Supporting Information

Regioselective C-C cross-coupling of 1,2,4-thiadiazoles with maleimide through iridium-catalyzed C-H activation

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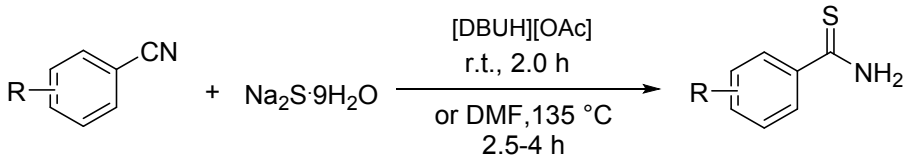
1. General Information

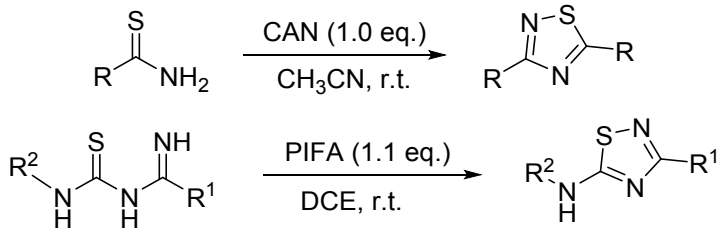
All the reagents were obtained commercially and used without any prior purification. ^{1}H NMR spectra were recorded on a BrukerAvanceII 500 spectrometer. All products were isolated by column chromatography on a silica gel (200–300 mesh) column using petroleum ether (60-90°C) and ethyl acetate. Chemical shifts were reported in parts per million (ppm, δ) downfield from tetramethylsilane. Proton coupling patterns are described as singlet (s), doublet (d), triplet (t), quartet (q), multiplet (m), doublet of doublets (dd).

2. Experimental Information

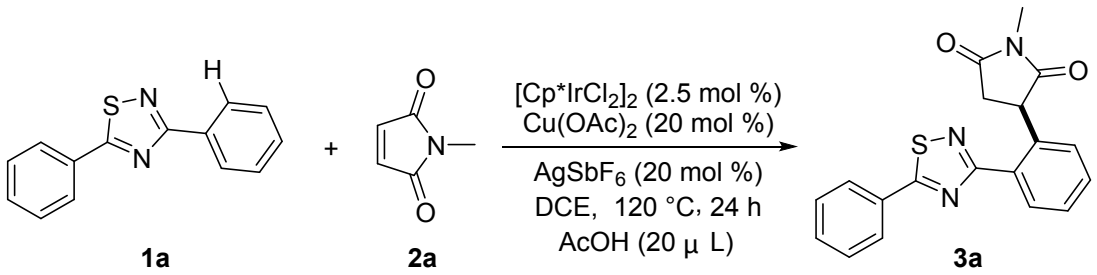
Preparation of the materials starting materials (Thioamides) were prepared according to our previous work. [1-2]



Preparation of the materials starting materials (1,2,4-Thiadiazoles) were prepared according to literature procedures. [3-4]



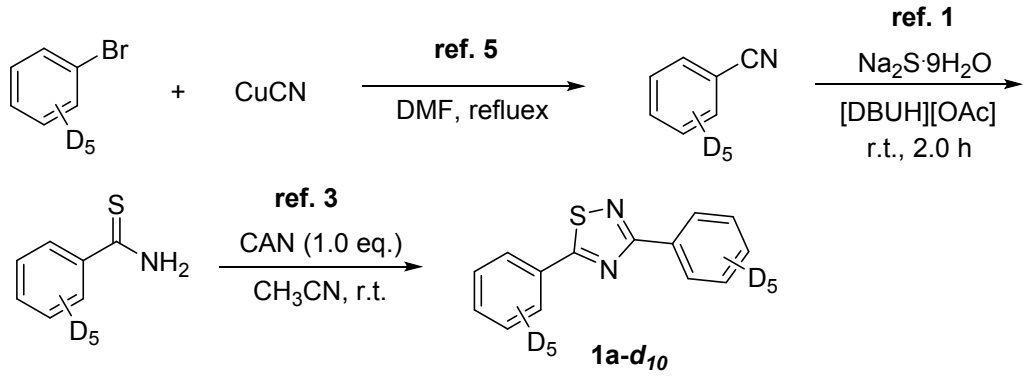
General procedure for the synthesis of product 3a-3w and 6a-6I (compound 3a as the example).



3,5-Diphenyl-1,2,4-thiadiazole (**1a**, 0.2 mmol), *N*-methylmaleimide (**2a**, 0.4 mmol),

$[Cp^*IrCl_2]_2$ (2.5 mol %), $Cu(OAc)_2$ (20 mol %), $AgSbF_6$ (20 mol %), AcOH (20 μL)were dissolved in DCE (1 mL) in a pressure tube. The mixture was stirred at 120 ^oC for 24 hours. After that, the solvent was removed under vacuum and the residue was purified by silica gel chromatography to afford product (**3a**).

Preparation of the Benzonitrile-d_5[5] and 3,5-diphenyl-1,2,4-thiadiazole-d_{10} [1, 3] (1,2,4-Thiadiazoles) were prepared according to literature.



[1] X.-T. Cao, L. Qiao, H. Zheng, H.-Y. Yang, P.-F. Zhang. *RSC Adv.*, 2018, **8**, 170.

[2] X.-T. Cao, H.-Y. Yang, H. Zheng, P.-F. Zhang. *Heterocycles*, 2018, **96,** 509.

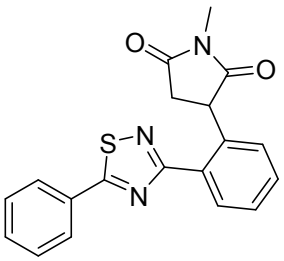
[3] G. Vanajatha, V. P. Reddy. *Tetrahedron Lett.*, 2016, **57**, 2356.

[4] A. Mariappan, K. Rajaguru, N. M. Chola,S. Muthusubramanian, N. Bhuvanesh. *J. Org. Chem.* 2016, **81**, 6573.

[5] Y. Koseki, K. Kitazawa, M. Miyake, T. Kochi, F. Kakiuchi. *J. Org. Chem.* 2017*,* **82***,* 6503.

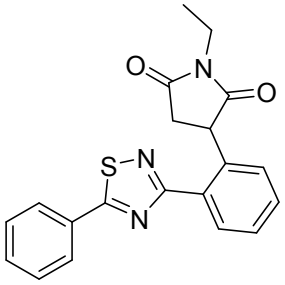
3. Characterization data of the products.

3a:

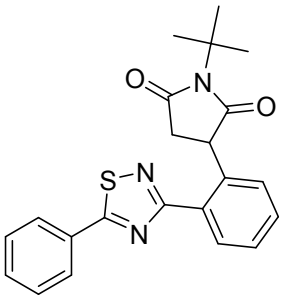


White solid; ^1H NMR (500 MHz, $CDCl_3$) δ 8.41-8.26 (m, 1H), 8.06-7.88 (m, 2H), 7.59-7.44 (m, 5H), 7.26-7.24 (m, 1H), 5.11-4.93 (m, 1H), 3.41-3.34 (m, 1H), 3.02 (s, 3H), 2.92-2.85 ppm (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.87, 178.54, 176.66, 173.39, 136.44, 132.25, 132.14, 132.01, 130.77, 130.30, 129.70, 129.41, 128.17, 127.56, 45.45, 38.52, 25.11 ppm. HRMS (ESI): Calculated for $C_{19}H_{15}N_3O_2S$: $[M+H]^+$

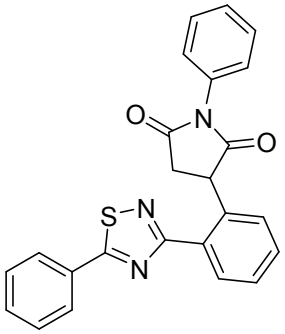
350.0958, Found 350.0937.

3b: 

White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.34-8.19 (m, 1H), 8.02-7.85 (m, 2H), 7.55-7.34 (m, 5H), 7.18-7.10 (m, 1H), 5.02-4.76 (m, 1H), 3.53 (q, *J* = 7.2 Hz, 2H), 3.32-3.23 (m, 1H), 2.80-2.71 (m, 1H), 1.15 ppm (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.79, 178.29, 176.46, 173.38, 136.72, 132.23, 132.13, 132.06, 130.80, 130.33, 129.41, 128.10, 127.55, 45.25, 38.53, 33.97, 13.14 ppm. HRMS (ESI): Calculated for $C_{20}H_{17}N_3O_2S_2$: $[M+H]^+$ 364.1114, Found 364.1091.

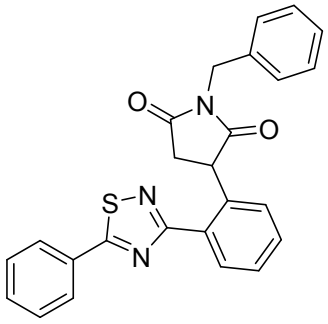
3c: 

White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.34 (d, *J* = 7.4 Hz, 1H), 8.00 (d, *J* = 8.0 Hz, 2H), 7.56-7.50 (m, 3H), 7.48-7.43 (m, 2H), 7.24 (d, *J* = 7.3 Hz, 1H), 4.95-4.80 (m, 1H), 3.25-3.18 (m, 1H), 2.79-2.72 (m, 1H), 1.63 ppm (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.63, 179.44, 177.56, 173.45, 137.37, 132.18, 132.16, 132.05, 130.71, 130.40, 129.44, 129.39, 127.92, 127.56, 58.44, 45.30, 38.69, 28.45 ppm. HRMS (ESI): Calculated for $C_{22}H_{21}N_3O_2S$: $[M+H]^+$ 392.1427, Found 392.1402.

3d: 

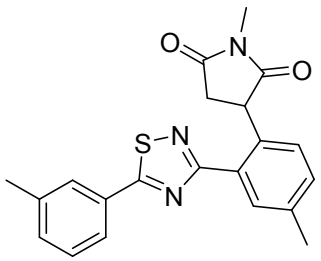
White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.45-8.27 (m, 1H), 8.00-7.86 (m, 2H), 7.51-7.36 (m, 7H), 7.34-7.22 (m, 4H), 5.10-4.91 (m, 1H), 3.48-3.37 (m, 1H), 3.08-2.94 ppm (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.83, 177.24, 175.51, 173.34, 136.13, 132.43, 132.28, 132.26, 131.84, 130.85, 130.32, 129.42, 129.14, 128.47, 128.38, 127.62, 126.38, 46.08, 38.32 ppm. HRMS (ESI): Calculated for $C_{24}H_{19}N_3O_2S$: $[M+H]^+$ 412.1114, Found 412.1090.

3e:

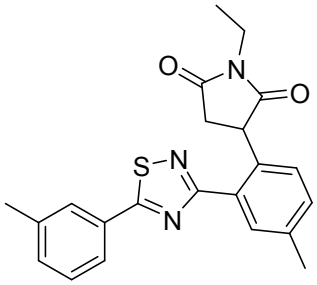


White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.32 (d, *J* = 7.2 Hz, 1H), 7.95 (d, *J* = 6.8 Hz, 2H), 7.57-7.39 (m, 7H), 7.35-7.27 (m, 3H), 7.19-7.12 (m, 1H), 5.02-4.91 (m, 1H), 4.69 (s, 2H), 3.38-3.30 (m, 1H), 2.88-2.81 ppm (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.82, 178.12, 176.19, 173.23, 136.46, 136.01, 132.20, 132.13, 132.00, 130.75, 130.33, 129.73, 129.39, 129.24, 128.73, 128.15, 127.98, 127.54, 45.48, 42.68, 38.44 ppm. HRMS (ESI): Calculated for $C_{25}H_{19}N_3O_2S$: $[M+H]^+$ 426.1271, Found 426.1258.

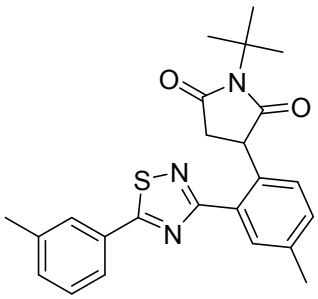
3f:



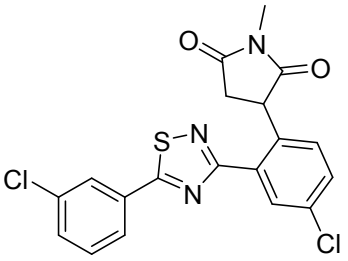
White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05 (s, 1H), 7.71 (s, 1H), 7.69 (d, *J* = 7.7 Hz, 1H), 7.33-7.26 (m, 2H), 7.20 (d, *J* = 7.9 Hz, 1H), 7.05 (d, *J* = 7.9 Hz, 1H), 4.90-4.77 (m, 1H), 3.28-3.21 (m, 1H), 2.91 (s, 3H), 2.82-2.75 (m, 1H), 2.37 (s, 3H), 2.36 ppm (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 188.04, 178.72, 176.77, 173.49, 139.35, 138.03, 133.39, 133.04, 132.57, 131.75, 131.46, 130.21, 129.82, 129.28, 128.02, 124.77, 45.23, 38.54, 25.06, 21.33, 21.04 ppm. HRMS (ESI): Calculated for $C_{21}H_{19}N_3O_2S$: $[M+H]^+$ 378.1271, Found 378.1250.

3g: 

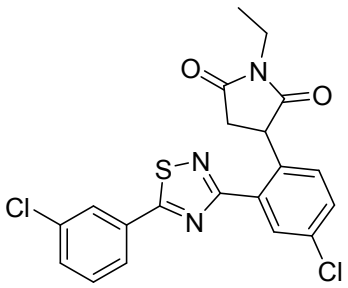
White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 (s, 1H), 7.79 (s, 1H), 7.77 (d, *J* = 7.5 Hz, 1H), 7.38 (t, *J* = 7.5 Hz, 1H), 7.34 (d, *J* = 7.6 Hz, 1H), 7.29-7.26 (m, 1H), 7.11 (d, *J* = 7.9 Hz, 1H), 5.05-4.85 (m, 1H), 3.63-3.56 (m, 2H), 3.34-3.27 (m, 1H), 2.85-2.78 (m, 1H), 2.44 (s, 3H), 2.43 (s, 3H), 1.22 ppm (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.93, 178.43, 176.53, 173.48, 139.30, 137.91, 133.69, 133.01, 132.57, 131.81, 131.48, 130.24, 129.54, 129.27, 128.01, 124.75, 45.03, 38.52, 33.90, 21.33, 21.05, 13.13 ppm. HRMS (ESI): Calculated for $C_{22}H_{21}N_3O_2S$: $[M+H]^+$ 392.1427, Found 392.1407.

3h: 

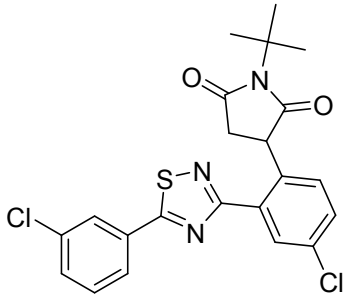
White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 (s, 1H), 7.82 (s, 1H), 7.79 (d, *J* = 7.6 Hz, 1H), 7.44-7.32 (m, 2H), 7.27 (d, *J* = 7.8 Hz, 1H), 7.12 (d, *J* = 7.8 Hz, 1H), 4.85-4.70 (m, 1H), 3.21-3.13 (m, 1H), 2.77-2.70 (m, 1H), 2.45 (s, 3H), 2.43 (s, 3H), 1.62 ppm (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.80, 179.60, 177.67, 173.56, 139.30, 137.70, 134.35, 132.96, 132.59, 131.82, 131.42, 130.33, 129.49, 129.27, 128.04, 124.77, 58.35, 45.02, 38.70, 28.45, 21.35, 21.04 ppm. HRMS (ESI): Calculated for $C_{24}H_{25}N_3O_2S$: $[M+H]^+$ 420.1740, Found 420.1725.

3i: 

White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.36 (s, 1H), 7.99 (s, 1H), 7.85 (d, *J* = 7.7 Hz, 1H), 7.55-7.51 (m, 1H), 7.49-7.43 (m, 2H), 7.20 (d, *J* = 8.3 Hz, 1H), 5.07-4.97 (m, 1H), 3.40-3.32 (m, 1H), 3.03 (s, 3H), 2.85-2.78 ppm (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 186.58, 178.07, 176.23, 172.14, 135.57, 134.89, 134.12, 133.09, 132.33, 132.07, 131.55, 131.24, 130.83, 130.75, 127.42, 125.76, 44.90, 38.18, 25.19 ppm. HRMS (ESI): Calculated for $C_{19}H_{13}Cl_2N_3O_2S$: $[M+H]^+$ 418.0179, Found 418.0190.

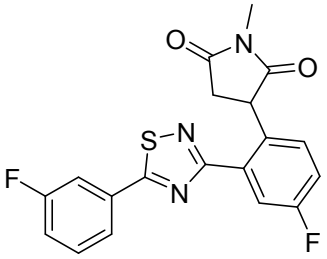
3j: 

White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.28 (s, 1H), 7.91 (s, 1H), 7.77 (d, *J* = 7.7 Hz, 1H), 7.46-7.41 (m, 1H), 7.40-7.34 (m, 2H), 7.09 (d, *J* = 8.3 Hz, 1H), 5.00-4.82 (m, 1H), 3.53 (q, *J* = 7.2 Hz, 2H), 3.28-3.20 (m, 1H), 2.74-2.64 (m, 1H), 1.15 ppm (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 186.48, 177.80, 176.00, 172.12, 135.55, 135.12, 134.05, 133.12, 132.30, 132.07, 131.57, 131.02, 130.84, 130.74, 127.40, 125.75, 44.76, 38.16, 34.05, 13.13 ppm. HRMS (ESI): Calculated for $C_{20}H_{15}Cl_2N_3O_2S$: $[M+H]^+$ 432.0335, Found 432.0350.

3k: 

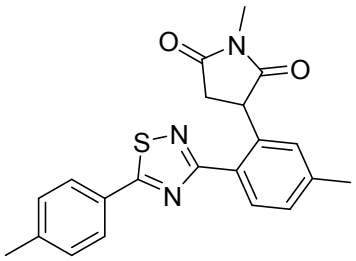
White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.38 (s, 1H), 8.01 (s, 1H), 7.87 (d, *J* = 8.3 Hz, 1H), 7.55-7.52 (m, 1H), 7.49-7.43 (m, 2H), 7.18 (d, *J* = 8.3 Hz, 1H), 4.90-4.80 (m, 1H), 3.23-3.16 (m, 1H), 2.74-2.67 (m, 1H), 1.63 ppm (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 186.35, 178.92, 177.12, 172.20, 135.72, 135.56, 133.87, 133.11, 132.26, 132.10, 131.65, 131.12, 130.77, 130.73, 127.43, 125.76, 58.55, 44.89, 38.30, 28.42 ppm. HRMS (ESI): Calculated for $C_{22}H_{19}Cl_2N_3O_2S$: $[M+H]^+$ 460.0648, Found 460.0662.

3l:



White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.09 (d, *J* = 9.7 Hz, 1H), 7.79-7.65 (m, 2H), 7.54-7.48 (m, 1H), 7.29-7.22 (m, 2H), 7.21-7.16 (m, 1H), 5.07-5.00 (m, 1H), 3.40-3.33 (m, 1H), 3.04 (s, 3H), 2.86-2.79 ppm (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 186.70, 186.67, 178.33, 176.35, 172.25, 172.23, 163.04 (d, *J* = 248.9 Hz), 161.95 (d, *J* = 247.7 Hz), 133.49 (d, *J* = 8.1 Hz), 132.31 (d, *J* = 3.4 Hz), 131.89 (d, *J* = 8.1 Hz), 131.69 (d, *J* = 8.1 Hz), 131.22 (d, *J* = 8.2 Hz), 123.45 (d, *J* = 3.1 Hz), 119.34 (d, *J* = 21.3 Hz), 119.00 (d, *J* = 23.9 Hz), 117.87 (d, *J* = 21.4 Hz), 114.35 (d, *J* = 23.5 Hz), 44.82, 38.29, 25.15 ppm. HRMS (ESI): Calculated for $C_{19}H_{13}F_2N_3O_2S$: $[M+H]^+$386.0770, Found 386.0746

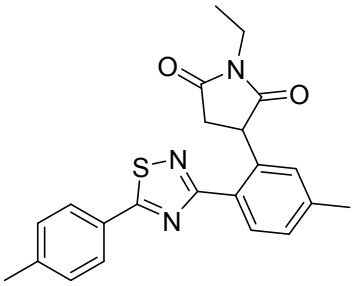
3m:



White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.23 (d, *J* = 8.0 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.24 (d, *J* = 5.6 Hz, 1H), 7.02 (s, 1H), 5.13-4.89 (m, 1H), 3.38-3.32 (m, 1H), 3.03 (s, 3H), 2.88-2.83 (m, 1H), 2.42 (s, 3H), 2.40 ppm (s,

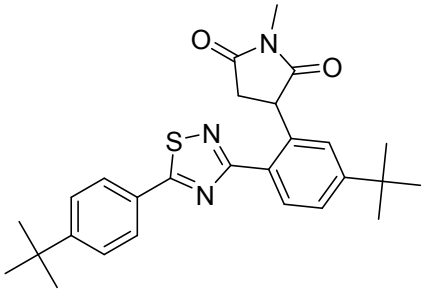
3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.65, 178.74, 176.85, 173.32, 142.84, 140.95, 136.24, 132.12, 130.39, 130.18, 130.03, 129.34, 129.17, 128.93, 127.73, 127.47, 45.44, 38.51, 25.12, 21.68, 21.38 ppm. HRMS (ESI): Calculated for $C_{21}H_{19}N_3O_2S$: $[M+H]^+$ 378.1271, Found 378.1266.

3n:

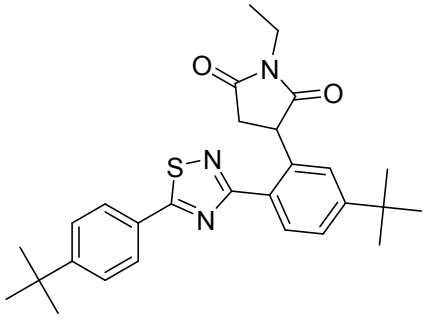


White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.24 (d, *J* = 8.0 Hz, 1H), 7.83 (d, *J* = 8.0 Hz, 2H), 7.34-7.26 (m, 3H), 7.01 (s, 1H), 5.05-4.90 (m, 1H), 3.62 (q, *J* = 7.1 Hz, 2H), 3.37-3.29 (m, 1H), 2.85-2.79 (m, 1H), 2.43 (s, 3H), 2.40 (s, 3H), 1.24 ppm (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.57, 178.44, 176.61, 173.33, 142.82, 140.94, 136.48, 132.13, 130.12, 130.03, 129.41, 128.87, 127.79, 127.47, 45.27, 38.51, 33.95, 21.68, 21.41, 13.13 ppm. HRMS (ESI): Calculated for $C_{22}H_{21}N_3O_2S$: $[M+H]^+$ 392.1427, Found392.1407.

3o:

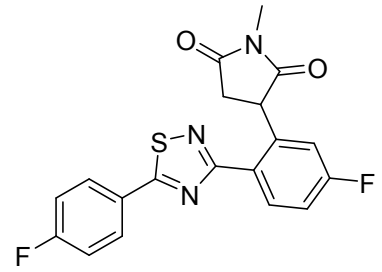


White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.18 (d, *J* = 8.3 Hz, 1H), 7.81 (d, *J* = 8.4 Hz, 2H), 7.44 (d, *J* = 8.4 Hz, 2H), 7.41 (d, *J* = 8.3, 1H), 7.15 (s, 1H), 4.85-4.75 (m, 1H), 3.29-3.21 (m, 1H), 2.92 (s, 3H), 2.89-2.82 (m, 1H), 1.28 (s, 9H), 1.27 ppm (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.57, 178.62, 176.83, 173.36, 155.92, 153.91, 135.63, 131.99, 129.28, 127.68, 127.37, 127.15, 126.32, 125.41, 46.20, 38.44, 35.16, 34.89, 31.17, 31.13, 25.09 ppm. HRMS (ESI): Calculated for $C_{27}H_{31}N_3O_2S$: $[M+H]^+$ 462.2210, Found 462.2188.



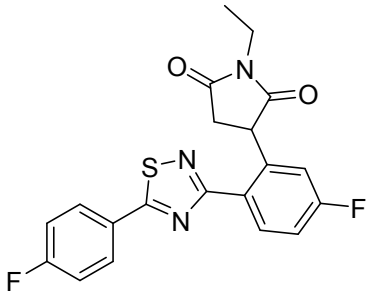
3p

White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.20 (d, *J* = 8.3 Hz, 1H), 7.83 (d, *J* = 8.3 Hz, 2H), 7.46 (d, *J* = 8.4 Hz, 2H), 7.41 (d, *J* = 8.3 Hz, 1H), 7.12 (s, 1H), 4.99-4.75 (m, 1H), 3.54 (dd, *J* = 14.2, 7.0 Hz, 2H), 3.29-3.21 (m, 1H), 2.83-2.76 (m, 1H), 1.29 (s, 9H), 1.27 (s, 9H), 1.16 ppm (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.49, 178.47, 176.68, 173.33, 155.90, 153.91, 136.15, 131.94, 129.31, 127.74, 127.36, 126.51, 126.32, 125.33, 45.81, 38.52, 35.16, 34.90, 33.88, 31.13, 13.14 ppm. HRMS (ESI): Calculated for $C_{28}H_{33}N_3O_2S$: $[M+H]^+$ 476.2336, Found 476.2311.

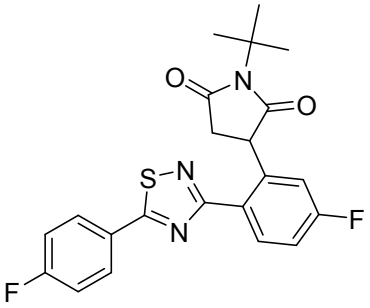


3q:

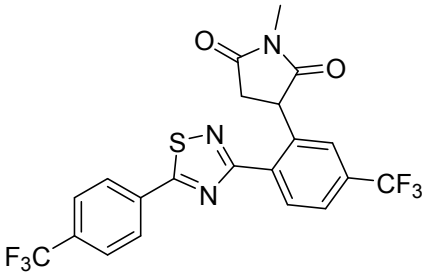
White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.30-8.25 (m, 1H), 7.98-7.80 (m, 2H), 7.13 (t, *J* = 8.5 Hz, 2H), 7.10-7.05 (m, 1H), 6.92-6.87 (m, 1H), 5.05-4.92 (m, 1H), 3.33-3.25 (m, 1H), 2.95 (s, 3H), 2.79-2.73 ppm (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 186.59, 177.84, 176.16, 172.45, 165.06 (d, *J* = 254.2 Hz), 163.65 (d, *J* = 252.2 Hz), 138.99 (d, *J* = 7.6 Hz), 134.45 (d, *J* = 8.7 Hz), 134.20, 129.75 (d, *J* = 9.0 Hz), 128.15 (d, *J* = 3.2 Hz), 126.58 (d, *J* = 3.3 Hz), 116.70 (d, *J* = 22.3 Hz), 115.27 (d, *J* = 21.1 Hz), 45.26, 38.15, 25.18 ppm. HRMS (ESI): Calculated for $C_{19}H_{13}F_2N_3O_2S$: $[M+H]^+$ 386.0760, Found 386.0746.

3r: 

White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.39-8.34 (m, 1H), 8.10-7.90 (m, 2H), 7.21 (t, *J* = 8.6 Hz, 2H), 7.17-7.13 (m, 1H), 6.96-6.93 (m, 1H), 5.15-4.96 (m, 1H), 3.62 (q, *J* = 6.8 Hz, 2H), 3.39-3.31 (m, 1H), 2.84-2.77 (m, 1H), 1.24 ppm (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 186.50, 177.59, 175.95, 172.43, 165.05 (d, *J* = 254.1 Hz), 163.64 (d, *J* = 252.1 Hz), 139.22 (d, *J* = 7.7 Hz), 134.45 (d, *J* = 8.8 Hz), 129.74 (d, *J* = 9.0 Hz), 128.19 (d, *J* = 3.3 Hz), 126.61 (d, *J* = 3.3 Hz), 116.68 (d, *J* = 22.3 Hz), 116.41, 115.20 (d, *J* = 21.1 Hz), 45.12, 38.13, 34.06, 13.10 ppm. HRMS (ESI): Calculated for $C_{20}H_{15}F_2N_3O_2S$: $[M+H]^+$400.0926, Found 400.0912.

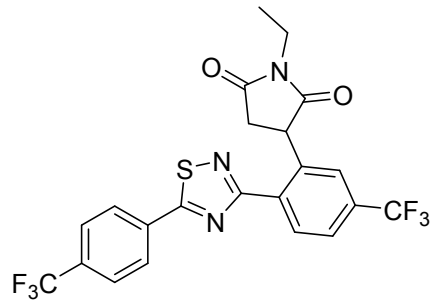
3s: 

White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.30-8.27 (m, 1H), 7.95-7.89 (m, 2H), 7.14 (t, *J* = 8.5 Hz, 2H), 7.06 (t, *J* = 8.2 Hz, 1H), 6.89-6.85 (m, 1H), 4.84-4.75 (m, 1H), 3.17-3.09 (m, 1H), 2.68-2.61 (m, 1H), 1.55 ppm (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 186.37, 178.72, 177.07, 172.51, 165.04 (d, *J* = 254.1 Hz), 163.62 (d, *J* = 251.9 Hz), 139.88 (d, *J* = 7.7 Hz), 134.47 (d, *J* = 8.7 Hz), 129.75 (d, *J* = 8.9 Hz), 128.19 (d, *J* = 3.2 Hz), 126.69 (d, *J* = 3.3 Hz), 116.67 (d, *J* = 22.3 Hz), 116.44, 115.02 (d, *J* = 21.1 Hz), 58.62, 45.22, 38.31, 28.41 ppm. HRMS (ESI): Calculated for $C_{22}H_{19}F_2N_3O_2S$: $[M+H]^+$428.1239, Found 428.1222.



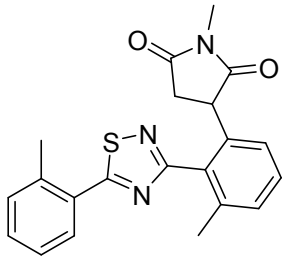
3t:

White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.50 (d, *J* = 8.2 Hz, 1H), 8.12 (d, *J* = 8.1 Hz, 2H), 7.82 (d, *J* = 8.2 Hz, 2H), 7.75 (d, *J* = 8.2 Hz, 1H), 7.53 (s, 1H), 5.07-4.98 (m, 1H), 3.43-3.36 (m, 1H), 3.04 (s, 3H), 2.95-2.88 ppm (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 186.72, 177.56, 175.91, 172.44, 137.11, 134.80, 134.02 (q, *J* = 32.9 Hz), 132.99, 132.93, 132.68 (q, *J* = 32.8 Hz), 127.98, 127.06, 126.57 (q, *J* = 3.7 Hz), 125.12 (q, *J* = 3.5 Hz), 123.49 (q, *J* = 272.7 Hz), 123.48 (q, *J* = 272.5 Hz), 45.49, 38.05, 25.28 ppm. HRMS (ESI): Calculated for $C_{21}H_{13}F_6N_3O_2S$: $[M+H]^+$ 486.0706, Found 486.0722.

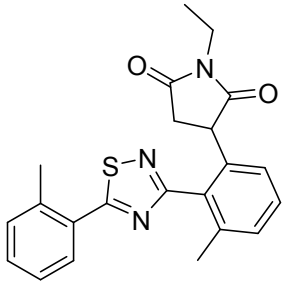


3u:

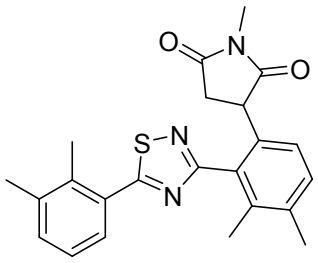
White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.51 (d, *J* = 8.2 Hz, 1H), 8.13 (d, *J* = 8.1 Hz, 2H), 7.82 (d, *J* = 8.2 Hz, 2H), 7.75 (d, *J* = 8.2 Hz, 1H), 7.51 (s, 1H), 5.07-4.02 (m, 1H), 3.66-3.62 (m, 1H), 3.58 (q, *J* = 7.2 Hz, 2H), 3.41-3.33 (m, 1H), 2.92-2.85 (m, 1H), 1.24 ppm (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 186.64, 177.34, 175.72, 172.43, 137.35, 134.81, 134.00 (q, *J* = 32.9 Hz), 133.03, 132.94, 132.67 (q, *J* = 32.9 Hz), 127.97, 126.84, 126.56 (q, *J* = 3.7 Hz), 125.07 (q, *J* = 3.6 Hz), 123.49 (q, *J* = 272.7 Hz), 45.39, 38.01, 34.16, 13.06 ppm. HRMS (ESI): Calculated for $C_{22}H_{15}F_6N_3O_2S$: $[M+H]^+$ 500.0862, Found 500.0879.

3w: 

White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07 (d, *J* = 7.6 Hz, 1H), 7.44 (t, *J* = 7.0 Hz, 1H), 7.39-7.34 (m, 3H), 7.29 (d, *J* = 7.6 Hz, 1H), 7.09 (d, *J* = 7.7 Hz, 1H), 4.10-4.04 (m, 1H), 3.06-2.98 (m, 1H), 2.92 (s, 3H), 2.82-2.75 (m, 1H), 2.67 (s, 3H), 2.26 ppm (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.42, 177.80, 176.19, 172.01, 138.92, 137.21, 136.91, 133.38, 131.91, 131.53, 130.15, 129.94, 129.90, 129.72, 126.70, 125.99, 45.04, 38.25, 25.08, 22.16, 20.73 ppm. HRMS (ESI): Calculated for $C_{21}H_{19}N_3O_2S$: $[M+H]^+$ 378.1271, Found 378.1276.

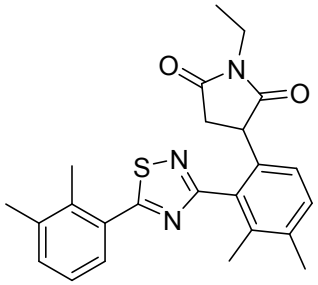
3x: 

White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.09 (d, *J* = 7.7 Hz, 1H), 7.45 (t, *J* = 7.1 Hz, 1H), 7.39-7.34 (m, 3H), 7.29 (d, *J* = 7.6 Hz, 1H), 7.06 (d, *J* = 7.7 Hz, 1H), 4.06-4.02 (m, 1H), 3.52 (q, *J* = 7.2 Hz, 2H), 3.04-2.96 (m, 1H), 2.77-2.70 (m, 1H), 2.67 (s, 3H), 2.26 (s, 3H), 1.16 ppm (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.40, 177.58, 176.04, 172.01, 138.84, 137.25, 137.21, 134.13, 133.55, 131.92, 131.51, 130.06, 129.99, 129.87, 129.75, 126.70, 125.34, 44.67, 38.40, 33.96, 22.19, 20.74, 13.11 ppm. HRMS (ESI): Calculated for $C_{22}H_{21}N_3O_2S$: $[M+H]^+$ 392.1425, Found 392.1441.

3y: 

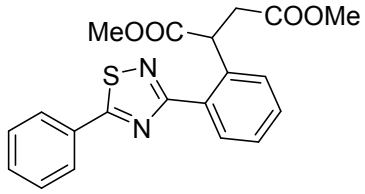
White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70 (d, *J* = 7.7 Hz, 1H), 7.34 (d, *J* = 7.5 Hz, 1H), 7.27-7.22 (m, 2H), 6.99 (d, *J* = 7.9 Hz, 1H), 3.99-3.90 (m, 1H), 3.00-2.92 (m, 1H), 2.92 (s, 3H), 2.78-2.71 (m, 1H), 2.52 (s, 3H), 2.40 (s, 3H), 2.33 ppm (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 188.64, 177.86, 176.26, 172.76, 138.46, 137.22, 137.16, 135.60, 134.42, 133.56, 132.96, 131.40, 130.06, 128.27, 126.09, 125.61, 44.98, 38.16, 25.07, 20.86, 20.33, 17.25, 17.13 ppm. HRMS (ESI): Calculated for $C_{23}H_{23}N_3O_2S$: $[M+H]^+$ 406.1584, Found 406.1589.

3z:

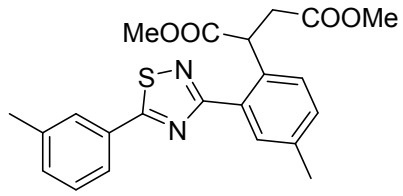


White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.71 (d, *J* = 7.7 Hz, 1H), 7.34 (d, *J* = 7.5 Hz, 1H), 7.27-7.24 (m, 2H), 6.96 (d, *J* = 7.9 Hz, 1H), 3.96-3.86 (m, 1H), 3.52 (q, *J* = 7.2 Hz, 2H), 2.98-2.90 (m, 1H), 2.73-2.66 (m, 1H), 2.53 (s, 3H), 2.40 (s, 3H), 2.33 (s, 3H), 2.08 (s, 3H), 1.16 ppm (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 188.62, 177.63, 176.10, 172.78, 138.46, 137.11, 137.05, 135.59, 134.78, 134.13, 133.73, 132.94, 131.45, 130.09, 128.25, 126.08, 124.94, 44.59, 38.31, 33.94, 20.87, 20.32, 17.26, 17.14, 13.12 ppm. HRMS (ESI): Calculated for $C_{24}H_{25}N_3O_2S$: $[M+H]^+$ 420.1740, Found 420.1756.

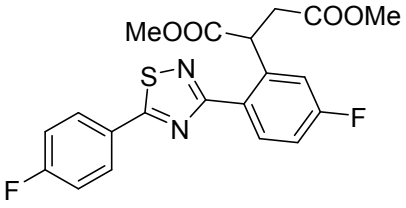
3aa:



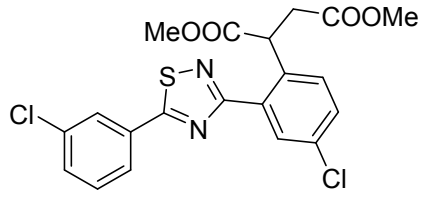
White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.21 (d, *J* = 7.4 Hz, 1H), 8.08-7.95 (m, 2H), 7.55-7.49 (m, 3H), 7.47-7.36 (m, 3H), 5.35- 5.28 (m, 1H), 3.68 (s, 3H), 3.64 (s, 3H), 3.26-3.19 (m, 1H), 3.00-2.94 ppm (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.92, 174.00, 173.48, 172.37, 137.33, 132.07, 131.84, 131.67, 130.52, 130.46, 129.33, 128.37, 127.67, 127.56, 52.27, 51.80, 44.23, 38.14 ppm. HRMS (ESI): Calculated for $C_{20}H_{18}N_2O_4S$: $[M+H]^+$ 383.1060, Found 383.1041.

3ab: 

White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.85 (s, 1H), 7.79 (d, *J* = 7.5 Hz, 1H), 7.41-7.32 (m, 2H), 5.28-5.23 (m, 1H), 3.67 (s, 3H), 3.623 (s, 3H), 3.24-3.17 (m, 1H), 2.98-2.92 (m, 1H), 2.45 (s, 3H), 2.41 ppm (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 188.08, 174.17, 173.57, 172.44, 139.22, 137.42, 134.39, 132.85, 132.07, 131.65, 131.25, 130.44, 129.19, 128.31, 128.05, 124.78, 52.21, 51.75, 43.89, 38.18, 21.31, 21.00 ppm. HRMS (ESI): Calculated for $C_{22}H_{22}N_2O_4S$: $[M+H]^+$ 411.1373, Found 411.1352.

3ac: 

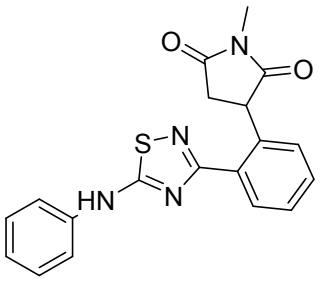
White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.28-8.20 (m, 1H), 8.08-7.96 (m, 2H), 7.21 (t, *J* = 8.5 Hz, 2H), 7.15-7.04 (m, 2H), 5.38-5.33 (m, 1H), 3.69 (s, 3H), 3.66 (s, 3H) 3.24-3.17 (m, 1H), 2.97-2.90 ppm (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 186.72, 173.44, 172.58, 172.10, 164.99 (d, *J* = 253.8 Hz), 163.65 (d, *J* = 251.4 Hz), 139.95 (d, *J* = 7.7 Hz), 133.86 (d, *J* = 8.7 Hz), 129.75 (d, *J* = 8.9 Hz), 127.95, 126.85, 116.61 (d, *J* = 22.3 Hz), 115.44 (d, *J* = 22.6 Hz), 114.89 (d, *J* = 21.3 Hz), 52.45, 51.90, 44.19, 37.90 ppm. HRMS (ESI): Calculated for $C_{20}H_{16}F_2N_4O_2S$: $[M+H]^+$ 419.0872, Found419.0855.

3ad: 

White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.16 (s, 1H), 7.97 (s, 1H), 7.80 (d, *J* = 7.7 Hz, 1H), 7.45 (d, *J* = 8.0 Hz, 1H), 7.39 (t, *J* = 7.9 Hz, 1H), 7.35 (d, *J* = 8.4 Hz, 1H), 7.26 (d, *J* = 8.4 Hz, 1H), 5.22-5.17 (m, 1H), 3.62 (s, 3H), 3.57 (s, 3H), 3.17-3.09 (m, 1H), 2.88-2.82 ppm (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 186.72, 173.56, 172.27,

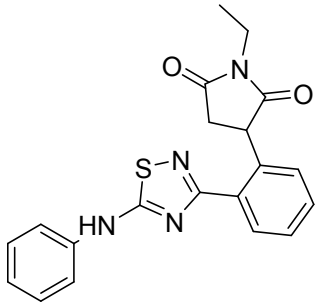
172.10, 135.82, 135.55, 133.64, 132.97, 132.14, 131.82, 131.52, 130.67, 130.58, 130.01, 127.37, 125.82, 52.40, 51.95, 43.79, 37.90 ppm. HRMS (ESI): Calculated for $C_{20}H_{16}Cl_2N_4O_2S$: $[M+H]^+$ 451.0281, Found 451.0267.

6a:

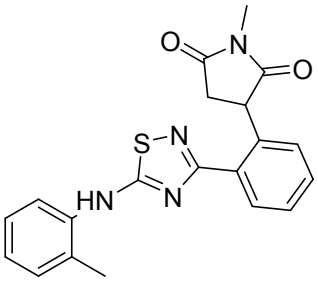


White solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.06 (s, 1H), 8.04-8.01 (m, 1H), 7.61 (d, J = 7.9 Hz, 2H), 7.52-7.34 (m, 5H), 7.10 (t, J = 7.3 Hz, 1H), 4.95-4.78 (m, 1H), 3.23-3.16 (m, 1H), 2.85 (s, 3H), 2.75-2.69 ppm (m, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 178.92, 178.72, 176.77, 169.36, 140.19, 137.15, 132.85, 131.41, 130.54, 129.86, 128.16, 123.52, 118.25, 45.32, 38.26, 25.18 ppm. HRMS (ESI): Calculated for $C_{19}H_{16}N_4O_2S$: $[M+H]^+$ 365.1067, Found 365.1046.

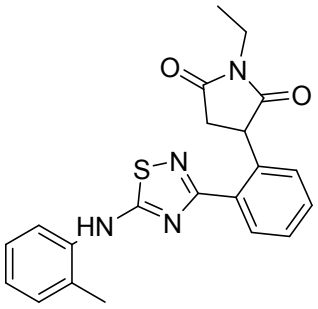
6b:



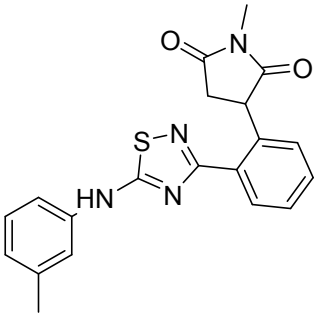
White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.13 (s, 1H), 8.02 (d, J = 7.8 Hz, 1H), 7.40-7.35 (m, 1H), 7.34-7.27 (m, 3H), 7.18 (d, J = 7.7 Hz, 1H), 7.15-7.08 (m, 3H), 4.97-4.81 (m, 1H), 3.68-3.58 (m, 2H), 3.31-3.24 (m, 1H), 2.87-2.81 (m, 1H), 1.24 ppm (t, J = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 180.21, 178.64, 176.83, 168.82, 139.04, 136.28, 132.22, 131.55, 130.41, 129.75, 129.69, 127.98, 124.31, 118.51, 45.35, 38.39, 34.02, 13.15 ppm. HRMS (ESI): Calculated for $C_{20}H_{18}N_4O_2S$: $[M+H]^+$ 379.1223, Found 379.1202.

6c: 

White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.41 (s, 1H), 8.01 (d, *J* = 7.8 Hz, 1H), 7.41 (d, *J* = 7.8 Hz, 1H), 7.36 (t, *J* = 7.6 Hz, 1H), 7.29 (t, *J* = 7.7 Hz, 1H), 7.26-7.22 (m, 2H), 7.22-7.14 (m, 2H), 4.86-4.79 (m, 1H), 3.30-3.22 (m, 1H), 3.04 (s, 3H), 2.89-2.83 (m, 1H), 2.29 ppm (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 182.22, 178.68, 177.13, 169.00, 137.58, 135.99, 131.97, 131.53, 131.41, 130.62, 130.31, 127.95, 127.56, 126.25, 120.81, 45.71, 38.36, 25.16, 17.66 ppm. HRMS (ESI): Calculated for $C_{20}H_{18}N_4O_2S$: $[M+H]^+$ 379.1223, Found 379.1212.

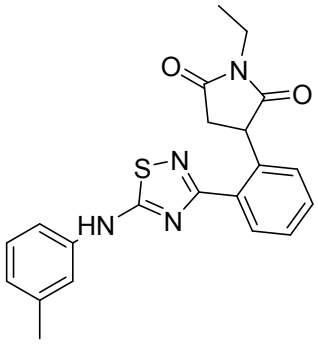
6d: 

White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.45 (s, 1H), 8.00 (d, *J* = 7.8 Hz, 1H), 7.42 (d, *J* = 7.9 Hz, 1H), 7.37-7.35 (m, 1H), 7.31-7.27 (m, 1H), 7.25-7.20 (m, 2H), 7.18-7.13 (m, 2H), 4.96-4.78 (m, 1H), 3.68-3.55 (m, 2H), 3.28-3.21 (m, 1H), 2.83-2.76 (m, 1H), 2.27 (s, 3H), 1.23 ppm (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 182.23, 178.44, 176.80, 169.06, 137.63, 136.24, 132.08, 131.51, 131.40, 130.68, 130.31, 129.86, 127.85, 127.54, 126.25, 120.96, 45.42, 38.36, 33.95, 17.64, 13.14 ppm. HRMS (ESI): Calculated for $C_{21}H_{20}N_4O_2S$: $[M+H]^+$ 93.1380, Found 393.1361.

6e: 

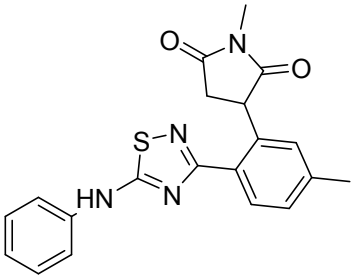
White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.15 (s, 1H), 8.03 (d, *J* = 7.7 Hz, 1H), 7.39 (t, *J* = 7.5 Hz, 1H), 7.29 (t, *J* = 7.6 Hz, 1H), 7.23-7.18 (m, 2H), 6.96-6.91 (m, 2H), 6.88 (s, 1H), 4.87-4.75 (m, 1H), 3.32-3.25 (m, 1H), 3.05 (s, 3H), 2.94-2.87 (m, 1H), 2.29 ppm (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 180.52, 178.74, 177.10, 168.74, 139.87, 138.97, 136.06, 132.11, 131.54, 130.33, 130.25, 129.52, 128.04, 125.34, 119.47, 115.47, 45.68, 38.41, 25.20, 21.47 ppm. HRMS (ESI): Calculated for $C_{20}H_{18}N_4O_2S$: $[M+H]^+$ 379.1223, Found 379.1202.

6f:



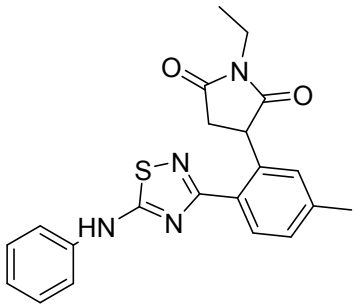
White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.98 (s, 1H), 8.04 (d, *J* = 7.8 Hz, 1H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.31 (t, *J* = 7.6 Hz, 1H), 7.25-7.18 (m, 2H), 6.99-6.91 (m, 2H), 6.90 (s, 1H), 4.96-4.82 (m, 1H), 3.68-3.58 (m, 2H), 3.31-3.24 (m, 1H), 2.88-2.81 (m, 1H), 2.31 (s, 3H), 1.24 ppm (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 180.42, 178.50, 176.82, 168.74, 139.90, 138.96, 136.31, 132.17, 131.54, 130.39, 129.81, 129.57, 127.98, 125.37, 119.44, 115.49, 45.38, 38.41, 33.99, 21.49, 13.15 ppm. HRMS (ESI): Calculated for $C_{21}H_{20}N_4O_2S$: $[M+H]^+$ 393.1380, Found 393.1361.

6g:

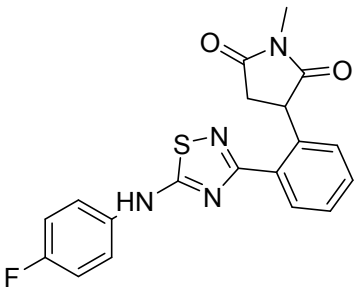


White solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.04 (s, 1H), 7.94 (d, *J* = 7.9 Hz, 1H), 7.60 (d, *J* = 7.9 Hz, 2H), 7.41 (t, *J* = 7.9 Hz, 2H), 7.28 (d, *J* = 7.9 Hz, 1H), 7.09 (t, *J* = 7.4 Hz, 1H), 4.93-4.80 (m, 1H), 3.22-3.14 (m, 1H), 2.86 (s, 3H), 2.74-2.68 (m, 1H), 2.35 ppm (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 178.77, 176.83, 169.40, 140.28, 140.23, 137.02, 131.91, 131.46, 130.09, 129.85, 128.77, 123.47, 118.21, 45.25, 38.23,

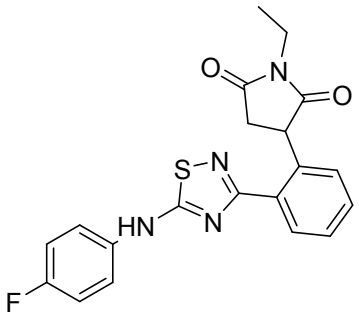
25.18, 21.23 ppm. HRMS (ESI): Calculated for $C_{20}H_{18}N_4O_2S$: $[M+H]^+$ 379.1223, Found 379.1202.

6h: 

White solid; ^1H NMR (500 MHz, $CDCl_3$) δ 9.12 (s, 1H), 7.92 (d, *J* = 8.0 Hz, 1H), 7.33-7.29 (m, 2H), 7.14-7.04 (m, 4H), 6.96 (s, 1H), 4.95-4.85 (m, 1H), 3.70 – 3.60 (m, 2H), 3.30-3.23 (m, 1H), 2.86-2.80 (m, 1H), 2.31 (s, 3H), 1.25 ppm (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 179.99, 178.82, 176.94, 168.83, 140.61, 139.09, 136.07, 131.56, 130.47, 129.62, 129.42, 128.75, 124.18, 118.49 , 45.35, 38.37, 34.01, 21.28, 13.15 ppm. HRMS (ESI): Calculated for $C_{21}H_{20}N_4O_2S$: $[M+H]^+$ 393.1380, Found 393.1361.

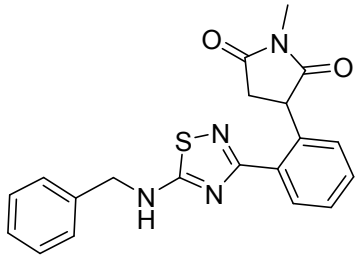
6i: 

White solid; ^1H NMR (500 MHz, $CDCl_3$) δ 9.14 (s, 1H), 7.90 (d, *J* = 7.6 Hz, 1H), 7.31 (t, *J* = 7.3 Hz, 1H), 7.25-7.18 (m, 2H), 7.14 (d, *J* = 7.5 Hz, 1H), 7.09-7.02 (m, 2H), 6.93 (t, *J* = 7.8 Hz, 2H), 4.82-4.63 (m, 1H), 3.24-3.16 (m, 1H), 2.97 (s, 3H), 2.88-2.81 ppm (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 180.90, 178.90, 176.98, 168.79, 159.58 (d, *J* = 245.0 Hz), 135.96, 135.17 (d, *J* = 2.8 Hz), 135.56 (d, *J* = 100.6 Hz), 131.94, 131.51, 130.47, 130.28, 128.08, 121.08 (d, *J* = 8.2 Hz), 116.44 (d, *J* = 22.8 Hz), 45.62, 38.33, 25.23 ppm. HRMS (ESI): Calculated for $C_{19}H_{15}FN_4O_2S$: $[M+H]^+$ 383.0973, Found 383.0954.



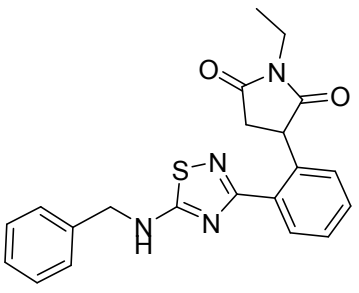
6j:

White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.35 (s, 1H), 7.86 (d, *J* = 7.8 Hz, 1H), 7.28 (t, *J* = 7.6 Hz, 1H), 7.16 (t, *J* = 7.6 Hz, 1H), 7.11 (d, *J* = 7.7 Hz, 1H), 7.05-7.00 (m, 2H), 6.91-6.86 (m, 2H), 4.86-4.75 (m, 1H), 3.58-3.50 (m, 2H), 3.22-3.15 (m, 1H), 2.82-2.76 (m, 1H), 1.16 ppm (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 180.92, 178.81, 176.73, 168.97, 159.44 (d, *J* = 244.6 Hz), 136.16, 135.29 (d, *J* = 2.7 Hz), 132.23, 131.48, 130.41, 129.80, 127.96, 120.96 (d, *J* = 8.2 Hz), 116.31 (d, *J* = 22.8 Hz), 45.33, 38.34, 34.06, 13.15 ppm. HRMS (ESI): Calculated for $C_{20}H_{17}FN_4O_2S$: $[M+H]^+$400.0926, Found 400.0910.



6k:

White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.7 Hz, 1H), 7.36-7.18 (m, 7H), 7.15-7.00 (m, 2H), 4.80-4.68 (m, 1H), 4.32 (s, 2H), 3.12-3.04 (m, 1H), 2.93 (s, 3H), 2.73-2.66 ppm (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 183.74, 178.74, 176.97, 169.12, 136.12, 136.07, 132.39, 131.39, 130.25, 129.90, 128.88, 128.11, 127.93, 127.60, 50.23, 45.43, 38.35, 25.11 ppm. HRMS (ESI): Calculated for $C_{20}H_{18}N_4O_2S$: $[M+H]^+$ 379.1223, Found 379.1201.

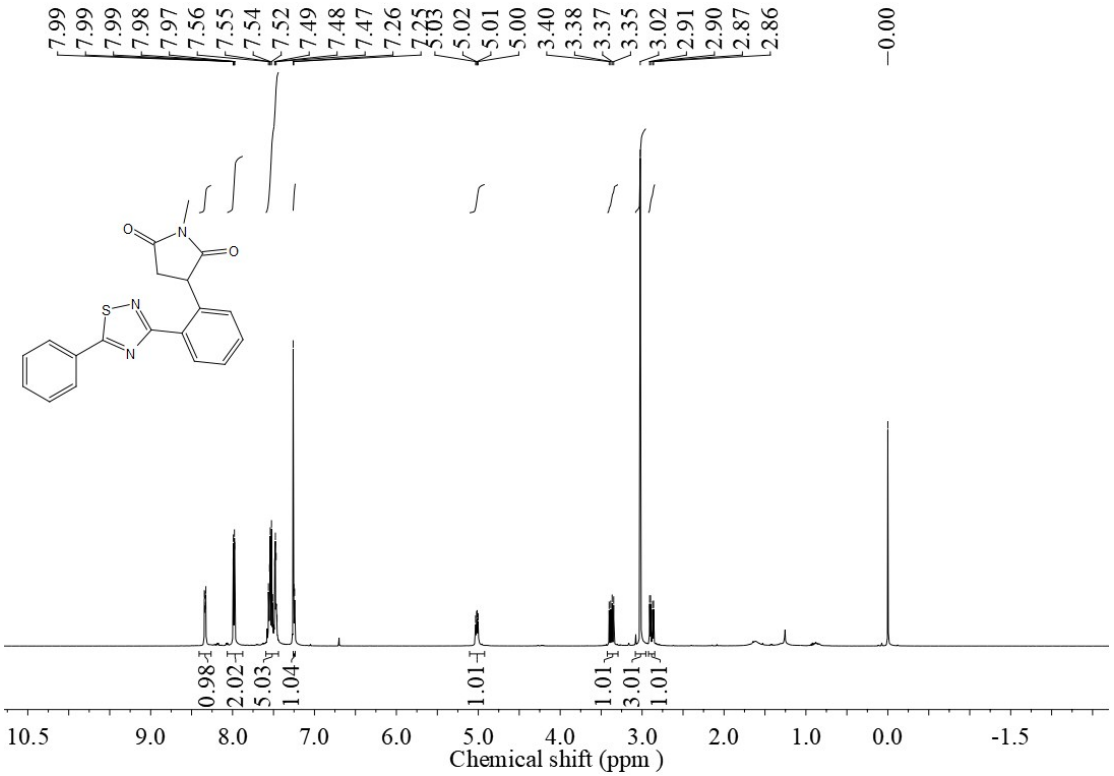


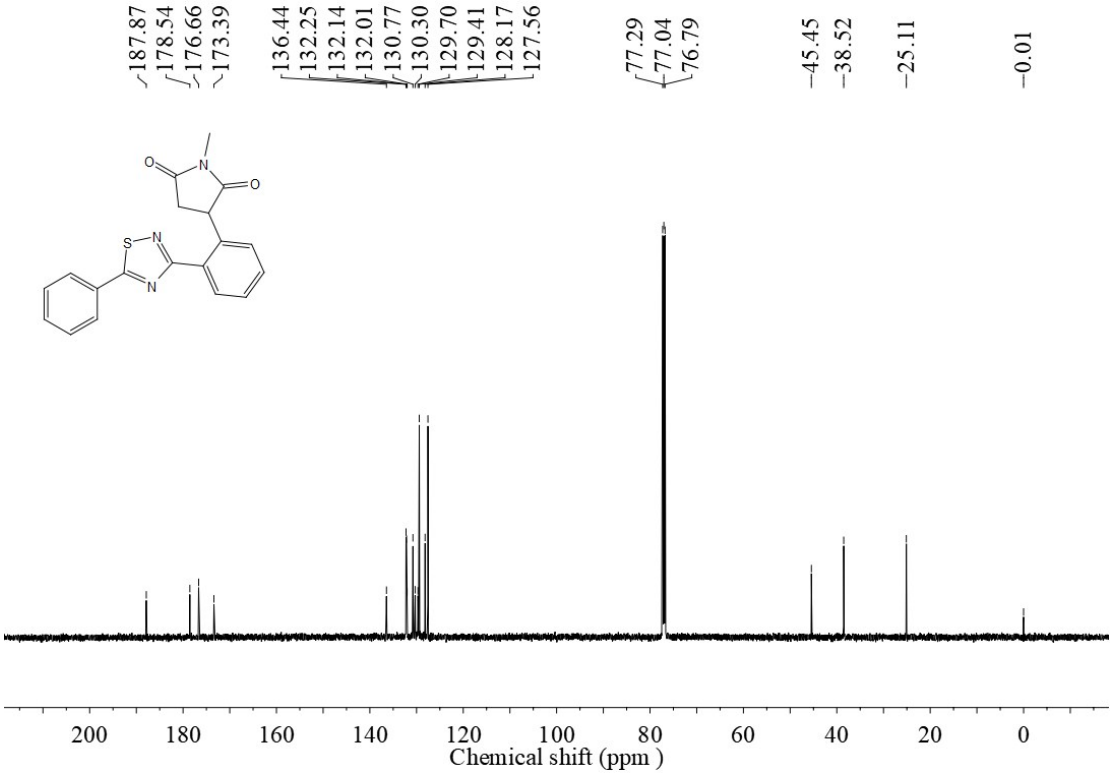
6l:

White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.96 (d, *J* = 7.6 Hz, 1H), 7.32-7.20 (m, 7H), 7.07 (d, *J* = 7.6 Hz, 1H), 6.96 (s, 1H), 4.82-4.72 (m, 1H), 4.33 (s, 2H), 3.55-3.48 (m, 2H), 3.11-3.03 (m, 1H), 2.68-2.61 (m, 1H), 1.14 ppm (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 183.65, 178.50, 176.72, 169.14, 136.37, 136.09, 132.45, 131.40, 130.28, 129.51, 128.89, 128.14, 127.87, 127.60, 50.24, 45.19, 38.36, 33.92, 13.14 ppm. HRMS (ESI): Calculated for $C_{21}H_{20}N_4O_2S$: $[M+H]^+$ 93.1380, Found 393.1362.

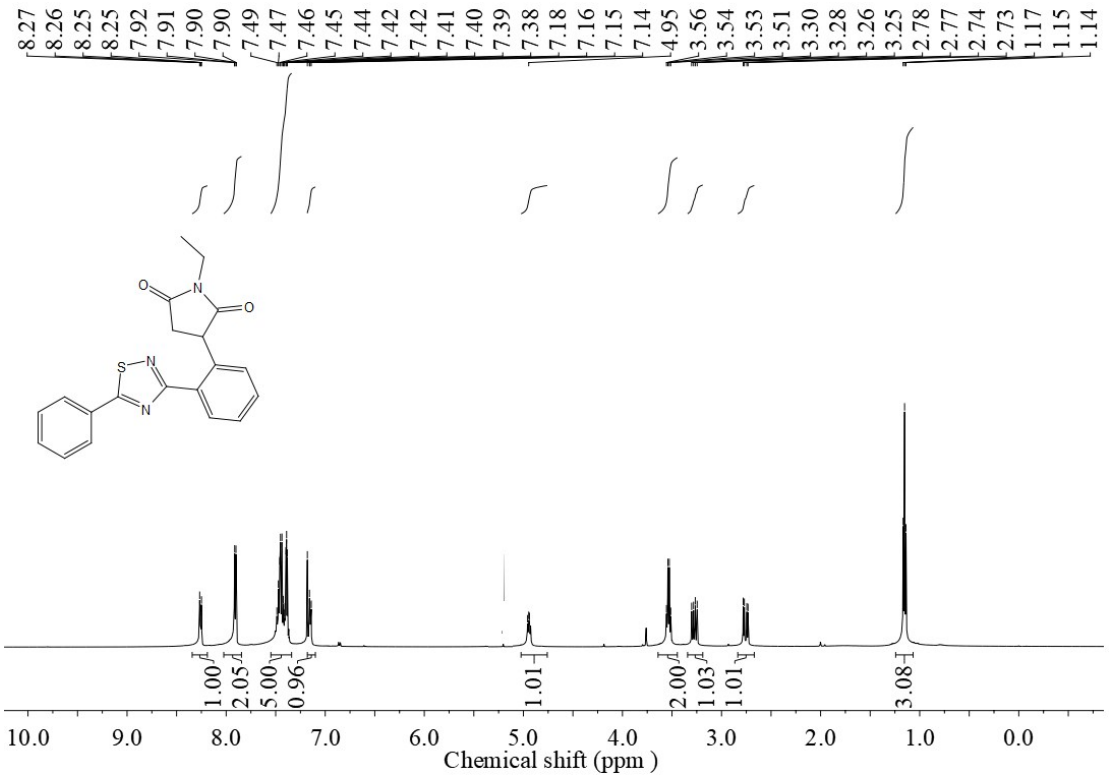
4. ^{1}H and ^{13}C NMR spectra of the products

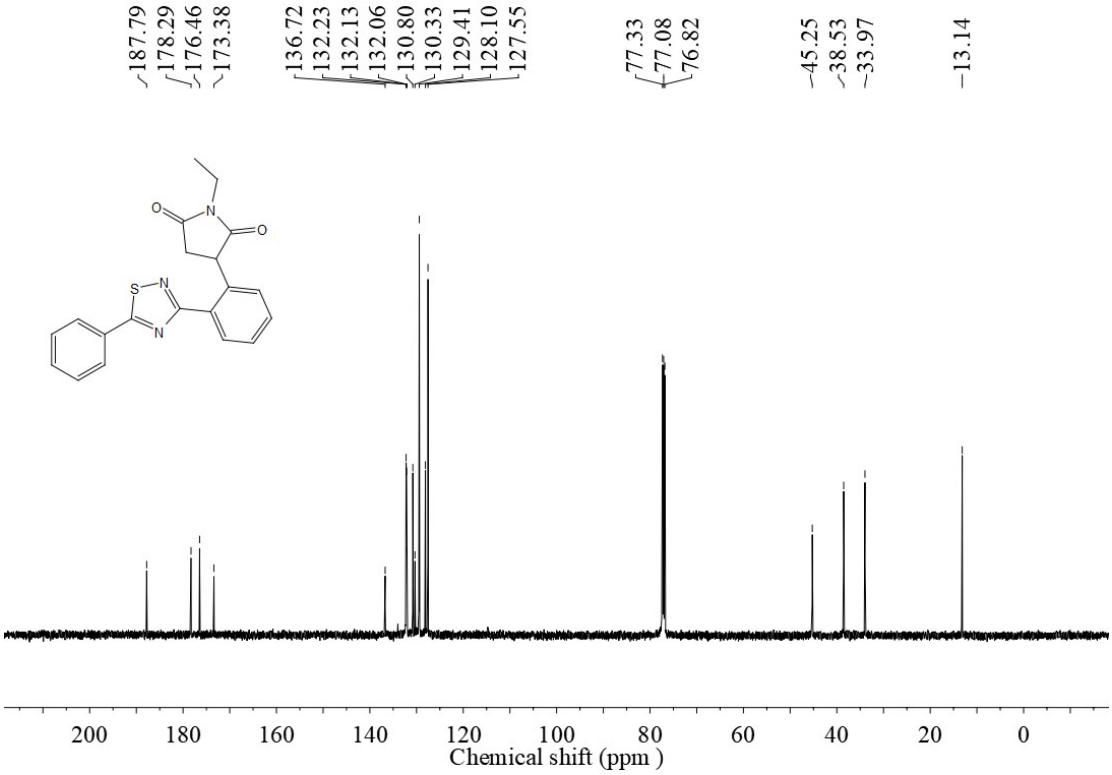
3a:


7.99
7.99
7.99
7.98
7.97
7.56
7.55
7.54
7.52
7.49
7.48
7.47
7.26
5.02
5.01
5.00
3.40
3.38
3.37
3.35
3.02
2.91
2.90
2.87
2.86
0.00
0.98
2.02
5.03
1.04
1.01
1.01
3.01
1.01
Chemical shift (ppm)

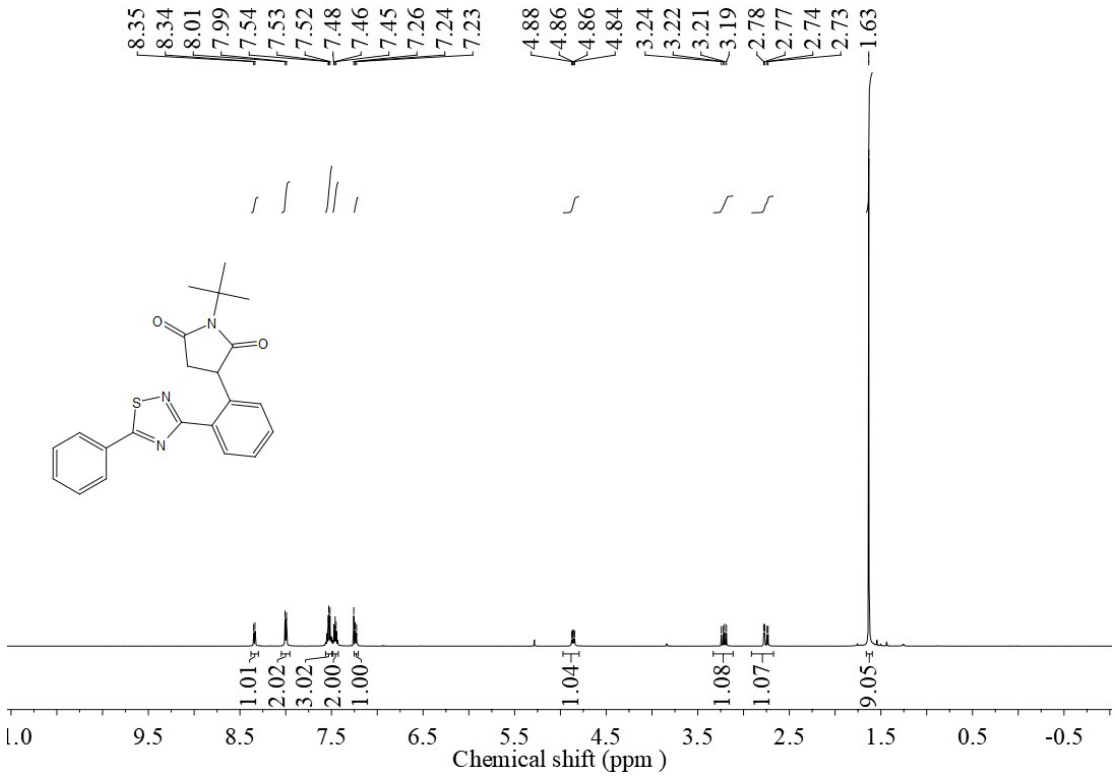

187.87
178.54
176.66
173.39
136.44
132.25
132.14
132.01
130.77
130.30
129.70
129.41
128.17
127.56
77.29
77.04
76.79
45.45
38.52
25.11
0.01
Chemical shift (ppm)

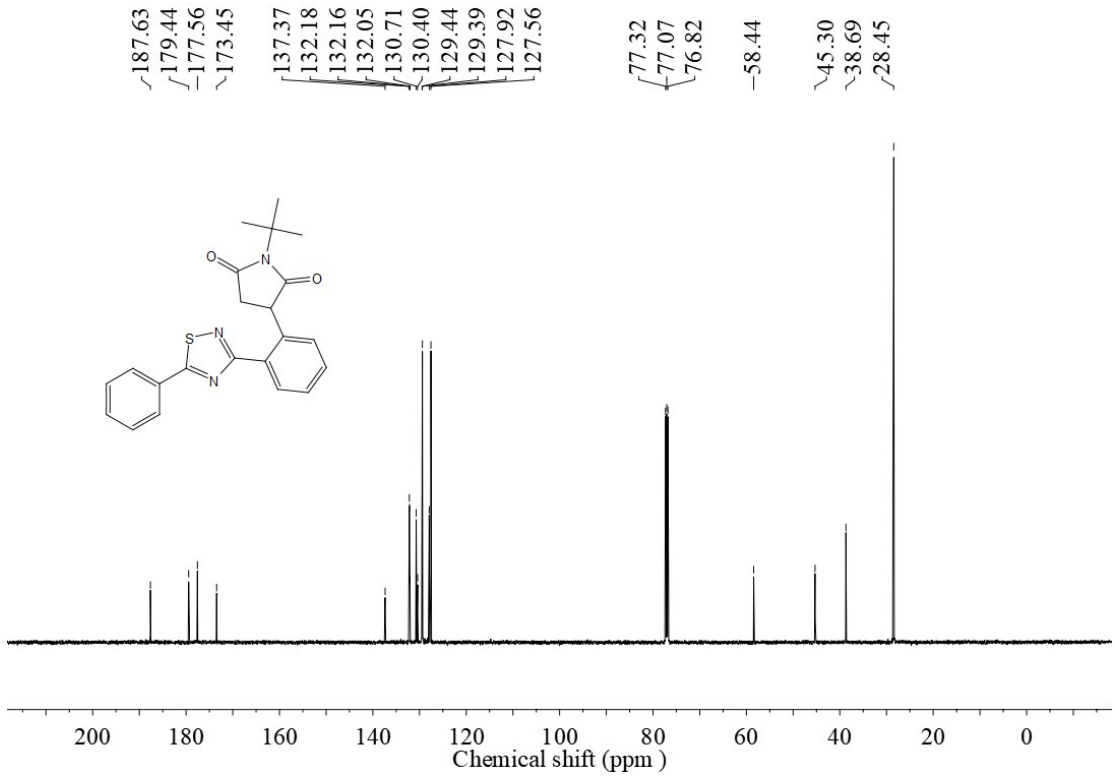
3b:


8.27
8.26
8.25
8.25
7.92
7.91
7.90
7.90
7.49
7.47
7.46
7.45
7.44
7.42
7.42
7.41
7.40
7.39
7.38
7.18
7.16
7.15
7.14
4.95
3.56
3.54
3.53
3.51
3.30
3.28
3.26
3.25
2.78
2.77
2.74
2.73
1.17
1.15
1.14
1.00
2.05
5.00
0.96
1.01
2.00
1.03
1.01
3.08
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
Chemical shift (ppm)

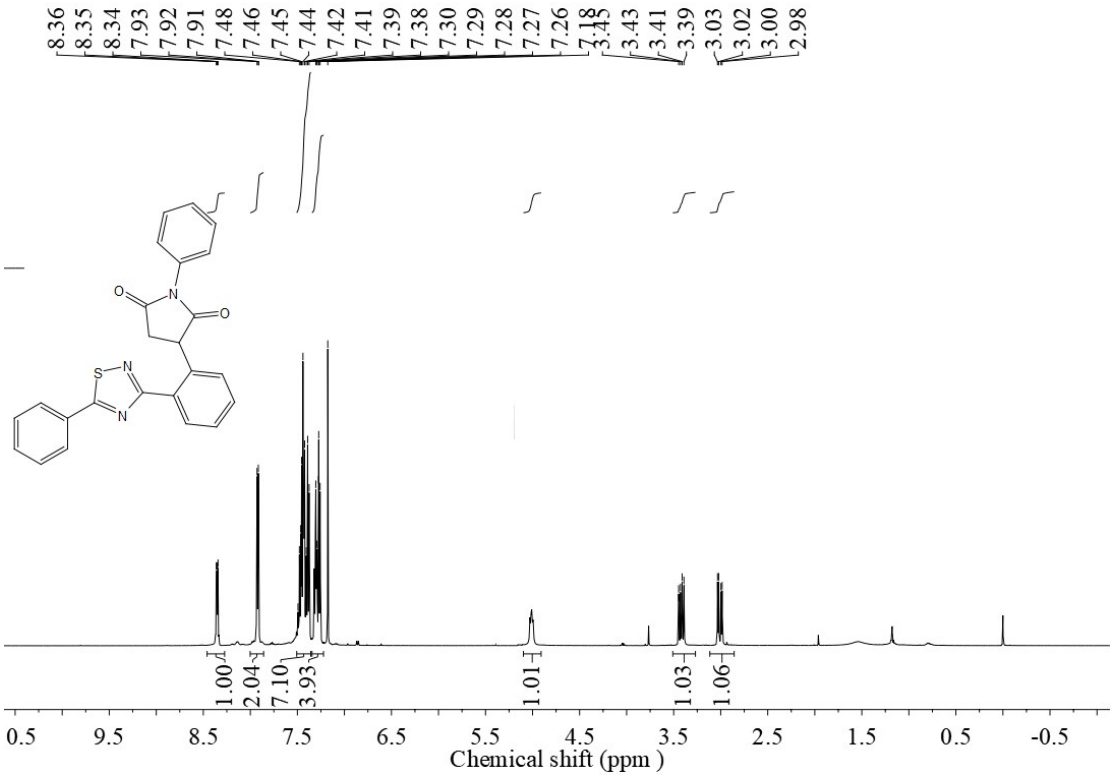

187.79
178.29
176.46
173.38
136.72
132.23
132.13
132.06
130.80
130.33
129.41
128.10
127.55
77.33
77.08
76.82
45.25
38.53
33.97
13.14
200
180
160
140
120
100
80
60
40
20
0
Chemical shift (ppm)

3c:


8.35
8.34
8.01
7.99
7.54
7.53
7.52
7.48
7.46
7.45
7.26
7.24
7.23
4.88
4.86
4.86
4.84
3.24
3.22
3.21
3.19
2.78
2.77
2.74
2.73
1.63
1.01
2.02
3.02
2.00
1.00
1.04
1.08
1.07
9.05
Chemical shift (ppm)


187.63
179.44
177.56
173.45
137.37
132.18
132.16
132.05
130.71
130.40
129.44
129.39
127.92
127.56
77.32
77.07
76.82
58.44
45.30
38.69
28.45
Chemical shift (ppm)

3d: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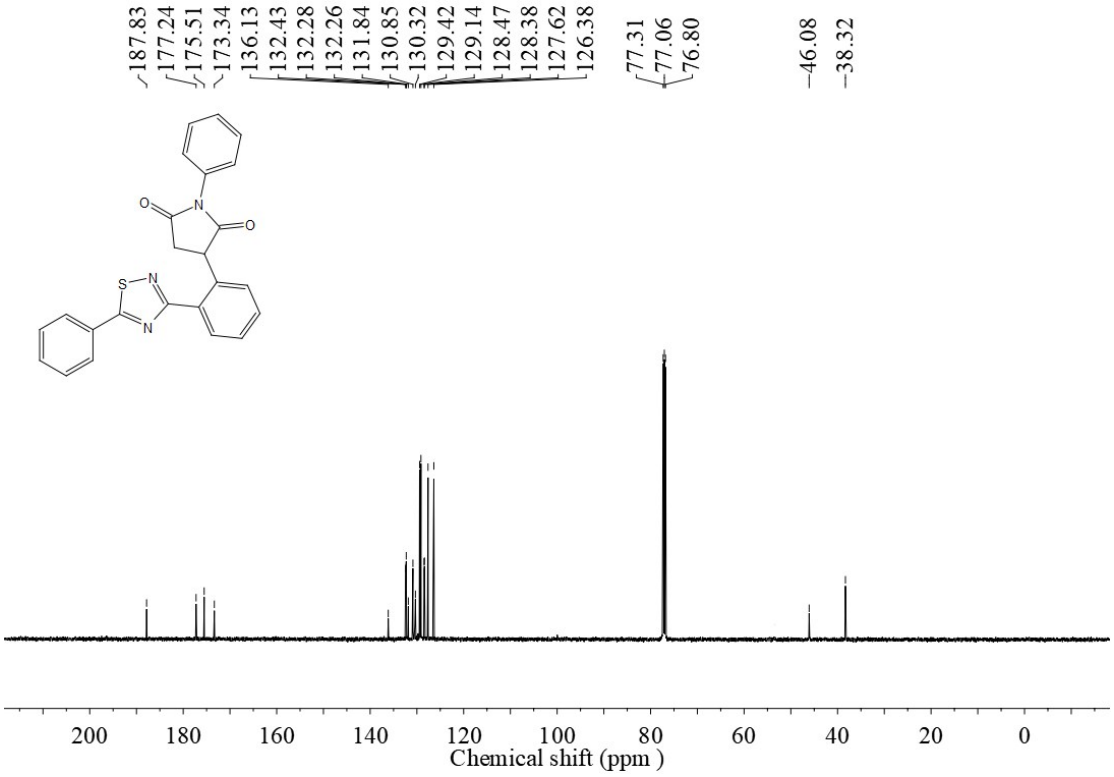
8.35
8.34
7.93
7.92
7.91
7.48
7.46
7.45
7.44
7.42
7.41
7.39
7.38
7.30
7.29
7.28
7.27
7.26
7.18
3.45
3.43
3.41
3.39
3.03
3.02
3.00
2.98
1.00
2.04
7.10
3.93
1.01
1.03
1.06
0.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
Chemical shift (ppm)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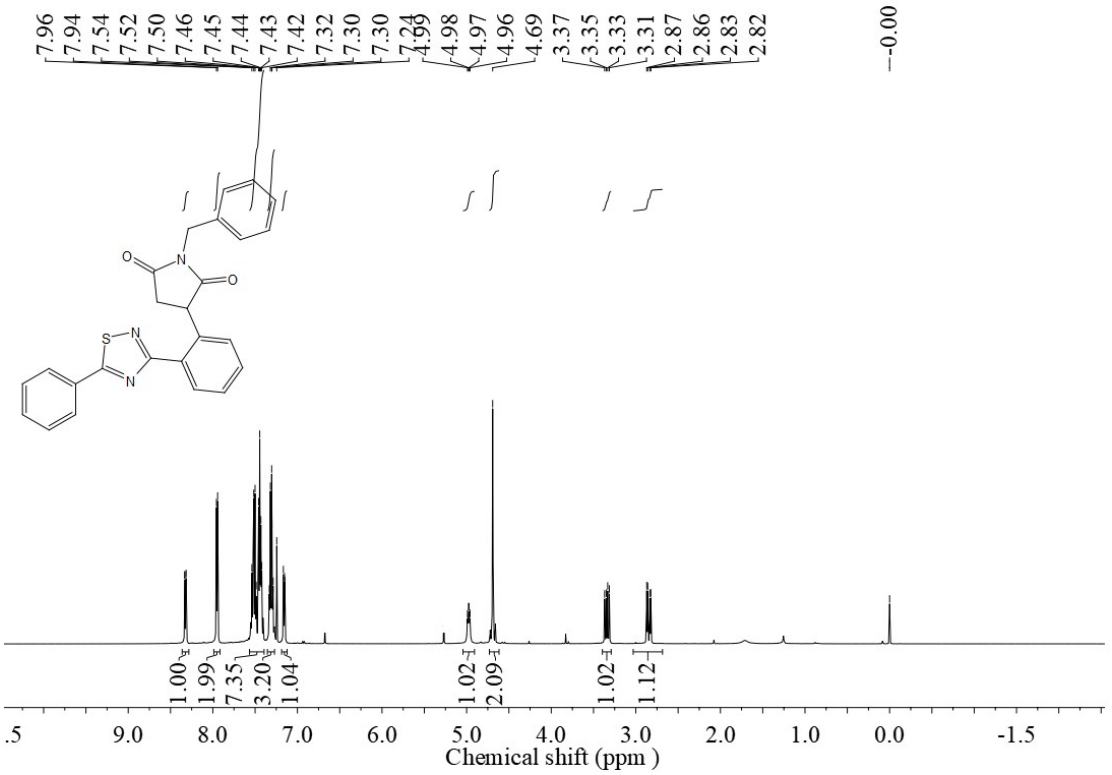
177.24
175.51
173.34
136.13
132.43
132.28
132.26
131.84
130.85
130.32
129.42
129.14
128.47
128.38
127.62
126.38
77.31
77.06
76.80
46.08
38.32
200
180
160
140
120
100
80
60
40
20
0
Chemical shift (ppm)

3e:


7.96
7.94
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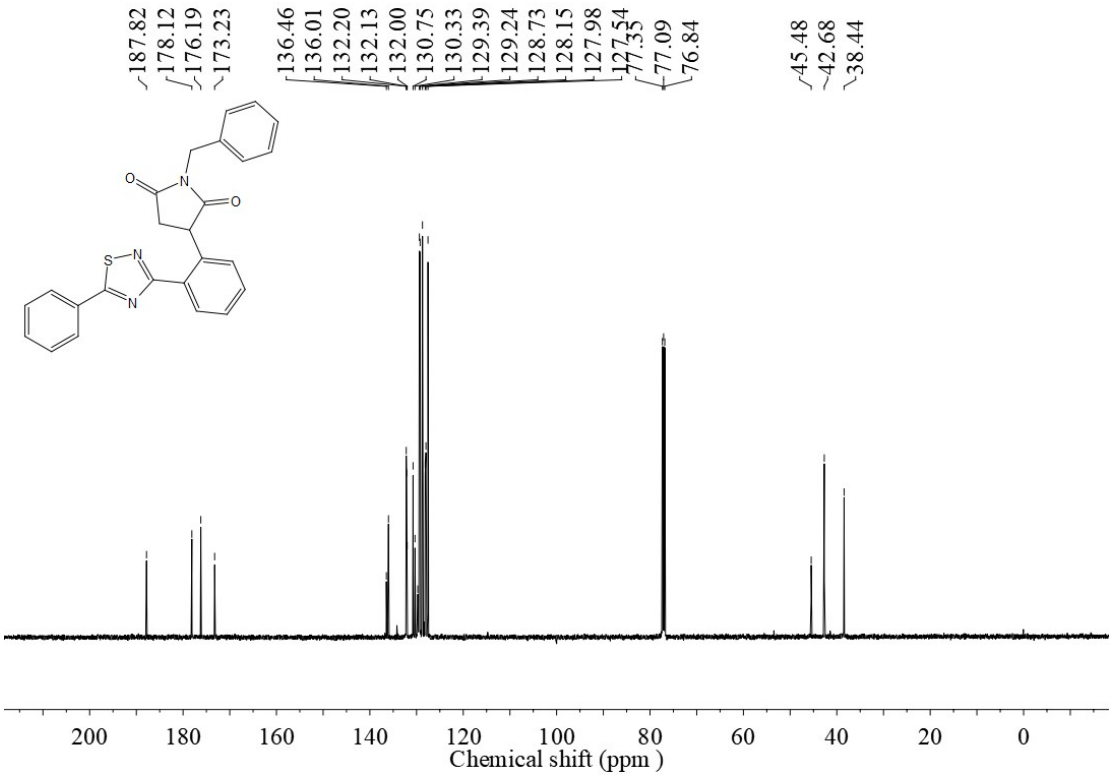
7.52
7.50
7.46
7.45
7.44
7.43
7.42
7.32
7.30
7.30
7.24
4.99
4.98
4.97
4.96
4.69
3.37
3.35
3.33
3.31
2.87
2.86
2.83
2.82
-0.00
1.00
1.99
7.35
3.20
1.04
1.02
2.09
1.02
1.12
Chemical shift (ppm)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173.23
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136.01
132.20
132.13
132.00
130.75
130.33
129.39
129.24
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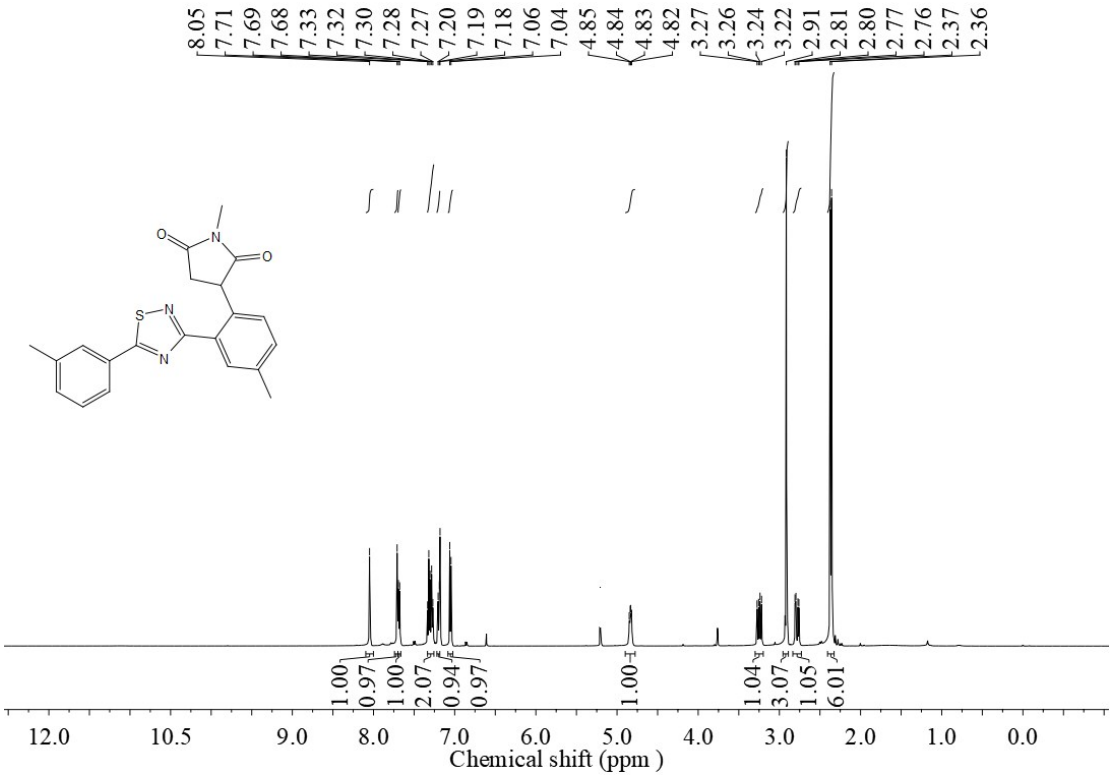
128.15
127.98
77.09
76.84
45.48
42.68
38.44
Chemical shift (ppm)

3f: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7.32
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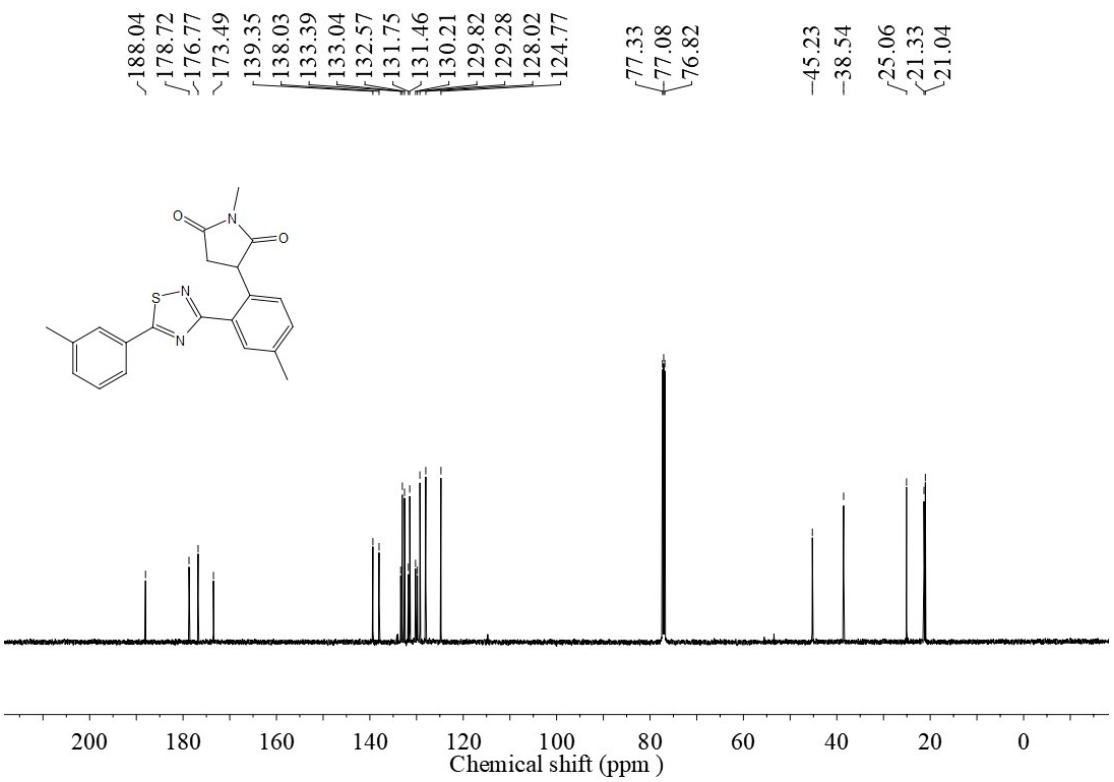
7.28
7.27
7.20
7.19
7.18
7.06
7.04
4.85
4.84
4.83
4.82
3.27
3.26
3.24
3.22
2.91
2.81
2.80
2.77
2.76
2.37
2.36
1.00
0.97
1.00
2.07
0.94
0.97
1.00
1.04
3.07
1.05
6.01
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
Chemical shift (ppm)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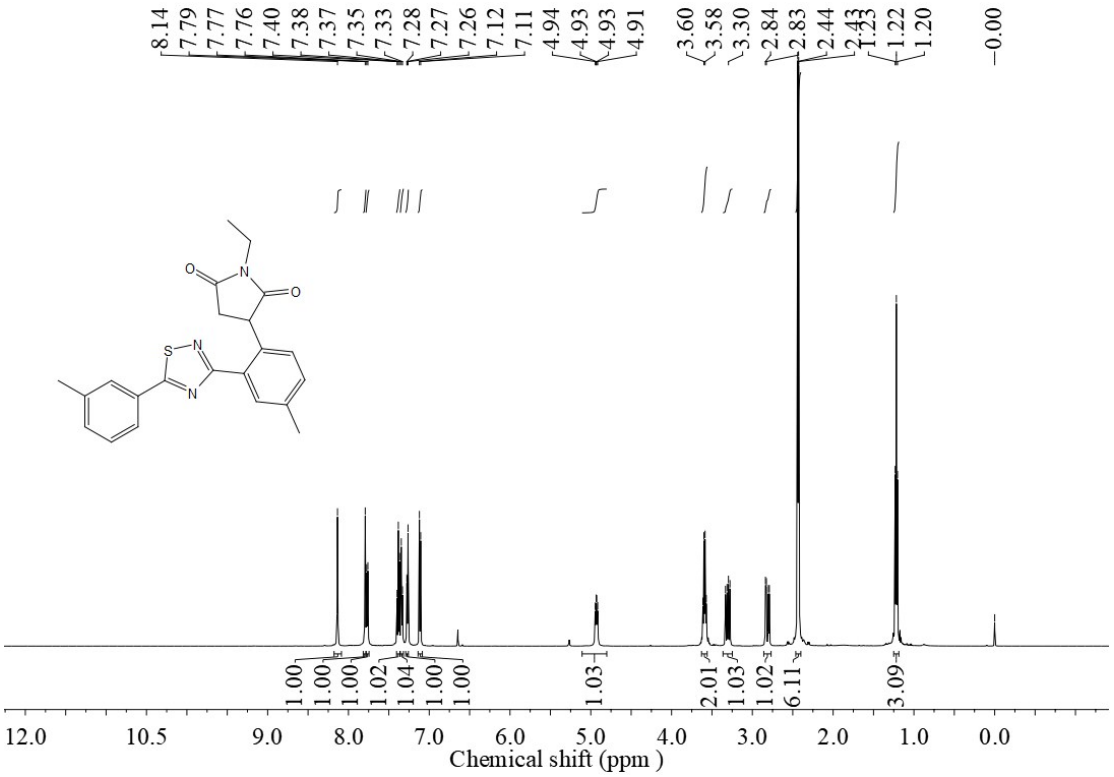
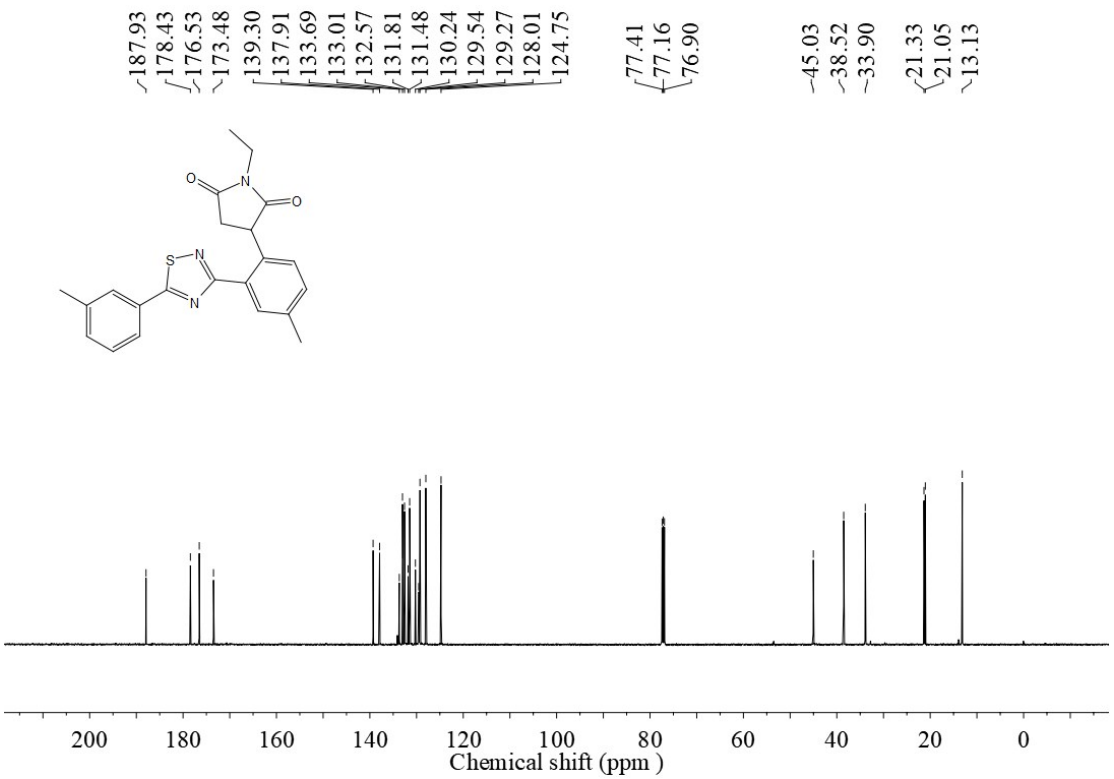
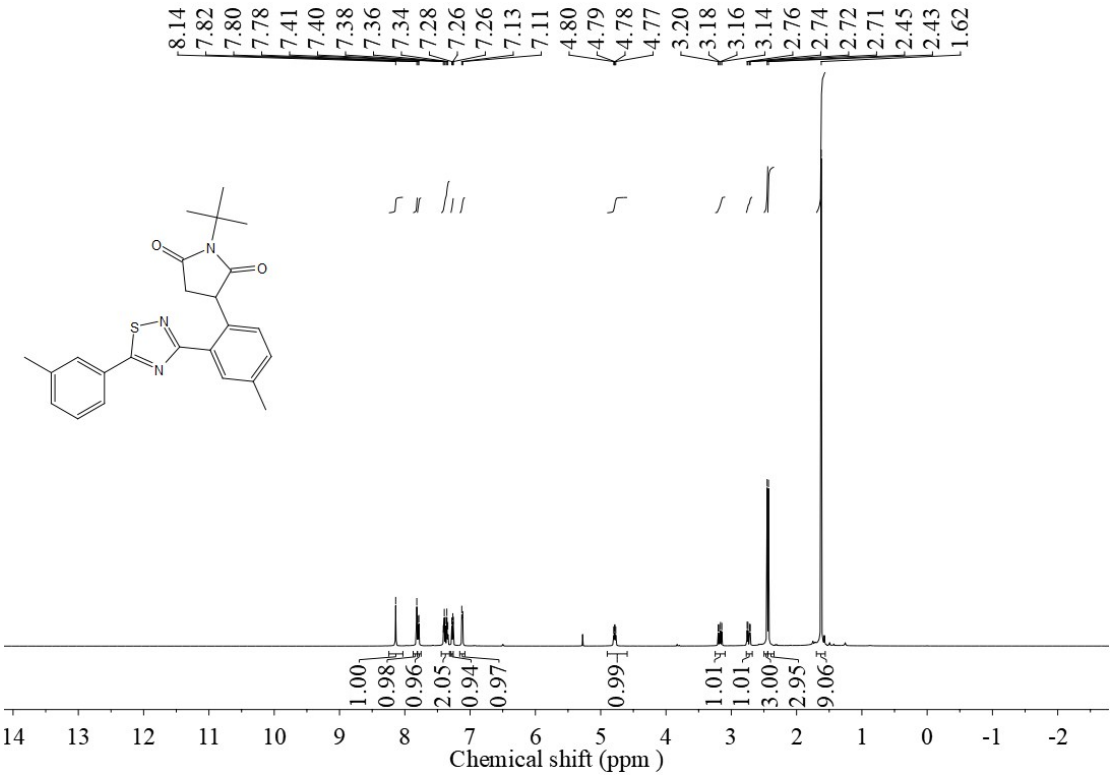
176.77
173.49
139.35
138.03
133.39
133.04
132.57
131.75
131.46
130.21
129.82
129.28
128.02
124.77
77.33
77.08
76.82
45.23
38.54
25.06
21.33
21.04
200
180
160
140
120
100
80
60
40
20
0
Chemical shift (ppm)

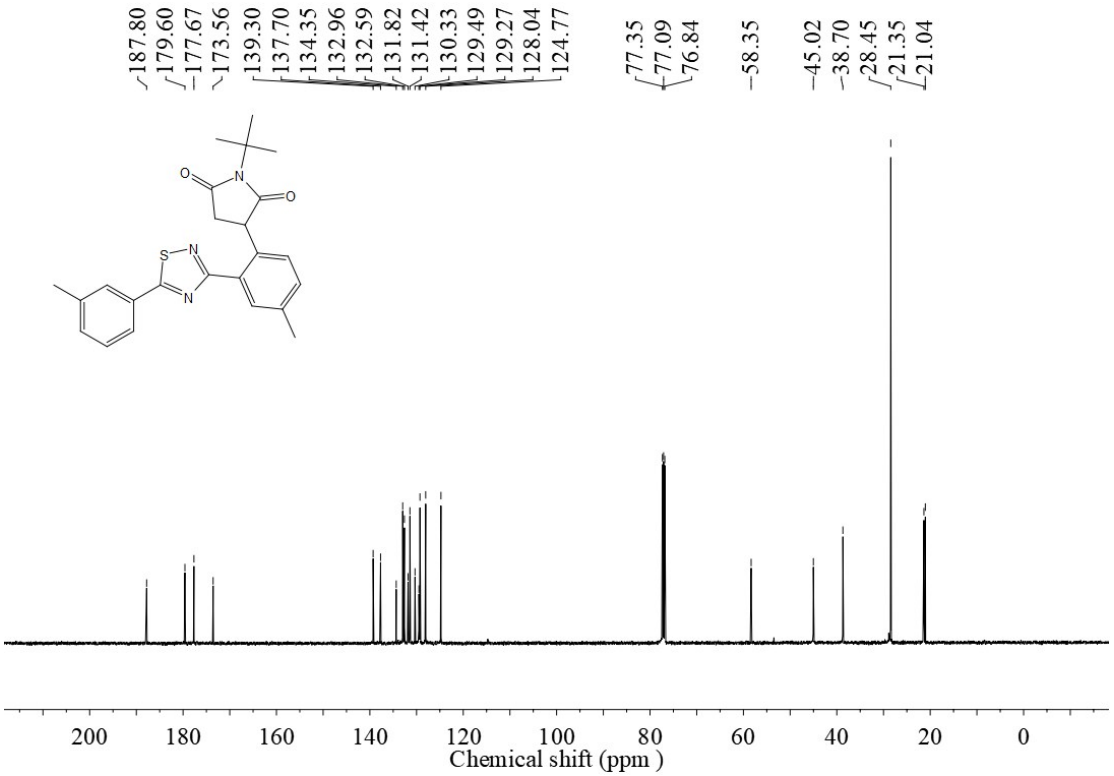
3g:


8.14
7.79
7.77
7.76
7.40
7.38
7.37
7.35
7.33
7.28
7.27
7.26
7.12
7.11
4.94
4.93
4.93
4.91
3.60
3.58
3.30
2.84
2.83
2.44
2.43
1.23
1.22
1.20
0.00
1.00
1.00
1.00
1.02
1.04
1.00
1.00
1.03
2.01
1.03
1.02
6.11
3.09
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
Chemical shift (ppm)

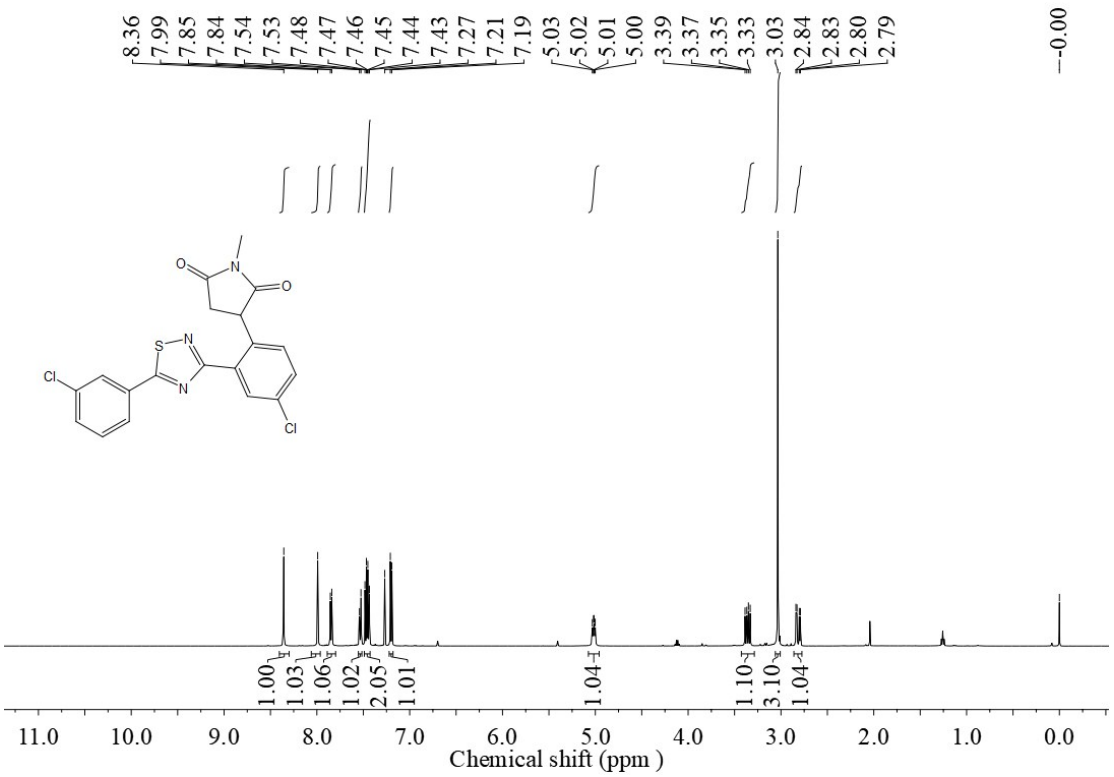

187.93
178.43
176.53
173.48
139.30
137.91
133.69
133.01
132.57
131.81
131.48
130.24
129.54
129.27
128.01
124.75
77.41
77.16
76.90
45.03
38.52
33.90
21.33
21.05
13.13
200
180
160
140
120
100
80
60
40
20
0
Chemical shift (ppm)

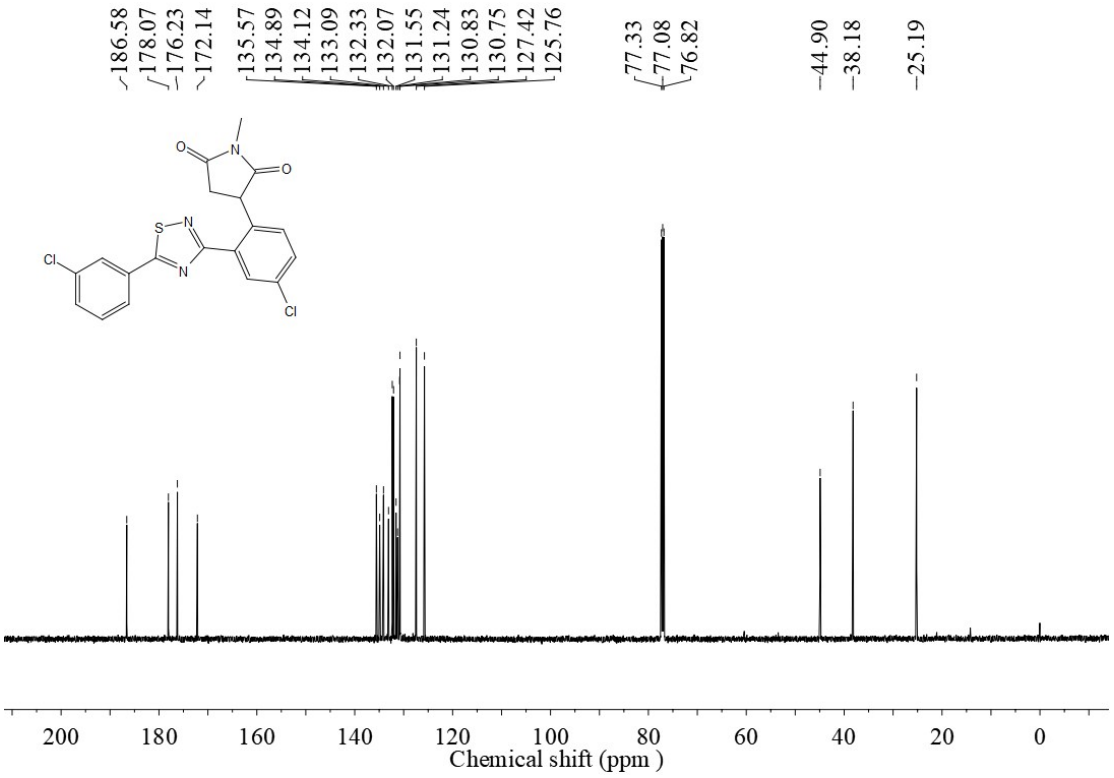
3h:


8.14
7.82
7.80
7.78
7.41
7.40
7.38
7.36
7.34
7.28
7.26
7.26
7.13
7.11
4.80
4.79
4.78
4.77
3.20
3.18
3.16
3.14
2.76
2.74
2.72
2.71
2.45
2.43
1.62
1.00
0.98
0.96
2.05
0.94
0.97
0.99
1.01
1.01
3.00
2.95
9.06
Chemical shift (ppm)

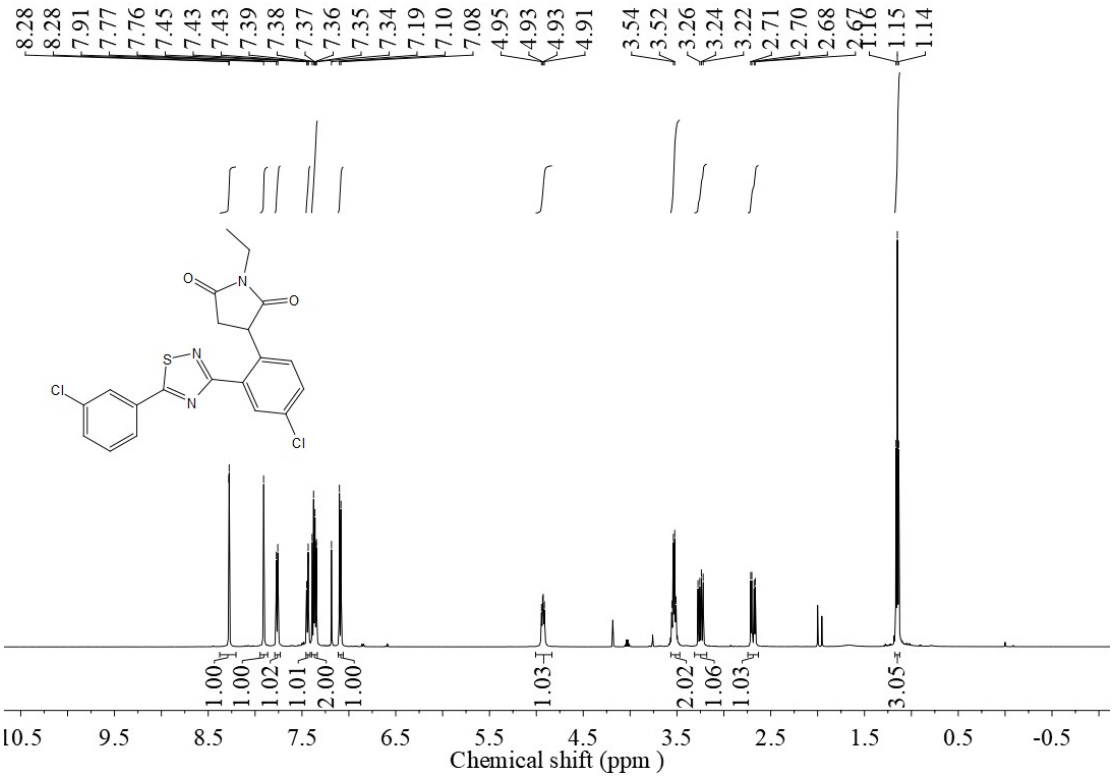

187.80
179.60
177.67
173.56
139.30
137.70
134.35
132.96
132.59
131.82
131.42
130.33
129.49
129.27
128.04
124.77
77.35
77.09
76.84
58.35
45.02
38.70
28.45
21.35
21.04
Chemical shift (ppm)

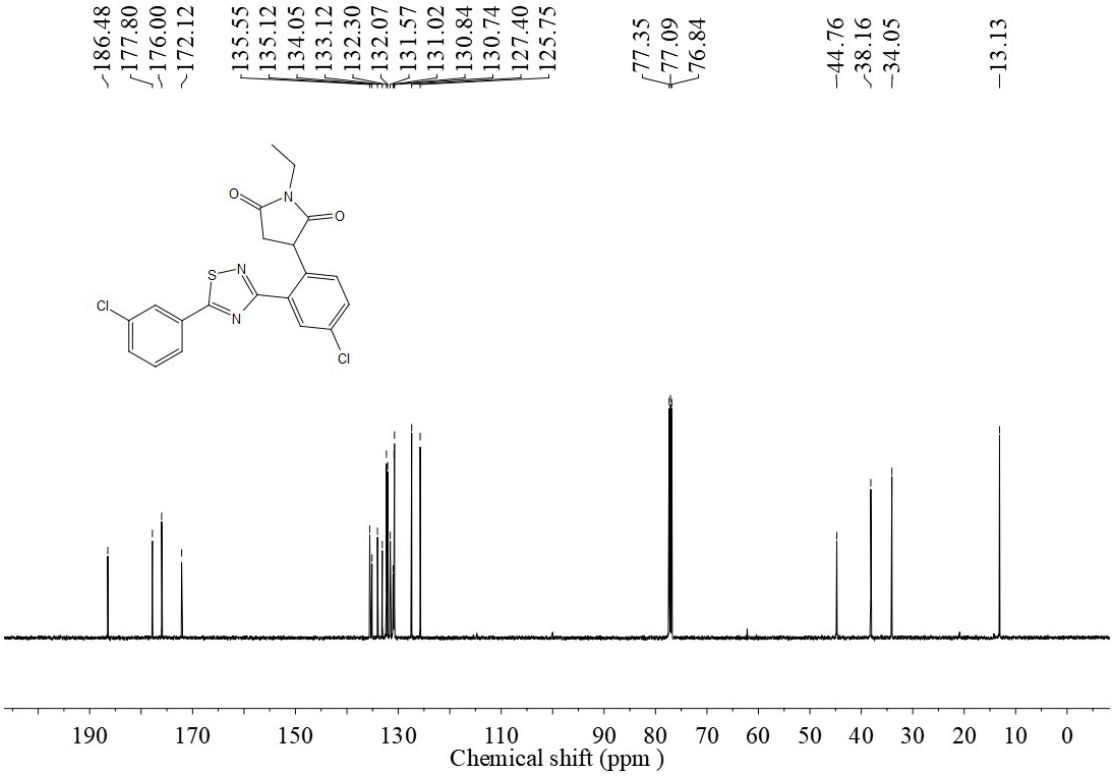
3i:


8.36
7.99
7.85
7.84
7.54
7.53
7.48
7.47
7.46
7.45
7.44
7.43
7.27
7.21
7.19
5.03
5.02
5.01
5.00
3.39
3.37
3.35
3.33
3.03
2.84
2.83
2.80
2.79
-0.00
1.00
1.03
1.06
1.02
2.05
1.01
1.04
1.10
3.10
1.04
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
Chemical shift (ppm)

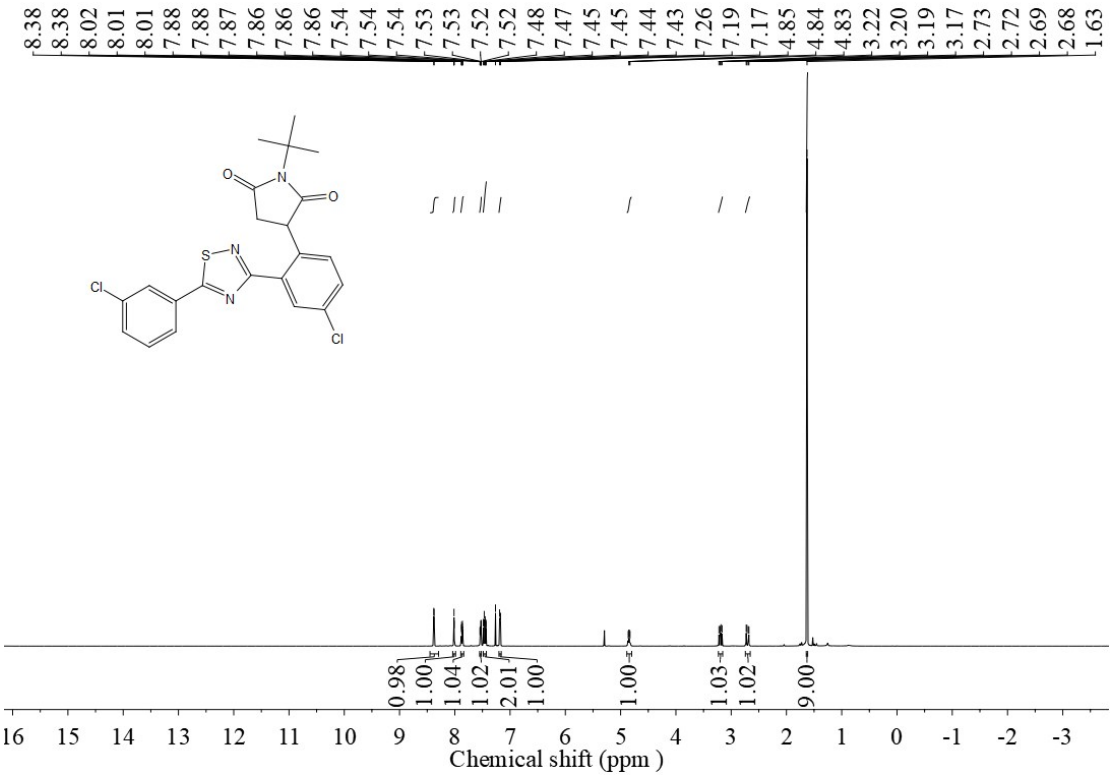

186.58
178.07
176.23
172.14
135.57
134.89
134.12
133.09
132.33
132.07
131.55
131.24
130.83
130.75
127.42
125.76
77.33
77.08
76.82
44.90
38.18
25.19
200
180
160
140
120
100
80
60
40
20
0
Chemical shift (ppm)

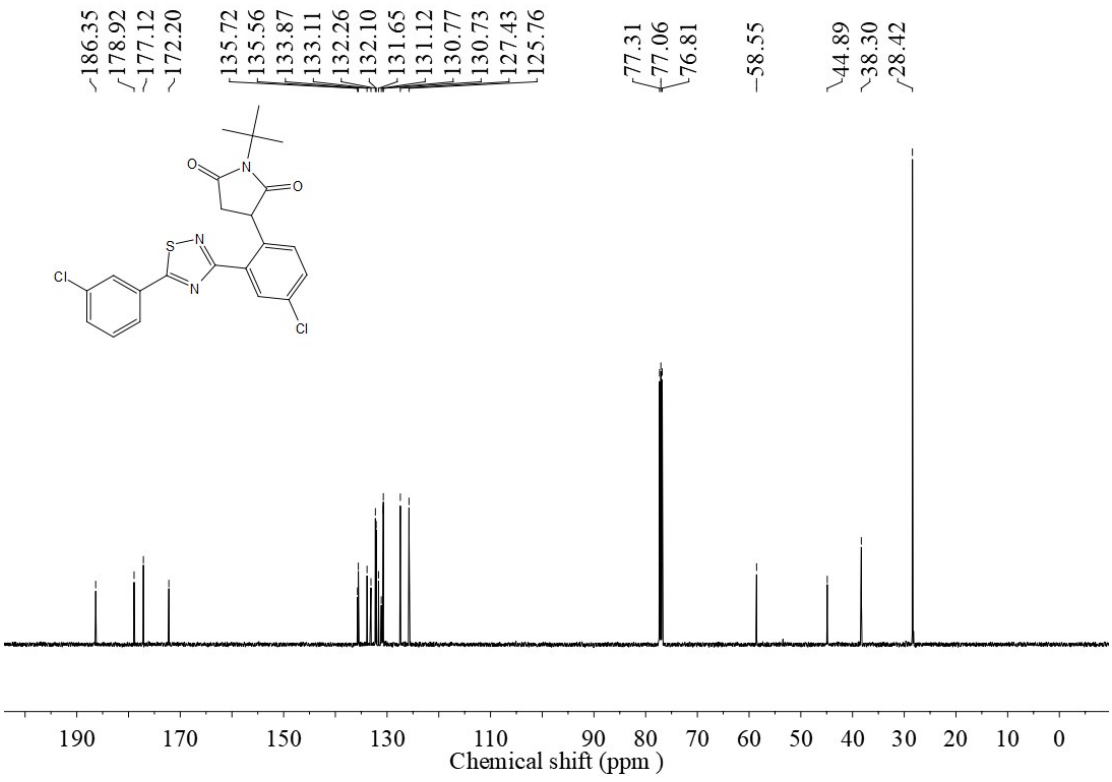
3j:


8.28
8.28
7.91
7.77
7.76
7.45
7.43
7.43
7.39
7.38
7.37
7.36
7.35
7.34
7.19
7.10
7.08
4.95
4.93
4.93
4.91
3.54
3.52
3.26
3.24
3.22
2.71
2.70
2.68
2.67
1.16
1.15
1.14
1.00
1.00
1.02
1.01
2.00
1.00
1.03
2.02
1.06
1.03
3.05
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
Chemical shift (ppm)

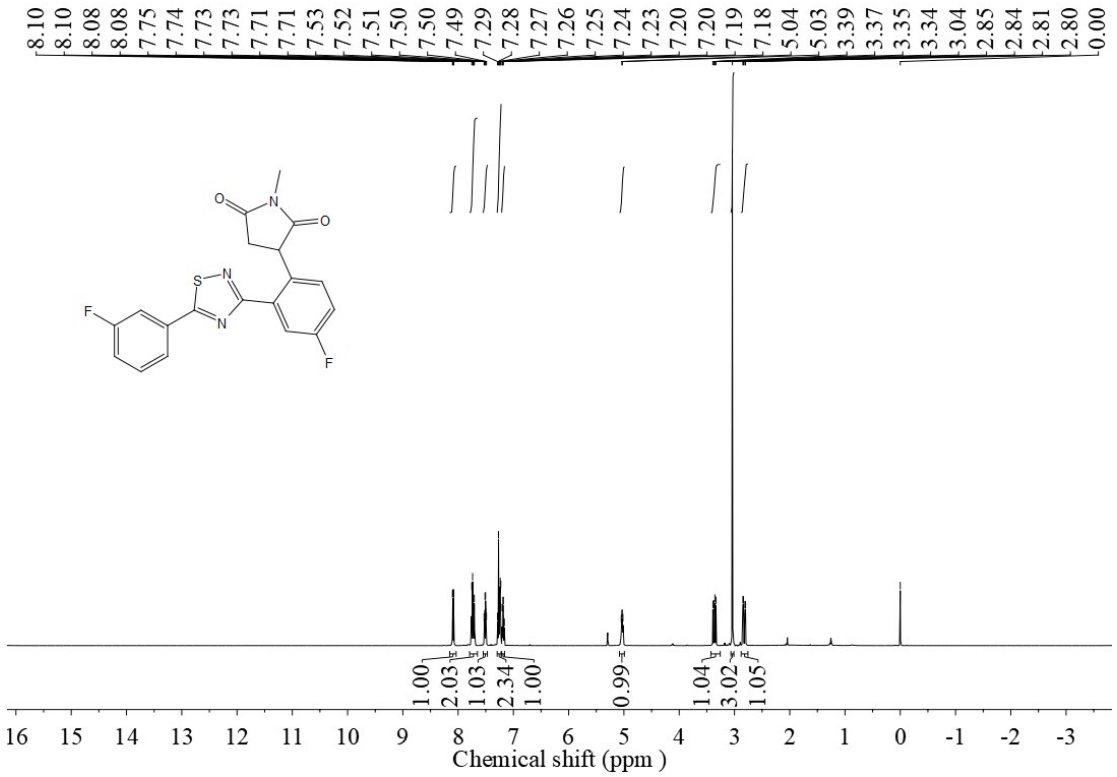

186.48
177.80
176.00
172.12
135.55
135.12
134.05
133.12
132.30
132.07
131.57
131.02
130.84
130.74
127.40
125.75
77.35
77.09
76.84
44.76
38.16
34.05
13.13
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
Chemical shift (ppm)

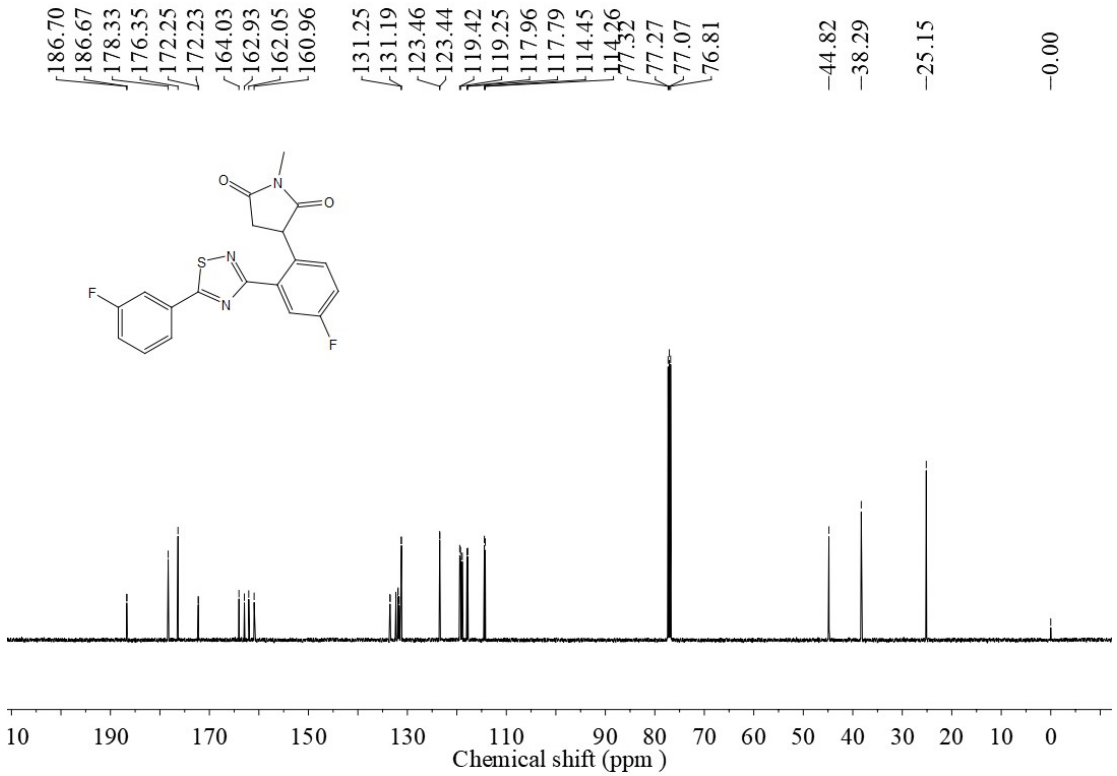
3k:


8.38
8.38
8.02
8.01
8.01
7.88
7.88
7.87
7.86
7.86
7.86
7.54
7.54
7.54
7.53
7.53
7.52
7.52
7.48
7.47
7.45
7.45
7.44
7.43
7.26
7.19
7.17
4.85
4.84
4.83
3.22
3.20
3.19
3.17
2.73
2.72
2.69
2.68
1.63
0.98
1.00
1.04
1.02
2.01
1.00
1.00
1.03
1.02
9.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
Chemical shift (ppm)

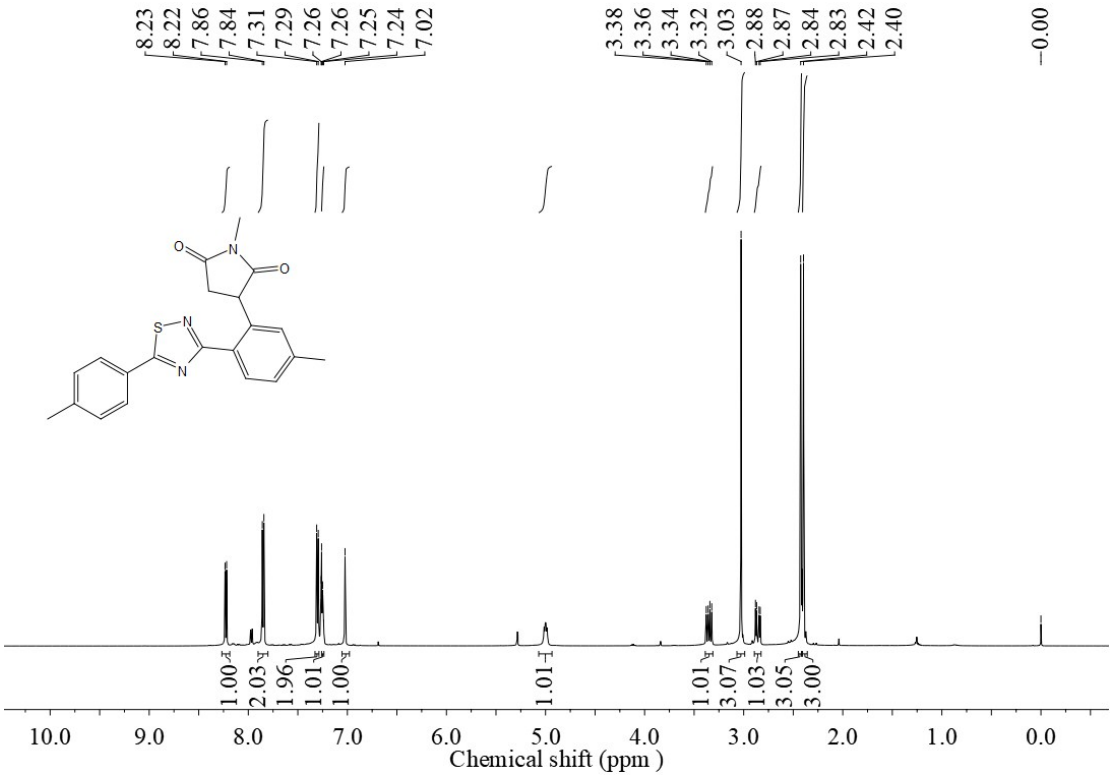

186.35
178.92
177.12
172.20
135.72
135.56
133.87
133.11
132.26
132.10
131.65
131.12
130.77
130.73
127.43
125.76
77.31
77.06
76.81
58.55
44.89
38.30
28.42
190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
Chemical shift (ppm)

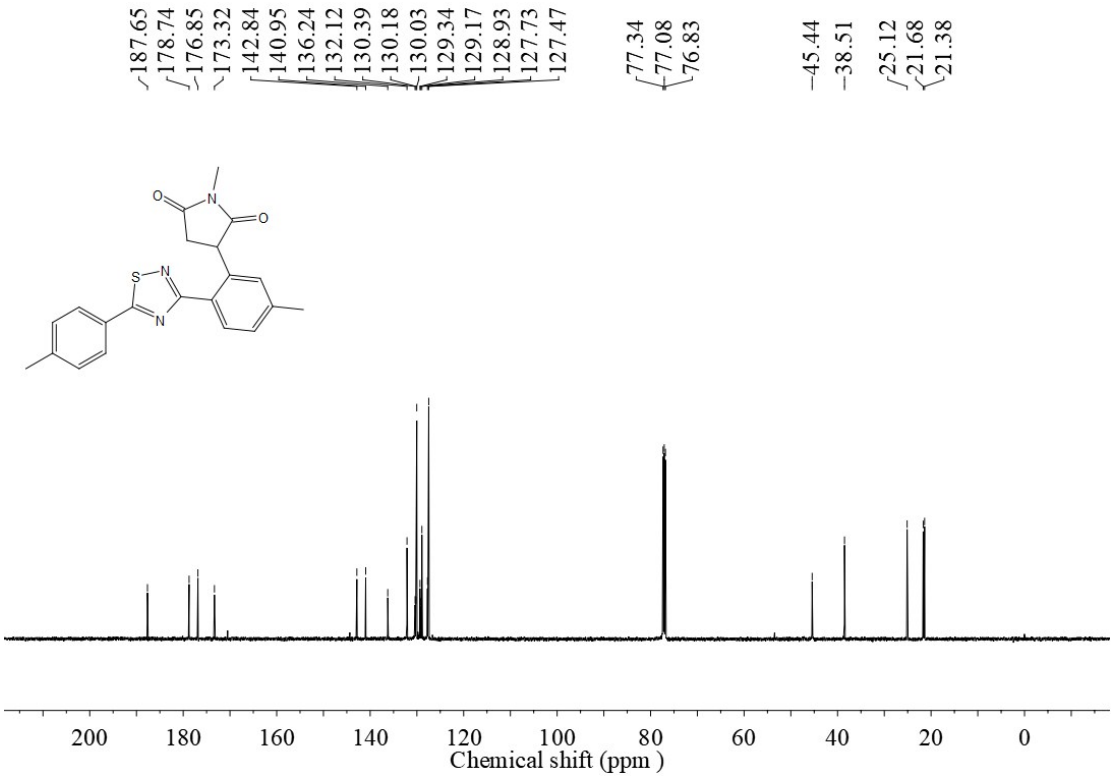
3l:


8.10 8.10 8.08 8.08 7.75 7.74 7.73 7.73 7.71 7.71 7.53 7.52 7.51 7.50 7.50 7.49 7.29 7.28 7.27 7.26 7.25 7.24 7.23 7.20 7.20 7.19 7.18 5.04 5.03 3.39 3.37 3.35 3.34 3.04 2.85 2.84 2.81 2.80 0.00
1.00 2.03 1.03 2.34 1.00 0.99 1.04 3.02 1.05
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
Chemical shift (ppm)

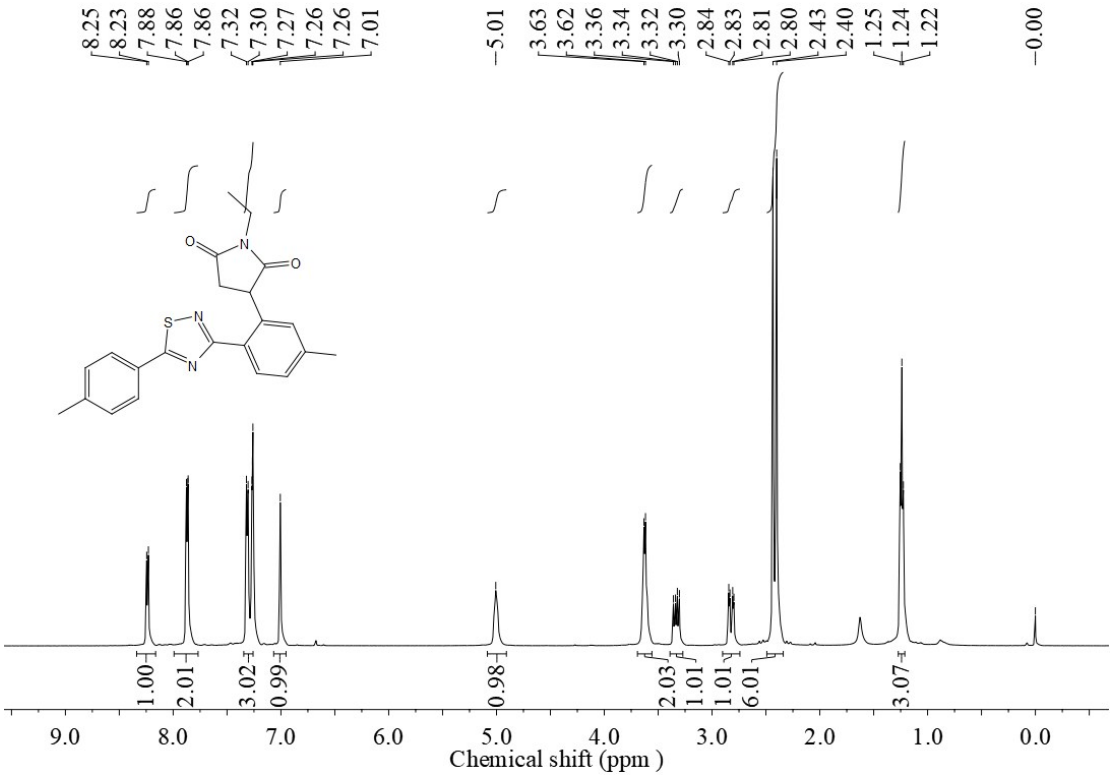

186.70 186.67 178.33 176.35 172.25 172.23 164.03 162.93 162.05 160.96 131.25 131.19 123.46 123.44 119.42 119.25 117.96 117.79 114.45 114.26 77.32 77.27 77.07 76.81 44.82 38.29 25.15 0.00
10 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
Chemical shift (ppm)

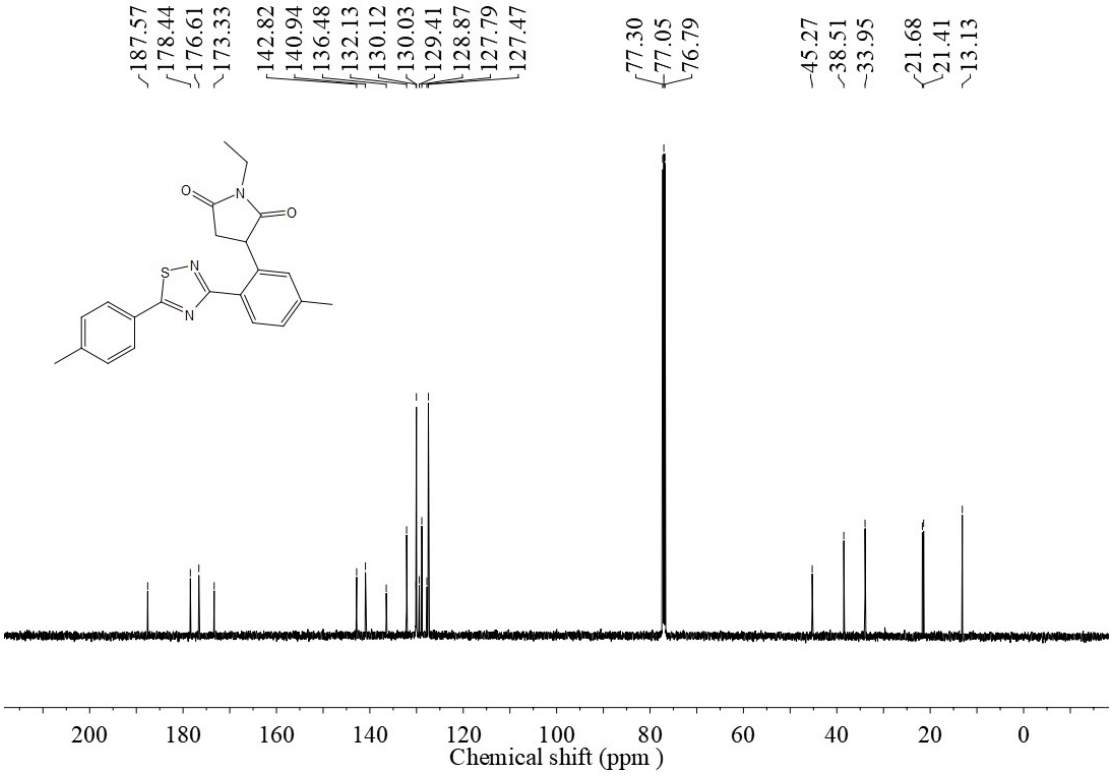
3m:


8.23
8.22
7.86
7.84
7.31
7.29
7.26
7.26
7.25
7.24
7.02
3.38
3.36
3.34
3.32
3.03
2.88
2.87
2.84
2.83
2.42
2.40
0.00
1.00
2.03
1.96
1.01
1.00
1.01
1.01
3.07
1.03
3.05
3.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
Chemical shift (ppm)

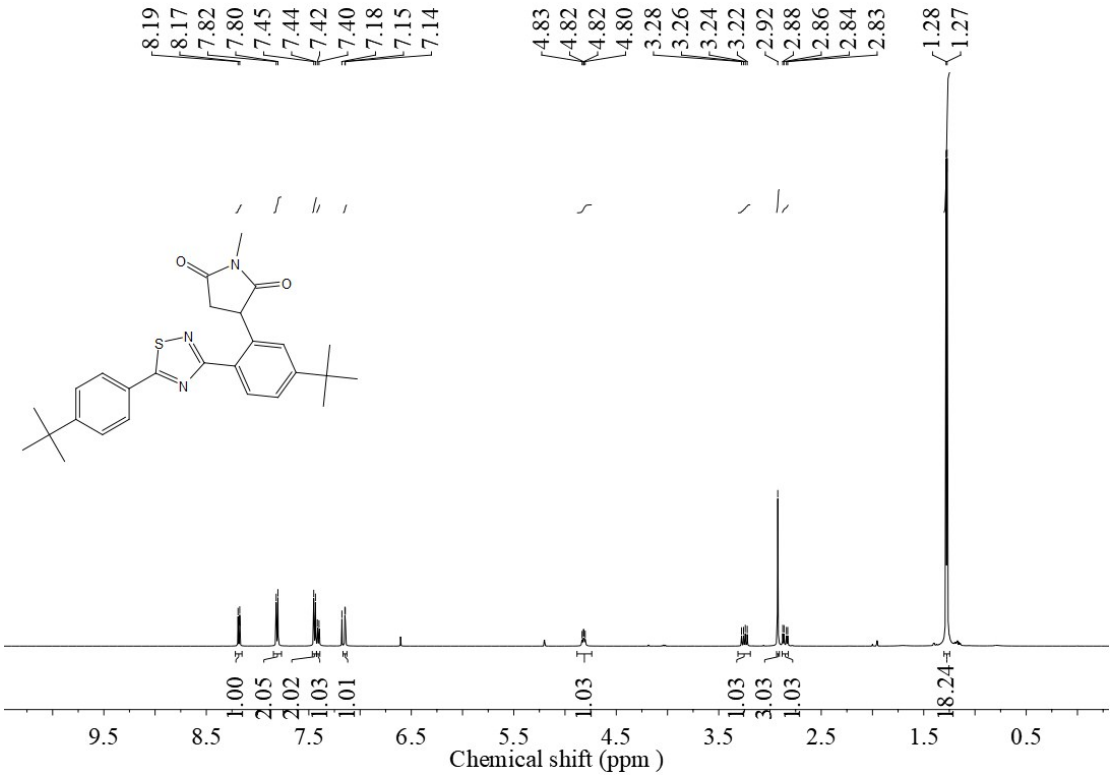

187.65
178.74
176.85
173.32
142.84
140.95
136.24
132.12
130.39
130.18
130.03
129.34
129.17
128.93
127.73
127.47
77.34
77.08
76.83
45.44
38.51
25.12
21.68
21.38
200
180
160
140
120
100
80
60
40
20
0
Chemical shift (ppm)

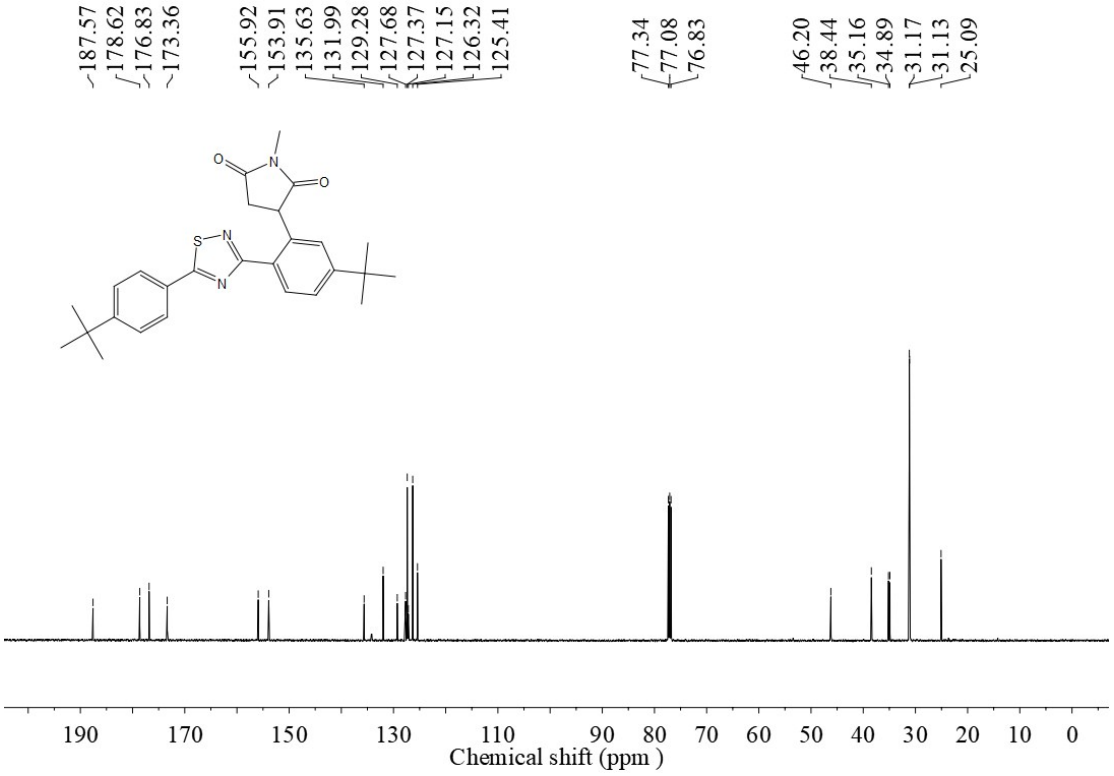
3n:


8.25
8.23
7.88
7.86
7.86
7.32
7.30
7.27
7.26
7.26
7.01
5.01
3.63
3.62
3.36
3.34
3.32
3.30
2.84
2.83
2.81
2.80
2.43
2.40
1.25
1.24
1.22
0.00
1.00
2.01
3.02
0.99
0.98
2.03
1.01
1.01
6.01
3.07
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
Chemical shift (ppm)

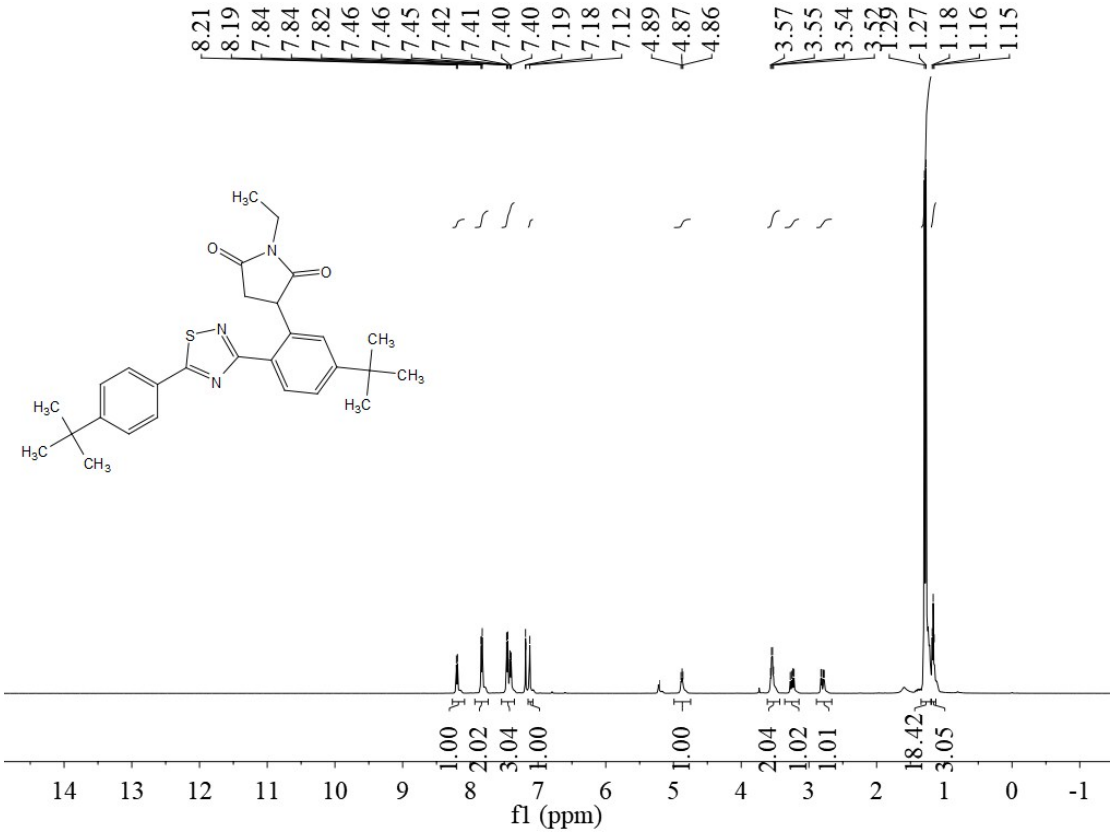

187.57
178.44
176.61
173.33
142.82
140.94
136.48
132.13
130.12
130.03
129.41
128.87
127.79
127.47
77.30
77.05
76.79
45.27
38.51
33.95
21.68
21.41
13.13
200
180
160
140
120
100
80
60
40
20
0
Chemical shift (ppm)

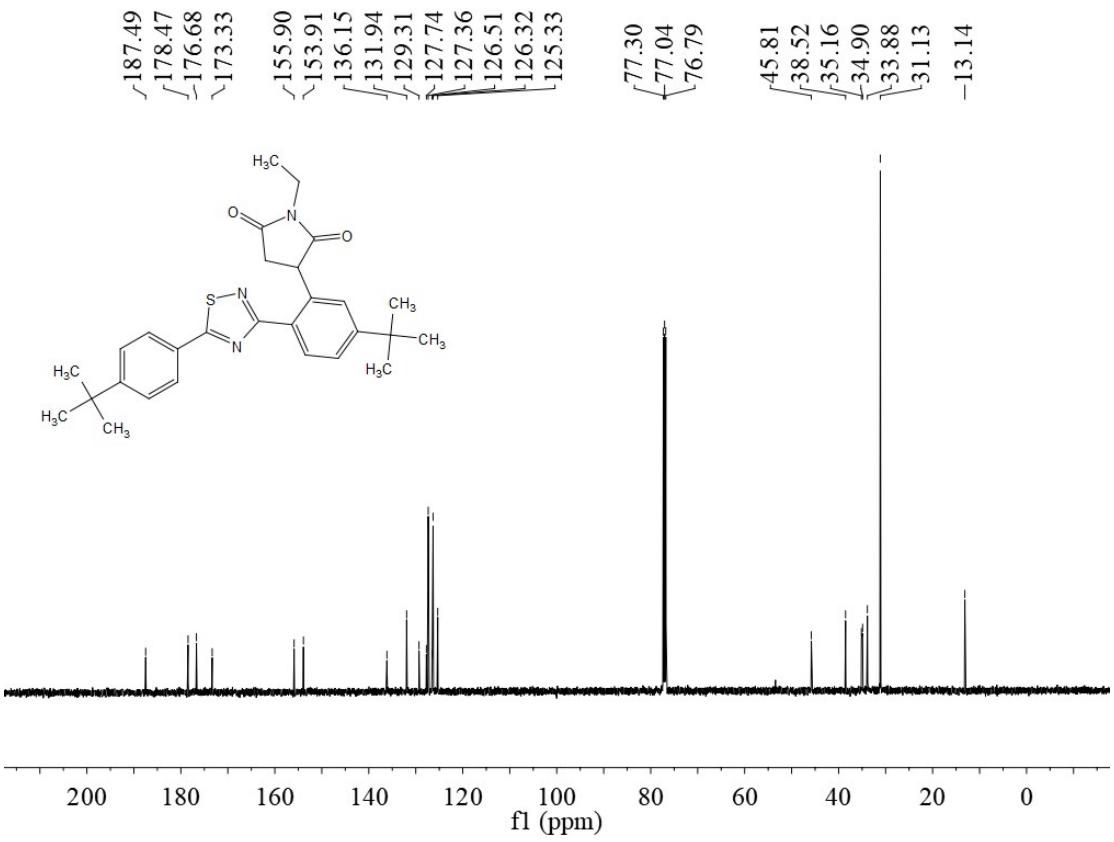
3o:


8.19
8.17
7.82
7.80
7.45
7.44
7.42
7.40
7.18
7.15
7.14
4.83
4.82
4.82
4.80
3.28
3.26
3.24
3.22
2.92
2.88
2.86
2.84
2.83
1.28
1.27
1.00
2.05
2.02
1.03
1.01
1.03
1.03
3.03
1.03
18.24
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
Chemical shift (ppm)

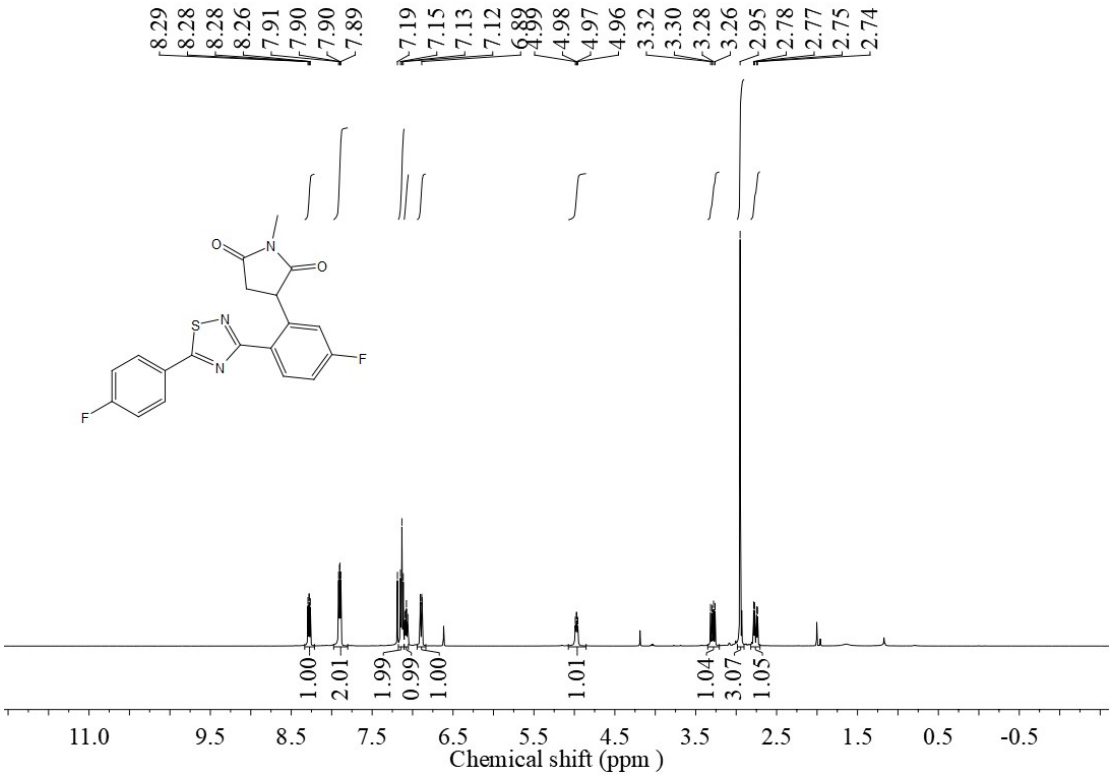

187.57
178.62
176.83
173.36
155.92
153.91
135.63
131.99
129.28
127.68
127.37
127.15
126.32
125.41
77.34
77.08
76.83
46.20
38.44
35.16
34.89
31.17
31.13
25.09
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
Chemical shift (ppm)

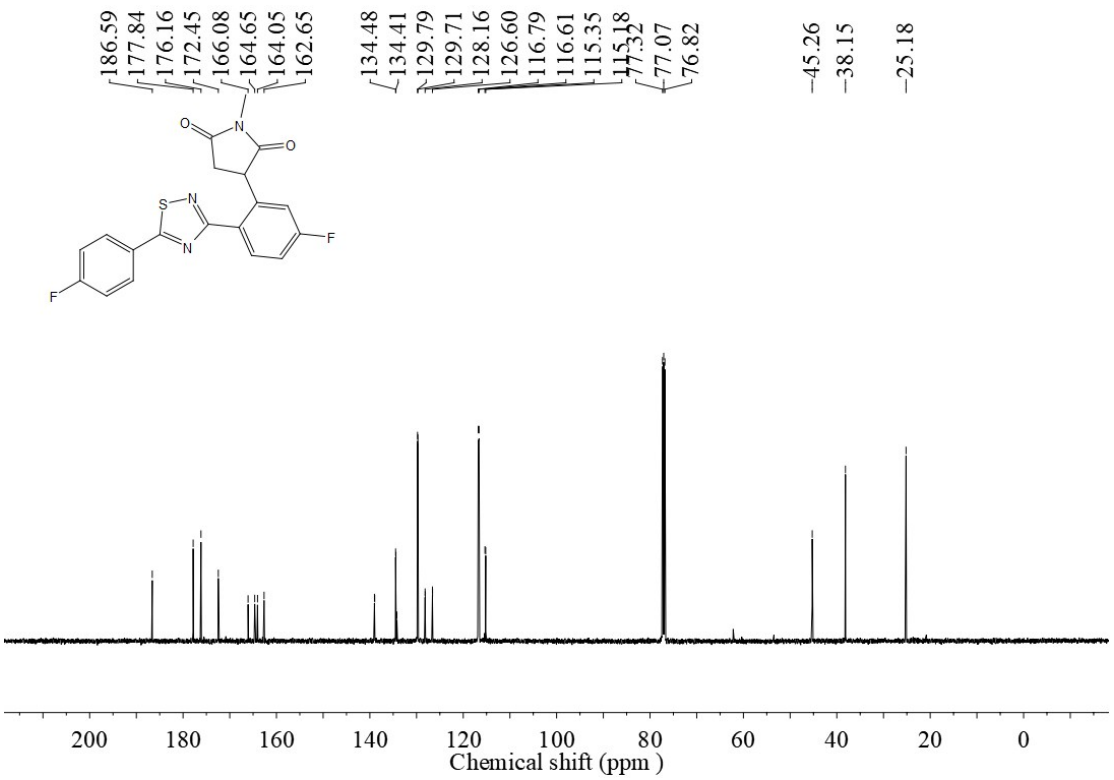
3p:


8.21
8.19
7.84
7.84
7.82
7.46
7.46
7.45
7.42
7.41
7.40
7.40
7.19
7.18
7.12
4.89
4.87
4.86
3.57
3.55
3.54
3.52
1.27
1.18
1.16
1.15
1.00
2.02
3.04
1.00
1.00
2.04
1.02
1.01
18.42
3.05
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

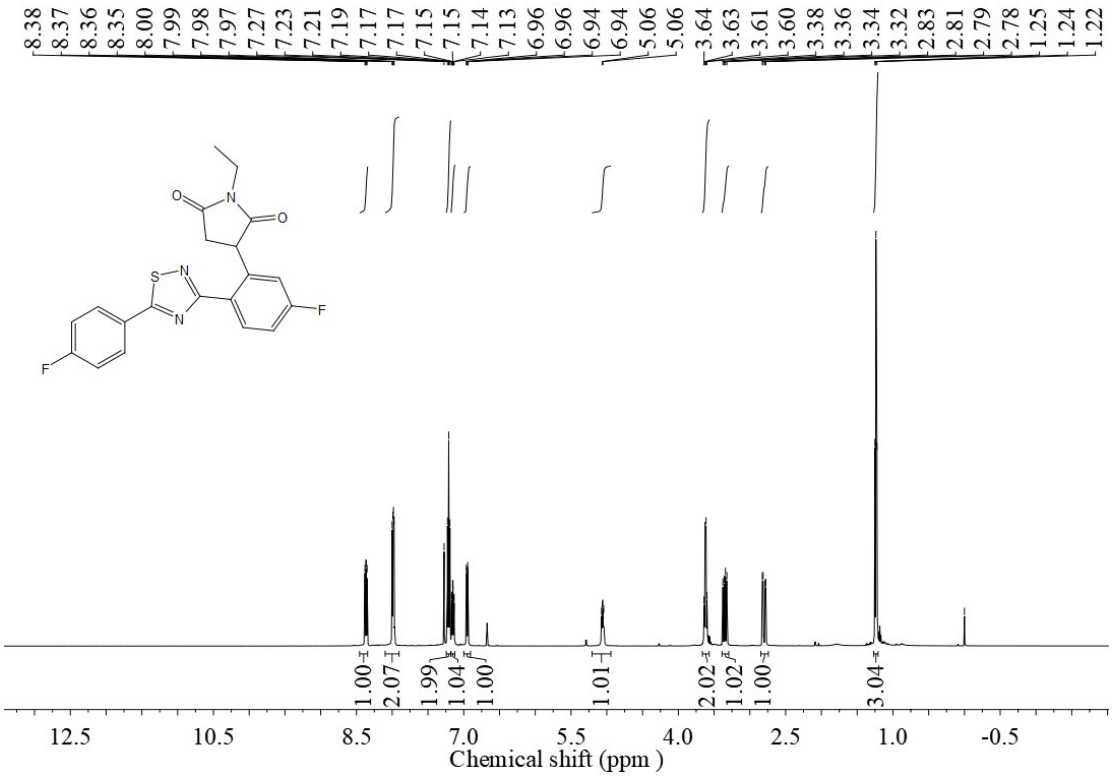

187.49
178.47
176.68
173.33
155.90
153.91
136.15
131.94
129.31
127.74
127.36
126.51
126.32
125.33
77.30
77.04
76.79
45.81
38.52
35.16
34.90
33.88
31.13
13.14
200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)

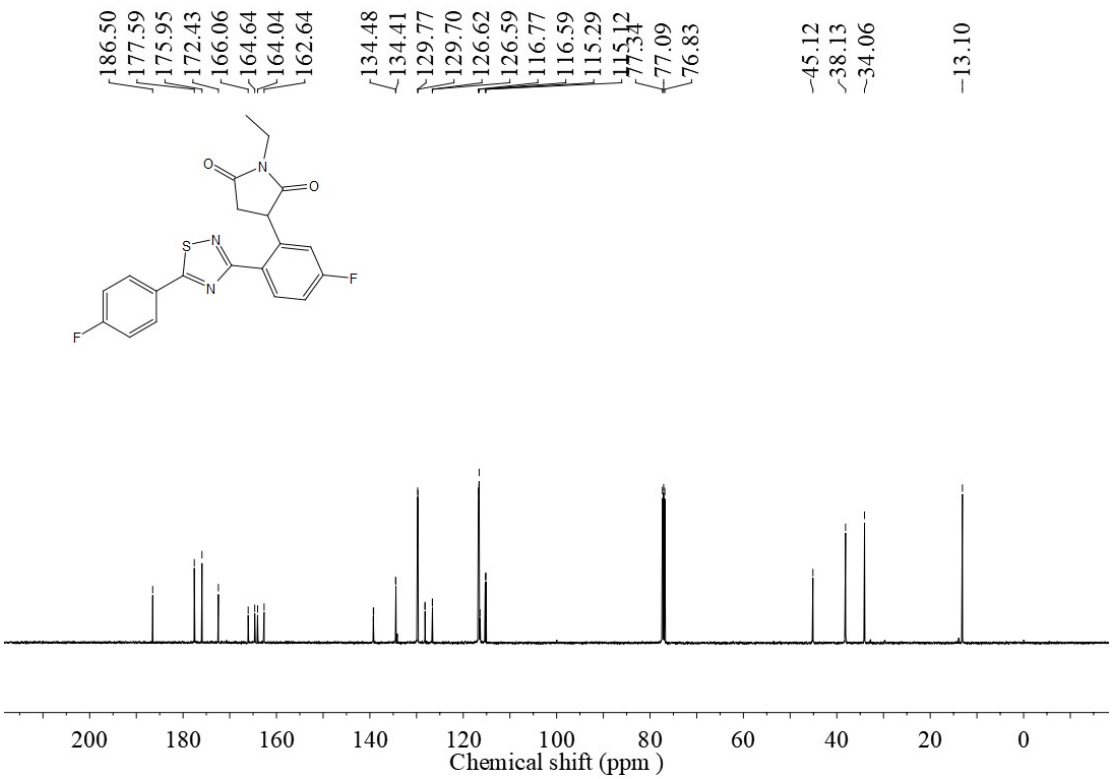
3q:


8.29
8.28
8.28
8.26
7.91
7.90
7.90
7.89
7.19
7.15
7.13
7.12
4.98
4.97
4.96
3.32
3.30
3.28
3.26
2.95
2.78
2.77
2.75
2.74
1.00
2.01
1.99
0.99
1.00
1.01
1.04
3.07
1.05
11.0
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
Chemical shift (ppm)

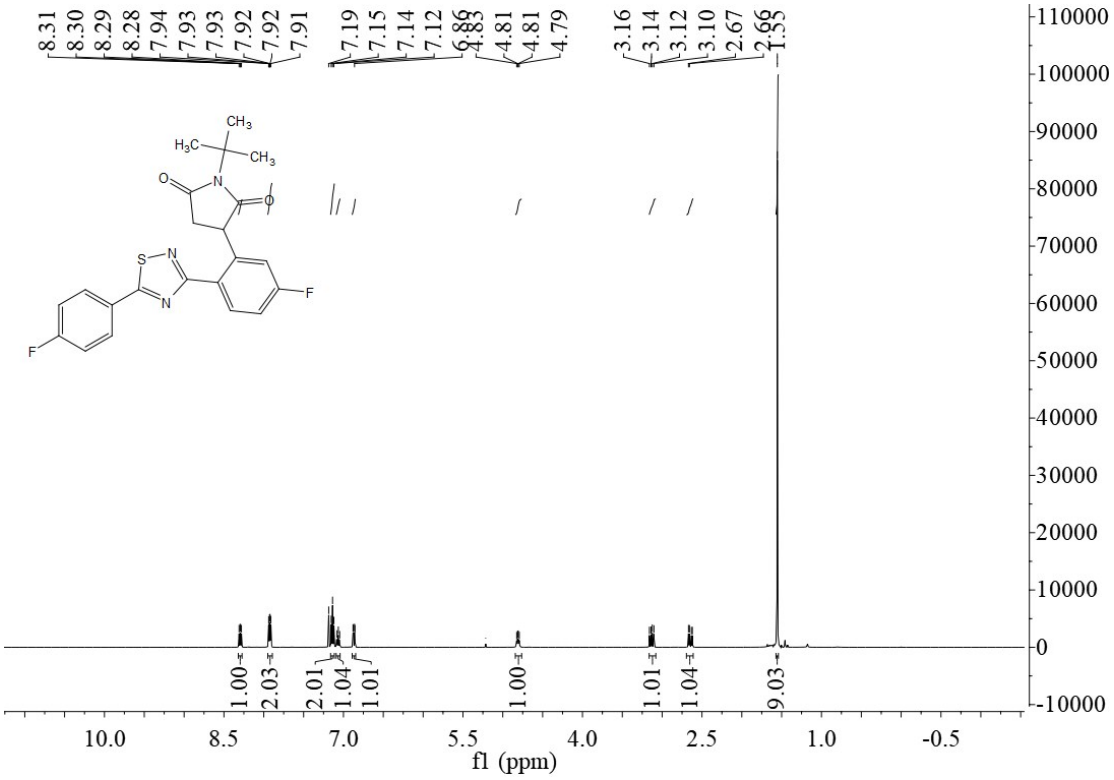

186.59
177.84
176.16
172.45
166.08
164.65
164.05
162.65
134.48
134.41
129.79
129.71
128.16
126.60
116.79
116.61
115.35
77.32
77.07
76.82
45.26
38.15
25.18
200
180
160
140
120
100
80
60
40
20
0
Chemical shift (ppm)

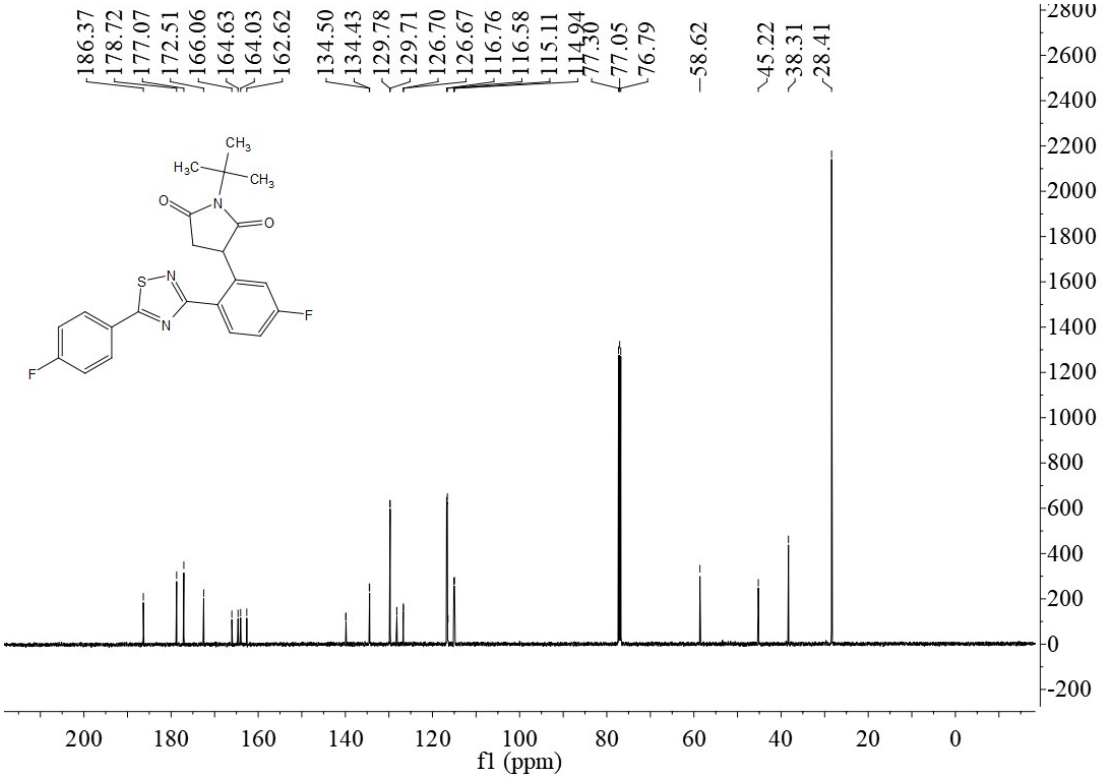
3r:


8.38
8.37
8.36
8.35
8.00
7.99
7.98
7.97
7.27
7.23
7.21
7.19
7.17
7.17
7.15
7.15
7.14
7.13
6.96
6.96
6.94
6.94
5.06
5.06
3.64
3.63
3.61
3.60
3.38
3.36
3.34
3.32
2.83
2.81
2.79
2.78
1.25
1.24
1.22
1.00
2.07
1.99
1.04
1.00
1.01
2.02
1.02
1.00
3.04
12.5
10.5
8.5
7.0
5.5
4.0
2.5
1.0
-0.5
Chemical shift (ppm)

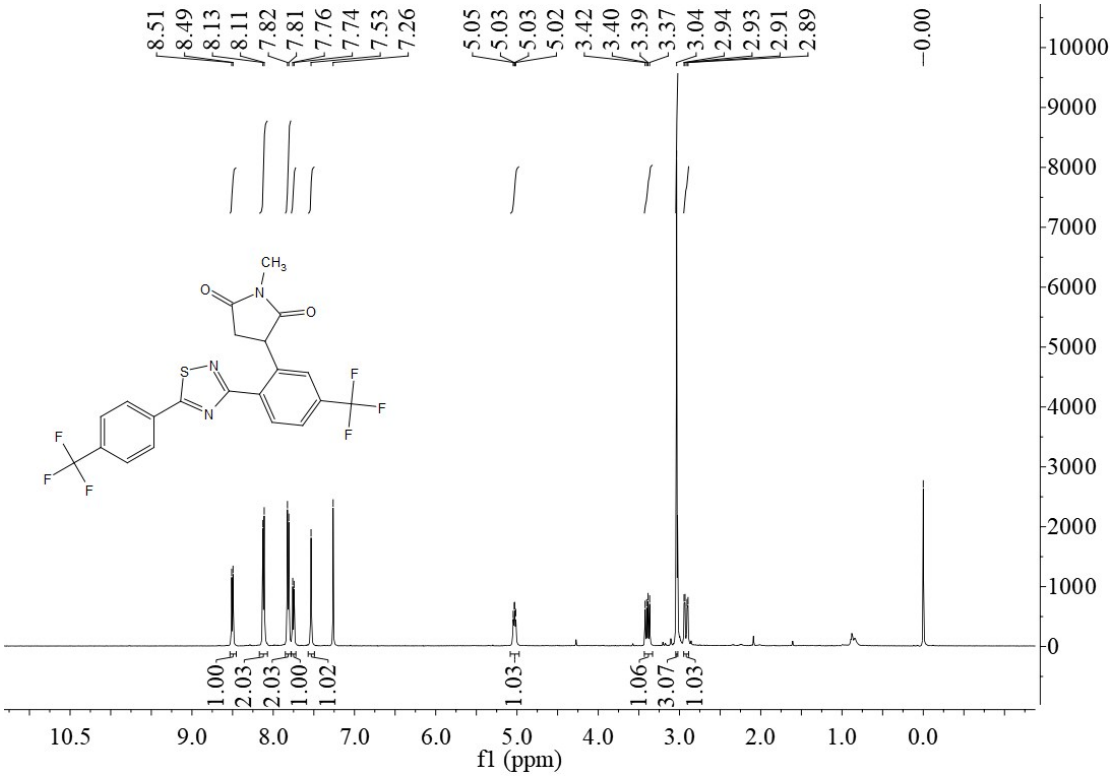

186.50
177.59
175.95
172.43
166.06
164.64
164.04
162.64
134.48
134.41
129.77
129.70
126.62
126.59
116.77
116.59
115.29
115.12
77.34
77.09
76.83
45.12
38.13
34.06
13.10
200
180
160
140
120
100
80
60
40
20
0
Chemical shift (ppm)

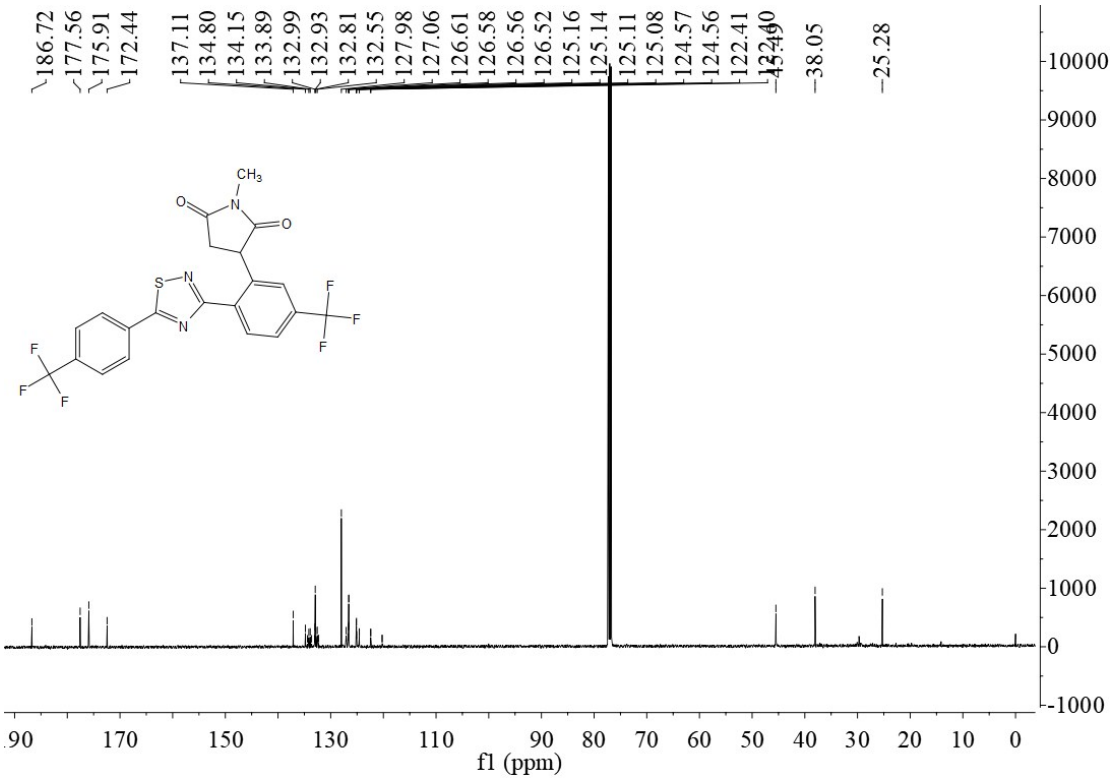
3s:


8.31
8.30
8.29
8.28
7.94
7.93
7.93
7.92
7.92
7.91
7.19
7.15
7.14
7.12
6.86
4.85
4.81
4.81
4.79
3.16
3.14
3.12
3.10
2.67
2.66
1.55
1.00
2.03
2.01
1.04
1.01
1.00
1.01
1.04
9.03
fl (ppm)

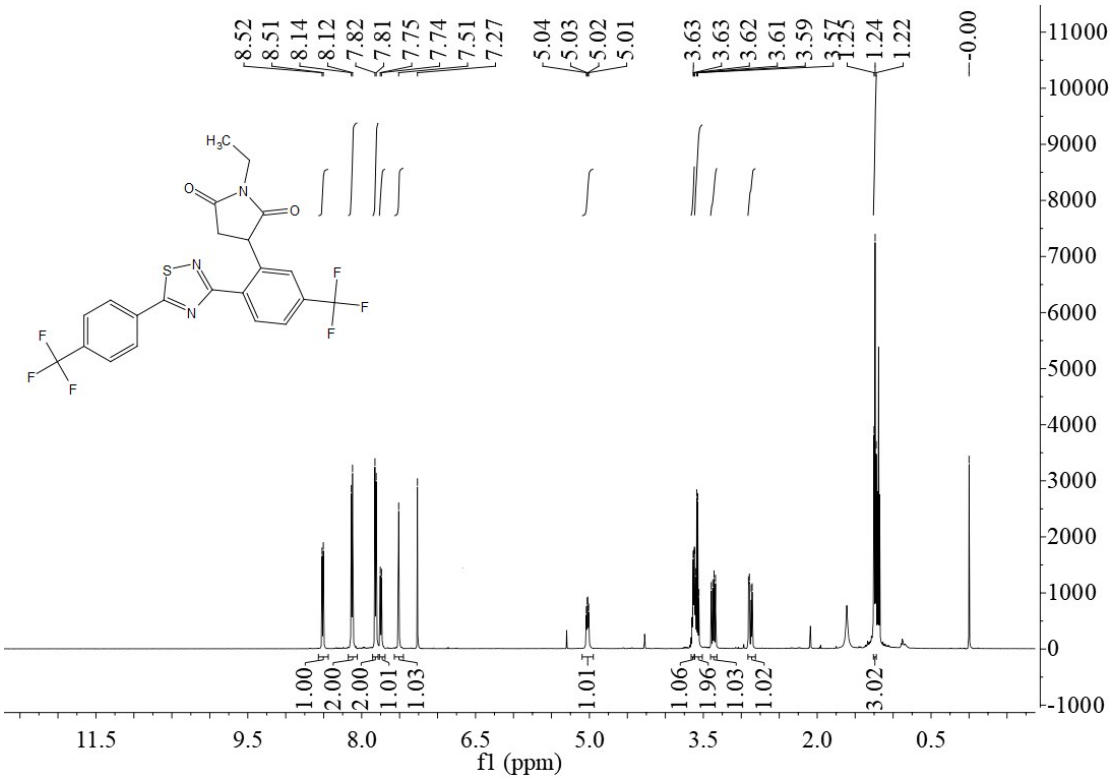

186.37
178.72
177.07
172.51
166.06
164.63
164.03
162.62
134.50
134.43
129.78
129.71
126.70
126.67
116.76
116.58
115.11
114.94
77.30
77.05
76.79
58.62
45.22
38.31
28.41
fl (ppm)

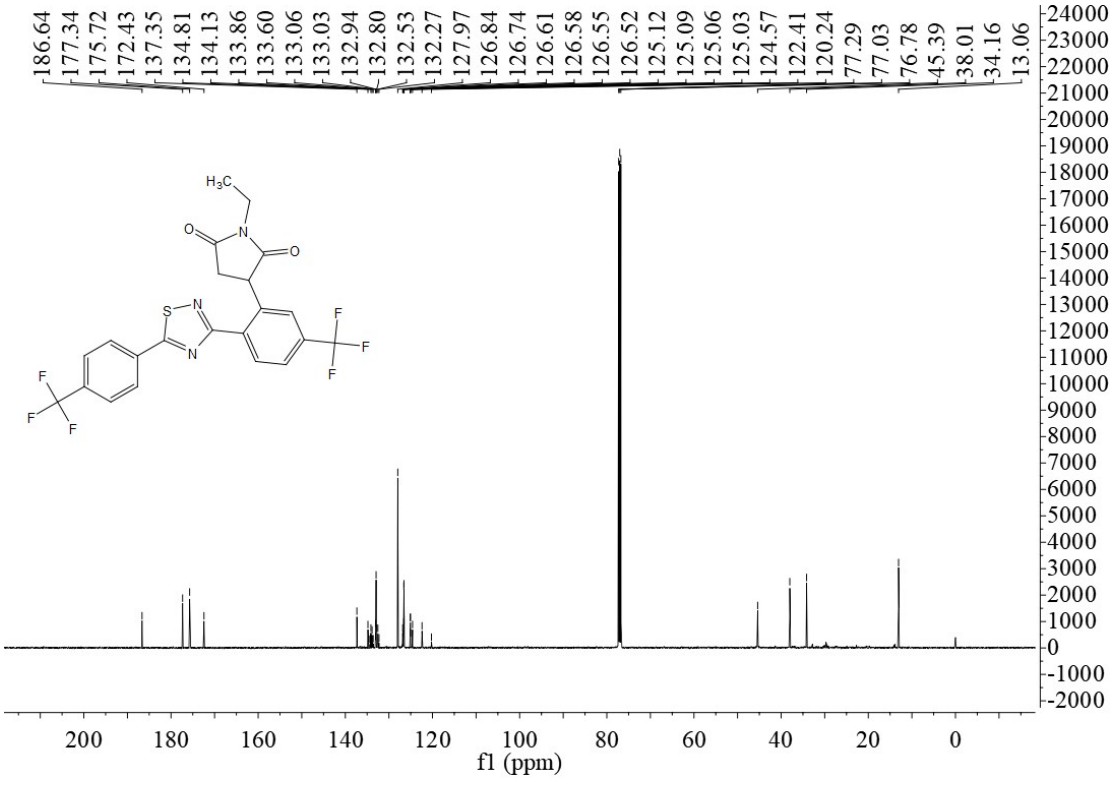
3t:


8.51
8.49
8.13
8.11
7.82
7.81
7.76
7.74
7.53
7.26
5.05
5.03
5.03
5.02
3.42
3.40
3.39
3.37
3.04
2.94
2.93
2.91
2.89
0.00
1.00
2.03
2.03
1.00
1.02
1.03
1.06
3.07
1.03
f1 (ppm)

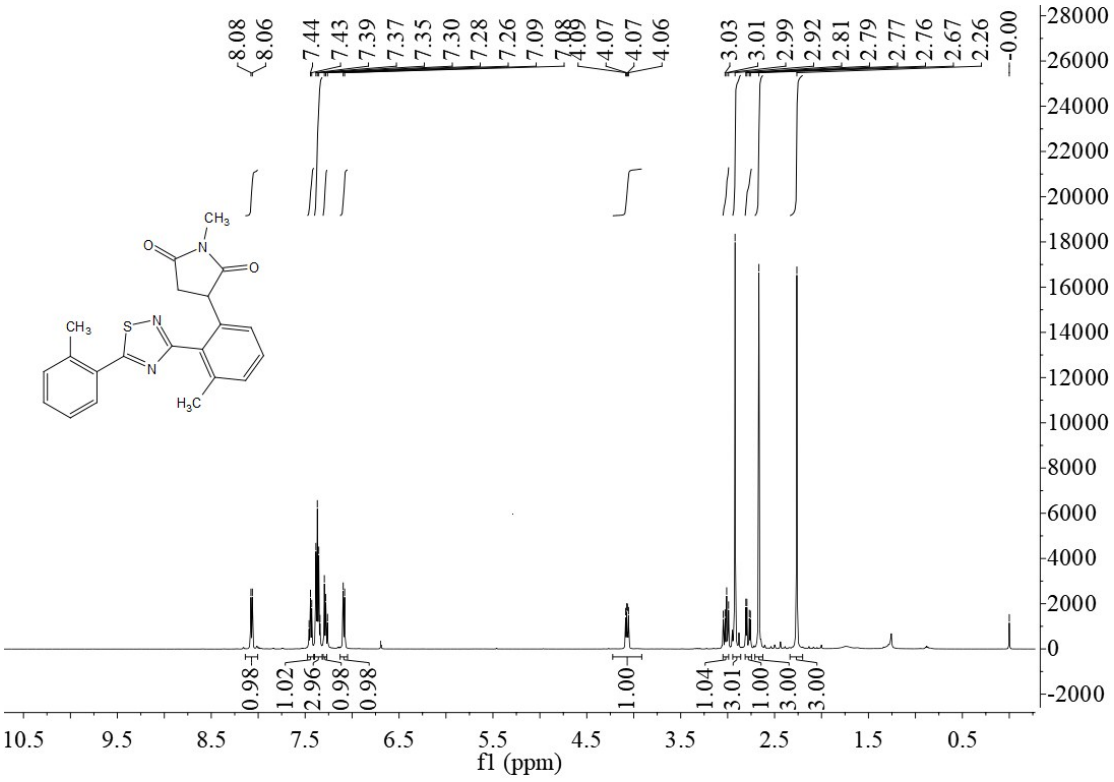

186.72
177.56
175.91
172.44
137.11
134.80
134.15
133.89
132.99
132.93
132.81
132.55
127.98
127.06
126.61
126.58
126.56
126.52
125.16
125.14
125.11
125.08
124.57
124.56
122.41
45.49
38.05
25.28
f1 (ppm)

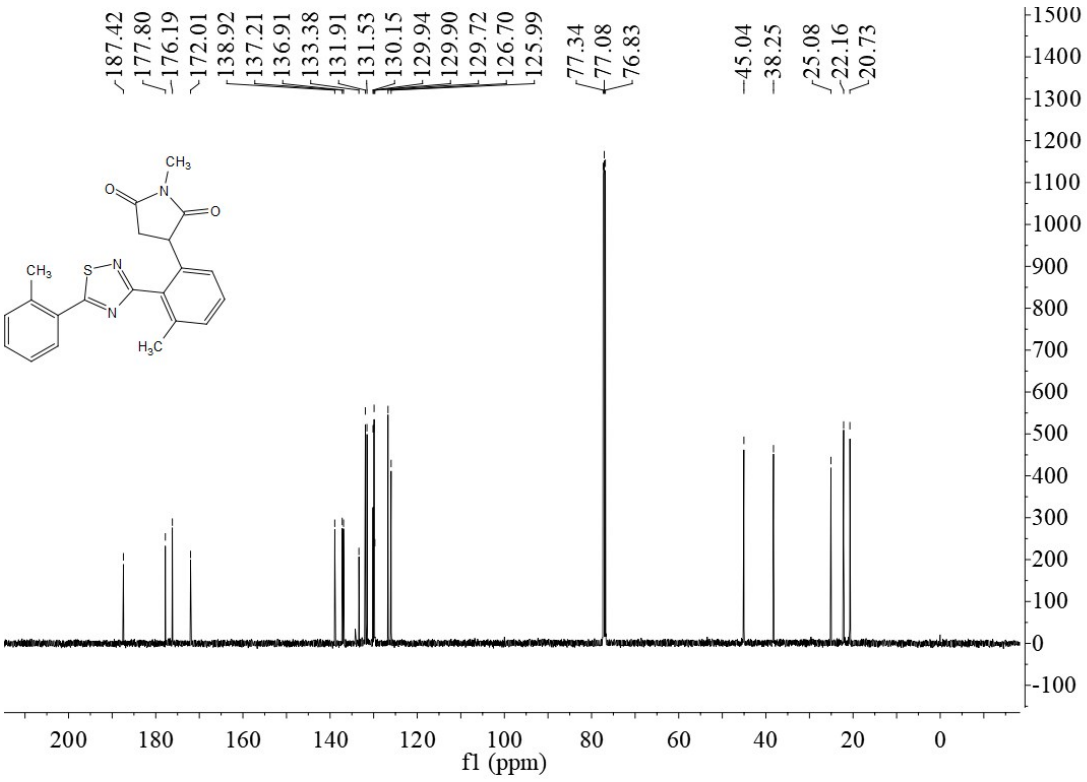
3u:


8.52
8.51
8.14
8.12
7.82
7.81
7.75
7.74
7.51
7.27
5.04
5.03
5.02
5.01
3.63
3.63
3.62
3.61
3.59
1.24
1.22
-0.00
1.00
2.00
2.00
1.01
1.03
1.01
1.06
1.96
1.03
1.02
3.02
f1 (ppm)

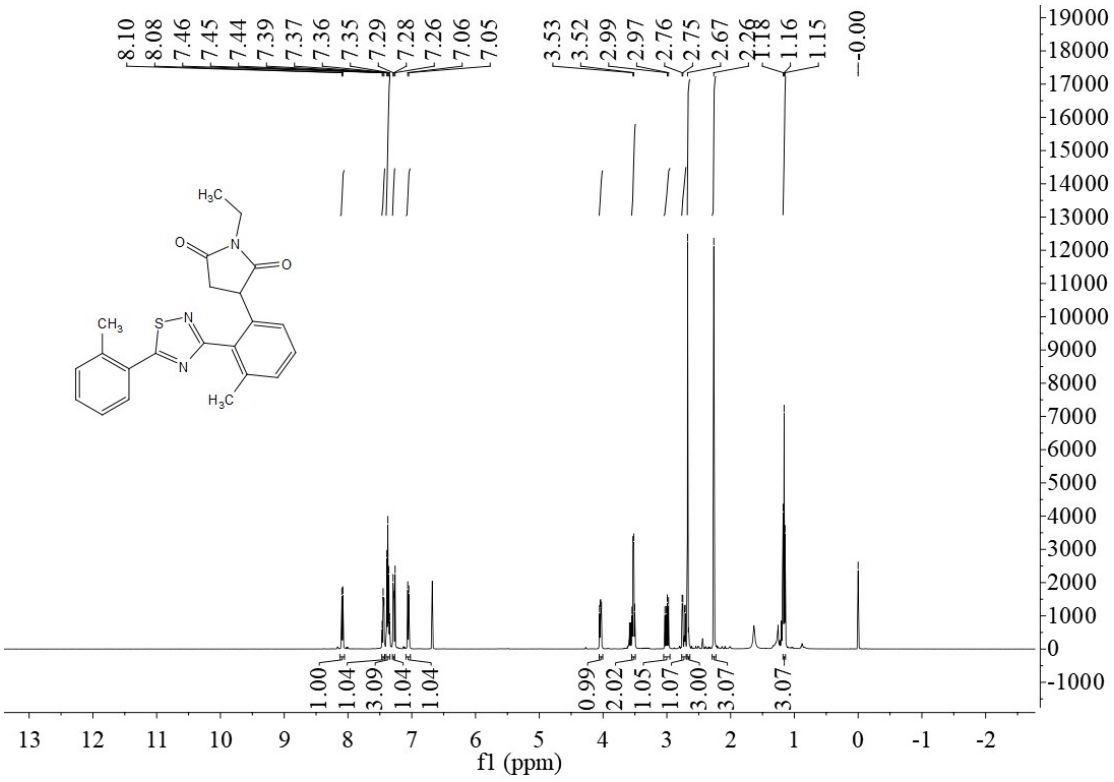

186.64
177.34
175.72
172.43
137.35
134.81
134.13
133.86
133.60
133.06
133.03
132.94
132.80
132.53
132.27
127.97
126.84
126.74
126.61
126.58
126.55
126.52
125.12
125.09
125.06
125.03
124.57
122.41
120.24
77.29
77.03
76.78
45.39
38.01
34.16
13.06
f1 (ppm)

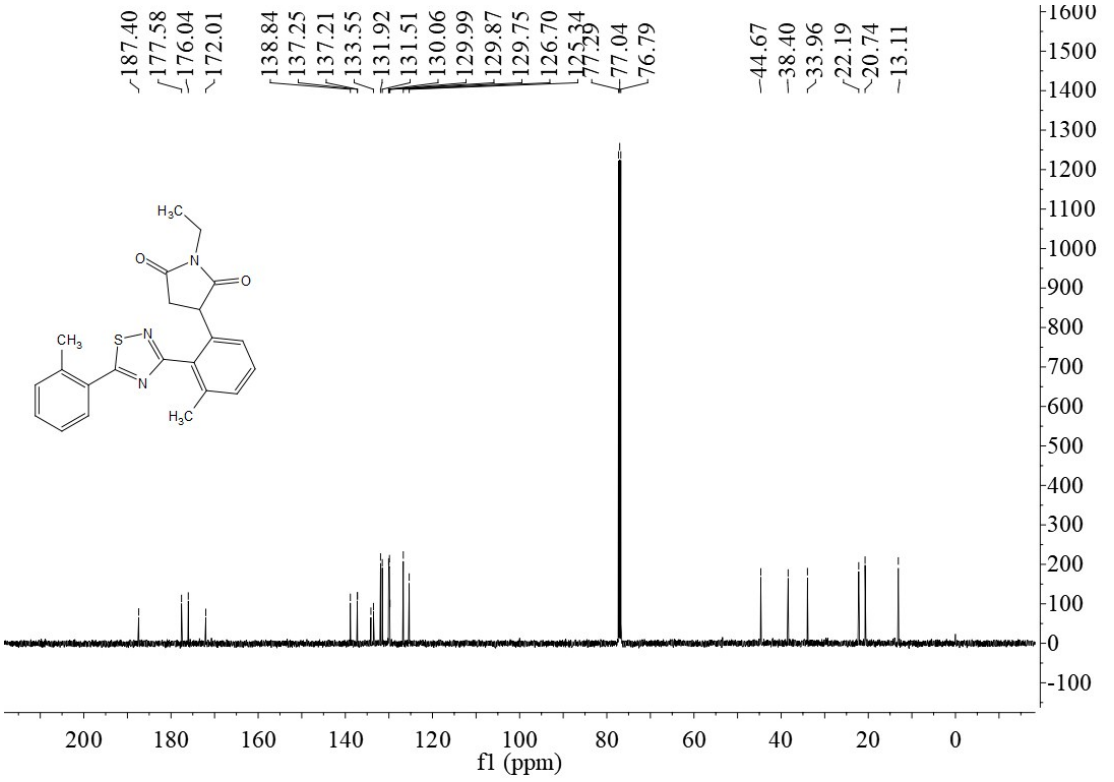
3w:


8.08
8.06
7.44
7.43
7.39
7.37
7.35
7.30
7.28
7.26
7.09
7.08
4.09
4.07
4.07
4.06
3.03
3.01
2.99
2.92
2.81
2.79
2.77
2.76
2.67
2.26
-0.00
0.98
1.02
2.96
0.98
0.98
1.00
1.04
3.01
1.00
3.00
3.00
f1 (ppm)

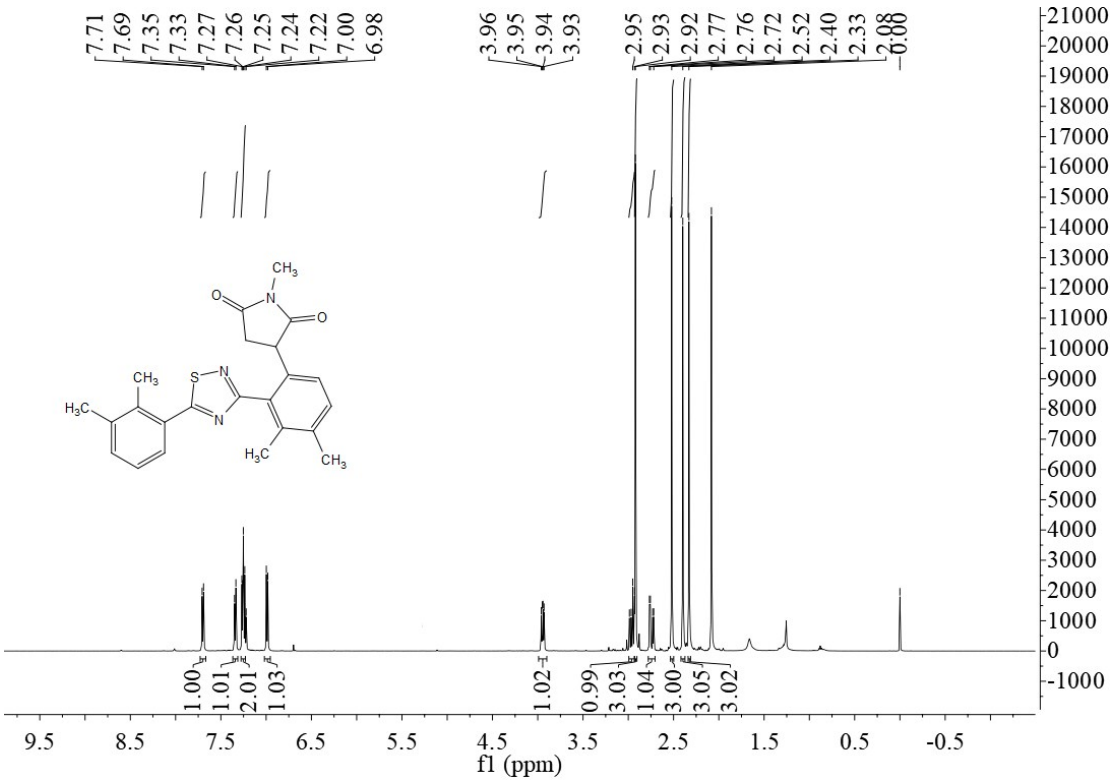

187.42
177.80
176.19
172.01
138.92
137.21
136.91
133.38
131.91
131.53
130.15
129.94
129.90
129.72
126.70
125.99
77.34
77.08
76.83
45.04
38.25
25.08
22.16
20.73
f1 (ppm)

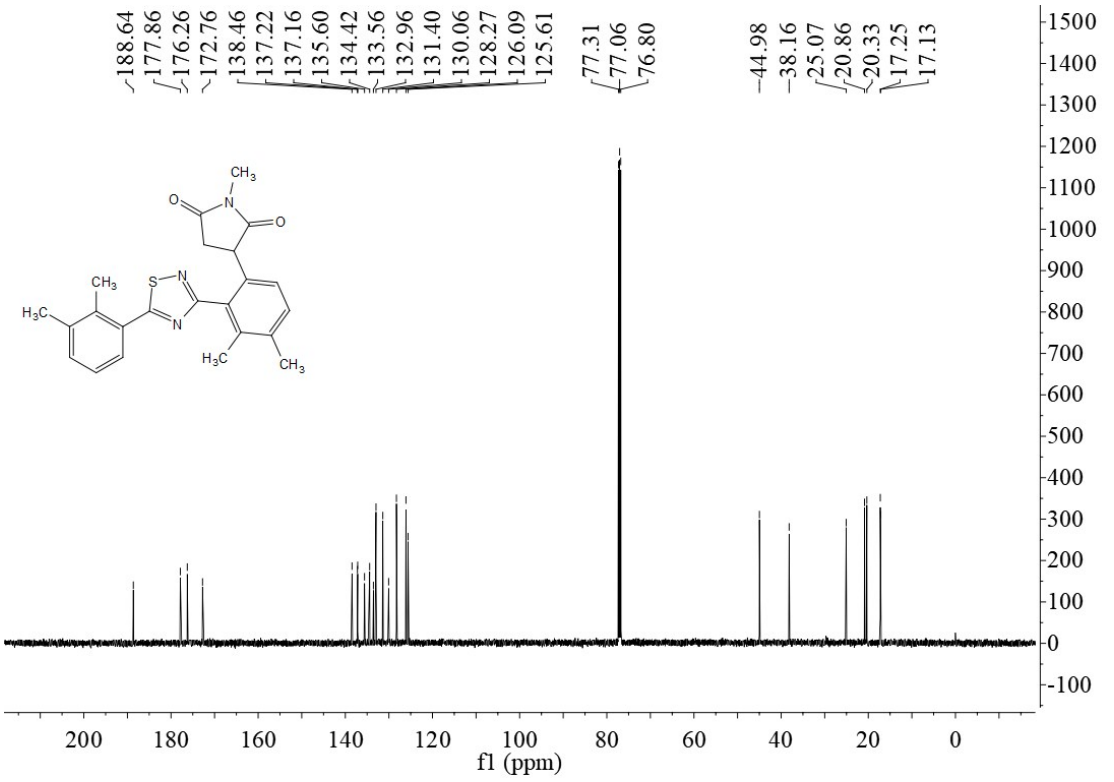
3x:


8.10
8.08
7.46
7.45
7.44
7.39
7.37
7.36
7.35
7.29
7.28
7.26
7.06
7.05
3.53
3.52
2.99
2.97
2.76
2.75
2.67
1.16
1.15
-0.00
1.00
1.04
3.09
1.04
1.04
0.99
2.02
1.05
1.07
3.00
3.07
3.07
f1 (ppm)

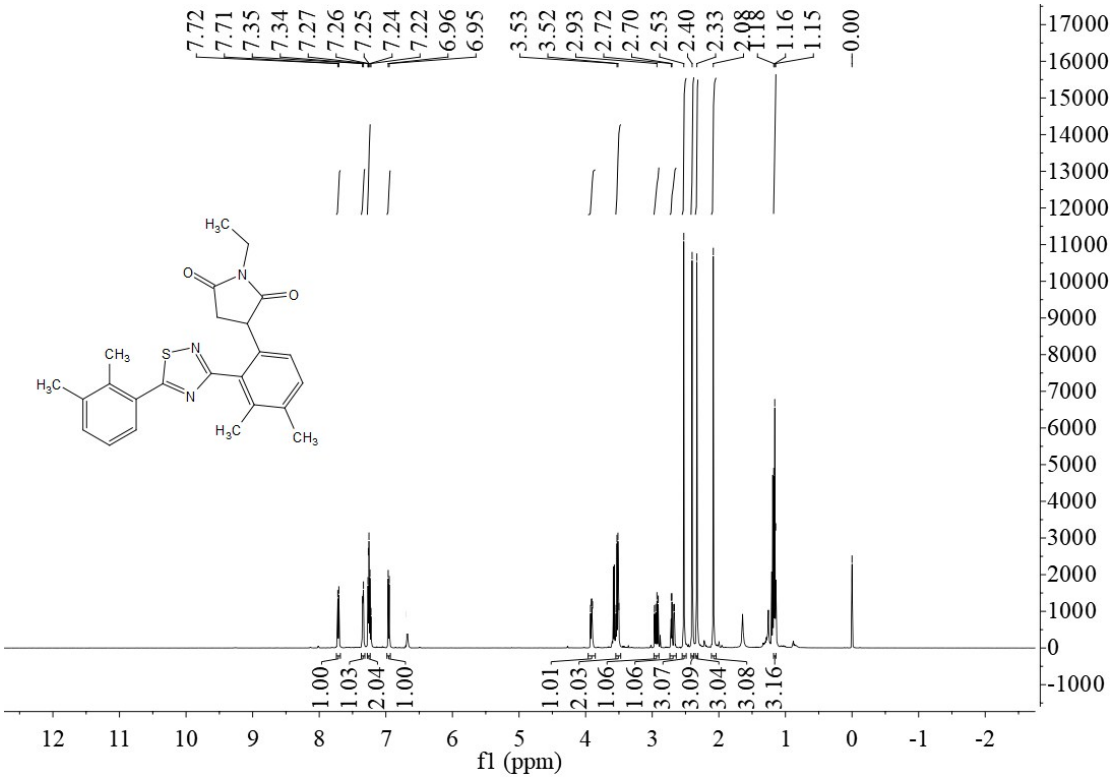

187.40
177.58
176.04
172.01
138.84
137.25
137.21
133.55
131.92
131.51
130.06
129.99
129.87
129.75
126.70
125.34
77.29
77.04
76.79
44.67
38.40
33.96
22.19
20.74
13.11
f1 (ppm)

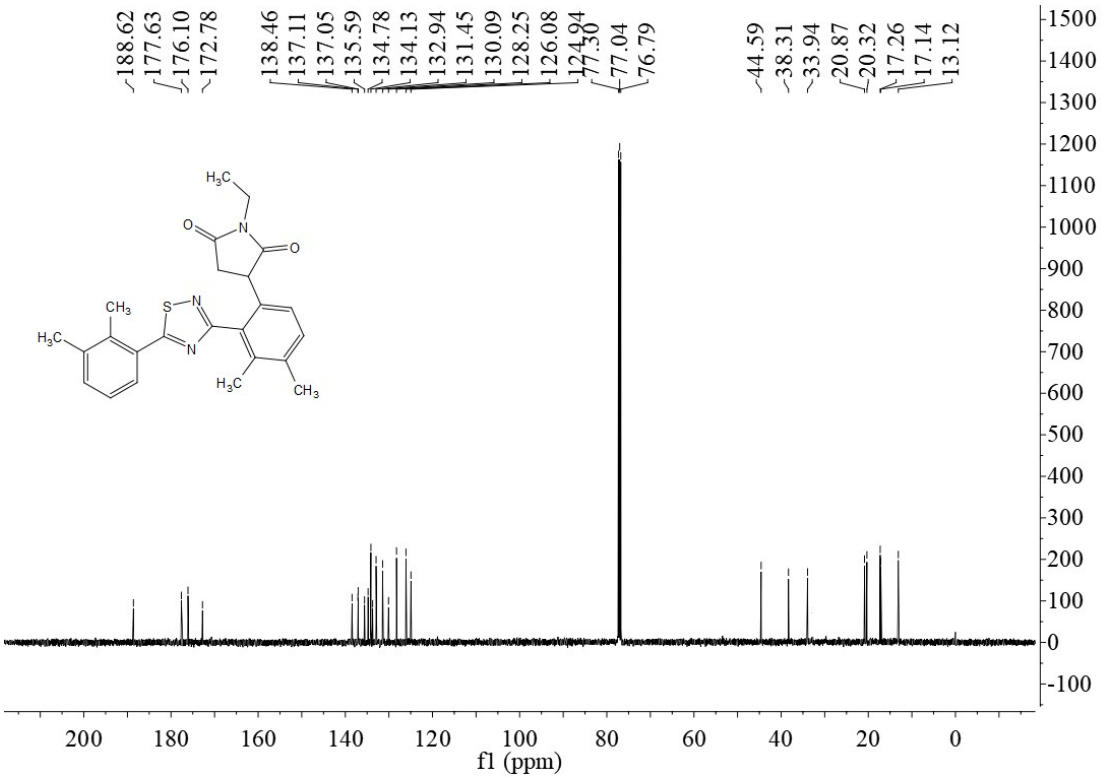
3y:


7.71
7.69
7.35
7.33
7.27
7.26
7.25
7.24
7.22
7.00
6.98
3.96
3.95
3.94
3.93
2.95
2.93
2.92
2.77
2.76
2.72
2.52
2.40
2.33
2.08
0.00
1.00
1.01
2.01
1.03
1.02
0.99
3.03
1.04
3.00
3.05
3.02
f1 (ppm)

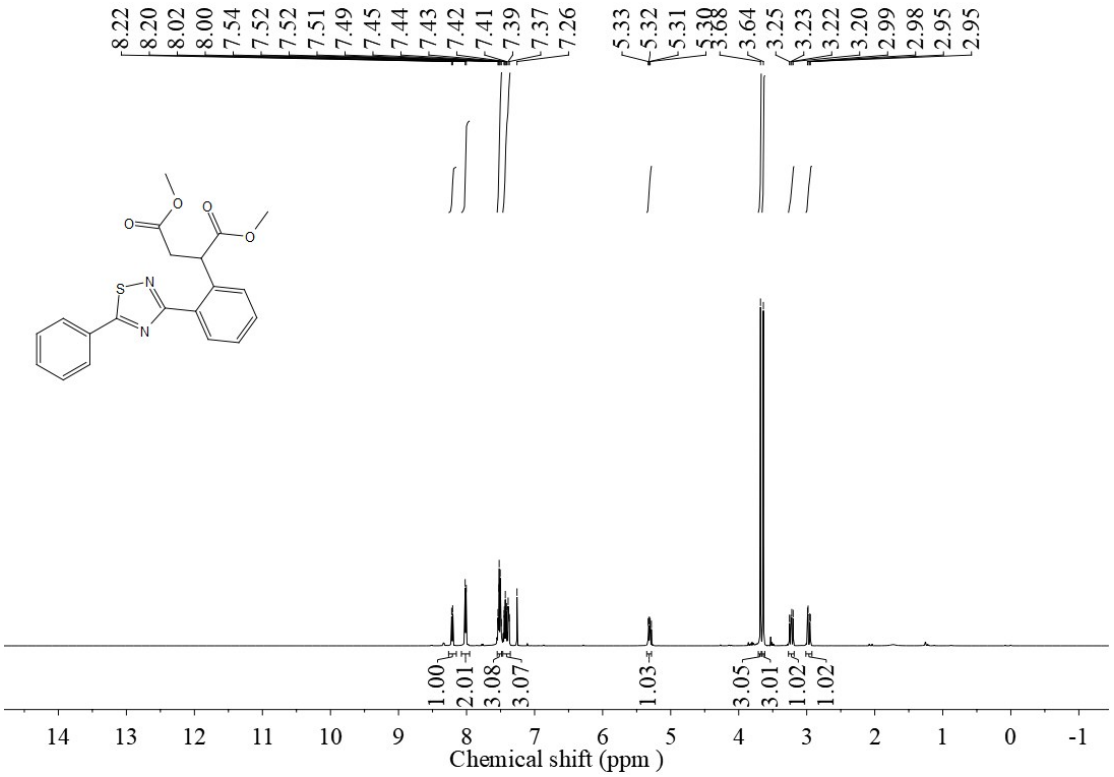

188.64
177.86
176.26
172.76
138.46
137.22
137.16
135.60
134.42
133.56
132.96
131.40
130.06
128.27
126.09
125.61
77.31
77.06
76.80
44.98
38.16
25.07
20.86
20.33
17.25
17.13
f1 (ppm)

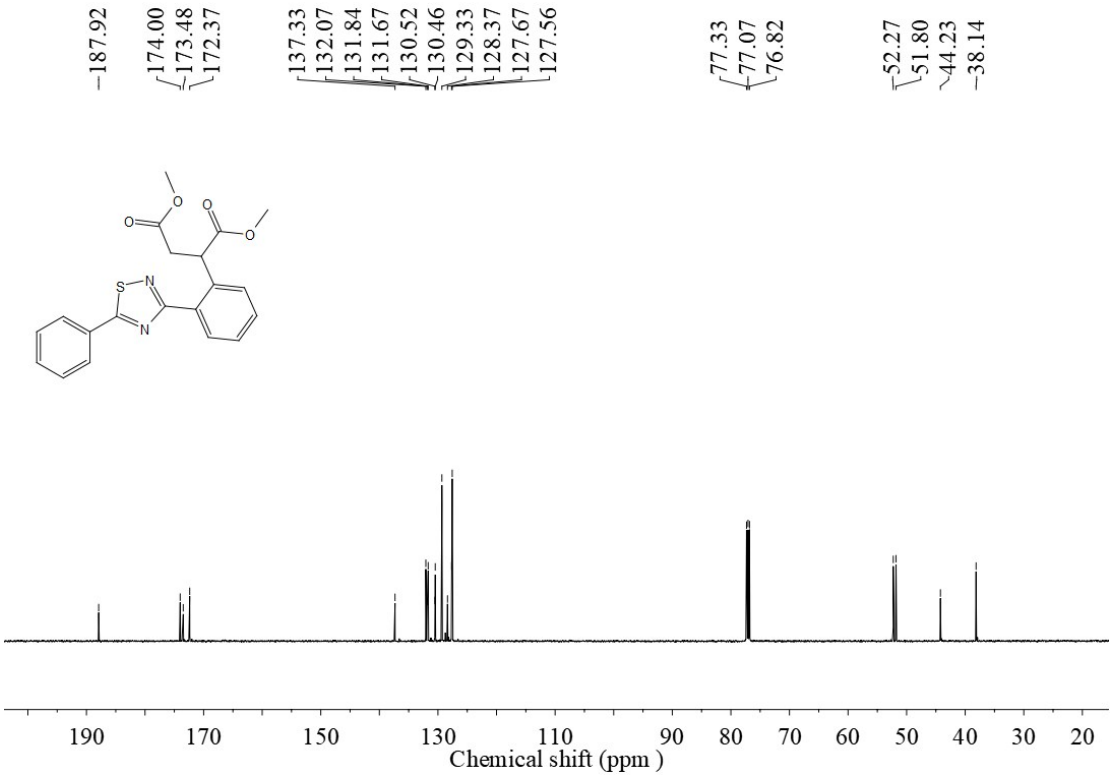
3z:


7.72
7.71
7.35
7.34
7.27
7.26
7.25
7.24
7.22
6.96
6.95
3.53
3.52
2.93
2.72
2.70
2.53
2.40
2.33
2.08
1.18
1.16
1.15
0.00
1.00
1.03
2.04
1.00
1.01
2.03
1.06
1.06
3.07
3.09
3.04
3.08
3.16
f1 (ppm)

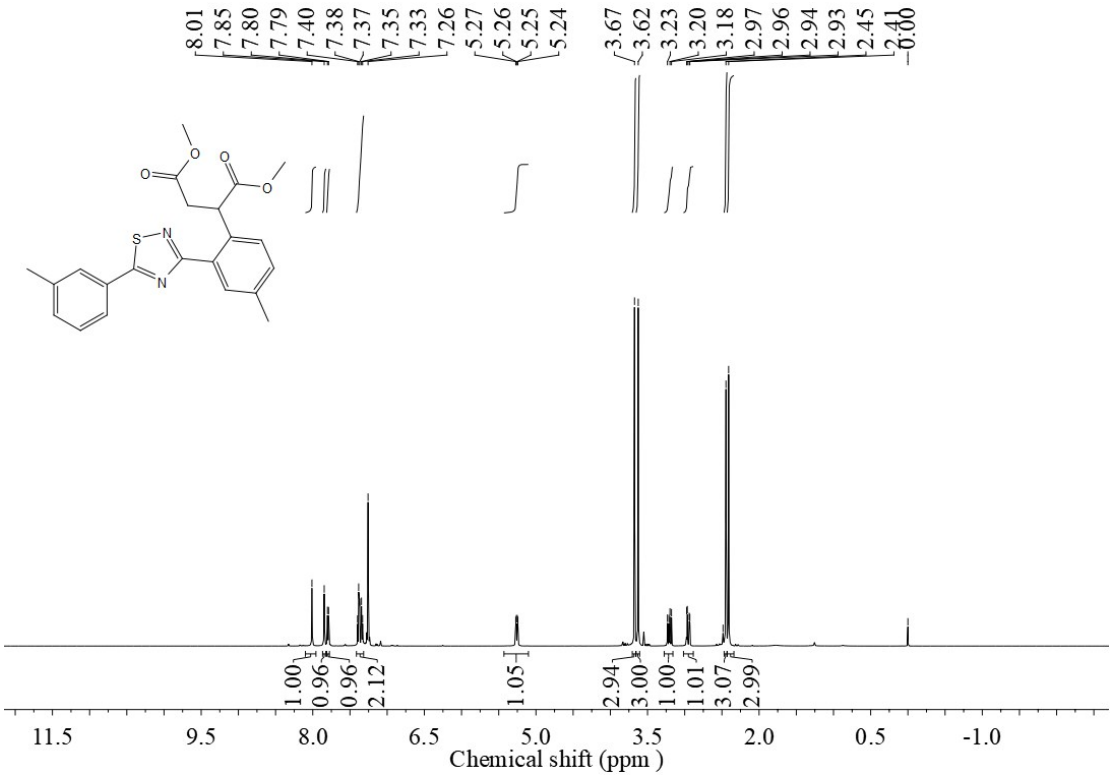

188.62
177.63
176.10
172.78
138.46
137.11
137.05
135.59
134.78
134.13
132.94
131.45
130.09
128.25
126.08
124.94
77.30
77.04
76.79
44.59
38.31
33.94
20.87
20.32
17.26
17.14
13.12
f1 (ppm)

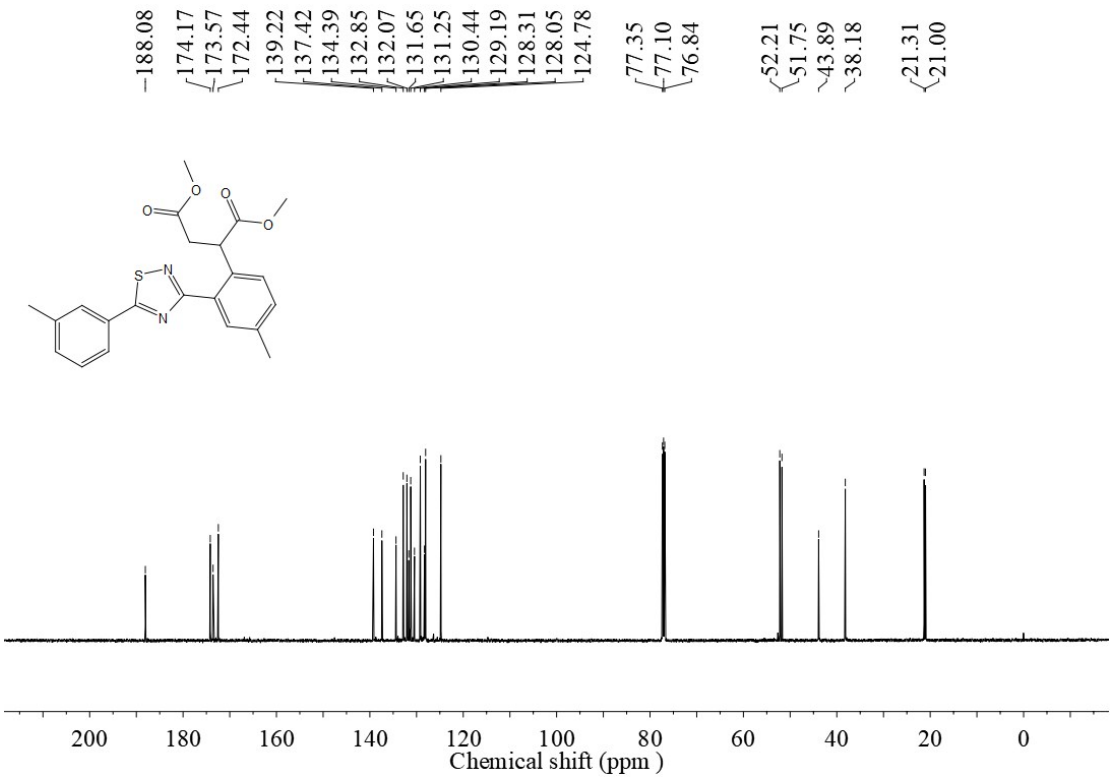
3aa:


8.22
8.20
8.02
8.00
7.54
7.52
7.52
7.51
7.49
7.45
7.44
7.43
7.42
7.41
7.39
7.37
7.26
5.33
5.32
5.31
3.68
3.64
3.25
3.23
3.22
3.20
2.99
2.98
2.95
2.95
1.00
2.01
3.08
3.07
1.03
3.05
3.01
1.02
1.02
Chemical shift (ppm)

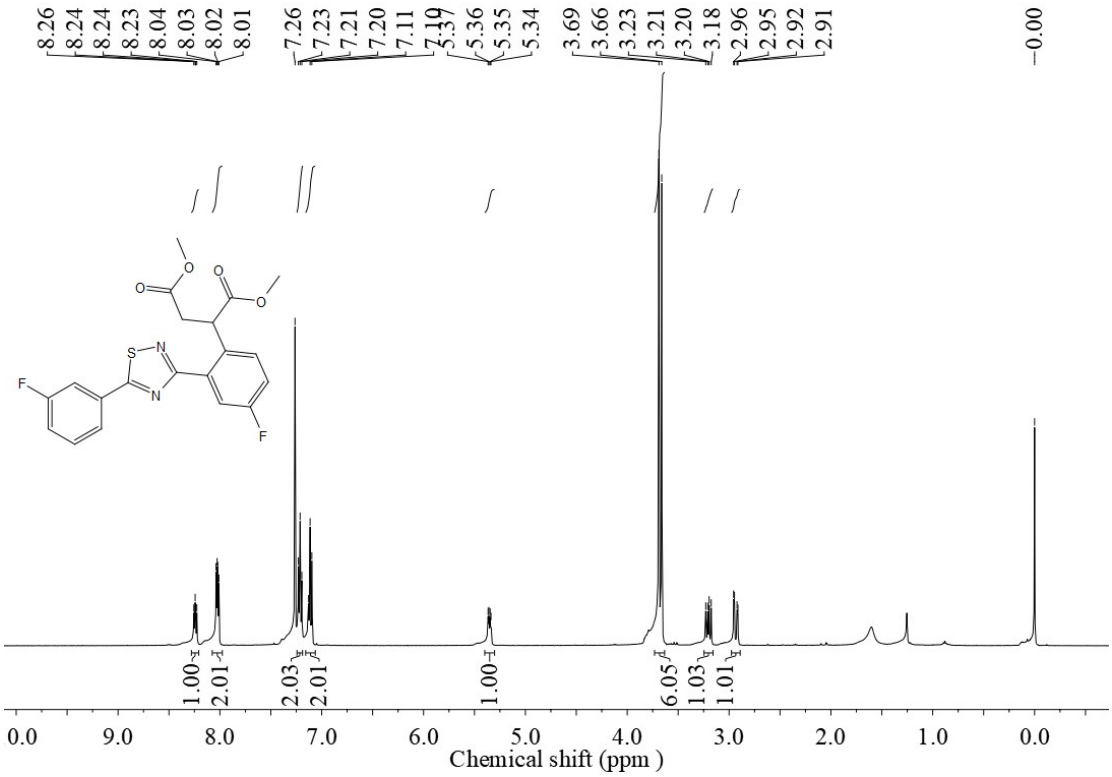

187.92
174.00
173.48
172.37
137.33
132.07
131.84
131.67
130.52
130.46
129.33
128.37
127.67
127.56
77.33
77.07
76.82
52.27
51.80
44.23
38.14
Chemical shift (ppm)

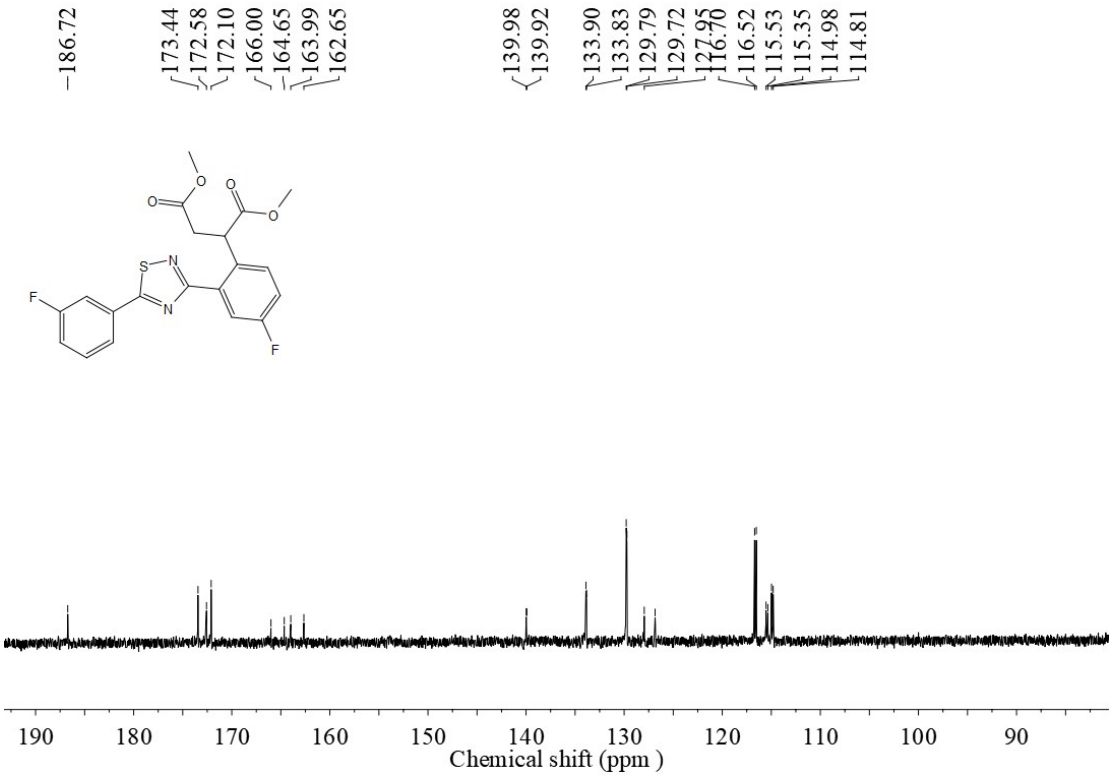
3ab:


8.01
7.85
7.80
7.79
7.40
7.38
7.37
7.35
7.33
7.26
5.27
5.26
5.25
5.24
3.67
3.62
3.23
3.20
3.18
2.97
2.96
2.94
2.93
2.45
2.41
0.00
1.00
0.96
0.96
2.12
1.05
2.94
3.00
1.00
1.01
3.07
2.99
11.5
9.5
8.0
6.5
5.0
3.5
2.0
0.5
-1.0
Chemical shift (ppm)

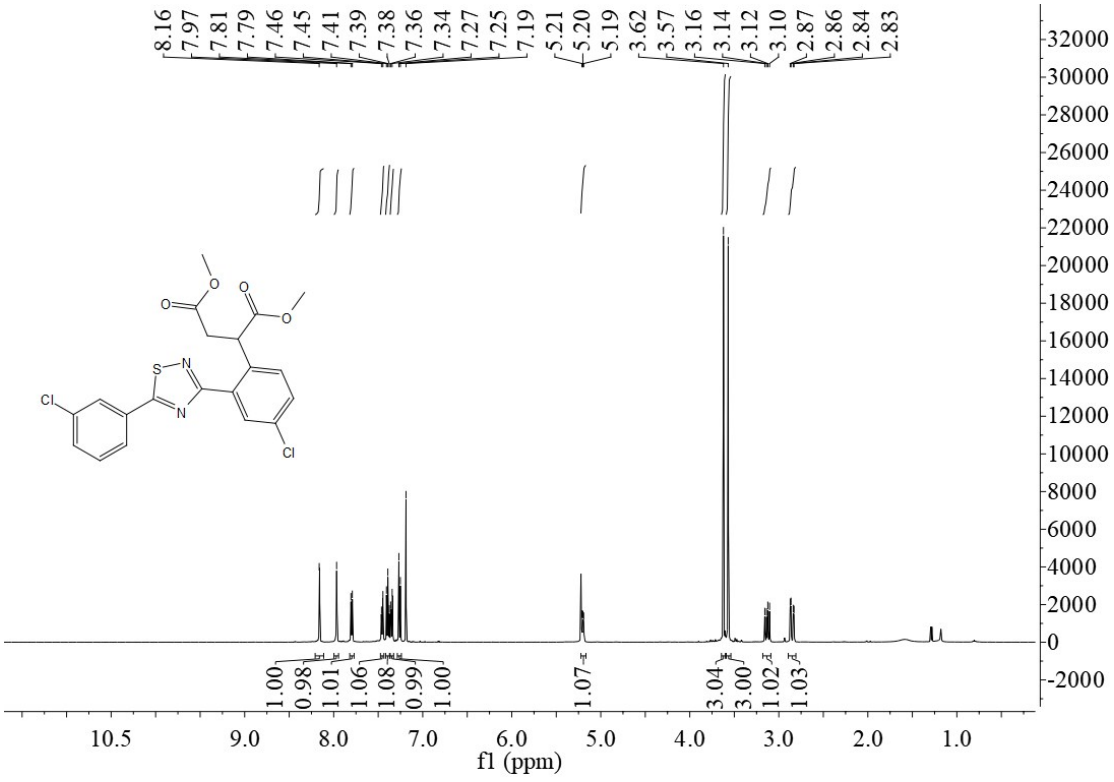

188.08
174.17
173.57
172.44
139.22
137.42
134.39
132.85
132.07
131.65
131.25
130.44
129.19
128.31
128.05
124.78
77.35
77.10
76.84
52.21
51.75
43.89
38.18
21.31
21.00
200
180
160
140
120
100
80
60
40
20
0
Chemical shift (ppm)

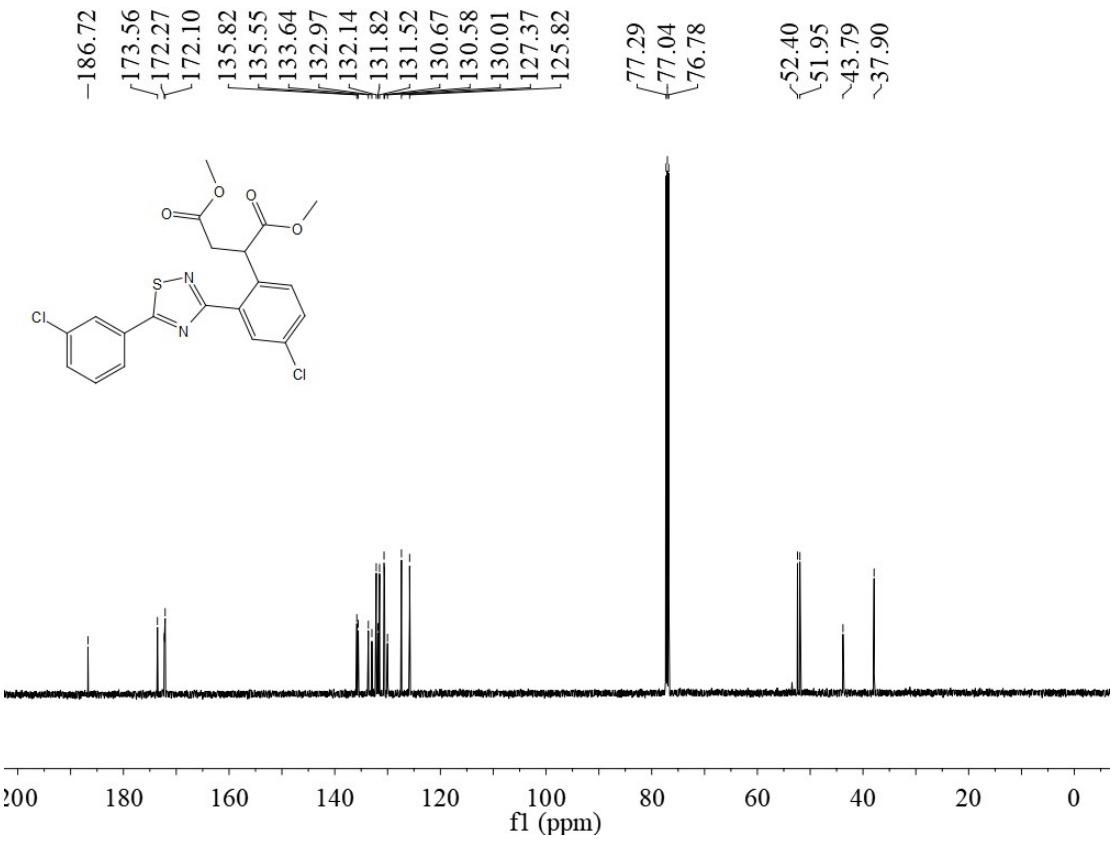
3ac:


8.26
8.24
8.24
8.23
8.04
8.03
8.02
8.01
7.26
7.23
7.21
7.20
7.11
5.36
5.35
5.34
3.69
3.66
3.23
3.21
3.20
3.18
2.96
2.95
2.92
2.91
0.00
1.00
2.01
2.03
2.01
1.00
6.05
1.03
1.01
Chemical shift (ppm)

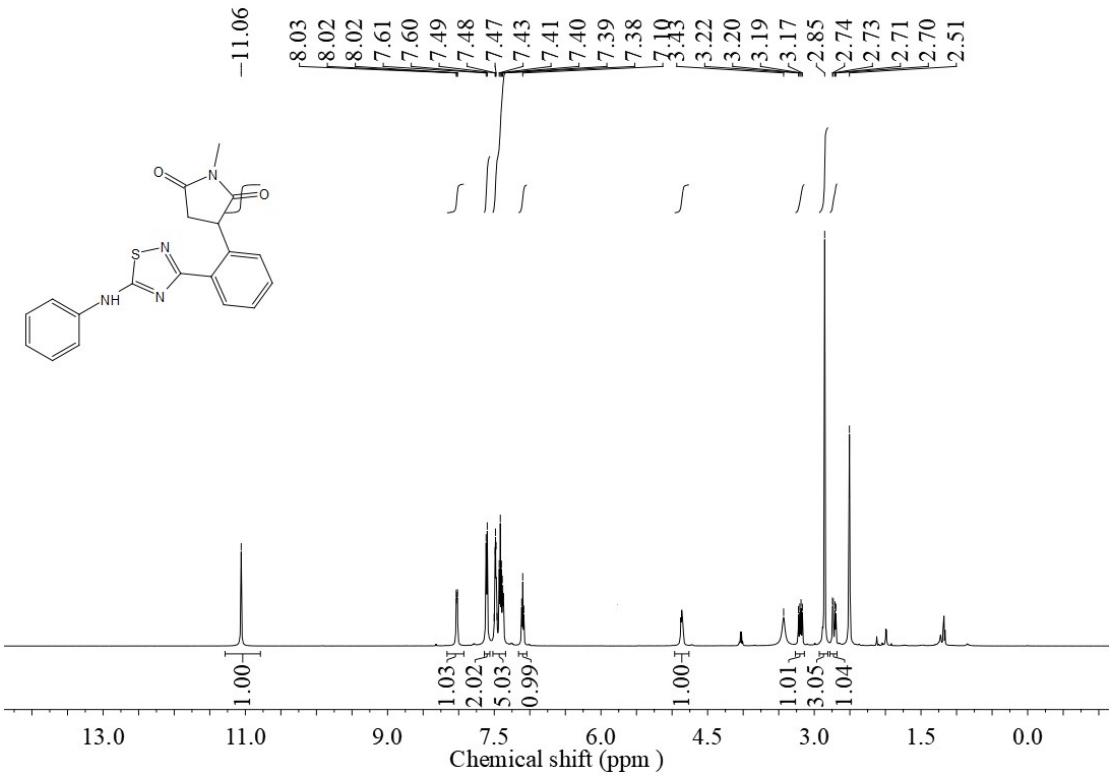

186.72
173.44
172.58
172.10
166.00
164.65
163.99
162.65
139.98
139.92
133.90
133.83
129.79
129.72
127.95
116.70
116.52
115.53
115.35
114.98
114.81
Chemical shift (ppm)

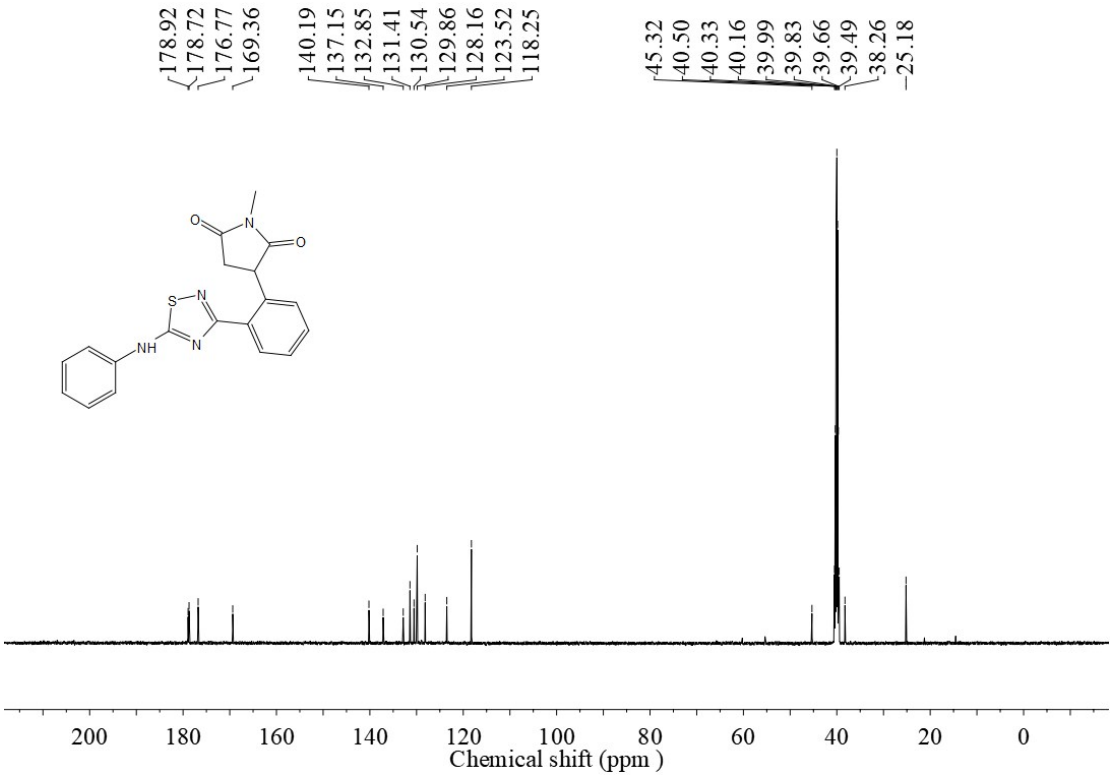
3ad:


8.16
7.97
7.81
7.79
7.46
7.45
7.41
7.39
7.38
7.36
7.34
7.27
7.25
7.19
5.21
5.20
5.19
3.62
3.57
3.16
3.14
3.12
3.10
2.87
2.86
2.84
2.83
1.00
0.98
1.01
1.06
1.08
0.99
1.00
1.07
3.04
3.00
1.02
1.03
f1 (ppm)

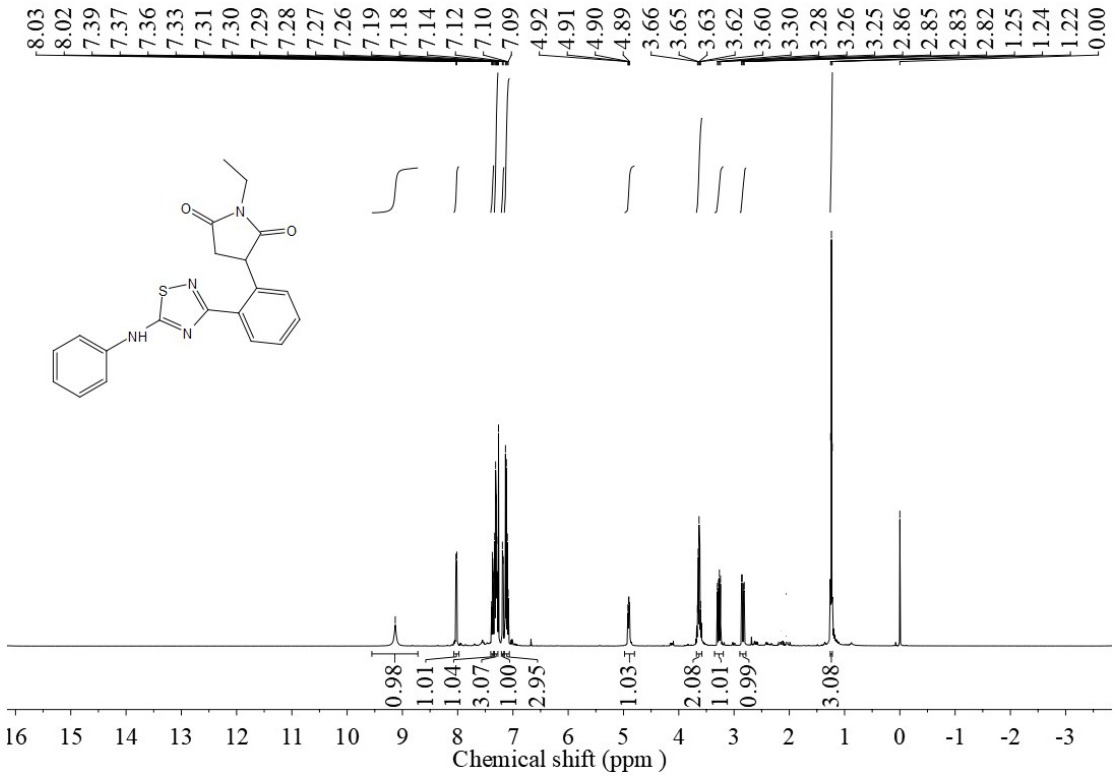

186.72
173.56
172.27
172.10
135.82
135.55
133.64
132.97
132.14
131.82
131.52
130.67
130.58
130.01
127.37
125.82
77.29
77.04
76.78
52.40
51.95
43.79
37.90
f1 (ppm)

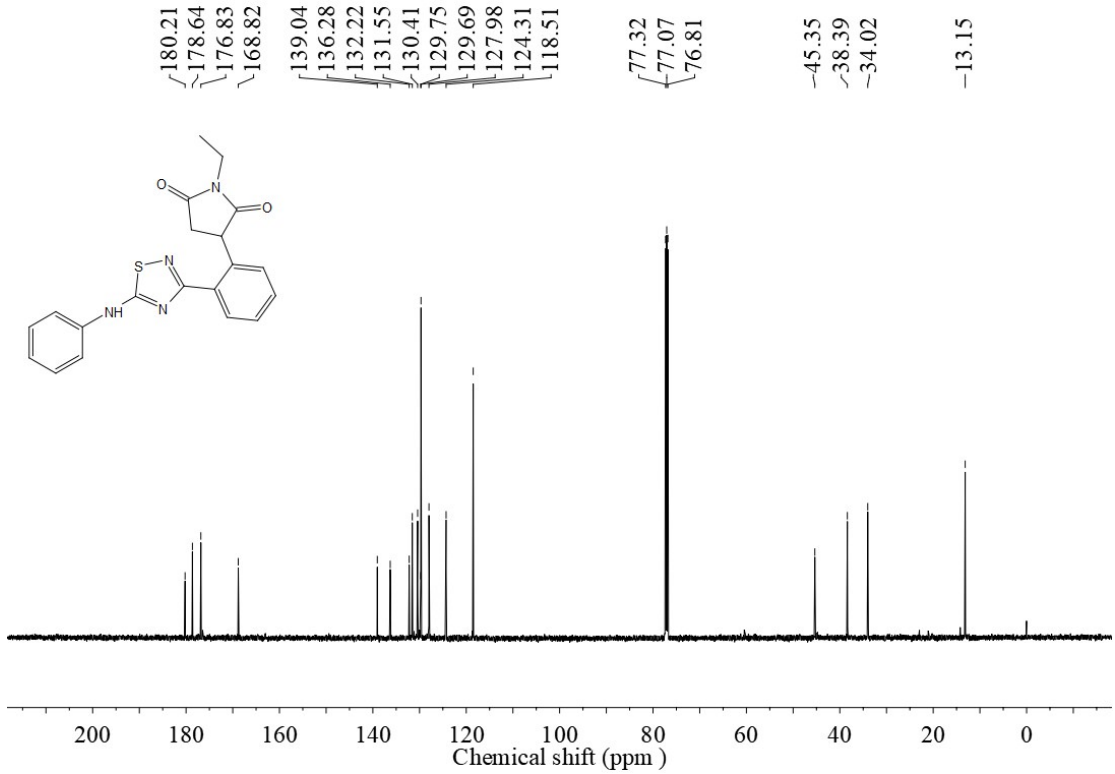
6a:


11.06
8.03
8.02
8.02
7.61
7.60
7.49
7.48
7.47
7.43
7.41
7.40
7.39
7.38
7.10
3.43
3.22
3.20
3.19
3.17
2.85
2.74
2.73
2.71
2.70
2.51
1.00
1.03
2.02
5.03
0.99
1.00
1.01
3.05
1.04
13.0
11.0
9.0
7.5
6.0
4.5
3.0
1.5
0.0
Chemical shift (ppm)

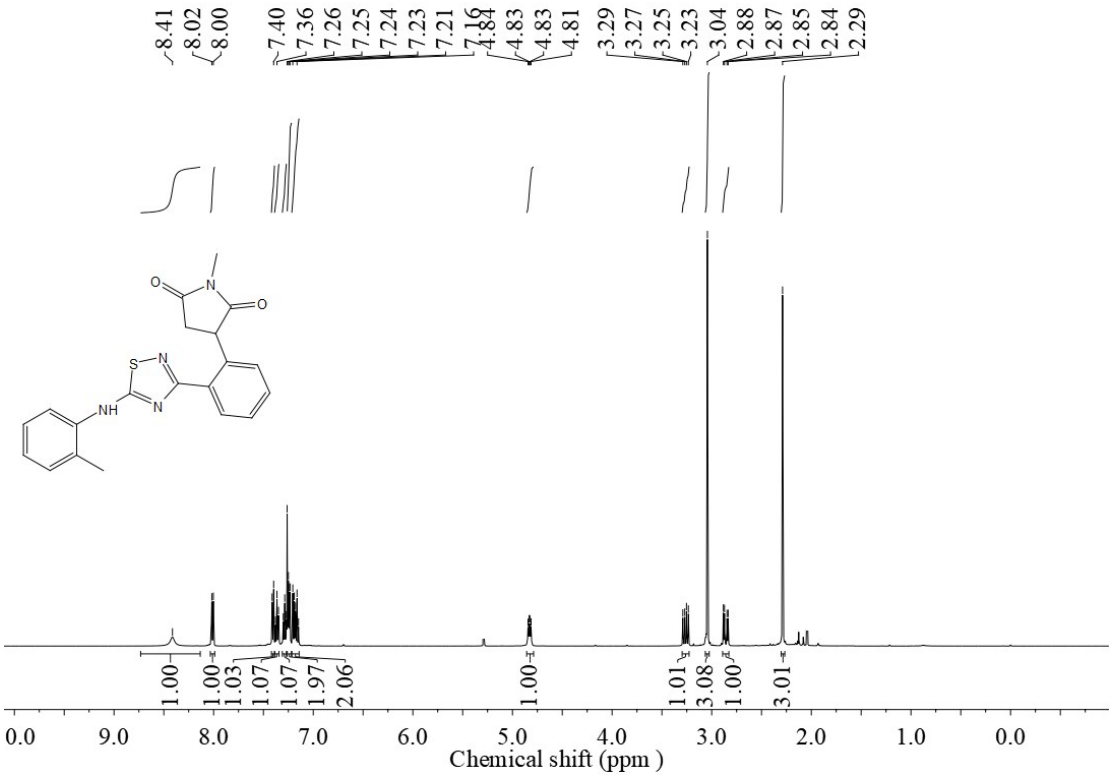

178.92
178.72
176.77
169.36
140.19
137.15
132.85
131.41
130.54
129.86
128.16
123.52
118.25
45.32
40.50
40.33
40.16
39.99
39.83
39.66
39.49
38.26
25.18
200
180
160
140
120
100
80
60
40
20
0
Chemical shift (ppm)

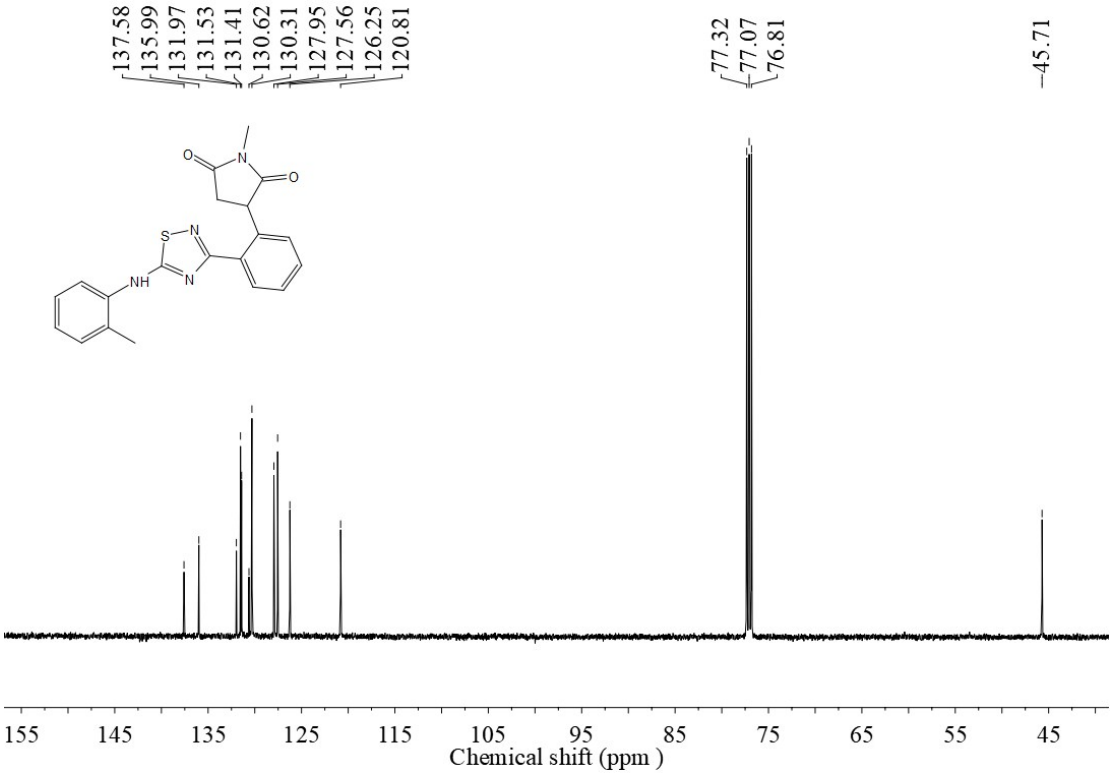
6b:


8.03
8.02
7.39
7.37
7.36
7.33
7.31
7.30
7.29
7.28
7.27
7.26
7.19
7.18
7.14
7.12
7.10
7.09
4.92
4.91
4.90
4.89
3.66
3.65
3.63
3.62
3.60
3.30
3.28
3.26
3.25
2.86
2.85
2.83
2.82
1.25
1.24
1.22
0.00
0.98
1.01
1.04
3.07
1.00
2.95
1.03
2.08
1.01
0.99
3.08
Chemical shift (ppm)

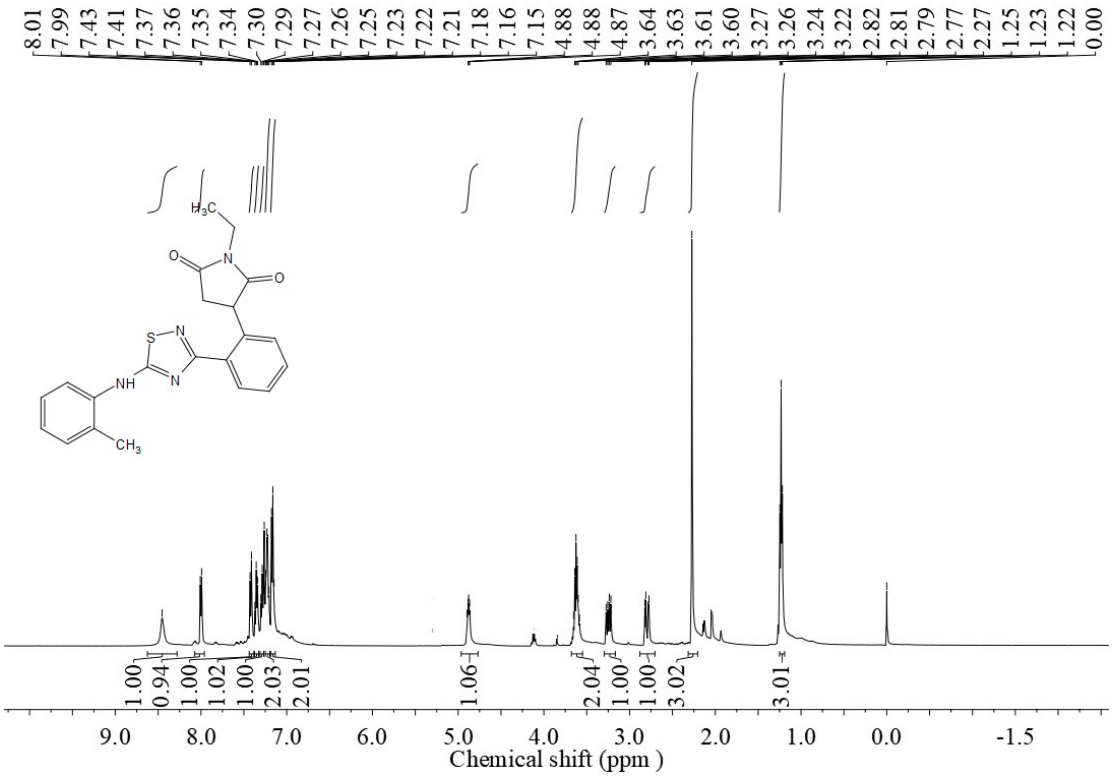

180.21
178.64
176.83
168.82
139.04
136.28
132.22
131.55
130.41
129.75
129.69
127.98
124.31
118.51
77.32
77.07
76.81
45.35
38.39
34.02
13.15
Chemical shift (ppm)

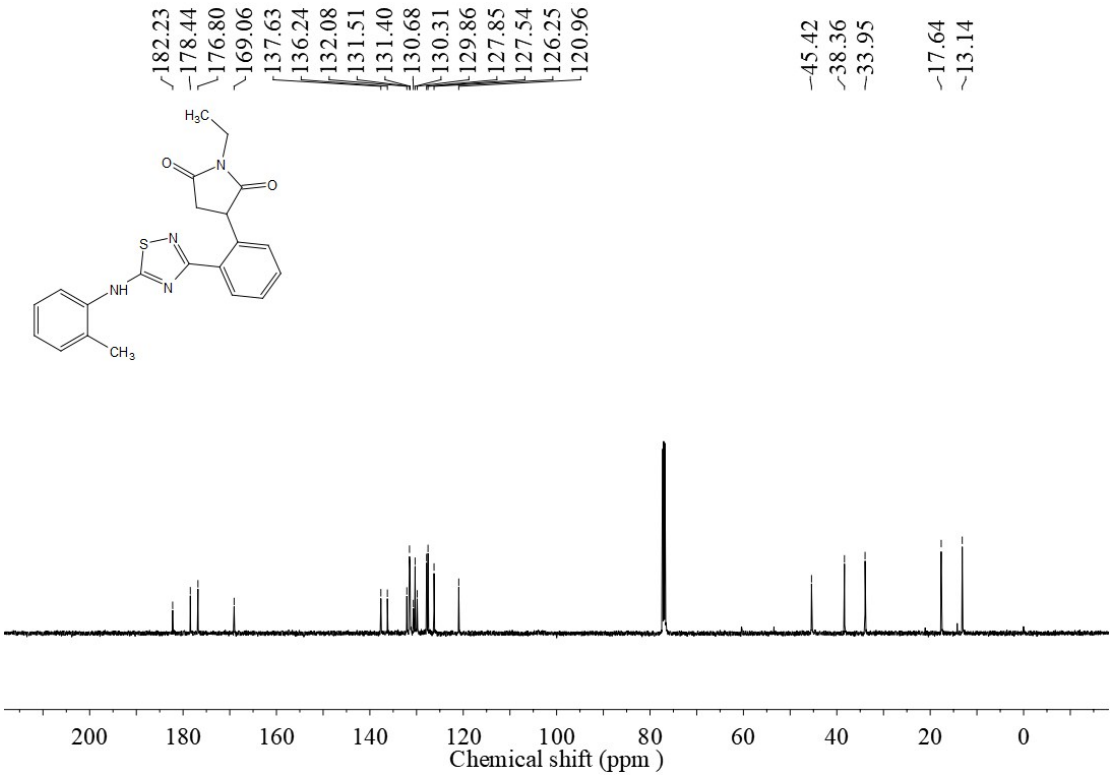
6c:


8.41
8.02
8.00
7.40
7.36
7.26
7.25
7.24
7.23
7.21
7.16
4.84
4.83
4.83
4.81
3.29
3.27
3.25
3.23
3.04
2.88
2.87
2.85
2.84
2.29
1.00
1.00
1.03
1.07
1.07
1.97
2.06
1.00
1.01
3.08
1.00
3.01
0.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
Chemical shift (ppm)

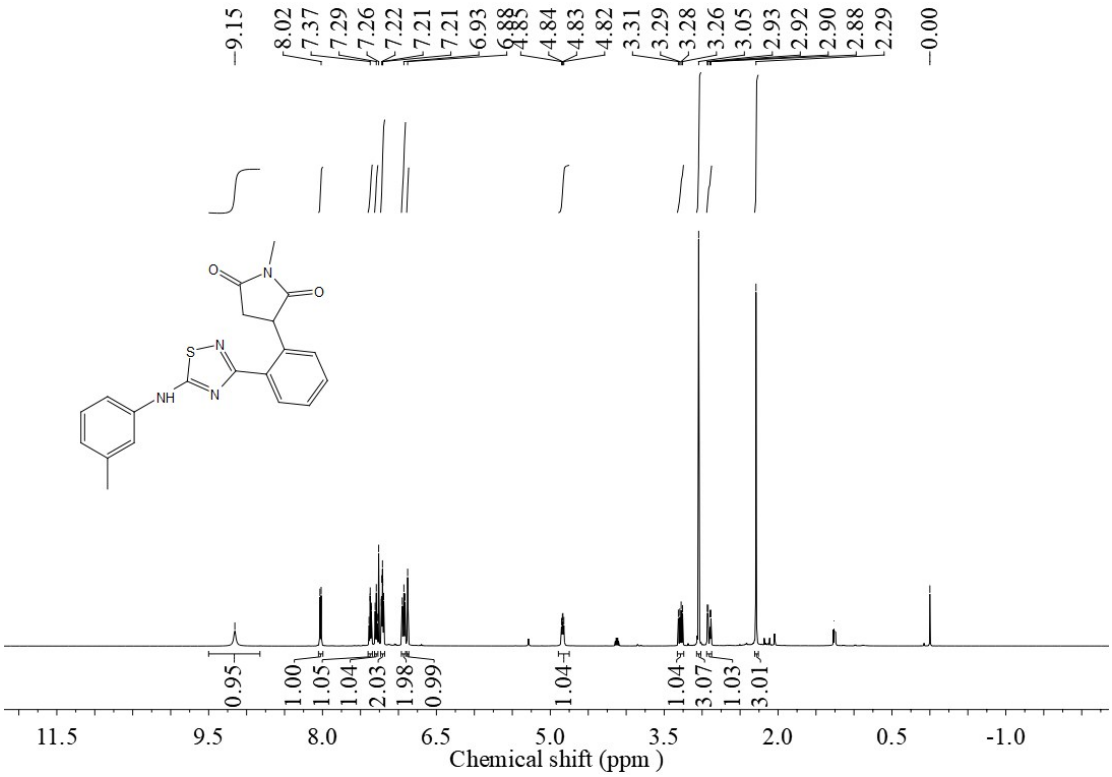

137.58
135.99
131.97
131.53
131.41
130.62
130.31
127.95
127.56
126.25
120.81
77.32
77.07
76.81
45.71
155
145
135
125
115
105
95
85
75
65
55
45
Chemical shift (ppm)

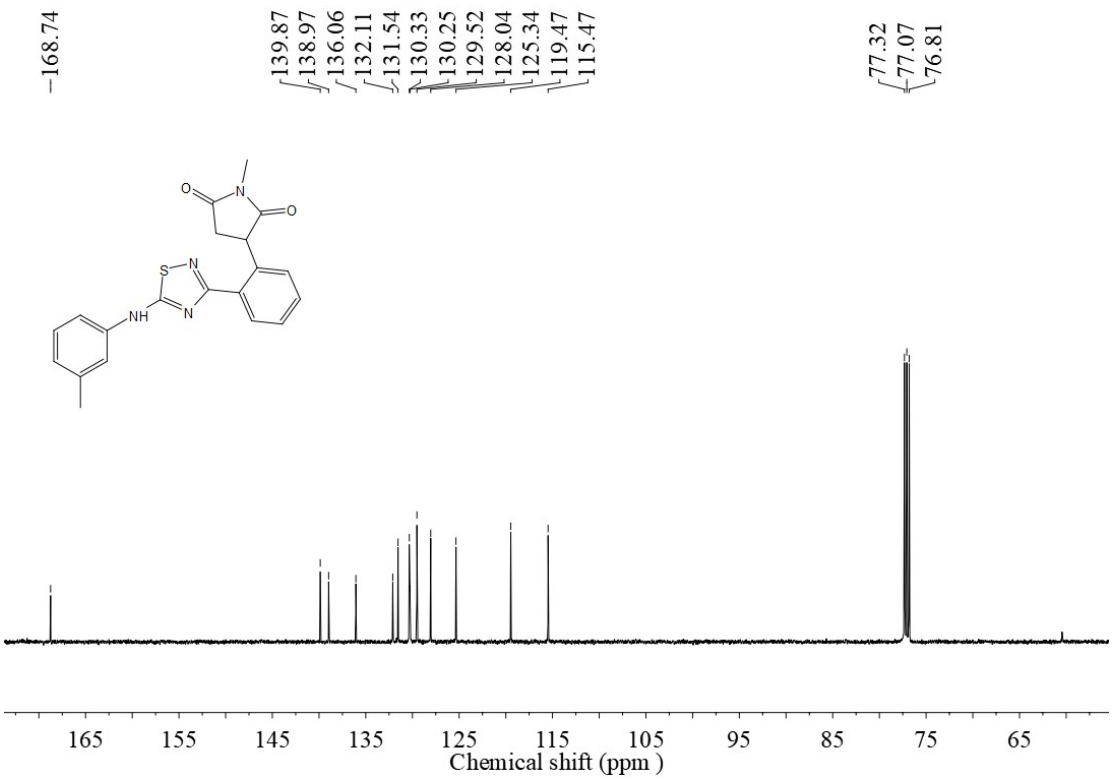
6d:


8.01
7.99
7.43
7.41
7.37
7.36
7.35
7.34
7.30
7.29
7.27
7.26
7.25
7.23
7.22
7.21
7.18
7.16
7.15
4.88
4.87
3.64
3.63
3.61
3.60
3.27
3.26
3.24
3.22
2.82
2.81
2.79
2.77
2.27
1.25
1.23
1.22
0.00
1.00
0.94
1.00
1.02
1.00
2.03
2.01
1.06
2.04
1.00
1.00
3.02
3.01
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.5
Chemical shift (ppm)

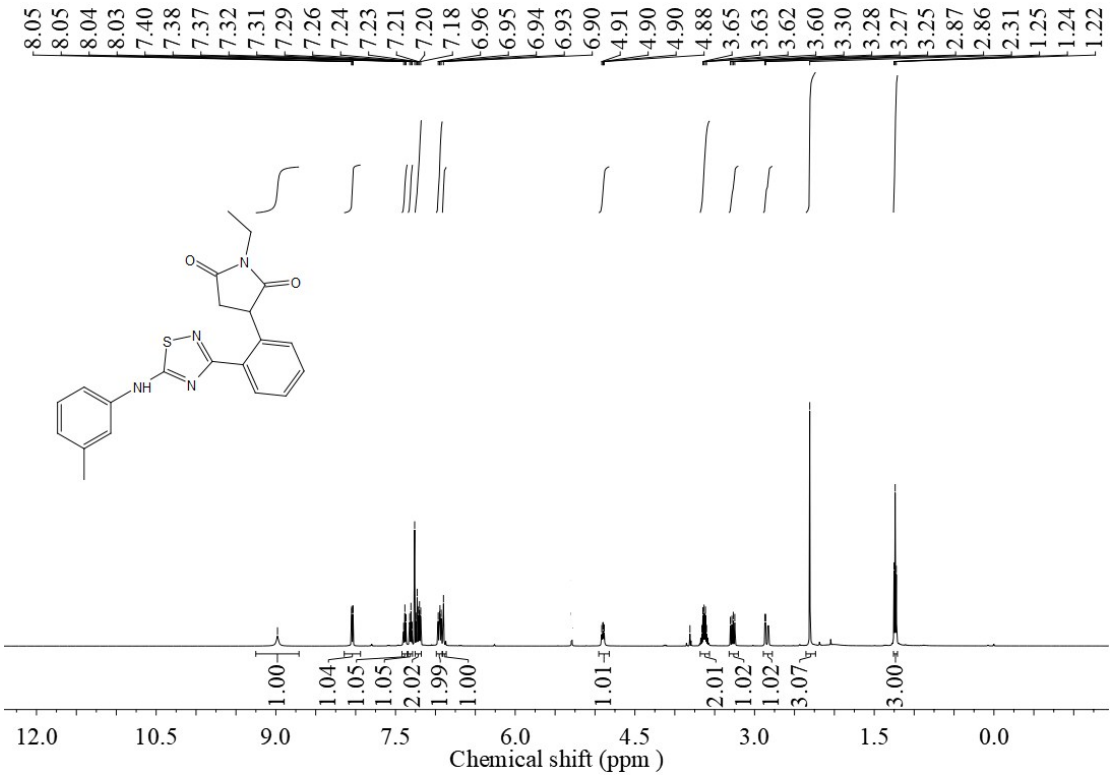

182.23
178.44
176.80
169.06
137.63
136.24
132.08
131.51
131.40
130.68
130.31
129.86
127.85
127.54
126.25
120.96
45.42
38.36
33.95
17.64
13.14
200
180
160
140
120
100
80
60
40
20
0
Chemical shift (ppm)

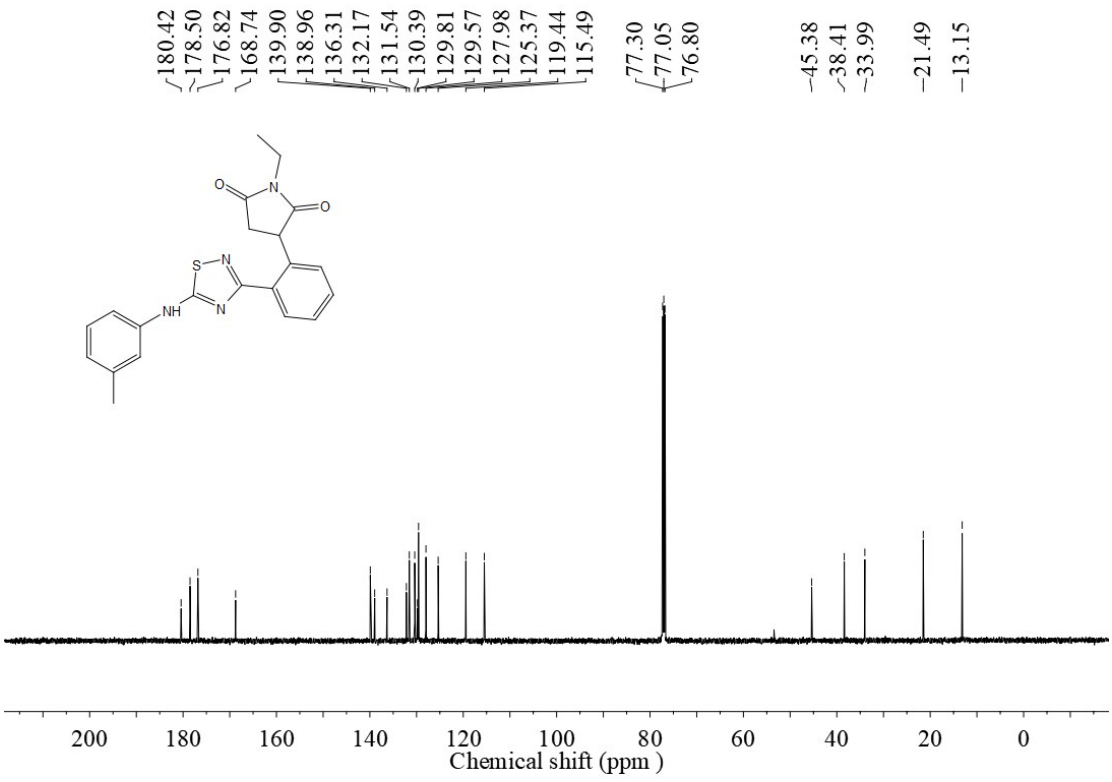
6e:


9.15
8.02
7.37
7.29
7.26
7.22
7.21
7.21
6.93
6.88
6.85
4.84
4.83
4.82
3.31
3.29
3.28
3.26
3.05
2.93
2.92
2.90
2.88
2.29
0.00
0.95
1.00
1.05
1.04
2.03
1.98
0.99
1.04
1.04
3.07
1.03
3.01
11.5
9.5
8.0
6.5
5.0
3.5
2.0
0.5
-1.0
Chemical shift (ppm)

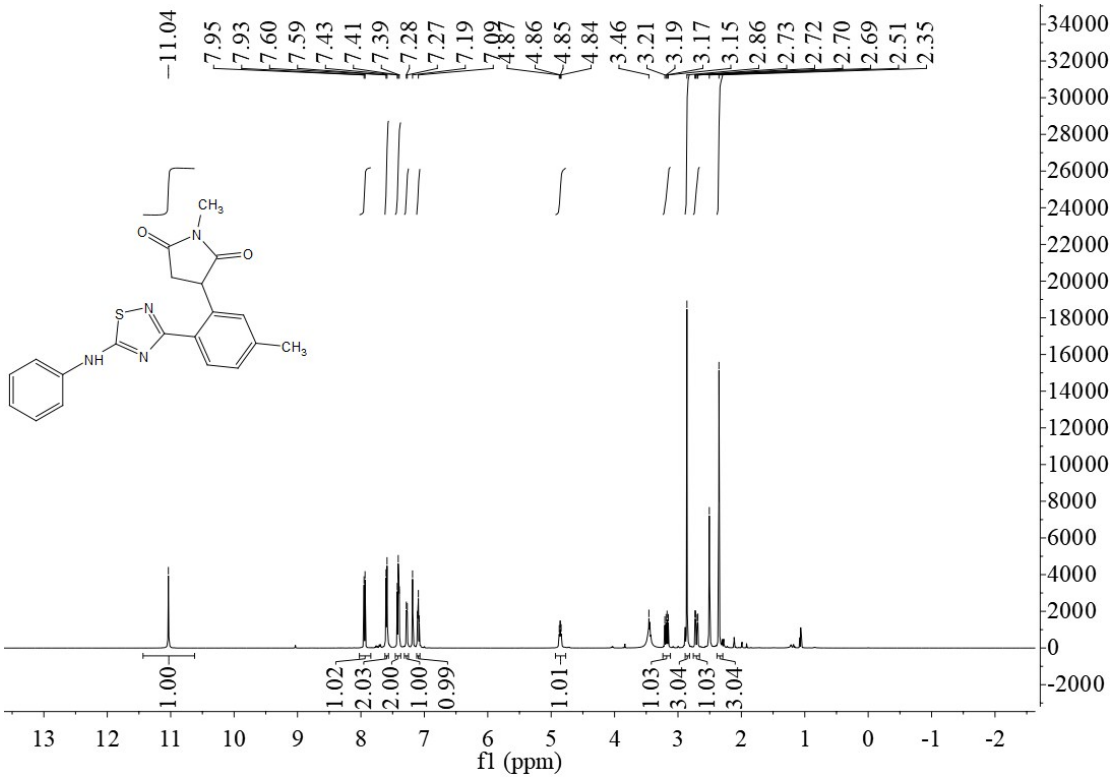

168.74
139.87
138.97
136.06
132.11
131.54
130.33
130.25
129.52
128.04
125.34
119.47
115.47
77.32
77.07
76.81
165
155
145
135
125
115
105
95
85
75
65
Chemical shift (ppm)

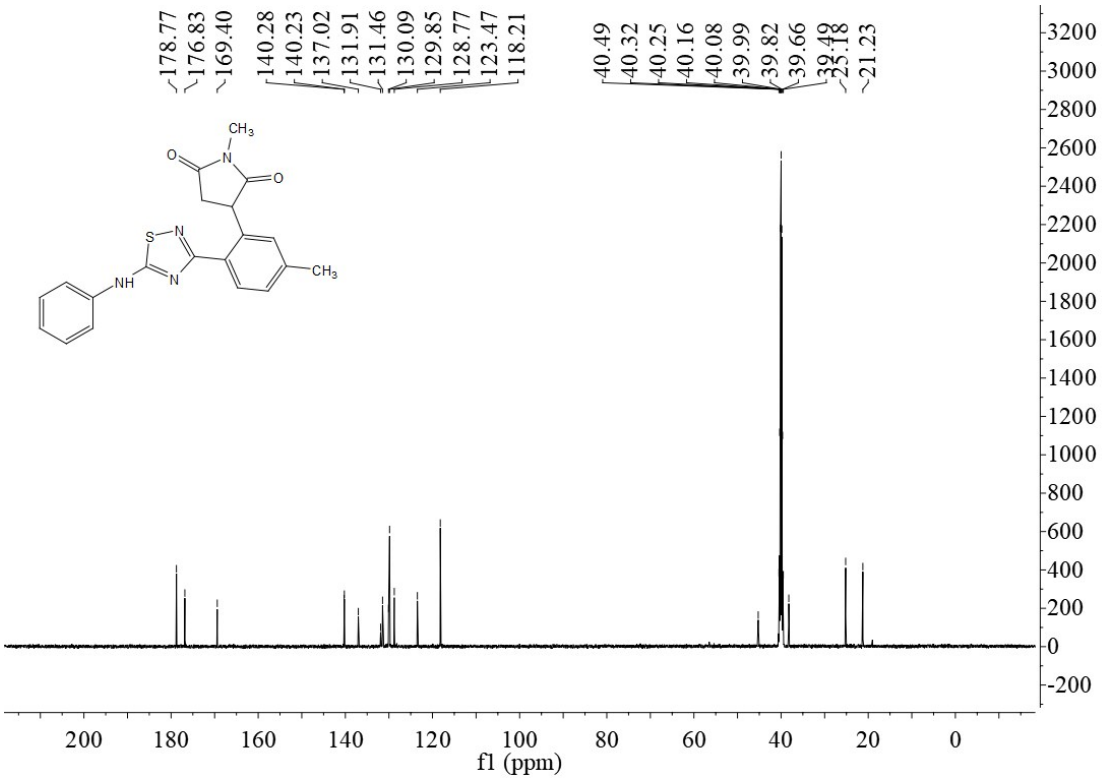
6f:


8.05
8.05
8.04
8.03
7.40
7.38
7.37
7.32
7.31
7.29
7.26
7.24
7.23
7.21
7.20
7.18
6.96
6.95
6.94
6.93
6.90
4.91
4.90
4.90
4.88
3.65
3.63
3.62
3.60
3.30
3.28
3.27
3.25
2.87
2.86
2.31
1.25
1.24
1.22
1.00
1.04
1.05
1.05
2.02
1.99
1.00
1.01
2.01
1.02
1.02
3.07
3.00
12.0
10.5
9.0
7.5
6.0
4.5
3.0
1.5
0.0
Chemical shift (ppm)

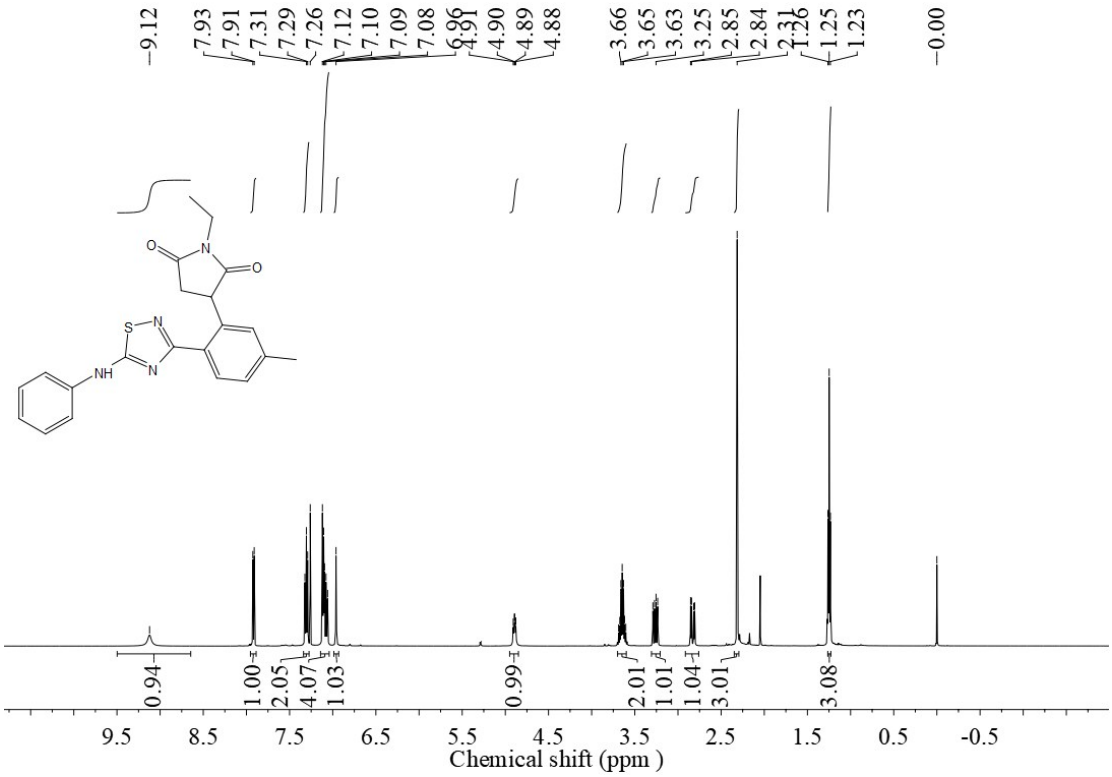

180.42
178.50
176.82
168.74
139.90
138.96
136.31
132.17
131.54
130.39
129.81
129.57
127.98
125.37
119.44
115.49
77.30
77.05
76.80
45.38
38.41
33.99
21.49
13.15
200
180
160
140
120
100
80
60
40
20
0
Chemical shift (ppm)

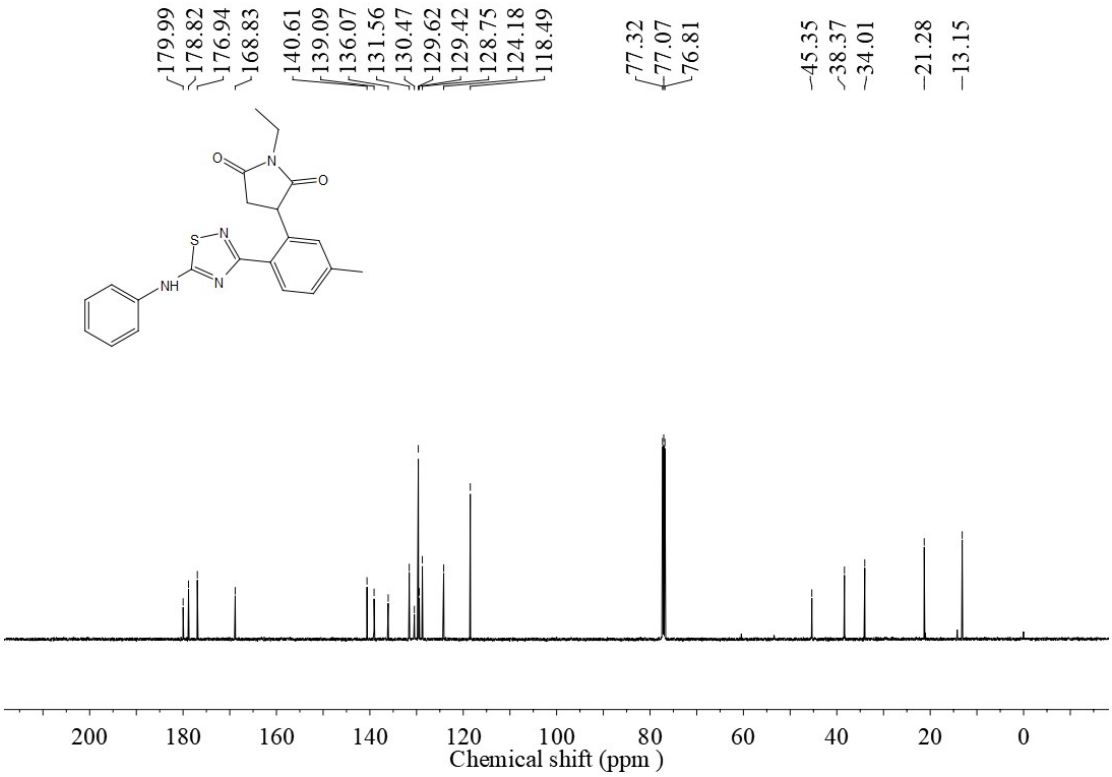
6g:


11.04
7.95
7.93
7.60
7.59
7.43
7.41
7.39
7.28
7.27
7.19
7.09
4.87
4.86
4.85
4.84
3.46
3.21
3.19
3.17
3.15
2.86
2.73
2.72
2.70
2.69
2.51
2.35
1.00
1.02
2.03
2.00
1.00
0.99
1.01
1.03
3.04
1.03
3.04
f1 (ppm)

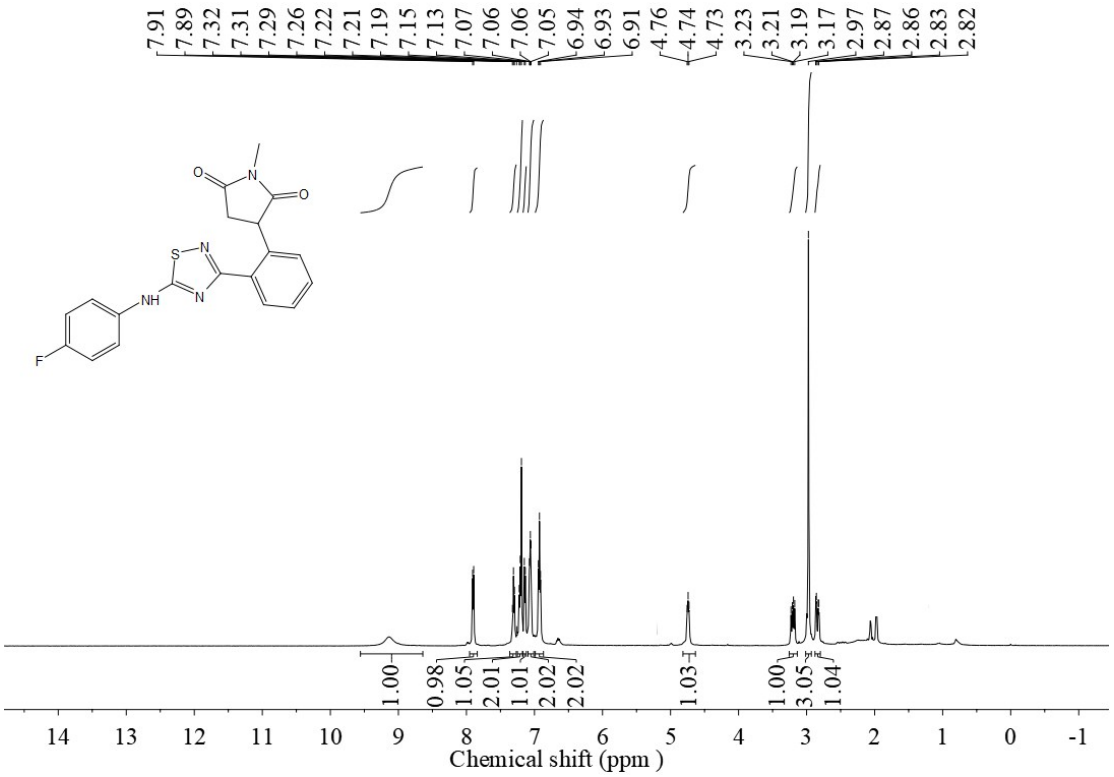

178.77
176.83
169.40
140.28
140.23
137.02
131.91
131.46
130.09
129.85
128.77
123.47
118.21
40.49
40.32
40.25
40.16
40.08
39.99
39.82
39.66
39.49
25.18
21.23
f1 (ppm)

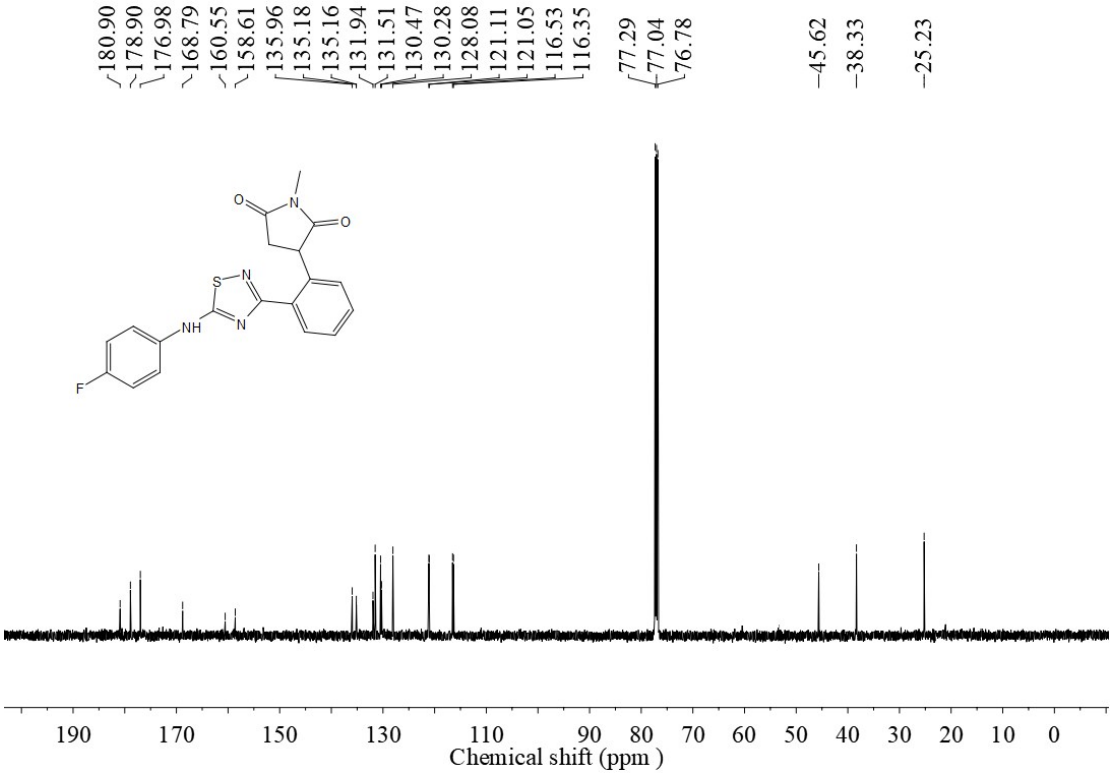
6h:


9.12
7.93
7.91
7.31
7.29
7.26
7.12
7.10
7.09
7.08
6.96
4.91
4.90
4.89
4.88
3.66
3.65
3.63
3.25
2.85
2.84
2.31
2.26
1.25
1.23
0.00
0.94
1.00
2.05
4.07
1.03
0.99
2.01
1.01
1.04
3.01
3.08
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
Chemical shift (ppm)

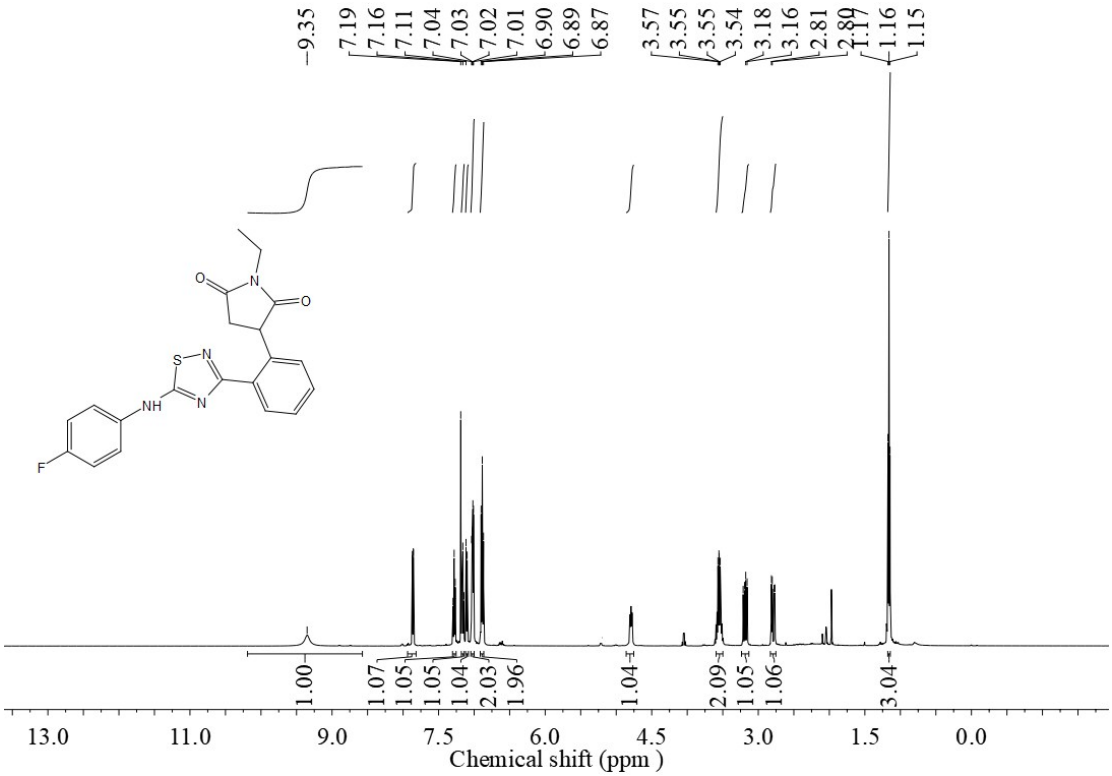

179.99
178.82
176.94
168.83
140.61
139.09
136.07
131.56
130.47
129.62
129.42
128.75
124.18
118.49
77.32
77.07
76.81
45.35
38.37
34.01
21.28
13.15
200
180
160
140
120
100
80
60
40
20
0
Chemical shift (ppm)

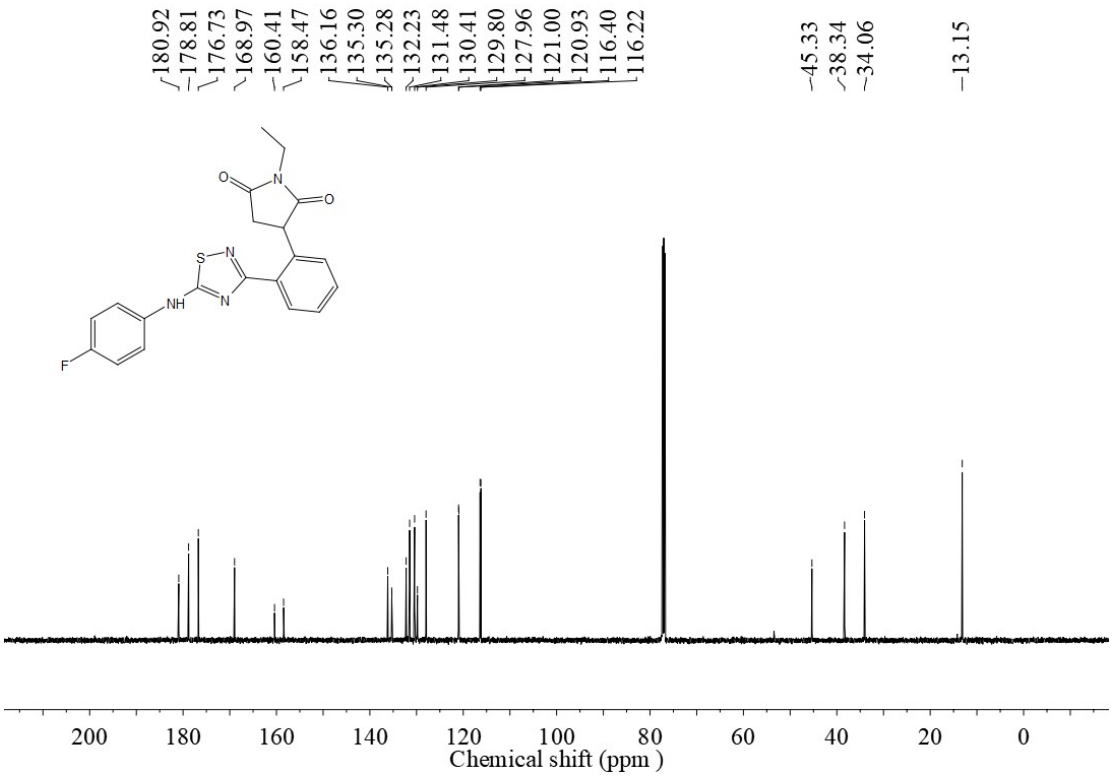
6i:


7.91
7.89
7.32
7.31
7.29
7.26
7.22
7.21
7.19
7.15
7.13
7.07
7.06
7.06
7.05
6.94
6.93
6.91
4.76
4.74
4.73
3.23
3.21
3.19
3.17
2.97
2.87
2.86
2.83
2.82
1.00
0.98
1.05
2.01
1.01
2.02
2.02
1.03
1.00
3.05
1.04
Chemical shift (ppm)

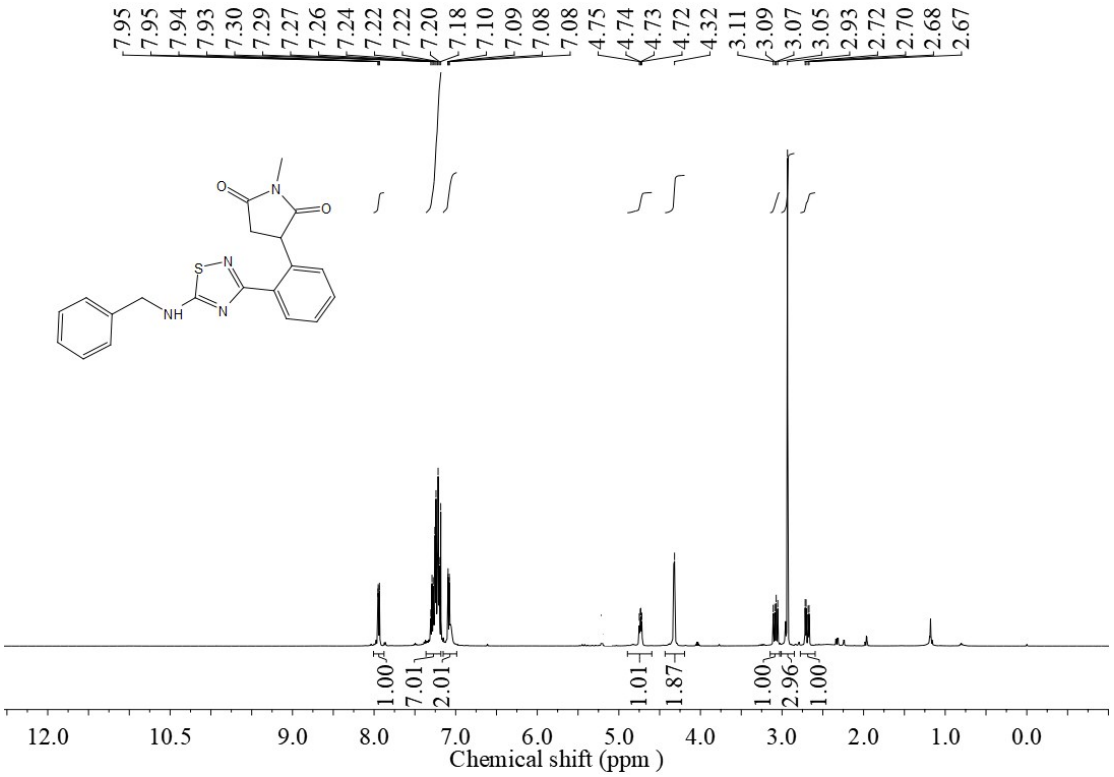

180.90
178.90
176.98
168.79
160.55
158.61
135.96
135.18
135.16
131.94
131.51
130.47
130.28
128.08
121.11
121.05
116.53
116.35
77.29
77.04
76.78
45.62
38.33
25.23
Chemical shift (ppm)

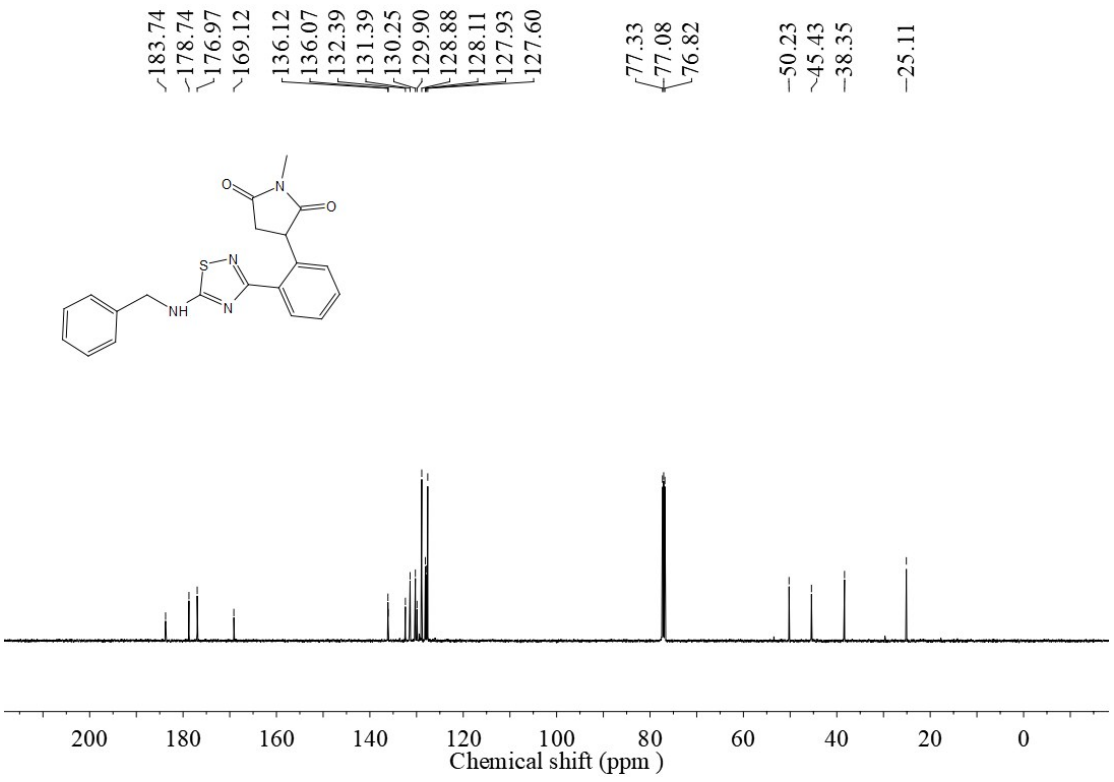
6j:


9.35
7.19
7.16
7.11
7.04
7.03
7.02
7.01
6.90
6.89
6.87
3.57
3.55
3.55
3.54
3.18
3.16
2.81
2.80
1.17
1.16
1.15
1.00
1.07
1.05
1.05
1.04
2.03
1.96
1.04
2.09
1.05
1.06
3.04
13.0
11.0
9.0
7.5
6.0
4.5
3.0
1.5
0.0
Chemical shift (ppm)

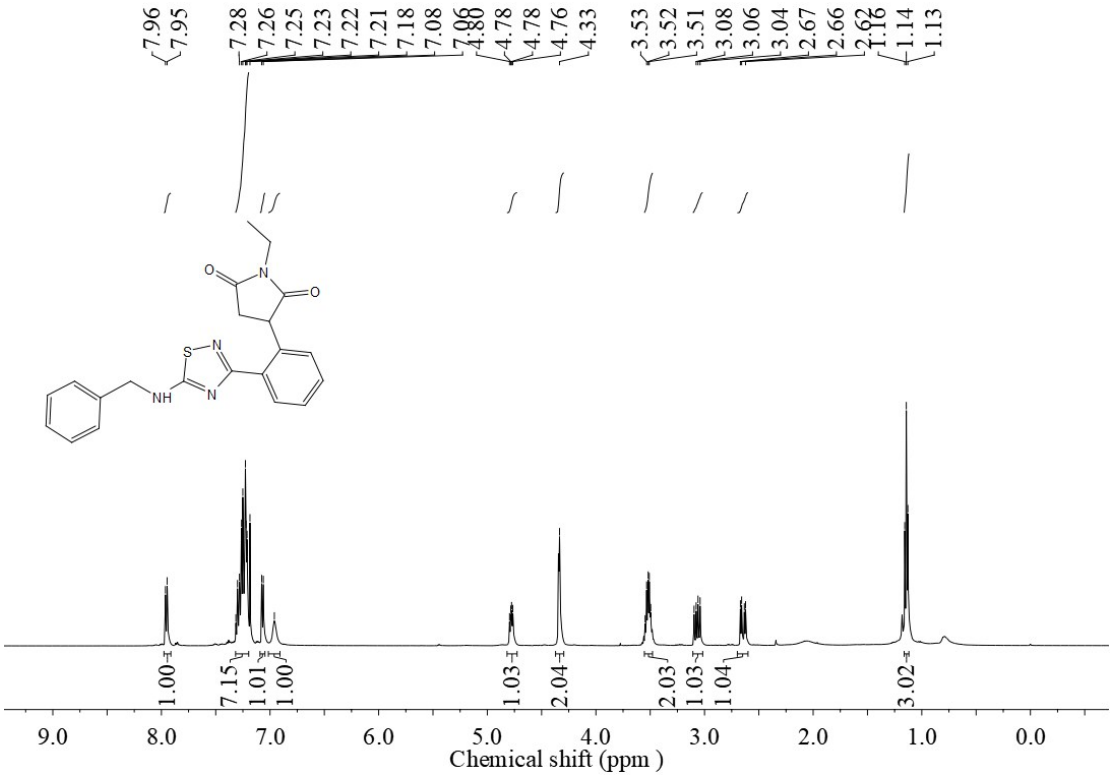

180.92
178.81
176.73
168.97
160.41
158.47
136.16
135.30
135.28
132.23
131.48
130.41
129.80
127.96
121.00
120.93
116.40
116.22
45.33
38.34
34.06
13.15
200
180
160
140
120
100
80
60
40
20
0
Chemical shift (ppm)

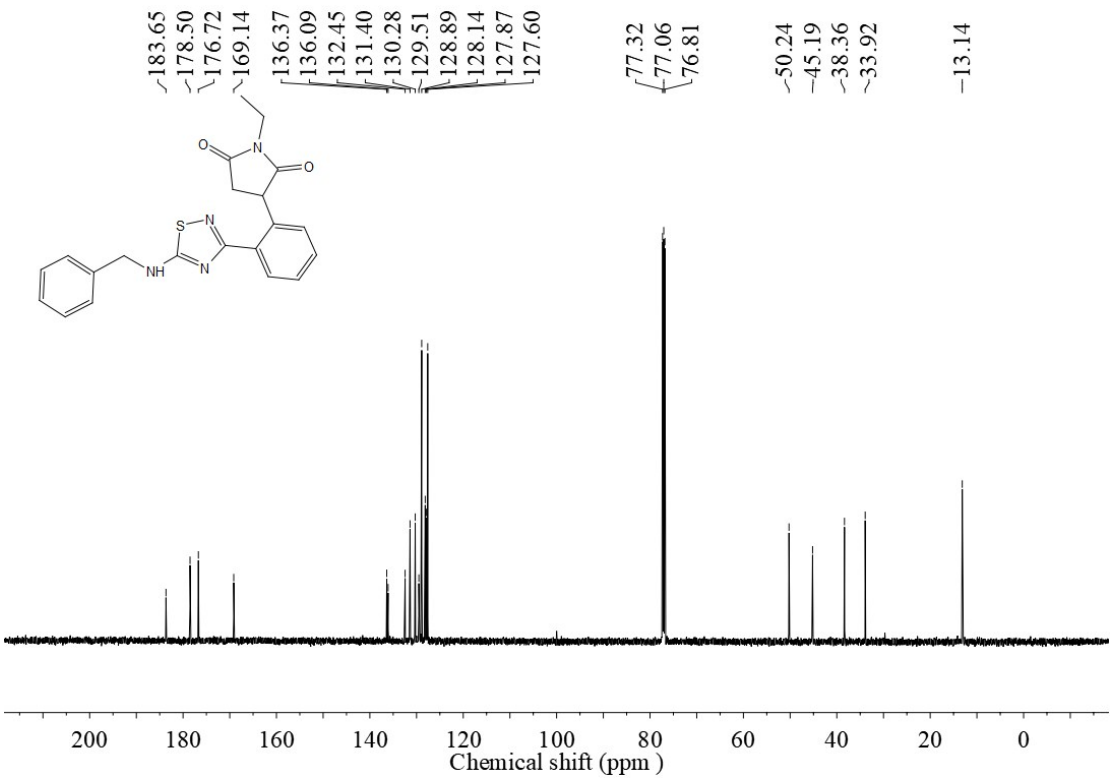
6k:


7.95
7.95
7.94
7.93
7.30
7.29
7.27
7.26
7.24
7.22
7.22
7.20
7.18
7.10
7.09
7.08
7.08
4.75
4.74
4.73
4.72
4.32
3.11
3.09
3.07
3.05
2.93
2.72
2.70
2.68
2.67
1.00
7.01
2.01
1.01
1.87
1.00
2.96
1.00
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
Chemical shift (ppm)


183.74
178.74
176.97
169.12
136.12
136.07
132.39
131.39
130.25
129.90
128.88
128.11
127.93
127.60
77.33
77.08
76.82
50.23
45.43
38.35
25.11
200
180
160
140
120
100
80
60
40
20
0
Chemical shift (ppm)

6l:


7.96
7.95
7.28
7.26
7.25
7.23
7.22
7.21
7.18
7.08
4.80
4.78
4.78
4.76
4.33
3.53
3.52
3.51
3.08
3.06
3.04
2.67
2.66
2.62
1.16
1.14
1.13
1.00
7.15
1.01
1.00
1.03
2.04
2.03
1.03
1.04
3.02
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
Chemical shift (ppm)


183.65
178.50
176.72
169.14
136.37
136.09
132.45
131.40
130.28
129.51
128.89
128.14
127.87
127.60
77.32
77.06
76.81
50.24
45.19
38.36
33.92
13.14
200
180
160
140
120
100
80
60
40
20
0
Chemical shift (ppm)