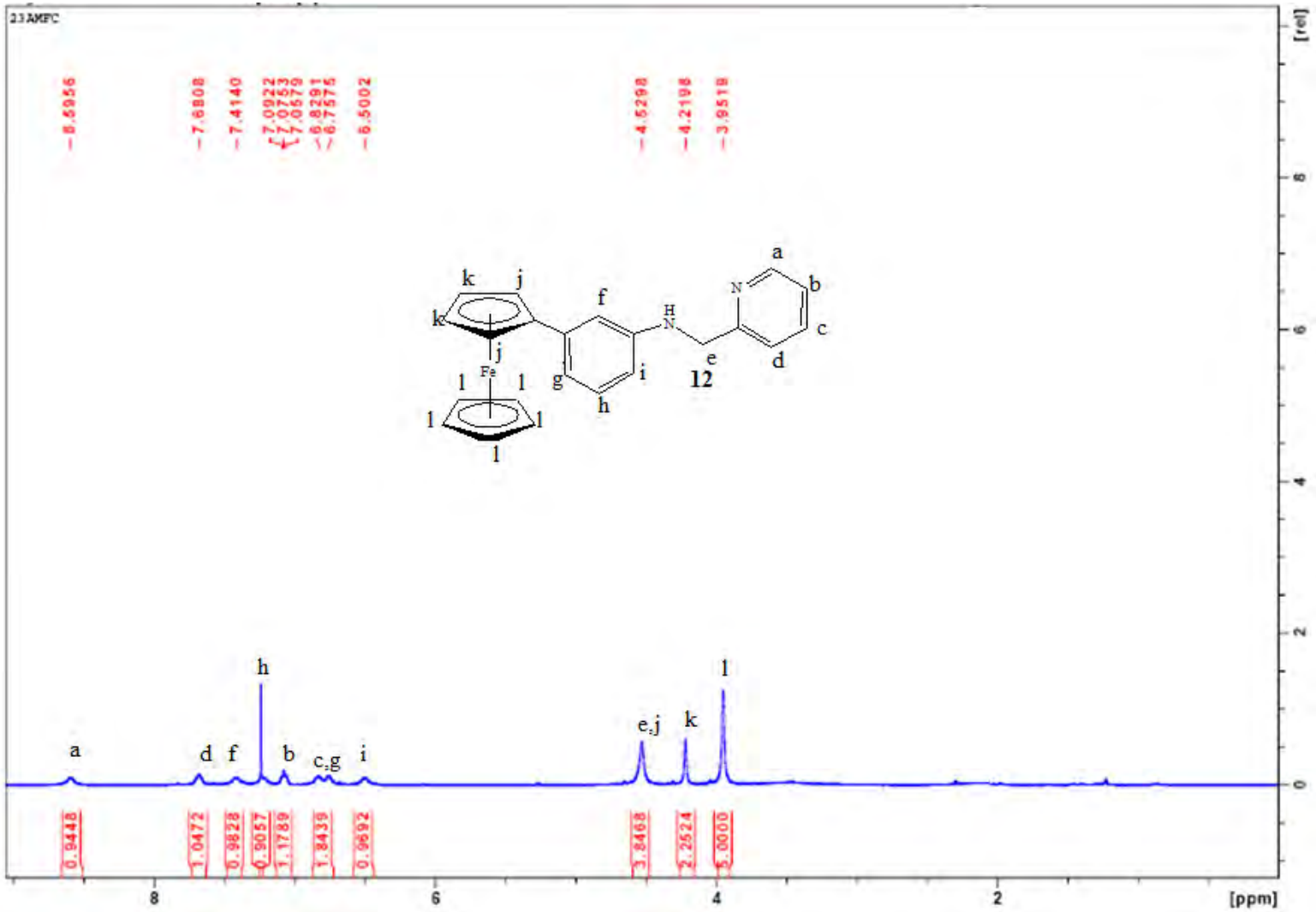


Figure S38: ^{1}H-NMR spectrum for compound **12**

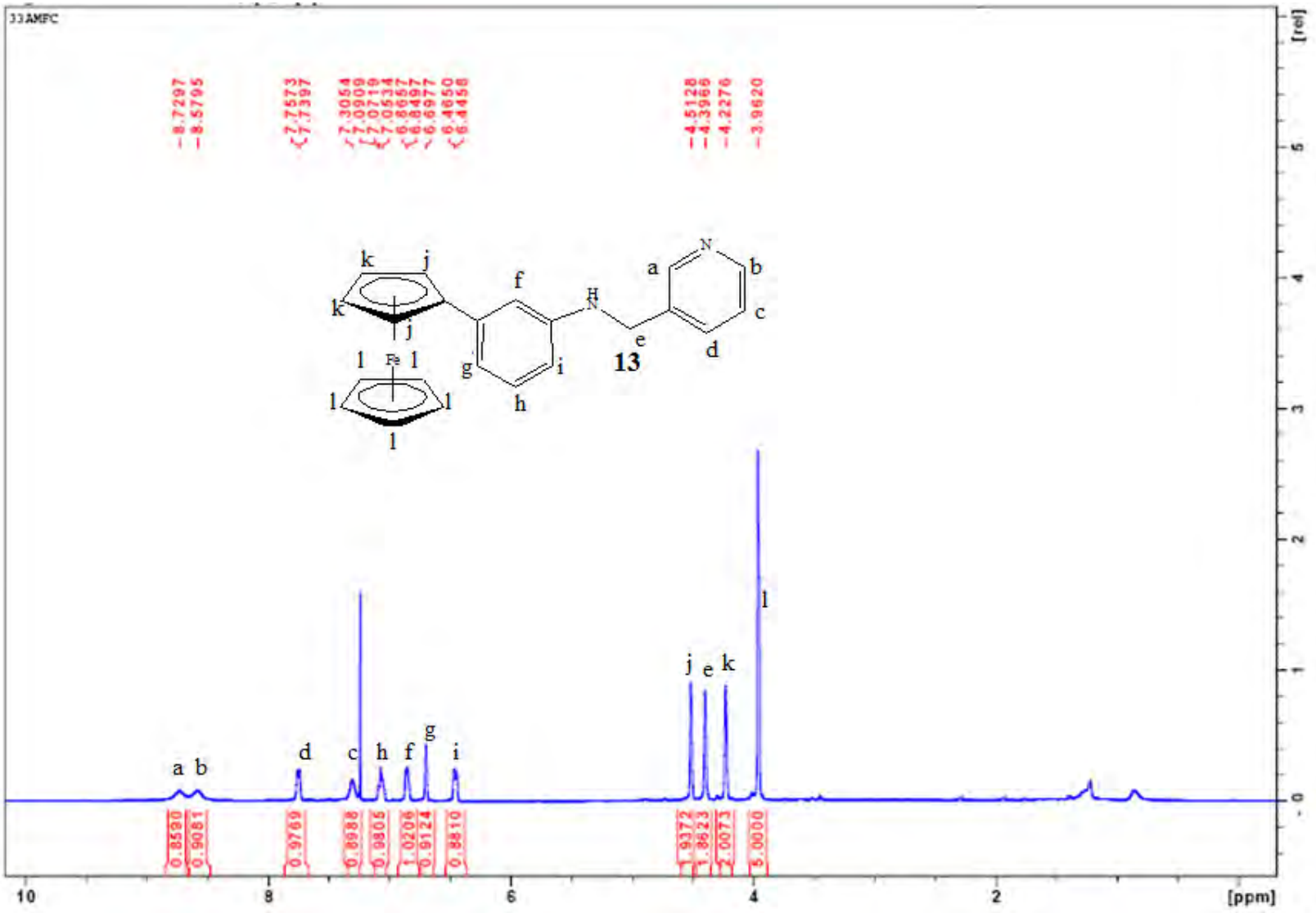


Figure S39: ^{1}H-NMR spectrum for compound **13**

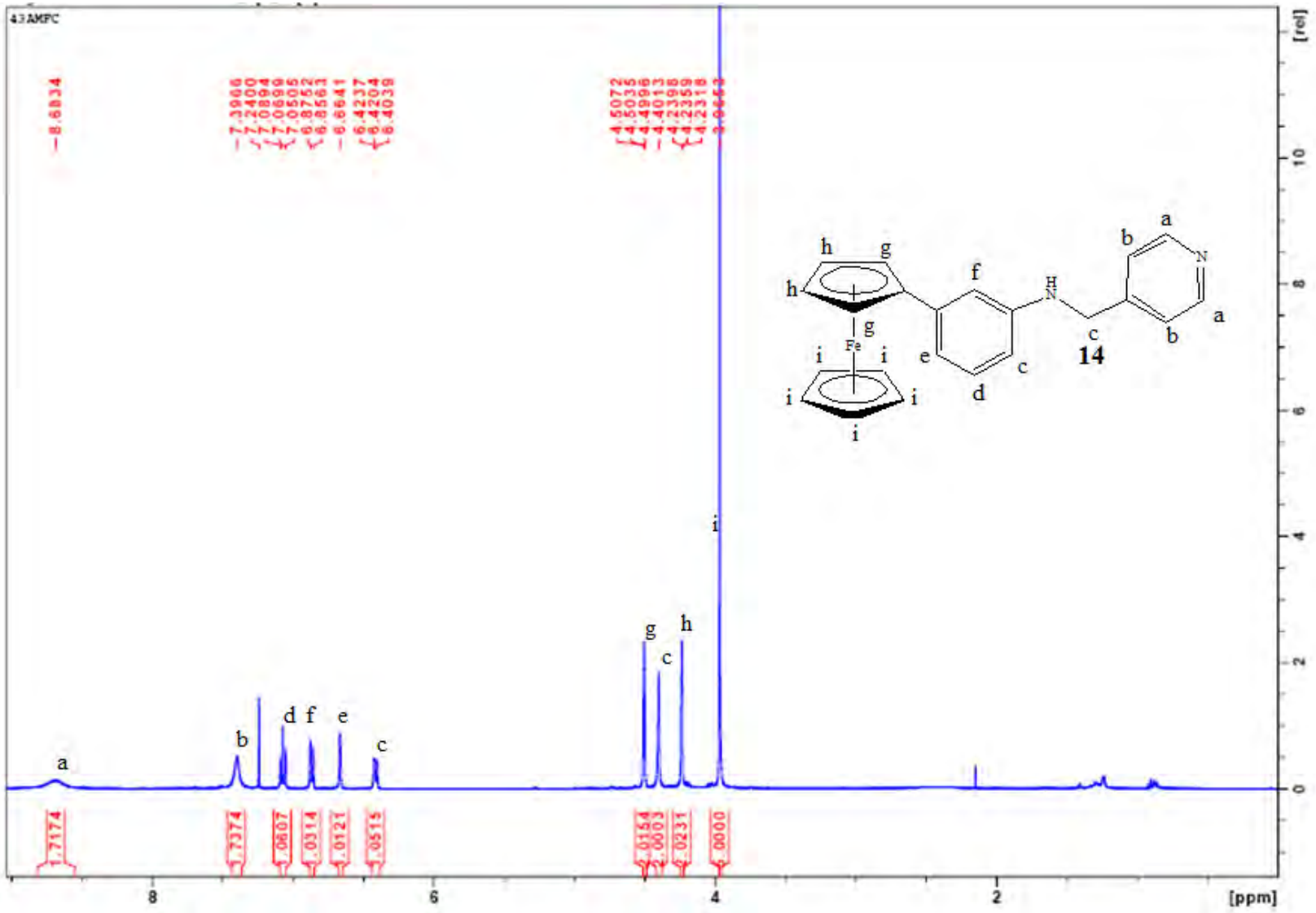


Figure 40: ^{1}H-NMR spectrum for compound **14**

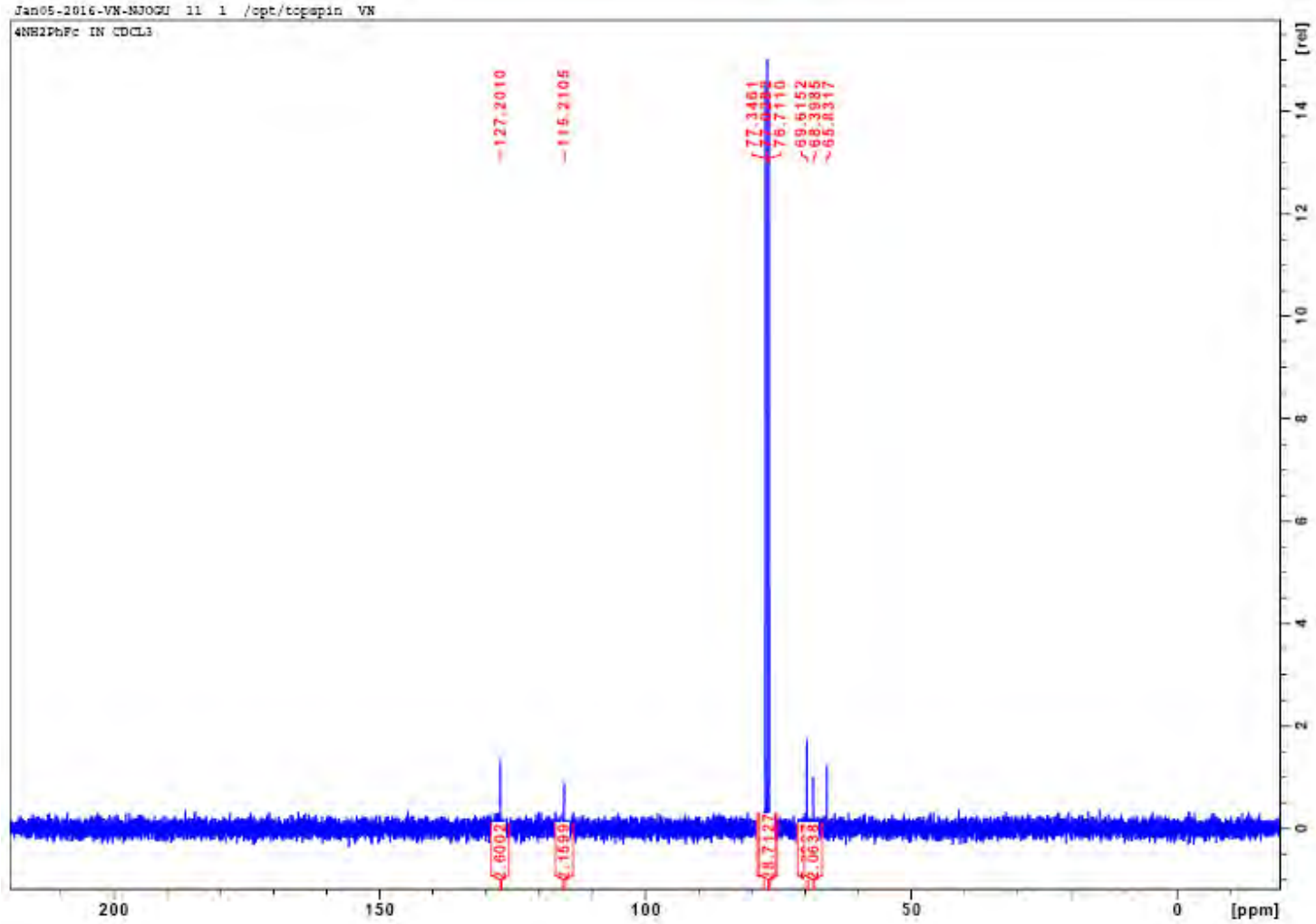


Figure S41: ^{13}C-NMR spectrum for compound **1**

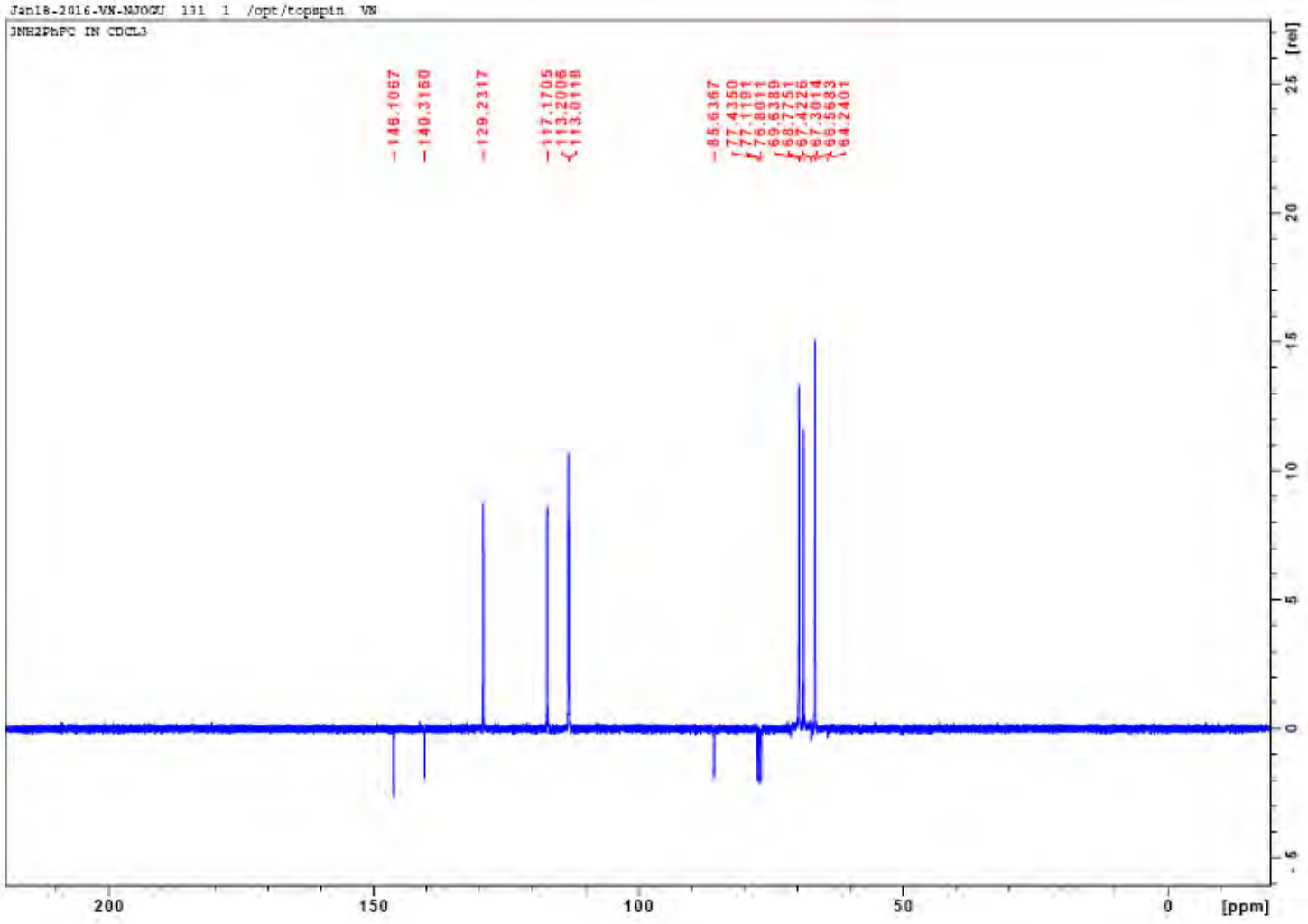


Figure S42: ^{13}C-NMR spectrum for compound **2**

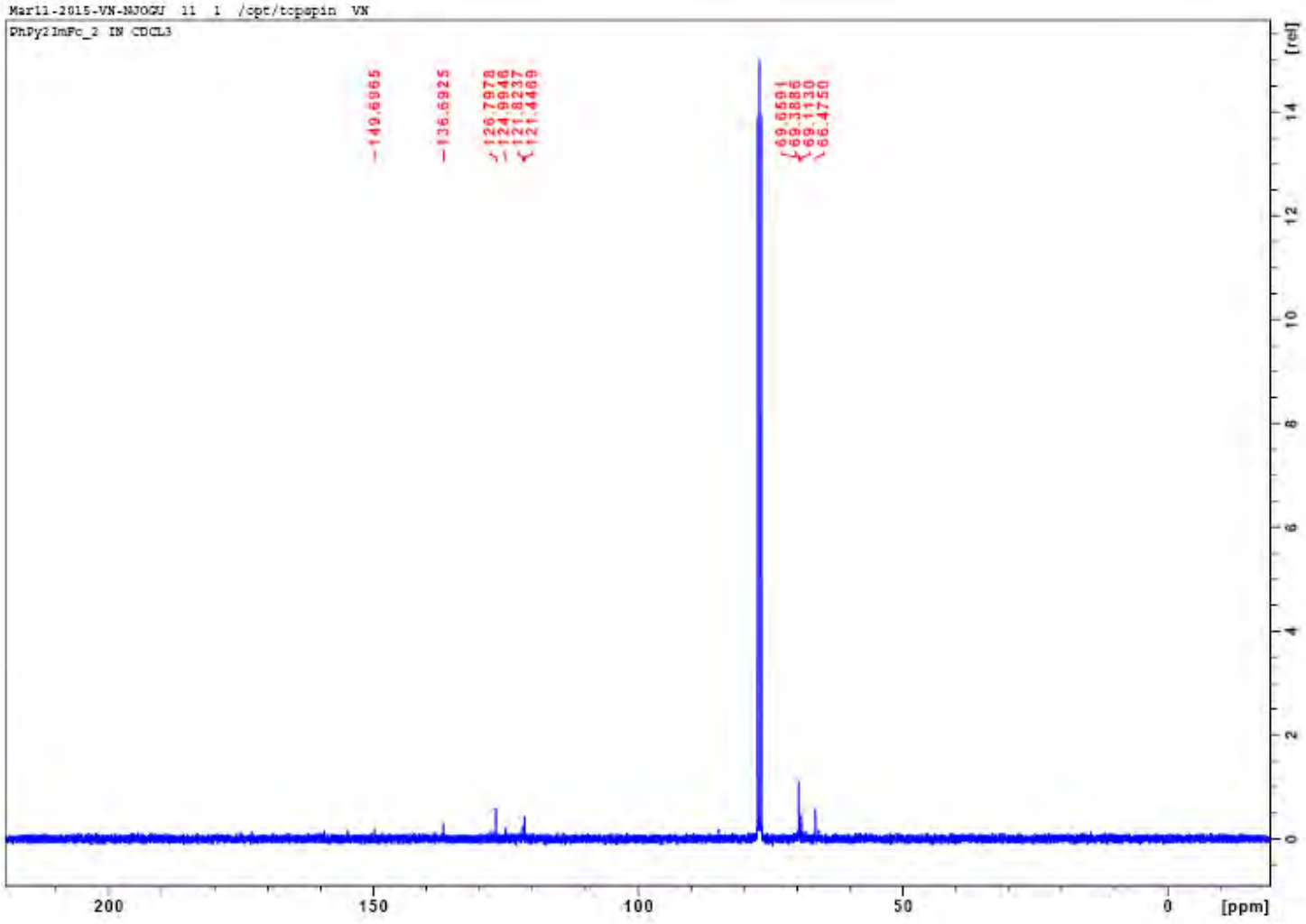


Figure S43: ^{13}C-NMR spectrum for compound **3**

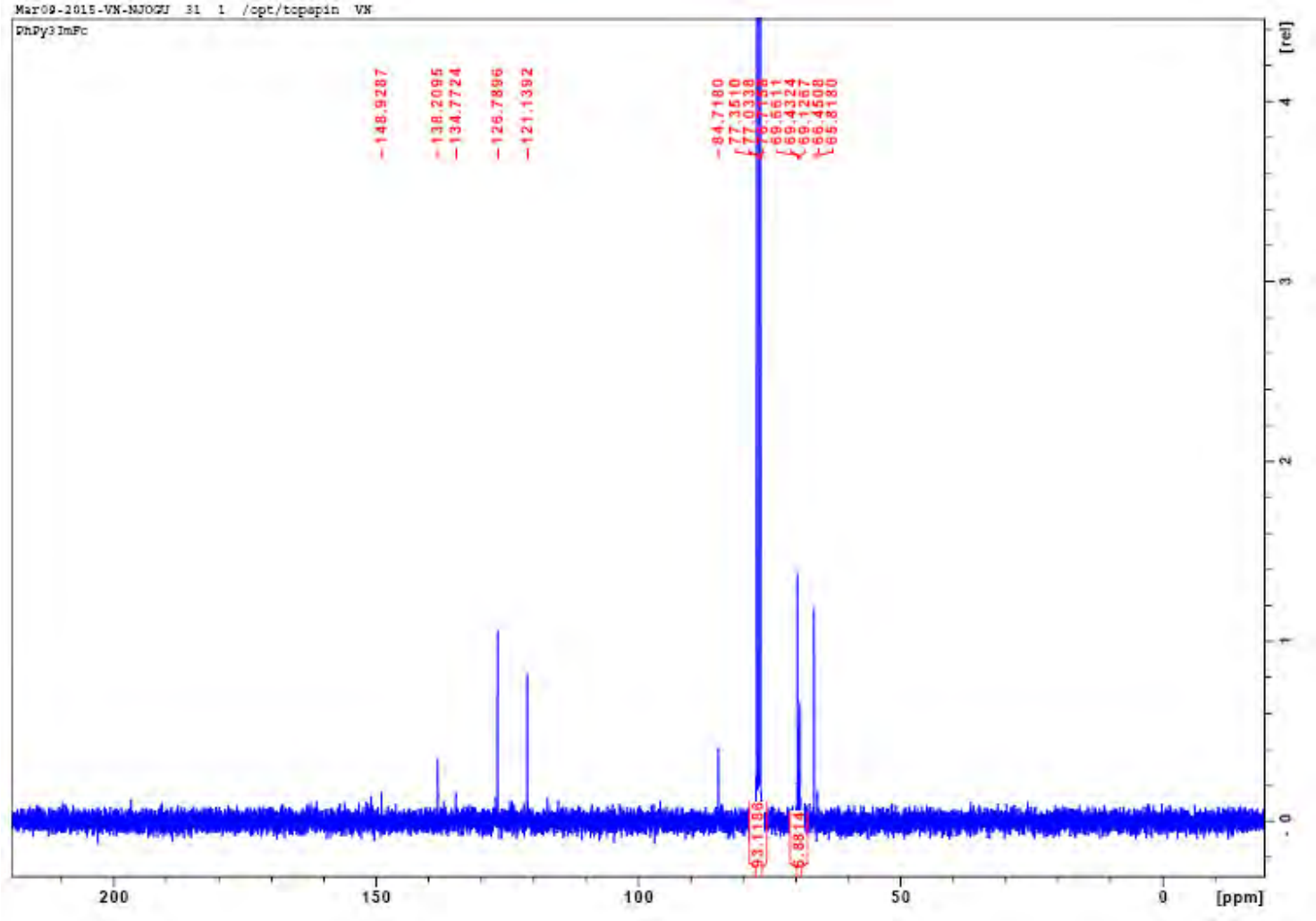


Figure S44: ^{13}C-NMR spectrum for compound **4**

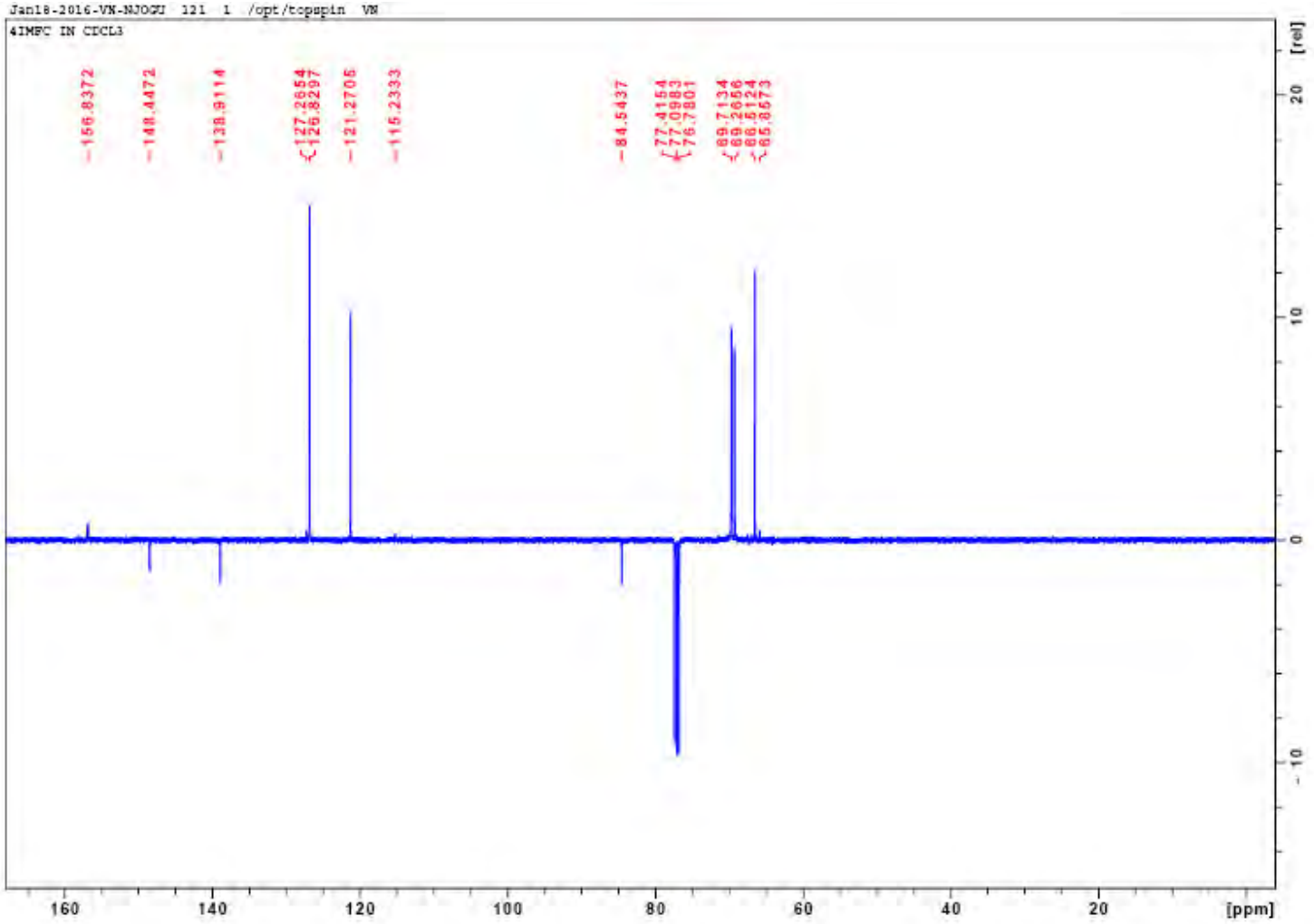


Figure S45: ^{13}C-NMR spectrum for compound **5**

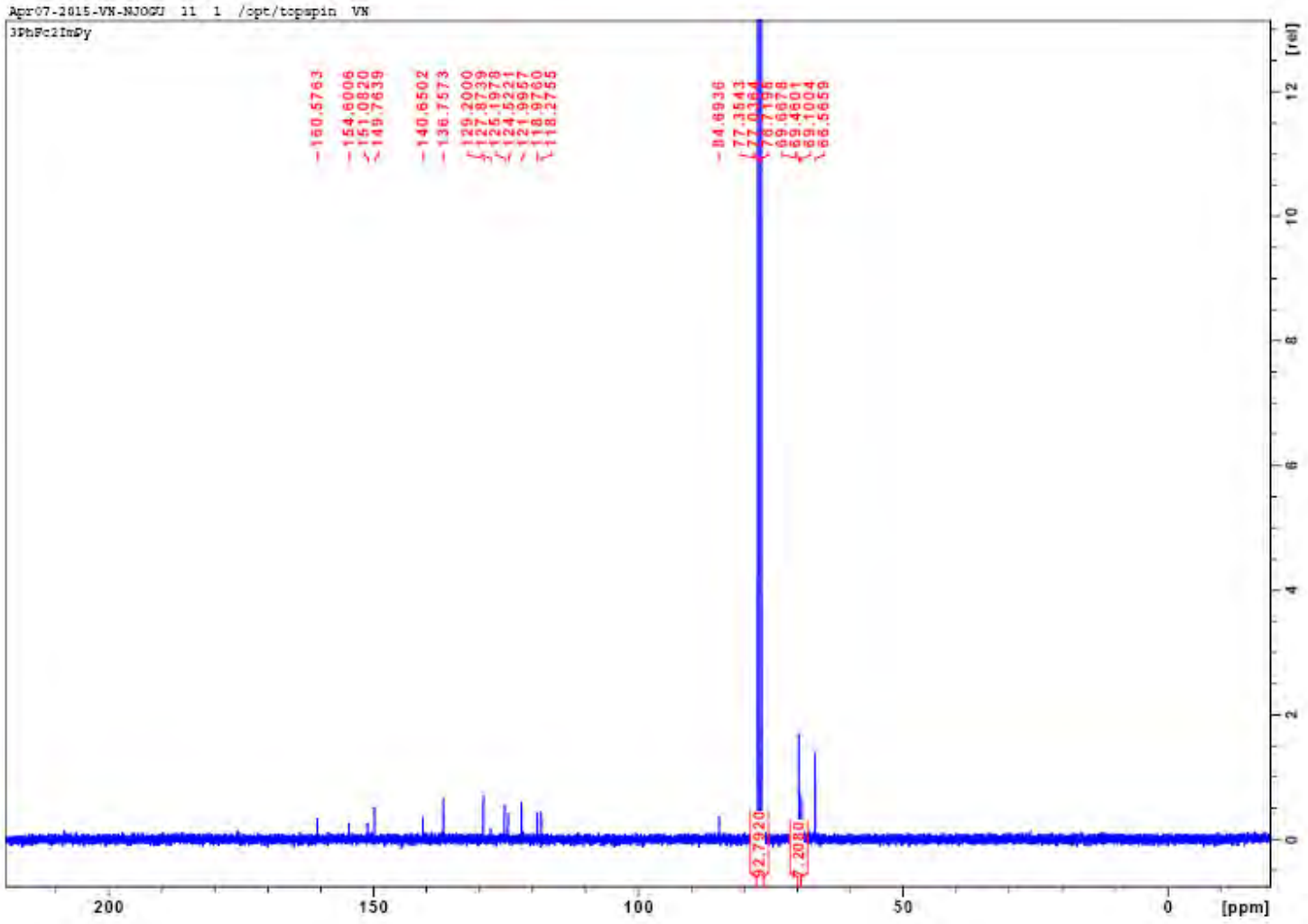


Figure S46: ^{13}C-NMR spectrum for compound **6**

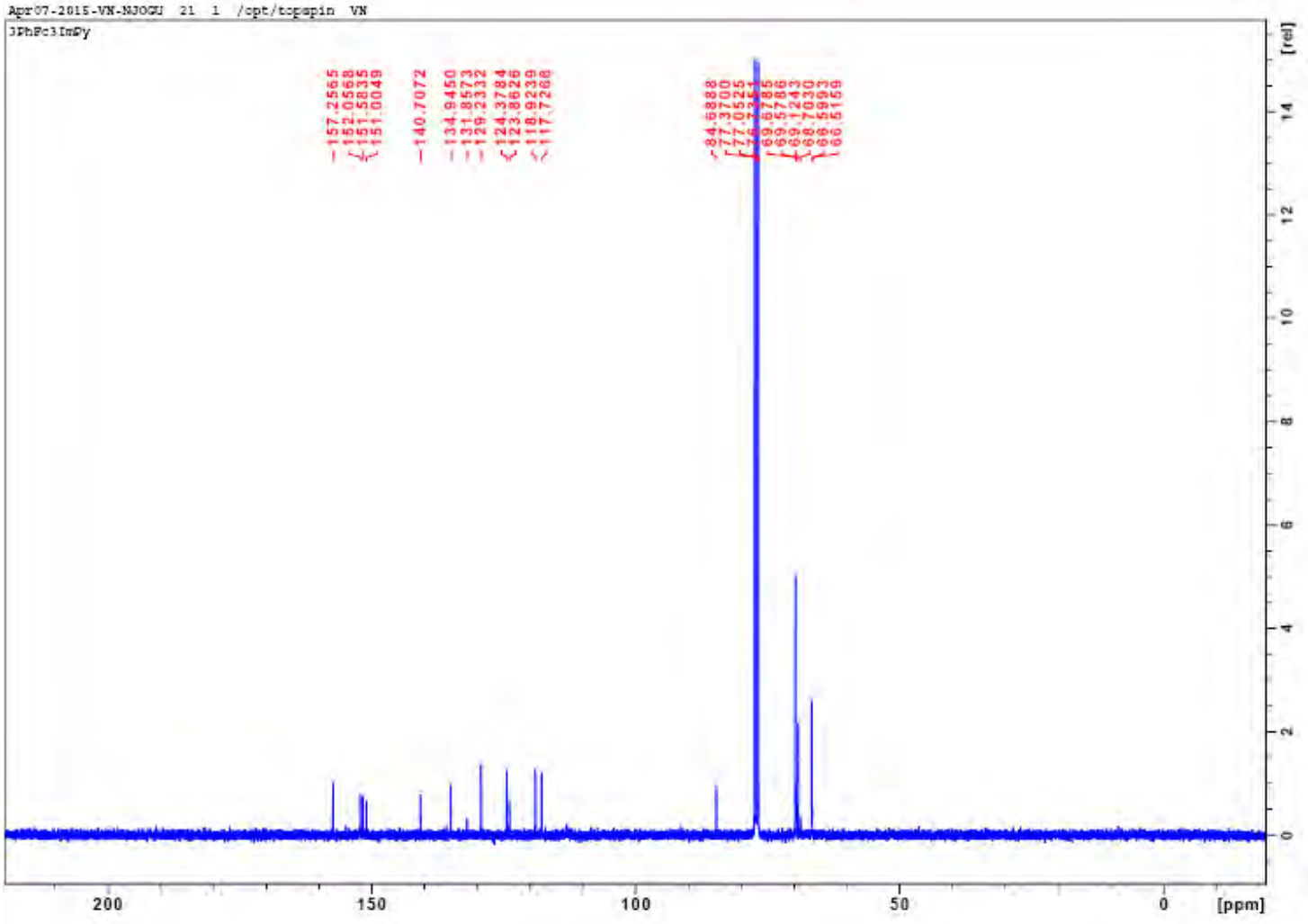


Figure S47: ^{13}C-NMR spectrum for compound **7**

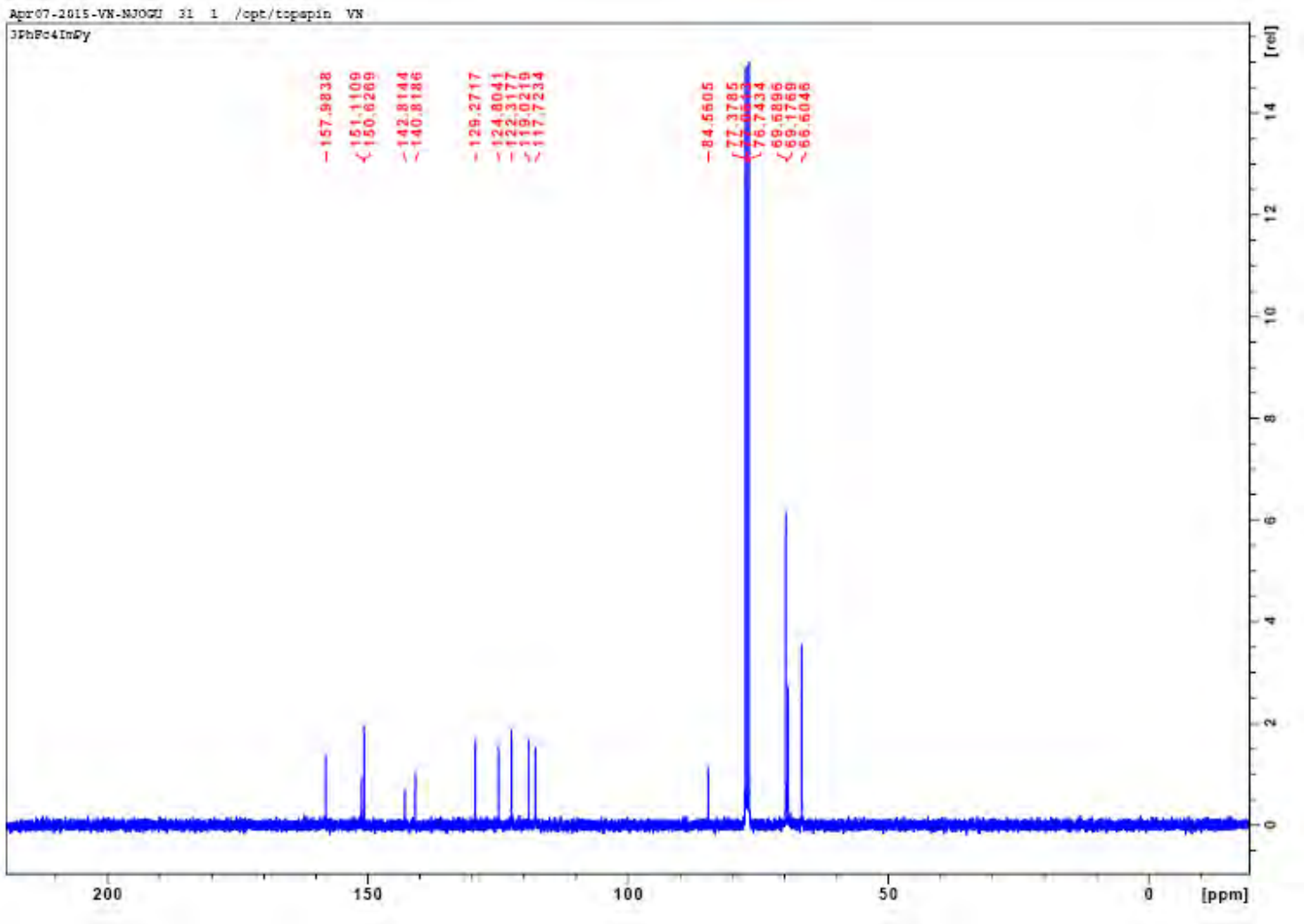


Figure S48: ^{13}C-NMR spectrum for compound **8**

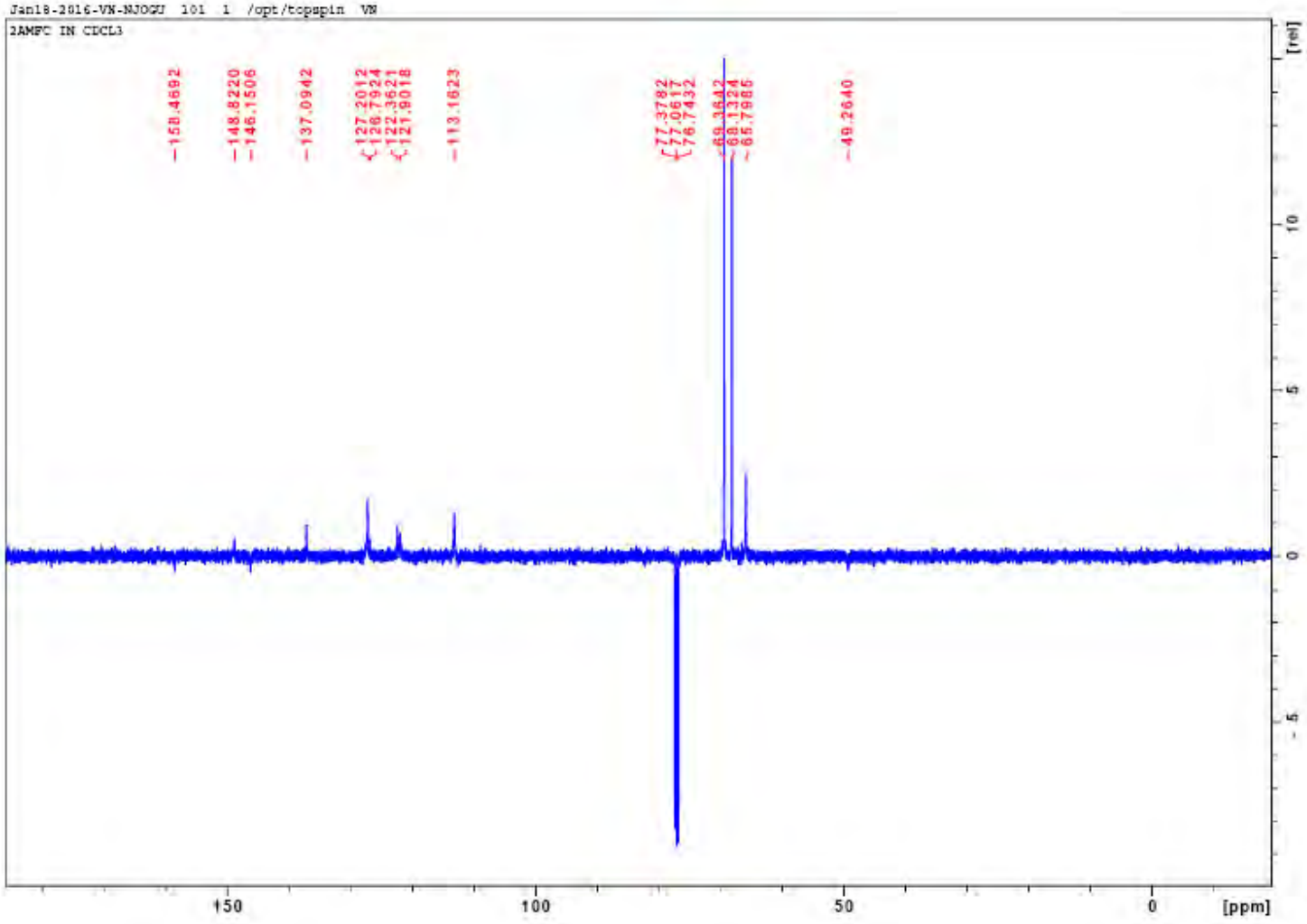


Figure S49: ^{13}C-NMR spectrum for compound **9**

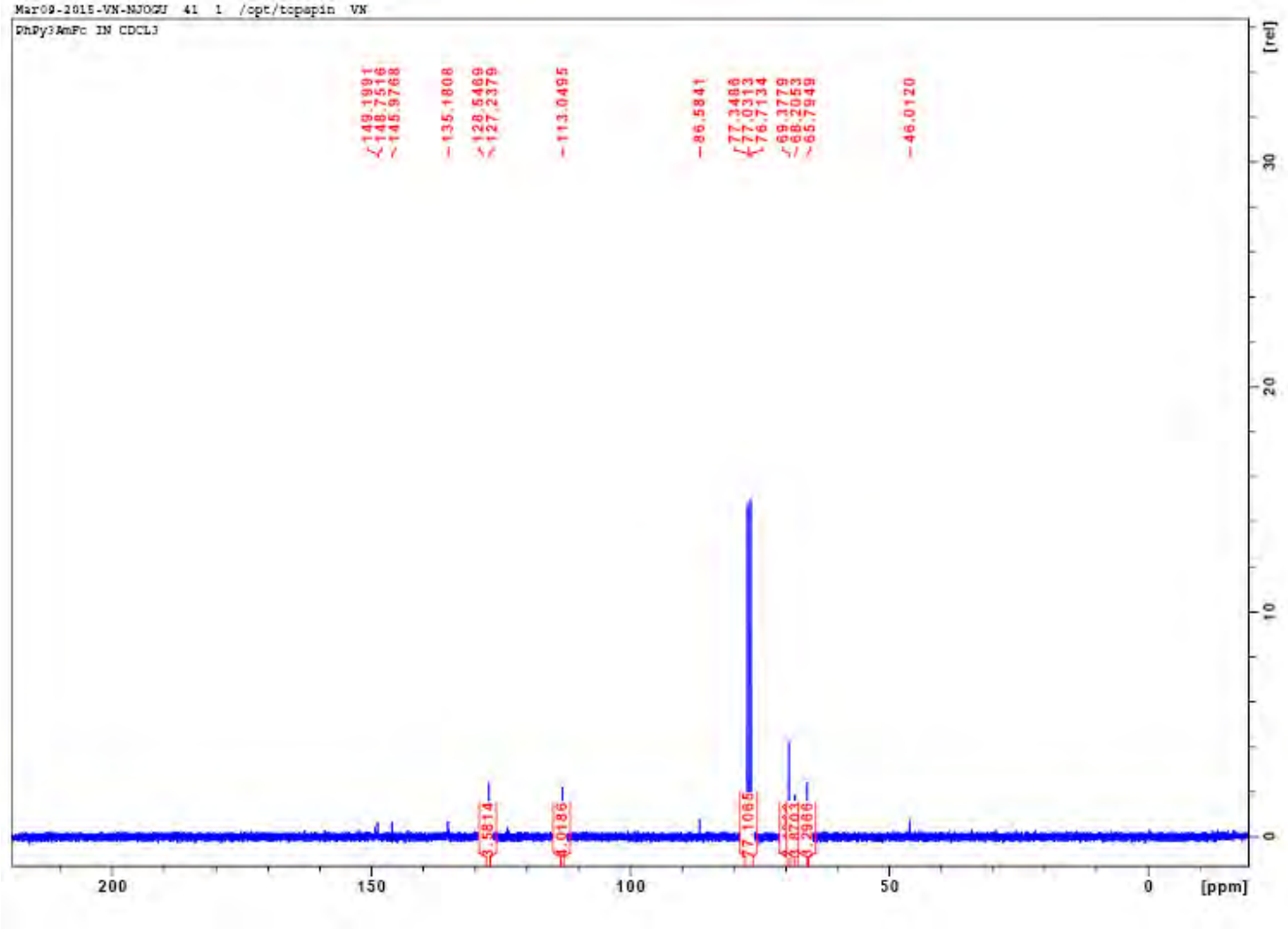


Figure S50: ^{13}C-NMR spectrum for compound **10**

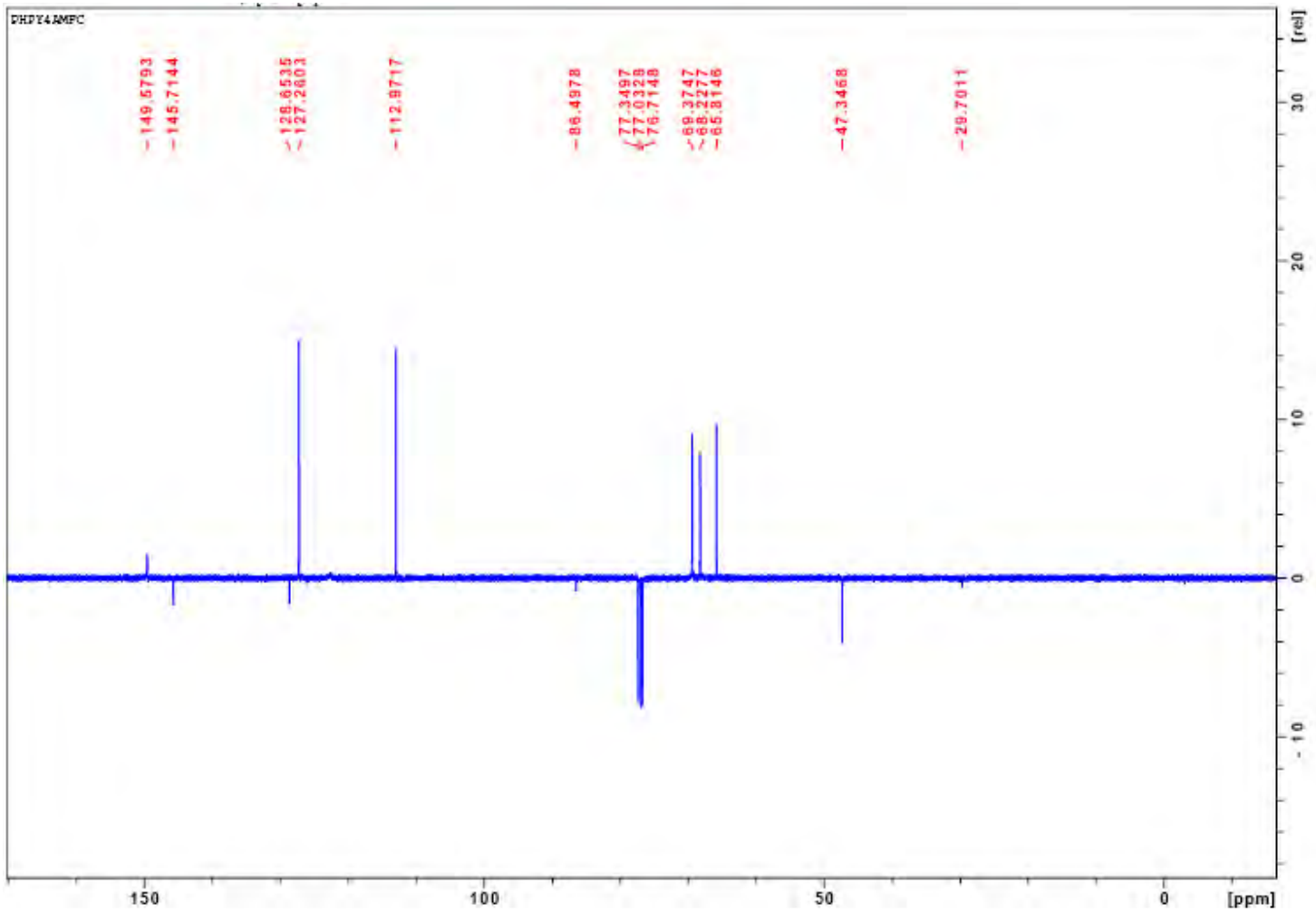


Figure S51: ^{13}C-NMR spectrum for compound **11**

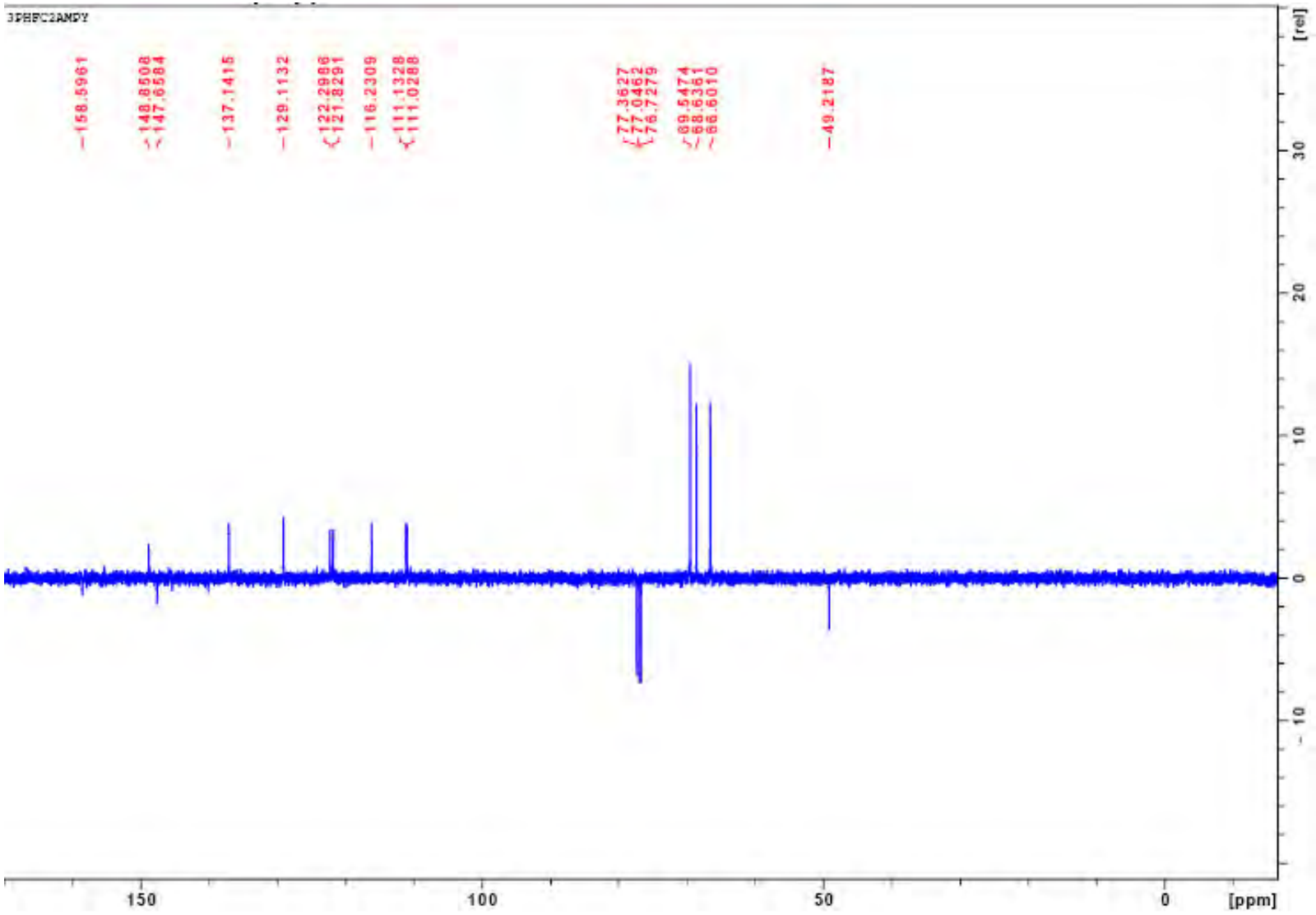


Figure S52: ^{13}C-NMR spectrum for compound **12**

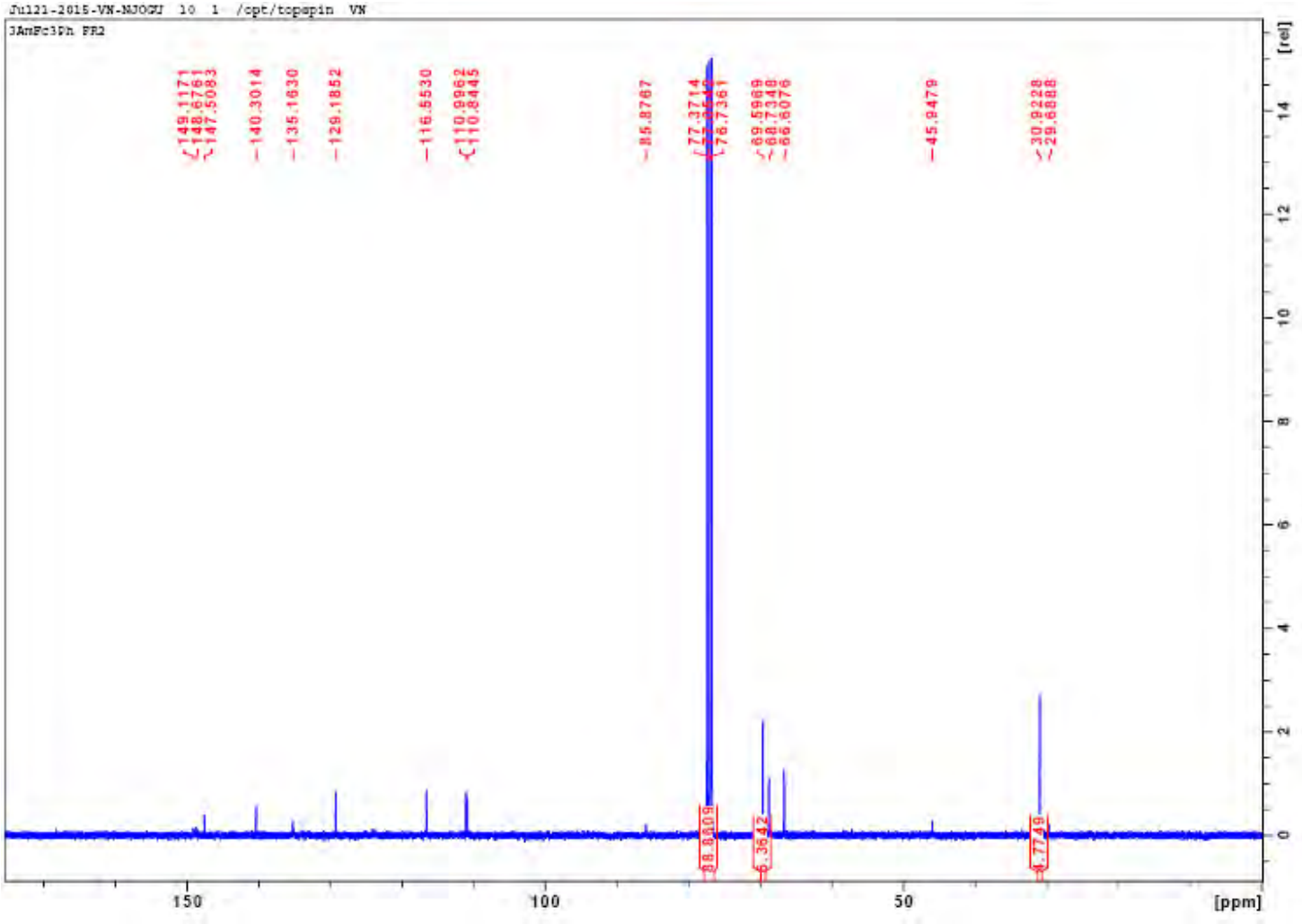


Figure S53: ^{13}C-NMR spectrum for compound **13**

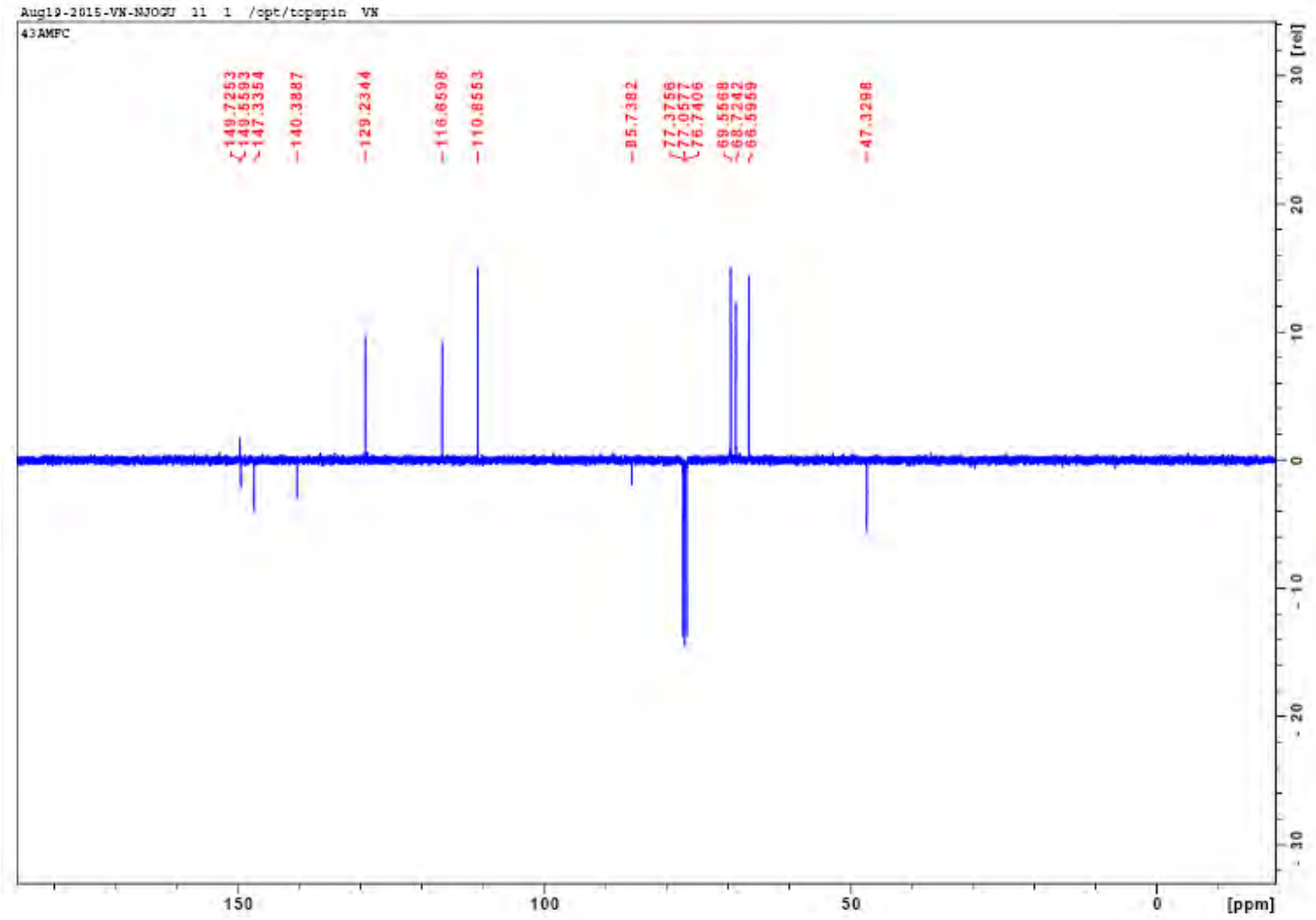


Figure S54: ^{13}C-NMR spectrum for compound **14**