Supporting Information

Polysubstituted imidazoles as Lysotracker Molecules: Their Syntheses via Iodine/H_2O and Cell-Imaging Studies

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Contents:

Figure S1: ^{1}H NMR spectrum of 1-Benzyl-2,4,5-triphenyl-1H-imidazole (3a) in $CDCl_3$.

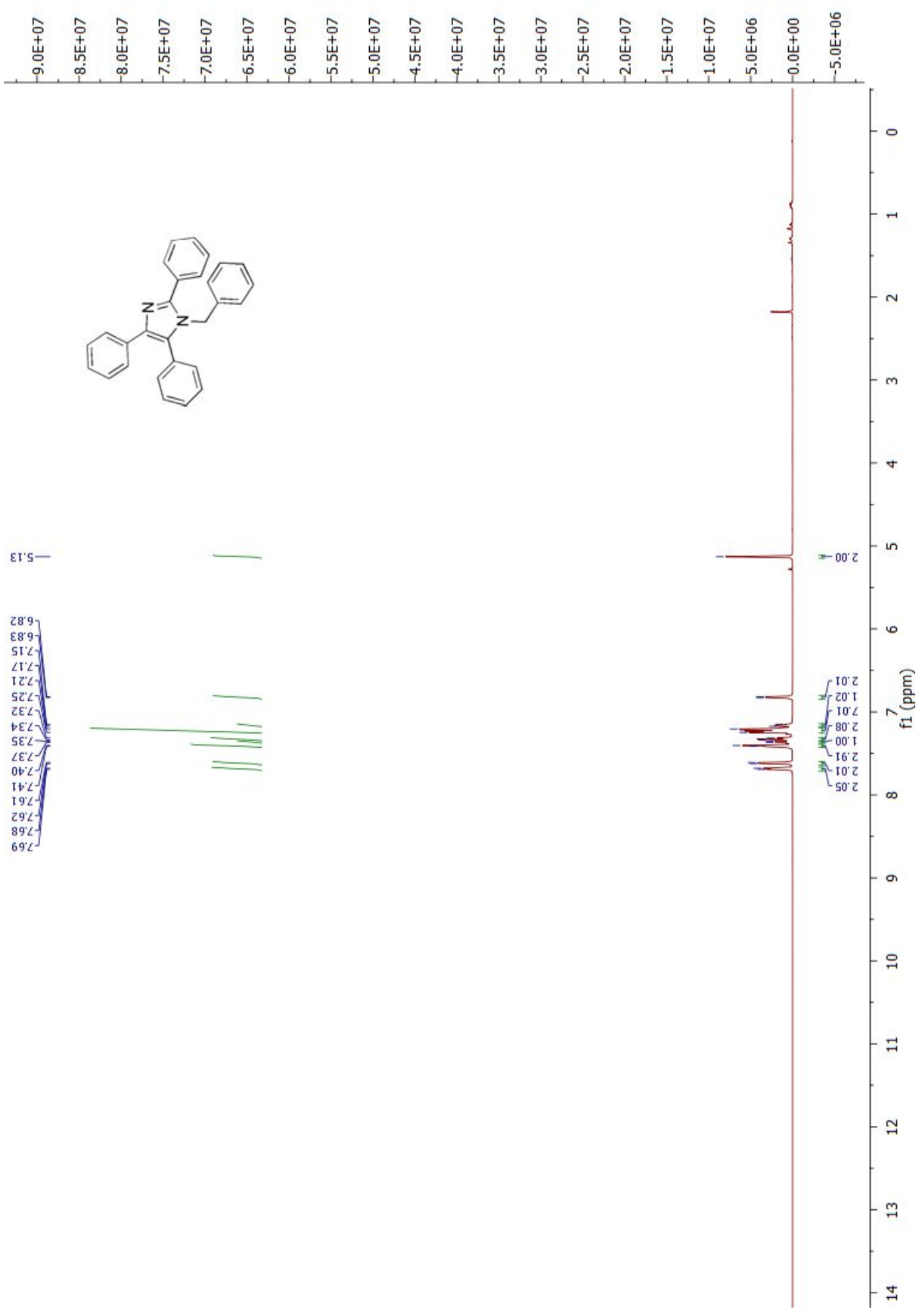


Figure S2: ^{13}C NMR spectrum of1-Benzyl-2,4,5-triphenyl-1H-imidazole (3a) in $CDCl_3$.

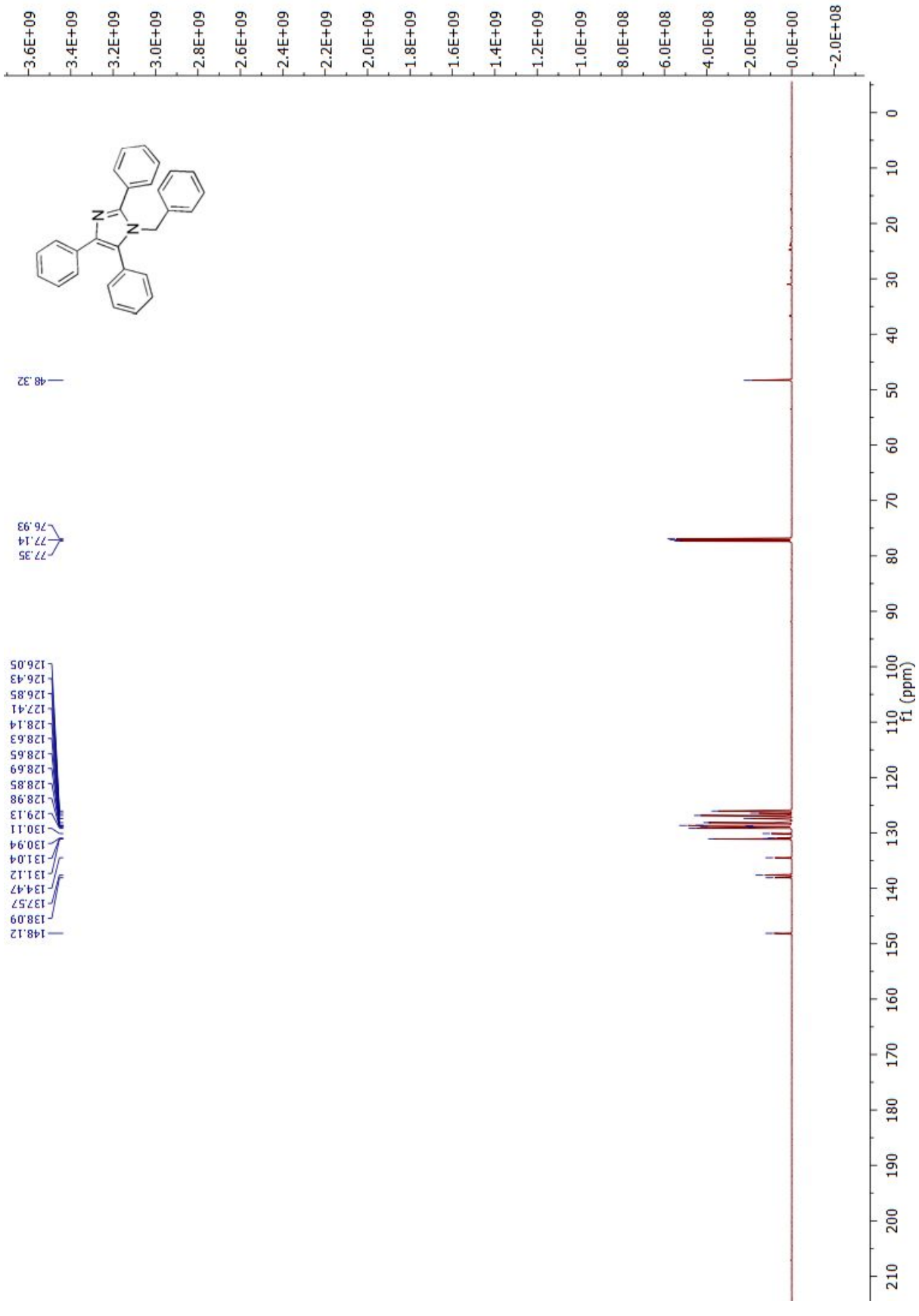


Figure S3: ^{1}H NMR spectrum of 1-(4-Methyl-benzyl)-4,5-diphenyl-2-p-tolyl-1H-imidazole (3b) in $CDCl_3$.

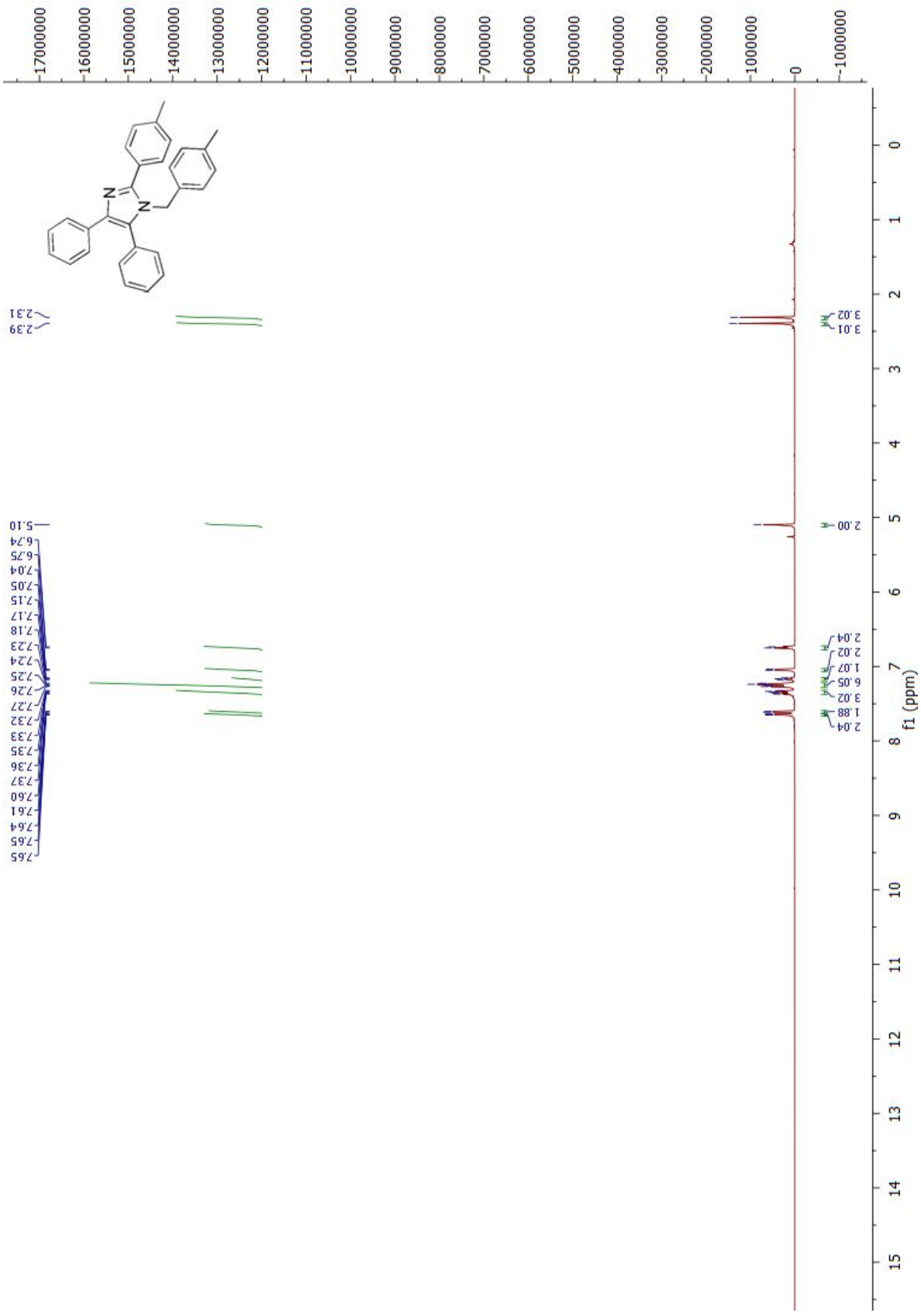


Figure S4: ^{13}C NMR spectrum of 1-(4-Methyl-benzyl)-4,5-diphenyl-2-p-tolyl-1H-imidazole (3b) in $CDCl_3$.

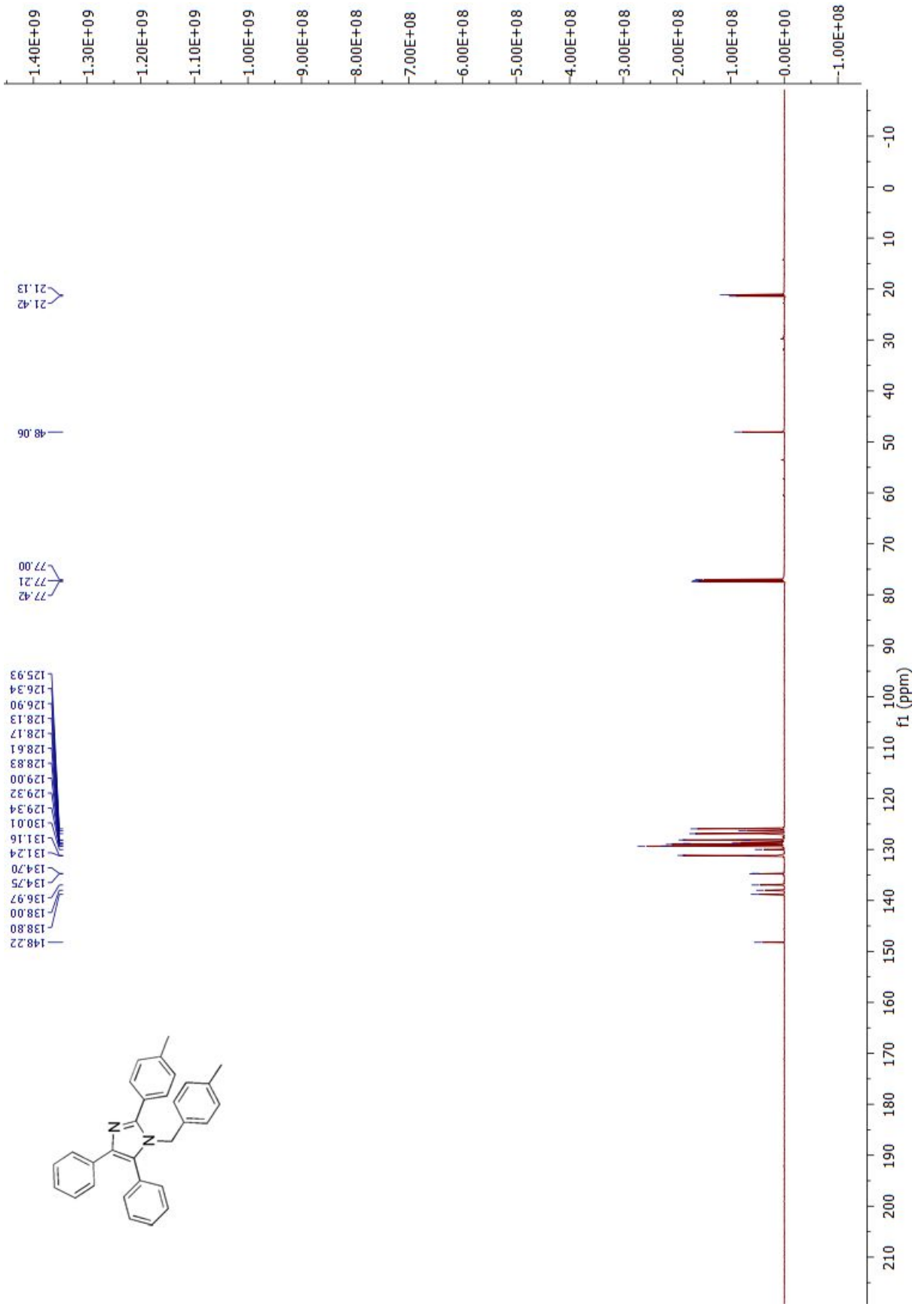


Figure S5: ^{1}H NMR spectrum of 1-(4-tert-Butyl-benzyl)-2-(4-tert-butyl-phenyl)-4,5-diphenyl-1H-imidazole (3c) in DMSO-d_6.

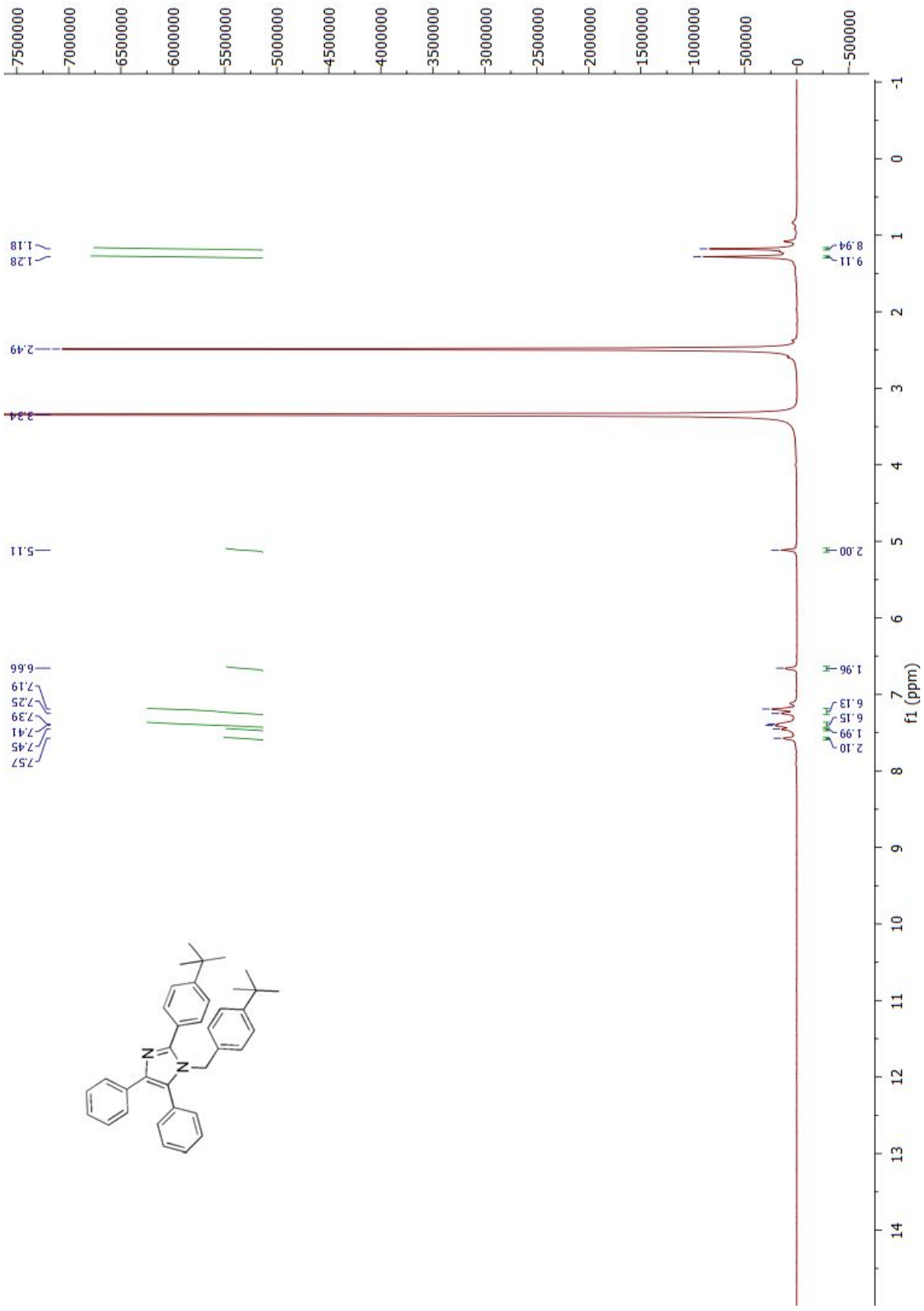


Figure S6: ^{13}C NMR spectrum of 1-(4-tert-Butyl-benzyl)-2-(4-tert-butyl-phenyl)-4,5-diphenyl-1H-imidazole (3c) in $CDCl_3$.

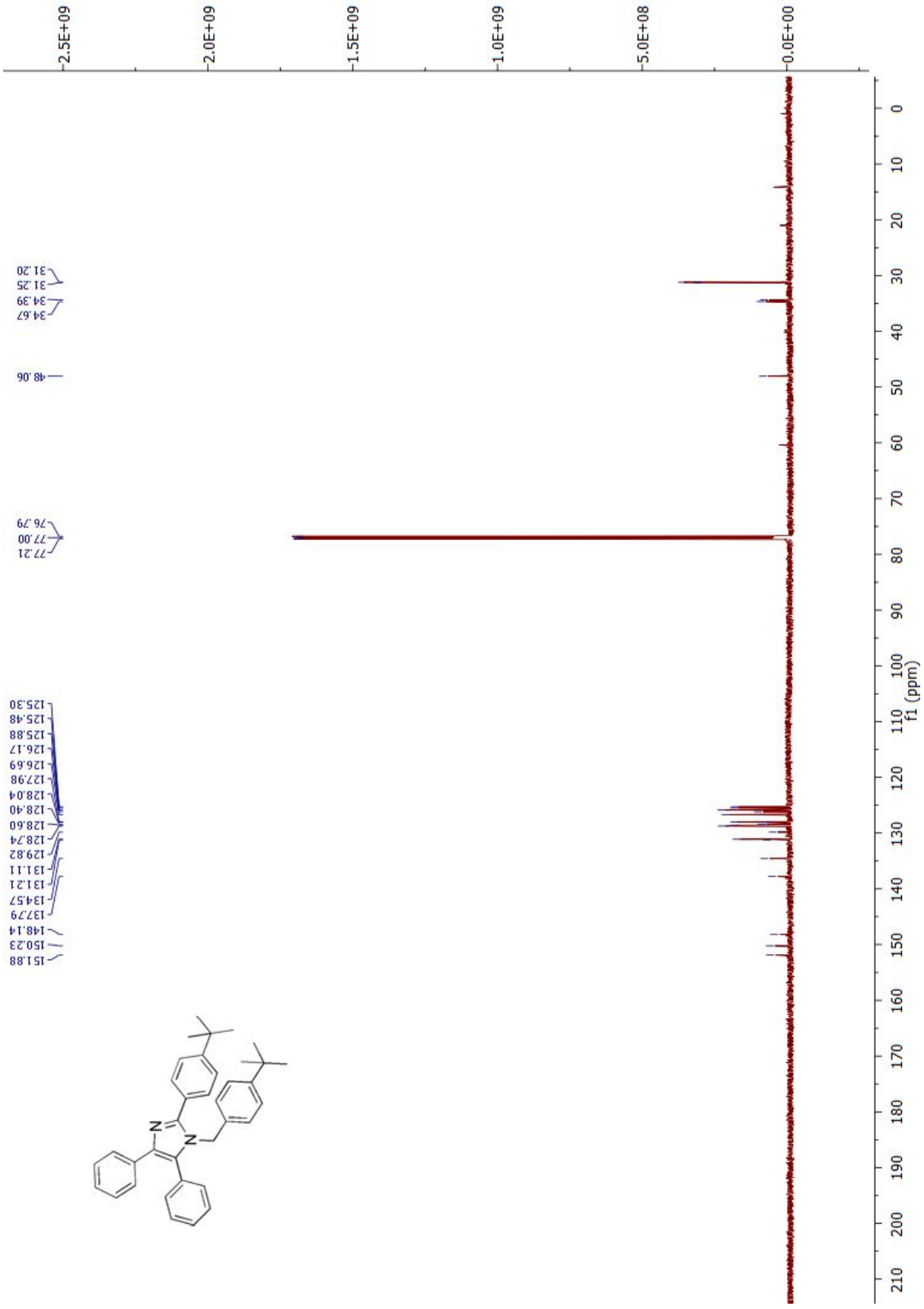


Figure S7: ^{1}H NMR spectrum of 1-(4-Fluoro-benzyl)-2-(4-fluoro-phenyl)-4,5-diphenyl-1H-imidazole (3d) in DMSO-d_6.

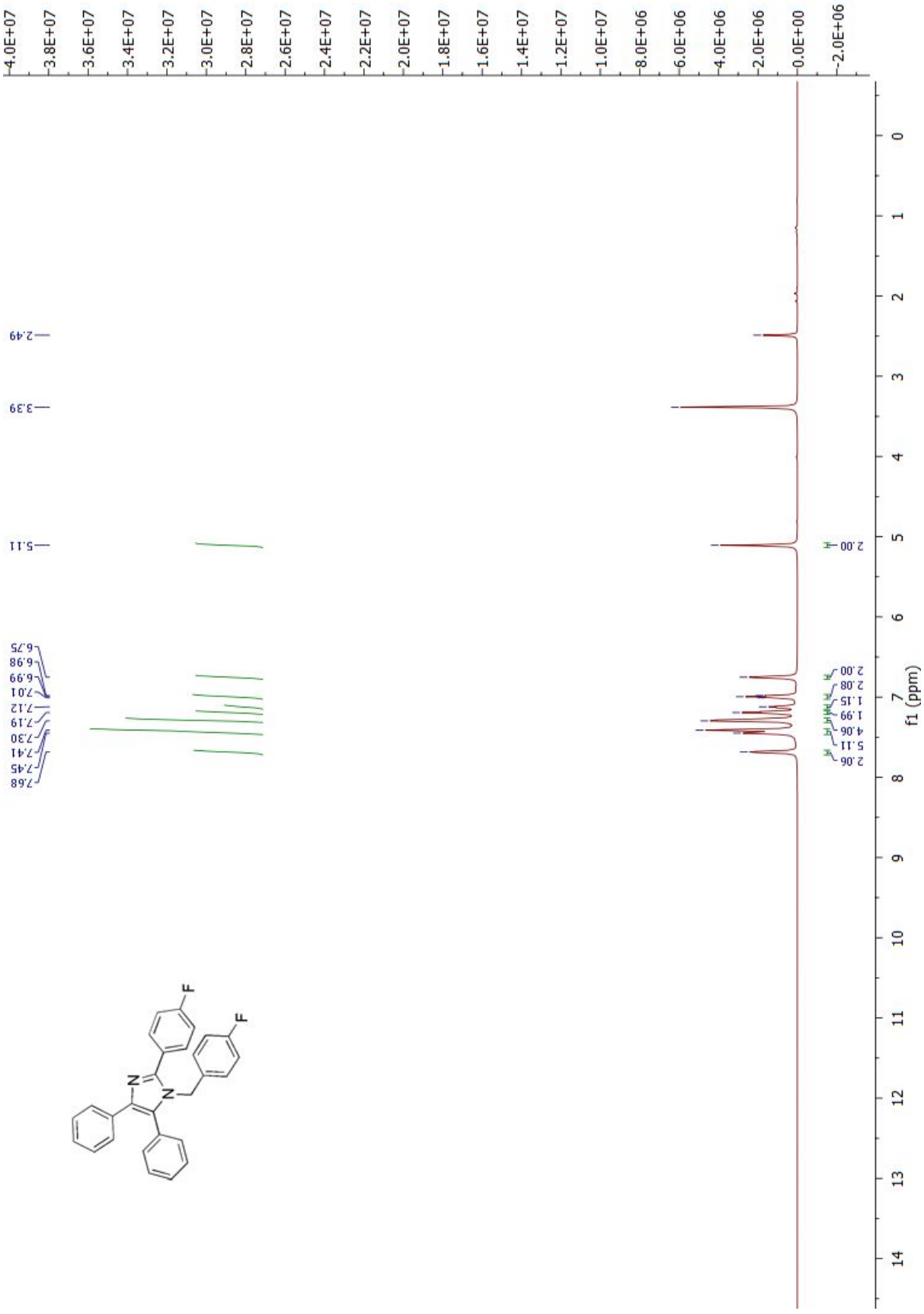


Figure S8: ^{13}C NMR spectrum of 1-(4-Fluoro-benzyl)-2-(4-fluoro-phenyl)-4,5-diphenyl-1H-imidazole (3d) in DMSO-d_6.

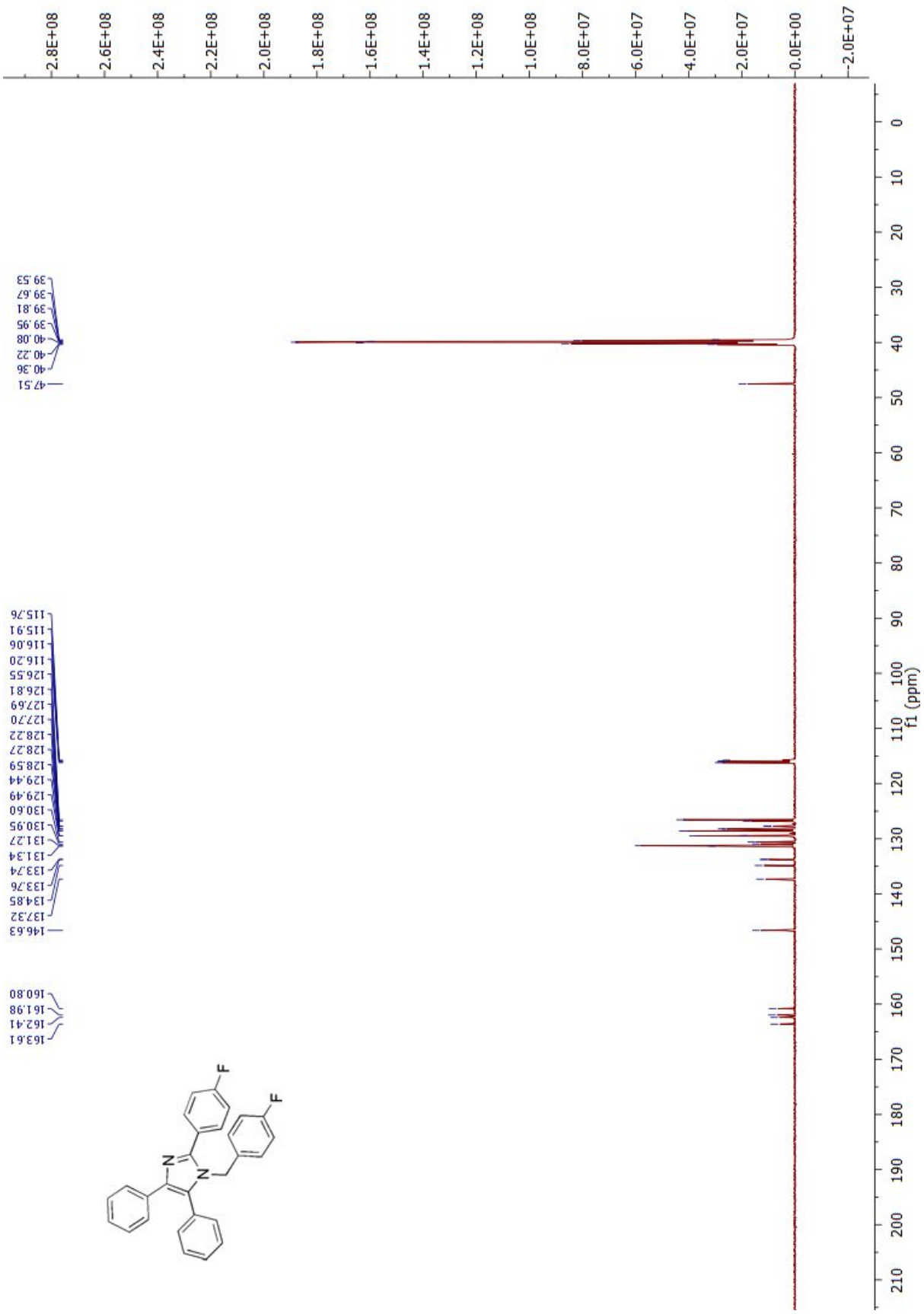


Figure S9: ^{1}H NMR spectrum of 1-(4-Bromo-benzyl)-2-(4-bromo-phenyl)-4,5-diphenyl-1H-imidazole (3e) in $CDCl_3$.

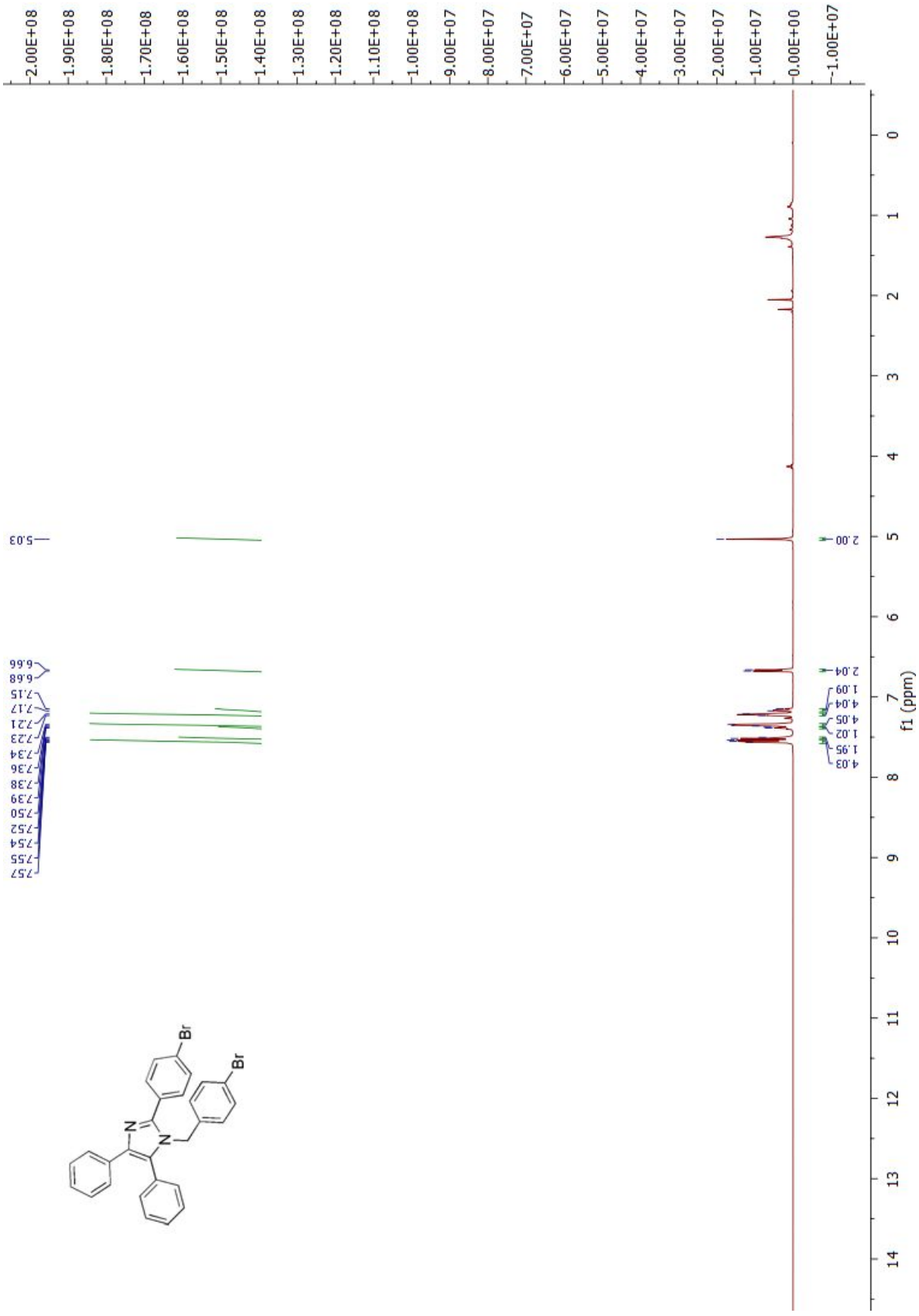


Figure S10: ^{13}C NMR spectrum of 1-(4-Bromo-benzyl)-2-(4-bromo-phenyl)-4,5-diphenyl-1H-imidazole (3e) in $CDCl_3$.

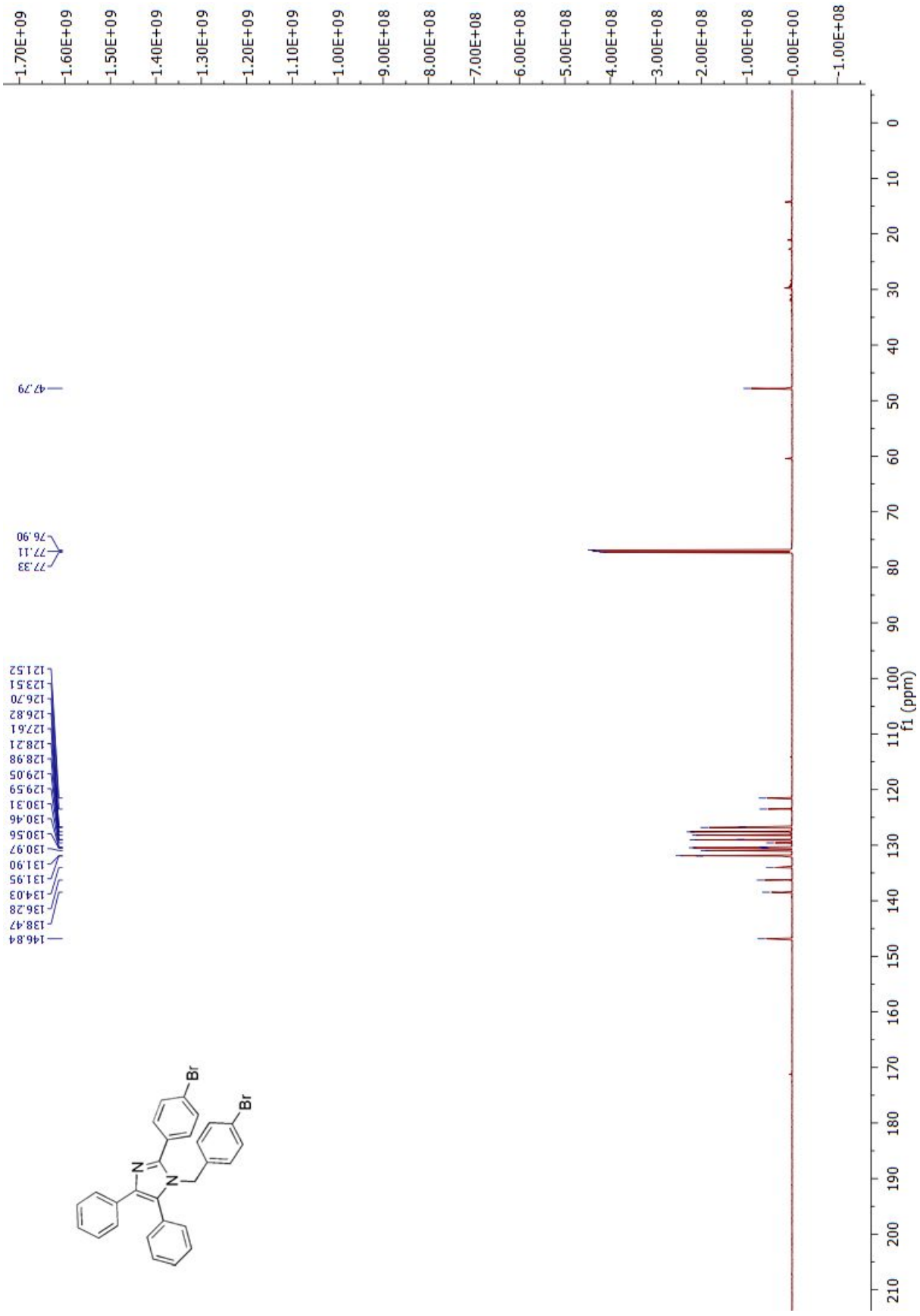


Figure S11: ^{1}H NMR spectrum of 1-(4-Chloro-benzyl)-2-(4-chloro-phenyl)-4,5-diphenyl-1H-imidazole (3f) in $CDCl_3$.

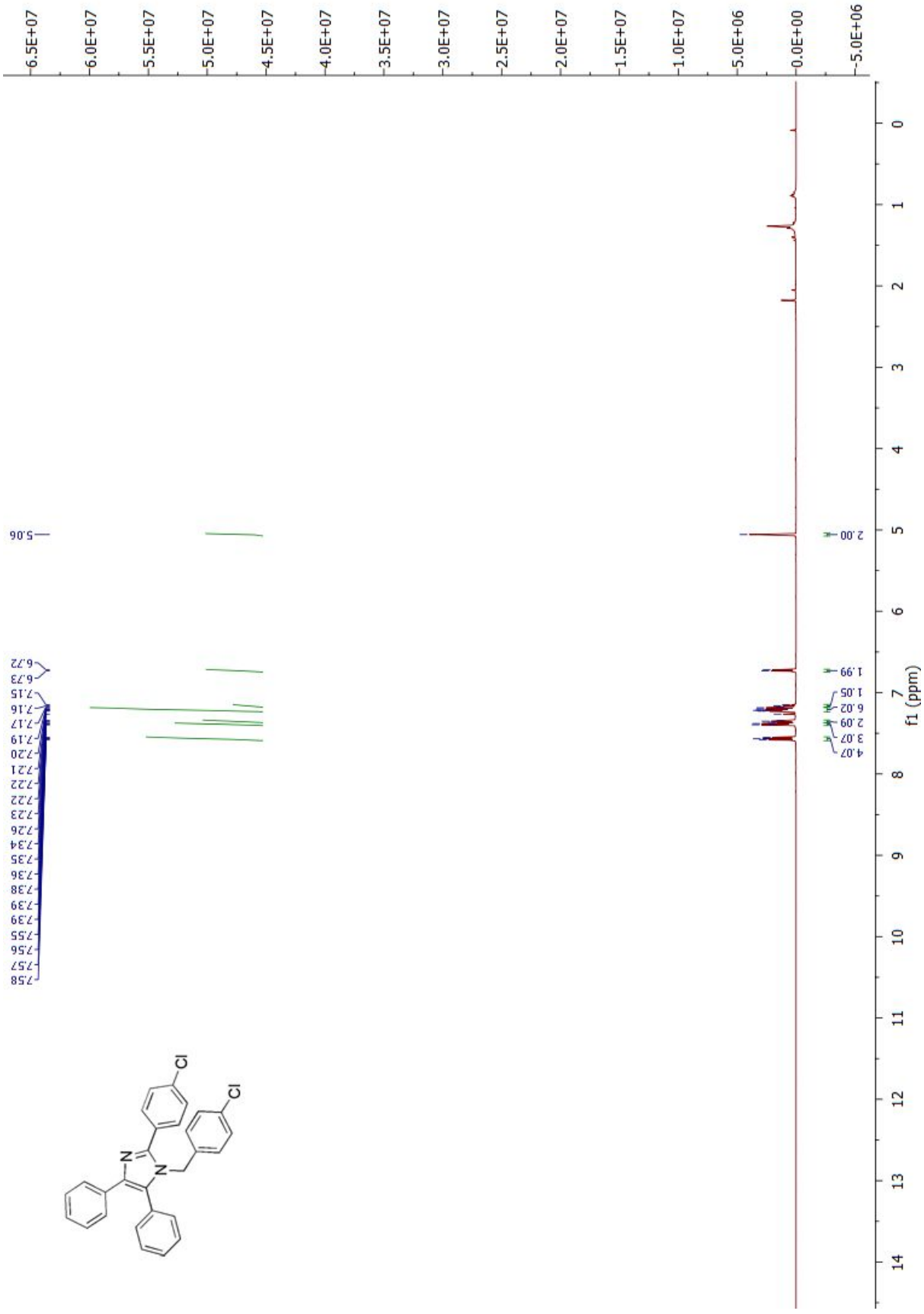


Figure S12: ^{13}CNMR spectra of 1-(4-Chloro-benzyl)-2-(4-chloro-phenyl)-4,5-diphenyl-1H-imidazole (3f) in $CDCl_3$.

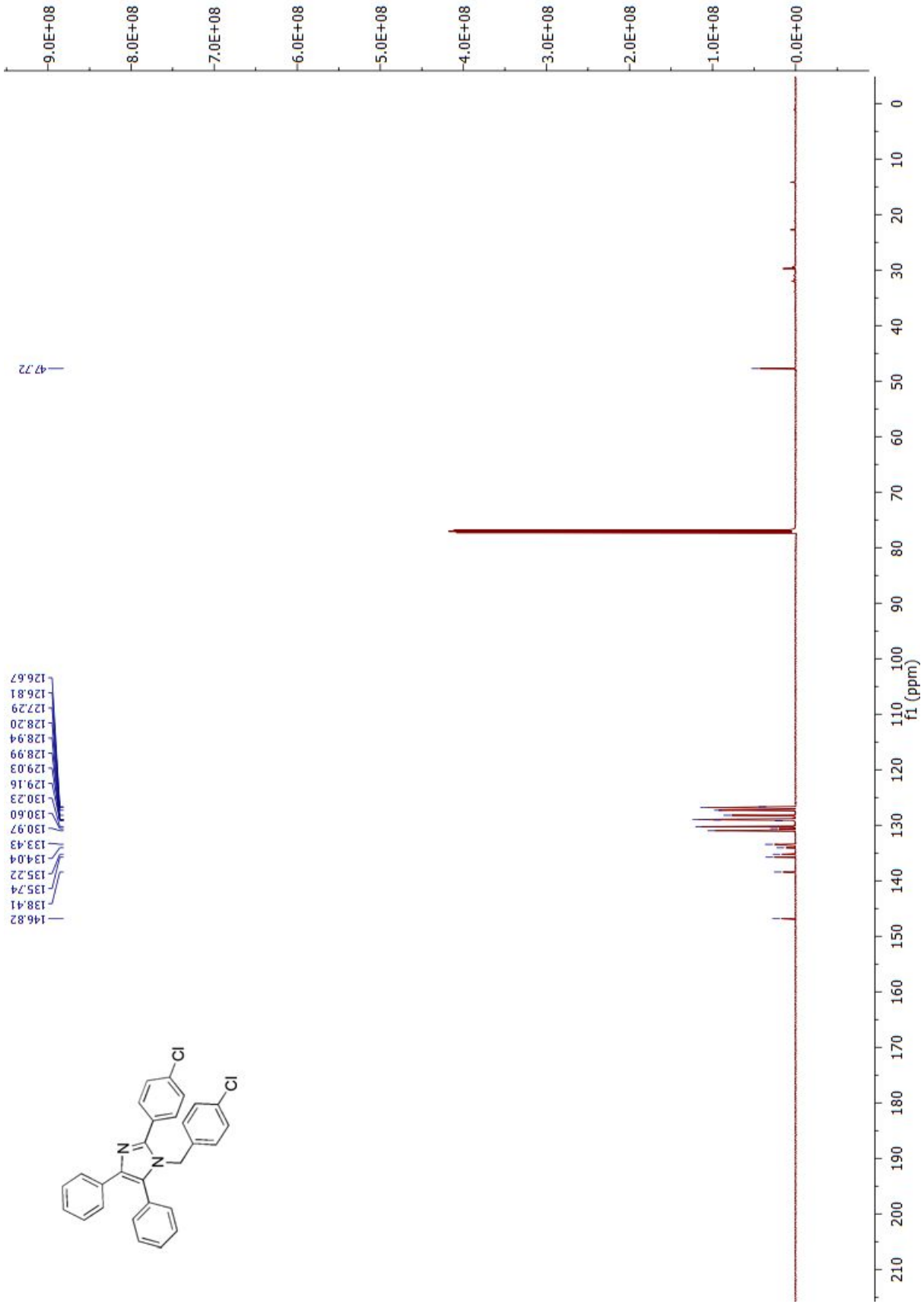


Figure S13: ^{1}H NMR spectrum of 4,5-Diphenyl-1-(4-trifluoromethyl-benzyl)-2-(4-trifluoromethyl-phenyl)-1H-imidazole (3g) in $CDCl_3$.

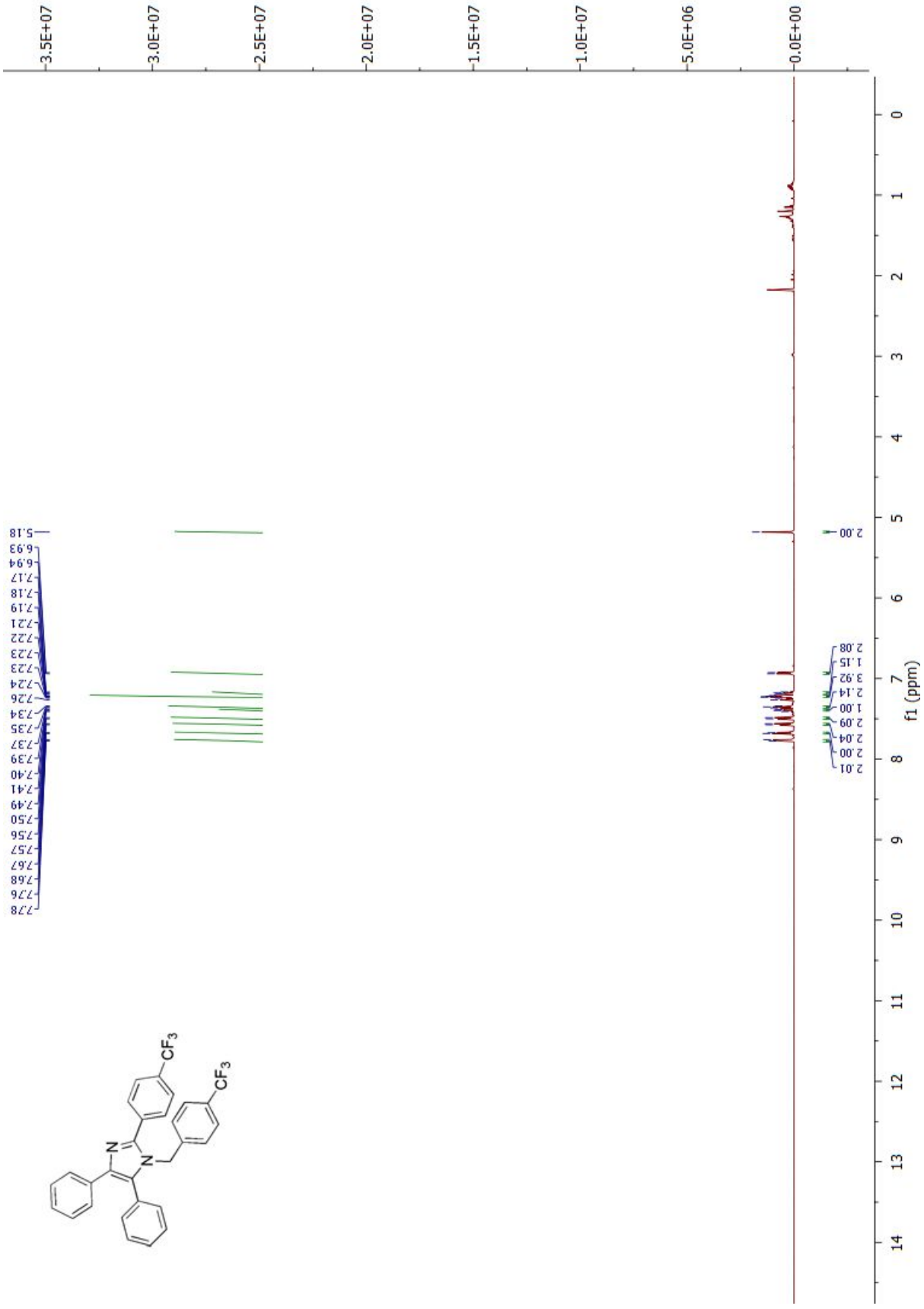


Figure S14: ^{13}C NMR spectrum of 4,5-Diphenyl-1-(4-trifluoromethyl-benzyl)-2-(4-trifluoromethyl-phenyl)-1H-imidazole (3g) in $CDCl_3$.

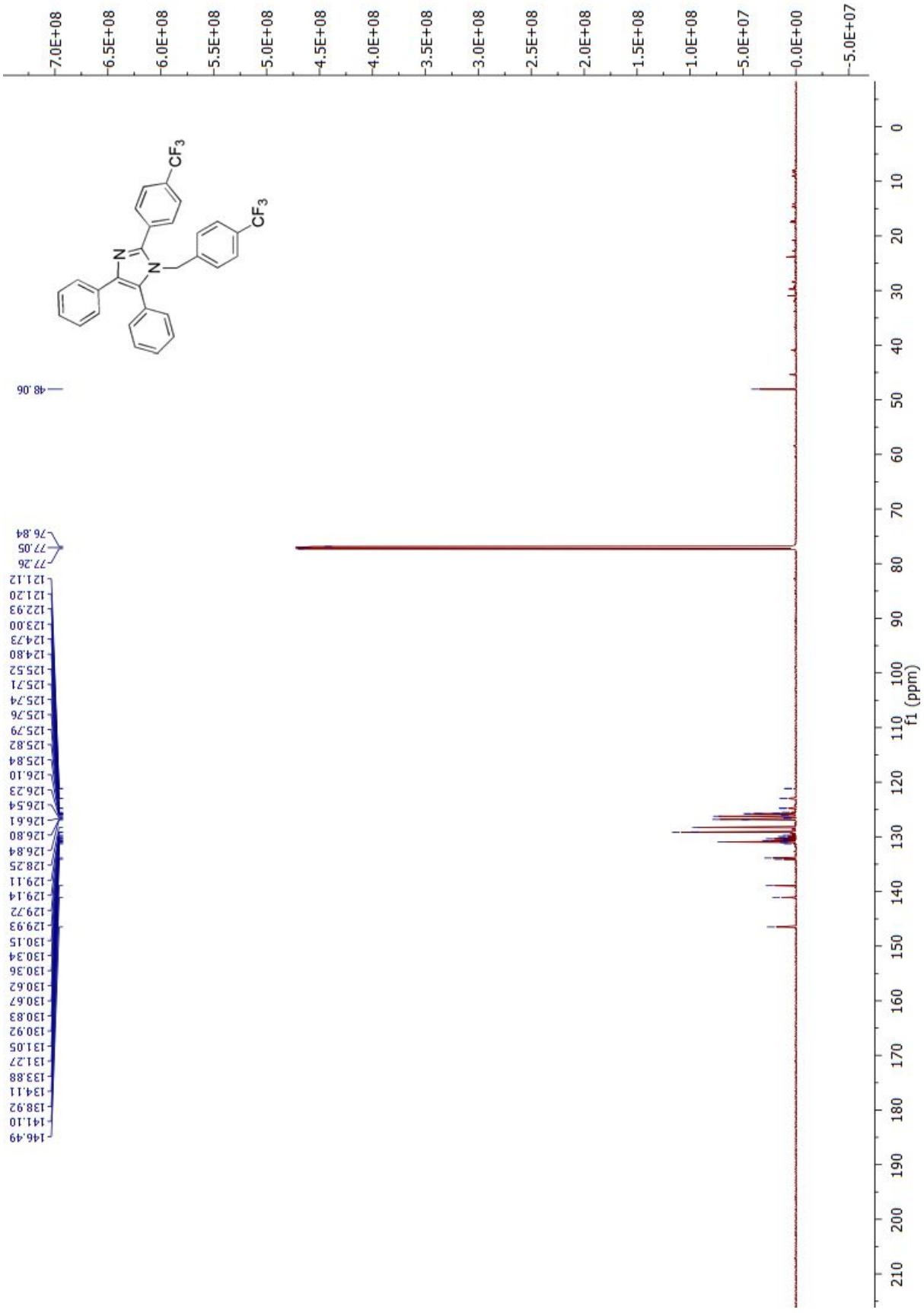


Figure S15: ^{1}H NMR spectrum of 4,5-Diphenyl-1-(4-trifluoromethoxy-benzyl)-2-(4-trifluoromethoxy-phenyl)-1H-imidazole (3h) in $CDCl_3$.

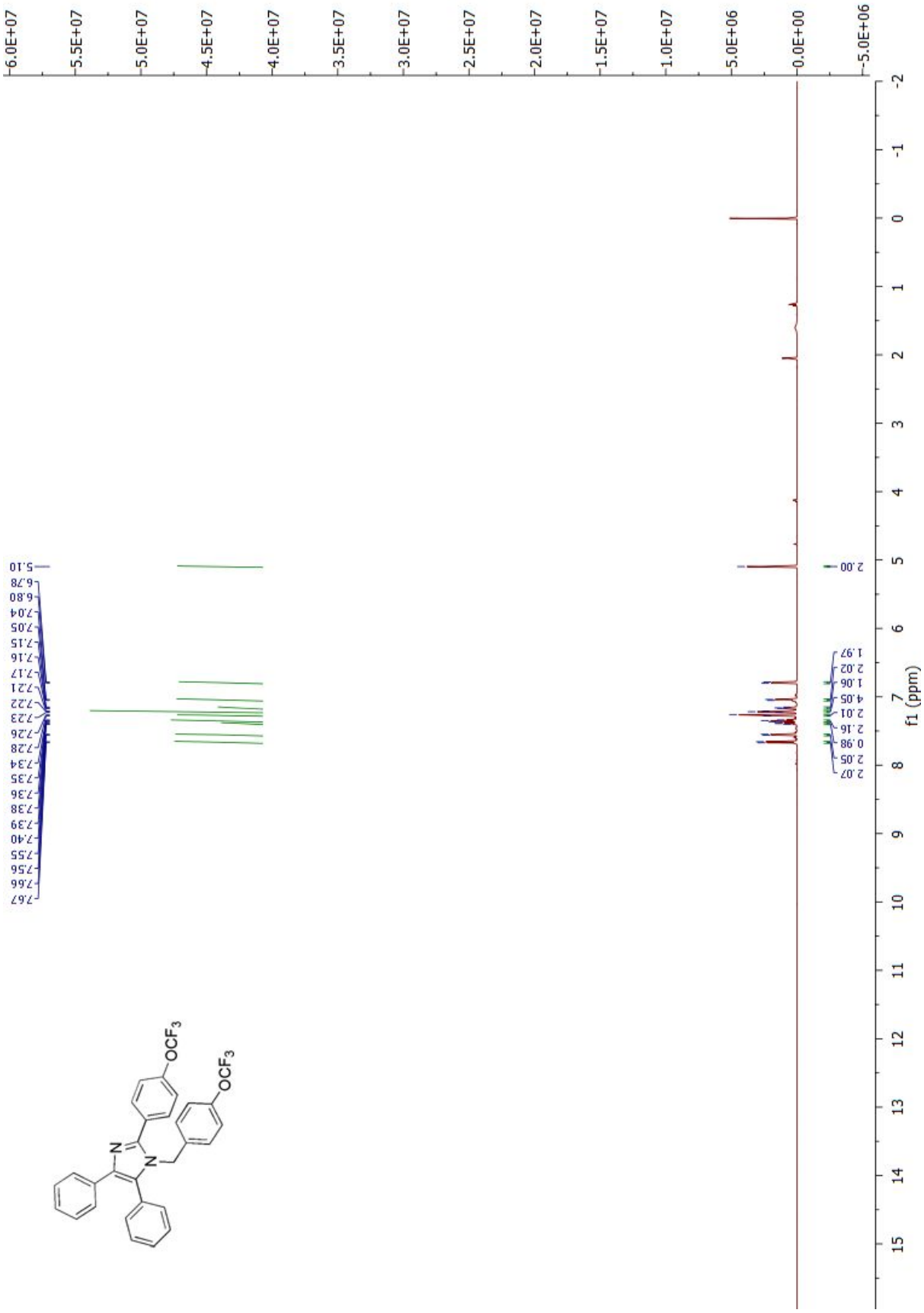


Figure S16: ^{13}CNMR spectrum of 4,5-Diphenyl-1-(4-trifluoromethoxy-benzyl)-2-(4-trifluoromethoxy-phenyl)-1H-imidazole (3h) in $CDCl_3$.

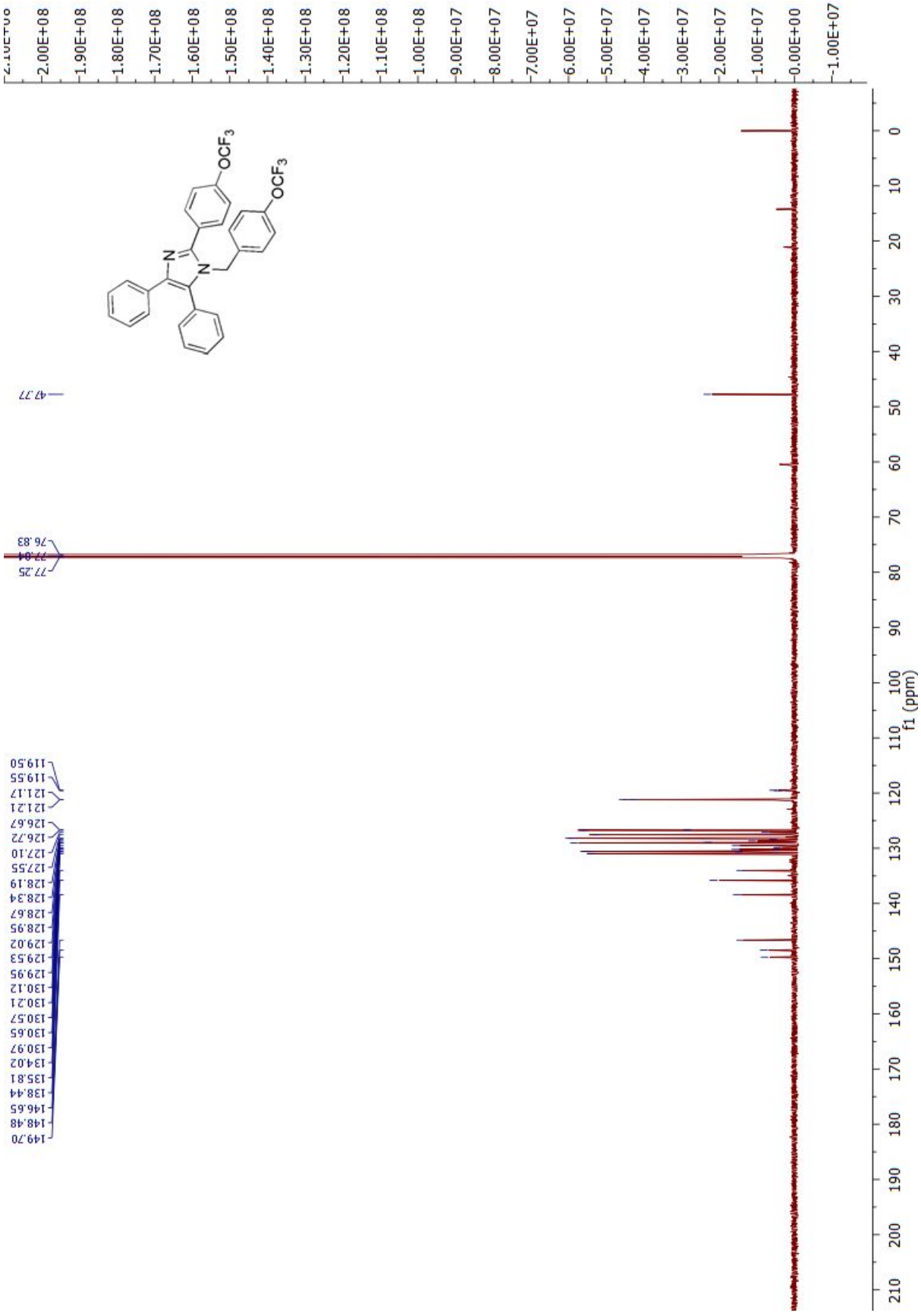


Figure S17: ^{1}H NMR spectrum of 2-(4,5-diphenyl-1-(pyridin-2-ylmethyl)-1H-imidazol-2-yl)pyridine (3i) in $CDCl_3$.

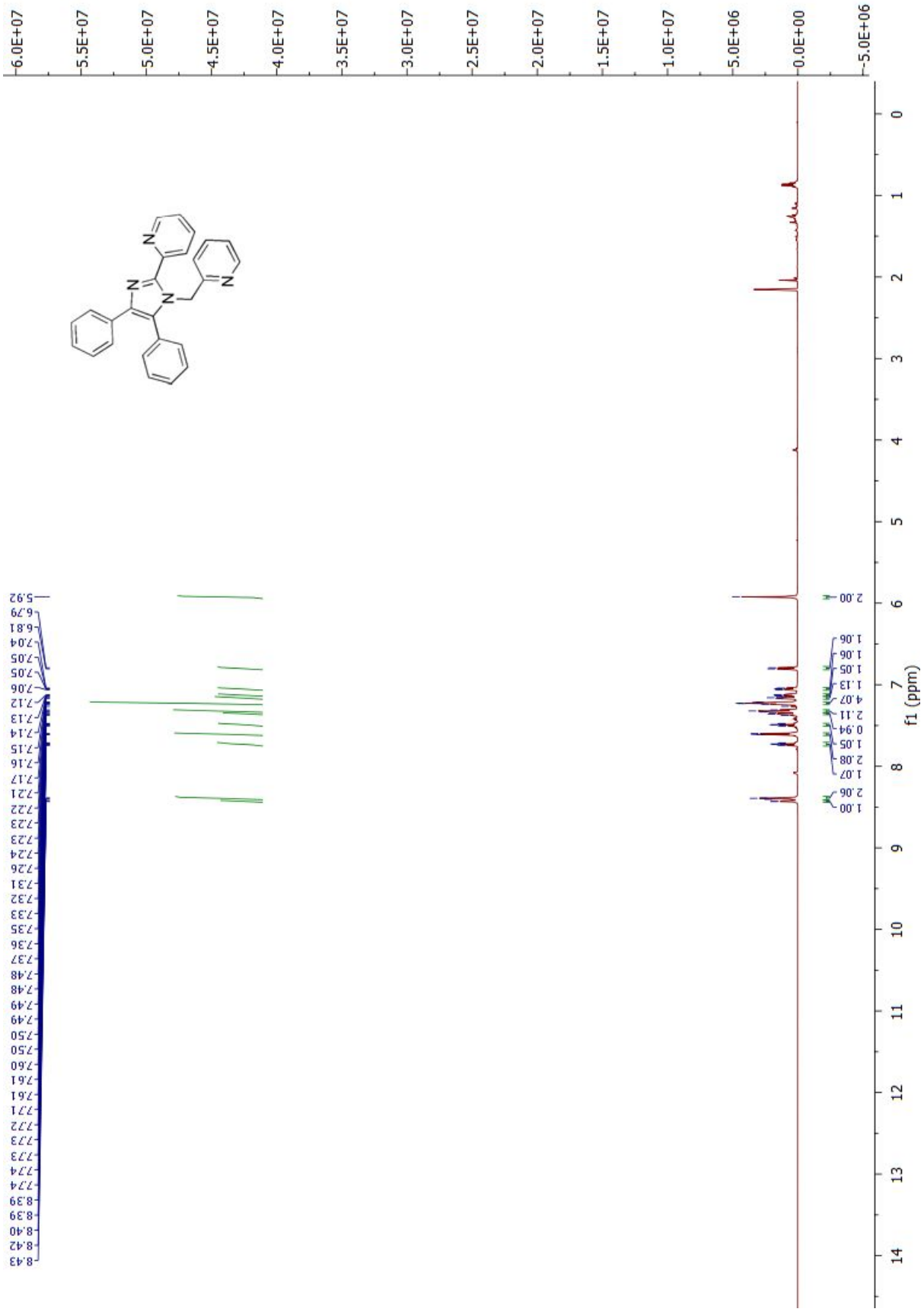


Figure S18: ^{13}C NMR spectrum of 2-(4,5-diphenyl-1-(pyridin-2-ylmethyl)-1H-imidazol-2-yl)pyridine (3i) in $CDCl_3$.

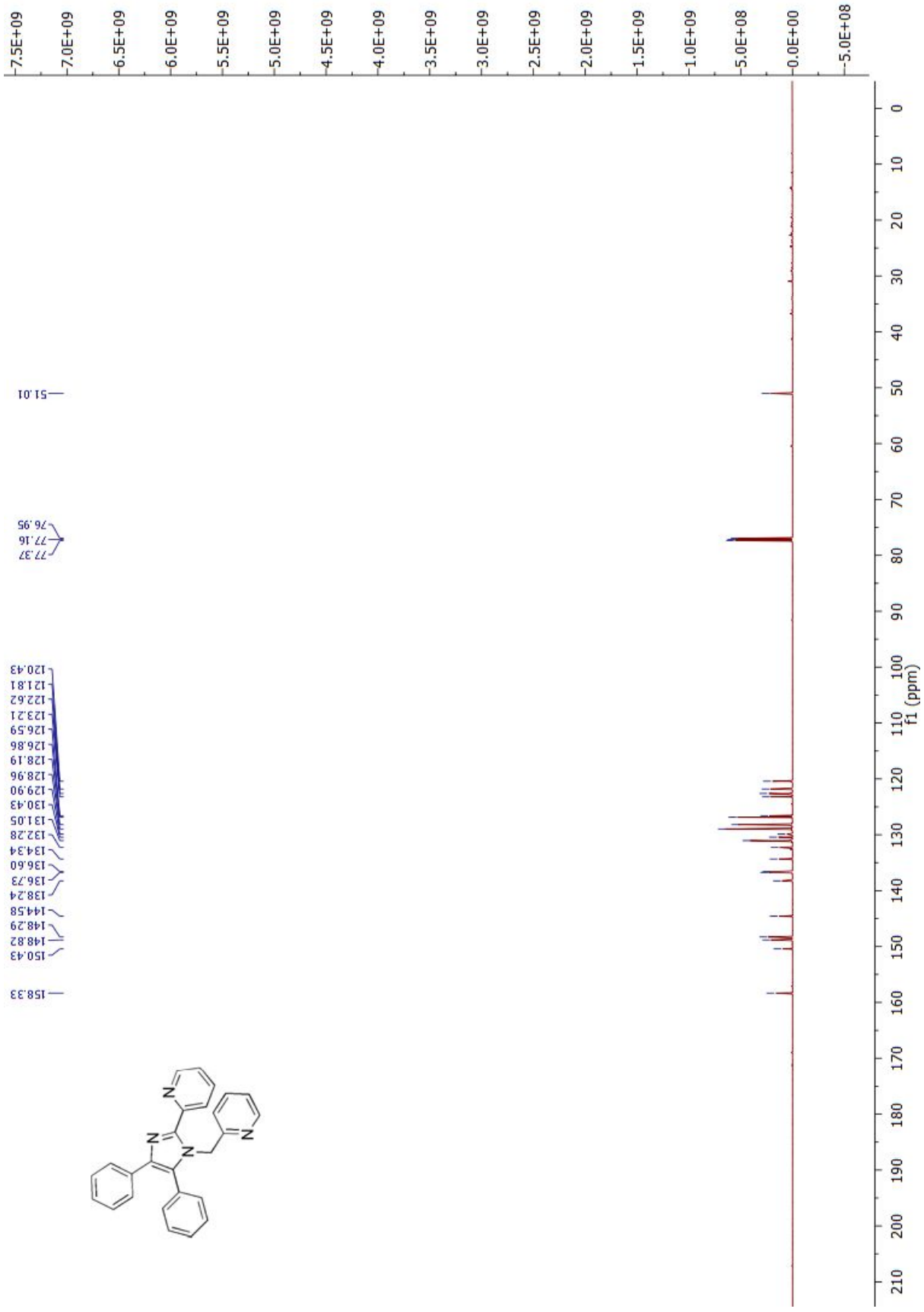


Figure S19: ^{1}H NMR spectrum of 2-Benzo[1,3]dioxol-5-yl-1-benzo[1,3]dioxol-5-ylmethyl-4,5-diphenyl-1H-imidazole (3j) in DMSO-d_6.

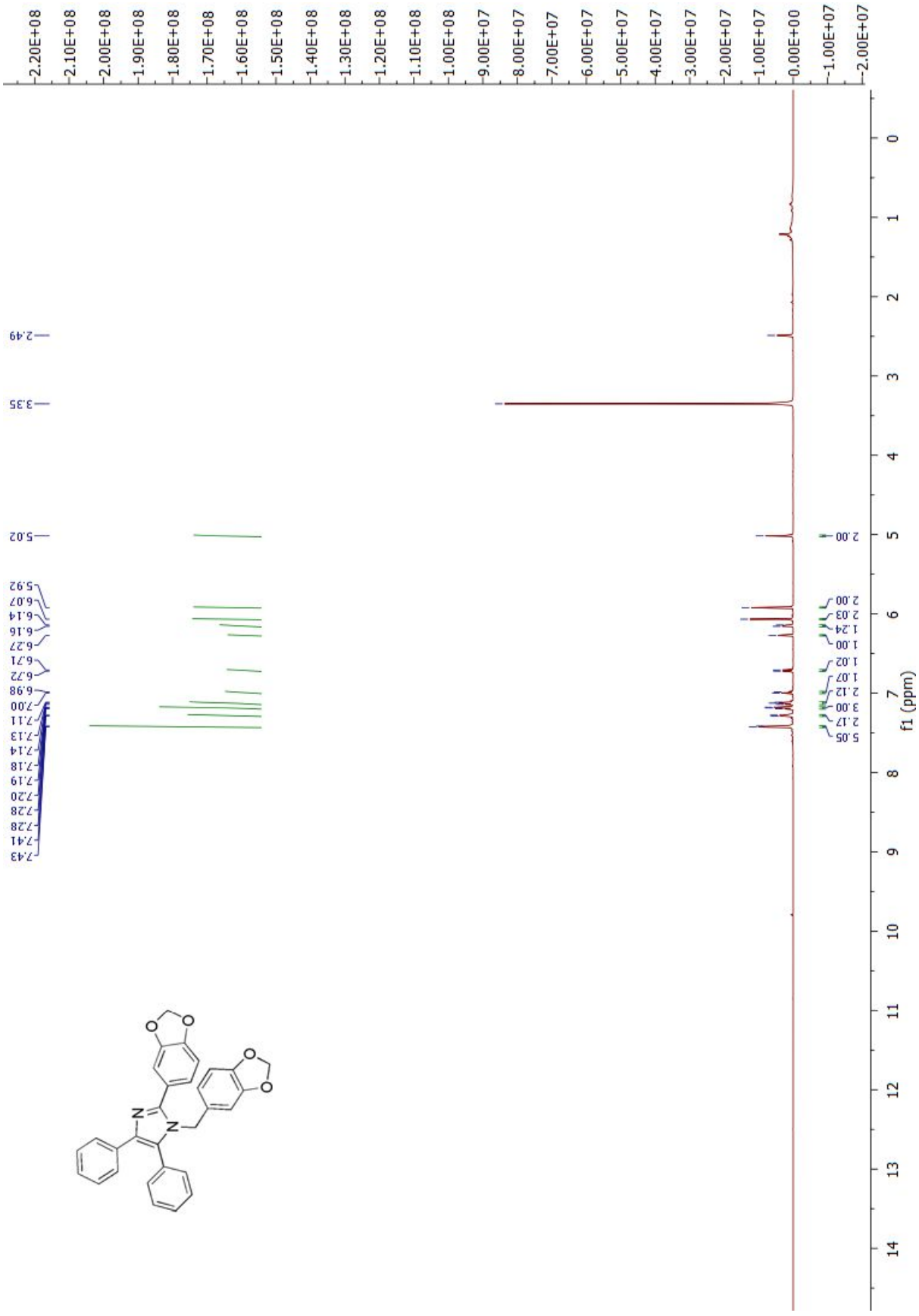


Figure S20: ^{13}C NMR spectrum of 2-Benzo[1,3]dioxol-5-yl-1-benzo[1,3]dioxol-5-ylmethyl-4,5-diphenyl-1H-imidazole (3j) in DMSO-d_6.

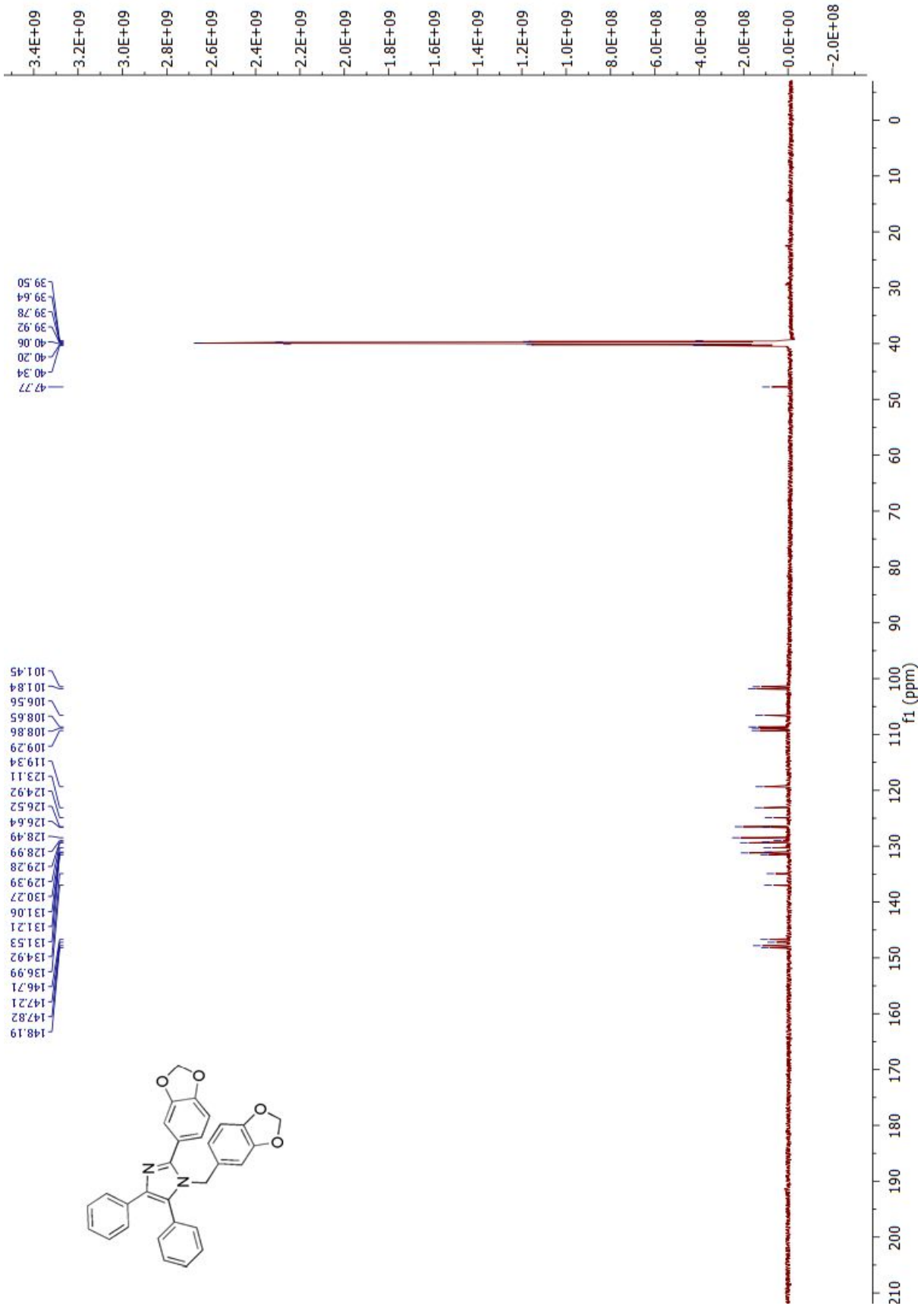


Figure S21: ^{1}H NMR spectrum of 4,5-Diphenyl-2-thiophen-2-yl-1-thiophen-2-ylmethyl-1H-imidazole (3k) in $CDCl_3$.

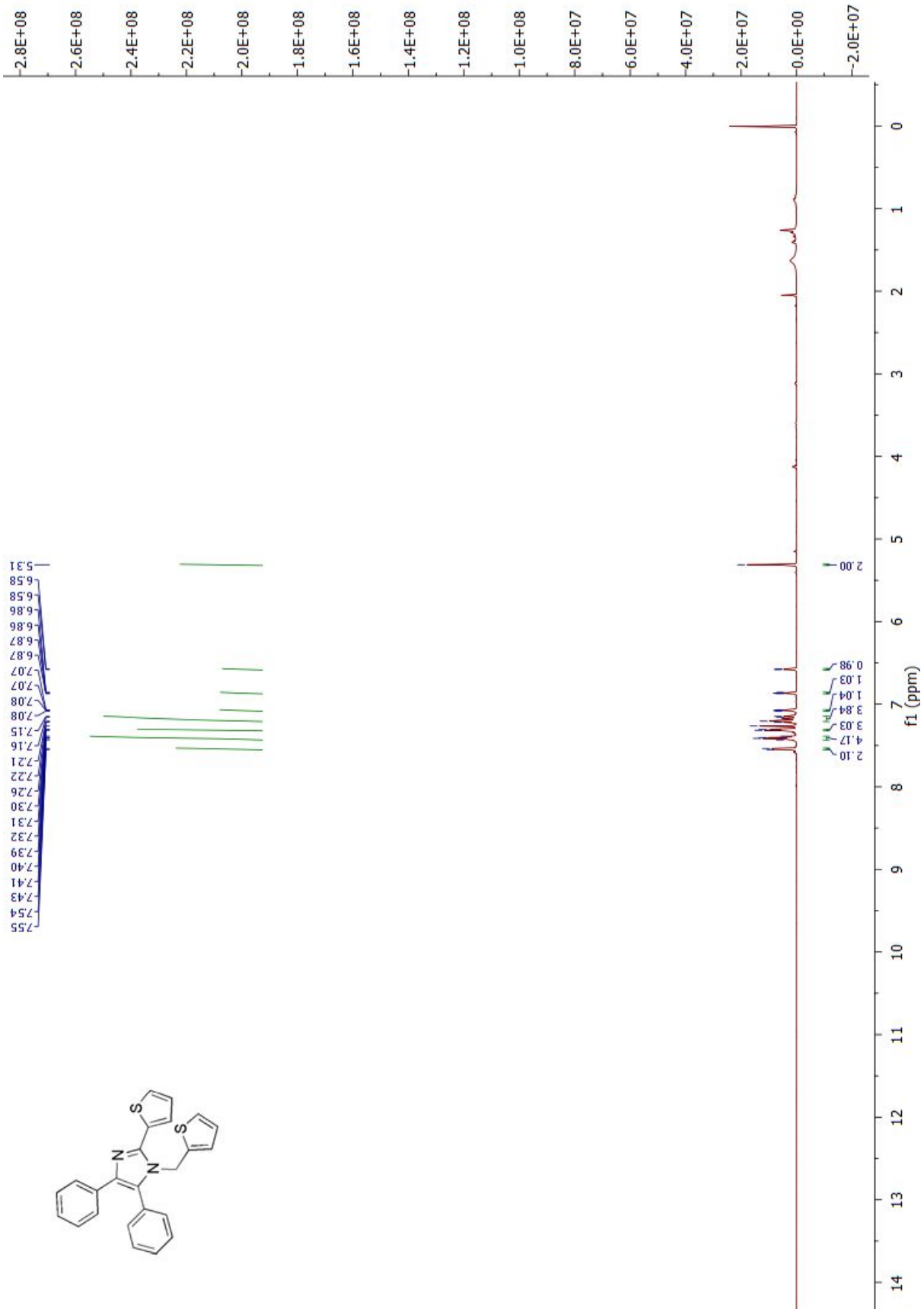


Figure S22: ^{13}C NMR spectrum of 4,5-Diphenyl-2-thiophen-2-yl-1-thiophen-2-ylmethyl-1H-imidazole (3k) in $CDCl_3$.

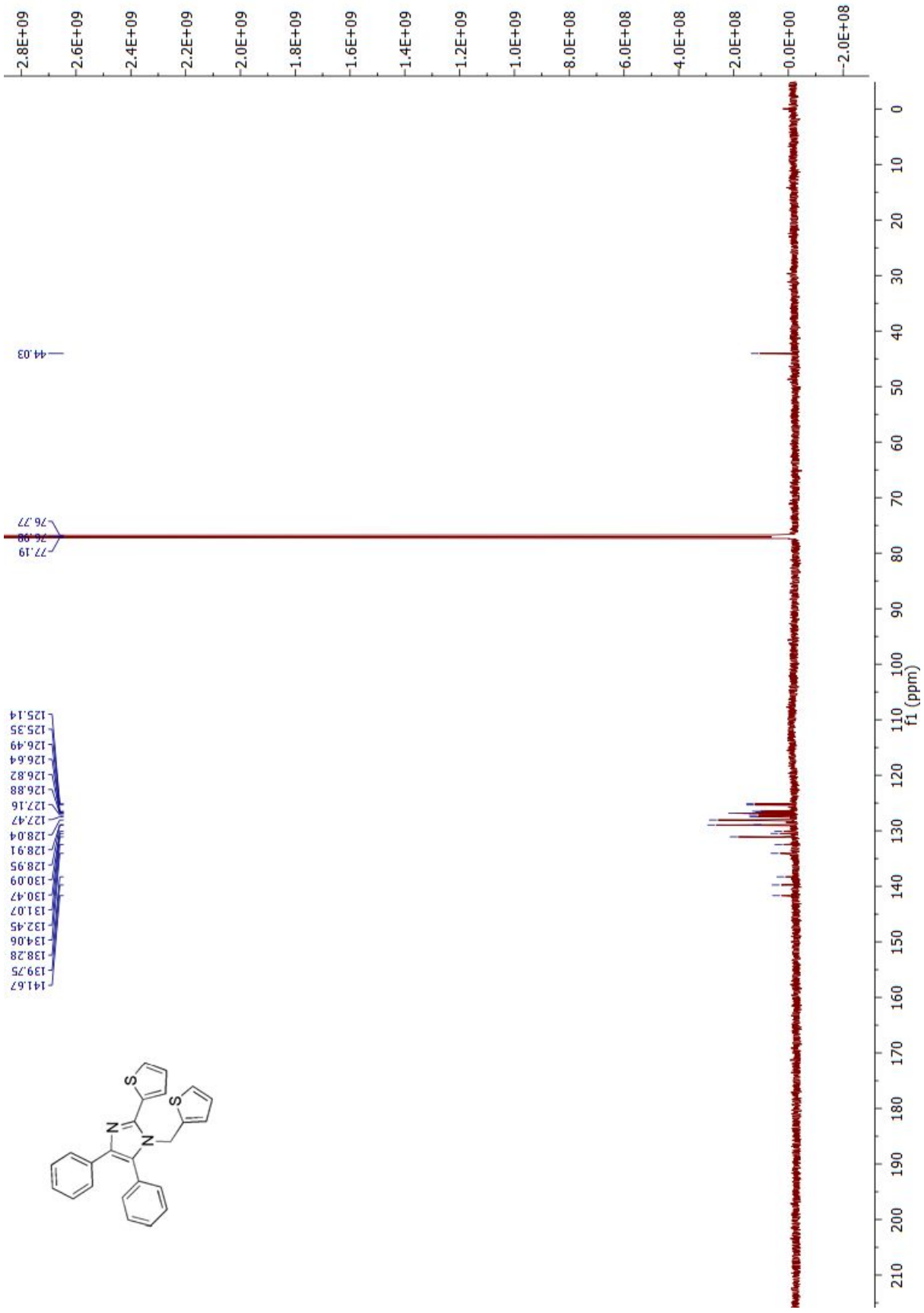


Figure S23: ^{1}H NMR spectrum of 2-Naphthalen-1-yl-1-naphthalen-1-ylmethyl-4,5-diphenyl-1H-imidazole (3l) in $CDCl_3$.

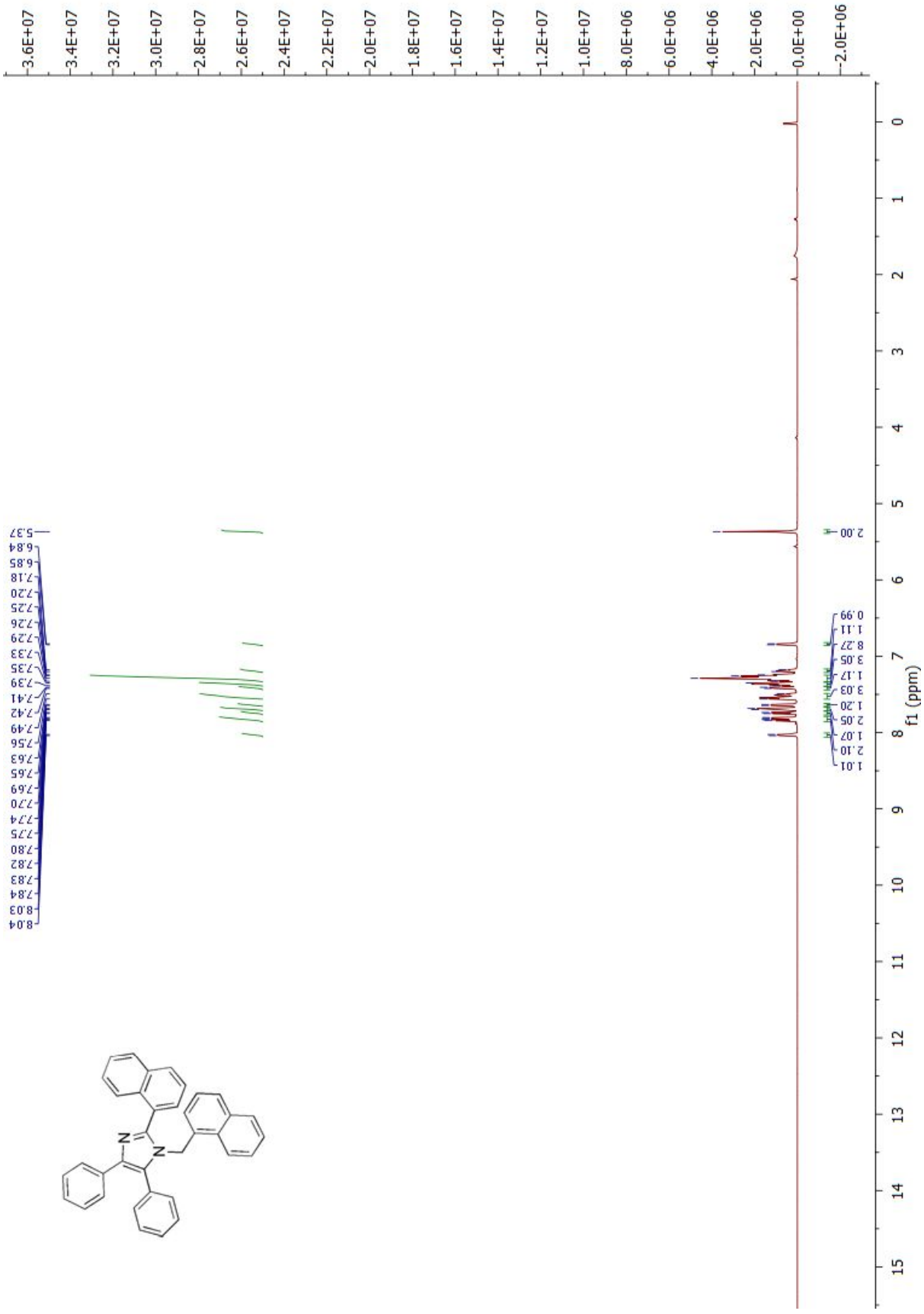


Figure S24: ^{13}C NMR spectrum of 2-Naphthalen-1-yl-1-naphthalen-1-ylmethyl-4,5-diphenyl-1H-imidazole (3l) in $CDCl_3$.

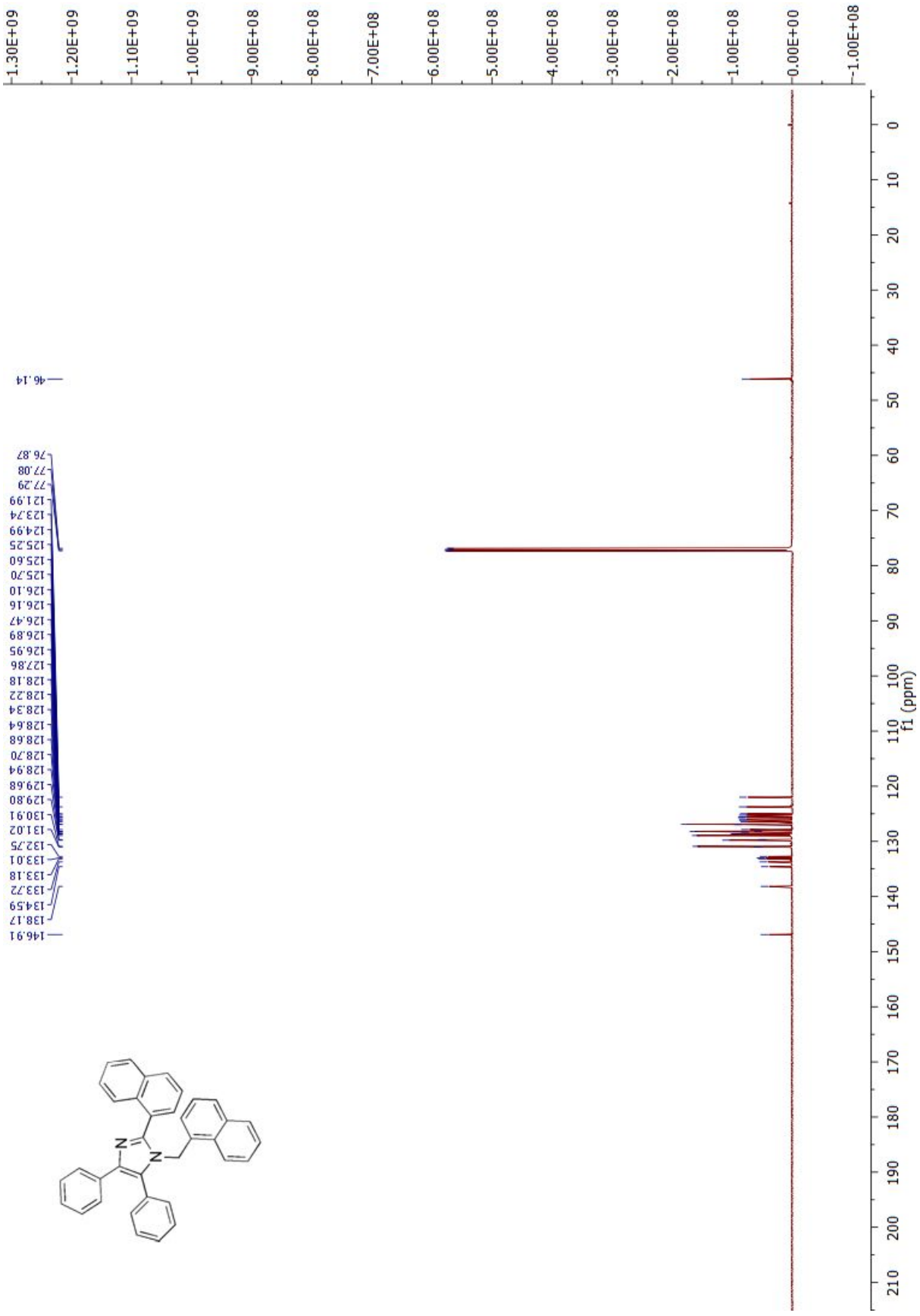


Figure S25: ^{1}H NMR spectrum of 1-Benzyl-4,5-bis-(4-methoxy-phenyl)-2-phenyl-1H-imidazole (3o) in DMSO-d_6.

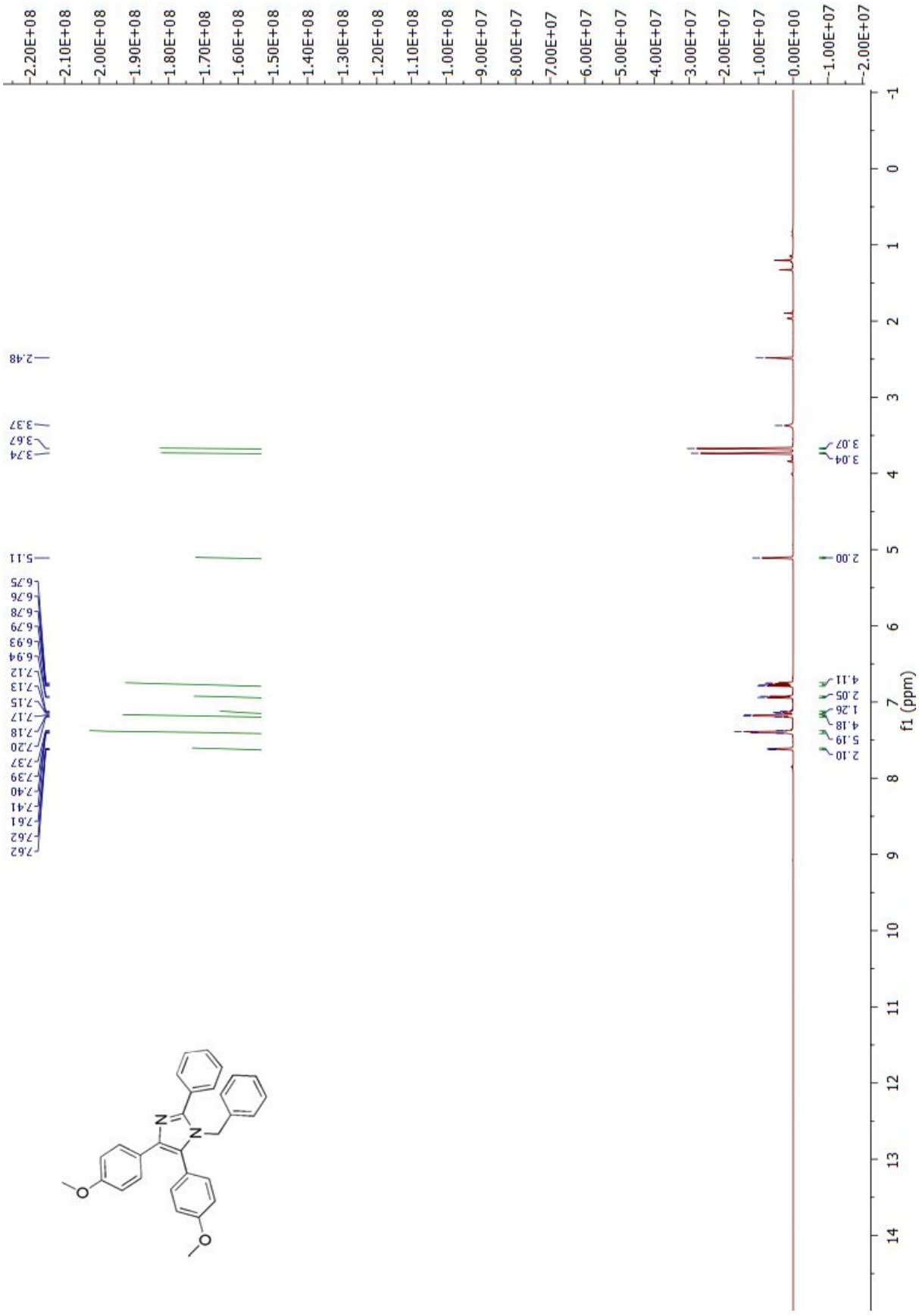


Figure S26: ^{13}C NMR spectrum of 1-Benzyl-4,5-bis-(4-methoxy-phenyl)-2-phenyl-1H-imidazole (3o) in DMSO-d_6.

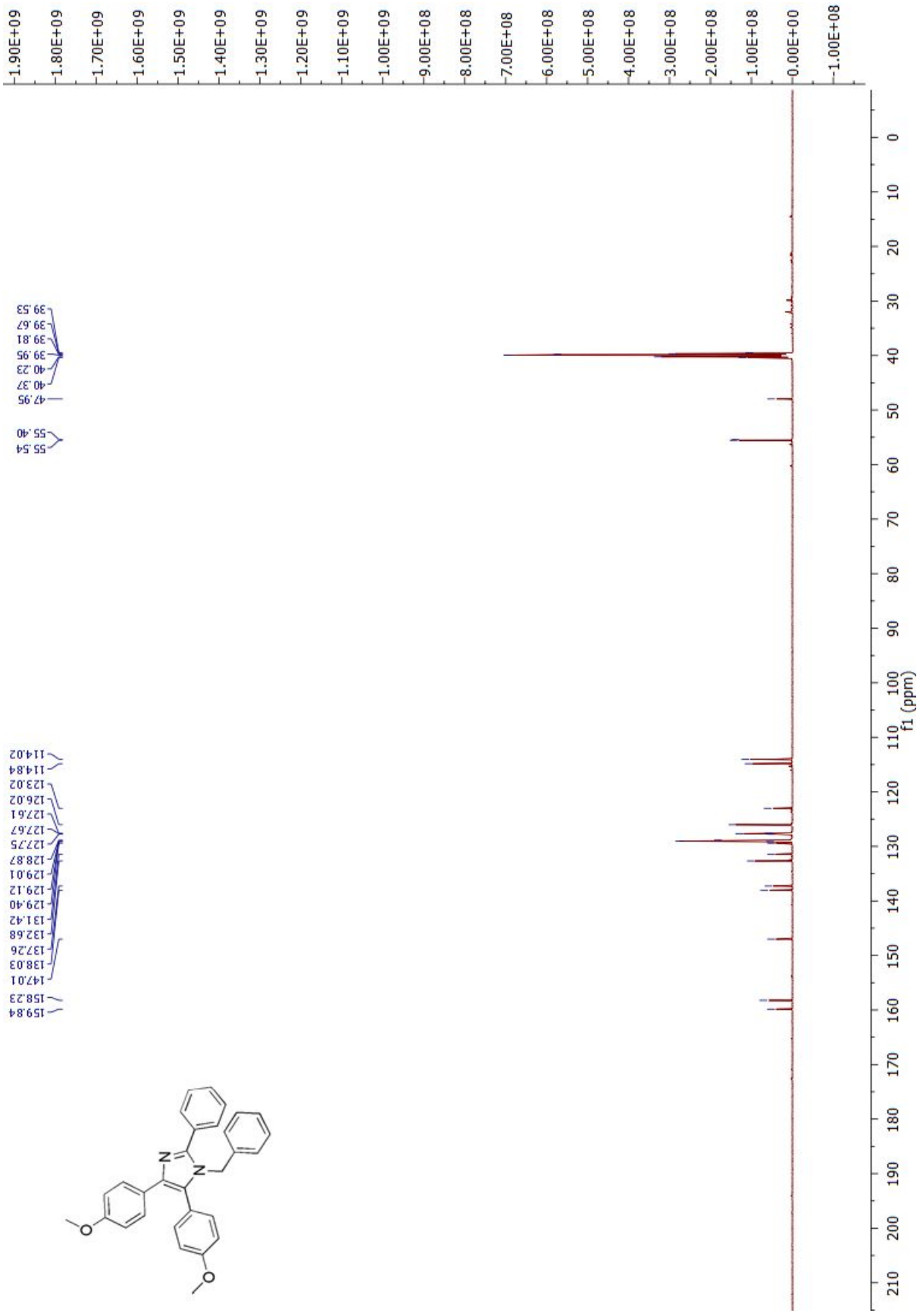


Figure S27: ^{1}H NMR spectrum of 2-(4,5-bis(4-methoxyphenyl)-1-(pyridin-2-ylmethyl)-1H-imidazol-2-yl)pyridine (3p) in DMSO-d_6.

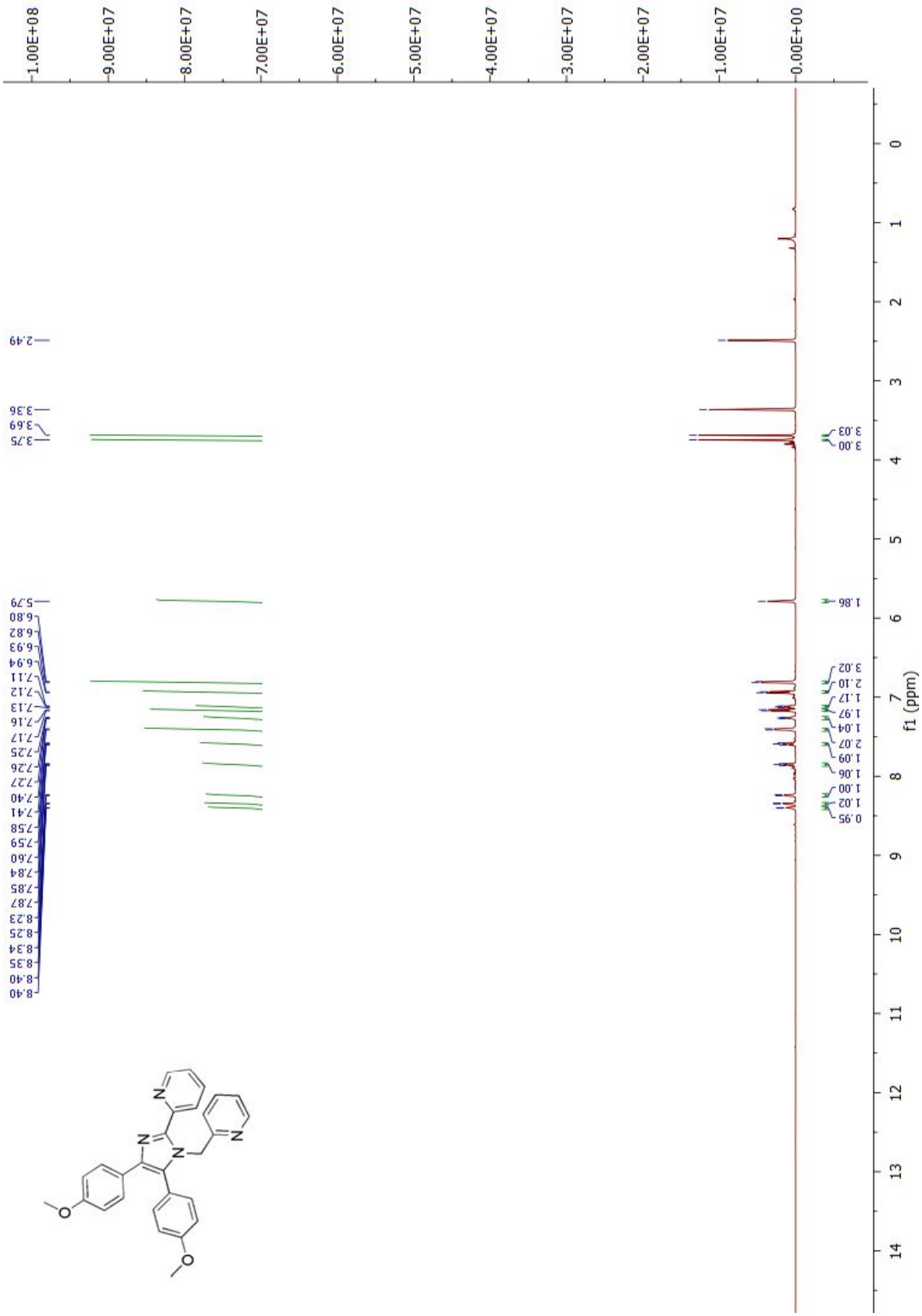


Figure S28: ^{13}C NMR spectrum of 2-(4,5-bis(4-methoxyphenyl)-1-(pyridin-2-ylmethyl)-1H-imidazol-2-yl)pyridine (3p) in DMSO-d_6.

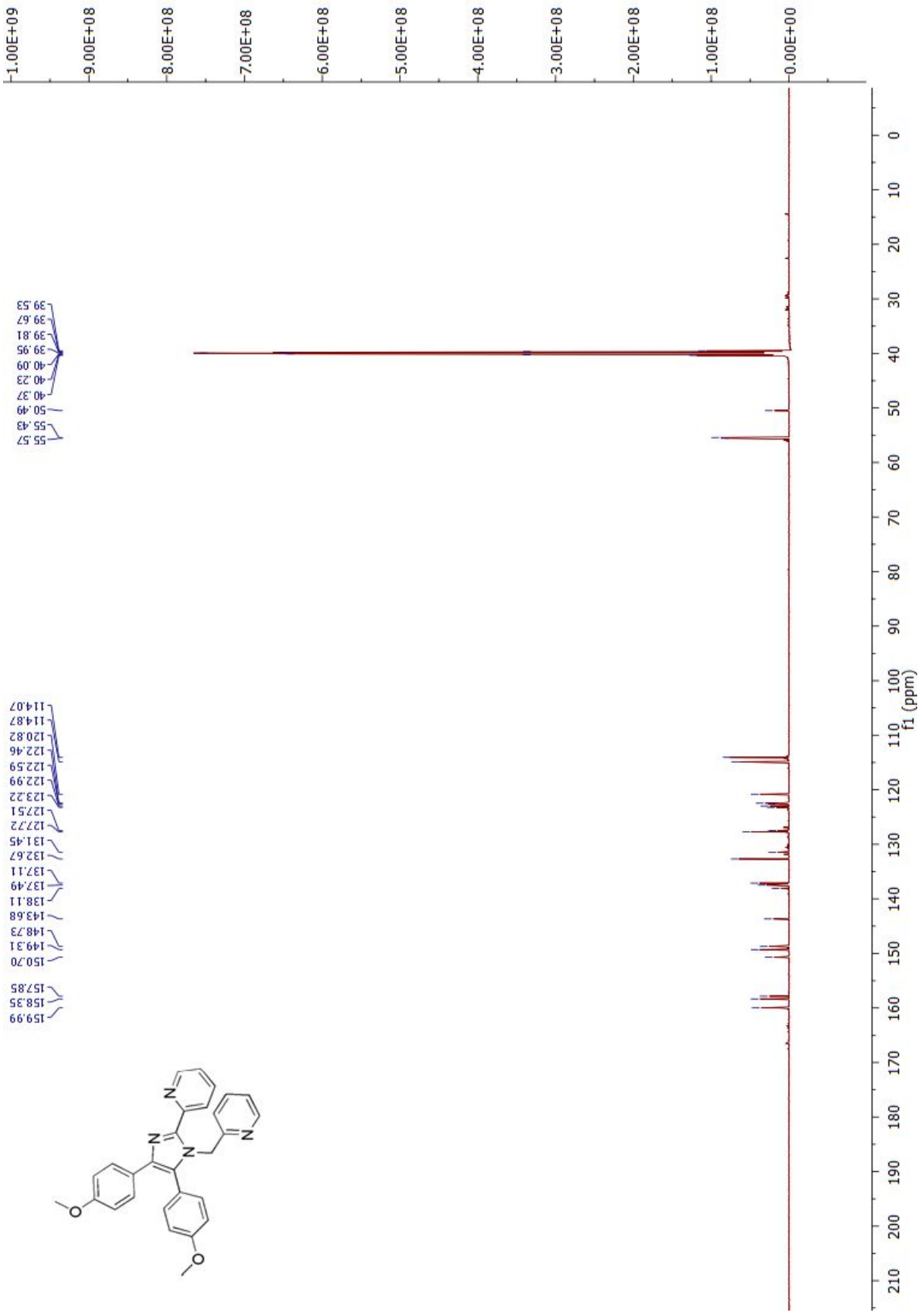


Figure S29: ^{1}H NMR spectrum of 1-Benzyl-5-methyl-2,4-diphenyl-1H-imidazole (5a) in $CDCl_3$.

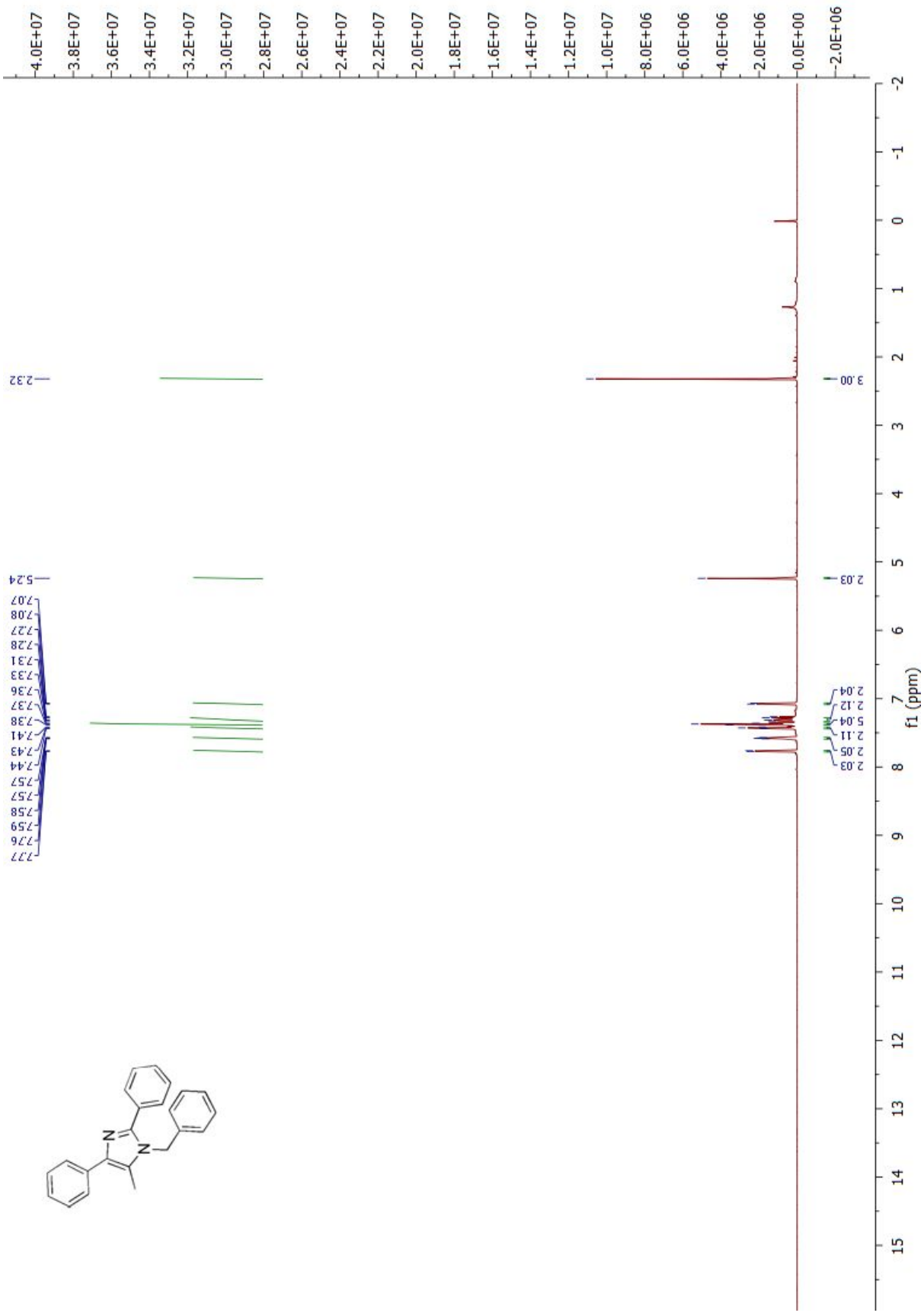


Figure S30: ^{13}C NMR spectrum of 1-Benzyl-5-methyl-2,4-diphenyl-1H-imidazole (5a) in $CDCl_3$.

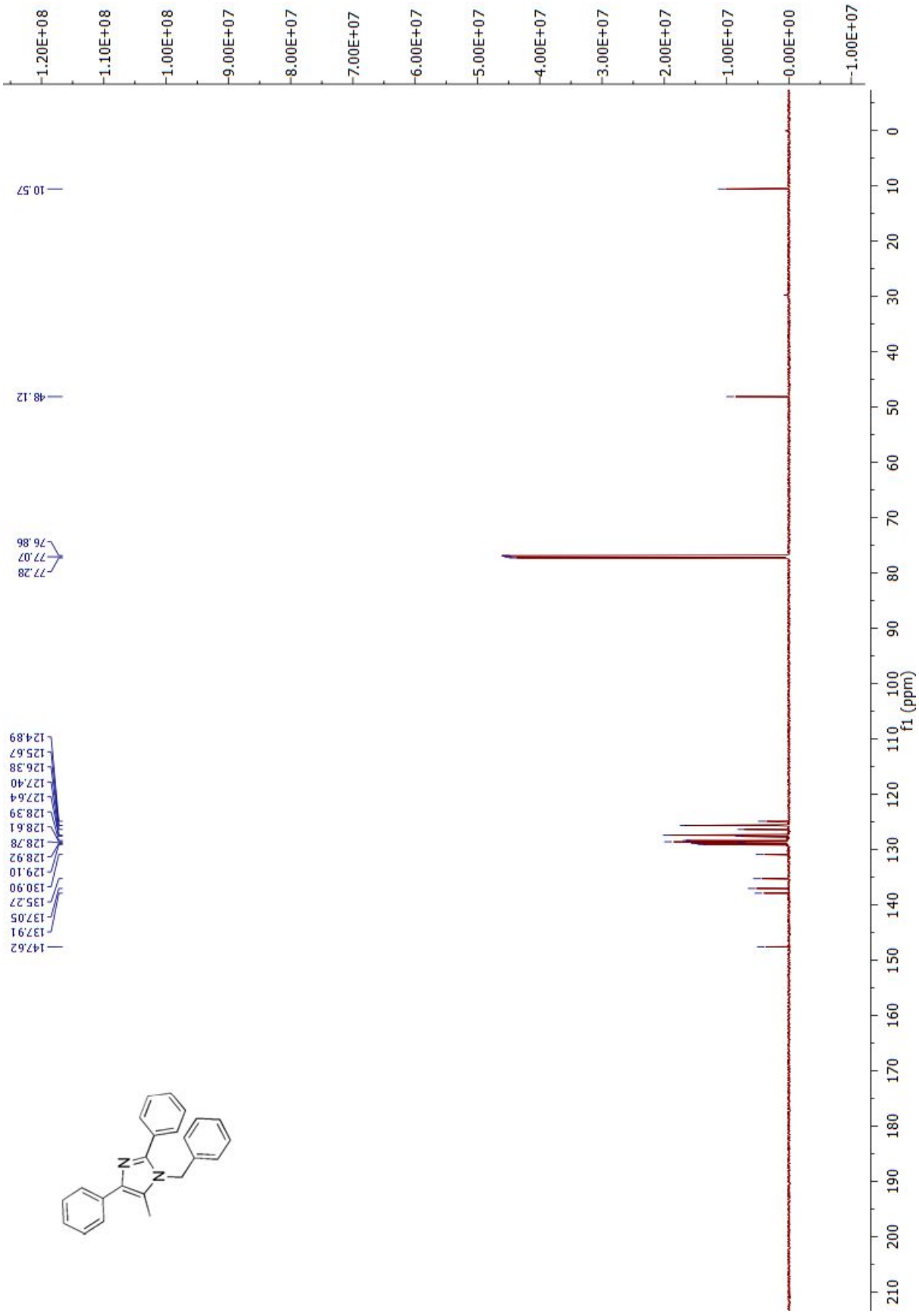


Figure S31: ^{1}H NMR spectrum of 1-(4-Methoxy-benzyl)-2-(4-methoxy-phenyl)-5-methyl-4-phenyl-1H-imidazole (5b) in $CDCl_3$.

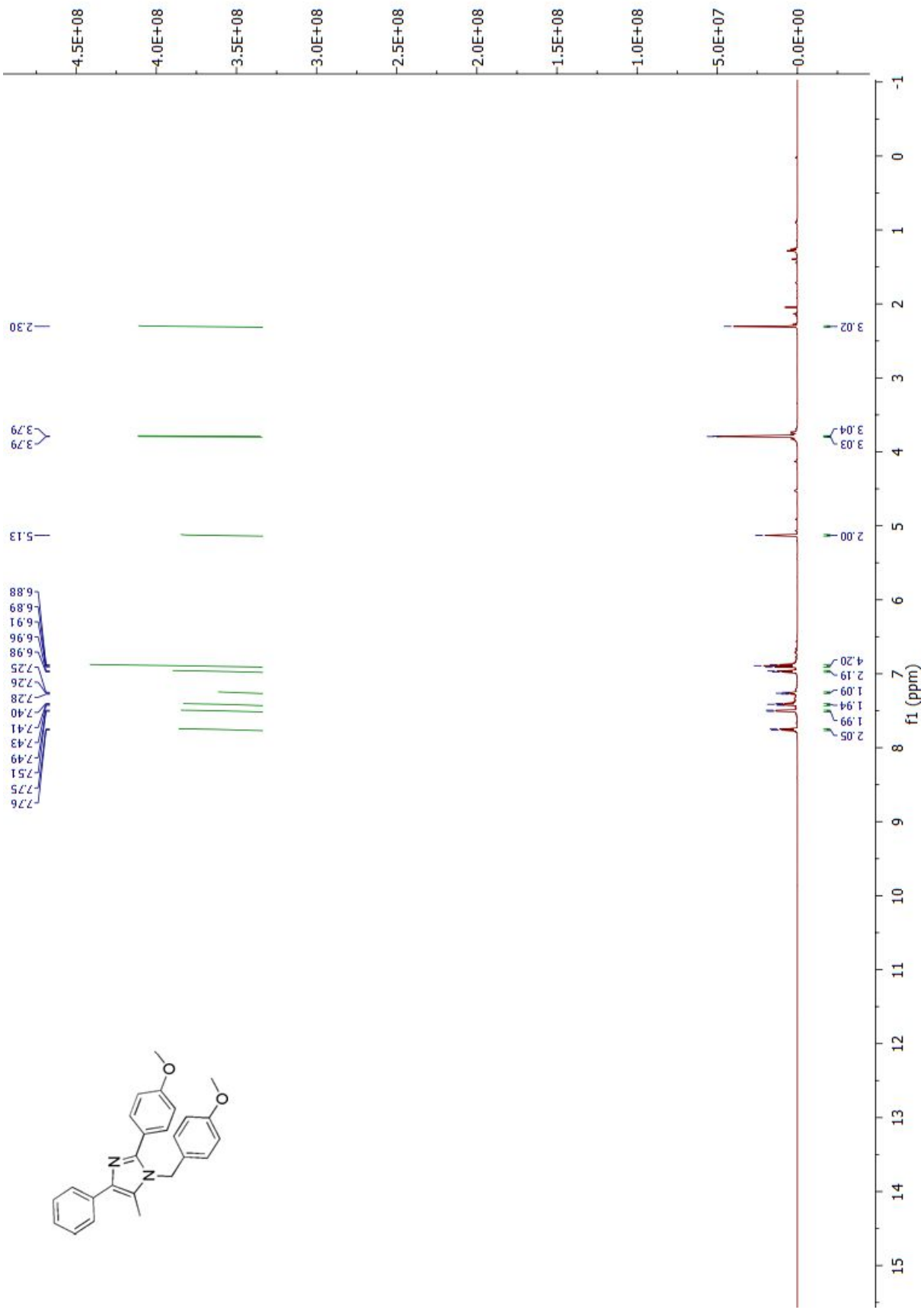


Figure S32: ^{13}C NMR spectrum of 1-(4-Methoxy-benzyl)-2-(4-methoxy-phenyl)-5-methyl-4-phenyl-1H-imidazole (5b) in $CDCl_3$.

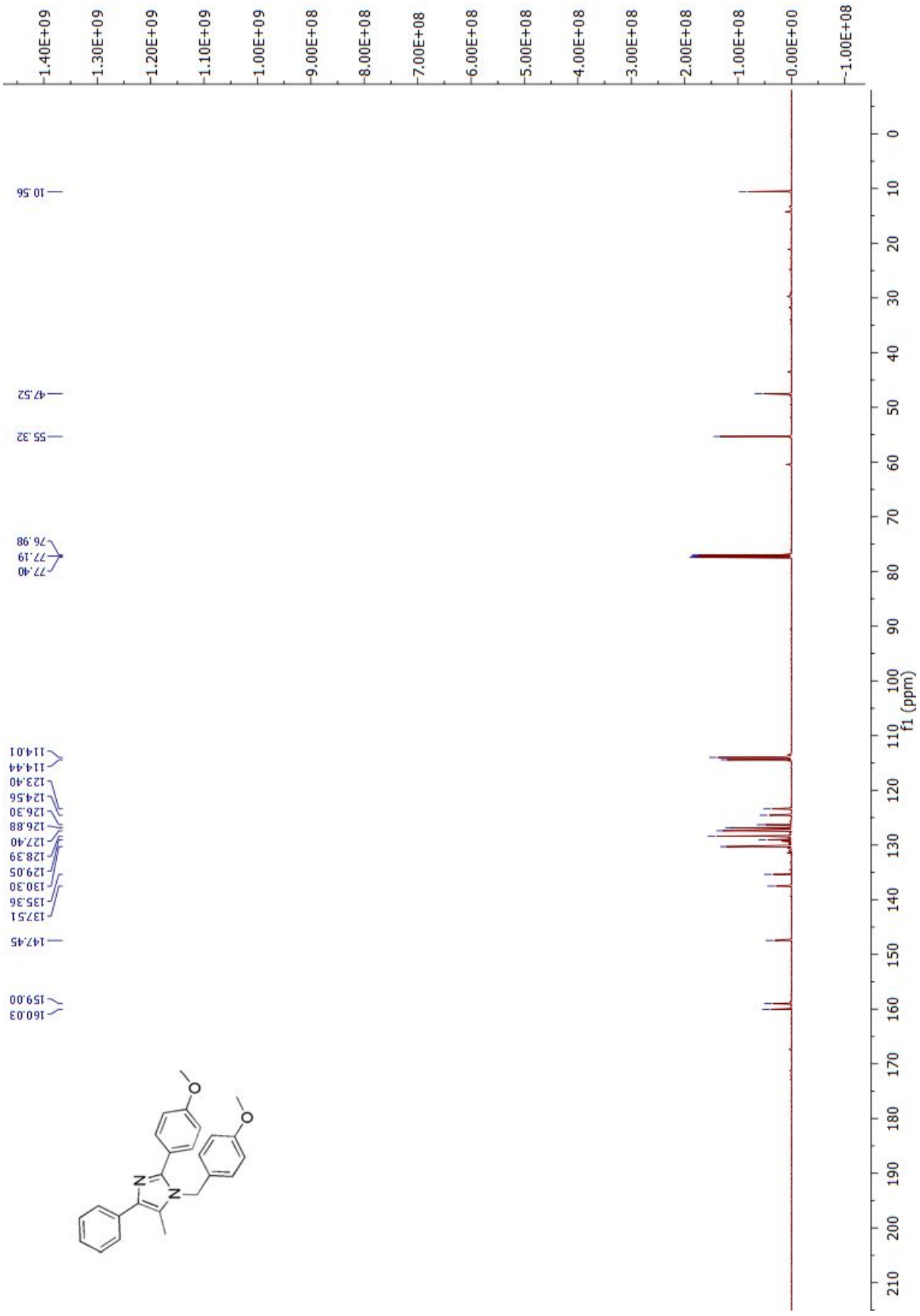


Figure S33: ^{1}H NMR spectrum of 1-Benzyl-4-(2-chloro-phenyl)-5-(3,4-dimethoxy-phenyl)-2-phenyl-1H-imidazole (5c) in DMSO-d_6.

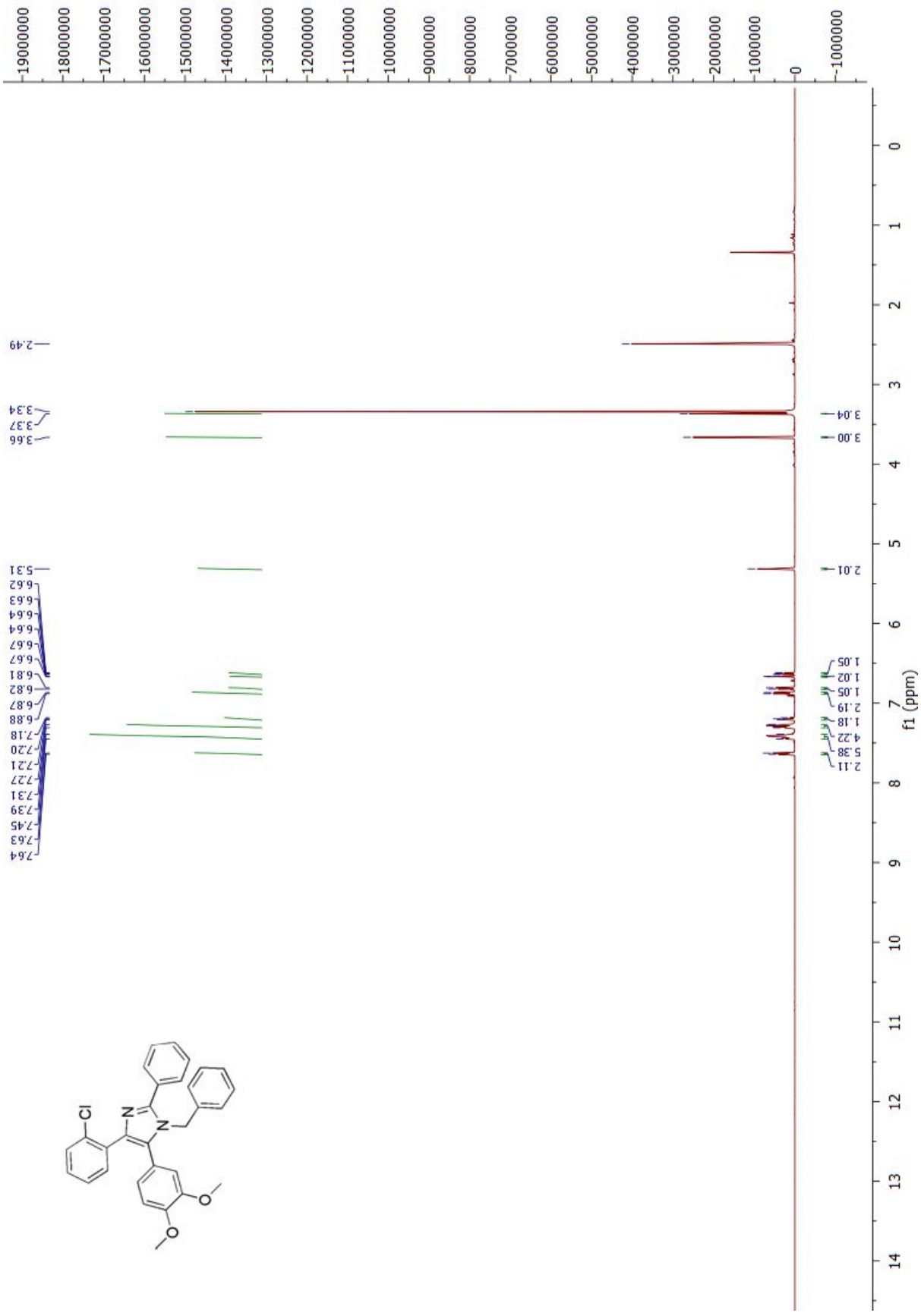


Figure S34: ^{13}C NMR spectrum of 1-Benzyl-4-(2-chloro-phenyl)-5-(3,4-dimethoxy-phenyl)-2-phenyl-1H-imidazole (5c) in DMSO-d_6.

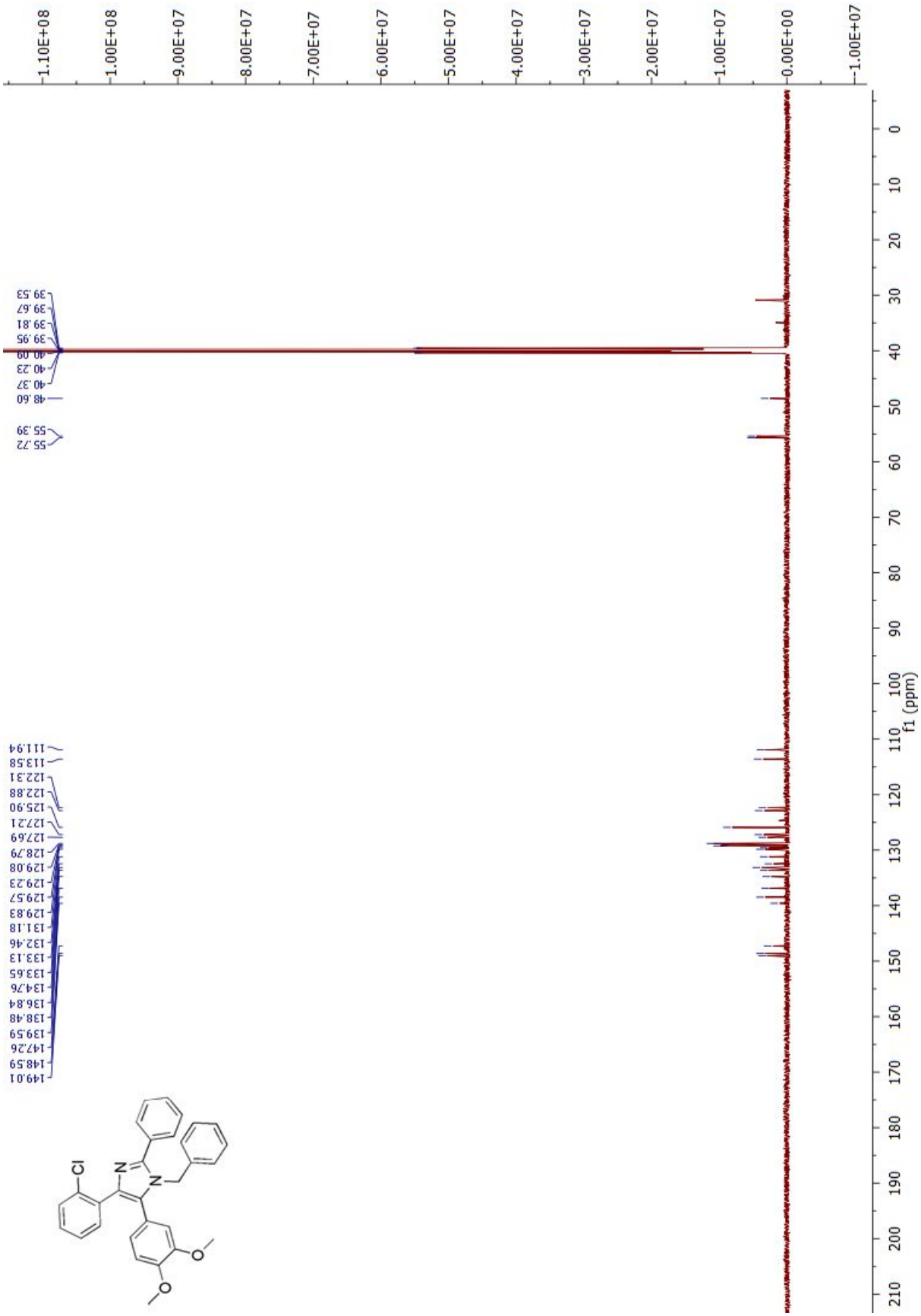


Figure S35: ^{1}H NMR spectrum of 2-(4-(2-chlorophenyl)-5-(3,4-dimethoxyphenyl)-1-(pyridin-2-ylmethyl)-1H-imidazol-2-yl)pyridine (5d) in DMSO-d_6.

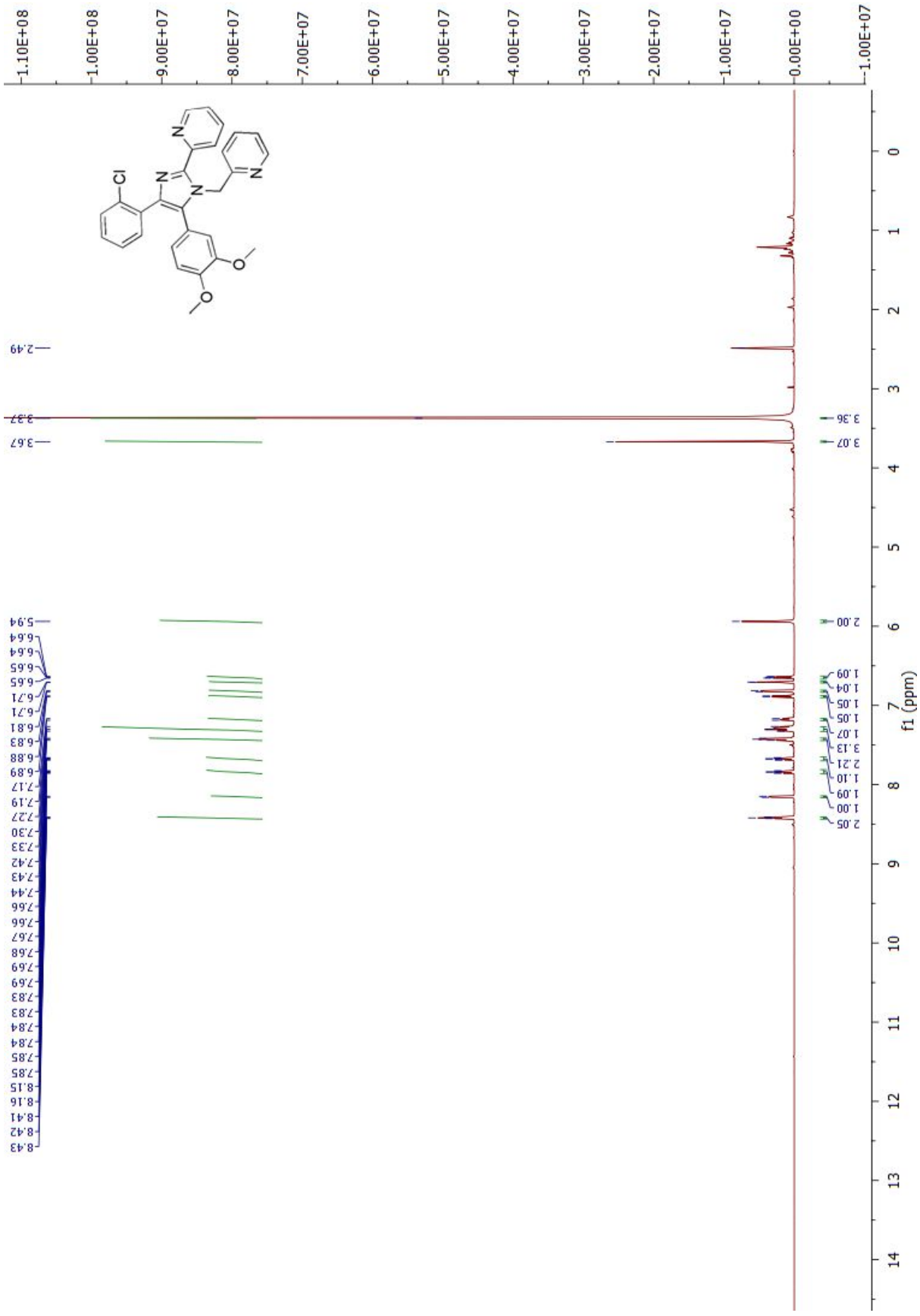


Figure S36: ^{13}C NMR spectrum of 2-(4-(2-chlorophenyl)-5-(3,4-dimethoxyphenyl)-1-(pyridin-2-ylmethyl)-1H-imidazol-2-yl)pyridine (5d) in DMSO-d_6.

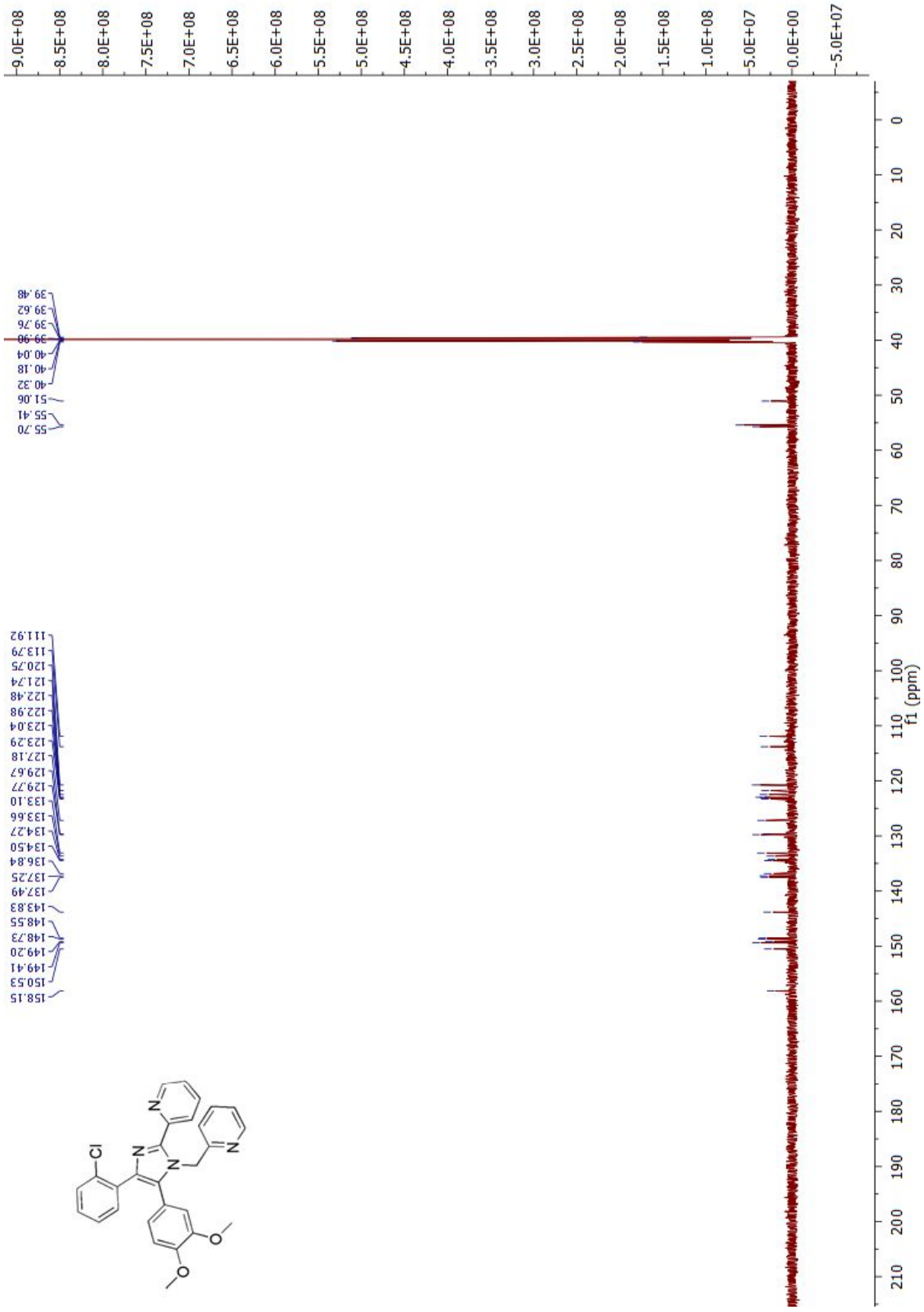


Figure S37: ^{1}H NMR spectrum of 2,4,5-Triphenyl-1H-imidazole (8a) in DMSO-d_6.

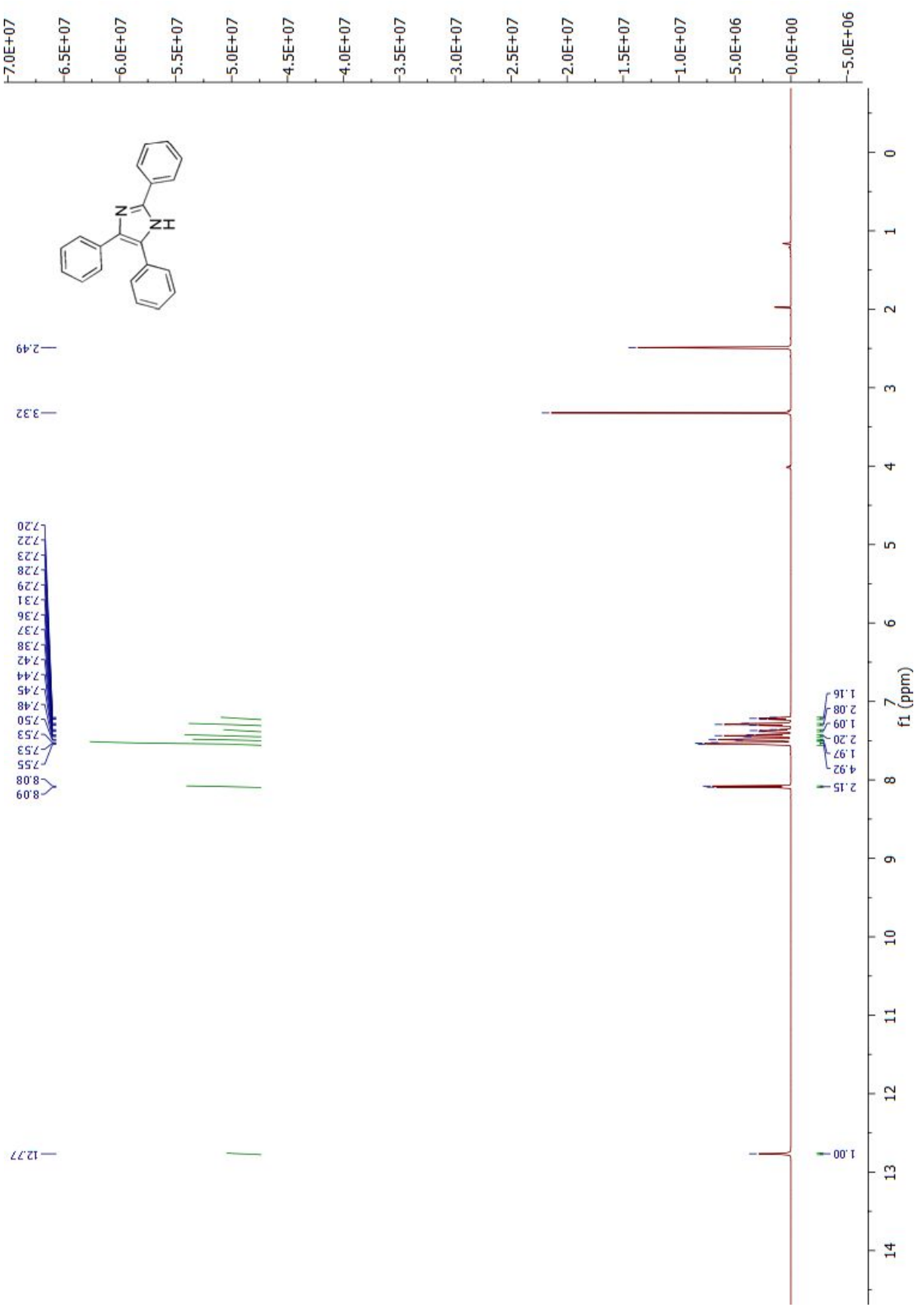


Figure S38: ^{13}C NMR spectrum of 2,4,5-Triphenyl-1H-imidazole(8a) in DMSO-d_6.

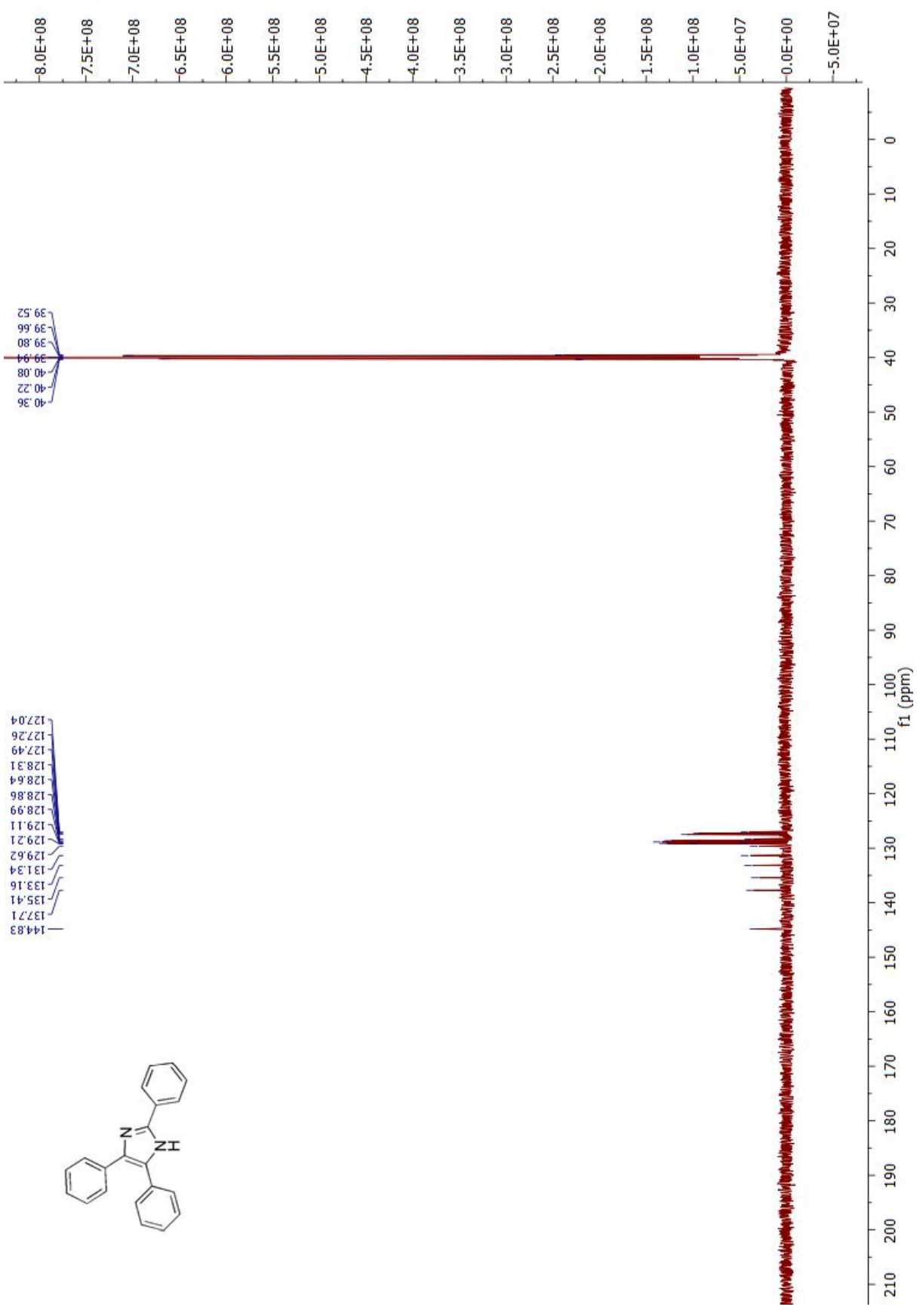


Figure S39: ^{1}H NMR spectrum of 2-(4-Chloro-phenyl)-4,5-diphenyl-1H-imidazole (8b) in DMSO-d_6.

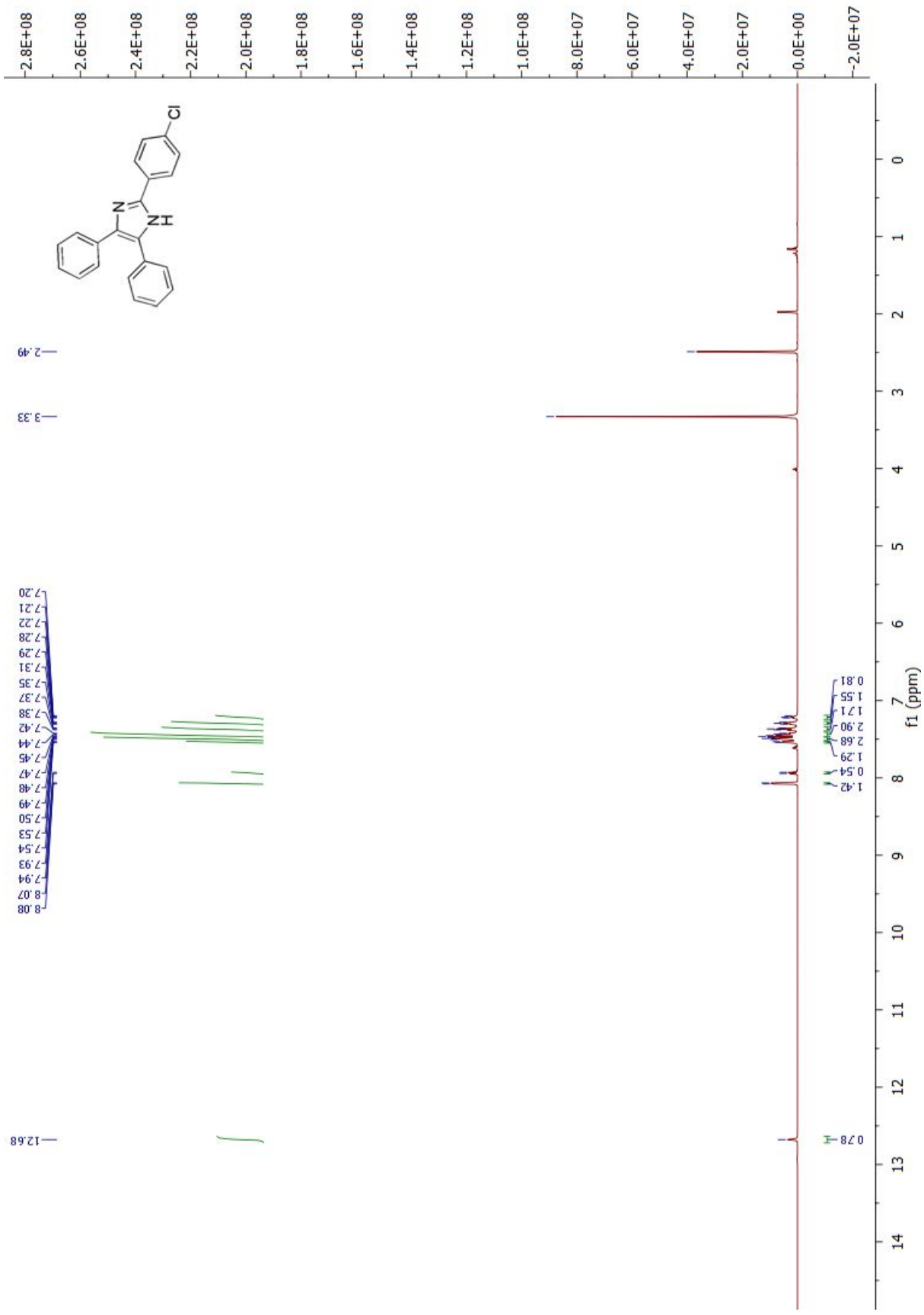


Figure S40: ^{13}C NMR spectrum of 2-(4-Chloro-phenyl)-4,5-diphenyl-1H-imidazole (8b) in DMSO-d_6.

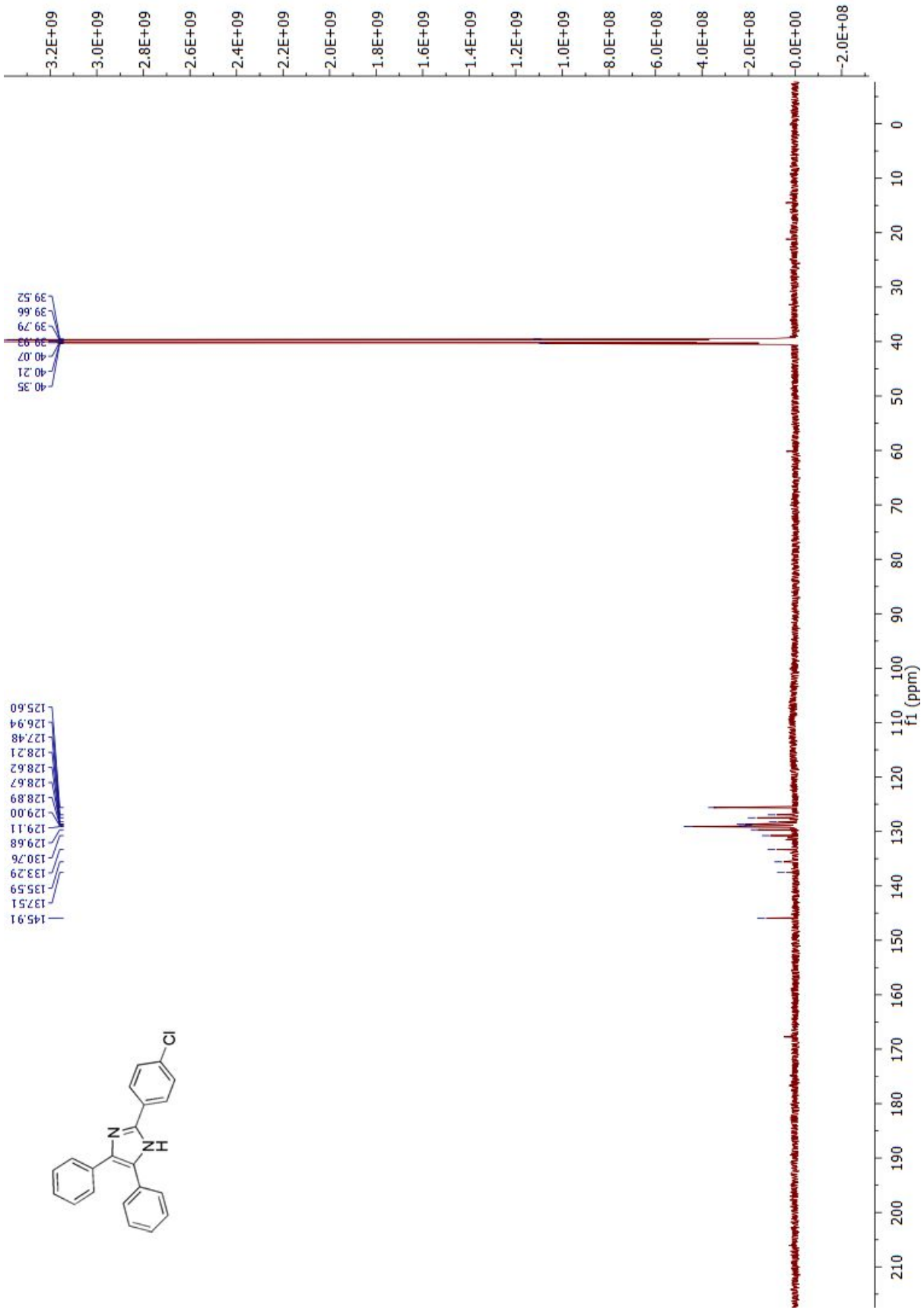


Figure S41: ^{1}H NMR spectrum of 2-(4,5-Diphenyl-1H-imidazol-2-yl)-phenol (8c) in DMSO-d_6.

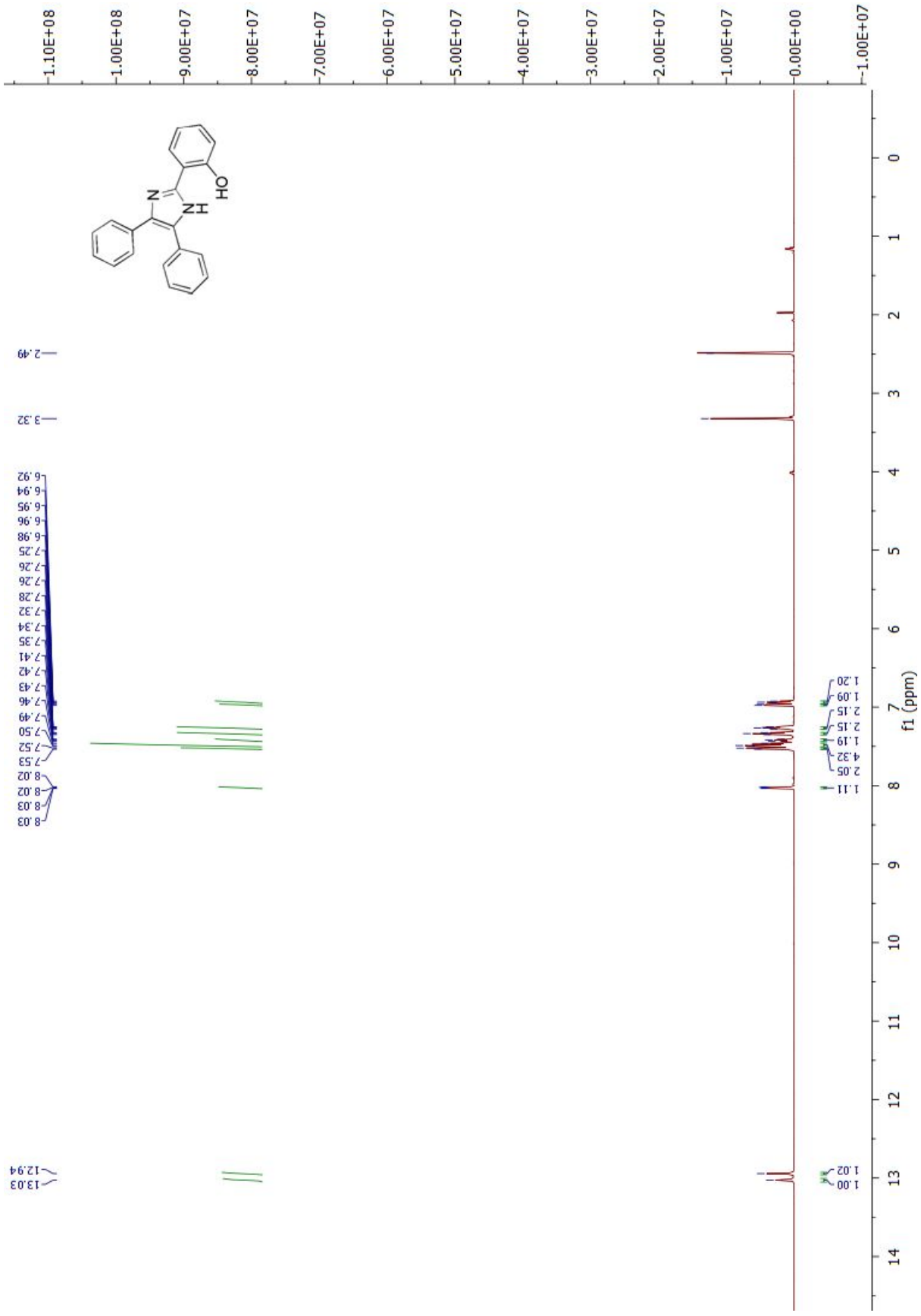


Figure S42: ^{13}C NMR spectrum of 2-(4,5-Diphenyl-1H-imidazol-2-yl)-phenol (8c) in DMSO-d_6:

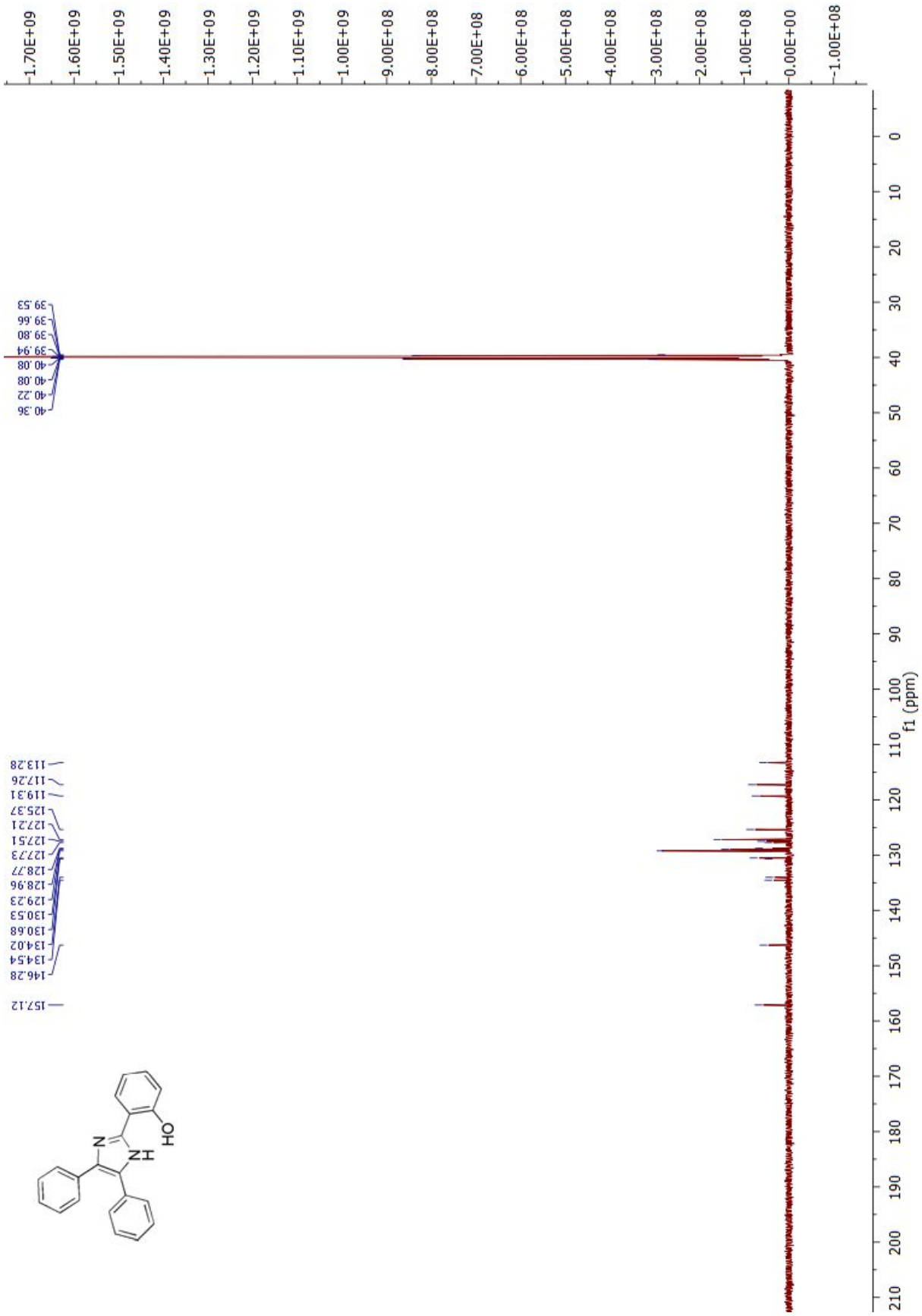


Figure S43: ^{1}H NMR spectrum of 4,5-Diphenyl-2-thiophen-2-yl-1H-imidazole (8d) in DMSO-d_6.

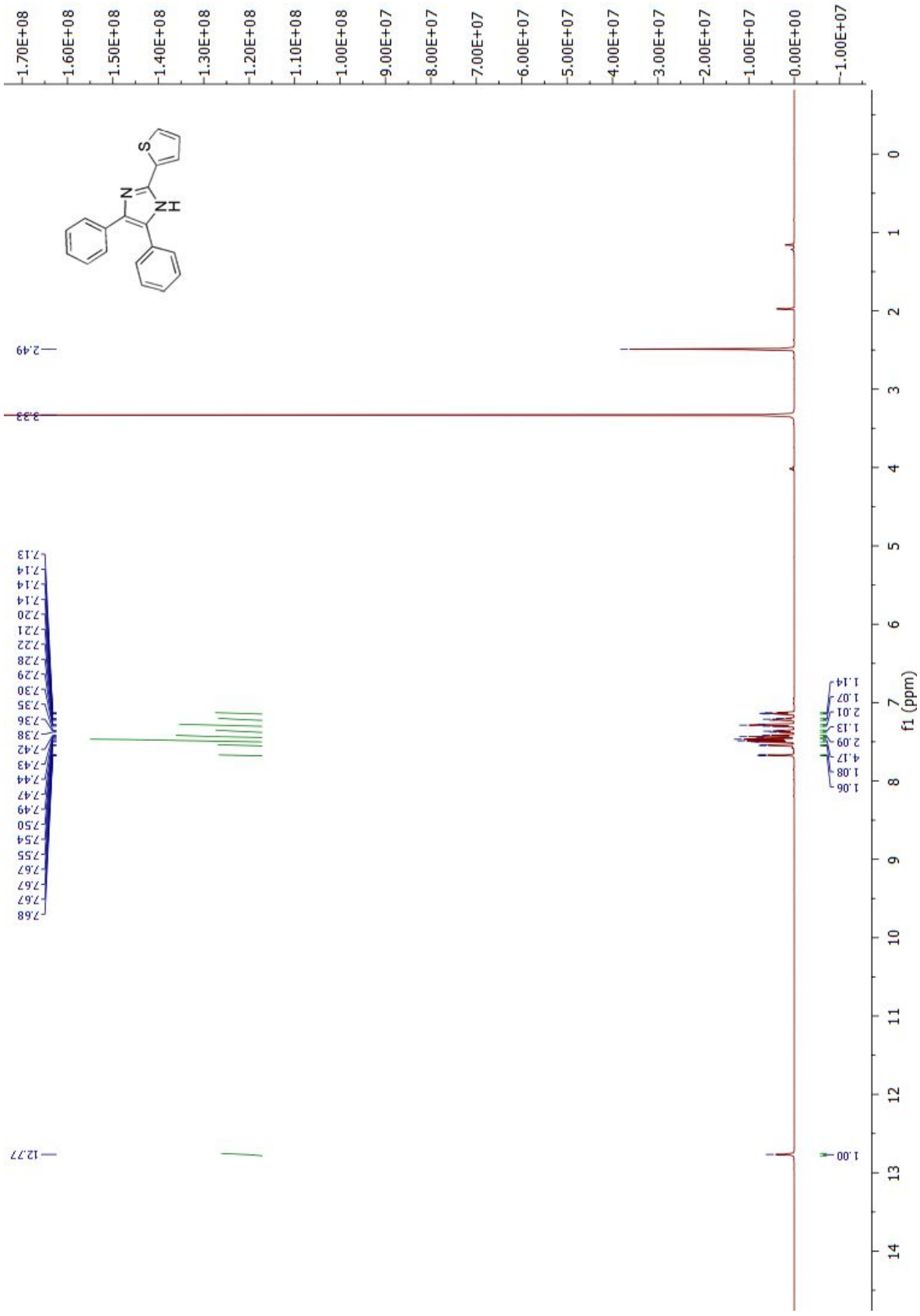


Figure S44: ^{13}C NMR spectrum of 4,5-Diphenyl-2-thiophen-2-yl-1H-imidazole (8d) in DMSO-d_6.

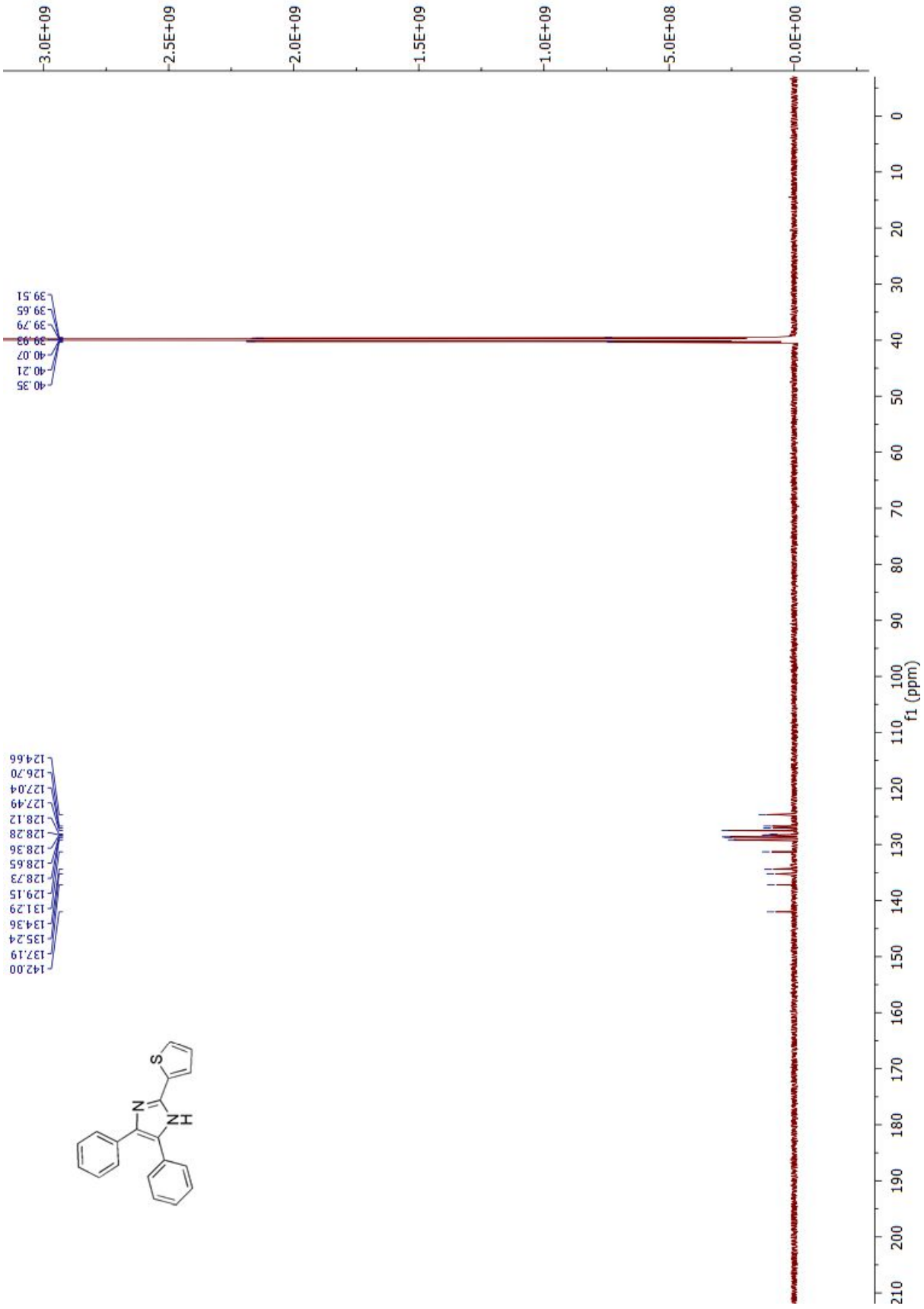


Figure S45: ^{1}H NMR spectrum of 2-(4,5-Diphenyl-1H-imidazol-2-yl)-pyridine (8e) in DMSO-d_6.

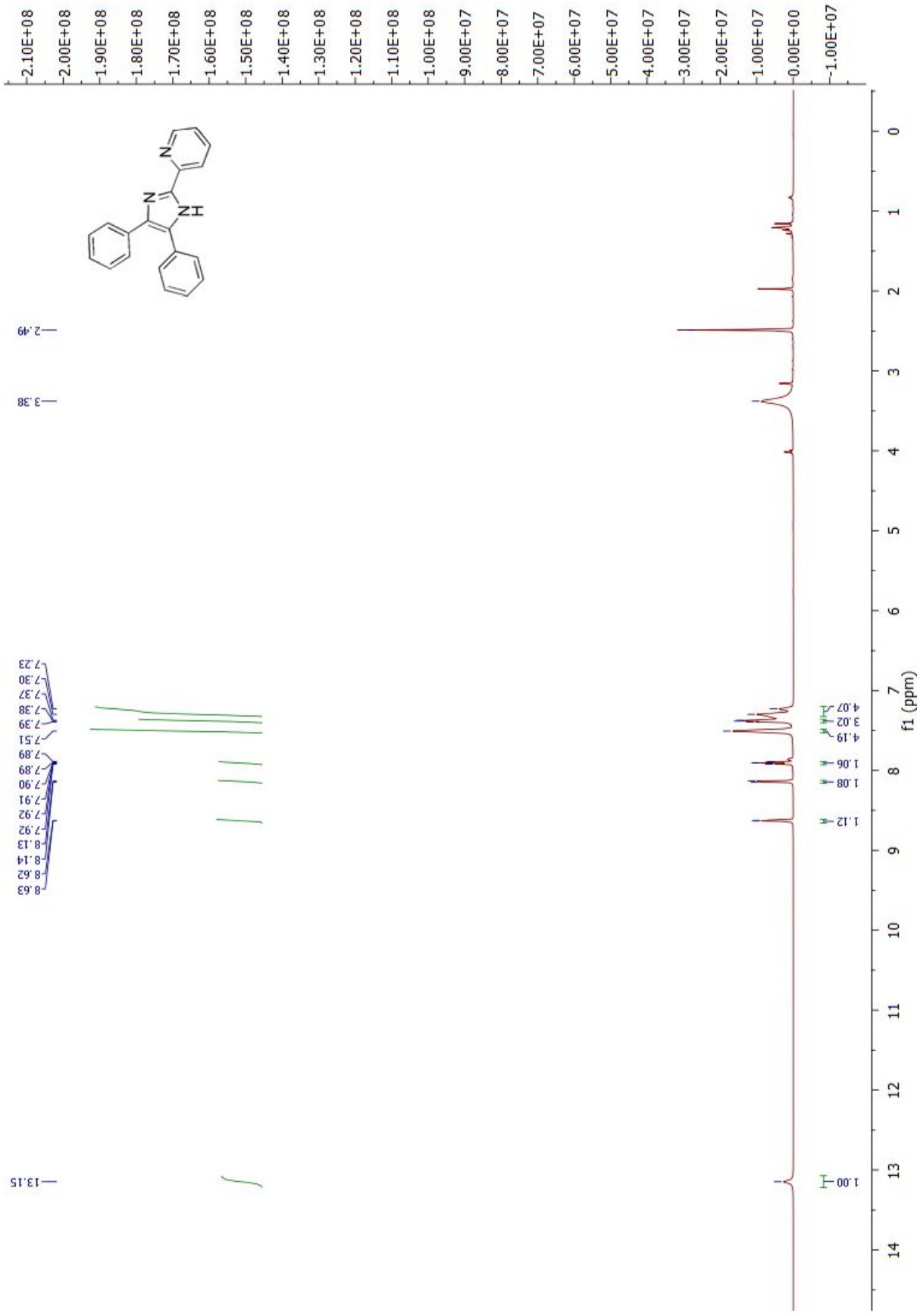


Figure S46: ^{13}C NMR spectrum of 2-(4,5-Diphenyl-1H-imidazol-2-yl)-pyridine (8e) in DMSO-d_6.

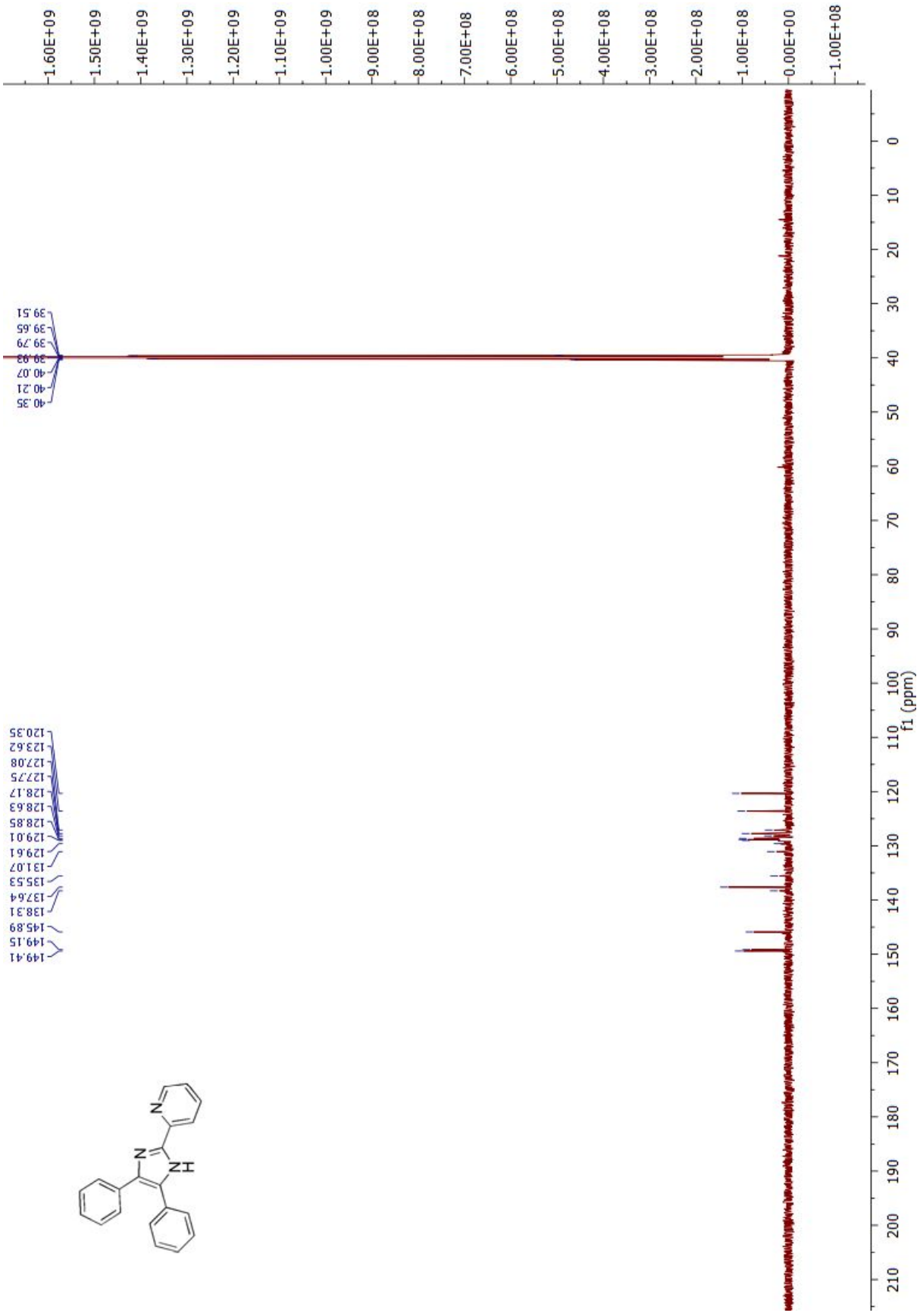


Figure S47: ^{1}H NMR spectrum of [4-(4,5-Diphenyl-1H-imidazol-2-yl)-phenyl]-dimethyl-amine (8f) in DMSO-d_6.

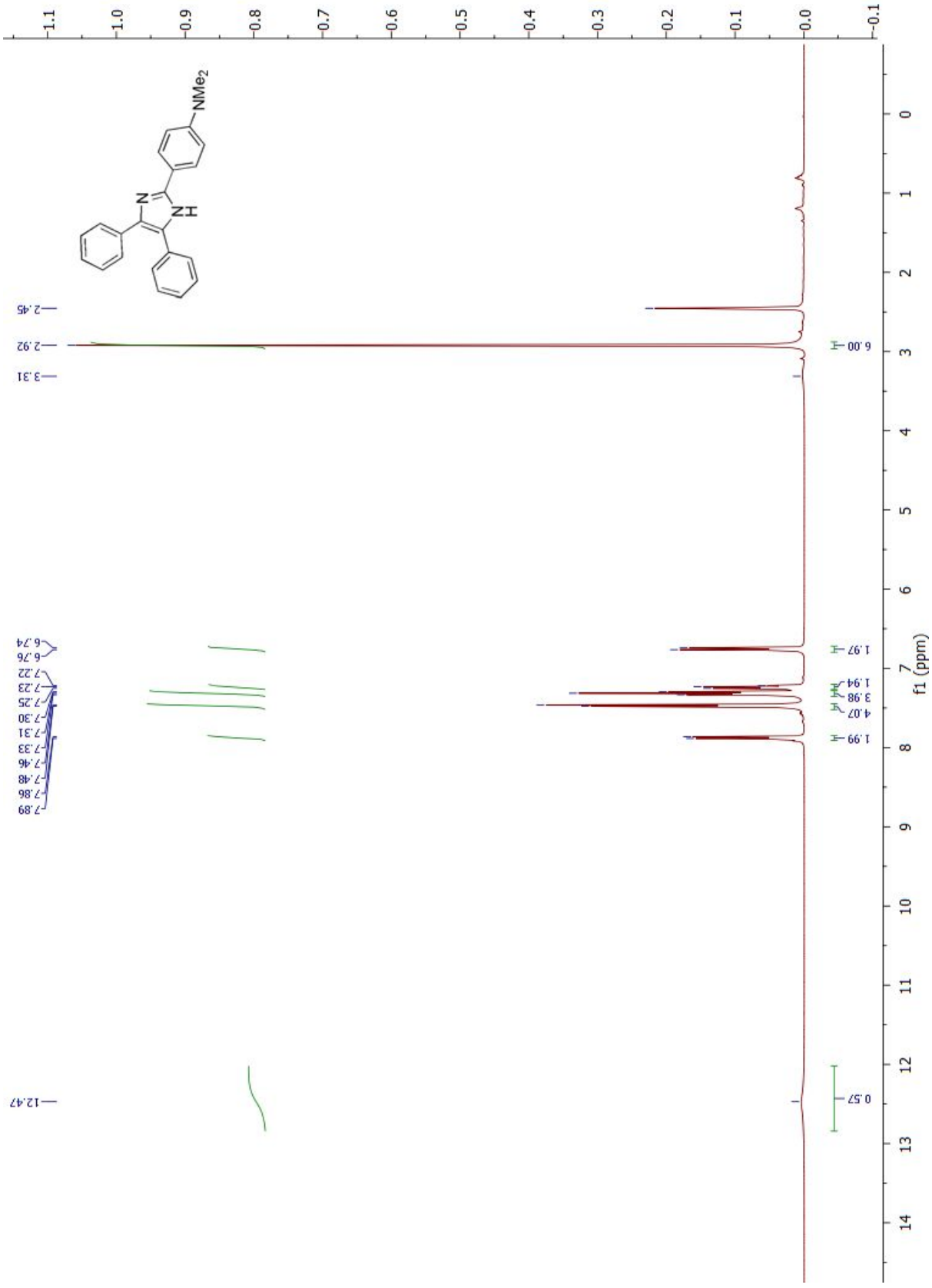


Figure S48: ^{13}C NMR spectrum of [4-(4,5-Diphenyl-1H-imidazol-2-yl)-phenyl]-dimethyl-amine (8f) in DMSO-d_6.

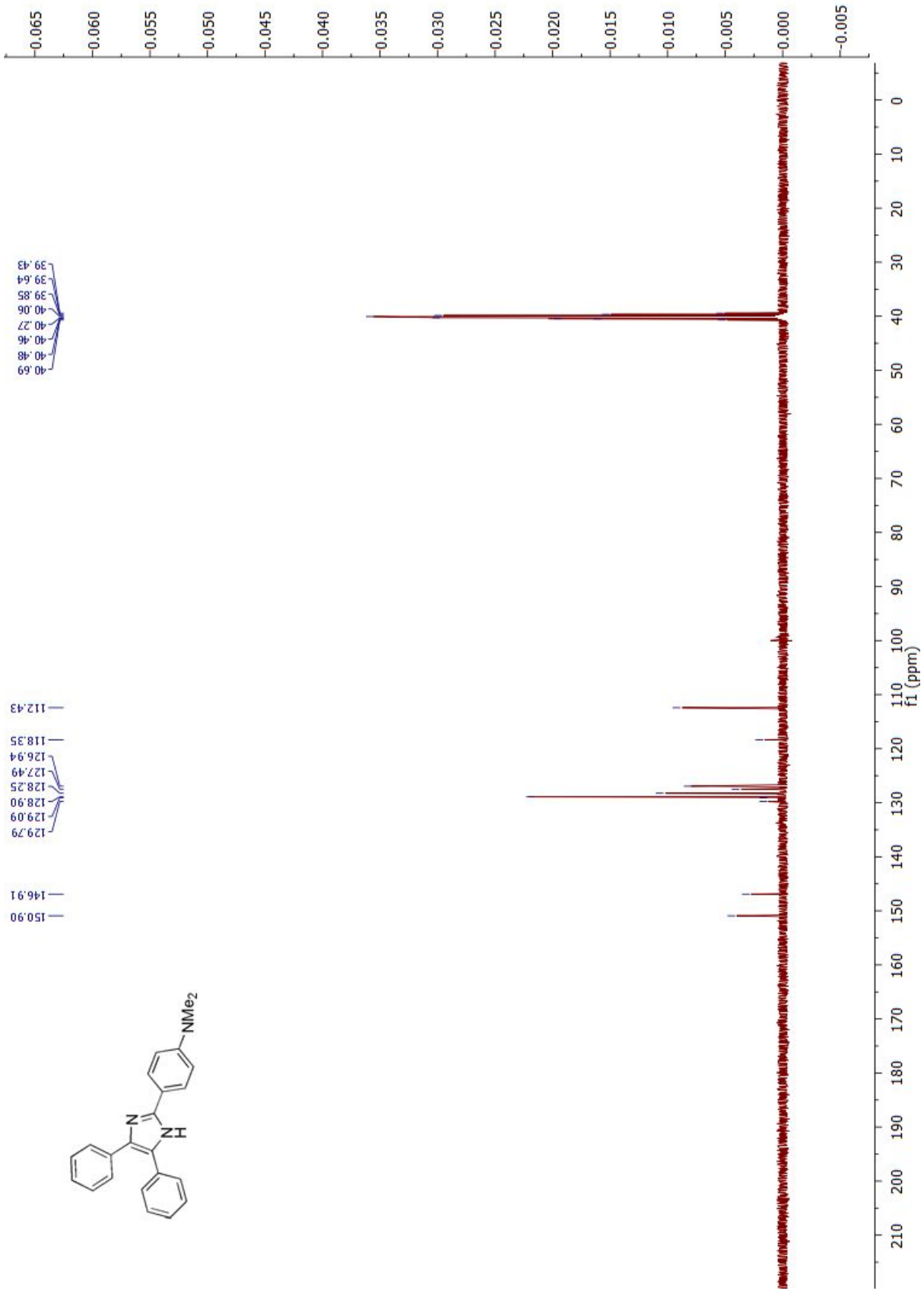


Figure S49: ^{1}H NMR spectrum of 2-[4,5-Bis-(4-methoxy-phenyl)-1H-imidazol-2-yl]-pyridine (8g) in DMSO-d_6.

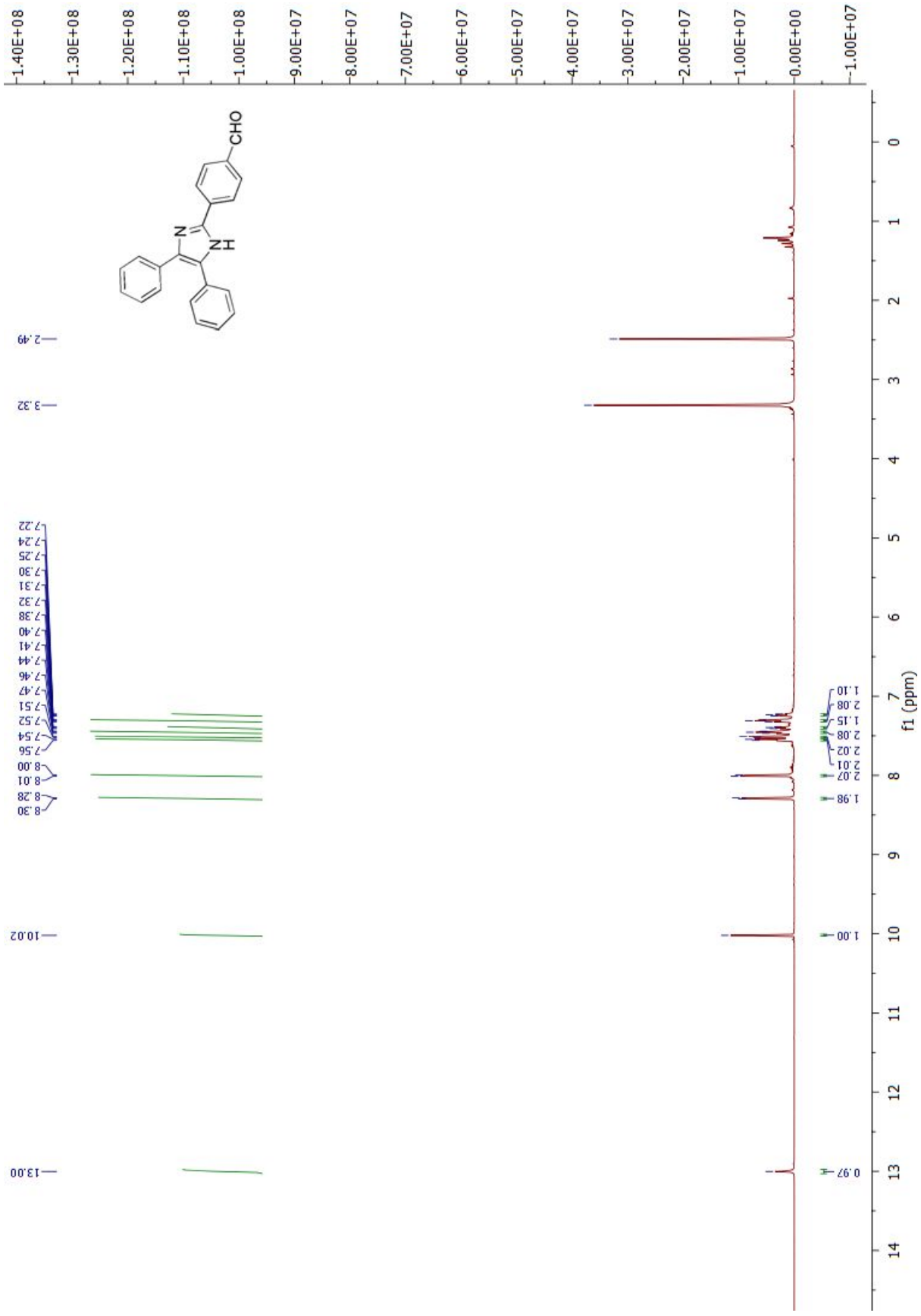


Figure S50: ^{13}C NMR spectrum of 2-[4,5-Bis-(4-methoxy-phenyl)-1H-imidazol-2-yl]-pyridine (8g) in DMSO-d_6.

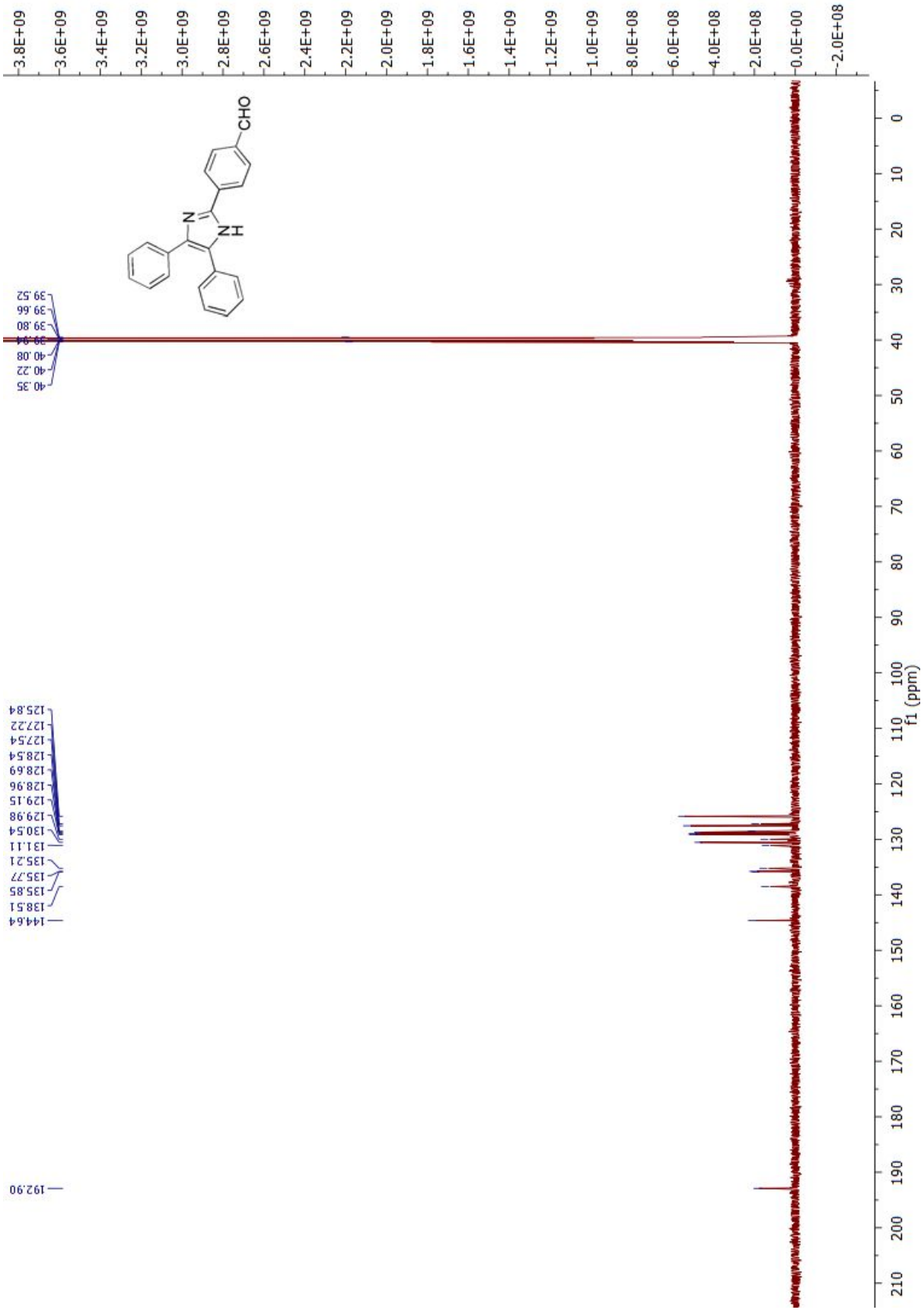


Figure S51: ^{1}H NMR spectrum of 2-[4,5-Bis-(4-methoxy-phenyl)-1H-imidazol-2-yl]-pyridine (8h) in DMSO-d_6.

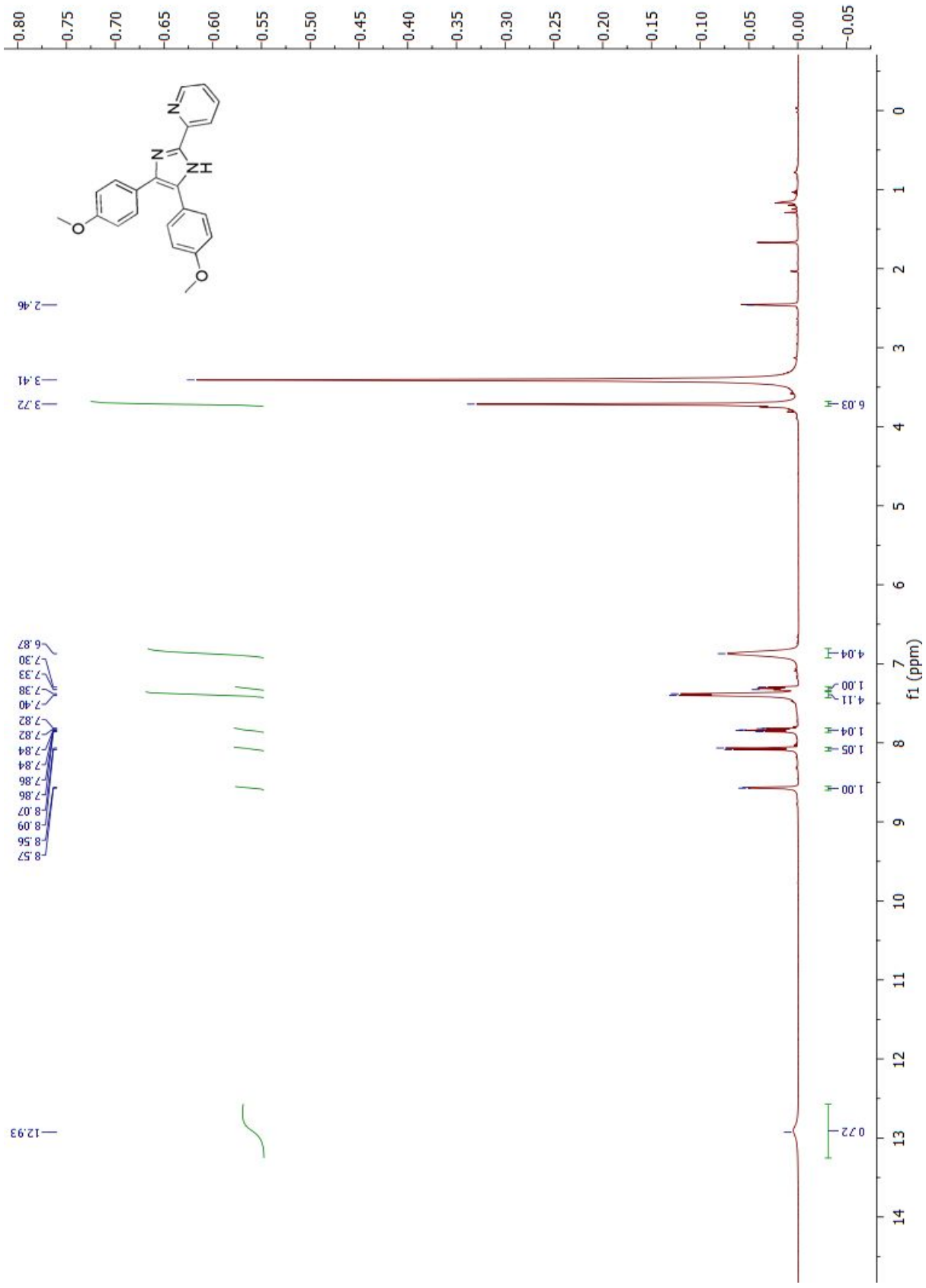


Figure S52: ^{13}C NMR spectrum of 2-[4,5-Bis-(4-methoxy-phenyl)-1H-imidazol-2-yl]-pyridine (8h) in DMSO-d_6.

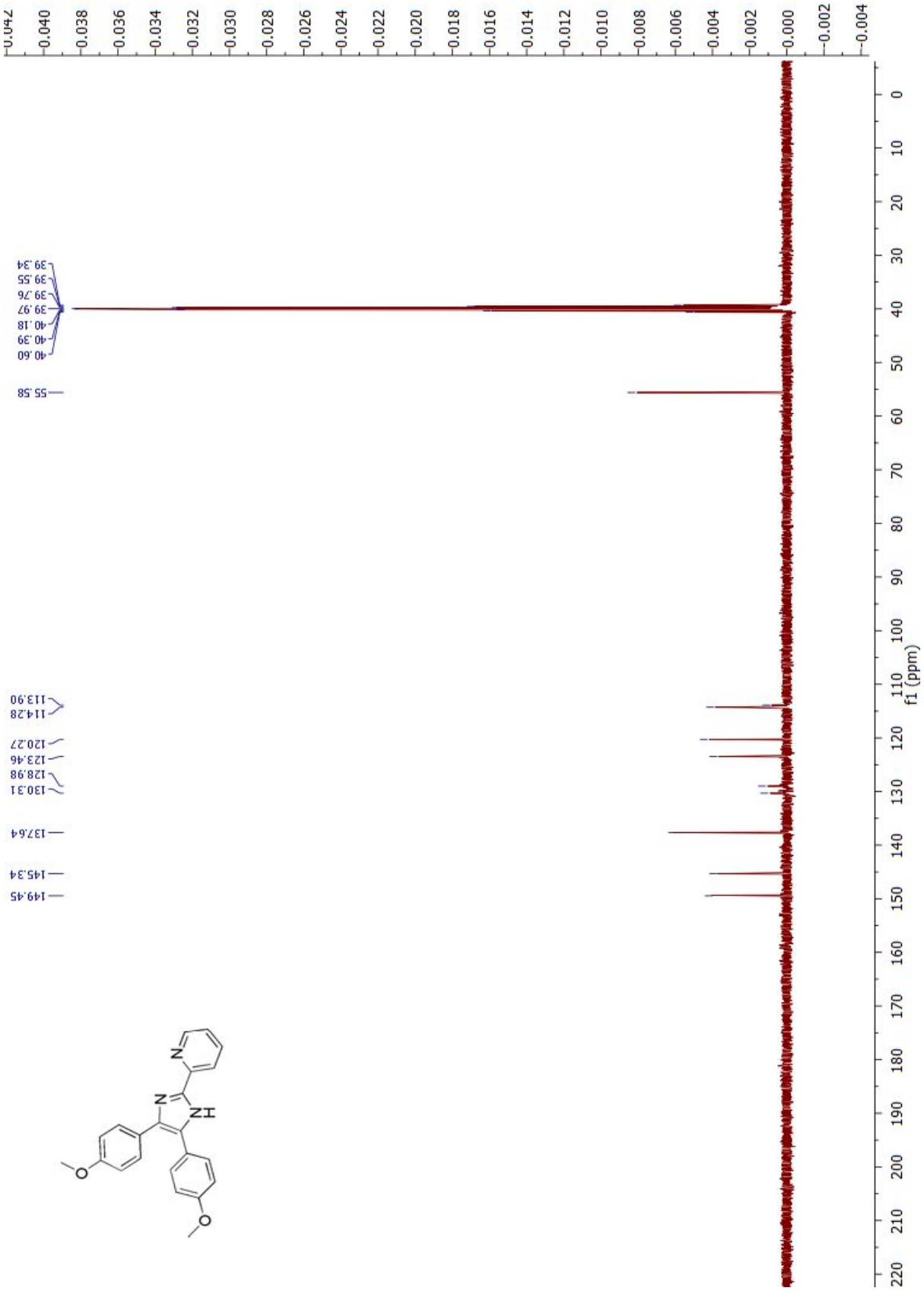


Figure S53: ^{1}H NMR spectrum of 1-(4-Bromo-phenyl)-2-(4-chloro-phenyl)-4,5-diphenyl-1H-imidazole (10a) in DMSO-d_6.

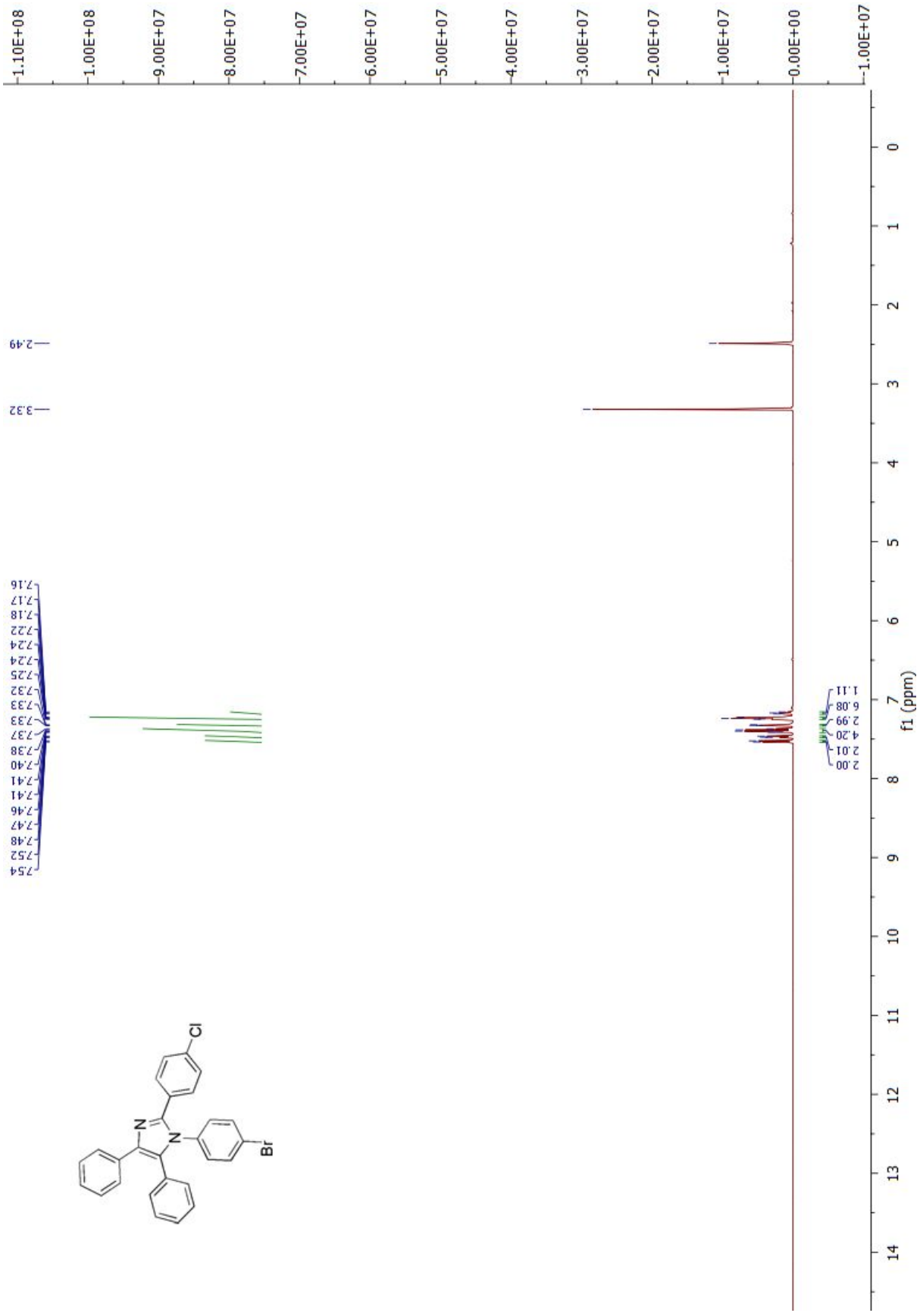


Figure S54: ^{13}C NMR spectrum of 1-(4-Bromo-phenyl)-2-(4-chloro-phenyl)-4,5-diphenyl-1H-imidazole (10a) in DMSO-d_6.

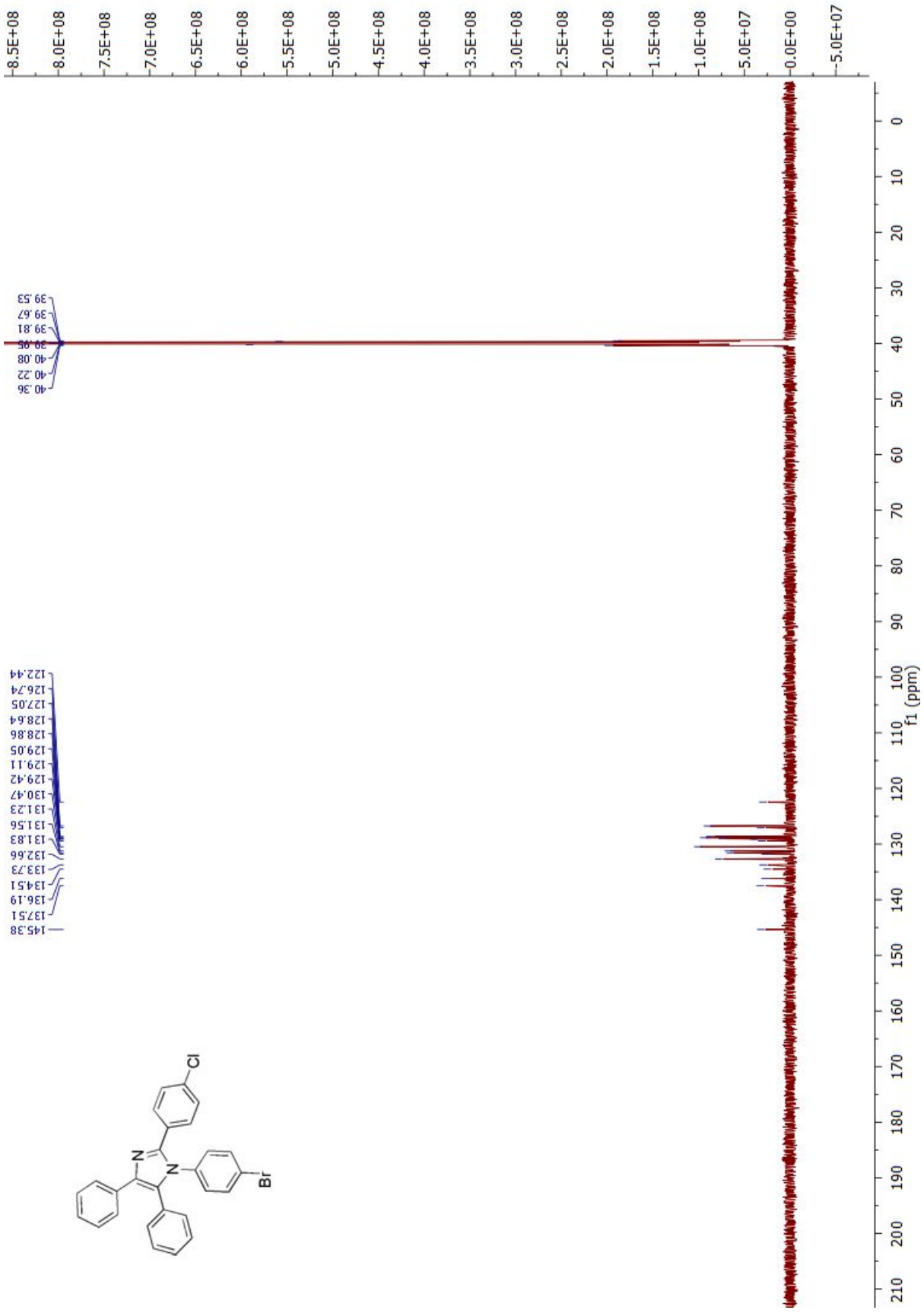


Figure S55: ^{1}H NMR spectrum of 1,2-bis(4-methoxyphenyl)ethane-1,2-dione (1c) in $CDCl_3$.

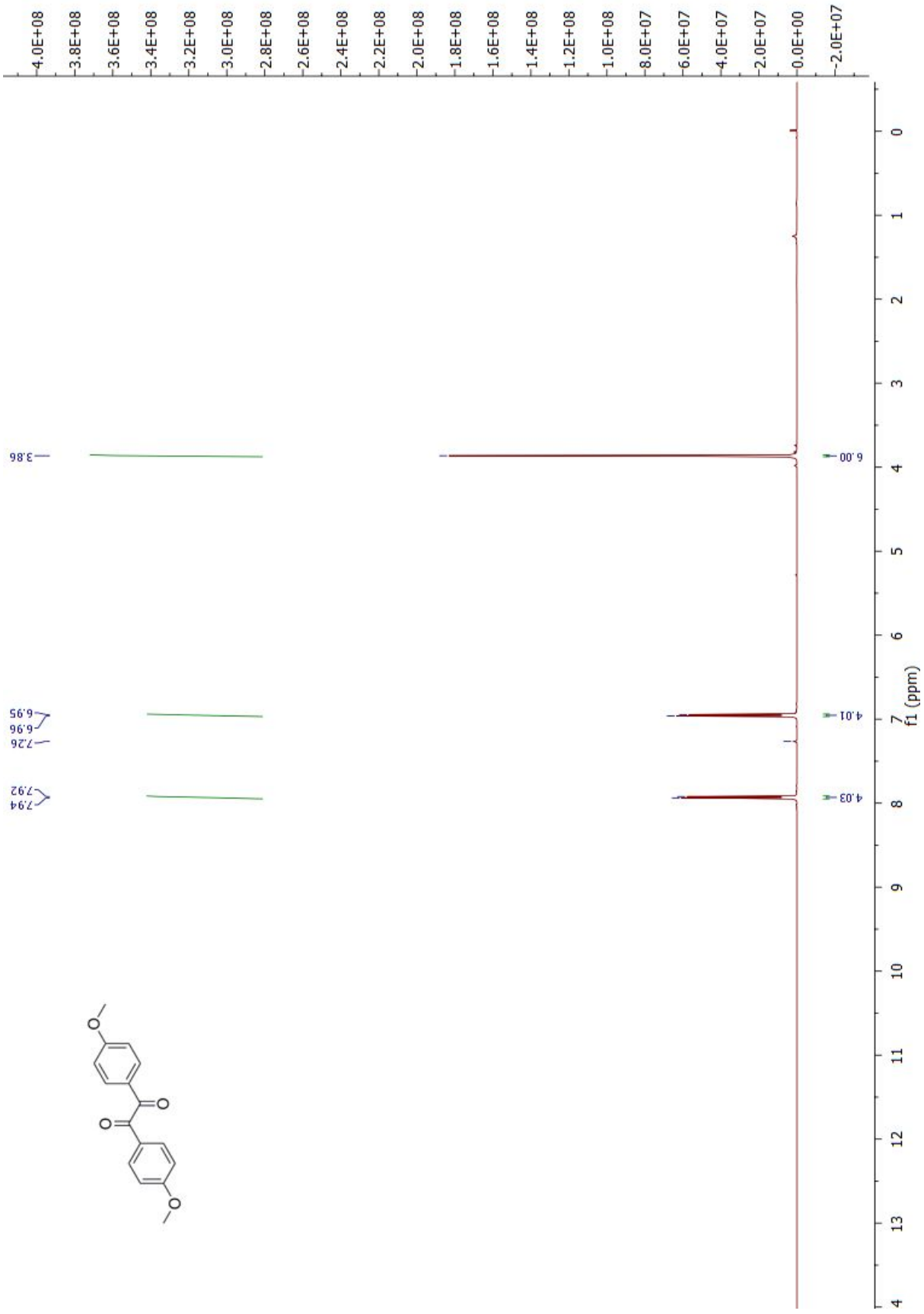


Figure S56: ^{13}C NMR spectrum of 1,2-bis(4-methoxyphenyl)ethane-1,2-dione (1c) in $CDCl_3$.

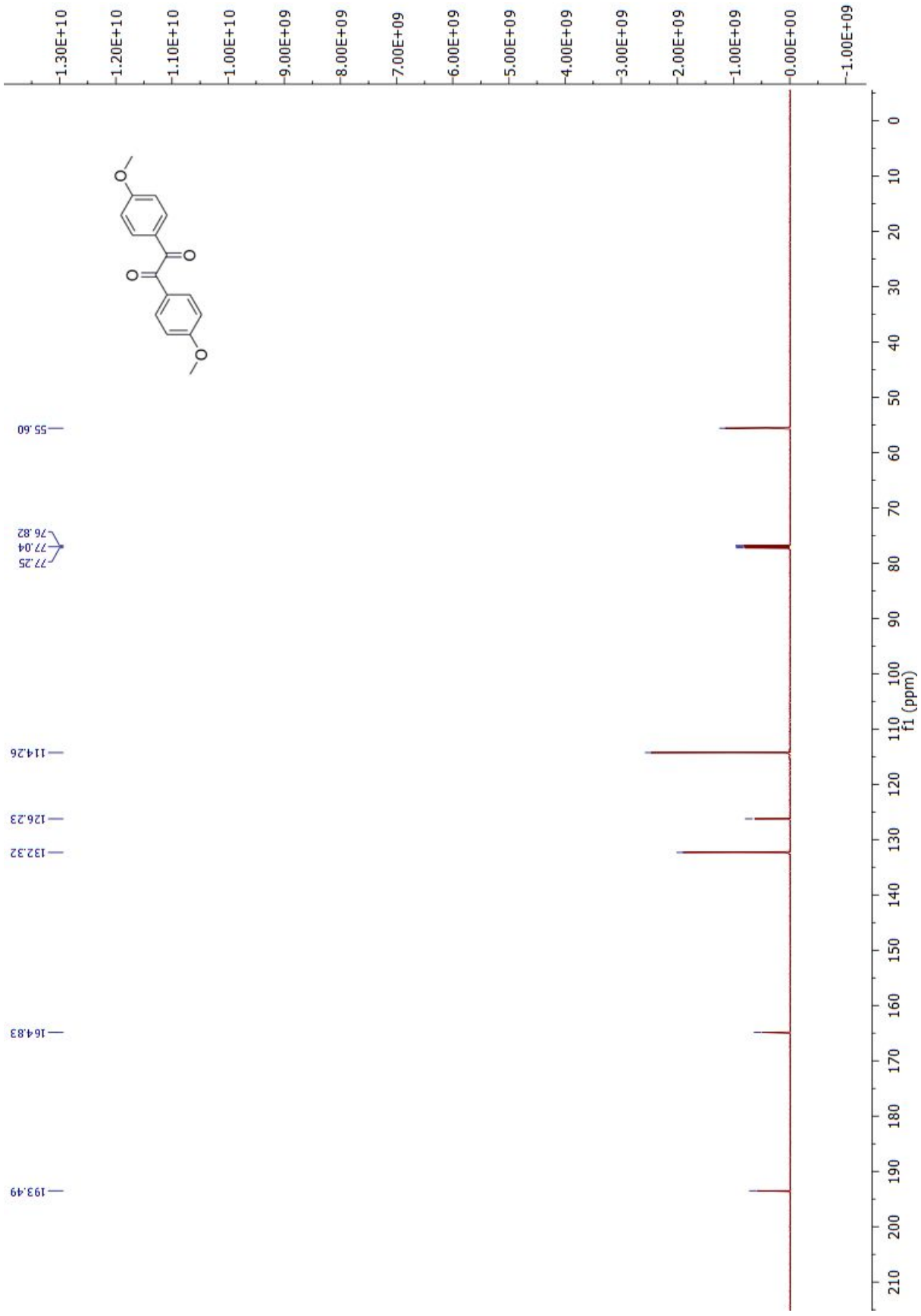


Figure S57: ^{1}H NMR spectrum of Benzyl-[2-benzylimino-1,2-bis-(4-methoxy-phenyl)-ethylidene]-amine (A) in $CDCl_3$.

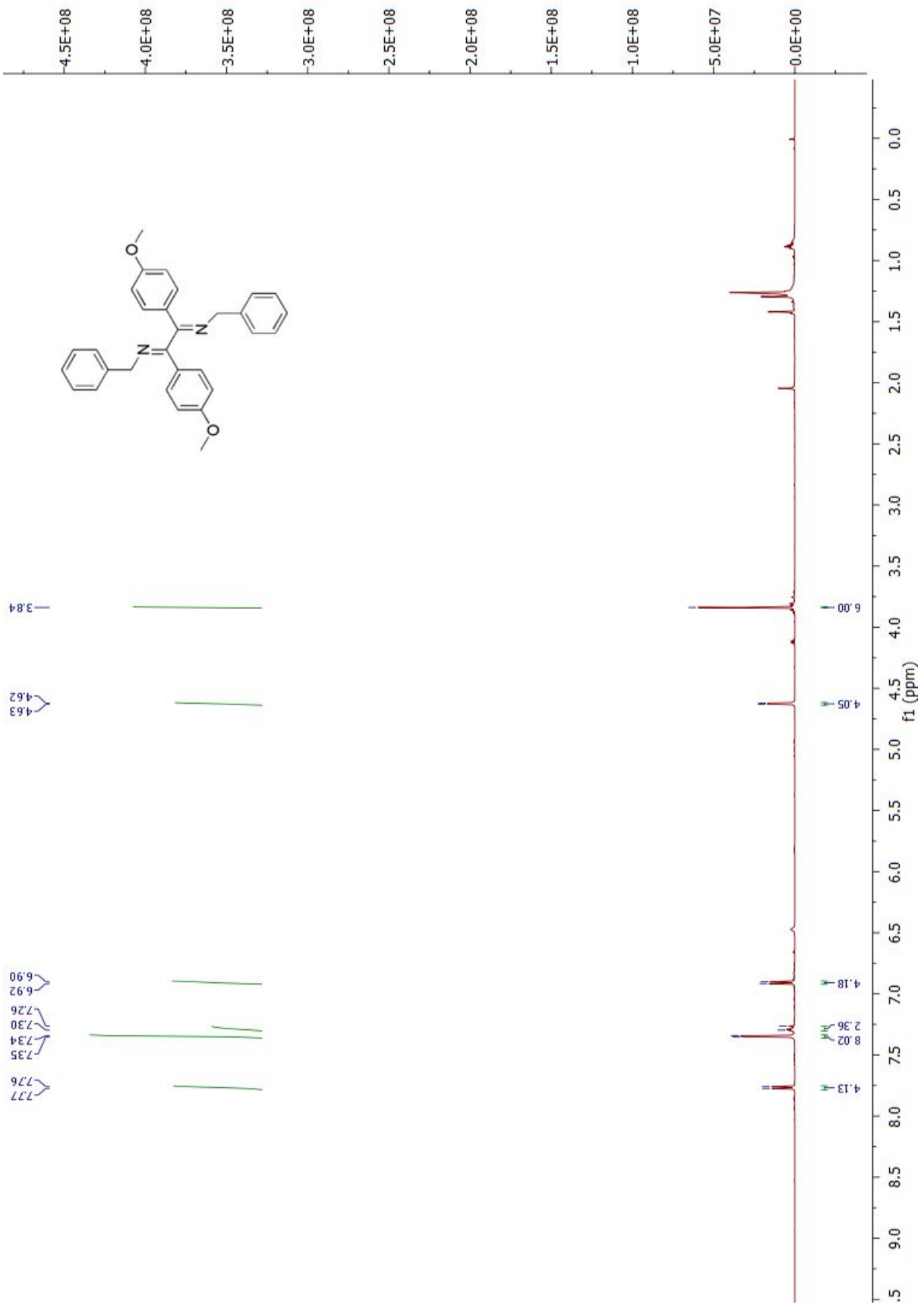
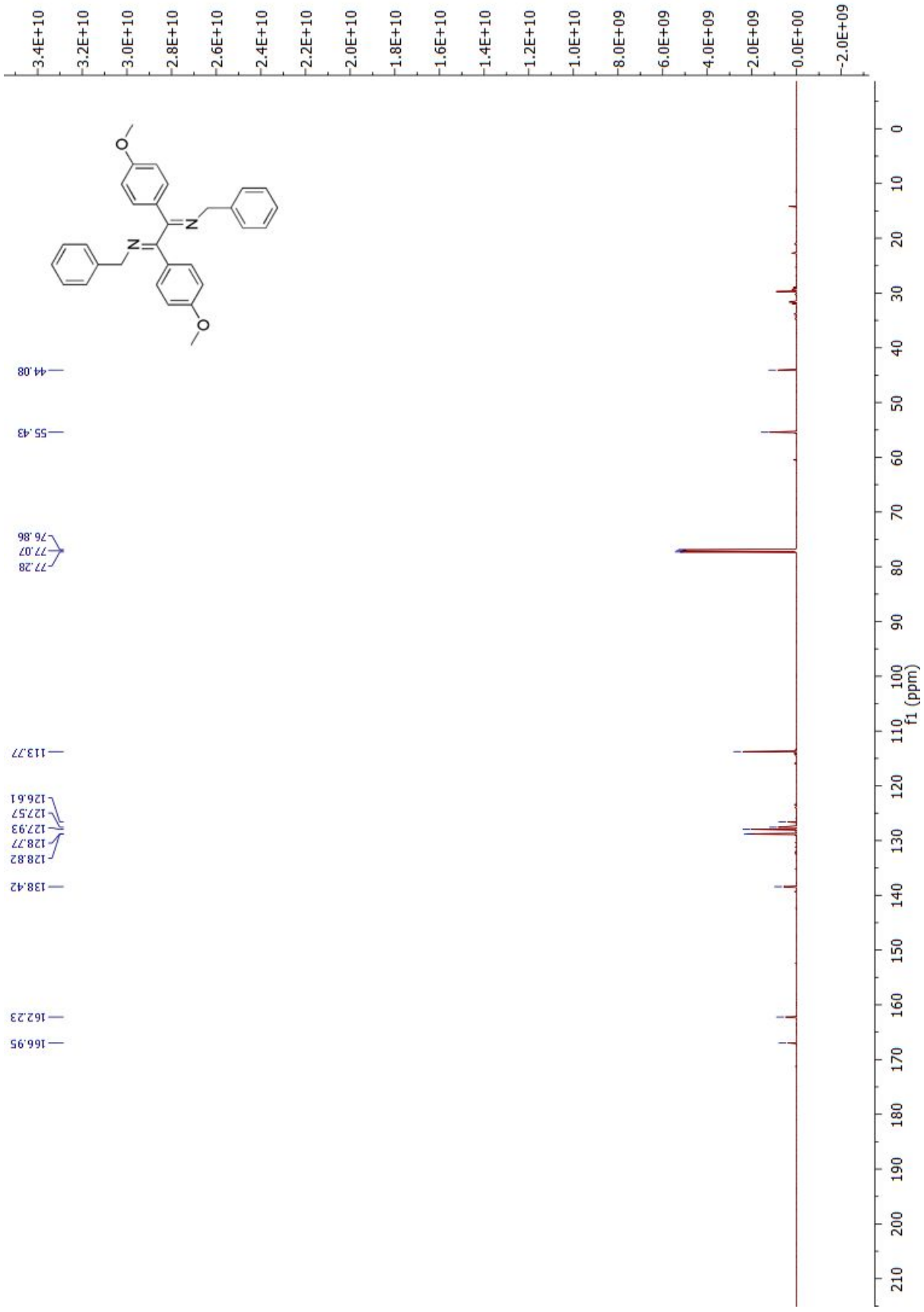


Figure S58: ^{13}C NMR spectrum of Benzyl-[2-benzylimino-1,2-bis-(4-methoxy-phenyl)-ethylidene]-amine (A) in $CDCl_3$.



X-ray Diffraction Analysis of Compound 3l :

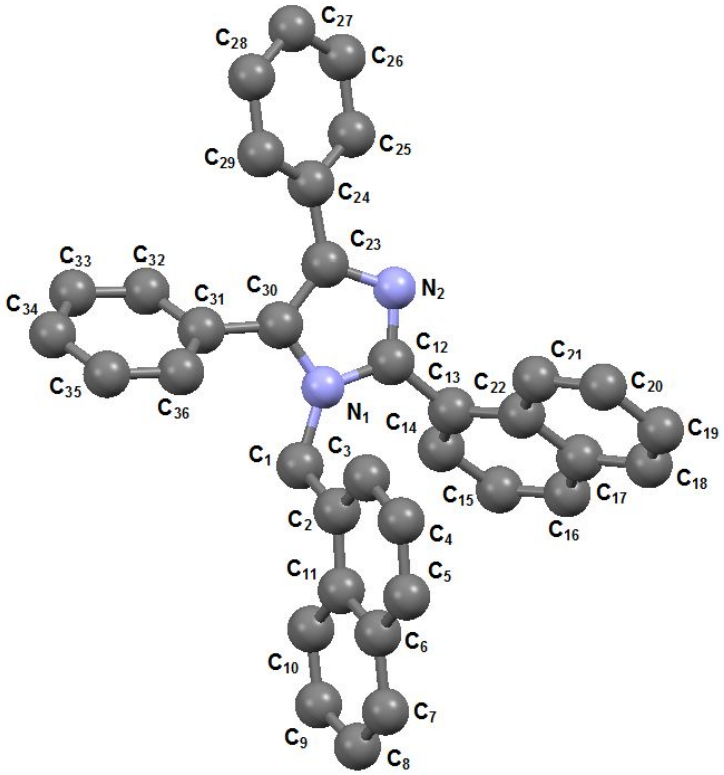


Figure S59. ORTEP diagram (ball and stick plot) of product **3l** (drawn at 50% probability level) and hydrogens are omitted for clarity. Colour code: nitrogen in blue and carbon in grey.

X-Ray Crystallographic Information of Product 3l:

The Single crystal of imidazole derivative **3l** was acquired by slow evaporation of petroleum ether at room temperature. The entire diffraction data of compound **3l** was measured with MoKα radiation (λ = 1.54178 Å) at 100 K. The structure of the single crystal of imidazole derivative **3l** was solved by using the SHELXS-97 program.[1] Refinements were carried out by full matrix least-squares process against F using SHELXL-97.2 and the non-hydrogen atoms were refined with anisotropic thermal parameters.[2] All the hydrogen atoms in the crystal structure (**3l**) were included in geometric positions and given thermal parameters equivalent to 1.2 times those of the atom to which they were attached. All the essential crystal data of the imidazole derivative **3l** is given below:

Table S1: Important crystal data of product **3l.**	
Empirical Formula	$C_{36}H_{26}N_2$
Formula weight	486.59
Temperature	100 K
Wave length	1.54178
Crystal system	Monoclinic
Space group	P 1 21/c 1
Unit cell dimensions	a = 9.9474(3) Å α = 90 b = 14.0292(4) Å β = 91.9680(10) c = 18.0762(6) Å γ = 90
Volume	2521.12(13) $Å^3$
Z	4
Density (calculated)	1.282 g/cm^3
Absorption coefficient (Mu)	0.571mm^{-1}
F(000)	1024
Theta range for data collection	5.826° to 66.630°
Index ranges	$-11 \leq h \leq 10$, $-16 \leq k \leq 16$, $-21 \leq l \leq 21$
Reflection collected	35722
Independent reflection	4337 [R_{int} = 0.0379, R_{sigma} = 0.0261]
Absorption correction	multi-scan
Data/restraints/parameters	4337/0/343
Good of fit on (F^2)	1.054
Final R indices [I>=2σ (I)]	R_1 = 0.0355, wR_2 = 0.0888
R indices (all data)	R_1 = 0.0364, wR_2 = 0.0896

The crystal data of product 3l was deposited at the Cambridge Crystallographic Data Centre. The CCDC reference number is 1948135.

X-ray Diffraction Analysis of Product 5a:

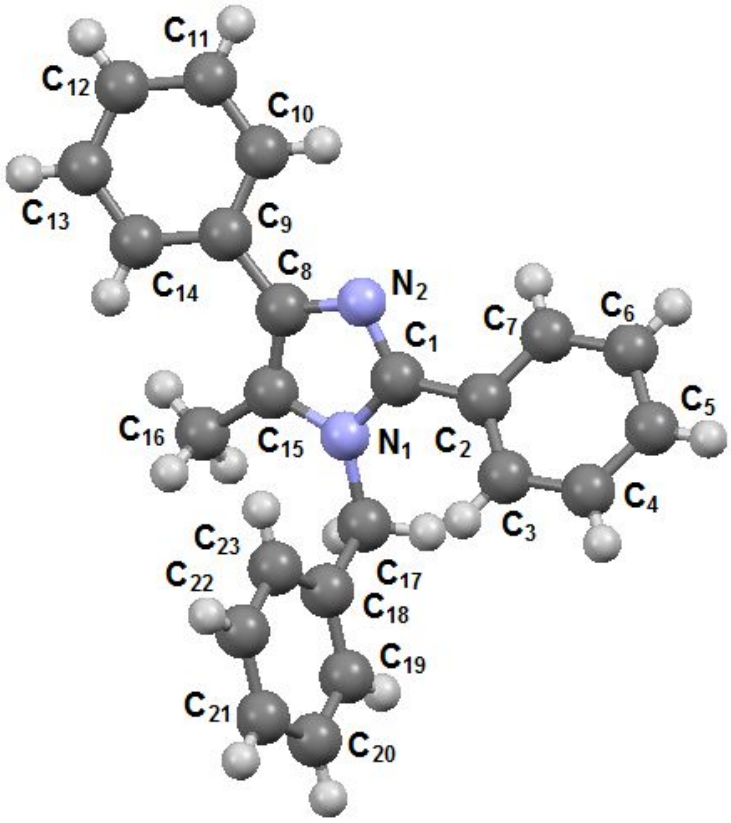


Figure S60. ORTEP diagram (ball and stick plot) of product **5a** (drawn at 50% probability level) and hydrogens are omitted for clarity. Colour code: nitrogen in blue and carbon in grey.

X-Ray Crystallographic Information of Product 5a:

The Single crystal of imidazole derivative **5a** was acquired by slow evaporation of petroleum ether at room temperature. The diffraction data of compound **5a** was measured by MoKα radiation (λ = 1.54178Å) at 101 K. The structure of the single crystal of imidazole derivative **5a** was solved by using the SHELXS-97 program.[1] Refinements were carried out by full matrix least-squares process against F using SHELXL-97.2 and the non-hydrogen atoms were refined with anisotropic thermal parameters.[2] All the hydrogen atoms in the crystal structure (**5a**) were included in geometric positions and given thermal parameters equivalent to 1.2 times those of the atom to which they were attached. All the necessary crystal data of the imidazole derivative **5a** is given below:

Table S2:Important crystal data of product **5a.**	
Empirical Formula	$C_{23}H_{20}N_2$
Formula weight	324.41
Temperature	101 K
Wave length	1.54178
Crystal system	monoclinic
Space group	C 1 c 1
Unit cell dimensions	a = 6.9727(11)Å α = 90 b = 19.869(3) Å β = 91.013(4) c = 12.956(2) Å γ = 90
Volume	1794.7(5) $Å^3$
Z	4
Density (calculated)	1.201g/cm^3
Absorption coefficient (Mu)	0.541 mm^{-1}
F(000)	688.0
Theta range for data collection	4.450° to 72.584°
Index ranges	$-8 \leq h \leq 8$, $-24 \leq k \leq 24$, $-16 \leq l \leq 15$
Reflection collected	12501
Independent reflection	3254 [R_{int} = 0.0431, R_{sigma} = 0.0385]
Absorption correction	multi-scan
Data/restraints/parameters	3254/2/227
Good of fit on (F^2)	1.104
Final R indices [I>=2σ (I)]	R_1 = 0.0353, wR_2 = 0.0871
R indices (all data)	R_1 = 0.0354, wR_2 = 0.0871

The crystal data of product 5a was deposited at the Cambridge Crystallographic Data Centre. The CCDC reference number is 1948126.

4. References:

1. Sheldrick, G. M.; Phase Annealing in SHELX-90: Direct Methods for Larger Structures. *Acta Cryst.* **1990**, *A46,* 467-473.

2. Sheldrick, G. M. *SHELXL-97, Program for Crystal Structure Refinement;* Universität Göttingen: Göttingen, Germany, 1997.