Supporting Information

for

Iodo-Sulphonylation of 1,6-Enynones: A Metal-Free Strategy to Synthesize N-Substituted Succinimides

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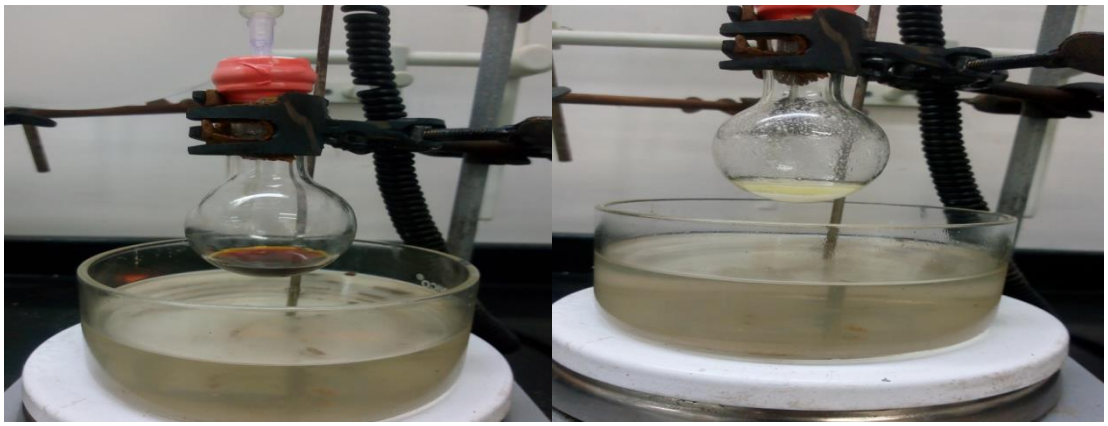
(1) General Information

^{1}H and ^{13}C NMR spectra were recorded on a Bruker BBFO (500 MHz) and Bruker Avance III (400 MHz). The chemical shift (δ) values are given in parts per million (ppm), and the coupling constants (J) are given in hertz (Hz). The spectra were recorded using $CDCl_3$ and DMSO- d_6 solvents. ^{1}H NMR chemical shifts are referenced to tetramethylsilane (TMS) (0 ppm) and ^{13}C NMR referenced to $CDCl_3$ (77.0 ppm) or DMSO-d_6 (39.51 ppm). HRMS recorded with QTOF-ESI source M/S Bruker Daltonik GmbH, Germany. The progress of the reaction was monitored by TLC using Merck pre-coated TLC sheets. The melting point of compounds was determined on digital melting point apparatus (Model 33/0112) from a VEEGO-VMP-DS spectrometer. X-ray diffractions were recorded on a Siemens P4 or Simart-1000 diffractometer. Column chromatography was performed on 100–120 mesh silica gel using hexane/ethyl acetate as eluting solvents and solvents were used without further distillation, methanol is dried over 5A molecular sieves. All commercial chemicals were purchased from Merck, Avra, Carbanio, and SRL. Starting materials **2a-m** and **3a-l** were prepared according to the previous literature methods[1,2] and used for the final reactions.

The geometry optimization and frequency calculation were carried out using the Gaussian 09[3] software using the B3LYP[4,5]/GENECP level of theory. The split basis set (GENECP) included LANL2DZ[6] for the iodine atom and 6-31[7] for all the other atoms (i.e., C, H, O, S, N). All positive frequencies indicate the lowest energy structure of these isomeric pairs. The FMO analysis was carried out at the same level of theory using the coordinates of the optimized geometries.

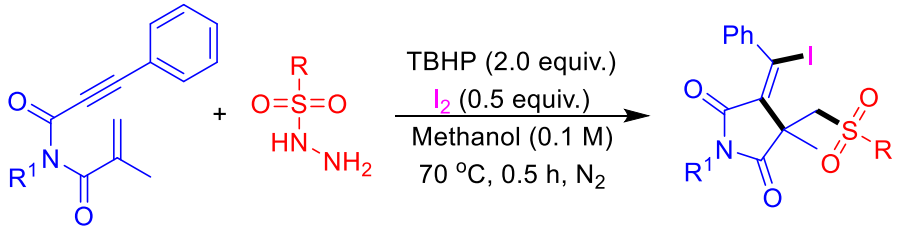
(2) Experimental Set up for 4aa.



A **B**

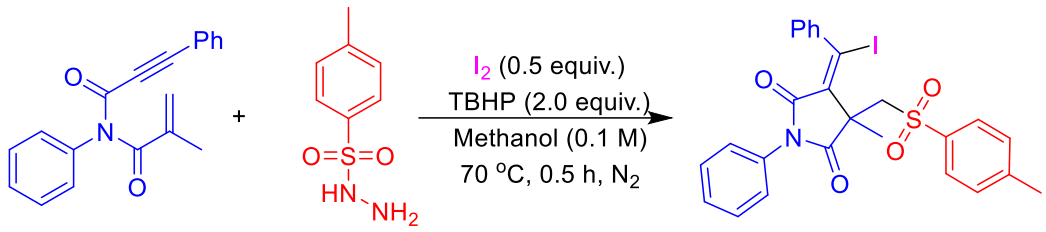
Figure S1. Model experimental setup for sulphonated succinimide synthesis: A) At the start of reaction; B) Reaction completion (After - 0.5 h)

(3) General procedure for the synthesis of 4aa-al and **4ba-ma**.



A round-bottom flask equipped with a magnetic stir bar was charged with **2a-l** (0.5mmol), **3a-l** (1.0mmol) and I_2 (0.25mmol), sealed with a septum, and degassed by alternating vacuum evacuation and N_2 back filling. Then TBHP (1.0 mmol) and methanol (5.0 mL, 0.1M) was charged under N_2 atmosphere. Then the reaction mixture was heated to 70 ^oC with stirring for 0.5 h (monitored reactions by TLC). After the completion, the precipitated solid was filtered and washed with methanol (2x3 mL) to afford the pure compounds **4aa-al** and **4ba-ma** as an off-white to white solid.

(4) Experimental procedure for the gram scale synthesis.



2a
1.0 g (3.46 mmol)

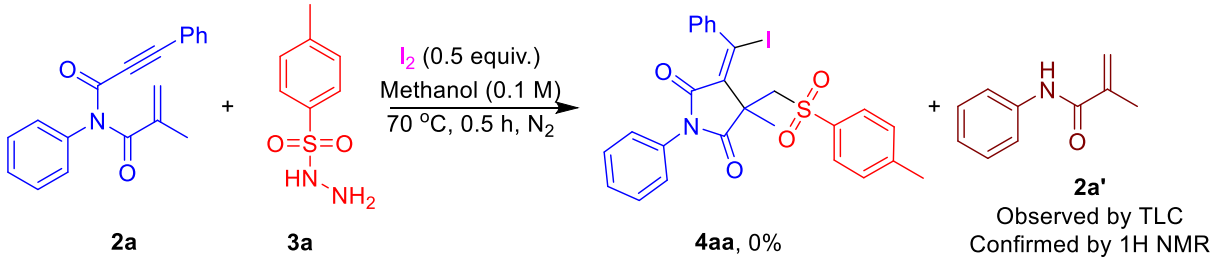
3a
1.28g (6.91 mmol)

4aa
1.2 g (65%)

A 100mL round-bottom flask equipped with a magnetic stir bar was charged with **2a** (3.46 mmol), **3a** (6.91 mmol) and I_2 (1.73 mmol) sealed with a septum, and degassed by alternating vacuum evacuation and N_2 back filling. Next TBHP (6.91 mmol) and methanol (34.6 mL) were charged under an N_2 atmosphere. Then the reaction mixture was heated to 70 °C with stirring for 0.5 h (monitored reactions by TLC). After the completion, the precipitated solid was filtered and washed with methanol (3x5 mL) to obtain the pure white solid compound **4aa** (1.2g, 65% yield).

(5) Control Studies.

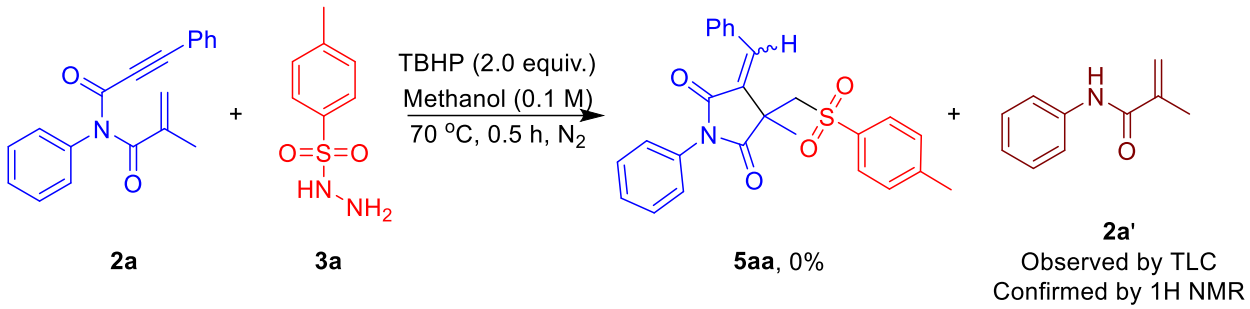
a) Without TBHP.



2a **3a** **4aa**, 0% **2a'**
Observed by TLC
Confirmed by 1H NMR

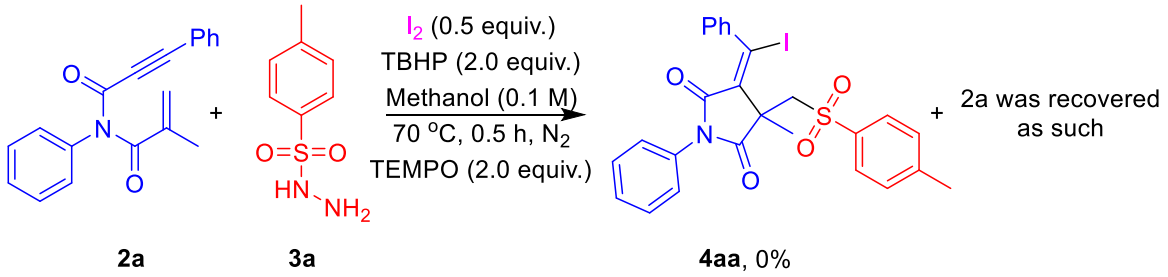
A round-bottom flask equipped with a magnetic stir bar was charged with **2** (1.0 equiv., 0.5 mmol), **3** (2.0 equiv., 1.0 mmol) and I_2 (0.5 equiv., 0.25 mmol), sealed with a septum, and degassed by alternating vacuum evacuation and N_2 back filling. Then methanol (5.0 mL, 0.1 M) was charged under N_2 atmosphere. Then the reaction mixture was heated to 70 °C with stirring for 0.5 h (monitored reactions by TLC). **4aa** was not observed, only cleavage product of **2a'**was observed.

b) Without Iodine.



To a round-bottom flask equipped with magnetic stir bar was charged with **2** (1.0 equiv., 0.5 mmol), **3** (2.0 equiv., 1.0 mmol), sealed with a septum, and degassed by alternating vacuum evacuation and N_2 back filling. Then TBHP (2.0 equiv., 1.0 mmol) and methanol (5.0 mL, 0.1 M) was charged under N_2 atmosphere. Then the reaction mixture was heated to 70 °C with stirring for 0.5 h (monitored reactions by TLC). **4aa**was not observed, only cleavage product of **2a'** was observed.

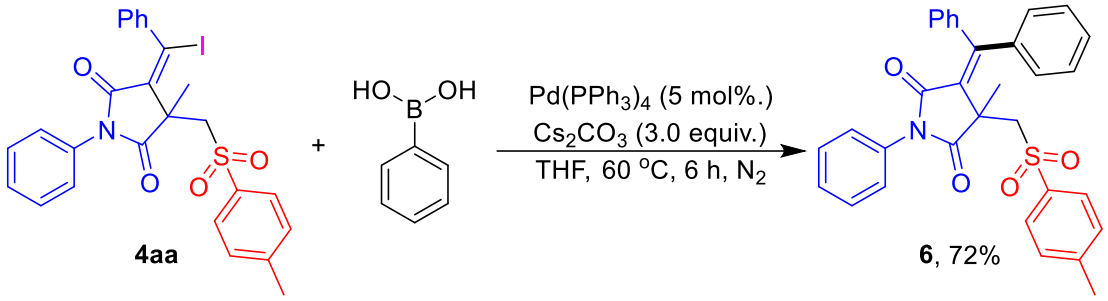
c) TEMPO Reaction.



To a round-bottom flask equipped with magnetic stir bar was charged with **2** (1.0 equiv., 0.5 mmol), **3** (2.0 equiv., 1.0 mmol), TEMPO (2.0 equiv., 1.0 mmol) and I_2 (0.5 equiv., 0.25 mmol), sealed with a septum, and degassed by alternating vacuum evacuation and N_2 back filling. Then TBHP (2.0 equiv., 1.0 mmol) and methanol (5.0 mL, 0.1 M) was charged under N_2 atmosphere. Then the reaction mixture was heated to 70 °C with stirring for 0.5 h (monitored reactions by TLC). **4aa** was not formed, starting material remains not involved in the reaction.

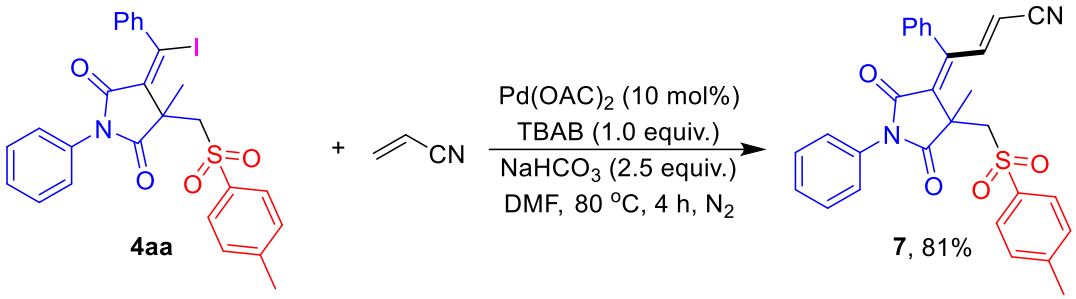
(6) Synthetic applications

Synthesis of 4-(diphenylmethylene)-3-methyl-1-phenyl-3-(tosylmethyl)pyrrolidine-2,5-dione (6).



To a round-bottom flask added **4aa** (0.1 mmol, 57.1 mg), phenyl boronic acid (0.2 mmol, 24.4 mg), $Pd(PPh_3)_4$ (5 mol %, 5.8 mg), Cs_2CO_3 (0.3 mmol, 105.8 mg) and degassed by alternating vacuum evacuation and N_2 back filling. Then, THF (1 mL) was added under N_2 atmosphere. Then the reaction mixture was heated to 60 ºC with stirring for 6 h (monitored reactions by TLC). The mixture was diluted with H_2O (20 mL) and extracted with ethyl acetate (3×25 mL). The organic layers were dried with Na_2SO_4 and the solvent was then removed under reduced pressure with the aid of a rotary evaporator. The crude material was purified by silica gel column chromatography (Hex:EA=8:2) to afford the corresponding product **6** as white solid in 72% yield (37.4 mg); mp: 178-181 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.2 Hz, 2H), 7.52 (d, *J* = 7.0 Hz, 2H), 7.45 (s, 1H), 7.44 (s, 3H), 7.41 (d, *J* = 7.3 Hz, 3H), 7.39 (s, 2H), 7.36 (s, 1H), 7.34 (s, 2H), 7.32 (d, *J* = 2.1 Hz, 2H), 7.31 - 7.28 (m, 1H), 3.56 (d, *J* = 14.0 Hz, 1H), 3.19 (d, *J* = 14.0 Hz, 1H), 2.43 (s, 3H), 1.45 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.27, 167.11, 157.04, 144.99, 141.02, 139.51, 137.80, 132.20, 130.00, 128.92, 128.63, 128.51, 128.49, 128.27, 128.25, 128.11, 127.88, 127.66, 126.93, 126.75, 60.82, 45.78, 27.01, 21.66; HRMS (ESI): Calc'd for $[M+H]^+$ $C_{32}H_{28}NO_4S$: 522.1734; found 522.1733.

Synthesis of (2*E*,4*Z*)-4-(4-methyl-2,5-dioxo-1-phenyl-4-(tosylmethyl)pyrrolidin-3-ylidene)-4-phenylbut-2-enenitrile (7).



To a round-bottom flask added compound **4aa** (57.1 mg, 0.1 mmol,), $Pd(OAc)_2$ (2.3 mg, 0.01 mmol), $(Bu)_4NBr$ (32.2 mg, 0.1 mmol), $NaHCO_3$ (21.0 mg, 0.25 mmol) and degassed by alternating vacuum evacuation and N_2 back filling. Then, acrylonirile (10.6 mg, 0.2 mmol), DMF (1.0 mL) were added under N_2 atmosphere and the reaction mixture was heated to 80 ºC with stirring for 4h (monitored reactions by TLC). The mixture was diluted with H_2O (20 mL) and extracted with ethyl acetate (3×25 mL). The organic layers were dried with Na_2SO_4 and the solvent was then removed under reduced pressure with the aid of a rotary evaporator. The crude material was purified by silica gel column chromatography (Hex:EA=7:3) to afford the corresponding product **7** as white solid in 81% yield (40.2 mg); mp: 202-204 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.3 Hz, 2H), 7.62 (d, *J* = 15.9 Hz, 1H), 7.44 (s, 1H), 7.42 (s, 3H), 7.40 (d, *J* = 5.4 Hz, 2H), 7.37 (s, 1H), 7.35 (d, *J* = 1.7 Hz, 2H), 7.33 (s, 1H), 7.24 (d, *J* = 7.5 Hz, 2H), 5.30 (d, *J* = 15.9 Hz, 1H), 4.18 (d, *J* = 14.4 Hz, 1H), 3.82 (d, *J* = 14.4 Hz, 1H), 2.46 (s, 3H), 1.76 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.74, 165.91, 146.71, 146.44, 145.55, 136.92, 134.51, 131.77, 131.44, 130.24, 129.04, 128.84, 128.74, 128.64, 128.28, 127.85, 126.80, 117.38, 108.95, 61.70, 45.31, 25.24, 21.73; HRMS (ESI): Calc'd for $[M+H]^+$ $C_{29}H_{25}N_2O_4S$: 497.1530; found 497.1518.

(7) Computational studies

To further understand the double bond stereochemistry, computational studies were performed. The optimized geometries of *E* and *Z* isomers of **4aa** and **4al** are shown in Figure S2. The energy of the molecules from the optimization, in Table S1, shows no difference indicating that the overall strength of the molecules is similar. This reveals that the non-bonding and steric parameters play a vital role in the pathway for formation of the products, thereby determining

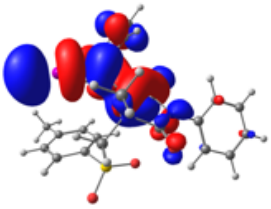
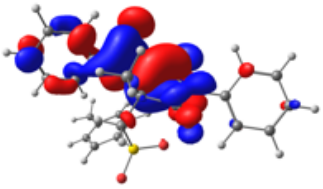
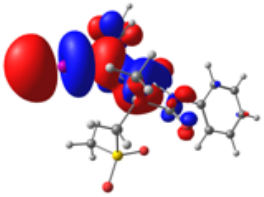
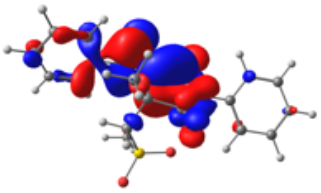
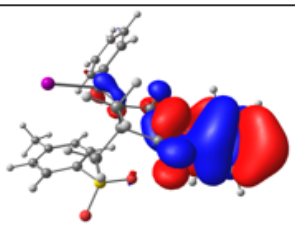
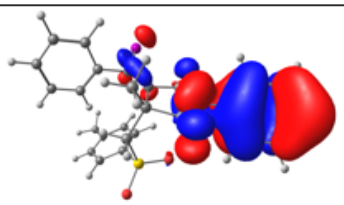
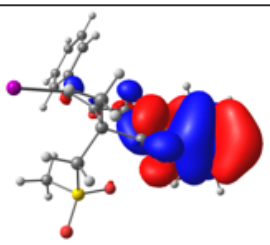
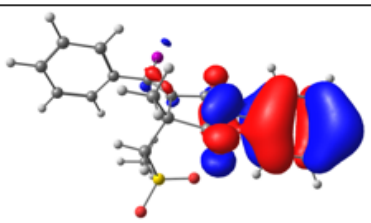
the nature of the products. From Table S2, it is evident that the distance between C atom of the phenyl ring (Cpy) connecting to the C=C and the S atom is larger in *E* isomers than the *Z* isomer. This indicates the presence of steric repulsion between the ring units (i.e., the toluene unit attached to the S atom and the phenyl unit attached to the C=C), where the two rings repel to exit in different planes on coming closer during the pentavalent ring formation. However, it can be seen that in the *E* isomer of **4aa**, a relatively shorter C-C bond length is formed indicating that the attraction between the C-C to form the ring is balanced by the repulsion of the phenyl ring units. Such a balance in the attraction and repulsion is not observed in the *Z*-isomer of **4aa**, where the Cpy-S distance is short, while the C-C ring formation has a bond length slightly longer than that of a single bond. In the case of *E* and *Z* isomers of **4al**, it can be seen that the difference in the Cpy-S distance (0.664 Å) is relatively less than in the isomers of **4aa** (0.772 Å), pointing to more similarity between the isomers. Further, the frontier molecular orbitals (FMO) were calculated and the contour plots are shown in Table S3 along with the energy values of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). The difference between the HOMO-LUMO gap values validates that the *E* and *Z* isomers of the **4al** (0.07) are quite similar (with *E* isomer having a slightly smaller gap, i.e., 4.44, than Z isomer, i.e., 4.51) compared to the isomers of **4aa** (0.21). This supports the experimental observation of obtaining both the *E* and *Z* isomers in the case of **4al**, with *E* isomer being stereoselective product in both **4aa**.

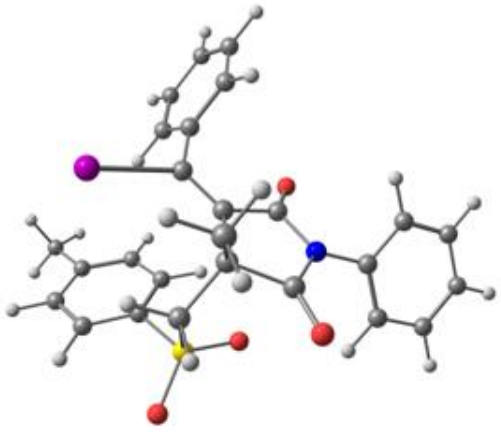
Table S1. Energy of the molecules

Complex	R = Methyl		R = Toluene	
	E isomer - **4al**	*Z* isomer - **4al**	*E* isomer - **4aa**	*Z* isomer - **4aa**
Energy (in $x10^3$ eV)	-41.854	-41.854	-48.141	-48.141
Energy (in $x10^4$ kcal/mol)	-96.518	-96.518	-111.016	-111.016

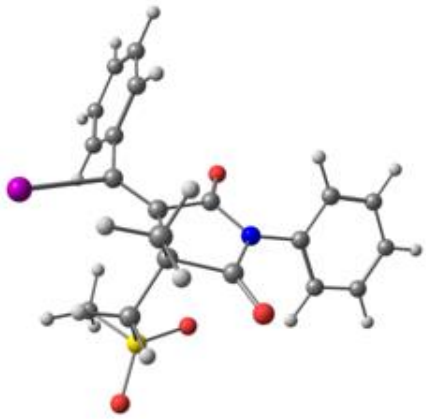
Table S2. Atom and distances

Complex	Atom distance between C_{py}-S (Å)	Pentavalent ring forming C-C (Å)
E isomer - **4aa**	5.400	1.525
Z isomer - **4aa**	4.682	1.534
E isomer - **4al**	5.297	1.525
Z isomer - **4al**	4.633	1.534

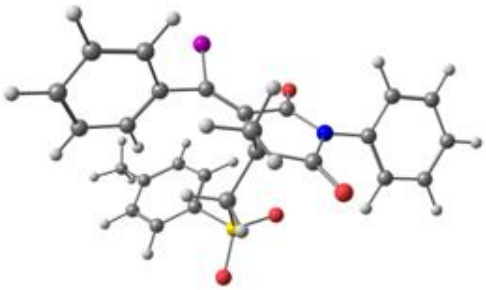
Table S3. HOMO-LUMO contour plots (isosurface 0.025)				
	E isomer - 4aa	**Z isomer - 4aa**	**E isomer - 4al**	**Z isomer - 4al**
LUMO	 -1.86	 -1.84	 -2.15	 -2.01
GAP	4.59	4.80	4.44	4.51
HOMO	 -6.45	 -6.64	 -6.60	 -6.52



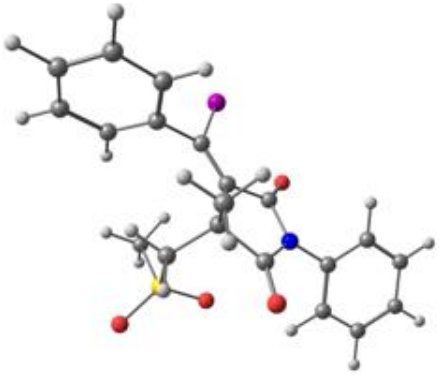
E isomer - **4aa**



E isomer - **4al**



Z isomer - **4aa**



Z isomer - **4al**

Figure S2. Optimized geometry of **4aa** and **4al** in the *E* and *Z* isomeric forms

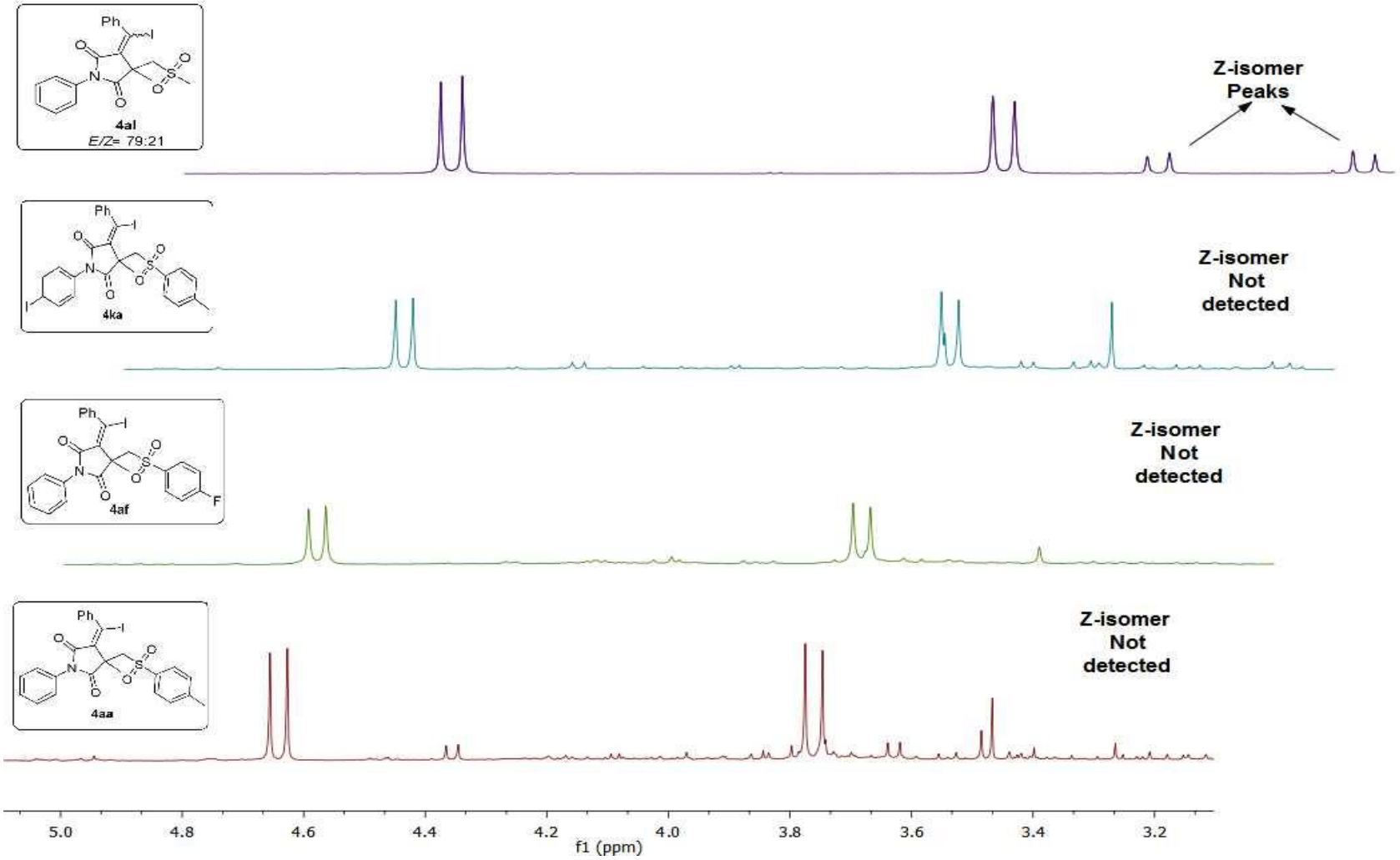


Figure S3: ^{1}H NMR spectra for Comparison of **4al** (***E***-isomer) with crude NMR of **4aa**, **4af** and **4ka**

(9) Characterization Data of the Products 4aa-al and 4ba-ma

(*E*)-4-(iodo(phenyl)methylene)-3-methyl-1-phenyl-3-(tosylmethyl)pyrrolidine-2,5-dione (4aa). The title compound was prepared according to the general procedure and the product was isolated by filtration to obtain as a white solid (192mg, yield = 74%); mp:236-239 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (d, *J* = 8.0 Hz, 2H), 7.41 (d, *J* = 7.2 Hz, 2H), 7.38 (s, 3H), 7.36 (d, *J* = 4.1 Hz, 6H), 7.31 – 7.27 (m, 1H), 4.64 (d, *J* = 14.2 Hz, 1H), 3.76 (d, *J* = 14.2 Hz, 1H), 2.46 (s, 3H), 1.80 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.09, 163.69, 145.20, 144.77, 137.40, 134.22, 131.62, 130.12, 129.12, 129.00, 128.76, 128.11, 127.92, 126.89, 126.68, 119.34, 58.12, 47.91, 22.42, 21.72; HRMS (ESI): Calc'd for $[M+H]^+$ $C_{26}H_{23}INO_4S$: 572.0387; found 572.0389.

(*E*)-4-(iodo(phenyl)methylene)-3-methyl-1-phenyl-3(phenylsulphonyl)methyl) pyrrolidine-2,5-dione (4ab). The title compound was prepared according to the general procedure and the product was isolated by filtration to obtain as a white solid (176mg, yield = 70%); mp:254.2-258 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.3 Hz, 2H), 7.69 (t, *J* = 7.5 Hz, 1H), 7.59 (t, *J* = 7.7 Hz, 2H), 7.43 (s, 1H), 7.41 (s, 1H), 7.39 (s, 2H), 7.37 (d, *J* = 4.3 Hz, 5H), 7.29 (dd, *J* = 8.7, 4.4 Hz, 1H), 4.67 (d, *J* = 14.2 Hz, 1H), 3.79 (d, *J* = 14.2 Hz, 1H), 1.81 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.08, 163.66, 144.72, 140.35, 134.22, 134.09, 131.61, 129.52, 129.15, 129.01, 128.78, 128.12, 127.88, 126.89, 126.67, 119.40, 58.08, 47.95, 22.41; HRMS (ESI): Calc'd for $[M+H]^+$ $C_{25}H_{21}INO_4S$: 558.0231; found 558.0231.

(*E*)-4-(iodo(phenyl)methylene)-3-(((4-methoxyphenyl)sulphonyl)methyl)-3-methyl-1-phenyl pyrrolidine-2,5-dione (4ac). The title compound was prepared according to the general procedure and the product was isolated by filtration to obtain as a white solid (188mg, yield = 70%); mp:266.4-268.4 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 9.0 Hz, 2H), 7.45 - 7.41 (m, 1H), 7.41 - 7. 37 (m, 3H) 7.36 (d, *J* = 4.4 Hz, 5H), 7.29 (dd, *J* = 8.7, 4.4 Hz, 1H), 7.02 (d, *J* = 8.9 Hz, 2H), 4.63 (d, *J* = 14.2 Hz, 1H), 3.89 (s, 3H), 3.76 (d, *J* = 14.2 Hz, 1H), 1.80

(s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.12, 164.05, 163.71, 144.77, 134.24, 131.90, 131.63, 130.15, 129.12, 128.99, 128.74, 128.09, 126.88, 126.71, 119.29, 114.66, 58.34, 55.78, 47.94, 22.40; HRMS (ESI): Calc'd for $[M+H]^+C_{26}H_{23}INO_5S$: 588.0336; found 588.0329.

(*E*)-3-(((4-(tert-butyl)phenyl)sulphonyl)methyl)-4-(iodo(phenyl)methylene)-3-methyl-1-phenyl pyrrolidine-2,5-dione (4ad). The title compound was prepared according to the general procedure and the product was isolated by filtration to obtain as a white solid (189mg, yield = 67%); mp:233.7-235.8 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.6 Hz, 2H), 7.58 (d, *J* = 8.6 Hz, 2H), 7.42 (s, 1H), 7.40 (s, 1H), 7.39 (s, 2H), 7.36 (d, *J* = 4.9 Hz, 5H), 7.29 (dd, *J* = 8.8, 4.5 Hz, 1H), 4.65 (d, *J* = 14.2 Hz, 1H), 3.78 (d, *J* = 14.2 Hz, 1H), 1.80 (s, 3H), 1.35 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.09, 163.70, 158.09, 144.76, 137.30, 134.25, 131.64, 129.11, 128.99, 128.74, 128.09, 127.78, 126.90, 126.69, 126.52, 119.28, 58.13, 47.91, 35.35, 31.07, 22.41; HRMS (ESI): Calc'd for $[M+H]^+C_{29}H_{29}INO_4S$: 614.0857; found 614.0856.

(*E*)-N-(4-(((4-(iodo(phenyl)methylene)-3-methyl-2,5-dioxo-1-phenylpyrrolidin-3-yl) methyl)sulphonyl)phenyl)acetamide (4ae). The title compound was prepared according to the general procedure and the product was isolated by filtration to obtain as a white solid (97mg, yield = 36%); mp:290.3-292.7 ºC; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.7 Hz, 2H), 7.72 (d, *J* = 8.1 Hz, 2H), 7.45 – 7.40 (m, 3H), 7.40 – 7.33 (m, 7H), 7.29 (d, *J* = 5.2 Hz, 1H), 4.65 (d, *J* = 14.2 Hz, 1H), 3.76 (d, *J* = 14.2 Hz, 1H), 2.21 (s, 3H), 1.81 (s, 3H); ^{13}C NMR (101 MHz, DMSO) δ 176.89, 169.81, 163.97, 145.61, 144.90, 134.08, 133.66, 132.33, 129.36, 129.30, 129.12, 128.89, 128.11, 127.53, 127.09, 119.67, 119.42, 58.57, 47.87, 24.67, 22.00; HRMS (ESI): Calc'd for $[M+H]^+ C_{27}H_{24}IN_2O_5S$: 615.0445; found 615.0445.

(*E*)-3-(((4-fluorophenyl)sulphonyl)methyl)-4-(iodo(phenyl)methylene)-3-methyl-1-phenyl pyrrolidine-2,5-dione (4af). The title compound was prepared according to the general procedure and the product was isolated by filtration to obtain as a white solid (202mg, yield = 74%); mp:274.2-277 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 – 7.95 (m, 2H), 7.43 (s, 1H), 7.41

(s, 1H), 7.37 (d, *J* = 6.0 Hz, 7H), 7.32 - 7.27 (m, 2H), 7.24 (s, 1H), 4.68 (d, *J* = 14.2 Hz, 1H), 3.78 (d, *J* = 14.2 Hz, 1H), 1.81 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.06, 166.07 (d, *J* = 253.9 Hz), 163.61, 144.64, 136.41 (d, *J* = 3.2 Hz), 134.14, 131.55, 130.85(d, *J* = 9.6 Hz), 129.22, 129.04, 128.83, 128.15, 126.85, 126.66, 119.52, 116.86 (d, *J* = 22.6 Hz), 58.26, 48.00, 22.38; HRMS (ESI): Calc'd for $[M+H]^+$ $C_{25}H_{20}FINO_4S$: 576.0136; found 576.0127.

(*E*)-3-(((4-chlorophenyl)sulphonyl)methyl)-4-(iodo(phenyl)methylene)-3-methyl-1-phenyl pyrrolidine-2,5-dione (4ag). The title compound was prepared according to the general procedure and the product was isolated by filtration to obtain as a white solid (197mg, yield = 72%); mp: 245.8-248 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.6 Hz, 2H), 7.56 (d, *J* = 8.6 Hz, 2H), 7.43 (s, 1H), 7.41 (s, 1H), 7.36 (d, *J* = 6.9 Hz, 7H), 7.32 – 7.27 (m, 1H), 4.68 (d, *J* = 14.2 Hz, 1H), 3.77 (d, *J* = 14.2 Hz, 1H), 1.81 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.99, 163.58, 144.61, 141.00, 138.71, 134.09, 131.53, 129.87, 129.42, 129.24, 129.05, 128.85, 128.16, 126.83, 126.67, 119.60, 58.16, 47.98, 22.40; HRMS (ESI): Calc'd for $[M+H]^+$ $C_{25}H_{20}ClINO_4S$: 591.9841; found 591.9841.

(*E*)-4-(iodo(phenyl)methylene)-3-methyl-1-phenyl-3-(((4(trifluoromethyl)phenyl) sulphonyl)methyl)pyrrolidine-2,5-dione (4ah). The title compound was prepared according to the general procedure and the product was isolated by filtration to obtain as a white solid (138mg, yield = 49%); mp:251.5-253.3 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, *J* = 8.2 Hz, 2H), 7.86 (d, *J* = 8.3 Hz, 2H), 7.47 – 7.41 (m, 2H), 7.40 - 7.38 (m, 1H), 7.37 (s, 2H), 7.35 (d, *J* = 3.4 Hz, 3H), 7.33 - 7.27 (m, 2H), 4.72 (d, *J* = 14.2 Hz, 1H), 3.80 (d, *J* = 14.2 Hz, 1H), 1.82 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.92, 163.53, 144.54, 143.66, 135.83 (d, *J* = 32.9 Hz), 134.03, 131.50, 129.31, 129.08, 128.91, 128.62, 128.18, 126.81, 126.70 (t, *J* = 3.8 Hz), 123.07 (d, *J* = 271.5 Hz), 119.76, 58.04, 48.01, 22.41; HRMS (ESI): Calc'd for $[M+H]^+$ $C_{26}H_{20}F_3INO_4S$: 626.0104; found 626.0093.

(*E*)-3-(((2,5-dichlorophenyl)sulphonyl)methyl)-4-(iodo(phenyl)methylene)-3-methyl-1-phenyl pyrrolidine-2,5-dione (4ai). The title compound was prepared according to the general procedure and the product was isolated by filtration to obtain as a white solid (96mg, yield = 36%); mp: 218-224 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 2.4 Hz, 1H), 7.59 - 7.55 (m, 1H), 7.54 - 7.50 (m, 1H), 7.44 (d, *J* = 7.8 Hz, 1H), 7.41 (s, 1H), 7.36 (d, *J* = 3.1 Hz, 3H), 7.34 (s, 2H), 7.31 - 7.28 (m, 2H), 7.27 (s, 1H), 5.07 (d, *J* = 14.5 Hz, 1H), 3.98 (d, *J* = 14.5 Hz, 1H), 1.84 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.45, 163.48, 144.42, 139.20, 135.17, 134.07, 134.05, 133.23, 131.48, 131.40, 130.89, 129.22, 129.04, 128.83, 128.14, 126.79, 126.63, 119.47, 56.47, 47.82, 22.58; HRMS (ESI): Calc'd for $[M+H]^+$ $C_{25}H_{19}Cl_2INO_4S$: 625.9451; found 625.9452.

(*E*)-4-(iodo(phenyl)methylene)-3-methyl-1-phenyl-3-(((4-(trifluoromethoxy)phenyl) sulphonyl)methyl)pyrrolidine-2,5-dione (4aj). The title compound was prepared according to the general procedure and the product was isolated by filtration to obtain as a white solid (153mg, yield = 53%); mp:231.2-234.6 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.8 Hz, 2H), 7.46 - 7.41 (m, 3H), 7.40 (s, 1H), 7.37 (t, *J* = 2.3 Hz, 3H), 7.36 (s, 4H), 7.33 - 7.27 (m, 1H), 4.70 (d, *J* = 14.2 Hz, 1H), 3.80 (d, *J* = 14.2 Hz, 1H), 1.81 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.01, 163.57, 153.29, 144.60, 138.51, 134.11, 131.54, 130.28, 129.25, 129.05, 128.85, 128.16, 126.83, 126.66, 121.25, 119.59, 58.22, 48.02, 22.38; HRMS (ESI): Calc'd for $[M+H]^+$ $C_{26}H_{20}F_3INO_5S$: 642.0054; found 642.0052.

(*E*)-4-(iodo(phenyl)methylene)-3-methyl-3-((naphthalen-2-ylsulphonyl)methyl)-1-phenyl pyrrolidine-2,5-dione (4ak). The title compound was prepared according to the general procedure and the product was isolated by filtration to obtain as a white solid (187mg, yield = 69%); mp: 245-248 ºC; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.53 (s, 1H), 8.03 (d, *J* = 8.7 Hz, 1H), 8.00 (d, *J* = 8.2 Hz, 1H), 7.95 (d, *J* = 8.2 Hz, 1H), 7.92 (dd, *J* = 8.7, 1.9 Hz, 1H), 7.70 (t, *J* = 7.5 Hz, 1H), 7.64 (t, *J* = 7.5 Hz, 1H), 7.46 – 7.27 (m, 10H), 4.73 (d, *J* = 14.3 Hz, 1H), 3.86 (d,

J = 14.3 Hz, 1H), 1.82 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.06, 163.69, 144.69, 137.01, 135.51, 134.19, 132.16, 131.64, 129.99, 129.81, 129.64, 129.58, 129.13, 129.03, 128.78, 128.09, 128.07, 127.90, 126.90, 126.68, 122.46, 119.52, 58.04, 47.96, 22.46; HRMS (ESI): Calc'd for $[M+H]^+$ $C_{29}H_{23}INO_4S$: 608.0387; found 608.0379.

(*E*)-4-(iodo(phenyl)methylene)-3-methyl-3-((methylsulphonyl)methyl)-1-phenyl pyrrolidine-2,5-dione (4al). The title compound was prepared according to the general procedure and the product was isolated by filtration to obtain as a white solid (103mg, yield = 46%, 79:21 E/Z mixture); mp: 244-249 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 7.7 Hz, 1H), 7.42 (d, *J* = 1.6 Hz, 1H), 7.40 (d, *J* = 1.6 Hz, 1H), 7.38 (s, 1H), 7.36 (s, 1H), 7.34 (s, 3H), 7.32 (d, *J* = 1.3 Hz, 1H), 7.30 (d, *J* = 1.6 Hz, 1H), 7.28 (s, 1H), 4.65 (d, *J* = 14.3 Hz, 1H), 3.75 (d, *J* = 14.3 Hz, 1H), 3.49 (d, *J* = 14.5 Hz, 0.26H), 3.15 (d, *J* = 14.6 Hz, 0.26H), 3.03 (s, 3H), 2.88 (s, 0.71H), 1.84 (s, 3H), 1.36 (s, 0.69H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.99, 163.51, 144.55, 143.66, 134.39, 131.45, 129.25, 129.20, 129.03, 128.84, 128.17, 126.78, 126.71, 126.67, 118.75, 59.53, 56.60, 47.72, 47.26, 44.20, 43.93, 25.42, 22.41; HRMS (ESI): Calc'd for $[M+H]^+$ $C_{20}H_{19}INO_4S$: 496.0074; found 496.0078.

(*E*)-4-(iodo(phenyl)methylene)-3-methyl-1-(p-tolyl)-3-(tosylmethyl)pyrrolidine-2,5-dione (4ba). The title compound was prepared according to the general procedure and the product was isolated by filtration to obtain as a white solid (174mg, yield = 65%); mp: 238-242 ºC; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.3 Hz, 2H), 7.37 (s, 1H), 7.35 (d, *J* = 4.4 Hz, 5H), 7.28 (dd, *J* = 8.9, 4.5 Hz, 1H), 7.25 – 7.19 (m, 4H), 4.63 (d, *J* = 14.2 Hz, 1H), 3.75 (d, *J* = 14.2 Hz, 1H), 2.46 (s, 3H), 2.34 (s, 3H), 1.79 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.17, 163.81, 145.16, 144.77, 138.77, 137.46, 134.30, 130.10, 129.63, 129.08, 128.97, 128.08, 127.92, 126.73, 126.62, 119.09, 58.12, 47.89, 22.42, 21.72, 21.26; HRMS (ESI): Calc'd for $[M+H]^+$ $C_{27}H_{25}INO_4S$: 586.0544; found 586.0546.

(*E*)-4-(iodo(phenyl)methylene)-1-(2-methoxyphenyl)-3-methyl-3-(tosylmethyl)

pyrrolidine-2,5-dione (4ca). The title compound was prepared according to the general procedure and the product was isolated by filtration to obtain as a white solid (192mg, yield = 70%); mp: 251.7-254 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.3 Hz, 2H), 7.40 – 7.30 (m, 8H), 7.29 – 7.23 (m, 2H), 7.00 (t, *J* = 7.6 Hz, 1H), 6.93 (d, *J* = 8.2 Hz, 1H), 4.64 (d, *J* = 14.2 Hz, 1H), 3.77 (d, *J* = 12.1 Hz, 4H), 2.45 (s, 3H), 1.80 (s, 3H);^{13}C NMR (101 MHz, $CDCl_3$) δ 176.83, 163.56, 154.75, 145.06, 144.73, 137.64, 134.62, 130.66, 130.06, 129.48, 129.01, 128.02, 127.92, 126.90, 120.98, 120.38, 118.52, 111.63, 58.06, 55.84, 48.27, 22.24, 21.70; HRMS (ESI): Calc'd for $[M+H]^+$ $C_{27}H_{25}INO_5S$: 602.0493; found 602.0492.

(*E*)-4-(iodo(phenyl)methylene)-1-(3-methoxyphenyl)-3-methyl-3-(tosylmethyl) pyrrolidine-2,5-dione (4da). The title compound was prepared according to the general procedure and the product was isolated by filtration to obtain as a white solid (178mg, yield = 65%); mp: 202.7-204.4 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.2 Hz, 2H), 7.38 (s, 1H), 7.36 (d, *J* = 4.6 Hz, 5H), 7.31 (d, *J* = 9.2 Hz, 1H), 7.30 – 7.27 (m, 1H), 6.95 (d, *J* = 9.0 Hz, 1H), 6.91 (s, 1H), 6.90 (s, 1H), 4.64 (d, *J* = 14.2 Hz, 1H), 3.78 (s, 3H), 3.75 (d, *J* = 14.2 Hz, 1H), 2.46 (s, 3H), 1.80 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.03, 163.61, 160.02, 145.19, 144.74, 137.43, 134.22, 132.61, 130.11, 129.72, 129.12, 128.09, 127.92, 126.71, 119.32, 119.24, 115.03, 112.49, 58.14, 55.45, 47.93, 22.41, 21.71; HRMS (ESI): Calc'd for $[M+H]^+$ $C_{27}H_{25}INO_5S$: 602.0493; found 602.0493.

(*E*)-4-(iodo(phenyl)methylene)-1-(4-methoxyphenyl)-3-methyl-3-(tosylmethyl) pyrrolidine-2,5-dione (4ea). The title compound was prepared according to the general procedure and the product was isolated by filtration to obtain as a white solid (193mg, yield = 72%); mp: 241.5-244.6 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.3 Hz, 2H), 7.38 (s, 2H), 7.35 (d, *J* = 5.8 Hz, 4H), 7.29 (d, *J* = 9.0 Hz, 3H), 6.93 (d, *J* = 9.0 Hz, 2H), 4.63 (d, *J* = 14.2 Hz, 1H), 3.79 (s, 3H), 3.75 (d, *J* = 14.2 Hz, 1H), 2.46 (s, 3H), 1.79 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.28, 163.94, 159.65, 145.17, 144.78, 137.45, 134.28, 130.10, 129.08,

128.08, 127.92, 126.71, 124.28, 119.06, 114.32, 58.13, 55.51, 47.84, 22.40, 21.71; HRMS (ESI): Calc'd for $[M+H]^+$ $C_{27}H_{25}INO_5S$: 602.0493; found 602.0491.

(*E*)-1-(3,5-dimethylphenyl)-4-(iodo(phenyl)methylene)-3-methyl-3-(tosylmethyl) pyrrolidine-2,5-dione (4fa). The title compound was prepared according to the general procedure and the product was isolated by filtration to obtain as a white solid (121mg, yield = 47%); mp: 236.5-239 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.3 Hz, 2H), 7.38 (s, 1H), 7.35 (d, *J* = 4.6 Hz, 5H), 7.30 – 7.26 (m, 1H), 6.98 (s, 1H), 6.95 (s, 2H), 4.63 (d, *J* = 14.2 Hz, 1H), 3.76 (d, *J* = 14.2 Hz, 1H), 2.46 (s, 3H), 2.30 (s, 6H), 1.79 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.21, 163.87, 145.15, 144.78, 138.82, 137.47, 134.35, 131.32, 130.70, 130.10, 129.07, 128.09, 127.94, 126.73, 124.51, 119.05, 58.03, 47.91, 22.46, 21.72, 21.24; HRMS (ESI): Calc'd for $[M+H]^+$ $C_{28}H_{27}INO_4S$: 600.0700; found 600.0700.

(*E*)-4-(iodo(phenyl)methylene)-3-methyl-3-(tosylmethyl)-1-(3,4,5-trimethoxyphenyl) pyrrolidine-2,5-dione (4ga). The title compound was prepared according to the general procedure and the product was isolated by filtration to obtain as a white solid (176mg, yield = 59%); mp: 163.3-166.6 ^oC; ^1H NMR (500 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.0 Hz, 2H), 7.39 (s, 1H), 7.37 (d, *J* = 6.1 Hz, 5H), 7.32 – 7.28 (m, 1H), 6.59 (s, 2H), 4.64 (d, *J* = 14.2 Hz, 1H), 3.83 (s, 6H), 3.81 (s, 3H), 3.74 (d, *J* = 14.2 Hz, 1H), 2.47 (s, 3H), 1.81 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.27, 163.84, 153.50, 145.27, 144.70, 138.35, 137.41, 134.17, 130.14, 129.14, 128.11, 127.88, 127.20, 126.67, 119.42, 104.68, 60.80, 58.19, 56.21, 47.91, 22.38, 21.72; HRMS (ESI): Calc'd for $[M+H]^+$ $C_{29}H_{29}INO_7S$: 662.0704; found 662.0705.

(*E*)-1-(4-fluorophenyl)-4-(iodo(phenyl)methylene)-3-methyl-3-(tosylmethyl)pyrrolidine-2,5-dione (4ha). The title compound was prepared according to the general procedure and the product was isolated by filtration to obtain as a white solid (117mg, yield = 43%); mp: 229-231.5 ^oC; ^1H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.3 Hz, 2H), 7.38 (s, 2H), 7.37 (t, *J* = 2.0 Hz, 3H), 7.36 (s, 3H), 7.32 – 7.28 (m, 1H), 7.11 (t, *J* = 8.7 Hz, 2H), 4.64 (d, *J* = 14.2 Hz, 1H),

3.74 (d, *J* = 14.2 Hz, 1H), 2.47 (s, 3H), 1.80 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.10, 163.63, 162.41 (d, *J* = 245.7 Hz), 145.29, 144.72, 137.32, 134.02, 130.15, 129.19, 128.85 (d, *J* = 88. Hz), 128.13, 127.90, 127.51 (d, *J* = 3.1 Hz), 126.62, 119.68, 116.01 (d, *J* = 22.8 Hz), 58.15, 47.89, 22.36, 21.72; HRMS (ESI): Calc'd for $[M+H]^+$ $C_{26}H_{22}FINO_4S$: 590.0293; found 590.0297.

(*E*)-1-(4-chlorophenyl)-4-(iodo(phenyl)methylene)-3-methyl-3-(tosylmethyl)pyrrolidine-2,5-dione (4ia). The title compound was prepared according to the general procedure and the product was isolated by filtration to obtain as a white solid (110mg, yield = 43%); mp: 219-221.4 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.1 Hz, 2H), 7.40 (s, 1H), 7.38 (d, *J* = 0.9 Hz, 3H), 7.37 (s, 2H), 7.36 (s, 1H), 7.35 (d, *J* = 1.0 Hz, 2H), 7.33 (d, *J* = 1.1 Hz, 1H), 7.31 (d, *J* = 7.6 Hz, 1H), 4.63 (d, *J* = 14.2 Hz, 1H), 3.74 (d, *J* = 14.2 Hz, 1H), 2.47 (s, 3H), 1.79 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.91, 163.40, 145.29, 144.69, 137.29, 134.59, 133.95, 130.14, 130.10, 129.21, 129.18, 128.21, 128.13, 127.89, 126.63, 119.85, 58.15, 47.91, 22.36, 21.71; HRMS (ESI): Calc'd for $[M+H]^+$ $C_{26}H_{22}ClINO_4S$: 605.9997; found 605.9997.

(*E*)-1-(4-bromophenyl)-4-(iodo(phenyl)methylene)-3-methyl-3-(tosylmethyl)pyrrolidine-2,5-dione (4ja). The title compound was prepared according to the general procedure and the product was isolated by filtration to obtain as a white solid (181mg, yield = 62%); mp: 224.5-225.9 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.3 Hz, 2H), 7.54(d, *J* = 8.7 Hz, 2H), 7.37(t, *J* = 6.9 Hz, 6H), 7.32 – 7.30 (m, 1H), 7.29 (s, 1H), 7.28-7.26 (m, 1H), 4.63 (d, *J* = 14.2 Hz, 1H), 3.73 (d, *J* = 14.2 Hz, 1H), 2.46 (s, 3H), 1.80 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.86, 163.35, 145.31, 144.69, 137.26, 133.93, 132.17, 130.63, 130.15, 129.23, 128.51, 128.14, 127.90, 126.62, 122.69, 119.92, 58.14, 47.92, 22.36, 21.73; HRMS (ESI): Calc'd for $[M+H]^+$ $C_{26}H_{22}BrINO_4S$: 649.9492; found 649.9495.

(*E*)-4-(iodo(phenyl)methylene)-1-(4-iodophenyl)-3-methyl-3-(tosylmethyl)pyrrolidine-2,5-dione (4ka). The title compound was prepared according to the general procedure and the

product was isolated by filtration to obtain as a white solid (160mg, yield = 53%); mp: 244.4-246.4 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.3 Hz, 2H), 7.75 (d, *J* = 8.6 Hz, 2H), 7.40 – 7.37 (t, *J* = 7.0 Hz, 6H), 7.32 – 7.27 (m, 1H), 7.14 (d, *J* = 8.6 Hz, 2H), 4.63 (d, *J* = 14.2 Hz, 1H), 3.73 (d, *J* = 14.2 Hz, 1H), 2.46 (s, 3H), 1.79 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.81, 163.29, 145.30, 144.67, 138.15, 137.27, 133.93, 131.35, 130.15, 129.23, 128.66, 128.14, 127.89, 126.62, 119.91, 94.32, 58.14, 47.93, 22.35, 21.73; HRMS (ESI): Calc'd for $[M+H]^+$ $C_{26}H_{22}I_2NO_4S$: 697.9354; found 697.9353.

(*E*)-1-(3-chlorophenyl)-4-(iodo(phenyl)methylene)-3-methyl-3-(tosylmethyl)pyrrolidine-2,5-dione (4la). The title compound was prepared according to the general procedure and the product was isolated by filtration to obtain as a white solid (174mg, yield = 63%); mp: 206.7-209.5 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.2 Hz, 2H), 7.41 – 7,38 (m, 2H), 7.37 (d, *J* = 5.4 Hz, 5H), 7.34 (s, 1H), 7.33 (d, *J* = 1.9 Hz, 1H), 7.32 (t, *J* = 1.8 Hz, 1H), 7.31 – 7.29 (m, 1H), 4.64 (d, *J* = 14.2 Hz, 1H), 3.74 (d, *J* = 14.2 Hz, 1H), 2.47 (s, 3H), 1.80 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.78, 163.27 145.30, 144.70, 137.28, 134.50, 133.90, 132.66, 130.15, 129.93, 129.23, 128.99, 128.15, 127.91, 127.18, 126.61, 125.20, 119.99, 58.13, 47.93, 22.39, 21.72; HRMS (ESI): Calc'd for $[M+H]^+$ $C_{26}H_{22}ClINO_4S$: 605.9997; found 605.9997.

(*E*)-1-(3,4-dichlorophenyl)-4-(iodo(phenyl)methylene)-3-methyl-3-(tosylmethyl) pyrrolidine-2,5-dione (4ma). The title compound was prepared according to the general procedure and the product was isolated by filtration to obtain as a white solid (85mg, yield = 32%); mp: 173-177.5^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 8.2, 1.7 Hz, 2H), 7.52 (s, 1H), 7.49 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.39 (d, *J* = 5.9 Hz, 4H), 7.36 – 7.28 (m, 4H), 4.64 (dd, *J* = 14.2, 1.8 Hz, 1H), 3.73 (dd, *J* = 14.2, 1.8 Hz, 1H), 2.47 (s, 3H), 1.80 (d, *J* = 1.8 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.68, 163.08, 145.38, 144.64, 137.16, 133.68, 133.00, 132.90, 130.84, 130.59, 130.18, 129.32, 128.84, 128.18, 127.89, 126.58, 126.28, 120.44, 58.14, 47.94, 22.33, 21.73; HRMS (ESI): Calc'd for $[M+H]^+$ $C_{26}H_{21}Cl_2INO_4S$: 639.9608; found 639.9608.

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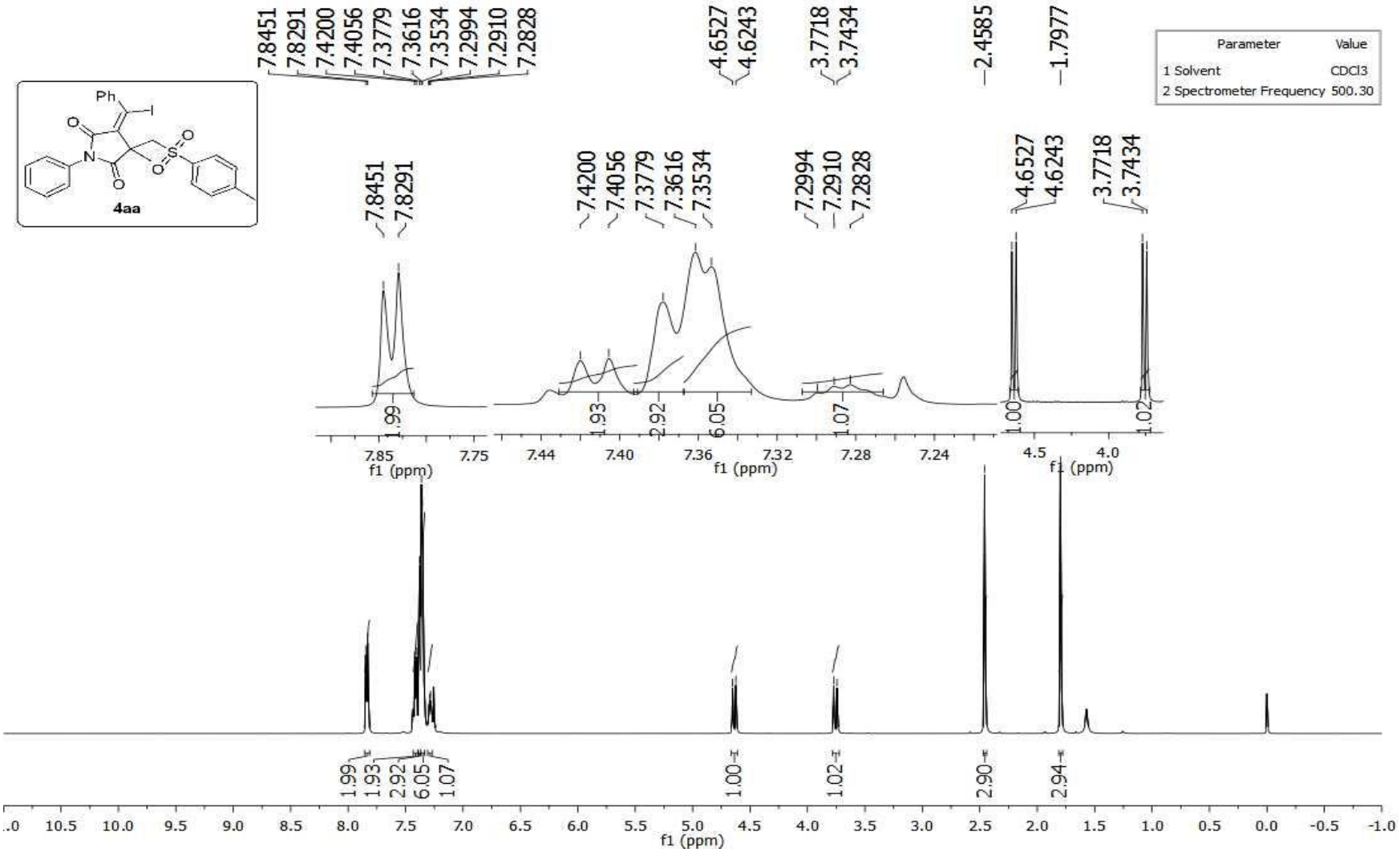

Figure S4. ^{1}H NMR spectra of (*E*)-4-(iodo(phenyl)methylene)-3-methyl-1-phenyl-3-(tosylmethyl)pyrrolidine-2,5-dione **(4aa)**

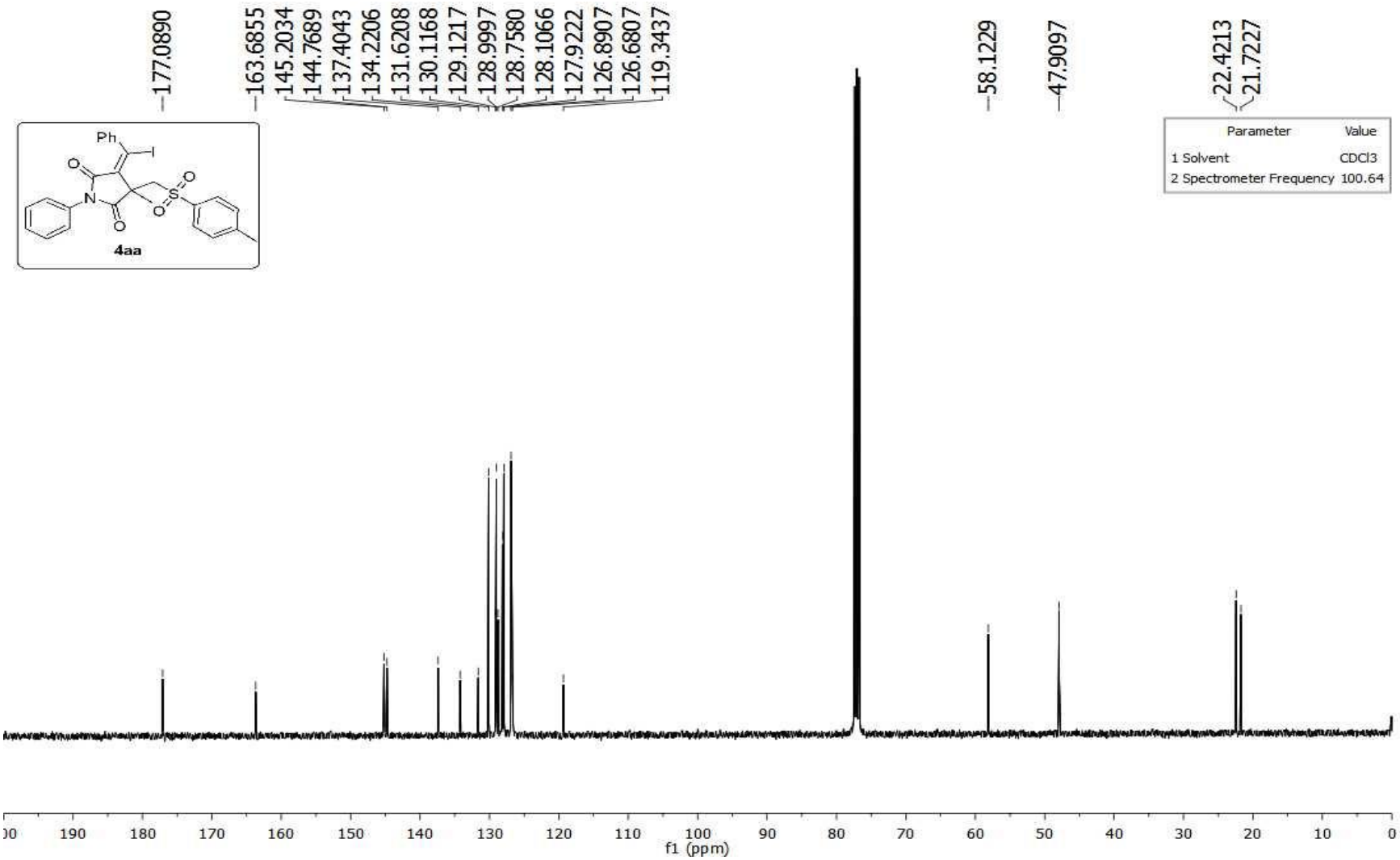

Figure S5. ^{13}C NMR spectra of (*E*)-4-(iodo(phenyl)methylene)-3-methyl-1-phenyl-3-(tosylmethyl)pyrrolidine-2,5-dione **(4aa)**

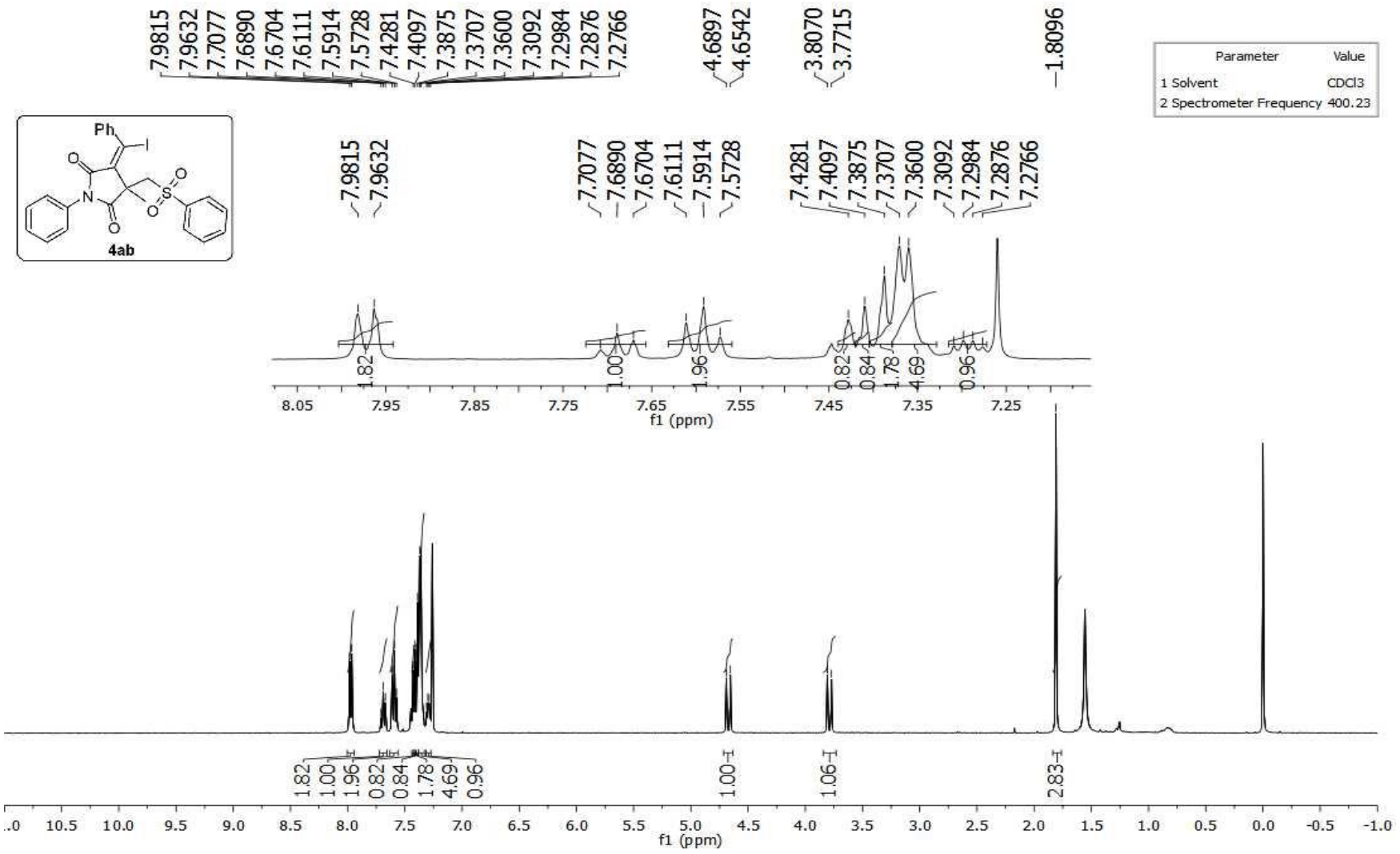

Figure S6. ^{1}H NMR spectra of (*E*)-4-(iodo(phenyl)methylene)-3-methyl-1-phenyl-3(phenylsulphonyl)methyl) pyrrolidine-2,5-dione **(4ab)**

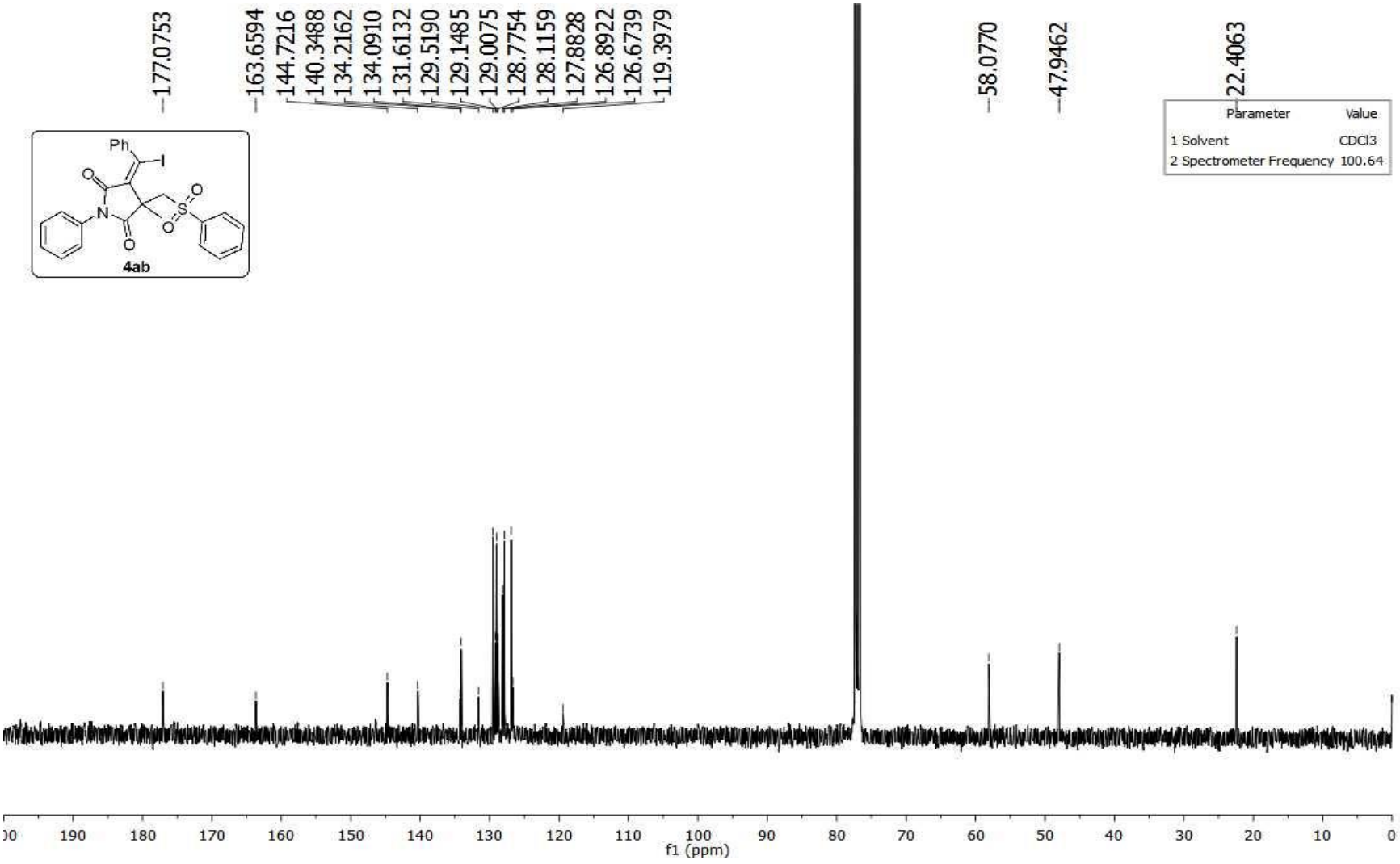

Figure S7. ^{13}C NMR spectra of (*E*)-4-(iodo(phenyl)methylene)-3-methyl-1-phenyl-3(phenylsulphonyl)methyl) pyrrolidine-2,5-dione **(4ab)**

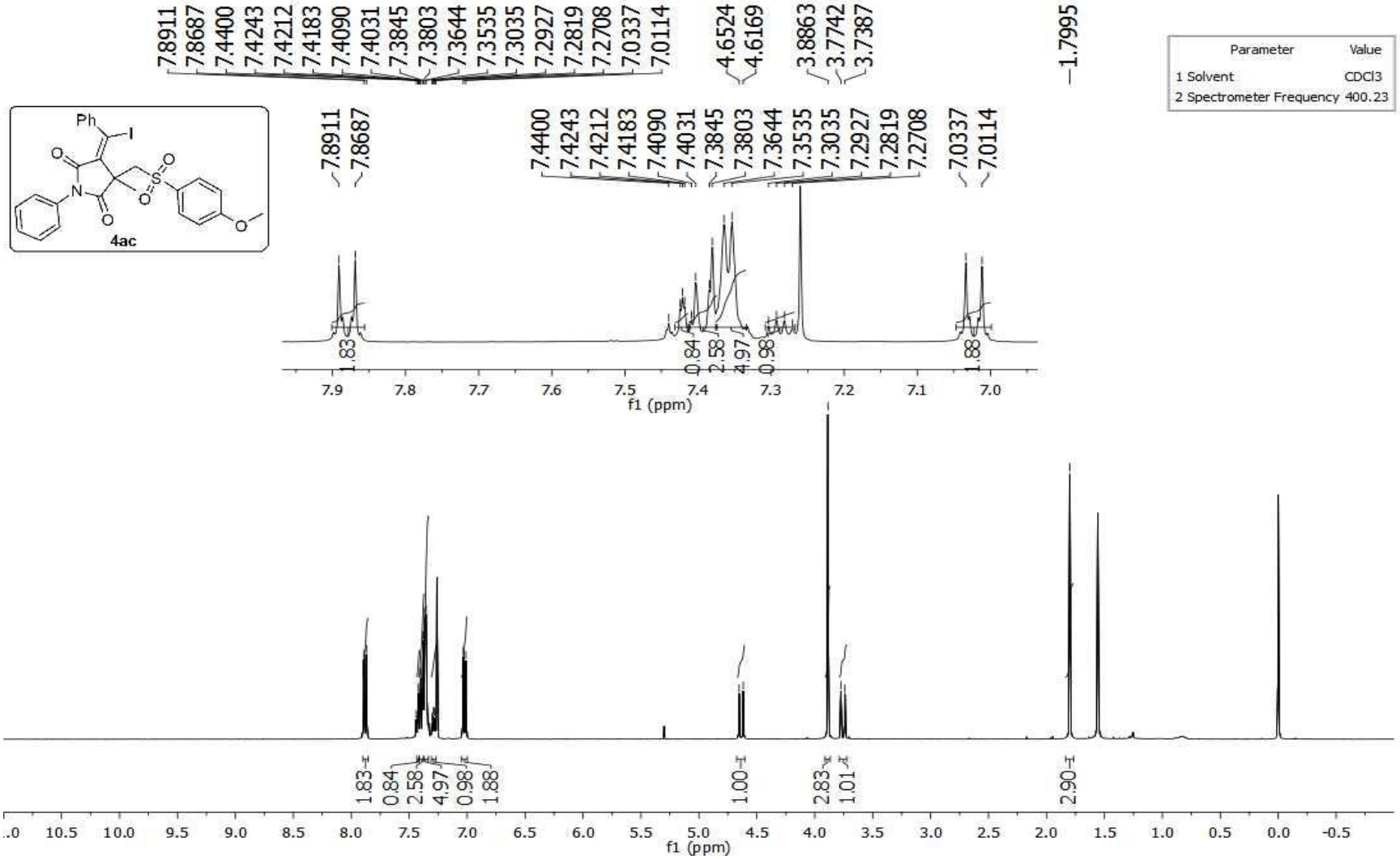

Figure S8. ^{1}H NMR spectra of (*E*)-4-(iodo(phenyl)methylene)-3-(((4-methoxyphenyl)sulphonyl)methyl)-3-methyl-1-phenyl pyrrolidine-2,5-dione **(4ac)**

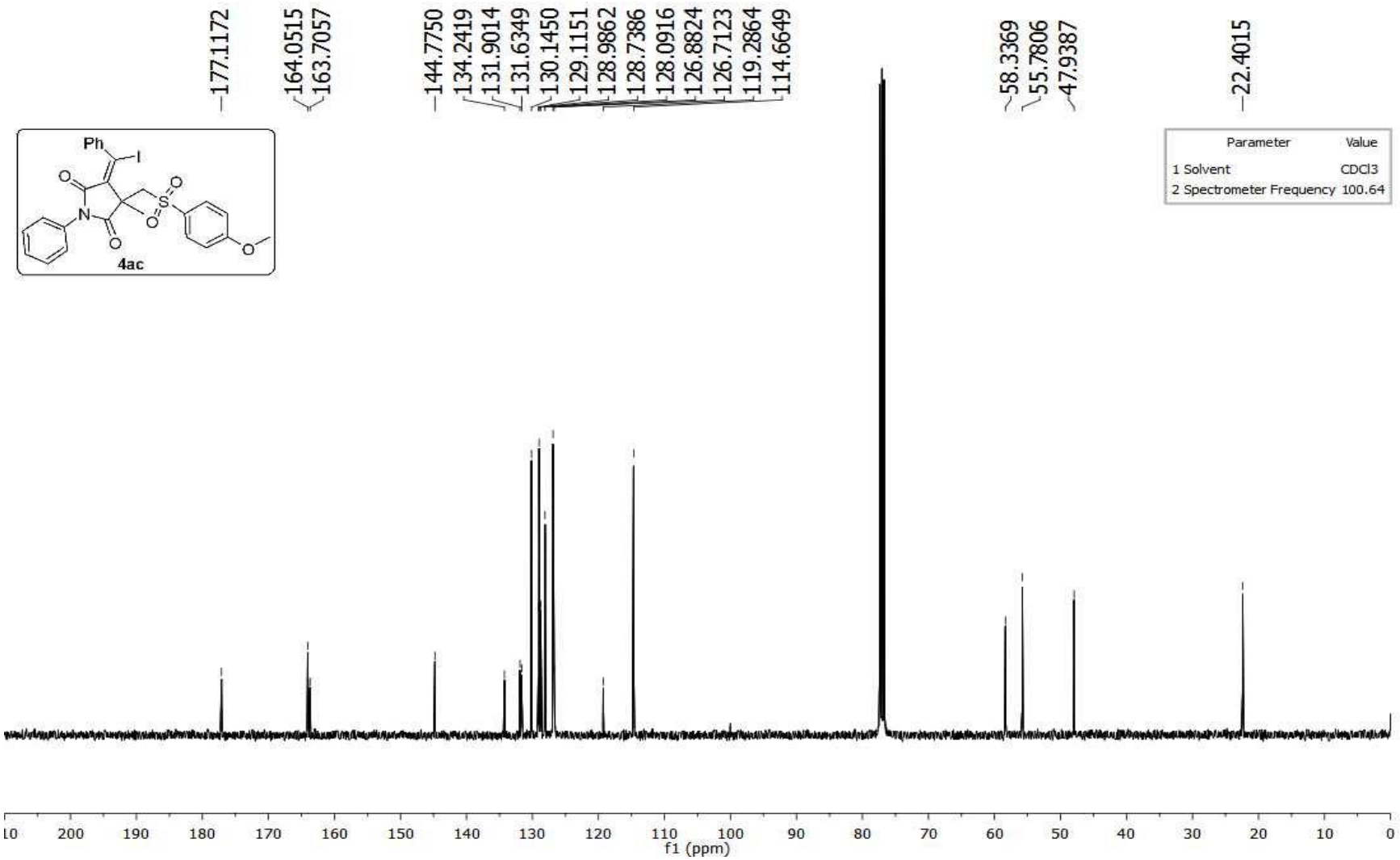

Figure S9. ^{13}C NMR spectra of (*E*)-4-(iodo(phenyl)methylene)-3-(((4-methoxyphenyl)sulphonyl)methyl)-3-methyl-1-phenyl pyrrolidine-2,5-dione **(4ac)**

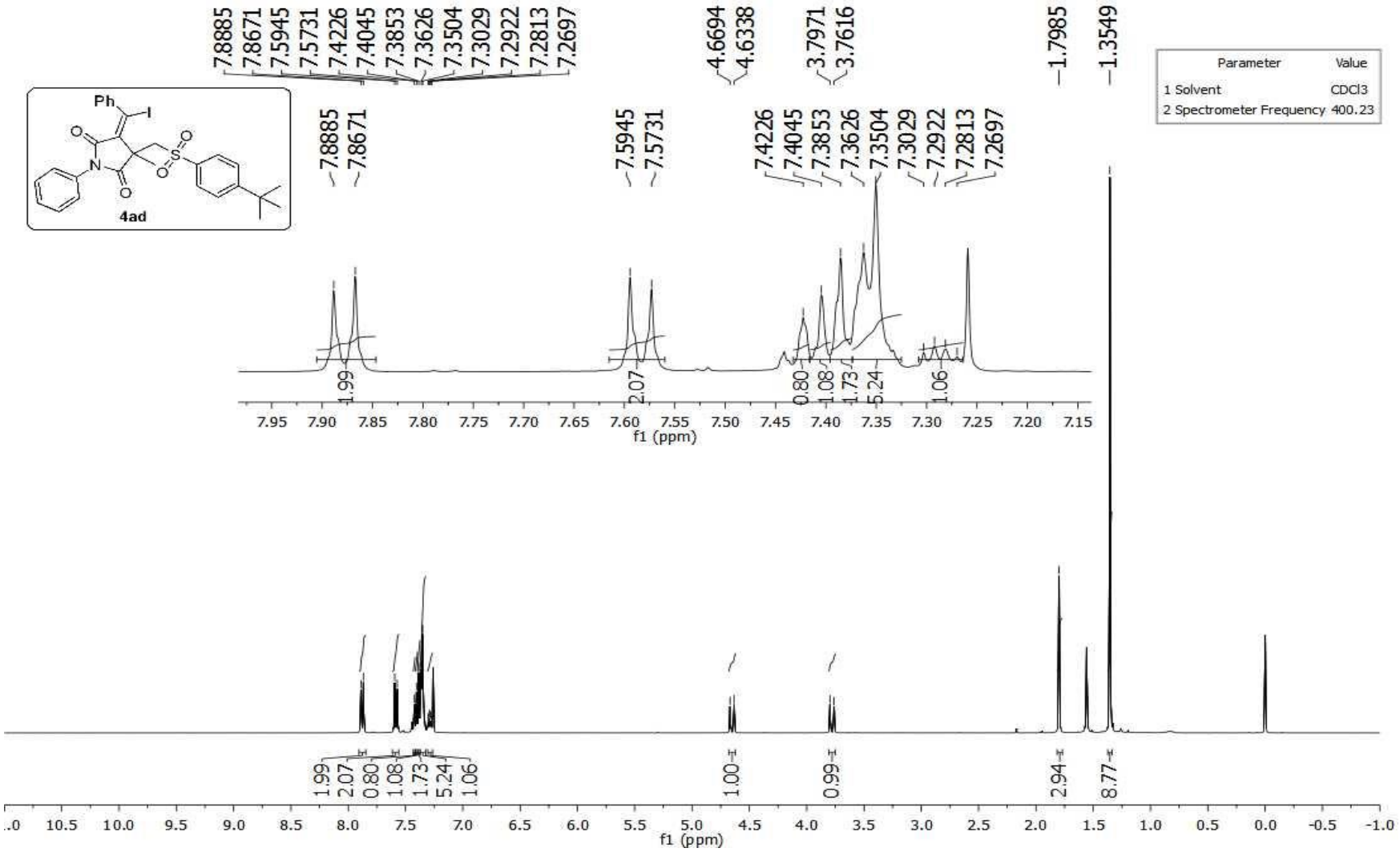

Figure S10. [1]H NMR spectra of (*E*)-3-(((4-(tert-butyl)phenyl)sulphonyl)methyl)-4-(iodo(phenyl)methylene)-3-methyl-1-phenyl pyrrolidine-2,5-dione **(4ad)**

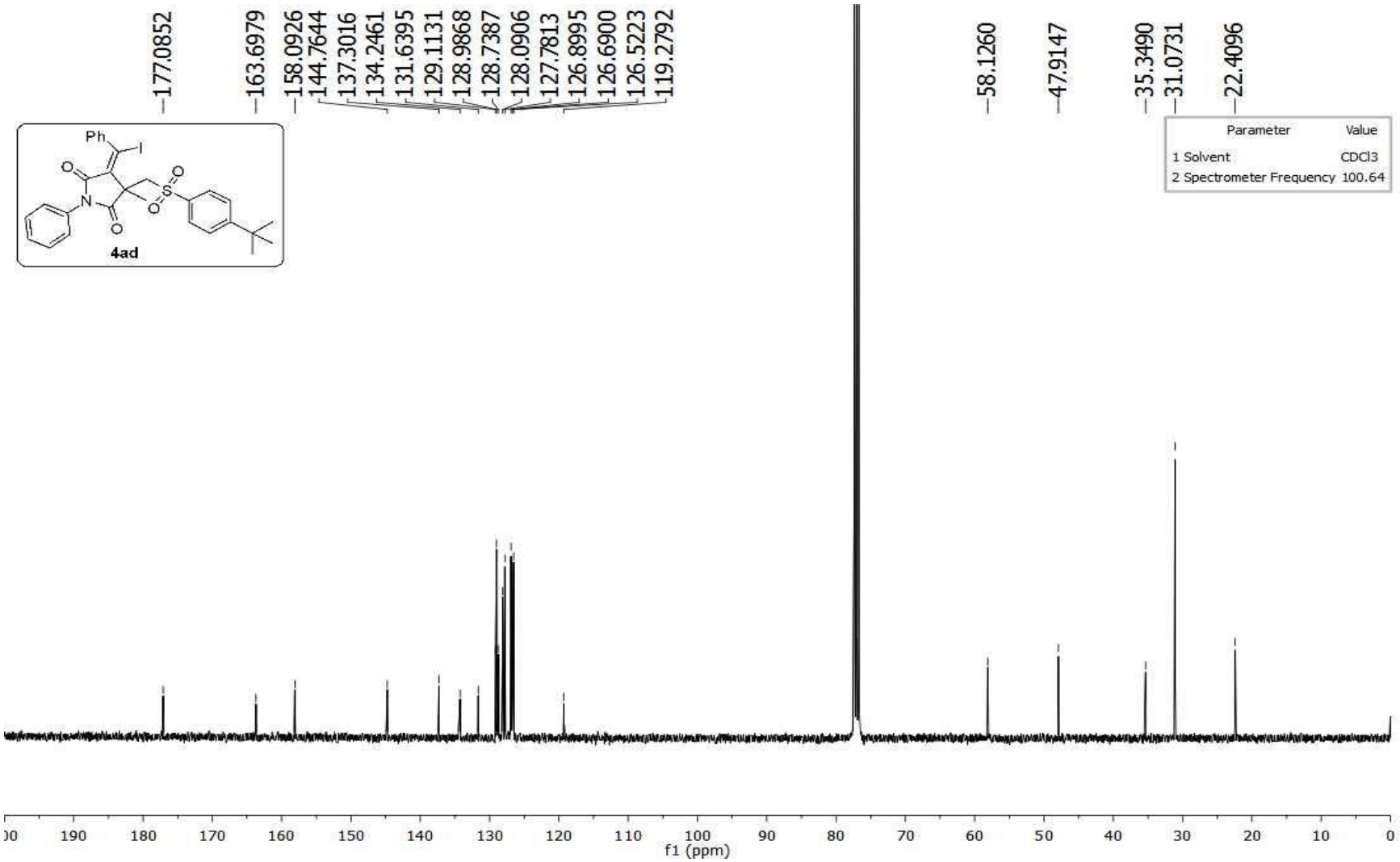

Figure S11. ^{13}C NMR spectra of (*E*)-3-(((4-(tert-butyl)phenyl)sulphonyl)methyl)-4-(iodo(phenyl)methylene)-3-methyl-1-phenyl pyrrolidine-2,5-dione **(4ad)**

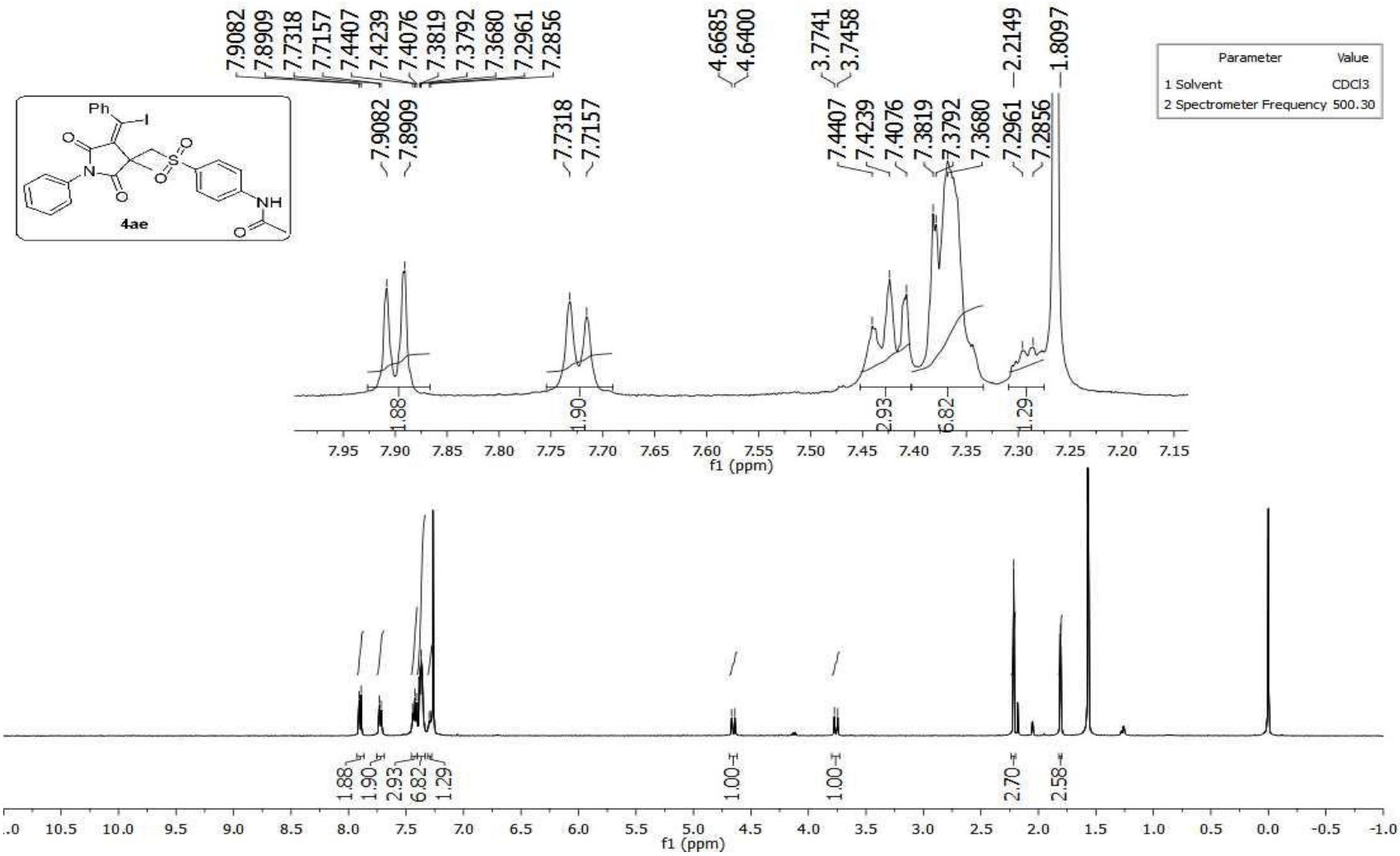

Figure S12. ^{1}H NMR spectra of (*E*)-N-(4-(((4-(iodo(phenyl)methylene)-3-methyl-2,5-dioxo-1-phenylpyrrolidin-3-yl) methyl)sulphonyl)phenyl)acetamide **(4ae)**

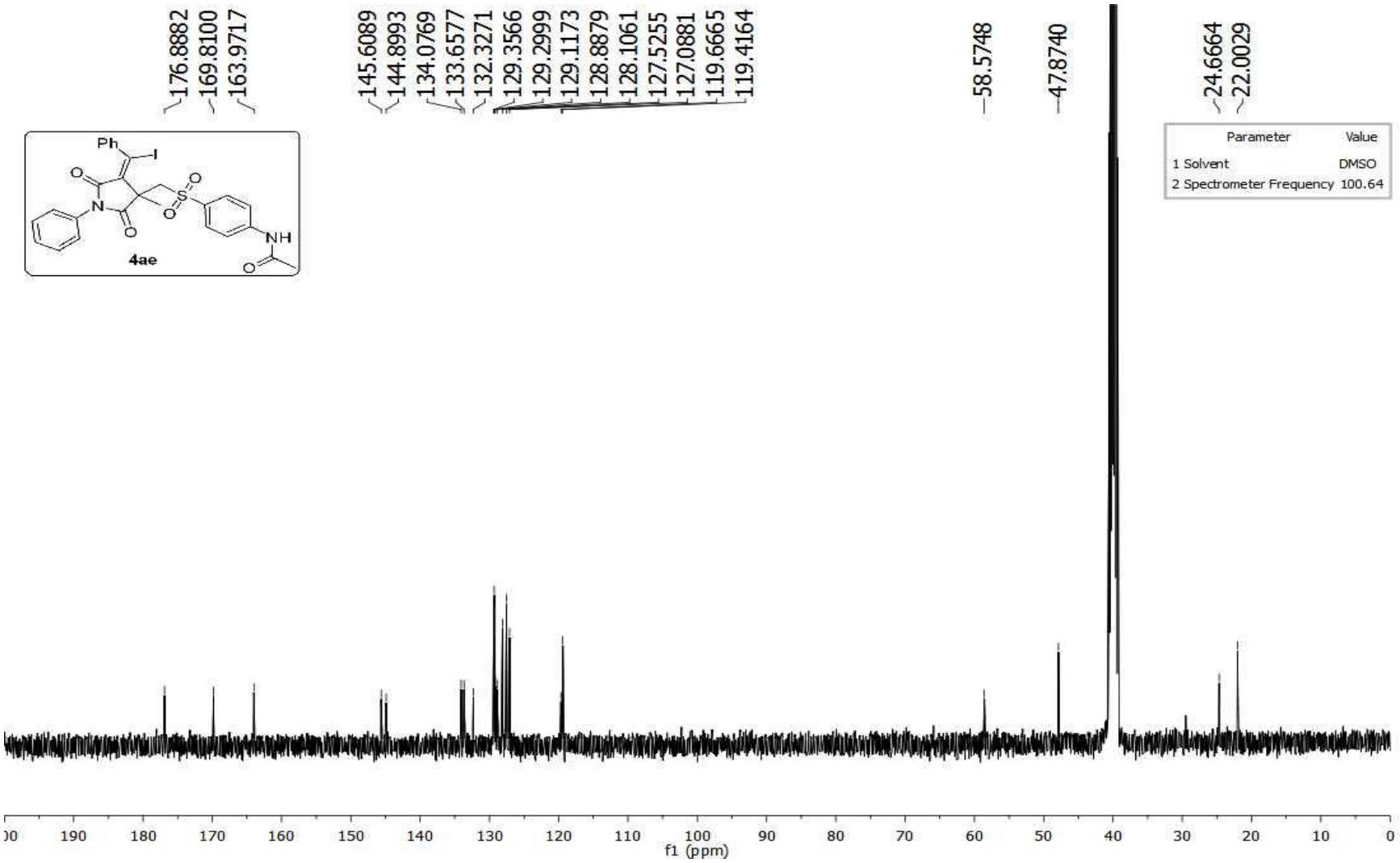

Figure S13. ^{13}C NMR spectra of (*E*)-N-(4-(((4-(iodo(phenyl)methylene)-3-methyl-2,5-dioxo-1-phenylpyrrolidin-3-yl) methyl)sulphonyl)phenyl)acetamide **(4ae)**

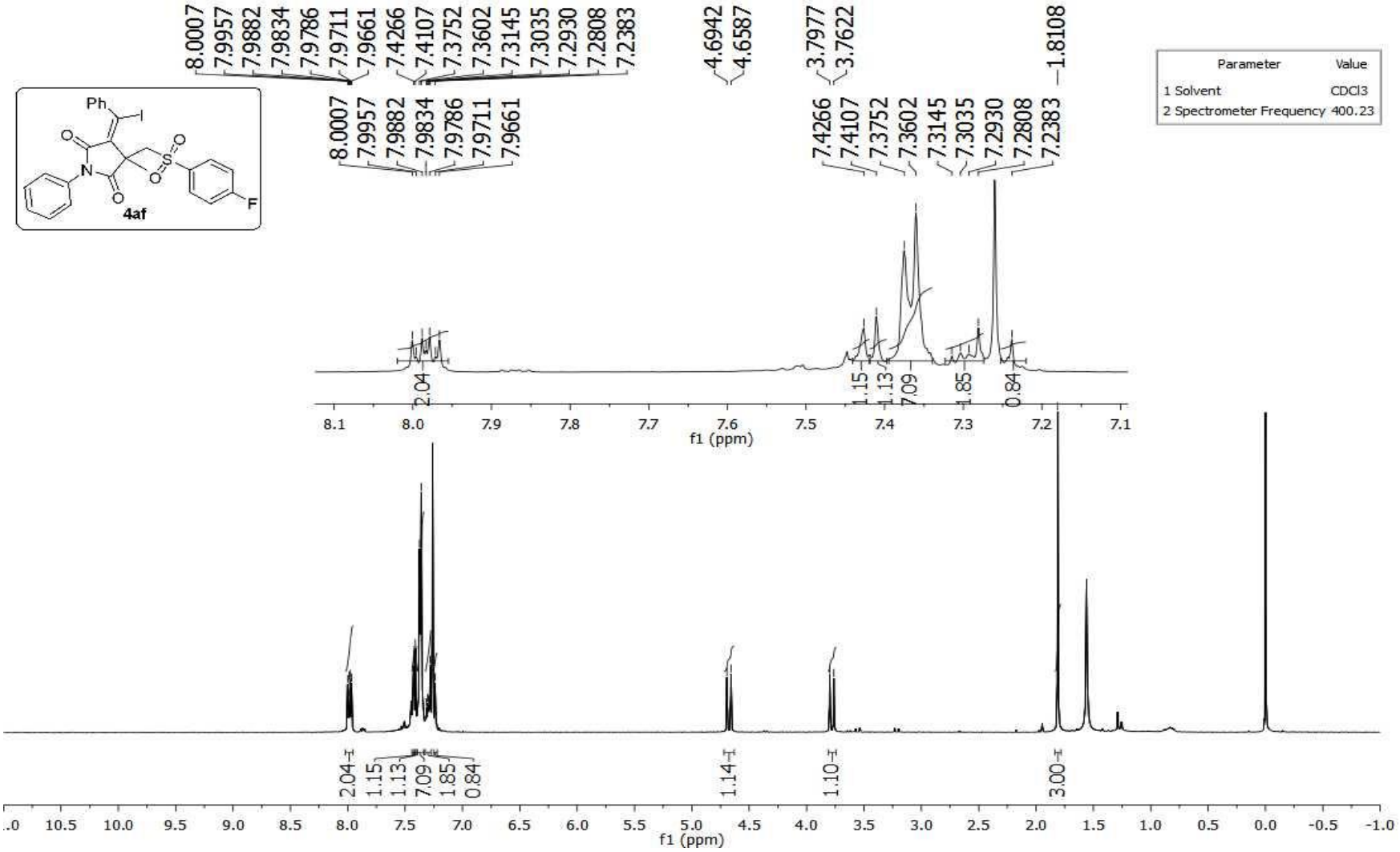

Figure S14. ^{1}H NMR spectra of (*E*)-3-(((4-fluorophenyl)sulphonyl)methyl)-4-(iodo(phenyl)methylene)-3-methyl-1-phenyl pyrrolidine-2,5-dione **(4af)**

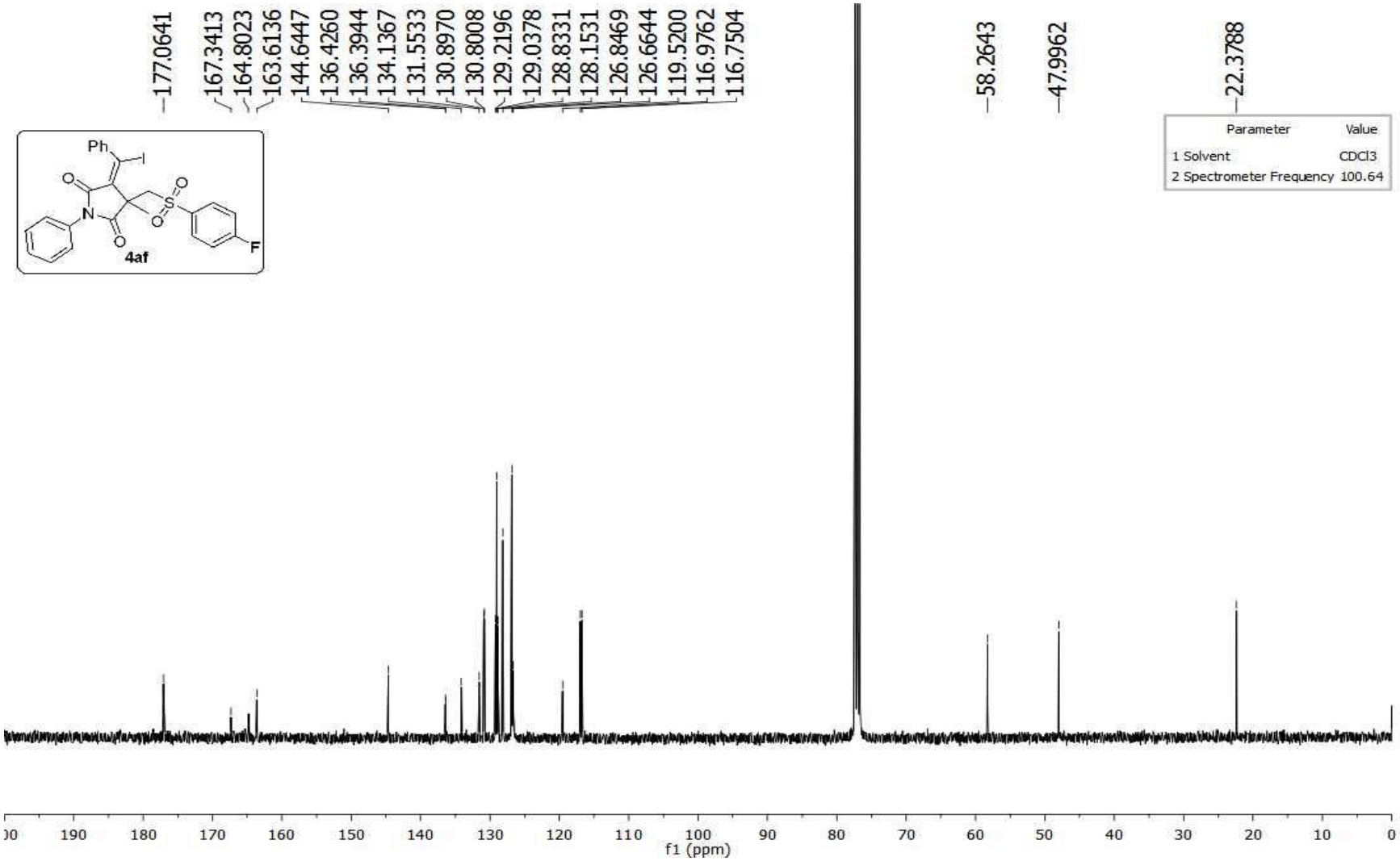

Figure S15. ^{13}C NMR spectra of (*E*)-3-(((4-fluorophenyl)sulphonyl)methyl)-4-(iodo(phenyl)methylene)-3-methyl-1-phenyl pyrrolidine-2,5-dione **(4af)**

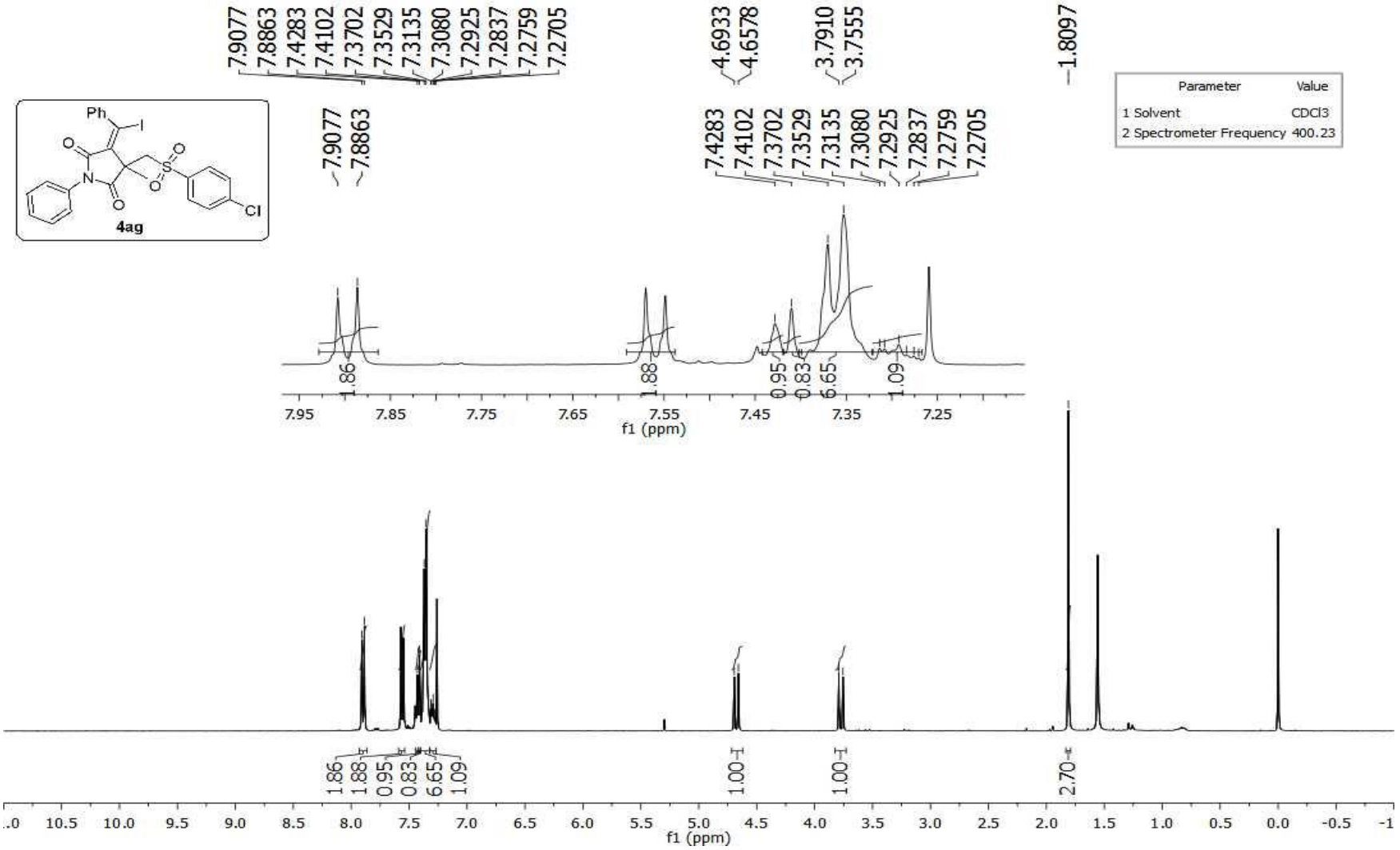

Figure S16. ^{1}H NMR spectra of (*E*)-3-(((4-chlorophenyl)sulphonyl)methyl)-4-(iodo(phenyl)methylene)-3-methyl-1-phenyl pyrrolidine-2,5-dione **(4ag)**

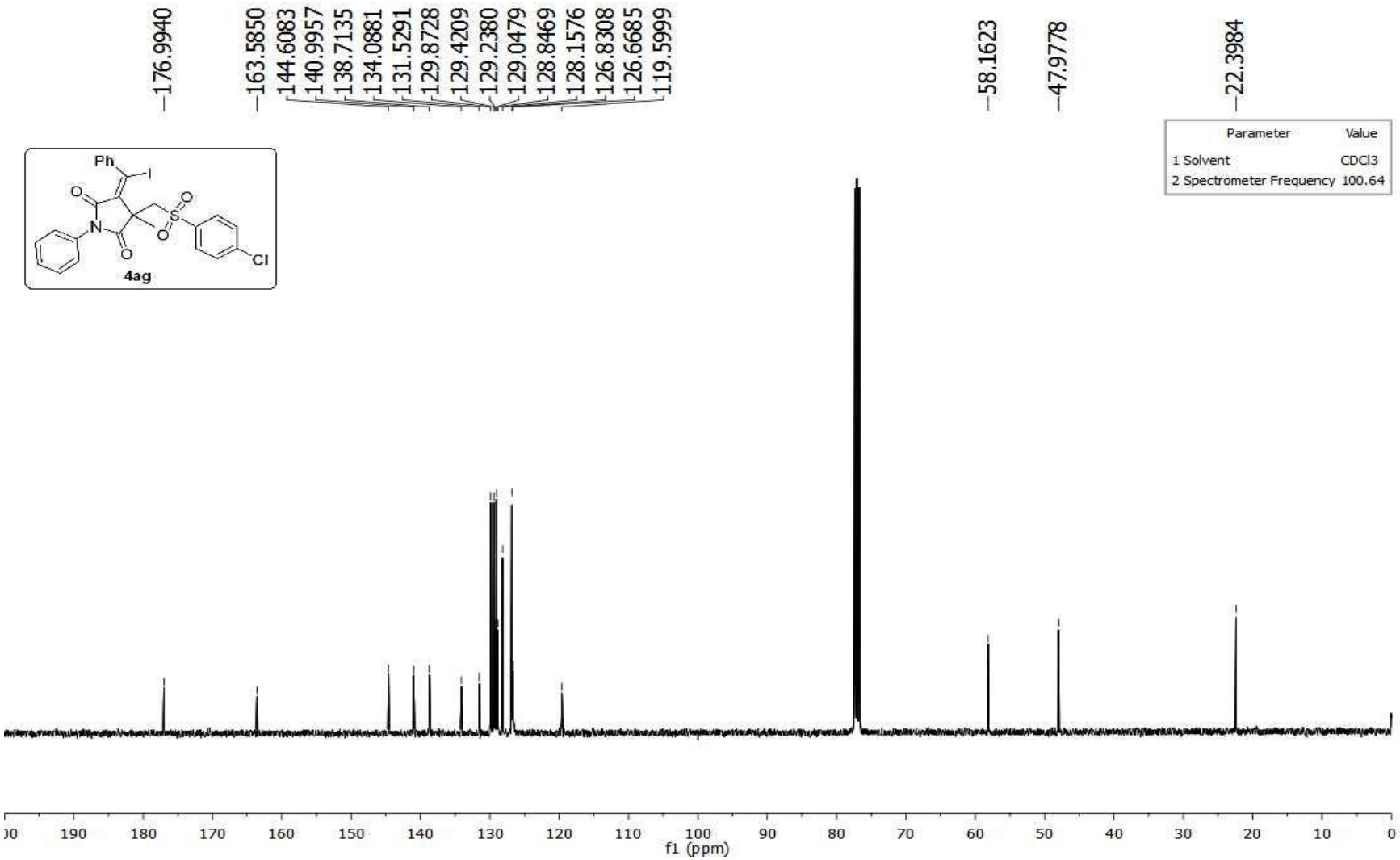

Figure S17. ^{13}C NMR spectra of (*E*)-3-(((4-chlorophenyl)sulphonyl)methyl)-4-(iodo(phenyl)methylene)-3-methyl-1-phenyl pyrrolidine-2,5-dione **(4ag)**

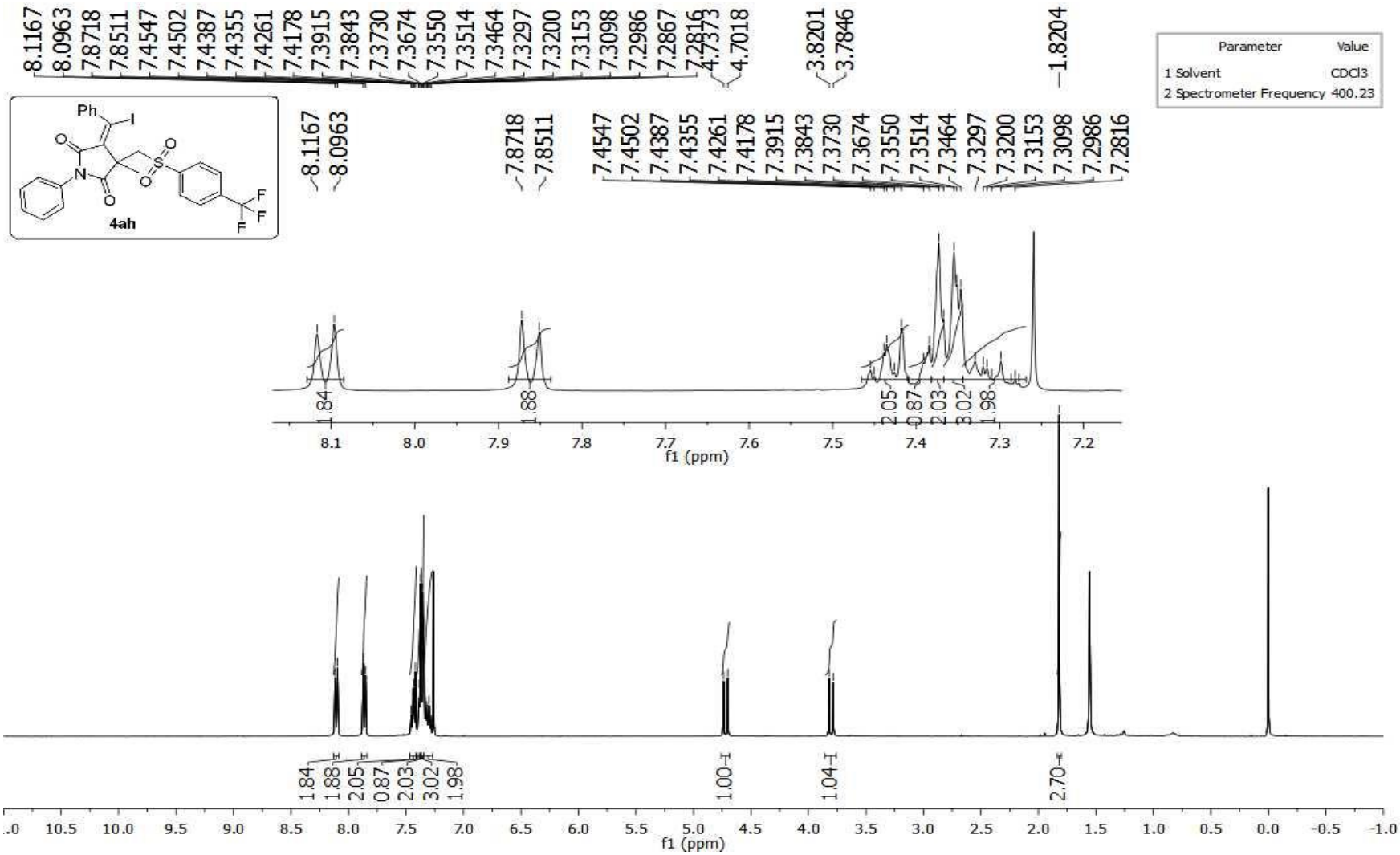

Figure S18. ^{1}H NMR spectra of (*E*)-4-(iodo(phenyl)methylene)-3-methyl-1-phenyl-3-(((4 (trifluoromethyl)phenyl) sulphonyl) methyl) pyrrolidine-2,5-dione **(4ah)**

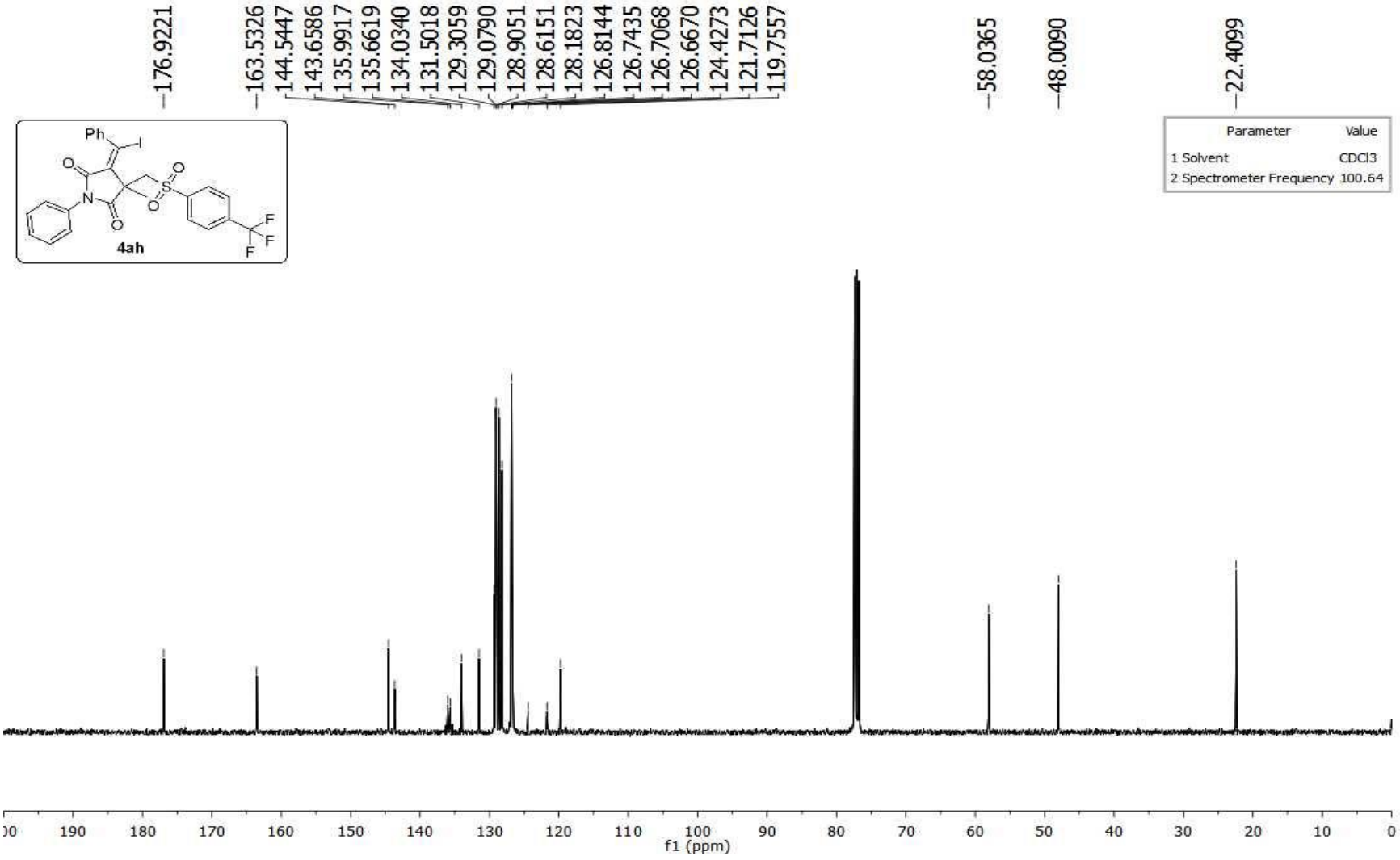

Figure S19. ^{13}C NMR spectra of (*E*)-4-(iodo(phenyl)methylene)-3-methyl-1-phenyl-3-(((4 (trifluoromethyl)phenyl)sulphonyl)methyl) pyrrolidine-2,5-dione **(4ah)**

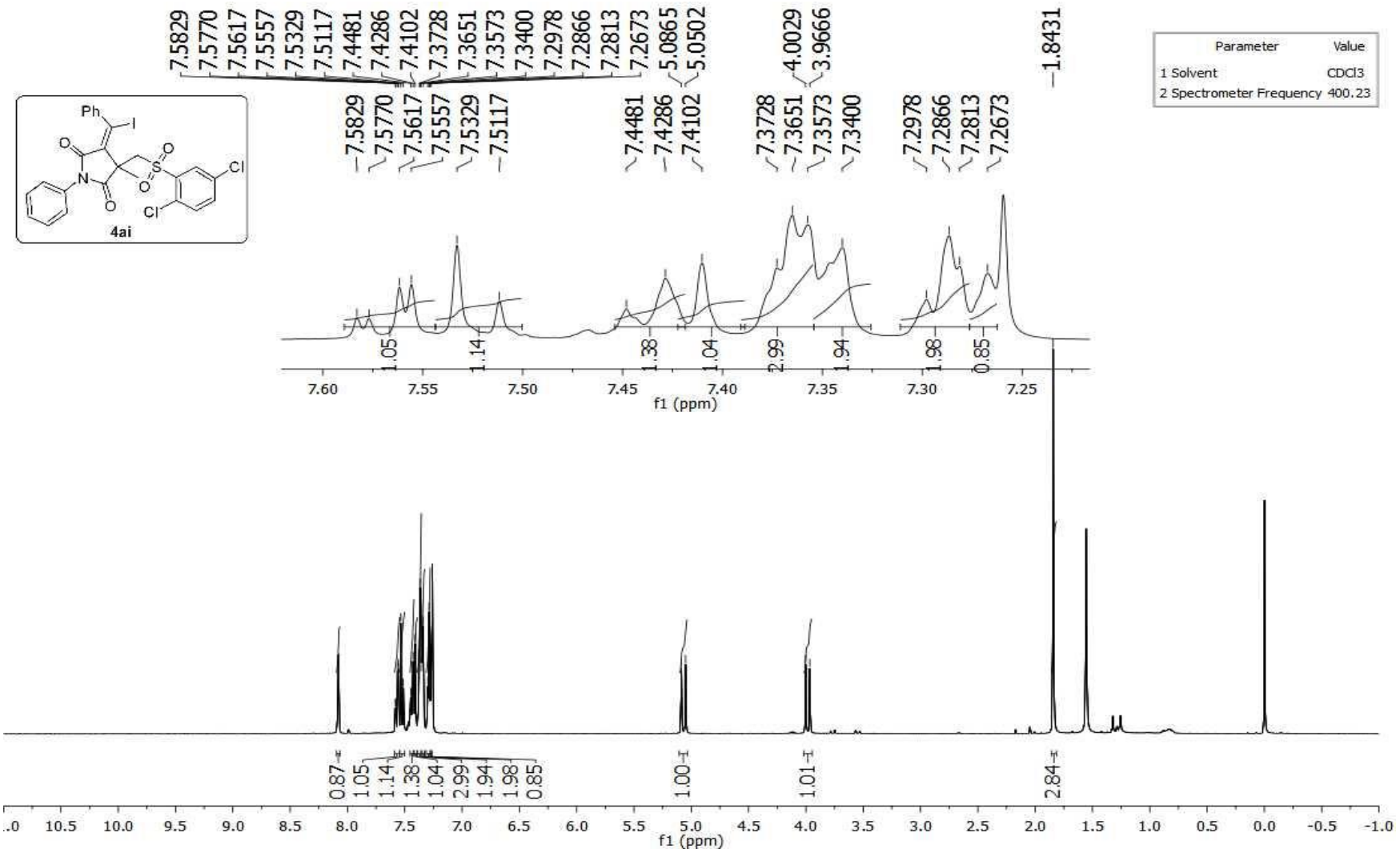

Figure S20. [1]H NMR spectra of (*E*)-3-(((2,5-dichlorophenyl)sulphonyl)methyl)-4-(iodo(phenyl)methylene)-3-methyl-1-phenyl pyrrolidine-2,5-dione **(4ai)**

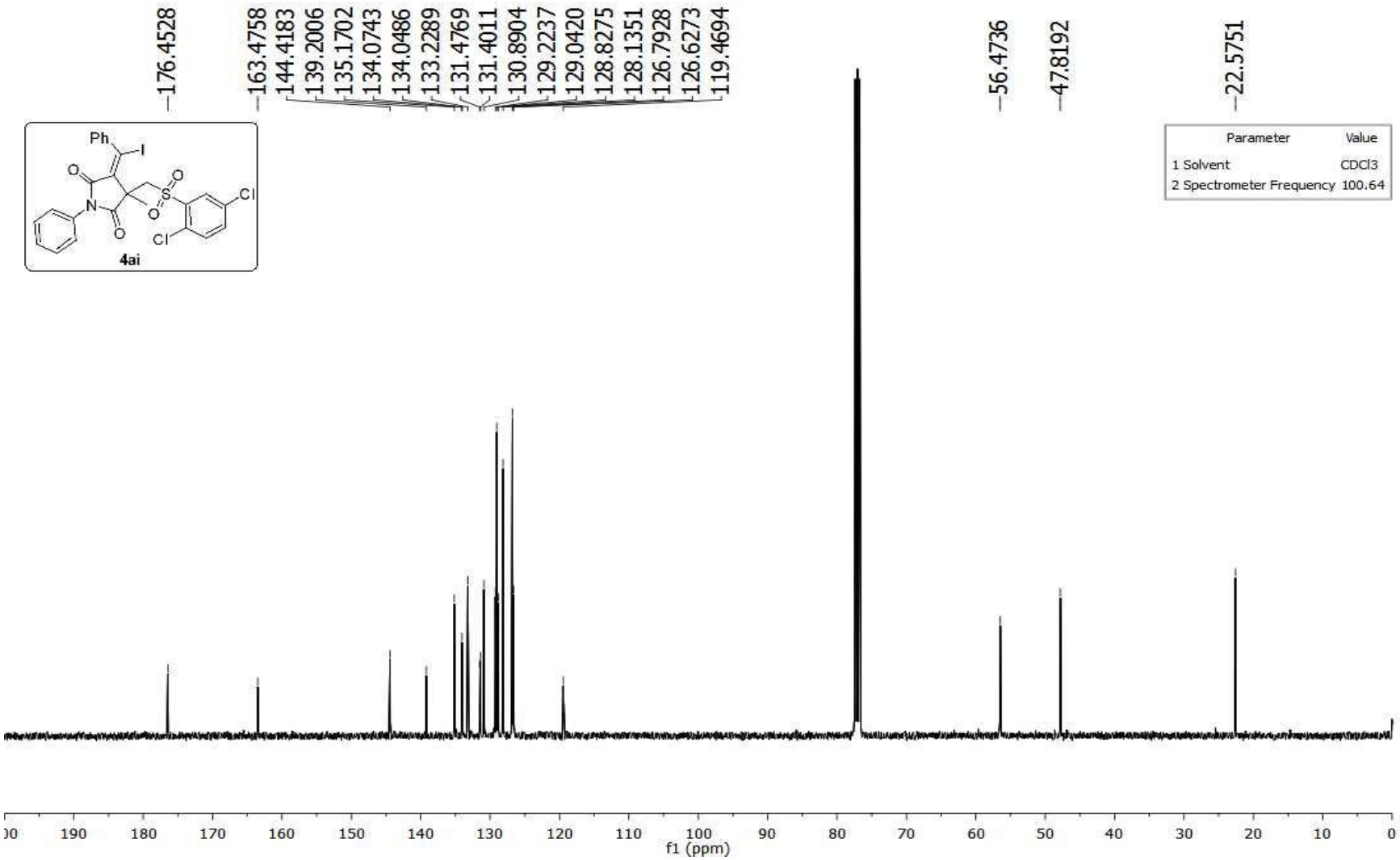

Figure S21. ^{13}C NMR spectra of (*E*)-3-(((2,5-dichlorophenyl)sulphonyl)methyl)-4-(iodo(phenyl)methylene)-3-methyl-1-phenyl pyrrolidine-2,5-dione **(4ai)**

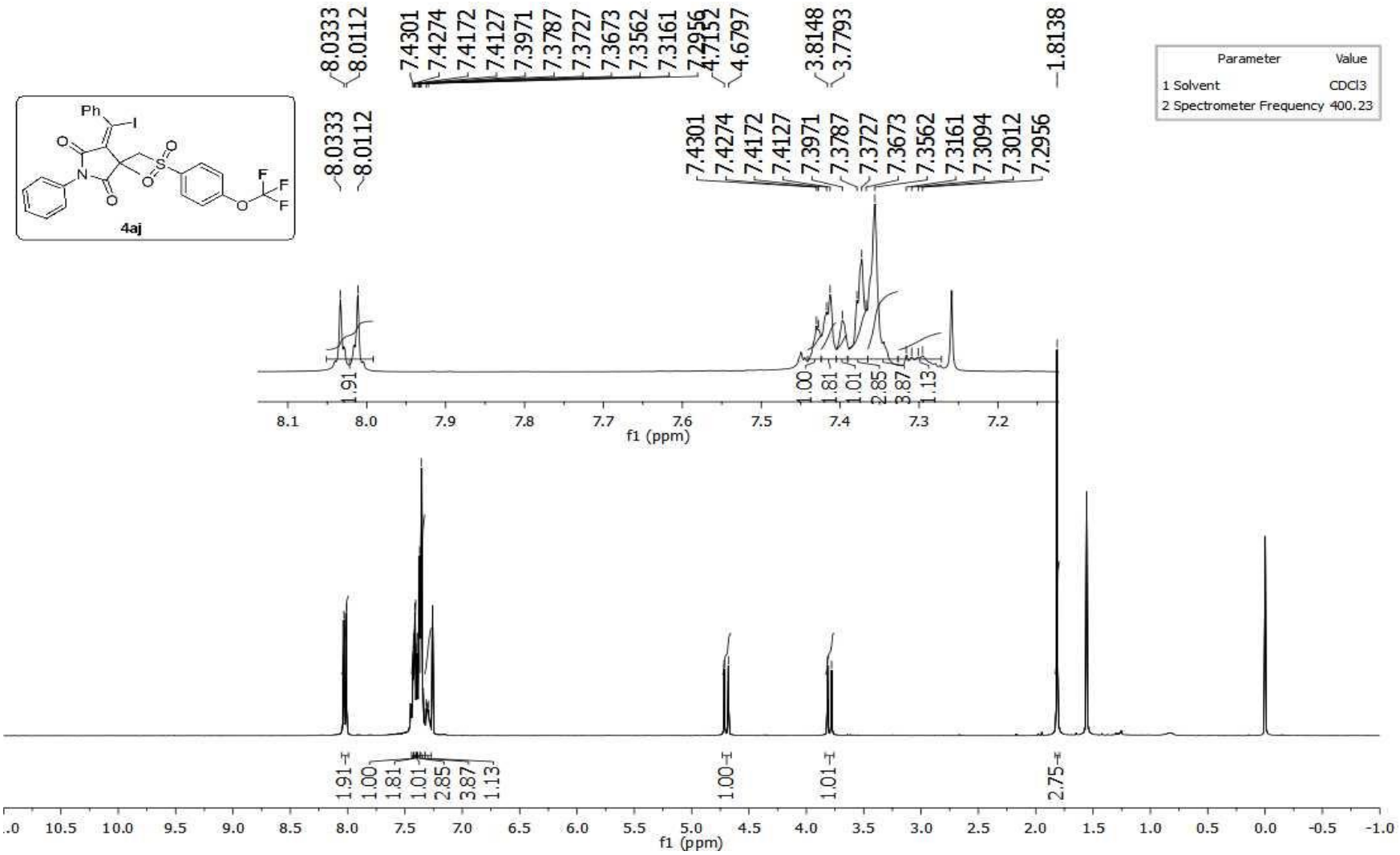

Figure S22. ^{1}H NMR spectra of (*E*)-4-(iodo(phenyl)methylene)-3-methyl-1-phenyl-3-(((4-(trifluoromethoxy)phenyl) sulphonyl)methyl) pyrrolidine-2,5-dione **(4aj)**

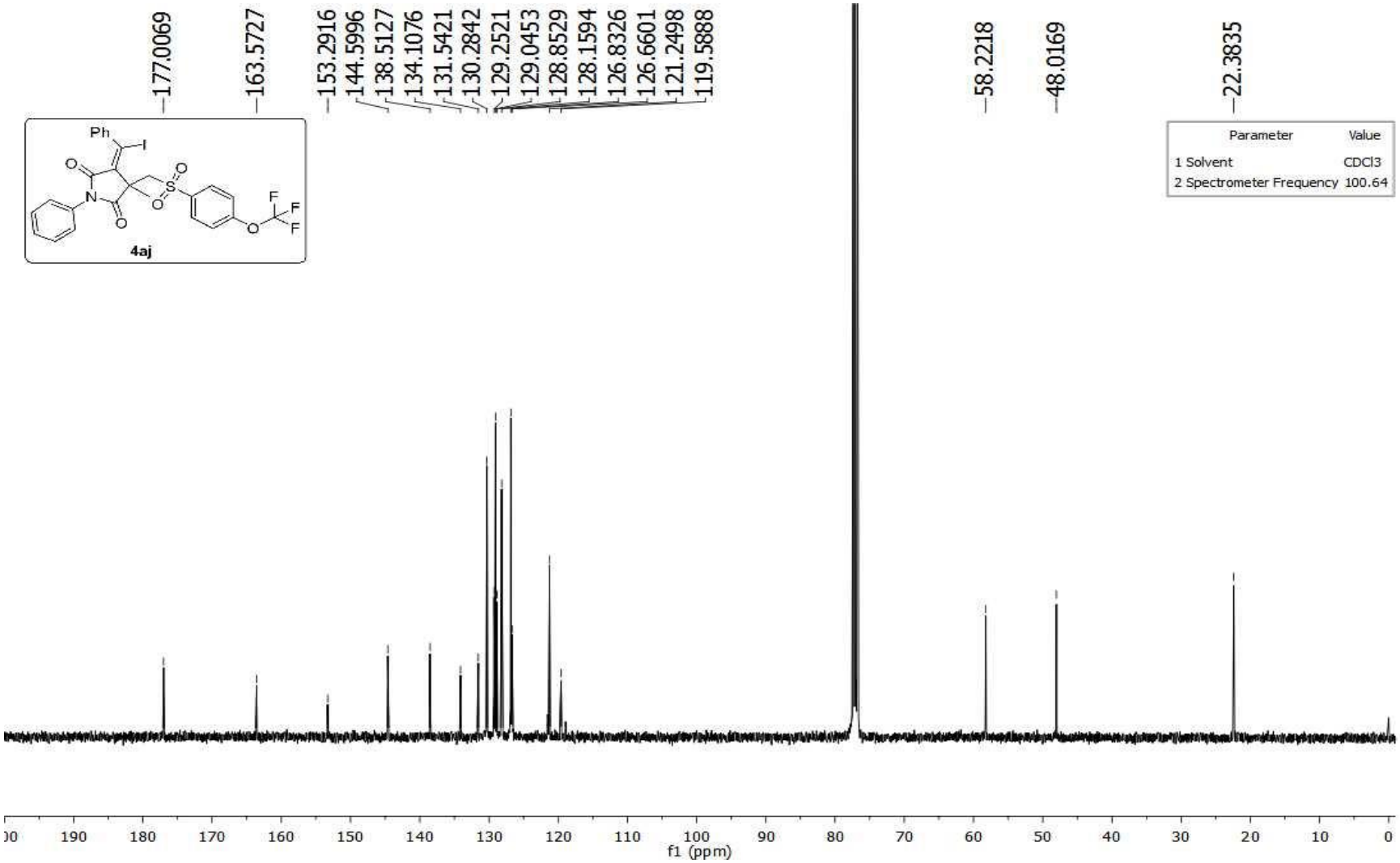

Figure S23. ^{13}C NMR spectra of (*E*)-4-(iodo(phenyl)methylene)-3-methyl-1-phenyl-3-(((4-(trifluoromethoxy)phenyl) sulphonyl)methyl)pyrrolidine-2,5-dione **(4aj)**

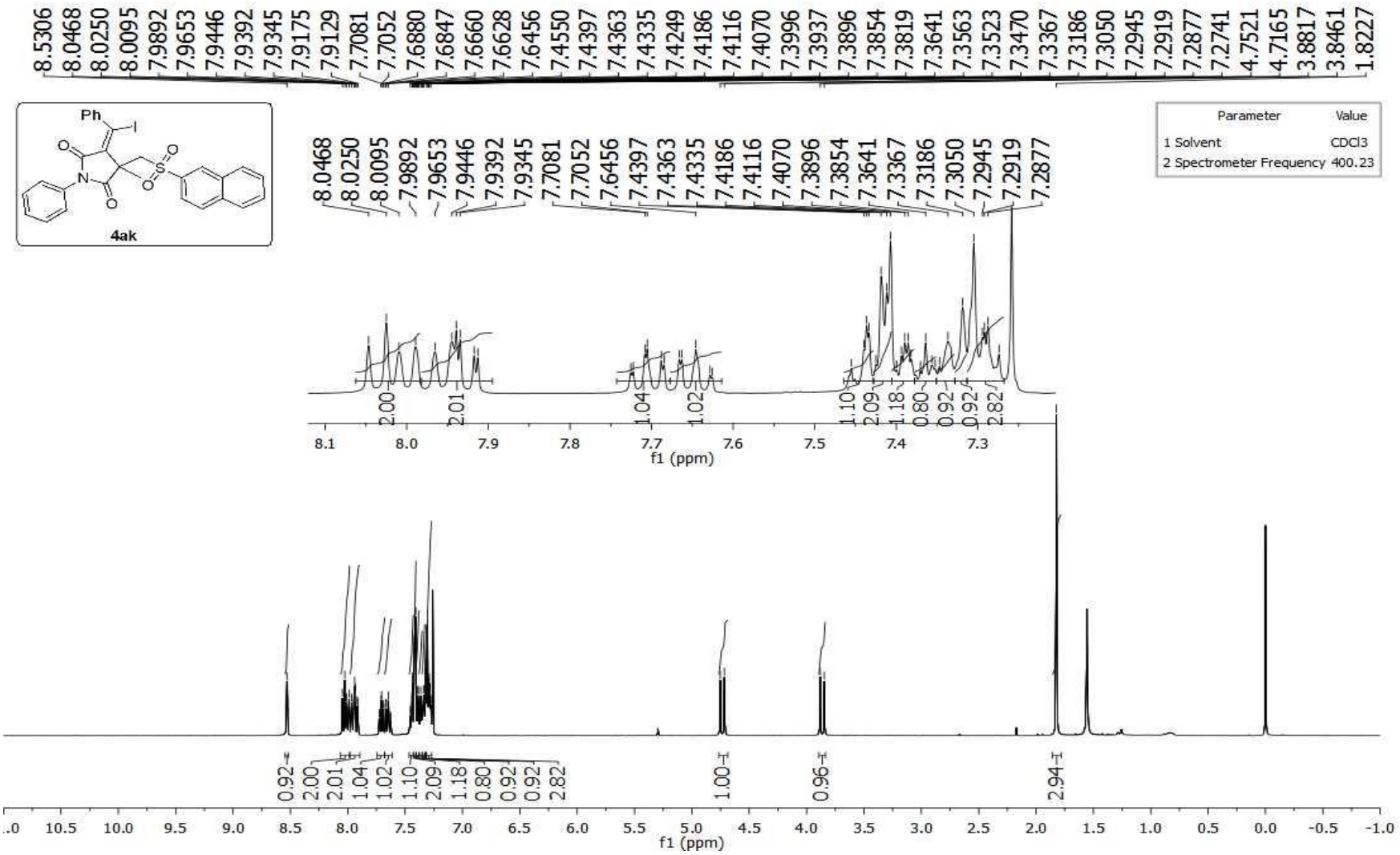

Figure S24. [1]H NMR spectra of (*E*)-4-(iodo(phenyl)methylene)-3-methyl-3-((naphthalen-2-ylsulphonyl)methyl)-1-phenyl pyrrolidine-2,5-dione **(4ak)**

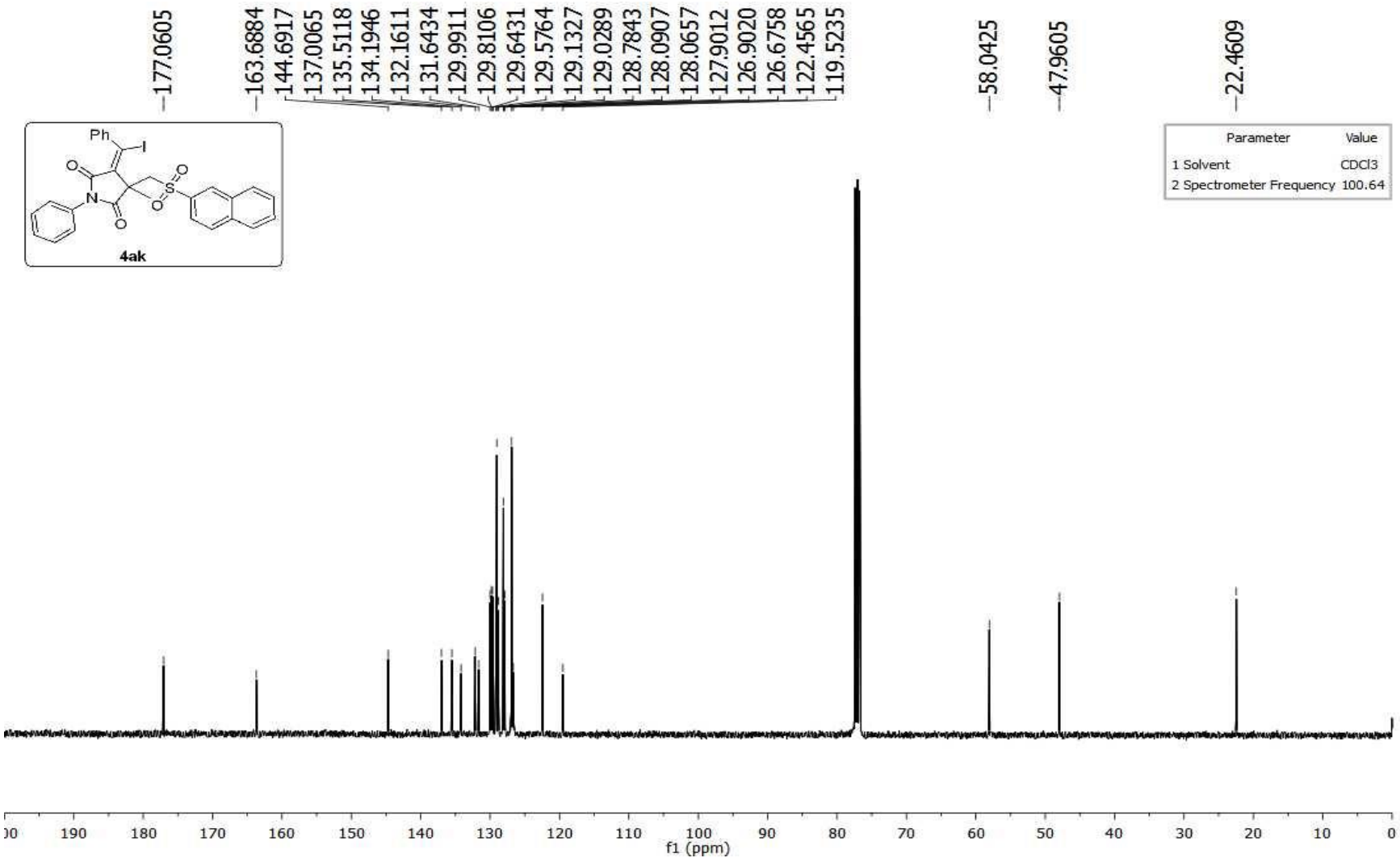

Figure S25. ^{13}C NMR spectra of (*E*)-4-(iodo(phenyl)methylene)-3-methyl-3-((naphthalen-2-ylsulphonyl)methyl)-1-phenyl pyrrolidine-2,5-dione **(4ak)**

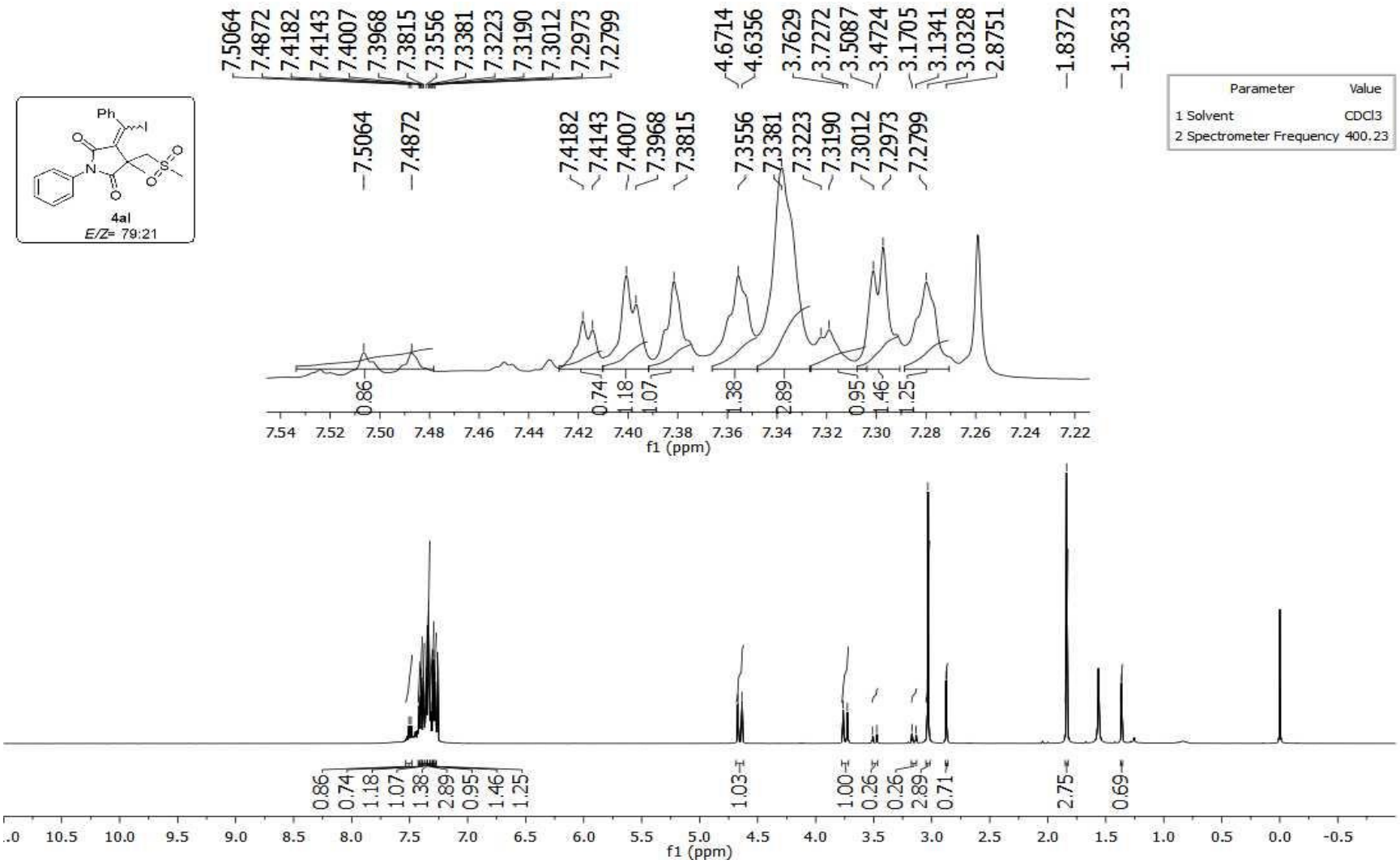

Figure S26. [1]H NMR spectra of **(*E*)**-4-(iodo(phenyl)methylene)-3-methyl-3-((methylsulphonyl)methyl)-1-phenyl pyrrolidine-2,5-dione **(4al)**

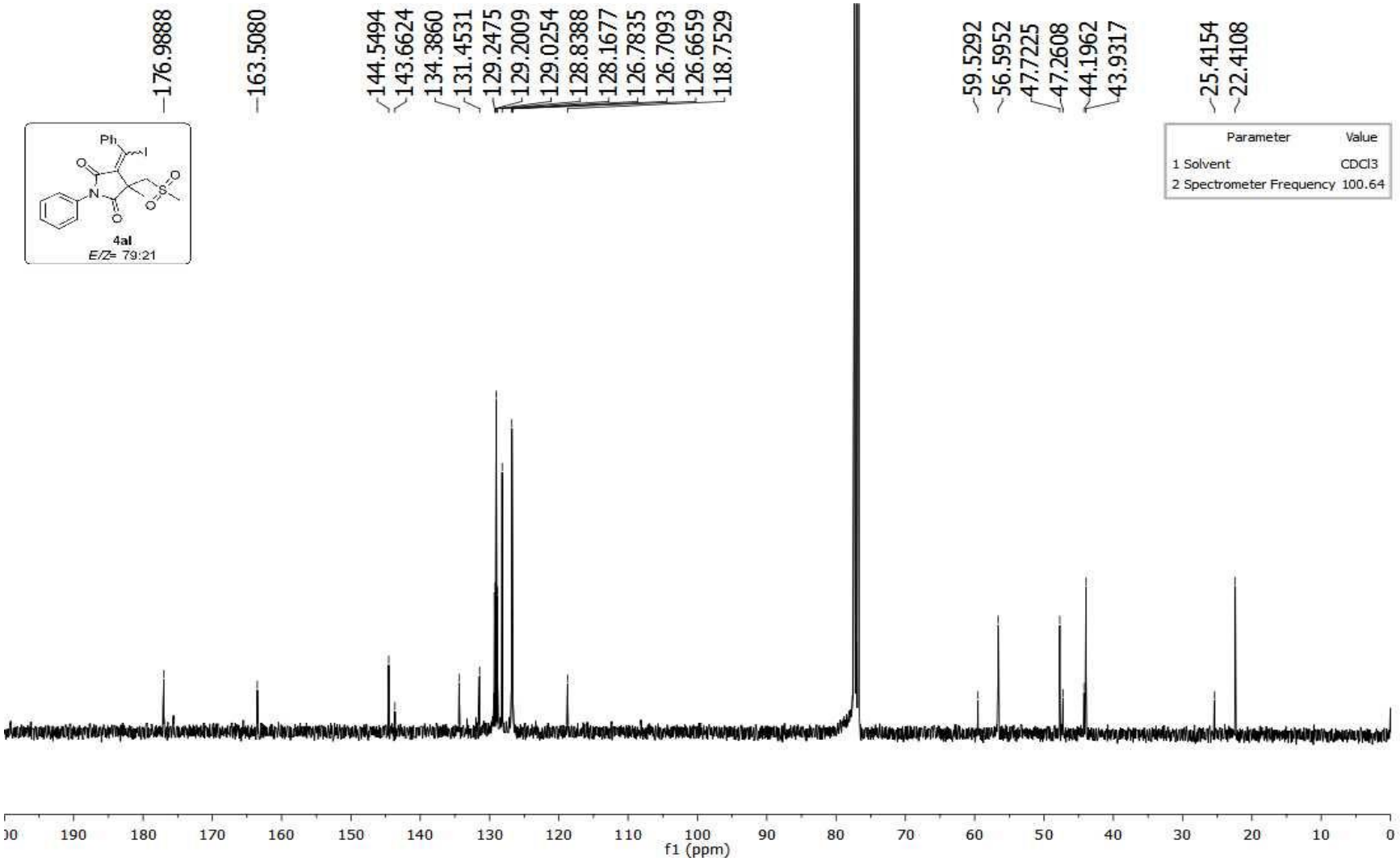

Figure S27. ^{13}C NMR spectra of **(*E*)**-4-(iodo(phenyl)methylene)-3-methyl-3-((methylsulphonyl)methyl)-1-phenyl pyrrolidine-2,5-dione **(4al)**

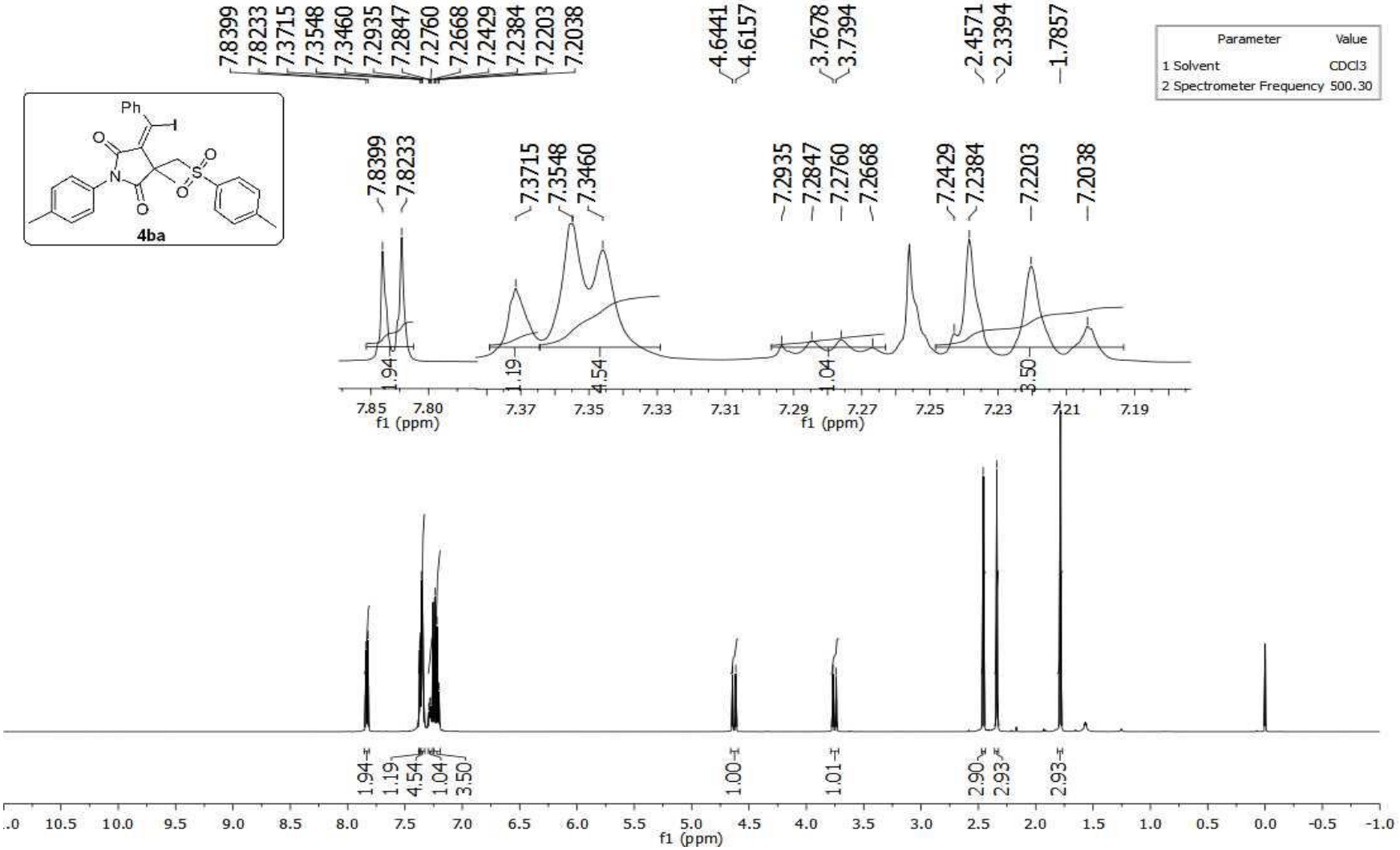

Figure S28. ^{1}H NMR spectra of **(*E*)**-4-(iodo(phenyl)methylene)-3-methyl-1-(p-tolyl)-3-(tosylmethyl)pyrrolidine-2,5-dione **(4ba)**

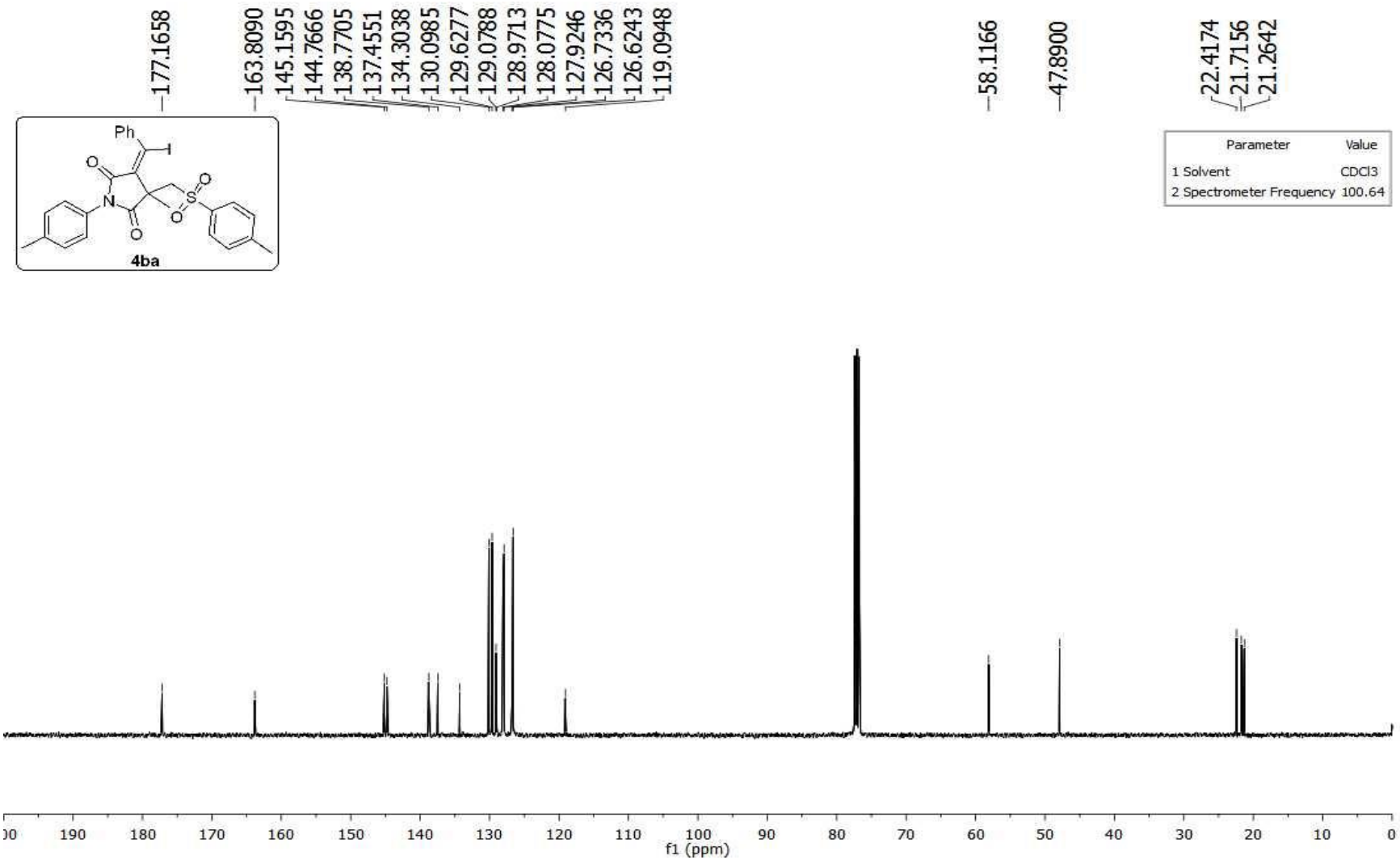

Figure S29. ^{13}C NMR spectra of **(*E*)**-4-(iodo(phenyl)methylene)-3-methyl-1-(p-tolyl)-3-(tosylmethyl)pyrrolidine-2,5-dione **(4ba)**

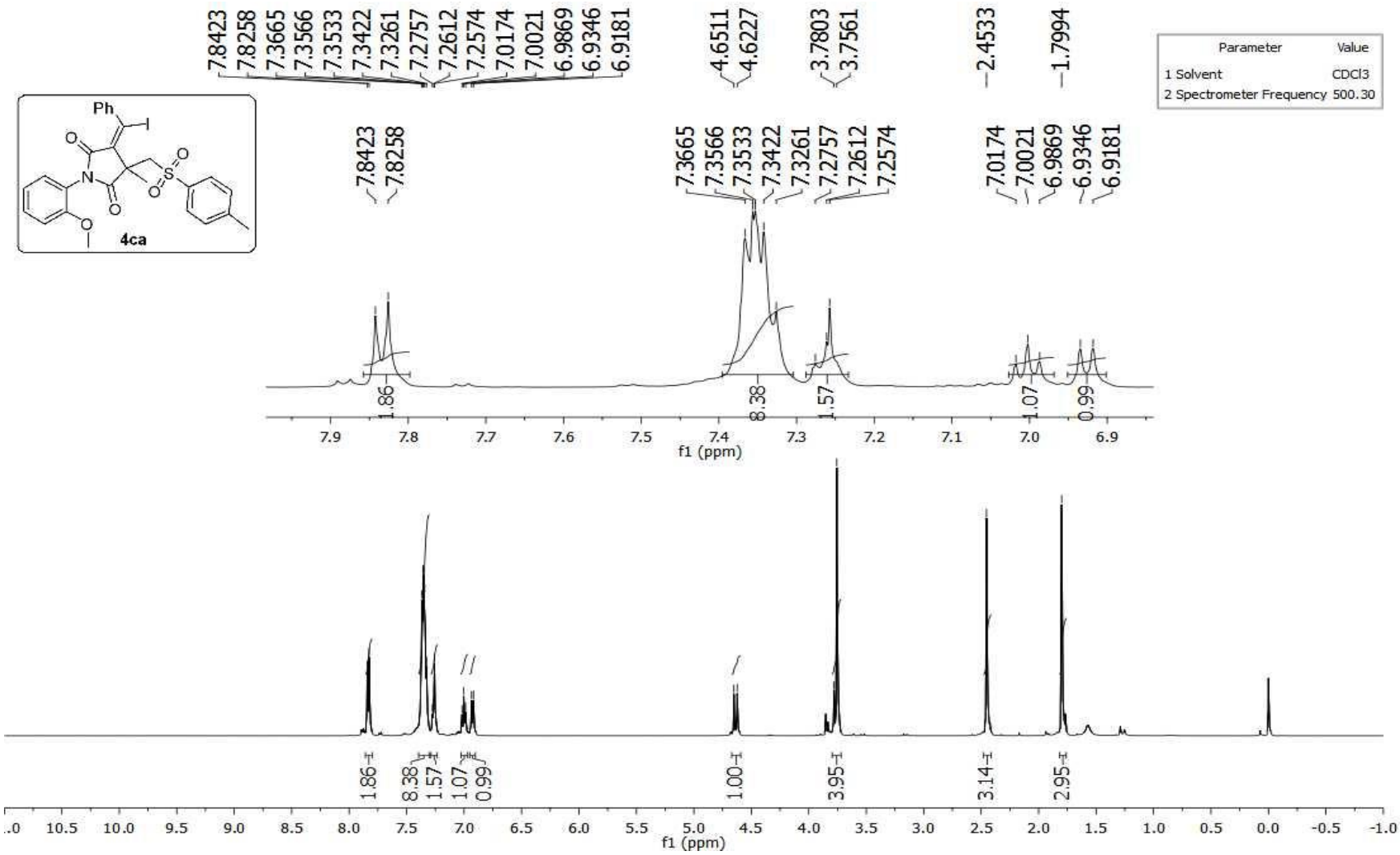

Figure S30. ^{1}H NMR spectra of (*E*)-4-(iodo(phenyl)methylene)-1-(2-methoxyphenyl)-3-methyl-3-(tosylmethyl) pyrrolidine-2,5-dione **(4ca)**

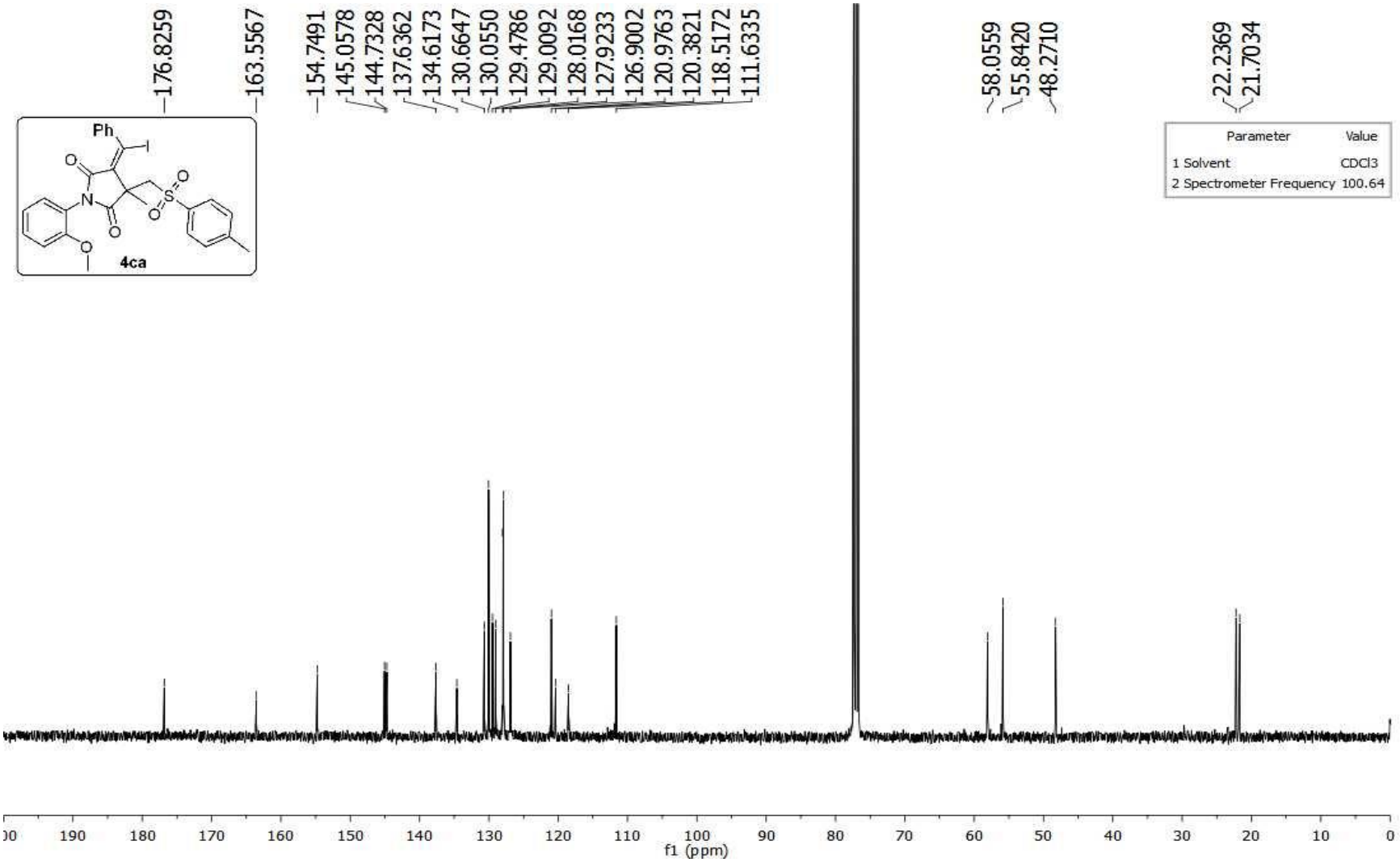

Figure S31. ^{13}C NMR spectra of (*E*)-4-(iodo(phenyl)methylene)-1-(2-methoxyphenyl)-3-methyl-3-(tosylmethyl) pyrrolidine-2,5-dione **(4ca)**

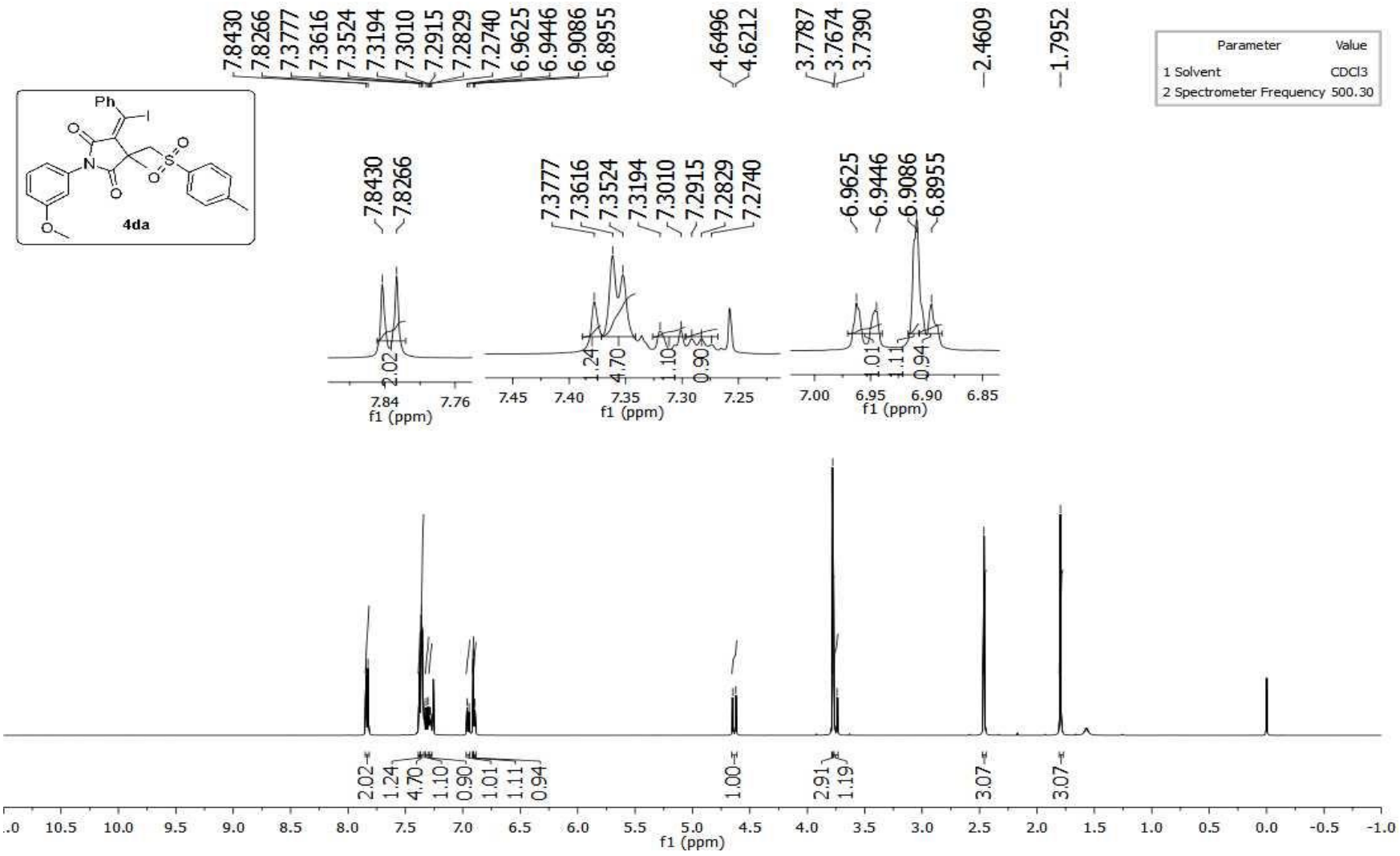

Figure S32. ^{1}H NMR spectra of (*E*)-4-(iodo(phenyl)methylene)-1-(3-methoxyphenyl)-3-methyl-3-(tosylmethyl) pyrrolidine-2,5-dione **(4da)**

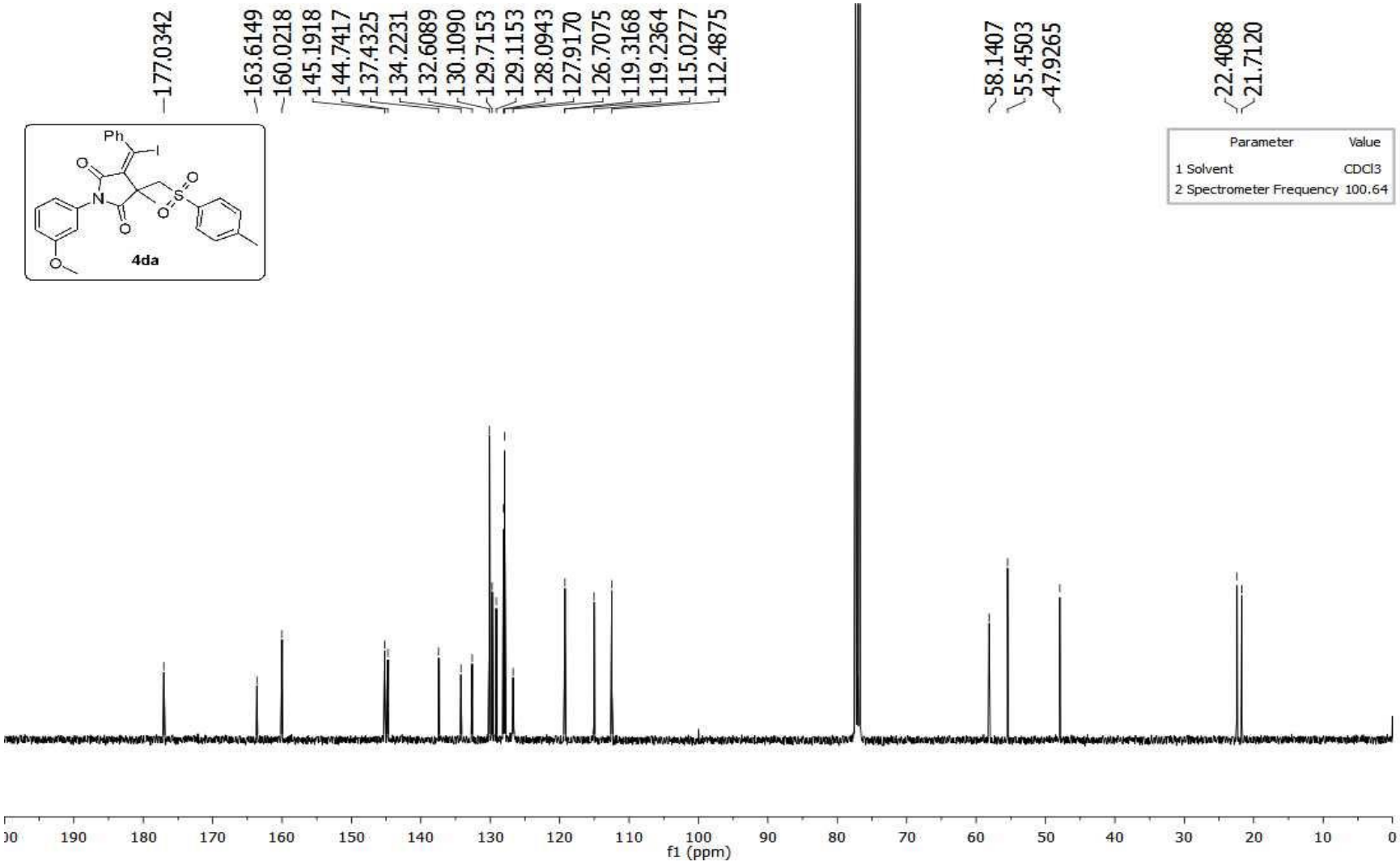

Figure S33. ^{13}C NMR spectra of (*E*)-4-(iodo(phenyl)methylene)-1-(3-methoxyphenyl)-3-methyl-3-(tosylmethyl) pyrrolidine-2,5-dione **(4da)**

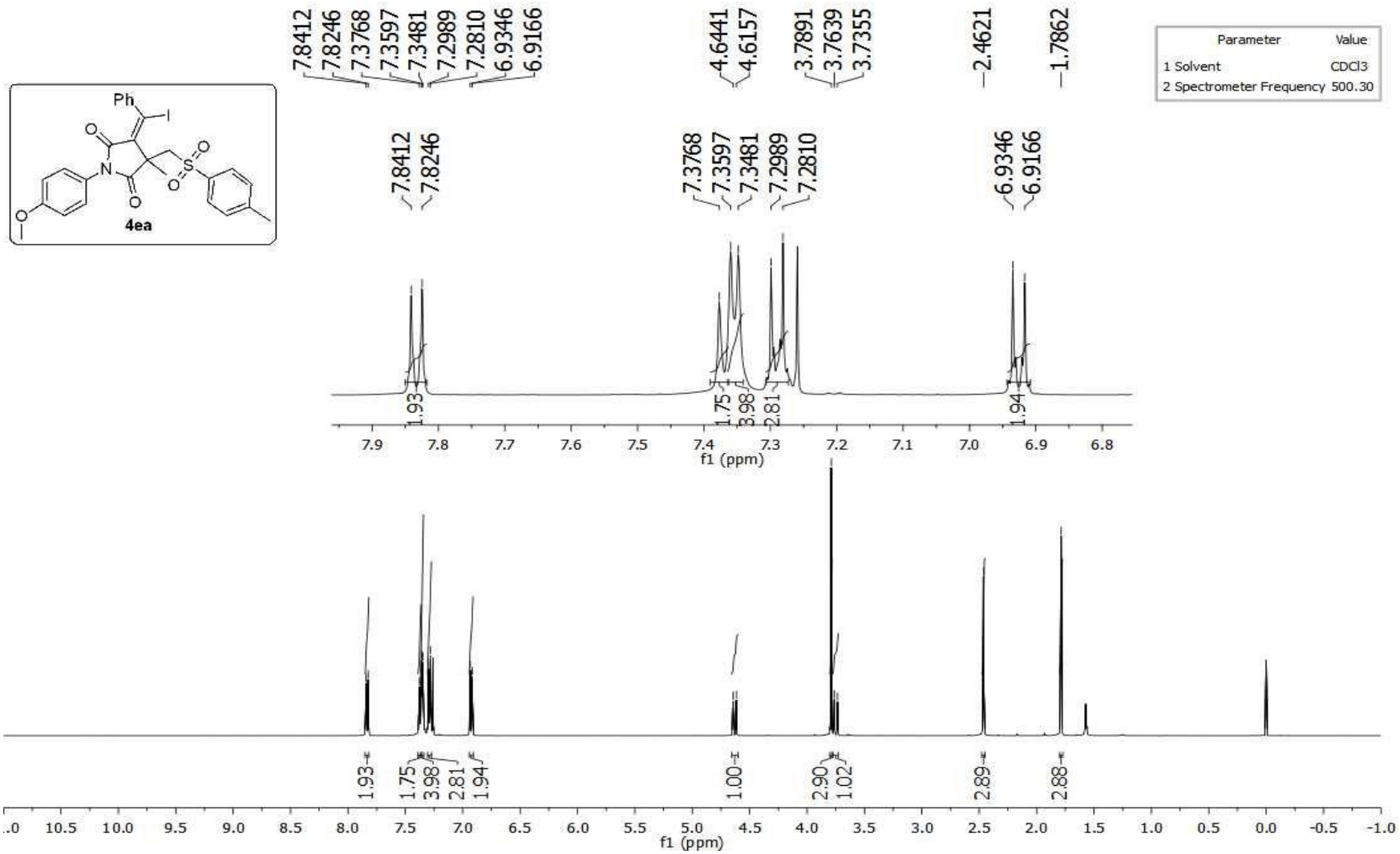

Figure S34. ^{1}H NMR spectra of (*E*)-4-(iodo(phenyl)methylene)-1-(4-methoxyphenyl)-3-methyl-3-(tosylmethyl) pyrrolidine-2,5-dione **(4ea)**

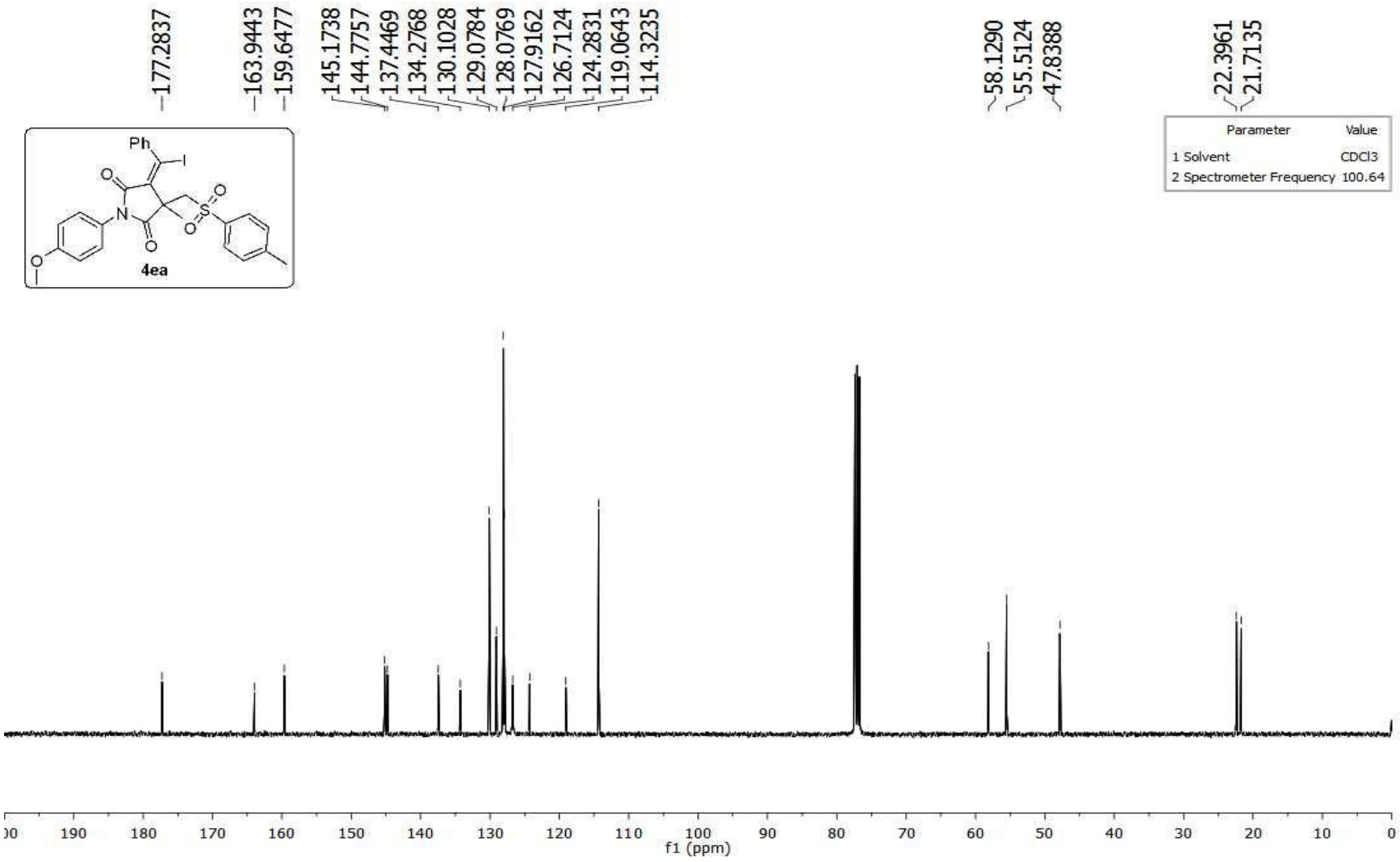

Figure S35. ^{13}C NMR spectra of (*E*)-4-(iodo(phenyl)methylene)-1-(4-methoxyphenyl)-3-methyl-3-(tosylmethyl) pyrrolidine-2,5-dione **(4ea)**

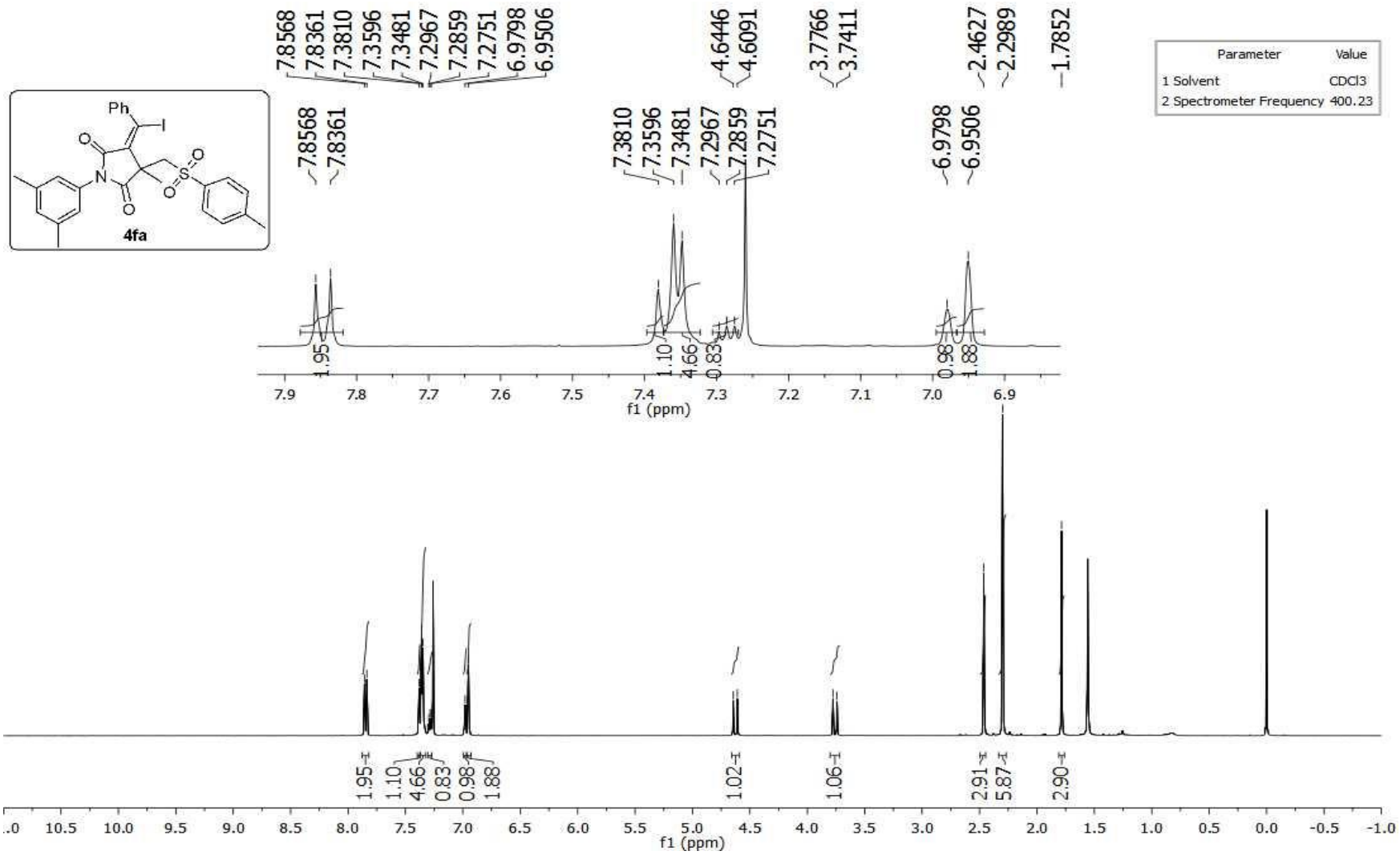

Figure S36. [1]H NMR spectra of (*E*)-1-(3,5-dimethylphenyl)-4-(iodo(phenyl)methylene)-3-methyl-3-(tosylmethyl) pyrrolidine-2,5-dione **(4fa)**

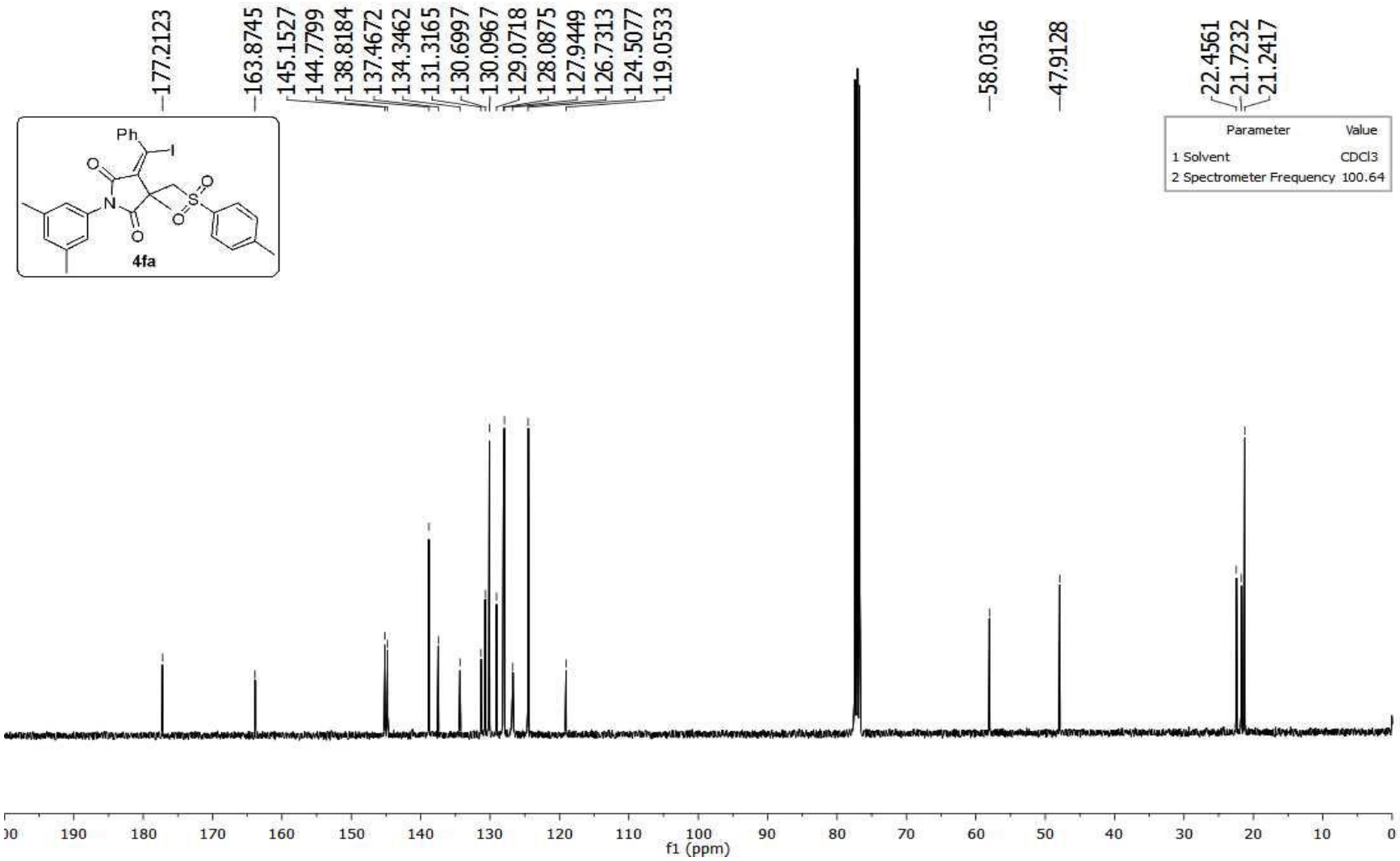

Figure S37. ^{13}C NMR spectra of (*E*)-1-(3,5-dimethylphenyl)-4-(iodo(phenyl)methylene)-3-methyl-3-(tosylmethyl) pyrrolidine-2,5-dione **(4fa)**

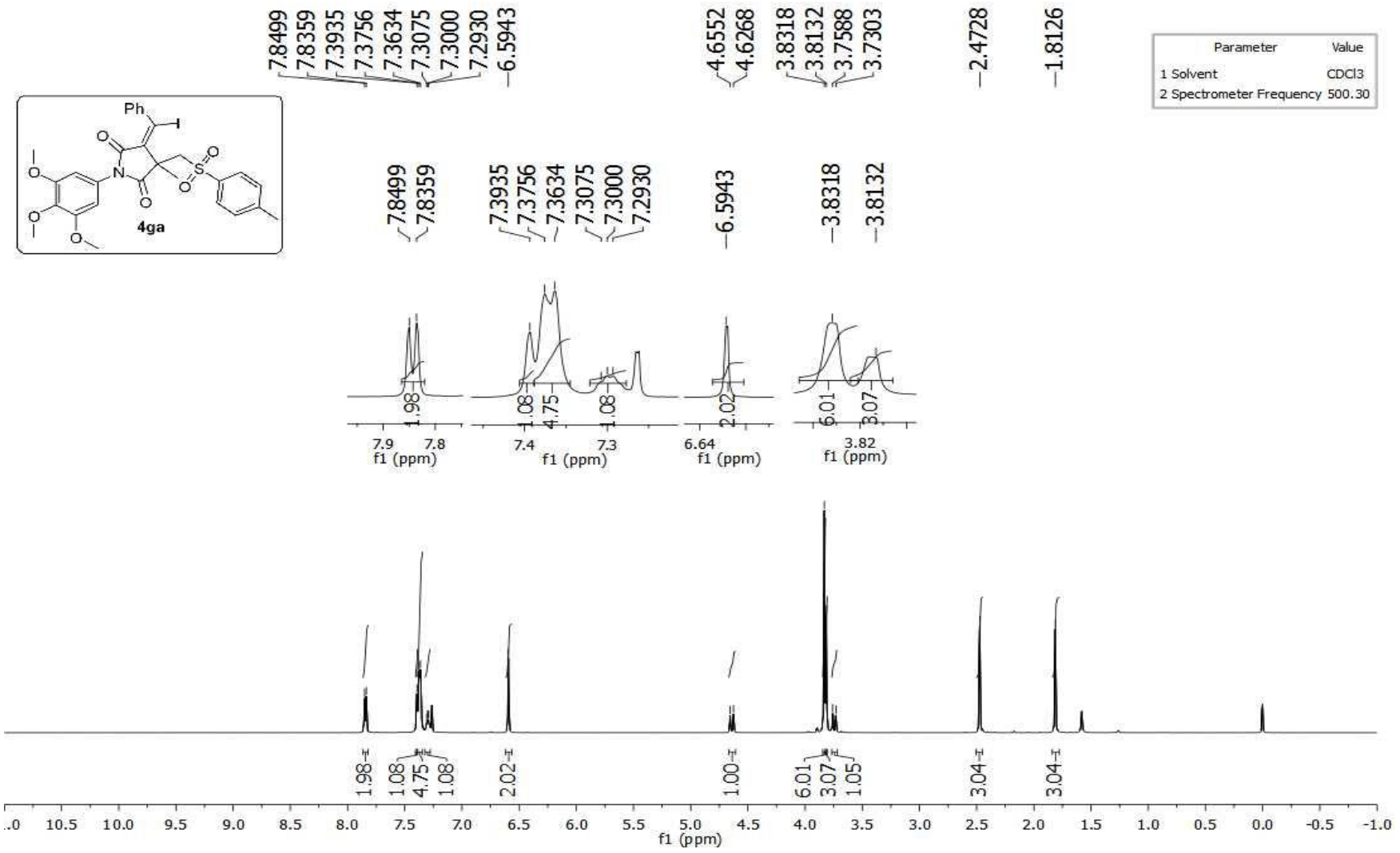

Figure S38. ^{1}H NMR spectra of (*E*)-4-(iodo(phenyl)methylene)-3-methyl-3-(tosylmethyl)-1-(3,4,5-trimethoxyphenyl) pyrrolidine-2,5-dione **(4ga)**

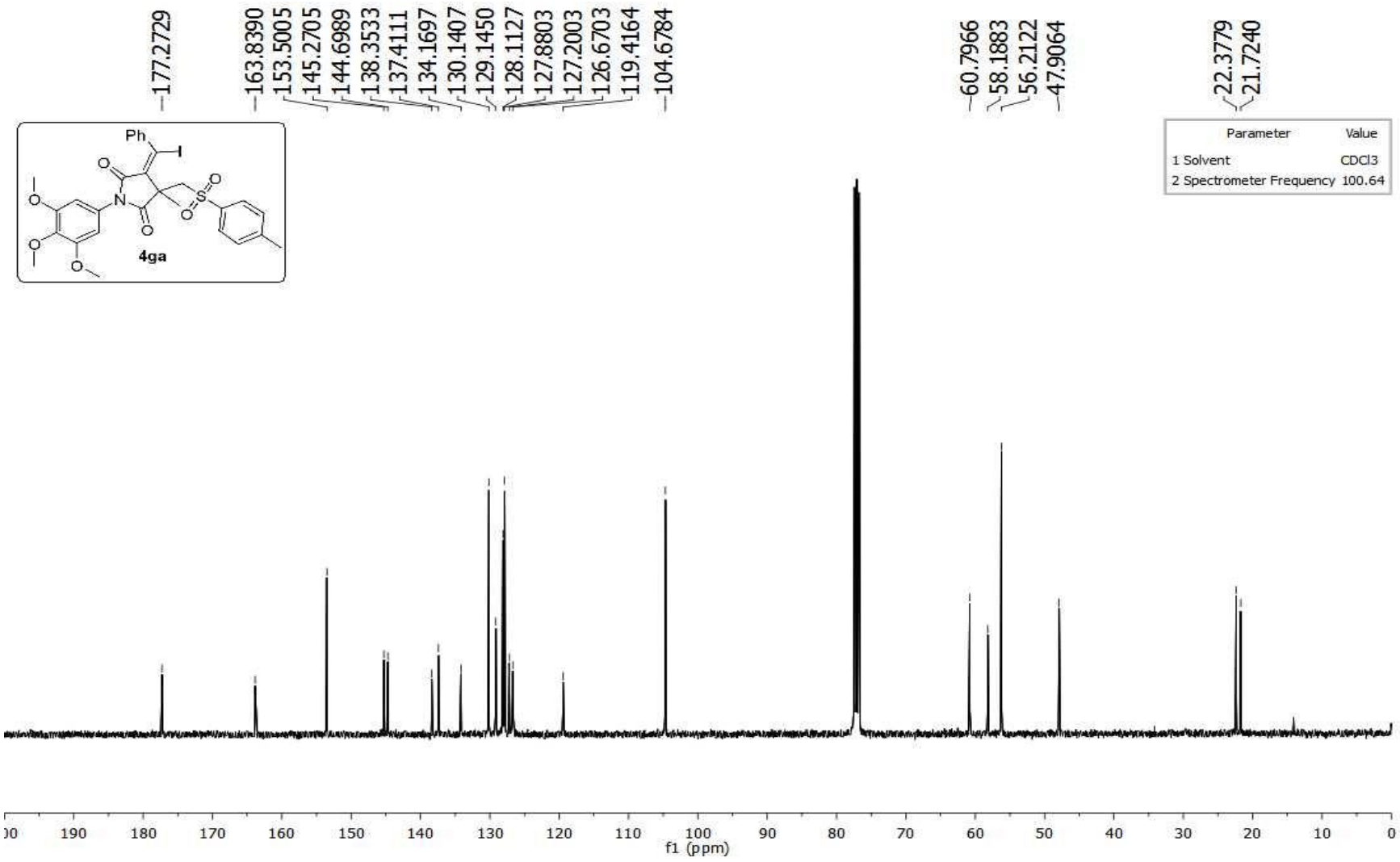

Figure S39. ^{13}C NMR spectra of (*E*)-4-(iodo(phenyl)methylene)-3-methyl-3-(tosylmethyl)-1-(3,4,5-trimethoxyphenyl) pyrrolidine-2,5-dione **(4ga)**

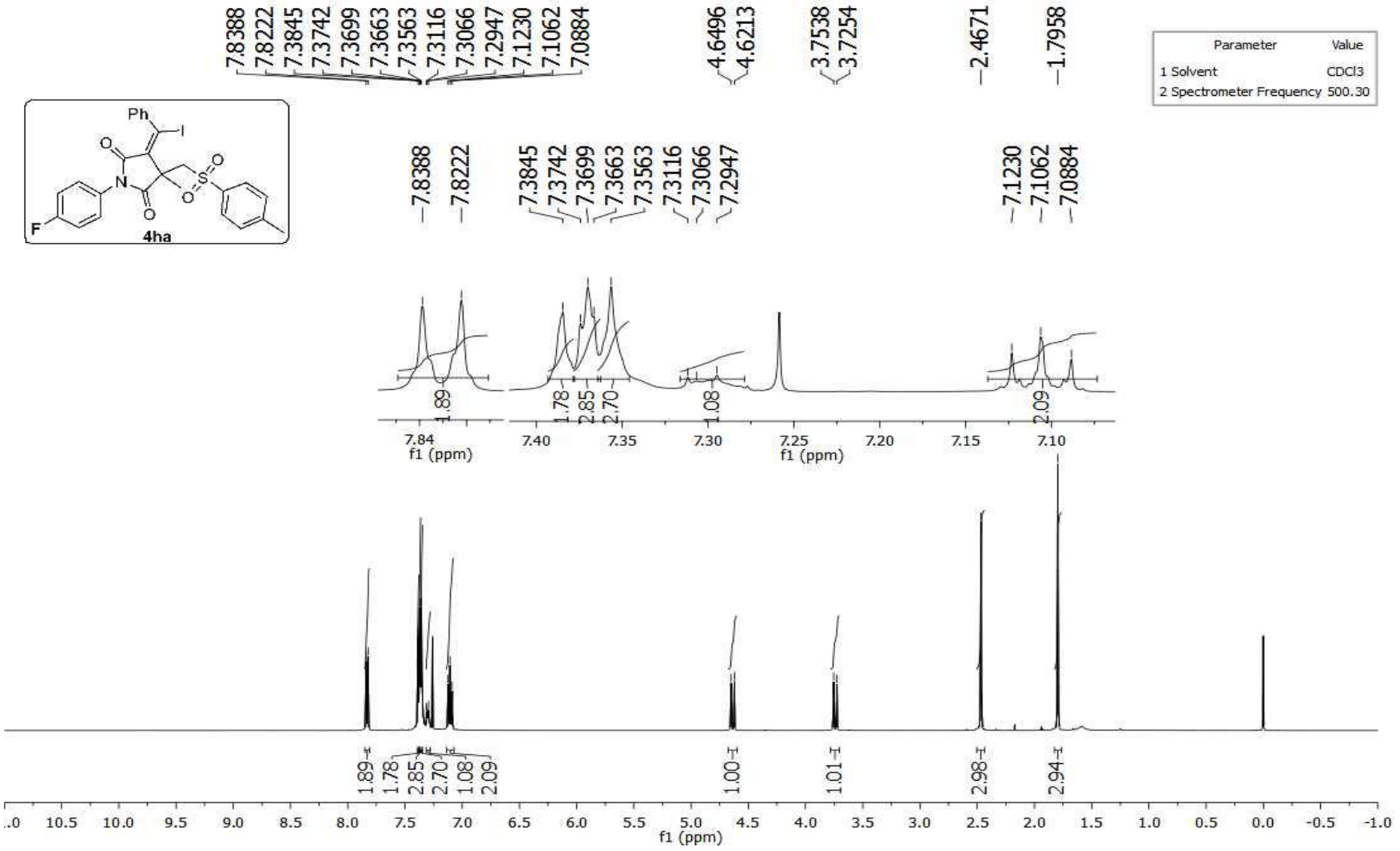

Figure S40. [1]H NMR spectra of (*E*)-1-(4-fluorophenyl)-4-(iodo(phenyl)methylene)-3-methyl-3-(tosylmethyl)pyrrolidine-2,5-dione **(4ha)**

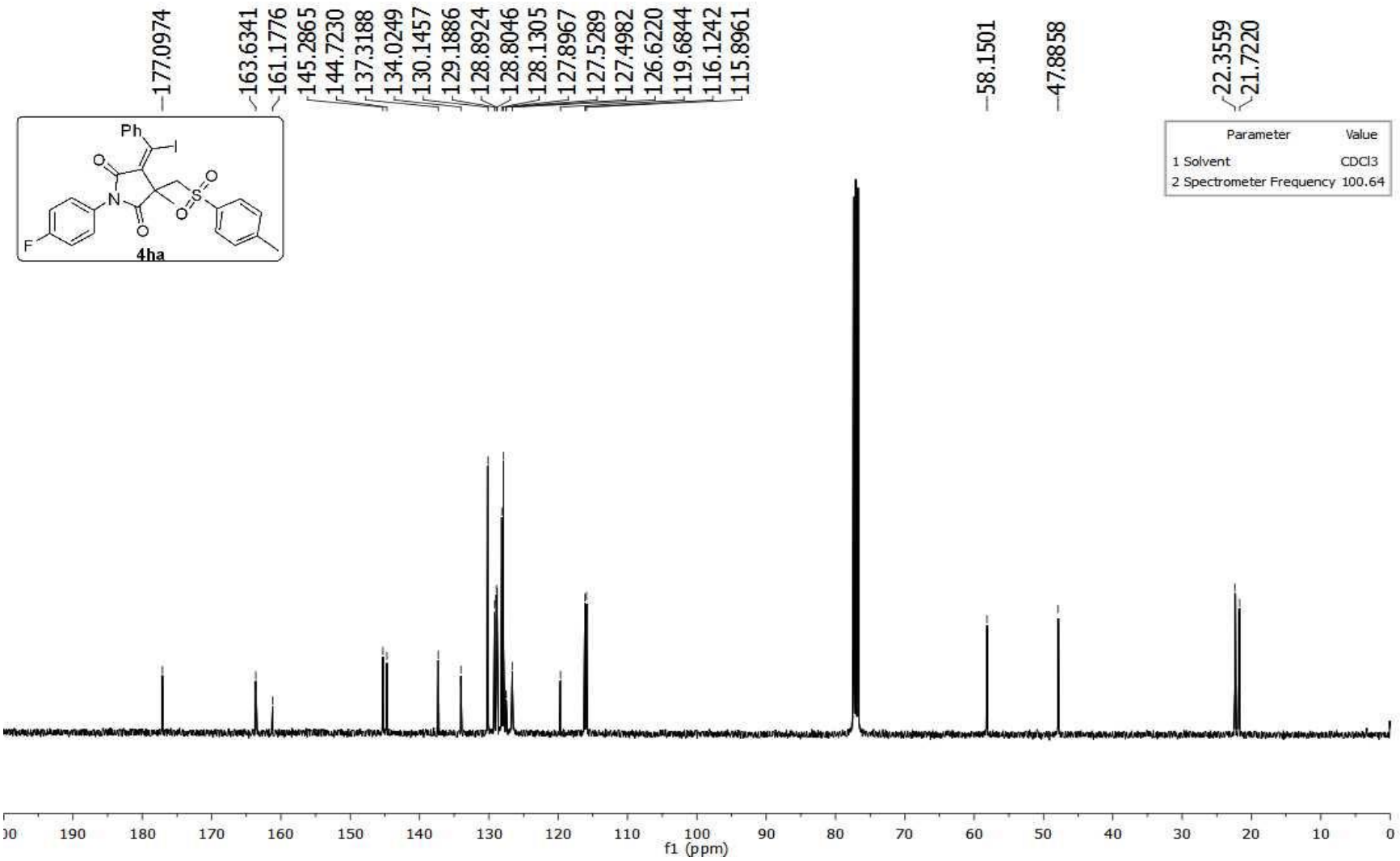

Figure S41. ^{13}C NMR spectra of (*E*)-1-(4-fluorophenyl)-4-(iodo(phenyl)methylene)-3-methyl-3-(tosylmethyl)pyrrolidine-2,5-dione **(4ha)**

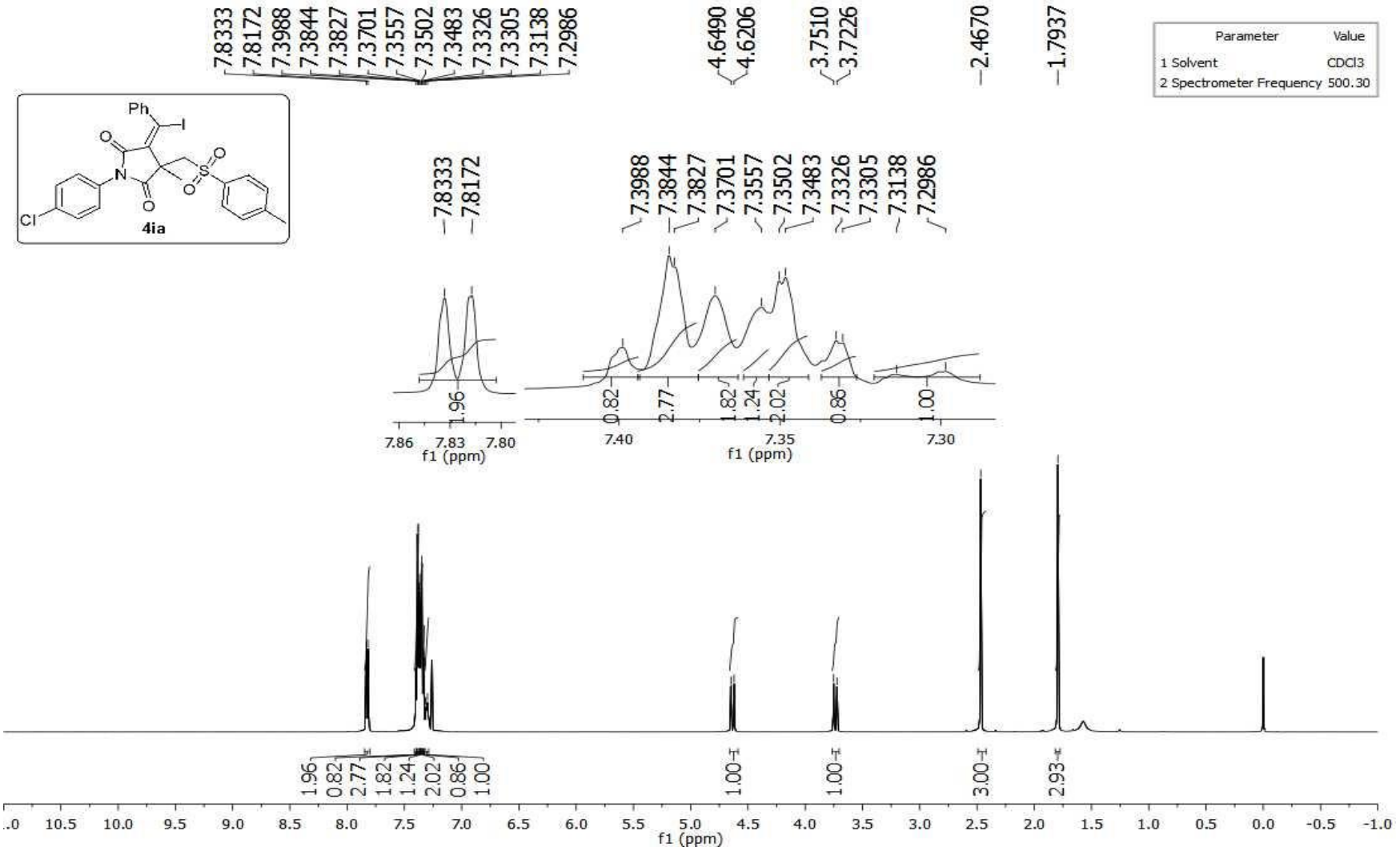

Figure S42. ^{1}H NMR spectra of (*E*)-1-(4-chlorophenyl)-4-(iodo(phenyl)methylene)-3-methyl-3-(tosylmethyl)pyrrolidine-2,5-dione **(4ia)**

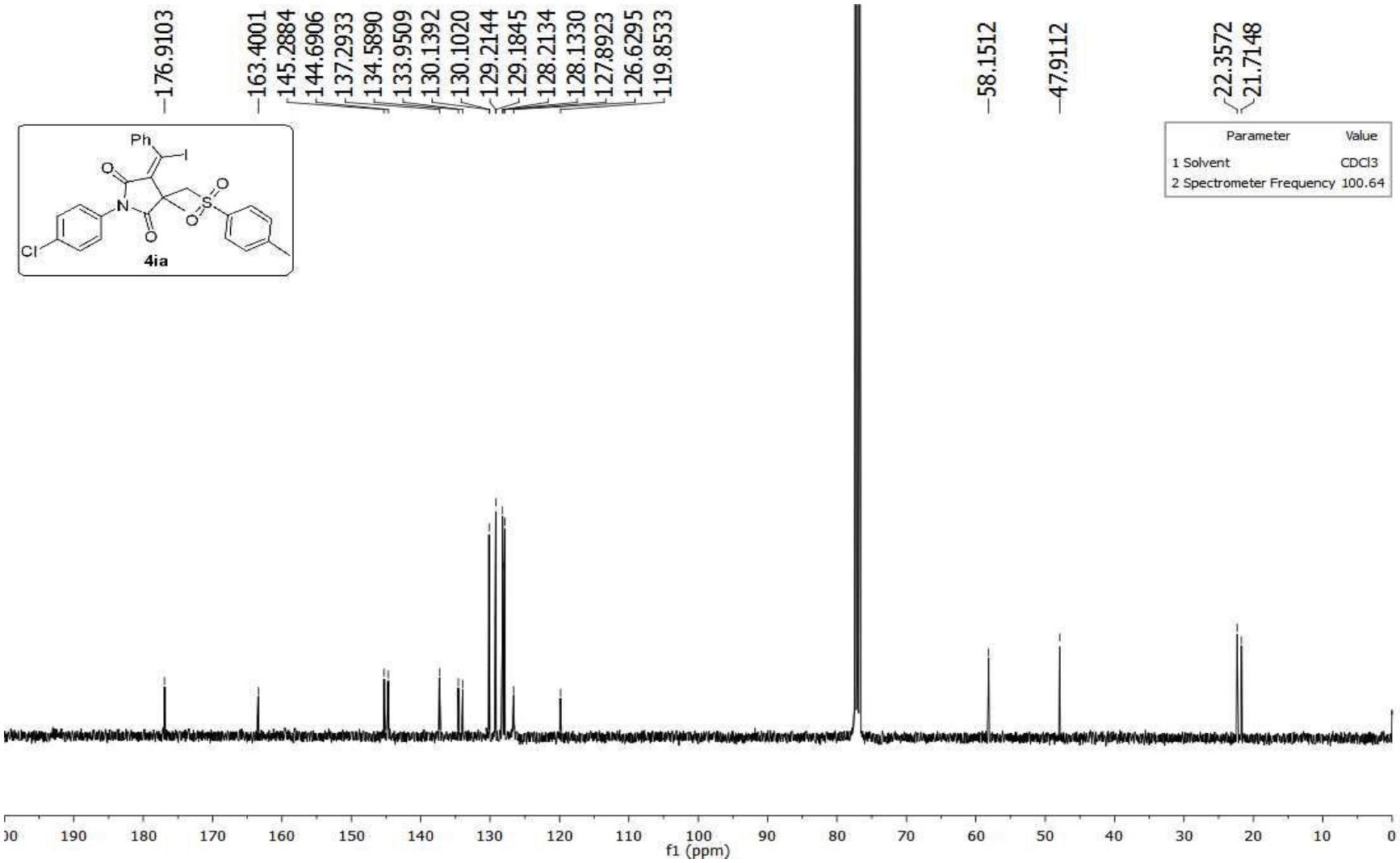

Figure S43. ^{13}C NMR spectra of (*E*)-1-(4-chlorophenyl)-4-(iodo(phenyl)methylene)-3-methyl-3-(tosylmethyl)pyrrolidine-2,5-dione **(4ia)**

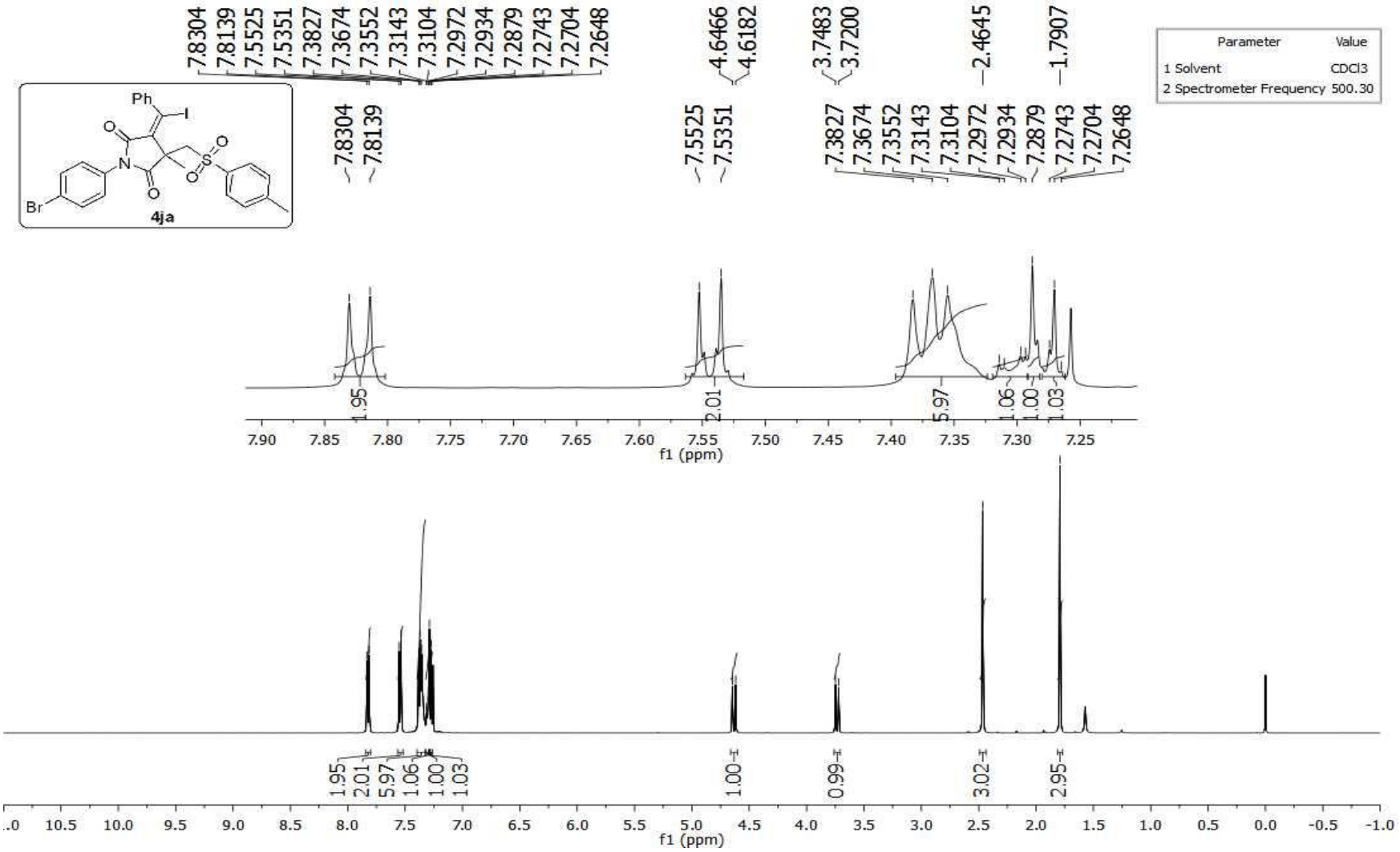

Figure S44. ^{1}H NMR spectra of (*E*)-1-(4-bromophenyl)-4-(iodo(phenyl)methylene)-3-methyl-3-(tosylmethyl)pyrrolidine-2,5-dione **(4ja)**

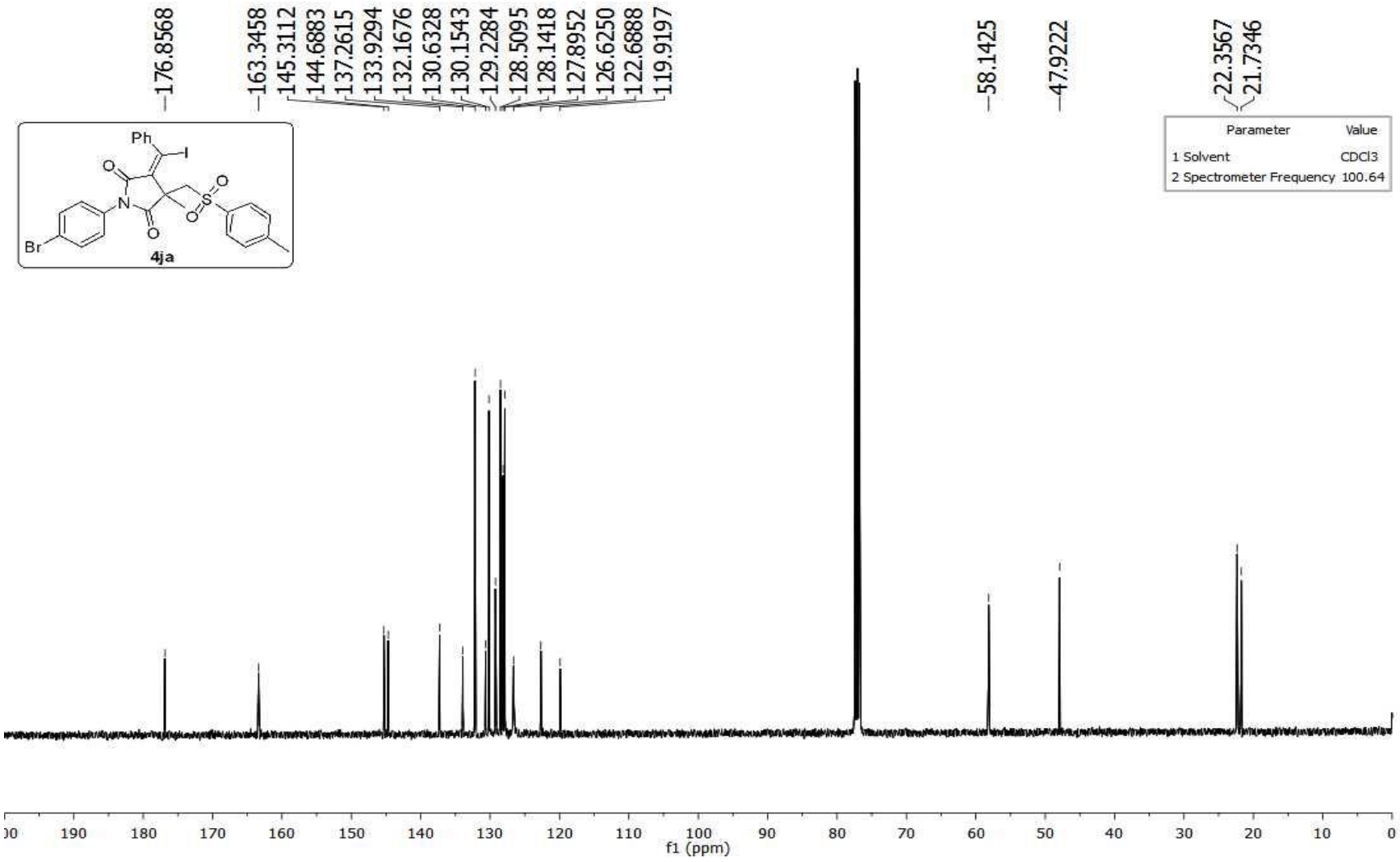

Figure S45. ^{13}C NMR spectra of (*E*)-1-(4-bromophenyl)-4-(iodo(phenyl)methylene)-3-methyl-3-(tosylmethyl)pyrrolidine-2,5-dione **(4ja)**

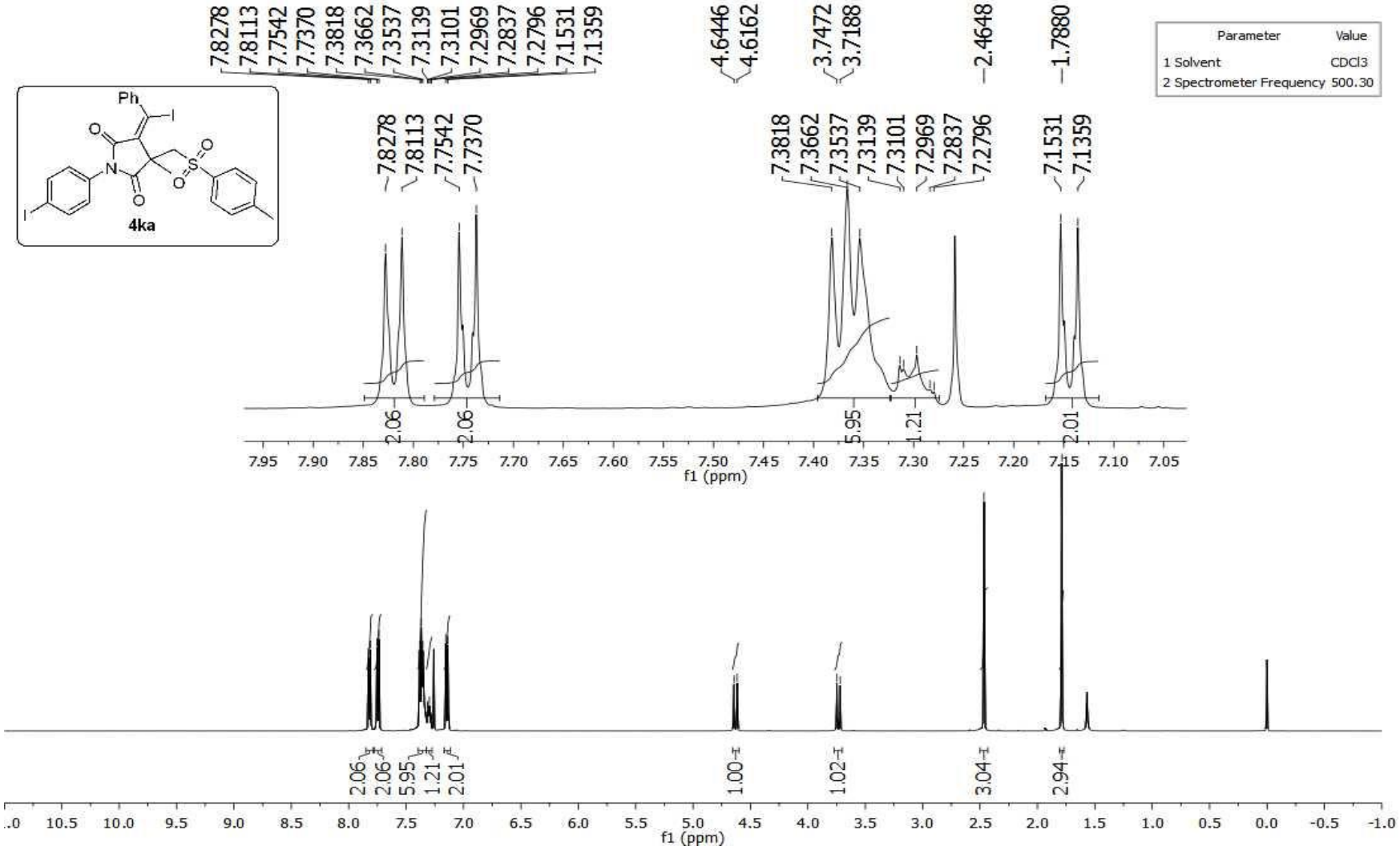

Figure S46. ^{1}H NMR spectra of **(*E*)**-4-(iodo(phenyl)methylene)-1-(4-iodophenyl)-3-methyl-3-(tosylmethyl)pyrrolidine-2,5-dione **(4ka)**

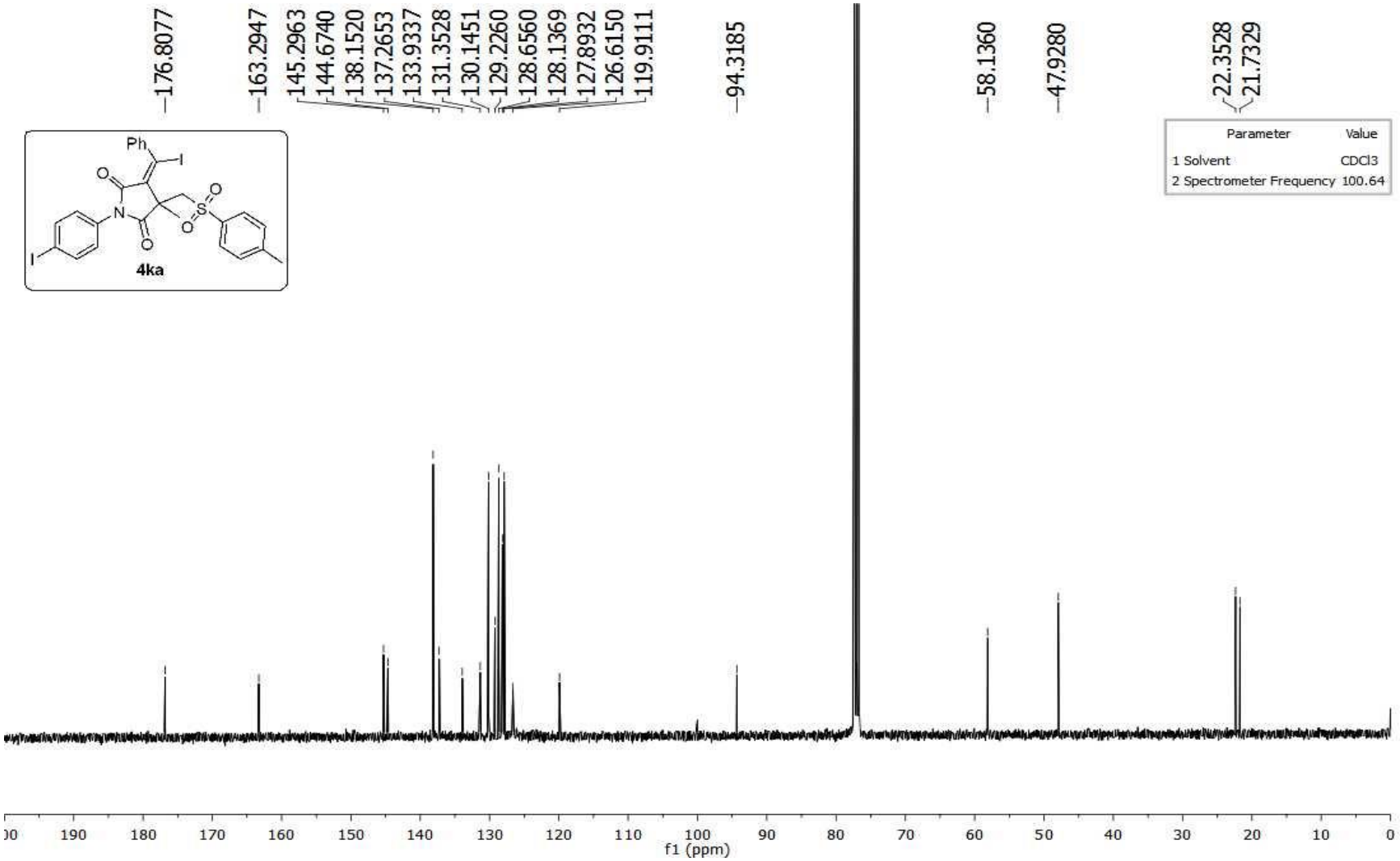

Figure S47. ^{13}C NMR spectra of **(*E*)**-4-(iodo(phenyl)methylene)-1-(4-iodophenyl)-3-methyl-3-(tosylmethyl)pyrrolidine-2,5-dione **(4ka)**

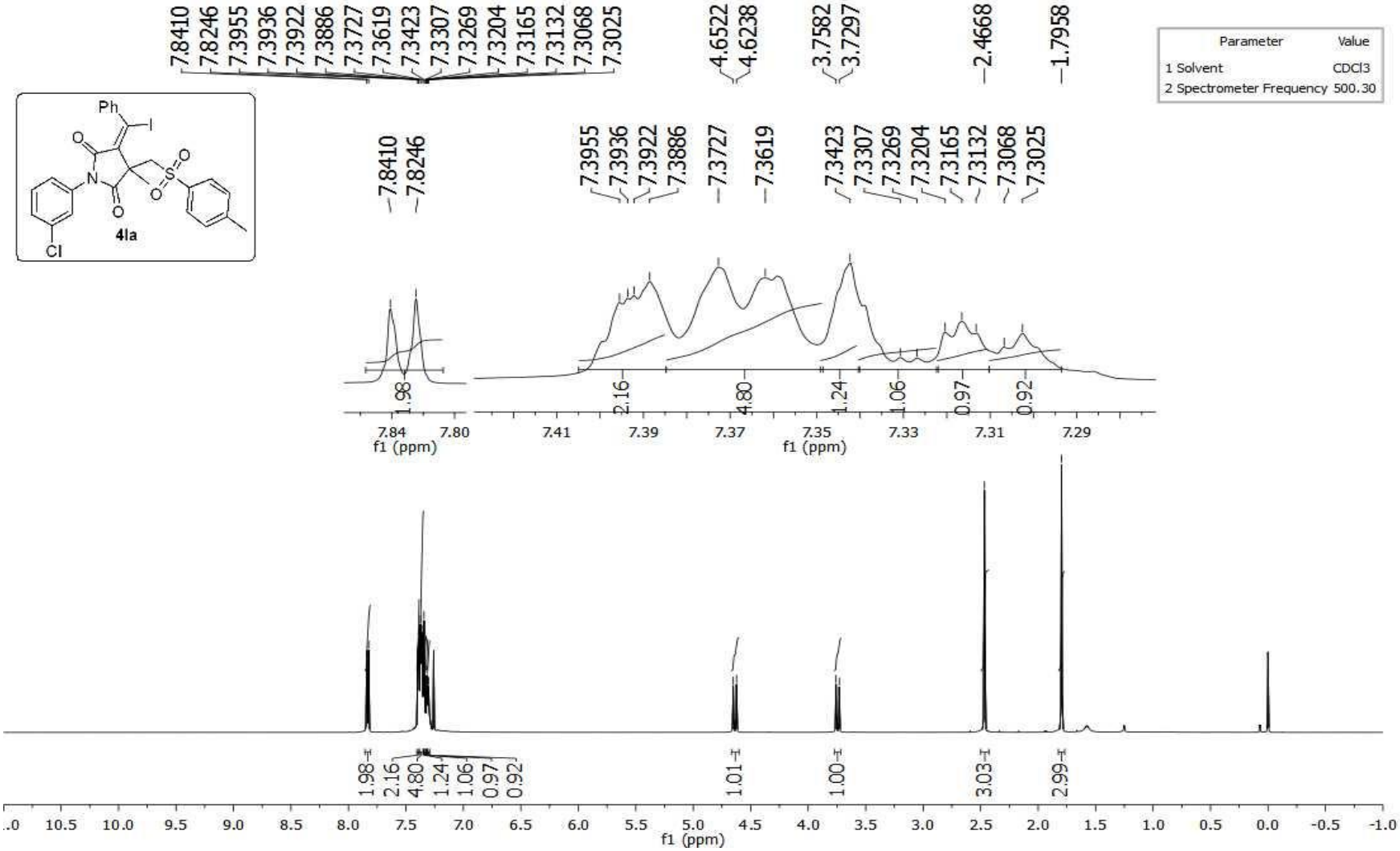

Figure S48. [1]H NMR spectra of (*E*)-1-(3-chlorophenyl)-4-(iodo(phenyl)methylene)-3-methyl-3-(tosylmethyl)pyrrolidine-2,5-dione **(4la)**

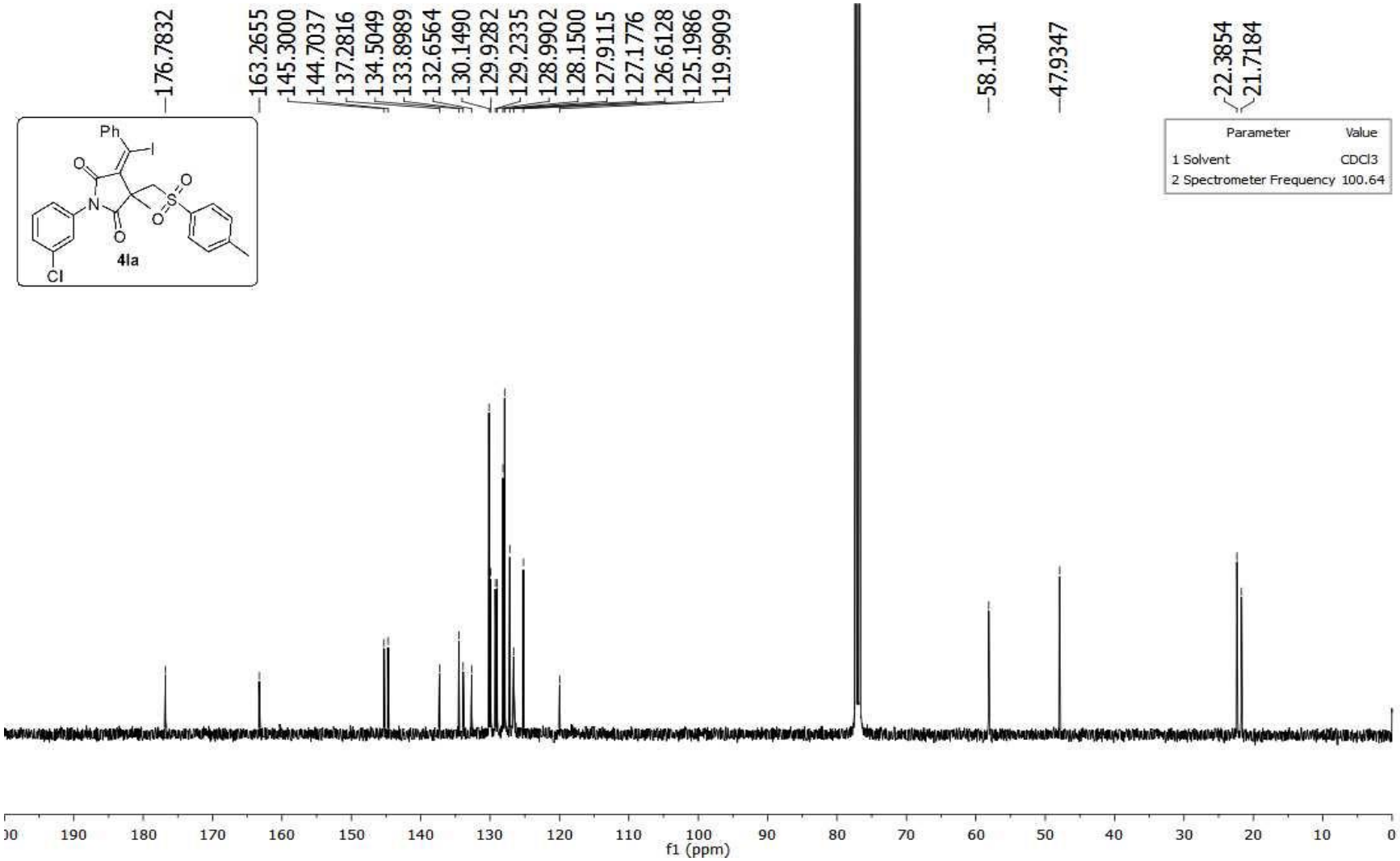

Figure S49. ^{13}C NMR spectra of (*E*)-1-(3-chlorophenyl)-4-(iodo(phenyl)methylene)-3-methyl-3-(tosylmethyl)pyrrolidine-2,5-dione **(4la)**

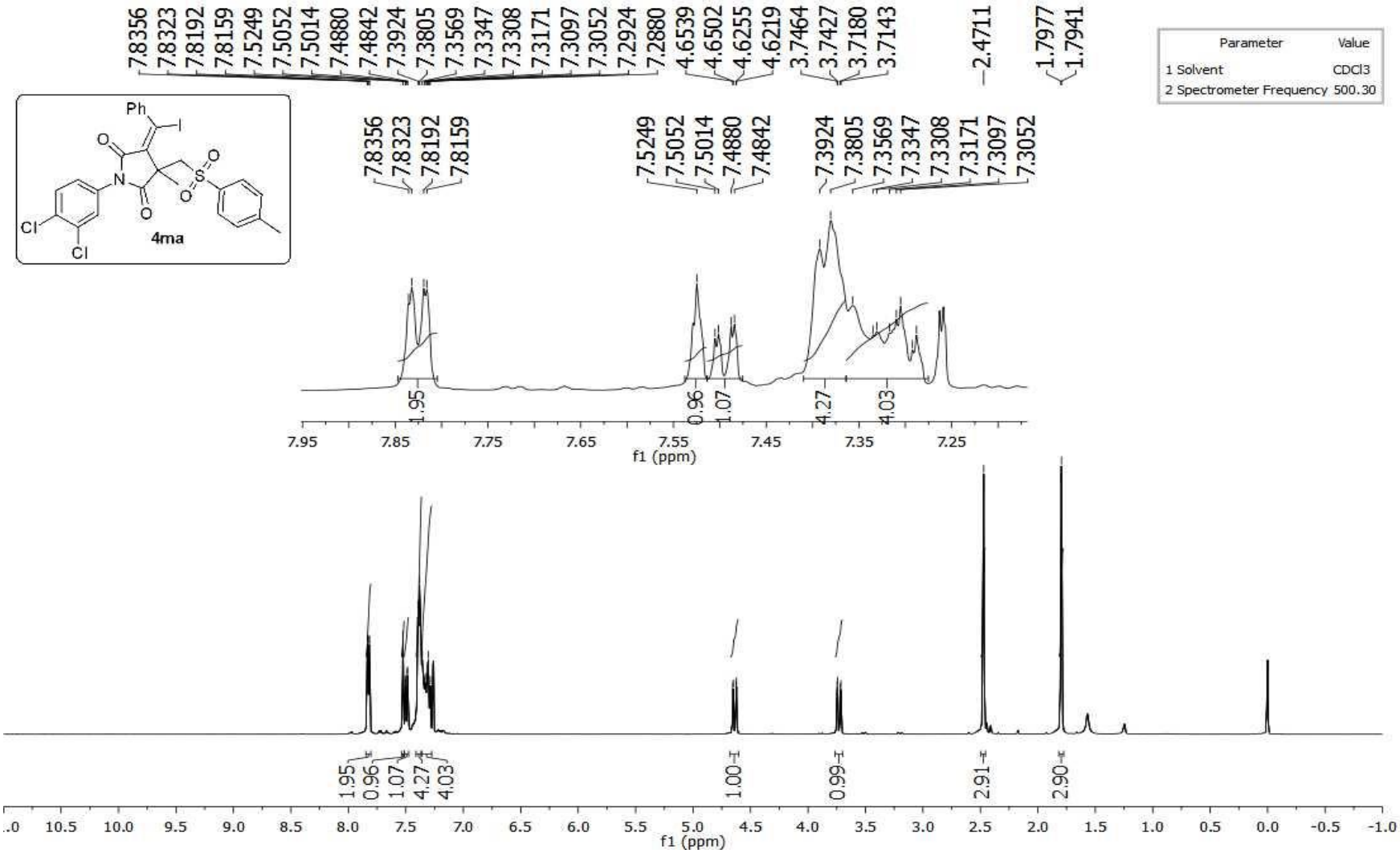

Figure S50. [1]H NMR spectra of (*E*)-1-(3,4-dichlorophenyl)-4-(iodo(phenyl)methylene)-3-methyl-3-(tosylmethyl) pyrrolidine-2,5-dione **(4ma)**

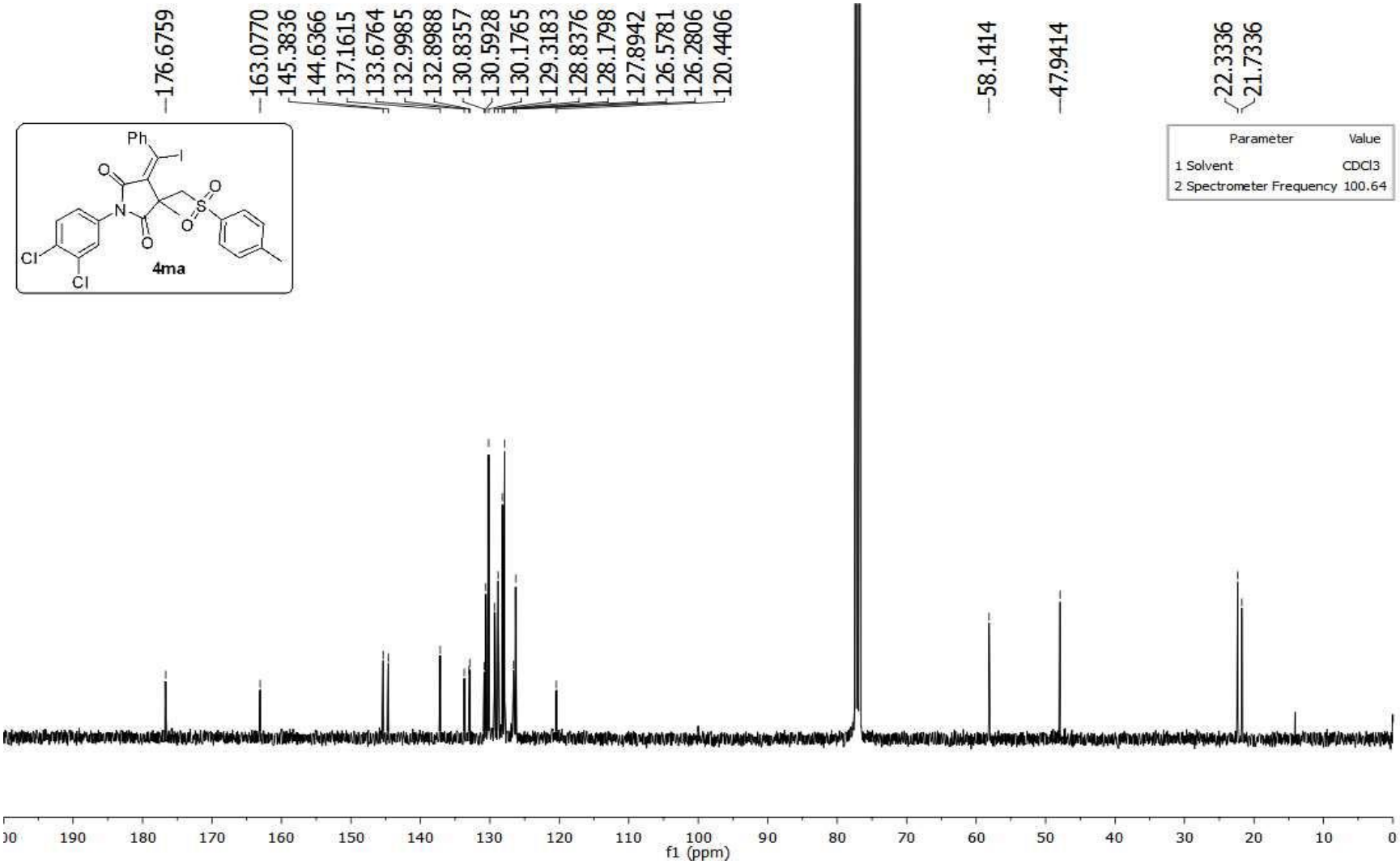

Figure S51. ^{13}C NMR spectra of (*E*)-1-(3,4-dichlorophenyl)-4-(iodo(phenyl)methylene)-3-methyl-3-(tosylmethyl) pyrrolidine-2,5-dione **(4ma)**

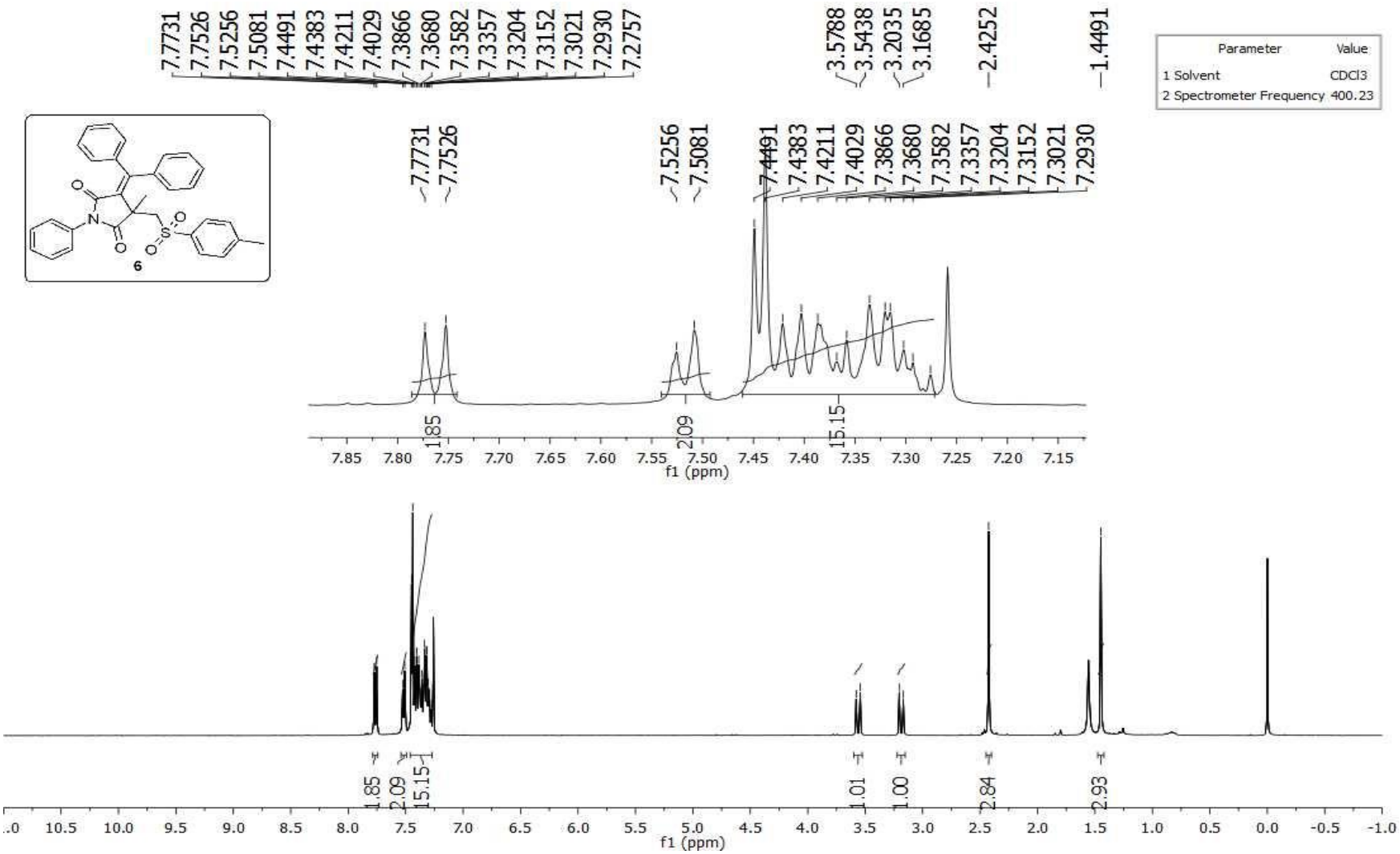

Figure S52. ^{1}H NMR spectra of 4-(diphenylmethylene)-3-methyl-1-phenyl-3-(tosylmethyl)pyrrolidine-2,5-dione **(6)**

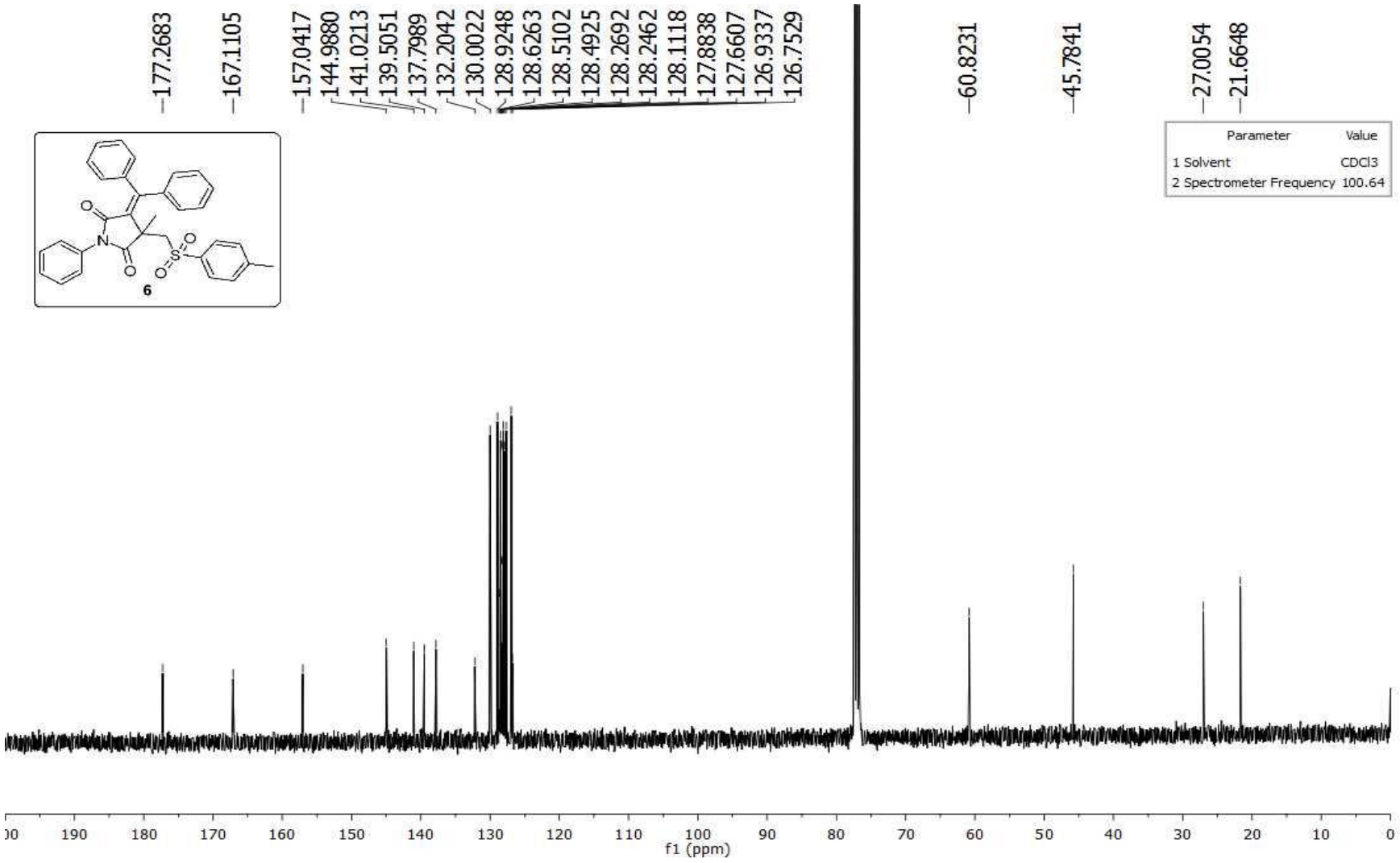

Figure S53. ^{13}C NMR spectra of 4-(diphenylmethylene)-3-methyl-1-phenyl-3-(tosylmethyl)pyrrolidine-2,5-dione **(6)**

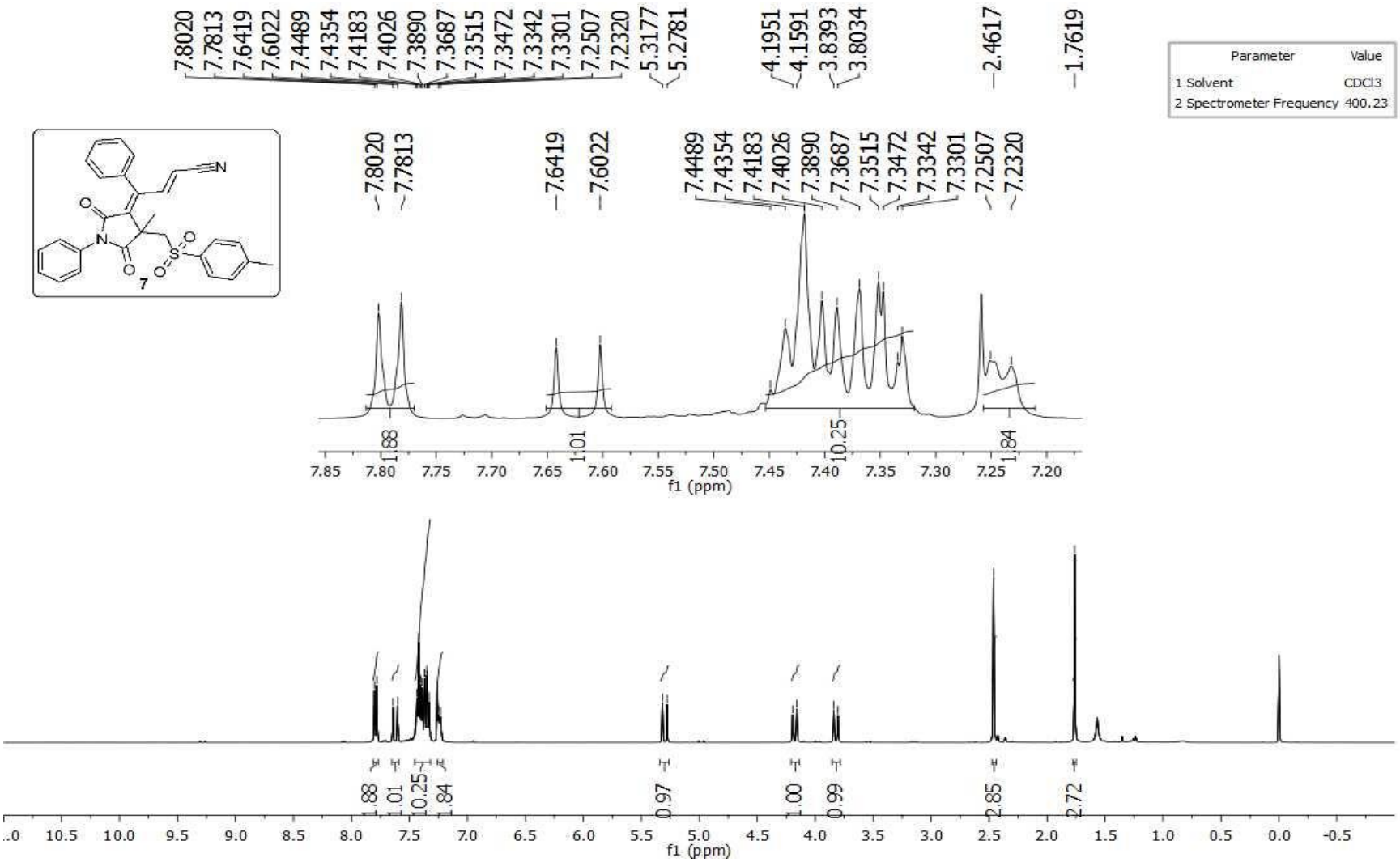

Figure S54. ^{1}H NMR spectra of (2*E*,4*Z*)-4-(4-methyl-2,5-dioxo-1-phenyl-4-(tosylmethyl)pyrrolidin-3-ylidene)-4-phenyl but-2-enenitrile **(7)**

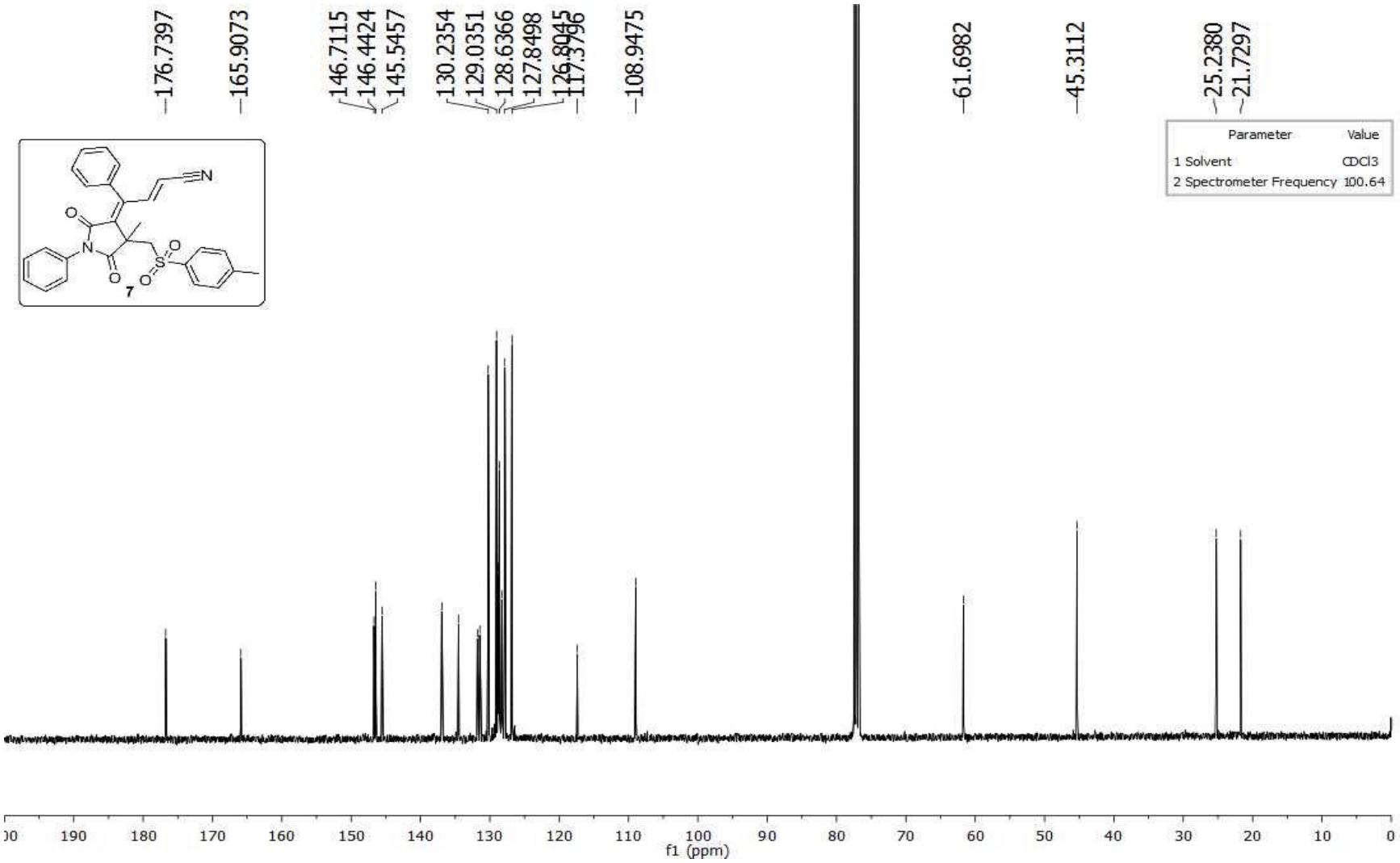

Figure S55. ^{13}C NMR spectra of (2*E*,4*Z*)-4-(4-methyl-2,5-dioxo-1-phenyl-4-(tosylmethyl)pyrrolidin-3-ylidene)-4-phenyl but-2-enenitrile **(7)**

12. X-Ray Crystallographic Data of 4aa

Table S4. Crystal data and structure refinement for **4aa.**

Identification code	RMK-SM- 232-21032022
Chemical formula	$C_{26}H_{22}INO_4S$
Formula weight	571.40 g/mol
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal size	0.230 x 0.270 x 0.310 mm
Crystal system	Monoclinic
Space group	P 1 21/n 1
Unit cell dimensions	a = 11.8903(6) Å α = 90° b = 15.0921(7) Å β = 113.6510(10)° c = 14.6135(7) Å γ = 90°
Volume	2402.1(2) $Å^3$
Z	4
Density (calculated)	1.580 g/cm^3
Absorption coefficient	1.453 mm^{-1}
F(000)	1144
Theta range for data collection	2.31 to 30.07°
Index ranges	-16<=h<=16, -20<=k<=21, -19<=l<=20
Reflections collected	39026
Independent reflections	6983 [R(int) = 0.0343]
Coverage of independent reflections	98.9%
Absorption correction	Multi-Scan
Max. and min. Transmission	0.7160 and 0.6440
Structure solution technique	direct methods
Structure solution program	SHELXT 2014/5 (Sheldrick, 2014)
Refinement method	Full-matrix least-squares on F2
Refinement program	SHELXL-2018/3 (Sheldrick, 2018)
Function minimized	Σ w(Fo2 - Fc2)2
Data / restraints / parameters	6983 / 0 / 300
Goodness-of-fit on F2	1.042
Δ/σmax	0.002

Final R indices	5438 data; I>2σ(I)	R1 = 0.0340, wR2 = 0.0733
	all data	R1 = 0.0510, wR2 = 0.0827
Weighting scheme	w=1/[$\sigma^2(F_o^2)$+(0.0277P)^2+1.7031P] where P=(F_o^2+2F_c^2)/3	
Largest diff. peak and hole	0.797 and -0.822 eÅ^{-3}	
R.M.S. deviation from mean	0.058 eÅ^{-3}	

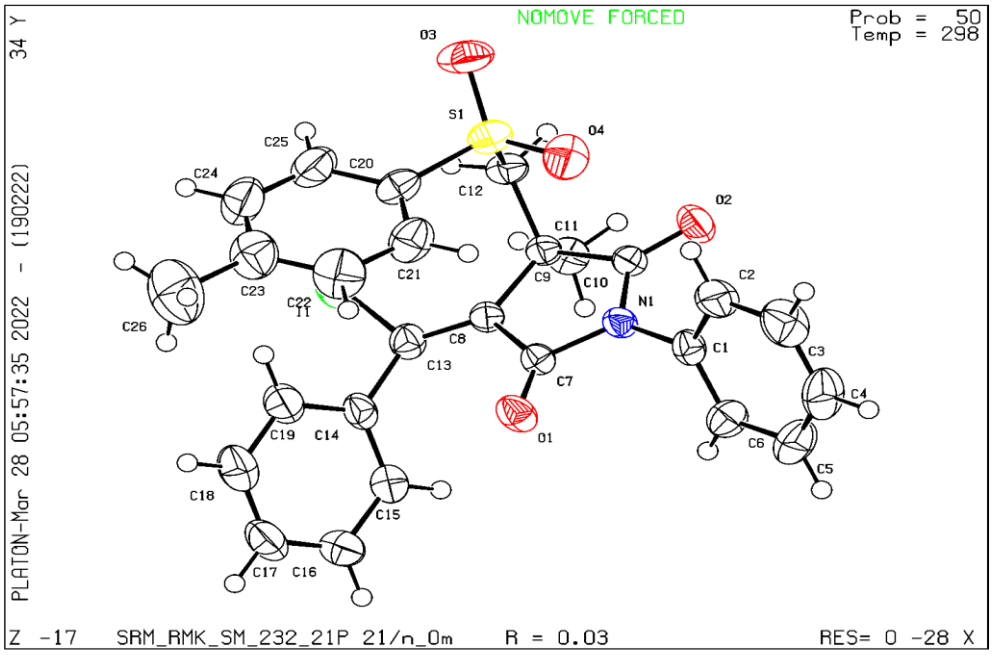

Figure S56. Single Crystal XRD image of compound(*E*)-4-(iodo(phenyl)methylene)-3-methyl-1-phenyl-3-(tosylmethyl)pyrrolidine-2,5-dione (**4aa**)

Crystal structure determination of 4aa

Crystal Data for $C_{26}H_{22}INO_4S$ (*M* =571.40 g/mol): monoclinic, space group P 1 21/n 1, *a* = 11.8903(6) Å, *b* = 15.0921(7) Å, *c* = 14.6135(7) Å, *β* = 113.6510(10)°, *V* = 2402.1(2) Å^3, *Z* = 4, *T* = 298(2) K, μ(Mo Kα) = 1.453 mm^{-1}, *Dcalc* = 1.580 g/cm^3 , 9903 reflections measured (6.299° < 2θ < 59.84°), 6983 unique (R(int) = 0.0343) which were used in all calculations. The final *R*1 was 0.0340(I > 2σ(I)) and *wR*2 was 0.0827(all data).