Effects of Non Covalent Interactions in Light Emitting Properties of *bis*-pyridyl-alkyl-*di*-imines

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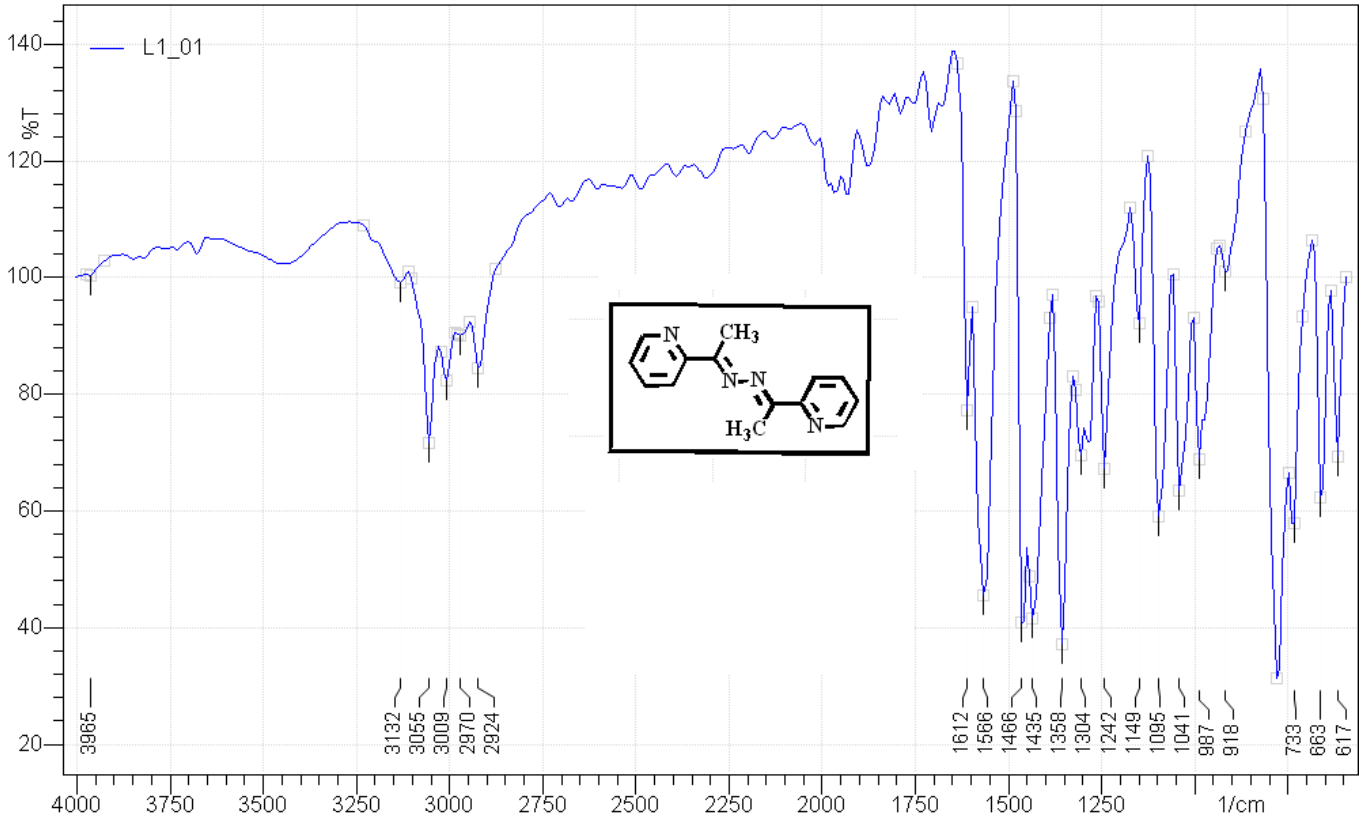
General

Infra-red spectrum was recorded in FTIR ABB Bomen MB-3000. UV-Vis absorption spectra were recorded in Shimadzu Spectrophotometer with model UV-2450. Fluorescence spectra were recorded in Shimadzu Spectrofluorophotometer with model RF-5301PC. ^{1}H and ^{13}C nuclear magnetic resonance spectra were measured on a 400 MHz NMR spectrometer (Bruker).

Figure S1: IR Spectra of (L1a):



IR: 3055(s), 3009(w), 2924(w), 1612(s), 1566(vs), 1466(vs), 1435(vs), 1358(vs), 1304(s), 1242(s), 1149(w), 1095(s), 1041(s), 987(s), 779(vs), 733(s), 663(s), 617(s).

Figure S2: ^{1}H NMR Spectra of L1a:

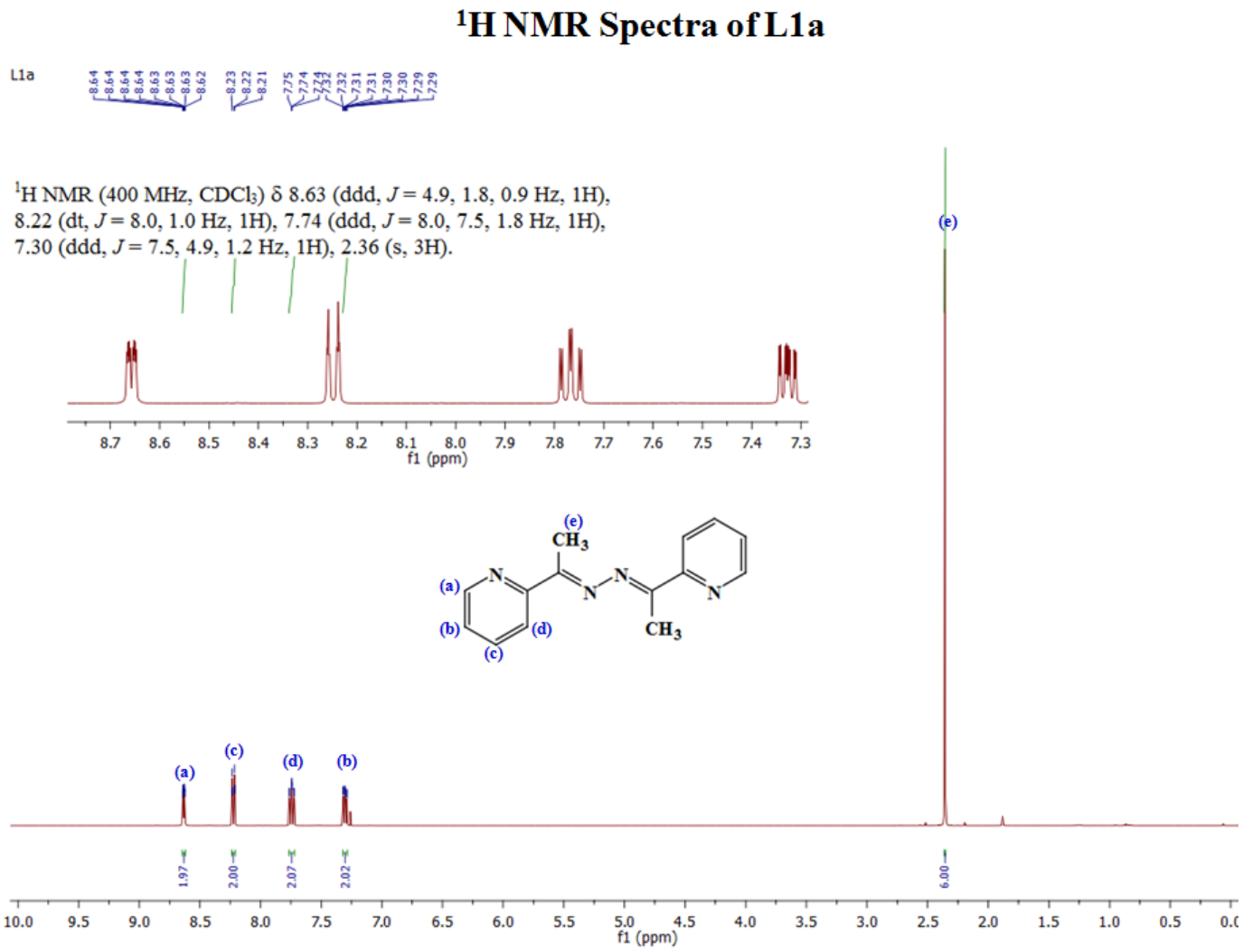


Figure S3: ^{13}C NMR Spectra of L1a:

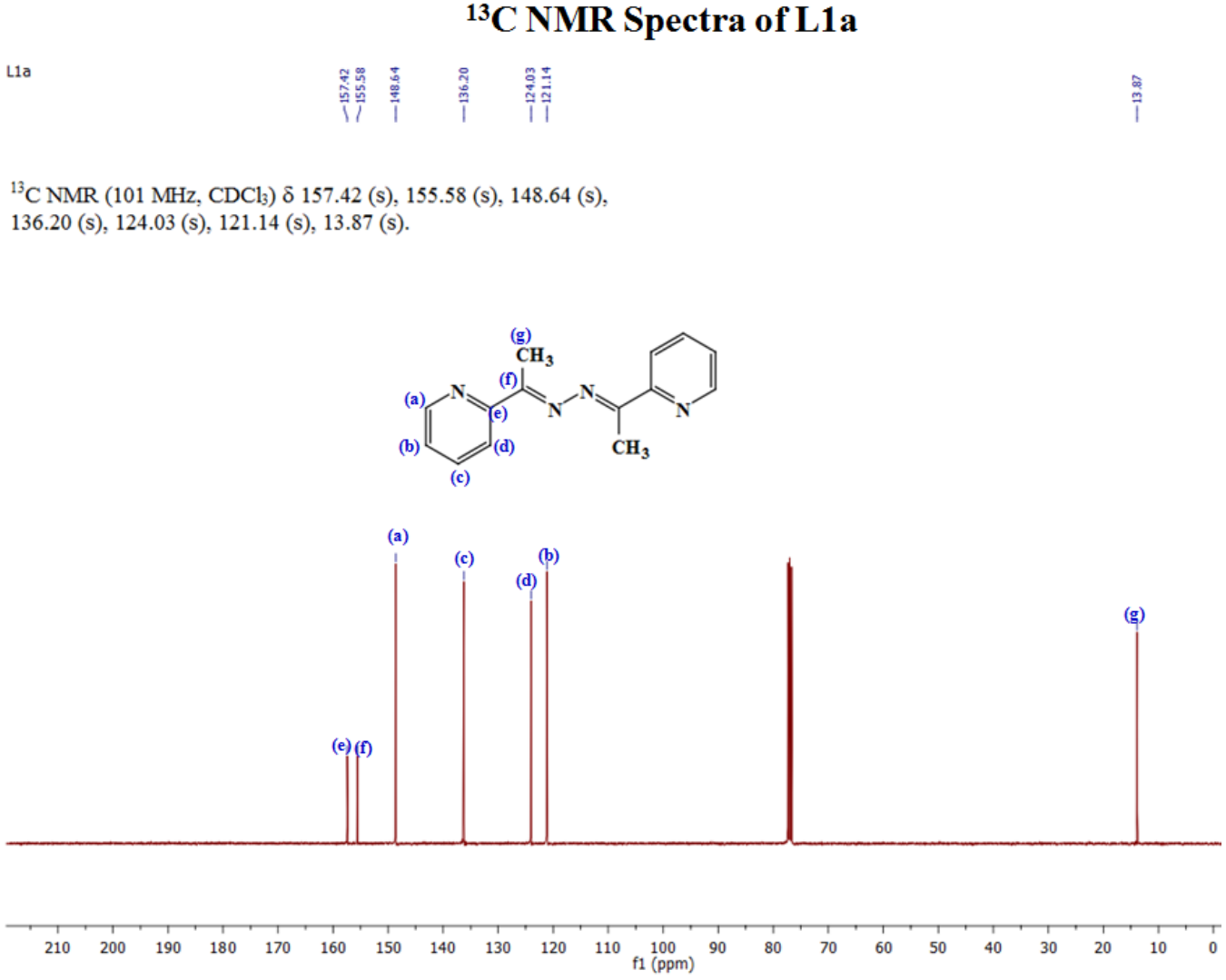
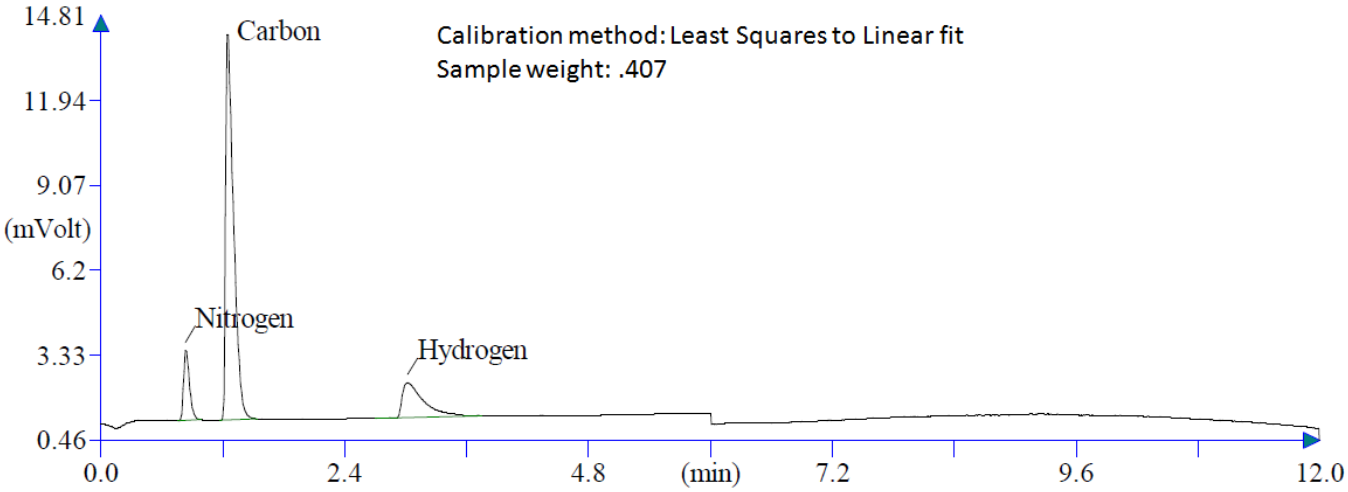


Figure S4: Elemental Analysis of L1a



Retention Time (min)	Component Name	Element %
0.833	Nitrogen	23.48
1.242	Carbon	70.63
3.017	Hydrogen	5.89

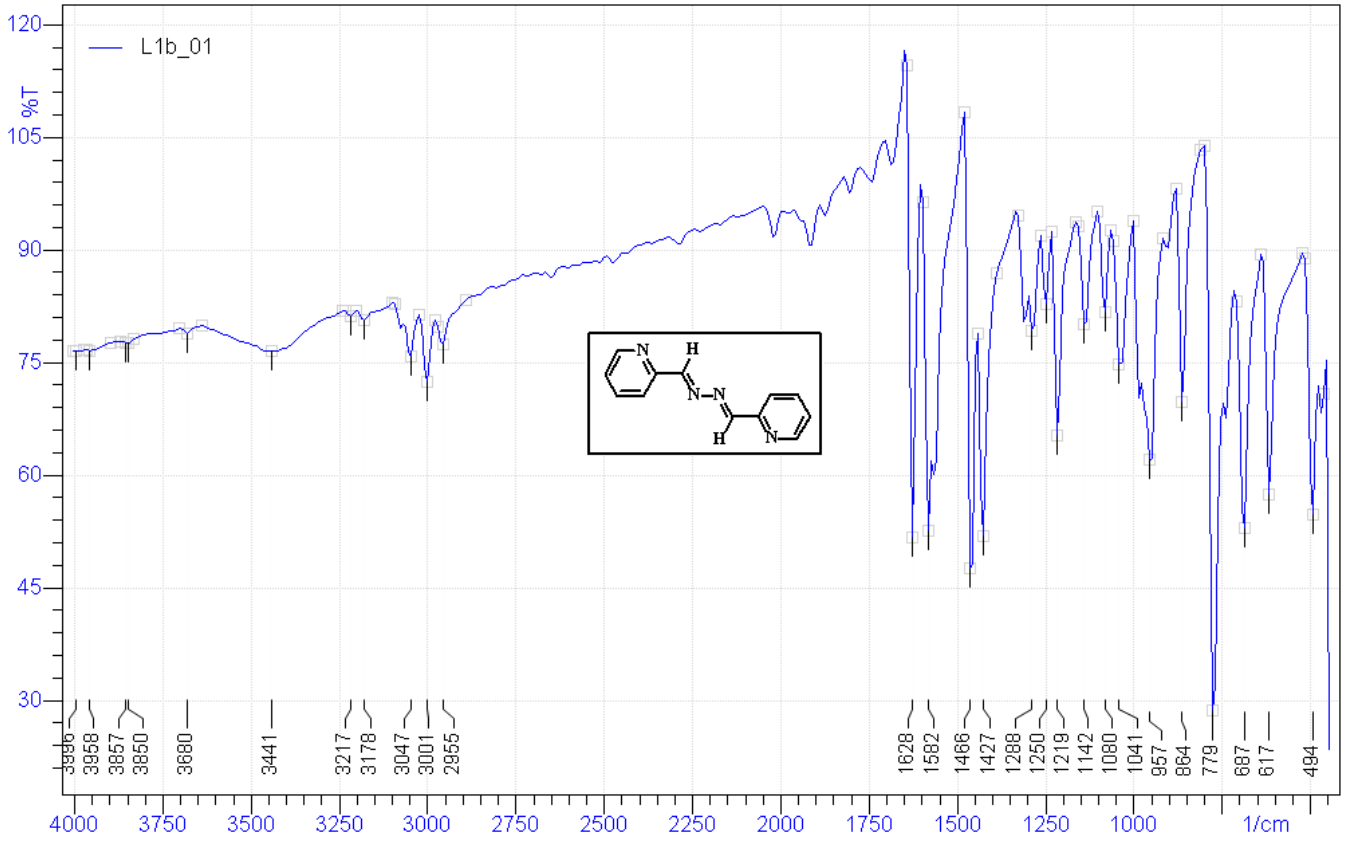
Calculated :

Chemical Formula: $C_{14}H_{14}N_4$

Molecular Weight: 238.29

Elemental Analysis: C, 70.57; H, 5.92; N, 23.51

Figure S5: IR Spectra of L1b:



IR: 3047(w), 3001(w), 2955(w), 1628(vs), 1582(vs), 1466(vs), 1427(vs), 1288(w), 1250(w), 1219(s), 1142(w), 1080(w), 957(s), 864(s), 779(vs), 687(vs), 617(vs), 494(vs)

Figure S6: ^{1}H NMR Spectra of L1b:

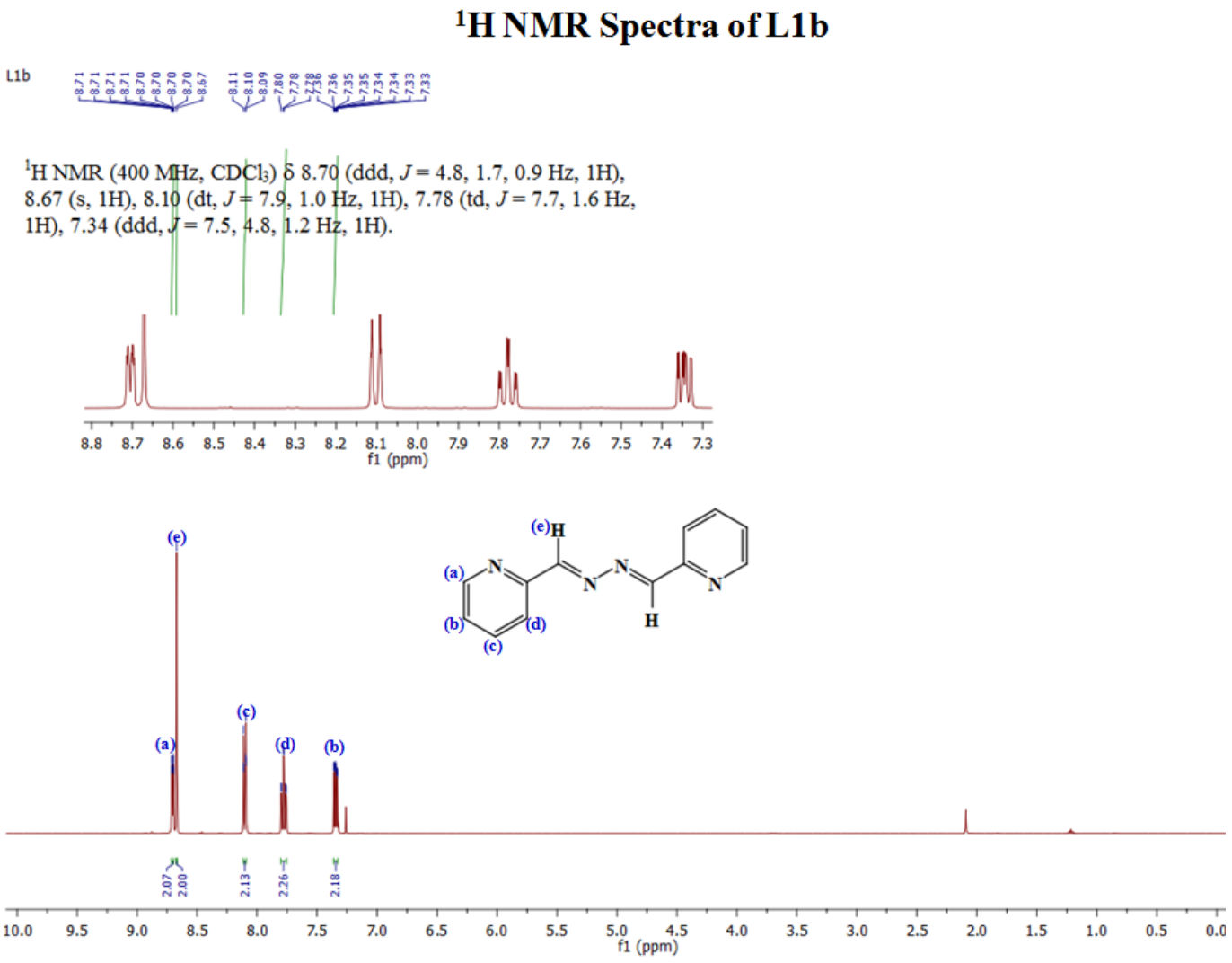


Figure S7: ^{13}C NMR Spectra of L1b:

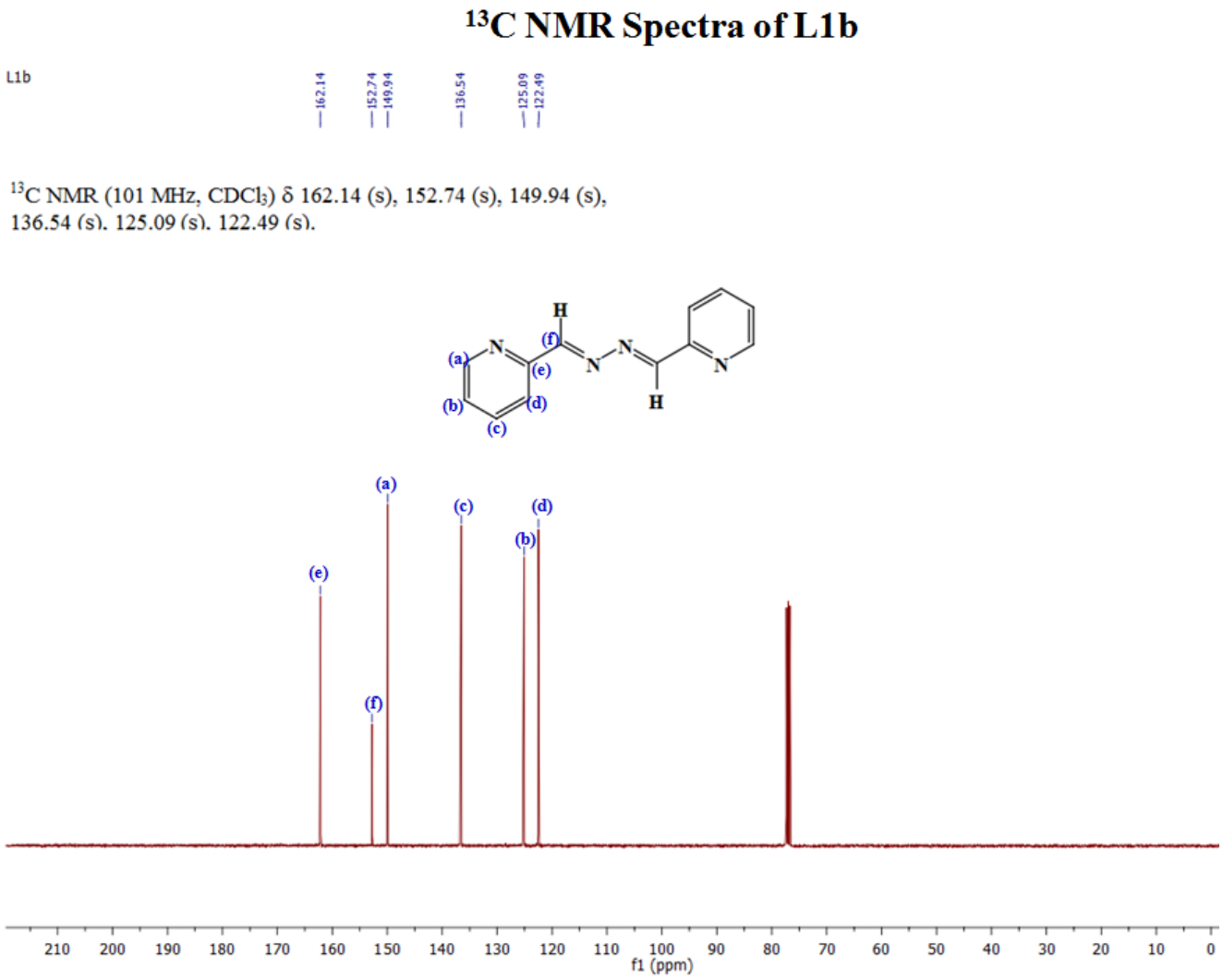
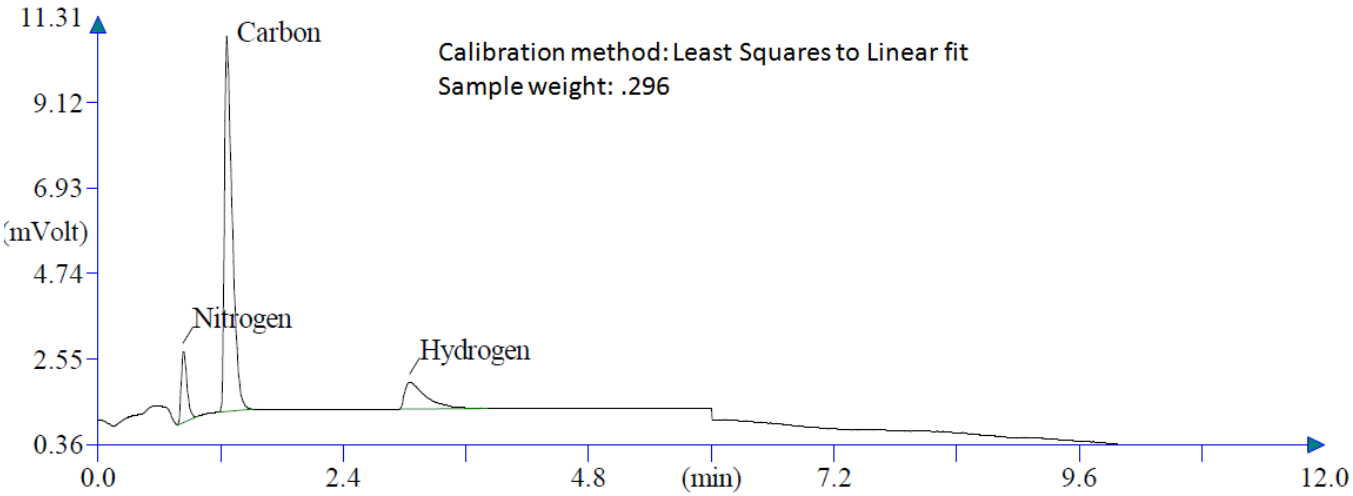


Figure S8: Elemental Analysis of L1b:

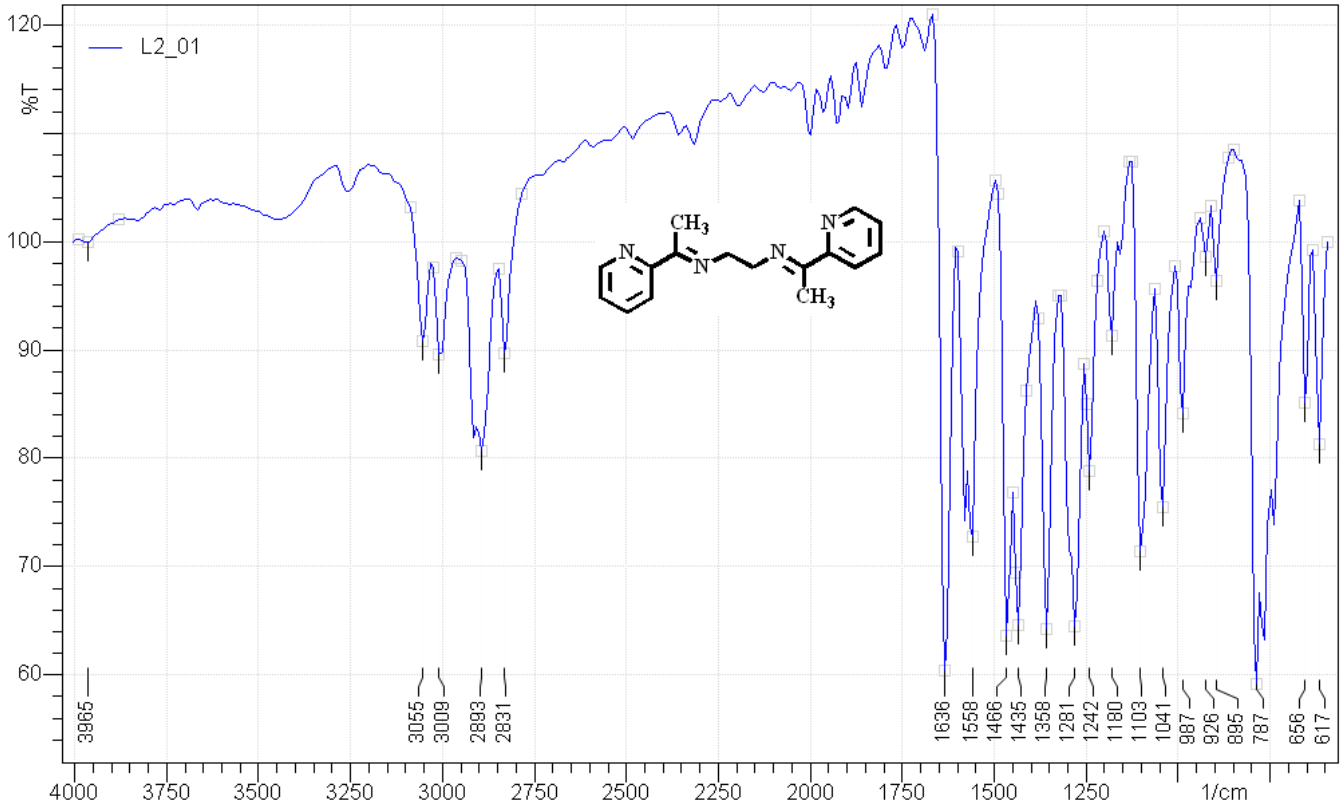


Retention Time (min)	Component Name	Element %
0.833	Nitrogen	26.61
1.258	Carbon	68.64
3.050	Hydrogen	4.75

Calculated:

Chemical Formula: $C_{12}H_{10}N_4$
Molecular Weight: 210.23
Elemental Analysis: C, 68.56; H, 4.79; N, 26.65

Figure S9: IR Spectra of L2a:



IR: 3055(s), 3009(s), 2893(s), 2831(s), 1636(vs), 1558(vs), 1466(vs), 1435(vs), 1358(vs), 1281(vs), 1242(s), 1180(w), 1103(vs), 1041(vs), 987(s), 926(w), 859(w), 787((vs), 656(s), 617(s).

Figure S10: ^{1}H NMR Spectra of L2a:

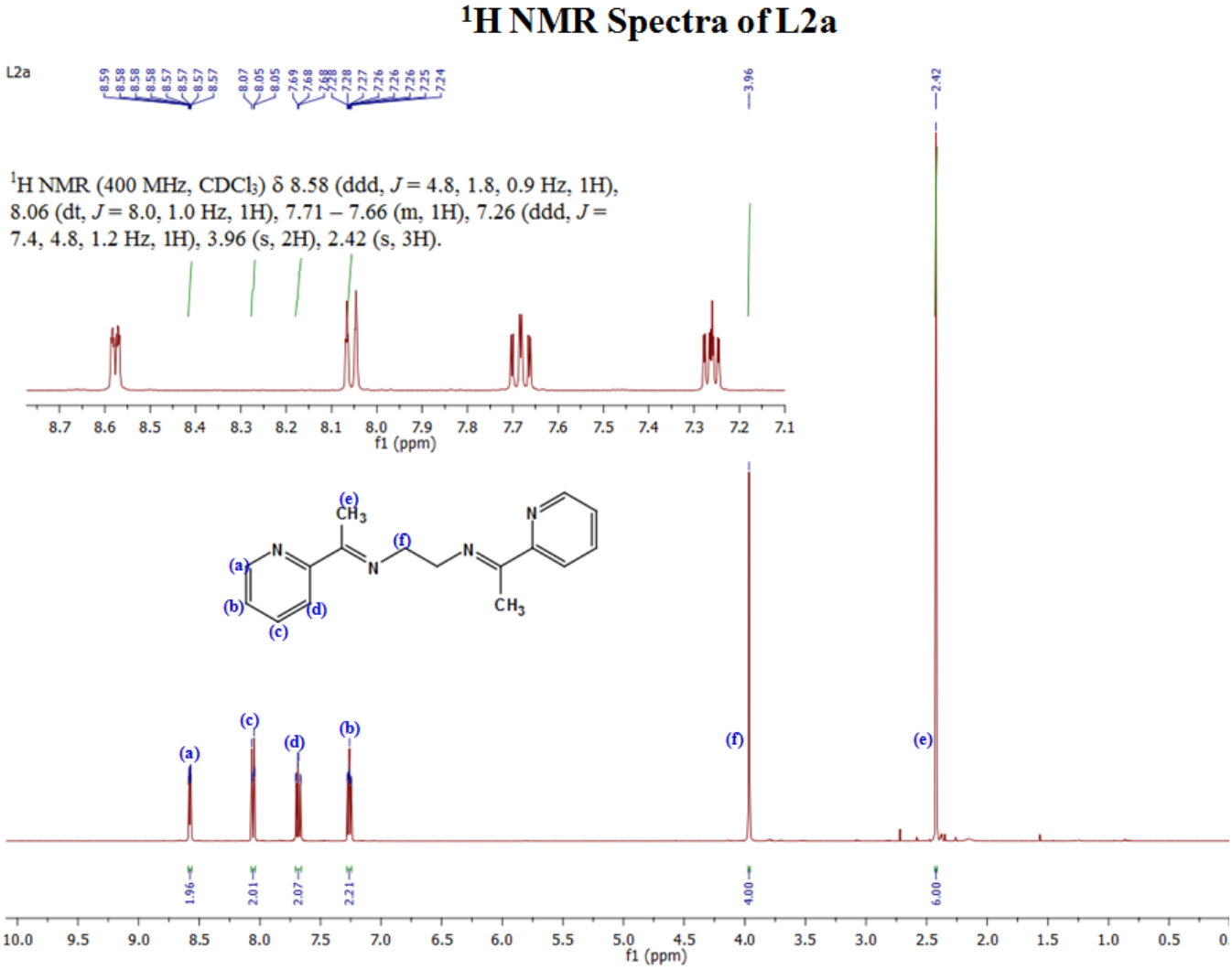


Figure S11: ^{13}C NMR Spectra of L2a:

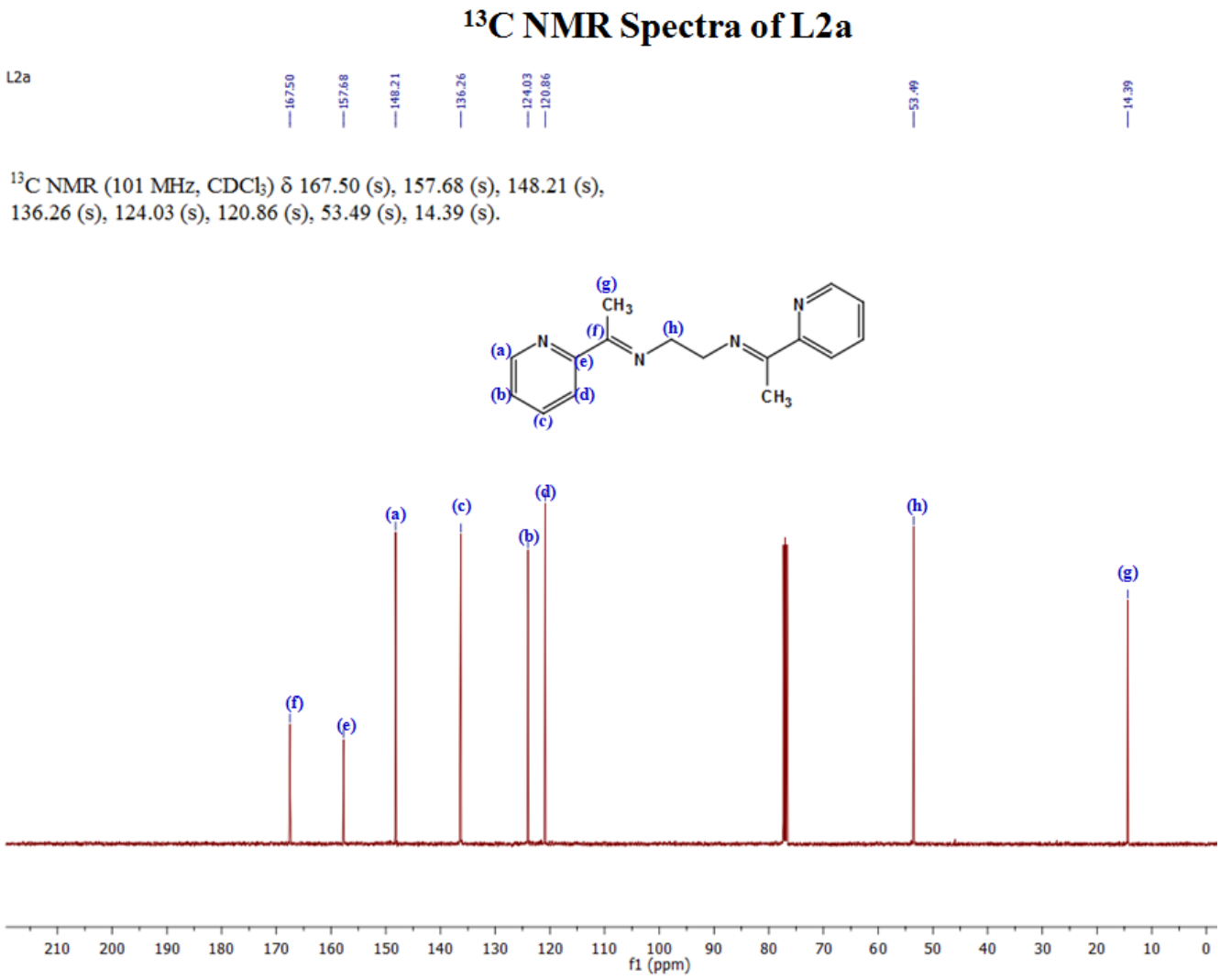
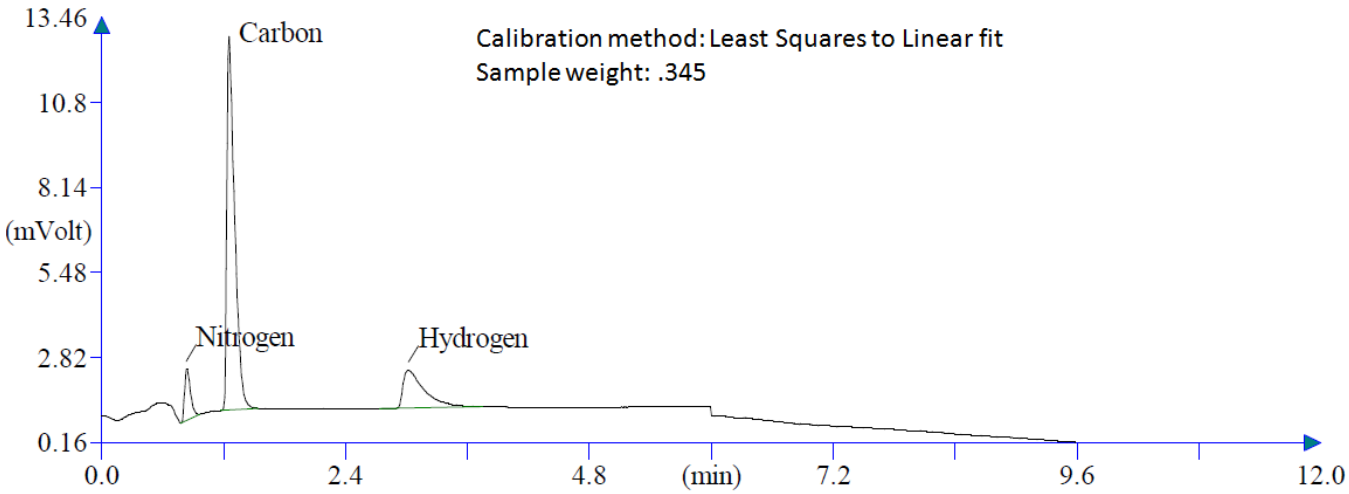


Figure S12: Elemental Analysis of L2a:

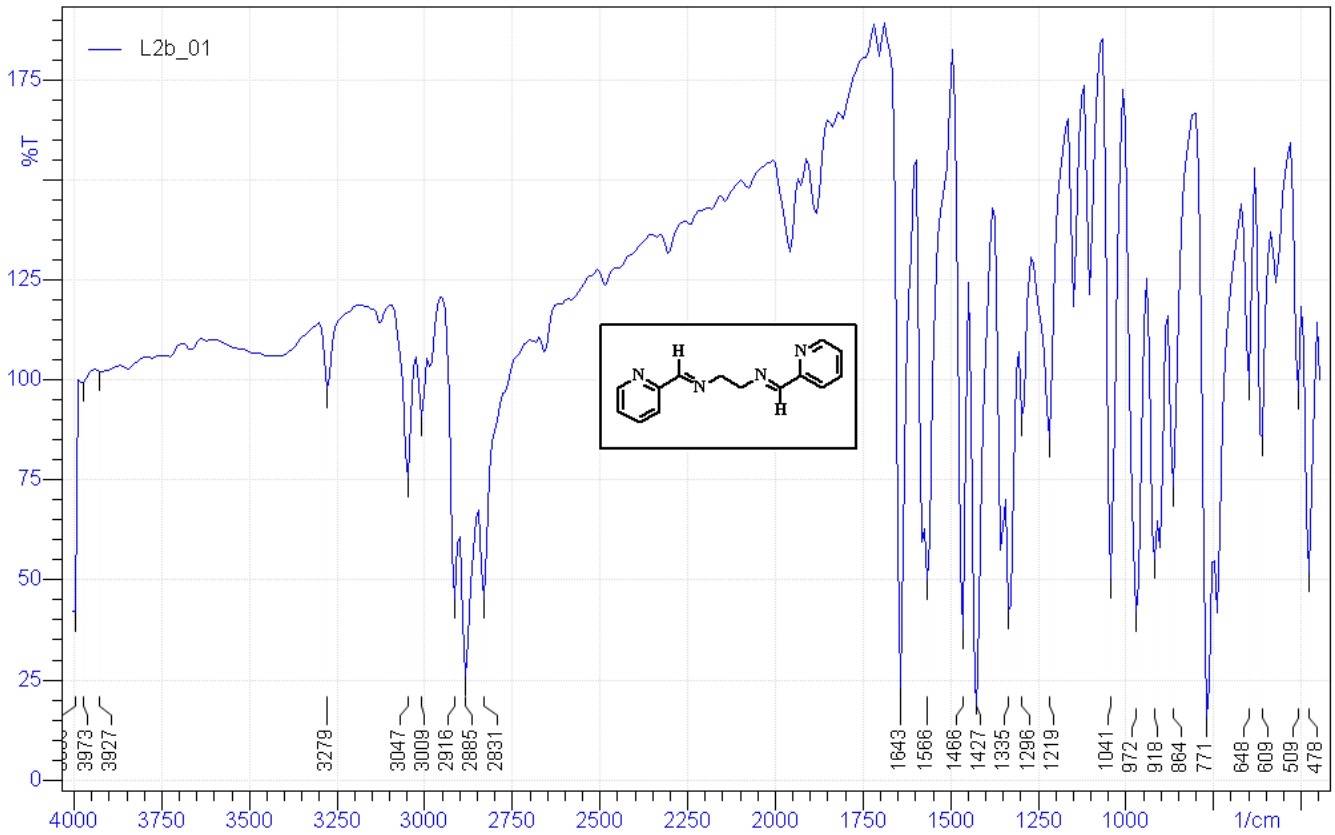


Retention Time (min)	Component Name	Element %
0.833	Nitrogen	20.98
1.250	Carbon	72.23
3.017	Hydrogen	6.79

Calculated:

Chemical Formula: $C_{16}H_{18}N_4$
Molecular Weight: 266.34
Elemental Analysis: C, 72.15; H, 6.81; N, 21.04

Figure S13: IR Spectra of L2b:



IR(cm^{-1} KBr pellet): 3047(s), 3009(w), 2916(s), 2885(vs), 2831(s), 1643(vs), 1566(vs), 1466(vs), 1427(vs), 1335(vs), 1296(s), 1219(s), 1041(vs), 972(vs), 918(vs), 864(vs), 771(vs).

Figure S14: ^{1}H NMR Spectra of L2b:

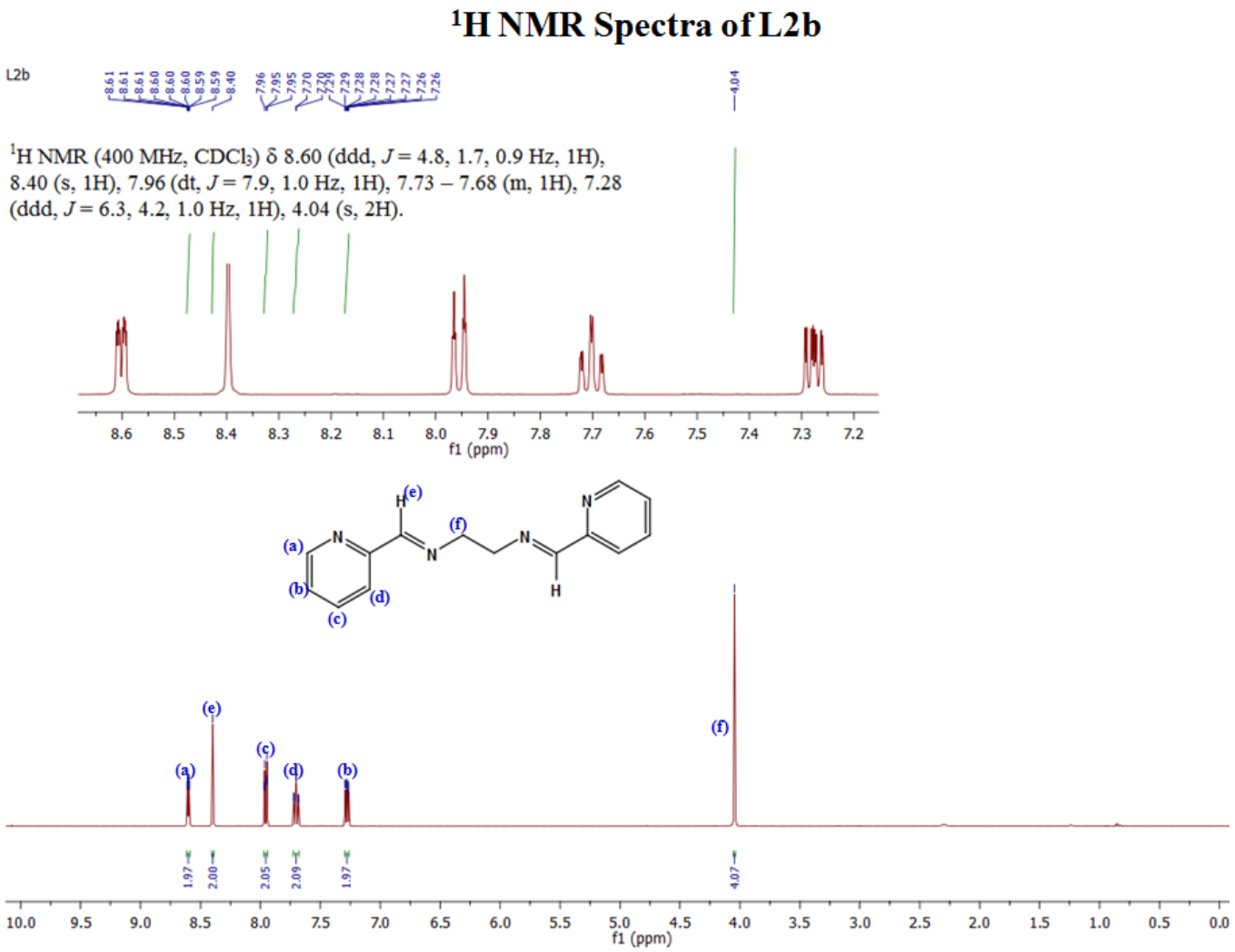


Figure S15: ^{13}C NMR Spectra of L2b:

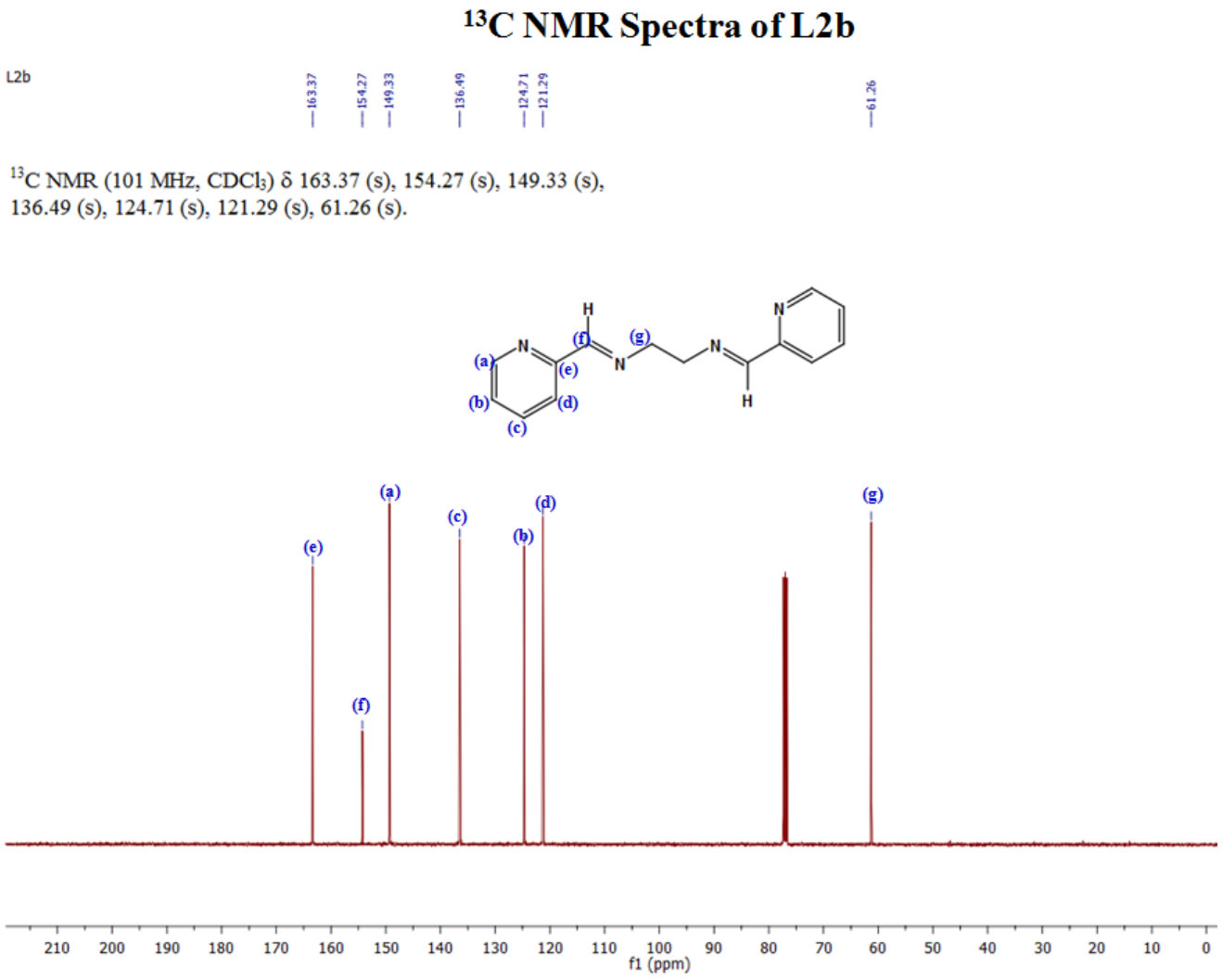
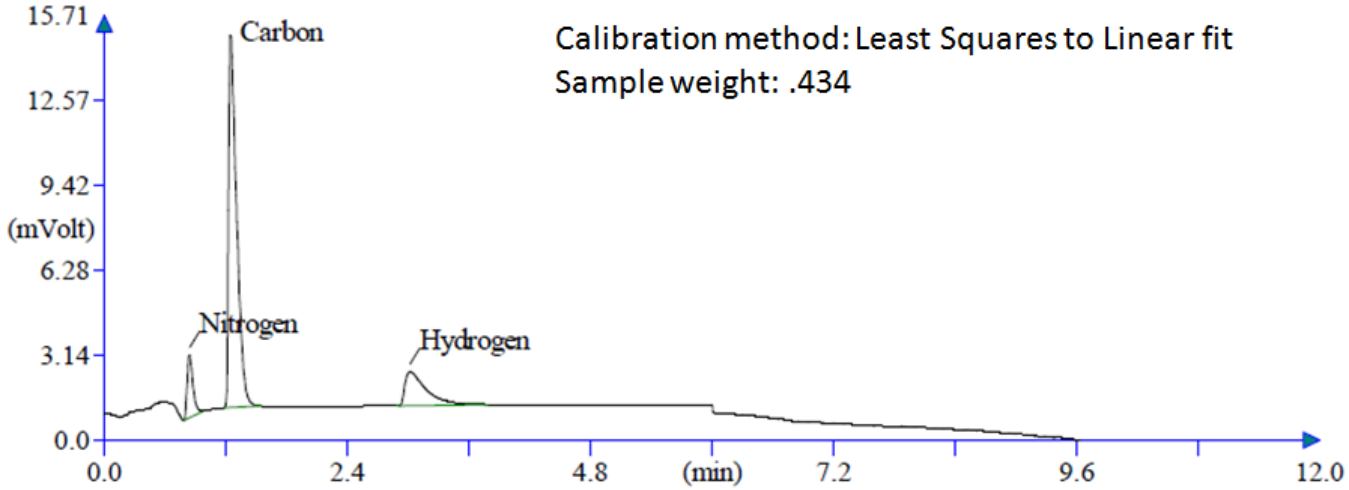


Figure S16: Elemental Analysis of L2b:

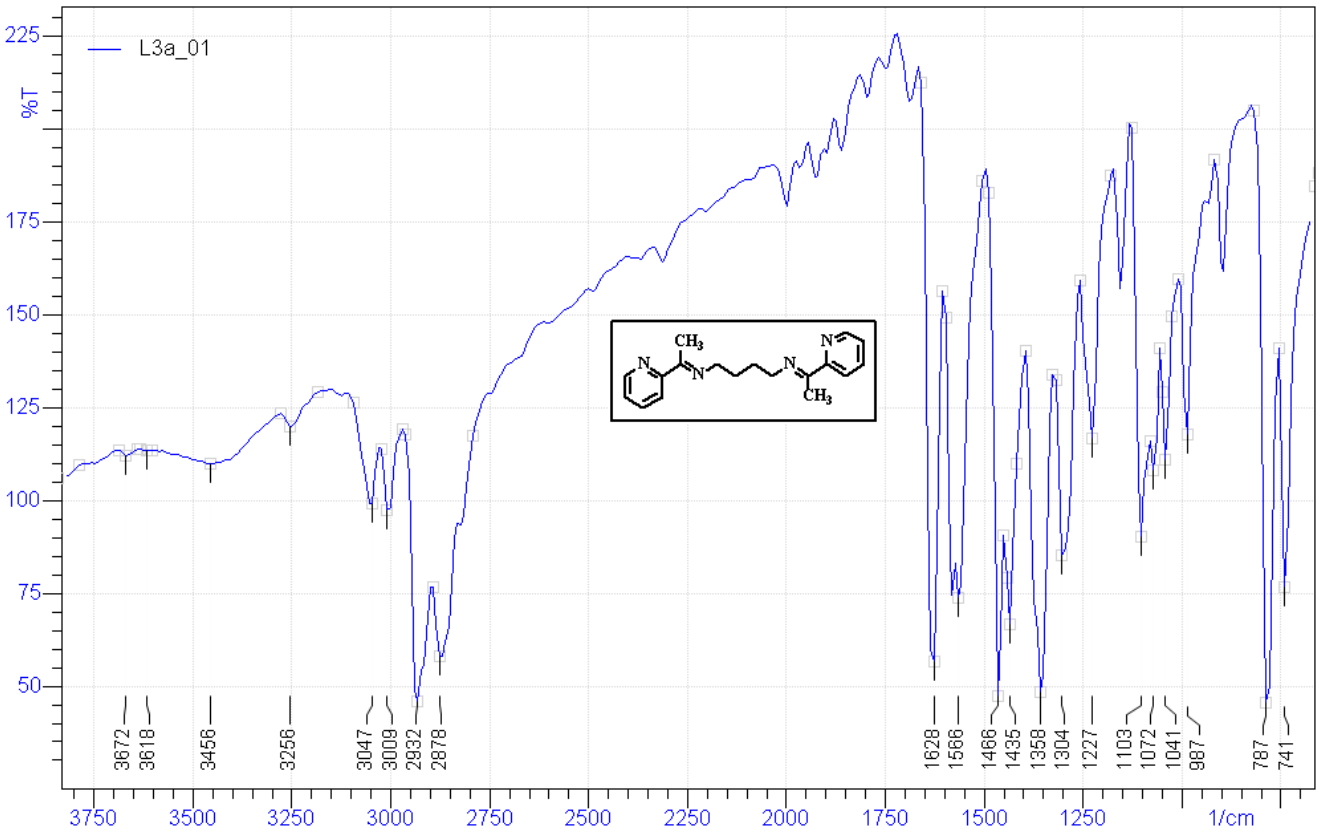


Retention Time (min)	Component Name	Element %
0.842	Nitrogen	23.48
1.242	Carbon	70.62
3.017	Hydrogen	5.90

Calculated:

Chemical Formula: $C_{14}H_{14}N_4$
Molecular Weight: 238.29
Elemental Analysis: C, 70.57; H, 5.92; N, 23.51

Figure S17: IR Spectra of L3a:



IR: 3047(w), 3009(w), 2932(vs), 2878(vs), 1628(vs), 1566(vs), 1466(vs), 1435(vs), 1358(vs), 1304(s), 1227(w), 1103(s), 1072(w), 1041(w), 987(w), 787(vs), 741(s),

Figure S18: ^{1}H NMR Spectra of L3a:

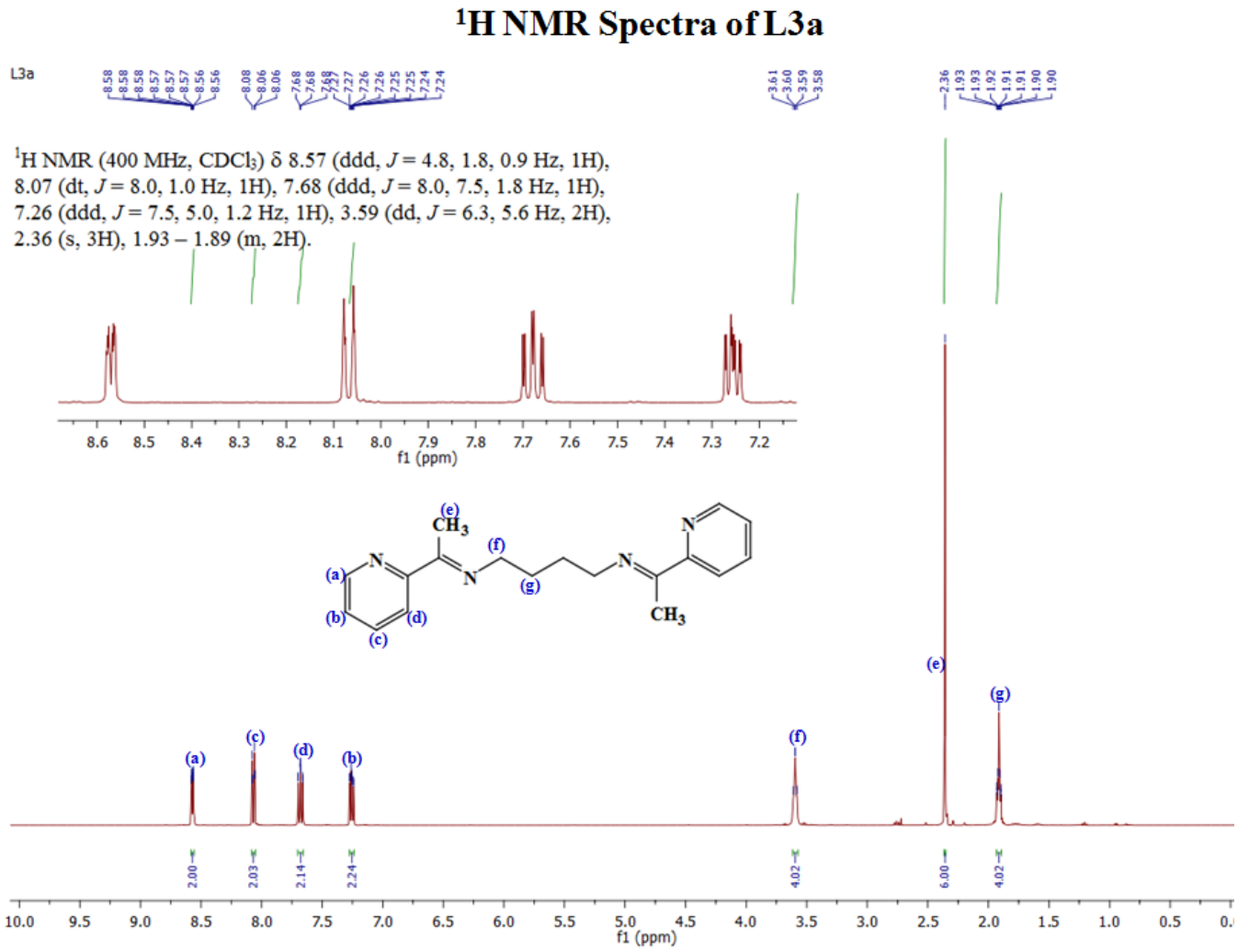


Figure S19: ^{13}C NMR Spectra of L3a:

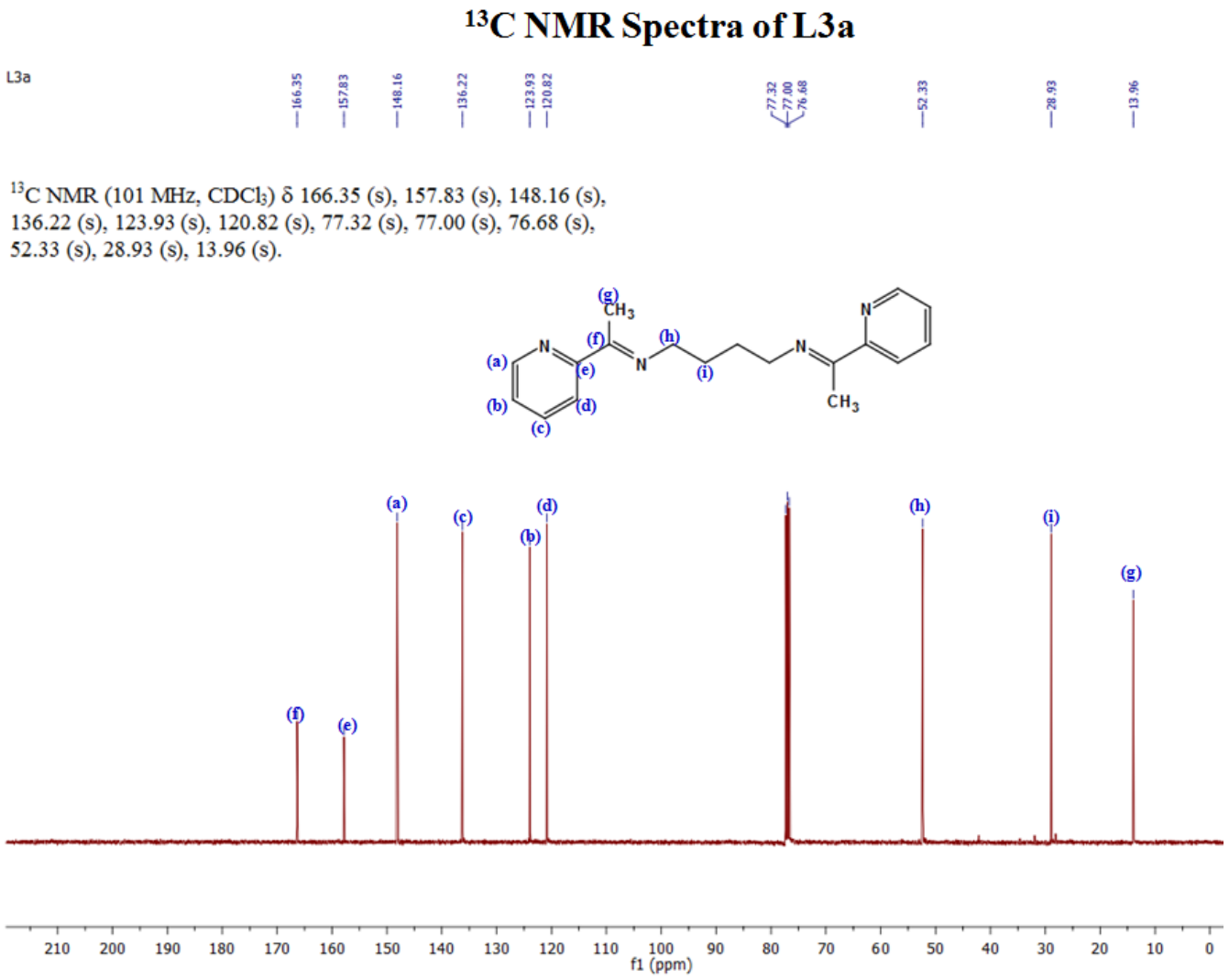
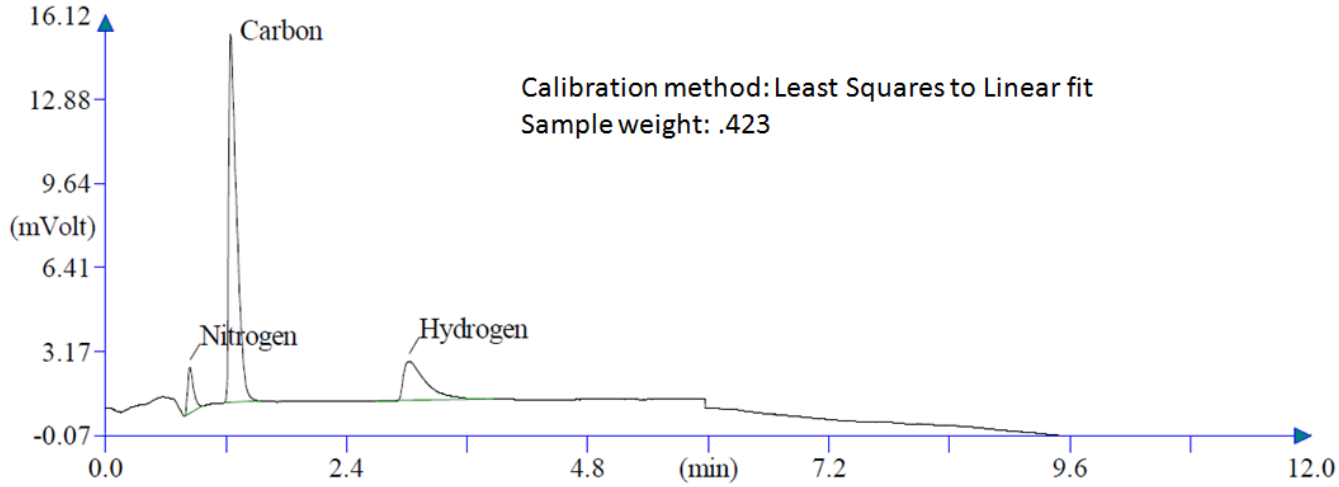


Figure S20: Elemental Analysis of L3a:

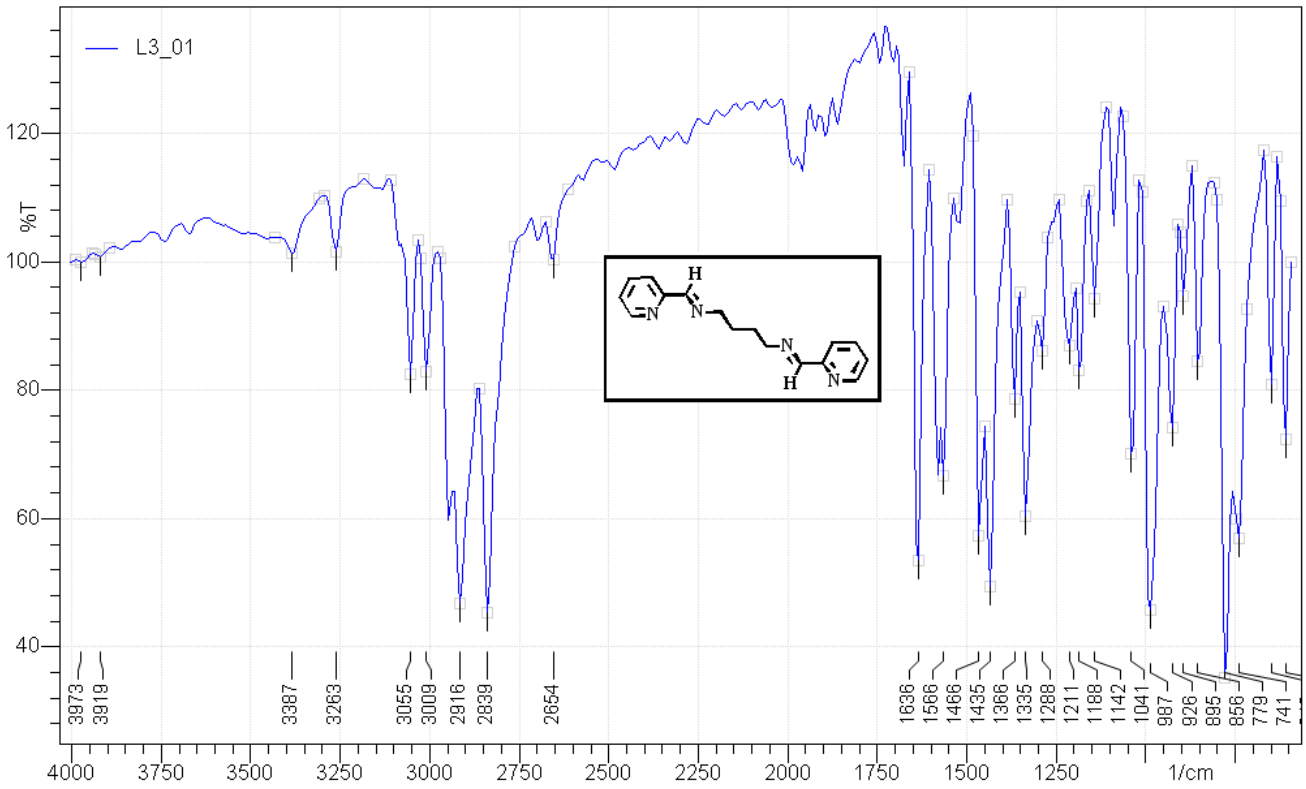


Retention Time (min)	Component Name	Element %
0.842	Nitrogen	19.00
1.242	Carbon	73.5
3.025	Hydrogen	7.50

Calculated:

Chemical Formula: $C_{18}H_{22}N_4$
Molecular Weight: 294.39
Elemental Analysis: C, 73.44; H, 7.53; N, 19.03

Figure S21: IR Spectra of L3b:



IR: 3055(s), 3009(s), 2916(vs), 2839(vs), 1636(vs), 1566(vs), 1466(vs), 1435(vs), 1366(s), 1335(vs), 1288(w), 1211(w), 1188(w), 1188(w), 1142(w), 1041(s), 987(vs), 926(s), 895(w), 856(s), 779(vs), 741(s),

Figure S22: ^{1}H NMR Spectra of L3b:

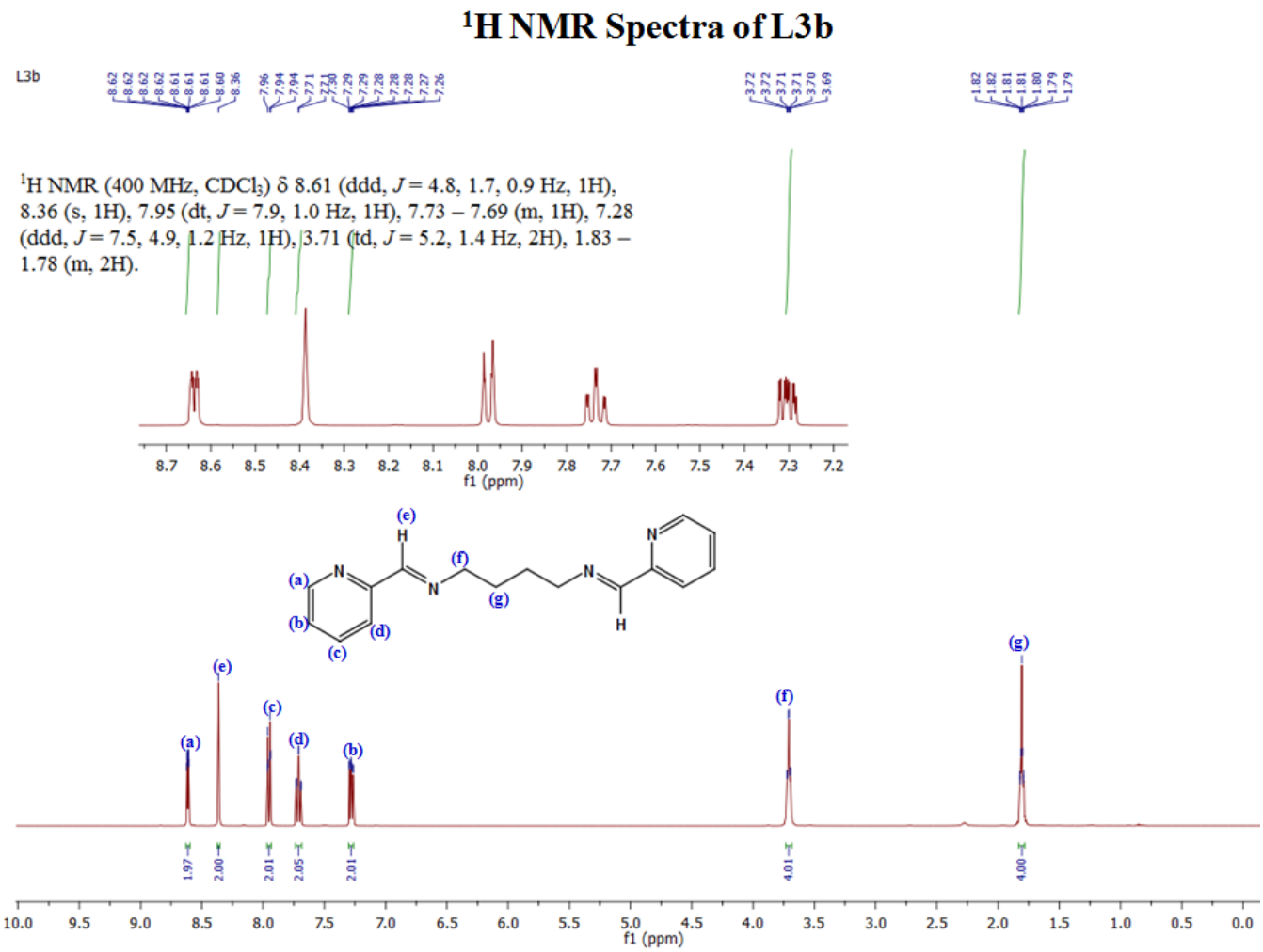


Figure S23: ^{13}C NMR Spectra of L3b:

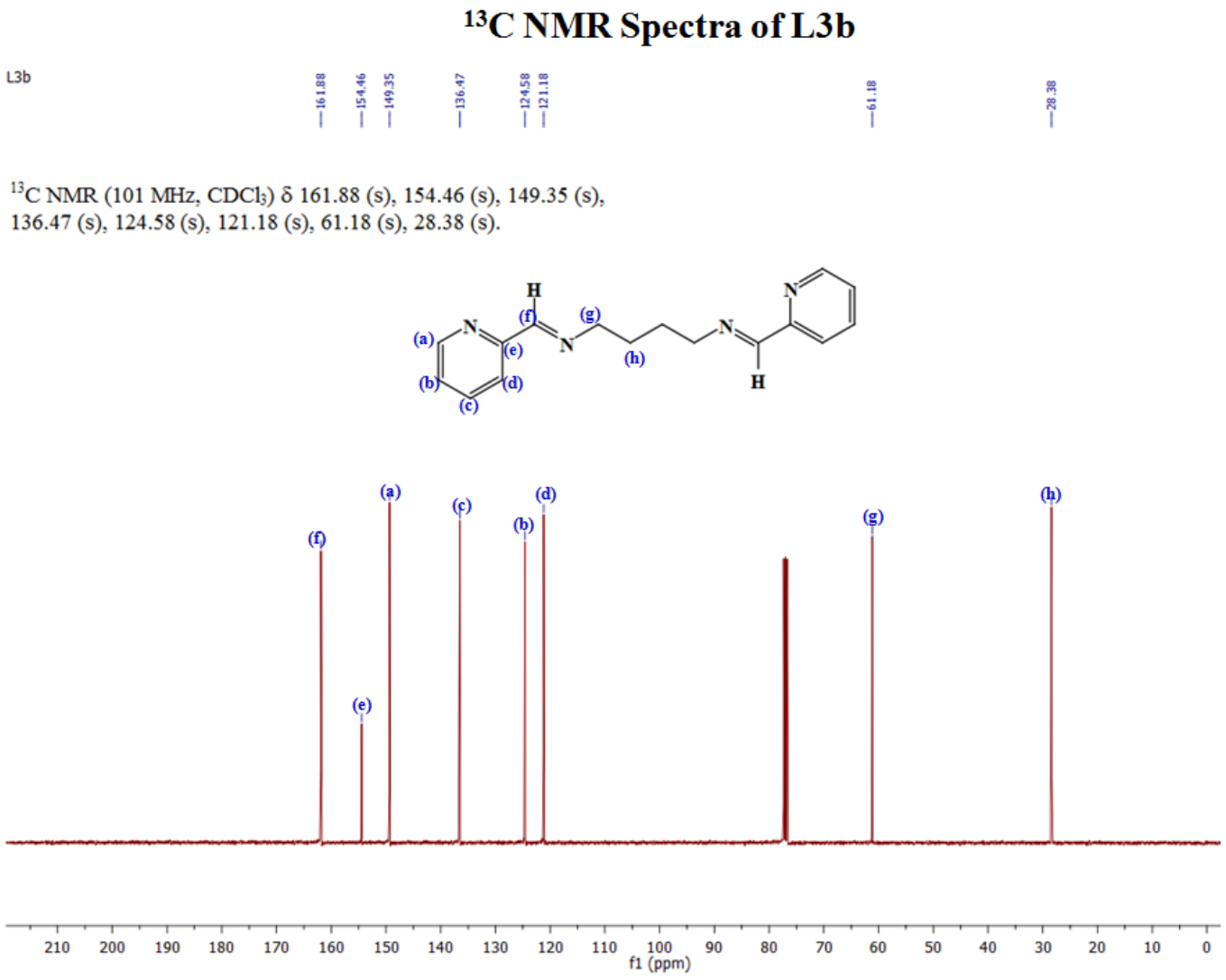
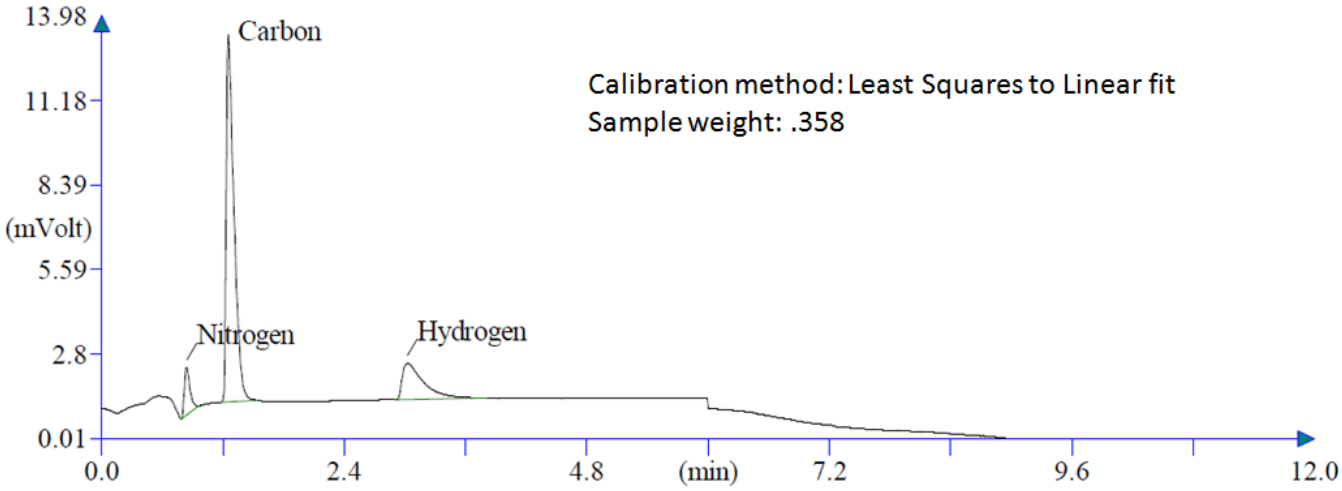


Figure S24: Elemental Analysis of L3b:



Retention Time (min)	Component Name	Element %
0.842	Nitrogen	21.01
1.250	Carbon	72.21
3.025	Hydrogen	6.78

Calculated:

Chemical Formula: $C_{16}H_{18}N_4$
Molecular Weight: 266.34
Elemental Analysis: C, 72.15; H, 6.81; N, 21.04

Figure S25: ORTEP of L1a

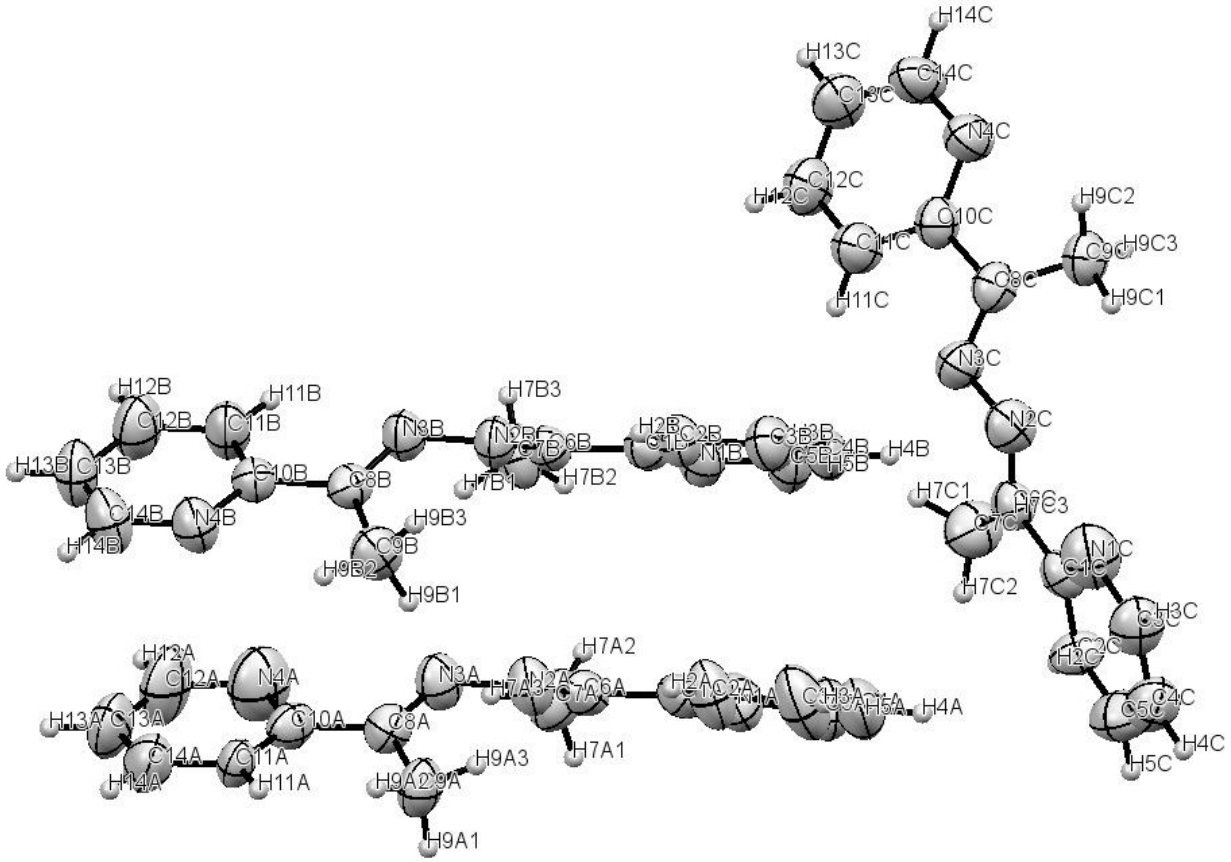


Figure S26: ORTEP of L2a

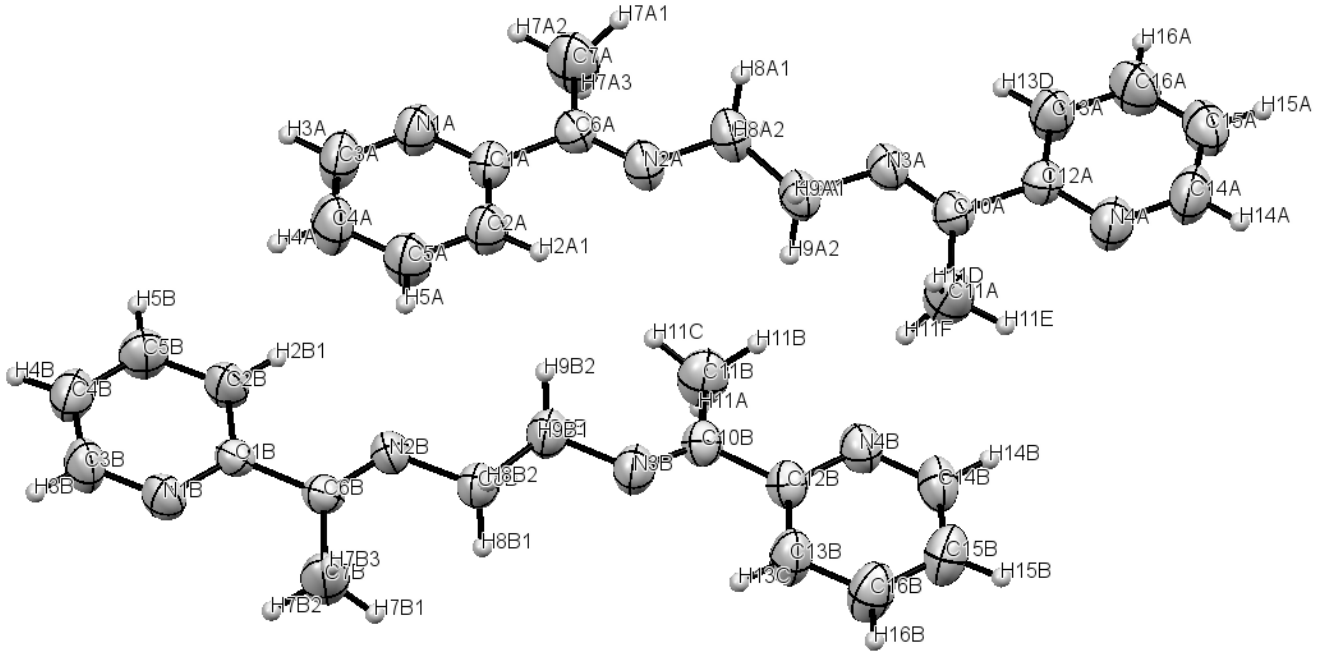


Figure S27: ORTEP of L3b:

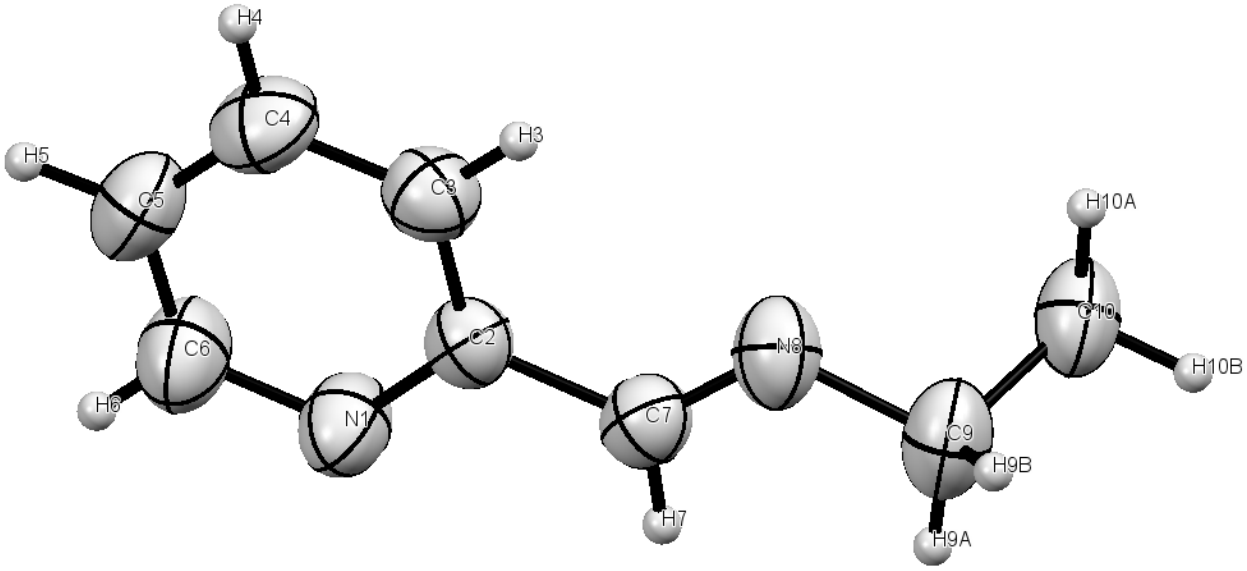


Figure S28: Solid State UV-Vis Spectrum of L1a:

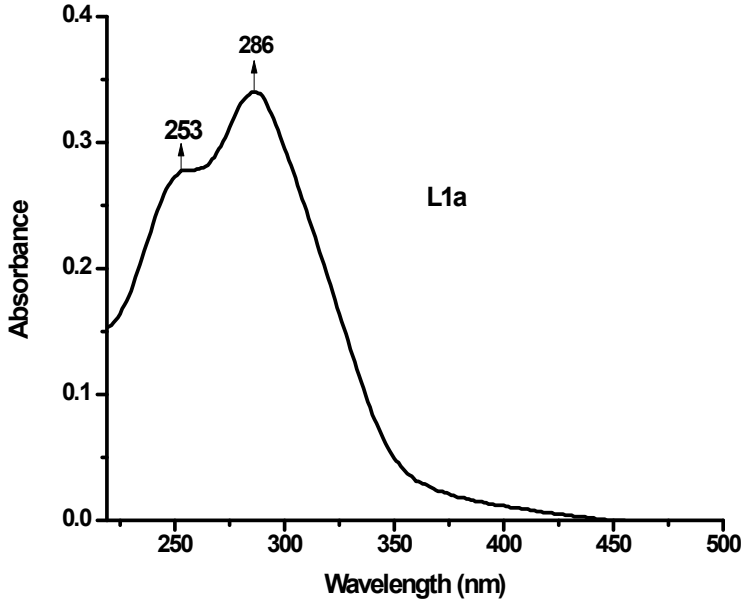


Figure S29: Solid State UV-Vis Spectrum of L2a:

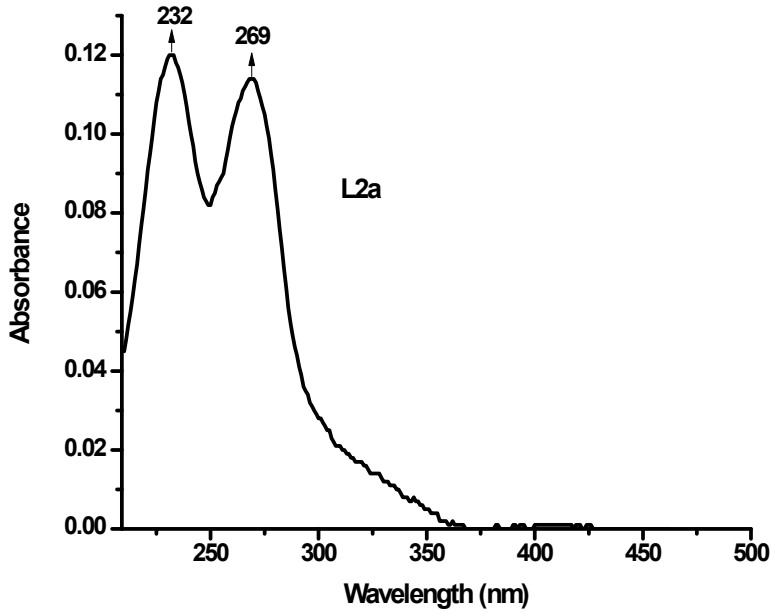


Figure S30: Solid State UV-Vis Spectrum of L3b:

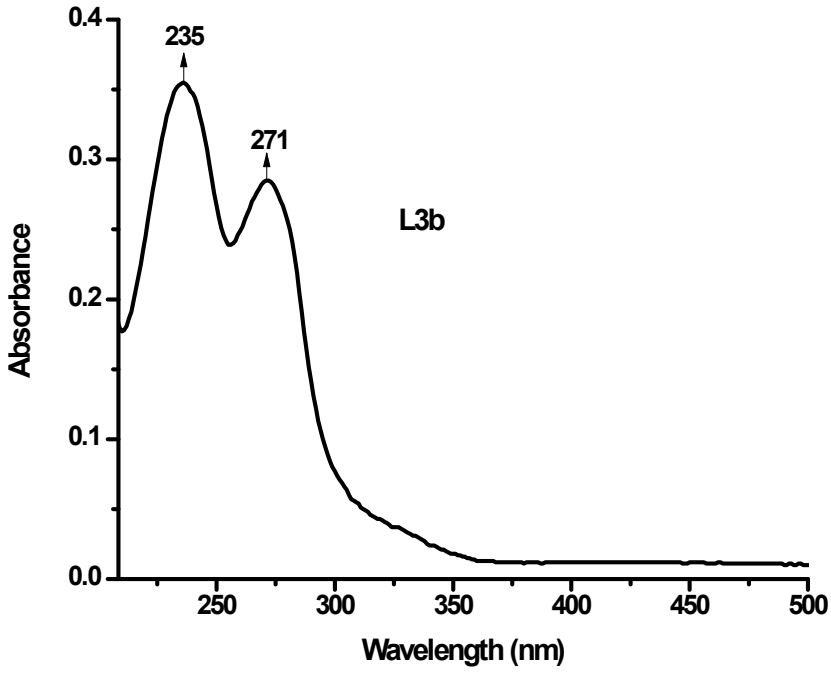


Figure S31: Excitation Spectra of L1b in $CHCl_3$ in different concentrations: (a) 10^{-3}M, (b) 10^{-4}M, (c) 10^{-5}M

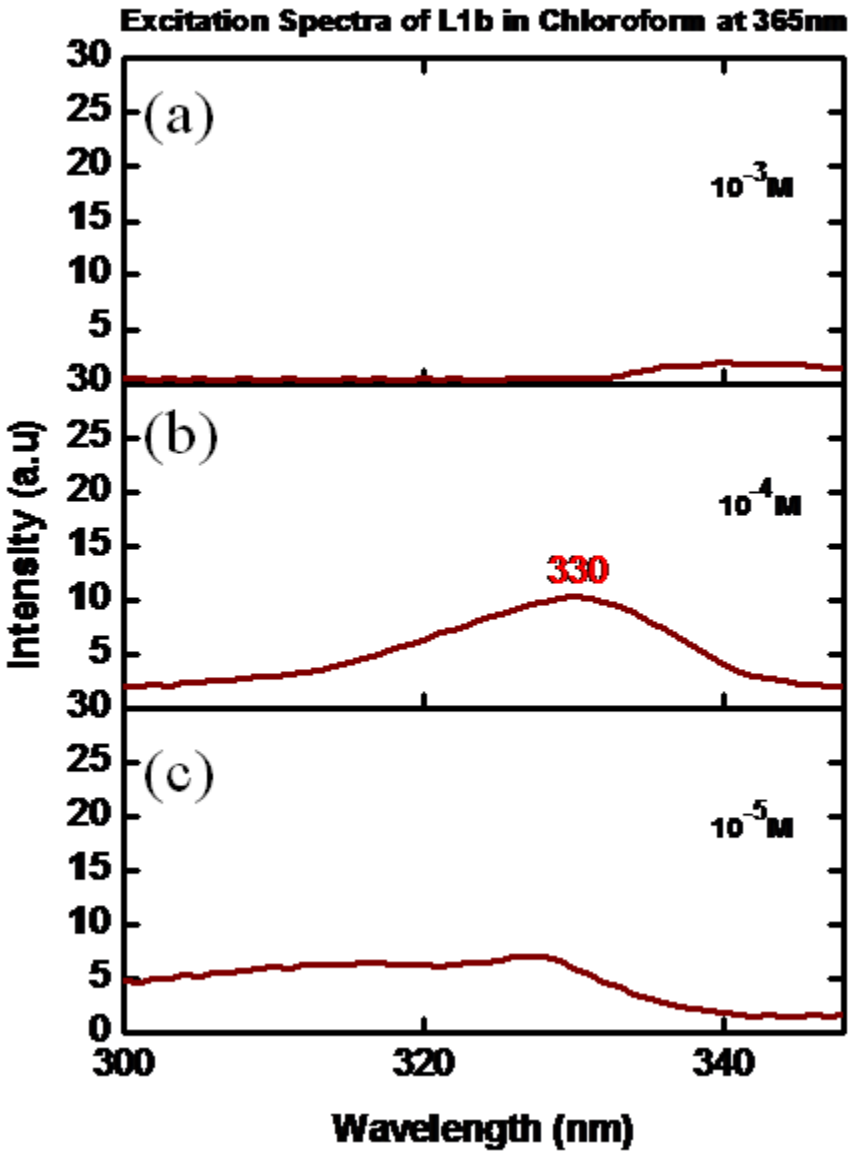


Figure S32: PL Spectra of L1b in CHCl3 in different Concentrations: (a) 10^{-4}M; (b) 10^{-5}M

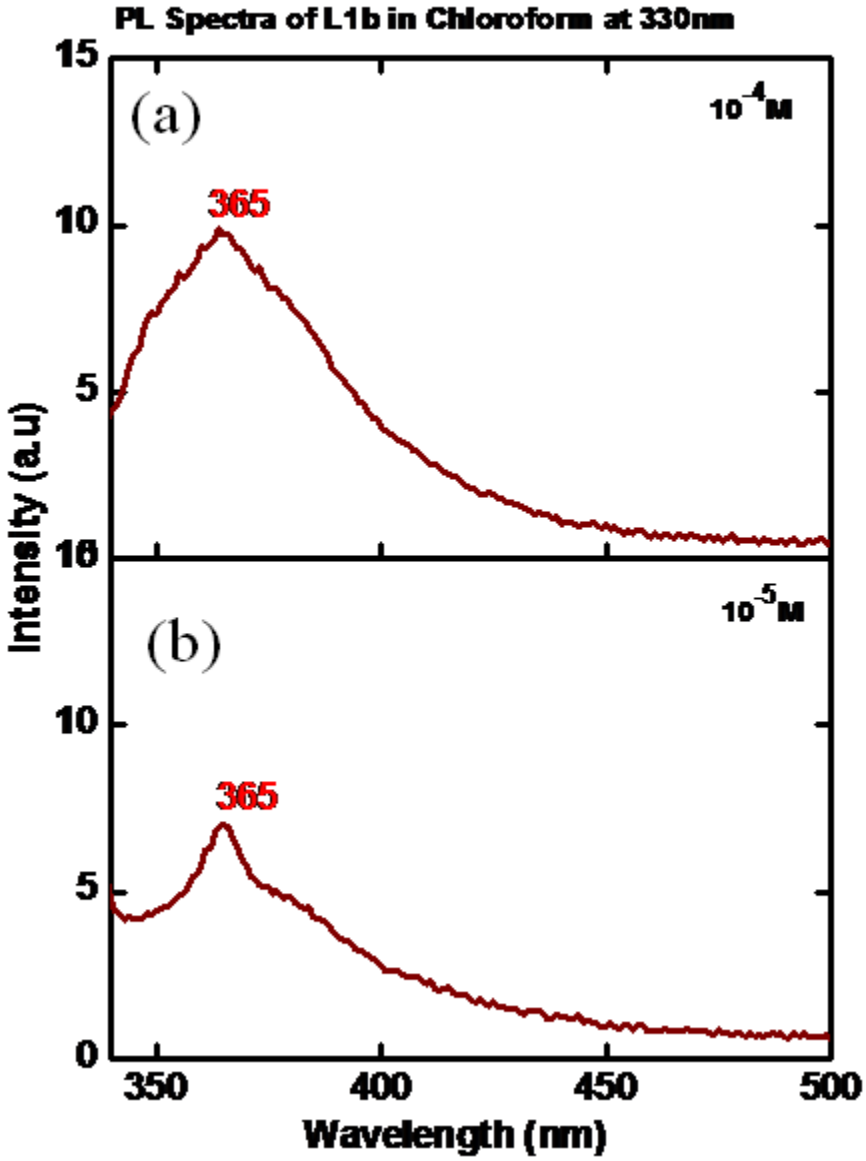


Figure S33: Excitation Spectra of L2a in $CHCl_3$ in different concentrations: (a) 5×10^{-2}M (b) 10^{-2}M (c) 5×10^{-3}M, (d) 10^{-3}M (Emission Wavelength is kept at 370 nm)

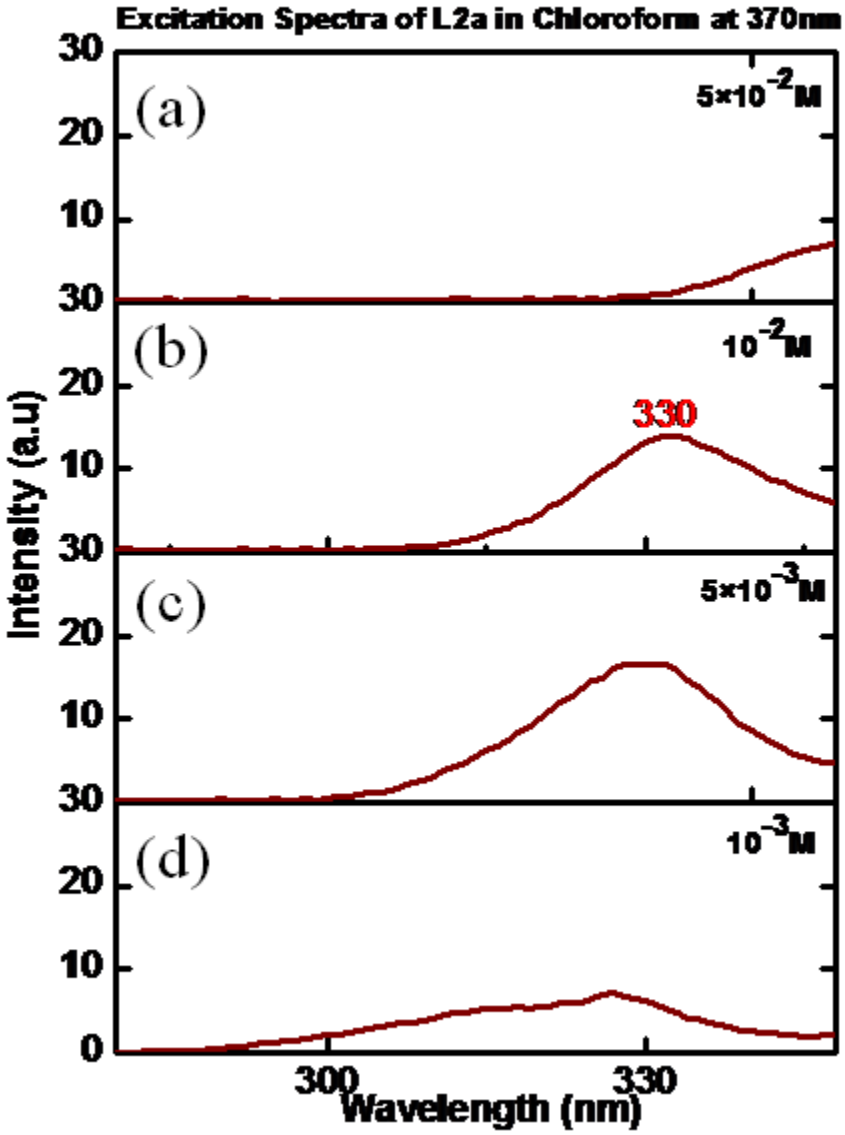


Figure S34: Excitation Spectra of L3a in $CHCl_3$ in different concentrations: (a) 5×10^{-1}M (b) (a) 2×10^{-1}M; (c) 10^{-1}M (d) 5×10^{-2}M, (e) 10^{-2}M, (f) 5×10^{-3}M; (g) 10^{-3} (Emission Wavelength is kept at 460 nm)

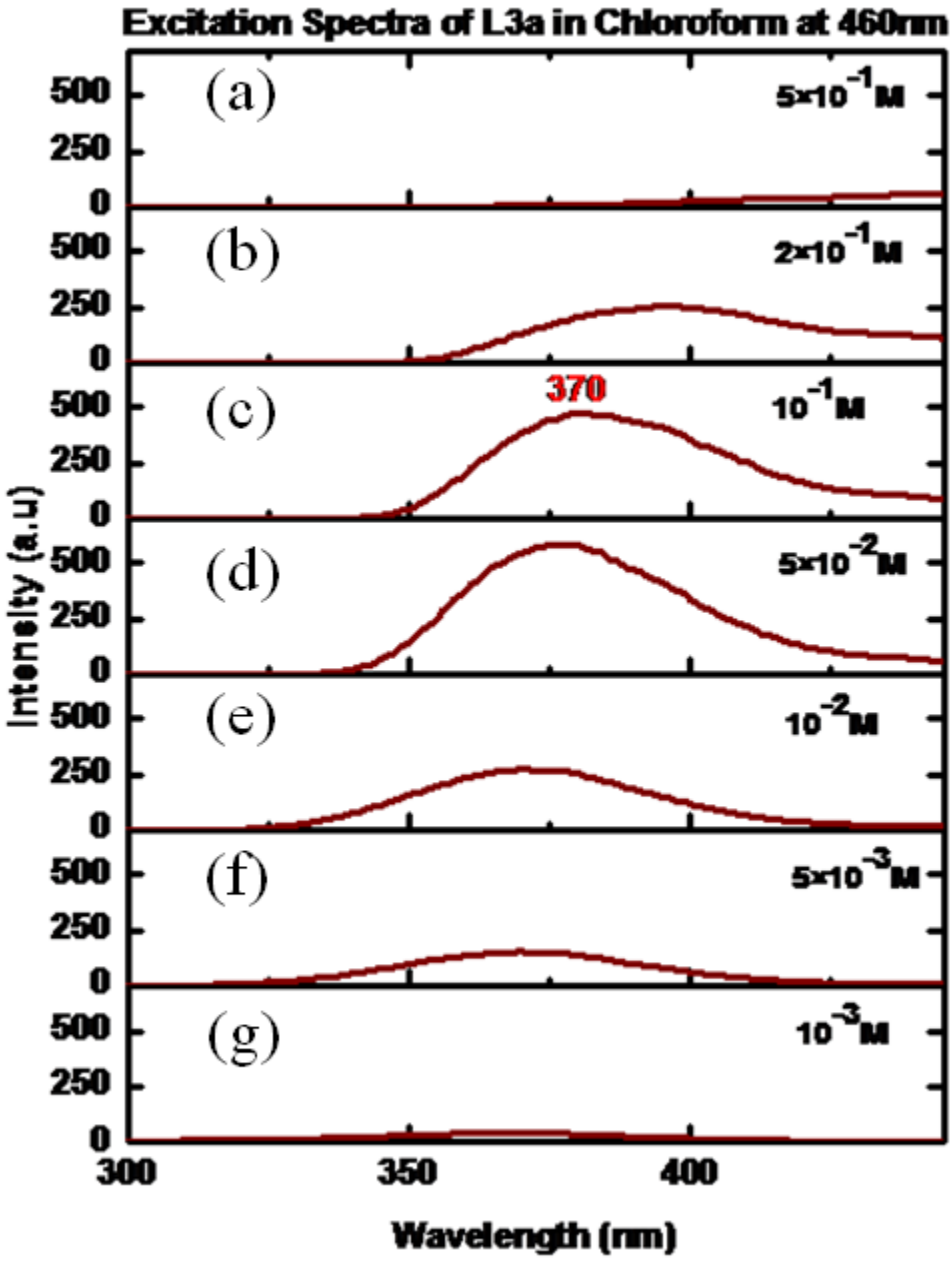


Figure S35: PL Spectra of L3a in $CHCl_3$ in different concentrations: (a) 5×10^{-1}M (b) (a) 2×10^{-1}M; (c) 10^{-1}M (d) 5×10^{-2}M, (e) 10^{-2}M, (f) 5×10^{-3}M; (g) 10^{-3} (Excitation Wavelength is kept at 420 nm)

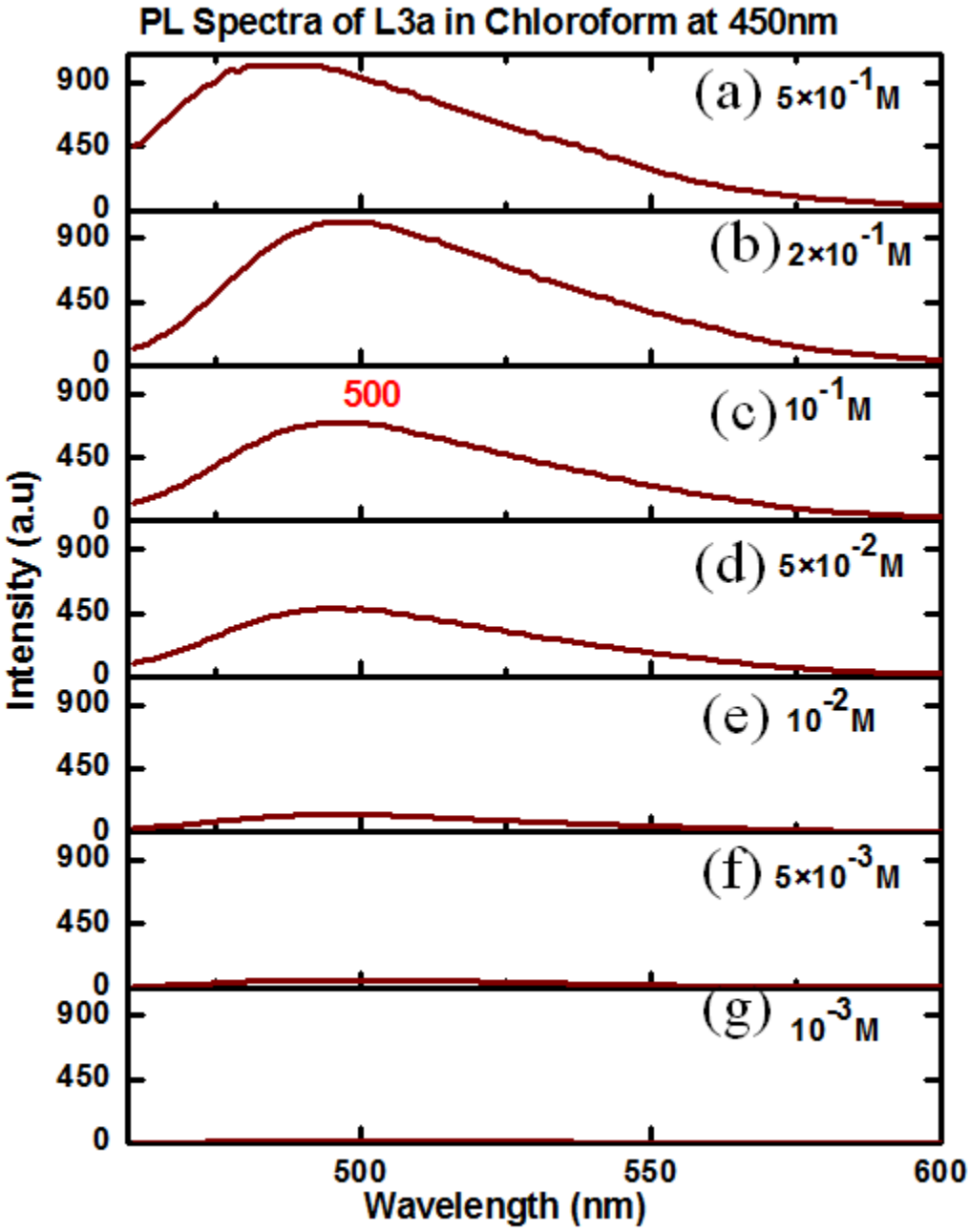


Figure S36: PL Spectra (at an excitation wavelength of 450 nm) of L3a in solid state

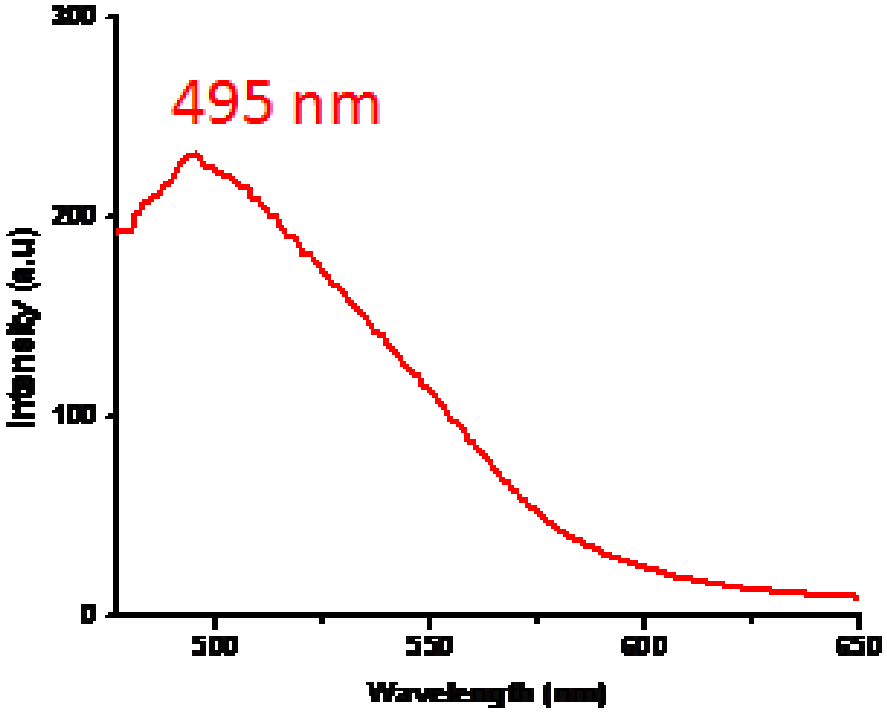


Figure S37: ^{1}H NMR spectra of L3b in $CDCl_3$ by changing the concentration of compound; (a) 1 M; (b) 10^{-1} M; (c) 10^{-2} M; (d) 10^{-3} M

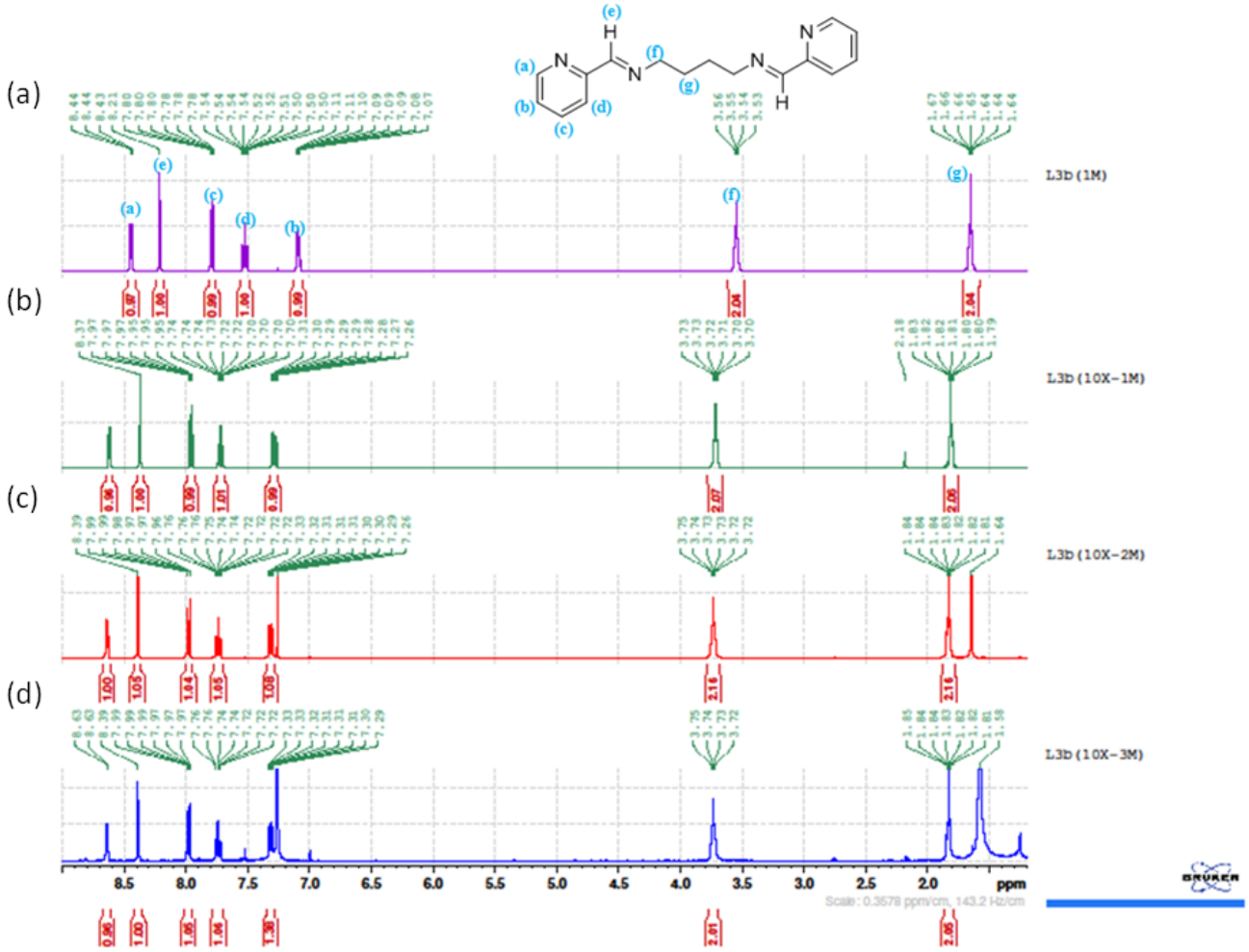


Figure S38: NOESY of L3b in $CDCl_3$ at a concentration of 1 M

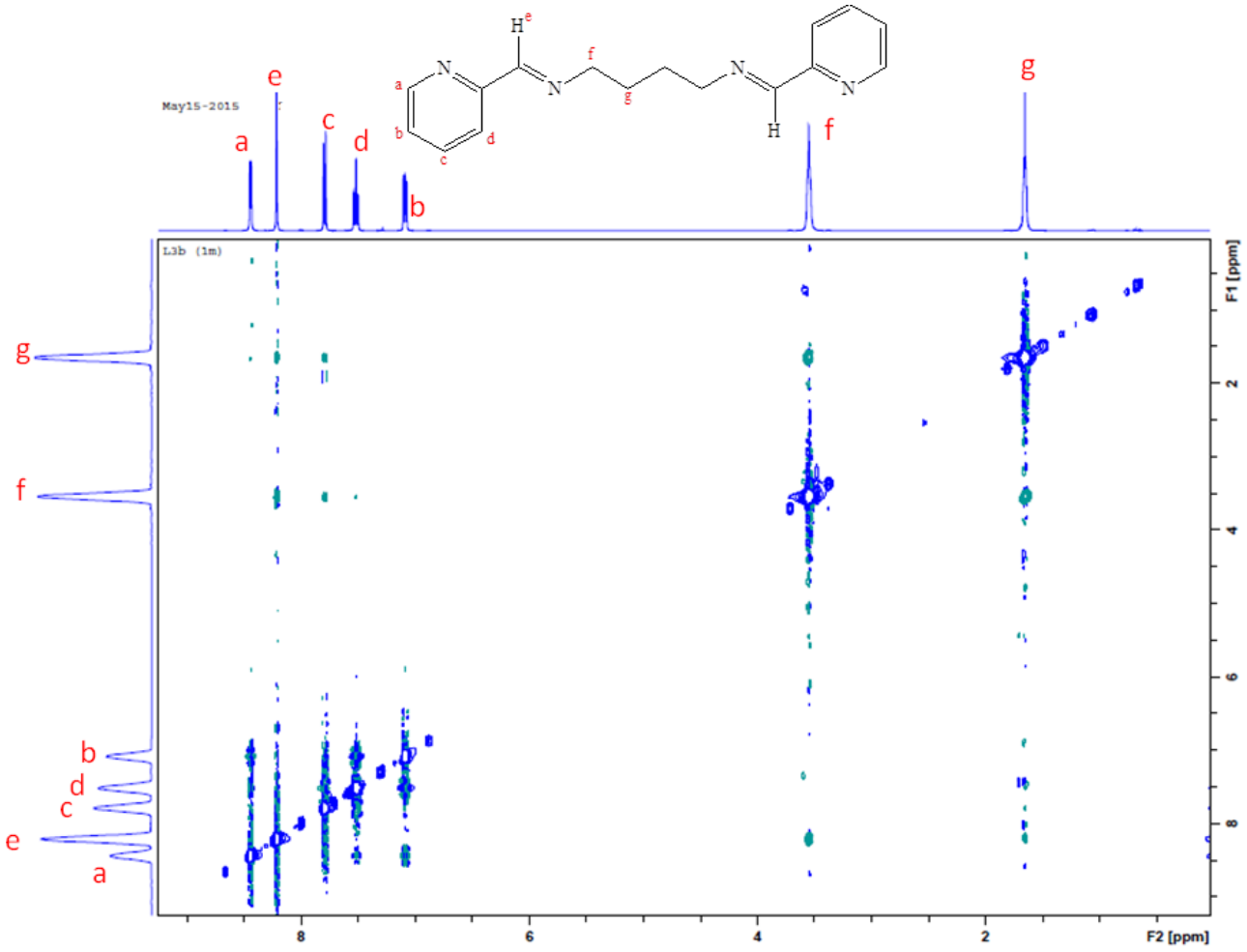
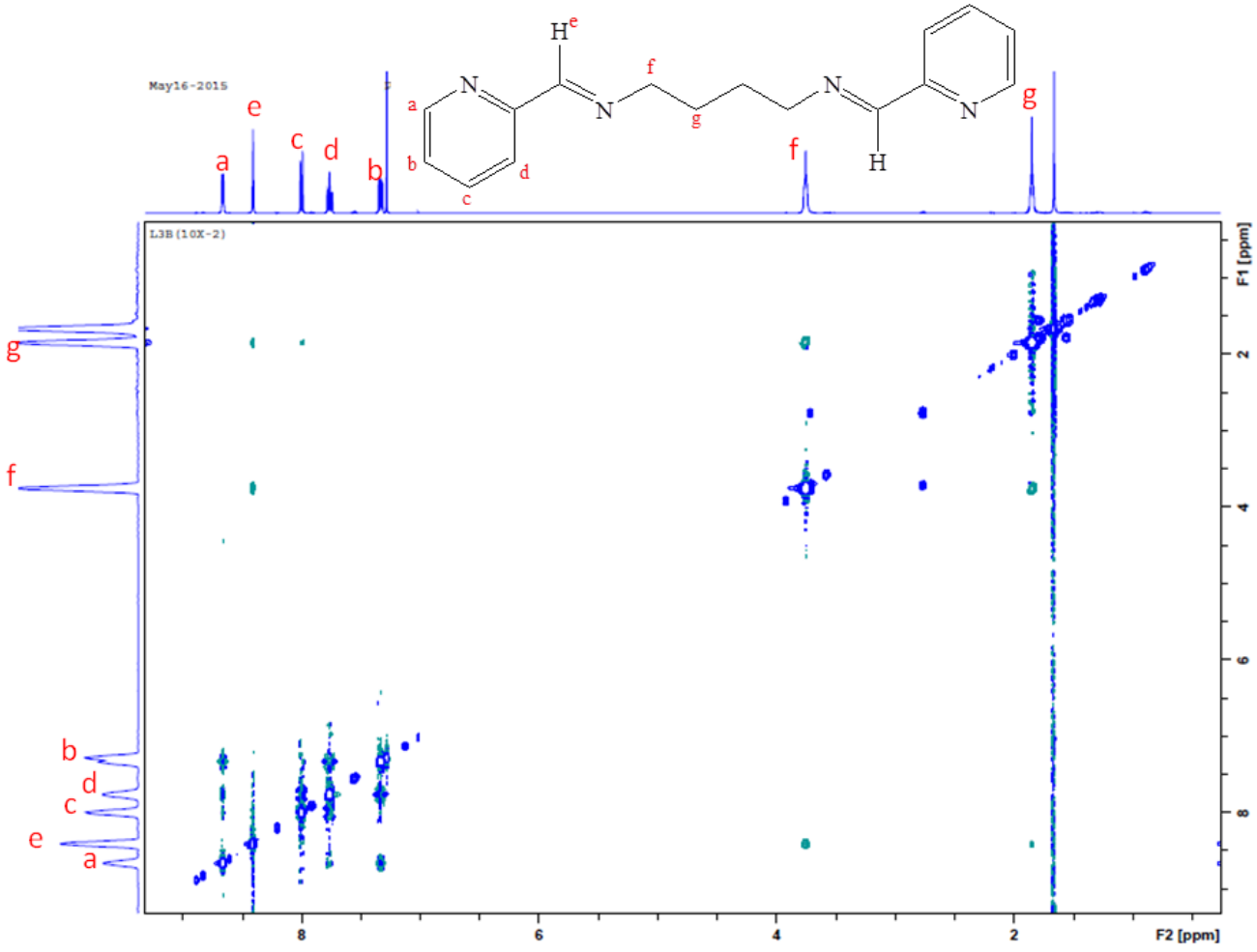


Figure S39: NOESY of L3b in $CDCl_3$ at a concentration of 10^{-2} M



Compound L1a

checkCIF/PLATON (full publication check)

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No syntax errors found. CIF dictionary

Please wait while processing .... Interpreting this report

Datablock: I

Bond precision: C-C = 0.0056 A Wavelength=0.71073

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alpha=90 beta=98.394(4) gamma=90

Temperature: 293 K

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Hall group	P 2yb	P 2yb
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Sum formula	C14 H14 N4	C14 H14 N4
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Dx,g cm-3	1.214	1.214
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Mu (mm-1)	0.076	0.076
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F000'	756.22	
h,k,lmax	10,21,15	10,21,15
Nref	7679[3970]	7598
Tmin,Tmax	0.982,0.985	0.843,1.000

Tmin' 0.977

Correction method= # Reported T Limits: Tmin=0.843 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 1.91/0.99 Theta(max)= 25.990

R(reflections)= 0.0637(4636) wR2(reflections)= 0.1900(7598)

S = 1.001 Npar= 493

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level B

PLAT230_ALERT_2_B Hirshfeld Test Diff for N4A -- C10A .. 7.2 su

And 3 other PLAT230 Alerts

More ...

Alert level C

STRVA01_ALERT_4_C Flack parameter is too small

From the CIF: _refine_ls_abs_structure_Flack -2.000

From the CIF: _refine_ls_abs_structure_Flack_su 3.000

And 4 other PLAT230 Alerts

More ...

PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... N4A Check

And 2 other PLAT241 Alerts

More ...

PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C11A Check

PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0056 Ang.

PLAT411_ALERT_2_C Short Inter H...H Contact H3B .. H11A .. 2.00 Ang.

PLAT412_ALERT_2_C Short Intra XH3 .. XHn H11A .. H9A2 .. 1.81 Ang.

PLAT412_ALERT_2_C Short Intra XH3 .. XHn H2C .. H7C2 .. 1.87 Ang.

PLAT413_ALERT_2_C Short Inter XH3 .. XHn H2C .. H9A1 .. 2.06 Ang.

Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF Please Do !

PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 3.000 Report

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large. 0.10 Report

PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check

PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 18 Note

PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

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14 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

7 **ALERT level G** = General information/check it is not something unexpected

Compound L2a

checkCIF/PLATON (full publication check)

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary

Please wait while processing .... Interpreting this report

Datablock: I

Bond precision: C-C = 0.0048 A Wavelength=0.71073

Cell: a=19.379(5) b=24.584(5) c=12.300(5)

alpha=90 beta=90 gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	5860(3)	5860(3)
Space group	P c a b	P c a b
Hall group	-P 2bc 2ac	-P 2bc 2ac
Moiety formula	C16 H18 N4	C16 H18 N4
Sum formula	C16 H18 N4	C16 H18 N4
Mr	266.34	266.34
Dx,g cm-3	1.208	1.208
Z	16	16
Mu (mm-1)	0.075	0.075
F000	2272.0	2272.0
F000'	2272.67	
h,k,lmax	23,30,15	23,30,15
Nref	5757	5740
Tmin,Tmax	0.982,0.985	0.900,1.000
Tmin'	0.978	

Correction method= # Reported T Limits: Tmin=0.900 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 26.000

R(reflections)= 0.0813(2710) wR2(reflections)= 0.2360(5740)

S = 1.038 Npar= 366

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level C

PLAT026_ALERT_3_C Ratio Observed / Unique Reflections too Low .... 47 %

PLAT147_ALERT_1_C su on Symmetry Constrained Cell Angle(s) ..... Please Check

PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C6A Check

PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0048 Ang.

PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note

C16 H18 N4

Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF Please Do !

PLAT128_ALERT_4_G Alternate Setting for Input Space Group Pcab Pbca Note

PLAT153_ALERT_1_G The su's on the Cell Axes are Equal ..... 0.00500 Ang.

PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check

PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 16 Note

PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

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Compound L3b

checkCIF/PLATON (full publication check)

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No syntax errors found. CIF dictionary

Please wait while processing .... Interpreting this report

Datablock: I

Bond precision: C-C = 0.0024 A Wavelength=0.71073

Cell: a=9.2157(5) b=8.9944(5) c=9.3471(5)

alpha=90 beta=107.344(6) gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	739.55(7)	739.55(7)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C16 H18 N4	C16 H18 N4
Sum formula	C16 H18 N4	C16 H18 N4
Mr	266.34	266.34
Dx,g cm-3	1.196	1.196
Z	2	2
Mu (mm-1)	0.074	0.074
F000	284.0	284.0
F000'	284.08	
h,k,lmax	11,11,11	11,11,11
Nref	1451	1448

Tmin,Tmax 0.982,0.985 0.926,1.000

Tmin' 0.978

Correction method= # Reported T Limits: Tmin=0.926 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 26.000

R(reflections)= 0.0445(993) wR2(reflections)= 0.1214(1448)

S = 1.042 Npar= 91

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF Please Do !

PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check

PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check

PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

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