Electronic Supplementary Information

The Effect of N-Heterocyclic Carbene in Palladium-Tin Heterobimetallic Catalysis: A DFT Supported Study on the C3-H Functionalization of Unprotected Indole

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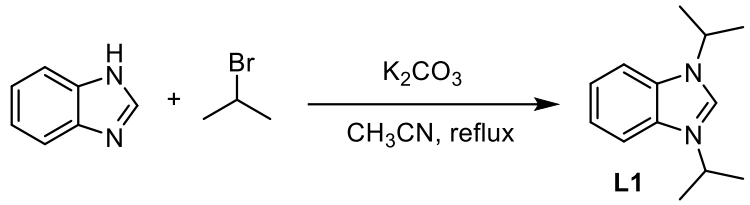
General Methods

All chemicals, reagents, and solvents were procured from Merck, Spectrochem, GLR, and SRL and purified as needed. All solvents used for the synthesis have been dried and distilled using standard methods.[1] All deuterated solvents ($CDCl_3$, DMSO-d6, and CD_3NO_2) are purchased from authorised suppliers. Pre-coated silica gel $60F_{254}$ from Merck was used for thin-layer chromatography, and silica gel 100-200 mesh (Spectrochem) was used for column chromatography. Single-crystal X-ray diffraction analysis was done on a Bruker APEXXII CCD diffractometer with graphite monochromated Mo-Kα radiation (0.71073 Å). ^{1}H (400 MHz) and ^{13}C NMR (100 MHz) spectra were recorded on Bruker-AC 400 MHz spectrometer at 300 K. Proton chemical shifts are reported in ppm with the residual solvent reference relative to tetramethylsilane employed as the internal standard ($CDCl_3$, δ = 7.26 ppm; CD_3NO_2, δ = 4.35 ppm; dmso-d_6, δ = 2.49). Carbon chemical shifts are reported in ppm with the residual solvent reference relative to tetramethylsilane employed as the internal standard ($CDCl_3$, δ = 77.3 ppm; CD_3NO_2, δ = 61.3 ppm; dmso-d_6, δ = 39.8). Coupling constants are expressed in Hertz (Hz) and Multiplicity is represented as; (s = singlet, d= doublet, t = triplet, q= quartet, m = multiplate, br = broad). High-resolution mass spectral analysis (HRMS) was performed on a Thermoscintific Exactive Plus ORBITRAP mass spectrometer using MeOH as a solvent with an electrospray ionization (ESI) positive method. N-heterocyclic carbene precursors and their palladium carbene complexes were synthesized using reported procedures. All the computational model structures at their ground electronic states were optimized at the level of density functional theory (DFT) using the hybrid meta-GGA exchange-correlation functional B3LYP.[2] The D3 version of Grimme's dispersion correction was included. LANL2DZ basis set for Pd and Sn atoms with electronic core potentials and 6-31G(d) for the other atoms, were used.[3,4] Solvation effects were accounted for by the integral equation formalism polarizable continuum model (IEFPCM).[5] To mimic the reaction conditions closely, a temperature of 90 ^{o}C was used for the solvent model. The character of the stationary points (minimum or saddle point) was ascertained by inspecting the harmonic frequencies computed at the optimized structures. The reaction path passing through the proposed transition state was confirmed in terms of the intrinsic reaction coordinate (IRC) calculation.[6] All the calculations were performed using the Gaussian 16 software package[7] at a High-Performance Computing Cluster (HPCC) provided by Quantum Chemistry Laboratory, IIT Bhubaneswar, Odisha, India.

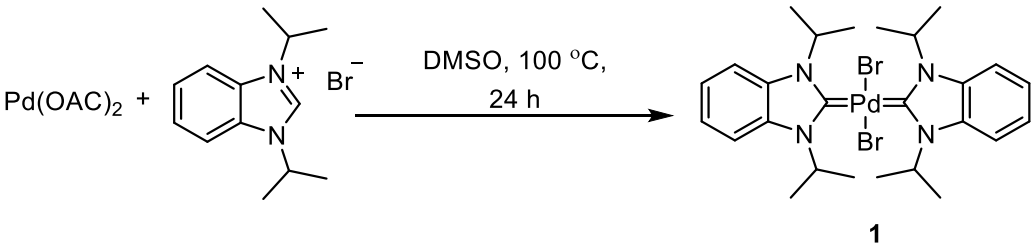
General Procedures for the Synthesis of Catalysts, Starting Materials, and Products

Synthesis of 1,3-diisopropyl-1H-benzo[d]imidazol-3-ium bromide (L1):[8]



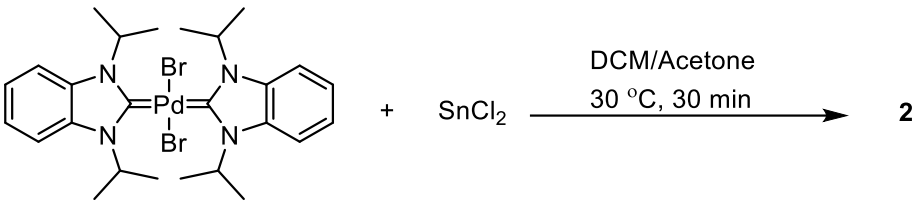
To a suspended mixture of benzimidazole (2 g, 5 mmol) in CH_3CN (15 mL), K_2CO_3 (760 mg, 5.5 mmol) was added and stirred at ambient temperature for 1 h. To the suspension, was added isopropyl bromide (1.40 mL, 15 mmol). The reaction mixture was stirred under reflux conditions for 24 h, followed by a second addition of isopropyl bromide (1.40 mL, 15 mmol). Stirring was continued for the next 72 hours. After removing the volatiles in vacuo, CH_2Cl_2 (50 mL) was added to the residue, and the resulting suspension was filtered over Celite. The remaining solid was washed with CH_2Cl_2 (5 × 20 mL), and the solvent of the filtrate was removed in vacuo to give a spongy solid. It was then thoroughly washed with ethyl acetate and diethyl ether several times until a white powder (1190 mg, 4.2 mmol, 84%) was obtained.

Bis(1,3-diisopropyl-1,3-dihydro-2H-benzo[d]imidazol-2-ylidene)palladium(II) bromide (1):[9]



To a mixture of salt **L1** (0.6 mmol) was added $Pd(OAc)_2$ (67 mg, 0.3 mmol) in DMSO (6 mL). It was then stirred at 100 °C for 24 h. The reaction mixture was then diluted with DCM and filtered over Celite. The clear solution was then washed with cold water several times to remove DMSO completely. The organic phase was dried over Na_2SO_4 followed by the removal of the solvent in vacuo, afforded the product as a yellow solid (131 mg, 0.14 mmol, 93%).

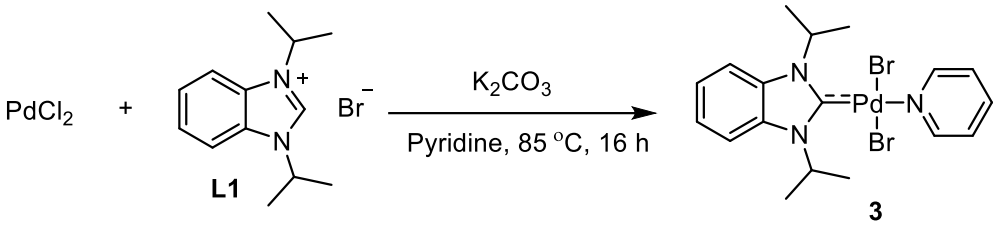
Procedure for the Synthesis of 2[10]



1

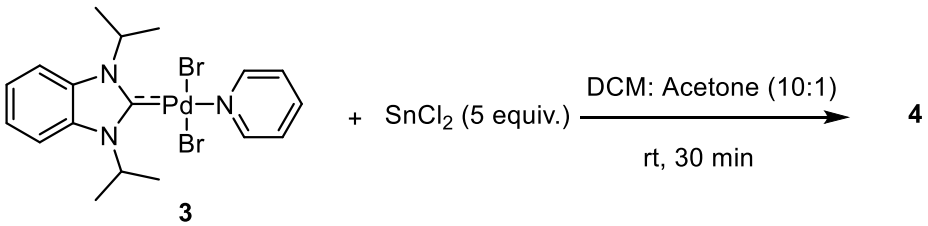
To a stirring solution of **1** (1 mmol) in dry DCM, was added a solution of $SnCl_2$ (3 mmol) in dry acetone at room temperature under an argon atmosphere. In addition to the solution of $SnCl_2$, a clear change in the color of the solution mixture was observed. The mixture was stirred for another 30 minutes and then was left undisturbed. Nice golden yellow crystals of **2** were obtained (yield 87%).

Procedure for the Synthesis of 3[11]



3 was prepared using a modified reported procedure. In a round bottom flask, $PdCl_2$ (1 mmol), **L1** (1 mmol), and K_2CO_3 (5 mmol) were taken. To it, added 4 ml of pyridine and the resulting solution was stirred at 85 ℃ for 16 h. After completion of the reaction, the reaction mixture was brought to room temperature followed by the addition of 20 ml of DCM. The insoluble components were removed by passing the solution through a short celite pad. The filtrate was concentrated in vacuo followed by the addition of 20 ml of hexane. A yellow precipitate was formed which was filtered and washed with hexane to remove extra pyridine. The pure product was isolated, dried under a vacuum, and characterized using NMR.

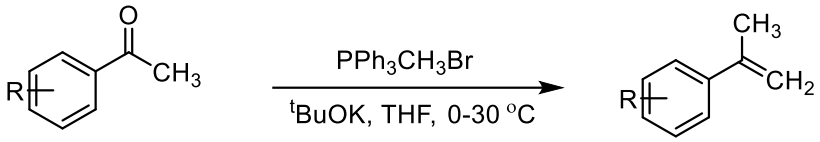
Procedure for the Synthesis of 4



To a solution of **3** (0.1 mmol) in dry DCM (10 ml), a solution of 0.5 mmol of $SnCl_2$ in acetone (1 ml) under argon atmosphere. The resultant solution was then stirred for 30 minutes. To it,

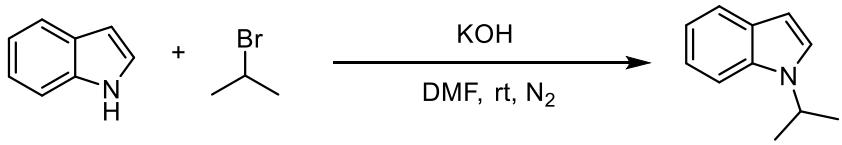
30 ml of freshly distilled hexane was added and it was stirred for another 5 minutes. The solution mixture was then passed through a cotton and the solvent was evaporated in vacuo at room temperature. 10 ml of DCM was then added to the crude where excess $SnCl_2$ gets precipitated. It was then filtered, and the solution was concentrated in vacuo at room temperature followed by the addition of 20 ml of hexane. The product gets precipitated. It was filtered, washed with hexane, and dried under vacuum to get product **4.** Later **4** was recrystallized in chloroform and characterized by NMR and Single crystal XRD.

Procedure for the Synthesis of α-Methyl Styrene[12]



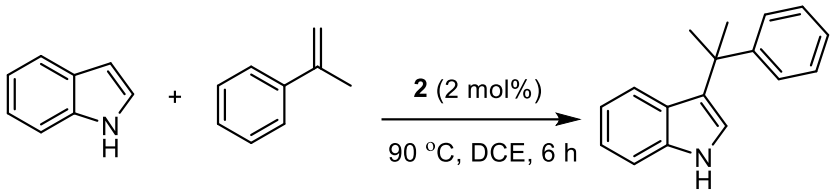
1.5 equivalent of methyltriphenylphosphonium bromide and ^tBuOK (3.0 equiv.) were taken in a double-necked round bottom flask under an argon atmosphere. 20 ml of dry THF was added to it and the temperature was maintained at 0 ºC. The reaction mixture was stirred for 1 hour at 0 ºC then it was brought to room temperature. Then the acetophenone (1.0 equiv.) dissolved in THF was added slowly and the reaction was stirred at rt for 1 h. After the starting material was fully consumed the reaction was quenched by the addition of sat. aq. NH_4Cl and extracted with ethyl acetate 3 times. The organic phases were dried over anhydrous Na_2SO_4, the solvent was removed and the resulting crude product was purified by silica gel column chromatography.

General Procedure for the Synthesis of N-Substituted Indoles[13]



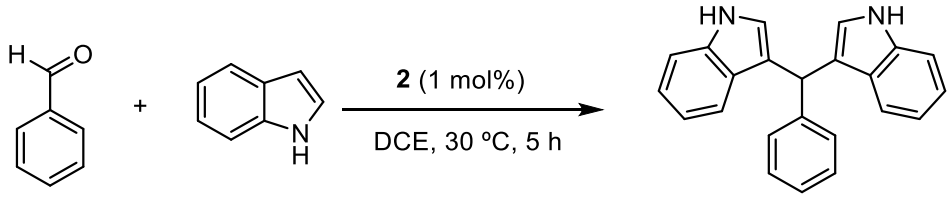
Indole (5 mmol) was taken in a round bottom flask; to it, KOH (6 mmol, 1.2 equivalent) was added, and argon gas was purged into the system. 10 ml of DMF was then added, and the mixture was stirred for 1 hour. When all KOH dissolved, 1.2 equivalent of isopropyl bromide (6 mmol) was added dropwise. After completion, the mixture was allowed to stir for another 24 hours. Then 20 ml of water was added to the reaction mixture, followed by 30 minutes of stirring. The organic part was then extracted with ethyl acetate, washed with water, and dried with Na_2SO_4. The solvent was removed in vacuo, and the pure product was isolated in column chromatography using 5% ethyl acetate in hexane as eluent.

Procedure for the Synthesis of 3-(2-phenylpropan-2-yl)-1H-indole



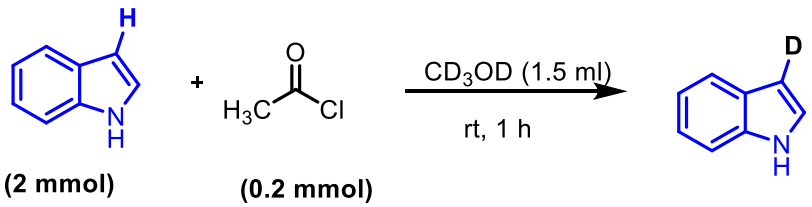
In a sealed tube, indole (0.25 mmol), styrene (0.50 mmol), and catalyst (**2**: 0.005 mmol, and **4**: 0.0025 mmol) were taken. To it, 1.5 ml of DCE was added. The mixture solution was then stirred at 90 ºC for 6 hours. The reaction was monitored using TLC. After completion of the reaction, the whole reaction mixture was dissolved with 20 ml of ethyl acetate. The inorganic part was removed by washing it with water. The organic layer was collected and dried using Na_2SO_4. The solvent was removed in vacuo. The pure product was obtained using column chromatography with petroleum ether and ethyl acetate as eluent.

Procedure for the Synthesis of Bis(indolyl)methane



In a Schlenk tube, indole (0.5 mmol), aldehyde (0.35 mmol), and catalyst (0.005 mmol) were taken. To it, 1.5 ml of DCE was added. The mixture solution was then stirred at room temperature for 5 hours. The reaction was monitored using TLC. After completion of the reaction, the whole reaction mixture was dissolved with 20 ml of ethyl acetate. The inorganic part was removed by washing it with water. The organic layer was collected and dried using Na_2SO_4. The solvent was removed in vacuo. The pure product was obtained using column chromatography with petroleum ether and ethyl acetate in 4:1 (v/v).

Procedure for the Synthesis of C3-D Indole[14]



Indole (2 mmol) was taken in a round bottom flask; to it, CD_3OD (1.5 ml) was added followed by the addition of acetyl chloride (10 mol%). The mixture was stirred for 1 hour and the

conversion of indole C3-H was monitored using ^{1}H NMR (figure S1). After completion of the reaction, the solvent was removed in a rotary evaporator and the product was isolated using column chromatography (yield 60 %).

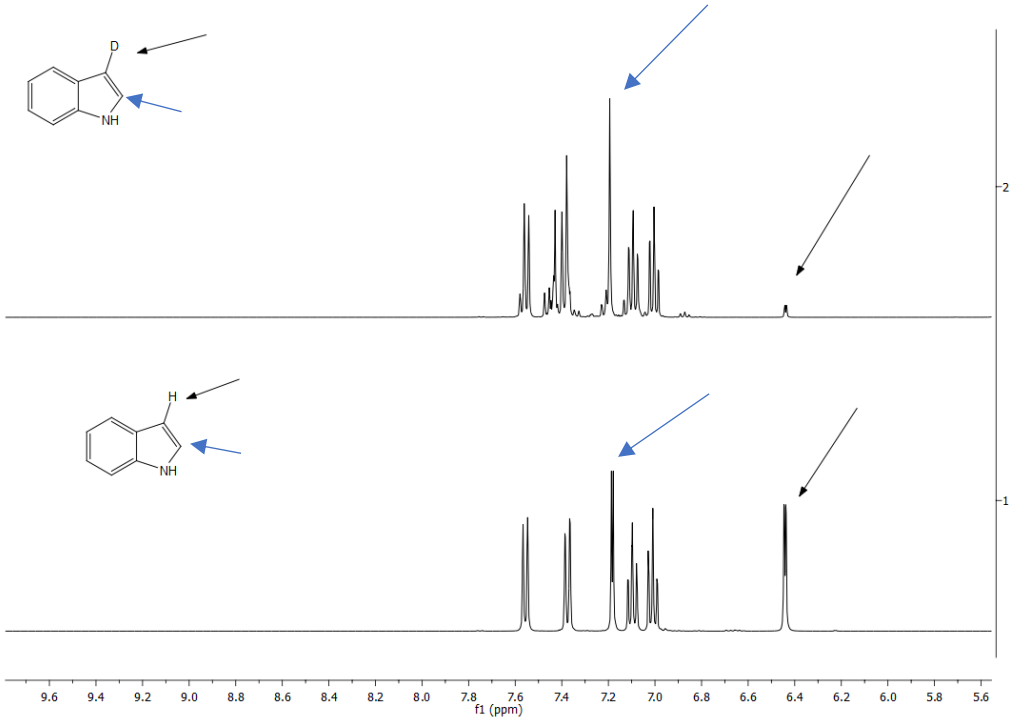
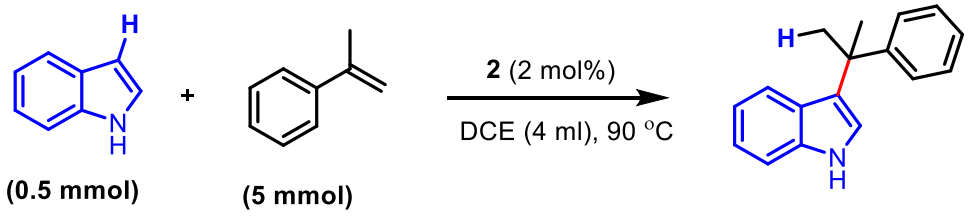


Figure S1. Conversion of indole C3-H to indole C3-D in CD_3OD

Procedure for the Study of Kinetic Isotopic Effect

Determination of k_H



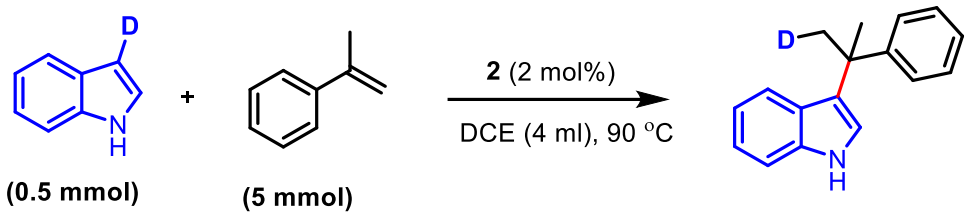
A round bottom flask was charged with indole C3-H (0.5 mmol) and **2** (2 mol % to indole) followed by the addition of 4 ml of DCE. Excess of α-methylstyrene (10 equivalent, 5 mmol) was added to follow the pseudo-first-order kinetics and the mixture was made homogenous by sonication. The whole reaction volume was divided into four equal parts and each part was transferred to a sealed tube (each tube contains 0.108 mmol of indole). All four sealed tubes were stirred at 90 °C and each tube was taken out from the oil bath periodically, filtered through

a short pad of celite and the solvent was removed using a rotary evaporator. The product concentration was analyzed with ^{1}H NMR in $CDCl_3$ against mesitylene (0.051 mmol) as the external standard to estimate the concentration of the product (Table S1).

Table S1. Change in Concentration of Reactant with Time

Sl. No.	Time (min)	$n_{product}$ (mmol)	n_{indole} (mmol)	C_0 (mmol)	$\ln C_0/C_t$
1	0	0	0.108	0.108	0
2	5	0.003	0.105	0.108	0.028
3	15	0.010	0.098	0.108	0.097
4	25	0.023	0.085	0.108	0.239
5	35	0.027	0.081	0.108	0.287

Determination of k_D



The same procedure was applied to measure k_D except indole C3-D was used instead of indole C3-H.

Table S2. Change in Concentration of Reactant with Time

Sl. No.	Time (min)	$n_{product}$ (mmol)	n_{indole} (mmol)	C_0 (mmol)	$\ln C_0/C_t$
1	0	0	0.108	0.108	0
2	5	0.007	0.101	0.108	0.067
3	15	0.027	0.081	0.108	0.287
4	25	0.044	0.064	0.108	0.523
5	35	0.048	0.060	0.108	0.587

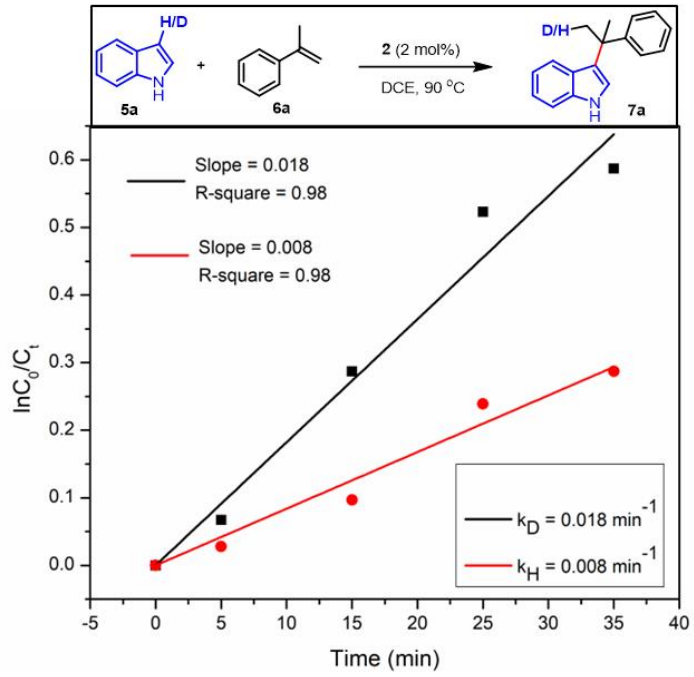
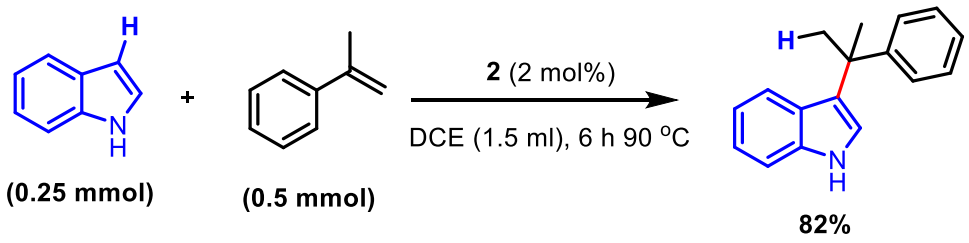


Figure S2. Study of kinetic isotopic effect

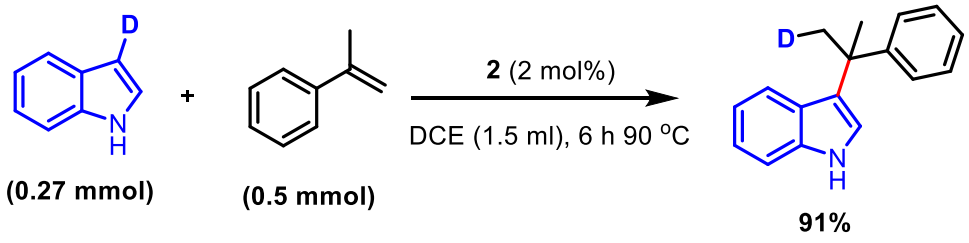
Calculation of Equilibrium Isotopic Effect

Calculation for K_H



K_H = [Product]/[Reactant] = 82/18 = 4.55

Calculation for K_D



K_D = [Product]/[Reactant] = 91/9 = 10.11

K_H/K_D = 0.45

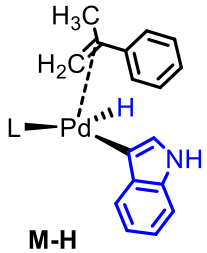
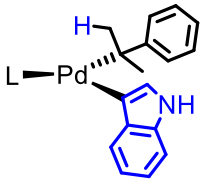
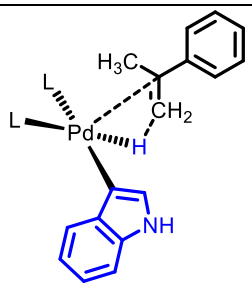
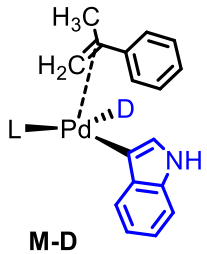
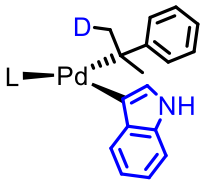
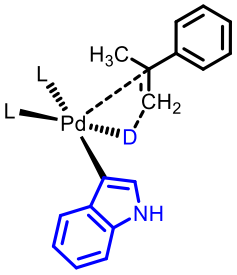
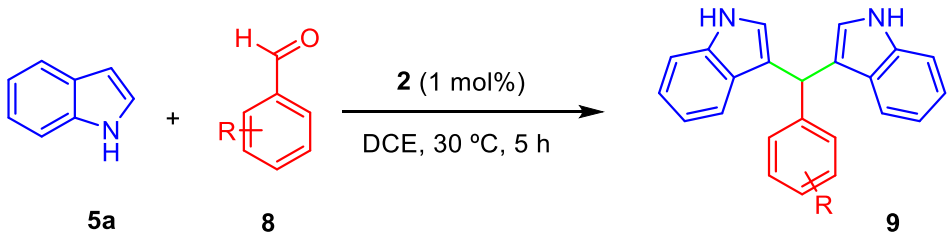
 **M-H** **E^{R}_{H} = -2070.278942 Hartrees**	 **C-H** **E^{P}_{H} = -2070.274807 Hartrees**	 **TS-H** **$E^{\#}_{H}$ = -2070.215305 Hartees**
 **M-D** **E^{R}_{D} = -2070.281193 Hartrees**	 **C-D** **E^{P}_{D} = -2070.278055 Hartrees**	 **TS-D** **$E^{\#}_{D}$ = -2070.218492 Hartees**

Figure S3. Zero-point correction energy of reactants and products involved in the rate limiting stage.

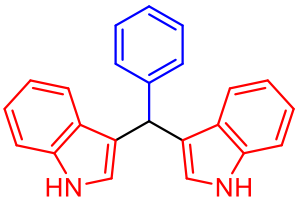
Substrates Scope for the Synthesis of Bis(indolyl)methane

The scope of the reaction was tested for various substituted aldehydes and indole derivatives with the optimized conditions. **Table S1** displays a variety of benzaldehydes used to synthesize the corresponding bis(indolyl)methanes. Electron-donating functionalities like -Me, -OMe, -iPr, and -NMe_2 on aldehyde afforded fairly good results for the corresponding Bis(indolyl)methane. Similarly, electron-withdrawing groups like -F, -Cl, -Br, and -NO_2 produced excellent results. The substitution at ortho and meta-position to aldehyde does not affect the reactivity. Next, the reactivity of different substituted indoles was explored (**Table S2**). Excellent reactivity was also observed in the case of N-substituted indoles. This concept can be applied to both electron-donating and electron-withdrawing functionalities on indole moieties.

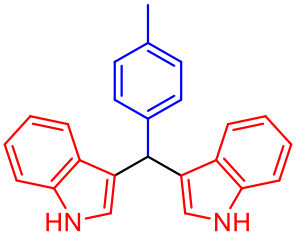
Table S3. Substrates Scope for Different Substituted Aldehydes[a]



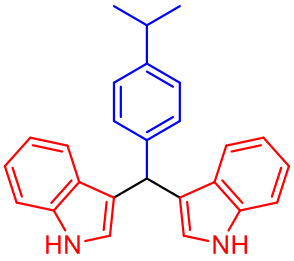
5a **8** **9**



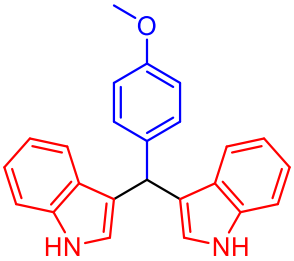
9a (92%)[b]



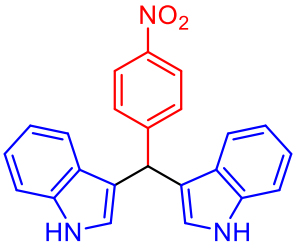
9b (77%)[b]



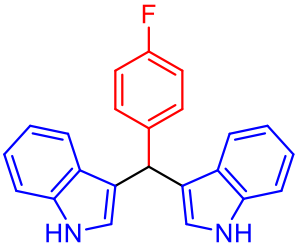
9c (76%)[b]



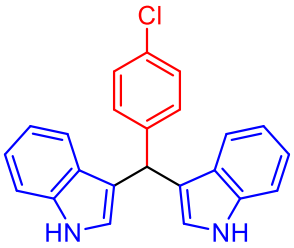
9d (80%)[b]



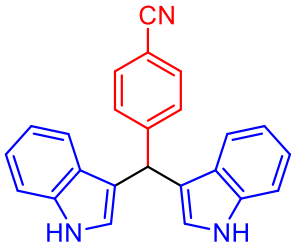
9e (98%)[b]



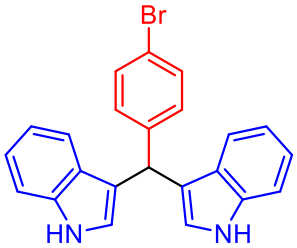
9f (93%)[b]



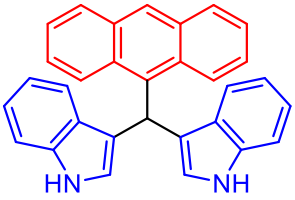
9g (96%)[b]



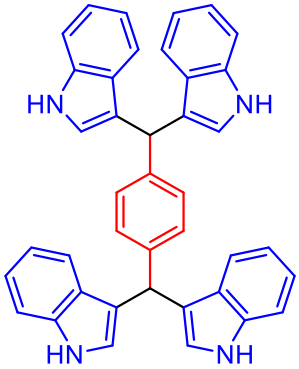
9h (94%)[b]



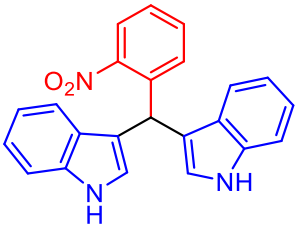
9i (90%)[b]



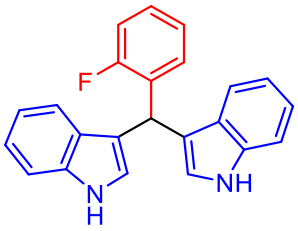
9j (80%)[b]



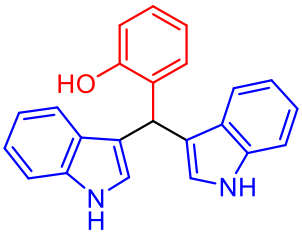
9k (76%)[b]



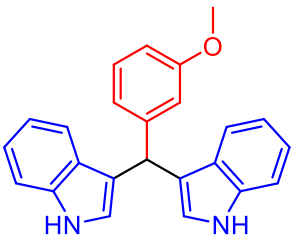
9l (95%)[b]



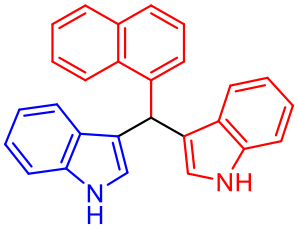
9m (96%)[b]



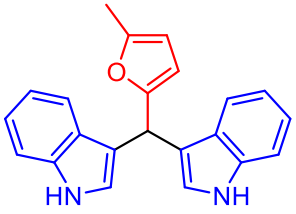
9n (66%)[b]



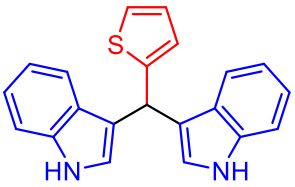
9o (82%)[b]



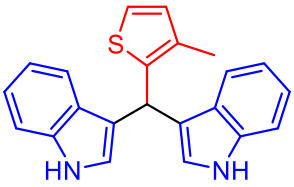
9p (80%)[b]



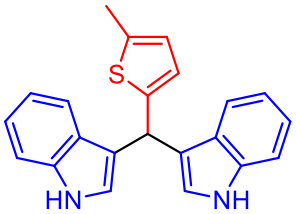
9q (80%)[b]



9r (77%)[b]



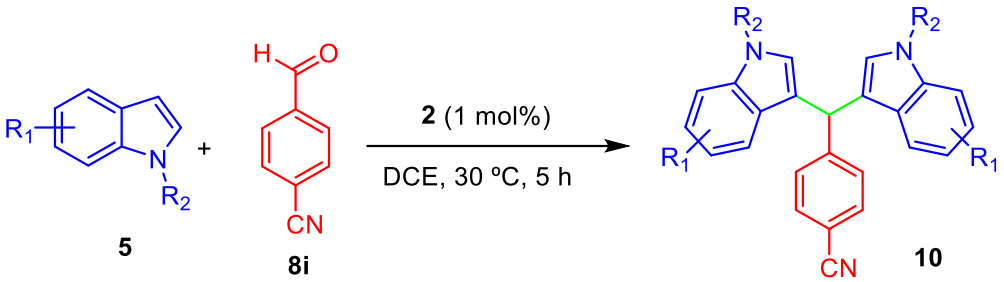
9s (85%)[b]



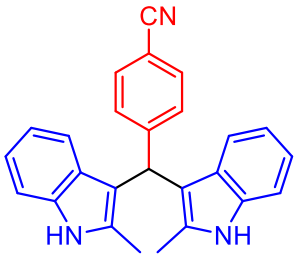
9t (80%)[b]

[a]**5a** (0.5 mmol), **8** (0.35 mmol), Catalyst (1 mol% with respect to **5a**, 0.005 mmol), DCE 1.5 ml. [b]refers to isolated yield.

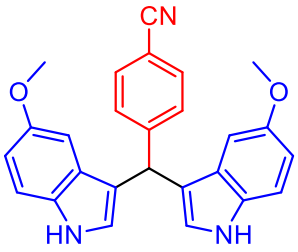
Table S4. Substrate Scope for Different Substituted Indoles



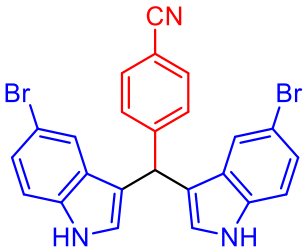
5 8i 10



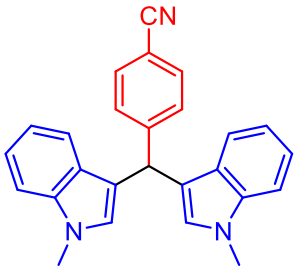
10a (94%)[b]



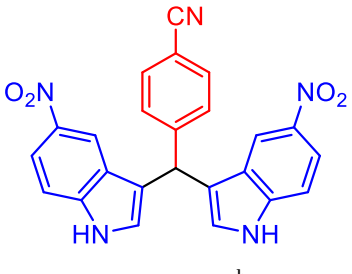
10b (96%)[b]



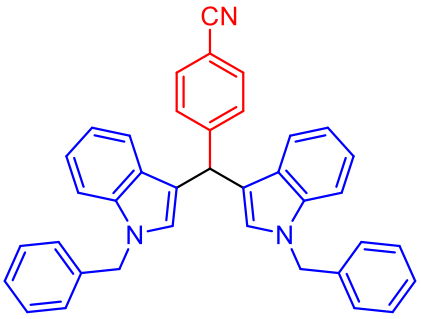
10c (95%)[b]



10d (99%)[b]



10e (88%)[b]



10f (80%)[b]

[a]**5** (0.5 mmol), **8** (0.35 mmol), Catalyst (1 mol% with respect to **5**, 0.005 mmol), [b]refers to isolated yield

Single Crystal Analysis of Complex 2 & 4

Single crystal X-ray diffraction data were collected on a Bruker APEXXII CCD diffractometer with graphite monochromated Mo-Kα radiation (0.71073 Å). The data collection was smooth without any complications, and the crystal was stable throughout the data collection period. The data sets were reduced in Bruker Apex2. Crystal structures were solved using direct methods and refined with full-matrix least-squares based on F2, using the SHELXL software package.

The molecular structure of **2** has been well established in our previous work[10] and is shown in figure S1.

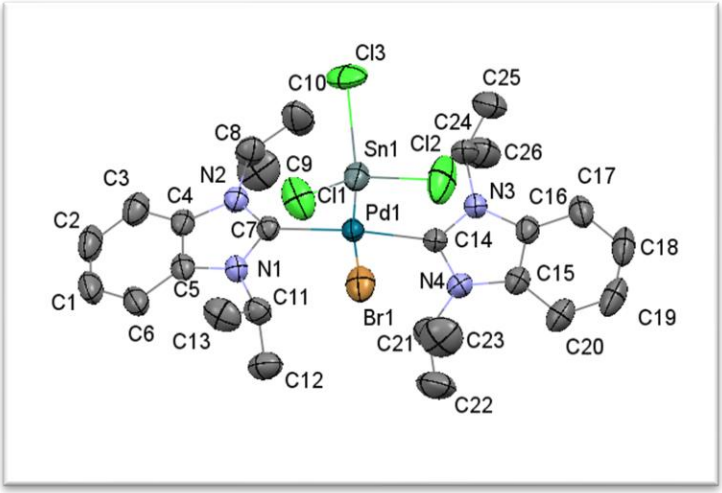


Figure S4. Solid-State Structure of **2**

Single Crystal Analysis of 4

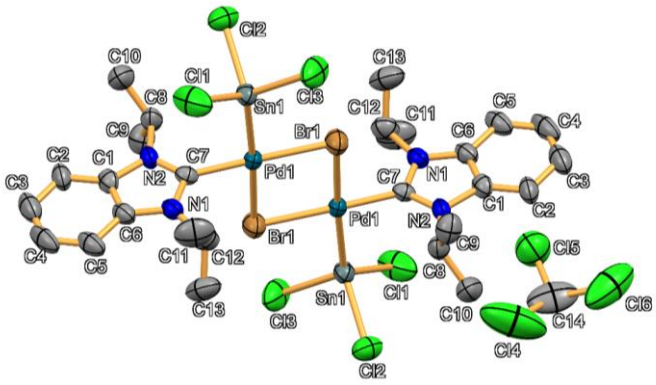


Figure S5. Solid state structure of **4**

Table S5. Crystal data and structure refinement for **4**

Identification code	**2291609**
Empirical formula	C14 H19 Br Cl6 N2 Pd Sn
Formula weight	733.01
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P -1
Unit cell dimensions	a = 9.03(2) Å, α= 103.95(11)°.
	b = 10.515(19) Å, β= 106.54(8)°
	c = 14.250(19) Å, γ = 97.14(12)°
Volume	1231(4) $Å^3$
Z	2
Density (calculated)	1.978 Mg/m^3
Absorption coefficient	4.022 mm^{-1}
F(000)	700
Crystal size	0.25 x 0.20 x 0.16 mm^3
Theta range for data collection	2.402 to 26.726°.
Index ranges	-11<=h<=11, -13<=k<=13, -17<=l<=17
Reflections collected	18945
Independent reflections	5150 [R(int) = 0.0606]
Completeness to theta = 25.242°	99.5 %
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	5150 / 0 / 230
Goodness-of-fit on F^2	1.052

Final R indices [I>2sigma(I)]	R1 = 0.0598, wR2 = 0.1652
R indices (all data)	R1 = 0.0899, wR2 = 0.2002
Extinction coefficient	n/a
Largest diff. peak and hole	1.476 and -2.446 e.Å^{-3}

Table S6. Crystal Data and Structure Refinement for **4**

	x	y	z	U(eq)
Sn(1)	2267(1)	4566(1)	1738(1)	43(1)
Pd(1)	4273(1)	5508(1)	1034(1)	35(1)
Br(1)	3733(1)	3398(1)	-381(1)	62(1)
Cl(2)	-404(3)	4787(3)	1147(2)	71(1)
Cl(3)	1737(4)	2236(3)	1474(4)	98(1)
Cl(1)	2619(4)	5361(5)	3505(2)	105(1)
Cl(5)	3552(5)	7342(5)	8058(3)	112(1)
Cl(6)	2012(8)	9505(7)	7865(6)	182(3)
N(2)	4022(8)	8219(7)	2150(5)	43(2)
Cl(4)	934(7)	6903(9)	6267(6)	217(4)
N(1)	5961(8)	7523(7)	3063(5)	45(2)
C(8)	2630(11)	8215(10)	1265(7)	53(2)
C(7)	4745(9)	7187(8)	2180(6)	38(2)
C(12)	7095(12)	6637(11)	3338(8)	61(3)
C(9)	3097(14)	9111(11)	662(8)	67(3)
C(2)	4560(13)	10611(9)	3342(8)	59(2)
C(10)	1222(13)	8525(12)	1616(11)	78(3)
C(13)	8729(13)	7247(16)	3381(11)	89(4)
C(6)	6038(11)	8843(10)	3614(7)	50(2)
C(1)	4810(11)	9313(9)	3038(6)	46(2)
C(11)	7043(16)	6346(17)	4333(11)	95(4)
C(5)	7087(13)	9696(12)	4576(7)	64(3)
C(3)	5622(15)	11439(12)	4295(9)	75(3)
C(4)	6824(15)	10991(13)	4876(8)	78(4)
C(14)	1795(19)	7710(20)	7558(15)	131(7)

Table S7. Bond lengths [Å] and angles [°] for **4**

Sn(1)-Cl(3)	2.353(5)
Sn(1)-Cl(1)	2.368(5)
Sn(1)-Cl(2)	2.378(6)
Sn(1)-Pd(1)	2.517(4)
Pd(1)-C(7)	1.998(9)
Pd(1)-Br(1)	2.498(5)
Pd(1)-Br(1)	2.526(4)
Cl(5)-C(14)	1.676(17)
Cl(6)-C(14)	1.81(2)
N(2)-C(7)	1.337(10)
N(2)-C(1)	1.418(11)
N(2)-C(8)	1.505(11)
Cl(4)-C(14)	1.73(2)
N(1)-C(7)	1.347(10)
N(1)-C(6)	1.403(12)
N(1)-C(12)	1.501(12)
C(8)-C(9)	1.518(15)
C(8)-C(10)	1.536(15)
C(8)-H(8)	0.9800
C(12)-C(13)	1.512(17)
C(12)-C(11)	1.534(17)
C(12)-H(12)	0.9800
C(9)-H(9A)	0.9600
C(9)-H(9B)	0.9600
C(9)-H(9C)	0.9600
C(2)-C(1)	1.396(13)
C(2)-C(3)	1.414(15)
C(2)-H(2)	0.9300
C(10)-H(10A)	0.9600
C(10)-H(10B)	0.9600
C(10)-H(10C)	0.9600

C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
C(6)-C(1)	1.400(13)
C(6)-C(5)	1.427(13)
C(11)-H(11A)	0.9600
C(11)-H(11B)	0.9600
C(11)-H(11C)	0.9600
C(5)-C(4)	1.396(17)
C(5)-H(5)	0.9300
C(3)-C(4)	1.374(18)
C(3)-H(3)	0.9300
C(4)-H(4)	0.9300
C(14)-H(14)	0.9800

Bond Angle

Cl(3)-Sn(1)-Cl(1)	101.0(2)
Cl(3)-Sn(1)-Cl(2)	96.85(19)
Cl(1)-Sn(1)-Cl(2)	96.30(16)
Cl(3)-Sn(1)-Pd(1)	117.71(14)
Cl(1)-Sn(1)-Pd(1)	119.76(15)
Cl(2)-Sn(1)-Pd(1)	120.57(15)
C(7)-Pd(1)-Br(1)	178.8(2)
C(7)-Pd(1)-Sn(1)	87.1(3)
Br(1)-Pd(1)-Sn(1)	93.15(14)
C(7)-Pd(1)-Br(1)#1	89.5(3)
Br(1)-Pd(1)-Br(1)#1	90.21(14)
Sn(1)-Pd(1)-Br(1)#1	176.33(3)
Pd(1)-Br(1)-Pd(1)#1	89.79(14)
C(7)-N(2)-C(1)	110.1(7)
C(7)-N(2)-C(8)	123.8(7)
C(1)-N(2)-C(8)	126.0(7)
C(7)-N(1)-C(6)	108.7(7)
C(7)-N(1)-C(12)	124.0(8)
C(6)-N(1)-C(12)	127.2(8)

N(2)-C(8)-C(9)	111.3(8)
N(2)-C(8)-C(10)	111.2(9)
C(9)-C(8)-C(10)	113.9(9)
N(2)-C(8)-H(8)	106.6
C(9)-C(8)-H(8)	106.6
C(10)-C(8)-H(8)	106.6
N(2)-C(7)-N(1)	108.9(7)
N(2)-C(7)-Pd(1)	125.6(6)
N(1)-C(7)-Pd(1)	125.1(6)
N(1)-C(12)-C(13)	110.5(10)
N(1)-C(12)-C(11)	109.5(9)
C(13)-C(12)-C(11)	113.6(10)
N(1)-C(12)-H(12)	107.7
C(13)-C(12)-H(12)	107.7
C(11)-C(12)-H(12)	107.7
C(8)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(1)-C(2)-C(3)	115.6(11)
C(1)-C(2)-H(2)	122.2
C(3)-C(2)-H(2)	122.2
C(8)-C(10)-H(10A)	109.5
C(8)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(8)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5

H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(1)-C(6)-N(1)	107.7(7)
C(1)-C(6)-C(5)	120.0(9)
N(1)-C(6)-C(5)	132.4(10)
C(2)-C(1)-C(6)	123.3(9)
C(2)-C(1)-N(2)	132.1(9)
C(6)-C(1)-N(2)	104.6(7)
C(12)-C(11)-H(11A)	109.5
C(12)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(12)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(4)-C(5)-C(6)	116.3(11)
C(4)-C(5)-H(5)	121.8
C(6)-C(5)-H(5)	121.8
C(4)-C(3)-C(2)	121.9(11)
C(4)-C(3)-H(3)	119.0
C(2)-C(3)-H(3)	119.0
C(3)-C(4)-C(5)	122.9(10)
C(3)-C(4)-H(4)	118.6
C(5)-C(4)-H(4)	118.6
Cl(5)-C(14)-Cl(4)	112.9(12)
Cl(5)-C(14)-Cl(6)	109.1(11)
Cl(4)-C(14)-Cl(6)	113.2(9)
Cl(5)-C(14)-H(14)	107.1
Cl(4)-C(14)-H(14)	107.1
Cl(6)-C(14)-H(14)	107.1

Table S8. Crystal Data and Structure Refinement for **4**

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Sn(1)	45(1)	38(1)	47(1)	10(1)	20(1)	5(1)

Pd(1)	35(1)	32(1)	36(1)	6(1)	13(1)	8(1)
Br(1)	65(1)	52(1)	66(1)	4(1)	32(1)	5(1)
Cl(2)	52(1)	81(2)	87(2)	34(2)	25(1)	21(1)
Cl(3)	98(2)	44(2)	178(4)	44(2)	70(3)	25(2)
Cl(1)	89(2)	158(4)	47(2)	6(2)	27(2)	-18(2)
Cl(5)	107(3)	108(3)	116(3)	36(2)	23(2)	31(2)
Cl(6)	190(6)	185(6)	317(9)	182(6)	178(6)	120(5)
N(2)	48(4)	32(3)	41(4)	0(3)	15(3)	3(3)
Cl(4)	123(4)	287(9)	186(6)	128(6)	-41(4)	-54(5)
N(1)	39(4)	47(4)	39(4)	2(3)	10(3)	0(3)
C(8)	49(5)	44(5)	55(5)	4(4)	5(4)	14(4)
C(7)	34(4)	38(4)	40(4)	15(3)	9(3)	2(3)
C(12)	48(5)	65(6)	60(6)	20(5)	3(4)	11(5)
C(9)	82(8)	67(7)	56(6)	21(5)	21(6)	28(6)
C(2)	70(6)	37(5)	62(6)	-3(4)	28(5)	3(4)
C(10)	53(6)	64(7)	106(10)	11(7)	20(6)	16(5)
C(13)	48(6)	123(12)	98(10)	33(9)	22(6)	25(7)
C(6)	44(5)	52(5)	42(4)	1(4)	12(4)	-4(4)
C(1)	53(5)	46(5)	36(4)	3(4)	20(4)	5(4)
C(11)	72(8)	132(13)	88(9)	61(9)	10(7)	33(8)
C(5)	59(6)	72(7)	42(5)	-3(5)	14(4)	-14(5)
C(3)	87(9)	52(6)	69(7)	-11(5)	35(7)	-10(6)
C(4)	76(8)	83(9)	44(5)	-18(5)	23(5)	-30(7)
C(14)	95(11)	200(20)	154(16)	125(16)	62(11)	39(12)

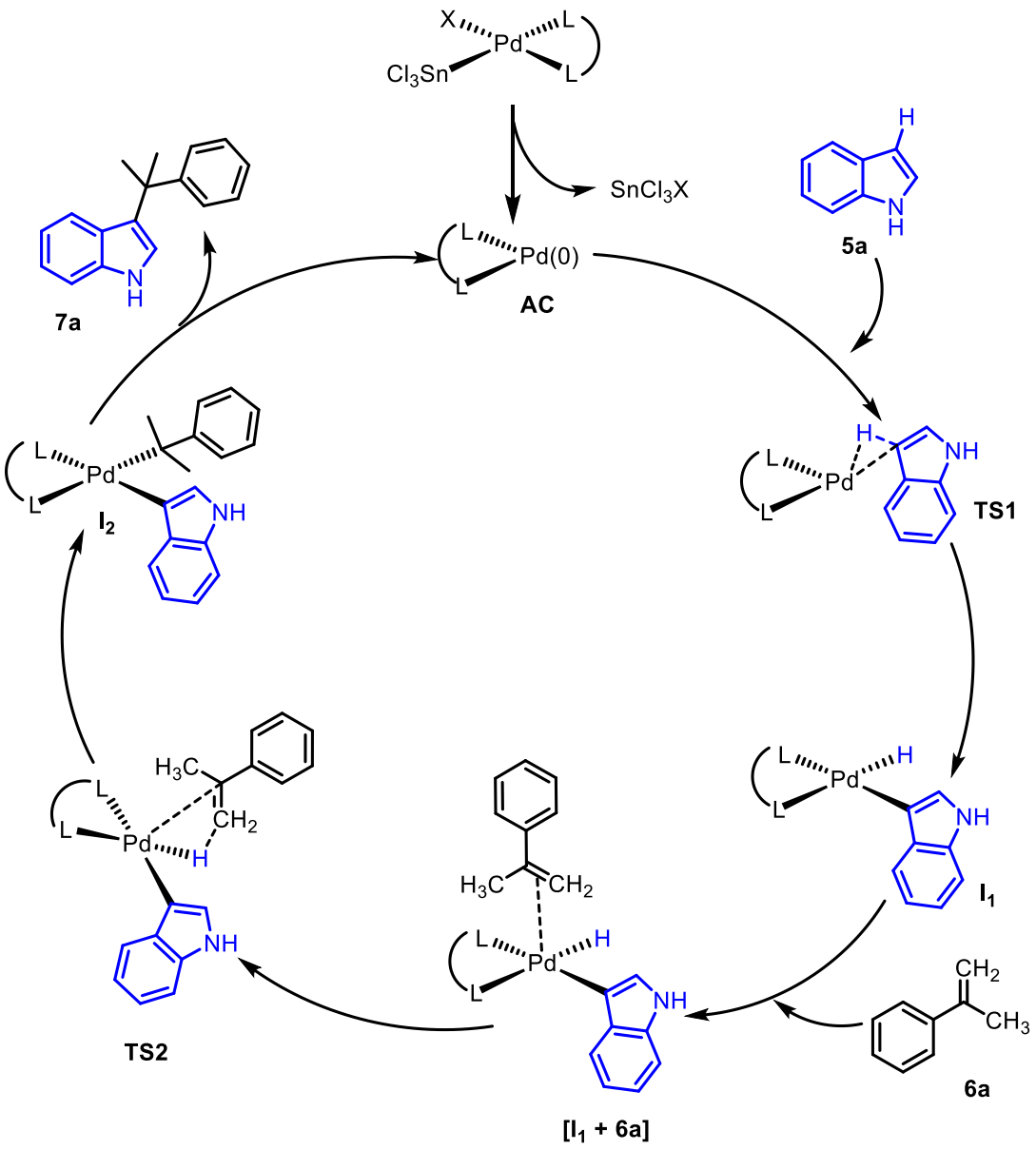


Figure S6. General catalytic cycle for C3-H functionalization of indole

Application of Energetic Span Model

The efficiency of a catalytic cycle can be evaluated by using the energetic span model. In this method the turnover frequency (TOF) of a catalytic cycle is expressed in terms of the energetics of various stationary points. In the catalytic cycle, the TOF can be determined by transition state and intermediate. Therefore, the TOF of the catalytic cycle depends on the TOF-determining intermediate (TDI) and TOF-determining transition state (TDTS). The energy span δE can be calculated using the following equations:

δE = TDTS – TDI (1), when the TDTS appear after the TDI.

δE= TDTS – TDI + $\Delta_r G$ (2), when TDTS appear before TDI.

where, $\Delta_r G$ is the Gibbs free energy of the reaction.

Table S9. Calculation of energetic span (δE, in kJ/mol) using different combinations of TDI and TDTS for complex **2**. Highlighted pair gives the maximum energetic span.

TDI	TDTS	δE	TDI	TDTS	δE
AC + 5a + 6a	**TS1 + 6a**	119.75	**[I_1 + 6a]**	**TS1 + 6a**	-44.28
	TS2	276.69		**TS2**	169.42
I_1 + 6a	**TS1 + 6a**	-04.7	**I_2**	**TS1 + 6a**	-13.46
	TS2	209		**TS2**	86.72

Table S10. Calculation of energetic span (δE, in kJ/mol) using different combinations of TDI and TDTS for complex **4**. Highlighted pair gives the maximum energetic span.

TDI	TDTS	δE	TDI	TDTS	δE
AC + 5a + 6a	**TS1 + 6a**	101.26	**[I_1 + 6a]**	**TS1 + 6a**	-21.3
	TS2	178.32		**TS2**	-55.76
I_1 + 6a	**TS1 + 6a**	-05.16	**I_2**	**TS1 + 6a**	-5.93
	TS2	87.21		**TS2**	55.82

Table S11. Calculation of energetic span (δE, in kJ/mol) using different combinations of TDI and TDTS for (COD)PdClSnCl_3. Highlighted pair gives the maximum energetic span.

TDI	TDTS	δE	TDI	TDTS	δE
AC + 5a + 6a	**TS1 + 6a**	94.07	**[I_1 + 6a]**	**TS1 + 6a**	-29.47
	TS2	262.78		**TS2**	139.24
I_1 + 6a	**TS1 + 6a**	23.52	**I_2**	**TS1 + 6a**	7.73
	TS2	184.63		**TS2**	176.44

Computational Results

1. Optimized structures related to Complex 2 (In DCE solvent)

1.1 Optimized geometry and the energies of complex 2

- SCF energy: -5314.00890368 Hartree
- Zero-point correction: 0.588001 (Hartree/Particle)
- Thermal correction to Energy: 0.647529 Hartree
- Thermal correction to Enthalpy: 0.648679 Hartree
- Thermal correction to Gibbs Free Energy: 0.479816 Hartree
- Sum of electronic and zero-point Energies: -5313.420903 Hartree
- Sum of electronic and thermal Energies: -5313.361375 Hartree
- Sum of electronic and thermal Enthalpies: -5313.360225 Hartree
- Sum of electronic and thermal Free Energies: -5313.529088 Hartree

Pd	0.01001148	-0.37117421	0.07916562
Sn	-0.03073627	2.03806090	-0.64466375
Br	0.03417881	-2.78395937	0.92579006
N	-2.84236421	-0.13773006	1.15584426
C	-6.52231693	-0.82600715	0.97823087
H	-7.45720490	-0.78451204	1.52845224
N	-2.83273614	-0.90301861	-0.89462670
Cl	0.04809455	3.58756076	1.19036974
C	-6.51640358	-1.31635770	-0.33992416
H	-7.44691828	-1.64695043	-0.79090806
C	-5.33917651	-1.39084635	-1.08118560
H	-5.34528565	-1.77735401	-2.09214953
N	2.86406745	-0.83393390	-0.91324991
N	2.86157430	-0.11477022	1.15426173
C	-4.16228673	-0.95644452	-0.46412373
C	-4.16855099	-0.46502296	0.85527239
C	-5.35126291	-0.39416329	1.59710485
H	-5.36660085	-0.02615698	2.61492991
C	-2.04571864	-0.42739356	0.09921194
C	-2.29774650	-1.37754437	-2.19082539
H	-1.23433973	-1.12681576	-2.14379071
C	-2.42059136	-2.89996247	-2.29433943
H	-1.89643675	-3.37221462	-1.45748685
H	-1.96665086	-3.23879693	-3.23141225
H	-3.46554704	-3.22501451	-2.28569745
C	-2.91160060	-0.61252885	-3.36542620
H	-3.96873469	-0.85105544	-3.51035082
H	-2.37948930	-0.88483575	-4.28259961
H	-2.81502089	0.46636489	-3.21257399
C	-2.32039395	0.36333776	2.44750145
H	-1.25727538	0.53289581	2.25526566
C	-2.43743038	-0.71625398	3.52659479
H	-1.90626949	-1.61856878	3.20733602
H	-3.48066186	-0.97479926	3.73291151
H	-1.98655252	-0.35260353	4.45572690

C	-2.95026390	1.70595280	2.82525794
H	-2.43026588	2.10881672	3.70001636
H	-4.00975069	1.61210276	3.07830588
H	-2.84933591	2.42469136	2.00639584
C	2.07015549	-0.38143805	0.08699724
C	4.18940381	-0.43475735	0.85354598
C	4.19080261	-0.89848986	-0.47570232
C	5.36993223	-1.32991359	-1.09094243
H	5.38133447	-1.70218289	-2.10704159
C	6.54199777	-1.27518545	-0.33996646
H	7.47369861	-1.60440933	-0.78949157
C	6.54080908	-0.80869632	0.98675117
H	7.47171616	-0.78251389	1.54462622
C	5.36708193	-0.38385449	1.60515465
H	5.37614959	-0.03750387	2.63054612
C	2.33653337	0.35968722	2.45530995
H	1.27194574	0.52477963	2.26833947
C	2.46447141	-0.73661943	3.51601404
H	1.94979714	-1.64155404	3.17792590
H	2.00264408	-0.39606241	4.44850838
H	3.51047815	-0.98205049	3.72436204
C	2.95683441	1.70105195	2.85228529
H	4.02288635	1.61600676	3.07914754
H	2.45125991	2.07600505	3.74763308
H	2.82535049	2.43630445	2.05286964
C	2.33863638	-1.27505657	-2.22554773
H	1.28290147	-0.99185927	-2.19471114
C	2.99189678	-0.51542744	-3.38307518
H	4.04451464	-0.77890099	-3.51544407
H	2.91727317	0.56420892	-3.22507982
H	2.46714261	-0.76801446	-4.31014617
C	2.42280461	-2.79881565	-2.34768766
H	1.96853838	-3.11481389	-3.29248702
H	1.88250846	-3.27000357	-1.52067907
H	3.46034839	-3.14736808	-2.33581928
Cl	-1.94557847	2.88728014	-1.80998329
Cl	1.72115383	2.92603868	-2.01574152

1.2 Optimized geometry and the energies of the isomer of the complex 2

- SCF energy: -5313.99841968 Hartree
- Zero-point correction: 0.588543 (Hartree/Particle)
- Thermal correction to Energy: 0.648003 Hartree
- Thermal correction to Enthalpy: 0.649153 Hartree
- Thermal correction to Gibbs Free Energy: 0.482063 Hartree
- Sum of electronic and zero-point Energies: -5313.409877 Hartree
- Sum of electronic and thermal Energies: -5313.350417 Hartree
- Sum of electronic and thermal Enthalpies: -5313.349267 Hartree
- Sum of electronic and thermal Free Energies: -5313.516356 Hartree

Pd	0.16365471	-0.67552697	-0.45360249
Sn	2.63475646	-1.08478073	0.22217798
Br	0.12928424	-3.00541644	-1.47333774
N	-2.67061298	-1.34803671	0.48192583
C	-6.38302689	-0.85233016	0.67124826
H	-7.29709581	-1.19568094	1.14547161
N	-2.76587816	0.26362179	-0.99647599
Cl	4.45177207	-1.51262442	-1.30265040
C	-6.44142769	0.19219218	-0.26913923
H	-7.39920040	0.64387058	-0.50764910
C	-5.29395953	0.65948635	-0.90400692
H	-5.35106204	1.46264391	-1.62698425
N	0.89255311	2.23636075	-0.73751414
N	-0.06017176	1.87678337	1.20478596
C	-4.08048572	0.05113180	-0.56690596
C	-4.01941128	-0.98759503	0.37801797
C	-5.17599017	-1.45818476	1.00946567
H	-5.14741475	-2.26267282	1.73217292
C	-1.92195841	-0.58380435	-0.35834954
C	-2.33071573	1.23950396	-2.01617196
H	-1.25819154	1.06441219	-2.09645858
C	-2.95343107	0.93315362	-3.38141082
H	-2.75601880	-0.10515495	-3.66568240
H	-2.50591050	1.58920836	-4.13505926
H	-4.03402696	1.09771256	-3.39382230
C	-2.55997039	2.67586622	-1.53522436
H	-3.62309395	2.90508197	-1.42326410
H	-2.14032701	3.37802059	-2.26161360
H	-2.06996908	2.84700157	-0.57232915
C	-2.13843372	-2.45854634	1.31348384
H	-1.06274259	-2.44029968	1.13299759
C	-2.67561339	-3.80395838	0.81695860
H	-2.43569229	-3.93533047	-0.24078819
H	-3.75742788	-3.89166626	0.95278889
H	-2.19596894	-4.60933008	1.38220771
C	-2.38171958	-2.22637485	2.80791173
H	-1.89631928	-3.03054142	3.36936850
H	-3.44332243	-2.23022524	3.06749408
H	-1.95390234	-1.27794830	3.14073741
C	0.35830164	1.27504816	0.06655086
C	0.20506213	3.24970408	1.14571245
C	0.82042496	3.47896444	-0.09729555
C	1.22293760	4.76256422	-0.47989572
H	1.70549480	4.95364175	-1.42903232
C	0.98310783	5.80173351	0.41510470
H	1.28463743	6.80935621	0.14694927
C	0.36052527	5.57268226	1.65534177
H	0.18698849	6.40648431	2.32818797
C	-0.03760364	4.29571750	2.04147672
H	-0.51402816	4.13178772	2.99909369
C	-0.66062136	1.15115048	2.34601248

H	-0.65113467	0.10843563	2.02478365
C	0.22203574	1.26288162	3.59227711
H	1.24567343	0.95243288	3.36108638
H	-0.17616354	0.60551164	4.37165884
H	0.24984665	2.27978216	3.99254644
C	-2.11402083	1.58390620	2.56115813
H	-2.19007525	2.63674082	2.84538645
H	-2.55929643	0.98818214	3.36331970
H	-2.70397517	1.42984635	1.65261627
C	1.55989632	1.96724788	-2.03809115
H	1.42304618	0.89308992	-2.19333723
C	0.88839358	2.70516605	-3.20051159
H	0.96723115	3.79068428	-3.10325985
H	-0.16861646	2.44668640	-3.28820898
H	1.38489058	2.41469034	-4.13130028
C	3.06135953	2.26273791	-1.94619505
H	3.55359305	1.90199326	-2.85412369
H	3.51249289	1.76304152	-1.08516536
H	3.25859701	3.33446787	-1.85509476
Cl	2.90525063	-2.93634739	1.73268487
Cl	3.69441459	0.62223796	1.59018648

1.3 Optimized geometry and the energies of the active Pd(0) catalyst generated from complex 2

- SCF energy: -1358.34417150 Hartree
- Zero-point correction: 0.580463 (Hartree/Particle)
- Thermal correction to Energy: 0.627368 Hartree
- Thermal correction to Enthalpy: 0.628518 Hartree
- Thermal correction to Gibbs Free Energy: 0.491283 Hartree
- Sum of electronic and zero-point Energies: -1357.763709 Hartree
- Sum of electronic and thermal Energies: -1357.716804 Hartree
- Sum of electronic and thermal Enthalpies: -1357.715654 Hartree
- Sum of electronic and thermal Free Energies: -1357.852888 Hartree

Pd	-0.00000922	-0.00011921	-0.00009450
N	-2.88732840	-0.95795852	0.52207453
C	-6.61785152	-0.61636618	0.33669075
H	-7.56254181	-1.08649776	0.59334410
N	-2.88719769	0.95793149	-0.52195077
C	-6.61776748	0.61684997	-0.33654891
H	-7.56239317	1.08711985	-0.59318645
C	-5.42514283	1.25202813	-0.68327963
H	-5.43806910	2.20241525	-1.20206476
N	2.88715807	0.95792078	0.52202330
N	2.88736095	-0.95792405	-0.52207366
C	-4.22736586	0.61868125	-0.33752686

C	-4.22745264	-0.61855423	0.33760733
C	-5.42531291	-1.25171602	0.68340660
H	-5.43837274	-2.20209116	1.20221294
C	-2.05642121	-0.00009493	0.00003692
C	-2.37203092	2.17076927	-1.18481949
H	-1.28487884	2.05115120	-1.11940856
C	-2.76413427	2.20592794	-2.66529183
H	-2.43091915	1.29193469	-3.16816047
H	-2.28371829	3.06239551	-3.15004760
H	-3.84501066	2.30208868	-2.80674929
C	-2.76399241	3.43594425	-0.41506768
H	-3.84457400	3.60855670	-0.42112335
H	-2.28175994	4.30596961	-0.87319783
H	-2.43277481	3.36484705	0.62635471
C	-2.37233958	-2.17100165	1.18471001
H	-1.28517697	-2.05159070	1.11917841
C	-2.76464562	-3.43598543	0.41480459
H	-2.43362462	-3.36475838	-0.62667215
H	-3.84524507	-3.60847508	0.42105191
H	-2.28243999	-4.30615579	0.87268738
C	-2.76429306	-2.20627952	2.66521890
H	-2.28416656	-3.06302457	3.14977802
H	-3.84519025	-2.30201939	2.80678081
H	-2.43066386	-1.29250987	3.16822070
C	2.05641381	-0.00007344	-0.00007367
C	4.22747370	-0.61853299	-0.33748579
C	4.22733543	0.61869139	0.33766969
C	5.42508743	1.25200983	0.68356212
H	5.43798046	2.20238082	1.20237985
C	6.61773679	0.61682418	0.33692949
H	7.56234268	1.08707953	0.59366669
C	6.61787221	-0.61637920	-0.33633460
H	7.56258092	-1.08652011	-0.59290141
C	5.42535789	-1.25170844	-0.68317406
H	5.43845238	-2.20207973	-1.20198661
C	2.37242075	-2.17093562	-1.18480627
H	1.28525244	-2.05154443	-1.11932797
C	2.76445769	-2.20612809	-2.66529679
H	2.43082998	-1.29234178	-3.16826880
H	2.28438161	-3.06286160	-3.14992505
H	3.84536589	-2.30183160	-2.80679792
C	2.76470107	-3.43596150	-0.41495797
H	3.84529734	-3.60847123	-0.42120602
H	2.28248507	-4.30610243	-0.87288714
H	2.43367509	-3.36478597	0.62652092
C	2.37196679	2.17085354	1.18468841
H	1.28482203	2.05128212	1.11912582
C	2.76387908	2.20613795	2.66521096
H	3.84476010	2.30203505	2.80680037
H	2.43036989	1.29230033	3.16816973
H	2.28360985	3.06279410	3.14978424

C	2.76409334	3.43594288	0.41486015
H	2.28170097	4.30600640	0.87275009
H	2.43315294	3.36470812	-0.62664197
H	3.84466021	3.60863260	0.42118532

1.4 Optimized geometry and the energies of the $SnCl_3Br$ complex

- SCF energy: -3955.53566029
- Zero-point correction: 0.004169 (Hartree/Particle)
- Thermal correction to Energy: 0.014527
- Thermal correction to Enthalpy: 0.015677
- Thermal correction to Gibbs Free Energy: -0.042796
- Sum of electronic and zero-point Energies: -3955.531492
- Sum of electronic and thermal Energies: -3955.521133
- Sum of electronic and thermal Enthalpies: -3955.519983
- Sum of electronic and thermal Free Energies: -3955.578456

Sn	-0.31827615	0.00049717	-0.00004344
Cl	-1.13683559	2.16939886	-0.04897810
Cl	-1.14323251	-1.12601076	-1.85138240
Cl	-1.14189268	-1.04065115	1.90114117
Br	2.11677545	-0.00203962	-0.00031713

1.5 Optimized geometry and the energies of the complex where active Pd(0) catalyst interacts with 5a

- SCF energy: -1722.18535601 Hartree
- Zero-point correction: 0.711610 (Hartree/Particle)
- Thermal correction to Energy: 0.769338 Hartree
- Thermal correction to Enthalpy: 0.770488 Hartree
- Thermal correction to Gibbs Free Energy: 0.610227 Hartree
- Sum of electronic and zero-point Energies: -1721.473747 Hartree
- Sum of electronic and thermal Energies: -1721.416018 Hartree
- Sum of electronic and thermal Enthalpies: -1721.414868 Hartree
- Sum of electronic and thermal Free Energies: -1721.575129 Hartree

Pd	0.59318653	-0.39685274	0.79616706
N	3.24442420	1.04380200	0.25162333
C	6.88988053	1.19698261	-0.61475634
H	7.72683754	1.86299864	-0.80256705
N	3.54407908	-1.11513175	0.15686525
C	7.08107391	-0.19311691	-0.68536006
H	8.06342041	-0.58698610	-0.92866756
C	6.03173829	-1.08118684	-0.44708039

H	6.19160559	-2.15073397	-0.50360281
N	-2.32679020	-1.43984057	0.65464994
N	-2.22573140	0.57005337	1.49989600
C	4.78062911	-0.53997633	-0.13583369
C	4.58758041	0.85491325	-0.07050410
C	5.64277354	1.74136860	-0.30683269
H	5.50829309	2.81457491	-0.25306954
C	2.59318839	-0.15745908	0.39699734
C	3.23421893	-2.55619329	0.20227837
H	2.17339658	-2.57591420	0.47334836
C	3.38982169	-3.19968205	-1.17925507
H	2.77198455	-2.67266470	-1.91404463
H	3.06181352	-4.24369870	-1.13620906
H	4.42702558	-3.18673809	-1.52837952
C	4.02720205	-3.26541978	1.30445835
H	5.10326582	-3.27127096	1.10594412
H	3.69400764	-4.30585876	1.38079596
H	3.85796262	-2.77634094	2.26957843
C	2.55709584	2.33555271	0.42927531
H	1.52309324	2.03986510	0.63864578
C	2.56947778	3.16484910	-0.85966913
H	2.20921533	2.56944286	-1.70510607
H	3.56827735	3.53285097	-1.11223703
H	1.91471866	4.03501044	-0.73984352
C	3.09798439	3.09416697	1.64459757
H	2.50997657	4.00510236	1.80027446
H	4.14501171	3.38637893	1.51674199
H	3.02027303	2.47356629	2.54340955
C	-1.44530605	-0.47202454	1.06291149
C	-3.58110006	0.28520279	1.34328304
C	-3.64720723	-1.01604822	0.80595303
C	-4.87769003	-1.61910149	0.52898356
H	-4.94204987	-2.61986004	0.12079450
C	-6.03415245	-0.88425892	0.79122504
H	-7.00276309	-1.32827882	0.58118311
C	-5.96752692	0.41712827	1.31637985
H	-6.88514069	0.96684252	1.50422909
C	-4.74214682	1.01997833	1.60057482
H	-4.70216411	2.02558898	2.00057399
C	-1.64941481	1.77390430	2.12730009
H	-0.57395605	1.56579346	2.12830026
C	-1.88844724	3.02602152	1.28124249
H	-1.45920275	2.88561570	0.28635108
H	-1.40288189	3.88737391	1.75233485
H	-2.95204887	3.25511239	1.16511699
C	-2.11206886	1.91879296	3.58097571
H	-3.18377920	2.12396551	3.66062699
H	-1.57512329	2.74909908	4.05174348
H	-1.89468636	1.00400040	4.14235212
C	-1.87891773	-2.77988898	0.22876573
H	-0.78739489	-2.69602339	0.24227861

C	-2.30036107	-3.84106321	1.25135331
H	-3.38889625	-3.94248501	1.30983608
H	-1.92498208	-3.58279301	2.24729916
H	-1.88534709	-4.81342313	0.96525337
C	-2.31395772	-3.10938868	-1.20105522
H	-1.85260860	-4.05427153	-1.50828845
H	-1.99083147	-2.32142502	-1.88373276
H	-3.39823476	-3.22088882	-1.29398197
C	-3.46163376	-0.30449470	-3.25799622
C	-4.57816570	0.43252020	-2.88068054
C	-0.84096649	-0.26734442	-3.20848496
C	-2.17933263	0.21047593	-2.99259855
C	-4.44278753	1.68829094	-2.24993856
C	0.01148215	0.68107261	-2.70190129
C	-2.06694389	1.47894517	-2.35133990
C	-3.18939896	2.22990175	-1.98278564
N	-0.71948560	1.74203497	-2.20474251
H	-3.57265830	-1.27165561	-3.74134347
H	-5.57282858	0.03706396	-3.06792155
H	-0.54992977	-1.19910922	-3.67379121
H	-5.33326692	2.23873332	-1.95970112
H	1.09039781	0.69104582	-2.65466408
H	-3.08659256	3.19525462	-1.49764296
H	-0.32498870	2.54341617	-1.73684348

1.6 Optimized geometry and the energies of the TS1

- SCF energy: -1722.13683082 Hartree
- Zero-point correction: 0.706487 (Hartree/Particle)
- Thermal correction to Energy: 0.764581 Hartree
- Thermal correction to Enthalpy: 0.765731 Hartree
- Thermal correction to Gibbs Free Energy: 0.607313 Hartree
- Sum of electronic and zero-point Energies: -1721.430344 Hartree
- Sum of electronic and thermal Energies: -1721.372250 Hartree
- Sum of electronic and thermal Enthalpies: -1721.371100 Hartree
- Sum of electronic and thermal Free Energies: -1721.529518 Hartree

Pd	-0.39358129	-1.16093521	-0.35248747
N	2.73655230	-1.61391736	-0.37061445
C	6.20204843	-1.01238954	0.94020118
H	7.25775842	-1.19676553	0.76477932
N	2.12169593	-0.46649970	1.37828963
C	5.80577854	-0.26630544	2.06207776
H	6.55898192	0.12044596	2.74206302
C	4.45867746	-0.01269354	2.32319446
H	4.16501442	0.56138956	3.19314940
N	-1.47985101	1.83342047	0.15263177

N	0.23550943	1.91292318	-1.18287490
C	3.51603174	-0.52518278	1.42722136
C	3.91341856	-1.26934348	0.29865559
C	5.26375920	-1.52458293	0.04305935
H	5.58275388	-2.10158721	-0.81577496
C	1.63366346	-1.13067399	0.28357329
C	1.24021056	0.20399910	2.35241504
H	0.23723550	0.01672909	1.95975893
C	1.34217140	-0.44640996	3.73578681
H	1.14489692	-1.52110969	3.66638392
H	0.59792325	-0.00060705	4.40427327
H	2.32800371	-0.30598889	4.18936108
C	1.47417246	1.71863476	2.36845753
H	2.48149517	1.97771352	2.70754221
H	0.75995508	2.19428191	3.04827909
H	1.32713746	2.13963506	1.37013825
C	2.63291221	-2.45426286	-1.57886114
H	1.55821865	-2.47553340	-1.78209158
C	3.09769182	-3.88578558	-1.28964456
H	2.53175742	-4.30536531	-0.45148458
H	4.16317345	-3.93041659	-1.04329640
H	2.92780296	-4.51273334	-2.17124818
C	3.33923671	-1.82197890	-2.78308512
H	3.14945229	-2.43122173	-3.67288190
H	4.42251649	-1.75776748	-2.64650319
H	2.96007383	-0.81395499	-2.97353771
C	-0.58842111	1.04555076	-0.52019148
C	-0.12199506	3.24178062	-0.93787217
C	-1.23736479	3.18835157	-0.07877711
C	-1.86815624	4.35593475	0.36054315
H	-2.73482235	4.32469693	1.00926154
C	-1.34570957	5.57500392	-0.07173859
H	-1.81510545	6.49843230	0.25434643
C	-0.22644678	5.62895127	-0.91991614
H	0.15880059	6.59350915	-1.23705444
C	0.40051666	4.46560021	-1.36699303
H	1.26029033	4.52027423	-2.02335189
C	1.33316804	1.44753427	-2.04891263
H	1.25796057	0.35984395	-1.98805475
C	1.10911425	1.86233725	-3.50674403
H	0.12684890	1.52413163	-3.85265043
H	1.87571316	1.40164096	-4.13907721
H	1.16796033	2.94620111	-3.64408189
C	2.69977956	1.86807990	-1.49746958
H	2.82528527	2.95501822	-1.49328517
H	3.49509997	1.44050571	-2.11652523
H	2.82989147	1.50162980	-0.47565352
C	-2.56952909	1.25877563	0.96277210
H	-2.37199974	0.18944098	0.92542793
C	-2.50288544	1.70044617	2.42736594
H	-2.72039087	2.76419274	2.56107328

H	-1.51361359	1.49759796	2.84903031
H	-3.24167118	1.13063727	3.00065701
C	-3.93427314	1.50284345	0.31428135
H	-4.70136150	0.95835193	0.87408163
H	-3.93352775	1.12644124	-0.71347317
H	-4.20114878	2.56500473	0.29953841
C	-3.51941761	-2.02259048	1.48879350
C	-4.77029509	-2.09733881	2.09476522
C	-2.30973663	-1.95482031	-0.83716998
C	-3.42487318	-2.05596880	0.08578198
C	-5.94539736	-2.21257410	1.31891534
C	-2.87753301	-2.08624958	-2.09039452
C	-4.62597136	-2.18993247	-0.67376463
C	-5.88809265	-2.26545220	-0.07171578
N	-4.26215897	-2.21201581	-1.99962580
H	-2.61549340	-1.92754834	2.08673586
H	-4.84825951	-2.06896683	3.17872927
H	-1.04568909	-2.67682614	-0.46356428
H	-6.91107276	-2.26695652	1.81509110
H	-2.40770161	-2.09058649	-3.06484435
H	-6.79112188	-2.35959683	-0.66970501
H	-4.89403421	-2.31429628	-2.77944439

1.7 Optimized geometry and the energies of the I_1

- SCF energy: -1722.16085788 Hartree
- Zero-point correction: 0.709062 (Hartree/Particle)
- Thermal correction to Energy: 0.767007 Hartree
- Thermal correction to Enthalpy: 0.768157 Hartree
- Thermal correction to Gibbs Free Energy: 0.611512 Hartree
- Sum of electronic and zero-point Energies: -1721.451796 Hartree
- Sum of electronic and thermal Energies: -1721.393851 Hartree
- Sum of electronic and thermal Enthalpies: -1721.392701 Hartree
- Sum of electronic and thermal Free Energies: -1721.549346 Hartree

Pd	-0.32456598	-1.19949426	-0.23017197
N	2.76424879	-1.53527147	-0.41872373
C	6.29883209	-0.85095016	0.63743541
H	7.34293780	-1.03244130	0.40099355
N	2.25052653	-0.32279739	1.32038920
C	5.96797365	-0.06024346	1.75097778
H	6.75975601	0.36267297	2.36185285
C	4.63929558	0.19193603	2.09015080
H	4.39706854	0.80082138	2.95194462
N	-1.47154094	1.65852639	0.40879768
N	0.05409037	1.78267456	-1.14455114
C	3.64696851	-0.36809143	1.27987204
C	3.97784098	-1.15449741	0.16040277
C	5.31157975	-1.40969314	-0.17327409

H	5.58048382	-2.01975895	-1.02608811
C	1.70850824	-1.03138852	0.28680904
C	1.43137291	0.37186702	2.33229457
H	0.40703997	0.14632455	2.03060939
C	1.65210337	-0.21632322	3.72947340
H	1.48467938	-1.29814411	3.71825442
H	0.94063878	0.23611030	4.42832325
H	2.66074582	-0.02669347	4.10762387
C	1.63603917	1.88929940	2.26494842
H	2.66046748	2.17758553	2.51761982
H	0.96504854	2.38406739	2.97401482
H	1.41041092	2.26439085	1.26276381
C	2.59907890	-2.42066327	-1.59108052
H	1.51658695	-2.46167297	-1.73165063
C	3.09300866	-3.83555165	-1.27327141
H	2.57350987	-4.22805986	-0.39318856
H	4.16988339	-3.86346752	-1.08033836
H	2.88347181	-4.49500646	-2.12181787
C	3.23082187	-1.82553601	-2.85373737
H	2.99117374	-2.46580867	-3.70885285
H	4.31979218	-1.75258691	-2.78526127
H	2.83514929	-0.82623274	-3.05603712
C	-0.61174014	0.90684348	-0.33808615
C	-0.37265762	3.09457143	-0.91860358
C	-1.36313698	3.01233784	0.07829415
C	-2.01824711	4.15831855	0.53953818
H	-2.79095836	4.10804648	1.29589718
C	-1.64616304	5.38267683	-0.01420083
H	-2.13834389	6.28876116	0.32614317
C	-0.64893937	5.46502380	-1.00107021
H	-0.37878978	6.43394470	-1.41000672
C	0.00125413	4.32390951	-1.46932851
H	0.76697862	4.39920062	-2.23106270
C	1.06550099	1.34918526	-2.12724779
H	1.07128678	0.26237527	-2.02322005
C	0.63195208	1.68234964	-3.55827072
H	-0.36386915	1.27352917	-3.75851880
H	1.33792414	1.23302905	-4.26456420
H	0.60754331	2.75928165	-3.74788739
C	2.45629870	1.87965156	-1.76403747
H	2.50193546	2.97207293	-1.80148933
H	3.19660307	1.48852879	-2.46912593
H	2.73941763	1.55702146	-0.75785498
C	-2.43316363	1.07346149	1.36909229
H	-2.20190700	0.00842291	1.35696887
C	-2.21813325	1.59701576	2.79282364
H	-2.43106864	2.66545694	2.88742813
H	-1.19096054	1.42428305	3.12607893
H	-2.88939084	1.06066439	3.47144255
C	-3.87068930	1.24687183	0.87004489
H	-4.54858709	0.68547071	1.52047080

H	-3.96261653	0.84728482	-0.14289976
H	-4.18309164	2.29626206	0.87109559
C	-3.45356713	-2.56749992	1.28244223
C	-4.68265075	-2.97192630	1.79675325
C	-2.29403383	-1.48004090	-0.79969744
C	-3.38203415	-2.02731137	-0.01486905
C	-5.86397031	-2.84848565	1.03199653
C	-2.89112681	-1.06483697	-1.96944620
C	-4.59597549	-1.90664575	-0.76272791
C	-5.83528854	-2.31668713	-0.25554591
N	-4.26765735	-1.32037562	-1.96106745
H	-2.54482586	-2.65867291	1.87420252
H	-4.73918101	-3.38945980	2.79932353
H	-0.21030360	-2.81110845	-0.13951220
H	-6.81211354	-3.17205119	1.45468160
H	-2.45775534	-0.57516345	-2.83273562
H	-6.74514251	-2.21493860	-0.84264218
H	-4.91073731	-1.12058425	-2.71210552

1.8 Optimized geometry and the energies of the complex where I_1 interacts with 6a

- SCF energy: -2071.15271736 Hartree
- Zero-point correction: 0.873775 (Hartree/Particle)
- Thermal correction to Energy: 0.945414 Hartree
- Thermal correction to Enthalpy: 0.946564 Hartree
- Thermal correction to Gibbs Free Energy: 0.758943 Hartree
- Sum of electronic and zero-point Energies: -2070.278942 Hartree
- Sum of electronic and thermal Energies: -2070.207304 Hartree
- Sum of electronic and thermal Enthalpies: -2070.206154 Hartree
- Sum of electronic and thermal Free Energies: -2070.393775 Hartree

Pd	0.47969533	0.63144422	-0.62331273
N	-2.18121779	-0.92012552	-1.03911046
C	-4.88882309	-3.30891618	-0.02816507
H	-5.80130758	-3.79929235	-0.35337886
N	-1.41788246	-1.28630958	0.97217385
C	-4.39490231	-3.55182573	1.26502171
H	-4.92780407	-4.23086742	1.92364558
C	-3.22972791	-2.93577063	1.72196883
H	-2.85950065	-3.13104372	2.72031930
N	2.88900169	-0.83445713	0.76952402
N	2.03517790	-2.09161787	-0.79458725
C	-2.57018528	-2.06786747	0.84650271
C	-3.06305076	-1.82768141	-0.44975700
C	-4.23193687	-2.44533596	-0.90326274
H	-4.63038396	-2.25550306	-1.89135340
C	-1.17477598	-0.58698616	-0.17835042
C	-0.52759194	-1.23196280	2.14868607

H	0.23278176	-0.50496667	1.85901203
C	-1.24693020	-0.69399627	3.39003485
H	-1.67027262	0.29518844	3.19582805
H	-0.52565208	-0.59845384	4.20850119
H	-2.05071897	-1.35337769	3.72837815
C	0.15442470	-2.58434332	2.38436318
H	-0.56653643	-3.36697744	2.63854493
H	0.86519126	-2.50073466	3.21238734
H	0.70437514	-2.89883157	1.49343594
C	-2.31213770	-0.33523581	-2.39150896
H	-1.42451015	0.29454916	-2.48428783
C	-3.54798538	0.56489082	-2.48006032
H	-3.49476517	1.35797296	-1.73066690
H	-4.47715113	0.01047136	-2.31823275
H	-3.59208749	1.02263889	-3.47406233
C	-2.25939079	-1.40985852	-3.48257830
H	-2.24017863	-0.92228237	-4.46264744
H	-3.12500197	-2.07779852	-3.45876757
H	-1.35662520	-2.02016313	-3.38840575
C	1.91343878	-0.87858812	-0.18347496
C	3.08388804	-2.82959207	-0.23798151
C	3.63922506	-2.01409370	0.76682079
C	4.72947506	-2.44899629	1.52649056
H	5.17389386	-1.82803841	2.29380575
C	5.23730472	-3.72020031	1.26014994
H	6.08364973	-4.08304683	1.83558651
C	4.67539924	-4.53747134	0.26457251
H	5.09123057	-5.52408728	0.08375072
C	3.59216216	-4.10516242	-0.49995762
H	3.16764362	-4.74302609	-1.26518325
C	1.16481877	-2.50697040	-1.91113337
H	0.52318543	-1.63742574	-2.06906124
C	1.97284267	-2.73438945	-3.19248358
H	2.57510279	-1.84941024	-3.42320525
H	1.28657457	-2.91158362	-4.02716819
H	2.64142614	-3.59682361	-3.11836305
C	0.28278695	-3.69577905	-1.51599517
H	0.87436016	-4.58281583	-1.27056423
H	-0.38248072	-3.95463275	-2.34584535
H	-0.33578603	-3.44296974	-0.64966934
C	3.13437323	0.35310678	1.61744796
H	2.34528058	1.04901869	1.32903970
C	2.98240050	0.03479617	3.10861536
H	3.74475361	-0.66118270	3.46988309
H	2.00049011	-0.39598288	3.32351398
H	3.07836758	0.96297300	3.68141206
C	4.47889496	1.00084210	1.27282172
H	4.57584662	1.94361215	1.82066111
H	4.52288468	1.22063364	0.20339820
H	5.32509441	0.36055167	1.54246978
C	1.79996167	3.91041590	0.51746286
C	2.40466145	5.09243817	0.93649345
C	2.02092325	1.90410301	-1.14791160
C	2.37745540	3.16146648	-0.52339503
C	3.59492876	5.55144442	0.32926754

C	3.01504457	1.69108782	-2.07754036
C	3.58674425	3.64547983	-1.11471425
C	4.19951271	4.83555678	-0.70230711
N	3.95626069	2.72818204	-2.06890394
H	0.88603110	3.55263148	0.98385777
H	1.95837892	5.67405019	1.73995767
H	-0.51291226	1.85537982	-0.96000914
H	4.04888962	6.47794129	0.67272314
H	3.16280815	0.85915558	-2.75513481
H	5.11859947	5.18593101	-1.16646317
H	4.75620953	2.80552759	-2.67852768
H	-7.33764688	2.47247246	-0.51461067
H	-5.38008799	3.94183083	-0.26288970
C	-6.43231462	2.08433955	-0.05495462
C	-5.31949132	2.91282995	0.07855198
H	-2.39868096	2.73793280	2.81136781
C	-6.39259150	0.76649441	0.41224924
H	-7.26071721	0.12092155	0.31003190
C	-4.12899162	2.44480533	0.66844542
C	-2.92169086	3.30651814	0.78035988
C	-1.91374262	2.95926076	1.85287810
C	-2.69498891	4.33119519	-0.05854772
H	-1.20709887	3.78017773	2.00431825
C	-5.22912621	0.29169178	1.01924929
C	-4.11494082	1.12227454	1.14681059
H	-3.35856044	4.56835522	-0.88491920
H	-1.80950217	4.95254128	0.04376904
H	-5.17887878	-0.72989004	1.38346899
H	-3.21494152	0.72112438	1.59637338
H	-1.33072603	2.07739985	1.55557850

1.9 Optimized geometry and the energies of the TS2

- SCF energy: -2071.08897222 Hartree
- Zero-point correction: 0.873667 (Hartree/Particle)
- Thermal correction to Energy: 0.945183 Hartree
- Thermal correction to Enthalpy: 0.946333 Hartree
- Thermal correction to Gibbs Free Energy: 0.759724 Hartree
- Sum of electronic and zero-point Energies: -2070.215305 Hartree
- Sum of electronic and thermal Energies: -2070.143789 Hartree
- Sum of electronic and thermal Enthalpies: -2070.142639 Hartree
- Sum of electronic and thermal Free Energies: -2070.329248 Hartree

Pd	0.57181504	-1.10245857	1.03469374
N	-0.35098156	1.79659752	1.44418479
C	-0.74015716	5.34591457	0.28963779
H	-0.97799930	6.35696475	0.60605106
N	0.10530983	1.40802655	-0.65949116
C	-0.41520534	5.09902405	-1.05506797
H	-0.40720256	5.92166032	-1.76353967
C	-0.12055965	3.81269547	-1.50361828

H	0.10286262	3.62860666	-2.54605856
N	3.12103060	-1.63712727	-0.61604943
N	3.48270115	0.10770464	0.64445568
C	-0.14473468	2.77998814	-0.56332270
C	-0.44934032	3.02894285	0.78789343
C	-0.76531199	4.31643439	1.23088964
H	-1.02256788	4.51952588	2.26245802
C	-0.00897884	0.81663647	0.56009453
C	0.38639108	0.65197372	-1.89747408
H	0.51405818	-0.37367756	-1.54353614
C	-0.82099573	0.68880167	-2.83742334
H	-1.71494697	0.31580528	-2.33044487
H	-0.61976321	0.05821463	-3.71047691
H	-1.04583460	1.69989790	-3.18669027
C	1.70022492	1.10333733	-2.54306248
H	1.64534408	2.12638884	-2.92499885
H	1.93497764	0.44624372	-3.38632763
H	2.52449909	1.04668492	-1.82633014
C	-0.62856828	1.53636774	2.87338866
H	-0.38265885	0.47852266	2.99396491
C	-2.11788029	1.72803722	3.17407934
H	-2.71536276	1.06123169	2.54791513
H	-2.43942608	2.75932093	2.99733690
H	-2.31420067	1.48662991	4.22415041
C	0.28307922	2.35077629	3.79762678
H	0.12245713	2.02501362	4.83032674
H	0.07724611	3.42327241	3.75093512
H	1.33752591	2.19582108	3.55346377
C	2.56920814	-0.87284622	0.37854716
C	4.61196925	-0.02509807	-0.16625483
C	4.37942716	-1.15336161	-0.97738506
C	5.32800854	-1.57686131	-1.91371141
H	5.16454449	-2.44466397	-2.54001900
C	6.50706297	-0.83912664	-2.01741427
H	7.26066609	-1.14484686	-2.73685744
C	6.73673732	0.28839771	-1.21095561
H	7.66460237	0.84226991	-1.31688612
C	5.79533412	0.71200041	-0.27317323
H	5.98422923	1.58117852	0.34412061
C	3.26677324	1.13003289	1.68423926
H	2.28256775	0.88032537	2.08340320
C	4.28759631	0.99482325	2.81854859
H	4.27520476	-0.02204189	3.22419674
H	4.03142341	1.69179310	3.62351200
H	5.30523243	1.22274973	2.48816725
C	3.20287081	2.53828839	1.08413906
H	4.16877772	2.85964049	0.68394962
H	2.90559791	3.25280248	1.85831853
H	2.46507636	2.58240978	0.27882026
C	2.47454232	-2.86326621	-1.12961873
H	1.51677969	-2.89867321	-0.59855320

C	2.18101427	-2.77541006	-2.62996861
H	3.09338782	-2.73084684	-3.23134515
H	1.57774929	-1.89289536	-2.85957008
H	1.61826303	-3.66257440	-2.93770914
C	3.27920119	-4.10737388	-0.73927430
H	2.73315720	-5.00594388	-1.04416170
H	3.42422287	-4.14080756	0.34556443
H	4.26194763	-4.12825888	-1.21991482
C	-1.75610927	-3.19650487	-0.65826016
C	-2.59112966	-4.15747032	-1.22069555
C	-1.24584657	-1.88352915	1.55811665
C	-1.94601319	-2.80933616	0.68133174
C	-3.62667105	-4.74981543	-0.46475643
C	-1.95635782	-1.93328094	2.74617398
C	-3.00863288	-3.41384210	1.41574830
C	-3.84832882	-4.38699661	0.86191803
N	-2.98360696	-2.86672388	2.68114153
H	-0.96274774	-2.73765782	-1.24443607
H	-2.45094284	-4.45640995	-2.25656808
H	-3.54836867	-0.57948250	1.13789545
H	-4.26414923	-5.49982144	-0.92598383
H	-1.81250213	-1.37891715	3.66476916
H	-4.64464073	-4.84274402	1.44515420
H	-3.65372286	-3.05503773	3.41199678
H	-2.95041592	3.92343927	-0.74408741
H	-3.63459167	1.92340005	0.44293522
C	-3.40087853	3.10939743	-1.30538435
C	-3.79708231	1.96928793	-0.62852725
H	-5.86006747	-1.28461781	-2.25045074
C	-3.54680188	3.22262638	-2.69813642
H	-3.22108123	4.11681504	-3.22203749
C	-4.40388779	0.84543797	-1.30115874
C	-4.83410076	-0.29365576	-0.59615078
C	-5.42389397	-1.50208318	-1.26951678
C	-4.61108090	-0.40463980	0.88261017
H	-6.22018265	-1.94319041	-0.65202958
C	-4.11161747	2.13881387	-3.39202590
C	-4.52368439	0.99238992	-2.73115282
H	-4.91371503	0.49910537	1.43340199
H	-5.16460693	-1.25002292	1.30588722
H	-4.22556976	2.19232655	-4.47397163
H	-4.94107884	0.17939670	-3.31713327
H	-4.68226570	-2.30614074	-1.41313706

1.10 Optimized geometry and the energies of the I_2

- SCF energy: -2071.15338884 Hartree
- Zero-point correction: 0.878582 (Hartree/Particle)
- Thermal correction to Energy: 0.948885 Hartree
- Thermal correction to Enthalpy: 0.950035 Hartree

- Thermal correction to Gibbs Free Energy: 0.769495 Hartree
- Sum of electronic and zero-point Energies: -2070.274807 Hartree
- Sum of electronic and thermal Energies: -2070.204503 Hartree
- Sum of electronic and thermal Enthalpies: -2070.203353 Hartree
- Sum of electronic and thermal Free Energies: -2070.383894 Hartree

Pd	-0.27942705	-0.83226147	-0.20416547
N	2.71999478	0.05188548	-0.84689223
C	5.69225330	2.30163282	-0.41769141
H	6.62229401	2.63258351	-0.87004870
N	2.06931478	0.93049641	1.03817603
C	5.29396863	2.83592830	0.81919460
H	5.92273106	3.57003785	1.31396395
C	4.09868358	2.44771952	1.42231369
H	3.80009293	2.87397161	2.37118858
N	-2.07094276	1.61599393	0.77514303
N	-0.90939549	2.19198700	-0.97408976
C	3.31186348	1.50303699	0.75519481
C	3.72290649	0.94868097	-0.46924822
C	4.91452813	1.35295086	-1.07975553
H	5.22854325	0.95752592	-2.03646569
C	1.69464830	0.04517900	0.06428741
C	1.23705100	1.24664641	2.21318243
H	0.34628635	0.63290144	2.06705360
C	1.91449848	0.81531956	3.51840198
H	2.21183215	-0.23450946	3.46930679
H	1.21272344	0.94141717	4.34980749
H	2.80394466	1.41290536	3.73808862
C	0.82539877	2.72430816	2.22043526
H	1.67499634	3.38440882	2.41401302
H	0.08494441	2.89750654	3.00655811
H	0.38284262	3.01175274	1.26444073
C	2.79657934	-0.85476054	-2.01313124
H	1.97699806	-1.55067804	-1.84753179
C	4.11691296	-1.64029623	-2.03773878
H	4.41474163	-1.94861431	-1.03507030
H	4.93033825	-1.06663733	-2.49072244
H	3.97660175	-2.54256798	-2.64121267
C	2.57233232	-0.12471645	-3.34286322
H	2.72672712	-0.82869209	-4.16752543
H	3.27836472	0.70241394	-3.47035155
H	1.55767883	0.26756598	-3.42680748
C	-1.16845720	1.14560727	-0.13793076
C	-1.63055400	3.32924194	-0.60266969
C	-2.37578961	2.95898372	0.53040331
C	-3.19860142	3.88282986	1.18330530
H	-3.77122890	3.61737185	2.06248566
C	-3.25959410	5.17510078	0.66389799
H	-3.89069203	5.91181625	1.15175291
C	-2.52139935	5.54055930	-0.47485065

H	-2.59106323	6.55492181	-0.85590616
C	-1.69560478	4.62472612	-1.12471918
H	-1.12854154	4.91751446	-1.99920434
C	-0.00769209	2.08018317	-2.13089533
H	0.34514855	1.05118625	-2.06669948
C	-0.77380981	2.24320856	-3.44737778
H	-1.60899435	1.53684047	-3.48954732
H	-0.10263350	2.03968971	-4.28857443
H	-1.17065342	3.25511391	-3.57193803
C	1.19749471	3.01664394	-2.00273518
H	0.91470541	4.06952711	-2.08948762
H	1.91612200	2.79587191	-2.79759330
H	1.69781266	2.87304606	-1.04146779
C	-2.73881934	0.76495297	1.78239613
H	-2.32077396	-0.22514235	1.60245337
C	-2.40297531	1.18259917	3.21812694
H	-2.71178167	2.20897095	3.43695937
H	-1.33209156	1.09816418	3.41751394
H	-2.92739235	0.51867622	3.91329409
C	-4.24834469	0.70869368	1.52162053
H	-4.69638406	-0.05133879	2.16692836
H	-4.44161940	0.41901483	0.48557914
H	-4.73926650	1.66490673	1.72294465
C	-3.66216173	-2.46910816	1.04839945
C	-4.92576439	-2.97822939	1.32938997
C	-2.15687015	-1.46734612	-0.87078284
C	-3.34264074	-2.04147624	-0.25650000
C	-5.90980553	-3.07839088	0.32130125
C	-2.51969681	-1.27677201	-2.18859960
C	-4.36233654	-2.16315837	-1.25609410
C	-5.63856192	-2.67245342	-0.98214061
N	-3.83150021	-1.69188308	-2.43064770
H	-2.91815830	-2.39852793	1.83656745
H	-5.16237372	-3.30395702	2.33956260
H	0.99397965	-3.20436519	-2.21487131
H	-6.89075066	-3.47890980	0.56489313
H	-1.94356946	-0.86945012	-3.01002803
H	-6.39090639	-2.74783482	-1.76393225
H	-4.30709340	-1.66276659	-3.31981136
H	4.81278265	-4.61556526	0.10604615
H	2.66472955	-4.31127530	-1.02609759
C	4.03264710	-4.03667520	0.59610177
C	2.80159187	-3.85940016	-0.04966492
H	-0.21663881	-4.78549003	0.96710965
C	4.26351078	-3.47572180	1.84991817
H	5.21841165	-3.60911585	2.35162892
C	1.76140994	-3.11064477	0.52760823
C	0.38912225	-2.97407141	-0.09821412
C	-0.57723692	-3.74973041	0.82658299
C	0.29280381	-3.62626299	-1.48445160
H	-1.57648982	-3.80186539	0.39509528

C	3.23557046	-2.73983874	2.45603679
C	2.01727873	-2.56832165	1.80753895
H	0.49054543	-4.71333939	-1.44256772
H	-0.71507169	-3.48732368	-1.88450252
H	3.39082883	-2.30120994	3.43949360
H	1.23403574	-1.98613221	2.28511482
H	-0.66429632	-3.30179424	1.82240815

2. Optimized structures related to Complex (COD)PdClSnCl$_3$ (In DCE solvent)

2.1 Optimized geometry and the energies of the complex (COD)PdClSnCl$_3$

- SCF energy: -2283.22145907 Hartree
- Zero-point correction: 0.188699 (Hartree/Particle)
- Thermal correction to Energy: 0.214244 Hartree
- Thermal correction to Enthalpy: 0.215394 Hartree
- Thermal correction to Gibbs Free Energy: 0.121496 Hartree
- Sum of electronic and zero-point Energies: -2283.032761 Hartree
- Sum of electronic and thermal Energies: -2283.007215 Hartree
- Sum of electronic and thermal Enthalpies: -2283.006065 Hartree
- Sum of electronic and thermal Free Energies: -2283.099963 Hartree

Sn	-1.59211872	0.14960666	0.01144538
Pd	0.89470629	-0.41347882	-0.06092030
Cl	-1.98752667	2.50431744	0.19081032
Cl	-2.94148195	-0.42088164	-1.84893610
Cl	-2.84081507	-0.67844040	1.84477200
Cl	0.04652020	-2.63015019	-0.19371996
C	1.61590616	1.62237046	-0.70107932
H	0.72988657	2.10667814	-1.11066891
C	1.71211571	1.58574238	0.68579029
H	0.87224310	2.00842986	1.23405594
C	3.24011725	-0.90226111	-0.65674439
H	3.07421864	-1.75637898	-1.31102714
C	2.69937133	1.35779551	-1.72129181
H	3.15935392	2.32023810	-1.98992811
H	2.20761694	0.99582416	-2.63113759
C	3.05535706	-1.10388169	0.68591567
H	2.80208320	-2.11515983	0.99951823
C	3.79478545	0.34875045	-1.30526463
H	4.52152620	0.82203076	-0.64152728
H	4.34251900	0.05683262	-2.20642487
C	2.98074481	1.35863844	1.49501835
H	3.82010954	1.82601680	0.97407792
H	2.87336818	1.89115171	2.44420823
C	3.29234355	-0.12332993	1.81357184
H	4.33207082	-0.21198455	2.15912177
H	2.66616198	-0.43930163	2.65455425

2.2 Optimized geometry and the energies of the active Pd(0) catalyst generated from complex (COD)PdClSnCl$_3$

- SCF energy: -438.804374213 Hartree
- Zero-point correction: 0.181435 (Hartree/Particle)
- Thermal correction to Energy: 0.194512 Hartree
- Thermal correction to Enthalpy: 0.195662 Hartree
- Thermal correction to Gibbs Free Energy: 0.135955 Hartree
- Sum of electronic and zero-point Energies: -438.622940 Hartree
- Sum of electronic and thermal Energies: -438.609862 Hartree
- Sum of electronic and thermal Enthalpies: -438.608712 Hartree
- Sum of electronic and thermal Free Energies: -438.668419 Hartree

Pd	-1.41186885	-0.06334919	-0.33947781
C	1.57947344	-1.11843008	-1.05614090
H	1.46222782	-1.73256332	-1.95050522
C	1.94854452	0.15583217	-1.24538603
H	2.07264156	0.48923424	-2.27629546
C	-0.21224227	-0.10935983	1.45027230
H	-0.94678297	-0.27581609	2.24089606
C	1.30603094	-1.87212772	0.22511511
H	2.16997294	-2.52131297	0.44349399
H	0.47360924	-2.56006469	0.02078571
C	-0.21742184	1.19322147	0.90566928
H	-0.96725461	1.86755679	1.33034395
C	0.95928865	-1.09015989	1.51115033
H	1.85083488	-0.57660474	1.88839601
H	0.71838537	-1.84342315	2.27119213
C	2.18354488	1.21018841	-0.19191990
H	2.67956086	0.78098005	0.68201248
H	2.88197744	1.95525009	-0.59362594
C	0.91870029	1.97357330	0.26208138
H	1.24175555	2.73982014	0.98591372
H	0.51352735	2.53457944	-0.59167756

2.3 Optimized geometry and the energies of the SnCl$_4$ complex

- SCF energy: -1844.31659480 Hartree
- Zero-point correction: 0.004427 (Hartree/Particle)
- Thermal correction to Energy: 0.014625 Hartree
- Thermal correction to Enthalpy: 0.015775 Hartree
- Thermal correction to Gibbs Free Energy: -0.039936 Hartree
- Sum of electronic and zero-point Energies: -1844.312168 Hartree
- Sum of electronic and thermal Energies: -1844.301970 Hartree
- Sum of electronic and thermal Enthalpies: -1844.300820 Hartree
- Sum of electronic and thermal Free Energies: -1844.356531 Hartree

Sn	-0.00000000	0.00000000	-0.00000000

Cl	0.00000000	1.88207883	1.34281655
Cl	-0.00000000	-1.88207883	1.34281655
Cl	1.88207883	-0.00000000	-1.34281655
Cl	-1.88207883	0.00000000	-1.34281655

2.4 Optimized geometry and the energies of the complex where active Pd(0) catalyst interacts with 5a

- SCF energy: -802.666083454 Hartree
- Zero-point correction: 0.312354 (Hartree/Particle)
- Thermal correction to Energy: 0.337168 Hartree
- Thermal correction to Enthalpy: 0.338318 Hartree
- Thermal correction to Gibbs Free Energy: 0.250908 Hartree
- Sum of electronic and zero-point Energies: -802.353730 Hartree
- Sum of electronic and thermal Energies: -802.328915 Hartree
- Sum of electronic and thermal Enthalpies: -802.327765 Hartree
- Sum of electronic and thermal Free Energies: -802.415175 Hartree

Pd	-0.74347648	-1.12012761	-0.36276339
C	-2.84871467	-0.48563802	-0.21761132
H	-3.33476212	-1.40376301	-0.55955355
C	-2.35737623	-0.51718677	1.08389846
H	-2.50524836	-1.45738581	1.61541879
C	-1.20608257	2.24535991	-0.62845555
H	-0.74442798	2.59625340	-1.55227652
C	-3.20960712	0.70728102	-1.08851610
H	-4.30918566	0.74851204	-1.15110287
H	-2.86905569	0.50163893	-2.11367195
C	-0.38074273	1.93445022	0.38047616
H	0.68477330	2.07820138	0.20512803
C	-2.70863781	2.10805207	-0.66957985
H	-3.15483730	2.38279808	0.28939718
H	-3.10771845	2.82427474	-1.39899097
C	-2.02732918	0.66033162	1.99809610
H	-2.85373470	1.37864122	1.98398639
H	-1.99256642	0.27892636	3.02581319
C	-0.68913069	1.39436406	1.75702085
H	-0.61689331	2.21724278	2.48718637
H	0.12577554	0.70539796	2.01505222
H	3.56833992	2.48657151	-1.78223718
C	3.25924606	1.68619024	-1.11564777
H	4.13119896	2.62679601	0.62542707
C	3.58106610	1.76612236	0.25523089
C	2.54652626	0.60273036	-1.62306363
C	3.20926417	0.76009488	1.14475204
H	2.28622592	0.55330365	-2.67707087
C	2.14949927	-0.41840999	-0.74797612

H	3.45712718	0.81909959	2.20068207
C	2.50722954	-0.33220867	0.62548238
C	1.36922473	-1.63473610	-0.90831820
N	2.02778896	-1.46551443	1.25811657
C	1.31129317	-2.23713858	0.35872627
H	1.17193942	-2.14231012	-1.84820785
H	2.02742429	-1.61033595	2.25724663
H	1.00665090	-3.23734348	0.63098601

2.5 Optimized geometry and the energies of the TS1

- SCF energy: -802.626700255 Hartree
- Zero-point correction: 0.307735 (Hartree/Particle)
- Thermal correction to Energy: 0.332182 Hartree
- Thermal correction to Enthalpy: 0.333332 Hartree
- Thermal correction to Gibbs Free Energy: 0.247353 Hartree
- Sum of electronic and zero-point Energies: -802.318965 Hartree
- Sum of electronic and thermal Energies: -802.294518 Hartree
- Sum of electronic and thermal Enthalpies: -802.293368 Hartree
- Sum of electronic and thermal Free Energies: -802.379347 Hartree

Pd	-0.71438864	-0.57389488	-0.52873708
C	-2.67761385	0.46261820	-1.39178748
H	-2.46599843	0.31992830	-2.45121834
C	-3.16724940	-0.61430469	-0.70631026
H	-3.27170941	-1.54479355	-1.26226642
C	-1.35340424	1.27958737	1.25532320
H	-0.36222840	1.72144668	1.34789357
C	-2.57180246	1.90170849	-0.93010470
H	-3.45493073	2.45709797	-1.28172697
H	-1.71412689	2.34751442	-1.44907902
C	-1.53861501	0.05554452	1.80693153
H	-0.69385909	-0.37661369	2.34222504
C	-2.40680958	2.14319342	0.59263177
H	-3.36693826	2.01663819	1.09820455
H	-2.13066125	3.19486035	0.72991236
C	-3.79556229	-0.59940177	0.67812189
H	-4.37484923	0.31822827	0.80735946
H	-4.51933127	-1.42017402	0.73348946
C	-2.80481175	-0.77251781	1.85769303
H	-3.33961518	-0.57500591	2.79913684
H	-2.50153463	-1.82573219	1.90291709
H	3.37744779	3.26520501	-0.25708918
C	3.38985409	2.18592320	-0.12872271
H	5.45446666	2.15920018	0.52127543
C	4.57381441	1.55658835	0.31492347
C	2.24403277	1.44464207	-0.39963343
C	4.63395264	0.17701283	0.49343246
H	1.33035343	1.92874196	-0.73652430
C	2.27067438	0.04863015	-0.23219255

H	5.54369970	-0.30856378	0.83675710
C	3.47882961	-0.56358515	0.21485089
C	1.28130006	-0.99763159	-0.39378962
N	3.24152726	-1.91837931	0.29976703
C	1.93354242	-2.17448598	-0.08162924
H	0.23487455	-1.24367599	-1.62960874
H	3.91589974	-2.61534395	0.57875044
H	1.56943660	-3.19226862	-0.10530118

2.6 Optimized geometry and the energies of the I_1

- SCF energy: -802.635365306 Hartree
- Zero-point correction: 0.309630 (Hartree/Particle)
- Thermal correction to Energy: 0.334277 Hartree
- Thermal correction to Enthalpy: 0.335427 Hartree
- Thermal correction to Gibbs Free Energy: 0.249958 Hartree
- Sum of electronic and zero-point Energies: -802.325735 Hartree
- Sum of electronic and thermal Energies: -802.301089 Hartree
- Sum of electronic and thermal Enthalpies: -802.299939 Hartree
- Sum of electronic and thermal Free Energies: -802.385408 Hartree

Pd	-0.78018070	-0.56293307	-0.61327621
C	-2.77868085	0.52122051	-1.29112523
H	-2.68736120	0.38315252	-2.36784352
C	-3.22392627	-0.54858114	-0.56512914
H	-3.41467164	-1.46937762	-1.11352750
C	-1.10783175	1.22042057	1.17069030
H	-0.09807856	1.62491020	1.18163460
C	-2.56464568	1.94769293	-0.82839456
H	-3.46398724	2.53885801	-1.05833293
H	-1.76316815	2.37144014	-1.44574243
C	-1.28192151	-0.00913949	1.72731837
H	-0.40287932	-0.47591692	2.16875646
C	-2.19534415	2.14855381	0.66293908
H	-3.08606590	2.05549733	1.28847158
H	-1.84926931	3.18118075	0.78091702
C	-3.68833868	-0.53331730	0.88238821
H	-4.20340384	0.40712389	1.09223451
H	-4.43790041	-1.32193649	1.00849665
C	-2.57121423	-0.77710103	1.92731800
H	-2.96869975	-0.56610556	2.93143407
H	-2.31780190	-1.84392776	1.92442099
H	3.44245694	3.23142513	-0.24723477
C	3.41746728	2.15197966	-0.12095565
H	5.50504696	2.04040522	0.44242169
C	4.59340119	1.47427132	0.26957408
C	2.23422034	1.45692768	-0.35080178
C	4.60710651	0.09122379	0.43020992
H	1.33541915	1.98106607	-0.66760025

C	2.20599198	0.05899490	-0.18644997
H	5.51315707	-0.43326750	0.72327436
C	3.41317353	-0.60302419	0.19779162
C	1.17635910	-0.94847323	-0.33061030
N	3.13313804	-1.94789999	0.26695075
C	1.79592525	-2.14860968	-0.06298685
H	-0.52469055	-1.36720743	-1.93272080
H	3.79148810	-2.67178142	0.51301034
H	1.39630327	-3.15355203	-0.07067594

2.7 Optimized geometry and the energies of the complex where I_1 interacts with 6a

- SCF energy: -1151.62180266 Hartree
- Zero-point correction: 0.473492 (Hartree/Particle)
- Thermal correction to Energy: 0.512170 Hartree
- Thermal correction to Enthalpy: 0.513320 Hartree
- Thermal correction to Gibbs Free Energy: 0.394176 Hartree
- Sum of electronic and zero-point Energies: -1151.148310 Hartree
- Sum of electronic and thermal Energies: -1151.109633 Hartree
- Sum of electronic and thermal Enthalpies: -1151.108483 Hartree
- Sum of electronic and thermal Free Energies: -1151.227626 Hartree

Pd	-0.43164729	-0.83044131	-0.50749323
C	-0.93652447	-3.10266817	-1.15954288
H	-0.75334930	-2.99257851	-2.22778967
C	0.15544869	-3.27350374	-0.35840067
H	1.12902901	-3.25020127	-0.84422325
C	-2.18502784	-1.61250983	1.21795075
H	-2.81804075	-0.72901230	1.17013347
C	-2.40139905	-3.21855642	-0.79033939
H	-2.75128835	-4.23291446	-1.03533482
H	-2.95713150	-2.54372933	-1.45272223
C	-0.98879646	-1.47985135	1.84957793
H	-0.76836035	-0.50790458	2.28891117
C	-2.78551409	-2.89599970	0.67638837
H	-2.52421150	-3.73370452	1.32711297
H	-3.87686904	-2.80998686	0.71799895
C	0.15417530	-3.70116486	1.09963127
H	-0.64626476	-4.42569451	1.26733558
H	1.08945265	-4.23563294	1.29897766
C	0.05035116	-2.54548275	2.12549251
H	-0.12198598	-2.97188045	3.12508676
H	1.02264781	-2.04445980	2.18096352
H	-5.39511874	1.90265574	-0.75021350
C	-4.38653929	2.24076839	-0.52565395
H	-5.02504895	4.26017306	-0.07565959
C	-4.17671897	3.58389240	-0.14330751
C	-3.32189909	1.34951919	-0.62122492
C	-2.89925597	4.05884532	0.14370450

H	-3.48641838	0.31829427	-0.92606167
C	-2.01715135	1.79064336	-0.32968986
H	-2.73517497	5.09387920	0.43340220
C	-1.83175497	3.15807645	0.04553176
C	-0.71882028	1.15056956	-0.31349540
N	-0.48473462	3.33874254	0.25864040
C	0.17784496	2.13597953	0.03197766
H	0.30522737	-0.37496136	-1.80908236
H	-0.04610799	4.20289479	0.53937861
H	1.24923712	2.08642795	0.15251285
H	4.32596770	-1.80018041	-1.20165915
C	3.59766055	-1.29989792	-1.85144767
C	3.82491824	2.44415392	1.43141670
C	3.96317440	1.96751790	0.12887347
H	4.44954150	2.59112755	-0.61496969
H	3.82972300	-1.54601807	-2.89168699
H	4.19086362	3.43639799	1.68168870
C	3.23105120	1.64654893	2.41505221
C	3.49857668	0.68776529	-0.23376115
C	3.59108936	0.19656241	-1.63462780
C	2.79191843	0.36493833	2.08041406
C	2.93017291	-0.11120079	0.77525728
H	3.12342975	2.01656954	3.43080524
C	3.62692878	1.03734612	-2.68198347
H	2.61133289	-1.72255262	-1.62364118
H	2.33566149	-0.26634851	2.83814196
H	3.70732560	0.66304817	-3.69885524
H	2.56463146	-1.10343848	0.53613307
H	3.55676438	2.11508369	-2.56924038

2.8 Optimized geometry and the energies of the TS2

- SCF energy: -1151.57082662 Hartree
- Zero-point correction: 0.472691 (Hartree/Particle)
- Thermal correction to Energy: 0.509876 Hartree
- Thermal correction to Enthalpy: 0.511026 Hartree
- Thermal correction to Gibbs Free Energy: 0.396237 Hartree
- Sum of electronic and zero-point Energies: -1151.098136 Hartree
- Sum of electronic and thermal Energies: -1151.060951 Hartree
- Sum of electronic and thermal Enthalpies: -1151.059801 Hartree
- Sum of electronic and thermal Free Energies: -1151.174590 Hartree

Pd	1.42926434	0.34530677	0.08109465
C	3.15697760	0.90028120	-1.38791624
H	2.56263141	1.39170286	-2.15833502
C	3.42655798	1.62745434	-0.25783266
H	2.99584330	2.62643664	-0.20554480
C	3.29966283	-1.59307683	0.41479330
H	2.64920495	-2.46126179	0.32330890

C	3.75612340	-0.42014269	-1.82901941
H	4.57527264	-0.22074925	-2.53743492
H	2.98634322	-0.94878516	-2.40572626
C	3.18058138	-0.84918729	1.54246313
H	2.48275640	-1.20848707	2.29749497
C	4.27615288	-1.36943815	-0.71935454
H	5.22940679	-1.00371331	-0.33025828
H	4.49347326	-2.33499824	-1.19028348
C	4.46228531	1.30102095	0.80840078
H	5.35068854	0.87429756	0.33581771
H	4.79033879	2.24166072	1.26469873
C	3.97202271	0.37592029	1.95060864
H	4.84036220	0.07069351	2.55441733
H	3.33484757	0.96411122	2.62218809
H	-0.92527646	-4.57839777	-1.62947372
C	-1.27087484	-3.80403040	-0.94872691
H	-3.20696877	-4.73289062	-0.67031237
C	-2.56960349	-3.89401679	-0.40175091
C	-0.43507336	-2.73565867	-0.63334831
C	-3.04951846	-2.92298492	0.47526608
H	0.55981621	-2.66003202	-1.06762865
C	-0.88697982	-1.73452191	0.24586071
H	-4.05147671	-2.98682865	0.89262362
C	-2.20146594	-1.85624604	0.79348275
C	-0.30993279	-0.49328104	0.72420655
N	-2.40134371	-0.77146687	1.61967000
C	-1.27565241	0.05169977	1.54103261
H	0.02746497	0.86792192	-1.40915983
H	-3.31447860	-0.44807450	1.90978879
H	-1.28161544	0.99083692	2.07574535
H	0.05251711	3.71479162	-0.56554647
C	-0.60080267	2.99287947	-0.06372911
C	-4.64532261	0.20768705	-0.76834835
C	-3.40326029	0.66633849	-1.19119051
H	-2.87566243	0.10162033	-1.95062832
H	0.14171984	2.18759197	0.32442567
H	-5.06314832	-0.68753610	-1.22053172
C	-5.34092872	0.86864413	0.24987895
C	-2.79150308	1.80317099	-0.60102096
C	-1.46519730	2.23976641	-0.97843560
C	-4.77530471	2.01428703	0.82604901
C	-3.53348199	2.47589813	0.40680063
H	-6.31045346	0.50713546	0.58051243
C	-0.68635627	1.58502510	-2.01621332
H	-1.07681098	3.45614520	0.80126811
H	-5.31063014	2.55152279	1.60472541
H	0.02507436	2.25217715	-2.51331261
H	-3.12910816	3.37318839	0.86312103
H	-1.22351792	0.99114518	-2.75574158

2.9 Optimized geometry and the energies of the I_2

- SCF energy: -1151.64164450 Hartree

- Zero-point correction: 0.478256 (Hartree/Particle)
- Thermal correction to Energy: 0.515769 Hartree
- Thermal correction to Enthalpy: 0.516919 Hartree
- Thermal correction to Gibbs Free Energy: 0.402747 Hartree
- Sum of electronic and zero-point Energies: -1151.163389 Hartree
- Sum of electronic and thermal Energies: -1151.125875 Hartree
- Sum of electronic and thermal Enthalpies: -1151.124725 Hartree
- Sum of electronic and thermal Free Energies: -1151.238897 Hartree

Pd	0.36051811	0.63077528	0.19826626
C	1.20977899	2.77496405	1.12831777
H	1.42898209	2.42107319	2.13234266
C	2.13040311	2.50242899	0.16283007
H	2.99944374	1.92066867	0.46056087
C	-0.88758377	2.49902234	-1.07379209
H	-1.87707038	2.05779944	-0.97659574
C	-0.01599226	3.65978948	1.04550513
H	0.23762558	4.65750592	1.43507114
H	-0.76016581	3.24931027	1.73917915
C	-0.01868013	1.87706601	-1.91635090
H	-0.39874000	1.01241515	-2.45722885
C	-0.67171162	3.81140714	-0.34705962
H	-0.08757672	4.49491630	-0.96759304
H	-1.64625026	4.29139896	-0.20417954
C	2.18483531	3.08151192	-1.23975243
H	1.85579645	4.12310666	-1.22227612
H	3.23236541	3.10237988	-1.56003832
C	1.38581504	2.28709105	-2.30005659
H	1.35512855	2.86813974	-3.23413191
H	1.93778283	1.36918308	-2.53627374
H	-5.16075420	0.83337041	1.49417263
C	-4.58284799	0.14943412	0.87748502
H	-6.32644303	-0.98449421	0.27550653
C	-5.24768774	-0.88621811	0.18423791
C	-3.20269036	0.30179099	0.78209476
C	-4.54473816	-1.78672340	-0.61293701
H	-2.68944118	1.09705572	1.31890957
C	-2.45936879	-0.58569514	-0.01832167
H	-5.05578866	-2.58518291	-1.14545295
C	-3.15642704	-1.62873628	-0.70542379
C	-1.05292319	-0.71099113	-0.33092782
N	-2.21479885	-2.35153301	-1.40063935
C	-0.95704517	-1.79351908	-1.17222140
H	-0.35992276	-0.62936781	3.04200574
H	-2.40432283	-3.15058952	-1.98669487
H	-0.08328526	-2.24854187	-1.61619021
H	2.71839242	-0.91321552	3.05987530
C	2.22721037	-0.14945267	2.43533743
C	2.06271524	-4.09194778	-0.30907850
C	1.43365648	-3.17888777	0.54324765
H	0.59872425	-3.52051307	1.14394724
H	1.75573856	0.56717750	3.11580398

H	1.70815113	-5.11953399	-0.34463266
C	3.13332490	-3.69439631	-1.11020331
C	1.85007344	-1.83722975	0.62330847
C	1.18179922	-0.83035225	1.53098308
C	3.57234740	-2.36701120	-1.04021504
C	2.94562610	-1.46272596	-0.18615708
H	3.62029517	-4.40267880	-1.77520681
C	0.10397917	-1.42295248	2.44585630
H	3.01955323	0.36800316	1.88908899
H	4.40693186	-2.03562472	-1.65371731
H	0.54638837	-2.14823675	3.15025728
H	3.29682924	-0.43511836	-0.16336432
H	-0.69182029	-1.92133909	1.89084463

3. Optimized structures related to Complex 4 (In DCE solvent)

3.1 Optimized geometry and the energies of complex 3 (bridged complex) in DCE

- SCF energy: -9396.41986060 Hartree
- Zero-point correction: 0.594959 (Hartree/Particle)
- Thermal correction to Energy: 0.669872 Hartree
- Thermal correction to Enthalpy: 0.671022 Hartree
- Thermal correction to Gibbs Free Energy: 0.463670 Hartree
- Sum of electronic and zero-point Energies: -9395.824902 Hartree
- Sum of electronic and thermal Energies: -9395.749988 Hartree
- Sum of electronic and thermal Enthalpies: -9395.748838 Hartree
- Sum of electronic and thermal Free Energies: -9395.956190 Hartree

Sn	2.89753780	2.39355990	-0.01883394
Pd	1.56636529	0.39173764	0.75767537
Br	-0.38550230	1.80562109	1.67236823
Cl	1.82812674	4.33586856	-0.86753996
Cl	4.21931160	3.30500363	1.74430935
Cl	4.56835612	2.04425303	-1.68667912
N	2.85323310	-1.27877441	-1.33295322
N	4.07340370	-1.26138093	0.49383666
C	1.72646270	-0.97763733	-2.24877139
H	1.19045205	-0.16892282	-1.74204990
C	2.97067256	-0.74781952	-0.09440324
C	4.49971249	-0.93174627	1.87669201
H	3.81545073	-0.13700678	2.18632150
C	0.79287900	-2.18467582	-2.34938923
H	1.28598671	-3.04062402	-2.81971179
H	-0.08235118	-1.92585399	-2.95424780
H	0.45299042	-2.48376884	-1.35478213
C	4.19954729	-3.03274956	-2.61819420
H	3.59535504	-3.06066898	-3.51546042
C	2.21668046	-0.44199678	-3.59552944
H	2.89986205	0.39982244	-3.45168660
H	1.35272814	-0.09577328	-4.17189429
H	2.72424699	-1.20629518	-4.18913323
C	4.28419826	-2.13452915	2.79855762
H	3.23718799	-2.45218291	2.76773355

H	4.53309553	-1.85217183	3.82624814
H	4.91506468	-2.98226170	2.51513342
C	4.67361174	-2.18126273	-0.37470672
C	3.89018088	-2.19315873	-1.54397606
C	5.92202688	-0.36563592	1.90331504
H	6.67538557	-1.11864398	1.65904296
H	6.13319506	0.00600498	2.91054730
H	6.02404056	0.46765877	1.20168688
C	5.79445431	-3.00706109	-0.24431218
H	6.39910562	-3.01591037	0.65293527
C	5.31869830	-3.85001503	-2.48632828
H	5.58642415	-4.51447835	-3.30171718
C	6.10366877	-3.83673091	-1.31868065
H	6.96701436	-4.49081535	-1.24895150
Sn	-2.89752256	-2.39343895	-0.01878858
Pd	-1.56628748	-0.39168595	0.75770516
Br	0.38563140	-1.80573104	1.67230130
Cl	-4.21847005	-3.30546161	1.74463912
Cl	-1.82869750	-4.33556662	-0.86863129
Cl	-4.56927015	-2.04355685	-1.68563908
N	-4.07322801	1.26139633	0.49391468
N	-2.85311261	1.27882524	-1.33290740
C	-4.49956563	0.93170543	1.87674564
H	-3.81520309	0.13707506	2.18644169
C	-2.97048813	0.74788429	-0.09437464
C	-1.72650838	0.97746891	-2.24888357
H	-1.19048081	0.16878077	-1.74214193
C	-4.28425474	2.13447428	2.79866285
H	-4.91541465	2.98207111	2.51548630
H	-4.53287713	1.85191235	3.82636881
H	-3.23733126	2.45241502	2.76770042
C	-5.79441674	3.00694438	-0.24425515
H	-6.39905297	3.01575957	0.65300233
C	-5.92180695	0.36539519	1.90324217
H	-6.02365818	-0.46792153	1.20160090
H	-6.13304451	-0.00628821	2.91044298
H	-6.67522063	1.11831601	1.65887272
C	-0.79287087	2.18443716	-2.34978395
H	-0.45248432	2.48339117	-1.35530449
H	0.08202578	1.92565918	-2.95512885
H	-1.28617616	3.04048773	-2.81970797
C	-3.89012609	2.19312378	-1.54393639
C	-4.67349777	2.18124843	-0.37462585
C	-2.21697880	0.44166794	-3.59549816
H	-2.72423443	1.20602079	-4.18930110
H	-1.35315161	0.09496622	-4.17177336
H	-2.90044558	-0.39986564	-3.45140452
C	-4.19960356	3.03261547	-2.61820109
H	-3.59548300	3.06048088	-3.51551926
C	-6.10373730	3.83652901	-1.31865981
H	-6.96714718	4.49052899	-1.24894605
C	-5.31881197	3.84980387	-2.48633838
H	-5.58661280	4.51420356	-3.30175485

3.2 Optimized geometry and the energies of complex 4 with one DCE molecule as a ligand

- SCF energy: -5697.21315834 Hartree
- Zero-point correction: 0.356577 (Hartree/Particle)
- Thermal correction to Energy: 0.401940 Hartree
- Thermal correction to Enthalpy: 0.403090 Hartree
- Thermal correction to Gibbs Free Energy: 0.261716 Hartree
- Sum of electronic and zero-point Energies: -5696.856581 Hartree
- Sum of electronic and thermal Energies: -5696.811218 Hartree
- Sum of electronic and thermal Enthalpies: -5696.810068 Hartree
- Sum of electronic and thermal Free Energies: -5696.951442 Hartree

Pd	0.69809922	0.10403894	0.50307235
Sn	0.11903406	-2.14347862	-0.40659270
Br	3.01782690	-0.82381250	0.82937298
N	-2.19803967	0.66343962	1.10428842
C	-5.56125283	2.08016670	0.26364399
H	-6.56233675	2.26430428	0.64057241
N	-1.68565945	1.27256640	-0.93971557
Cl	1.19365411	-2.73516701	-2.43249170
C	-5.23261813	2.47249967	-1.04728196
H	-5.98466083	2.95424281	-1.66411170
C	-3.96161418	2.25739860	-1.57279550
H	-3.71999828	2.56742278	-2.58101921
C	-3.02387395	1.63016208	-0.74632312
C	-3.35252670	1.23861127	0.56494655
C	-4.62907173	1.46062517	1.09116674
H	-4.89185114	1.16694114	2.09903976
C	-1.20294799	0.69752539	0.18730106
C	-0.87454475	1.49614435	-2.16038917
H	0.09439803	1.04680764	-1.92313453
C	-0.66234867	2.99385335	-2.39794189
H	0.02840540	3.13358043	-3.23514121
H	-0.23405269	3.46655662	-1.50812961
H	-1.59801752	3.50547159	-2.64111666
C	-1.45944518	0.74886213	-3.36200633
H	-1.60888387	-0.30833638	-3.12368526
H	-0.75996937	0.82172762	-4.20034091
H	-2.41635830	1.16758998	-3.68478381
C	-2.03369876	0.11032871	2.47018687
H	-1.00474608	-0.26142772	2.48290308
C	-2.97172017	-1.07702372	2.70371199
H	-2.85409932	-1.82389631	1.91291890
H	-4.02202008	-0.77519540	2.73790400
H	-2.72378825	-1.54216276	3.66273923
C	-2.15317826	1.21856689	3.51954191
H	-1.93406695	0.80398678	4.50835198
H	-3.15797112	1.64998601	3.54797236
H	-1.43776021	2.02135131	3.31320163
Cl	-2.16782245	-2.44009969	-1.02604663

Cl	0.43679321	-4.04054877	0.96937566
H	2.30602626	2.47292990	-0.90546589
H	4.06578812	1.79311498	0.73650640
Cl	1.29136124	2.62157740	1.25214231
Cl	5.10422082	3.31884806	-0.77728053
C	2.51973961	3.09364120	-0.03593207
C	3.91162474	2.84846135	0.51276049
H	2.33142231	4.14401971	-0.25671515
H	4.11756977	3.46321161	1.38935446

3.3 Optimized geometry and the energies of the active Pd(0) catalyst generated from complex 4

- SCF energy: -1741.57279224 Hartree
- Zero-point correction: 0.349474 (Hartree/Particle)
- Thermal correction to Energy: 0.382205 Hartree
- Thermal correction to Enthalpy: 0.383355 Hartree
- Thermal correction to Gibbs Free Energy: 0.273469 Hartree
- Sum of electronic and zero-point Energies: -1741.223318 Hartree
- Sum of electronic and thermal Energies: -1741.190587 Hartree
- Sum of electronic and thermal Enthalpies: -1741.189437 Hartree
- Sum of electronic and thermal Free Energies: -1741.299323 Hartree

Pd	-0.99520705	-1.01301431	-0.25582651
N	2.01972750	-0.90286502	0.09255506
C	5.26599598	0.95376130	0.37693652
H	6.33419923	0.84571623	0.53971637
N	1.17214422	1.08879467	-0.21946330
C	4.72052570	2.23334210	0.18143276
H	5.37239757	3.10172614	0.19573492
C	3.35326123	2.41260476	-0.03053646
H	2.94404932	3.40425320	-0.17738778
C	2.54306497	1.27323166	-0.04245060
C	3.08977567	-0.01024034	0.15644495
C	4.46066521	-0.18552630	0.36792622
H	4.89289648	-1.16623381	0.52207688
C	0.83951897	-0.24040639	-0.13270432
C	0.17052054	2.14459029	-0.46133793
H	-0.76531043	1.58406503	-0.56413977
C	0.43675275	2.87747570	-1.77991208
H	-0.38316822	3.57539597	-1.97952421
H	0.49251167	2.16266594	-2.60765423
H	1.36780951	3.45154283	-1.75820626
C	0.04204373	3.07569361	0.74808805
H	-0.18822172	2.49663624	1.64867855
H	-0.77179730	3.78814558	0.57655078
H	0.95747034	3.64687273	0.93085080
C	2.09108349	-2.36788110	0.24937875
H	1.04930403	-2.68506287	0.13110900

C	2.55421591	-2.75453412	1.65760152
H	1.90508484	-2.29467826	2.41015727
H	3.58450397	-2.44400994	1.85601887
H	2.50210437	-3.84226488	1.77308157
C	2.91955299	-3.00843113	-0.86886100
H	2.86589193	-4.09881339	-0.78310636
H	3.97389227	-2.71947092	-0.82346289
H	2.52515140	-2.71818203	-1.84835796
H	-4.15598188	0.11920477	-1.32520985
H	-3.00236759	0.74704825	0.81847675
Cl	-3.31943399	-1.90675089	-0.38436068
Cl	-5.07601805	1.93990832	0.77553617
C	-4.37968228	-0.40263351	-0.39551535
C	-4.04938162	0.43656762	0.82474336
H	-5.40914019	-0.76058493	-0.38993069
H	-4.27965248	-0.08618254	1.75351579

3.4 Optimized geometry and the energies of the complex where active Pd(0) catalyst interacts with 5a

- SCF energy: -2105.39198441 Hartree
- Zero-point correction: 0.476821 (Hartree/Particle)
- Thermal correction to Energy: 0.521186 Hartree
- Thermal correction to Enthalpy: 0.522336 Hartree
- Thermal correction to Gibbs Free Energy: 0.389333 Hartree
- Sum of electronic and zero-point Energies: -2104.915163 Hartree
- Sum of electronic and thermal Energies: -2104.870799 Hartree
- Sum of electronic and thermal Enthalpies: -2104.869649 Hartree
- Sum of electronic and thermal Free Energies: -2105.002652 Hartree

Pd	0.40498194	-0.64948935	-1.34175838
N	-2.33351564	-1.06721066	0.02829260
C	-5.71026316	0.12219371	1.14874209
H	-6.63406191	-0.17322822	1.63719435
N	-2.10248024	0.98215455	-0.68912550
C	-5.56128162	1.44055114	0.68687159
H	-6.37139573	2.15078944	0.82298976
C	-4.39111283	1.85694873	0.05183958
H	-4.29037120	2.87428480	-0.30482478
C	-3.36903957	0.91624389	-0.10801597
C	-3.51817478	-0.40606216	0.35535433
C	-4.69361398	-0.81974826	0.98981302
H	-4.82304578	-1.83426116	1.34526930
C	-1.46397743	-0.23032371	-0.62135636
C	-1.49588823	2.16228313	-1.33527534
H	-0.50326115	1.80570901	-1.63241632
C	-1.31431240	3.31797714	-0.34630457
H	-0.76204165	4.12761373	-0.83487231
H	-0.74070729	2.99460082	0.52752186

H	-2.26889164	3.72539081	-0.00045894
C	-2.26609324	2.55433044	-2.60019985
H	-2.32855130	1.70268077	-3.28579294
H	-1.74407994	3.37168677	-3.10878778
H	-3.28302812	2.89113930	-2.37611934
C	-2.01689547	-2.48160255	0.30317565
H	-0.99604129	-2.59060823	-0.07778890
C	-2.93323859	-3.41647036	-0.49291966
H	-2.87285247	-3.18808192	-1.56226866
H	-3.97912336	-3.33227801	-0.18169810
H	-2.61890404	-4.45454751	-0.34140720
C	-2.00273399	-2.77160628	1.80742684
H	-1.65098286	-3.79527748	1.97481161
H	-2.99518176	-2.68125065	2.25867351
H	-1.32086841	-2.08720231	2.32036805
H	1.34192835	0.30116074	3.77871506
H	0.30559839	0.91542538	1.54318167
Cl	1.56721240	-1.60173522	2.36735101
Cl	1.62435290	2.77327648	2.26860151
C	1.87008303	0.13252850	2.83990375
C	1.37006776	1.04443857	1.73608190
H	2.94513453	0.23904439	2.98233391
H	1.92814934	0.91167363	0.81143983
H	3.51209228	2.15696434	-2.02439560
H	2.20302831	-0.25362074	-3.30116048
C	3.79856578	1.41970137	-1.27909392
C	2.45479931	-0.59291319	-2.30327589
C	3.33837159	0.09794240	-1.37732600
C	4.60356909	1.77486457	-0.19920169
H	4.95578027	2.79795654	-0.10385114
C	2.34540875	-1.90993457	-1.83689833
H	1.96669086	-2.78578462	-2.34573338
C	3.72741105	-0.84849783	-0.39029814
C	4.96150907	0.82676261	0.78122143
N	3.16514789	-2.06738005	-0.72159837
C	4.53073613	-0.49628965	0.69924839
H	5.58466564	1.13241823	1.61706939
H	3.06639232	-2.82762990	-0.06375963
H	4.80070842	-1.22731195	1.45540165

3.5 Optimized geometry and the energies of the TS1

- SCF energy: -2105.38442702 Hartree
- Zero-point correction: 0.474963 (Hartree/Particle)
- Thermal correction to Energy: 0.519301 Hartree
- Thermal correction to Enthalpy: 0.520451 Hartree
- Thermal correction to Gibbs Free Energy: 0.385643 Hartree
- Sum of electronic and zero-point Energies: -2104.909464 Hartree
- Sum of electronic and thermal Energies: -2104.865126 Hartree
- Sum of electronic and thermal Enthalpies: -2104.863976 Hartree

- Sum of electronic and thermal Free Energies: -2104.998784 Hartree

Pd	0.01921810	-0.76855466	0.50230977
N	3.10198431	-1.04492515	-0.08821491
C	6.55760776	0.35500338	-0.49476108
H	7.59444564	0.10600245	-0.69973460
N	2.54660486	1.03376890	0.26401861
C	6.19916425	1.69530865	-0.26777698
H	6.96320963	2.46617385	-0.30002787
C	4.87954913	2.05682408	-0.00100344
H	4.61611564	3.09265888	0.17260499
C	3.92307075	1.03691476	0.03337791
C	4.28213372	-0.30637183	-0.19392564
C	5.60741243	-0.66447373	-0.46163453
H	5.89626785	-1.69304275	-0.63761573
C	2.04145720	-0.23365093	0.19470834
C	1.69900286	2.20870043	0.54984095
H	0.69644322	1.78438352	0.66351514
C	1.67694981	3.17970579	-0.63479505
H	0.94662162	3.97220465	-0.44178201
H	1.38689175	2.65771094	-1.55221159
H	2.65001642	3.65142513	-0.80122168
C	2.09028757	2.86717319	1.87635571
H	2.06071477	2.13398851	2.68890729
H	1.38163274	3.66929179	2.10723187
H	3.09305646	3.30343908	1.84174455
C	2.96084361	-2.50512577	-0.25227162
H	1.89211284	-2.67847697	-0.09376290
C	3.73641202	-3.26301278	0.82991313
H	3.42613575	-2.92883697	1.82541210
H	4.81770550	-3.12197527	0.74070844
H	3.52852964	-4.33457348	0.74367506
C	3.31265243	-2.93935274	-1.67882129
H	3.09911848	-4.00668582	-1.79754398
H	4.36974046	-2.77985835	-1.91172490
H	2.71237925	-2.38285935	-2.40627034
H	-2.59564343	0.07894500	-3.19789121
H	-4.09611962	1.96700692	-2.43490821
Cl	-1.29396570	1.45723726	-1.75882294
Cl	-5.36438625	-0.04463838	-2.30762986
C	-2.68384252	0.33958851	-2.14283336
C	-3.98676059	1.05732209	-1.84366203
H	-2.55255556	-0.54024127	-1.51296877
H	-4.09573006	1.27429797	-0.78173783
H	-1.88489997	1.54556892	1.85442388
H	-0.40835954	-1.54941856	1.79812175
C	-2.85176880	1.06507177	1.72854666
C	-1.90765539	-1.24785184	0.92072180
C	-2.91307357	-0.27402495	1.30274458
C	-4.03332522	1.76036839	1.96536812
H	-3.99428219	2.79647190	2.29130856
C	-2.61509774	-2.39104475	0.59411408
H	-2.25345841	-3.36272591	0.28661165

C	-4.19373319	-0.87765781	1.13215853
C	-5.29045083	1.14192212	1.77841496
N	-3.97875781	-2.17072786	0.70542044
C	-5.38736042	-0.18246544	1.36048500
H	-6.19825137	1.71086133	1.96047392
H	-4.70094705	-2.83619566	0.47275411
H	-6.35261095	-0.65624146	1.20519924

3.6 Optimized geometry and the energies of the I_1

- SCF energy: -2105.39198441 Hartree
- Zero-point correction: 0.476821 (Hartree/Particle)
- Thermal correction to Energy: 0.521186 Hartree
- Thermal correction to Enthalpy: 0.522336 Hartree
- Thermal correction to Gibbs Free Energy: 0.389333 Hartree
- Sum of electronic and zero-point Energies: -2104.915163 Hartree
- Sum of electronic and thermal Energies: -2104.870799 Hartree
- Sum of electronic and thermal Enthalpies: -2104.869649 Hartree
- Sum of electronic and thermal Free Energies: -2105.002652 Hartree

Pd	0.18043562	-0.86213447	-0.29558312
N	-2.94503599	-0.99449573	-0.09191596
C	-6.34584150	0.58576698	-0.01788995
H	-7.40670430	0.39607574	0.11447285
N	-2.25770811	1.03972971	-0.47468649
C	-5.90239403	1.89685430	-0.26472498
H	-6.62592210	2.70456329	-0.32006137
C	-4.54930773	2.18339585	-0.43888225
H	-4.21934417	3.19775821	-0.62503935
C	-3.64768515	1.11750215	-0.36058150
C	-4.09190404	-0.19625702	-0.11346218
C	-5.44989631	-0.47917566	0.06244639
H	-5.80316854	-1.48413976	0.25618911
C	-1.83019435	-0.24311511	-0.30499955
C	-1.32532844	2.15919502	-0.72033638
H	-0.34466264	1.67462952	-0.75677769
C	-1.32936701	3.14782348	0.44948082
H	-0.56134680	3.91074733	0.28403548
H	-1.10568884	2.62743637	1.38609296
H	-2.29243276	3.65622980	0.55617228
C	-1.58325640	2.81112542	-2.08186123
H	-1.55135668	2.05954080	-2.87729939
H	-0.80644242	3.55709582	-2.27881707
H	-2.55257515	3.31651633	-2.12352834
C	-2.88464536	-2.44998785	0.15188702
H	-1.81838265	-2.68072215	0.07055112
C	-3.62740614	-3.22829262	-0.93837942
H	-3.24606588	-2.95691334	-1.92815687
H	-4.70520992	-3.04178605	-0.92103483

H	-3.46954003	-4.30129978	-0.78876248
C	-3.34466423	-2.78849625	1.57340286
H	-3.19691014	-3.85715031	1.76012609
H	-4.40389105	-2.56195526	1.72875559
H	-2.76015382	-2.22428681	2.30779644
H	2.31435677	0.75983897	3.45551916
H	1.78539865	2.60438619	1.80224137
Cl	0.37930461	0.07054733	2.25361483
Cl	4.13611132	2.22447612	1.67382950
C	2.14246612	0.54310883	2.40139547
C	2.38904021	1.74464772	1.50993138
H	2.71111897	-0.32546365	2.07187244
H	2.22627168	1.49480289	0.46222256
H	2.33346009	0.95515285	-2.12296406
H	0.12424428	-1.40517961	-1.74080350
C	3.26682688	0.48275248	-1.82213035
C	2.15132298	-1.38890573	-0.36281263
C	3.23170797	-0.65053118	-0.98787310
C	4.49201781	0.98492597	-2.25021368
H	4.52291785	1.86008567	-2.89455083
C	2.78053899	-2.40154562	0.33332095
H	2.35856231	-3.19236109	0.94063495
C	4.47194956	-1.25026217	-0.60866012
C	5.70300364	0.37231714	-1.85825049
N	4.16695054	-2.32084641	0.19949718
C	5.70909823	-0.75034673	-1.03407558
H	6.64745337	0.78456997	-2.20440693
H	4.83683201	-2.94986258	0.61627658
H	6.64113733	-1.22123178	-0.73113846

3.7 Optimized geometry and the energies of the complex where I_1 interacts with 6a

- SCF energy: -2454.38437392 Hartree
- Zero-point correction: 0.641082 (Hartree/Particle)
- Thermal correction to Energy: 0.699407 Hartree
- Thermal correction to Enthalpy: 0.700557 Hartree
- Thermal correction to Gibbs Free Energy: 0.534197 Hartree
- Sum of electronic and zero-point Energies: -2453.743292 Hartree
- Sum of electronic and thermal Energies: -2453.684967 Hartree
- Sum of electronic and thermal Enthalpies: -2453.683817 Hartree
- Sum of electronic and thermal Free Energies: -2453.850177 Hartree

Pd	-0.04375638	-0.44714554	0.67686016
N	2.73697177	-1.82581519	0.46505706
C	6.31989626	-2.01261155	-0.62670809
H	7.20347954	-2.64292989	-0.65807198
N	2.82262367	0.18807643	-0.37049334
C	6.36960770	-0.72199881	-1.18210153
H	7.29027715	-0.37131095	-1.63862530
C	5.25858968	0.11937687	-1.16006846
H	5.30791536	1.10943192	-1.59523323

C	4.09046408	-0.36600533	-0.56333256
C	4.03761645	-1.66323274	-0.01717831
C	5.15560758	-2.50321888	-0.03801396
H	5.12889178	-3.50015080	0.38339921
C	1.99626676	-0.70167831	0.24556629
C	2.39096179	1.55054133	-0.74988804
H	1.36539834	1.61758387	-0.37851070
C	2.36067008	1.71932154	-2.27134101
H	1.93129755	2.69603607	-2.51379176
H	1.73455977	0.94502965	-2.72774650
H	3.35997064	1.66056582	-2.71446498
C	3.22555002	2.61357744	-0.03014646
H	3.17380483	2.46739555	1.05326368
H	2.81669669	3.60048890	-0.26221214
H	4.27616637	2.59787964	-0.33360742
C	2.19237893	-3.01796161	1.14678864
H	1.15273745	-2.74630182	1.35315767
C	2.90013391	-3.25598506	2.48453474
H	2.84100697	-2.36083370	3.11224743
H	3.95491713	-3.51508036	2.35190070
H	2.41354334	-4.08270579	3.01233152
C	2.19496582	-4.24198219	0.22578047
H	1.68197220	-5.07036127	0.72558542
H	3.20789877	-4.57429808	-0.01947004
H	1.66589217	-4.01957516	-0.70546172
H	-1.92940257	-4.16390508	-0.35209762
H	-3.13279085	-3.51358021	-2.46221504
Cl	-0.70214878	-2.31862649	-1.22671567
Cl	-4.81999791	-3.73704219	-0.79220873
C	-2.19807989	-3.12350969	-0.53526319
C	-3.33361406	-2.98371337	-1.53051685
H	-2.40606300	-2.59751108	0.39600511
H	-3.56822327	-1.93805786	-1.72467923
H	-1.98369957	0.56779057	-1.73279962
H	0.24096015	0.56428454	1.80385823
C	-2.95211740	0.52190670	-1.24211179
C	-2.01891990	-0.16711522	1.11395774
C	-3.02326666	0.18184919	0.12266502
C	-4.12221122	0.78348627	-1.94995544
H	-4.06933045	1.04493910	-3.00385302
C	-2.74275740	-0.39799134	2.26675784
H	-2.39832398	-0.66681099	3.25699475
C	-4.31159260	0.12092131	0.73741075
C	-5.38330798	0.70748392	-1.31729775
N	-4.11007188	-0.23133074	2.05104679
C	-5.49384671	0.37625716	0.03080615
H	-6.28319988	0.91050025	-1.89200387
H	-4.83550344	-0.36283699	2.74000749
H	-6.46431984	0.31394258	0.51664003
H	-2.27910005	3.88841336	2.38396737
C	-1.41428506	3.26548305	2.64513026
C	0.54720642	5.34457475	-1.40273139
C	0.57213875	5.10267437	-0.02908445
H	1.17641165	5.73547375	0.61455901
H	-1.31865334	3.23961827	3.73529436

H	1.14420247	6.15273578	-1.81728478
C	-0.25529419	4.56347204	-2.24046760
C	-0.19164397	4.06695951	0.54143517
C	-0.15057854	3.79192903	2.00340089
C	-1.03460497	3.54516547	-1.68637658
C	-1.00842387	3.30276337	-0.31183922
H	-0.28169650	4.75586008	-3.30967439
C	0.96633665	3.98789752	2.72418943
H	-1.63295253	2.24618272	2.30451048
H	-1.67356387	2.93610305	-2.31953242
H	0.98331862	3.80711091	3.79576411
H	-1.61256654	2.49912170	0.09226818
H	1.89761378	4.31649013	2.27245081

3.8 Optimized geometry and the energies of the TS2

- SCF energy: -2454.36690903 Hartree
- Zero-point correction: 0.642727 (Hartree/Particle)
- Thermal correction to Energy: 0.700171 Hartree
- Thermal correction to Enthalpy: 0.701321 Hartree
- Thermal correction to Gibbs Free Energy: 0.537972 Hartree
- Sum of electronic and zero-point Energies: -2453.724182 Hartree
- Sum of electronic and thermal Energies: -2453.666738 Hartree
- Sum of electronic and thermal Enthalpies: -2453.665588 Hartree
- Sum of electronic and thermal Free Energies: -2453.828937 Hartree

Pd	-0.08077363	-0.35317473	-0.21977998
N	3.05815267	-0.62515989	-0.51654477
C	6.56300880	0.50494094	0.19654555
H	7.60967505	0.34878869	-0.04658510
N	2.51119471	0.89335796	0.94845528
C	6.20892535	1.49559009	1.12886158
H	6.98606765	2.09496329	1.59343871
C	4.87696689	1.72691599	1.47009784
H	4.61653663	2.49691402	2.18529579
C	3.90391162	0.93593638	0.85163900
C	4.25837898	-0.05068363	-0.08969632
C	5.59529851	-0.28145157	-0.42733763
H	5.87968190	-1.03855294	-1.14742993
C	1.99234025	-0.04794658	0.10632771
C	1.65216835	1.77399322	1.76698825
H	0.64413998	1.38364123	1.59045313
C	1.70958909	3.21668714	1.25502307
H	0.98438187	3.82964845	1.80055505
H	1.46294043	3.24900673	0.18927936
H	2.70104559	3.65932618	1.39470928
C	1.95827599	1.64589752	3.26223526
H	1.91897859	0.59970692	3.58025268
H	1.20789653	2.20531927	3.83027081

H	2.94182600	2.04679552	3.52303793
C	2.89726909	-1.67564082	-1.54001153
H	1.81547261	-1.81810520	-1.59273156
C	3.54001638	-2.99269680	-1.09423228
H	3.15294201	-3.29716695	-0.11586621
H	4.62934889	-2.91920760	-1.02278837
H	3.30204409	-3.77797550	-1.81904050
C	3.37465529	-1.18894818	-2.91186748
H	3.14828358	-1.94913947	-3.66672315
H	4.45234898	-1.00184981	-2.93367081
H	2.85692235	-0.26377029	-3.18626000
H	-1.34708021	3.23104620	-3.25165179
H	-0.79962688	4.08212437	-0.89810612
Cl	0.54961022	2.04272567	-2.43580179
Cl	-3.16484543	3.92693710	-1.12386773
C	-1.20084838	2.56193436	-2.40367371
C	-1.47643189	3.24650732	-1.07812340
H	-1.79586690	1.65317785	-2.50285601
H	-1.44361304	2.53381688	-0.25359619
H	-2.07078250	1.06452948	2.01231293
H	-0.27582458	-2.79126519	-1.92427554
C	-3.02835967	0.97281031	1.50452522
C	-2.09449152	-0.32981932	-0.57017910
C	-3.09498185	0.30772887	0.26662529
C	-4.19011436	1.48430049	2.07604878
H	-4.14219205	1.99573630	3.03464532
C	-2.80876806	-0.81301213	-1.64784697
H	-2.47187433	-1.39906862	-2.49385893
C	-4.37165197	0.17786002	-0.36251172
C	-5.43779805	1.34779262	1.42791524
N	-4.16935645	-0.52017932	-1.53146638
C	-5.54463613	0.69368448	0.20213180
H	-6.33072677	1.75836225	1.89303003
H	-4.87906341	-0.72988652	-2.21744636
H	-6.50492821	0.58818527	-0.29740202
H	-2.63014319	-5.61254085	-0.27145335
C	-2.64257109	-4.62196321	-0.75073779
C	0.06620118	-1.66006151	2.29378905
C	-0.10891131	-2.18922743	0.94681059
H	0.81028054	-2.57734419	0.51107152
H	-2.71512095	-4.79496353	-1.83005147
H	1.03433785	-1.23680210	2.54459256
C	-0.94539339	-1.67222318	3.20522645
C	-1.30886316	-3.02634177	0.69599625
C	-1.40703311	-3.81673619	-0.42206530
C	-2.20788419	-2.27346570	2.86133660
C	-2.37690184	-2.92200839	1.67720229
H	-0.80874035	-1.23788989	4.19234603
C	-0.32162560	-3.79610260	-1.46103176
H	-3.56804294	-4.12659920	-0.43848565
H	-3.02862396	-2.22227705	3.57259958
H	-0.49422031	-4.53076121	-2.25295668
H	-3.33069915	-3.39492948	1.46809234
H	0.67822641	-3.98085835	-1.04766031

3.9 Optimized geometry and the energies of the I_2

- SCF energy: -2454.39805355
- Zero-point correction: 0.645604 (Hartree/Particle)
- Thermal correction to Energy: 0.702905
- Thermal correction to Enthalpy: 0.704055
- Thermal correction to Gibbs Free Energy: 0.542025
- Sum of electronic and zero-point Energies: -2453.752449
- Sum of electronic and thermal Energies: -2453.695148
- Sum of electronic and thermal Enthalpies: -2453.693998
- Sum of electronic and thermal Free Energies: -2453.856028

Pd	-0.20720179	0.33100152	0.83197423
N	2.54911679	-1.13618011	0.87477840
C	5.50141479	-2.62273694	-0.89494046
H	6.29963840	-3.35531464	-0.82233515
N	2.37142643	0.08899864	-0.92063805
C	5.37229602	-1.85227830	-2.06364198
H	6.06985974	-2.00127903	-2.88236144
C	4.36146546	-0.90150032	-2.19687876
H	4.26453502	-0.32493201	-3.10783698
C	3.47940617	-0.73791108	-1.12386110
C	3.59974479	-1.52186964	0.04089935
C	4.61744945	-2.47198899	0.17234274
H	4.71903378	-3.07951376	1.06288917
C	1.78568379	-0.17082893	0.28488507
C	1.84695427	1.10673638	-1.85717268
H	1.08378780	1.62953530	-1.27725732
C	1.17665645	0.44621457	-3.06540147
H	0.76732090	1.21883507	-3.72505657
H	0.35664557	-0.20168414	-2.74144938
H	1.88627336	-0.15466521	-3.64412401
C	2.92348228	2.12536810	-2.24553746
H	3.42607912	2.51150921	-1.35451530
H	2.44390437	2.96856002	-2.75082727
H	3.67507860	1.70786704	-2.92093857
C	2.21655577	-1.70627591	2.19545308
H	1.33285578	-1.13945824	2.50278534
C	3.33434265	-1.45164090	3.21115463
H	3.56685967	-0.38339604	3.26492921
H	4.25238407	-1.99222631	2.96241282
H	3.00678123	-1.78421565	4.20162085
C	1.81597575	-3.18037513	2.07569001
H	1.47661160	-3.54651049	3.05033680
H	2.65015984	-3.80939926	1.75037675
H	0.99955036	-3.29128408	1.35520837
H	-1.86536307	-4.26164076	-1.75835510
H	-3.15294394	-2.11538787	-1.38578200
Cl	-0.24677074	-2.58320031	-1.26361490
Cl	-4.29991409	-3.81842714	-0.17098128
C	-1.68282366	-3.64163109	-0.88019829

C	-2.86728116	-2.75318283	-0.55002655
H	-1.39769642	-4.26784635	-0.03401412
H	-2.68099929	-2.13774468	0.32897986
H	-1.79697615	1.20915947	-1.82083150
H	1.24704395	1.08159356	3.48959459
C	-2.80627092	0.91992013	-1.53767095
C	-2.23608994	0.38725524	0.97007156
C	-3.07551260	0.54515916	-0.20704278
C	-3.83456834	0.91278429	-2.47562038
H	-3.62989331	1.19981491	-3.50420293
C	-3.10450973	-0.04173187	1.95397905
H	-2.91422711	-0.26439201	2.99631242
C	-4.41354621	0.17690969	0.13336977
C	-5.14694674	0.53565991	-2.11168475
N	-4.40492669	-0.16762183	1.46583159
C	-5.45343905	0.16501211	-0.80458647
H	-5.93146280	0.53442499	-2.86420503
H	-5.20267384	-0.49596492	1.98949659
H	-6.46089162	-0.13281220	-0.52476152
H	-0.71031943	3.35194669	3.46924847
C	-0.99598975	2.45650777	2.89175929
C	1.62400019	4.74080952	-0.44956284
C	1.51327914	3.78224323	0.56327629
H	2.39656366	3.53904790	1.14308307
H	-1.17241380	1.64154975	3.60080793
H	2.58497883	5.21575748	-0.63086283
C	0.51892467	5.07912561	-1.22895705
C	0.29197118	3.13867596	0.83258401
C	0.14586741	2.10679400	1.92560087
C	-0.70799260	4.45295970	-0.97356311
C	-0.81926350	3.50884208	0.04228704
H	0.60757635	5.81639723	-2.02235909
C	1.41224782	1.87689405	2.75607599
H	-1.93701340	2.66107998	2.38362913
H	-1.58125015	4.69844217	-1.57308201
H	1.66511534	2.79139284	3.31793660
H	-1.76785647	3.00850773	0.20281617
H	2.27804898	1.59994874	2.15172070

4.1 Optimized geometry and the energies of Indole (5a) in DCE solvent

- SCF energy: -363.832070783
- Zero-point correction: 0.130049 (Hartree/Particle)
- Thermal correction to Energy: 0.139378
- Thermal correction to Enthalpy: 0.140528
- Thermal correction to Gibbs Free Energy: 0.091267
- Sum of electronic and zero-point Energies: -363.702022
- Sum of electronic and thermal Energies: -363.692693
- Sum of electronic and thermal Enthalpies: -363.691543
- Sum of electronic and thermal Free Energies: -363.740804

C	0.42430388	-1.68365299	0.00000000
C	1.78502182	-1.39982506	0.00000000
C	-0.49676324	-0.61983739	0.00000000
C	2.25313883	-0.06729365	0.00000000
C	0.00000000	0.71688192	0.00000000
C	1.36962610	1.00704231	0.00000000
C	-1.93091970	-0.53032672	0.00000000
C	-2.25012670	0.80436752	0.00000000
N	-1.09269887	1.55765037	0.00000000
H	0.07292818	-2.71247572	0.00000000
H	2.50431202	-2.21457399	0.00000000
H	3.32312031	0.12239789	0.00000000
H	1.72626109	2.03347595	0.00000000
H	-2.63300579	-1.35297670	0.00000000
H	-3.21575319	1.29045196	0.00000000
H	-1.05465637	2.56601239	0.00000000

4.2 Optimized geometry and the energies of Styrene (6a) in DCE solvent

- SCF energy: -348.979533870 Hartree
- Zero-point correction: 0.162262 (Hartree/Particle)
- Thermal correction to Energy: 0.173854 Hartree
- Thermal correction to Enthalpy: 0.175004 Hartree
- Thermal correction to Gibbs Free Energy: 0.120031 Hartree
- Sum of electronic and zero-point Energies: -348.817271 Hartree
- Sum of electronic and thermal Energies: -348.805680 Hartree
- Sum of electronic and thermal Enthalpies: -348.804530 Hartree
- Sum of electronic and thermal Free Energies: -348.859503 Hartree

C	-0.46545604	-1.16310423	-0.20304123
C	-1.86003278	-1.22643290	-0.20506460
C	0.20766830	0.05733733	-0.01168785
C	-2.61830507	-0.07215701	-0.00283646
C	-0.57405132	1.20813281	0.20739971
C	-1.96610847	1.14646399	0.20711863
C	1.69497733	0.12406901	-0.02697405
C	2.45498019	-1.12509745	0.36363740
C	2.35208735	1.23842412	-0.38704349
H	0.10060671	-2.07463583	-0.36614569
H	-2.35287685	-2.18195154	-0.36429318
H	-3.70372211	-0.12158545	0.00165625
H	-0.08438330	2.15704598	0.40494419
H	-2.54345676	2.05015633	0.38408298
H	2.09118233	-1.53179093	1.31499578
H	3.52525422	-0.92068272	0.45814105
H	2.33574438	-1.91753349	-0.38642922
H	1.83924715	2.13523366	-0.72227486
H	3.43784736	1.27992994	-0.37372568

4.3 Optimized geometry and the energies of substituted indole (7a) in DCE solvent

- SCF energy: -712.845194057 Hartree
- Zero-point correction: 0.296694 (Hartree/Particle)
- Thermal correction to Energy: 0.318588 Hartree
- Thermal correction to Enthalpy: 0.319738 Hartree
- Thermal correction to Gibbs Free Energy: 0.241830 Hartree
- Sum of electronic and zero-point Energies: -712.548500 Hartree
- Sum of electronic and thermal Energies: -712.526606 Hartree
- Sum of electronic and thermal Enthalpies: -712.525456 Hartree
- Sum of electronic and thermal Free Energies: -712.603364 Hartree

C	-2.72778801	1.22098657	0.23229922
C	-4.10547599	1.03365465	0.24483046
C	-0.44037971	-0.07195082	-0.06780858
C	-1.87661447	0.11838348	0.01439944
C	-4.67243826	-0.24208639	0.04142539
C	-0.25297372	-1.40934078	-0.33149465
C	-2.48117556	-1.15666124	-0.19806463
C	-3.86681313	-1.35249259	-0.18356077
N	-1.46610368	-2.06175076	-0.40725248
H	-2.32241104	2.21547021	0.38673460
H	-4.75879172	1.88563103	0.41332022
H	0.54818469	1.13636025	2.23757282
H	-5.75269868	-0.35828968	0.05809362
H	0.66654029	-1.95743979	-0.47103829
H	-4.29258818	-2.33890121	-0.34630034
H	-1.58568054	-3.04944315	-0.57454341
H	4.94622465	0.16497918	-1.76383895
H	2.73615389	1.21602948	-1.82653492
C	4.24140666	-0.03200218	-0.96000146
C	2.97719545	0.56714816	-0.99236545
H	1.20810252	2.79531231	-1.08945876
C	4.59683295	-0.87486006	0.09169084
H	5.57844739	-1.34037947	0.11746401
C	2.03960503	0.34213125	0.02403416
C	0.64445530	0.99658192	0.03782780
C	0.46423375	1.99140897	-1.13280053
C	0.50179975	1.79292987	1.36427838
H	-0.52754204	2.44912315	-1.08558620
C	3.67237127	-1.11539075	1.11247629
C	2.41560949	-0.51376884	1.07573716
H	1.30831294	2.53029924	1.44651839
H	-0.45093244	2.32743981	1.40381297
H	3.92977631	-1.77283340	1.93902903
H	1.70555158	-0.72677625	1.86923745
H	0.54697137	1.48764626	-2.10113321

In Gas Phase

5. Optimized structures related to Complex 2

5.1 Optimized geometry and the energies of complex 2

- SCF energy: -5313.98757566 Hartree
- Zero-point correction: 0.588638 (Hartree/Particle)
- Thermal correction to Energy: 0.630858 Hartree
- Thermal correction to Enthalpy: 0.631802 Hartree
- Thermal correction to Gibbs Free Energy: 0.509486 Hartree
- Sum of electronic and zero-point Energies: -5313.398938 Hartree
- Sum of electronic and thermal Energies: -5313.356718 Hartree
- Sum of electronic and thermal Enthalpies: -5313.355774 Hartree
- Sum of electronic and thermal Free Energies: -5313.478089 Hartree

Pd	-0.00313516	-0.38708156	0.00435494
Sn	-0.16817391	2.03745102	-0.67437100
Br	0.15805300	-2.73284916	0.99128994
N	-2.81915129	-0.25356061	1.06060991
C	-6.50789785	-0.90890476	1.02554697
H	-7.42201329	-0.85978044	1.60939578
N	-2.89634128	-1.00926798	-0.98905903
Cl	0.25613134	3.50470231	1.15902708
C	-6.55524577	-1.39514121	-0.29240620
H	-7.50497971	-1.71528772	-0.70997204
C	-5.40546770	-1.47798592	-1.07448356
H	-5.45042443	-1.86146105	-2.08784048
N	2.87565921	-0.78364628	-0.87457515
N	2.82046359	0.02819412	1.15621171
C	-4.20547996	-1.05536741	-0.49913909
C	-4.15673582	-0.56825657	0.81757402
C	-5.31099141	-0.48935468	1.60140396
H	-5.28443072	-0.12150782	2.61910300
C	-2.05898216	-0.53799448	-0.02832817
C	-2.52657072	-1.50906973	-2.33538184
H	-3.48291336	-1.61448410	-2.85429567
C	-1.86727655	-2.88779634	-2.23946272
H	-1.67485787	-3.27460530	-3.24657174
H	-2.51685414	-3.59396962	-1.71241467
H	-0.92387495	-2.83314749	-1.69070481
C	-1.69765845	-0.50004033	-3.13142731
H	-2.16693198	0.48756515	-3.13287761
H	-1.60758452	-0.84981062	-4.16535961
H	-0.68764364	-0.40449259	-2.72391299
C	-2.25970336	0.27987118	2.32251572
H	-1.19982151	0.42821099	2.09816424
C	-2.35320192	-0.76496799	3.43679428
H	-1.82973838	-1.67646922	3.13168936
H	-3.39108776	-1.01491418	3.67867217
H	-1.87885193	-0.37331536	4.34317250
C	-2.86314516	1.64482819	2.66420237
H	-2.31595165	2.07783363	3.50743193

H	-3.91786709	1.57530586	2.94535489
H	-2.77630892	2.32964451	1.81521978
C	2.05158173	-0.30148517	0.08862919
C	4.15691471	-0.29349032	0.89889887
C	4.19250408	-0.80971072	-0.41013736
C	5.38944496	-1.24286375	-0.98640333
H	5.42405622	-1.64584206	-1.99055642
C	6.54534630	-1.14847609	-0.21516797
H	7.49070759	-1.47902123	-0.63465276
C	6.50937214	-0.64113044	1.09474017
H	7.42715398	-0.58788842	1.67246987
C	5.31796496	-0.20798083	1.67193258
H	5.29981133	0.16920417	2.68600164
C	2.26147115	0.53225185	2.43111574
H	1.21689461	0.74799520	2.19333408
C	2.29985408	-0.56620427	3.49723926
H	1.75934303	-1.44947945	3.14402252
H	1.82567841	-0.20187826	4.41524502
H	3.32866901	-0.85442758	3.73830799
C	2.91954401	1.84560078	2.86202072
H	3.94673397	1.70461608	3.20937744
H	2.34317416	2.27350492	3.68810091
H	2.91671078	2.57005013	2.04387098
C	2.37973229	-1.31405269	-2.16194183
H	1.30909867	-1.09409337	-2.13610342
C	2.98715633	-0.56563796	-3.35079697
H	4.06115018	-0.74734282	-3.45130441
H	2.82178380	0.51116185	-3.25145130
H	2.50412682	-0.90637057	-4.27283064
C	2.54203954	-2.83584458	-2.21216828
H	2.09018715	-3.22072607	-3.13285595
H	2.03729079	-3.29054335	-1.35401423
H	3.59523956	-3.13401627	-2.20133426
Cl	-2.29981990	2.83230446	-1.38529207
Cl	1.28389766	2.83686941	-2.37910758

5.2 Optimized geometry and the energies of the isomer of the complex 2

- SCF energy: -5313.96473780 Hartree
- Zero-point correction: 0.589072 (Hartree/Particle)
- Thermal correction to Energy: 0.631132 Hartree
- Thermal correction to Enthalpy: 0.632076 Hartree
- Thermal correction to Gibbs Free Energy: 0.512311 Hartree
- Sum of electronic and zero-point Energies: -5313.375665 Hartree
- Sum of electronic and thermal Energies: -5313.333606 Hartree
- Sum of electronic and thermal Enthalpies: -5313.332662 Hartree
- Sum of electronic and thermal Free Energies: -5313.452427 Hartree

Pd	-0.03285277	0.57481932	0.64410272
Sn	2.08015894	1.70870290	-0.29058915
Br	-0.71770315	2.73869274	1.72614964

N	-2.84838303	0.57700750	-0.51235992
C	-6.39467535	-0.55760347	-0.97355431
H	-7.30266874	-0.41102034	-1.55062268
N	-2.83636701	-0.90370770	1.09415252
Cl	3.52184720	3.36399721	0.58527983
C	-6.37156618	-1.53025376	0.04110860
H	-7.25904469	-2.12608119	0.23136858
C	-5.22866052	-1.74341820	0.80864363
H	-5.21271636	-2.49700159	1.58870694
N	1.64739375	-1.93206746	0.82843462
N	0.61631650	-1.85736489	-1.10154218
C	-4.11220240	-0.95401406	0.52585472
C	-4.12483352	0.00735977	-0.49658147
C	-5.27743842	0.22470507	-1.25816620
H	-5.31167987	0.97261470	-2.03912540
C	-2.06480792	0.01292276	0.45383736
C	-2.44636804	-1.75037614	2.24142421
H	-3.39449460	-2.01517424	2.71988480
C	-1.62609903	-0.97175321	3.26981645
H	-1.47973753	-1.59351860	4.15944190
H	-2.13689306	-0.04918154	3.55885342
H	-0.64777210	-0.69014858	2.87616588
C	-1.77877959	-3.03881368	1.74893550
H	-2.42821869	-3.56548408	1.04130412
H	-1.57697144	-3.70744340	2.59269714
H	-0.83360091	-2.81942546	1.24883709
C	-2.44475886	1.74121676	-1.34750033
H	-1.39506384	1.90540808	-1.10265072
C	-3.22611386	2.99161880	-0.93563664
H	-3.08072511	3.19101700	0.12798731
H	-4.29653751	2.89304827	-1.14482172
H	-2.84369110	3.84875538	-1.49893676
C	-2.54121167	1.45292435	-2.84884270
H	-2.03821163	2.26359156	-3.38419321
H	-3.57439059	1.40163713	-3.20442650
H	-2.04269407	0.51947026	-3.11767441
C	0.79756166	-1.18737497	0.06317605
C	1.35143006	-3.04475201	-1.09760365
C	2.01895943	-3.08967540	0.13911118
C	2.85360554	-4.16103140	0.46988632
H	3.38258284	-4.20216054	1.41302734
C	2.99258701	-5.18130269	-0.46759942
H	3.63805898	-6.02415433	-0.24020177
C	2.31797559	-5.13966985	-1.69972147
H	2.44822327	-5.95200382	-2.40812382
C	1.48804723	-4.07278673	-2.03407071
H	0.97527752	-4.04667664	-2.98689119
C	-0.21121031	-1.34028070	-2.20945888
H	-0.53105032	-0.36102558	-1.85300073
C	0.61842167	-1.11991581	-3.47715011
H	1.50157052	-0.51533845	-3.25376044
H	0.00997512	-0.58066439	-4.21027861
H	0.94371875	-2.05893158	-3.93370233
C	-1.45056886	-2.21968904	-2.40322434
H	-1.18404283	-3.23975840	-2.69633685

H	-2.08744045	-1.80031551	-3.18810652
H	-2.03469187	-2.26872420	-1.47848310
C	2.14844670	-1.51296718	2.15893481
H	1.64371596	-0.56012133	2.34459312
C	1.73368243	-2.50344327	3.25232501
H	2.23774811	-3.46802495	3.14447047
H	0.65601597	-2.67878706	3.24167816
H	2.00518620	-2.09125147	4.22954491
C	3.65932753	-1.25798802	2.13261183
H	3.96387274	-0.81431873	3.08600186
H	3.93174526	-0.57578046	1.32452873
H	4.22629309	-2.18319664	1.99340788
Cl	1.14314451	2.69169469	-2.27574074
Cl	3.66524480	0.21843703	-1.34752706

5.3 Optimized geometry and the energies of the active Pd(0) catalyst generated from complex 2

- SCF energy: -1358.33159721 Hartree
- Zero-point correction: 0.580240 (Hartree/Particle)
- Thermal correction to Energy: 0.613119 Hartree
- Thermal correction to Enthalpy: 0.614063 Hartree
- Thermal correction to Gibbs Free Energy: 0.512834 Hartree
- Sum of electronic and zero-point Energies: -1357.751357 Hartree
- Sum of electronic and thermal Energies: -1357.718479 Hartree
- Sum of electronic and thermal Enthalpies: -1357.717535 Hartree
- Sum of electronic and thermal Free Energies: -1357.818763 Hartree

Pd	0.06249928	-0.04782017	-0.00448625
N	2.95927106	0.95875149	-0.12438144
C	6.68999229	0.57636213	-0.02145892
H	7.63633817	1.10672479	-0.07565881
N	2.95962679	-1.20009958	0.16034114
C	6.68663503	-0.81631210	0.15565858
H	7.63009203	-1.34849641	0.23571673
C	5.49096698	-1.53133110	0.23130995
H	5.49706410	-2.60760761	0.36826849
N	-2.85091373	-1.02497672	-0.11798360
N	-2.78237187	1.14131708	0.11799858
C	4.29821840	-0.81359624	0.12459052
C	4.29909292	0.58284156	-0.05619622
C	5.49918436	1.29545713	-0.12980968
H	5.51456887	2.36990954	-0.26579332
C	2.12133743	-0.12276257	0.00706643
C	2.51406756	-2.60170018	0.30257051
H	3.43187469	-3.18091627	0.44147942
C	1.83002596	-3.08512414	-0.98130080
H	1.54641183	-4.13926524	-0.88097781
H	2.50257521	-2.98448989	-1.84032566

H	0.93334078	-2.48689226	-1.17293452
C	1.64231909	-2.78635941	1.54882845
H	2.17506071	-2.45557389	2.44697979
H	1.38247925	-3.84510628	1.66487393
H	0.72384242	-2.19578417	1.45592791
C	2.44674541	2.32575716	-0.31759533
H	1.36041658	2.18311606	-0.32848940
C	2.86957113	2.89305306	-1.67629652
H	2.54994747	2.22123734	-2.47959006
H	3.95255480	3.03165122	-1.75470281
H	2.39380873	3.86780022	-1.83142792
C	2.80402221	3.22603841	0.86907651
H	2.33600467	4.20851099	0.74066182
H	3.88361848	3.37856206	0.96790550
H	2.43280627	2.78463363	1.79982934
C	-1.98104794	0.03221203	-0.00055965
C	-4.13304001	0.80119234	0.07246229
C	-4.17726539	-0.59993524	-0.07980821
C	-5.39693779	-1.27687175	-0.16174542
H	-5.44183425	-2.35274532	-0.27922096
C	-6.56723164	-0.52068195	-0.08827330
H	-7.52824721	-1.02311569	-0.14974260
C	-6.52333998	0.87393138	0.06238809
H	-7.45084980	1.43664870	0.11573078
C	-5.30792208	1.55423948	0.14472765
H	-5.28540852	2.63103235	0.25981503
C	-2.22125835	2.49246976	0.27653213
H	-1.14059023	2.31283042	0.27631437
C	-2.56403431	3.38173172	-0.92288549
H	-2.22302010	2.90956432	-1.85004918
H	-2.06039757	4.34957692	-0.82095605
H	-3.63910310	3.56986228	-1.00876459
C	-2.60579572	3.10152000	1.62870862
H	-3.68233698	3.27921071	1.71678278
H	-2.09480452	4.06207633	1.75825403
H	-2.29992272	2.43503360	2.44169239
C	-2.37559633	-2.41066444	-0.25664154
H	-1.28633296	-2.30230049	-0.23445093
C	-2.79546918	-3.26738074	0.94196380
H	-3.88104522	-3.39276885	1.00661438
H	-2.44720777	-2.80796814	1.87284562
H	-2.34579756	-4.26300271	0.85820141
C	-2.77113601	-3.00453341	-1.61203590
H	-2.32329431	-3.99823701	-1.72377521
H	-2.40416826	-2.36663402	-2.42266601
H	-3.85532101	-3.10961235	-1.72148217

5.4 Optimized geometry and the energies of the $SnCl_3Br$ complex

- SCF energy: -3955.53018660 Hartree
- Zero-point correction: 0.004326 (Hartree/Particle)
- Thermal correction to Energy: 0.012266 Hartree

- Thermal correction to Enthalpy: 0.013210 Hartree
- Thermal correction to Gibbs Free Energy: -0.032192 Hartree
- Sum of electronic and zero-point Energies: -3955.525860 Hartree
- Sum of electronic and thermal Energies: -3955.517921 Hartree
- Sum of electronic and thermal Enthalpies: -3955.516977 Hartree
- Sum of electronic and thermal Free Energies: -3955.562379 Hartree

Sn	-0.32502370	-0.00000007	0.00003024
Cl	-1.12969703	-1.87554280	1.08636318
Cl	-1.12969097	1.87860546	1.08106323
Cl	-1.12993944	-0.00305876	-2.16732911
Br	2.11056433	-0.00000179	-0.00009047

5.5 Optimized geometry and the energies of the complex where active Pd(0) catalyst interacts with 5a

- SCF energy: -1722.16976324 Hartree
- Zero-point correction: 0.711620 (Hartree/Particle)
- Thermal correction to Energy: 0.752745 Hartree
- Thermal correction to Enthalpy: 0.753689 Hartree
- Thermal correction to Gibbs Free Energy: 0.632352 Hartree
- Sum of electronic and zero-point Energies: -1721.458143 Hartree
- Sum of electronic and thermal Energies: -1721.417018 Hartree
- Sum of electronic and thermal Enthalpies: -1721.416074 Hartree
- Sum of electronic and thermal Free Energies: -1721.537411 Hartree

Pd	0.00817572	0.89681086	0.11421423
N	2.91631333	0.96284090	-0.87483253
C	6.63328143	1.23965094	-0.44091666
H	7.58312649	1.30604371	-0.96360346
N	2.89087700	0.99867281	1.30295042
C	6.61357418	1.25240329	0.96255132
H	7.54806675	1.32695888	1.51109409
C	5.41221112	1.17447396	1.66786833
H	5.40485952	1.19049281	2.75265963
N	-2.91030764	-0.13002133	0.18880594
N	-2.84006845	2.01539574	-0.19678695
C	4.23152143	1.08053288	0.92913682
C	4.24897735	1.06094537	-0.47851054
C	5.45412714	1.14466115	-1.18105007
H	5.48228355	1.14144496	-2.26365923
C	2.06674769	0.93845144	0.20633319
C	2.42865596	1.03174380	2.70605042

H	3.34263059	1.03087772	3.30737670
C	1.62627735	-0.22449928	3.05755289
H	1.36701831	-0.21321968	4.12243807
H	2.20901031	-1.12803065	2.84789022
H	0.70426496	-0.25342362	2.46551253
C	1.65758933	2.32410642	2.99619533
H	2.26642122	3.20174982	2.75198111
H	1.38877838	2.36842324	4.05792533
H	0.74335862	2.35291426	2.39327377
C	2.41945422	0.94603220	-2.26196129
H	1.33732560	0.82153665	-2.13848124
C	2.96346983	-0.25176496	-3.04881682
H	2.76483891	-1.18650634	-2.51645949
H	4.04021912	-0.18120442	-3.23079273
H	2.46501896	-0.29786935	-4.02395053
C	2.67099547	2.29306152	-2.94732900
H	2.23007683	2.28766092	-3.95037968
H	3.73944350	2.51131231	-3.04800276
H	2.20721466	3.09894734	-2.36911317
C	-2.04201662	0.91791480	0.01731041
C	-4.19105014	1.67620917	-0.15483303
C	-4.23589254	0.28953585	0.09636724
C	-5.45607615	-0.38195396	0.20917722
H	-5.50059165	-1.44571666	0.40748419
C	-6.62568974	0.36418969	0.06100940
H	-7.58711982	-0.13436107	0.14467765
C	-6.58102771	1.74395920	-0.19222075
H	-7.50817784	2.29901079	-0.30280753
C	-5.36511566	2.41937471	-0.30303043
H	-5.34165348	3.48506311	-0.49567039
C	-2.27570200	3.35575121	-0.42260524
H	-1.19432115	3.18177728	-0.37944298
C	-2.62465300	3.88002656	-1.81922761
H	-2.29642291	3.16617711	-2.58197840
H	-2.11232177	4.83269865	-1.99366064
H	-3.69896316	4.04755252	-1.94672558
C	-2.65369851	4.31616536	0.70955289
H	-3.73074653	4.50790817	0.75221596
H	-2.14545235	5.27593470	0.56462876
H	-2.34063584	3.90144074	1.67339976
C	-2.43995426	-1.50168952	0.45286732
H	-1.35193606	-1.40523392	0.42687628
C	-2.84357115	-1.97139492	1.85350222
H	-3.92801166	-2.07942913	1.96122594
H	-2.49355290	-1.25659388	2.60619321
H	-2.37806614	-2.94173604	2.05354720
C	-2.85641605	-2.46664391	-0.66025768
H	-2.41045315	-3.44741757	-0.46995895
H	-2.48708248	-2.10824906	-1.62587288
H	-3.94263810	-2.58785822	-0.72372568
C	0.41745974	-3.47794601	1.17563344
C	0.13800797	-4.64519256	1.87707762
C	0.64337119	-2.52310674	-1.24828148
C	0.43348551	-3.51398093	-0.22945894
C	-0.12497832	-5.85652093	1.20133866

C	0.50396440	-3.15736582	-2.45501014
C	0.16409347	-4.74658521	-0.89012486
C	-0.11475097	-5.92475405	-0.18834736
N	0.21851961	-4.49817124	-2.24732570
H	0.60983156	-2.54448630	1.69464603
H	0.12166748	-4.62875092	2.96361398
H	0.81527184	-1.46718694	-1.08110112
H	-0.34016335	-6.75292607	1.77663131
H	0.57862966	-2.76368725	-3.45922347
H	-0.32047851	-6.85718722	-0.70793885
H	0.07597947	-5.18391365	-2.97153271

5.6 Optimized geometry and the energies of the TS1

- SCF energy: -1722.11917362 Hartree
- Zero-point correction: 0.705621 (Hartree/Particle)
- Thermal correction to Energy: 0.746219 Hartree
- Thermal correction to Enthalpy: 0.747163 Hartree
- Thermal correction to Gibbs Free Energy: 0.631907 Hartree
- Sum of electronic and zero-point Energies: -1721.413553 Hartree
- Sum of electronic and thermal Energies: -1721.372954 Hartree
- Sum of electronic and thermal Enthalpies: -1721.372010 Hartree
- Sum of electronic and thermal Free Energies: -1721.487267 Hartree

Pd	-0.10535184	-0.96881085	-0.39626546
N	3.01127724	-1.04459722	-0.57117204
C	6.52295670	-0.73009136	0.71951209
H	7.57376413	-0.79939286	0.45356050
N	2.46126461	-0.57752650	1.48268805
C	6.16305600	-0.39049679	2.03261475
H	6.93842175	-0.19446586	2.76744144
C	4.82285889	-0.30183166	2.41276384
H	4.55020093	-0.03814367	3.42926052
N	-1.87490662	1.60313488	0.40614872
N	-0.18926069	2.22214020	-0.82078236
C	3.85645993	-0.56095015	1.44008409
C	4.21367882	-0.88142936	0.11761811
C	5.55627221	-0.98045587	-0.25614267
H	5.84828857	-1.24665526	-1.26441445
C	1.92517727	-0.86182445	0.25233103
C	1.70126361	-0.24659494	2.70541167
H	2.40563394	-0.41081567	3.52771268
C	0.51444420	-1.18632345	2.92262946
H	0.04655457	-0.96044406	3.88755198
H	0.83804841	-2.23166493	2.92190096
H	-0.22789045	-1.06321695	2.12769859
C	1.29346105	1.23095854	2.69787033
H	2.17017968	1.87689746	2.57589528
H	0.80060269	1.49406056	3.64069441
H	0.60028959	1.42234455	1.87587810

C	2.86417980	-1.47700486	-1.97256743
H	1.78169698	-1.44737825	-2.13441304
C	3.33176134	-2.92585776	-2.14297166
H	2.76532790	-3.57944863	-1.47236925
H	4.39854447	-3.04001597	-1.92256457
H	3.15970490	-3.25441935	-3.17379949
C	3.53239660	-0.50434164	-2.95089373
H	3.26009915	-0.77853685	-3.97583157
H	4.62411850	-0.52016818	-2.88193422
H	3.19824690	0.52170749	-2.77114821
C	-0.77559826	1.12399839	-0.24940311
C	-0.89892801	3.38890275	-0.53054653
C	-1.99651396	2.98480780	0.25568242
C	-2.93411051	3.91278296	0.71555628
H	-3.78780162	3.60809239	1.30840708
C	-2.73848089	5.25286089	0.38130886
H	-3.45217168	5.99548774	0.72613707
C	-1.63731677	5.65753277	-0.39011333
H	-1.50898136	6.70912242	-0.62988983
C	-0.70311791	4.73304837	-0.85809008
H	0.14326419	5.05592902	-1.45226199
C	1.04157955	2.11490467	-1.61781910
H	1.23122178	1.03973460	-1.63891844
C	0.82472699	2.58974234	-3.05825228
H	-0.02093173	2.05921012	-3.50774150
H	1.72019282	2.37893872	-3.65332326
H	0.62722915	3.66414715	-3.12069808
C	2.22035942	2.79427391	-0.91302934
H	2.06591676	3.87205303	-0.79777771
H	3.13915724	2.64341320	-1.49024904
H	2.36551639	2.35790989	0.07975870
C	-2.79069743	0.71279776	1.14237709
H	-2.32449235	-0.26572477	1.04668203
C	-2.85154384	1.06358684	2.63182923
H	-3.33678780	2.02626079	2.82154030
H	-1.84381242	1.09773293	3.05917982
H	-3.42160026	0.28826975	3.15461638
C	-4.16128404	0.63436213	0.46674792
H	-4.76036573	-0.14107935	0.95438511
H	-4.04031847	0.35155831	-0.58298174
H	-4.70519706	1.58421643	0.51877916
C	-2.93973158	-2.78847818	1.15881097
C	-4.13648777	-3.21711065	1.72442508
C	-1.84730635	-1.96103901	-1.07411728
C	-2.89086834	-2.48180341	-0.21191156
C	-5.30011518	-3.35700183	0.93756840
C	-2.42634293	-1.88346342	-2.32262370
C	-4.07717173	-2.64453654	-0.98683963
C	-5.28365209	-3.07807201	-0.42641639
N	-3.76716154	-2.27280367	-2.27486250
H	-2.04231371	-2.68248262	1.76362197
H	-4.17906407	-3.45489858	2.78443825
H	-0.42422289	-2.52286615	-0.84339844
H	-6.22348820	-3.69373383	1.40194841
H	-1.99907318	-1.55806536	-3.26145323

H	-6.18014044	-3.18768246	-1.03247159
H	-4.38806308	-2.33803820	-3.06579976

5.7 Optimized geometry and the energies of the I_1

- SCF energy: -1722.13728803 Hartree
- Zero-point correction: 0.708891 (Hartree/Particle)
- Thermal correction to Energy: 0.749173 Hartree
- Thermal correction to Enthalpy: 0.750118 Hartree
- Thermal correction to Gibbs Free Energy: 0.636614 Hartree
- Sum of electronic and zero-point Energies: -1721.428397 Hartree
- Sum of electronic and thermal Energies: -1721.388115 Hartree
- Sum of electronic and thermal Enthalpies: -1721.387170 Hartree
- Sum of electronic and thermal Free Energies: -1721.500674 Hartree

Pd	-0.11084708	-1.00863775	-0.30613442
N	2.94396085	-1.05188368	-0.59147462
C	6.51036011	-0.78082694	0.54646380
H	7.54725700	-0.89797030	0.24542796
N	2.48947841	-0.45885627	1.45499651
C	6.21324090	-0.35964303	1.85239795
H	7.02287891	-0.14935296	2.54494033
C	4.89346153	-0.20878852	2.27828825
H	4.66965369	0.11682963	3.28862784
N	-1.78553686	1.53967188	0.52485906
N	-0.20081368	2.09292781	-0.86371440
C	3.88265107	-0.48963764	1.35789698
C	4.17664403	-0.89105166	0.04309485
C	5.49989123	-1.05275229	-0.37624494
H	5.74332679	-1.38351211	-1.37795997
C	1.90445680	-0.79335376	0.26523174
C	1.78794959	-0.06490777	2.69468711
H	2.53349701	-0.18559639	3.48710402
C	0.62264509	-1.00110100	3.01899991
H	0.19429969	-0.72275983	3.98828738
H	0.96265259	-2.03996662	3.06821426
H	-0.15623535	-0.94339988	2.25354273
C	1.38475621	1.41213005	2.63212785
H	2.25738821	2.04449134	2.43384230
H	0.94230053	1.72549933	3.58416982
H	0.65214634	1.57204054	1.83909874
C	2.73296836	-1.57487230	-1.95747413
H	1.64830421	-1.52117240	-2.08905448
C	3.13997751	-3.04884733	-2.03295114
H	2.55876276	-3.62693957	-1.30833363
H	4.20622211	-3.19091260	-1.82620307
H	2.93026411	-3.44002700	-3.03429266
C	3.40206903	-0.69938489	-3.02243576

H	3.07979978	-1.03424221	-4.01410539
H	4.49411545	-0.75503546	-2.99282078
H	3.11512929	0.34999734	-2.90688621
C	-0.74381382	1.02961998	-0.19636859
C	-0.88127222	3.27593851	-0.56951385
C	-1.91062618	2.91538680	0.32099133
C	-2.79937280	3.87291517	0.81748470
H	-3.60153091	3.60509757	1.49332435
C	-2.62404330	5.19449191	0.40916434
H	-3.30133164	5.95808830	0.78028162
C	-1.59023027	5.55491371	-0.47016759
H	-1.47658167	6.59357710	-0.76650946
C	-0.70502963	4.60209147	-0.97310430
H	0.09000847	4.89003122	-1.65002704
C	0.96278716	1.95015953	-1.75222566
H	1.15110843	0.87562615	-1.74927341
C	0.63106390	2.36505585	-3.18913556
H	-0.24912783	1.82015755	-3.54539046
H	1.47514058	2.12160455	-3.84363730
H	0.43250534	3.43669229	-3.28310563
C	2.19099807	2.65550898	-1.16736399
H	2.04020702	3.73586864	-1.07628090
H	3.06169301	2.48875205	-1.81044671
H	2.41727251	2.25420696	-0.17469829
C	-2.66000064	0.70688284	1.37843837
H	-2.24857754	-0.29620865	1.27720292
C	-2.56632805	1.12313584	2.84993679
H	-2.97626188	2.12145587	3.03211333
H	-1.52673436	1.11356533	3.19045319
H	-3.13338745	0.41065350	3.45828395
C	-4.09291276	0.67061577	0.84083232
H	-4.65988563	-0.09138649	1.38438345
H	-4.08645136	0.39221585	-0.21551755
H	-4.60484313	1.63222649	0.95560962
C	-2.91363202	-3.03117109	0.97767016
C	-4.04758420	-3.69530499	1.43522016
C	-1.98535478	-1.54524003	-0.96247252
C	-2.95367390	-2.35506892	-0.25385800
C	-5.23764901	-3.70253017	0.67636220
C	-2.64363148	-1.12672512	-2.09341941
C	-4.17187860	-2.37365639	-0.99853909
C	-5.31429941	-3.04488804	-0.54899838
N	-3.96277282	-1.60596189	-2.12172589
H	-1.98977577	-3.03083278	1.55206222
H	-4.02007372	-4.22343329	2.38545067
H	0.19182932	-2.57834692	-0.42785705
H	-6.10983458	-4.23161225	1.05279323
H	-2.30067717	-0.49004942	-2.89948138
H	-6.23385775	-3.04791651	-1.13053607
H	-4.60136622	-1.52651965	-2.89729313

5.8 Optimized geometry and the energies of the complex where I_1 interacts with 6a

- SCF energy: -2071.12902661 Hartree
- Zero-point correction: 0.872936 (Hartree/Particle)
- Thermal correction to Energy: 0.923044 Hartree
- Thermal correction to Enthalpy: 0.923988 Hartree
- Thermal correction to Gibbs Free Energy: 0.787929 Hartree
- Sum of electronic and zero-point Energies: -2070.256091 Hartree
- Sum of electronic and thermal Energies: -2070.205982 Hartree
- Sum of electronic and thermal Enthalpies: -2070.205038 Hartree
- Sum of electronic and thermal Free Energies: -2070.341098 Hartree

Pd	0.38580917	0.40870330	-0.41333137
N	-2.12141059	-1.32824321	-0.74646871
C	-5.02085722	-3.41905974	0.38931664
H	-5.94229992	-3.89983363	0.07442095
N	-1.52665324	-1.42815475	1.34771600
C	-4.61429240	-3.51547303	1.73004828
H	-5.21985549	-4.07708735	2.43518300
C	-3.44492619	-2.89688740	2.17467253
H	-3.13851426	-2.97101166	3.21268130
N	3.21274649	-0.60652780	0.60114142
N	2.33287140	-2.04919024	-0.77259688
C	-2.69720867	-2.18207410	1.23754749
C	-3.09096241	-2.10184478	-0.10955935
C	-4.26766833	-2.71318842	-0.54836922
H	-4.60377465	-2.62782945	-1.57353814
C	-1.16211152	-0.90523729	0.13544774
C	-0.77420892	-1.30603492	2.61413962
H	-1.47979696	-1.61853991	3.39008024
C	-0.37842685	0.14087861	2.91281728
H	0.13931403	0.18506309	3.87722182
H	-1.26240562	0.78357608	2.96350153
H	0.28084865	0.53606154	2.13408729
C	0.41331533	-2.27435437	2.62581668
H	0.07772446	-3.30038022	2.43809704
H	0.91345183	-2.24894081	3.60032756
H	1.13629280	-1.99792698	1.85643542
C	-2.14232465	-0.90881000	-2.16483857
H	-1.19701074	-0.37242374	-2.28822110
C	-3.27740925	0.08512642	-2.42128327
H	-3.11509693	0.98853561	-1.83090621
H	-4.25746991	-0.32536076	-2.15837817
H	-3.29053852	0.36033459	-3.48185147
C	-2.14941762	-2.11374428	-3.11241116
H	-1.98665347	-1.76264244	-4.13691017
H	-3.09706287	-2.65977197	-3.09694207
H	-1.35064493	-2.81834519	-2.86106896
C	2.10221042	-0.85022904	-0.15527466
C	3.57701587	-2.57189772	-0.41439235
C	4.14785678	-1.63448159	0.46762921
C	5.41435883	-1.84474102	1.01973188
H	5.86704012	-1.12495753	1.68989264
C	6.08606722	-3.01674174	0.67430855

H	7.07211679	-3.20446737	1.08903516
C	5.51210338	-3.95585498	-0.19778882
H	6.05872612	-4.86112067	-0.44530986
C	4.25117314	-3.74741151	-0.75560644
H	3.81722085	-4.47797669	-1.42730903
C	1.35001728	-2.67102318	-1.67341370
H	0.54690862	-1.93427302	-1.71848238
C	1.90976782	-2.84333158	-3.08891321
H	2.28757443	-1.88660482	-3.46382836
H	1.11198015	-3.18484914	-3.75744767
H	2.72211302	-3.57469362	-3.13451478
C	0.78631349	-3.95955781	-1.06495091
H	1.56063989	-4.71928426	-0.91930156
H	0.01928715	-4.38153819	-1.72298876
H	0.32619274	-3.74638915	-0.09511289
C	3.37367775	0.61270827	1.42008057
H	2.44415931	1.15700895	1.26333793
C	3.48955460	0.27482414	2.90987207
H	4.41098412	-0.26511307	3.14932426
H	2.64164442	-0.33608673	3.23468206
H	3.48467816	1.20497834	3.48788901
C	4.51279981	1.49079451	0.89609838
H	4.48681164	2.45605631	1.41100617
H	4.37449883	1.67799375	-0.17155680
H	5.49647783	1.03646508	1.05680808
C	1.45127852	3.68970049	0.89569377
C	1.94306731	4.91129796	1.34586374
C	1.58510229	1.95337623	-1.05637118
C	1.86902746	3.18375318	-0.34754594
C	2.85938345	5.65192555	0.56876226
C	2.34391598	2.03009367	-2.19924784
C	2.80757621	3.94780431	-1.10626375
C	3.30302656	5.17954980	-0.66406153
N	3.09396252	3.21607342	-2.23509657
H	0.74506129	3.11825897	1.49182923
H	1.61744292	5.30607218	2.30543505
H	-0.77177772	1.46684142	-0.69270076
H	3.22736560	6.60597101	0.93825040
H	2.43906394	1.32622077	-3.01665929
H	4.01680001	5.74710655	-1.25746474
H	3.64539695	3.54045046	-3.01369230
H	-7.42060012	1.78620847	-1.03972487
H	-5.58007064	3.42567437	-1.12830962
C	-6.50760061	1.60006877	-0.47932910
C	-5.46436301	2.52216918	-0.53697133
H	-2.72911552	3.47696263	2.18453127
C	-6.38882143	0.45014500	0.30600216
H	-7.20007995	-0.27153428	0.35317067
C	-4.26747526	2.31461391	0.17341637
C	-3.12730189	3.26220652	0.06316596
C	-2.18487793	3.36146376	1.23850574
C	-2.90095978	3.96308694	-1.05933417
H	-1.49200080	4.19830964	1.11886273
C	-5.21950137	0.24021187	1.03817557
C	-4.17428432	1.16210505	0.97435700

H	-3.51702921	3.85292047	-1.94728773
H	-2.05750783	4.64298375	-1.13421076
H	-5.11361317	-0.65186251	1.64770771
H	-3.26106694	0.96332895	1.52481413
H	-1.57332803	2.45385421	1.30222383

5.9 Optimized geometry and the energies of the TS2

- SCF energy: -2071.06435138 Hartree
- Zero-point correction: 0.875185 (Hartree/Particle)
- Thermal correction to Energy: 0.924378 Hartree
- Thermal correction to Enthalpy: 0.925322 Hartree
- Thermal correction to Gibbs Free Energy: 0.793381 Hartree
- Sum of electronic and zero-point Energies: -2070.189166 Hartree
- Sum of electronic and thermal Energies: -2070.139973 Hartree
- Sum of electronic and thermal Enthalpies: -2070.139029 Hartree
- Sum of electronic and thermal Free Energies: -2070.270971 Hartree

Pd	0.83743860	-0.29939858	0.40019838
N	-1.98033471	-0.44277394	1.26345463
C	-5.43664106	1.02011110	1.39627088
H	-6.30158196	1.18660526	2.03193699
N	-1.99205398	0.33972317	-0.78811704
C	-5.46721893	1.44244916	0.06113870
H	-6.35951491	1.92135806	-0.33125784
C	-4.36299788	1.26089240	-0.77670374
H	-4.39039009	1.58097753	-1.81161229
N	2.09458928	2.18622193	-0.72009184
N	0.51476612	2.84624877	0.64098160
C	-3.23623489	0.64319882	-0.23667138
C	-3.21774262	0.17783525	1.09039400
C	-4.31304429	0.38102121	1.93177943
H	-4.30604314	0.05860640	2.96442597
C	-1.19843947	-0.32224085	0.12067246
C	-1.67423410	0.73104248	-2.18034344
H	-2.53604897	0.38529097	-2.76329580
C	-0.43165929	0.04713570	-2.73499258
H	-0.39865394	0.20926290	-3.81833603
H	-0.45092233	-1.01858688	-2.53667963
H	0.47391729	0.45685131	-2.28962953
C	-1.54749030	2.25648927	-2.31832222
H	-2.43875704	2.78441943	-1.96920562
H	-1.39762727	2.51206564	-3.37327283
H	-0.68730177	2.62232078	-1.75234069
C	-1.51318451	-1.13424356	2.48607226
H	-0.68714987	-1.75062280	2.13135043
C	-2.58285862	-2.04554288	3.11188479
H	-3.22448330	-2.51148596	2.36205001
H	-3.22419257	-1.50814391	3.81718441
H	-2.08022061	-2.84044322	3.67234005

C	-0.96089936	-0.15855920	3.53178647
H	-0.70842955	-0.70656083	4.44703531
H	-1.70222071	0.60688974	3.79020666
H	-0.05303969	0.32522720	3.16477184
C	1.08481177	1.72400918	0.09209277
C	1.18100484	4.00172073	0.22382367
C	2.20167082	3.57395310	-0.64695790
C	3.08395380	4.48908166	-1.22729913
H	3.88551711	4.16813993	-1.88003464
C	2.90979687	5.83994519	-0.92579736
H	3.58302399	6.57144574	-1.36303525
C	1.88693383	6.26723180	-0.06584452
H	1.77604023	7.32545188	0.15168926
C	1.01069952	5.35549861	0.52393876
H	0.23356511	5.69552499	1.19647576
C	-0.55980758	2.79176049	1.64698779
H	-0.82953000	1.73978475	1.68176656
C	-0.02577687	3.20187317	3.02410501
H	0.84066033	2.59021660	3.29476879
H	-0.80298780	3.05665667	3.78169890
H	0.27739061	4.25329265	3.04590732
C	-1.80823437	3.57707004	1.23041244
H	-1.64357094	4.65828727	1.22091147
H	-2.61480240	3.36347361	1.93939958
H	-2.14879023	3.26827663	0.24104060
C	3.03158406	1.27179970	-1.40649164
H	2.57108411	0.28874570	-1.27384831
C	3.13033902	1.55545256	-2.90814455
H	3.67201054	2.47950789	-3.12988029
H	2.13706990	1.62435282	-3.36180324
H	3.67108805	0.73284101	-3.38833931
C	4.38449250	1.24303960	-0.69158855
H	5.02791675	0.48797556	-1.15462937
H	4.24002860	0.96426636	0.35671349
H	4.89145148	2.21315975	-0.73781419
C	3.65275269	-2.46412687	-0.90197601
C	4.76182787	-3.21640407	-1.27971079
C	2.05621134	-1.88316486	1.10258328
C	3.15857357	-2.55092043	0.41081236
C	5.40177235	-4.07200409	-0.36023844
C	2.12199045	-2.42002416	2.38232746
C	3.82606247	-3.43044314	1.31277646
C	4.94072681	-4.19147771	0.94903708
N	3.15990088	-3.33502952	2.51847021
H	3.14916981	-1.82245807	-1.62145889
H	5.13907029	-3.15111960	-2.29747455
H	-0.00948145	-3.54098787	1.05593613
H	6.26644120	-4.64986454	-0.67676705
H	1.50140992	-2.21194132	3.24673250
H	5.43350822	-4.85217717	1.65897694
H	3.40249961	-3.83989996	3.35750294
H	-5.51425035	-2.12078977	-0.60233814
H	-3.43831243	-2.88321171	0.40793859
C	-4.64323801	-2.27621662	-1.23389355
C	-3.45844890	-2.70655173	-0.65886566

H	0.20499166	-4.47624225	-2.06670782
C	-4.72056704	-2.01617377	-2.60862302
H	-5.64878219	-1.67292479	-3.05619855
C	-2.26272685	-2.87360986	-1.41723523
C	-1.00692104	-3.21455773	-0.81446288
C	0.22079937	-3.45360185	-1.64835172
C	-0.90834869	-3.88332957	0.52262415
H	1.11596265	-3.37196805	-1.02850481
C	-3.58459962	-2.23861220	-3.39563669
C	-2.39152973	-2.66256536	-2.82277813
H	-1.77948210	-3.74757539	1.16306511
H	-0.78227249	-4.97144245	0.38052778
H	-3.63184341	-2.08689546	-4.47191843
H	-1.54192941	-2.84552732	-3.47093154
H	0.33958724	-2.76824828	-2.49059353

5.10 Optimized geometry and the energies of the I_2

- SCF energy: -2071.12894135 Hartree
- Zero-point correction: 0.880020 (Hartree/Particle)
- Thermal correction to Energy: 0.928049 Hartree
- Thermal correction to Enthalpy: 0.928993 Hartree
- Thermal correction to Gibbs Free Energy: 0.802149 Hartree
- Sum of electronic and zero-point Energies: -2070.248921 Hartree
- Sum of electronic and thermal Energies: -2070.200893 Hartree
- Sum of electronic and thermal Enthalpies: -2070.199948 Hartree
- Sum of electronic and thermal Free Energies: -2070.326793 Hartree

Pd	-0.14553764	-0.79466055	-0.16228364
N	2.72958436	0.46161132	-0.57238685
C	5.40711075	3.00559846	0.10286266
H	6.29631728	3.48230764	-0.29902655
N	1.97350377	1.08834316	1.37345197
C	4.92636853	3.39080717	1.36457826
H	5.44868265	4.15956350	1.92625712
C	3.78011116	2.80907033	1.90471462
H	3.40170003	3.12132666	2.87185201
N	-2.39275138	1.44821190	0.59405830
N	-1.03798998	2.16739022	-0.94649037
C	3.13696847	1.82763999	1.14703452
C	3.62152112	1.42946667	-0.10575292
C	4.76418659	2.02360845	-0.65006621
H	5.14304635	1.74392543	-1.62418478
C	1.69563128	0.25854137	0.31504636
C	1.21279013	1.30956535	2.62451513
H	1.98803336	1.47516333	3.38233590
C	0.40712925	0.09651050	3.08127113
H	-0.12049544	0.35291977	4.00573090
H	1.06164311	-0.75153823	3.29291936
H	-0.31899512	-0.21688318	2.32718738
C	0.37769141	2.59341240	2.51989342

H	0.99715820	3.43913521	2.20467158
H	-0.05952738	2.83562352	3.49482171
H	-0.43159732	2.47593384	1.80043988
C	2.99375964	-0.39292104	-1.75320773
H	2.23783094	-1.17229403	-1.68654979
C	4.38245292	-1.03902642	-1.65508406
H	4.58115277	-1.39172008	-0.64258570
H	5.17994514	-0.35242970	-1.95449435
H	4.41809325	-1.90359880	-2.32301468
C	2.82427053	0.34960300	-3.08427629
H	3.14273973	-0.30926911	-3.89926377
H	3.43750745	1.25575116	-3.12858346
H	1.78524797	0.62351695	-3.27020251
C	-1.29243476	1.09076305	-0.14046442
C	-1.95004792	3.20060132	-0.72960175
C	-2.82595462	2.73534450	0.26434335
C	-3.87260939	3.53718124	0.73151666
H	-4.55778376	3.19135113	1.49396448
C	-4.01396273	4.80790187	0.17790244
H	-4.81889980	5.44967639	0.52377167
C	-3.13718493	5.27153063	-0.81648757
H	-3.27198498	6.26723682	-1.22860551
C	-2.09405143	4.47573785	-1.28523713
H	-1.42329466	4.84270343	-2.05164432
C	0.02206491	2.17300396	-1.96206477
H	0.48654839	1.19595261	-1.83984648
C	-0.57200429	2.24440378	-3.37357238
H	-1.28510466	1.42730267	-3.52260692
H	0.22642413	2.14990848	-4.11726683
H	-1.09102277	3.18927604	-3.55921015
C	1.07184786	3.25155920	-1.67856711
H	0.67716867	4.26251431	-1.81623802
H	1.92049519	3.12628542	-2.35742090
H	1.44328953	3.16565445	-0.65407843
C	-3.10482711	0.54578772	1.52066764
H	-2.52404364	-0.37295586	1.49040213
C	-3.10925121	1.07547551	2.95926920
H	-3.72476088	1.97260853	3.07352680
H	-2.09937004	1.31215655	3.29915036
H	-3.52161269	0.30306517	3.61721183
C	-4.51557208	0.24084406	1.00372962
H	-4.93072585	-0.60112599	1.56416634
H	-4.47926319	-0.04909591	-0.04810995
H	-5.18722671	1.09815400	1.11230192
C	-3.17276730	-2.82184823	1.14954383
C	-4.34739790	-3.47689382	1.50164130
C	-1.93827128	-1.60750802	-0.83221262
C	-2.99471230	-2.34957167	-0.16577561
C	-5.37444553	-3.68387269	0.55568357
C	-2.41037568	-1.41774980	-2.11149005
C	-4.05592058	-2.57127167	-1.09749148
C	-5.23987762	-3.23379341	-0.75355942
N	-3.67862780	-1.98318670	-2.28146226
H	-2.38571342	-2.67453373	1.88413982
H	-4.47664678	-3.84320306	2.51709719

H	1.18522646	-2.82792520	-2.46688368
H	-6.28192821	-4.20322011	0.85283644
H	-1.94098881	-0.92124451	-2.95143007
H	-6.03197118	-3.38512455	-1.48364122
H	-4.18511834	-2.04692169	-3.15040849
H	5.12285577	-4.63819017	-0.59063757
H	2.88459798	-4.23707644	-1.48317876
C	4.42744120	-4.02463303	-0.02164412
C	3.14567016	-3.78970496	-0.53090255
H	0.42437867	-4.80549167	0.64418309
C	4.82105841	-3.47084414	1.19483756
H	5.81975348	-3.64411956	1.58733137
C	2.20254241	-3.00365831	0.15905405
C	0.75569990	-2.86376318	-0.30073067
C	-0.03843080	-3.80342690	0.63620867
C	0.56814310	-3.37301938	-1.73902566
H	-1.06870391	-3.91850914	0.30341537
C	3.90097856	-2.69007055	1.90380664
C	2.62269017	-2.47727073	1.39546176
H	0.82543387	-4.44253419	-1.83171867
H	-0.47234671	-3.26410400	-2.04564255
H	4.17948304	-2.25219418	2.86023707
H	1.91283070	-1.88922254	1.96105266
H	-0.04793290	-3.44535416	1.67211423

6. Optimized structures related to Complex (COD)PdClSnCl$_3$ (In gas phase)

6.1 Optimized geometry and the energies of the complex (COD)PdClSnCl$_3$

- SCF energy: -2283.19949334 Hartree
- Zero-point correction: 0.189137 (Hartree/Particle)
- Thermal correction to Energy: 0.207587 Hartree
- Thermal correction to Enthalpy: 0.208531 Hartree
- Thermal correction to Gibbs Free Energy: 0.138672 Hartree
- Sum of electronic and zero-point Energies: -2283.010357 Hartree
- Sum of electronic and thermal Energies: -2282.991907 Hartree
- Sum of electronic and thermal Enthalpies: -2282.990963 Hartree
- Sum of electronic and thermal Free Energies: -2283.060821 Hartree

Sn	-1.62225110	0.13297648	0.01591200
Pd	0.85965400	-0.40891672	-0.06078010
Cl	-1.78384836	2.49900716	0.27789416
Cl	-2.86110068	-0.27032253	-1.92435635
Cl	-2.86302493	-0.67488198	1.82223226
Cl	-0.08907781	-2.54781557	-0.22159090
C	1.64236680	1.61003181	-0.66277528
H	0.76491749	2.12215604	-1.05630247
C	1.73955740	1.54298426	0.72009632
H	0.91017254	1.97881138	1.27392559

C	3.25569006	-0.95159146	-0.68411763
H	3.06241797	-1.77970432	-1.36436770
C	2.71964752	1.34308534	-1.69272883
H	3.19365445	2.30095181	-1.95657929
H	2.21860322	0.99807684	-2.60502836
C	3.06279023	-1.18520150	0.64471165
H	2.76824932	-2.19445021	0.92806544
C	3.81051008	0.31585301	-1.30146234
H	4.53941283	0.77228182	-0.62755348
H	4.36092873	0.04919405	-2.21005750
C	3.00361866	1.26273305	1.52372853
H	3.85553616	1.72893458	1.02114237
H	2.90863378	1.76923993	2.48951875
C	3.29289481	-0.23454493	1.80176164
H	4.32491206	-0.34047276	2.16729159
H	2.64845973	-0.56555214	2.62389941

6.2 Optimized geometry and the energies of the active Pd(0) catalyst generated from complex (COD)PdClSnCl$_3$

- SCF energy: -438.797582398 Hartree
- Zero-point correction: 0.180700 (Hartree/Particle)
- Thermal correction to Energy: 0.190062 Hartree
- Thermal correction to Enthalpy: 0.191006 Hartree
- Thermal correction to Gibbs Free Energy: 0.145485 Hartree
- Sum of electronic and zero-point Energies: -438.616883 Hartree
- Sum of electronic and thermal Energies: -438.607521 Hartree
- Sum of electronic and thermal Enthalpies: -438.606576 Hartree
- Sum of electronic and thermal Free Energies: -438.652098 Hartree

Pd	-1.21493448	-0.00165317	0.00069585
C	0.34711524	1.34040561	1.05492434
H	-0.27037103	2.06821488	1.58355957
C	0.52686206	0.11575240	1.65419241
H	0.01183207	-0.06504209	2.59644752
C	0.52379191	-0.11481323	-1.65440197
H	0.00718427	0.06320137	-2.59632902
C	1.12177216	1.91042644	-0.12080489
H	2.02220968	2.43011239	0.24579073
H	0.49427401	2.68692760	-0.57528814
C	0.35066647	-1.34041661	-1.05509984
H	-0.26465913	-2.07070662	-1.58279817
C	1.55812377	0.91921746	-1.24199515
H	2.47852051	0.40869087	-0.94195730
H	1.82651940	1.51910223	-2.11976871
C	1.56438743	-0.91385168	1.23943537
H	2.48178137	-0.39970232	0.93643159
H	1.83785119	-1.51246555	2.11652717
C	1.12864616	-1.90714019	0.11990372

H	2.02975006	-2.42495342	-0.24776269
H	0.50390252	-2.68481466	0.57621443

6.3 Optimized geometry and the energies of the $SnCl_4$ complex

- SCF energy: -1844.31082920 Hartree
- Zero-point correction: 0.004685 (Hartree/Particle)
- Thermal correction to Energy: 0.012406 Hartree
- Thermal correction to Enthalpy: 0.013350 Hartree
- Thermal correction to Gibbs Free Energy: -0.029478 Hartree
- Sum of electronic and zero-point Energies: -1844.306144 Hartree
- Sum of electronic and thermal Energies: -1844.298423 Hartree
- Sum of electronic and thermal Enthalpies: -1844.297479 Hartree
- Sum of electronic and thermal Free Energies: -1844.340307 Hartree

Sn	0.00000000	0.00000000	0.00000000
Cl	-0.00000000	1.88351818	1.33183341
Cl	-0.00000000	-1.88351818	1.33183341
Cl	1.88351818	-0.00000000	-1.33183341
Cl	-1.88351818	0.00000000	-1.33183341

6.4 Optimized geometry and the energies of the complex where active Pd(0) catalyst interacts with 5a

- SCF energy: -802.658979826 Hartree
- Zero-point correction: 0.312748 (Hartree/Particle)
- Thermal correction to Energy: 0.329785 Hartree
- Thermal correction to Enthalpy: 0.330730 Hartree
- Thermal correction to Gibbs Free Energy: 0.266751 Hartree
- Sum of electronic and zero-point Energies: -802.346232 Hartree
- Sum of electronic and thermal Energies: -802.329194 Hartree
- Sum of electronic and thermal Enthalpies: -802.328250 Hartree
- Sum of electronic and thermal Free Energies: -802.392229 Hartree

Pd	-0.73764954	-1.10243218	-0.34662808
C	-2.86042001	-0.51673235	-0.10883835
H	-3.32309761	-1.46548776	-0.39282830
C	-2.30933037	-0.47380993	1.16449240
H	-2.38534340	-1.39602687	1.73967493
C	-1.25570088	2.17654381	-0.74524157
H	-0.83180444	2.46001265	-1.70884240
C	-3.28239919	0.62506868	-1.01875221
H	-4.38428156	0.66159934	-1.01731553
H	-3.00220434	0.36127238	-2.04874453

C	-0.38971079	1.92887620	0.24672913
H	0.66737429	2.05621199	0.01959159
C	-2.75903588	2.04708293	-0.71199194
H	-3.16052969	2.38626993	0.24621473
H	-3.18816741	2.71910620	-1.46630364
C	-1.96722368	0.75639022	1.99974078
H	-2.80219280	1.46398399	1.97058305
H	-1.89618868	0.43667817	3.04694192
C	-0.64655349	1.48788480	1.66856585
H	-0.56302003	2.36188944	2.33547104
H	0.18479816	0.82764772	1.94774458
H	3.64889114	2.47375291	-1.72461324
C	3.31469175	1.67057073	-1.07385283
H	4.16686750	2.57548038	0.69408292
C	3.61059324	1.72864690	0.30192040
C	2.59226977	0.60587939	-1.60706914
C	3.20591176	0.71664171	1.17045263
H	2.34697283	0.57563976	-2.66525015
C	2.16044741	-0.41673213	-0.75320199
H	3.43735363	0.75919724	2.23143477
C	2.49774604	-0.35706407	0.62524444
C	1.35079892	-1.61011093	-0.94279112
N	1.99325046	-1.49446904	1.23638150
C	1.24779636	-2.22744449	0.31511285
H	1.16568801	-2.10161173	-1.89328132
H	1.89719145	-1.59734956	2.23547508
H	0.94153292	-3.23525143	0.55706947

2.5 Optimized geometry and the energies of the TS1

- SCF energy: -802.616878042 Hartree
- Zero-point correction: 0.308020 (Hartree/Particle)
- Thermal correction to Energy: 0.324801 Hartree
- Thermal correction to Enthalpy: 0.325745 Hartree
- Thermal correction to Gibbs Free Energy: 0.262464 Hartree
- Sum of electronic and zero-point Energies: -802.308858 Hartree
- Sum of electronic and thermal Energies: -802.292077 Hartree
- Sum of electronic and thermal Enthalpies: -802.291133 Hartree
- Sum of electronic and thermal Free Energies: -802.354414 Hartree

Pd	-0.72108570	-0.59861397	-0.53548978
C	-2.66850534	0.46064883	-1.38378163
H	-2.46381981	0.29850295	-2.44136940
C	-3.17291564	-0.59692349	-0.67896432
H	-3.29509259	-1.53428877	-1.21891522
C	-1.29933079	1.28385306	1.23779793
H	-0.29526573	1.69976561	1.30499253
C	-2.53171467	1.90377457	-0.94135460
H	-3.40731526	2.47396999	-1.29005774
H	-1.67020153	2.32464817	-1.47461788

C	-1.50410499	0.07165503	1.80661080
H	-0.65763815	-0.37697132	2.32461439
C	-2.34290482	2.16105584	0.57695692
H	-3.29966851	2.06118473	1.09563062
H	-2.04519504	3.20928357	0.69849778
C	-3.78716253	-0.55013960	0.71123382
H	-4.34693772	0.38087519	0.83422425
H	-4.52898440	-1.35389547	0.78564193
C	-2.78752475	-0.72772309	1.88347471
H	-3.30844654	-0.50872356	2.82860144
H	-2.50516403	-1.78640427	1.93669620
H	3.34804318	3.26183885	-0.29011059
C	3.36209392	2.18438105	-0.14764207
H	5.42003966	2.17247802	0.51993012
C	4.54314296	1.56485821	0.31244360
C	2.22255815	1.43613295	-0.42154082
C	4.60644264	0.18784937	0.50362752
H	1.31247319	1.91070593	-0.78066155
C	2.25144643	0.04344544	-0.23821125
H	5.51688878	-0.28944989	0.85823946
C	3.45726093	-0.55874517	0.22314427
C	1.26744925	-1.00707850	-0.39757620
N	3.22252553	-1.91446264	0.31976343
C	1.91627347	-2.17819215	-0.07124332
H	0.19112624	-1.27820674	-1.65421452
H	3.90193746	-2.60563246	0.59574141
H	1.55045911	-3.19531345	-0.08852933

6.6 Optimized geometry and the energies of the I_1

- SCF energy: -802.623268265 Hartree
- Zero-point correction: 0.309662 (Hartree/Particle)
- Thermal correction to Energy: 0.326647 Hartree
- Thermal correction to Enthalpy: 0.327592 Hartree
- Thermal correction to Gibbs Free Energy: 0.264454 Hartree
- Sum of electronic and zero-point Energies: -802.313606 Hartree
- Sum of electronic and thermal Energies: -802.296621 Hartree
- Sum of electronic and thermal Enthalpies: -802.295677 Hartree
- Sum of electronic and thermal Free Energies: -802.358815 Hartree

Pd	-0.77863573	-0.58247783	-0.59978144
C	-2.76036292	0.48713735	-1.30213904
H	-2.65765685	0.32106681	-2.37357790
C	-3.20907185	-0.56442025	-0.55161993
H	-3.39213440	-1.49994265	-1.07662714
C	-1.10663433	1.25613487	1.15245643
H	-0.09540117	1.65688233	1.14643006
C	-2.55310800	1.92629524	-0.87430816
H	-3.45021359	2.51302784	-1.12684524
H	-1.74547751	2.33304537	-1.49529006

C	-1.27952805	0.04061902	1.73542369
H	-0.39712322	-0.42012866	2.17599381
C	-2.19427174	2.16706944	0.61473488
H	-3.08990489	2.08784287	1.23610598
H	-1.85470544	3.20492125	0.70933748
C	-3.68116417	-0.51251296	0.89305951
H	-4.20036894	0.43169684	1.07676319
H	-4.43156951	-1.29821596	1.03732116
C	-2.56814846	-0.72542214	1.95022620
H	-2.97283547	-0.49323190	2.94752057
H	-2.31068386	-1.79116257	1.97206212
H	3.41941297	3.23224877	-0.27623678
C	3.39817924	2.15439160	-0.13680384
H	5.48167997	2.05930779	0.43962608
C	4.57379888	1.48733672	0.26666021
C	2.22109503	1.45092097	-0.36770325
C	4.59345760	0.10626601	0.43685321
H	1.32405973	1.96488488	-0.70542415
C	2.19818239	0.05597523	-0.18996943
H	5.50231032	-0.40967611	0.73795969
C	3.40595963	-0.59534222	0.20295580
C	1.17543955	-0.95819599	-0.33009653
N	3.13189149	-1.94266421	0.28001746
C	1.79690631	-2.15328177	-0.05761857
H	-0.49885278	-1.41813757	-1.88698136
H	3.80011744	-2.66112049	0.50956654
H	1.39897548	-3.15850582	-0.07054722

6.7 Optimized geometry and the energies of the complex where I_1 interacts with 6a

- SCF energy: -1151.61300268 Hartree
- Zero-point correction: 0.474371 (Hartree/Particle)
- Thermal correction to Energy: 0.500891 Hartree
- Thermal correction to Enthalpy: 0.501835 Hartree
- Thermal correction to Gibbs Free Energy: 0.416254 Hartree
- Sum of electronic and zero-point Energies: -1151.138631 Hartree
- Sum of electronic and thermal Energies: -1151.112112 Hartree
- Sum of electronic and thermal Enthalpies: -1151.111167 Hartree
- Sum of electronic and thermal Free Energies: -1151.196749 Hartree

Pd	-0.34092766	-0.63438159	-0.67696723
C	0.50486910	-2.85876617	-0.97902561
H	0.39906537	-2.88275953	-2.06296748
C	1.59859182	-2.21586038	-0.47521345
H	2.26016067	-1.72356719	-1.18492693
C	-0.97255565	-1.85753080	1.51659293
H	-2.00061831	-1.50542730	1.55899831
C	-0.51387158	-3.70108322	-0.23587755
H	-0.22211776	-4.76135226	-0.29680083
H	-1.46039946	-3.61958291	-0.78420877

C	0.00288472	-0.96060015	1.81207855
H	-0.31446447	0.04312222	2.09102386
C	-0.77563918	-3.33833295	1.24986774
H	0.03210160	-3.72353650	1.87763120
H	-1.68072211	-3.87104322	1.56423269
C	2.09358366	-2.26781942	0.95949767
H	1.93123636	-3.27041463	1.36530973
H	3.17935242	-2.11843018	0.94856383
C	1.49378225	-1.19700134	1.90483508
H	1.75646189	-1.45251966	2.94327558
H	1.98652434	-0.24585589	1.69862258
H	-5.87945140	-1.18209036	0.36544040
C	-5.25195367	-0.30948504	0.20284258
H	-6.87285849	1.08046632	0.55410352
C	-5.81965749	0.97778359	0.30606923
C	-3.90800282	-0.47463369	-0.11284269
C	-5.05569581	2.11913576	0.08344605
H	-3.48082901	-1.46891939	-0.21845201
C	-3.09900429	0.65622387	-0.32667603
H	-5.49529136	3.11164365	0.15056782
C	-3.70474578	1.94551093	-0.23651917
C	-1.70184531	0.84437619	-0.65739498
N	-2.72731248	2.87198843	-0.52207573
C	-1.53589097	2.20248063	-0.79484896
H	-0.27239889	-0.17673623	-2.16620982
H	-2.86582723	3.86874803	-0.57394959
H	-0.65932666	2.77180090	-1.07049853
H	5.96419892	1.59528535	-1.25232451
C	5.45218305	0.65521787	-1.49252925
C	1.53083486	2.37850320	1.08285412
C	2.06168761	1.86306053	-0.09713240
H	1.44142430	1.84182430	-0.98496138
H	5.76134332	0.34171378	-2.49358402
H	0.50171963	2.72491493	1.09191707
C	2.30922836	2.43164932	2.24261168
C	3.37999955	1.36941604	-0.15579836
C	3.94813766	0.80794098	-1.41236775
C	3.62100360	1.95690551	2.20490077
C	4.14830572	1.43422178	1.02202553
H	1.89701354	2.83658311	3.16284408
C	3.17981453	0.43470223	-2.45064776
H	5.81881017	-0.09823672	-0.78281192
H	4.23911616	1.98854925	3.09841734
H	3.62834774	0.04871698	-3.36219865
H	5.16953397	1.06801927	1.02597859
H	2.09549084	0.48062640	-2.43249721

6.8 Optimized geometry and the energies of the TS2

- SCF energy: -1151.55348967 Hartree
- Zero-point correction: 0.473981 (Hartree/Particle)
- Thermal correction to Energy: 0.500778 Hartree

- Thermal correction to Enthalpy: 0.501722 Hartree
- Thermal correction to Gibbs Free Energy: 0.413834 Hartree
- Sum of electronic and zero-point Energies: -1151.079508 Hartree
- Sum of electronic and thermal Energies: -1151.052712 Hartree
- Sum of electronic and thermal Enthalpies: -1151.051768 Hartree
- Sum of electronic and thermal Free Energies: -1151.139655 Hartree

Pd	-2.07386466	-0.69161568	0.16953110
C	-3.65522184	-0.91151517	-1.47712309
H	-3.16547711	-1.67998237	-2.07690799
C	-4.26237581	-1.33113605	-0.31526750
H	-4.18130641	-2.39226871	-0.08275301
C	-3.39329871	1.87968879	-0.14477107
H	-2.52547699	2.52401903	-0.27197127
C	-3.80081952	0.41129774	-2.20424636
H	-4.51258490	0.28125806	-3.03587973
H	-2.83267276	0.63319432	-2.67290069
C	-3.57544694	1.33442459	1.07753383
H	-2.87590667	1.63319075	1.85640396
C	-4.23519103	1.64799843	-1.37500873
H	-5.29208084	1.56532369	-1.10908346
H	-4.15903718	2.52444482	-2.03045145
C	-5.28277097	-0.56054187	0.51356290
H	-5.97689637	-0.03725596	-0.15064920
H	-5.89412035	-1.28577363	1.06371127
C	-4.69238919	0.42752649	1.55030805
H	-5.51216476	1.03724405	1.96293378
H	-4.30006932	-0.15544038	2.39221591
H	1.57915641	3.50442745	-1.14995373
C	1.62892722	2.70407420	-0.41577044
H	3.61330486	3.26477778	0.24938241
C	2.78647167	2.57307479	0.38644485
C	0.56467069	1.82204325	-0.27656476
C	2.89176810	1.57034555	1.34450698
H	-0.31834115	1.90502400	-0.90542472
C	0.63180085	0.79087293	0.67934916
H	3.79496266	1.45687120	1.93778811
C	1.81298328	0.69048513	1.47845584
C	-0.26814559	-0.28612196	1.03055786
N	1.64778349	-0.40456708	2.29607534
C	0.38931481	-0.96504707	2.04126220
H	0.81913807	-1.04029504	-2.48220536
H	2.29342198	-0.69445482	3.01441700
H	0.06244018	-1.80996988	2.63431119
H	2.64092588	-3.28153995	-0.36645790
C	1.92089155	-2.48501897	-0.59165461
C	5.69216874	0.75090654	-1.04015460
C	4.46338518	0.27162184	-1.47014853
H	3.98320019	0.74338685	-2.31913928
H	1.11666137	-2.89584143	-1.21022610
H	6.15351859	1.58487465	-1.56234550
C	6.33133961	0.17987252	0.06590037

C	3.82186488	-0.82304311	-0.81643365
C	2.55488699	-1.30337373	-1.24082076
C	5.71908725	-0.89026345	0.73744003
C	4.49945976	-1.38527752	0.30944998
H	7.28996764	0.56248252	0.40440047
C	1.83251899	-0.64663943	-2.38153464
H	1.44397473	-2.18880126	0.35866993
H	6.20592640	-1.33517294	1.60168266
H	2.36562747	-0.81530544	-3.33211395
H	4.03598536	-2.19556503	0.86056381
H	1.75593305	0.43591139	-2.24061525

6.9 Optimized geometry and the energies of the I_2

- SCF energy: -1151.63211281 Hartree
- Zero-point correction: 0.478692 (Hartree/Particle)
- Thermal correction to Energy: 0.504322 Hartree
- Thermal correction to Enthalpy: 0.505266 Hartree
- Thermal correction to Gibbs Free Energy: 0.423210 Hartree
- Sum of electronic and zero-point Energies: -1151.153421 Hartree
- Sum of electronic and thermal Energies: -1151.127791 Hartree
- Sum of electronic and thermal Enthalpies: -1151.126847 Hartree
- Sum of electronic and thermal Free Energies: -1151.208903 Hartree

Pd	-0.79998509	0.31128454	0.11600672
C	-3.01961665	0.49153953	1.17688076
H	-2.67502361	0.80587078	2.15969287
C	-3.09591610	1.44920645	0.21122894
H	-2.77166273	2.44987111	0.48527527
C	-2.29174193	-1.45512046	-1.06396506
H	-1.57117255	-2.26705550	-0.99619491
C	-3.51165037	-0.94045363	1.13596728
H	-4.51034624	-0.98890580	1.59772202
H	-2.85227238	-1.52718116	1.78760113
C	-2.00121725	-0.44684167	-1.92816228
H	-1.09076037	-0.55703649	-2.51438251
C	-3.56030893	-1.62269560	-0.25225210
H	-4.42417796	-1.26594719	-0.81867541
H	-3.72873370	-2.69346686	-0.08977400
C	-3.75208441	1.31801767	-1.15250246
H	-4.64912032	0.69875870	-1.07346180
H	-4.10140046	2.30981347	-1.46225102
C	-2.82658216	0.77525657	-2.26924227
H	-3.43052650	0.57397307	-3.16758029
H	-2.12450999	1.56927213	-2.55277171
H	0.43315223	-4.97180745	1.69769686
C	0.93532373	-4.27883586	1.02731638
H	2.46682572	-5.70960296	0.48939038
C	2.09408695	-4.69945161	0.34109313
C	0.43478571	-2.99195731	0.86132763

C	2.77161467	-3.84100482	-0.52049070
H	-0.45175869	-2.66274421	1.39951737
C	1.09048161	-2.09816346	-0.00454601
H	3.66587650	-4.16583950	-1.04748046
C	2.26396479	-2.54797702	-0.68371399
C	0.85246297	-0.72710031	-0.39675631
N	2.70807124	-1.49734895	-1.45583979
C	1.86197429	-0.40589932	-1.26988851
H	0.00247029	0.18897550	3.09735858
H	3.55208177	-1.49348564	-2.00645327
H	2.08095517	0.53443321	-1.75606872
H	0.18427681	3.25288492	2.64978880
C	-0.43665281	2.63675090	1.98026732
C	3.92864159	2.37192100	0.10661709
C	2.90399346	1.82447778	0.88286610
H	3.16853830	1.17275346	1.70755287
H	-1.27757622	2.26668790	2.57607861
H	4.96340848	2.14536139	0.35302975
C	3.63397415	3.19566994	-0.97930126
C	1.55257513	2.07999566	0.59819027
C	0.42099607	1.48987709	1.41025851
C	2.29473046	3.47199234	-1.27423686
C	1.27766534	2.92727344	-0.49402626
H	4.43077503	3.61768540	-1.58617171
C	0.87244117	0.59328594	2.56721718
H	-0.82877664	3.30617250	1.20908061
H	2.04245063	4.11163711	-2.11692014
H	1.46270811	1.16517148	3.30356089
H	0.24233007	3.13140879	-0.75633836
H	1.47113560	-0.25388367	2.22486831

7.1 Optimized geometry and the energies of Indole (5a) in gas phase

- SCF energy: -363.825875251 Hartree
- Zero-point correction: 0.129887 (Hartree/Particle)
- Thermal correction to Energy: 0.136225 Hartree
- Thermal correction to Enthalpy: 0.137169 Hartree
- Thermal correction to Gibbs Free Energy: 0.099540 Hartree
- Sum of electronic and zero-point Energies: -363.695988 Hartree
- Sum of electronic and thermal Energies: -363.689650 Hartree
- Sum of electronic and thermal Enthalpies: -363.688706 Hartree
- Sum of electronic and thermal Free Energies: -363.726335 Hartree

C	-0.42695024	-1.68064771	0.00000000
C	-1.78637260	-1.39574704	0.00000000
C	0.49434260	-0.61888973	0.00000000
C	-2.25237074	-0.06397026	0.00000000
C	0.00000000	0.71634325	0.00000000

C	-1.36786669	1.00848573	0.00000000
C	1.92855012	-0.53306238	0.00000000
C	2.25309806	0.79775021	0.00000000
N	1.09564759	1.55590244	0.00000000
H	-0.07633621	-2.70956467	0.00000000
H	-2.50651153	-2.20952347	0.00000000
H	-3.32198975	0.12739639	0.00000000
H	-1.72576439	2.03494917	0.00000000
H	2.62728006	-1.35827252	0.00000000
H	3.22116795	1.27929235	0.00000000
H	1.05803763	2.56283321	0.00000000

7.2 Optimized geometry and the energies of Styrene (6a) in gas phase

- SCF energy: -348.976888923 Hartree
- Zero-point correction: 0.162313 (Hartree/Particle)
- Thermal correction to Energy: 0.170313 Hartree
- Thermal correction to Enthalpy: 0.171258 Hartree
- Thermal correction to Gibbs Free Energy: 0.129502 Hartree
- Sum of electronic and zero-point Energies: -348.814576 Hartree
- Sum of electronic and thermal Energies: -348.806576 Hartree
- Sum of electronic and thermal Enthalpies: -348.805631 Hartree
- Sum of electronic and thermal Free Energies: -348.847387 Hartree

C	0.46686898	-1.16142805	0.21476677
C	1.86064406	-1.22291712	0.21562249
C	-0.20747491	0.05561798	0.01338790
C	2.61649173	-0.07012800	0.00173412
C	0.57157896	1.20459059	-0.21780547
C	1.96295789	1.14485021	-0.21873489
C	-1.69385206	0.12296130	0.02950543
C	-2.45395114	-1.11785458	-0.38524701
C	-2.34927190	1.23066594	0.40913925
H	-0.09891685	-2.07146331	0.38815414
H	2.35539446	-2.17611583	0.38350042
H	3.70207797	-0.11823788	-0.00381469
H	0.07750542	2.14898190	-0.42579297
H	2.53916051	2.04743510	-0.40556840
H	-2.08759521	-1.50804615	-1.34250270
H	-3.52398720	-0.91136089	-0.47975628
H	-2.33910152	-1.92334315	0.35181101
H	-1.83371436	2.11793326	0.76430169
H	-3.43477281	1.27606730	0.39545615

7.3 Optimized geometry and the energies of substituted indole (7a) in gas phase

- SCF energy: -712.838357601
- Zero-point correction: 0.296712 (Hartree/Particle)
- Thermal correction to Energy: 0.311599
- Thermal correction to Enthalpy: 0.312543
- Thermal correction to Gibbs Free Energy: 0.255028
- Sum of electronic and zero-point Energies: -712.541646
- Sum of electronic and thermal Energies: -712.526759
- Sum of electronic and thermal Enthalpies: -712.525815
- Sum of electronic and thermal Free Energies: -712.583329

C	2.72695709	1.21813085	-0.23609630
C	4.10358087	1.03068848	-0.25059626
C	0.43986097	-0.07118281	0.06972374
C	1.87620796	0.11735181	-0.01529617
C	4.66998894	-0.24354044	-0.04643338
C	0.24892371	-1.40559883	0.33649520
C	2.48021108	-1.15552716	0.19855385
C	3.86444866	-1.35222530	0.18197544
N	1.46318035	-2.05970939	0.41215045
H	2.32090868	2.21210953	-0.39136535
H	4.75692025	1.88196407	-0.42160692
H	-0.54142945	1.14480549	-2.23194861
H	5.75006973	-0.36031936	-0.06480626
H	-0.67377464	-1.94761246	0.47975356
H	4.29236930	-2.33803671	0.34594992
H	1.58363380	-3.04590889	0.57928026
H	-4.94780363	0.15870615	1.75752249
H	-2.73836603	1.21191838	1.82640880
C	-4.24099882	-0.03574111	0.95471139
C	-2.97826750	0.56453140	0.99075888
H	-1.20402100	2.79344684	1.10052230
C	-4.59321130	-0.87629689	-0.09873006
H	-5.57450152	-1.34249009	-0.12754730
C	-2.03887678	0.34306646	-0.02372449
C	-0.64406723	0.99751847	-0.03353862
C	-0.46320579	1.98633044	1.14176374
C	-0.50058541	1.79874537	-1.35666812
H	0.53104143	2.43903007	1.10025688
C	-3.66715907	-1.11330794	-1.11783723
C	-2.41179402	-0.51064687	-1.07769420
H	-1.31024191	2.53246223	-1.43945606
H	0.45085419	2.33559672	-1.39304436
H	-3.92297089	-1.76847756	-1.94686636
H	-1.69861017	-0.72031517	-1.86928651
H	-0.54842091	1.47731093	2.10697584

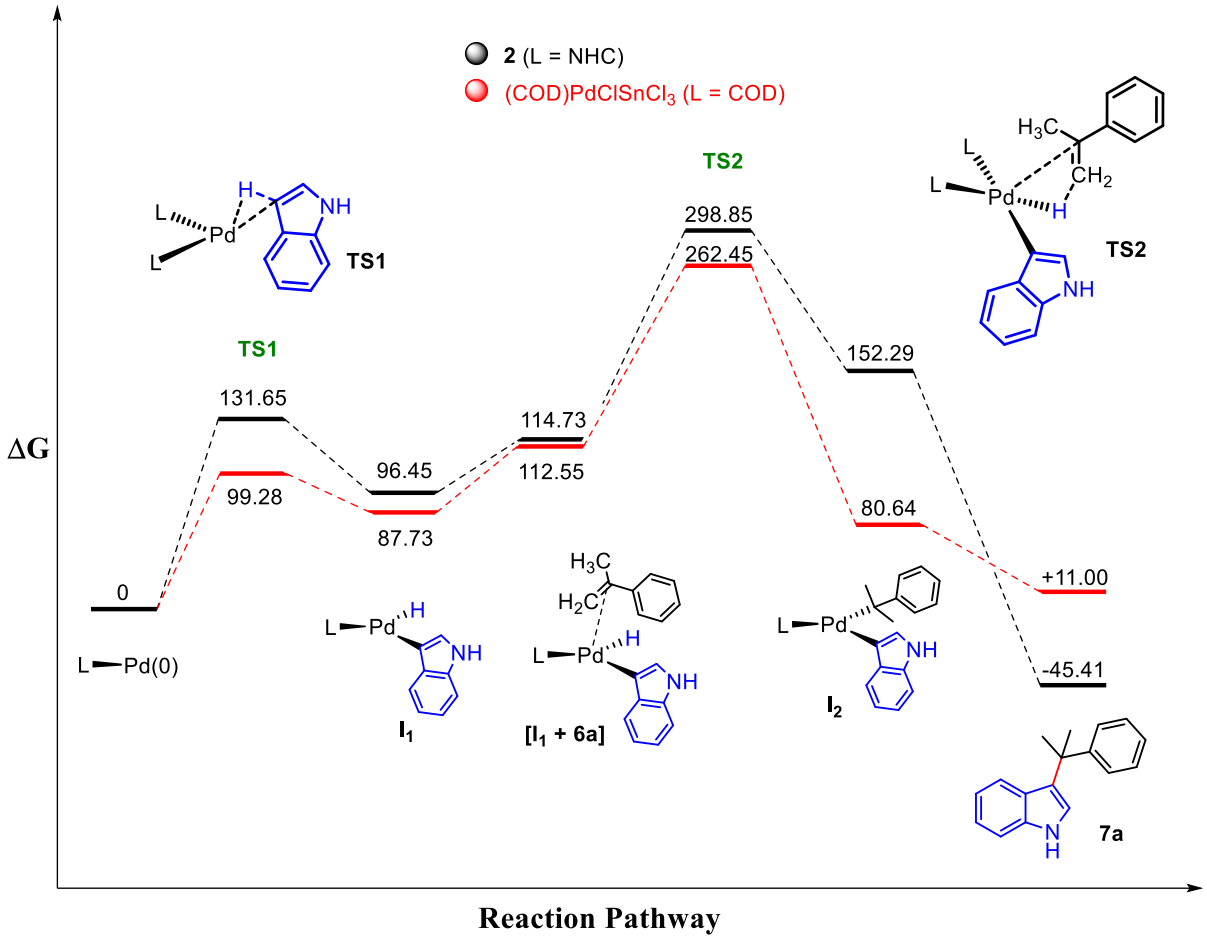


Figure S7. Gibbs free energy (ΔG) profile for the C3-H functionalization of indole with α-methyl styrene using two different catalysts [Black lines for complex **2**, and red lines for (COD)PdClSnCl$_3$] in gas phase. ΔG values are reported relative to the total Gibbs free energy of the active catalyst, **5a** and **6a**.

NMR Data of Catalysts and Products

bis(1,3-diisopropyl-1,3-dihydro-2H-benzo[d]imidazol-2-ylidene)(trichlorostannyl)palladium(II) bromide (2)[10]**:** Yield: 82% (335 mg), 1H NMR (400 MHz, CD_3NO_2): δ 7.88 (dd, J = 6.2, 3.2 Hz, 4H), 7.48 – 7.35 (m, 4H), 5.66 (m, J = 6.8 Hz, 4H), 1.92 (d, J = 6.9 Hz, 12H), 1.84 (d, J = 7.0 Hz, 12H). ^{13}C NMR (100 MHz, CD_3NO_2): δ 133.75, 123.07, 113.26, 55.04, 20.06, 19.61.

Di-μ-bromobis(1,3-diisopropylbenzimidazolin-2-ylidene)bis(trichlorostannyl)dipalladium(II) (4): Yield 75 %, ^{1}H NMR (400 MHz, $CDCl_3$)

δ 7.69 – 7.61 (m, 2H), 7.40 – 7.31 (m, 2H), 5.96 – 5.74 (m, 2H), 1.88 (dd, *J* = 25.1, 6.7 Hz, 12H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 133.74, 123.88, 113.22, 55.52, 21.64, 21.10.

3-(2-Phenylpropan-2-yl)-1H-indole (7a): Yield 82%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (s, 1H), 7.43 – 7.34 (m, 3H), 7.34 – 7.25 (m, 2H), 7.21 (ddd, *J* = 7.3, 4.2, 1.2 Hz, 1H), 7.17 (dd, *J* = 5.9, 5.0 Hz, 1H), 7.14 (d, *J* = 2.4 Hz, 1H), 7.10 (d, *J* = 8.0 Hz, 1H), 6.97 – 6.87 (m, 1H), 1.82 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.94, 137.13, 128.07, 126.44, 126.10, 126.03, 125.61, 121.66, 121.35, 120.64, 118.93, 111.12, 38.96, 30.69.

HRMS (ESI-ORBITRAP): m/z $[M + H]^+$ calculated for $C_{17}H_{17}N$ 236.1439, found 236.1430

5-Nitro-3-(2-phenylpropan-2-yl)-1H-indole (7b): Yield 96%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (s, 1H), 8.07 – 7.99 (m, 2H), 7.42 – 7.28 (m, 6H), 7.22 (t, *J* = 7.1 Hz, 1H), 1.82 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.74, 141.22, 140.08, 128.93, 128.31, 126.18, 126.13, 125.38, 123.44, 118.41, 117.56, 110.99, 38.89, 30.59.

HRMS (ESI-ORBITRAP): m/z $[M + Na]^+$ calculated for $C_{17}H_{16}N_2O_2$ 303.1109, found 303.1093

2-Methyl-3-(2-phenylpropan-2-yl)-1H-indole (7c): Yield 43%, Inseparable reaction mixture (**5c** + **3c;** spectra attached)

HRMS (ESI-ORBITRAP): m/z $[M]^+$ calculated for $C_{18}H_{19}N$ 249.1517, found 249.1509

5-Bromo-1-isopropyl-3-(2-phenylpropan-2-yl)-1H-indole (7d): Yield 92%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (dd, *J* = 5.3, 3.4 Hz, 2H), 7.36 – 7.30 (m, 2H), 7.27 – 7.23 (m, 3H), 7.23 (d, *J* = 1.2 Hz, 1H), 7.20 (s, 1H), 4.67 (hept, *J* = 6.7 Hz, 1H), 1.82 (s, 6H), 1.60 (d, *J* = 6.7 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.64, 135.37, 128.18, 128.16, 126.34, 125.76, 124.39, 123.80, 123.79, 121.31, 111.63, 110.86, 47.18, 39.00, 30.84, 22.81.

HRMS (ESI-ORBITRAP): m/z $[M + H]^+$ calculated for $C_{20}H_{22}BrN$ 358.0993, found 358.0974

3-(2-(3-Methoxyphenyl)propan-2-yl)-1H-indole (7e): Yield: 94%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (s, 1H), 7.40 – 7.33 (m, 1H), 7.22 (dd, *J* = 11.6, 4.7 Hz, 1H), 7.20 – 7.10 (m, 3H), 7.05 – 6.91 (m, 3H), 6.81 – 6.73 (m, 1H), 3.79 (s, 3H), 1.82 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.38, 151.85, 137.15, 128.94, 126.05, 125.95, 121.63, 121.33, 120.57, 119.22, 118.92, 113.11, 111.08, 110.12, 55.14, 39.00, 30.60.

HRMS (ESI-ORBITRAP): m/z $[M + Na]^+$ calculated for $C_{18}H_{19}NO$ 288.1364, found 288.1349

4-(2-(1H-indol-3-yl)propan-2-yl)aniline (7f): Yield: 95%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (s, 1H), 7.33 (d, *J* = 8.1 Hz, 1H), 7.20 – 7.10 (m, 4H), 7.08 (d, *J* = 2.4 Hz, 1H), 6.97 – 6.89 (m, 1H), 6.69 – 6.55 (m, 2H), 1.76 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.78, 140.40, 137.14, 127.29, 126.48, 126.12, 121.52, 120.56, 118.79, 115.07, 111.07, 38.23, 30.83.

HRMS (ESI-ORBITRAP): m/z $[M + H]^+$ calculated for $C_{17}H_{18}N_2$ 251.1548, found 251.1536

3,3'-(Phenylmethylene)bis(1H-indole) (9a)[15]**:** White Solid; Yield: 92%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (s, 2H), 7.44 (d, *J* = 7.9 Hz, 2H), 7.38 (d, *J* = 7.1 Hz, 2H), 7.36 – 7.29 (m, 4H), 7.26 (dd, *J* = 4.2, 2.9 Hz, 1H), 7.24 – 7.18 (m, 2H), 7.10 – 7.00 (m, 2H), 6.58 (d, *J* = 1.5 Hz, 2H), 5.92 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.08, 136.69, 128.79, 128.30, 127.10, 126.22, 123.72, 121.96, 119.98, 119.65, 119.27, 111.15, 40.22.

3,3'-(p-Tolylmethylene)bis(1H-indole) (9b)[16]**:** White Solid; Yield: 77%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (s, 2H), 7.43 (d, *J* = 7.9 Hz, 2H), 7.34 (d, *J* = 8.1 Hz, 2H), 7.26 (d, *J* = 7.8 Hz, 2H), 7.19 (t, *J* = 7.6 Hz, 2H), 7.11 (d, *J* = 7.9 Hz, 2H), 7.04 (t, *J* = 7.5 Hz, 2H), 6.61 (d, *J* = 1.6 Hz, 2H), 5.87 (s, 1H), 2.36 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.03, 136.70, 135.54, 128.97, 128.61, 127.12, 123.62, 121.90, 120.00, 119.88, 119.22, 111.08, 39.79, 21.14.

3,3'-((4-Isopropylphenyl)methylene)bis(1H-indole) (9c)[17]**:** White Solid; Yield: 76% ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (s, 2H), 7.42 (d, *J* = 7.9 Hz, 2H), 7.35 (d, *J* = 8.1 Hz, 2H), 7.29 – 7.24 (m, 2H), 7.23 – 7.09 (m, 4H), 7.01 (dd, *J* = 11.1, 3.9 Hz, 2H), 6.67 (d, *J* = 1.5 Hz, 2H), 5.87 (s, 1H), 2.89 (dt, *J* = 13.8, 6.9 Hz, 1H), 1.24 (d, *J* = 6.9 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.50, 141.27, 136.68, 128.55, 127.15, 126.25, 123.61, 121.87, 120.02, 119.96, 119.16, 111.06, 39.75, 33.69, 24.11.

3,3'-((4-Methoxyphenyl)methylene)bis(1H-indole) (9d)[15]**:** White Solid; Yield: 80% ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (s, 2H), 7.42 (d, *J* = 7.9 Hz, 2H), 7.33 (d, *J* = 8.1 Hz, 2H), 7.27 (d, *J* = 8.5 Hz, 2H), 7.19 (t, *J* = 7.5 Hz, 2H), 7.03 (t, *J* = 7.5 Hz, 2H), 6.84 (d, *J* = 8.6 Hz, 2H), 6.60 (s, 2H), 5.86 (s, 1H), 3.80 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.90, 136.71, 136.29, 129.65, 127.08, 123.60, 121.91, 120.01, 119.21, 113.61, 111.10, 55.25, 39.35.

3,3'-((4-Nitrophenyl)methylene)bis(1H-indole) (9e)[15]**:** Yellow solid; Yield: 98%, ^{1}H NMR (400 MHz, DMSO) δ 10.93 (s, 2H), 8.14 (d, *J* = 8.7 Hz, 2H), 7.60 (d, *J* = 8.7 Hz, 2H), 7.35 (d, *J* = 8.1 Hz, 2H), 7.27 (d, *J* = 7.9 Hz, 2H), 7.04 (t, *J* = 7.5 Hz, 2H), 6.87 (dd, *J* = 10.2, 4.6 Hz, 4H), 6.01 (s, 1H). ^{13}C NMR (100 MHz, DMSO) δ 153.61, 146.21, 137.04, 129.92, 126.81, 124.32, 123.91, 121.57, 119.38, 118.88, 117.12, 112.05.

3,3'-((4-Fluorophenyl)methylene)bis(1H-indole) (9f)[18]**:** White solid; Yield: 93% ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (s, 2H), 7.38 (dd, *J* = 16.0, 8.0 Hz, 4H), 7.33 – 7.27 (m, 2H), 7.24 – 7.17 (m, 2H), 7.07 – 7.01 (m, 2H), 6.97 (dd, *J* = 12.1, 5.3 Hz, 2H), 6.60 (d, *J* = 1.5 Hz, 2H), 5.89 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.64, 160.22, 139.73, 139.70, 136.71, 130.14, 130.06, 126.94, 123.62, 122.07, 119.89, 119.54, 119.34, 115.11, 114.90, 111.17, 39.47.

3,3'-((4-Chlorophenyl)methylene)bis(1H-indole) (9g)[15]: Yield: 96%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (s, 2H), 7.37 (d, *J* = 8.6 Hz, 4H), 7.30 – 7.23 (m, 4H), 7.19 (t, *J* = 7.6 Hz, 2H),

7.03 (t, *J* = 7.6 Hz, 2H), 6.65 (d, *J* = 1.7 Hz, 2H), 5.87 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.56, 136.70, 131.81, 130.09, 128.38, 126.89, 123.60, 122.10, 119.84, 119.38, 119.23, 111.11, 39.63.

4-(Di(1H-indol-3-yl)methyl)benzonitrile (9h)[15]**:** White solid; Yield: 94%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (s, 2H), 7.57 (d, *J* = 8.2 Hz, 2H), 7.45 (d, *J* = 8.2 Hz, 2H), 7.39 (d, *J* = 8.2 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 7.21 (t, *J* = 7.5 Hz, 2H), 7.04 (t, *J* = 7.5 Hz, 2H), 6.66 (d, *J* = 1.9 Hz, 2H), 5.95 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.73, 136.68, 132.21, 129.53, 126.69, 123.68, 122.32, 119.61, 119.57, 119.22, 118.24, 111.26, 110.02, 77.37, 77.05, 76.73, 40.36.

3,3'-((4-Bromophenyl)methylene)bis(1H-indole) (9i)[15]**:** White solid; Yield: 90%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (s, 2H), 7.46 – 7.30 (m, 6H), 7.21 (t, *J* = 8.1 Hz, 4H), 7.05 (t, *J* = 7.5 Hz, 2H), 6.59 (d, *J* = 1.5 Hz, 2H), 5.86 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.12, 136.69, 131.37, 130.54, 126.89, 123.68, 122.14, 119.97, 119.85, 119.41, 119.08, 111.20, 39.70.

3,3'-(Anthracen-9-ylmethylene)bis(1H-indole) (9j)[19]**:** Yield: 80%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (d, *J* = 9.1 Hz, 2H), 8.46 (s, 1H), 8.02 (d, *J* = 7.3 Hz, 2H), 7.88 (s, 2H), 7.47 – 7.29 (m, 6H), 7.12 (t, *J* = 7.8 Hz, 4H), 6.88 (t, *J* = 7.5 Hz, 2H), 6.78 (d, *J* = 1.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.56, 135.15, 131.95, 129.17, 127.33, 127.29, 124.69, 123.98, 121.86, 120.01, 119.20, 118.89, 111.01, 35.05.

1,4-Bis(di(1H-indol-3-yl)methyl)benzene (9k)[15]: White solid, Yield: 76%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, *J* = 7.9 Hz, 4H), 7.24 – 7.07 (m, 16H), 7.03 (t, *J* = 7.4 Hz, 4H), 6.05 (s, 4H), 5.72 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.51, 136.57, 128.54, 127.00, 123.74, 121.72, 119.93, 119.45, 118.92, 111.23, 39.90.

3,3'-((2-Nitrophenyl)methylene)bis(1H-indole) (9l)[15]**:** Yellow solid: Yield: 95%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (s, 2H), 7.88 – 7.82 (m, 1H), 7.44 – 7.32 (m, 7H), 7.22 – 7.16 (m, 2H), 7.07 – 7.00 (m, 2H), 6.68 (s, 1H), 6.62 (d, *J* = 1.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.80, 138.01, 136.67, 132.39, 131.09, 127.24, 126.75, 124.41, 123.86, 122.24, 119.74, 119.55, 117.66, 111.19, 34.79.

3,3'-((2-Fluorophenyl)methylene)bis(1H-indole) (9m)[20]**:** White solid; Yield: 96%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (s, 2H), 7.43 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 8.1 Hz, 2H), 7.25 – 7.16 (m, 4H), 7.14 – 7.07 (m, 1H), 7.07 – 6.98 (m, 3H), 6.68 (d, *J* = 1.6 Hz, 2H), 6.25 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.96, 159.51, 136.72, 130.95, 130.81, 130.42, 130.37, 127.88, 127.80, 126.93, 123.90, 123.86, 123.62, 122.03, 119.82, 119.33, 118.30, 115.38, 115.16, 111.11, 32.53, 32.49.

2-(Di(1H-indol-3-yl)methyl)phenol (9n)[15]**:** Yield: 66%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (s, 2H), 7.46 – 7.35 (m, 4H), 7.24 – 7.14 (m, 4H), 7.09 – 6.99 (m, 2H), 6.91 – 6.83 (m, 2H), 6.77 (dd, *J* = 2.3, 0.8 Hz, 2H), 6.01 (s, 1H), 5.41 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.53, 136.91, 129.97, 129.06, 128.04, 126.85, 123.64, 122.38, 120.80, 119.92, 119.60, 117.19, 116.63, 111.23, 35.90.

3,3'-((3-Methoxyphenyl)methylene)bis(1H-indole) (9o)[20]**:** White Solid; Yield: 82%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (s, 2H), 7.44 (d, *J* = 7.9 Hz, 2H), 7.32 (d, *J* = 8.1 Hz, 2H), 7.21 (ddd, *J* = 13.4, 10.5, 4.4 Hz, 3H), 7.07 – 7.01 (m, 2H), 6.97 (dd, *J* = 11.0, 4.9 Hz, 2H), 6.80 (dd, *J* = 8.2, 2.0 Hz, 1H), 6.58 (d, *J* = 1.6 Hz, 2H), 5.88 (s, 1H), 3.76 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.56, 145.83, 136.67, 129.21, 127.08, 123.67, 121.93, 121.38, 119.92, 119.46, 119.24, 114.85, 111.22, 111.12, 55.16, 40.22.

3,3'-(Naphthalen-1-ylmethylene)bis(1H-indole) (9p)[18]: Yield: 80%, ^{1}H NMR (400 MHz, DMSO) δ 10.79 (s, 2H), 8.25 (d, *J* = 8.1 Hz, 1H), 7.91 (d, *J* = 7.7 Hz, 1H), 7.76 (d, *J* = 8.2 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.34 (d, *J* = 8.3 Hz, 3H), 7.25 (d, *J* = 7.6 Hz, 3H), 7.02 (t, *J* = 7.6 Hz, 2H), 6.83 (t, *J* = 7.5 Hz, 2H), 6.72 (s, 2H), 6.62 (s, 1H). ^{13}C NMR (100 MHz, DMSO) δ 140.76, 137.12, 134.07, 131.79, 129.03, 127.08, 127.03, 126.29, 125.99, 125.81, 125.76, 124.72, 124.45, 121.35, 119.43, 118.73, 118.14, 111.99, 35.81.

3,3'-((5-Methylfuran-2-yl)methylene)bis(1H-indole) (9q)[21]**:** Yield: 80%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (s, 2H), 7.52 (d, *J* = 7.9 Hz, 2H), 7.35 (d, *J* = 8.1 Hz, 2H), 7.18 (t, *J* = 7.4 Hz, 2H), 7.05 (t, *J* = 7.5 Hz, 2H), 6.86 (d, *J* = 2.0 Hz, 2H), 5.89 (t, *J* = 4.9 Hz, 3H), 2.26 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.75, 34.11, 105.98, 107.32, 111.07, 117.47, 119.27, 119.80, 121.89, 123.07, 126.86, 136.55, 150.68, 155.13.

3,3'-(Thiophen-2-ylmethylene)bis(1H-indole) (9r)[15]**:** Yield: 77% ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (s, 2H), 7.48 (d, *J* = 7.9 Hz, 2H), 7.36 (d, *J* = 8.1 Hz, 2H), 7.18 (dd, *J* = 14.3, 6.4 Hz, 3H), 7.05 (t, *J* = 7.5 Hz, 2H), 6.96 – 6.88 (m, 2H), 6.83 (d, *J* = 1.5 Hz, 2H), 6.17 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.64, 136.58, 126.76, 126.45, 125.16, 123.64, 123.20, 122.05, 119.79, 119.71, 119.39, 111.14, 35.32.

3,3'-((3-Methylthiophen-2-yl)methylene)bis(1H-indole) (9s): Yield: 85%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (s, 2H), 7.46 (d, *J* = 7.9 Hz, 2H), 7.35 (d, *J* = 8.1 Hz, 2H), 7.20 (t, *J* = 7.6 Hz, 2H), 7.06 (dd, *J* = 9.7, 6.1 Hz, 3H), 6.88 (d, *J* = 5.1 Hz, 1H), 6.71 (d, *J* = 1.9 Hz, 2H), 6.13 (s, 1H), 2.25 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.55, 136.60, 132.59, 129.96, 126.87, 123.40, 122.01, 121.97, 119.70, 119.35, 119.24, 111.19, 33.27, 13.97.

3,3'-((5-Methylthiophen-2-yl)methylene)bis(1H-indole) (9t): Yield: 80% ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (s, 2H), 7.51 (d, *J* = 7.9 Hz, 2H), 7.34 (d, *J* = 8.2 Hz, 2H), 7.19 (dd, *J* =

11.2, 3.9 Hz, 2H), 7.06 (dd, *J* = 11.1, 3.9 Hz, 2H), 6.82 (d, *J* = 1.8 Hz, 2H), 6.69 (d, *J* = 3.3 Hz, 1H), 6.58 (dd, *J* = 3.3, 0.9 Hz, 1H), 6.09 (s, 1H), 2.43 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.11, 137.95, 136.57, 126.81, 124.84, 124.44, 123.19, 122.00, 119.85, 119.72, 119.34, 111.16, 35.46, 15.50.

4-(Bis(2-methyl-1H-indol-3-yl)methyl)benzonitrile (10a)[16]**:** Yield: 94%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (s, 2H), 7.52 (d, *J* = 8.3 Hz, 2H), 7.37 (d, *J* = 8.1 Hz, 2H), 7.25 (d, *J* = 8.1 Hz, 2H), 7.13 – 7.04 (m, 2H), 6.96 – 6.85 (m, 4H), 6.02 (s, 1H), 2.05 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.85, 135.08, 132.21, 132.03, 129.85, 128.46, 120.95, 119.38, 119.03, 111.90, 110.33, 109.66, 39.48, 12.39.

4-(Bis(5-methoxy-1H-indol-3-yl)methyl)benzonitrile (10b)[18]: Yield: 96%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (s, 2H), 7.56 (d, *J* = 8.3 Hz, 2H), 7.44 (d, *J* = 8.2 Hz, 2H), 7.30 – 7.23 (m, 2H), 6.87 (dd, *J* = 8.8, 2.4 Hz, 2H), 6.75 (d, *J* = 2.3 Hz, 2H), 6.63 (d, *J* = 2.0 Hz, 2H), 5.83 (s, 1H), 3.71 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.86, 149.74, 132.17, 131.86, 129.52, 127.13, 124.56, 119.25, 117.70, 112.11, 111.99, 109.90, 101.68, 55.91, 40.40.

4-(Bis(5-bromo-1H-indol-3-yl)methyl)benzonitrile (10c)[20]: Yield: 95%, ^{1}H NMR (400 MHz, DMSO) δ 11.16 (s, 2H), 7.75 (d, *J* = 8.2 Hz, 2H), 7.52 (d, *J* = 8.2 Hz, 2H), 7.45 (d, *J* = 1.5 Hz, 2H), 7.33 (d, *J* = 8.6 Hz, 2H), 7.16 (dd, *J* = 8.6, 1.8 Hz, 2H), 6.94 (d, *J* = 2.1 Hz, 2H), 6.01 (s, 1H). ^{13}C NMR (100 MHz, DMSO) δ 150.76, 135.67, 132.79, 129.67, 128.65, 125.93, 124.12, 121.47, 119.48, 116.95, 114.16, 111.56, 109.37, 40.66, 40.61, 40.45, 40.40, 40.24, 40.19, 39.99, 39.78, 39.57, 39.36.

4-(Bis(1-methyl-1H-indol-3-yl)methyl)benzonitrile (10d)[13]: White solid; Yield: 99%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.2 Hz, 2H), 7.48 (d, *J* = 8.2 Hz, 2H), 7.35 (dd, *J* = 8.0, 4.9 Hz, 4H), 7.26 (t, *J* = 7.6 Hz, 2H), 7.05 (t, *J* = 7.4 Hz, 2H), 6.56 (s, 2H), 5.96 (s, 1H), 3.73 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.22, 137.48, 132.19, 129.51, 128.33, 127.14, 121.83, 119.72, 119.27, 119.03, 116.79, 109.94, 109.35, 40.29, 32.78.

4-(Bis(5-nitro-1H-indol-3-yl)methyl)benzonitrile (10e): Yield: 88%, ^{1}H NMR (400 MHz, DMSO) δ 11.74 (s, 2H), 8.35 (d, *J* = 2.2 Hz, 2H), 7.97 (dd, *J* = 9.0, 2.3 Hz, 2H), 7.79 (d, *J* = 8.3 Hz, 2H), 7.56 (dd, *J* = 17.1, 8.6 Hz, 4H), 7.19 (d, *J* = 2.1 Hz, 2H), 6.39 (s, 1H). ^{13}C NMR (100 MHz, DMSO) δ 150.15, 140.81, 140.20, 133.01, 129.69, 128.36, 126.10, 119.85, 119.38, 117.25, 116.51, 112.69, 109.71, 38.65.

4-(Bis(1-benzyl-1H-indol-3-yl)methyl)benzonitrile (10f): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.2 Hz, 2H), 7.53 (d, *J* = 8.2 Hz, 2H), 7.41 (d, *J* = 7.9 Hz, 2H), 7.36 – 7.24 (m, 8H), 7.21 (t, *J* = 7.4 Hz, 2H), 7.07 (dd, *J* = 14.5, 6.9 Hz, 6H), 6.71 (s, 2H), 6.04 (s, 1H), 5.27 (s, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.89, 137.65, 137.16, 132.29, 129.56, 128.79,

127.92, 127.61, 127.47, 126.57, 122.12, 119.92, 119.36, 119.25, 117.40, 110.08, 110.00, 50.06, 40.51.

[3,3':3',3''-Terindolin]-2'-one (11)[15]: Yield: 95 %, ^{1}H NMR (400 MHz, DMSO) δ 10.94 (s, 2H), 10.58 (s, 1H), 7.33 (d, *J* = 8.1 Hz, 2H), 7.21 (t, *J* = 7.2 Hz, 4H), 6.99 (dd, *J* = 15.1, 7.7 Hz, 3H), 6.91 (t, *J* = 7.5 Hz, 1H), 6.83 (d, *J* = 2.5 Hz, 2H), 6.78 (t, *J* = 7.6 Hz, 2H). ^{13}C NMR (100 MHz, DMSO) δ 179.20, 141.78, 137.38, 135.06, 128.30, 126.16, 125.37, 124.74, 121.91, 121.38, 121.23, 118.67, 114.75, 112.06, 110.02, 53.01.

4-(1H-Indol-3-yl)butan-2-one (12a)[22]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (s, 1H), 7.63 (d, *J* = 7.9 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.28 – 7.20 (m, 1H), 7.20 – 7.14 (m, 1H), 7.04 – 6.91 (m, 1H), 3.09 (t, *J* = 7.5 Hz, 2H), 2.87 (t, *J* = 7.5 Hz, 2H), 2.17 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 209.25, 136.37, 127.20, 122.04, 121.65, 119.29, 118.69, 115.00, 111.32, 44.13, 30.13, 19.41.

3-(1H-Indol-3-yl)-1-phenyl-3-(p-tolyl)propan-1-one (12b)[23]**:** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (dd, *J* = 12.4, 5.2 Hz, 3H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.46 (dd, *J* = 15.5, 7.7 Hz, 3H), 7.32 (d, *J* = 8.1 Hz, 1H), 7.29 – 7.22 (m, 2H), 7.21 – 7.12 (m, 1H), 7.12 – 7.01 (m, 3H), 6.97 (d, *J* = 1.9 Hz, 1H), 5.06 (t, *J* = 7.2 Hz, 1H), 3.78 (ddd, *J* = 24.4, 16.7, 7.2 Hz, 2H), 2.30 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.75, 141.24, 137.19, 136.66, 135.75, 133.01, 129.17, 128.60, 128.15, 127.70, 126.68, 122.13, 121.42, 119.59, 119.50, 119.39, 111.15, 45.34, 37.86, 21.04.

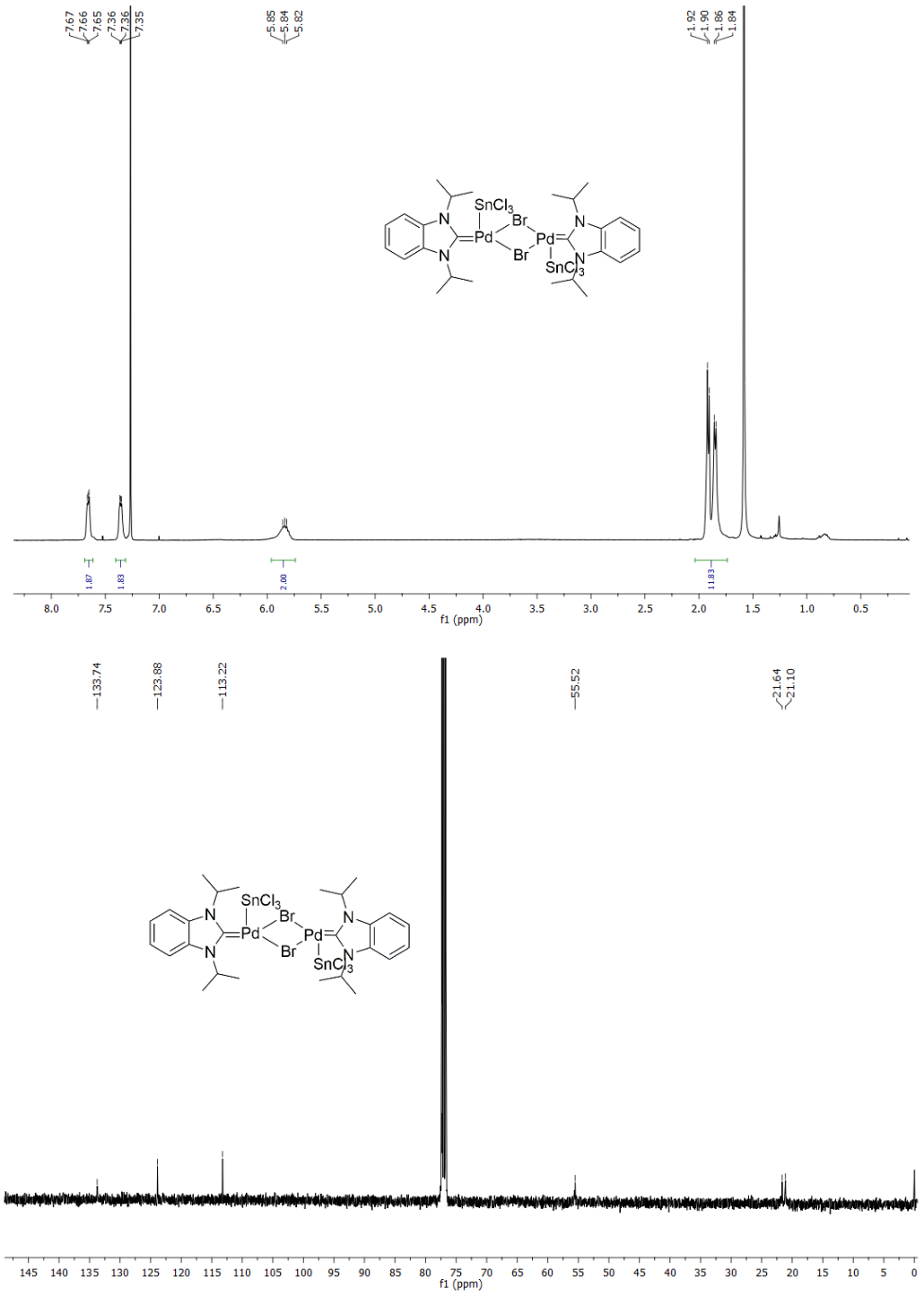


Figure S8. ^{1}H and ^{13}C Spectra of **4**

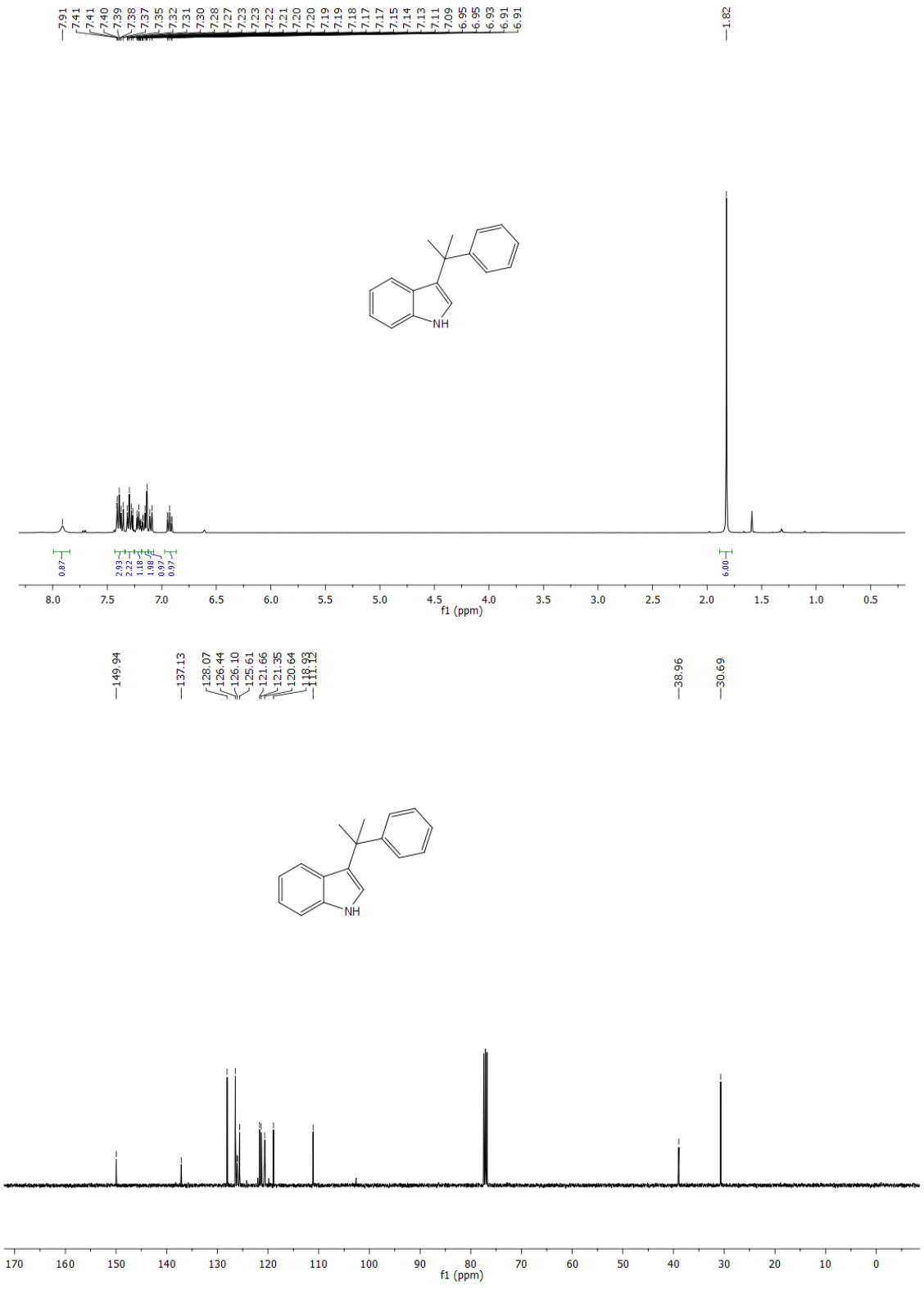


Figure S9. ^{1}H and ^{13}C Spectra of **5a**

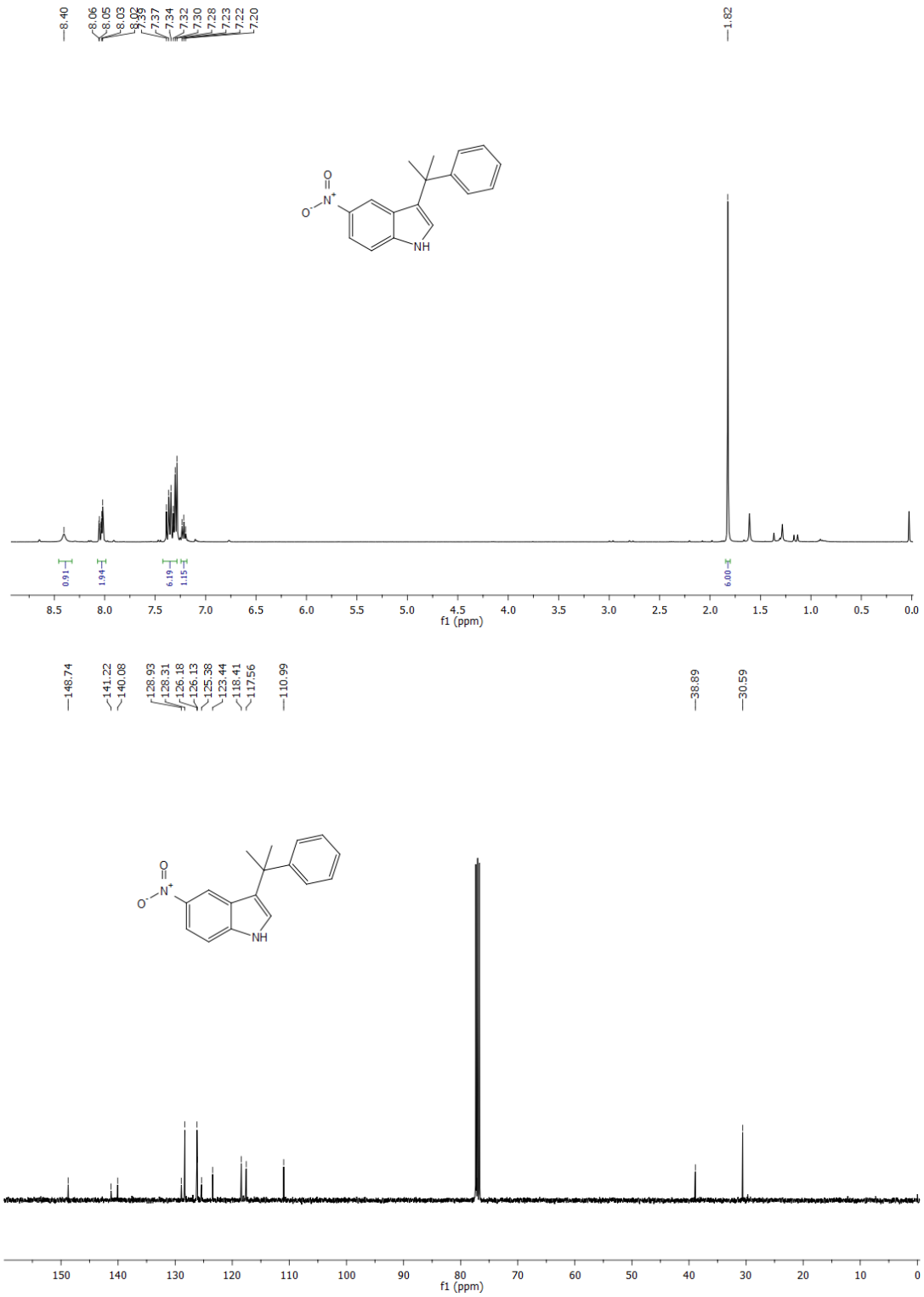


Figure S10. ^{1}H and ^{13}C Spectra of **5b**

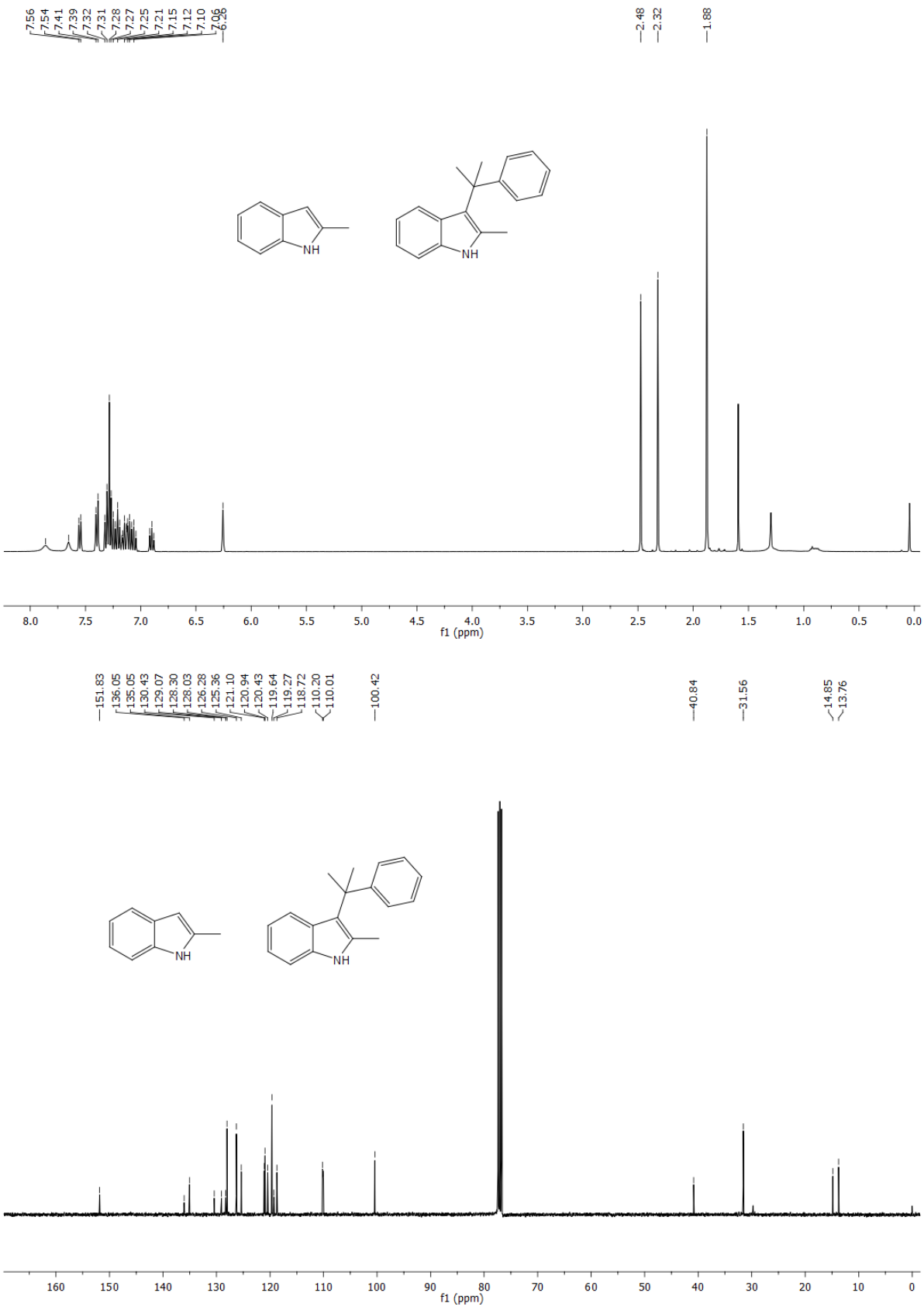


Figure S11. ^{1}H and ^{13}C Spectra of **5c**

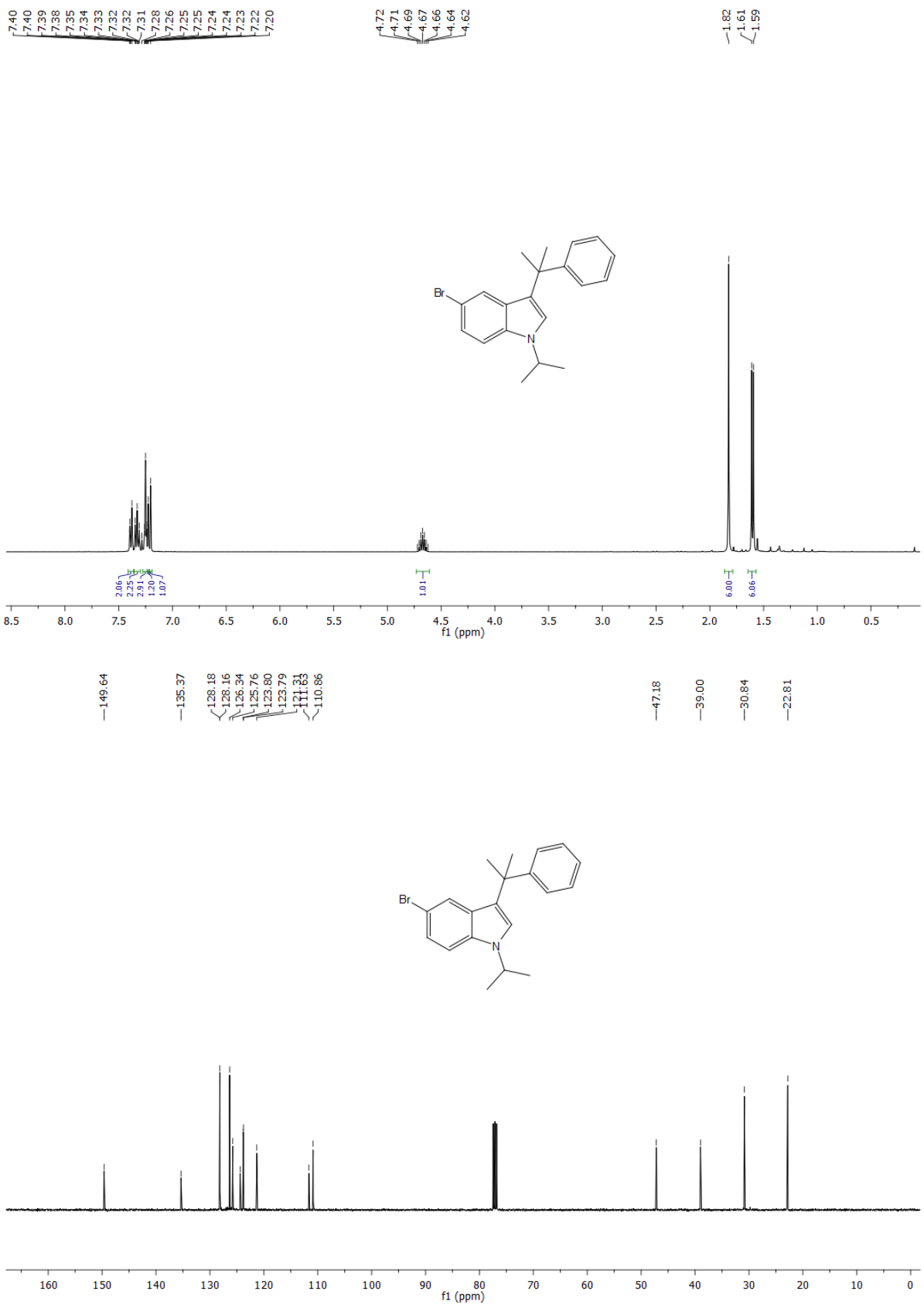


Figure S12. ^{1}H and ^{13}C Spectra of **5d**

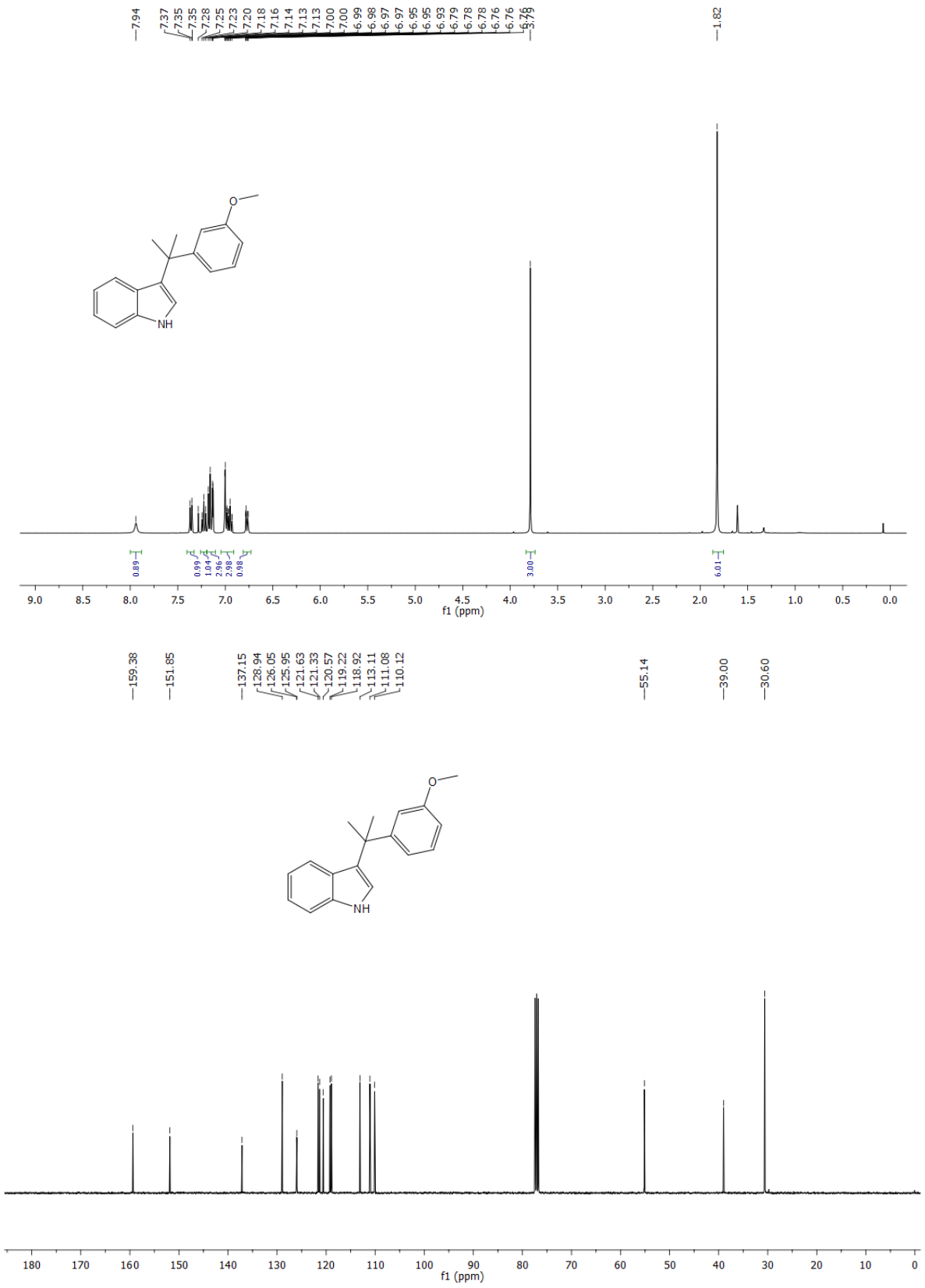


Figure S13. ^{1}H and ^{13}C Spectra of **5e**

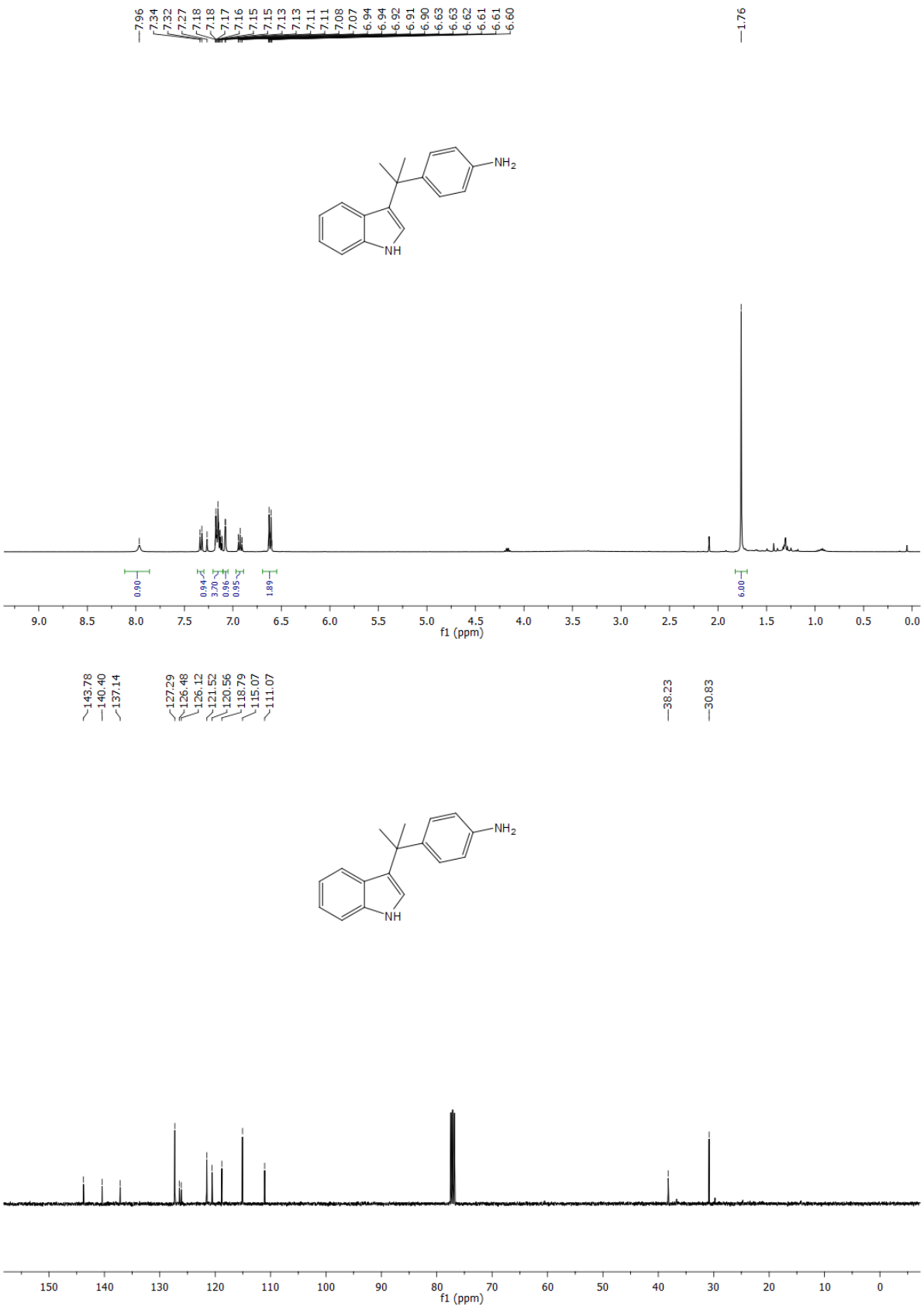


Figure S14. ^{1}H and ^{13}C Spectra of **5f**

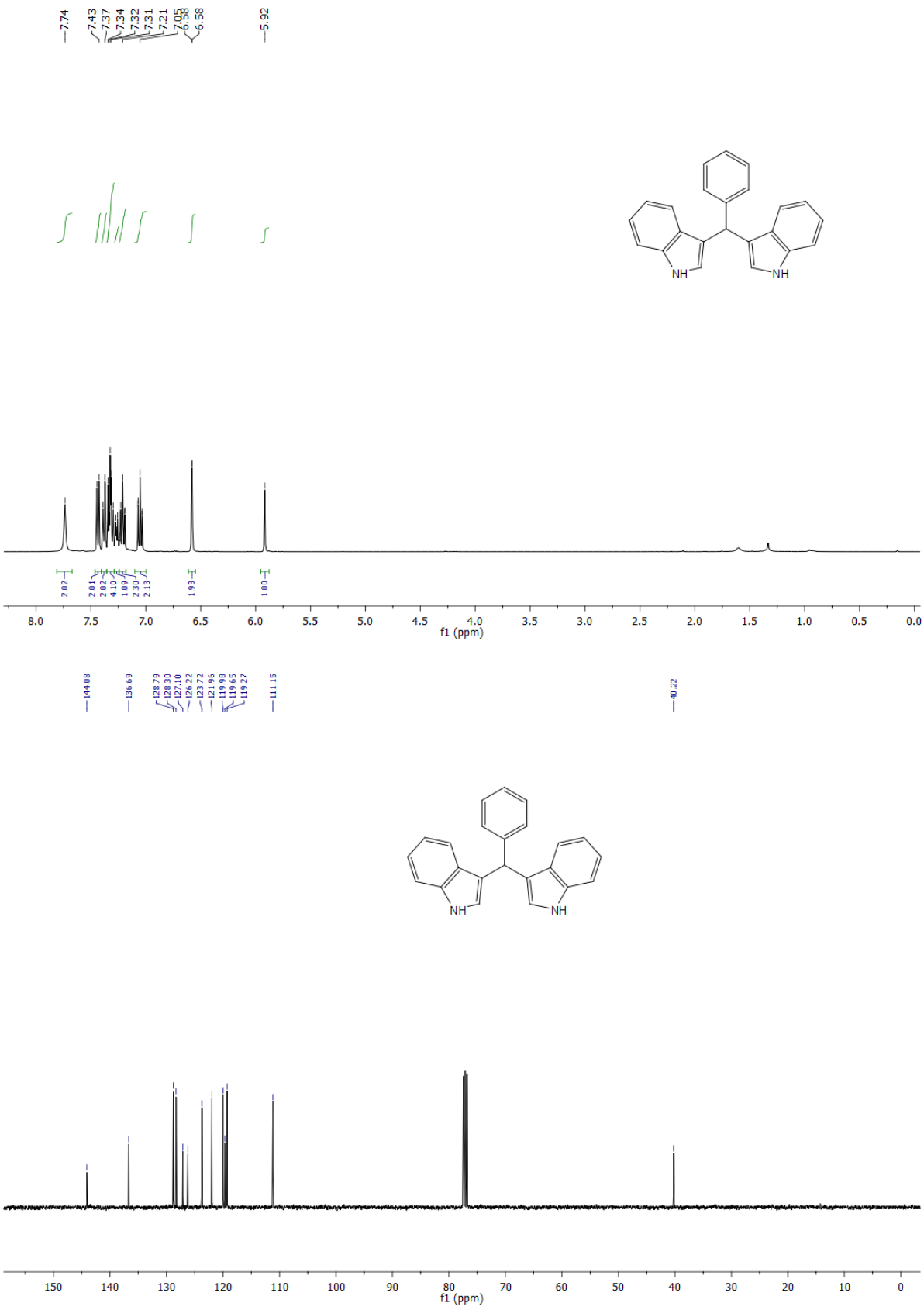


Figure S15. ^{1}H and ^{13}C Spectra of **9a**

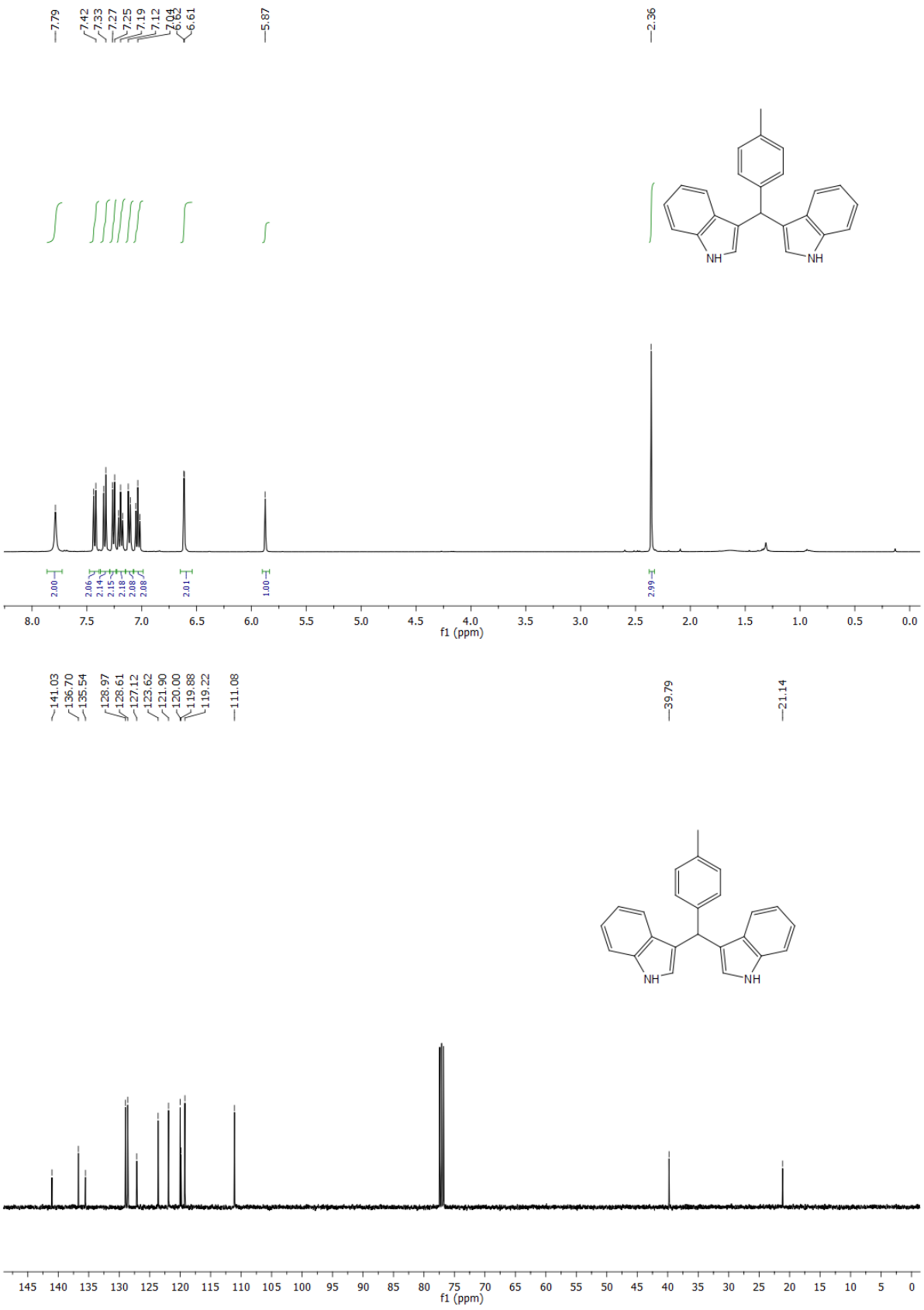


Figure S16. ^{1}H and ^{13}C Spectra of **9b**

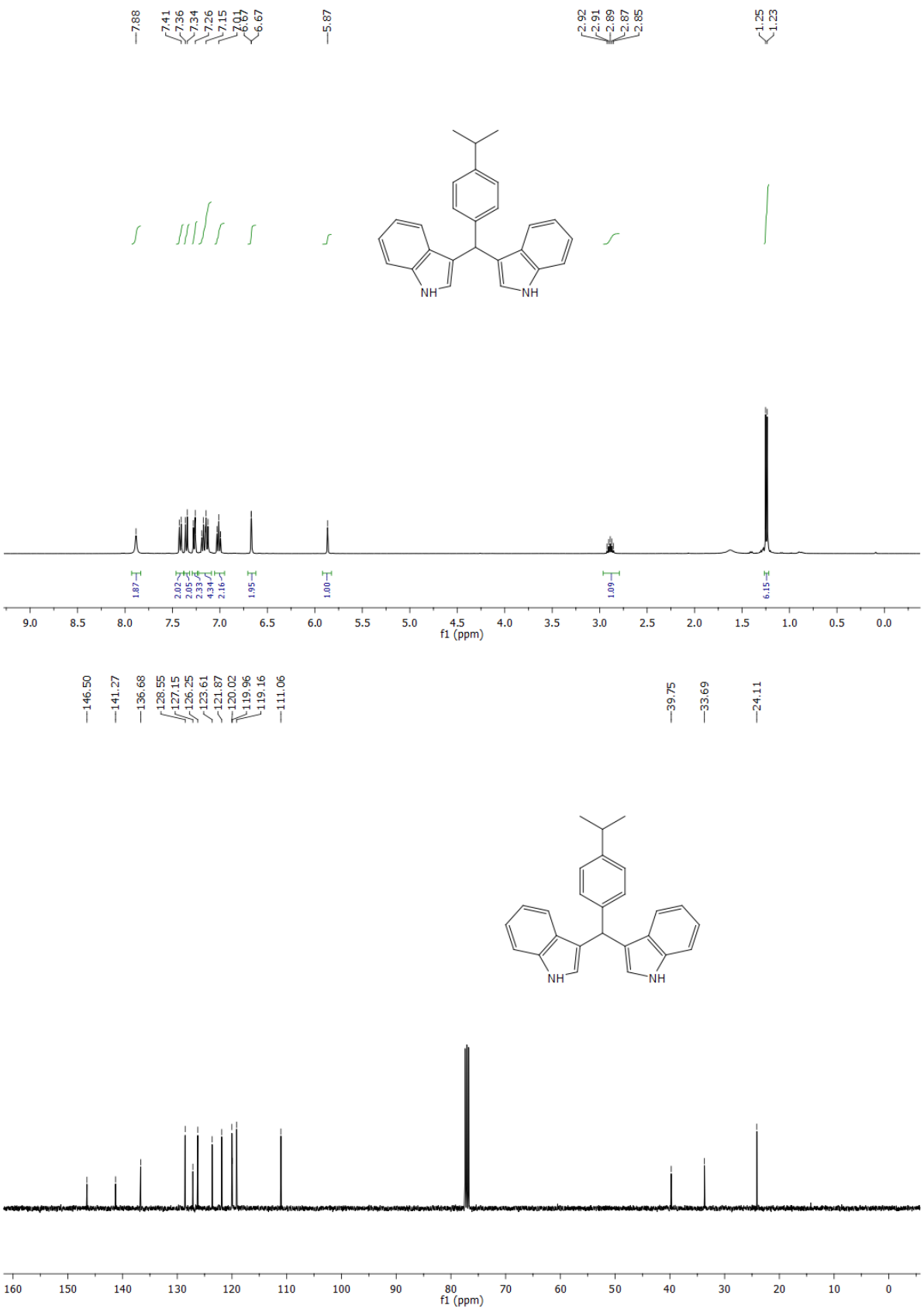


Figure S17. ^{1}H and ^{13}C Spectra of **9c**

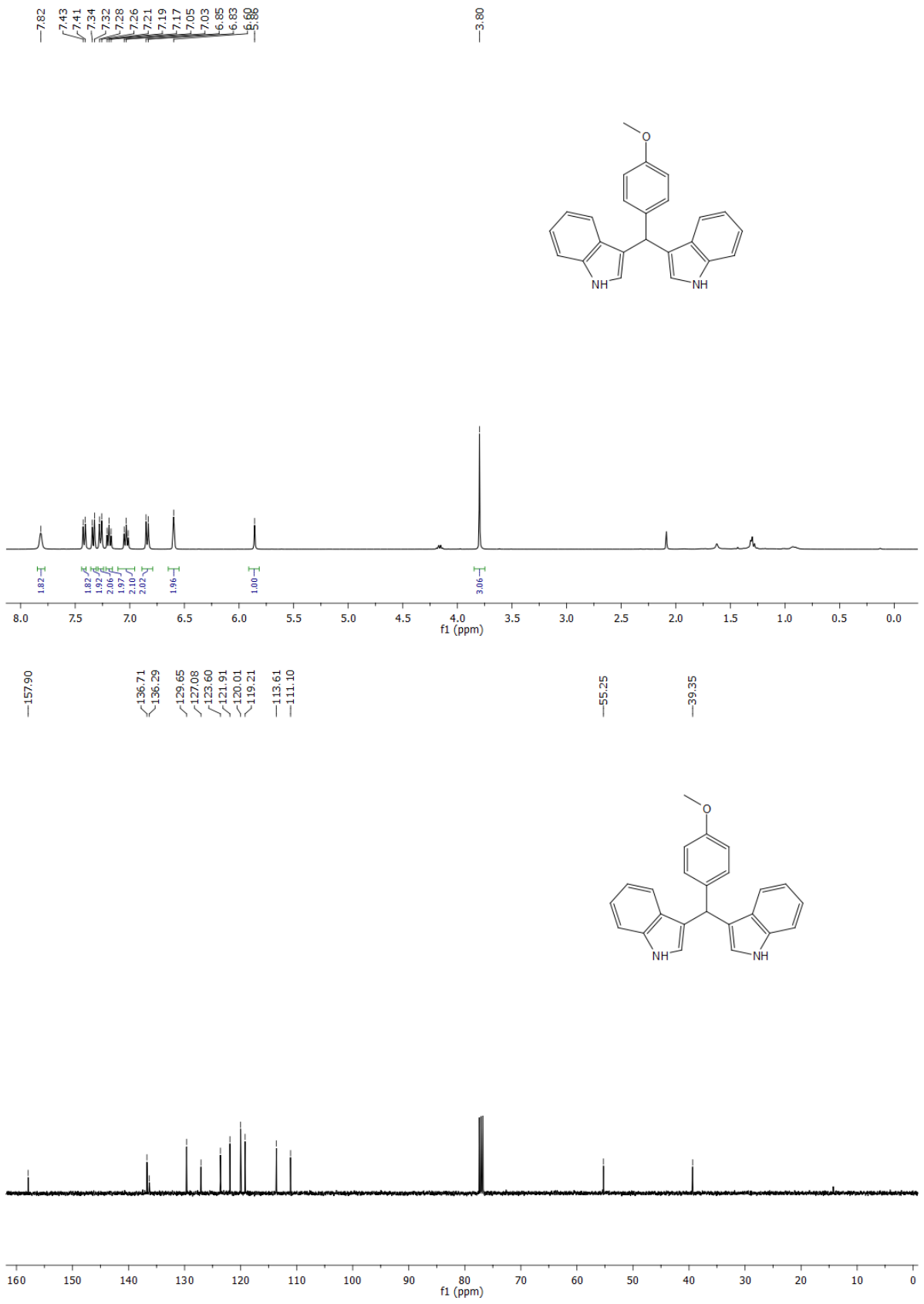


Figure S18. ^{1}H and ^{13}C Spectra of **9d**

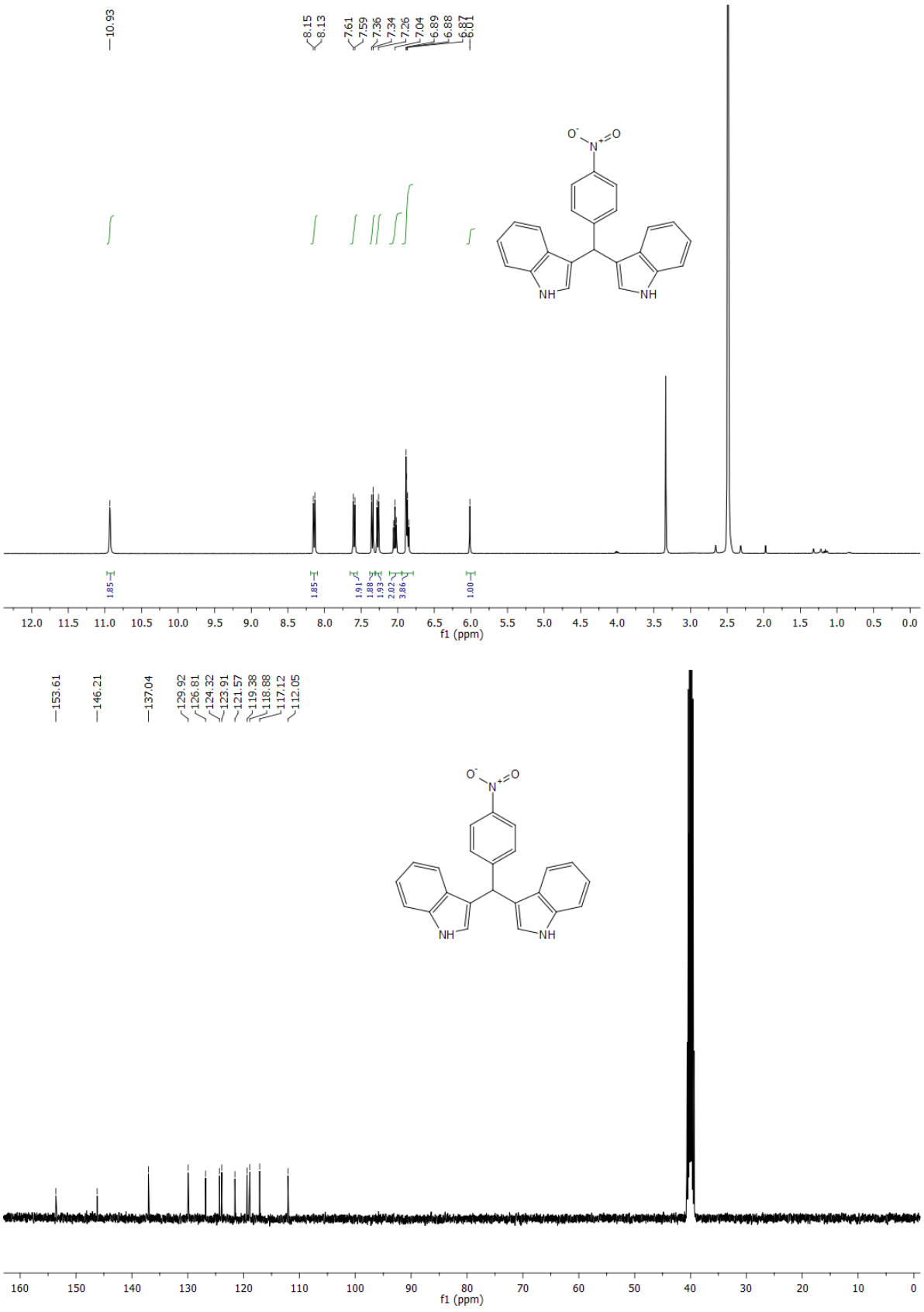


Figure S19. ^{1}H and ^{13}C Spectra of **9e**

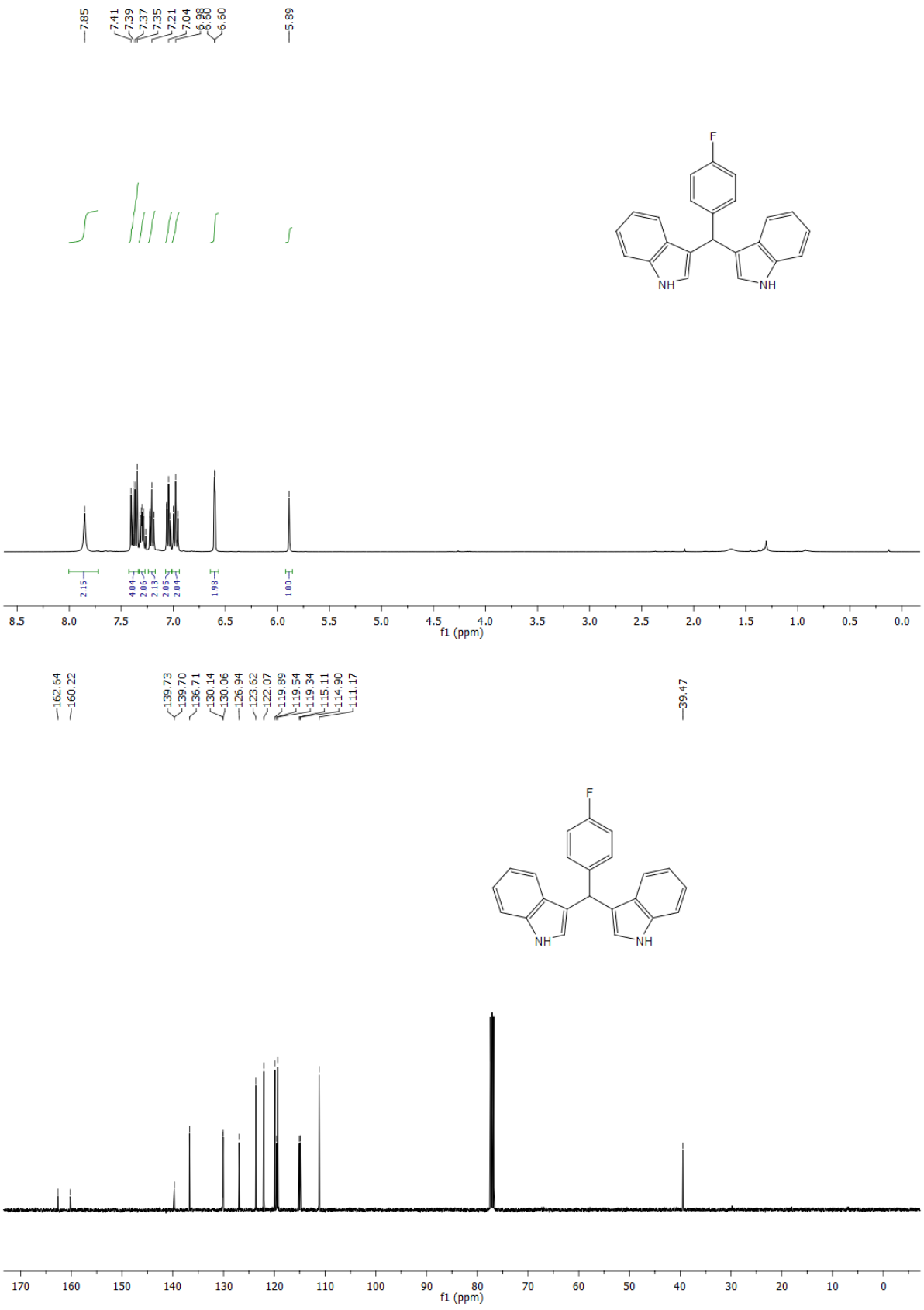


Figure S20. ^{1}H and ^{13}C Spectra of **9f**

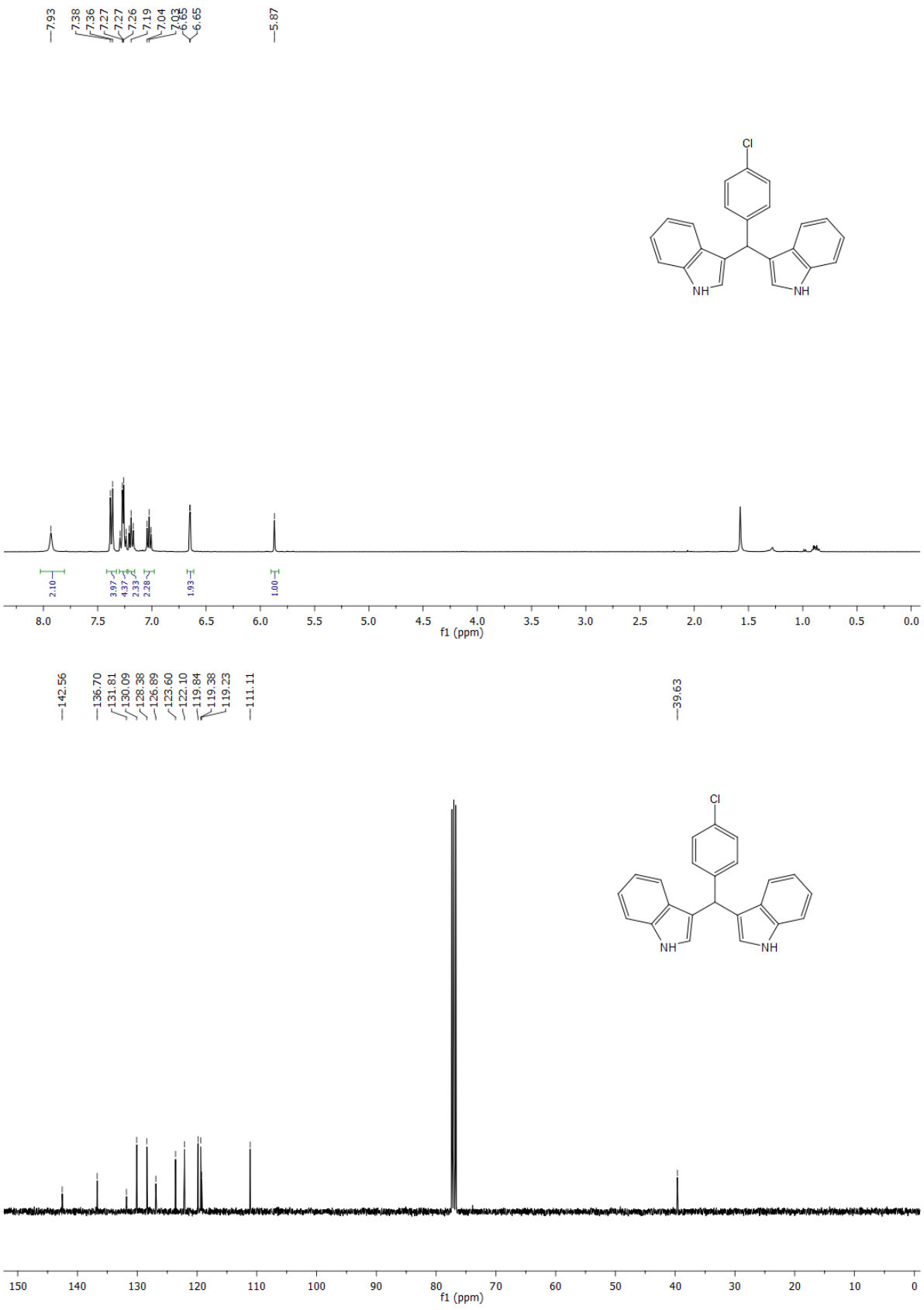


Figure S21. ^{1}H and ^{13}C Spectra of **9g**

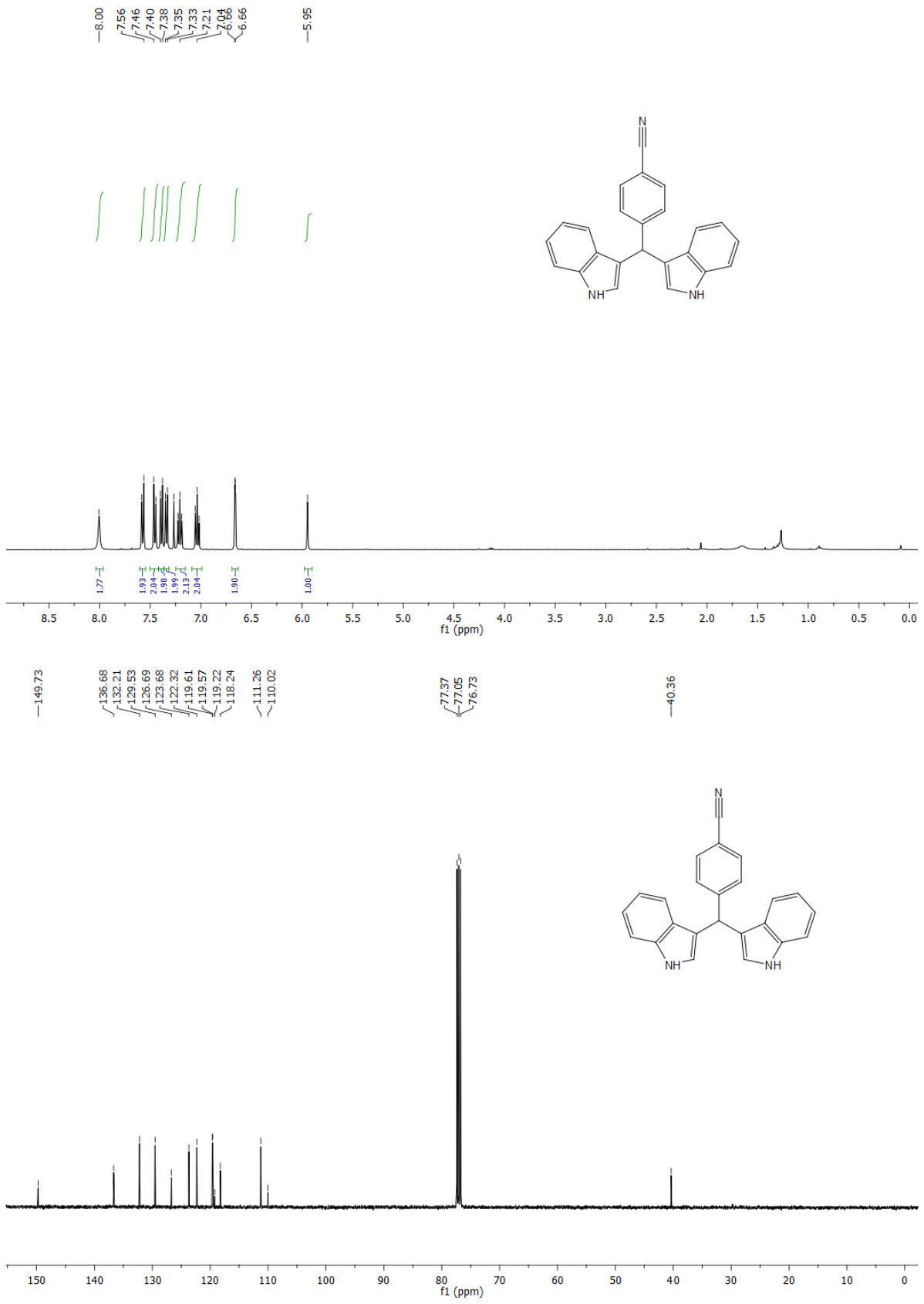


Figure S22. ^{1}H and ^{13}C Spectra of **9h**

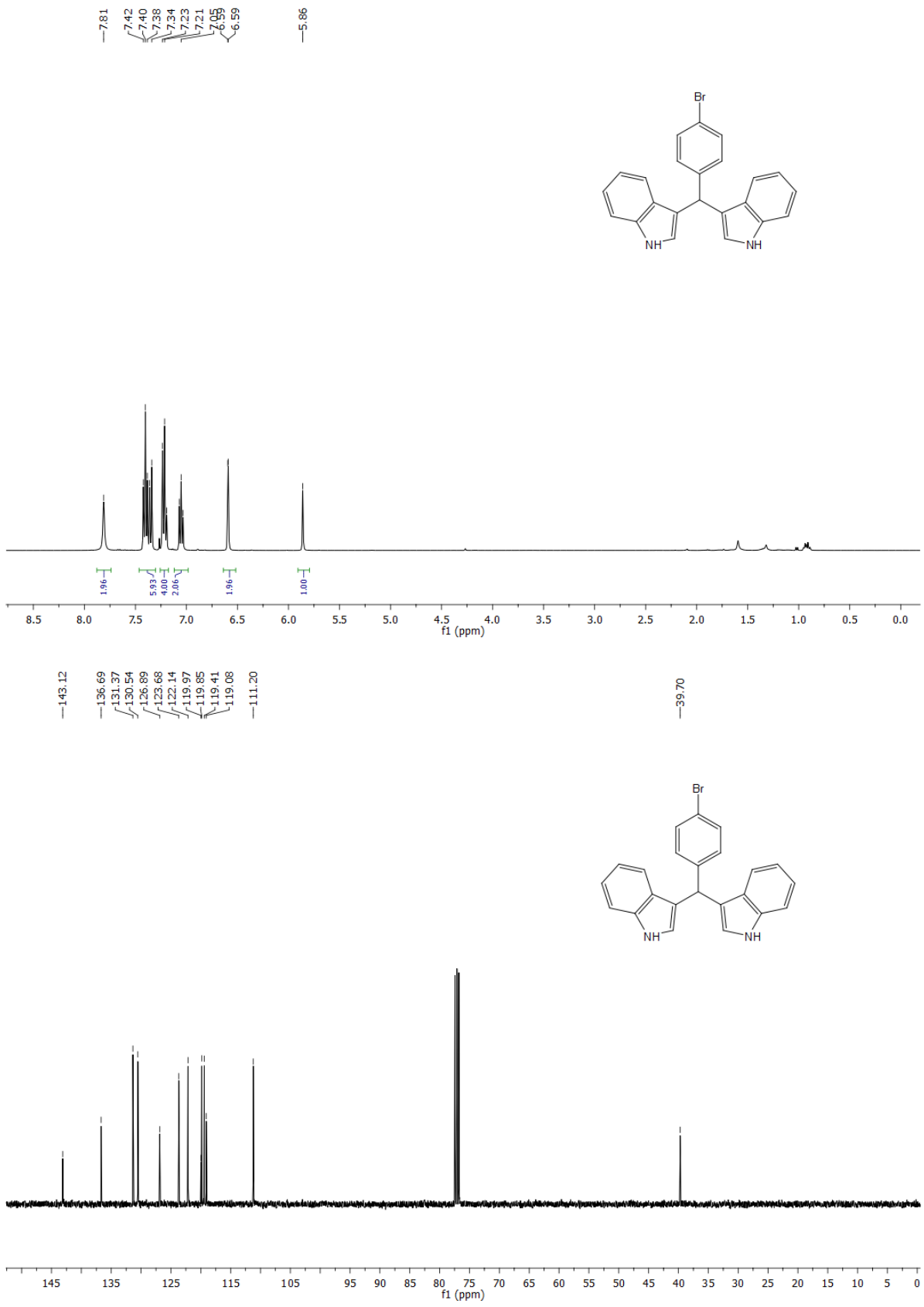


Figure S23. ^{1}H and ^{13}C Spectra of **9i**

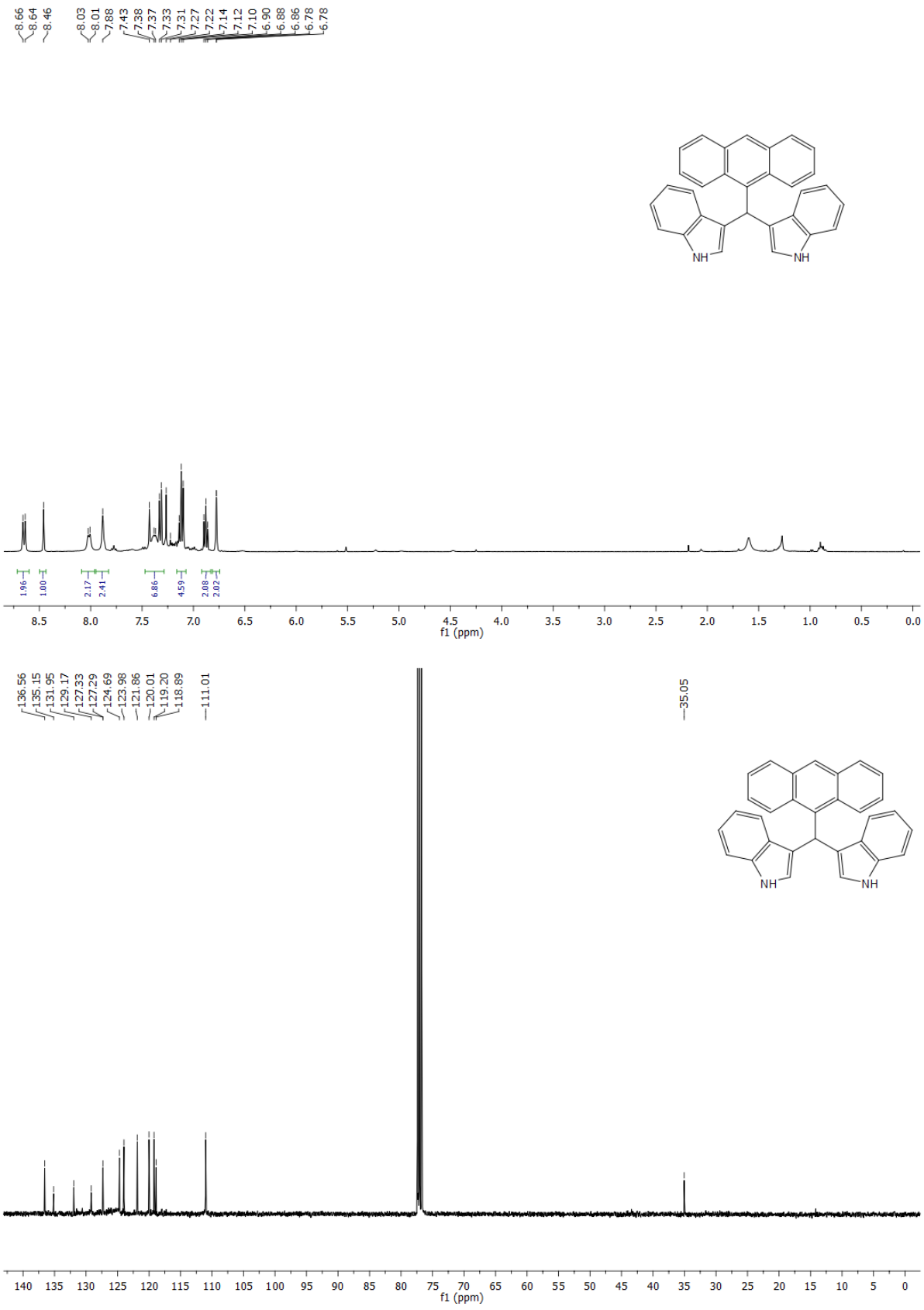


Figure S24. ^{1}H and ^{13}C Spectra of **9j**

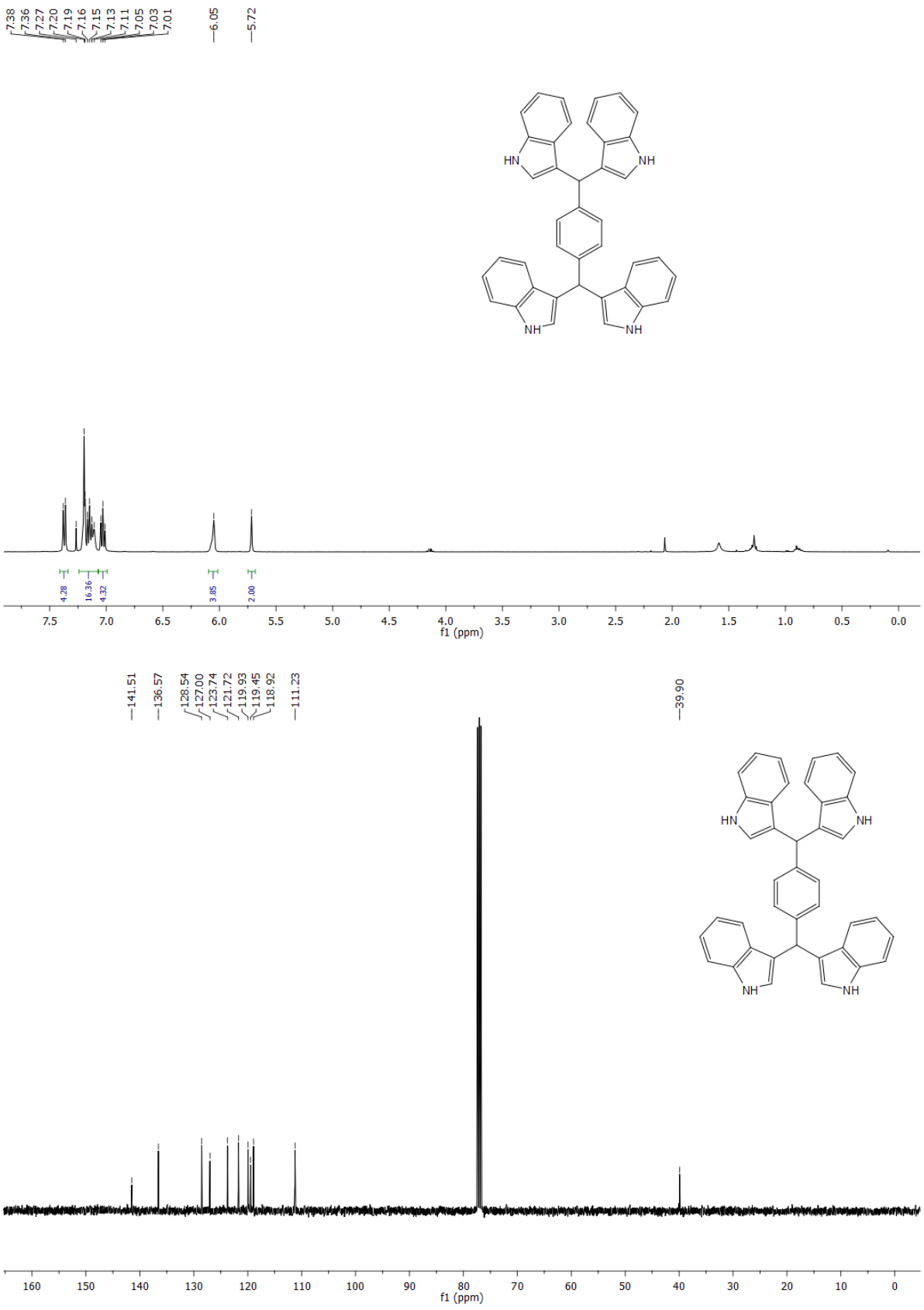


Figure S25. ^{1}H and ^{13}C Spectra of **9k**

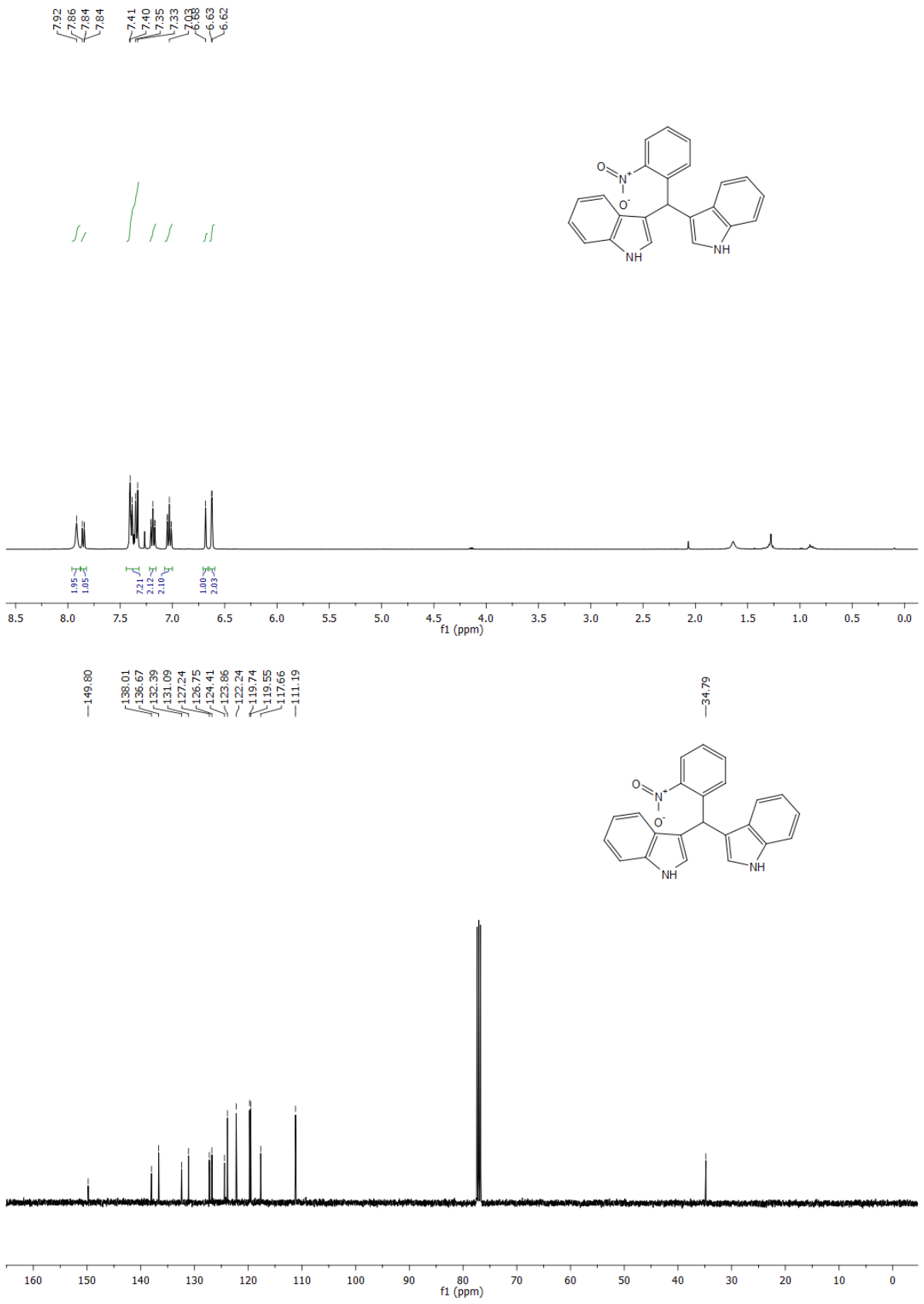


Figure S26. ^{1}H and ^{13}C Spectra of **9l**

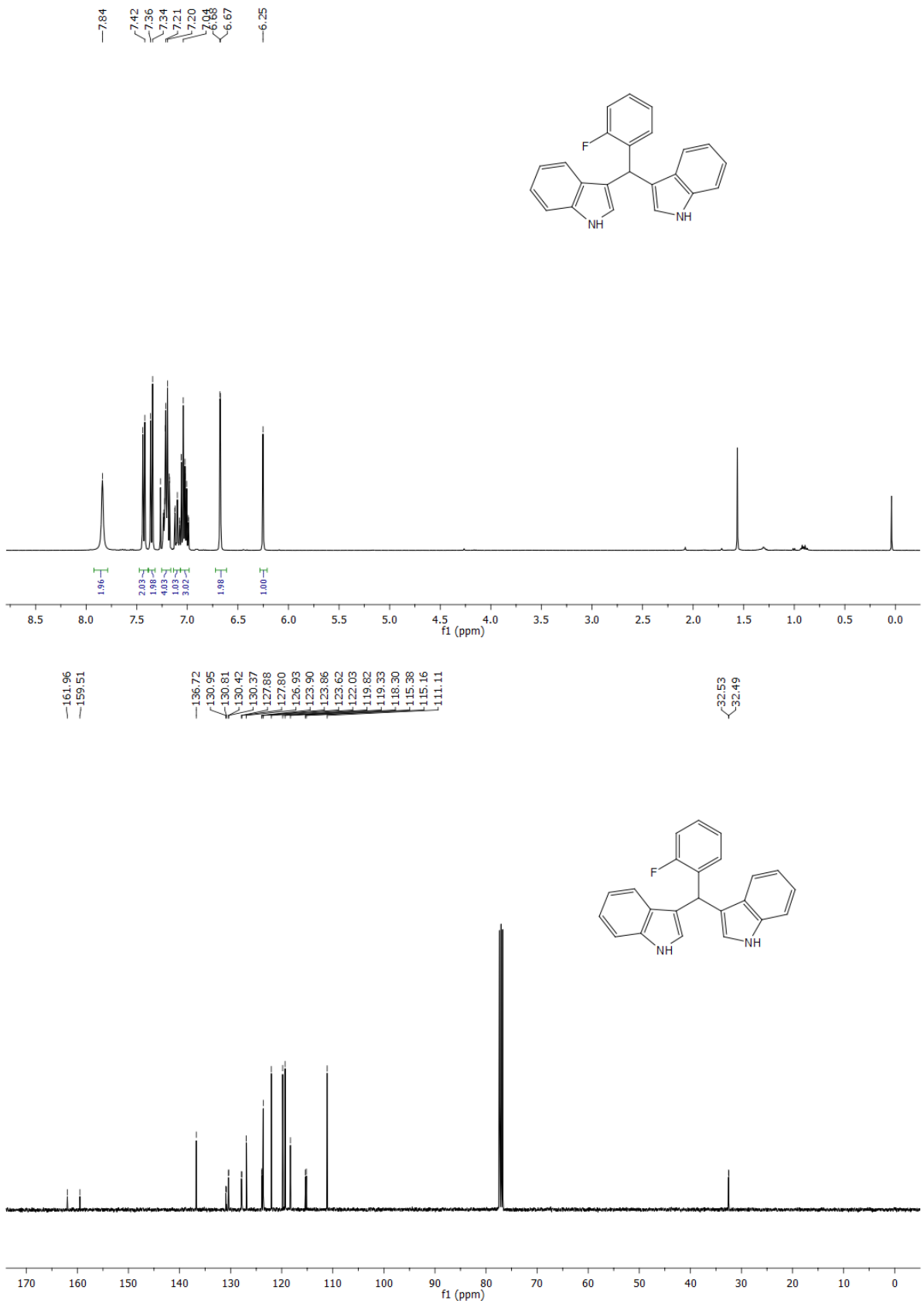


Figure S27. ^{1}H and ^{13}C Spectra of **9m**

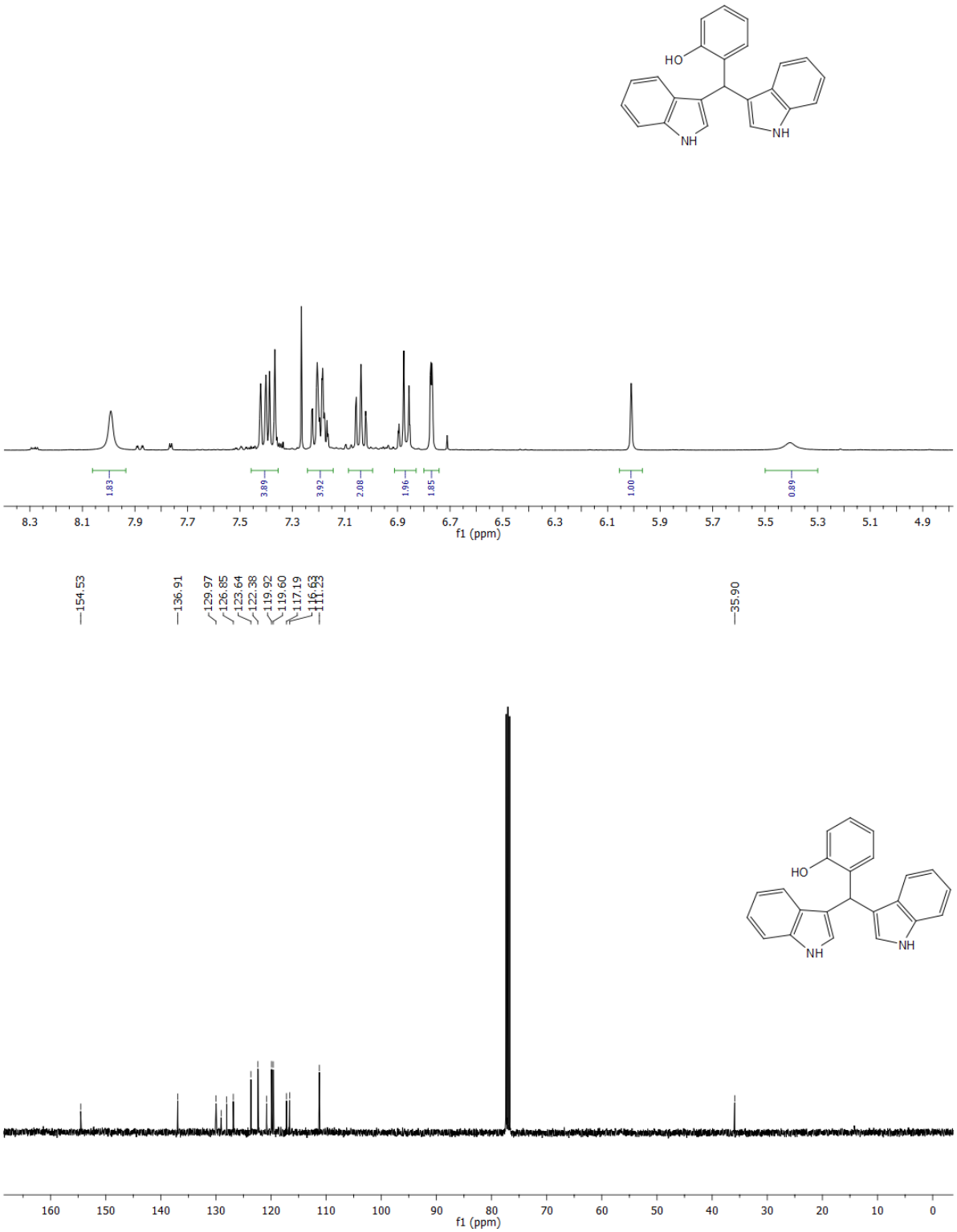


Figure S28. ^{1}H and ^{13}C Spectra of **9n**

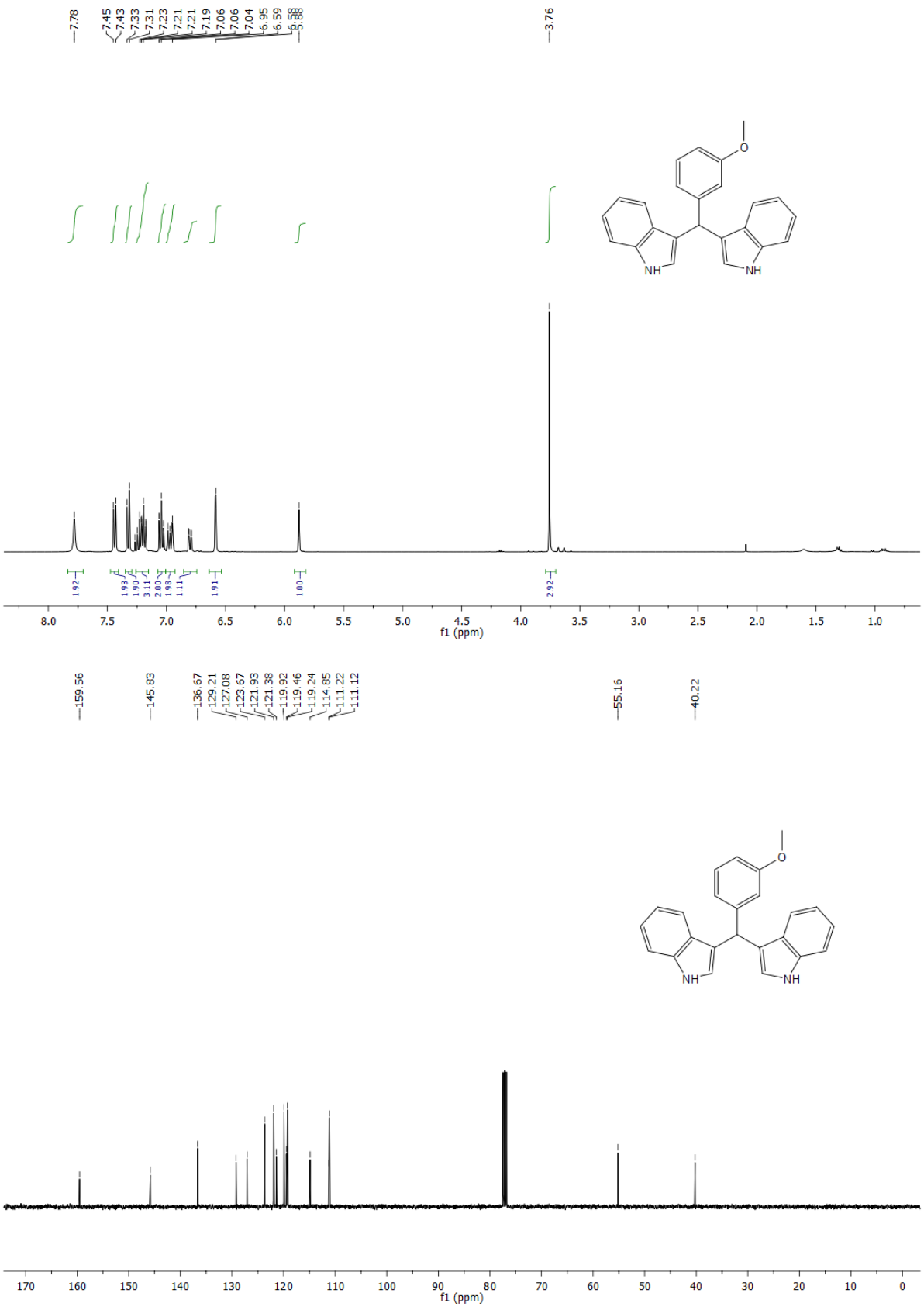


Figure S29. ^{1}H and ^{13}C Spectra of **9o**

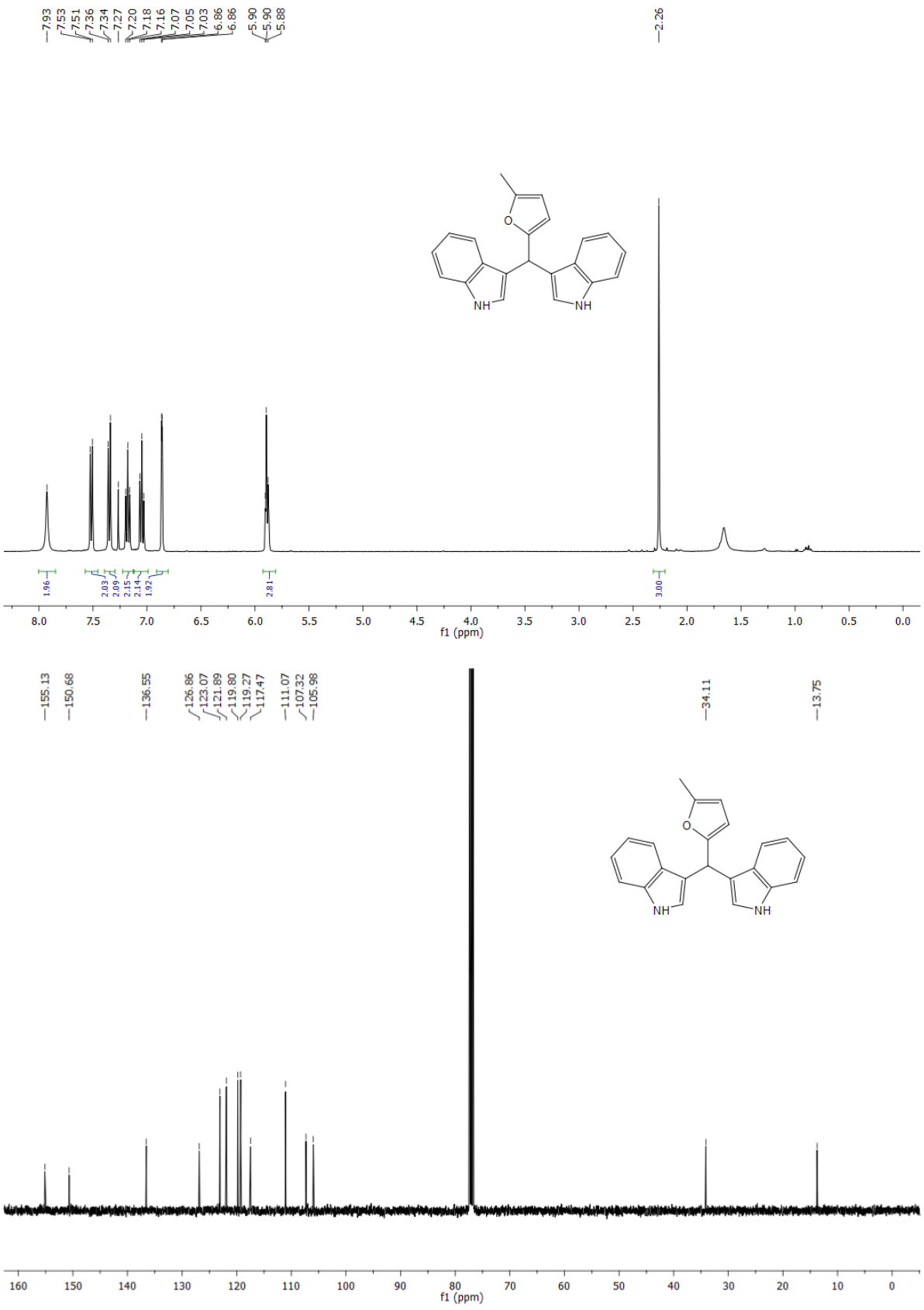


Figure S30. ^{1}H and ^{13}C Spectra of **9q**

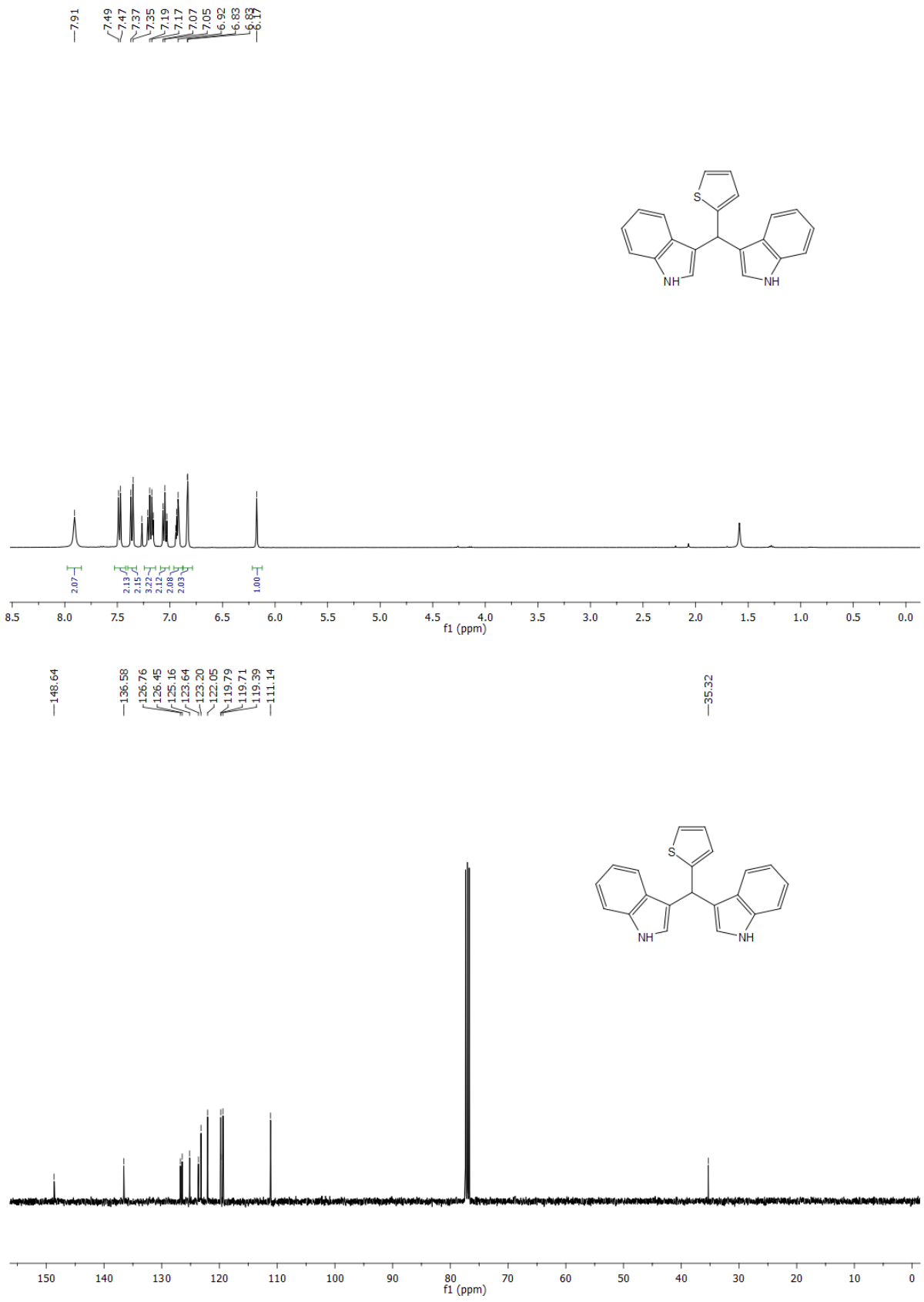


Figure S31. ^{1}H and ^{13}C Spectra of **9r**

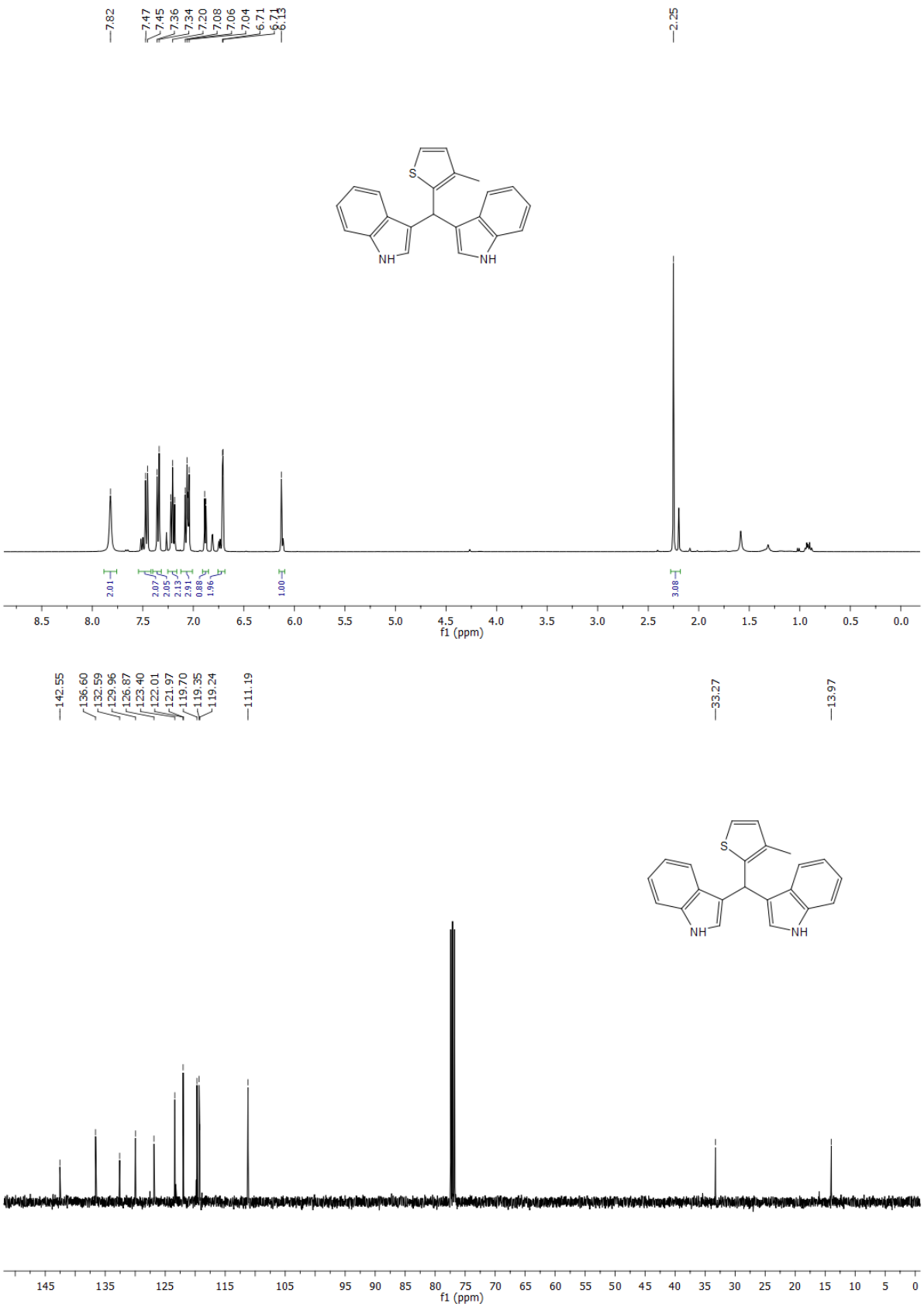


Figure S32. ^{1}H and ^{13}C Spectra of **9s**

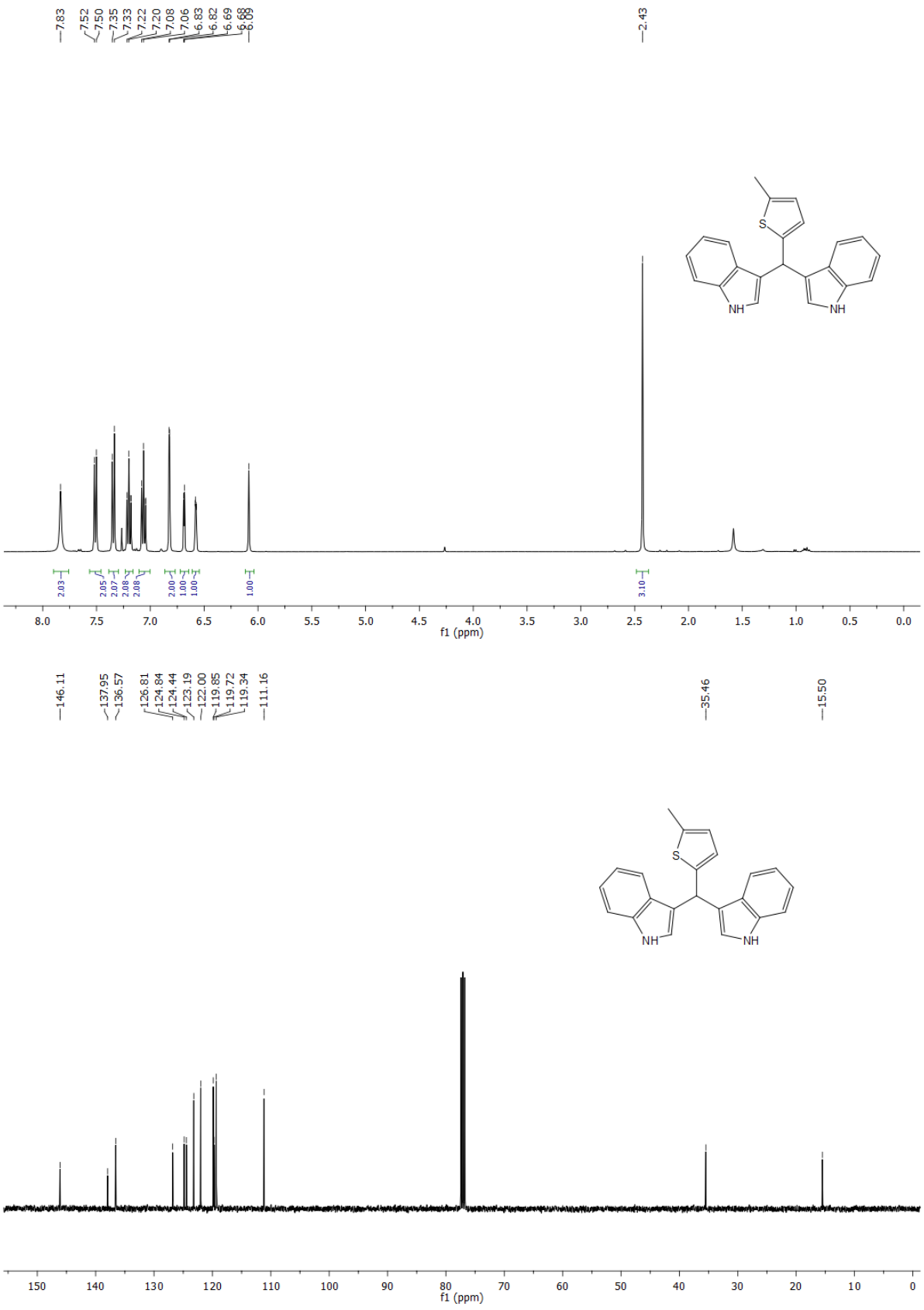


Figure S33. ^{1}H and ^{13}C Spectra of **9t**

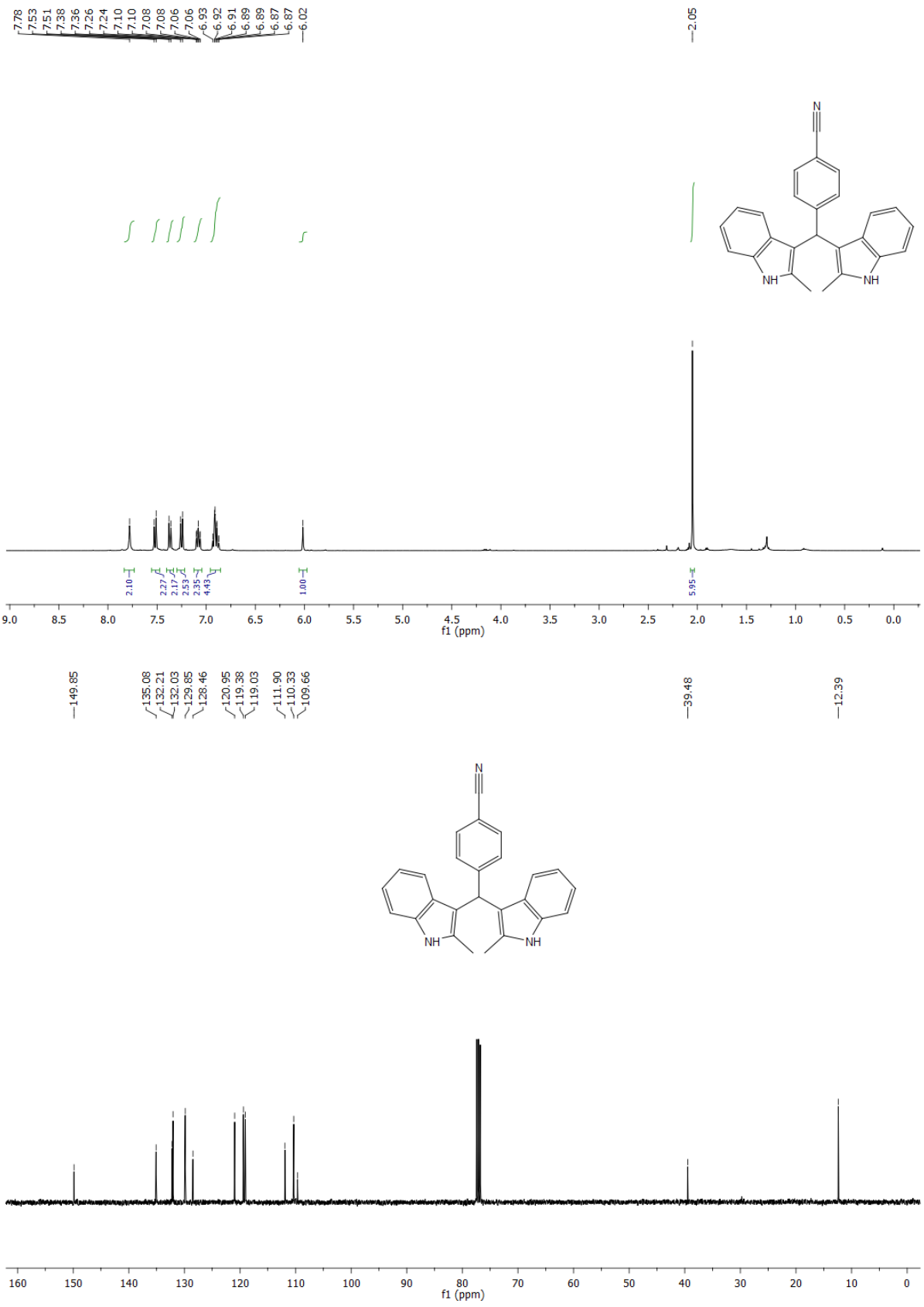


Figure S34. ^{1}H and ^{13}C Spectra of **10a**

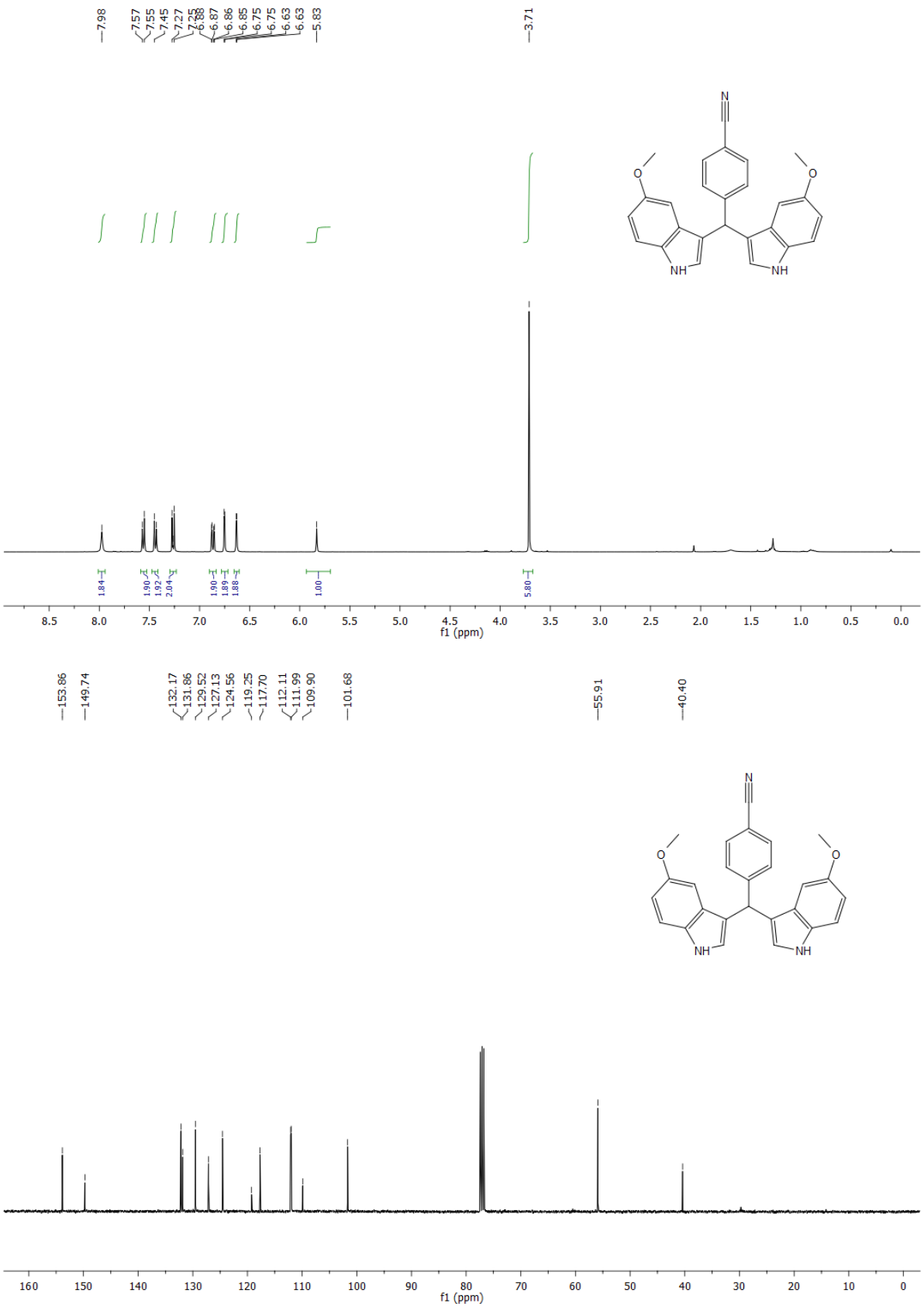


Figure S35. ^{1}H and ^{13}C Spectra of **10b**

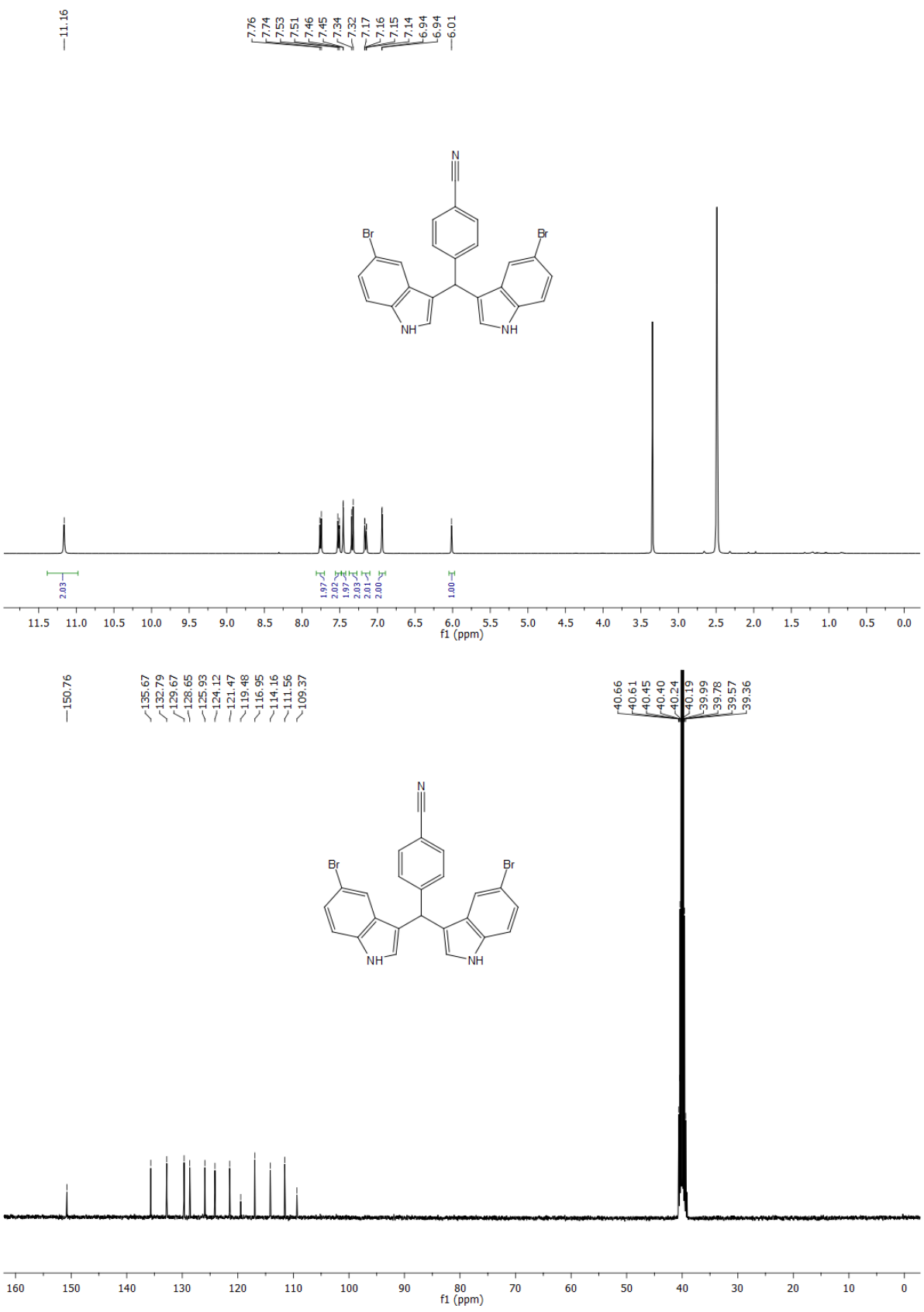


Figure S36. ^{1}H and ^{13}C Spectra of **10c**

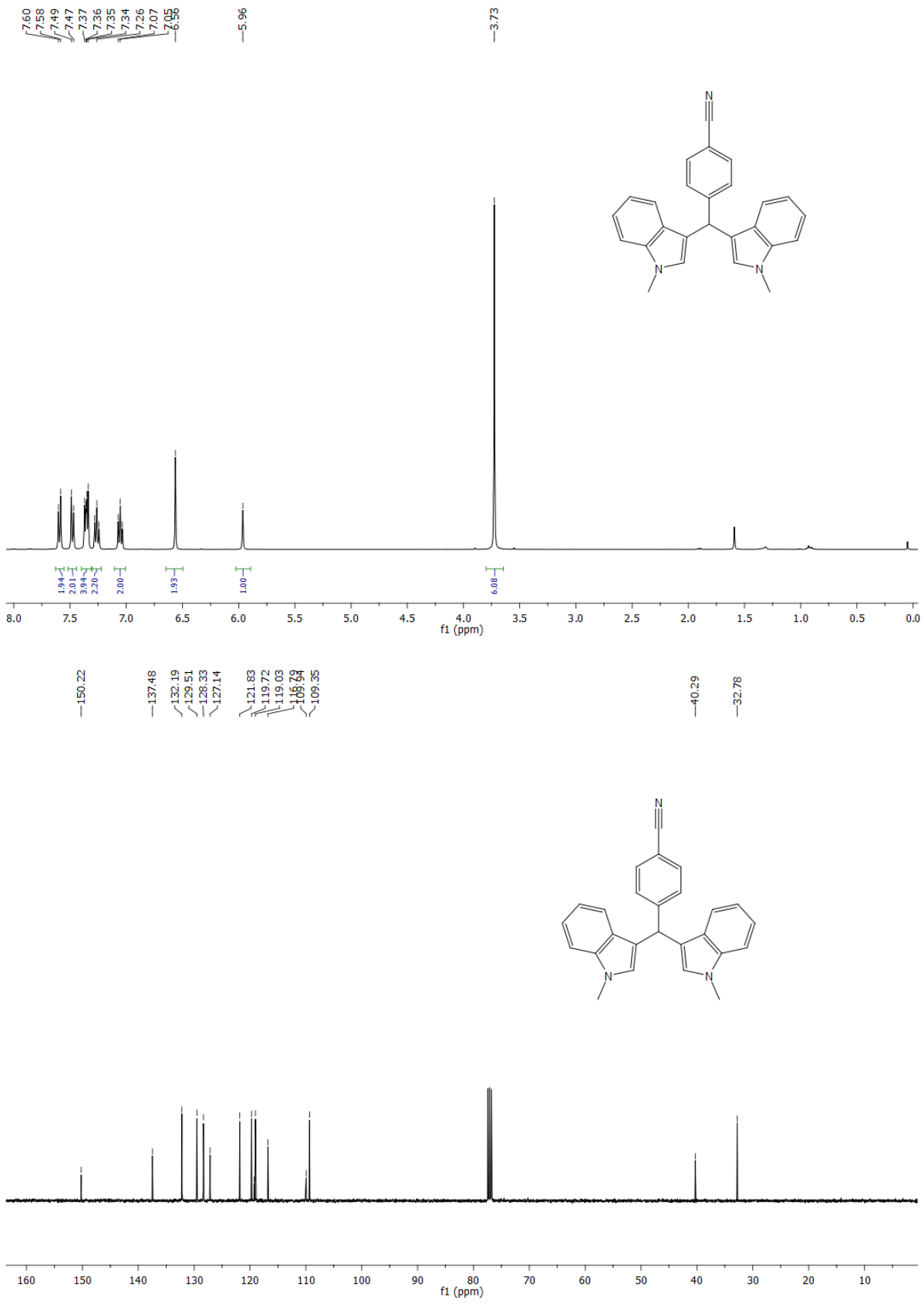


Figure S37. ^{1}H and ^{13}C Spectra of **10d**

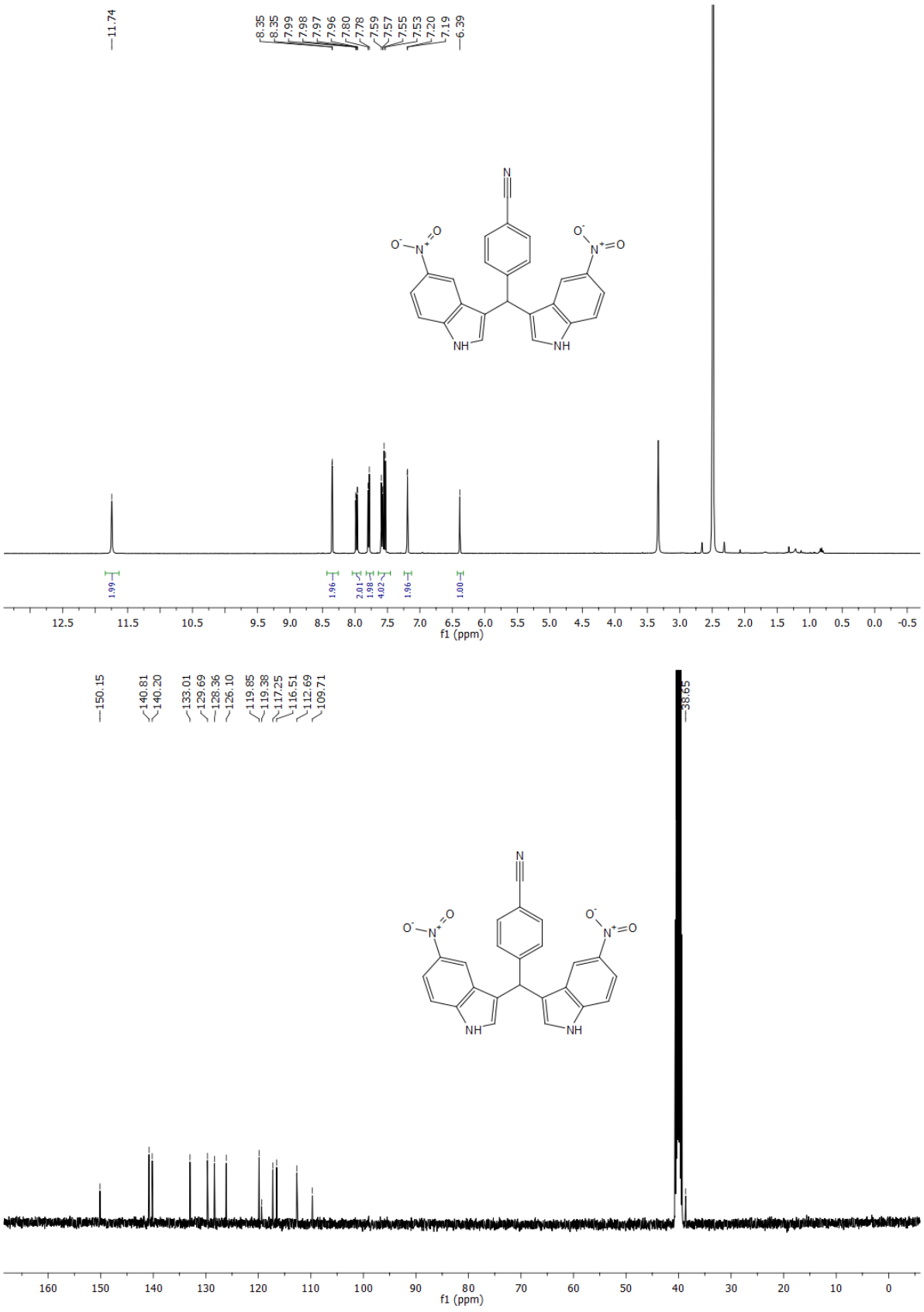


Figure S38. ^{1}H and ^{13}C Spectra of **10e**

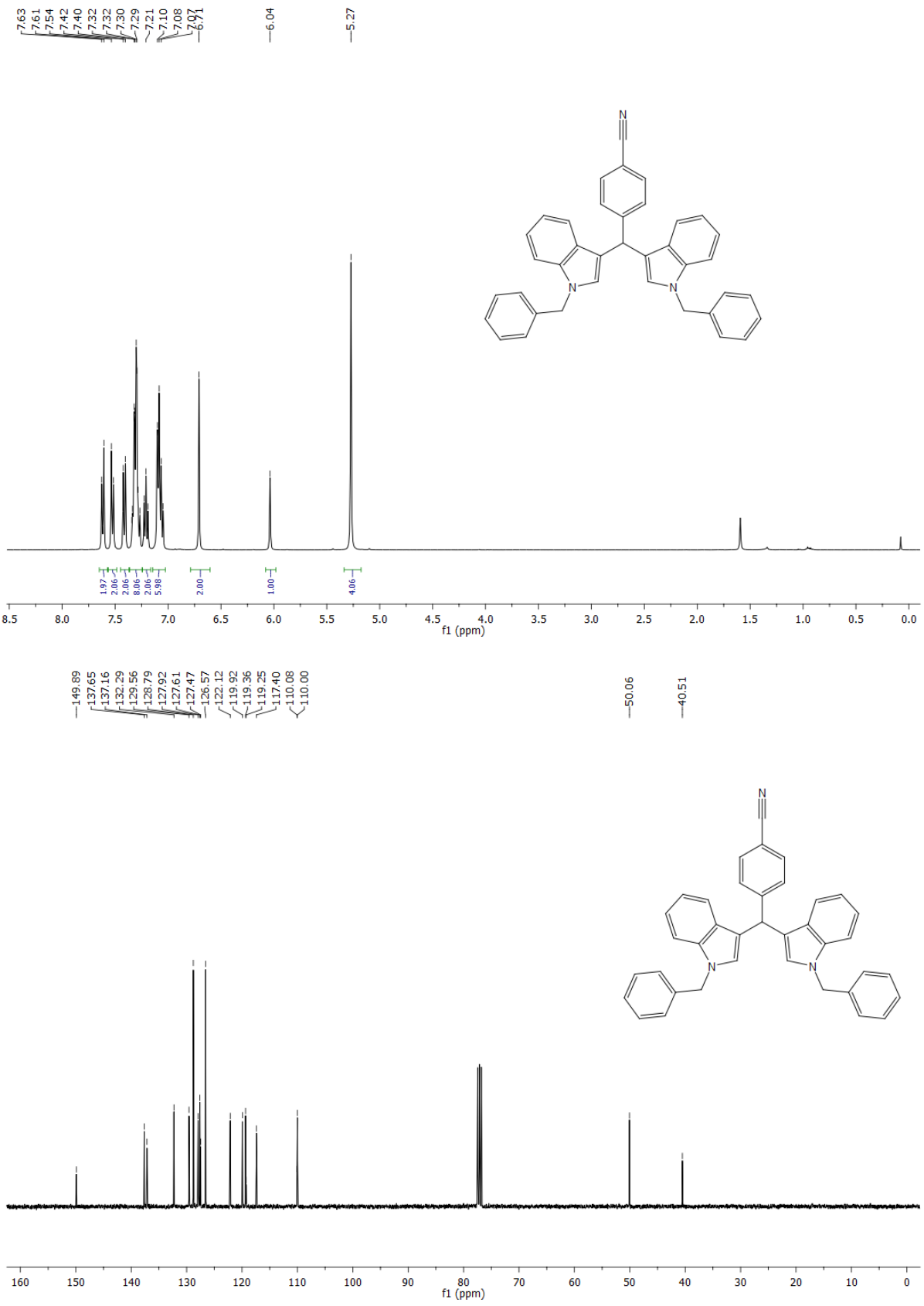


Figure S39. ^{1}H and ^{13}C Spectra of **10f**

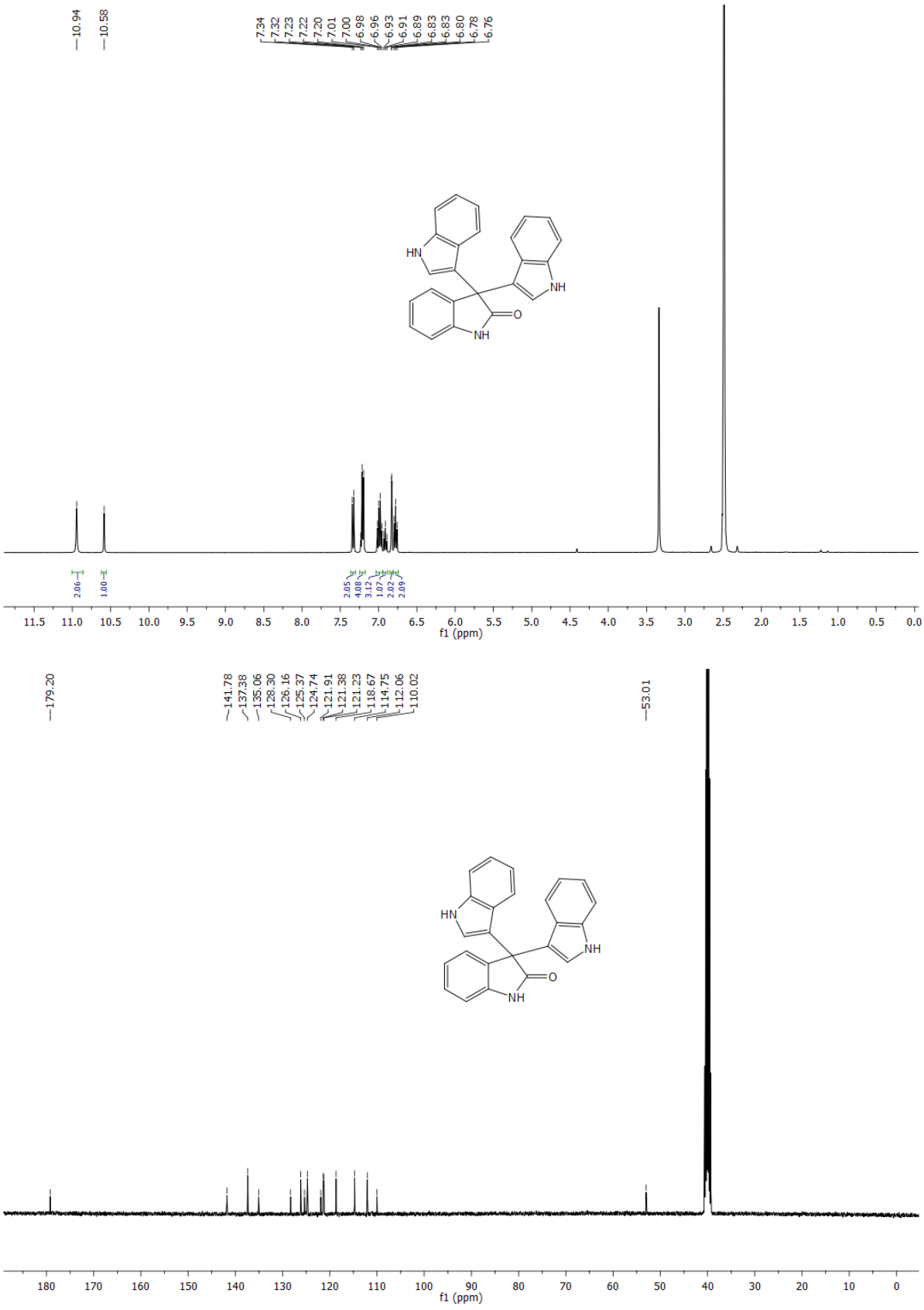


Figure S40. ^{1}H and ^{13}C Spectra of **11**

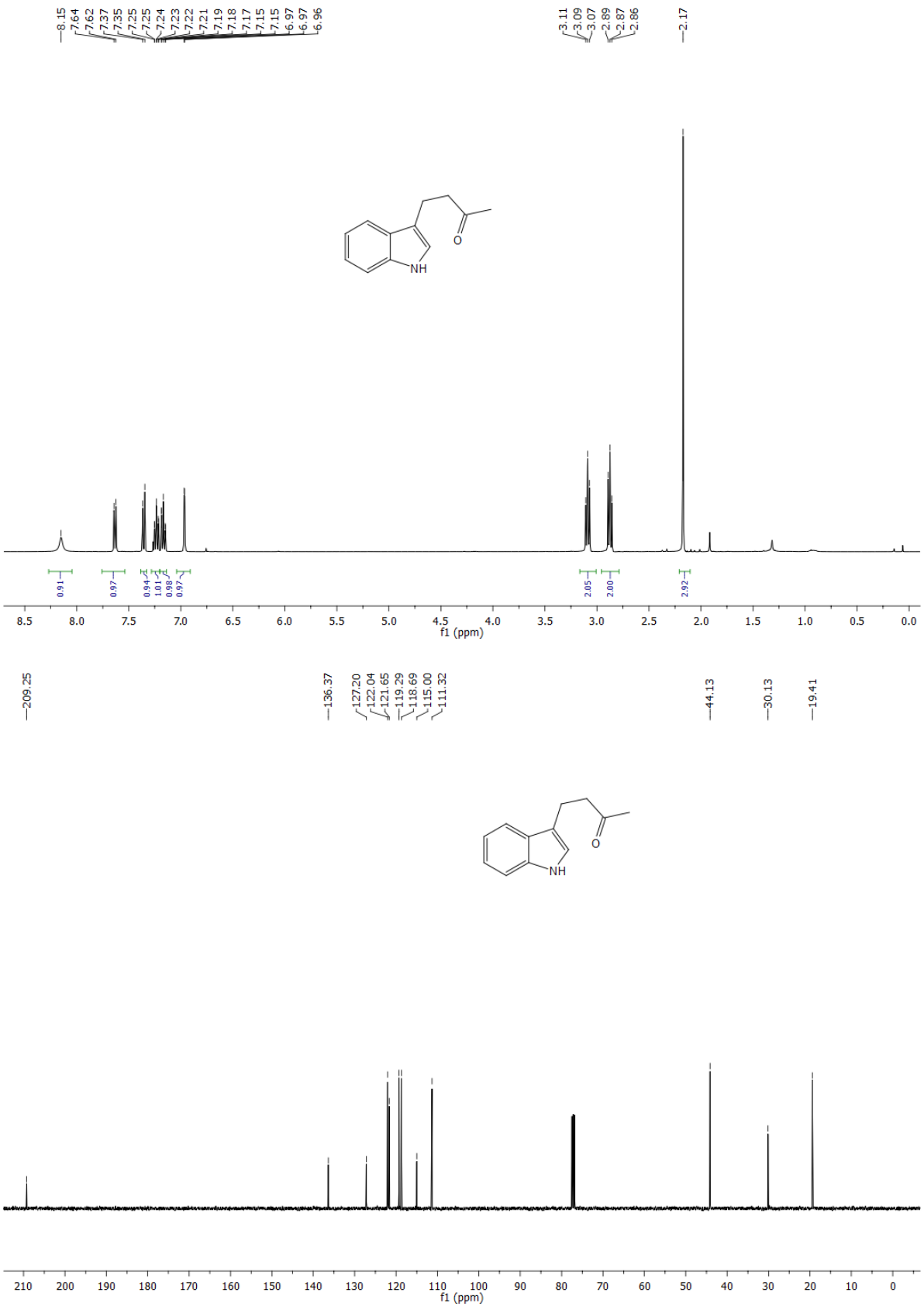


Figure S41. ^{1}H and ^{13}C Spectra of **12a**

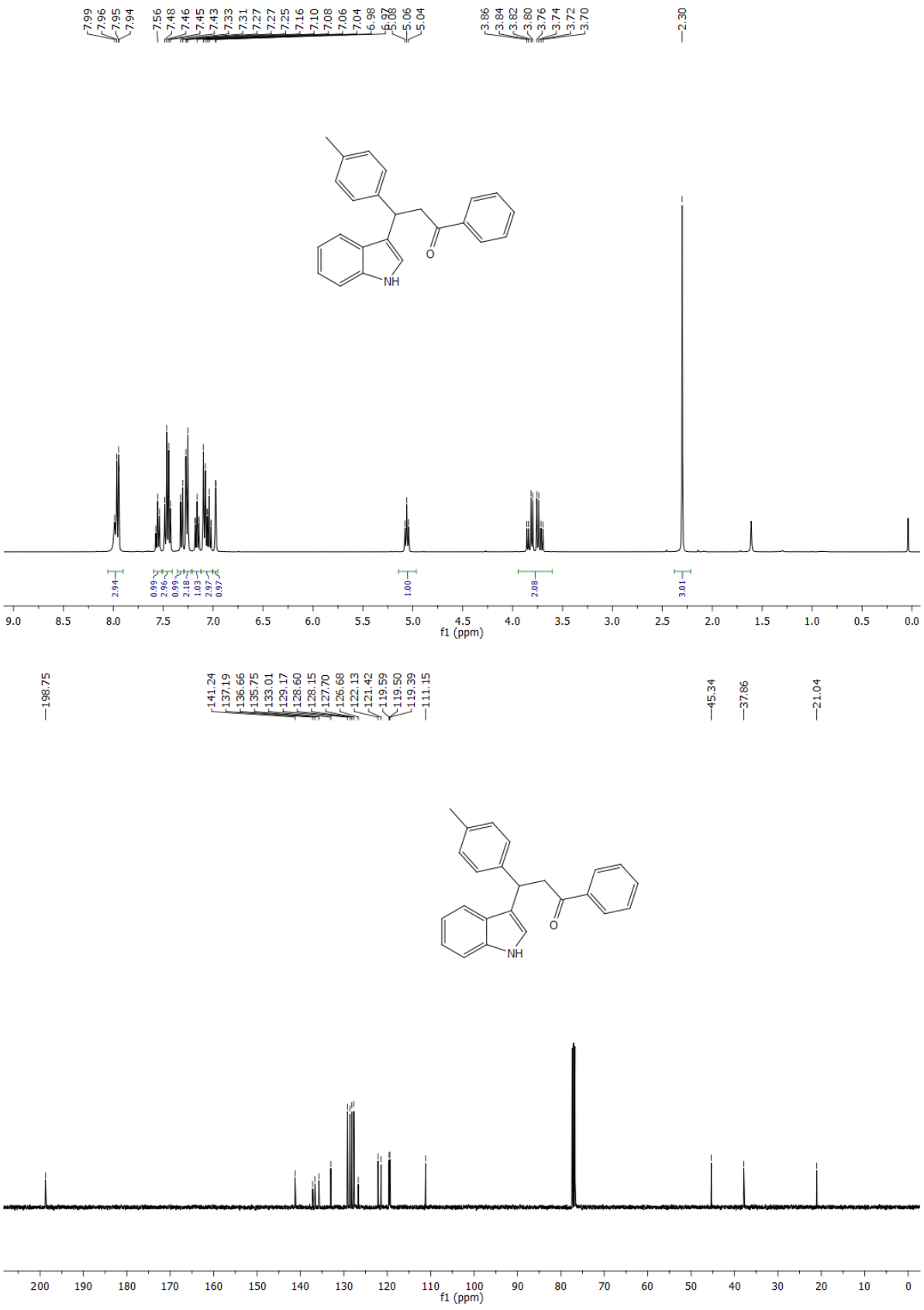


Figure S42. ^{1}H and ^{13}C Spectra of **12b**

References

1 D. B. G. Williams and M. Lawton, *J. Org. Chem.*, 2010, **75**, 8351–8354.

2 J. Tirado-Rives and W. L. Jorgensen, *J. Chem. Theory Comput.*, 2008, **4**, 297–306.

3 V. A. Rassolov, M. A. Ratner, J. A. Pople, P. C. Redfern and L. A. Curtiss, *J. Comput. Chem.*, 2001, **22**, 976–984.

4 M. Su and S. Chu, *Inorg. Chem.*, 1998, **4**, 3400–3406.

5 E. Cancès, B. Mennucci and J. Tomasi, *J. Chem. Phys.*, 1997, **107**, 3032–3041.

6 S. Maeda, Y. Harabuchi, Y. Ono, T. Taketsugu and K. Morokuma, *Int. J. Quantum Chem.*, 2015, **115**, 258–269.

7 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. a. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. a. Petersson, H. Nakatsuji, X. Li, M. Caricato, a. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, a. F. Izmaylov, J. L. Sonnenberg, Williams, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. a. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. a. Keith, R. Kobayashi, J. Normand, K. Raghavachari, a. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, 2016, Gaussian 16, Revision C.01, Gaussian, Inc., Wallin.

8 H. V. Huynh, Y. Han, J. H. H. Ho and G. K. Tan, *Organometallics*, 2006, **25**, 3267–3274.

9 Y. Han, H. V. Huynh and L. L. Koh, *J. Organomet. Chem.*, 2007, **692**, 3606–3613.

10 M. K. Nayak, A. Mohanty and S. Roy, *Organometallics*, 2023, **42**, 1927–1933.

11 W. Mansour, R. Suleiman, M. Fettouhi and B. El Ali, *ACS Omega*, 2020, **5**, 23687–23702.

12 S. J. Chen, W. Q. Zhong and J. M. Huang, *J. Org. Chem.*, ,

DOI:10.1021/acs.joc.3c01310.

13 X. Qi, H. J. Ai, N. Zhang, J. B. Peng, J. Ying and X. F. Wu, *J. Catal.*, 2018, **362**, 74–77.

14 J. Diego Pizarro, L. Morán-González, I. González-Fernández, F. Maseras, M. R. Fructos and P. J. Pérez, *Adv. Synth. Catal.*, 2023, 1–9.

15 S. Mathavan, K. Kannan and R. B. R. D. Yamajala, *Org. Biomol. Chem.*, 2019, **17**, 9620–9626.

16 A. K. Das, N. Sepay, S. Nandy, A. Ghatak and S. Bhar, *Tetrahedron Lett.*, 2020, **61**, 152231.

17 E. M. Galathri, L. Di Terlizzi, M. Fagnoni, S. Protti and C. G. Kokotos, *Org. Biomol. Chem.*, 2022, **21**, 365–369.

18 Q. Xing, Y. Shen, X. Zhang, H. Shao, C. Wang and X. Zhang, *Tetrahedron Lett.*, 2023, **122**, 154512.

19 S. Sri, V. Prasanna, T. Unit, B. Division, A. Lincoln, P. Muralidhar and S. Reddy, 2023, 0–10.

20 V. D. Kadu, M. S. Gund and A. S. Godage, *ChemistrySelect*, 2021, **6**, 11954–11960.

21 K. Griffiths, P. Kumar, G. R. Akien, N. F. Chilton, A. Abdul-Sada, G. J. Tizzard, S. J. Coles and G. E. Kostakis, *Chem. Commun.*, 2016, **52**, 7866–7869.

22 K. Wen, M. Feng, Q. Gao, C. Chen, Y. Wu, J. Zhou, L. Huang and X. Tang, *Adv. Synth. Catal.*, 2023, **365**, 1140–1146.

23 D. Liang, X. Li, W. Zhang, Y. Li, M. Zhang and P. Cheng, *Tetrahedron Lett.*, 2016, **57**, 1027–1030.