Supporting information

Molecular-iodine catalyzed selective construction of cyclopenta[*b*]indoles from indoles and acetone: a green gateway to indole-fused cycles

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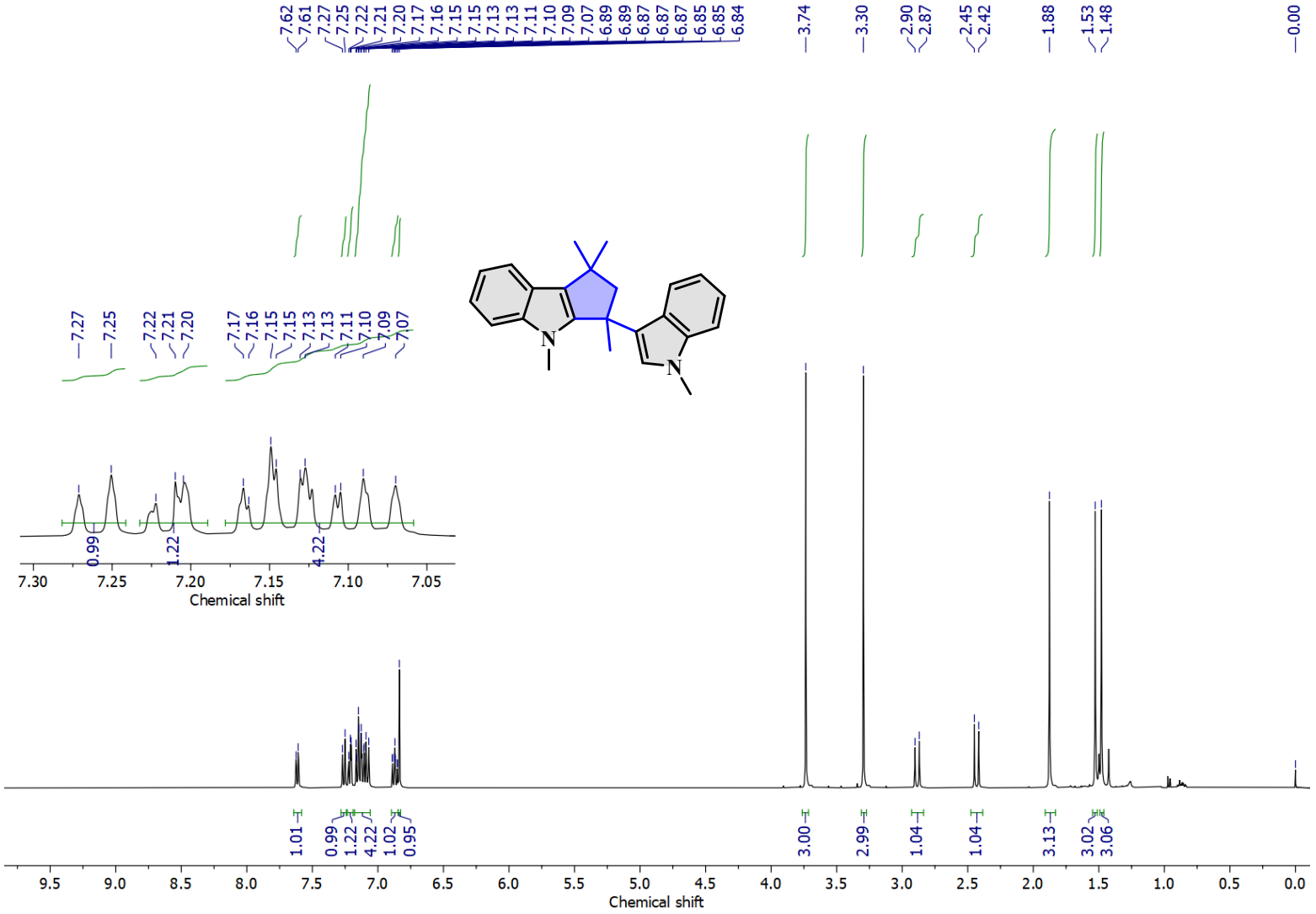


Fig. S1 400 MHz ^{1}H NMR spectrum of (**2a**)[1] in $CDCl_3$

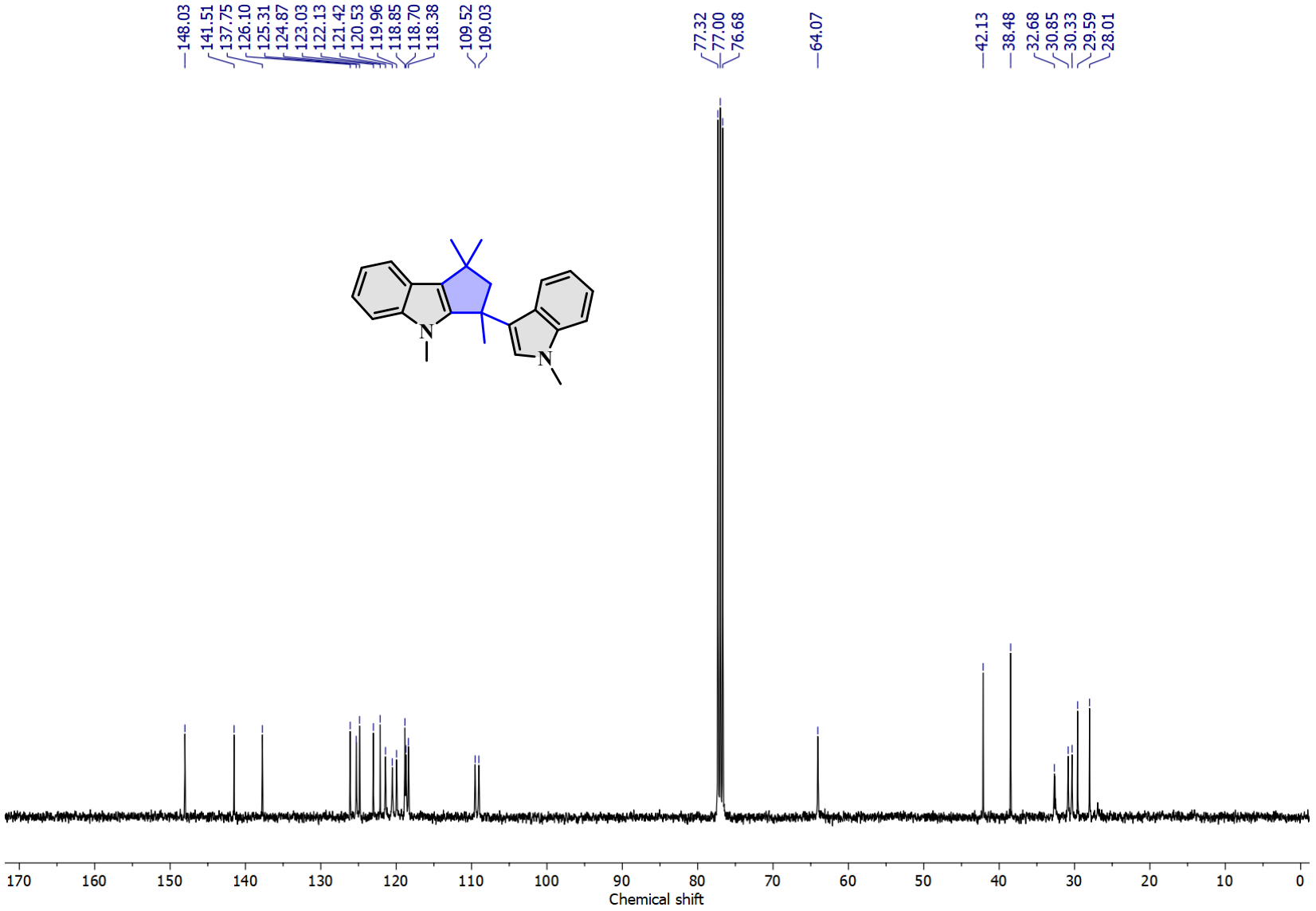
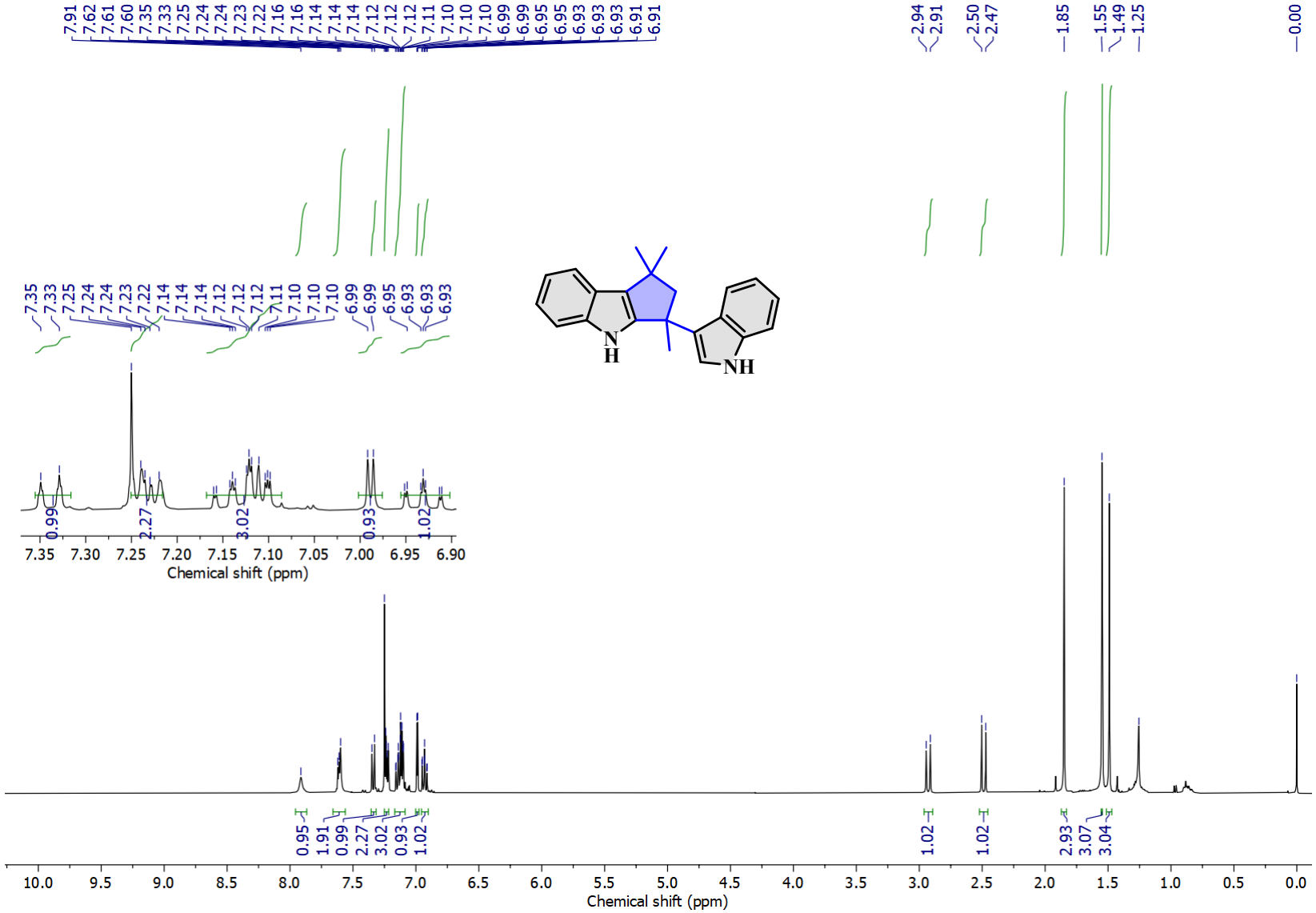


Fig. S2 100 MHz ^{13}C NMR spectrum of (**2a**)[1] in $CDCl_3$



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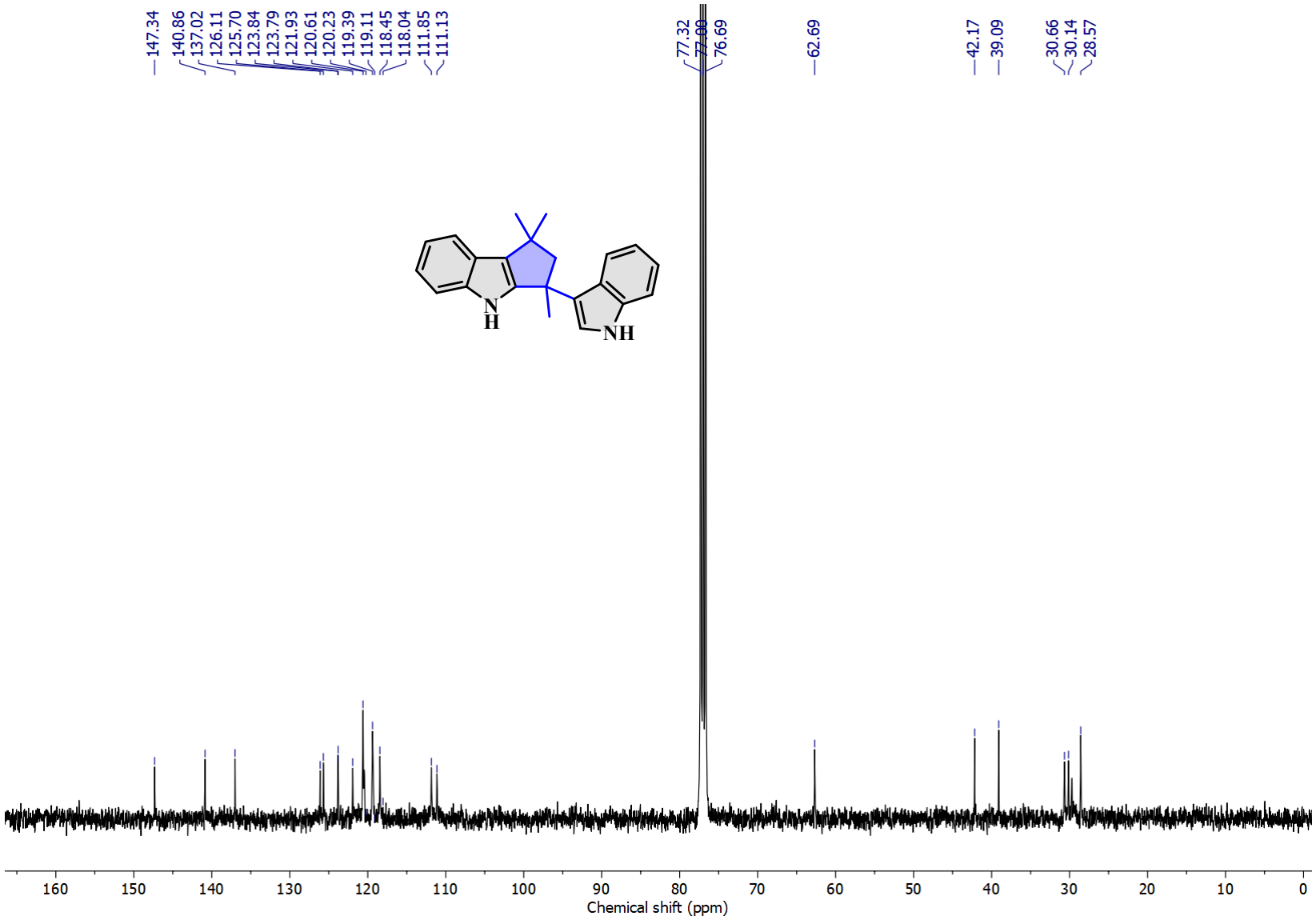

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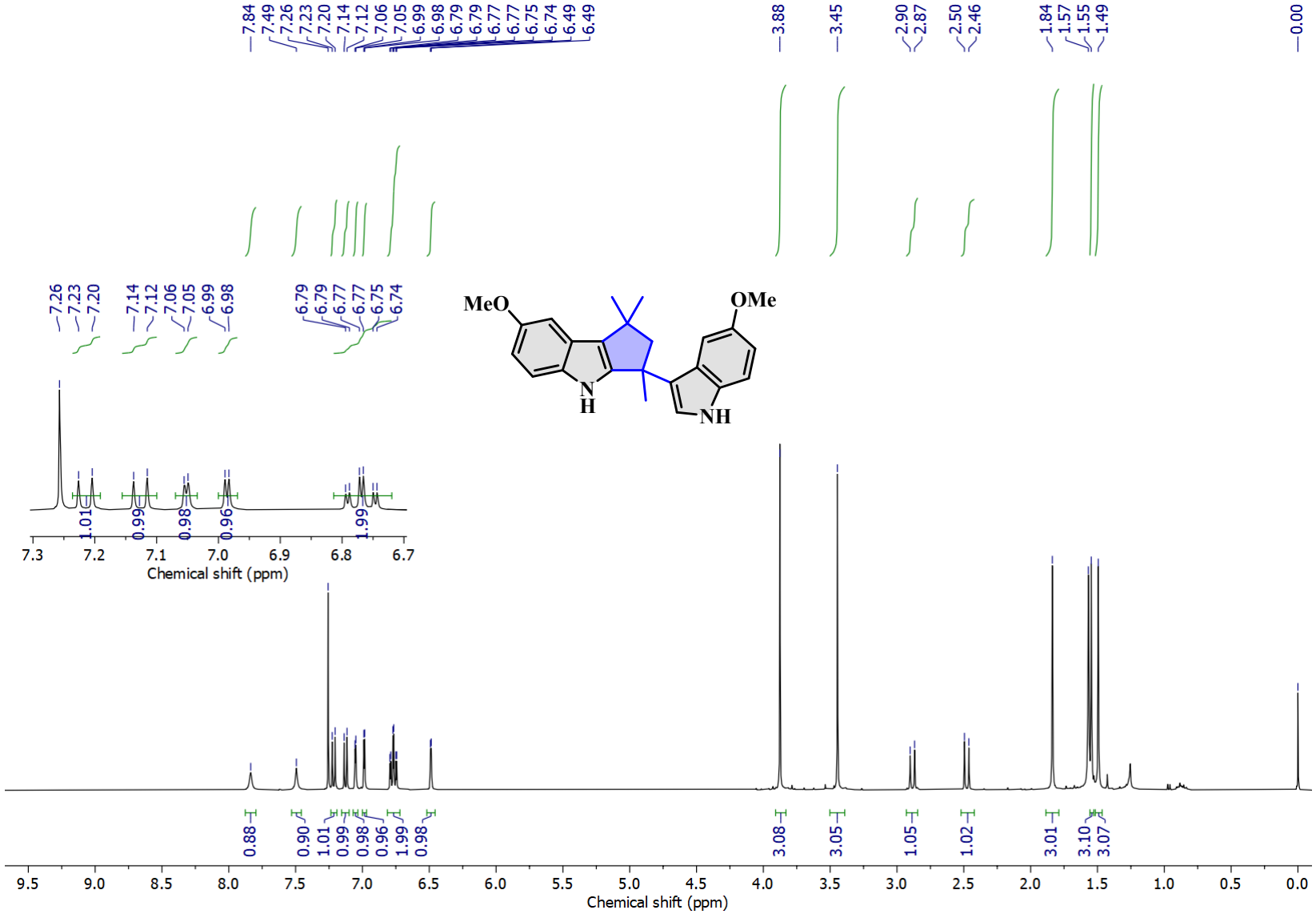
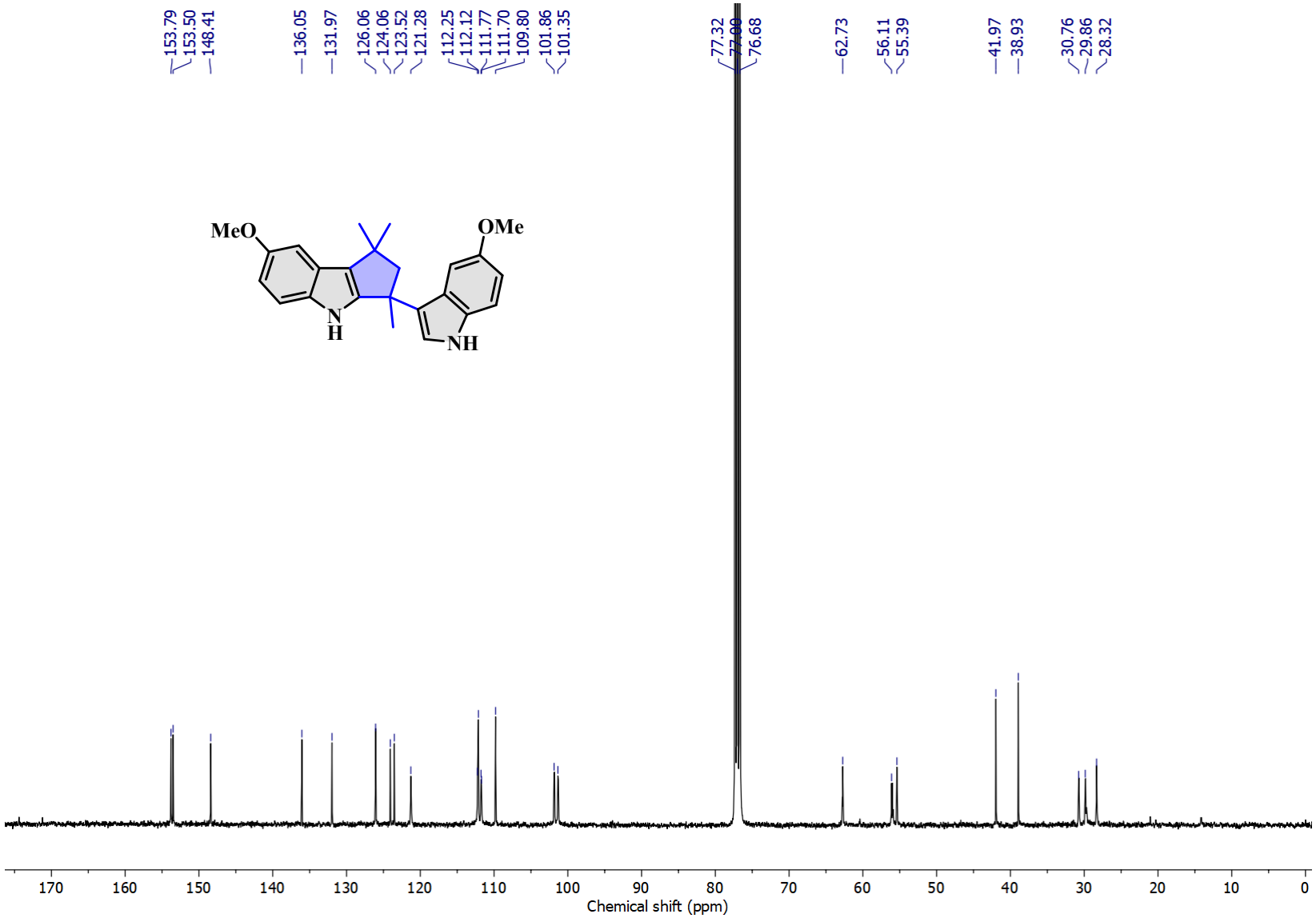


Fig. S5 400 MHz ^{1}H NMR spectrum of **(2c)²** in $CDCl_3$



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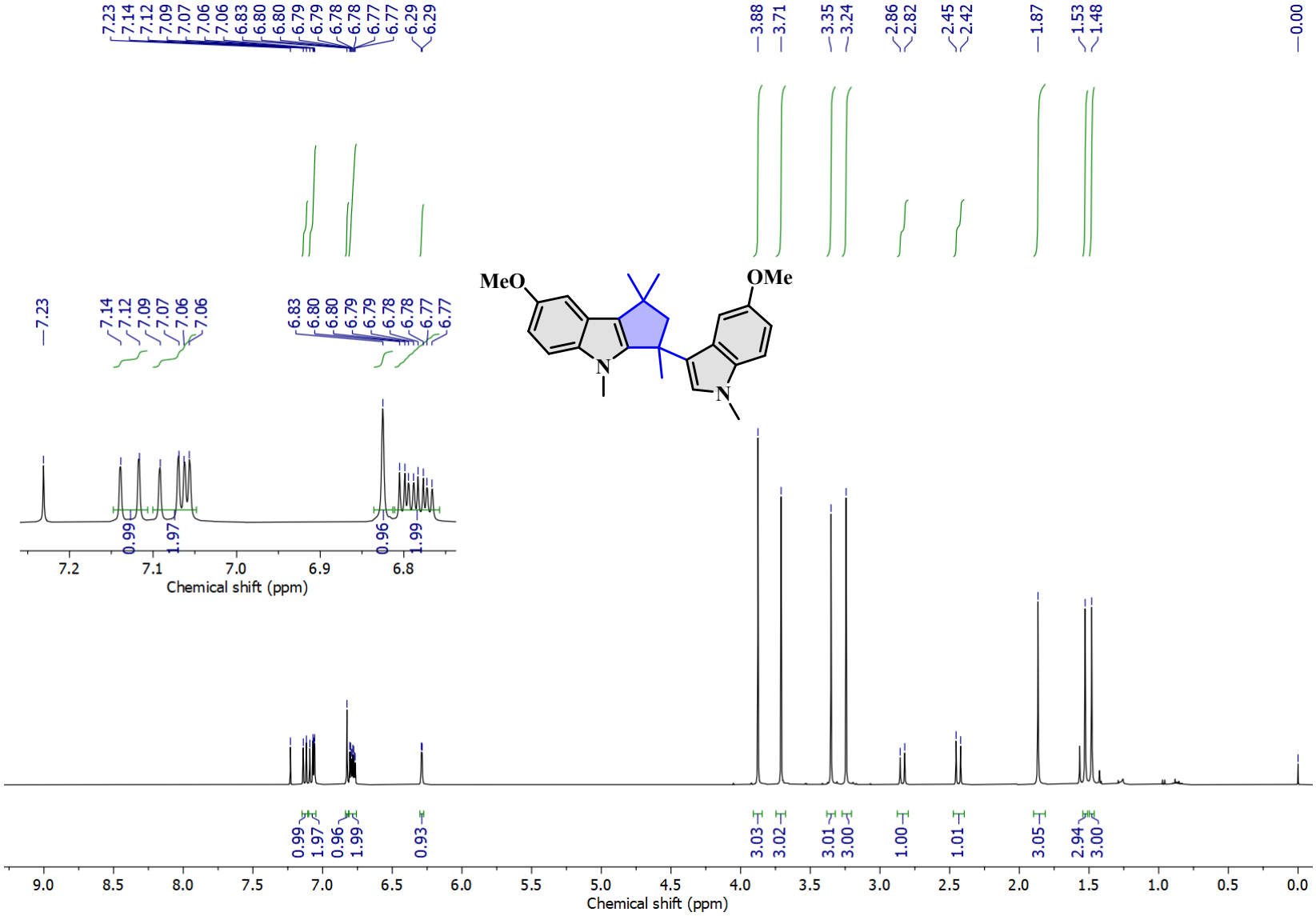

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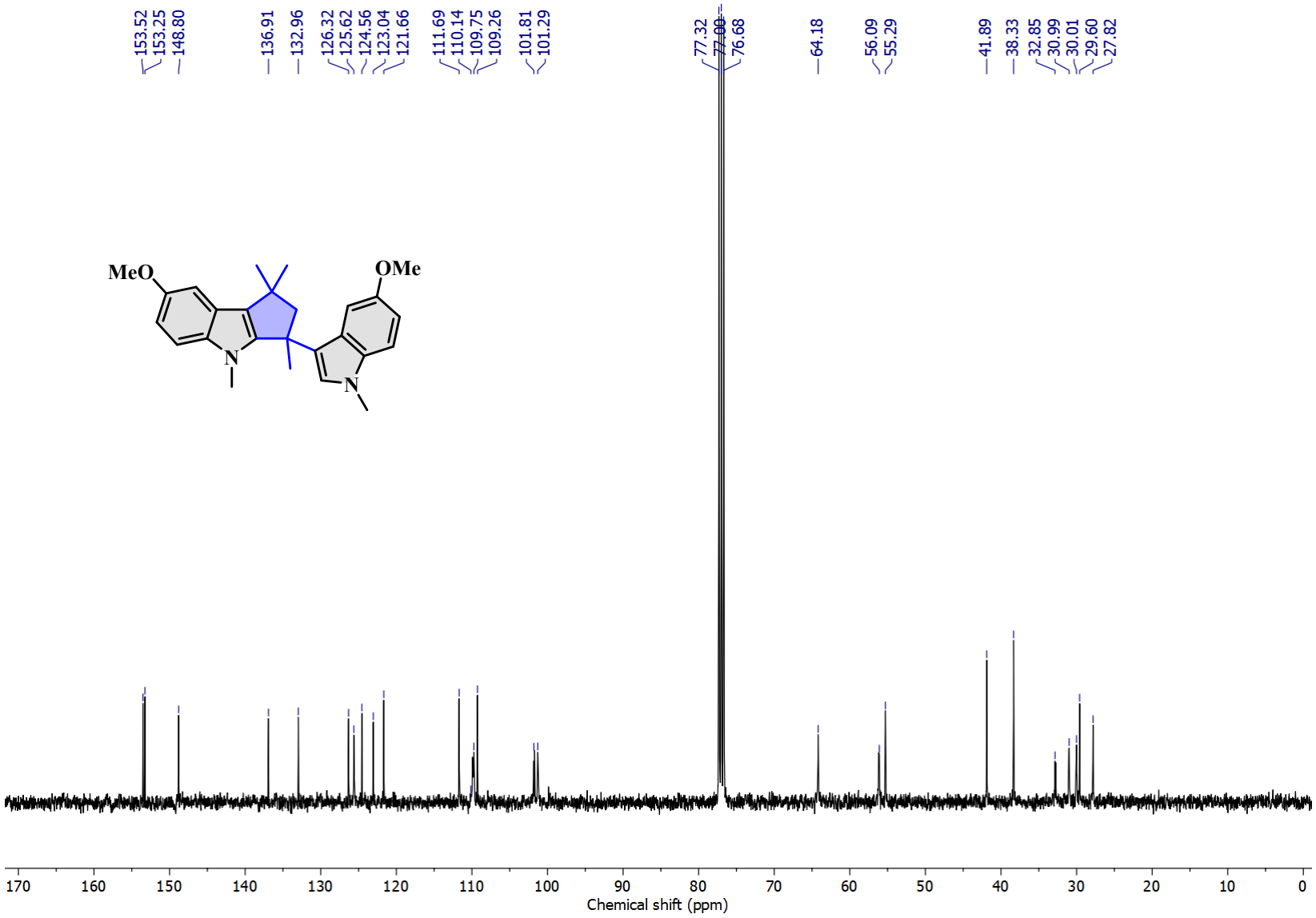

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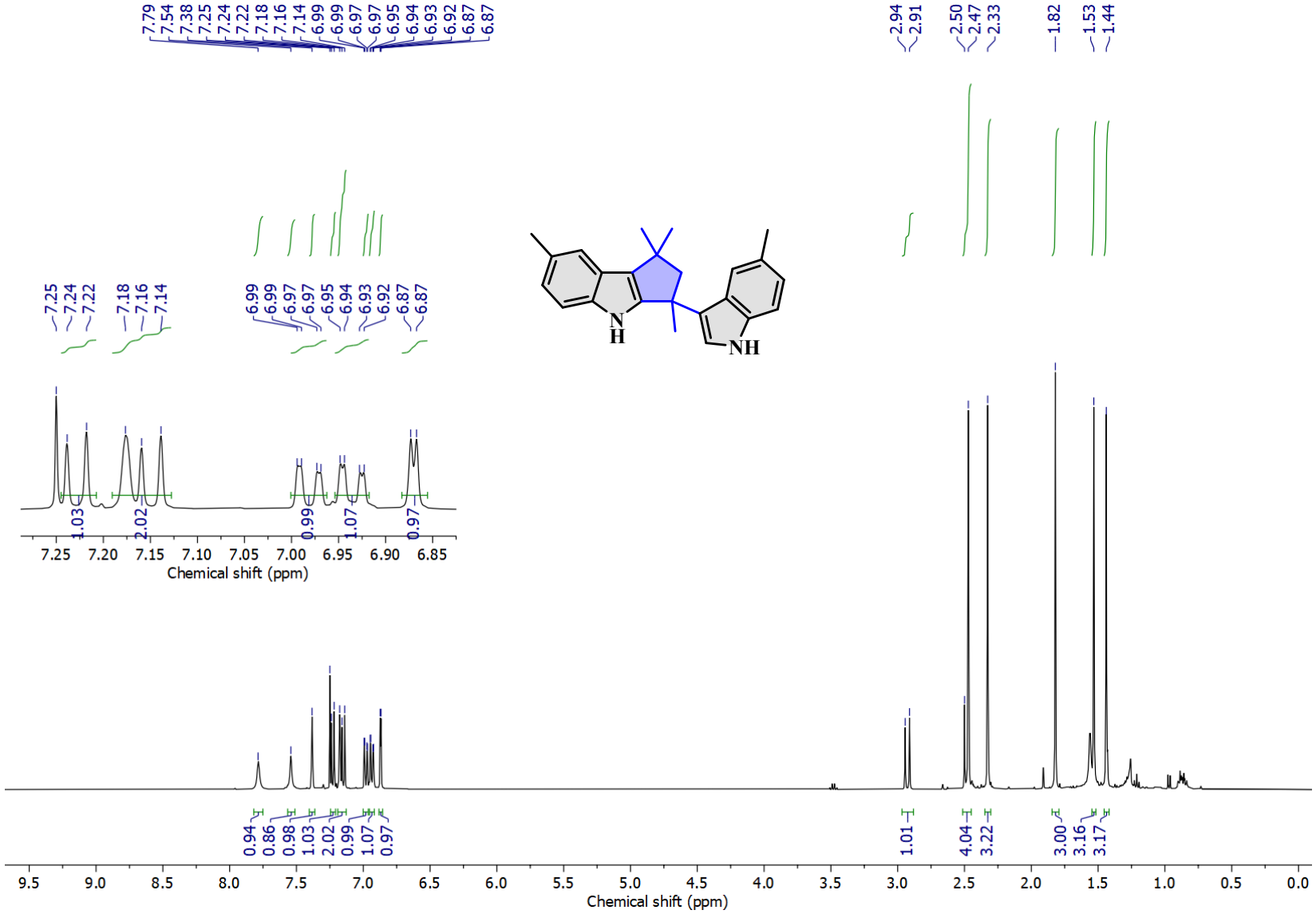

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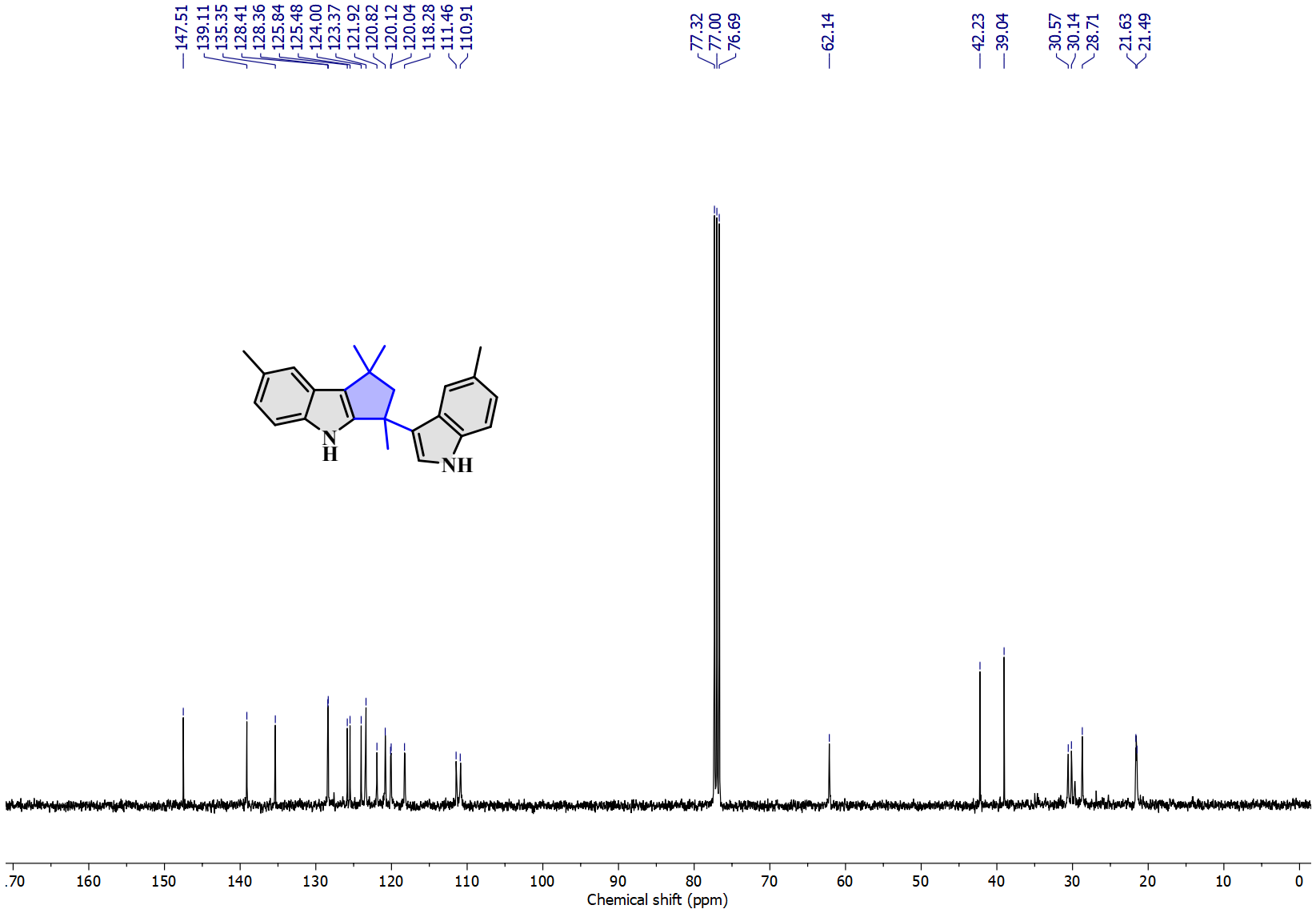

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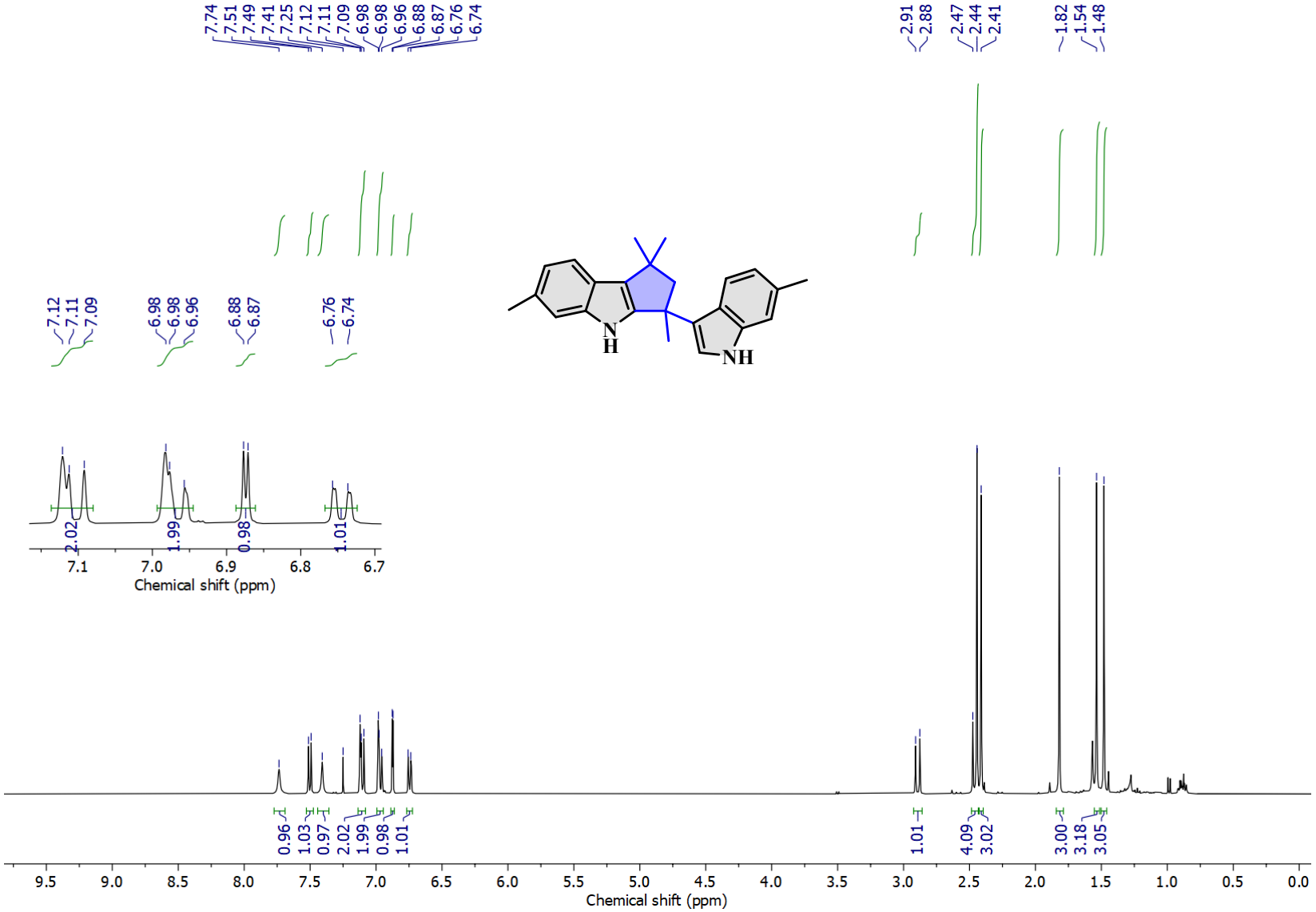

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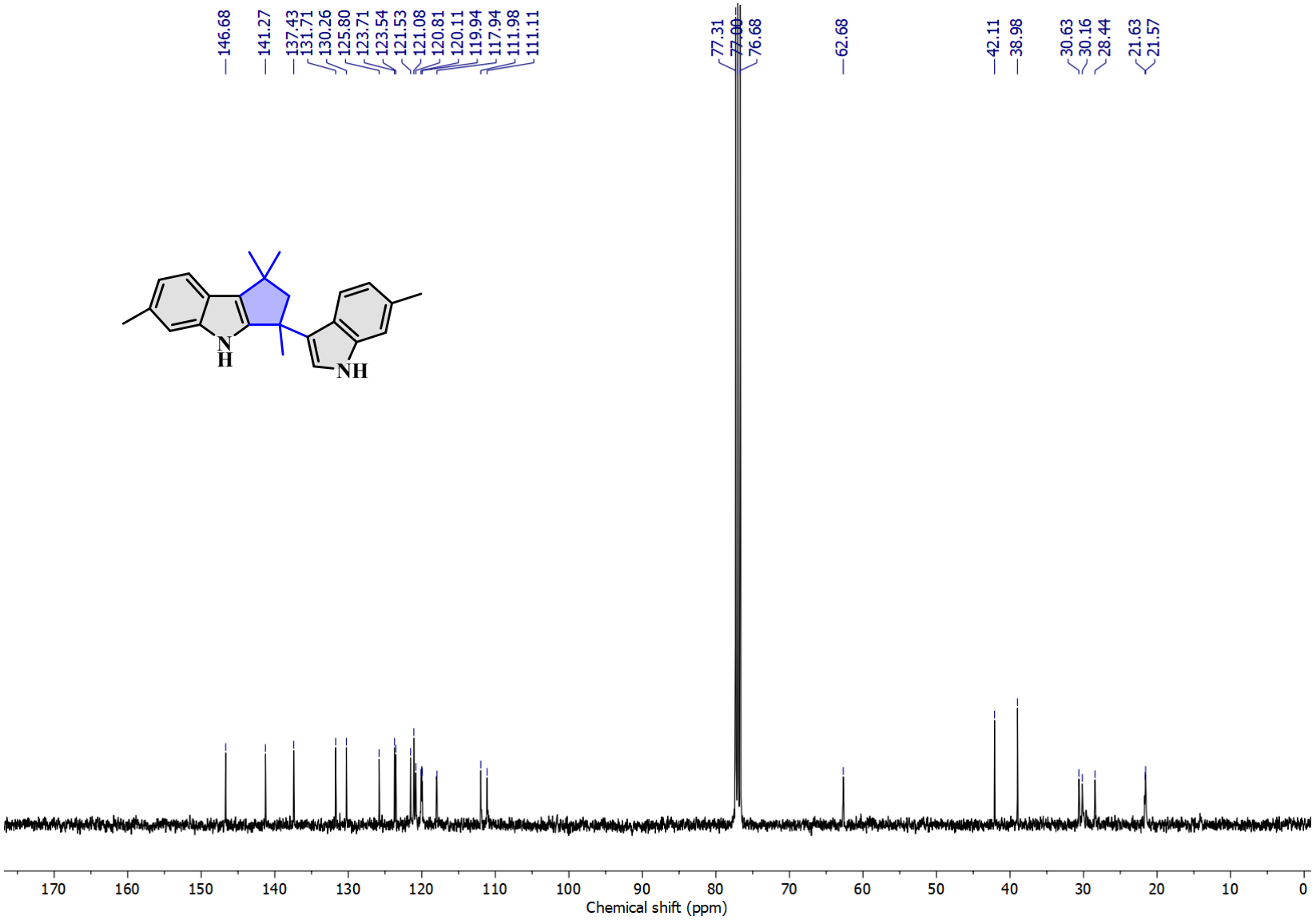

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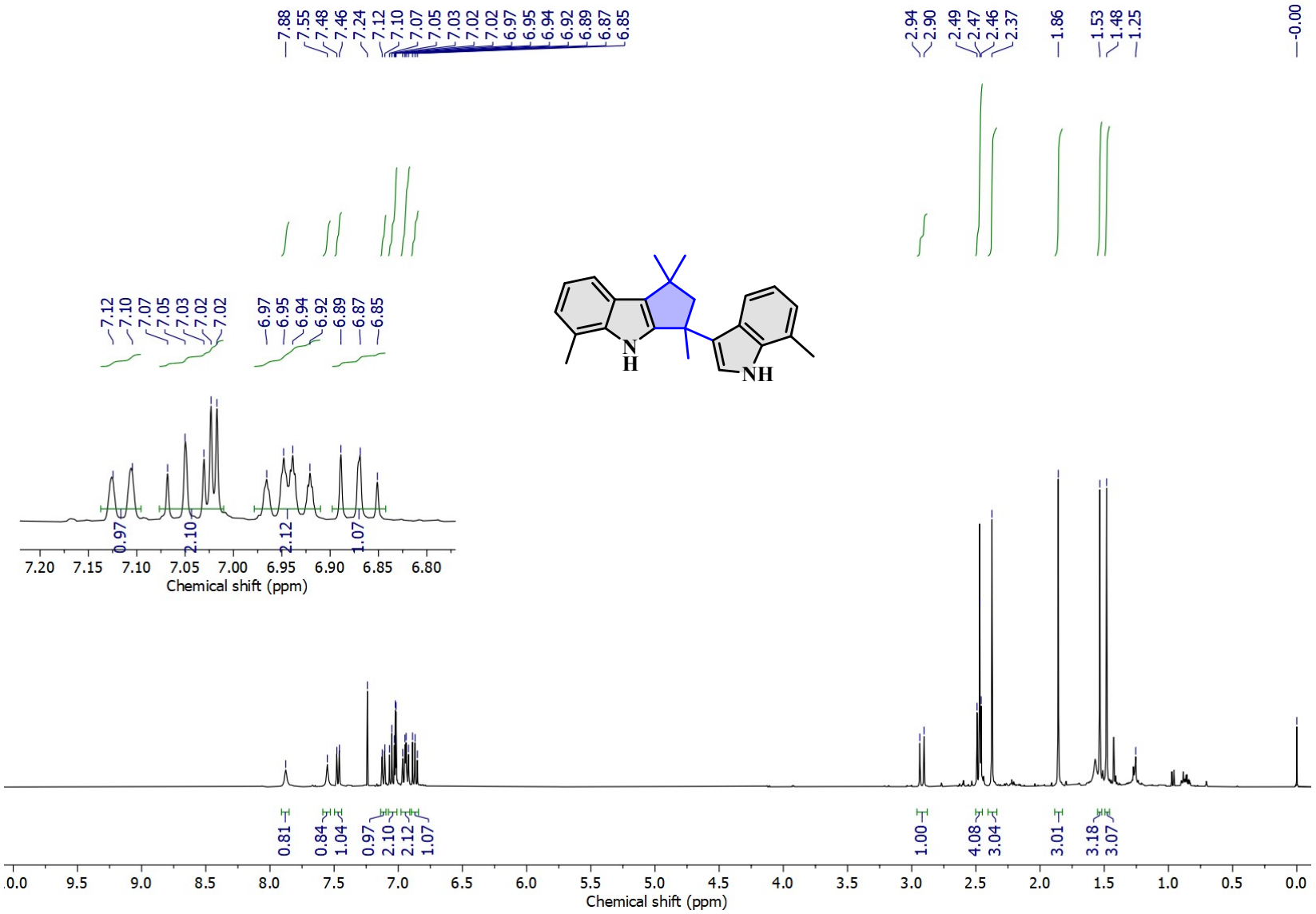

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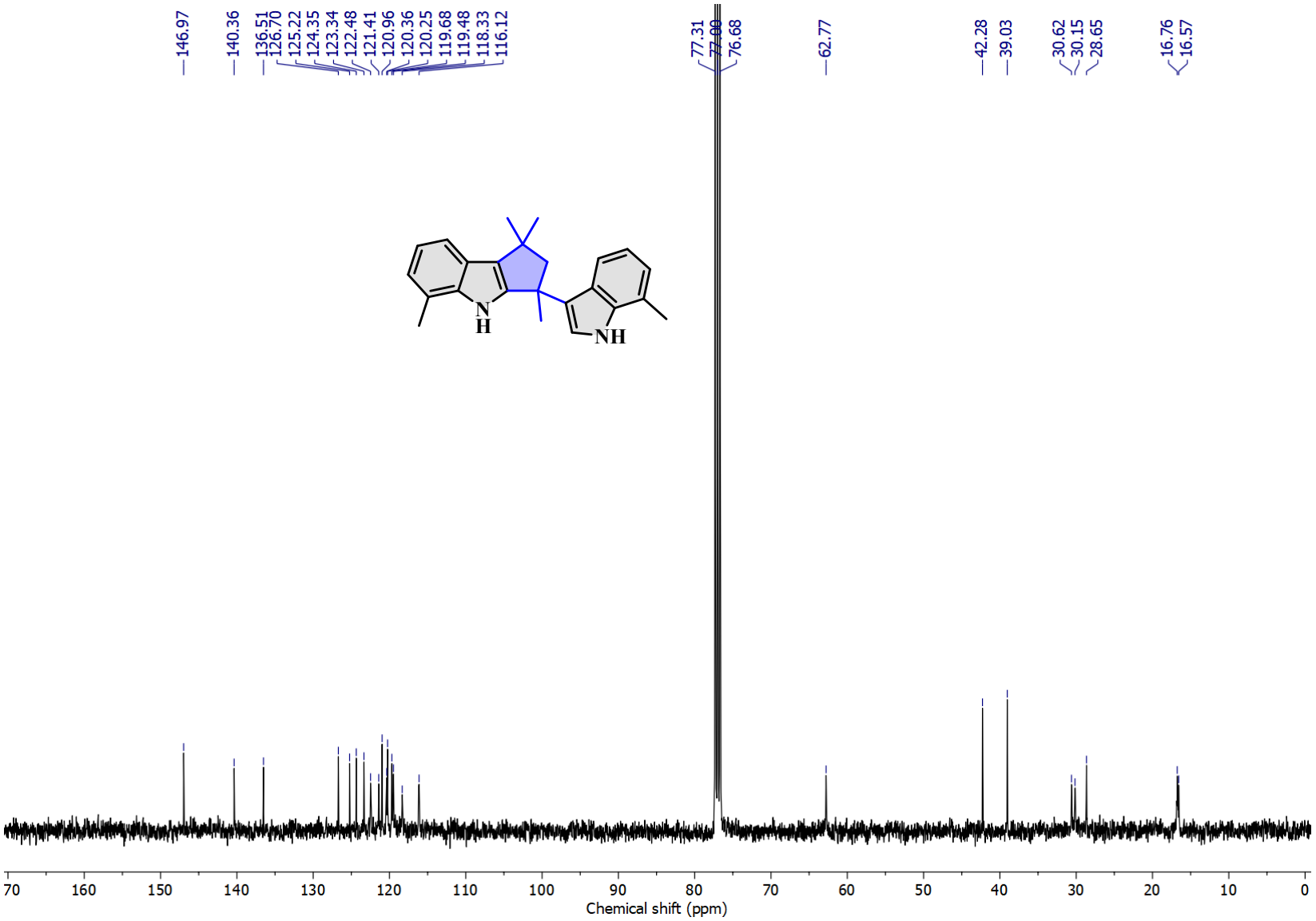

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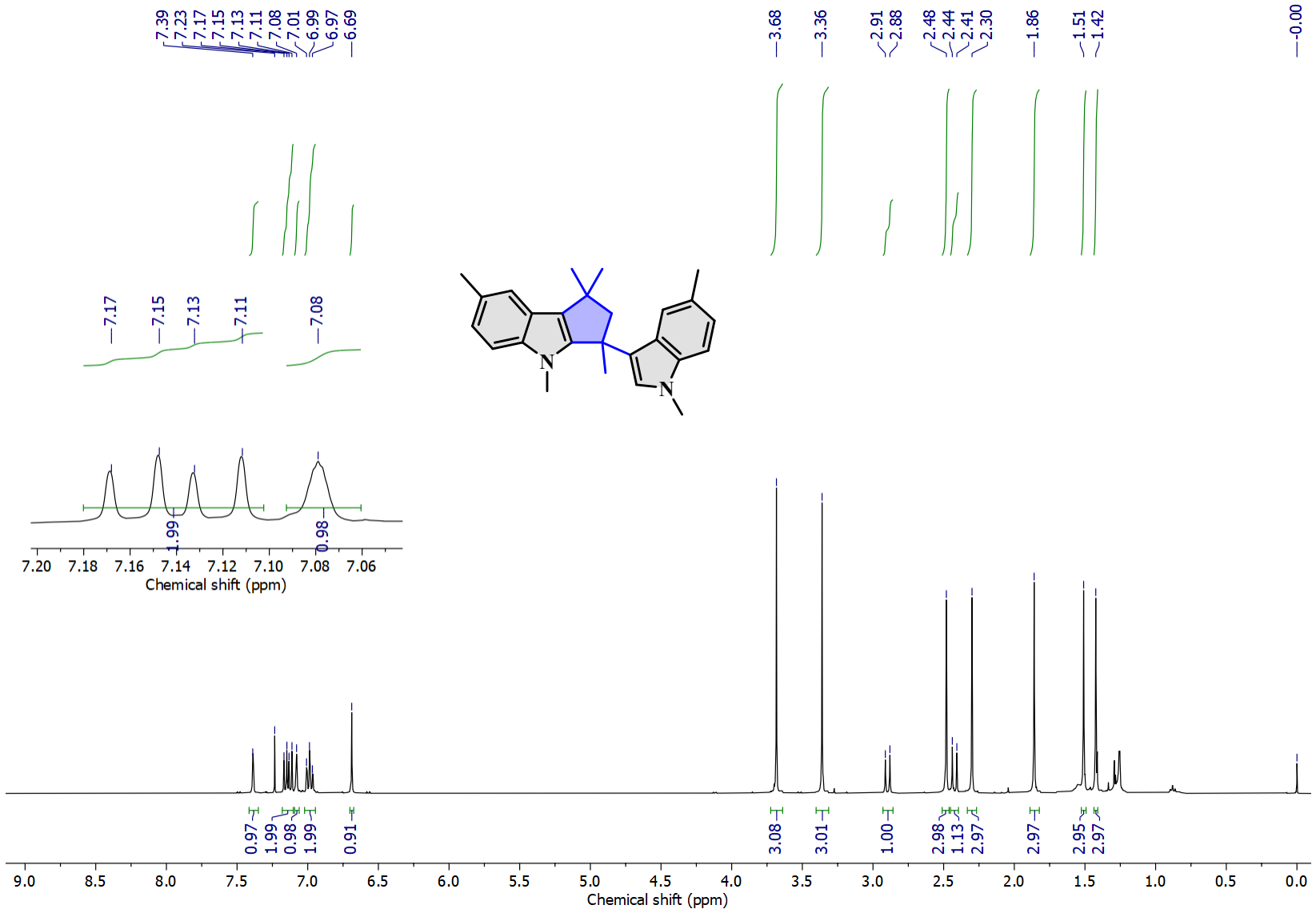

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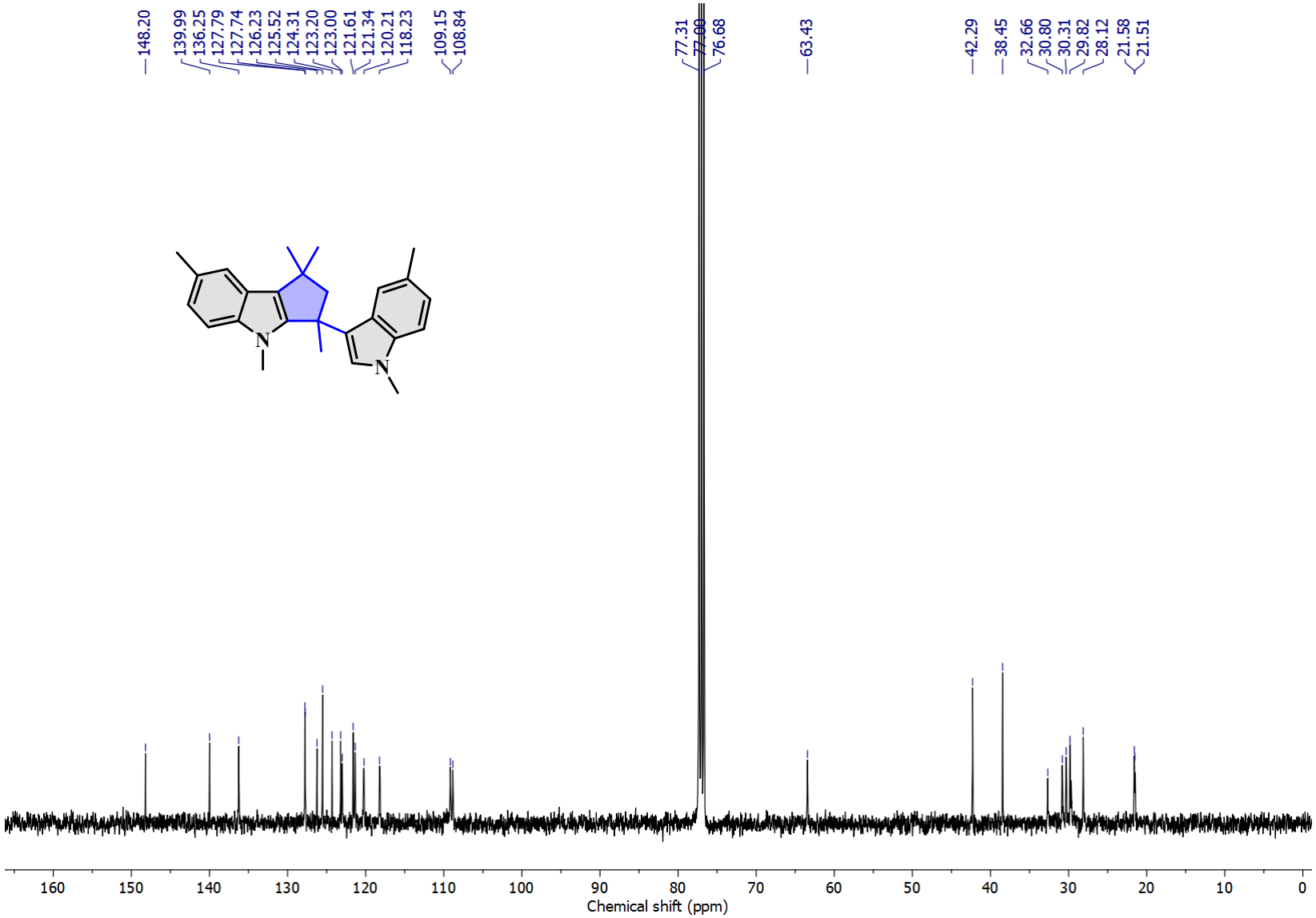
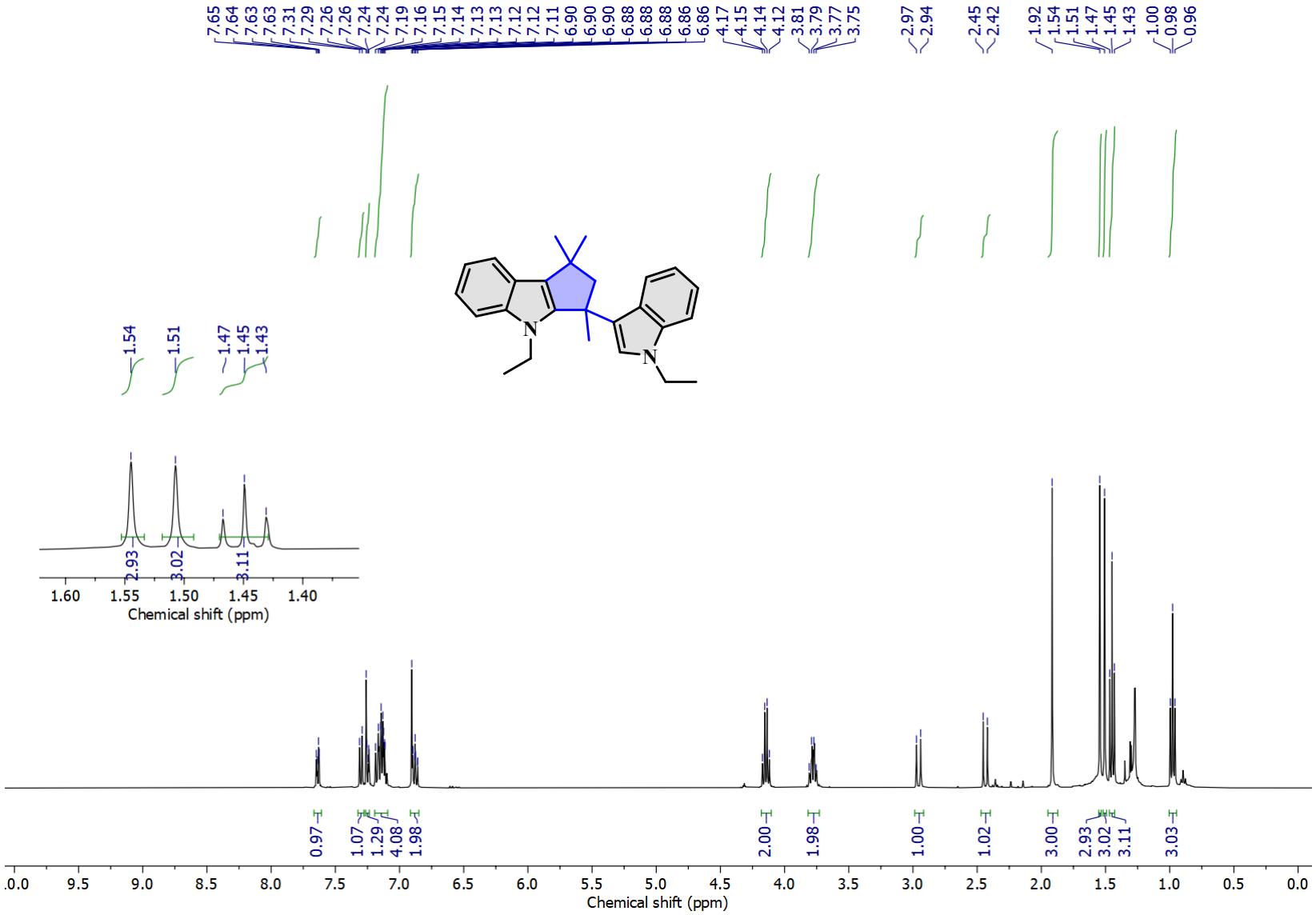


Fig. S16 100 MHz ^{13}C NMR spectrum of (**2h**)^2 in $CDCl_3$



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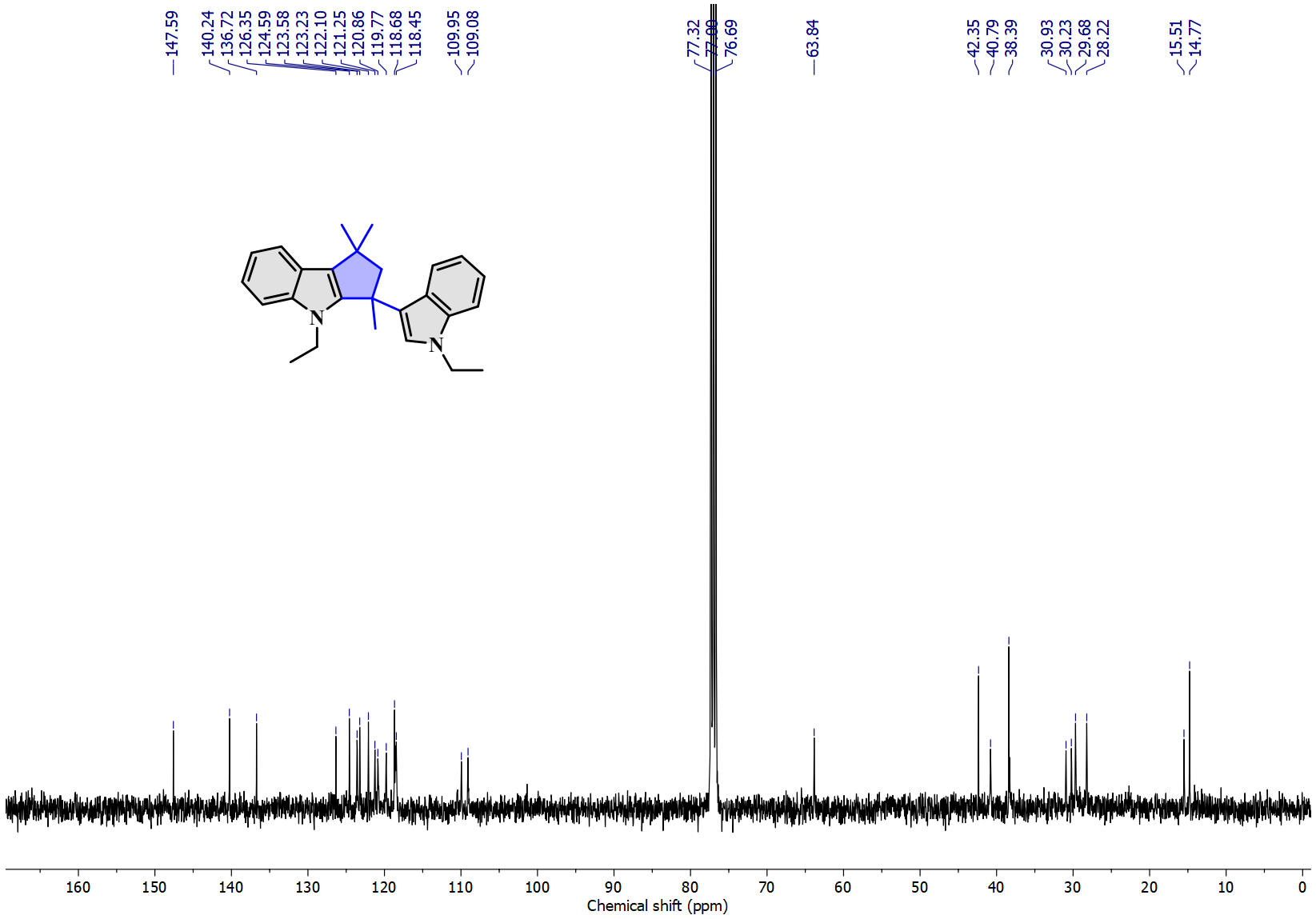

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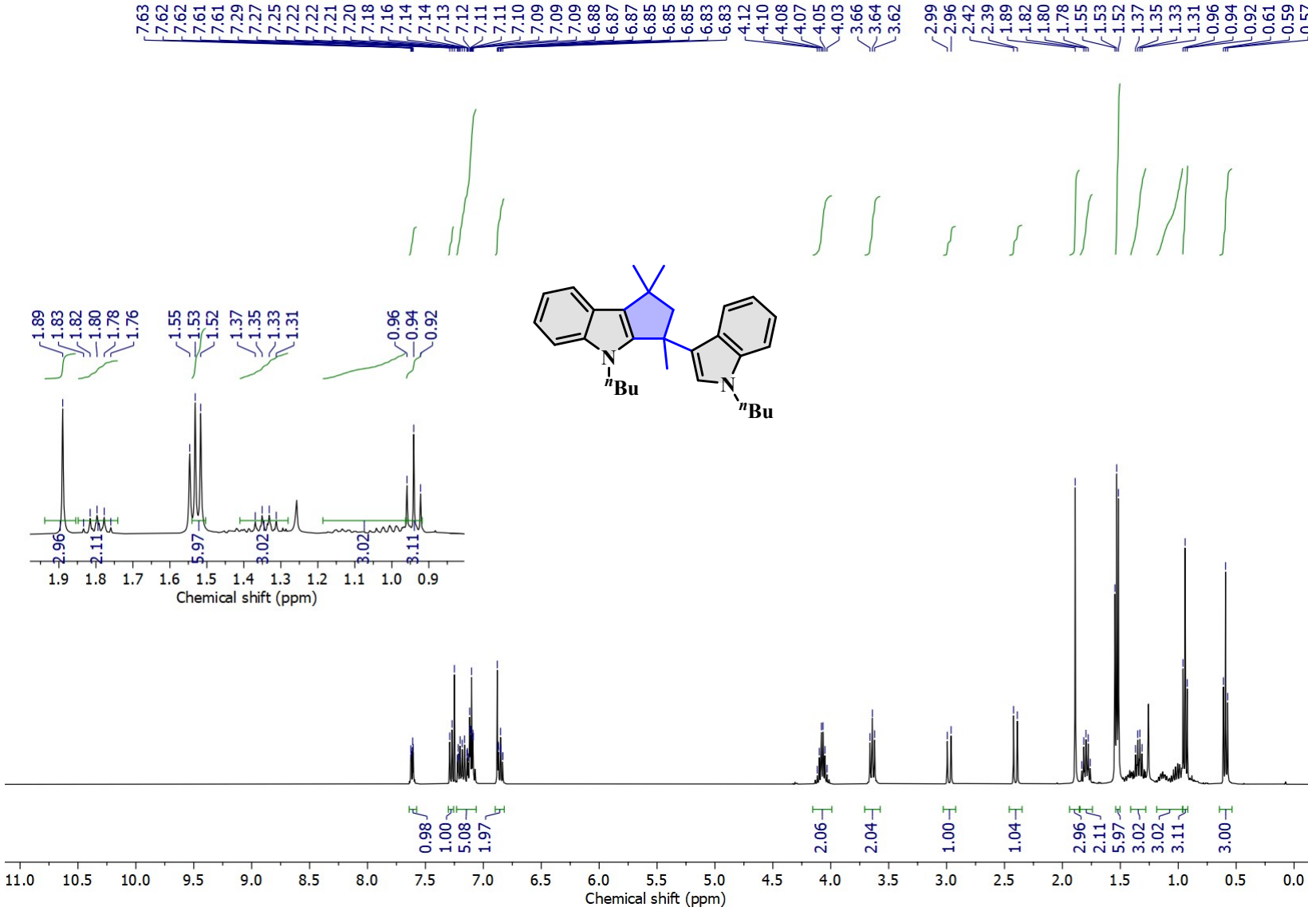


Fig. S19 400 MHz ^{1}H NMR spectrum of **2j** in $CDCl_3$

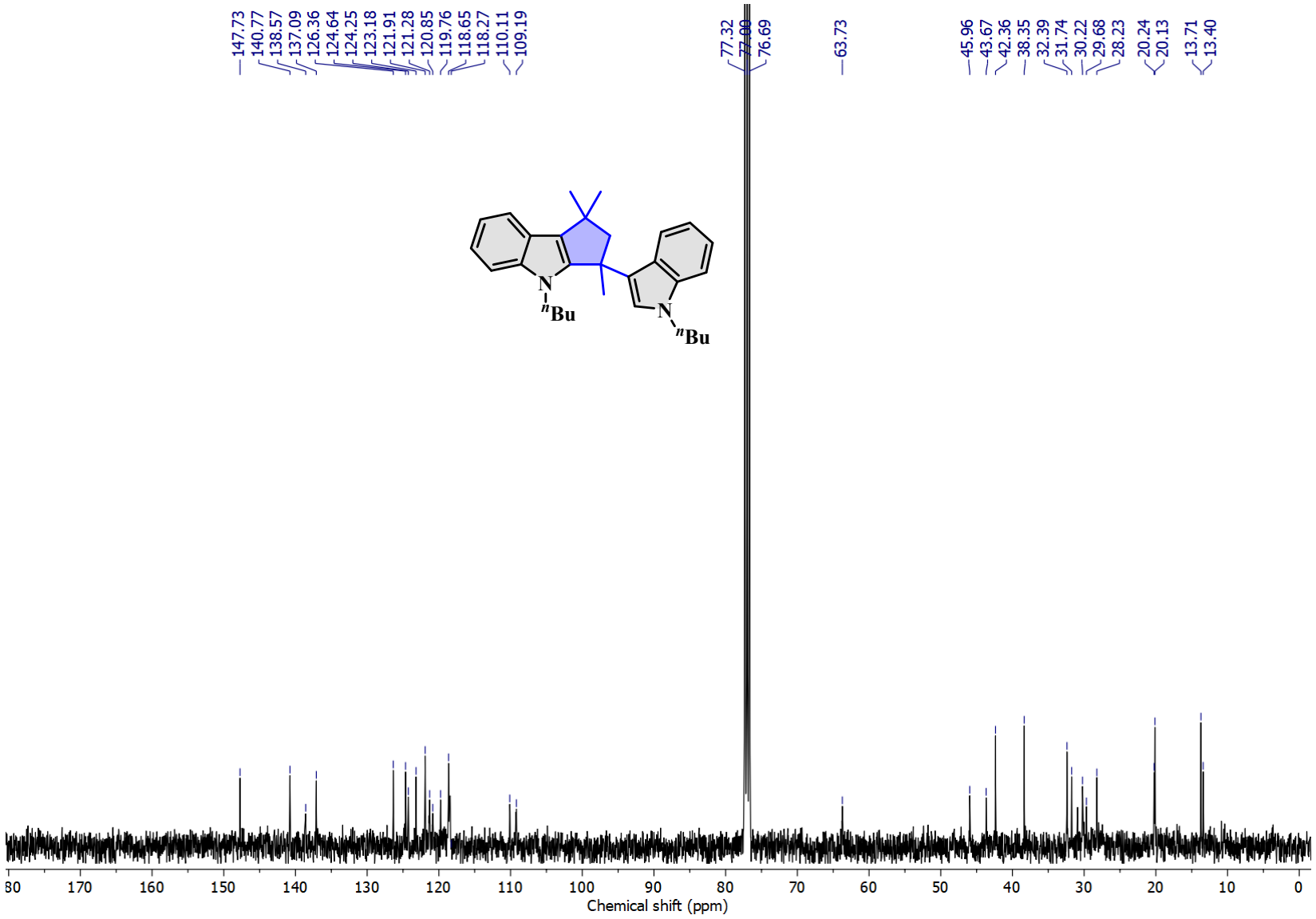


Fig. S20 100 MHz ^{13}C NMR spectrum of **2j** in $CDCl_3$

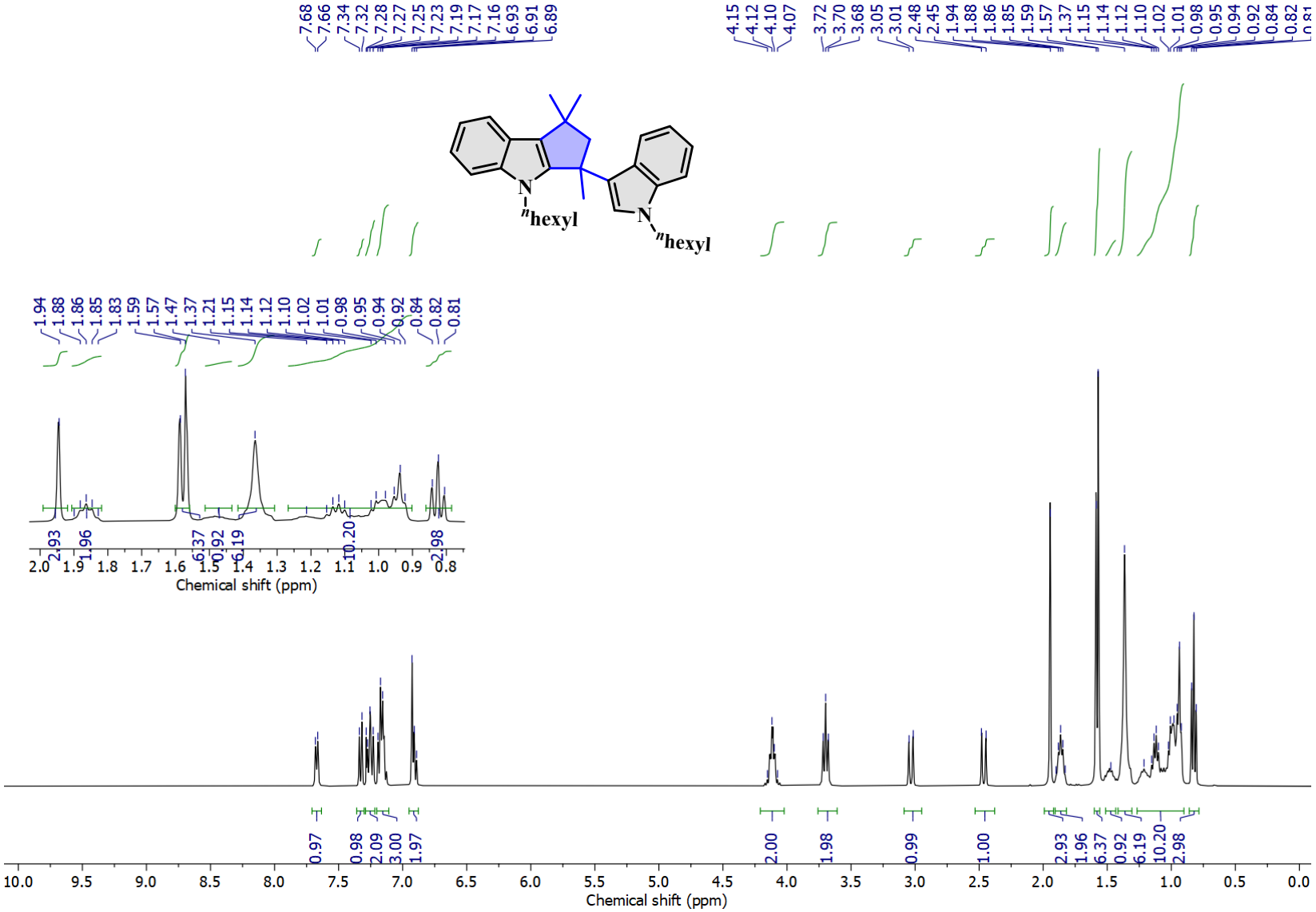


Fig. S21 400 MHz ^{1}H NMR spectrum of **2k** in $CDCl_3$

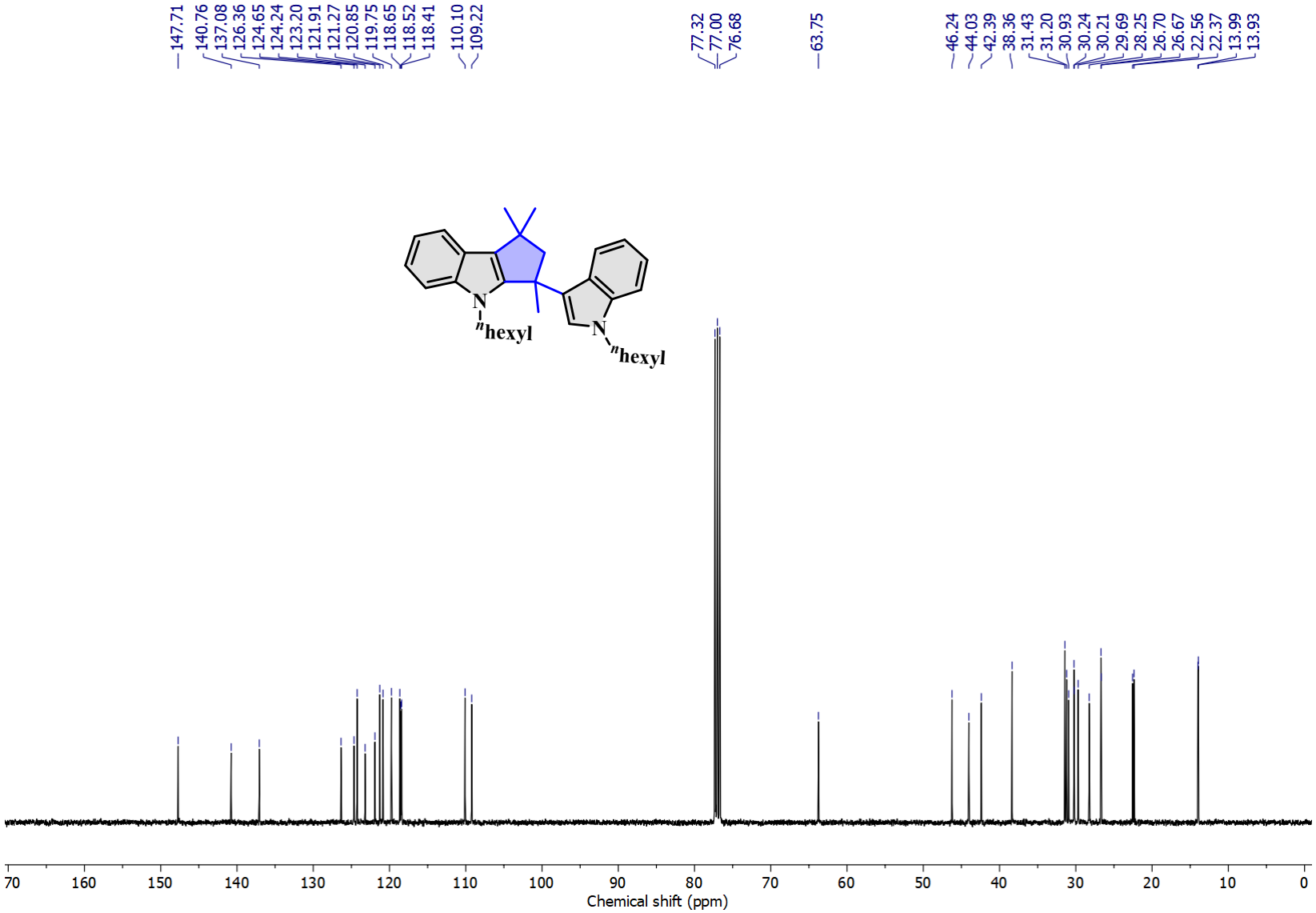
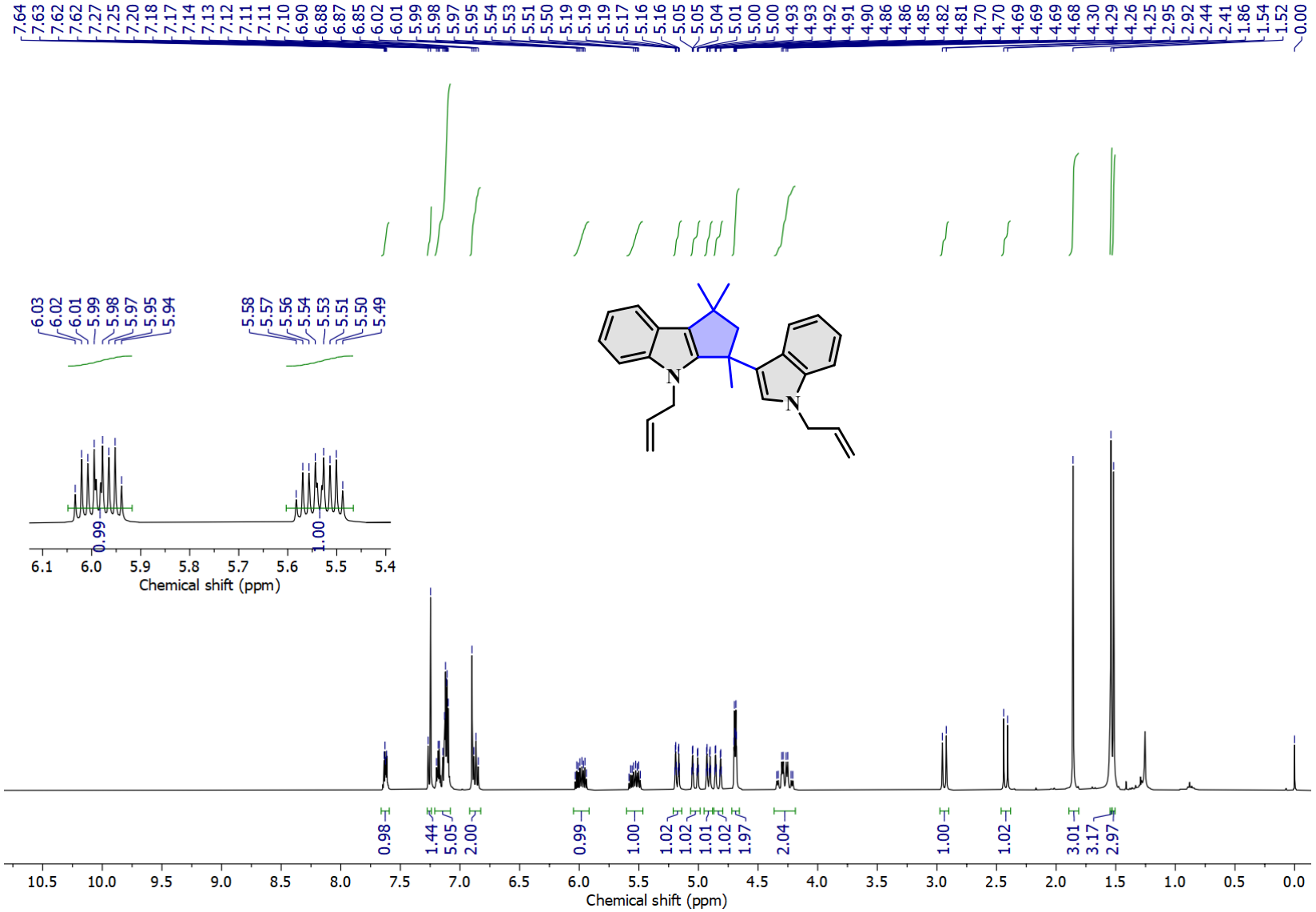


Fig. S22 100 MHz ^{13}C NMR spectrum of **2k** in $CDCl_3$



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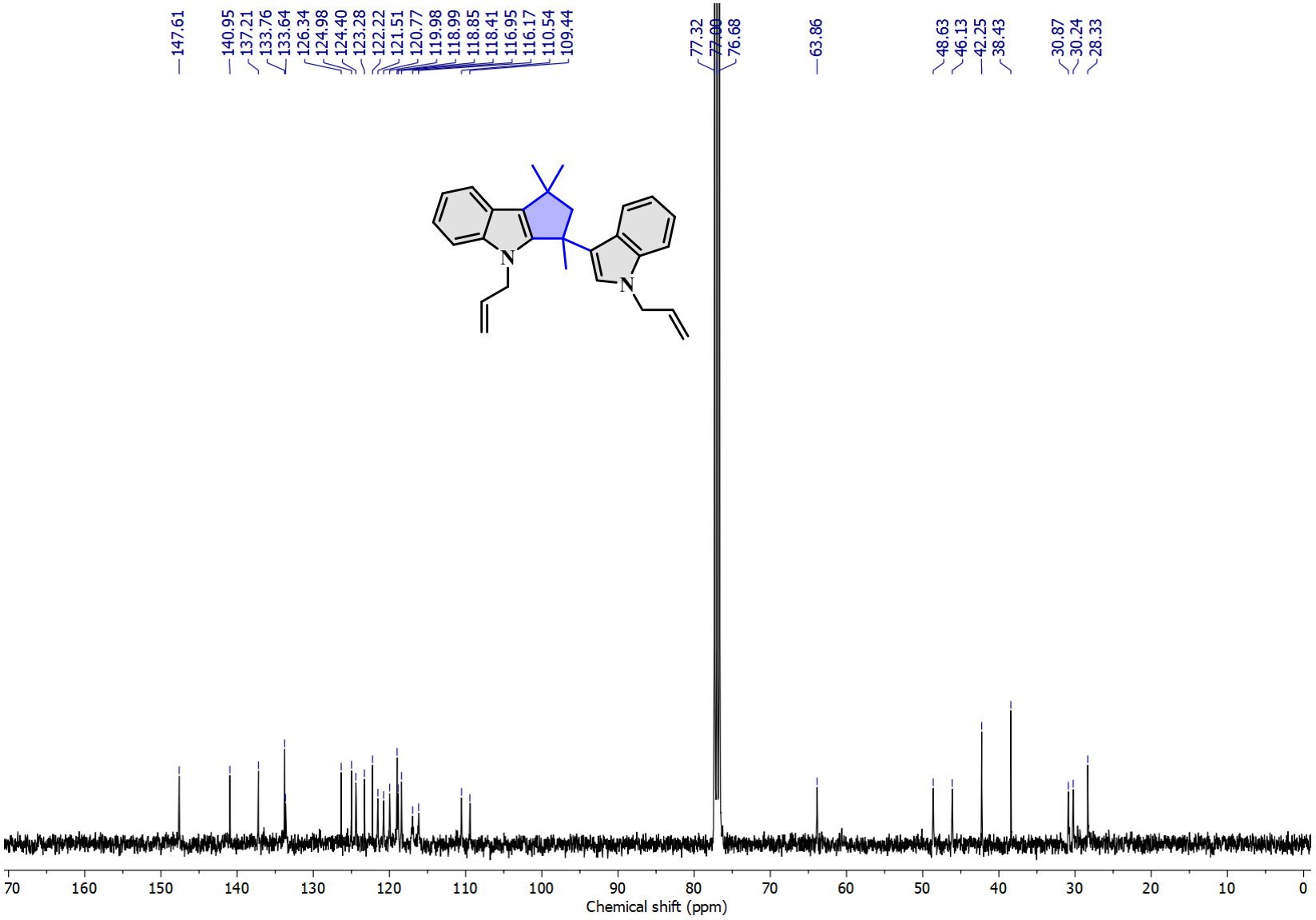
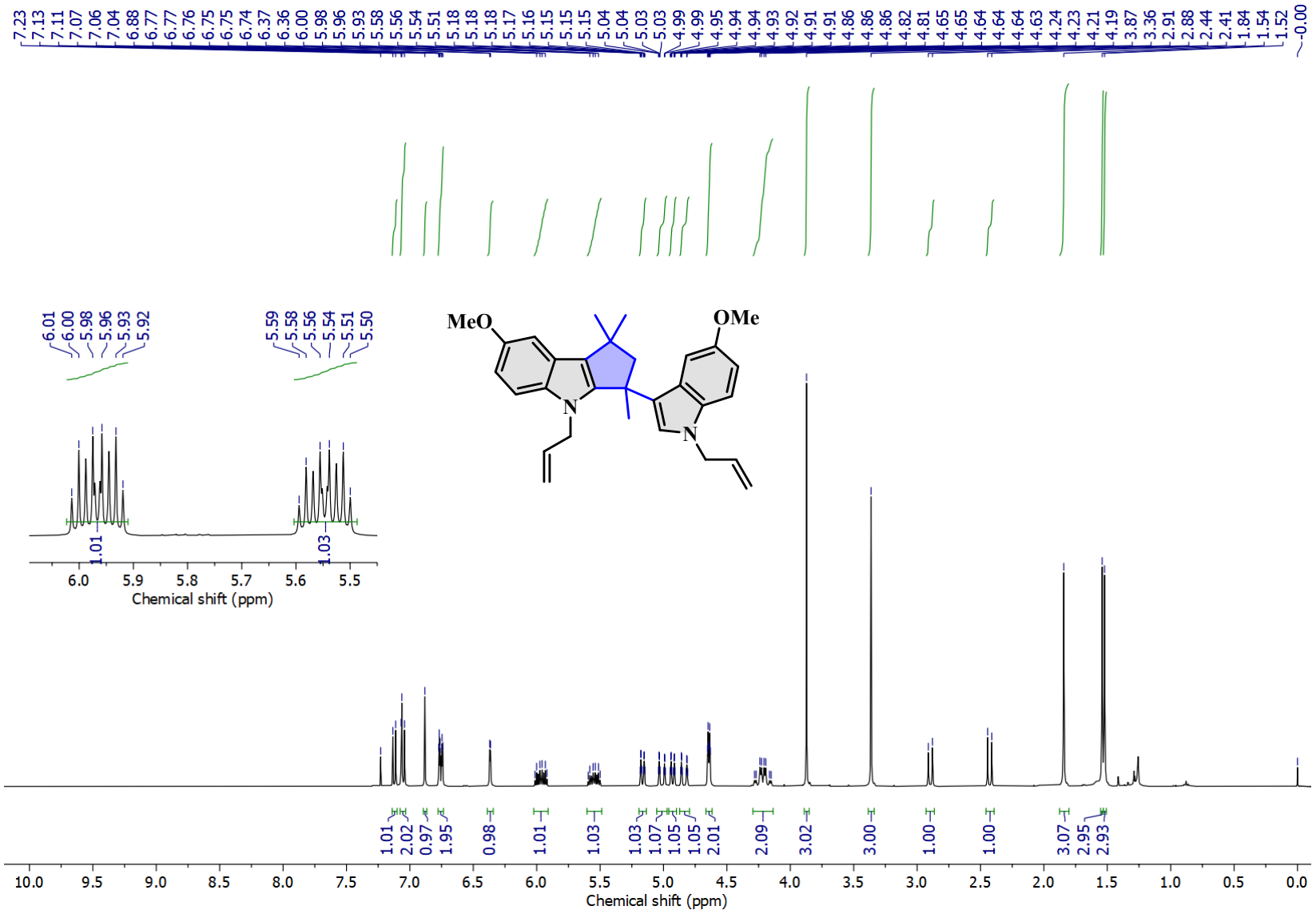


Fig. S24 100 MHz ^{13}C NMR spectrum of **2l** in $CDCl_3$



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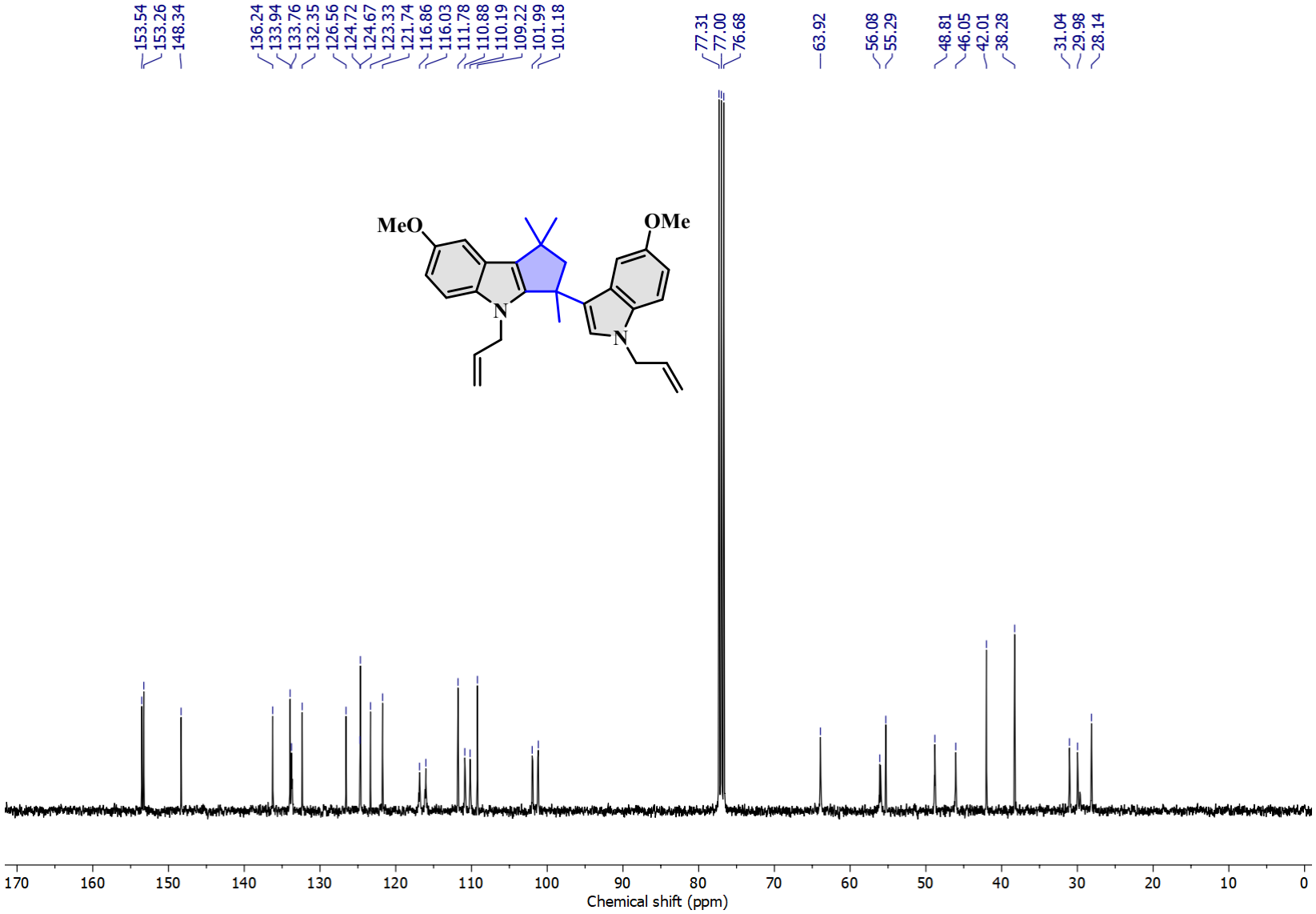

Fig. S26 100 MHz ^{13}C NMR spectrum of **2m** in $CDCl_3$

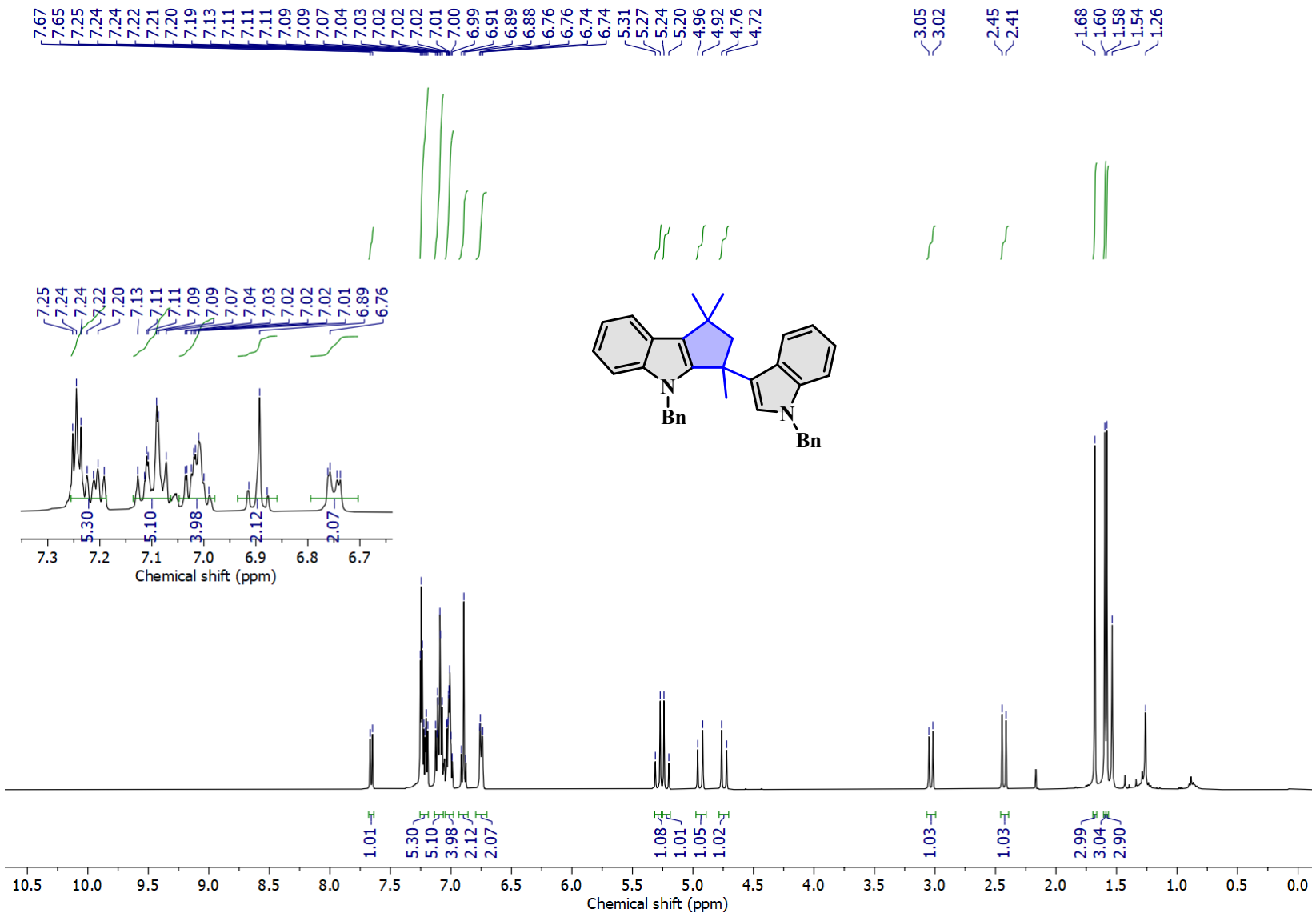

Fig. S27 400 MHz ^{1}H NMR spectrum of **2n** in $CDCl_3$

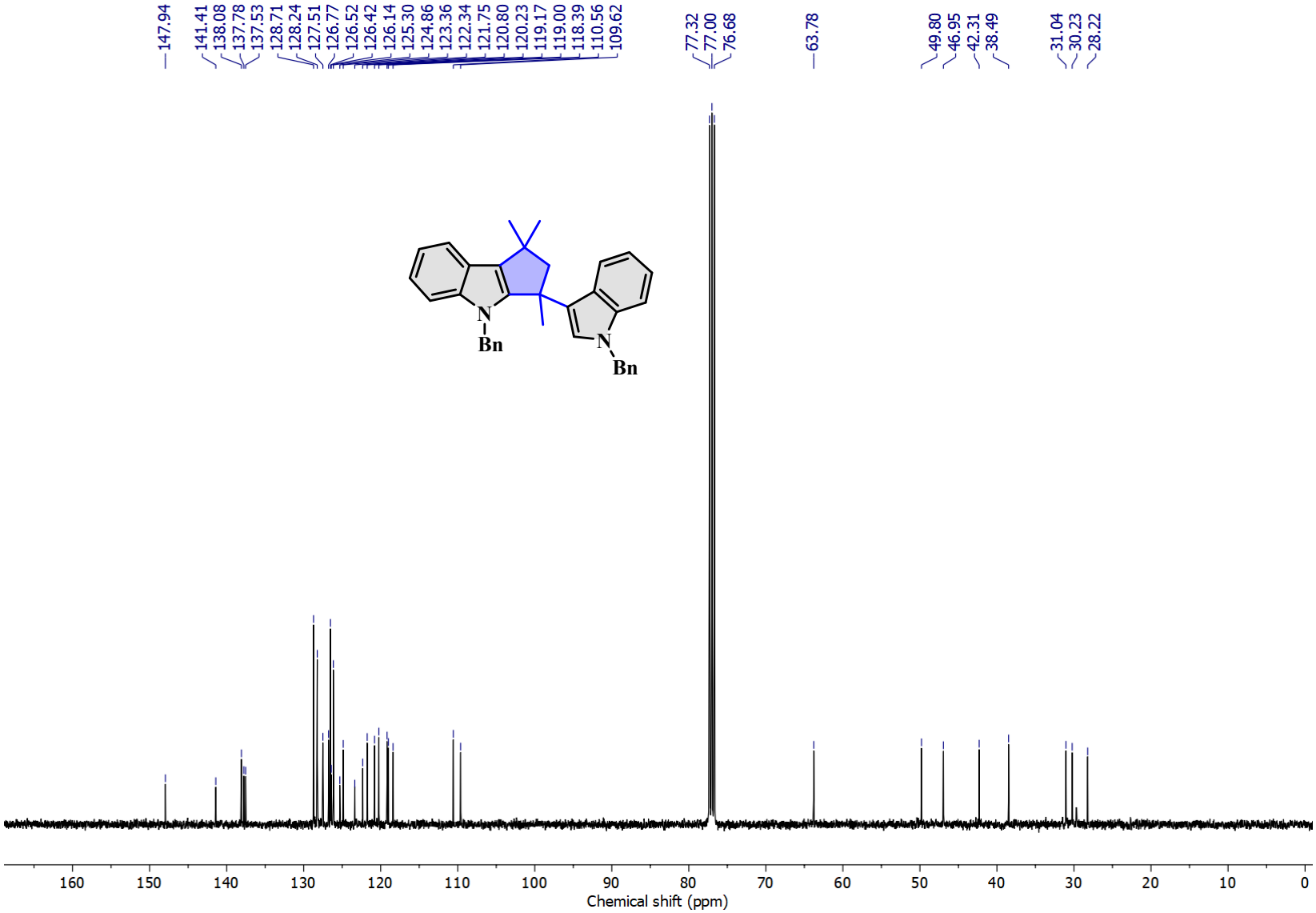

Fig. S28 100 MHz ^{13}C NMR spectrum of **2n** in $CDCl_3$

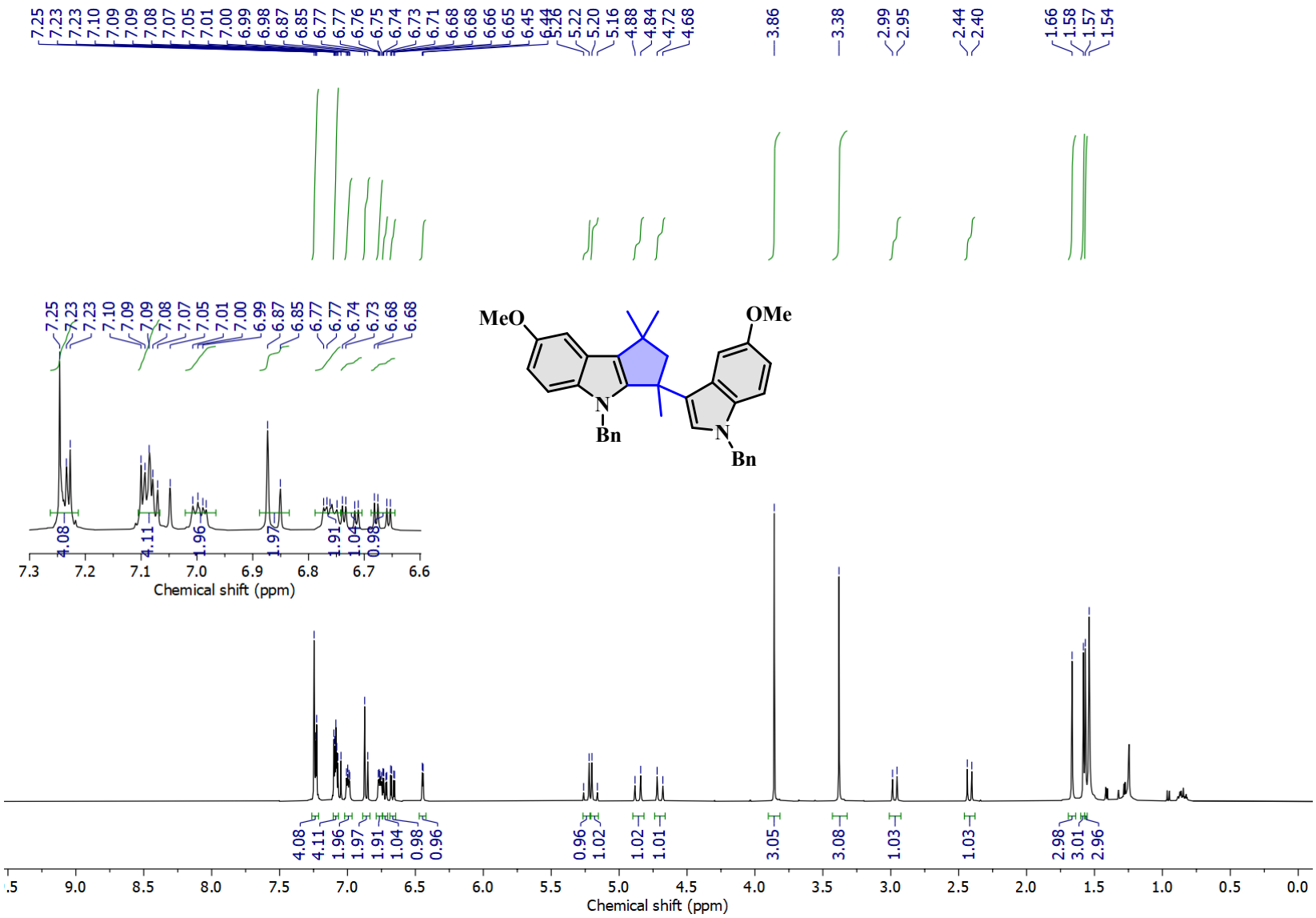

Fig. S29 400 MHz ^{1}H NMR spectrum of **2o** in $CDCl_3$

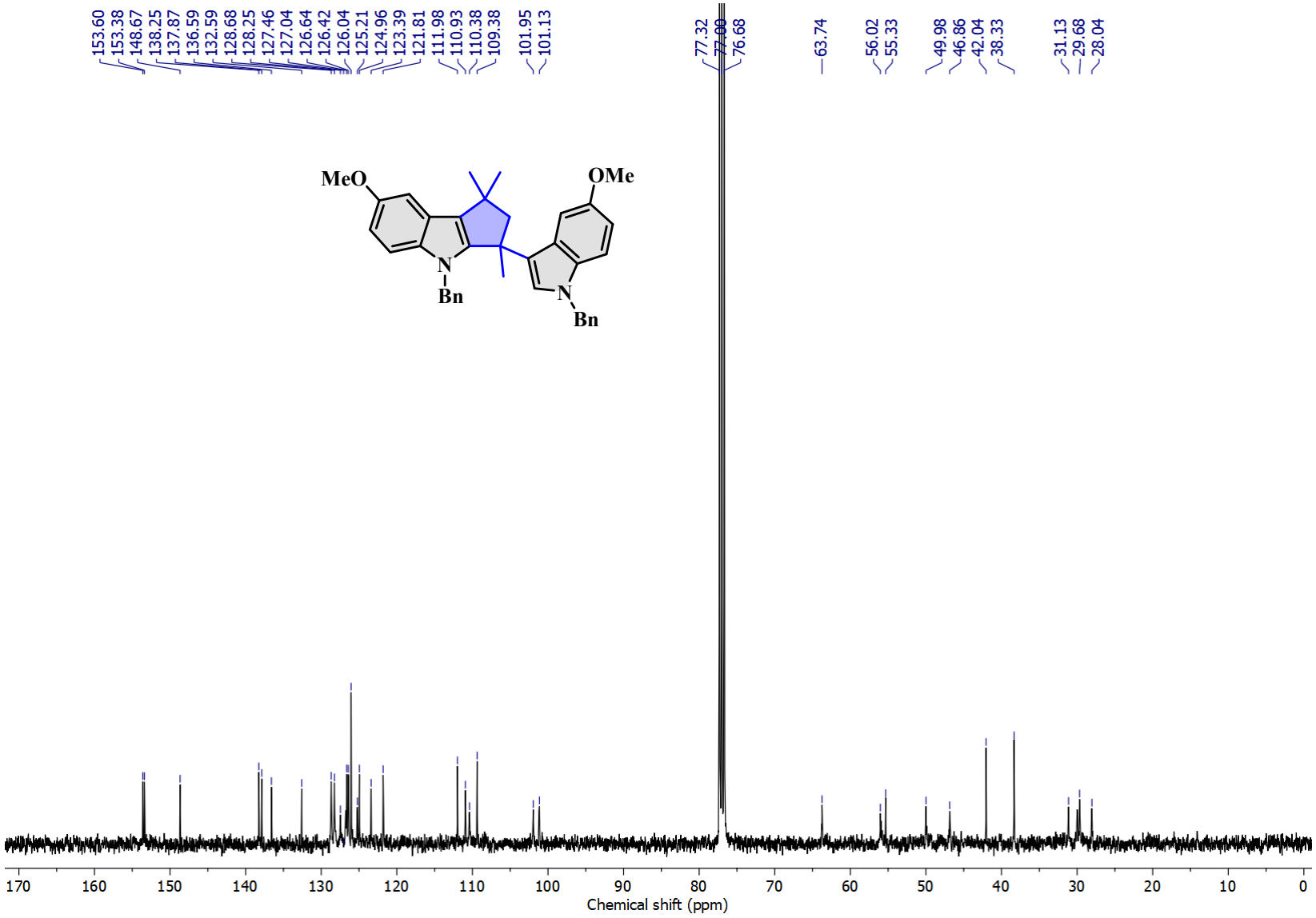

Fig. S30 100 MHz ^{13}C NMR spectrum of **2o** in $CDCl_3$

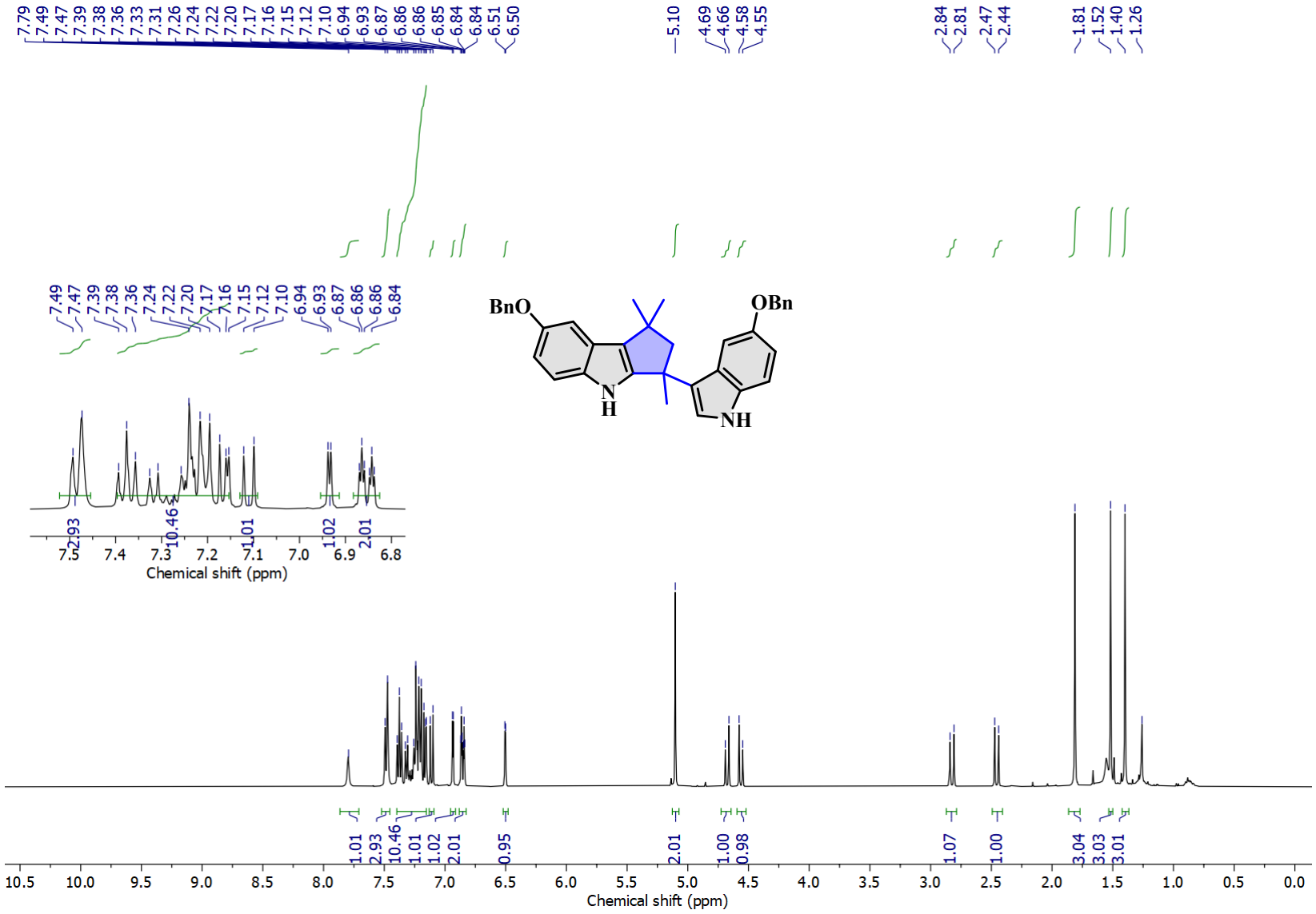

Fig. S31 400 MHz ^{1}H NMR spectrum of **2p** in $CDCl_3$

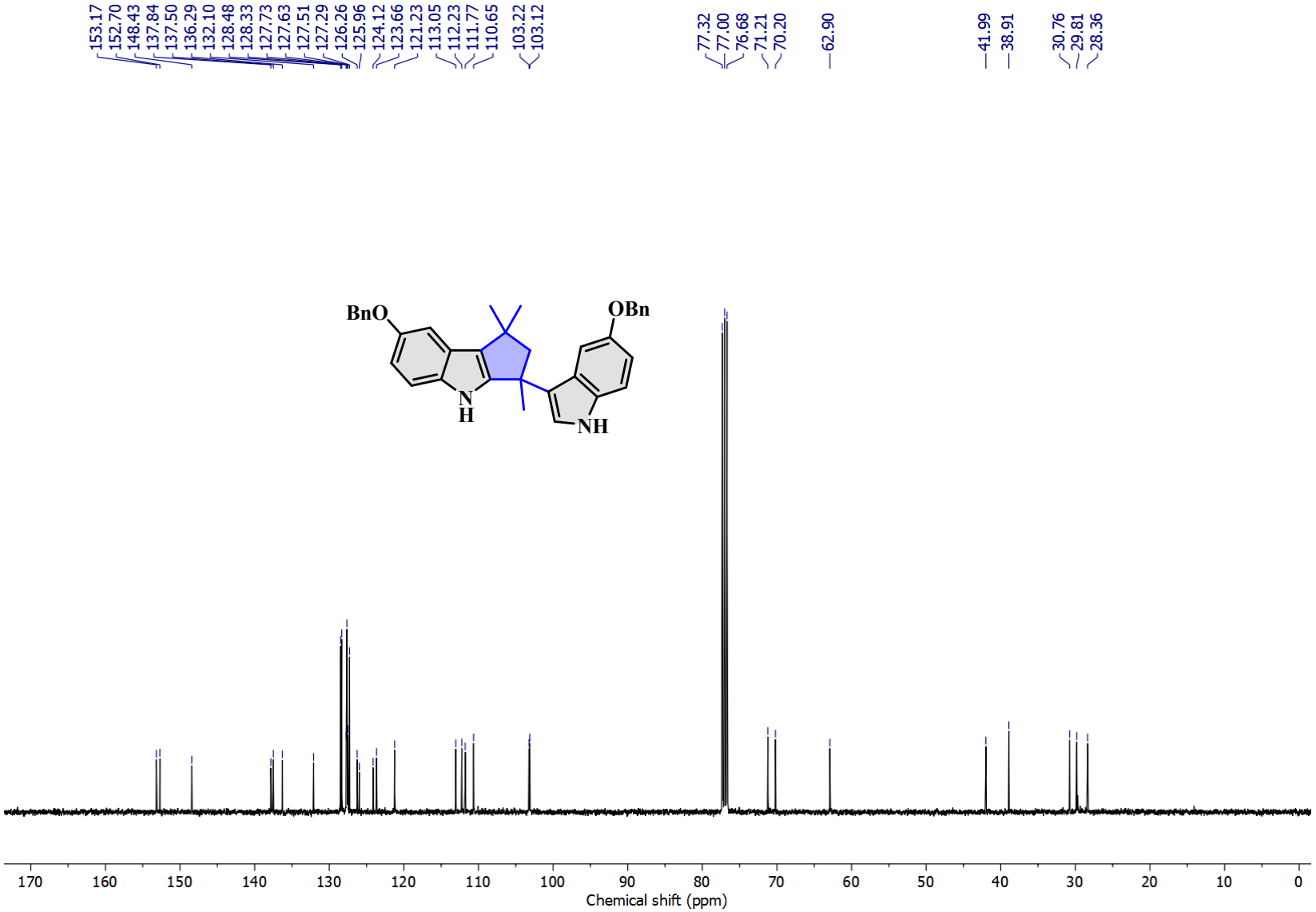

Fig. S32 100 MHz ^{13}C NMR spectrum of **2p** in $CDCl_3$

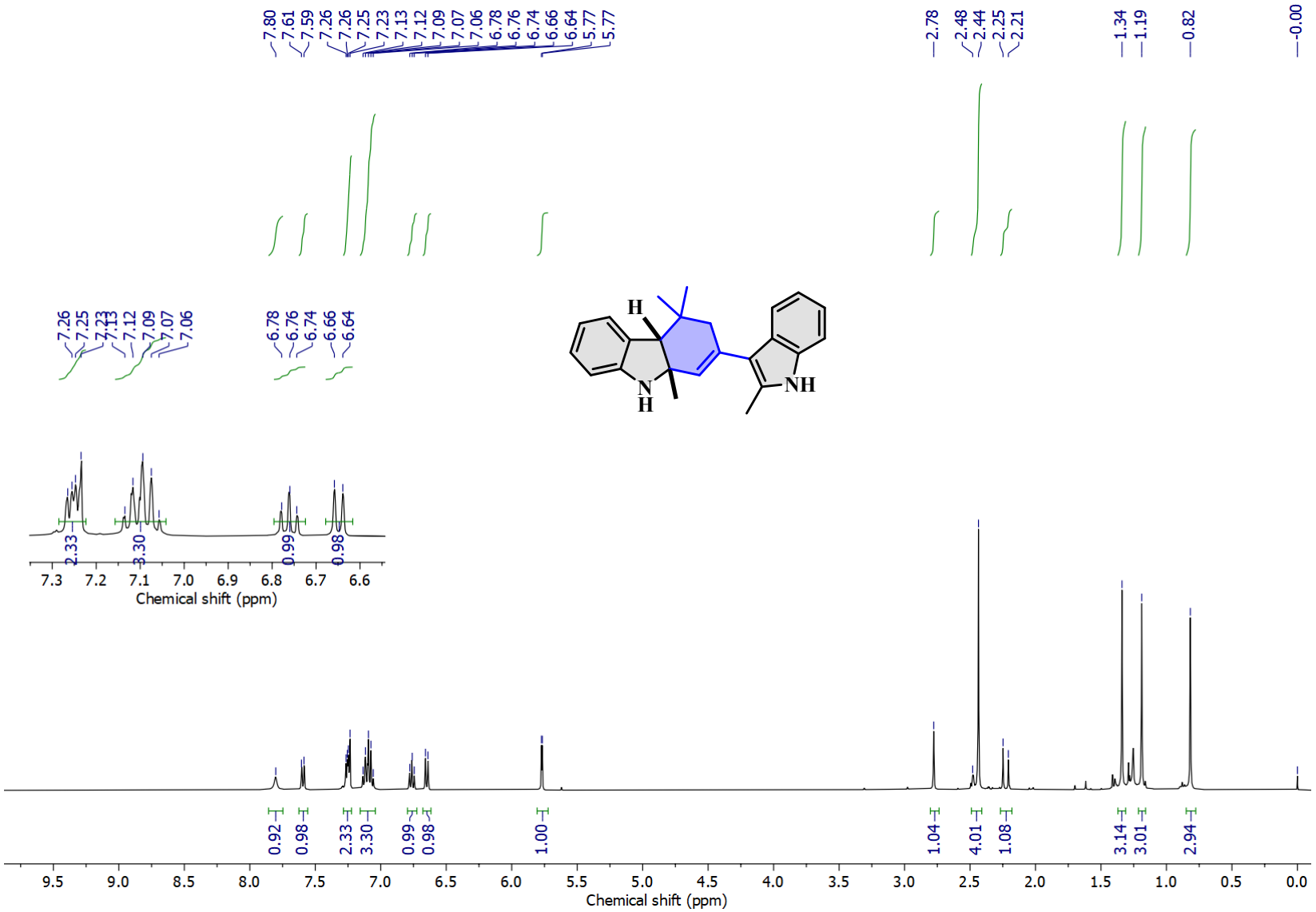

Fig. S33 400 MHz ^{1}H NMR spectrum of (**2q**)[3] in $CDCl_3$

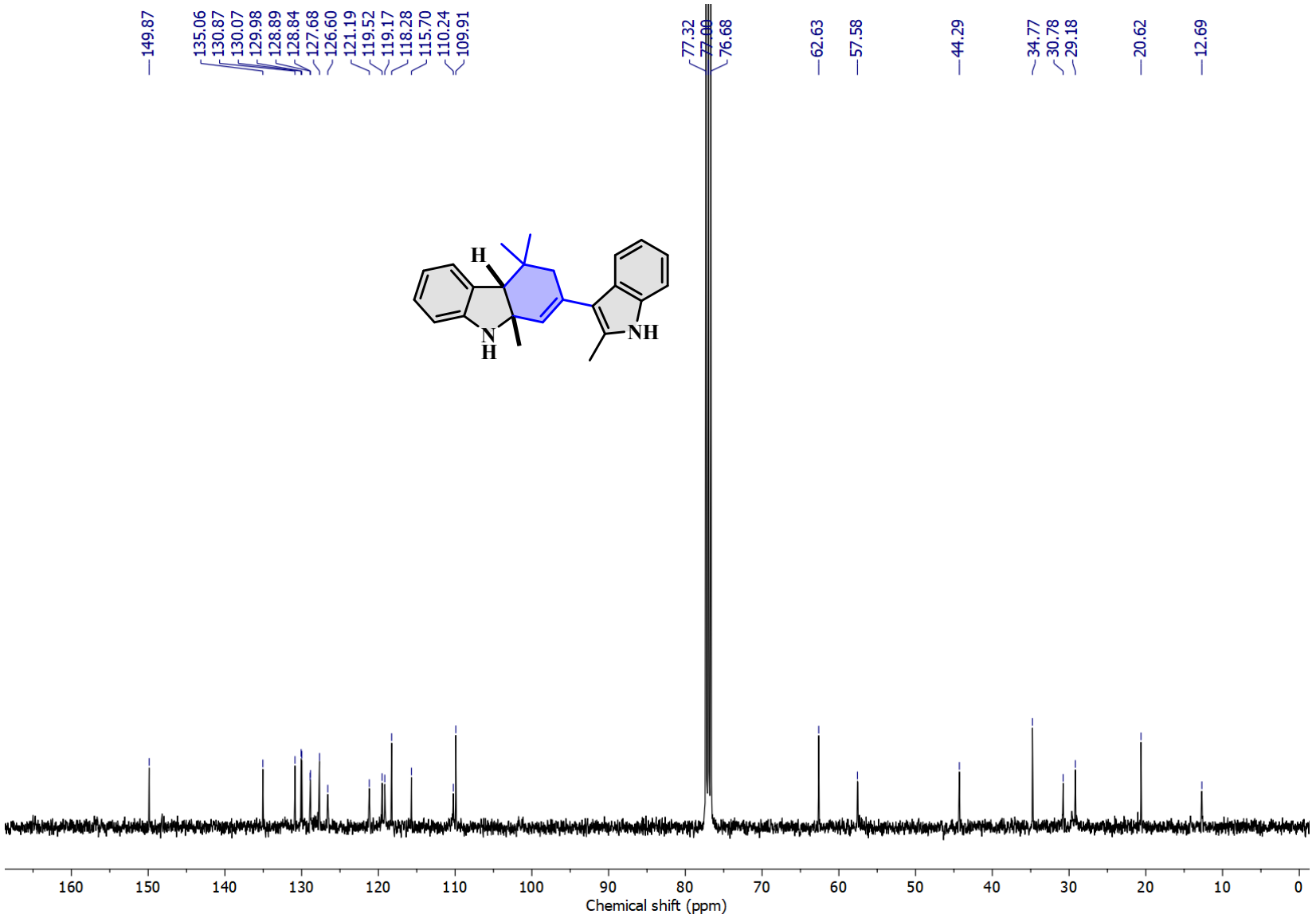

Fig. S34 100 MHz ^{13}C NMR spectrum of (**2q**)^3 in $CDCl_3$

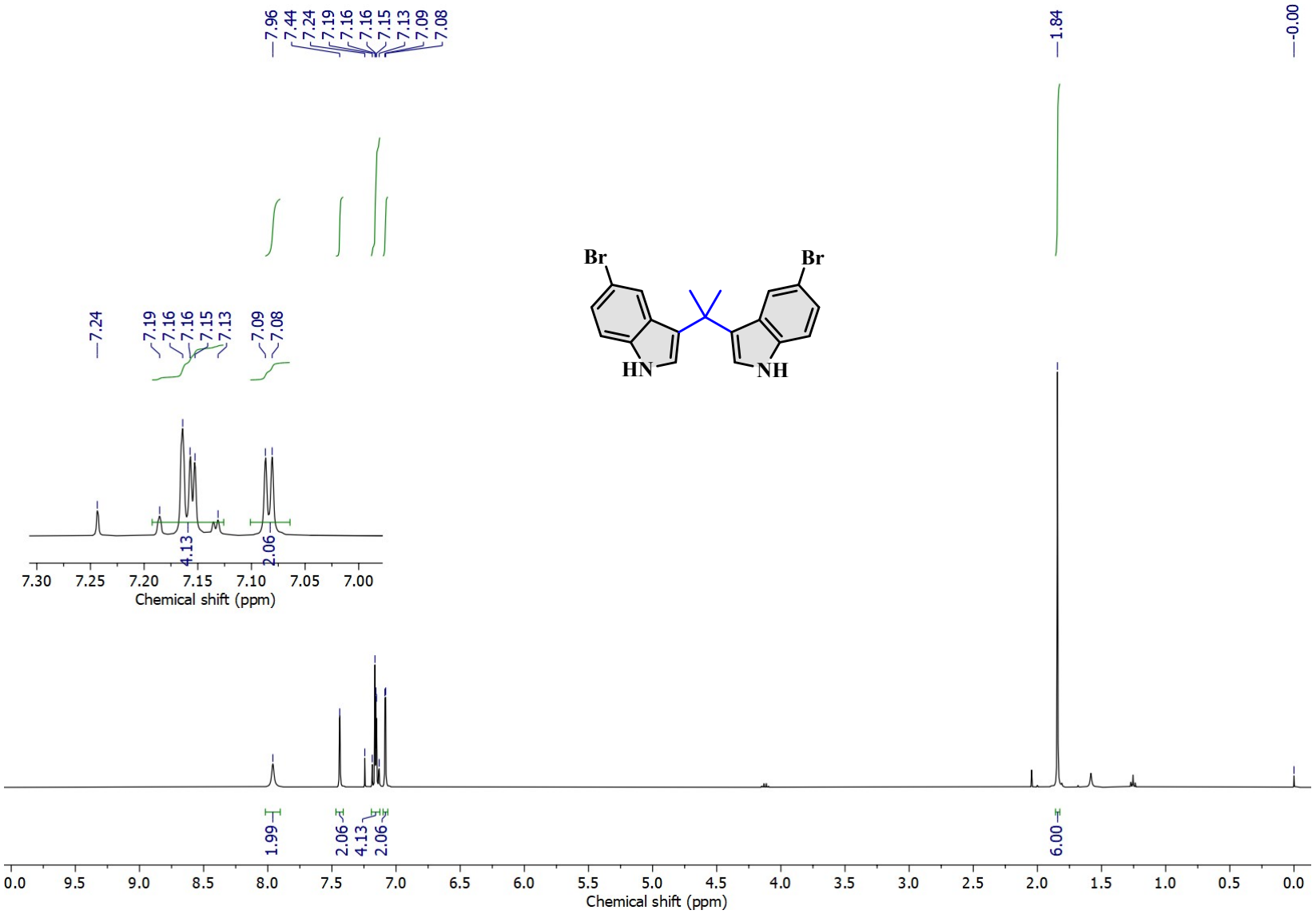

Fig. S35 400 MHz ^{1}H NMR spectrum of (**3a**)[2] in $CDCl_3$

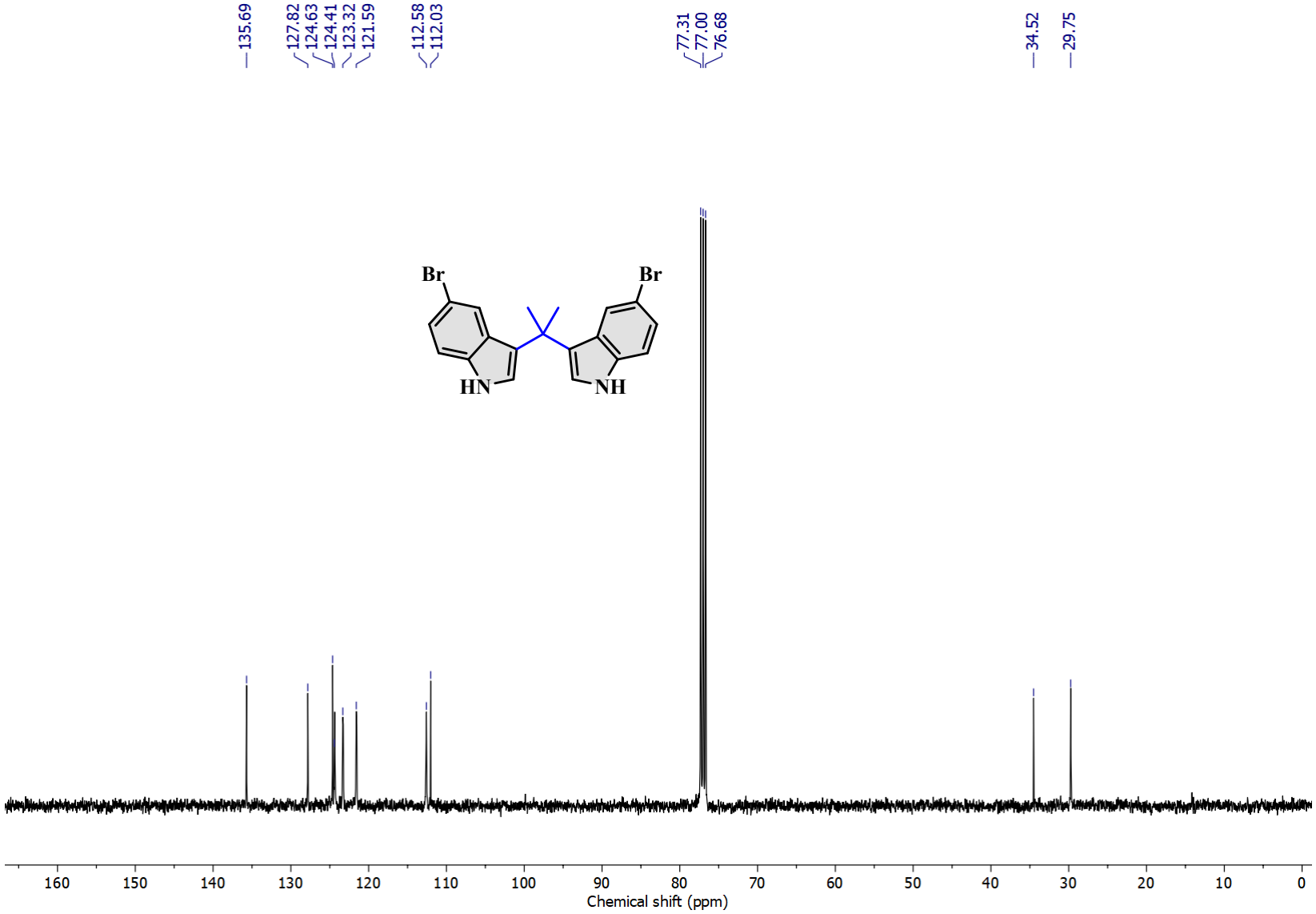

Fig. S36 100 MHz ^{13}C NMR spectrum of (**3a**)^2 in $CDCl_3$

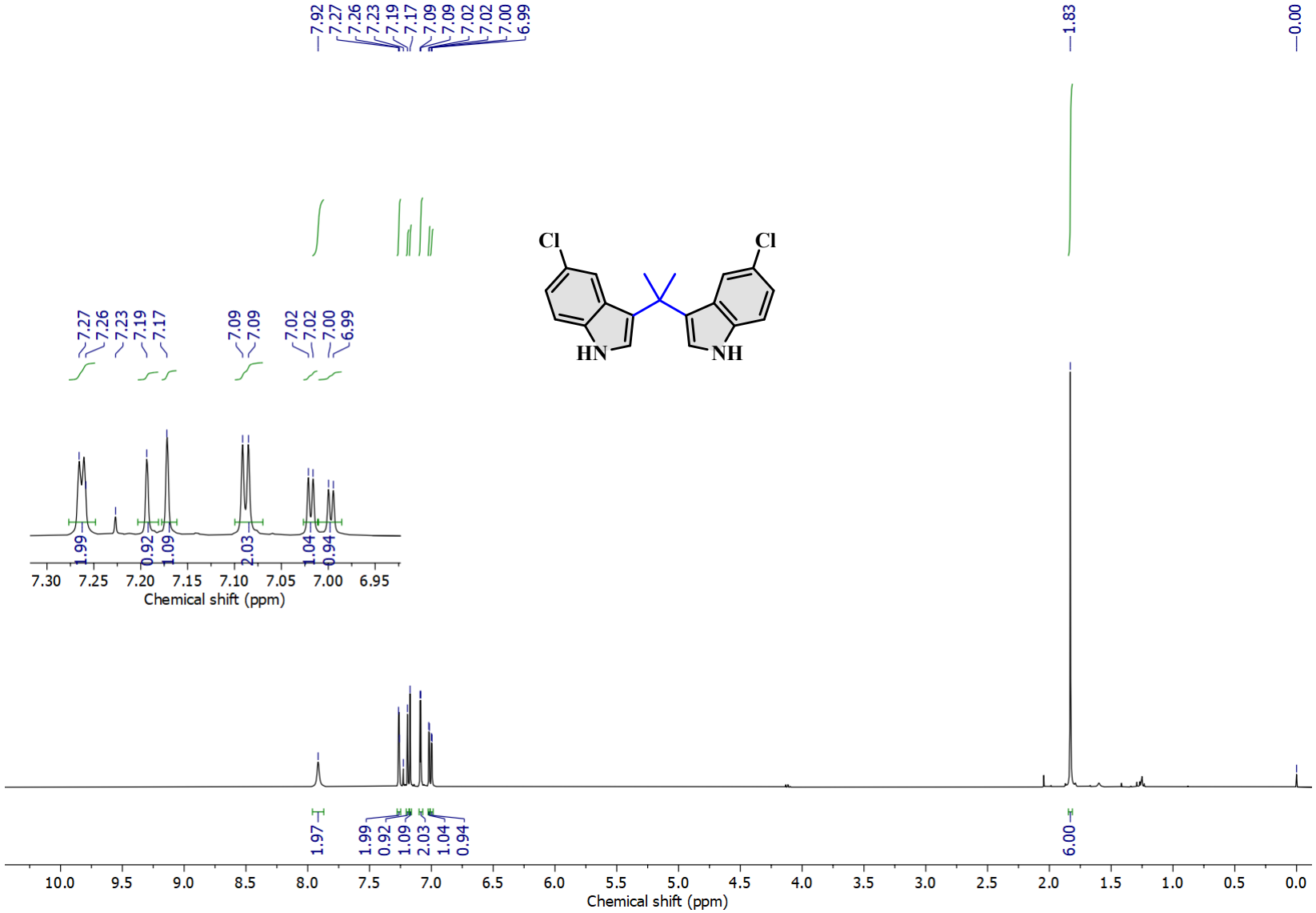

Fig. S37 400 MHz ^{1}H NMR spectrum of (**3b**)[2] in $CDCl_3$

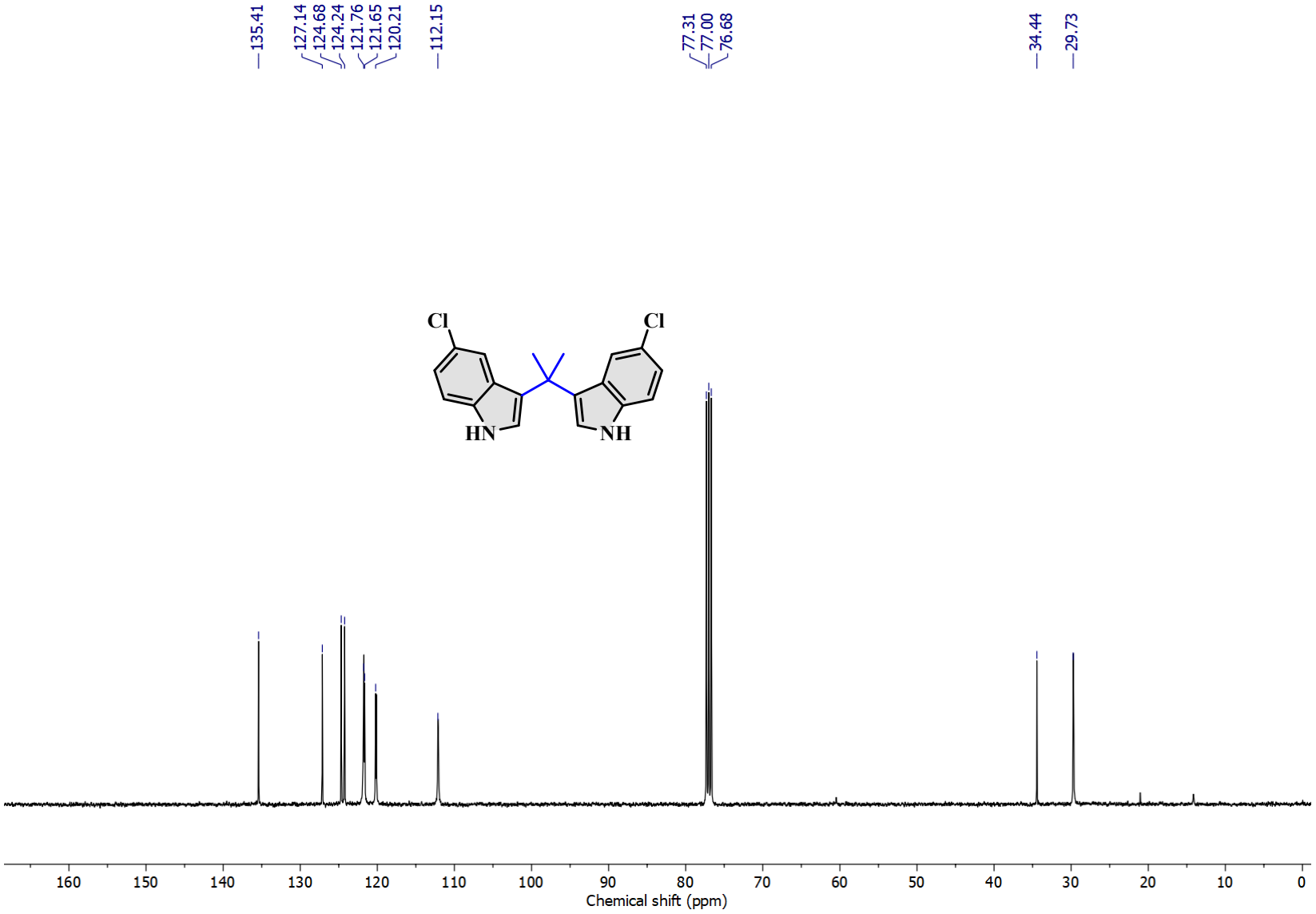

Fig. S38 100 MHz ^{13}C NMR spectrum of (**3b**)^2 in $CDCl_3$

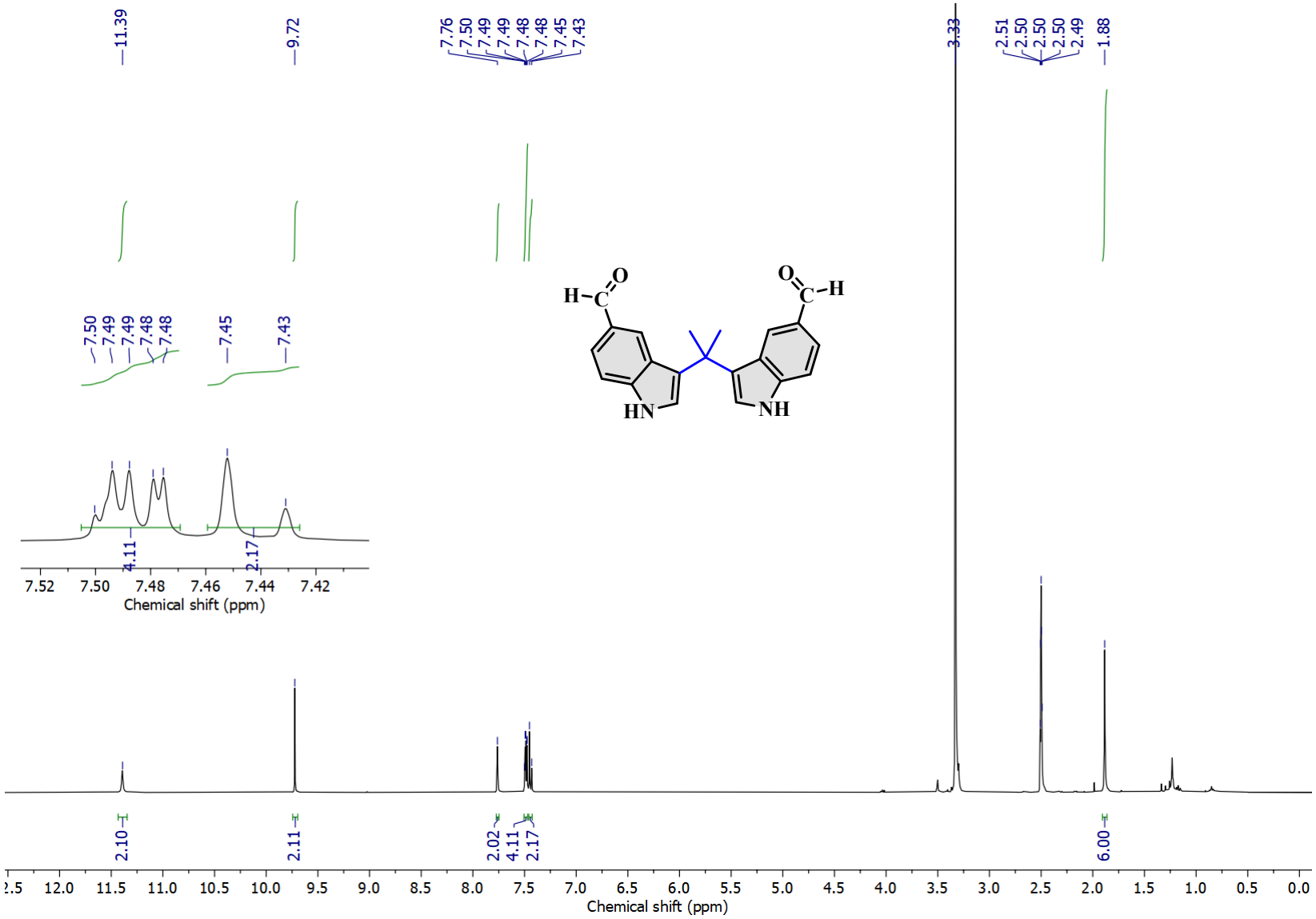

Fig. S39 400 MHz ^{1}H NMR spectrum of **3c** in DMSO-d_6

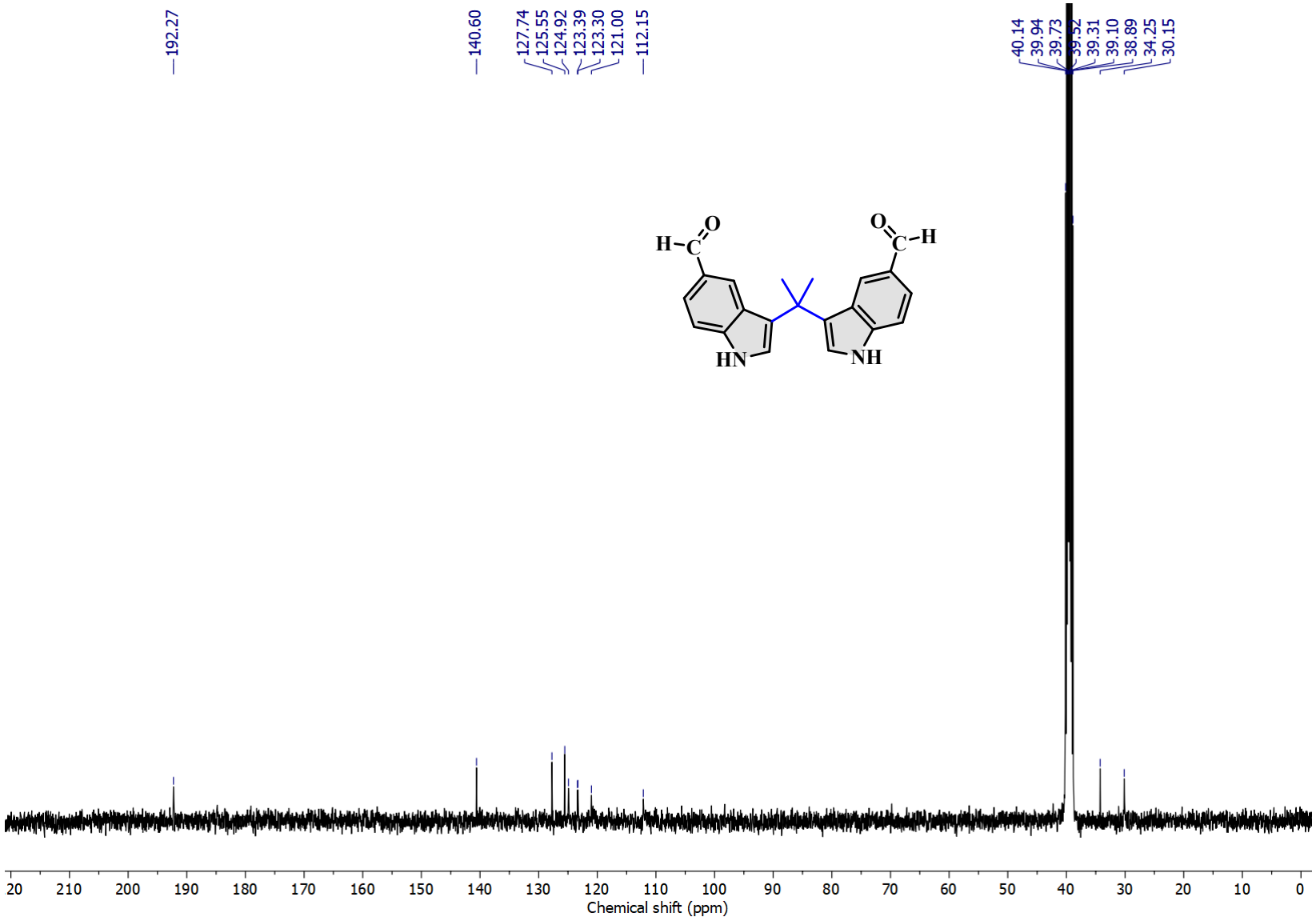

Fig. S40 100 MHz ^{13}C NMR spectrum of **3c** in DMSO-d_6

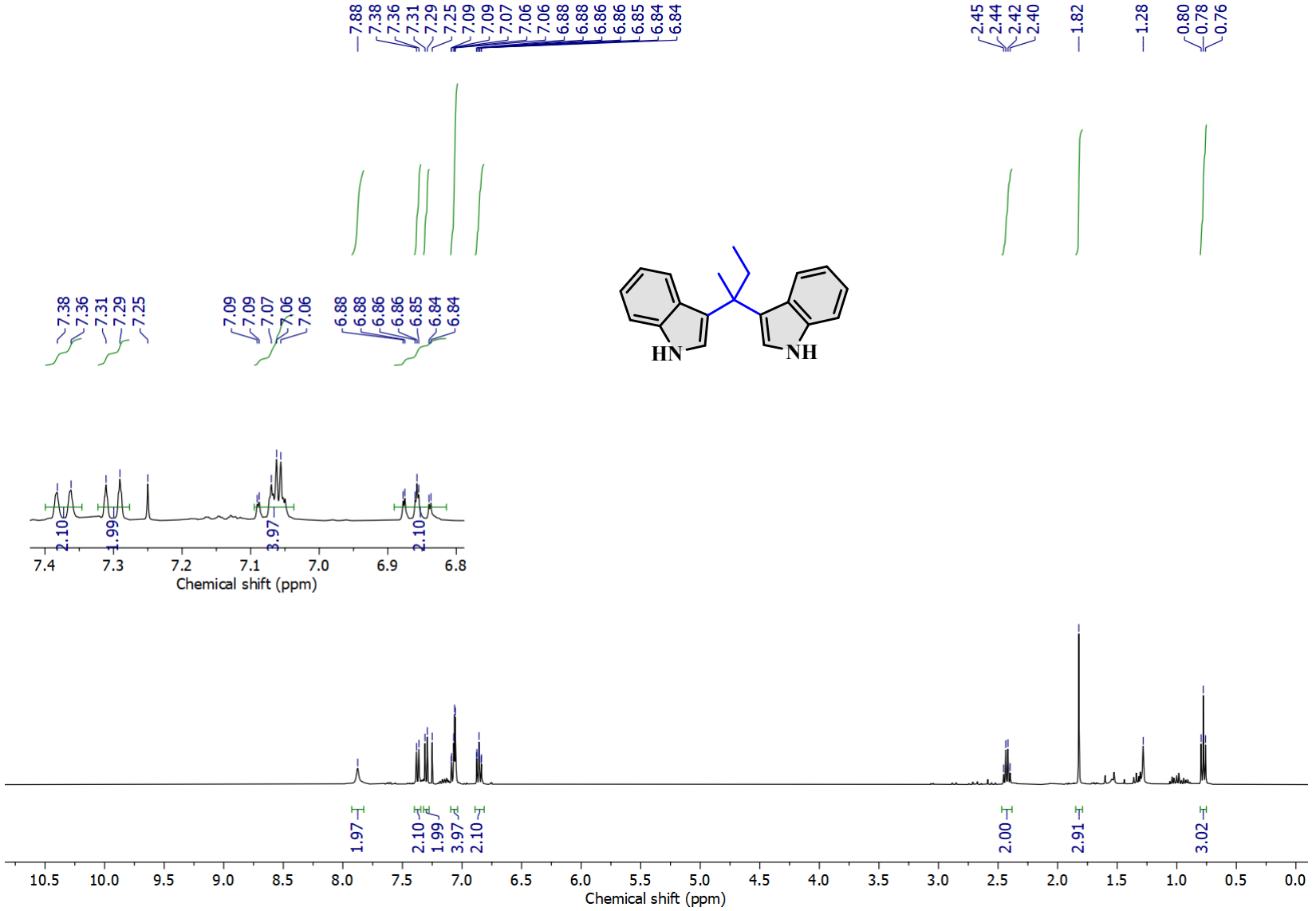

Fig. S41 400 MHz ^{1}H NMR spectrum of (**3d**)[4] in $CDCl_3$

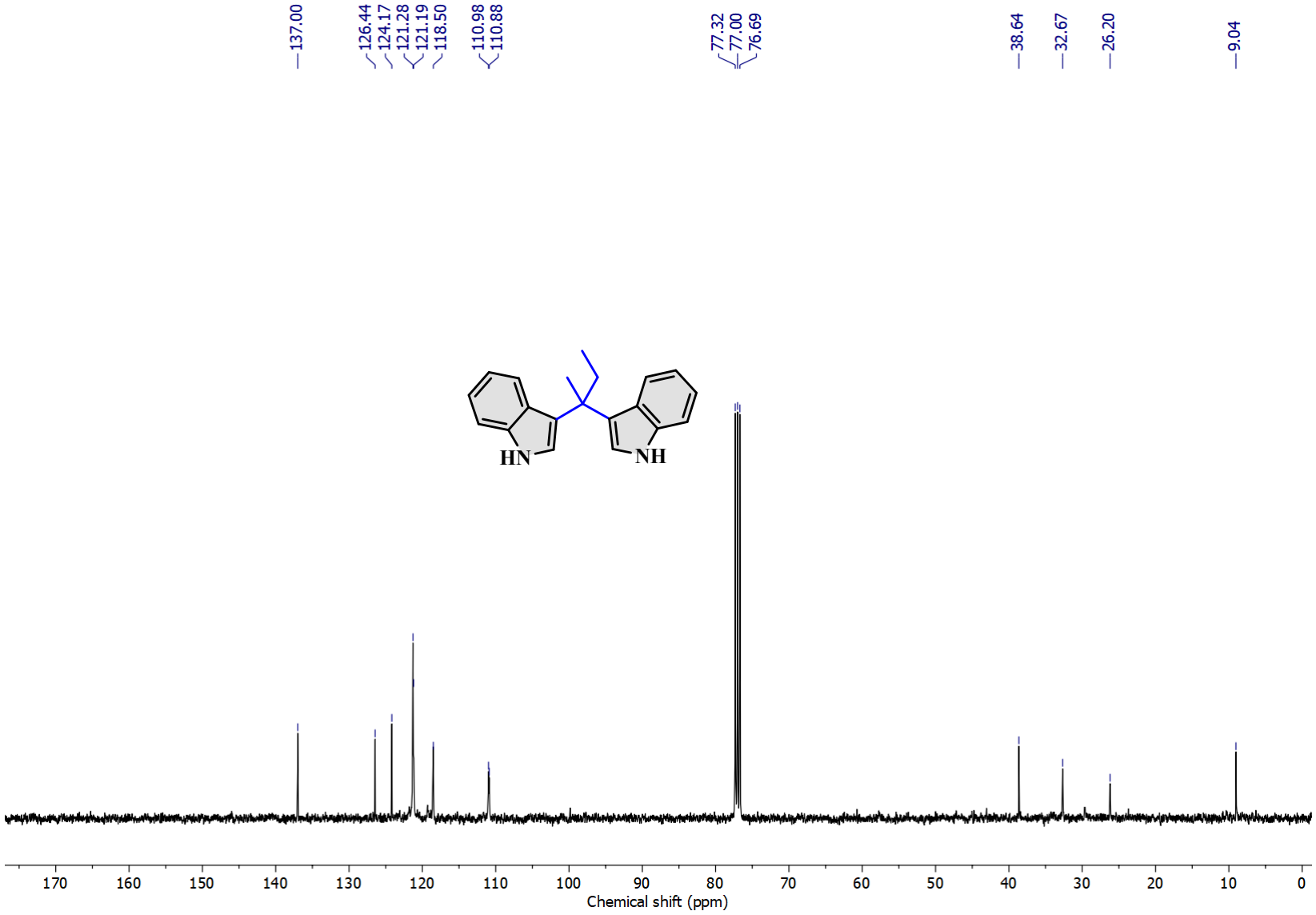

Fig. S42 100 MHz ^{13}C NMR spectrum of (**3d**)[4] in $CDCl_3$

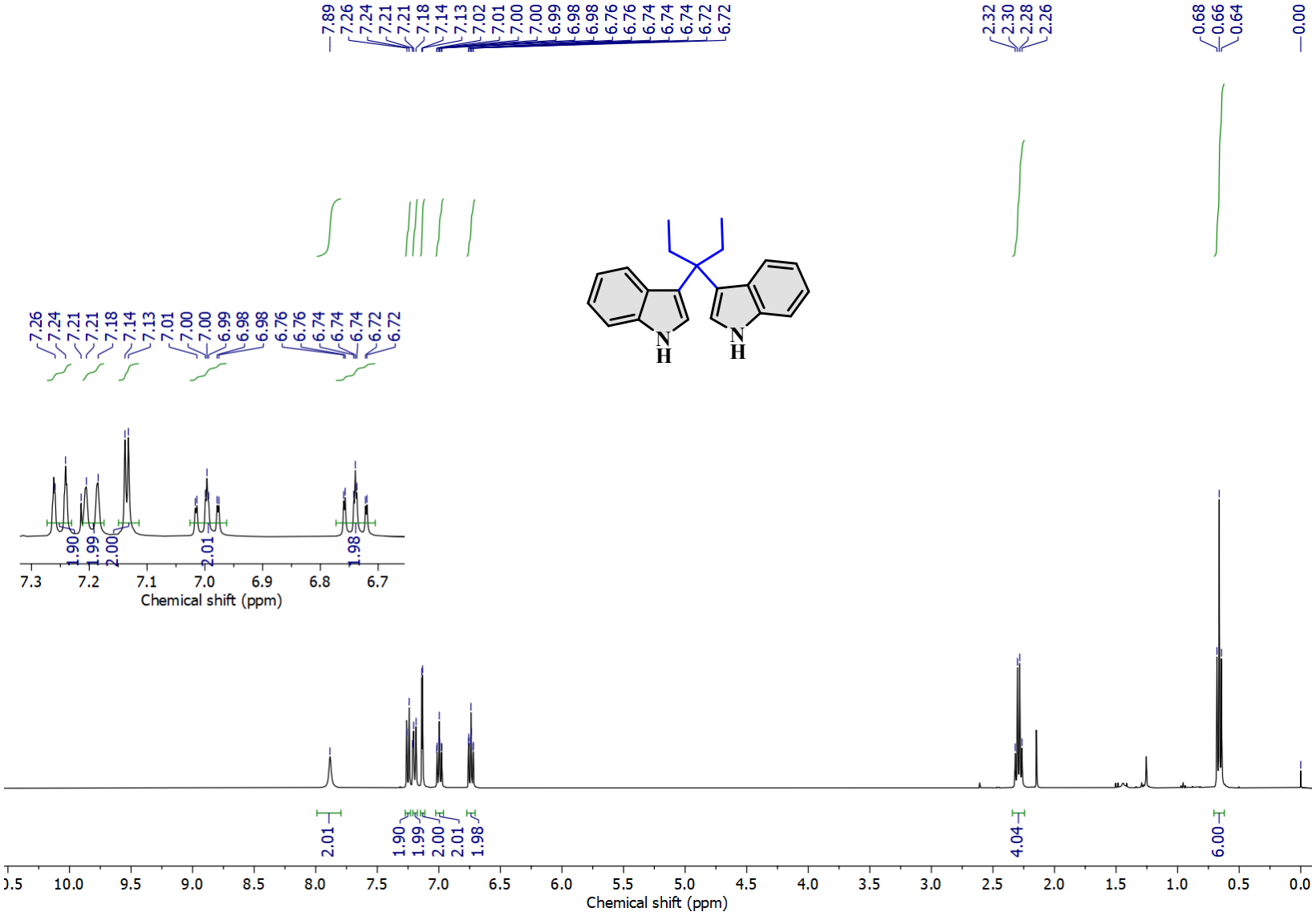

Fig. S43 400 MHz ^{1}H NMR spectrum of (**3e**)[4] in $CDCl_3$

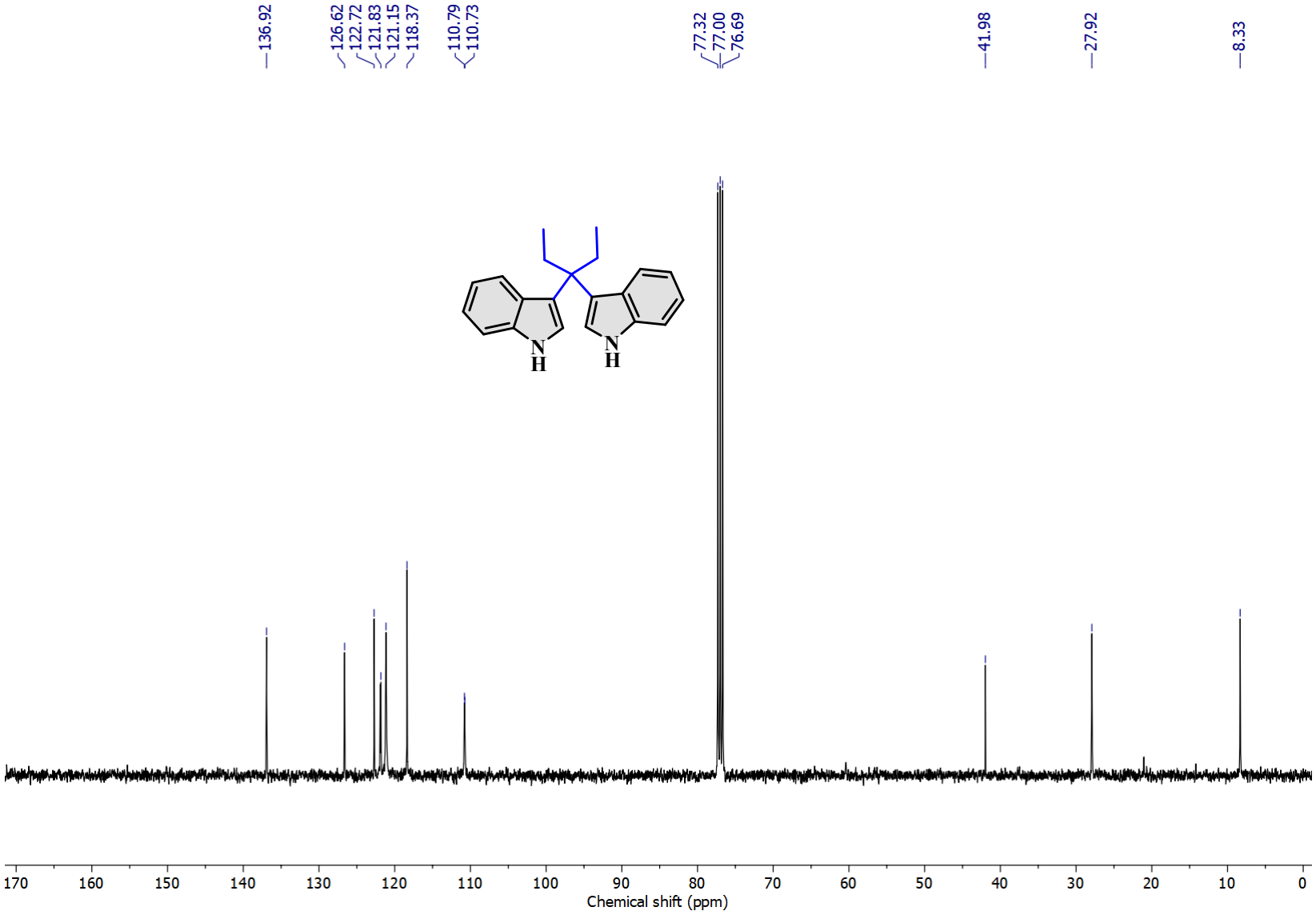

Fig. S44 100 MHz ^{13}C NMR spectrum of (**3e**)[4] in $CDCl_3$

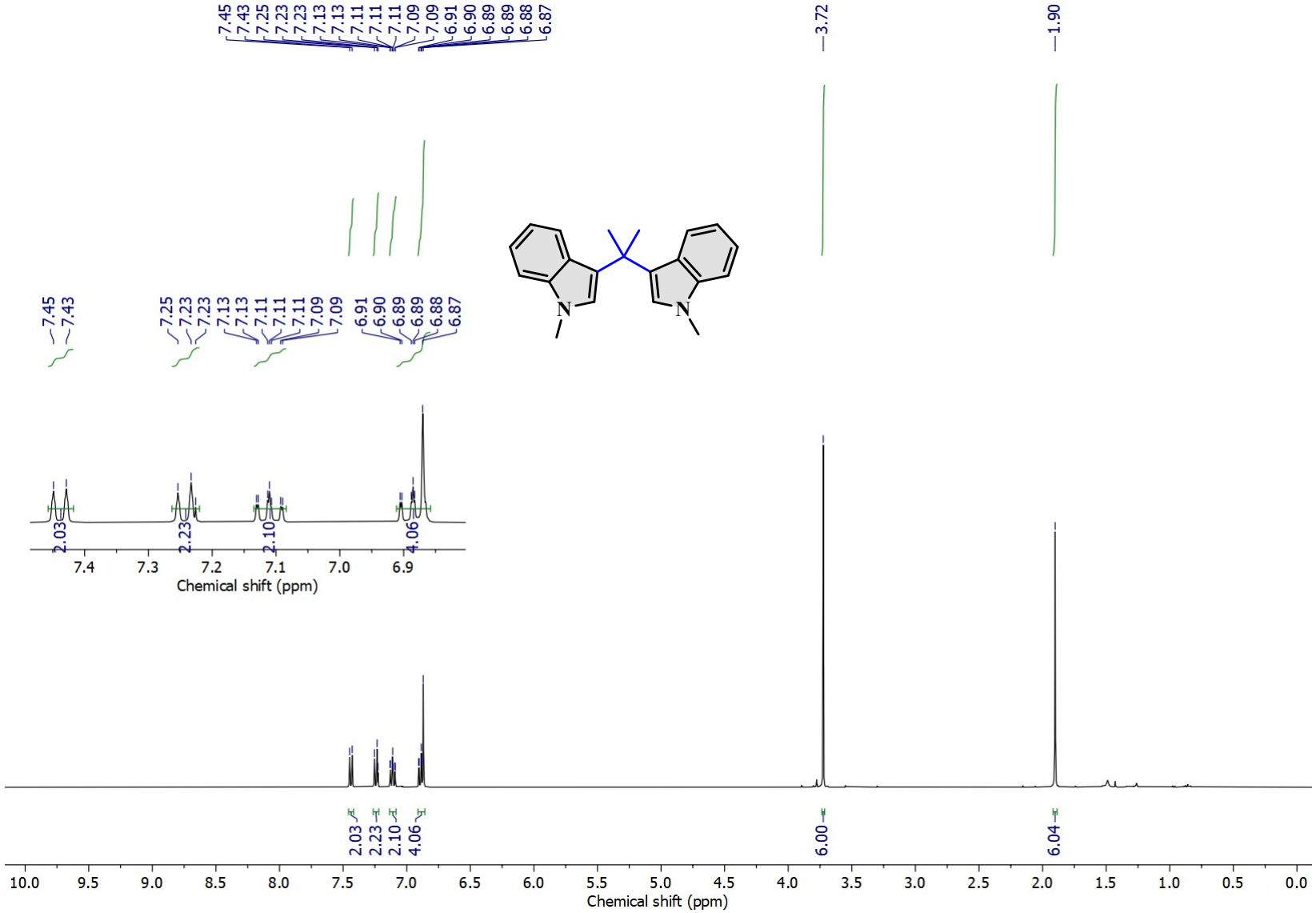

Fig. S45 400 MHz ^{1}H NMR spectrum of (**3a′**)[5] in $CDCl_3$

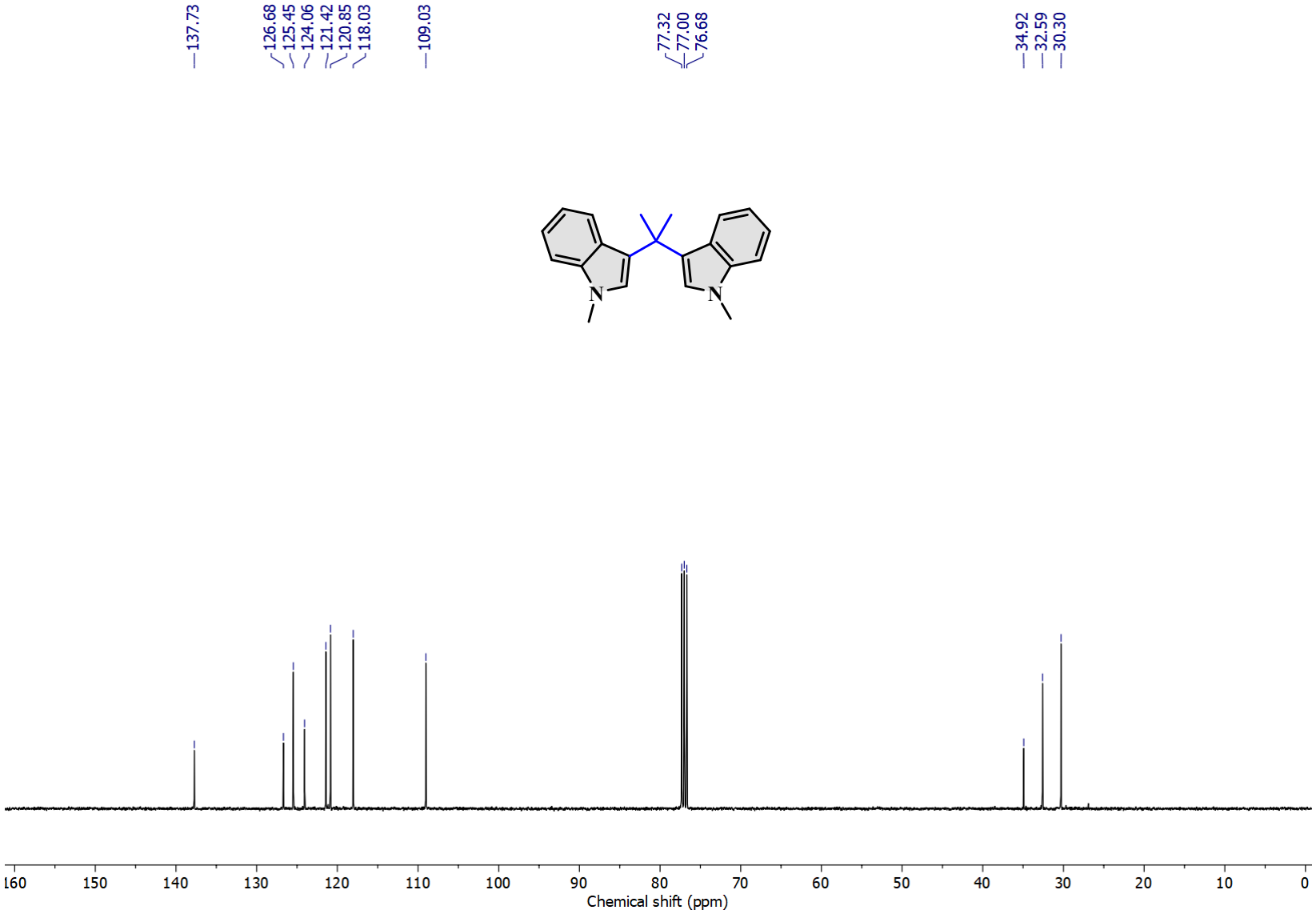

Fig. S46 100 MHz ^{13}C NMR spectrum of (**3a′**)[5] in $CDCl_3$

2. Copies of HRMS spectra

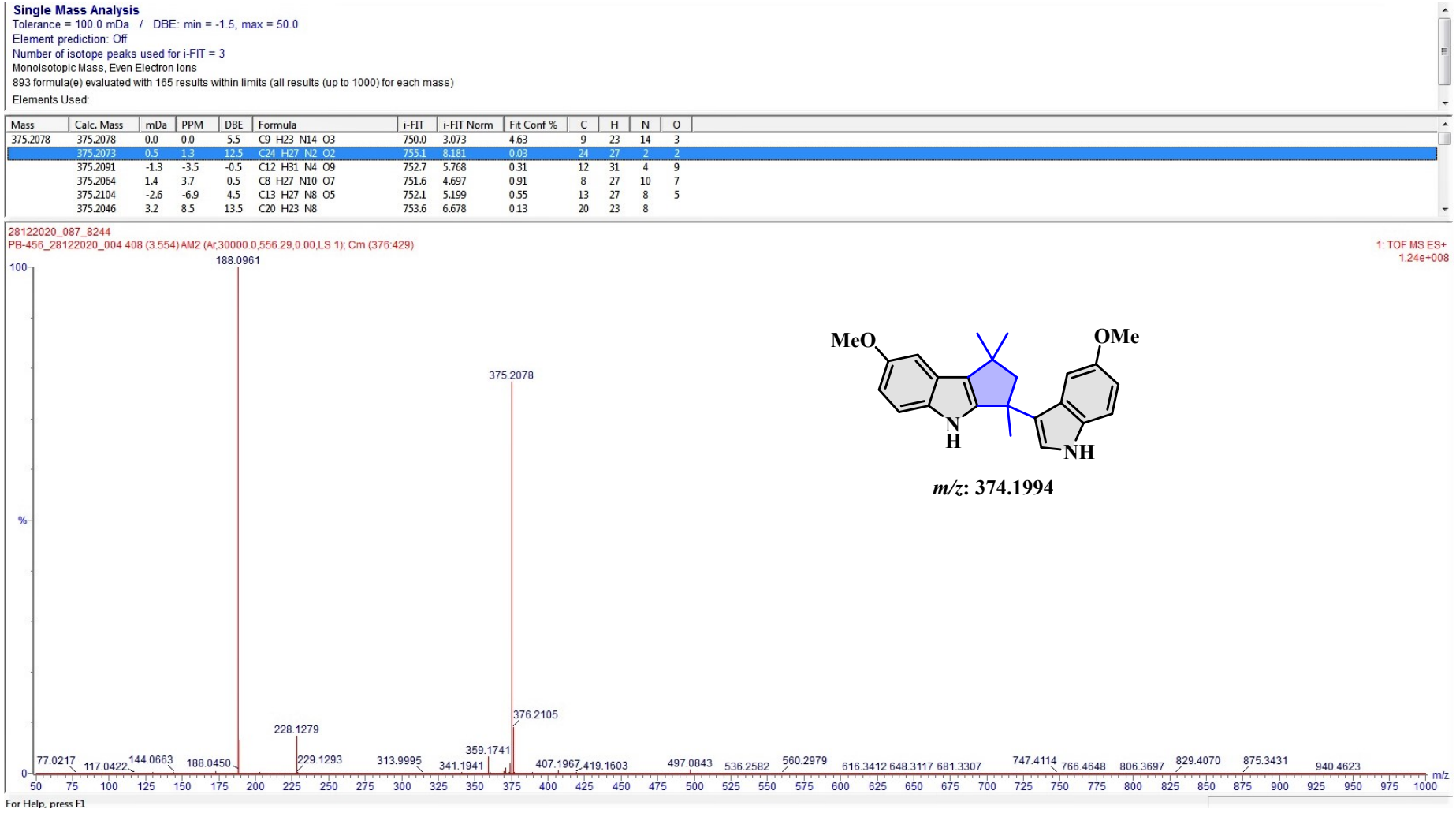

Fig. S47 HRMS spectrum of **2c**

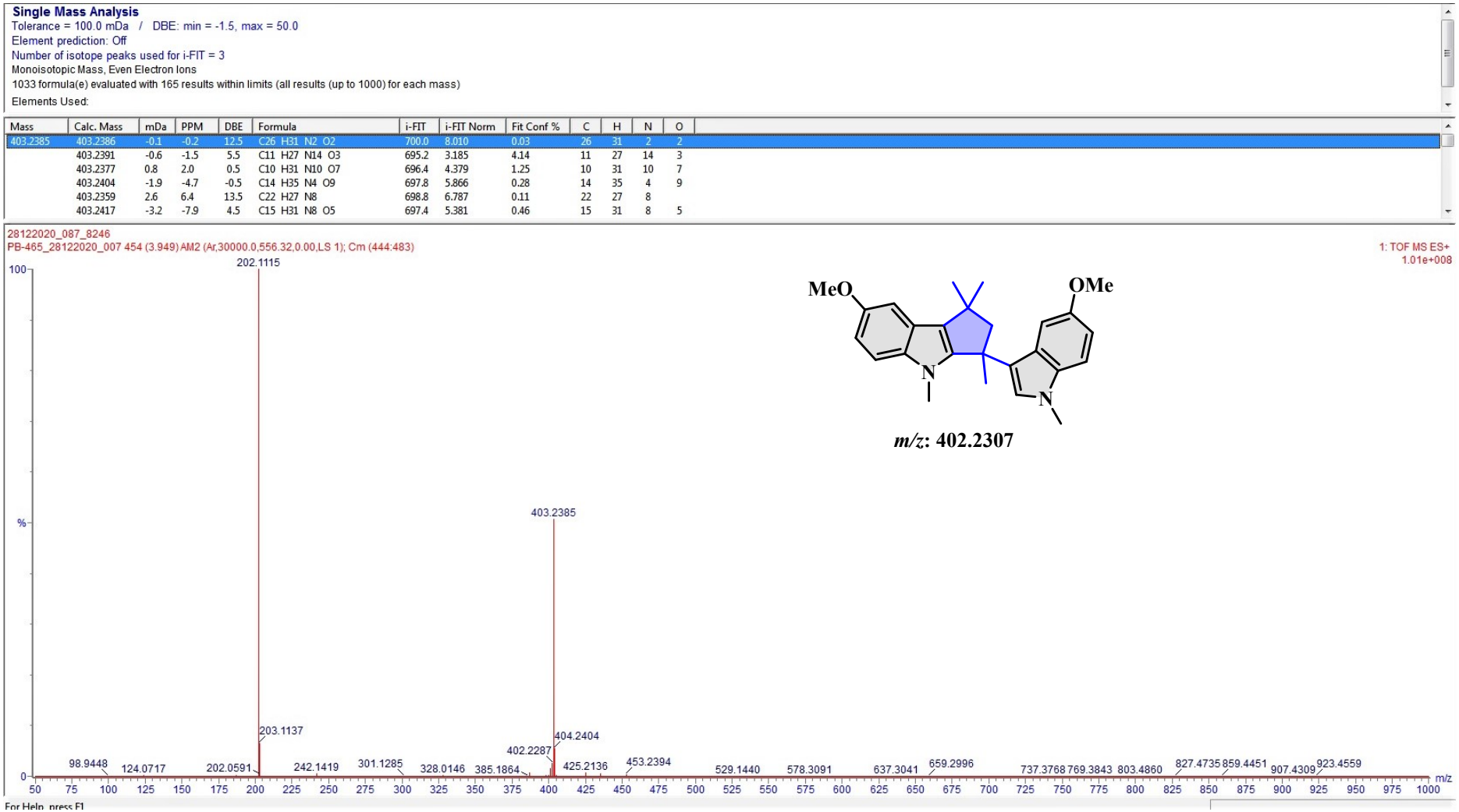

Fig. S48 HRMS spectrum of **2d**

3. Single crystal XRD data of 2d

(CCDC 2254620)

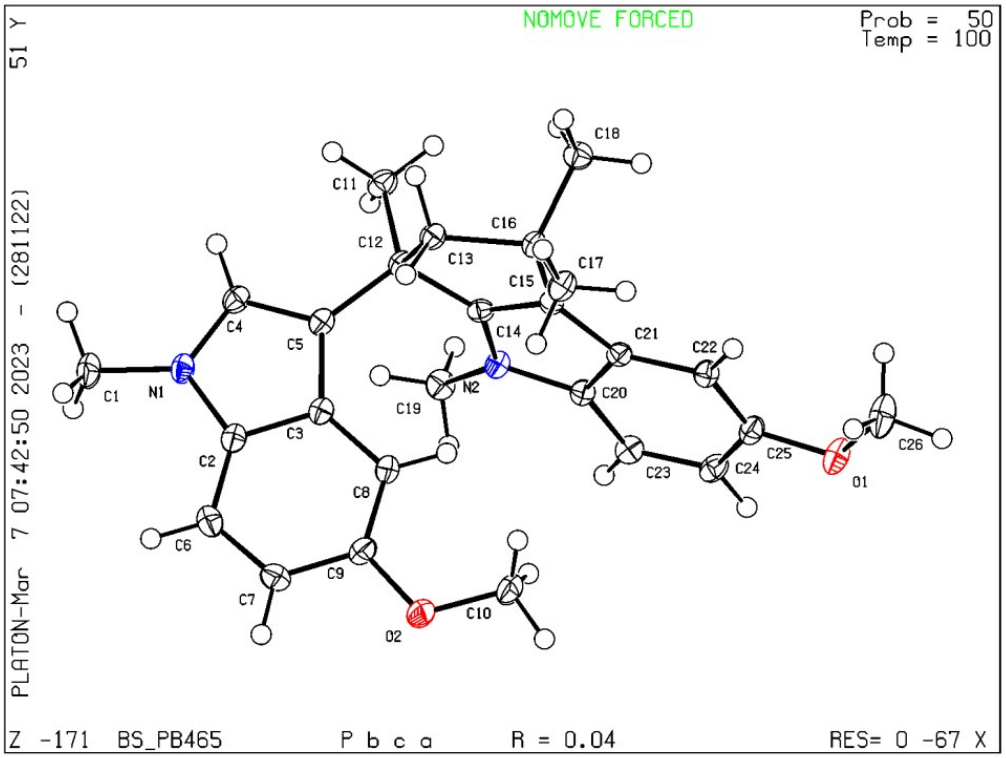

Fig. S49 ORTEP diagram of **2d** with 50% probability ellipsoids

Table S1 Crystallographic parameters of structures **2d**

Crystal data	**2d**
Formula unit	$C_{26}H_{30}N_2O_2$
Formula weight ($gmol^{-1}$)	402.52
Crystal system	orthorhombic
T [K]	100 K
a [Å]	8.0818(7)
b [Å]	16.4868(15)
c [Å]	32.475(3)
α [°]	90
β [°]	90
γ [°]	90
Volume [$Å^3$]	4327.1(7)
Space group	*Pbca*
Z	8
D_{cal} [g/cm^3]	1.236
R_1, *w*R2	0.0429, 0.0941
Instrument	Bruker CCD Apex II
CCDC No	CCDC 2254620

Single crystal X-ray diffraction. Single crystal X-ray diffractions were collected on a Bruker SMART APEX-II CCD diffractometer using Mo Kα (λ = 0.71073 Å) radiation. Bruker SAINT software has been employed for reducing the data and SADABS for correcting the intensities of absorption. Structure was solved and refined using SHELXL with anisotropic displacement parameters for non-H atoms. In the crystal structure H-atoms are located experimentally, whereas C–H atoms were fixed geometrically using the HFIX command in SHELX-TL. No missed symmetry observed in the final check of CIF file using PLATON. Information of crystallographic parameters for the structure is furnished in **Table S1**.

4. References

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