Spirocyclization and Michael addition of 3-benzylidene succinimides: Route to spirocyclopentapyrrolidine-tetraones and benzylidene *N*-arylpyrrolidine-diones

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SUPPORTING INFORMATION

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General information:

Unless otherwise noted, chemicals were purchased from commercial suppliers at the highest purity grade available and were used without further purification. The 2-hydroxy-2-(2-oxo-2-phenylethyl)-1*H*-indene-1,3(2*H*)-diones **1a**−**1d** and 3-benzylidene succinimides **2a**–**2f** and (*E*)-4-benzylidene-5-methyl-2-phenyl-2,4-dihydro-3*H*-pyrazol-3-ones **4a-4d** were synthesized by literature methods. Thin layer chromatography was performed on pre-coated 0.25 mm silica gel plates ($60F_{254}$) using UV light as visualizing agent. Silica gel (100–200 mesh) was used for column chromatography. NMR spectra were recorded in $CDCl_3$ and using TMS as an internal standard on 500 MHz instrument. Chemical shifts (δ) were reported as parts per million (ppm) in δ scale downfield from TMS. ^{1}H NMR spectra were referenced to $CDCl_3$ (7.26 ppm) and ^{13}C NMR spectra were referenced to $CDCl_3$ (77.0 ppm, the middle peak). Coupling constants were expressed in Hz. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, dt = doublet of triplets, m = multiplet. High-resolution mass spectra (HRMS) were obtained on a Xevo XS QTOF mass spectrometer (ESI-MS).

NMR studies of compounds 3c and 5o:

The structures of spiro compounds **3a-3p** were established by NMR and HRMS spectral analysis. Further to gain a deeper understanding, the structure of the product **3c** was corroborated by 2D NMR such as COSY, NOESY, HMBC, HSQC. From 2D experiments, the stereochemical correlation between H_a, H_b, H_c and H_d was established. In **3c**, H_a and H_c protons appear as doublets at 4.77 and 4.58 ppm while H_b and H_d appear as doublet of doublet at 3.96 and 4.56 ppm, respectively. We performed the 2D NMR experiments to know the spatial correlation between protons H_a, H_b, H_c, H_d from which we found that H_a and H_b are in same plane and H_c and H_d is in opposite plane w.r.t. H_a, H_b protons.

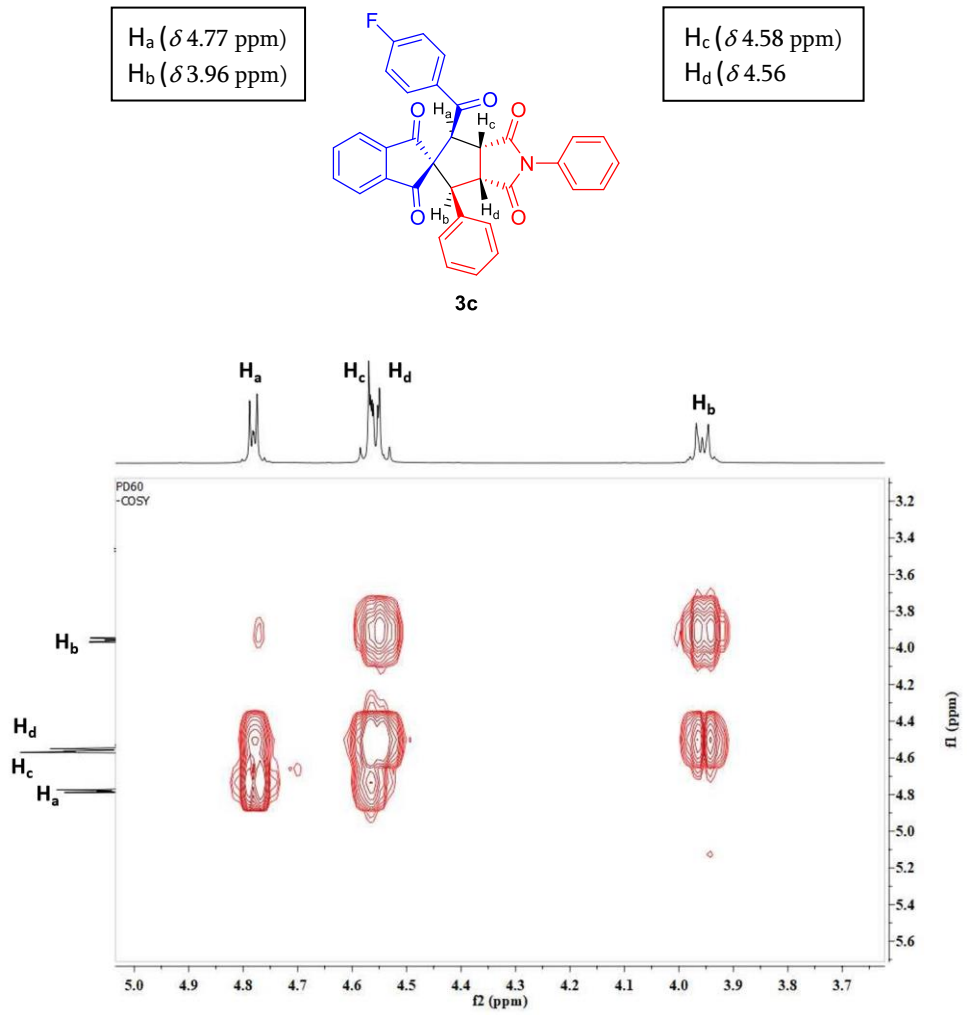


Figure S1: ^{1}H–^{1}H COSY spectrum of **3c**

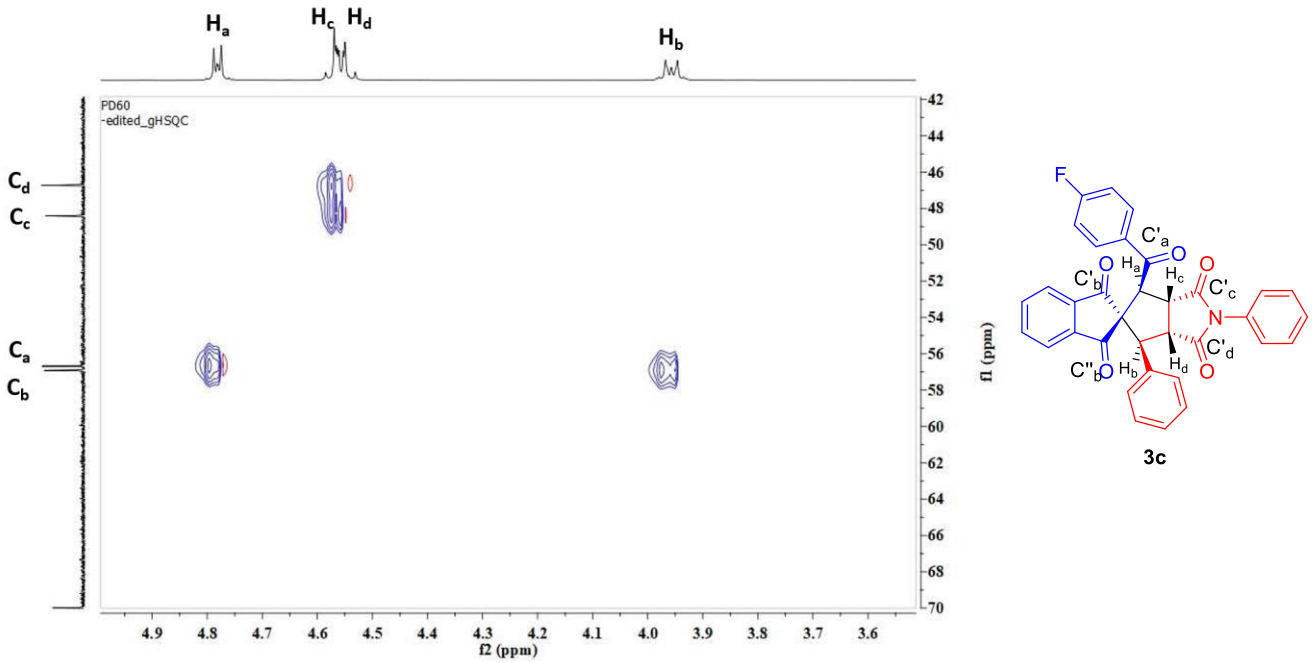


Figure S2: $^{1}H–^{13}C$ HSQC spectrum of **3c**

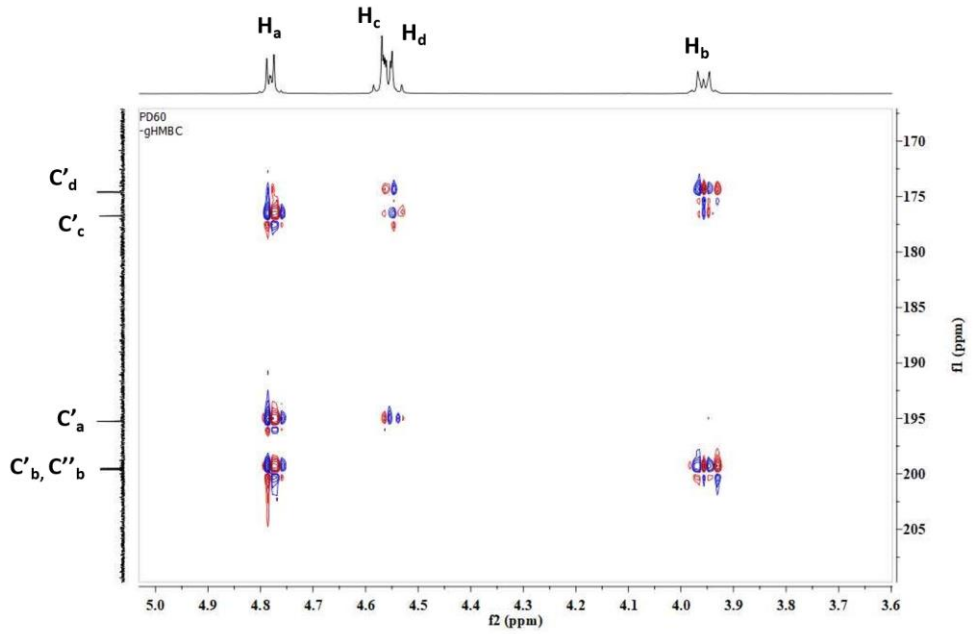
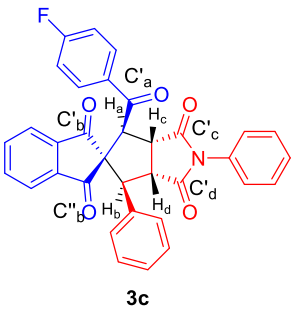


Figure S3: $^{1}H–^{13}C$ HMBC spectrum of **3c**



3c

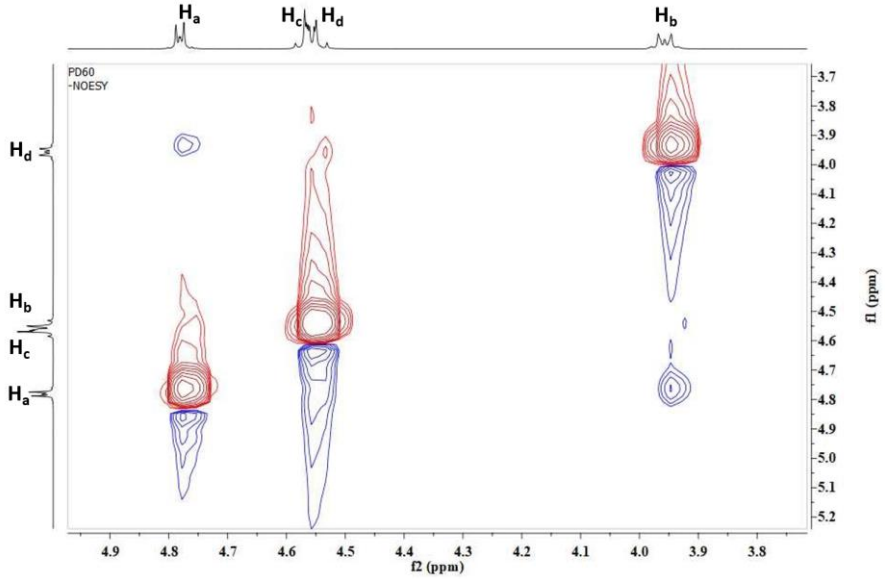


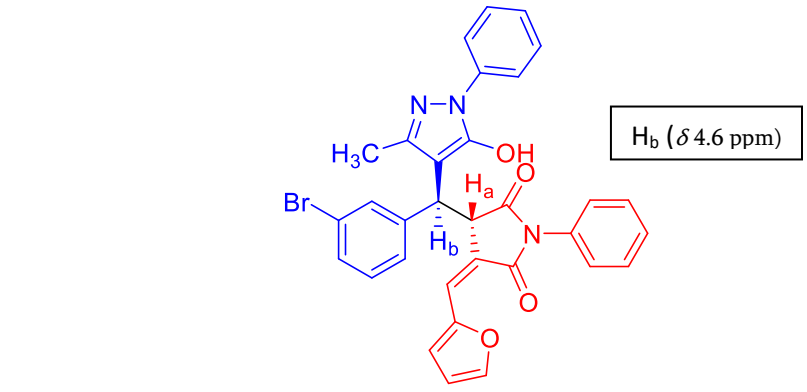
Figure S4: $^{1}H–^{1}H$ NOESY spectrum of **3c**

The COSY experiment of **3c** revealed that proton H_b at 3.96 ppm is correlated with protons H_d, H_a at 4.56 and 4.77, respectively, while the proton H_d at 4.54 ppm is showing correlation with protons H_b, H_c, H_a at 3.96, 4.58 and 4.77 ppm, respectively.

The HSQC experiment of **3c** revealed connectivity between proton H_a at 4.77 ppm and carbon C_a having chemical shift at 56.6 ppm. Similarly, it disclosed that the proton H_b at 3.96 ppm is directly bonded to carbon C_b at 56.9 ppm and the proton H_c at 4.58 ppm is connected directly to carbon C_c having chemical shift at 46.8 ppm while the proton H_d at 4.56 ppm is directly bonded to carbon C_d of chemical shift 48.4 ppm.

NOESY experiment of **3c** revealed that H_a at 4.77 ppm is connected weakly with H_b at 3.96 ppm while the H_c at 4.58 ppm is connected very weakly with H_d at 4.56 ppm. The HMBC experiment revealed the correlation between H_a at 4.77 ppm with four carbonyl groups at 176.7, 174.6 and 195.2, 199.6 ppm and numerous carbon centres that exist nearby. Thus, the H_b at 3.96 ppm shows correlation with four carbonyl groups at 176.7, 174.6 and 195.2, 199.6 ppm, the H_c at 4.58 ppm shows correlation with three carbonyl groups at 174.6, 176.7, 195.2 ppm while the H_d at 4.56 ppm shows correlation with three carbonyl groups at 174.6, 176.7 and 195.2 ppm.

We also performed two-dimensional experiments for **5o**. HSQC spectrum of **5o** showed connectivity between the proton H_a at 4.73 ppm to the carbon C_a bound directly to it at 49.3 ppm and correlation between H_b at 4.64 ppm and C_b at 43.4 ppm. The HMBC spectral studies of **5o** showed the correlation of H_a having resonance at 4.73 ppm with two carbonyls C_a' and C_b' resonating at 179.9 and 168.4 ppm. The NOESY spectrum of **5o** indicated that H_a and H_b are on opposite side *i.e.*, trans as H_a proton showing its correlation with OH proton and H_b proton is showing its correlation with H_c proton. This confirmed that both H_a and H_b protons are in opposite direction.



5o

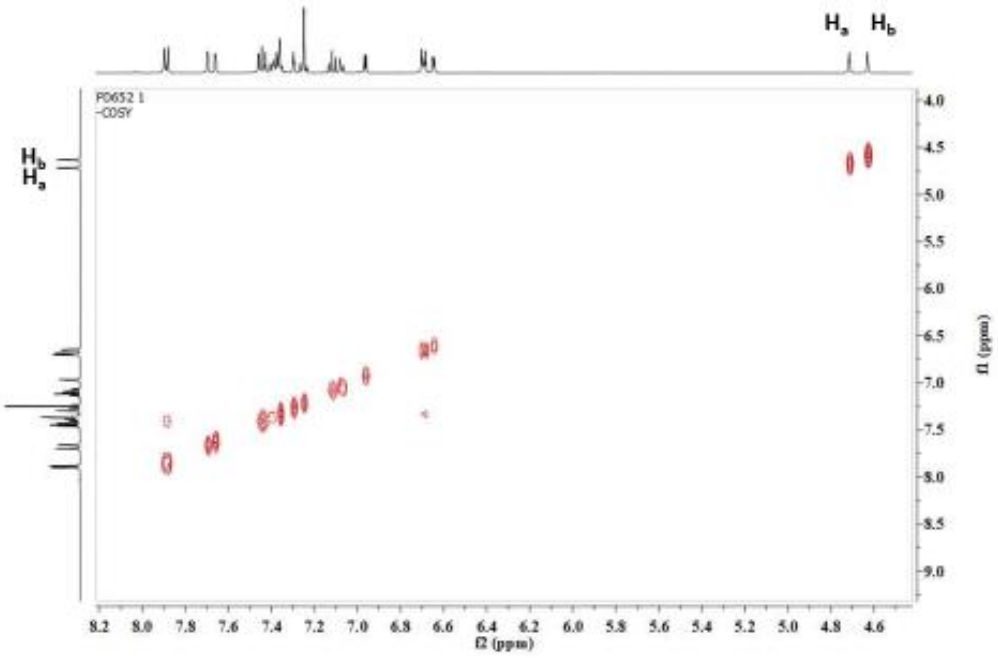


Figure S5: $^{1}H–^{1}H$ COSY spectrum of **5o**

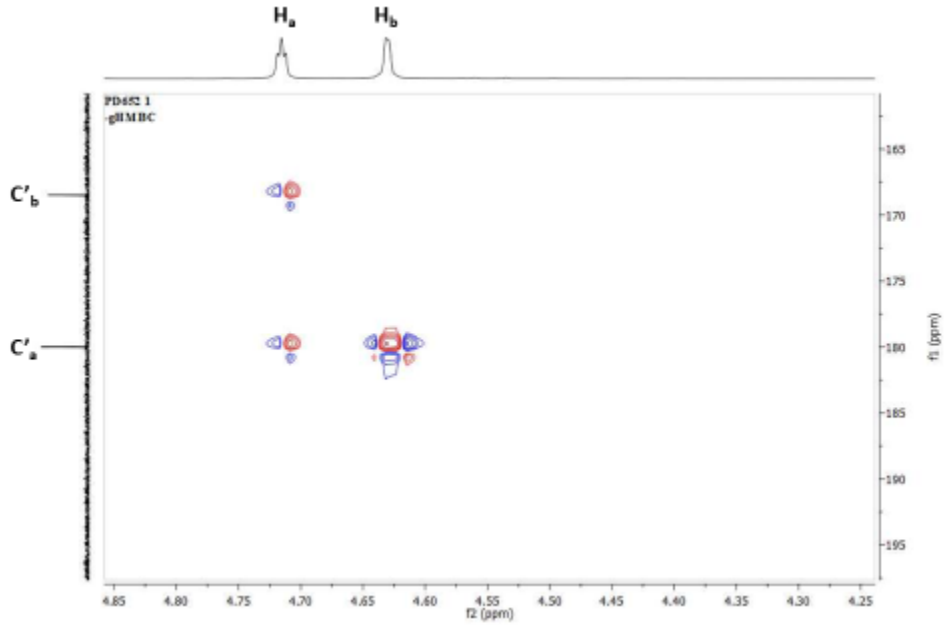
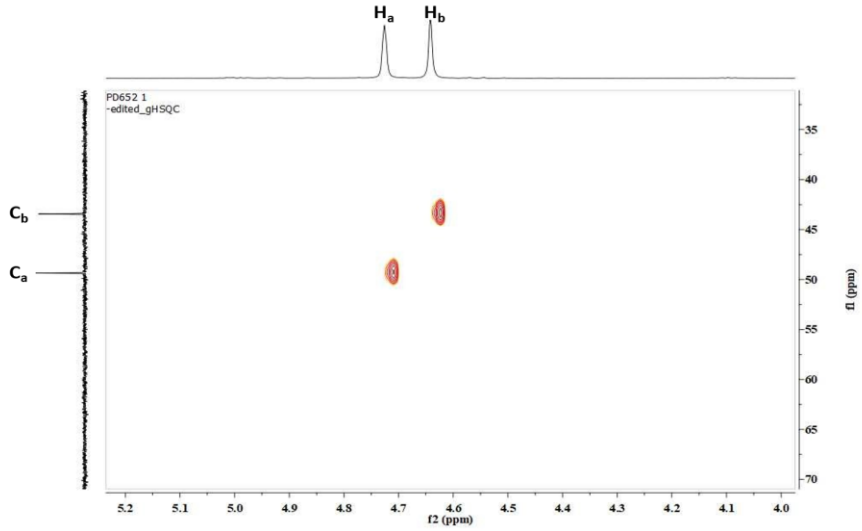
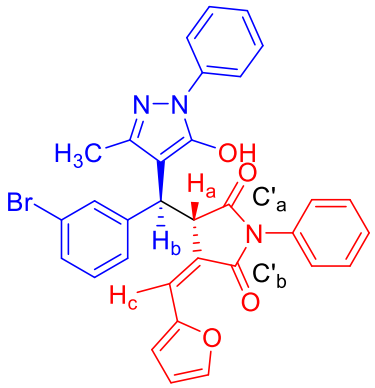


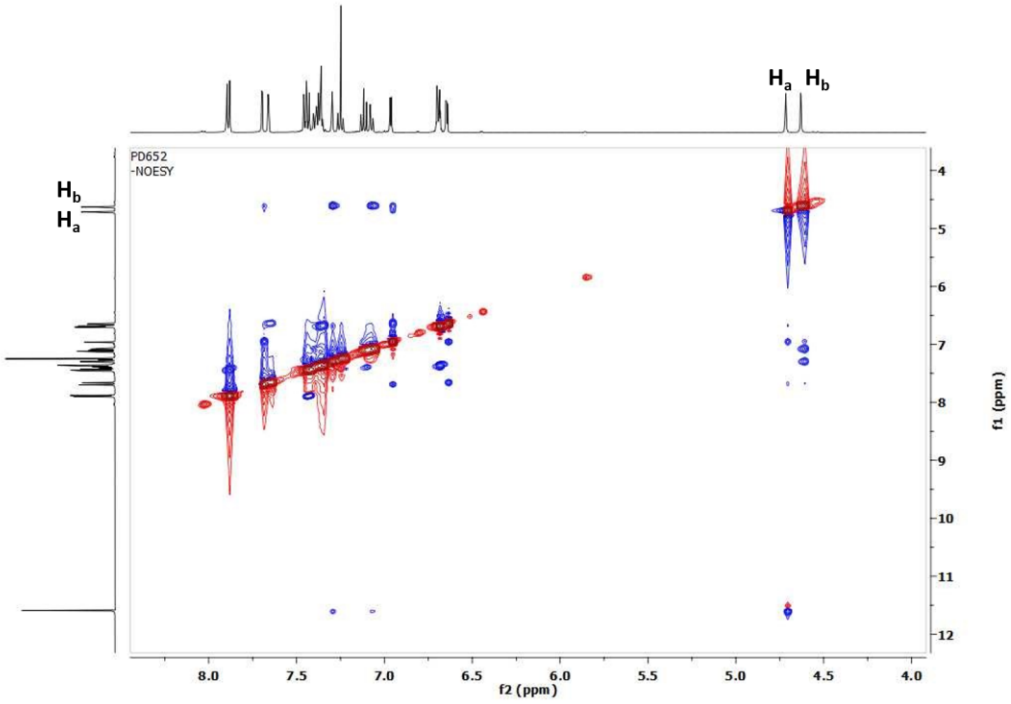
Figure S6: $^{1}H–^{13}C$ HMBC spectrum of **5o**

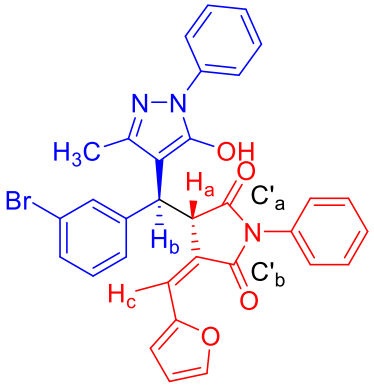




5o

Figure S7: $^{1}H–^{13}C$ HSQC spectrum of **5o**





5o

Figure S8: ^{1}H–^{1}H NOESY spectrum of **5o**

General procedures:

General procedure for the synthesis of indanediones 1a-1d:

Ninhydrin (10 mmol), acetophenone (10 mmol) were dissolved in 20 mL glacial acetic acid in a 100 mL RB flask, and the reaction mixture was refluxed for 1 hour. After completion of the reaction, as checked by

TLC, the contents were diluted with EtOAc and washed with brine solution. The organic layer was collected, dried over anhydrous Na_2SO_4, and concentrated by evaporation. The crude material was purified by column chromatography on silica gel (25% EtOAc/hexanes) to obtain pure indanedione **1**.

Synthesis of benzylidene succinimides 2a-2f:

A solution of an *N*-arylmaleimide (10 mmol) and triphenylphosphine (10 mmol) in ethanol (60 mL) was stirred at room temperature for 30 min. To the reaction mixture was added an aromatic aldehyde (10 mmol), and the reaction mixture was kept on stirring at room temperature for overnight, and the solid product was isolated by filtration and dried under vacuum.

General procedure for the synthesis of arylidene pyrazolidinones 4a-4d:

Arylaldehyde (10 mmol), pyrazolone (10 mmol) and MgO (0.20 g, 5 mmol) were dissolved in 80 mL of acetonitrile in a 150 mL RB and the contents were stirred at reflux temperature. After completion of the reaction, as checked by TLC, the reaction mixture was concentrated and the residue was dissolved in ethyl acetate and washed with brine solution. The organic layer was collected, dried over anhydrous Na_2SO_4, filtered and concentrated in vacuo. The resulting crude mixture was subjected to column chromatography on silica gel (10% EtOAc/hexanes) to obtain pure arylidene pyrazolidinones **4**.

Characterization data:

(3a*S*,4*S*,6*S*,6a*R*)-4-Benzoyl-2,6-diphenyl-3a,4,6,6a-tetrahydro-1*H*-spiro[cyclopenta[*c*]pyrrole-5,2'-indene]-1,1',3,3'(2*H*)-tetraone (3a)

Yield: 106 mg (81%) as white solid; mp: 229–231 ºC.

^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.74 (dd, J = 8.3, 1.1 Hz, 2H), 7.63 (dd, J = 12.8, 7.5, 2H), 7.59–7.52 (m,

2H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.39 (ddd, *J* = 12.8, 7.3, 1.1 Hz, 4H), 7.28 (s, 1H), 7.25 (s, 1H), 7.13–7.10 (m, 2H), 7.04 (ddd, *J* = 8.3, 7.6, 3.6 Hz, 3H), 4.84 (d, *J* = 7.4 Hz, 1H, H_a), 4.66–4.63 (m, 1H, H_c), 4.55 (dd, *J* = 11.3, 9.5 Hz, 1H, H_d), 3.99 (d, *J* = 11.4 Hz, 1H, H_b) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 199.64, 199.62, 196.8, 176.7, 174.7, 142.3, 141.4, 136.1, 135.9, 135.4, 133.5, 132.5, 131.7, 130.2, 129.24, 129.23, 128.82, 128.81, 128.7, 128.6, 128.55, 128.50, 128.4, 128.2, 126.51, 126.50, 126.49, 122.9, 122.8, 70.0, 57.0, 56.7, 48.4, 46.6 ppm.

HRMS (ESI): *m/z* calcd for $C_{34}H_{24}NO_5$ [M + H] $^+$: 526.1649; found: 526.1657.

(3a*S*,4*S*,6*S*,6a*R*)-4-Benzoyl-6-(4-methoxyphenyl)-2-phenyl-3a,4,6,6a-tetrahydro-1*H*-spiro[cyclopenta[*c*]pyrrole-5,2'-indene]-1,1',3,3'(2*H*)-tetraone (3b)

Yield: 106 mg (76%) as white solid; mp:195–197 ^{o}C.

^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.76 (d, *J* = 7.3 Hz, 2H), 7.69 (d, *J* = 7.4Hz, 1H), 7.65–7.63 (m, 2H), 7.59 (d, *J* = 7.1 Hz, 2H), 7.51 (t, *J* = 7.5 Hz, 2H), 7.43 (d, *J* = 7.4 Hz, 1H), 7.39 (d, *J* = 7.8 Hz, 3H), 7.29 (s, 1H), 7.07 (d, *J* = 8.3 Hz, 2H), 6.61 (d, *J* = 8.3 Hz, 2H), 4.83 (d, *J* = 7.3Hz, 1H, H_a), 4.64 (t, *J* = 8.3Hz, 1H, H_c), 4.51 (t, *J* = 10.4 Hz, 1H, H_d), 3.97 (d, *J* = 11.4 Hz, 1H, H_b), 3.64 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 199.7, 196.7, 176.7, 174.7, 159.3, 142.3, 141.4, 136.0, 135.9, 135.3, 133.3, 129.3, 129.1, 128.7, 128.6, 128.4, 126.4, 124.4, 122.9, 122.7, 113.9, 69.9, 56.6, 56.5, 55.0, 48.6, 46.4 ppm.

HRMS (ESI): *m/z* calcd for $C_{35}H_{26}NO_6$ [M + H] $^+$: 556.1755; found: 556.1756.

(3a*S*,4*S*,6*S*,6a*R*)-4-(4-Fluorobenzoyl)-2,6-diphenyl-3a,4,6,6a-tetrahydro-1*H*-spiro[cyclopenta[*c*]-pyrrole-5,2'-indene]-1,1',3,3'(2*H*)-tetraone (3c)

Yield: 99 mg (73%) as white solid; mp: 218–220 ^{o}C.

^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.86 (dd, *J* = 9.2, 5.4 Hz, 2H), 7.68–7.65 (m, 2H), 7.63–7.57 (m, 2H), 7.49 (d, *J* = 7.8 Hz, 1H), 7.48–4.87 (m, 1H), 7.43–7.35 (m, 3H), 7.12 (dd, J = 8.6, 1.5 Hz, 2H), 7.06 (s, 1H), 7.05–7.01(m, 2H), 6.97 (t, *J* = 8.8 Hz, 2H), 4.81–4.78 (m, 1H, H_a), 4.58 (dd, *J* = 3.0, 1.3 Hz, 1H, H_c), 4.56 (t, *J* = 2.8 Hz, 1H, H_d), 3.99–3.95 (m, 1H, H_b) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 199.6, 199.5, 195.2,

176.7, 174.6, 166.9, 164.9, 142.3, 141.3, 136.1, 135.5, 132.3, 132.2, 131.8, 131.7, 131.6, 129.2, 128.8, 128.6, 128.4, 128.25, 128.22, 126.49, 126.47, 126.46, 123.0, 122.9, 115.8, 115.6, 70.0, 56.9, 56.6, 48.4, 46.7 ppm.

^{19}F NMR (470 MHz, $CDCl_3$): –103.58 (1F) ppm.

HRMS (ESI): *m/z* calcd for $C_{34}H_{23}NO_5F$ [M + H] $^+$: 544.1555; found: 544.1557.

(3a*S*,4*S*,6*S*,6a*R*)-4-(4-Fluorobenzoyl)-6-(4-methoxyphenyl)-2-phenyl-3a,4,6,6a-tetrahydro-1*H*-spiro[cyclopenta[*c*]pyrrole-5,2'-indene]-1,1',3,3'(2*H*)-tetraone (3d)

Yield: 102 mg (71%) as white solid; mp: 202–204 ^{o}C.

^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.84–7.81 (m, 2H), 7.67 (t, *J* = 6.5Hz, 1H), 7.65–7.56 (m, 3H), 7.46 (t, *J* = 7.7, 2H), 7.39 (d, *J* = 7.3 Hz, 1H), 7.37–7.34 (m, 2H), 7.03 (d, *J* = 8.7 Hz, 2H), 6.94 (t, *J* = 8.6 Hz, 2H), 6.58 (d, *J* = 8.8 Hz, 2H), 4.76 (d, *J* = 7.3 Hz, 1H, H_a), 4.54 (d, *J* = 7.4 Hz, 1H, H_c), 452–4.4 (m, 1H, H_d), 3.93 (d, *J* = 11.3 Hz, 1H, H_b), 3.60 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 199.8, 199.7, 195.2, 176.8, 174.6, 166.9, 164.9, 159.4, 142.4, 141.4, 136.1, 135.5, 132.3, 132.2, 131.7, 131.7, 131.6, 129.4, 129.25, 129.23, 128.7, 126.4, 124.3, 123.0, 122.9, 115.8, 115.6, 114.0, 69.9, 56.5, 56.4, 55.1, 48.7, 46.6 ppm.

^{19}F NMR (470 MHz, $CDCl_3$): –103.63 (1F) ppm.

HRMS (ESI): *m/z* calcd for $C_{35}H_{25}NO_6F$ [M + H] $^+$: 574.1660; found: 574.1668.

(3a*S*,4*S*,6*S*,6a*R*)-4-(4-Methylbenzoyl)-2,6-diphenyl-3a,4,6,6a-tetrahydro-1*H*-spiro[cyclopenta[*c*]pyrrole-5,2'-indene]-1,1',3,3'(2*H*)-tetraone (3e)

Yield: 98 mg (73%) as white solid; mp: 158–160 ^{o}C.

^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.68 (d, *J* = 1.7 Hz, 1H), 7.67 (dd, *J* = 1.8, 1.3 Hz, 1H), 7.66–7.65 (m, 1H), 7.63 (ddd, *J* = 7.2, 1.3, 0.8 Hz, 1H), 7.60 (dd, *J* = 7.2, 1.4 Hz, 1H), 7.58 (dd, *J* = 4.1, 1.5 Hz, 1H), 7.55 (dd, *J* = 7.2, 1.3 Hz, 1H), 7.49 (dd, *J* = 7.0, 1.0 Hz, 1H), 7.47 (d, *J* = 1.6 Hz, 1H), 7.42–7.39 (m, 1H), 7.39–7.37 (m, 1H), 7.36 (t, *J* = 1.1, 1H), 7.13 (d, *J* = 1.6 Hz, 1H), 7.12 (s, 1H), 7.08 (s, 1H), 7.06 (dd, *J* = 2.9, 1.1 Hz, 1H), 7.05 (d, *J* = 1.2 Hz, 1H), 7.03 (dd, *J* = 5.0, 3.5 Hz, 1H), 4.82 (d, *J* = 7.2 Hz, 1H, H_a), 4.62–4.58 (m,

1H, H_c), 4.55 (d, *J* = 9.4 Hz, 1H, H_d), 3.98 (d, *J* = 10.7 Hz, 1H, H_b), 2.28 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 199.7, 199.5, 196.3, 176.7, 174.8, 144.5, 142.4, 141.4, 135.9, 135.3, 133.4, 132.5, 131.7, 129.2, 129.2, 129.2, 129.19, 129.15, 129.0, 128.7, 128.6, 128.36, 128.30, 126.5, 126.5, 122.9, 122.8, 69.9, 65.9, 56.8, 56.7, 48.4, 46.7, 21.6 ppm.

HRMS (ESI): *m/z* calcd for $C_{35}H_{26}NO_5$ $[M + H]^+$: 540.1805; found: 540.1815.

(3a*R*,4*S*,6*S*,6a*S*)-4-(4-Methoxyphenyl)-6-(4-methylbenzoyl)-2-phenyl-3a,4,6,6a-tetrahydro-1*H*-spiro[cyclopenta[*c*]pyrrole-5,2'-indene]-1,1',3,3'(2*H*)-tetraone (3f)

Yield: 102 mg (72%) as white solid; mp: 232–234 ^{o}C.

^{1}H NMR ($CDCl_3$, 500 MHz) : δ 7.67 (m, 2H), 7.64 (m, 1H), 7.62 (s, 1H), 7.58 (m, 2H), 7.48 (m, 2H), 7.40 (dt, *J* = 3.7, 1.6 Hz, 1H), 7.37 (q, *J* = 2.1 Hz, 1H), 7.35 (d, *J* = 1.1 Hz, 1H), 7.05 (m, 4H), 6.59 (d, *J* = 8.8 Hz, 2H), 4.79 (d, *J* = 7.5 Hz, 1H, H_a), 4.58 (dd, *J* = 9.4, 7.5 Hz, 1H, H_d), 4.5 (dd, *J* = 11.4, 9.4 Hz, 1H), 3.95 (d, *J* = 11.4 Hz, 1H, H_b), 3.61 (s, 3H, H_c), 2.27 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 199.89, 199.80, 196.2, 176.7, 174.88, 174.86, 159.3, 144.5, 142.5, 141.4, 136.0, 135.3, 133.4, 131.7, 129.5, 129.4, 129.2, 129.1, 129.0, 128.7, 126.50, 124.57, 122.98, 122.90, 114.0, 69.9, 56.6, 56.4, 55.1, 48.7, 46.7, 21.6 ppm.

HRMS (ESI): *m/z* calcd for $C_{36}H_{28}NO_6$ $[M + H]^+$: 570.1911; found: 570.1934.

(3a*S*,4*S*,6*S*,6a*R*)-4-(4-Bromobenzoyl)-2,6-diphenyl-3a,4,6,6a-tetrahydro-1*H*-spiro[cyclopenta[*c*]-pyrrole-5,2'-indene]-1,1',3,3'(2*H*)-tetraone (3g)

Yield: 98 mg (64%) as white solid; mp: 222–224 ^{o}C.

^{1}H NMR ($CDCl_3$, 500 MHz) : δ 7.99 (d, *J* = 8.0 Hz, 1H), 7.81 (dd, *J* = 11.9, 4.4 Hz, 1H), 7.75 (t, *J* = 8.2 Hz, 1H), 7.71 (d, *J* = 7.8 Hz, 1H), 7.46 (t, *J* = 8.0 Hz, 2H), 7.38 (d, *J* = 7.5 Hz, 1H), 7.33 (m, 4H), 7.23 (d, *J* = 3.1 Hz, 1H), 7.21 (s, 2H), 7.18 (d, *J* = 7.2Hz, 2H), 7.14 (s, 1H), 7.13(s, 1H), 4.75 (d, *J* = 12.3 Hz, 1H, H_a), 4.54 (dd, *J* = 12.6, 8.7 Hz, 1H, H_c), 4.17 (d, *J* = 10.5 Hz, 1H, H_d), 3.93 (dd, *J* = 10.6, 8.7Hz, 1H, H_b) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 198.9, 198.8, 195.5, 175.5, 173.9, 142.6, 140.9, 138.4, 136.7, 135.8, 134.7, 131.7, 131.6, 129.6, 129.2, 129.1, 129.0, 128.9, 128.0, 127.7, 126.9, 123.7, 123.6, 64.1, 63.2, 51.5,

50.8, 50.3 ppm.

HRMS (ESI): *m/z* calcd for $C_{34}H_{23}NO_5Br$ $[M + H]^+$: 604.0754; found: 604.0750.

(3a*S*,4*S*,6*S*,6a*R*)-4-(4-Bromobenzoyl)-6-(4-methoxyphenyl)-2-phenyl-3a,4,6,6a-tetrahydro-1*H*-spiro[cyclopenta[*c*]pyrrole-5,2'-indene]-1,1',3,3'(2*H*)-tetraone (3h)

Yield: 100 mg (63%) as white solid; mp: 216–218 ºC.

^{1}H NMR ($CDCl_3$, 500 MHz) : δ 7.68 (m, 2H), 7.65 (m, 3H), 7.62 (dd, *J* = 7.0, 1.8 Hz, 1H), 7.48 (m, 2H), 7.42 (m, 3H), 7.35 (m, 2H), 7.03 (d, *J* = 8.7 Hz, 2H), 6.59 (d, *J* = 8.8 Hz, 2H), 4.75 (d, *J* = 7.2 Hz, 1H, H_a), 4.54 (dd, *J* = 9.4, 7.2 Hz, 1H, H_c), 4.48 (dd, *J* = 11.2, 9.4 Hz, 1H, H_d), 3.93 (d, *J* = 11.2 Hz, 1H, H_b), 3.61 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 199.8, 199.7, 196.1, 176.7, 174.6, 159.4, 142.4, 141.4, 136.3, 136.2, 135.5, 134.7, 132.2, 131.8, 131.6, 130.3, 129.8, 129.4, 129.2, 128.9, 128.8, 126.5, 126.4, 126.4, 126.47, 126.45, 126.44, 126.43, 126.42, 124.3, 124.2, 123.0, 122.9, 114.0, 69.9, 56.6, 56.4, 55.1, 48.6, 46.5 ppm.

HRMS (ESI): *m/z* calcd for $C_{35}H_{24}NO_6BrNa$ $[M + Na]^+$: 656.0679; found: 656.0685.

(3a*S*,4*S*,6*S*,6a*R*)-4-benzoyl-2,6-bis(4-methoxyphenyl)-3a,4,6,6a-tetrahydro-1*H*-spiro[cyclopenta[*c*]pyrrole-5,2'-indene]-1,1',3,3'(2*H*)-tetraone (3i)

Yield: 109 mg (75%) as white solid; mp: 129–131 ºC

^{1}H NMR ($CDCl_3$, 500 MHz) : δ 7.74 (d, *J* = 1.1 Hz, 1H), 7.72 (t, *J* = 1.6 Hz, 1H), 7.66 (dt, *J* = 7.5, 0.9 Hz, 1H), 7.62–7.61 (m, 1H), 7.61–7.60(m, 1H), 7.56 (ddd, *J* = 8.5, 7.8, 1.3 Hz, 1H), 7.39–7.36 (m, 1H), 7.29-7.28 (m, 1H), 7.27–7.26 (m, 1H), 7.26–7.23 (m, 2H), 7.05–7.04 (m, 1H), 7.03–7.02 (m, 1H), 7.00–6.98 (m, 1H), 7.00–6.98 (m, 1H), 6.60–6.58 (m, 1H), 6.58–6.56 (m, 1H), 4.79 (d, *J* = 7.4 Hz, 1H, H_a), 4.59 (dd, *J* = 9.4, 7.4 Hz, 1H, H_c), 4.46 (dd, *J* = 11.5, 9.4 Hz, 1H, H_d), 3.93 (d, *J* =11.5 Hz, 1H, H_b), 3.82 (s, 3 H), 3.61 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 199.8, 196.9, 177.0, 175.0, 159.5, 159.3, 142.3, 141.4, 136.08, 136.04, 135.4, 133.4, 129.47, 129.45, 129.43, 129.40, 128.87, 128.82, 128.7, 128.5, 128.48, 128.44, 127.78, 127.76, 127.74, 127.71, 127.69, 127.67, 124.4, 124.3, 122.97, 122.8, 114.56, 114.53, 114.51, 114.48, 114.46, 114.05, 114.03, 114.00, 113.97, 113.95, 69.9, 56.6, 56.5, 55.6, 55.59, 55.56, 55.15, 55.12, 48.6,

46.4 ppm.

HRMS (ESI): *m/z* calcd for $C_{36}H_{27}NO_7$ $[M + H]^+$: 586.1866; found: 586.1848.

(3a*S*,4*S*,6*S*,6a*R*)-4-(4-bromobenzoyl)-2,6-bis(4-methoxyphenyl)-3a,4,6,6a-tetrahydro-1*H*-spiro[cyclopenta[*c*]pyrrole-5,2'-indene]-1,1',3,3'(*2H*)-tetraone (3j)

Yield: 110 mg (67%) as white solid; mp: 214–216 ºC.

^{1}H NMR ($CDCl_3$, 500 MHz) : δ 7.68 (dd, *J* = 6.7, 1.6 Hz, 2H), 7.67–7.64 (m, 3H), 7.63 (dd, *J* = 7.1, 1.9 Hz, 1H), 7.44–7.40 (m, 2H), 7.27 (s, 1H), 7.25 (s, 1H), 7.03 (d, *J* = 9.1 Hz, 2H), 7.00–6.96 (m, 2H), 6.60-6.57 (m, 2H), 4.73 (d, *J* = 7.2 Hz, 1H, H_a), 4.50 (dd, *J* = 9.3, 6.9 Hz, 1H, H_c), 4.45 (d, *J* = 9.5 Hz, 1H, H_d), 3.91 (d, *J* = 11.0 Hz, 1H, H_b), 3.83 (s, 3H), 3.61 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 199.8, 199.7, 196.1, 176.9, 174.8, 159.6, 159.3, 142.4, 141.3, 136.2, 135.5, 134.6, 131.83, 131.81, 130.46, 130.41, 130.3, 129.43, 129.41, 129.3, 128.91, 127.7, 124.28, 124.22, 123.0, 122.9, 114.57, 114.54, 114.51, 114.0, 69.9, 56.6, 56.4, 55.6, 55.1, 48.6, 46.5 ppm.

HRMS (ESI): *m/z* calcd for $C_{36}H_{26}NO_7Br$ $[M + H]^+$: 664.0971; found: 664.0955.

(3a*S*,4*S*,6*R*,6a*R*)-4-Benzoyl-6-(furan-2-yl)-2-(*p*-tolyl)-3a,4,6,6a-tetrahydro-1*H*-spiro[cyclopenta[*c*]-pyrrole-5,2'-indene]-1,1',3,3'(2*H*)-tetraone (3k)

Yield: 104 mg (79%) as white solid; mp: 225–227 ºC.

^{1}H NMR ($CDCl_3$, 500 MHz) : δ 7.77–7.74 (m, 1H), 7.73–7.68 (m, 4H), 7.66 (dd, *J* = 7.5, 1.3 Hz, 1H), 7.63 (dd, *J* = 7.3, 1.2 Hz, 1H), 7.40 (ddd, *J* = 7.4, 4.2, 1.2 Hz, 1H), 7.29 (dd, *J* = 10.5, 2.3 Hz, 3H), 7.25–7.20 (m, 2H), 6.90 (dd, *J* = 1.8, 0.7 Hz, 1H), 6.29 (dt, *J* = 3.3, 0.8 Hz, 1H), 6.07 (dd, *J* = 3.3, 1.8 Hz, 1H), 4.76 (d, *J* = 7.9 Hz, 1H, H_a), 4.58(dd, *J* = 9.6, 7.9 Hz, 1H, H_c), 4.36 (dd, *J* = 11.1, 9.6 Hz, 1H, H_d), 4.10 (d, *J* = 11.1 Hz, 1H, H_b), 2.39(s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 198.7, 198.6, 196.4, 176.3, 174.6, 148.0, 142.5, 141.9, 141.4, 138.9, 136.0, 135.9, 135.4, 133.5, 129.93, 129.92, 129.90, 128.9, 128.8, 128.5, 126.31, 126.30, 123.2, 123.0, 110.4, 109.3, 68.2, 56.2, 49.6, 48.2, 46.7, 21.3 ppm.

HRMS (ESI): *m/z* calcd for $C_{33}H_{24}NO_6$ $[M + H]^+$: 530.1598; found: 530.1614.

(3a*S*,4*S*,6*R*,6a*S*)-4-Benzoyl-6-(thiophen-2-yl)-2-(*p*-tolyl)-3a,4,6,6a-tetrahydro-1*H*-spiro[cyclopenta[*c*]pyrrole-5,2'-indene]-1,1',3,3'(2*H*)-tetraone (3l)

Yield: 110 mg (81%) as white solid; mp: 275–277 ^{o}C.

^{1}H NMR ($CDCl_3$, 500 MHz) : δ 7.73–7.71 (m, 1H), 7.70 (d, *J* = 1.1 Hz, 1H), 7.68 (d, *J* = 1.8 Hz, 1H), 7.65 (m, 1H), 7.63 (dd, *J* = 7.2, 1.2 Hz, 2H), 7.60–7.57 (m, 1H), 7.40–7.36 (m, 1H), 7.28 (s, 1H), 7.24 (d, *J* = 1.7 Hz, 2H), 7.23 (s, 1H), 7.22 (dd, *J* = 4.3, 1.9 Hz, 1H), 6.93 (dd, *J* = 5.1, 1.2 Hz, 1H), 6.87–6.86 (m, 1H), 6.68 (dd, *J* = 5.1, 3.6 Hz, 1H), 4.77 (d, *J* = 7.8 Hz, 1H, H_a), 4.58 (dd, *J* = 9.4, 7.8 Hz, 1H, H_c), 4.41 (dd, *J* =11.2, 9.5 Hz, 1H, H_d), 4.27 (d, *J* = 11.2 Hz, 1H, H_b), 2.37 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 199.29, 199.26, 196.4, 176.40, 174.44, 142.5, 141.6, 138.8, 136.1, 136.0, 135.5, 135.3, 133.6, 129.8, 129.0, 128.82, 128.81, 128.5, 127.4, 126.9, 126.29, 126.28, 126.27, 125.4, 123.1, 123.0, 69.6, 56.4, 51.8, 50.5, 46.6, 21.3 ppm.

HRMS (ESI): *m/z* calcd for $C_{33}H_{24}NO_5S$ $[M + H]^+$: 546.1370; found: 546.1378.

(3a*S*,4*S*,6*R*,6a*R*)-4-(4-Fluorobenzoyl)-6-(furan-2-yl)-2-(*p*-tolyl)-3a,4,6,6a-tetrahydro-1*H*-spiro[cyclopenta[*c*]pyrrole-5,2'-indene]-1,1',3,3'(2*H*)-tetraone (3m)

Yield: 103 mg (75%) as white solid; mp: 200–202 ^{o}C.

^{1}H NMR ($CDCl_3$, 500 MHz) : δ 7.82–7.76 (m, 4H), 7.70 (ddd, *J* = 8.7, 7.1, 1.4 Hz, 2H), 7.29 (d, J = 8.1 Hz, 2H), 7.24–7.22 (m, 2H), 6.95 (d, *J* = 8.7 Hz, 2H), 6.90 (dd, *J* = 1.8, 0.6 Hz, 1H), 6.29 (dd, *J* = 2.6, 0.8 Hz, 1H), 6.07 (dd, *J* = 3.3, 1.9 Hz, 1H), 4.72 (d, *J* = 7.9 Hz, 1H, H_a), 4.54–4.50 (m, 1H, H_c), 4.37 (dd, *J* = 11.1, 9.6 Hz, 1H, H_d), 4.08 (d, *J* = 11.1 Hz, 1H, H_b), 2.39 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 198.7, 198.6, 194.88, 194.86, 176.4, 174.5, 167.0, 165.0, 147.8, 142.5, 141.9, 141.3, 139.0, 136.1, 135.6, 131.8, 131.7, 129.97, 129.96, 128.8, 126.2, 123.2, 123.0, 115.8, 115.6, 110.5, 109.4, 68.2, 56.0, 49.5, 48.2, 46.8, 21.3 ppm.

^{19}F NMR (470 MHz, $CDCl_3$): –103.40 (1F) ppm.

HRMS (ESI): *m/z* calcd for $C_{33}H_{23}NO_6F$ $[M + H]^+$: 548.1504; found: 548.1529.

(3a*S*,4*S*,6*R*,6a*S*)-4-(4-Fluorobenzoyl)-6-(thiophen-2-yl)-2-(p-tolyl)-3a,4,6,6a-tetrahydro-1*H*-spiro[cyclopenta[*c*]pyrrole-5,2'-indene]-1,1',3,3'(2*H*)-tetraone (3n)

Yield: 110 mg (78%) as white solid; mp: 208–210 ^{o}C.

^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.81 (dd, J = 8.5, 5.3 Hz, 2H), 7.76(d, J = 7.4, 1H), 7.70 (t, J = 7.7 Hz, 1H), 7.67 (d, J = 6.9 Hz, 1H), 7.64 (d, J = 7.2 Hz, 1H), 7.31–7.27 (m, 3H), 7.23 (d, J = 8.2 Hz, 2H), 6.96 (t, J = 7.8 Hz, 2H), 6.88 (d, J = 3.2 Hz, 1H), 6.71–6.69 (m, 1H),4.75 (d, J = 7.8 Hz, 1H, H_a), 4.53 (d, J = 7.9 Hz, 1H, H_c), 4.47–4.42 (m, 1H, H_d), 4.27 (d, J = 11.1 Hz, 1H, H_b), 2.38 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 199.29, 199.26, 194.9, 176.4, 174.3, 142.5, 141.5, 138.9, 136.3, 135.6, 135.2, 131.8, 131.7, 129.9, 128.9, 127.4, 126.9, 126.3, 126.2, 125.4, 123.17, 123.13, 115.8, 115.6, 69.6, 56.3, 51.7, 50.5, 46.7, 21.3 ppm.

HRMS (ESI): *m/z* calcd for $C_{33}H_{23}NFO_5S$ $[M + H]^+$: 564.1275; found: 564.1282.

(3a*R*,4*R*,6*S*,6a*S*)-4-(Furan-2-yl)-6-(4-methylbenzoyl)-2-(*p*-tolyl)-3a,4,6,6a-tetrahydro-1*H*-spiro[cyclopenta[*c*]pyrrole-5,2'-indene]-1,1',3,3'(2*H*)-tetraone (3o)

Yield: 110 mg (81%) as white solid; mp: 247–249 ^{o}C.

^{1}H NMR ($CDCl_3$, 500 MHz) δ: 7.78–7.76 (m, 1H), 7.75–7.73 (m, 1H), 7.69 (dt, J = 7.5, 3.7 Hz, 1H), 7.66 (dd, J = 7.3, 1.3 Hz, 1H), 7.63 (d, J = 1.7 Hz, 1H), 7.61 (d, J = 1.7 Hz, 1H), 7.30 (m, 2H), 7.25–7.24 (m, 1H), 7.23 (s, 1H), 7.07 (dd, J = 8.4, 0.5 Hz, 2H), 6.90 (dd, J =1.8, 0.7 Hz, 1H), 6.30 (dt, J = 3.3, 0.9 Hz, 1H), 6.07 (dd, J = 3.3, 1.8 Hz, 1H), 4.74 (d, J = 8.0 Hz, 1H, H_a), 4.54 (dd, J = 9.6, 8.1 Hz, 1H, H_c), 4.37 (dd, J = 11.1, 9.6 Hz, 1H, H_d), 4.09 (d, J = 11.1 Hz, 1H, H_b), 2.39 (s, 3H), 2.28 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 198.8, 198.7, 195.8, 176.3, 174.7, 148.1, 144.7, 142.4, 142.0, 141.3, 138.9, 135.9, 135.3, 133.3, 129.9, 129.2, 129.0, 128.9, 126.31, 126.30, 126.29, 126.28, 123.2, 123.0, 110.5, 109.2, 68.1, 56.1, 49.4, 48.3, 46.9, 21.6, 21.3 ppm.

HRMS (ESI): *m/z* calcd for $C_{34}H_{26}NO_6$ $[M + H]^+$: 544.1755; found: 544.1757.

(3a*S*,4*S*,6*R*,6a*S*)-4-(4-Methylbenzoyl)-6-(thiophen-2-yl)-2-(*p*-tolyl)-3a,4,6,6a-tetrahydro-1*H*-spiro[cyclopenta[*c*]pyrrole-5,2'-indene]-1,1',3,3'(2*H*)-tetraone (3p)

Yield: 116 mg (82%) as white solid; mp: 245–247 °C.

^{1}H NMR ($CDCl_3$, 500 MHz) δ: 7.77–7.74 (m, 1H), 7.69–7.65 (m, 2H), 7.64–7.58 (m, 3H), 7.29–7.26 (m, 2H), 7.25–7.21 (m, 2H), 7.06 (dd, *J* = 8.5, 0.5 Hz, 2H), 6.95 (dd, *J* = 5.1, 1.2 Hz, 1H), 6.90–6.88 (m, 1H), 6.70 (dd, *J* = 5.1, 3.6 Hz 1H), 4.76 (d, *J* = 7.9 Hz, 1H, H_a), 4.55 (dd, *J* = 9.5, 7.9 Hz, 1H, H_c), 4.44 (dd, *J* = 11.1, 9.5 Hz, 1H, H_d), 4.09 (d, *J* = 11.1 Hz, 1H, H_b), 2.39 (s, 3H), 2.28 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 199.3, 199.2, 195.8, 176.3, 174.5, 144.7, 142.6, 141.6, 138.8, 136.2, 136.1, 135.48, 135.41, 133.3, 129.9, 129.89, 129.86, 129.5, 129.2, 129.0, 128.9, 128.5, 127.3, 126.9, 126.2, 125.3, 124.2, 123.1, 123.0, 69.6, 56.3, 51.6, 50.5, 46.7, 21.6, 21.3 ppm.

HRMS (ESI): *m/z* calcd for $C_{34}H_{26}NO_5S$ $[M + H]^+$: 560.1526; found: 560.1530.

(3a*S*,4*S*,6*R*,6a*R*)-4-(4-Bromobenzoyl)-6-(furan-2-yl)-2-(*p*-tolyl)-3a,4,6,6a-tetrahydro-1*H*-spiro[cyclopenta[*c*]pyrrole-5,2'-indene]-1,1',3,3'(2*H*)-tetraone (3q)

Yield: 110 mg (73%) as white solid; mp: 233–235 °C.

^{1}H NMR ($CDCl_3$, 500 MHz) δ: 7.78 (dd, *J* = 8.5, 0.5 Hz, 2H), 7.74–7.69 (m, 2H), 7.63–7.56 (m, 2H), 7.29–7.44–7.41(m, 2H), 7.30 (d, *J* = 8.1, 2H), 7.23 (d, *J* = 8.3, 2H), 6.90 (d, *J* = 1.1 Hz, 1H), 6.29 (d, *J* = 3.3 Hz, 1H), 6.07 (dd, *J* = 3.3, 1.8 Hz, 1H), 4.69 (d, *J* = 7.9 Hz, 1H, H_a), 4.50 (dd, *J* = 9.5, 7.9 Hz, 1H, H_c), 4.35 (dd, *J* = 11.0, 9.6 Hz, 1H, H_d), 4.06 (d, *J* = 11.1 Hz, 1H, H_b), 2.40 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 198.6, 195.7, 176.3, 174.4, 147.7, 142.5, 141.9, 141.3, 139.0, 136.1, 135.5, 134.6, 131.8, 130.3, 129.9, 129.0, 128.8, 126.27, 126.26, 123.3, 123.0, 110.5, 109.4, 68.2, 56.1, 49.5, 48.2, 46.7, 21.3 ppm.

HRMS (ESI): *m/z* calcd for $C_{33}H_{23}NO_6Br$ $[M + H]^+$: 608.0703; found: 608.0705.

(3a*S*,4*S*,6*R*,6a*S*)-4-(4-Bromobenzoyl)-6-(thiophen-2-yl)-2-(*p*-tolyl)-3a,4,6,6a-tetrahydro-1*H*-spiro[cyclopenta[*c*]pyrrole-5,2'-indene]-1,1',3,3'(2*H*)-tetraone (3r)

Yield: 118 mg (76%) as white solid; mp: 156–158 °C.

^{1}H NMR ($CDCl_3$, 500 MHz) δ: ^{1}H NMR ($CDCl_3$, 500 MHz) δ: 7.97 (dd, *J* = 6.9, 0.8 Hz, 1H), 7.83–7.79 (m, 1H), 7.74–7.71 (m, 2H), 7.33 (s, 1H), 7.32 (d, *J* = 2.0, 1H), 7.27 (t, *J* = 2.2 Hz, 3H), 7.25 (s, 1H), 7.23

(d, *J* = 2.0, 1H), 7.21 (d, *J* = 1.8, 1H), 7.13 (dd, *J* = 5.1, 1.0 Hz, 1H), 6.93–6.92 (m, 1H), 6.81 (dd, *J* = 5.1, 3.5 Hz, 1H), 4.92 (dd, *J* = 11.9, 8.8 Hz, 1H, H_a), 4.72 (d, *J* = 11.9 Hz, 1H, H_c), 4.16 (d, *J* = 10.4 Hz, 1H, H_d), 3.93–3.89 (m, 1H, H_b), 2.37 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): *δ* 198.6, 198.4, 195.0, 175.1, 173.9, 142.4, 141.7, 141.0, 139.0, 136.7, 135.9, 134.8, 131.8, 129.9, 129.6, 129.3, 129.0, 127.5, 126.76, 126.71, 124.7, 123.7, 123.6, 64.7, 63.3, 52.0, 49.8, 46.0, 21.3 ppm.

HRMS (ESI): *m/z* calcd for $C_{33}H_{23}SNO_5Br$ $[M + H]^+$: 624.0475; found: 624.0388.

(*Z*)-3-Benzylidene-4-((3-methyl-5-oxo-1-phenyl-4,5-dihydro-1*H*-pyrazol-4-yl)(phenyl)methyl)-1-phenylpyrrolidine-2,5-dione (5a)

Yield: 107 mg (82%) as white solid; mp: 110–112 ^oC.

^{1}H NMR ($CDCl_3$, 500 MHz) *δ*: 11.68 (s, 1H, OH), 7.98 (d, *J* = 1.7 Hz, 1H), 7.91 (d, *J* = 7.7 Hz, 2H), 7.68–7.65 (m, 3H), 7.54 (d, *J* = 6.0 Hz, 4H), 7.46 (t, *J* = 8.0 Hz, 3H), 7.36–7.34 (m, 4H), 7.13 (dd, *J* = 6.5, 2.8 Hz, 2H), 6.62–6.59 (m, 2H), 4.76 (s, 1H, H_a), 4.56 (s, 1H, H_b), 1.74 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): *δ* 180.0, 168.9, 150.5, 147.4, 139.1, 138.1, 137.1, 132.7, 131.27, 130.7, 129.6, 129.2, 129.1, 128.7, 128.6, 128.5, 127.8, 127.2, 126.3, 125.6, 121.8, 115.0, 98.7, 77.2, 76.7, 49.0, 41.8, 12.6 ppm.

HRMS (ESI): *m/z* calcd for $C_{34}H_{27}N_3O_3Na$ $[M + Na]^+$: 548.1945; found: 548.1952.

(*Z*)-3-Benzylidene-4-((2-methoxyphenyl)(3-methyl-5-oxo-1-phenyl-4,5-dihydro-1*H*-pyrazol-4-yl)methyl)-1-phenylpyrrolidine-2,5-dione (5b)

Yield: 108 mg (78%) as white solid; mp: 104–106 ^oC.

^{1}H NMR ($CDCl_3$, 500 MHz) *δ*: 11.57 (s, 1H, OH), 7.92 (d, *J* = 7.8 Hz, 2H), 7.78 (d, *J* = 1.2 Hz, 1H), 7.64 (d, *J* = 6.9 Hz, 2H), 7.52–7.44 (m, 6H), 7.36–7.34 (m, 3H), 7.25–7.21 (m, 1H), 7.16 (d, *J* = 7.6 Hz, 1H), 6.90 (t, *J* = 7.4 Hz, 1H), 6.78 (d, *J* = 8.2 Hz, 1H), 6.63 (dd, *J* = 6.6, 2.8 Hz, 2H), 5.13 (s, 1H, H_a), 4.71 (s, 1H, H_b), 3.63 (s, 3H), 1.82 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): *δ* 180.3, 169.3, 156.6, 150.7, 147.2, 139.2, 134.8, 133.4, 131.3, 130.9, 130.6, 130.5, 129.4, 129.1, 129.0, 128.8, 127.9, 126.4, 126.3, 125.6, 121.7, 120.8, 110.0, 100.1, 54.8, 49.5, 35.0, 12.5 ppm.

HRMS (ESI): *m/z* calcd for $C_{35}H_{30}N_3O_4$ $[M + H]^+$: 556.2231; found: 556.2257.

(*Z*)-3-(4-Methoxybenzylidene)-4-((2-methoxyphenyl)(3-methyl-5-oxo-1-phenyl-4,5-dihydro-1*H*-pyrazol-4-yl)methyl)-1-phenylpyrrolidine-2,5-dione (5c)

Yield: 112 mg (77%) as white solid; mp: 195–197 ^oC.

^1H NMR ($CDCl_3$, 500 MHz) δ: 11.76 (s, 1H, OH), 7.93 (d, J =8.3 Hz, 2H), 7.72 (s, 1H), 7.59 (d, J = 8.6 Hz, 2H), 7.46 (t, J = 7.9 Hz, 3H), 7.35–7.33 (m, 2H), 7.25–7.21 (m, 2H), 7.16 (d, J = 7.7 Hz, 1H), 7.01 (d, J = 8.6Hz, 2H), 6.89 (t, J = 7.5 Hz, 1H), 6.78 (d, J = 8.2Hz, 1H), 6.65–6.61 (m, 2H), 5.19 (s, 1H, H_a), 4.64 (s, 1H, H_b), 3.85 (s, 3H), 3.61 (s, 3H), 1.89 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 180.5, 169.5, 161.6, 156.7, 150.9, 147.4, 139.1, 134.7, 132.6, 131.3, 131.0, 129.1, 128.9, 128.8, 128.7, 126.5, 126.4, 126.0, 125.7, 124.8, 121.7, 120.8, 119.0, 115.0, 114.3, 110.0, 100.2, 55.6, 54.9, 49.4, 34.5, 12.6 ppm.

HRMS (ESI): *m/z* calcd for $C_{36}H_{31}N_3O_5Na$ $[M + Na]^+$: 608.2156; found: 608.2162.

(*Z*)-3-(2,6-Dimethoxybenzylidene)-1-(3,5-dimethylphenyl)-4-((2-methoxyphenyl)(3-methyl-5-oxo-1-phenyl-4,5-dihydro-1*H*-pyrazol-4-yl)methyl)pyrrolidine-2,5-dione (5d)

Yield: 111 mg (69%) as white solid; mp: 210–212 ^oC.

^1H NMR ($CDCl_3$, 500 MHz) δ: 11.53 (s, 1H, OH), 8.13 (d, J = 1.8 Hz, 1H), 7.84 (d, J = 7.7 Hz, 2H), 7.44 (t, J = 7.9 Hz, 2H), 7.25–7.20 (m, 2H), 7.15–7.12 (m, 1H), 7.05 (d, J = 2.7 Hz, 1H), 7.00 (dd, J = 9.0, 2.9 Hz, 1H), 6.97–6.92 (m, 2H), 6.89 (t, J = 7.4 Hz, 1H), 6.79 (d, J = 8.1 Hz, 1H), 6.16 (s, 2H), 4.96 (s, 1H, H_a), 4.76 (s, 1H, H_b), 3.83 (s, 3H), 3.66 (s, 3H), 3.55 (s, 3H), 2.25 (s, 6H), 1.67 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 180.6, 169.4, 156.8, 153.6, 152.9, 150.5, 147.3, 139.2, 138.9, 131.4, 130.8, 130.2, 128.8, 128.5, 128.1, 126.7, 125.6, 124.1, 122.8, 121.8, 120.6, 118.4, 113.7, 112.6, 110.0, 100.6, 55.8, 55.5, 54.7, 49.6, 34.9, 21.1, 12.2 ppm.

HRMS (ESI): *m/z* calcd for $C_{39}H_{37}N_3O_6Na$ $[M + Na]^+$: 666.2575; found: 666.2576.

(*Z*)-3-(4-Methoxybenzylidene)-4-((3-methyl-5-oxo-1-phenyl-4,5-dihydro-1*H*-pyrazol-4-yl)(phenyl)methyl)-1-phenylpyrrolidine-2,5-dione (5e)

Yield: 111 mg (80%) as white solid; mp: 178–180 °C.

^{1}H NMR ($CDCl_3$, 500 MHz) δ: 11.80 (s, 1H, OH), 7.93–7.90 (m, 3H), 7.61 (d, J = 8.7 Hz, 2H), 7.46 (t, J = 7.9 Hz, 3H), 7.35–7.33 (m, 3H), 7.27 (d, J = 7.1 Hz, 2H), 7.25 (s, 1H), 7.14 (dd, J = 6.3, 2.6 Hz, 2H), 7.04 (d, J = 8.7 Hz, 2H), 6.59 (dd, J = 6.3, 3.0 Hz, 2H), 4.68 (s, 1H, H_a), 4.60 (s, 1H, H_b), 3.87 (s, 3H), 1.83 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 180.1, 169.2, 162.1, 150.6, 147.5, 139.1, 138.2, 136.7, 133.0, 132.2, 130.8, 129.1, 128.8, 128.6, 128.6, 127.8, 126.5, 126.3, 125.7, 125.3, 123.9, 121.7, 115.2, 114.7, 98.8, 55.6, 49.0, 41.5, 12.8 ppm.

HRMS (ESI): *m/z* calcd for $C_{33}H_{30}N_3O_4$ $[M + H]^+$: 556.2231; found: 556.2031.

(*Z*)-3-((2,5-Dimethoxyphenyl) (3-methyl-5-oxo-1-phenyl-4,5-dihydro-1*H*-pyrazol-4-yl)methyl)-4-(4-methoxybenzylidene)-1-phenylpyrrolidine-2,5-dione (5f)

Yield: 125 mg (81%) as white solid; mp: 188–190 °C.

^{1}H NMR ($CDCl_3$, 500 MHz) δ: 11.68 (s, 1H, OH), 7.91 (d, J = 7.7 Hz, 2H), 7.72 (d, J = 1.4 Hz, 1H), 7.58 (d, J = 8.8 Hz, 2H), 7.45 (t, J = 8.0 Hz, 2H), 7.37 (td, J = 4.8, 2.5 Hz, 3H), 7.01 (d, J = 8.7 Hz, 2H), 6.72 (qd, J = 8.7, 5.6 Hz, 6H), 5.17 (s, 1H, H_a), 4.65 (s, 1H, H_b), 3.86 (s, 3H), 3.63 (s, 3H), 3.57 (s, 3H), 1.88 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 180.5, 169.5, 161.5, 153.5, 150.8, 150.6, 147.4, 139.1, 134.9, 132.6, 131.1, 129.0, 128.9, 128.8, 127.7, 126.4, 126.0, 125.6, 124.5, 121.7, 117.4, 115.0, 113.2, 110.9, 100.0, 55.7, 55.5, 55.3, 49.3, 34.6, 12.7 ppm.

HRMS (ESI): *m/z* calcd for $C_{37}H_{33}N_3O_6Na$ $[M + Na]^+$: 638.2262; found: 638.2265.

(*Z*)-3-Benzylidene-4-((3-bromophenyl) (3-methyl-5-oxo-1-phenyl-4,5-dihydro-1*H*-pyrazol-4-yl)-methyl)-1-phenylpyrrolidine-2,5-dione (5g)

Yield: 130 mg (86%) as white solid; mp: 126–128 °C.

^{1}H NMR ($CDCl_3$, 500 MHz) δ: 11.65 (s, 1H, OH), 7.99 (s, 1H), 7.91 (d, J = 8.0, 2H), 7.64 (d, J = 4.3, 2H), 7.53 (d, J = 4.5, 2H), 7.46 (t, J = 7.7, 3H), 7.40 (d, J = 10.7, 4H), 7.28 (d, J = 7.1, 2H), 7.12 (t, J = 7.8 , 1H), 7.04 (d, J = 7.7, 1H), 6.74 (d, J = 7.4, 2H), 4.76 (s, 1H, H_a), 4.51 (s, 1H, H_b), 1.74 (s, 3H) ppm; ^{13}C NMR

($CDCl_3$, 125 MHz): δ 179.7, 168.6, 150.4, 147.4, 140.6, 138.9, 137.6, 132.5, 131.4, 131.3, 131.1, 130.8, 130.6, 130.2, 129.7, 129.3, 128.8, 127.2, 126.5, 126.2, 125.8, 122.8, 121.8, 98.1, 48.7, 41.2, 12.7 ppm.

HRMS (ESI): *m/z* calcd for $C_{34}H_{27}N_3O_3Br$ $[M + H]^+$: 604.1230; found: 604.1271.

(*Z*)-3-(Furan-2-ylmethylene)-4-((3-methyl-5-oxo-1-phenyl-4,5-dihydro-1*H*-pyrazol-4-yl)(phenyl)-methyl)-1-phenylpyrrolidine-2,5-dione (5h)

Yield: 106 mg (82%) as white solid; mp: 198–200 ^oC.

^1H NMR ($CDCl_3$, 500 MHz) δ: 11.70 (s, 1H, OH), 7.91 (d, J = 8.0 Hz, 2H), 7.67 (s, 1H), 7.64 (s, 1H), 7.44 (t, J = 7.9 Hz, 2H), 7.33–7.30 (m, 3H), 7.24 (dd, J = 10.8, 5.3 Hz, 4H), 7.18–7.15 (m, 2H), 6.93 (d, J = 3.1, 1H), 6.61 (d, J = 1.4 Hz, 1H), 6.59–6.55 (m, 2H), 4.70 (s, 1H, H_a), 4.67 (s, 1H, H_b), 1.91 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 180.1, 168.7, 150.3, 149.9, 147.6, 147.3, 139.2, 138.3, 130.7, 129.13, 129.10, 128.8, 128.6, 128.6, 127.7, 126.3, 125.6, 124.4, 122.4, 121.8, 119.3, 115.0, 114.9, 113.4, 99.4, 77.3, 77.0, 76.8, 49.6, 43.8, 12.8 ppm.

HRMS (ESI): *m/z* calcd for $C_{32}H_{25}N_3O_4Na$ $[M + Na]^+$: 538.1737; found: 538.1740.

(*Z*)-3-(Furan-2-ylmethylene)-4-((3-methyl-5-oxo-1-phenyl-4,5-dihydro-1*H*-pyrazol-4-yl)(phenyl)-methyl)-1-(*p*-tolyl)pyrrolidine-2,5-dione (5i)

Yield: 105 mg (80%) as white solid; mp: 101–103 ^oC.

^1H NMR ($CDCl_3$, 500 MHz) δ: 11.73 (s, 1H, OH), 7.91 (d, J = 7.7 Hz, 2H), 7.68 (dd, J = 7.1, 1.4 Hz, 2H), 7.45 (t, J = 8.0 Hz, 2H), 7.27 (s, 1H), 7.25 (s, 2H), 7.15 (m, 5H), 6.95 (d, J = 3.5 Hz, 1H), 6.64 (m, 1H), 6.45 (d, J = 8.2 Hz, 2H), 4.70 (s, 1H, H_a), 4.67 (s, 1H, H_b), 2.32 (s, 3H), 1.92 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 180.2, 168.8, 150.4, 150.0, 147.6, 147.2, 139.28, 139.21, 138.4, 129.7, 128.7, 128.66, 128.61, 128.0, 127.7, 126.1, 125.6, 124.5, 122.2, 121.8, 119.2, 113.3, 99.5, 49.6, 43.7, 21.2, 12.8 ppm.

HRMS (ESI): *m/z* calcd for $C_{33}H_{27}N_3O_4Na$ $[M + Na]^+$: 552.1894; found: 552.1899.

(*Z*)-3-((3-Methyl-5-oxo-1-phenyl-4,5-dihydro-1*H*-pyrazol-4-yl)(phenyl)methyl)-4-(thiophen-2-

ylmethylene)-1-(*p*-tolyl)pyrrolidine-2,5-dione (5j)

Yield: 117 mg (86%) as white solid; mp: 117–119 °C.

^{1}H NMR ($CDCl_3$, 500 MHz) δ: 11.66 (s, 1H, OH), 8.10 (s, 1H), 7.92 (d, J = 8.0 Hz, 2H), 7.69 (d, J = 5.0 Hz, 1H), 7.53 (d, J = 3.4 Hz, 1H), 7.46 (t, J = 7.9 Hz, 2H), 7.28 (dd, J = 7.9, 6.6 Hz, 3H), 7.25 (d, J = 3.4 Hz, 1H), 7.17–7.14 (m, 4H), 7.13 (d, J = 7.8 Hz, 1H), 6.44 (d, J = 8.1 Hz, 2H), 4.70 (s, 1H, H_a), 4.61 (s, 1H, H_b), 2.33 (s, 3H), 1.89 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 179.8, 168.8, 150.4, 147.7, 139.3, 139.1, 138.2, 136.6, 134.5, 132.8, 129.8, 129.79 129.0, 128.9, 128.8, 128.75, 128.71, 128.3, 128.0, 127.8, 126.2, 126.1, 125.6, 124.5, 121.8, 115.0, 99.0, 48.7, 42.6, 21.2, 13.0 ppm.

HRMS (ESI): *m/z* calcd for $C_{33}H_{28}N_3O_3S$ $[M + H]^+$: 546.1846; found: 546.1694.

(*Z*)-3-(Furan-2-ylmethylene)-4-((2-methoxyphenyl)(3-methyl-5-oxo-1-phenyl-4,5-dihydro-1*H*-pyrazol-4-yl)methyl)-1-phenylpyrrolidine-2,5-dione(5k)

Yield: 106 mg (78%) as white solid; mp: 110–112 °C.

^{1}H NMR ($CDCl_3$, 500 MHz) δ: 11.57 (s, 1H, OH), 7.92 (d, J = 8.4 Hz, 2H), 7.60 (s, 1H), 7.53 (s, 1H), 7.45 (t, J = 7.9 Hz, 2H), 7.35–7.33 (m, 1H), 7.33 (d, J = 2.2 Hz, 2H), 7.25–7.21 (m, 2H), 7.17 (d, J = 7.6 Hz,1H), 6.89 (d, J = 7.5 Hz, 1H), 6.86 (d, J = 3.3 Hz, 1H), 6.79 (d, J = 8.2 Hz, 1H), 6.62–6.59 (m, 3H), 5.22 (s, 1H, H_a), 4.69 (s, 1H, H_b), 3.64 (s, 3H), 1.96 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 180.5, 169.0, 156.7, 150.6, 150.5, 147.4, 146.6, 139.2, 131.3, 130.9, 129.0, 128.9, 128.8, 128.7, 126.8, 126.3, 125.6, 125.5, 121.7, 120.8, 120.3, 119.0, 117.8, 115.0, 113.0, 109.9, 100.9, 54.8, 50.0, 36.4, 12.7 ppm.

HRMS (ESI): *m/z* calcd for $C_{33}H_{27}N_3O_5Na$ $[M + Na]^+$: 568.1843; found: 568.1849.

(*Z*)-3-(Furan-2-ylmethylene)-4-((2-methoxyphenyl)(3-methyl-5-oxo-1-phenyl-4,5-dihydro-1*H*-pyrazol-4-yl)methyl)-1-(*p*-tolyl)pyrrolidine-2,5-dione (5l)

Yield: 116 mg (83%) as white solid; mp: 102–104 °C.

^{1}H NMR ($CDCl_3$, 500 MHz) δ: 11.59 (s, 1H, OH), 7.92 (d, J = 7.7 Hz, 2H), 7.60 (s, 1H), 7.52 (d, J = 1.4 Hz, 1H), 7.45 (t, J = 8.0 Hz, 2H), 7.26–7.20 (m, 3H), 7.17–7.12 (m, 3H), 6.88 (d, J = 7.1 Hz, 1H), 6.85 (d,

J = 3.3 Hz, 1H), 6.79 (d, *J* = 8.1 Hz, 1H), 6.60 (dd, *J* = 3.2, 1.7 Hz, 1H), 6.49 (d, *J* = 8.2 Hz, 1H), 5.22 (s, 1H, H_a), 4.68 (s, 1H, H_b), 3.64 (s, 3H), 2.33 (s, 3H), 1.95 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 180.5, 169.1, 156.7, 150.6, 150.5, 147.4, 146.4, 139.3, 139.0, 131.3, 129.7, 128.7, 128.6, 128.3, 126.8, 126.1, 125.7, 125.4, 121.6, 120.8, 120.1, 117.6, 113.0, 109.9, 100.8, 54.8, 50.0, 36.3, 21.1, 12.6 ppm.

HRMS (ESI): *m/z* calcd for $C_{34}H_{30}N_3O_5$ $[M + H]^+$: 560.2180; found: 560.2183.

(*Z*)-3-((2,5-Dimethoxyphenyl)(3-methyl-5-oxo-1-phenyl-4,5-dihydro-1*H*-pyrazol-4-yl)methyl)-4-(furan-2-ylmethylene)-1-phenylpyrrolidine-2,5-dione (5m)

Yield: 109 mg (76%) as white solid; mp: 101–103 ^{o}C.

^{1}H NMR ($CDCl_3$, 500 MHz) δ: 11.53 (s, 1H, OH), 7.90 (d, *J* = 7.9 Hz, 2H), 7.61 (s, 1H), 7.52 (s, 1H), 7.44 (t, *J* = 7.9 Hz, 2H), 7.38–7.35 (m, 1H), 7.35 (d, *J* = 1.1 Hz, 2H), 7.24 (d, *J* = 7.4 Hz, 1H), 6.86 (d, *J* = 3.3 Hz, 1H), 6.76–6.68 (m, 5H), 6.61–6.59 (m, 1H), 5.21 (s, 1H, H_a), 4.68 (s, 1H, H_b), 3.63 (s, 3H), 3.59 (s, 3H), 1.95 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 180.5, 169.0, 153.6, 150.8, 150.4, 147.5, 146.6, 139.2, 131.0, 129.0, 128.9, 128.7, 127.9, 126.3, 125.5, 125.2, 121.7, 120.5, 117.8, 117.3, 113.1, 113.0, 110.8, 100.7, 55.7, 55.2, 49.9, 36.4, 12.7 ppm.

HRMS (ESI): *m/z* calcd for $C_{34}H_{29}N_3O_6Na$ $[M + Na]^+$: 598.1949; found: 598.1952.

(*Z*)-3-((2,5-Dimethoxyphenyl)(3-methyl-5-oxo-1-phenyl-4,5-dihydro-1*H*-pyrazol-4-yl)methyl)-4-(furan-2-ylmethylene)-1-(*p*-tolyl)pyrrolidine-2,5-dione (5n)

Yield: 106 mg (72%) as white solid; mp: 102–104 ^{o}C.

^{1}H NMR ($CDCl_3$, 500 MHz) δ: 11.58 (s, 1H, OH), 7.90 (d, *J* = 7.8 Hz, 2H), 7.60 (s, 1H), 7.50 (d, *J* = 1.3 Hz,1H), 7.43 (d, *J* = 8.1 Hz, 2H), 7.24 (d, *J* = 7.4 Hz, 1H), 7.16 (d, *J* = 8.1 Hz, 2H), 6.85 (d, *J* = 3.4 Hz, 1H), 6.75–6.70 (m, 3H), 6.61–6.56 (m, 3H), 5.20 (s, 1H, H_a), 4.67 (s, 1H, H_b), 3.64 (s, 3H), 3.59 (s, 3H), 2.34 (s, 3H), 1.95 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 180.6, 169.1, 153.6, 150.8, 150.5, 147.5, 146.5, 139.2, 139.1, 129.7, 128.7, 128.3, 127.9, 126.1, 125.5, 125.3, 121.8, 120.4, 117.7, 117.3, 113.1, 113.0, 110.8, 100.7, 55.7, 55.2, 49.9, 36.3, 21.2, 12.7 ppm.

HRMS (ESI): *m/z* calcd for $C_{35}H_{32}N_3O_6$ [M + H] $^+$: 590.2286; found: 590.2114.

(*Z*)-3-((3-Bromophenyl)(3-methyl-5-oxo-1-phenyl-4,5-dihydro-1*H*-pyrazol-4-yl)methyl)-4-(furan-2-ylmethylene)-1-phenylpyrrolidine-2,5-dione (5o)

Yield: 123 mg (83%) as white solid; mp: 168–170 ^{o}C.

^{1}H NMR ($CDCl_3$, 500 MHz) δ: 11.61 (s, 1H, OH), 7.90 (d, *J* = 7.8 Hz, 2H), 7.71 (d, *J* = 1.4 Hz,1H), 7.67 (s, 1H), 7.46 (t, *J* = 7.9 Hz, 3H), 7.42–7.38 (m, 3H), 7.37 (s, 1H), 7.31 (s, 1H), 7.13 (t, *J* = 7.7 Hz, 1H), 7.08 (d, *J* = 7.8 Hz, 1H), 6.98 (d, *J* = 3.4 Hz,1H), 6.70 (dd, *J* = 7.6, 1.7, 2H), 6.66 (dd, *J* = 3.3, 1.7 Hz, 1H), 4.73 (s, 1H, H_a), 4.64 (s, 1H, H_b), 1.91(s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 179.9, 168.4, 150.2, 149.8, 147.49, 147.45, 140.8, 139.0, 131.3, 130.9, 130.6, 130.2, 129.2, 128.8, 127.3, 126.1, 125.7, 123.7, 122.8, 122.7, 121.8, 119.7, 114.9, 113.5, 98.7, 49.3, 43.4, 12.9 ppm.

HRMS (ESI): *m/z* calcd for $C_{32}H_{24}N_3O_4BrNa$ [M + Na] $^+$: 616.0842; found: 616.0846.

(*Z*)-3-((3-Bromophenyl)(3-methyl-5-oxo-1-phenyl-4,5-dihydro-1*H*-pyrazol-4-yl)methyl)-4-(furan-2-ylmethylene)-1-(*p*-tolyl)pyrrolidine-2,5-dione (5p)

Yield: 120 mg (79%) as white solid; mp: 116–118 ^{o}C.

^{1}H NMR ($CDCl_3$, 500 MHz) δ: 11.64 (s, 1H, OH), 7.86 (d, *J* = 7.8 Hz, 2H), 7.63 (d, *J* =1.5 Hz, 1H), 7.59 (s, 1H), 7.41–7.38 (m, 2H), 7.22–7.18 (m, 1H), 7.13 (s, 1H), 7.11(s, 1H), 7.08(d, J = 7.7 Hz, 1H), 7.06 (s, 1H), 7.03 (dd, *J* = 9.8, 3.2 Hz, 2H), 6.89 (d, *J* = 3.5 Hz, 1H), 6.57 (dd, *J* = 3.4, 1.7 Hz, 1H), 6.53 (d, *J* = 8.3 Hz, 2H), 4.64 (s, 1H, H_a), 4.58 (s, 1H, H_b), 2.28 (s, 3H), 1.86 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 180.1, 168.6, 150.4, 149.9, 147.6, 147.4, 141.0, 139.4, 139.1, 131.4, 131.0, 130.3, 129.9, 128.94, 128.93, 128.9, 128.8, 128.1, 127.4, 126.0, 125.8, 123.9, 122.9, 122.6, 121.9, 119.7, 113.5, 98.9, 49.4, 43.4, 21.3, 13.0 ppm.

HRMS (ESI): *m/z* calcd for $C_{33}H_{27}N_3O_4Br$ [M + H] $^+$: 608.1179; found: 608.0943.

(*Z*)-3-((3-Bromophenyl)(3-methyl-5-oxo-1-phenyl-4,5-dihydro-1*H*-pyrazol-4-yl)methyl)-4-(thiophen-2-ylmethylene)-1-(*p*-tolyl)pyrrolidine-2,5-dione (5q)

Yield: 133 mg (85%) as white solid; mp: 138–140 ºC.

^{1}H NMR ($CDCl_3$, 500 MHz) δ: 11.61 (s, 1H, OH), 8.12 (s, 1H), 7.90 (dd, J = 8.8, 1.1 Hz, 1H), 7.70 (d, J = 5.6 Hz, 1H), 7.53 (d, J = 4.1 Hz, 1H), 7.48–7.46 (m, 1H), 7.44 (s, 1H), 7.41 (m, 1H), 7.33 (s, 1H), 7.31–7.28 (m, 2H), 7.24 (s, 1H), 7.18 (d, J = 8.6 Hz, 2H), 7.12 (d, J = 7.9 Hz, 1H), 7.07 (dd, J = 8.1, 0.9 Hz, 1H), 6.57 (d, J = 8.7 Hz, 2H), 4.66 (s, 1H, H_a), 4.61 (s, 1H, H_b), 2.35 (s, 3H), 1.88 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 179.6, 168.6, 150.4, 147.7, 140.8, 139.5, 139.1, 136.5, 134.8, 133.1, 131.6, 131.2, 130.3, 129.9, 129.5, 129.1, 128.94, 128.93, 128.91, 128.8, 128.0, 127.5, 126.0, 125.8, 123.9, 122.9, 121.9, 98.4, 48.5, 42.3, 21.3, 13.1 ppm.

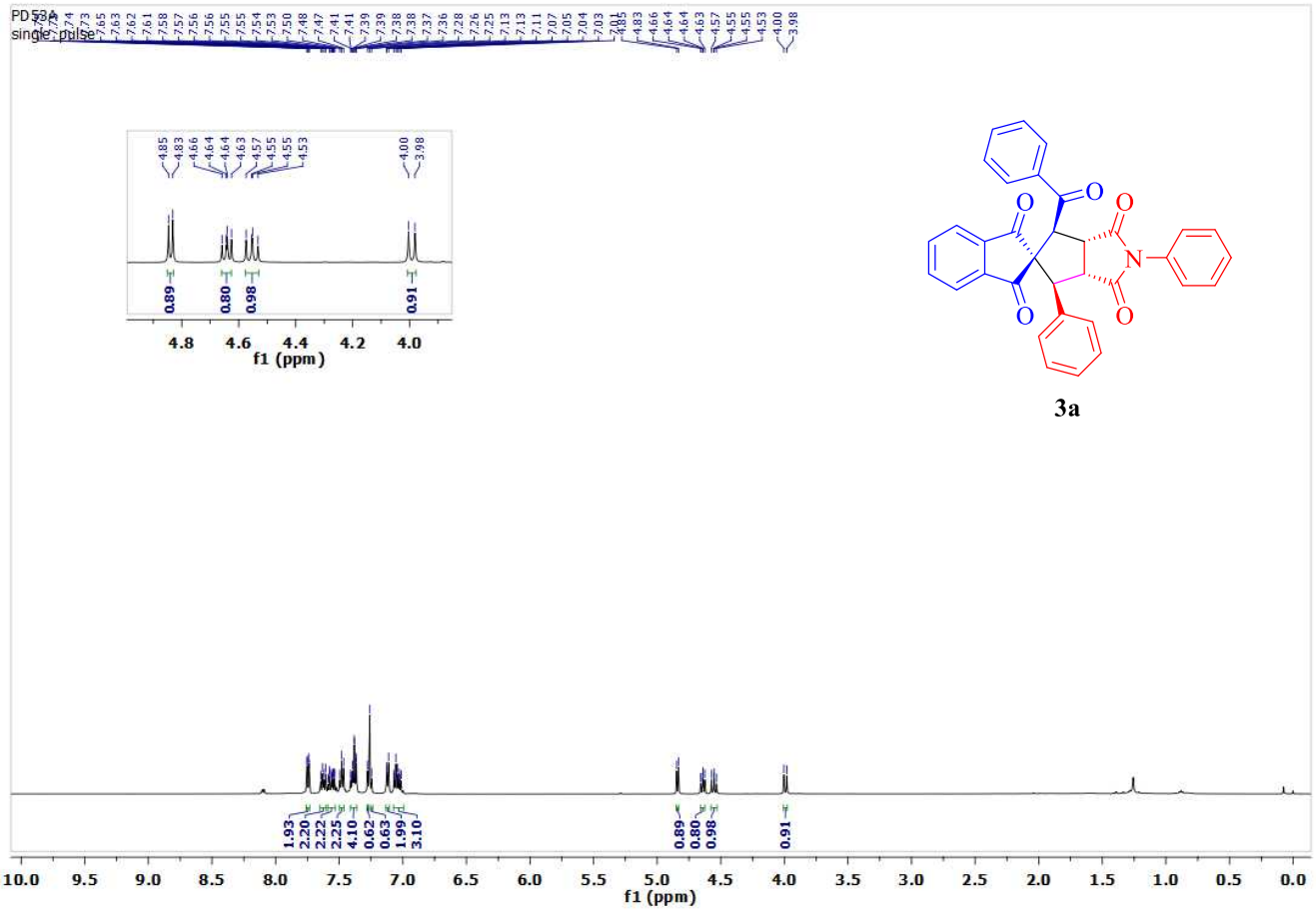
HRMS (ESI): *m/z* calcd for $C_{33}H_{27}N_3O_3Br$ $[M + H]^+$: 624.0951; found: 624.0746.

(*Z*)-3-(Furan-2-ylmethylene)-4-((3-methyl-5-oxo-1-phenyl-4,5-dihydro-1*H*-pyrazol-4-yl)(thiophen-2-yl)methyl)-1-(*p*-tolyl)pyrrolidine-2,5-dione (5r)

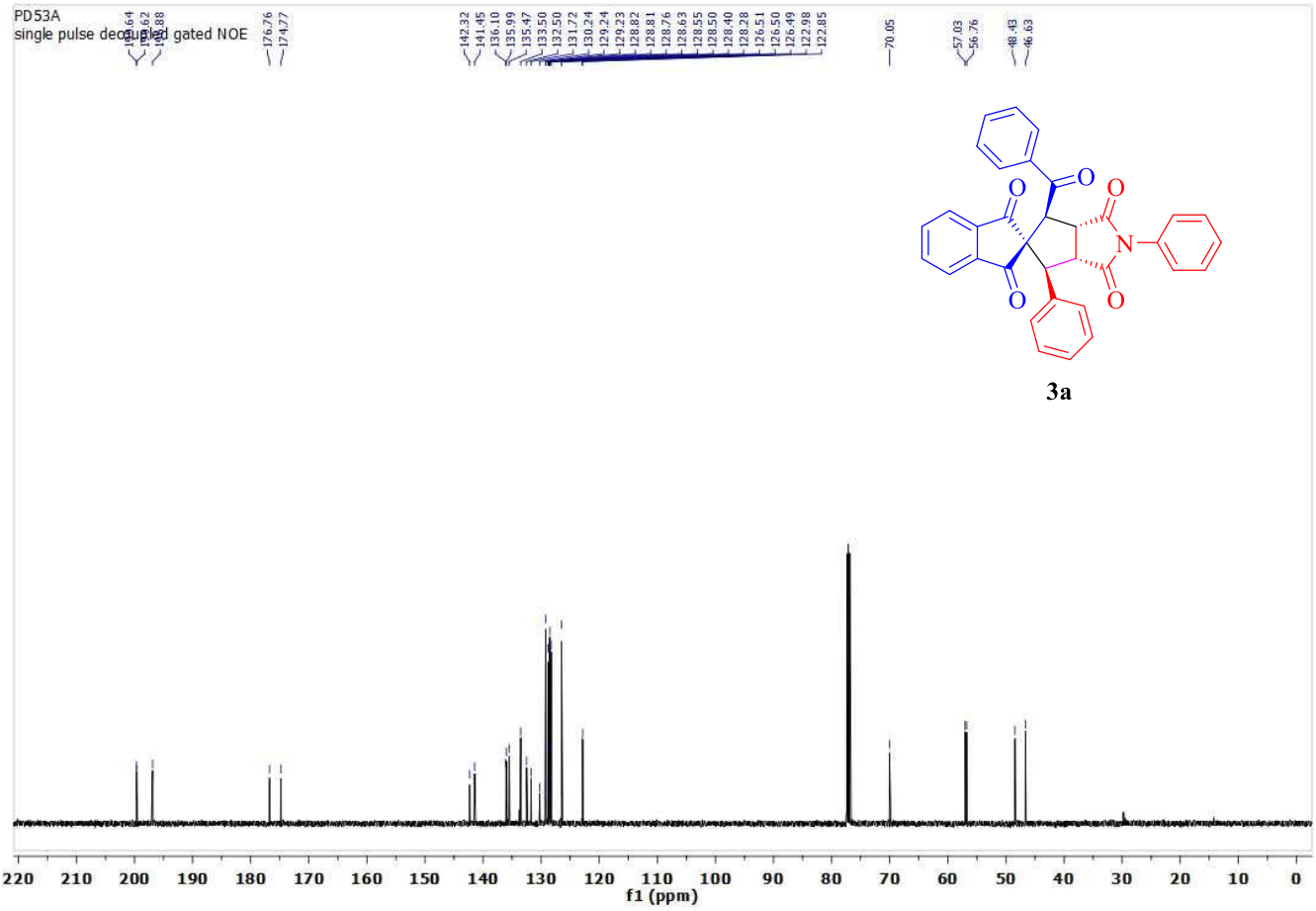
Yield: 87 mg (65%) as white solid; mp: 120–122 ºC.

^{1}H NMR ($CDCl_3$, 500 MHz) δ: 11.73 (s, 1H, OH), 7.89 (d, J = 7.9 Hz, 2H), 7.71 (s, 1H), 7.66 (s, 1H), 7.44 (t, J = 7.8 Hz, 2H), 7.24 (d, J = 7.5 Hz, 1H), 7.19 (d, J = 8.0 Hz, 2H), 7.16 (d, J = 4.9 Hz, 1H), 6.94 (d, J = 3.2 Hz, 1H), 6.93-6.90 (m, 1H), 6.82 (d, J = 2.9 Hz, 1H), 6.67 (d, J = 8.1 Hz, 2H), 6.64 (s, 1H), 4.88 (s, 1H, H_a), 4.69 (s, 1H, H_b), 2.35 (s, 3H), 1.98 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 180.0, 168.8, 149.99, 149.96, 147.4, 147.2, 141.6, 139.3, 139.1, 129.8, 128.7, 128.3, 127.1, 126.5, 126.1, 125.6, 124.8, 124.2, 122.6, 121.8, 119.4, 113.4, 99.8, 49.7, 39.0, 21.2, 12.7 ppm.

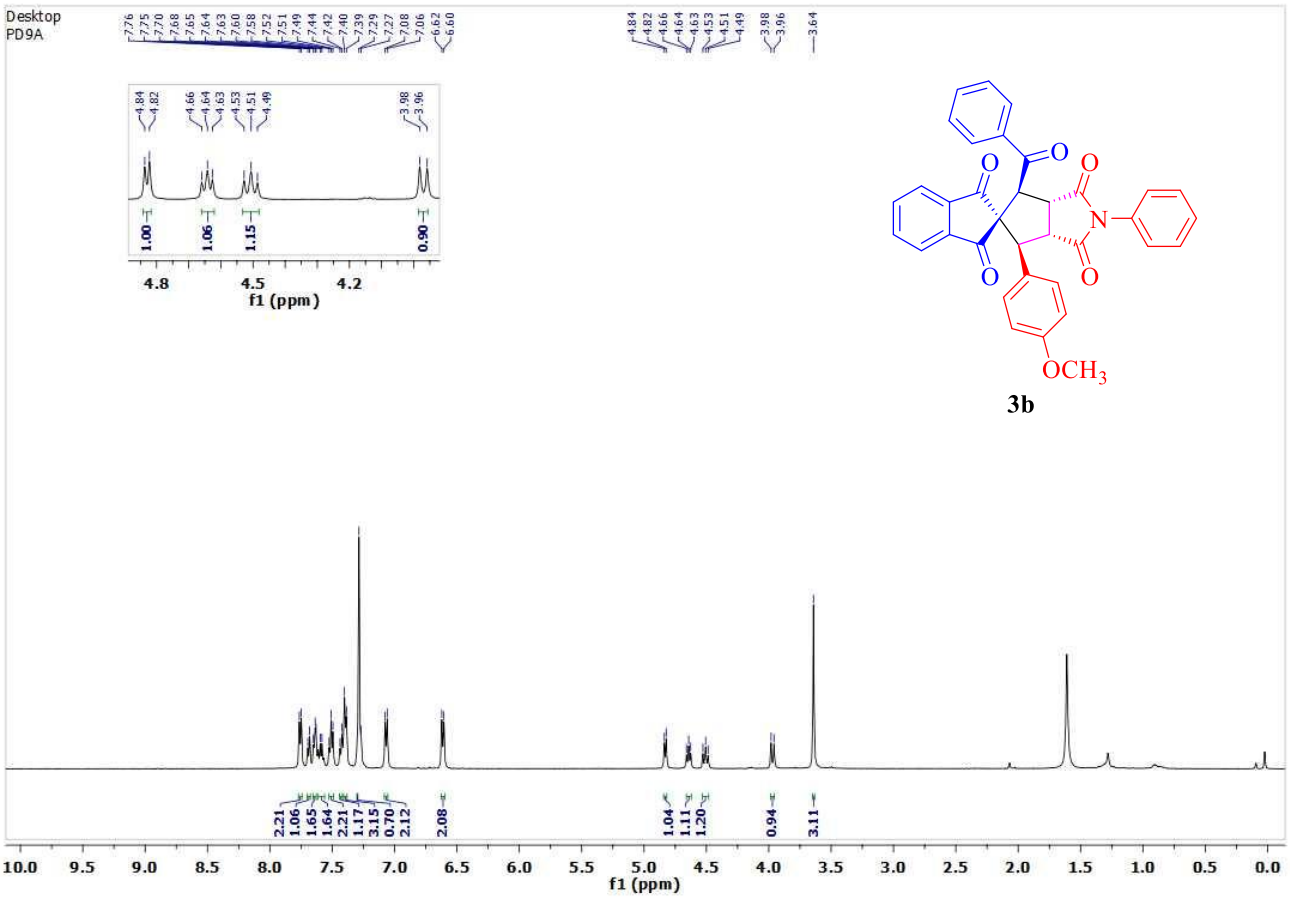
HRMS (ESI): *m/z* calcd for $C_{31}H_{25}SN_3O_4Na$ $[M + Na]^+$: 558.1458; found: 558.1464.

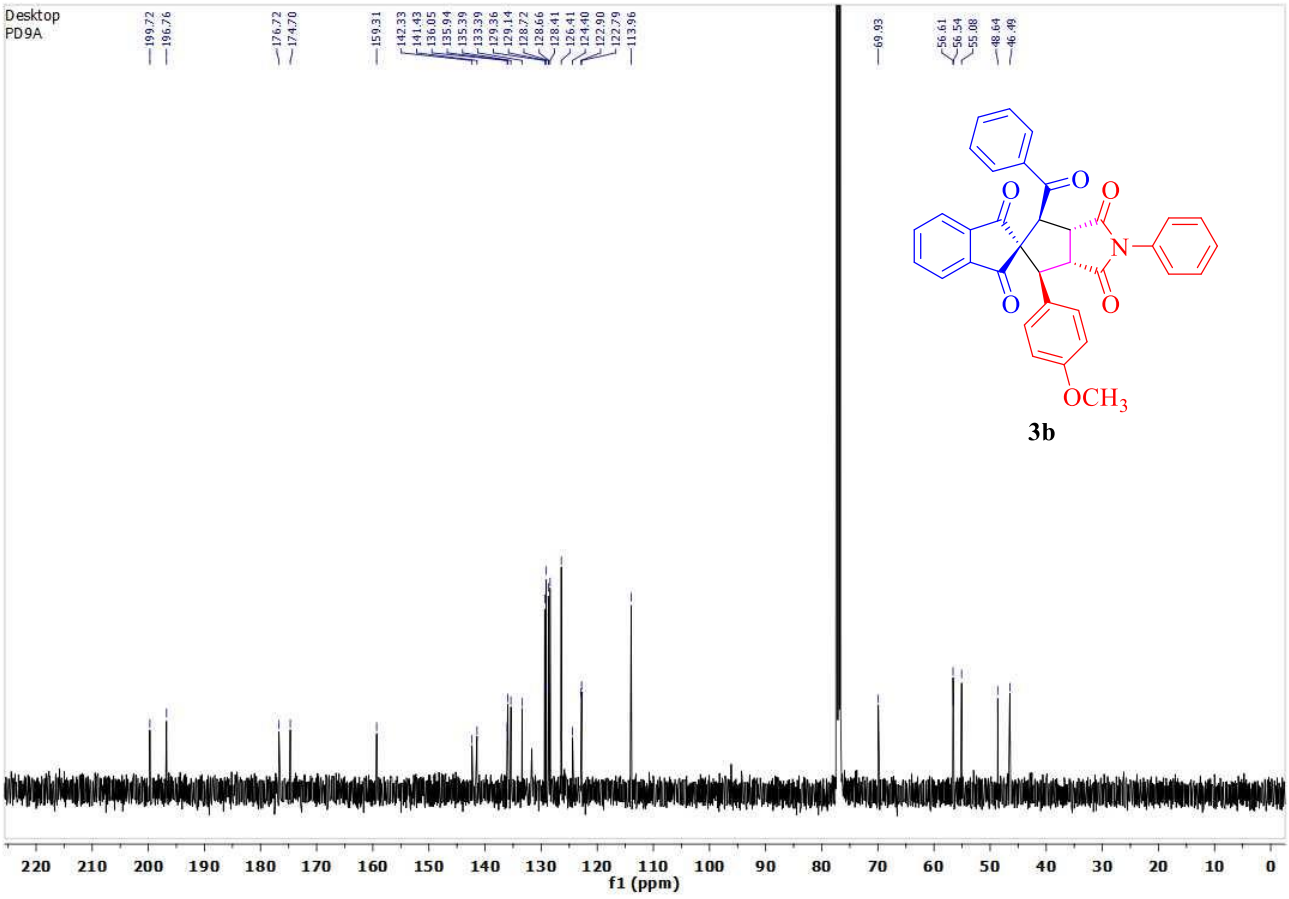

PD53A
single pulse
4.8
4.6
4.4
4.2
4.0
f1 (ppm)
0.89
0.80
0.98
0.91
1.93
2.20
2.22
2.25
4.10
0.62
0.63
1.99
3.10
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

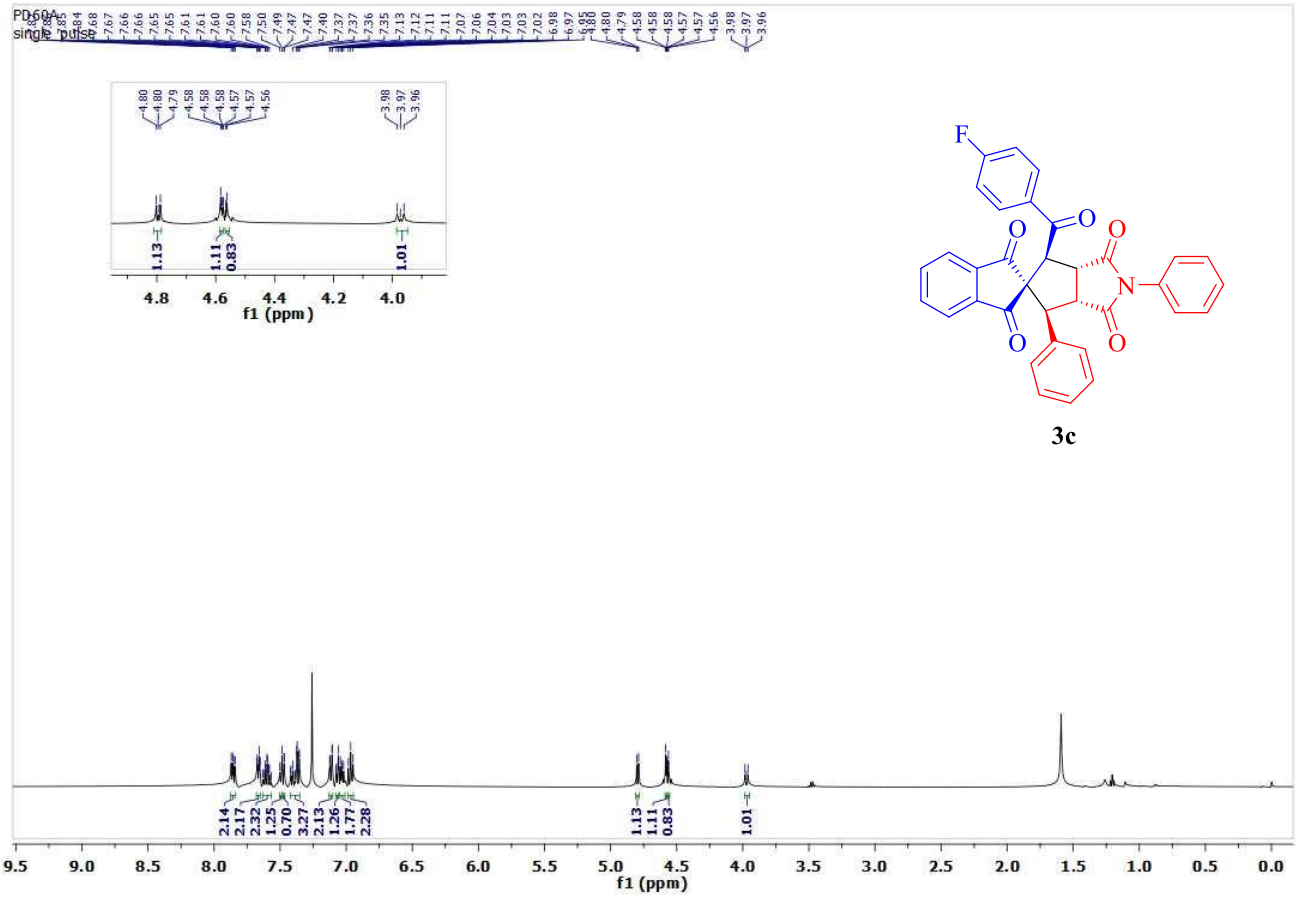
3a


PD53A
single pulse decoupled gated NOE
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

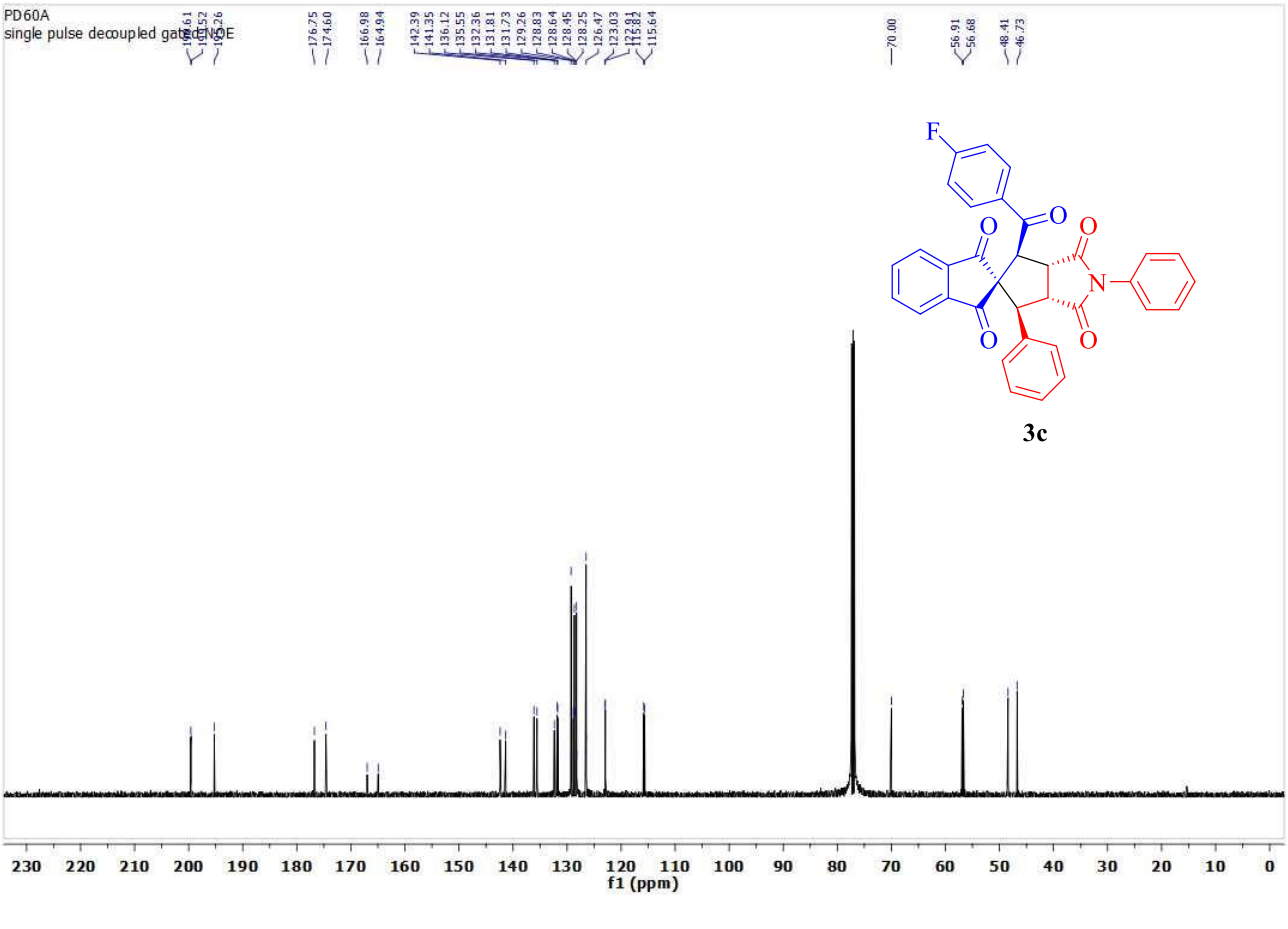
3a


Desktop
PD9A
f1 (ppm)
3b

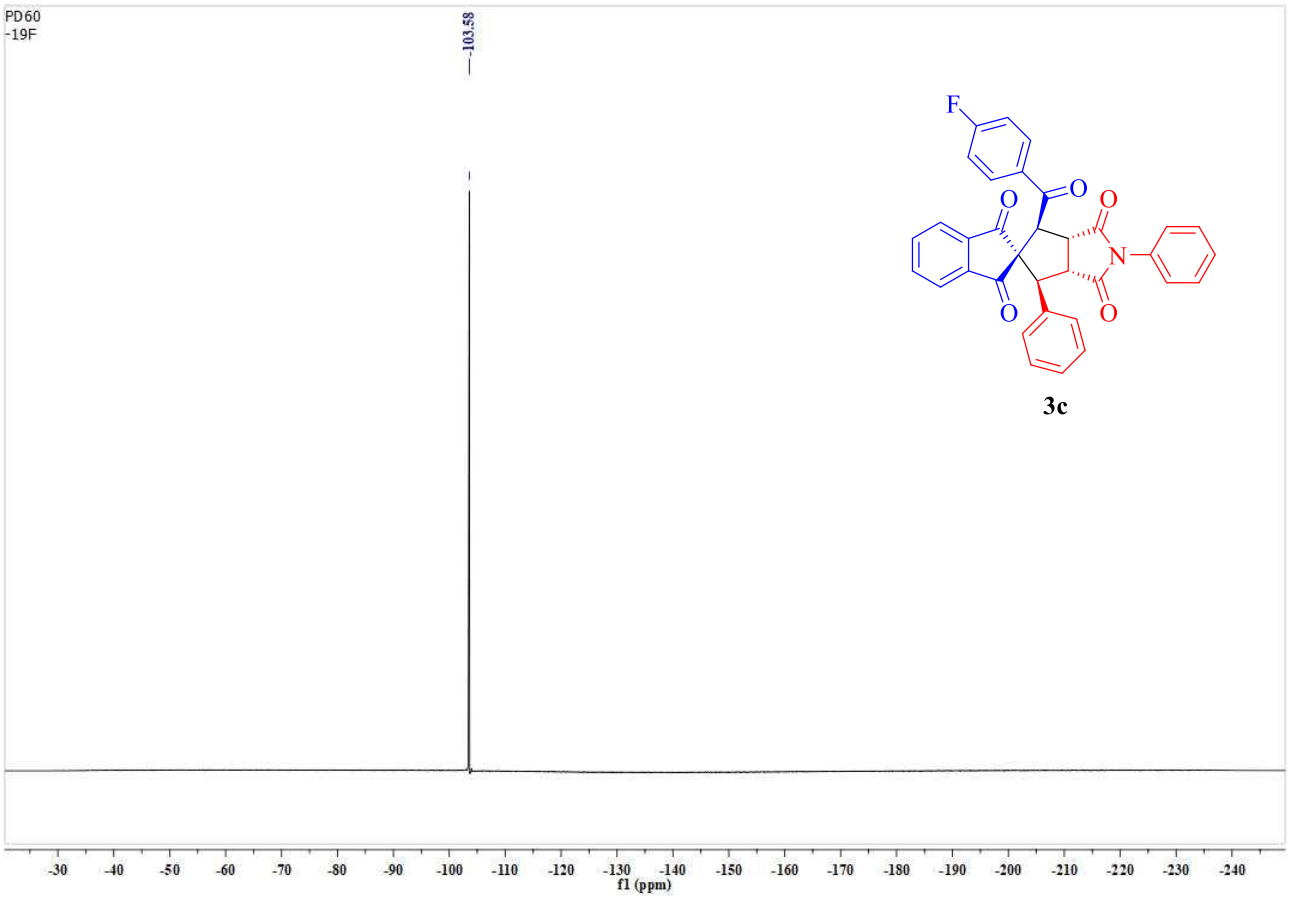

Desktop
PD9A
f1 (ppm)
3b


PD60A
single pulse
f1 (ppm)

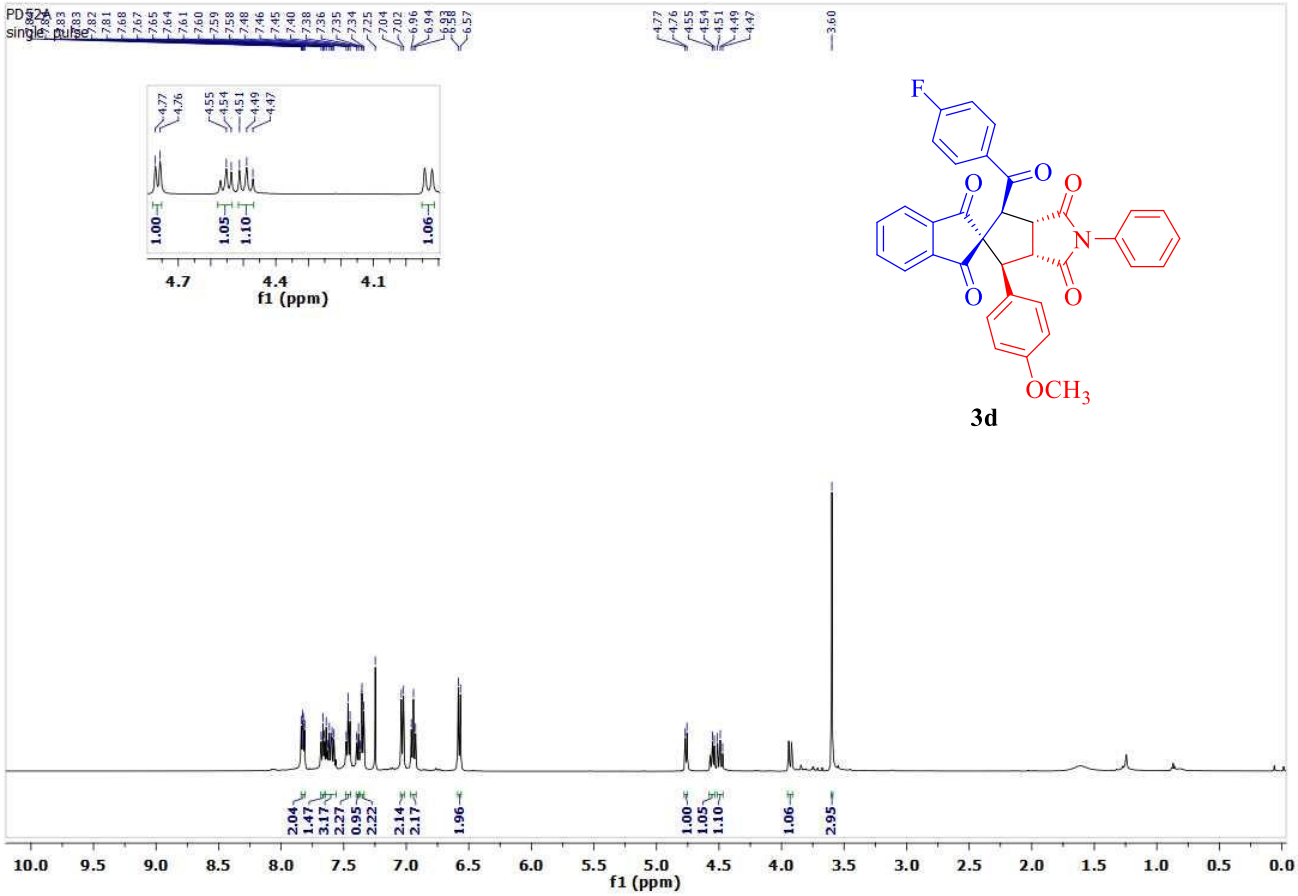
3c


PD60A
single pulse decoupled gated NOE
f1 (ppm)

3c

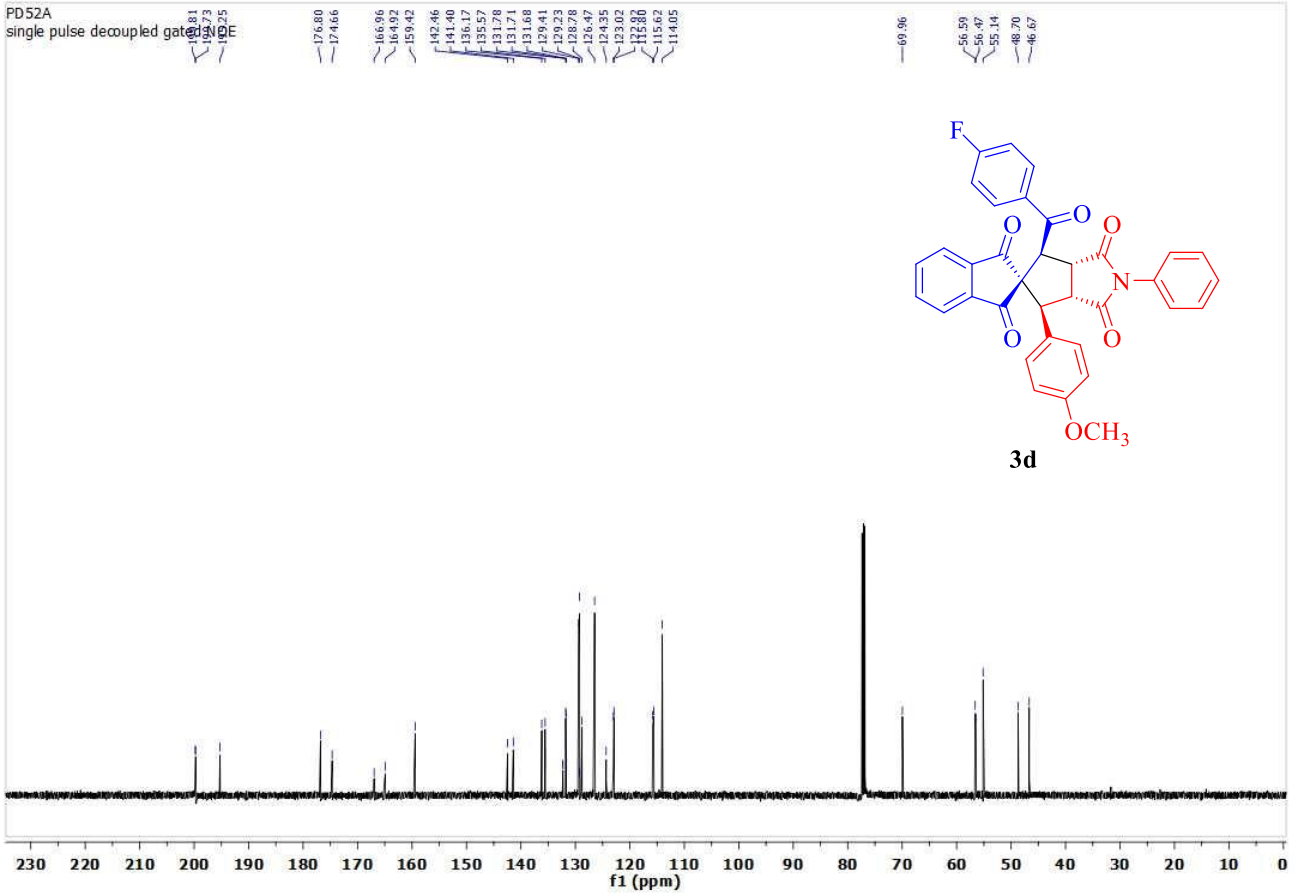

PD60
-19F
-103.58
F
O
O
O
O
N
O
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-220
-230
-240
f1 (ppm)

3c


PD52A
single pulse
f1 (ppm)

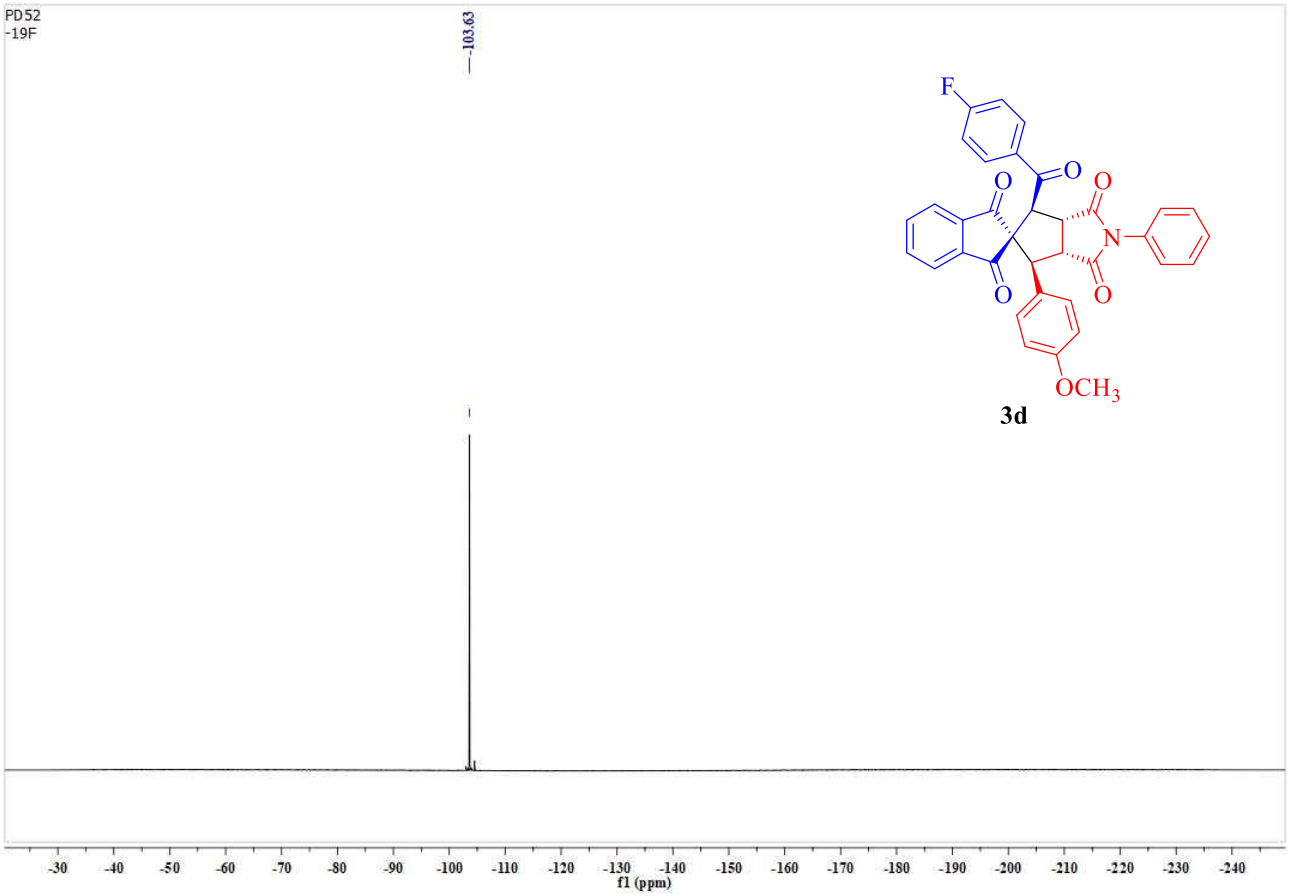
F
O
O
O
O
O
N
O
OCH3

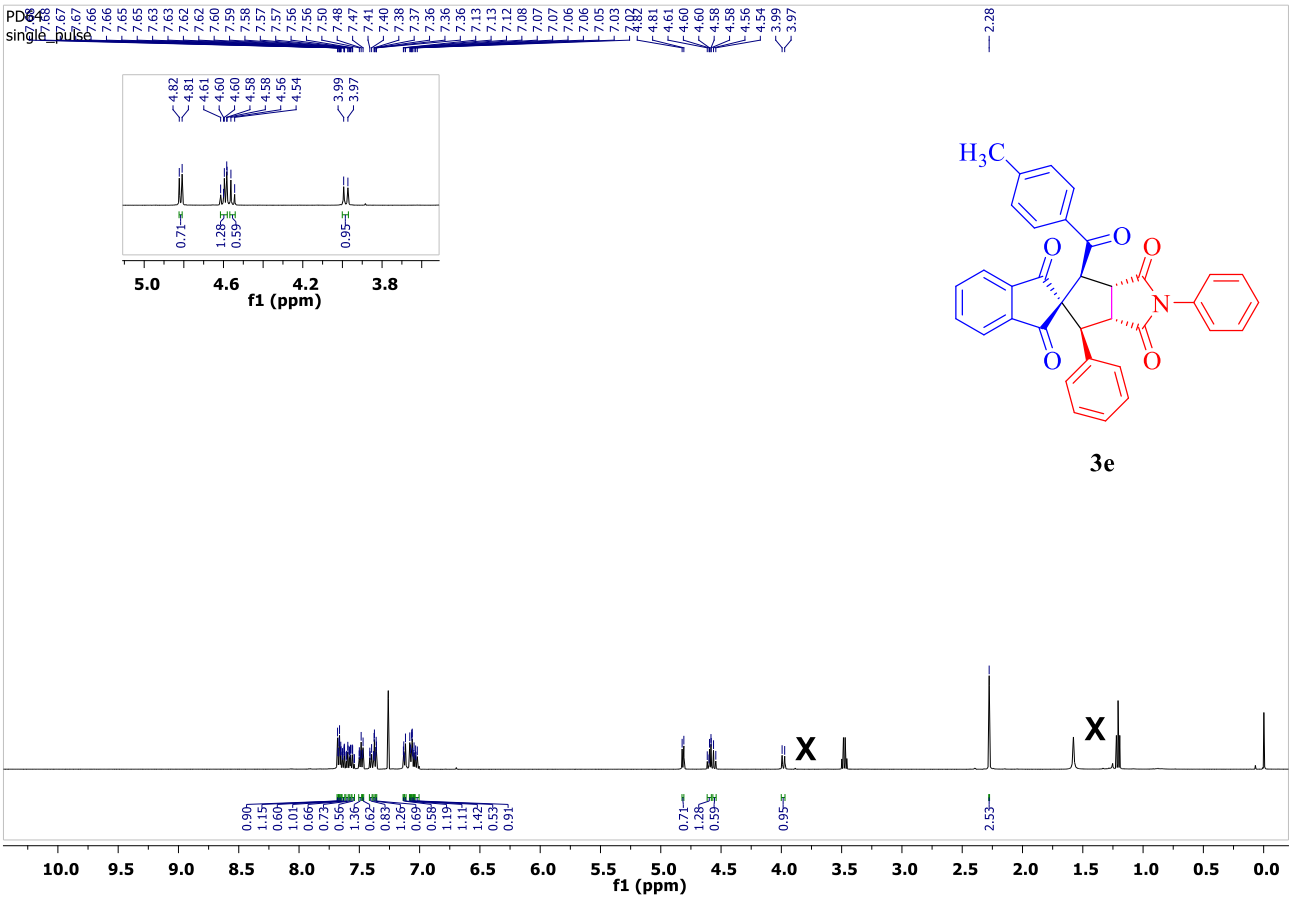
3d

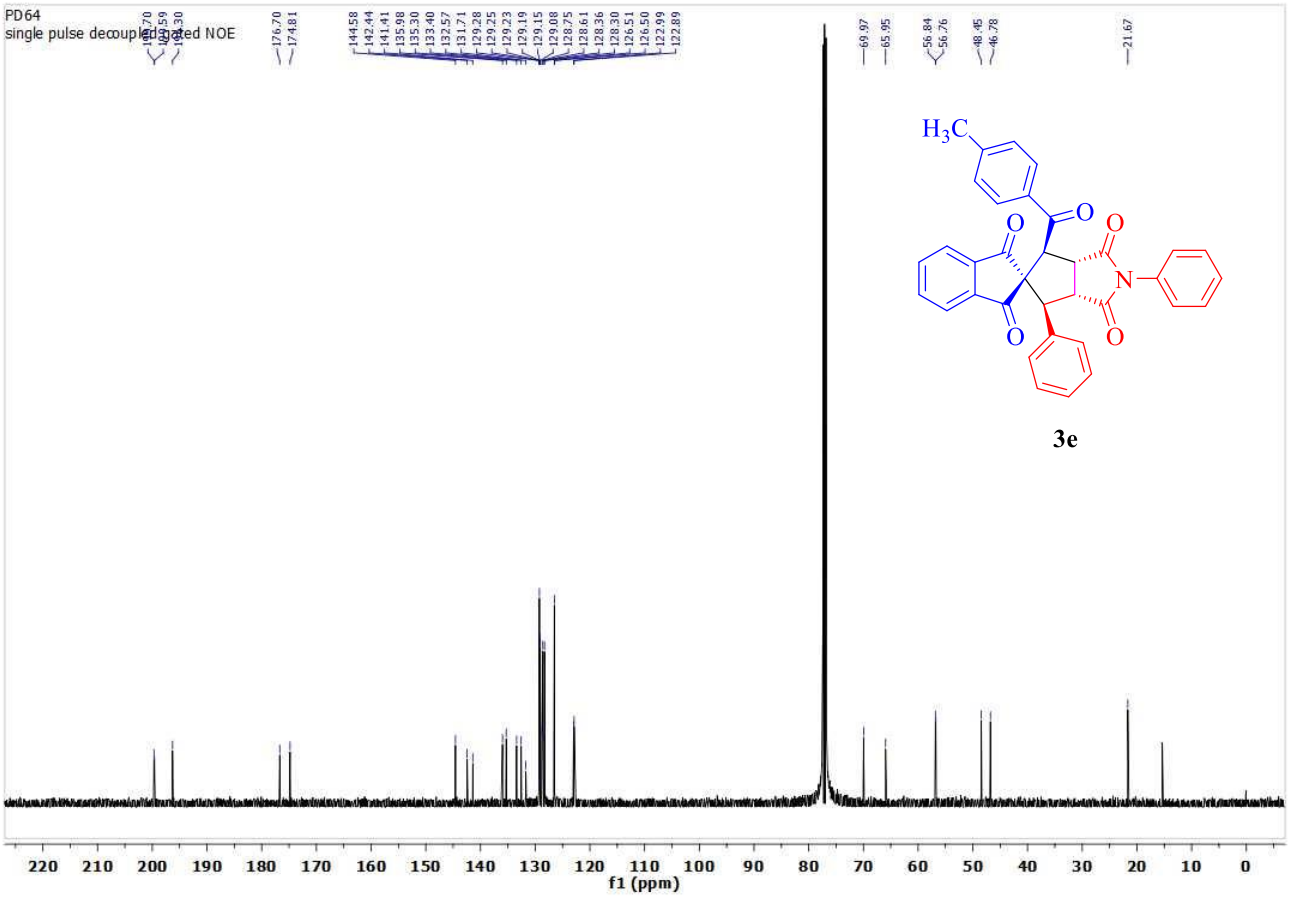

PD52A
single pulse decoupled gated NOE
f1 (ppm)

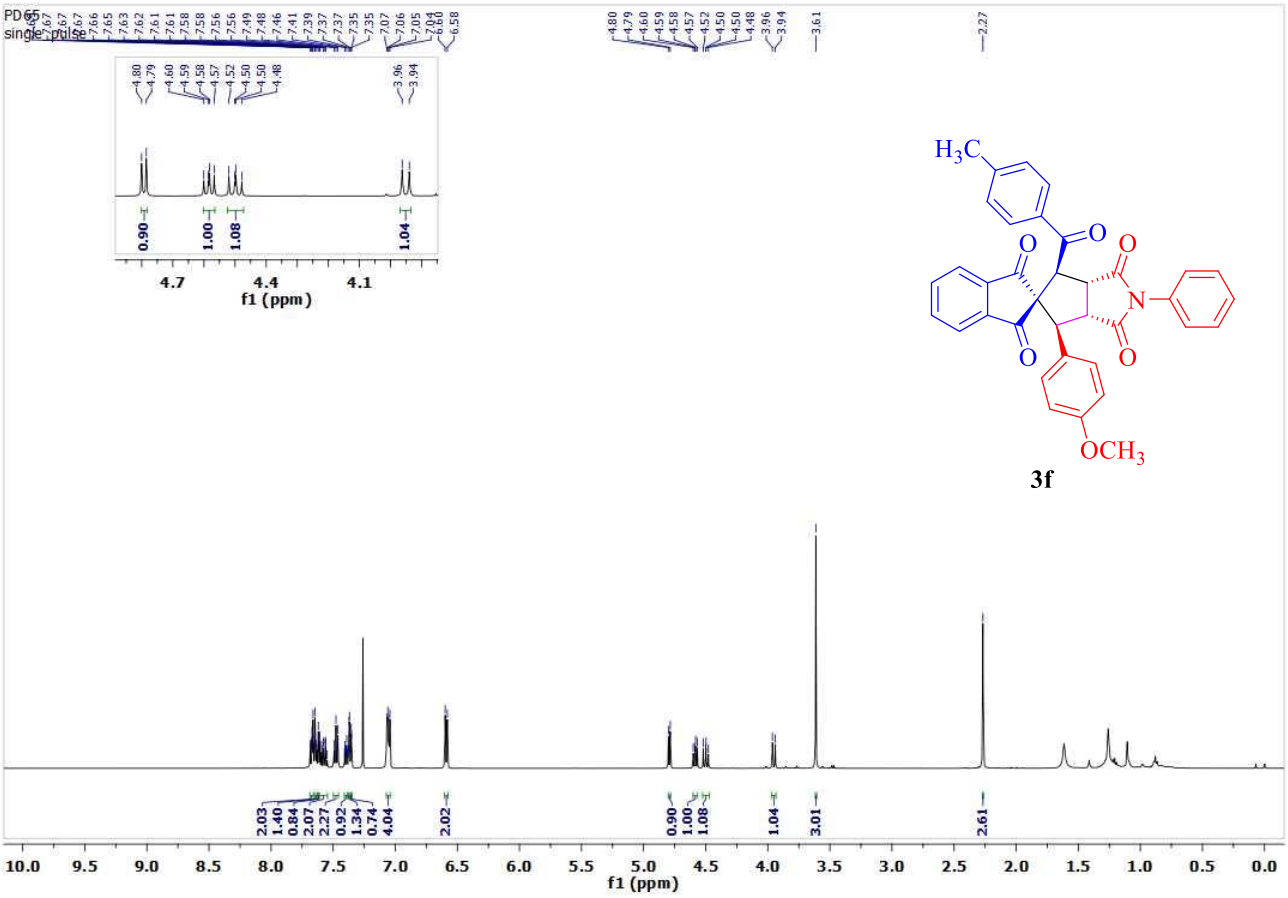
F
O
O
O
O
O
N
O
OCH3

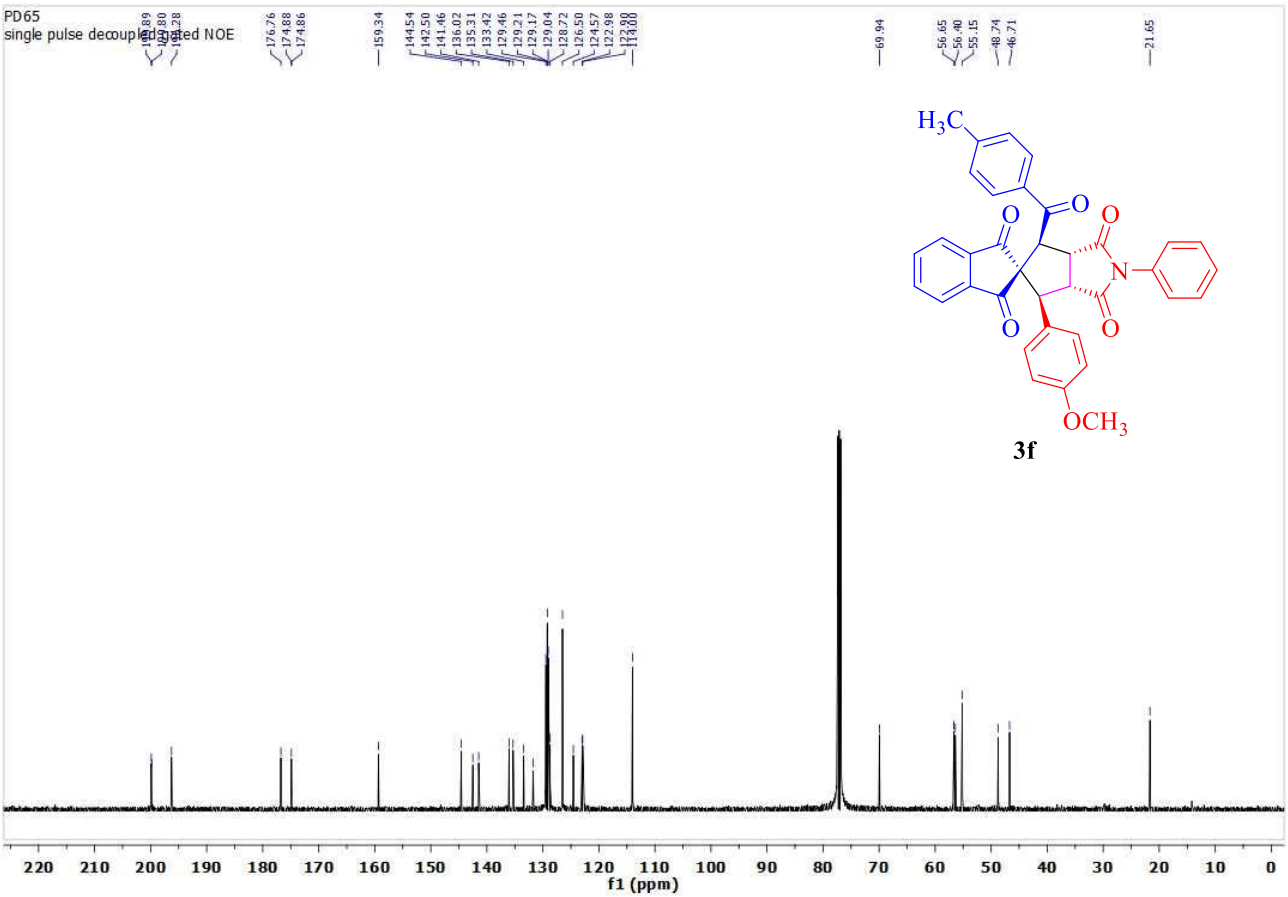
3d

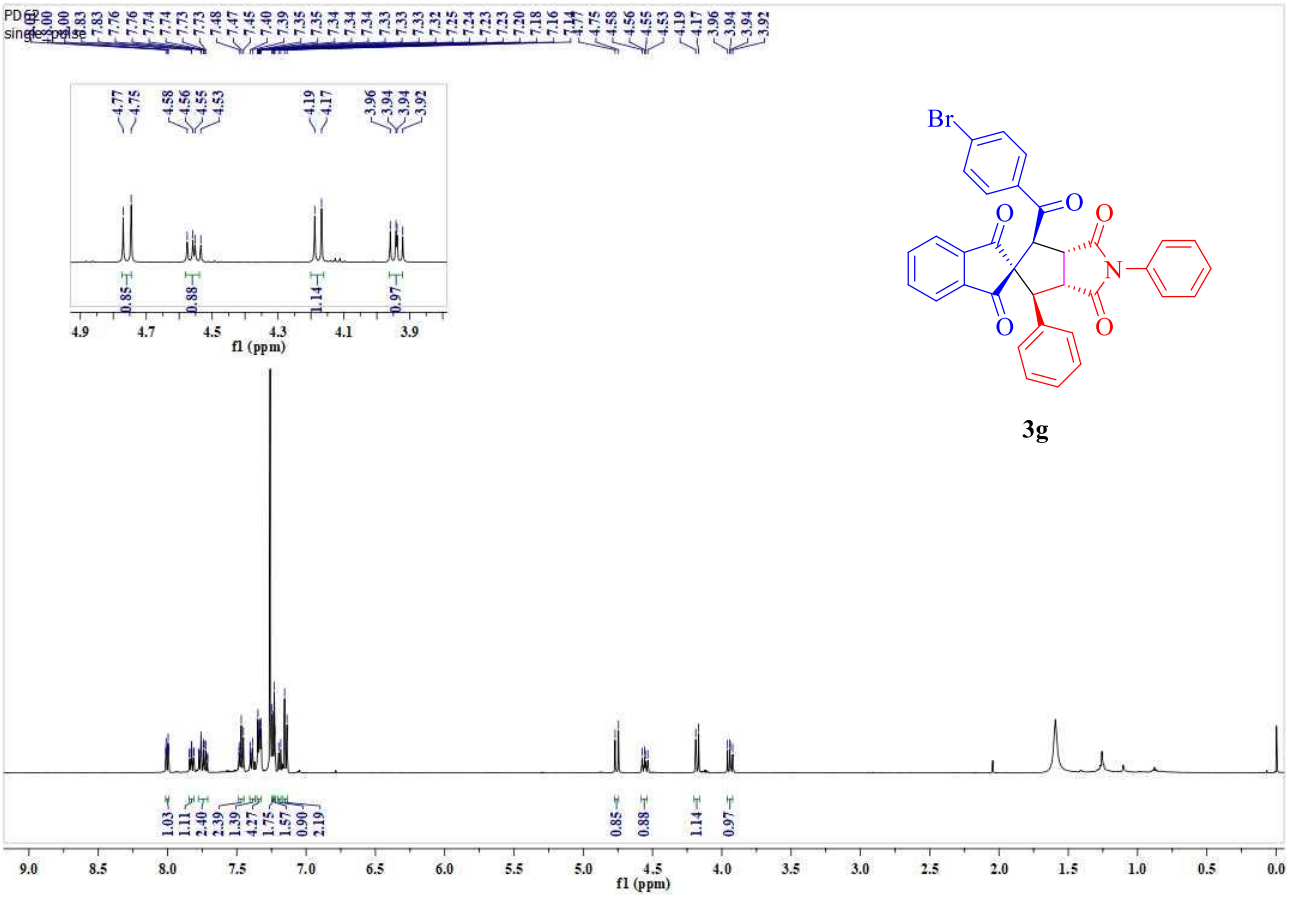

PD52
-19F
-103.63
F
O
O
O
O
N
O
O
OCH3
3d
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-220
-230
-240
f1 (ppm)

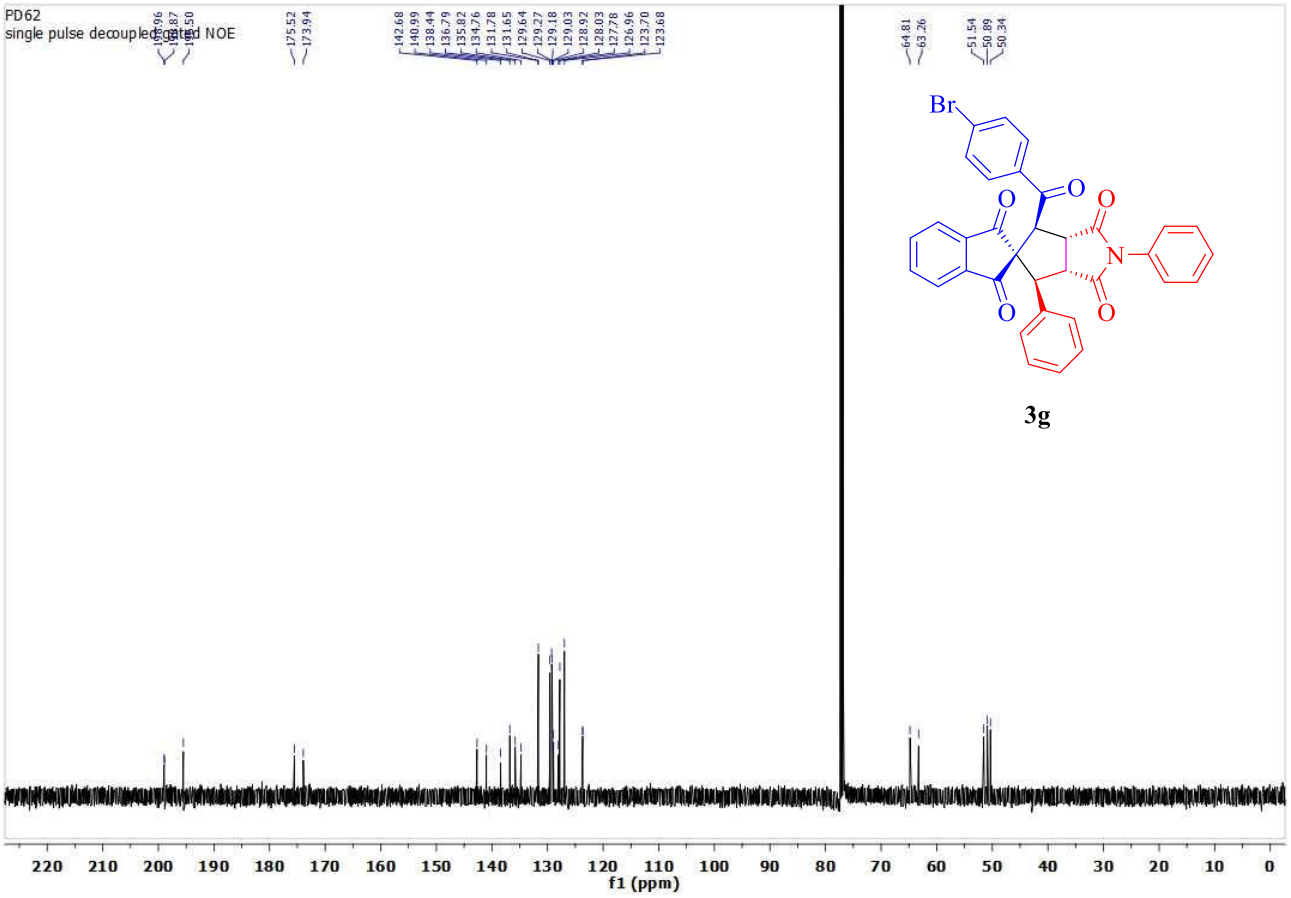

PD64
single_pulse
f1 (ppm)
3e

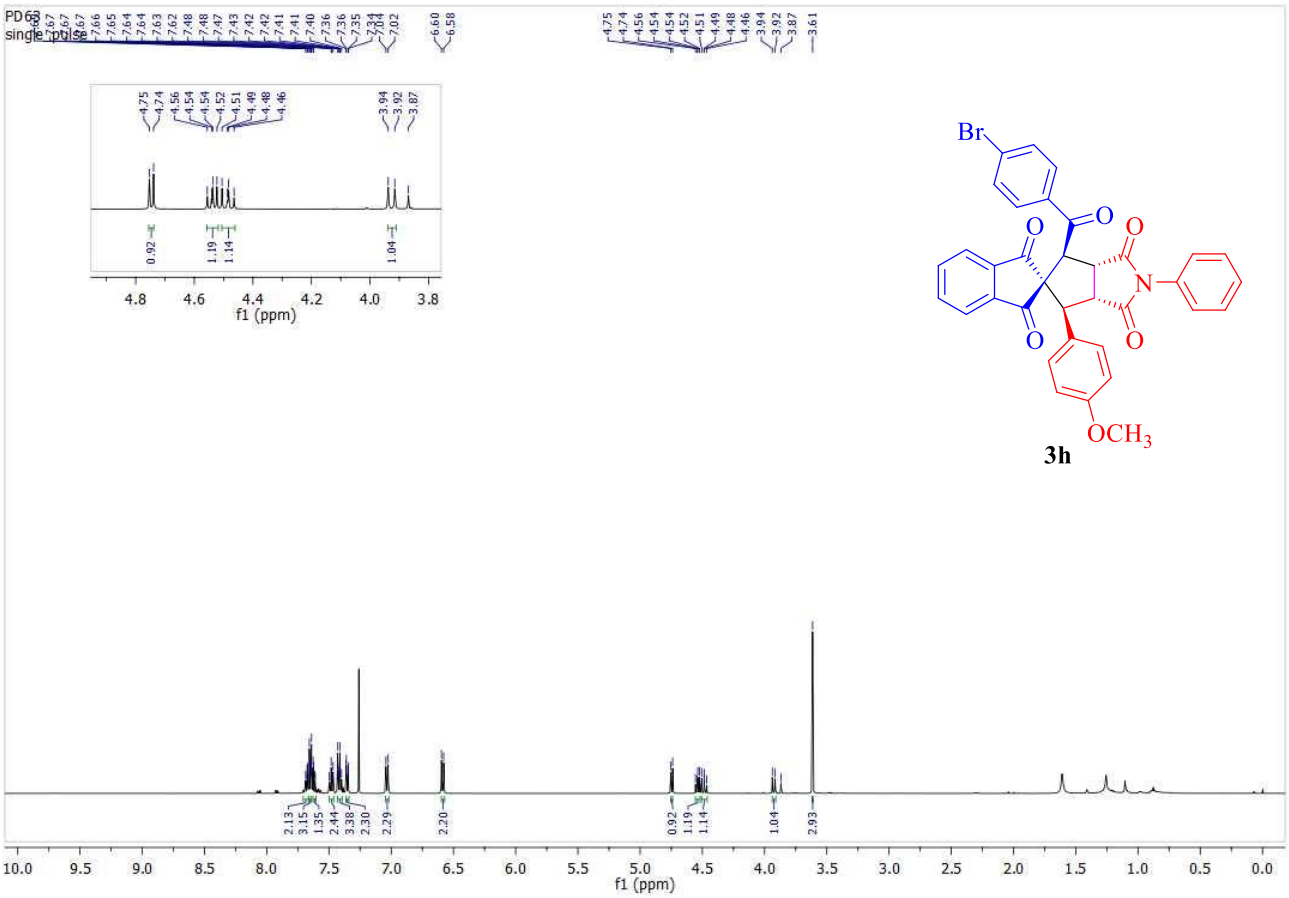

PD64
single pulse decoupled gated NOE
f1 (ppm)
3e

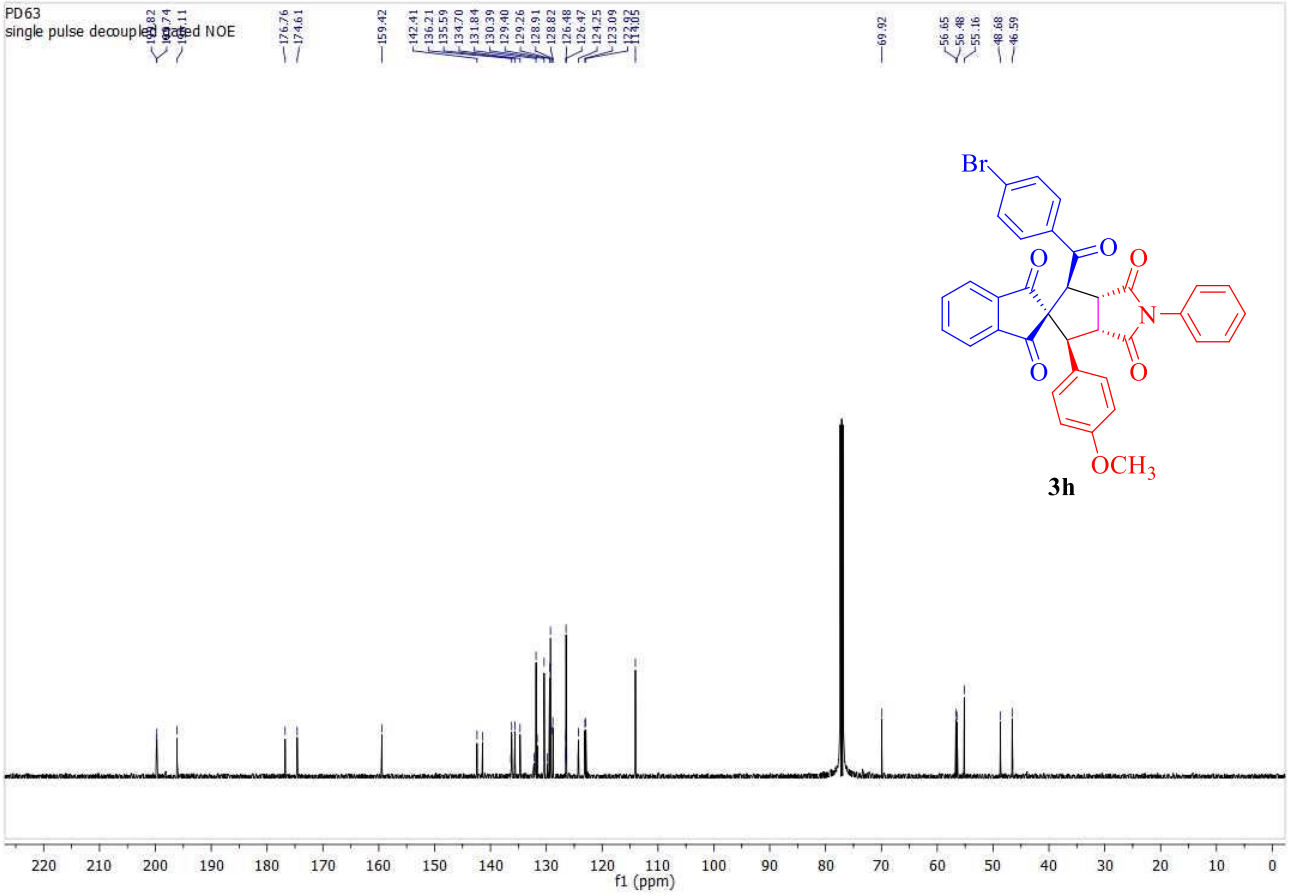

PD65
single pulse
f1 (ppm)
3f

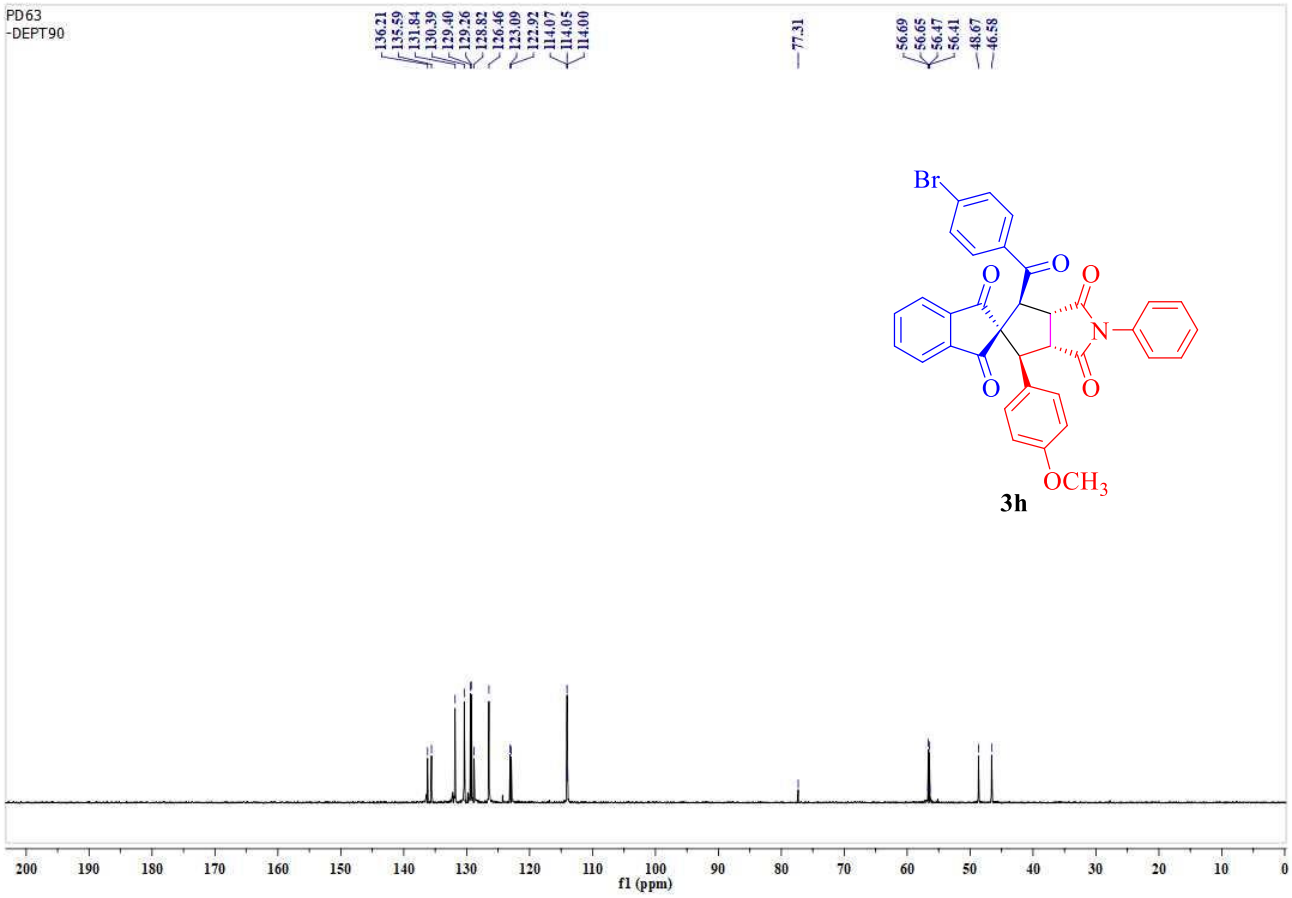

PD65
single pulse decoupled gated NOE
f1 (ppm)
3f

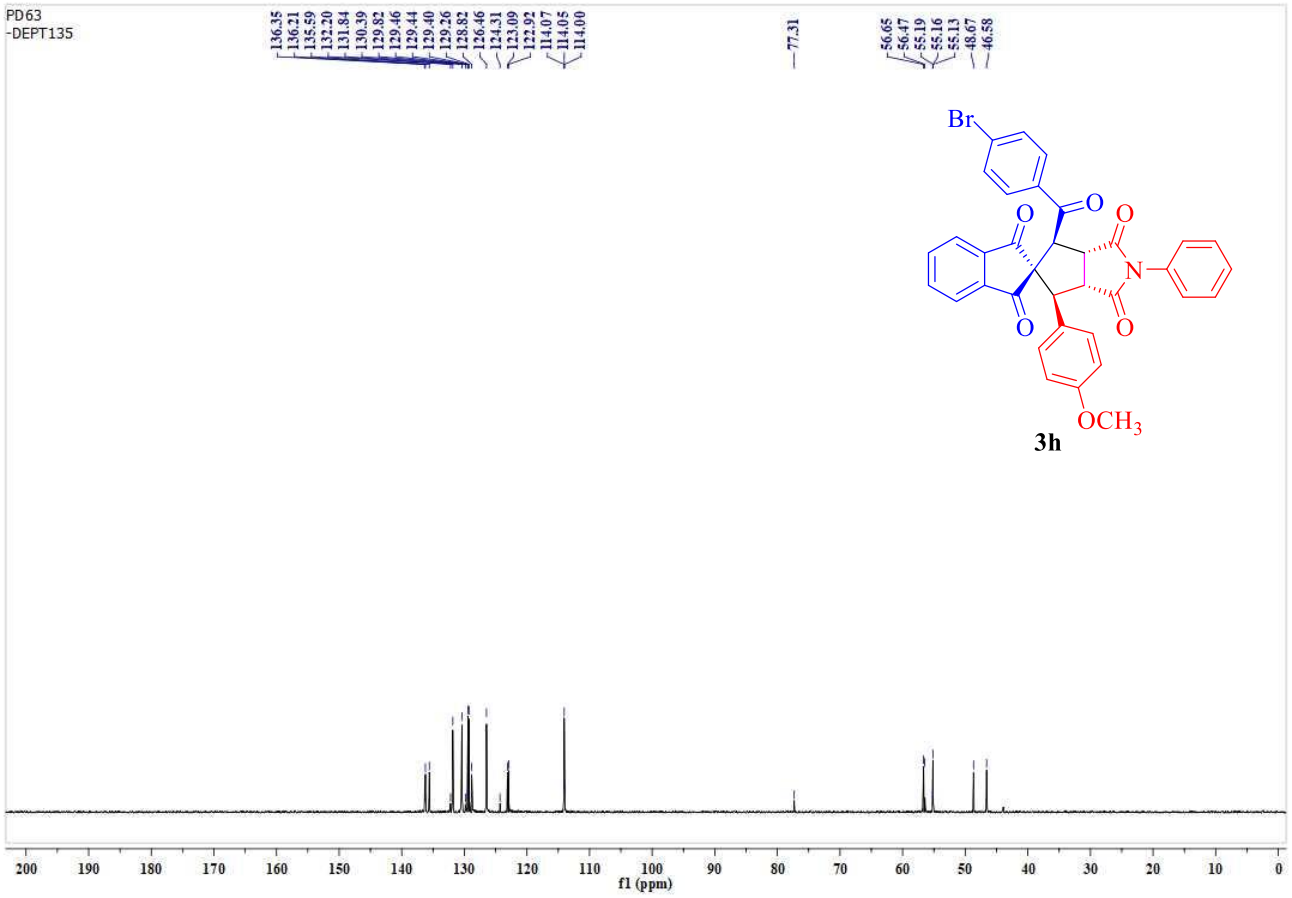

PD62
single pulse
Br
O
O
O
O
N
O
O
3g
f1 (ppm)

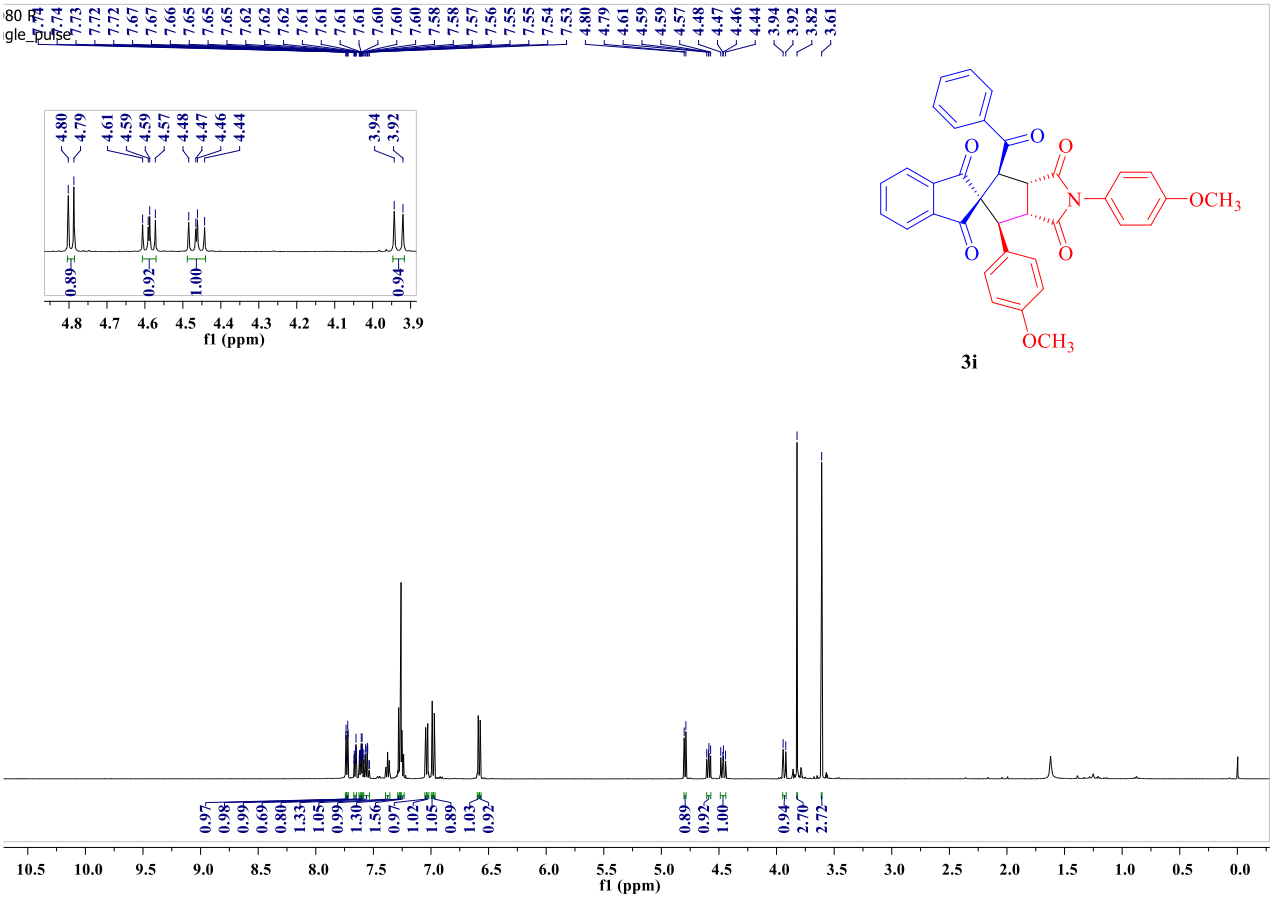

PD62
single pulse decoupled gated NOE
Br
O
O
O
O
N
O
O
3g
f1 (ppm)

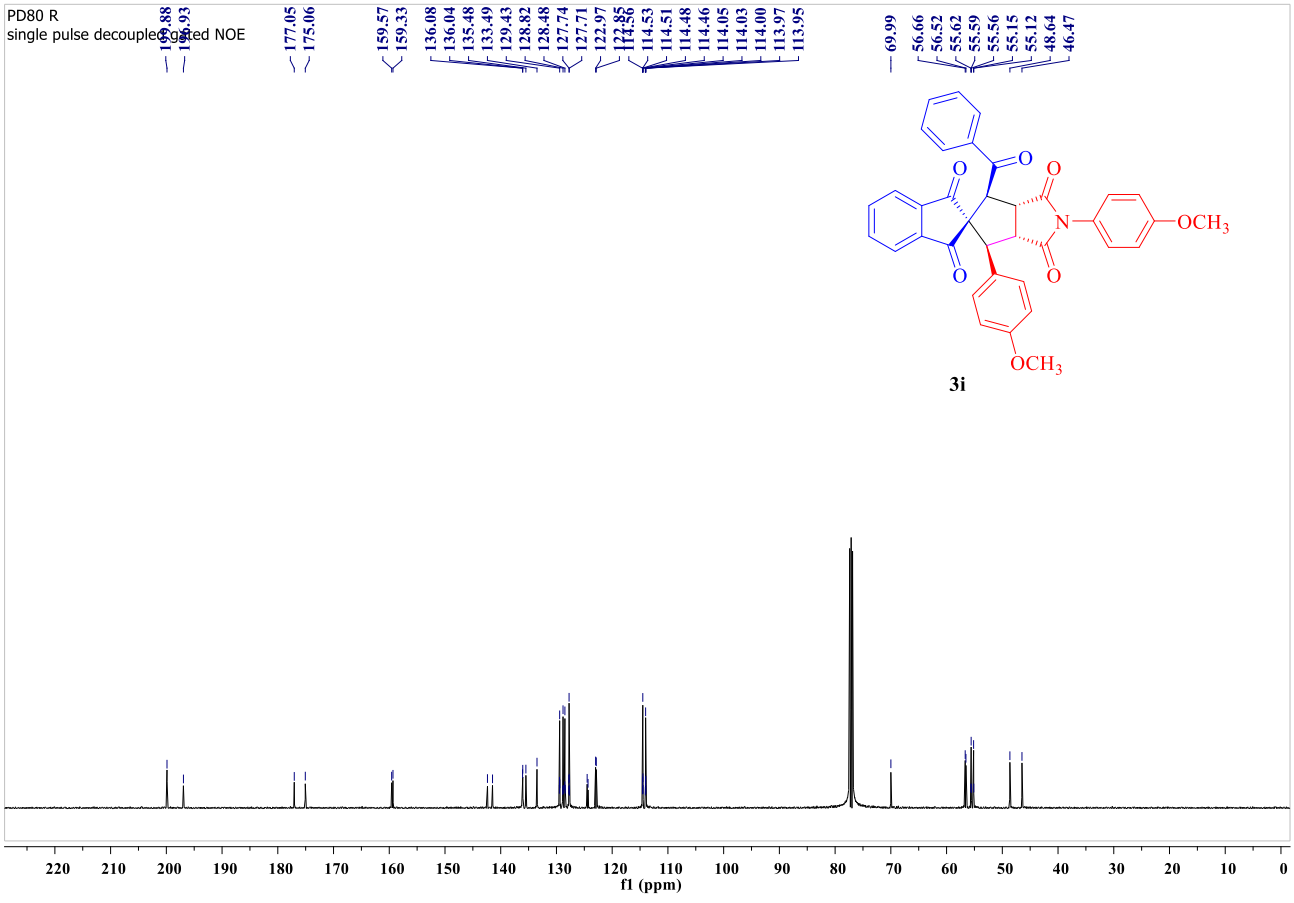

PD63
single pulse
f1 (ppm)
Br
O
N
OCH3
3h

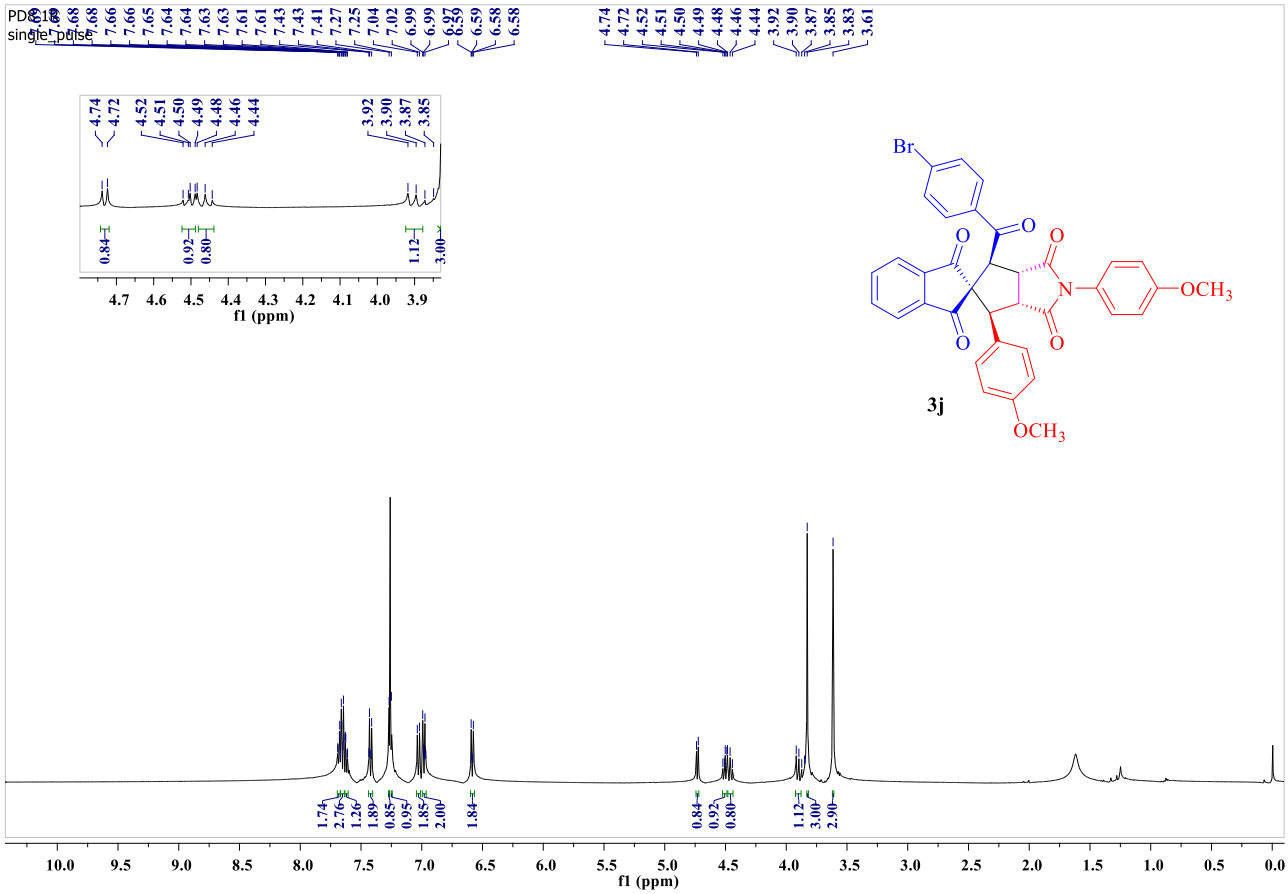

PD63
single pulse decoupled gated NOE
f1 (ppm)
Br
O
N
OCH3
3h

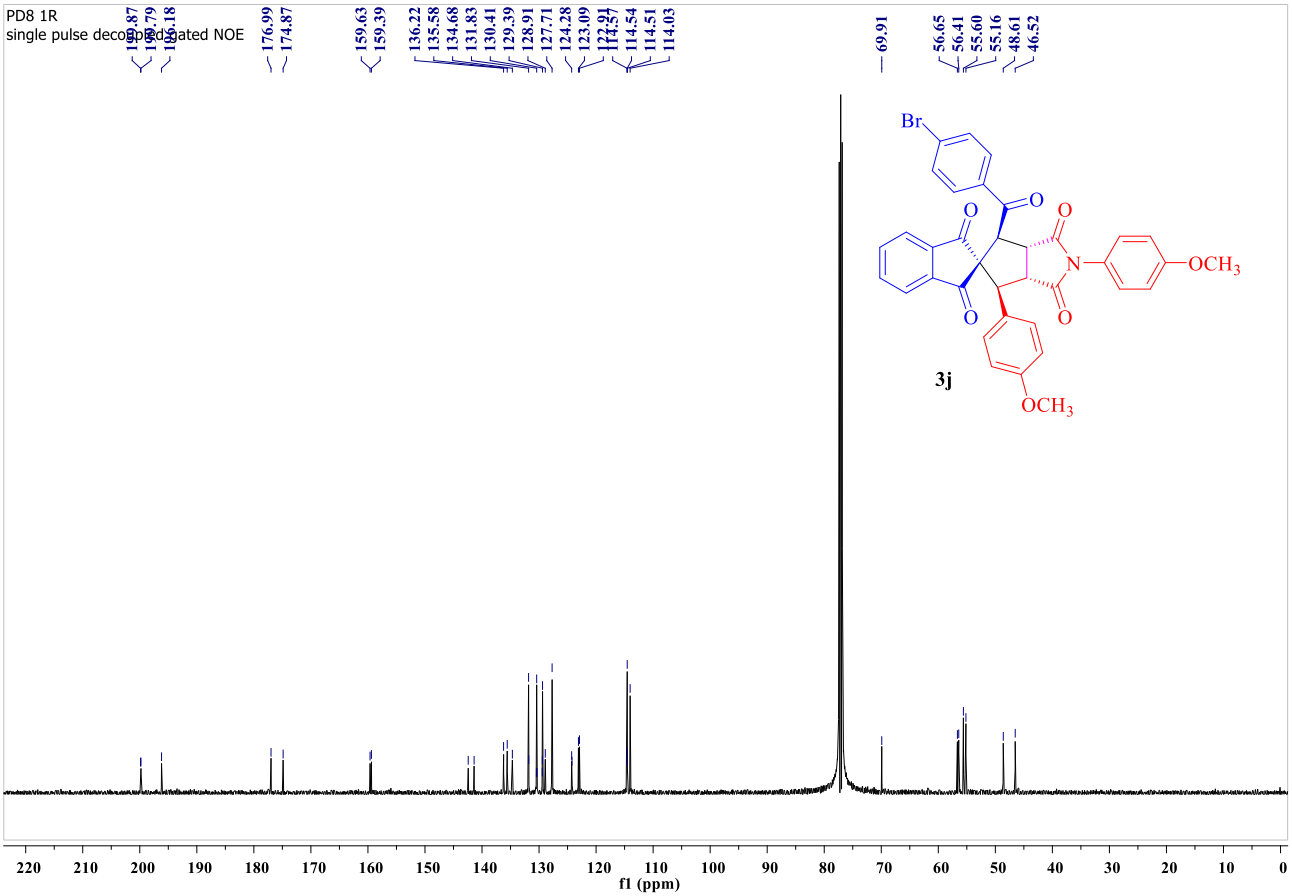

PD63
-DEPT90
136.21
135.59
131.84
130.39
129.40
129.26
128.82
126.46
123.09
122.92
114.07
114.05
114.00
77.31
56.69
56.65
56.47
56.41
48.67
46.58
Br
O
O
O
O
O
N
O
OCH3
3h
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

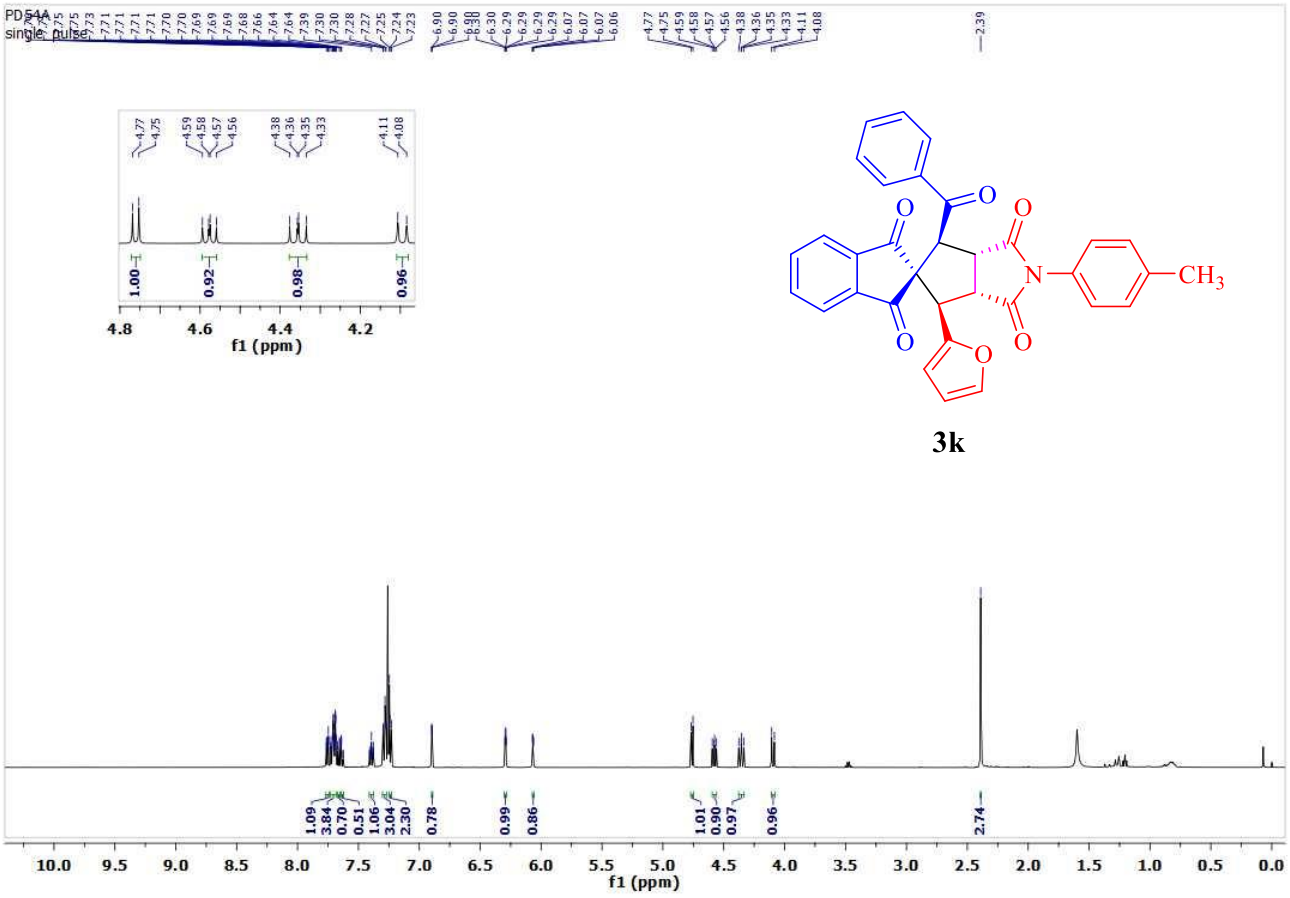

PD63
-DEPT135
136.35
136.21
135.59
132.20
131.84
130.39
129.82
129.46
129.44
129.40
129.26
128.82
126.46
124.31
123.09
122.92
114.07
114.05
114.00
77.31
56.65
56.47
55.19
55.16
55.13
48.67
46.58
Br
O
O
O
O
O
N
O
OCH3
3h
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


gle_pulse
f1 (ppm)
3i

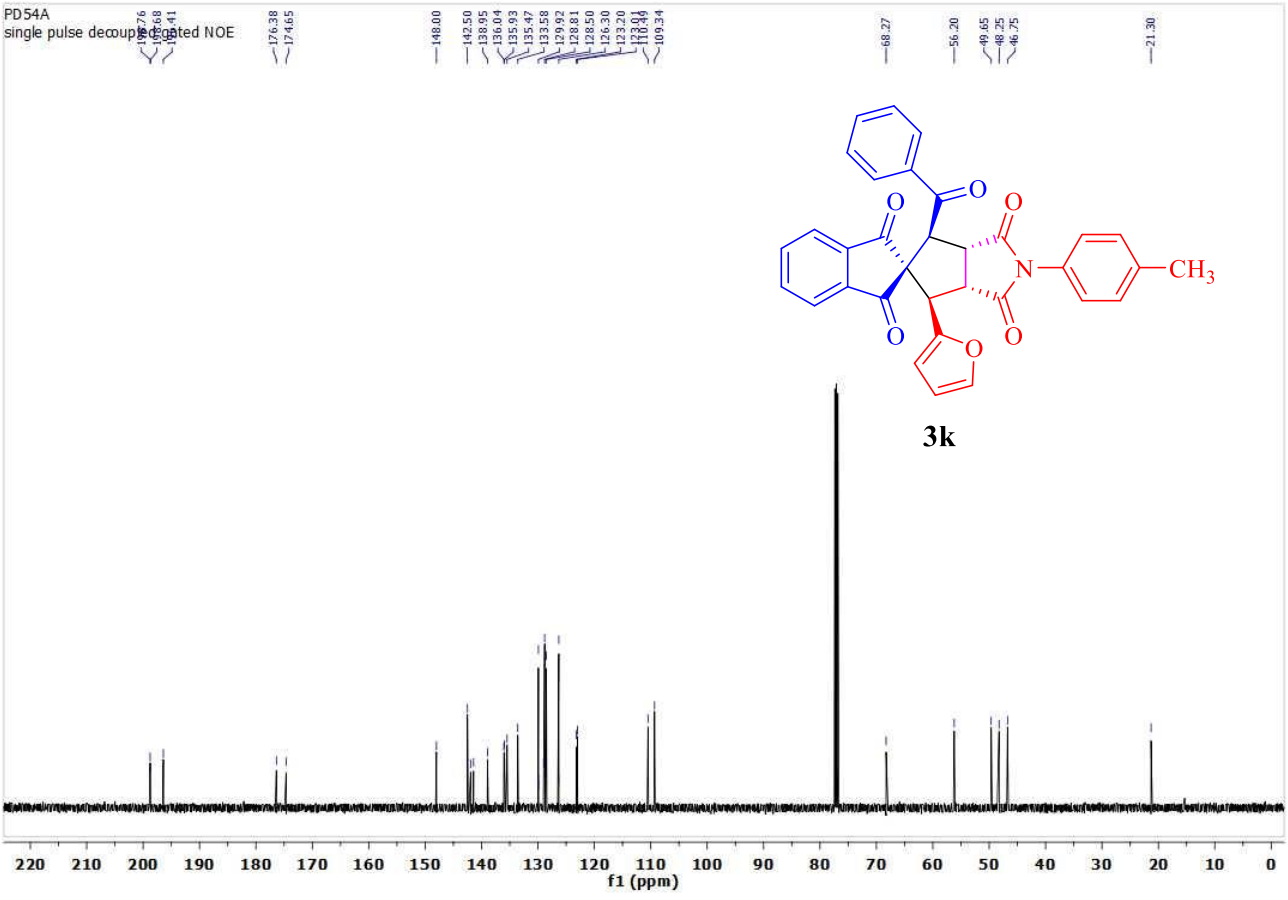

PD80 R
single pulse decoupled gated NOE
f1 (ppm)
3i


PD8 1H
single pulse
Br
O
N
OCH3
3j

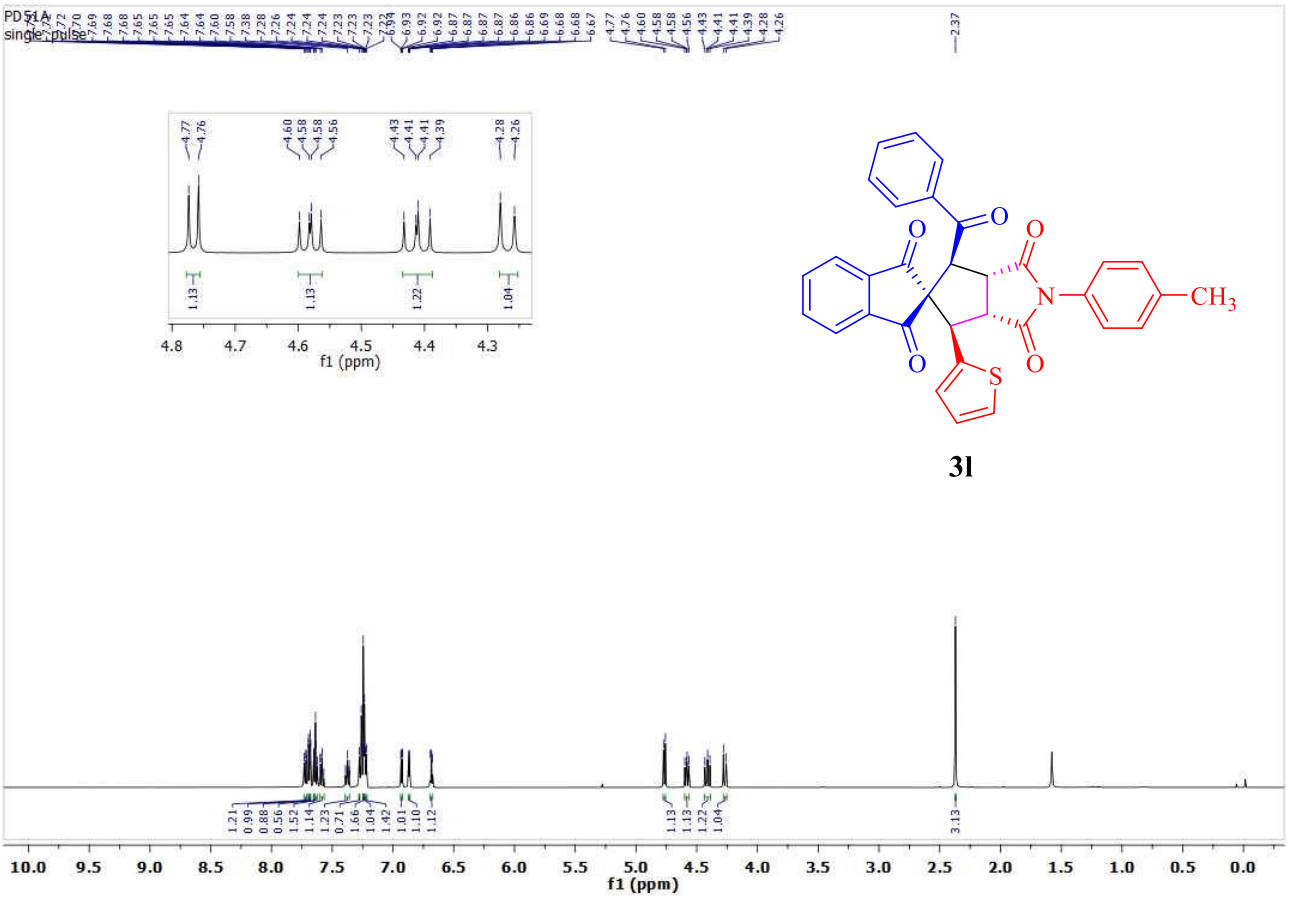

PD8 1R
single pulse decoupled gated NOE
Br
O
N
OCH3
3j


PD54A
single pulse
1.00
0.92
0.98
0.96
4.8
4.6
4.4
4.2
f1 (ppm)
O
O
O
O
O
O
N
CH3
1.09
3.84
0.70
0.51
1.06
3.04
2.30
0.78
0.99
0.86
1.01
0.90
0.97
0.96
2.74
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

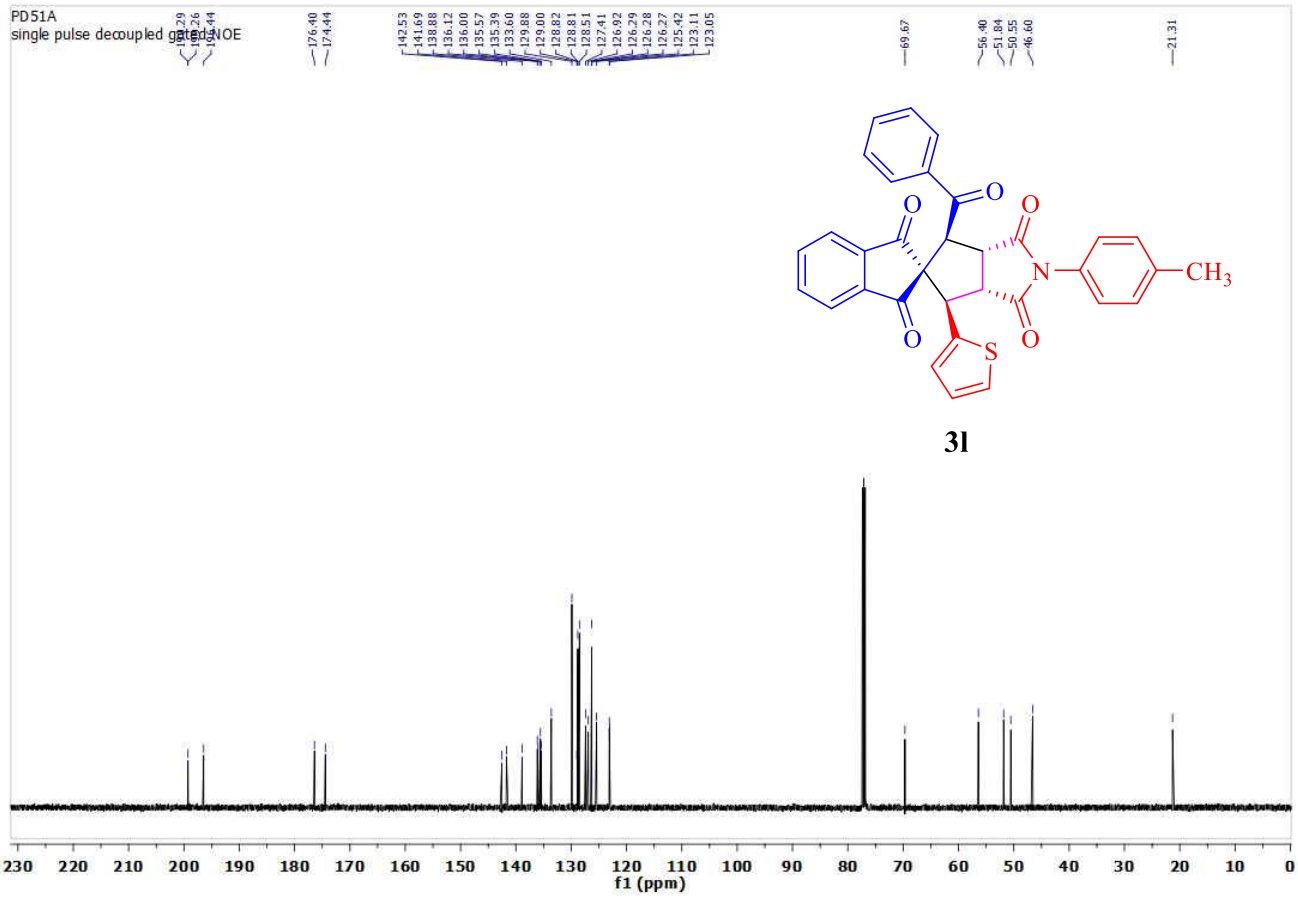
3k


PD54A
single pulse decoupled gated NOE
176.38
174.65
148.00
142.50
138.95
136.04
135.93
135.47
133.58
129.92
128.81
128.50
126.30
123.20
109.34
68.27
56.20
49.65
48.25
46.75
21.30
O
O
O
O
O
O
N
CH3
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

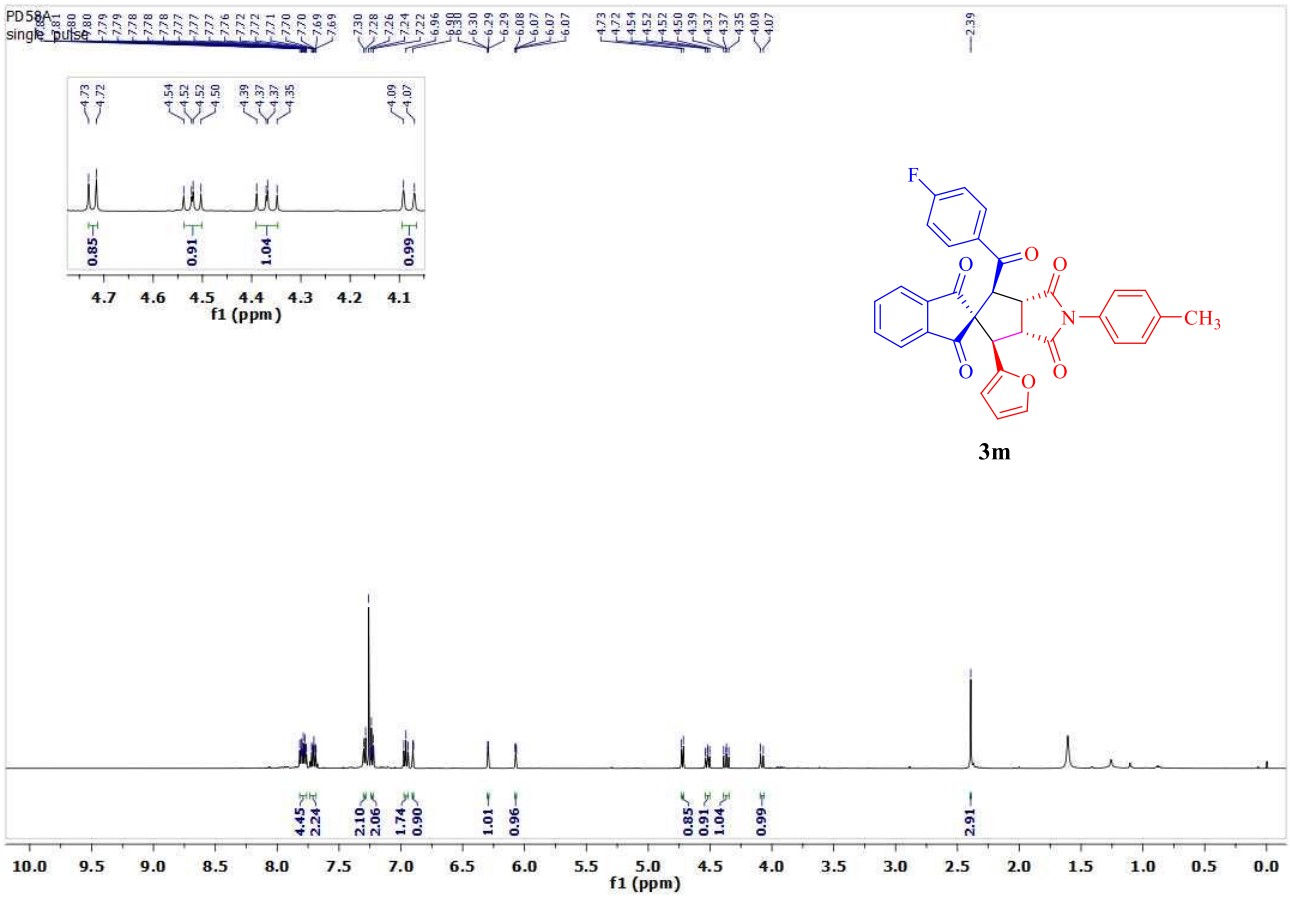
3k


PD51A
single pulse
f1 (ppm)

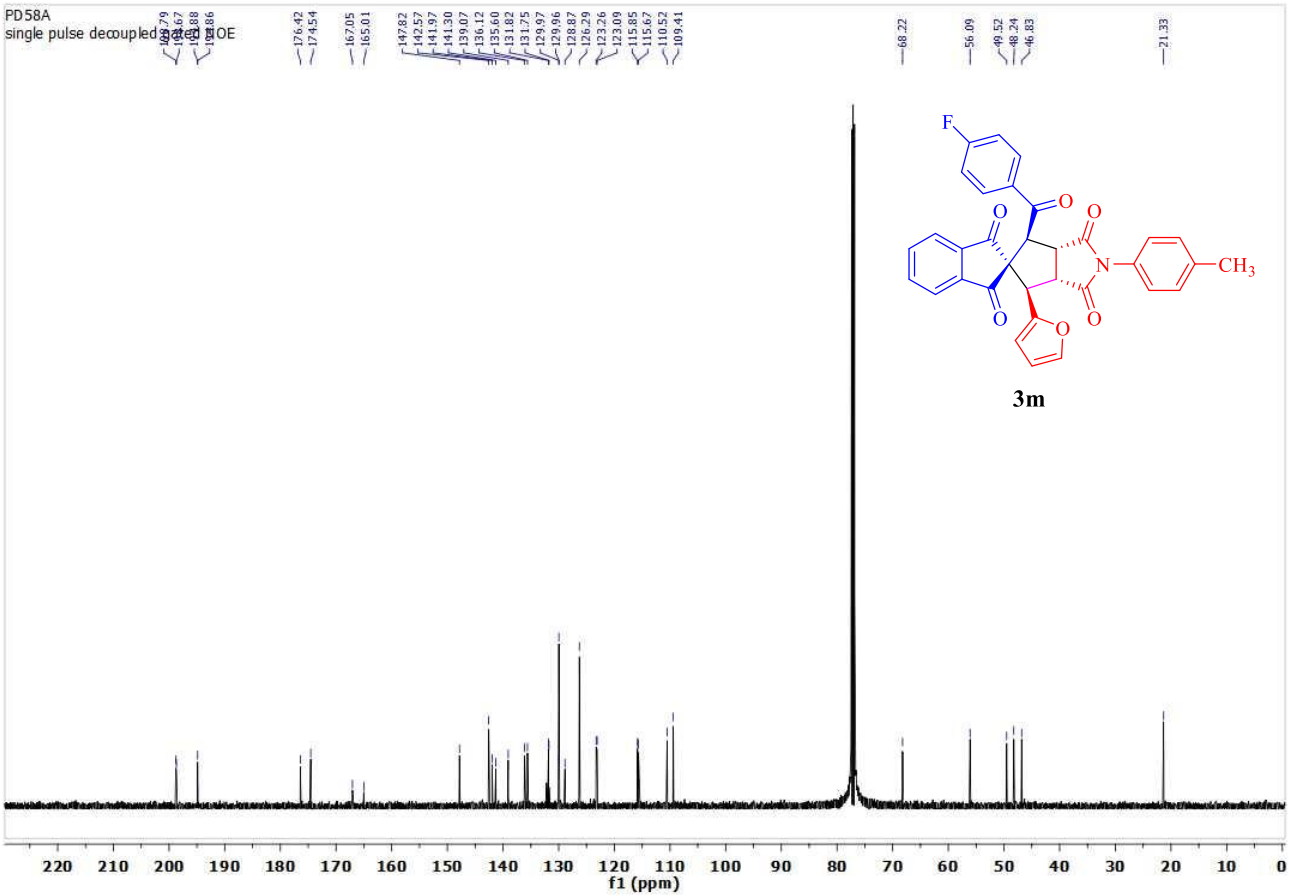
3l


PD51A
single pulse decoupled gated NOE
f1 (ppm)

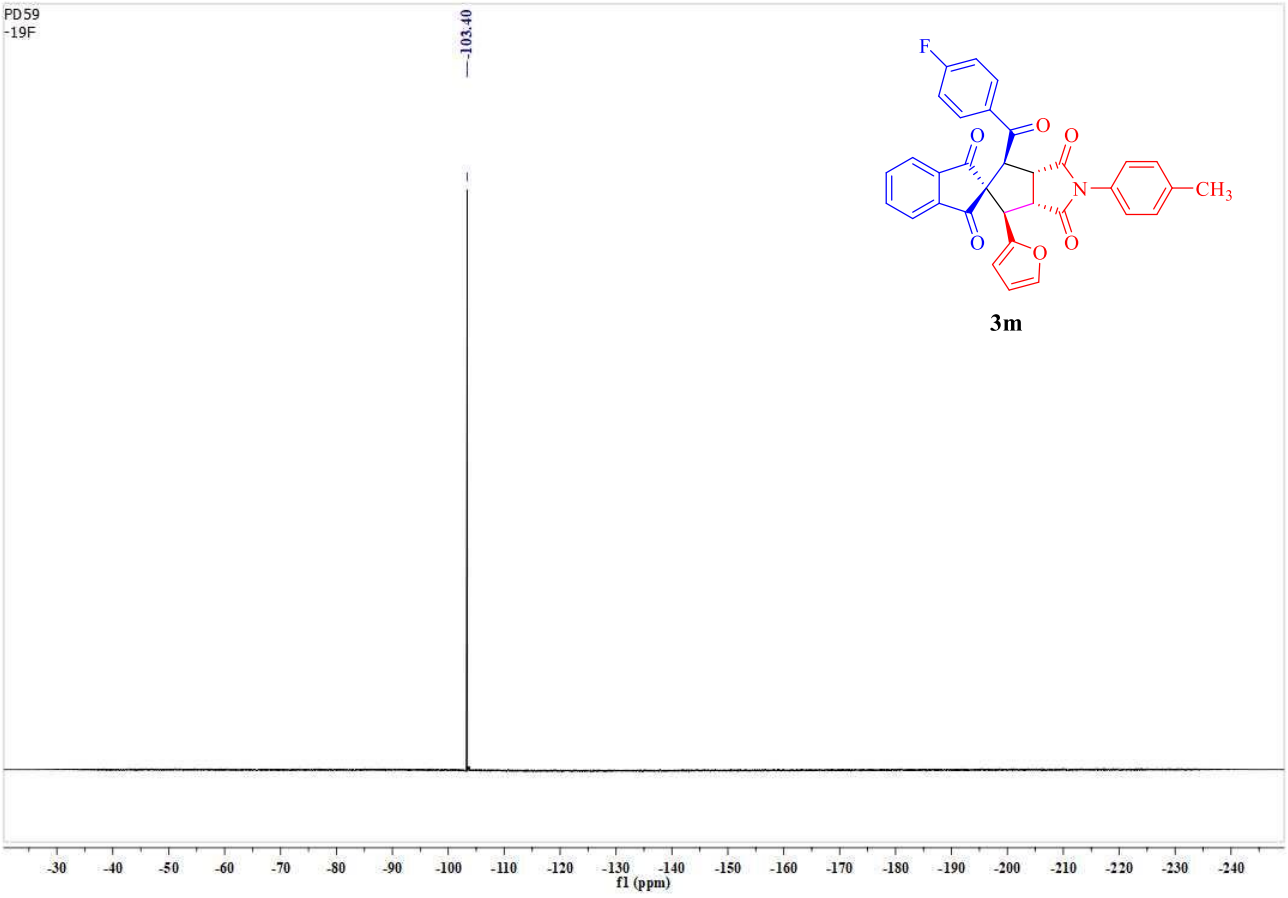
3l


PD58A
single pulse
f1 (ppm)

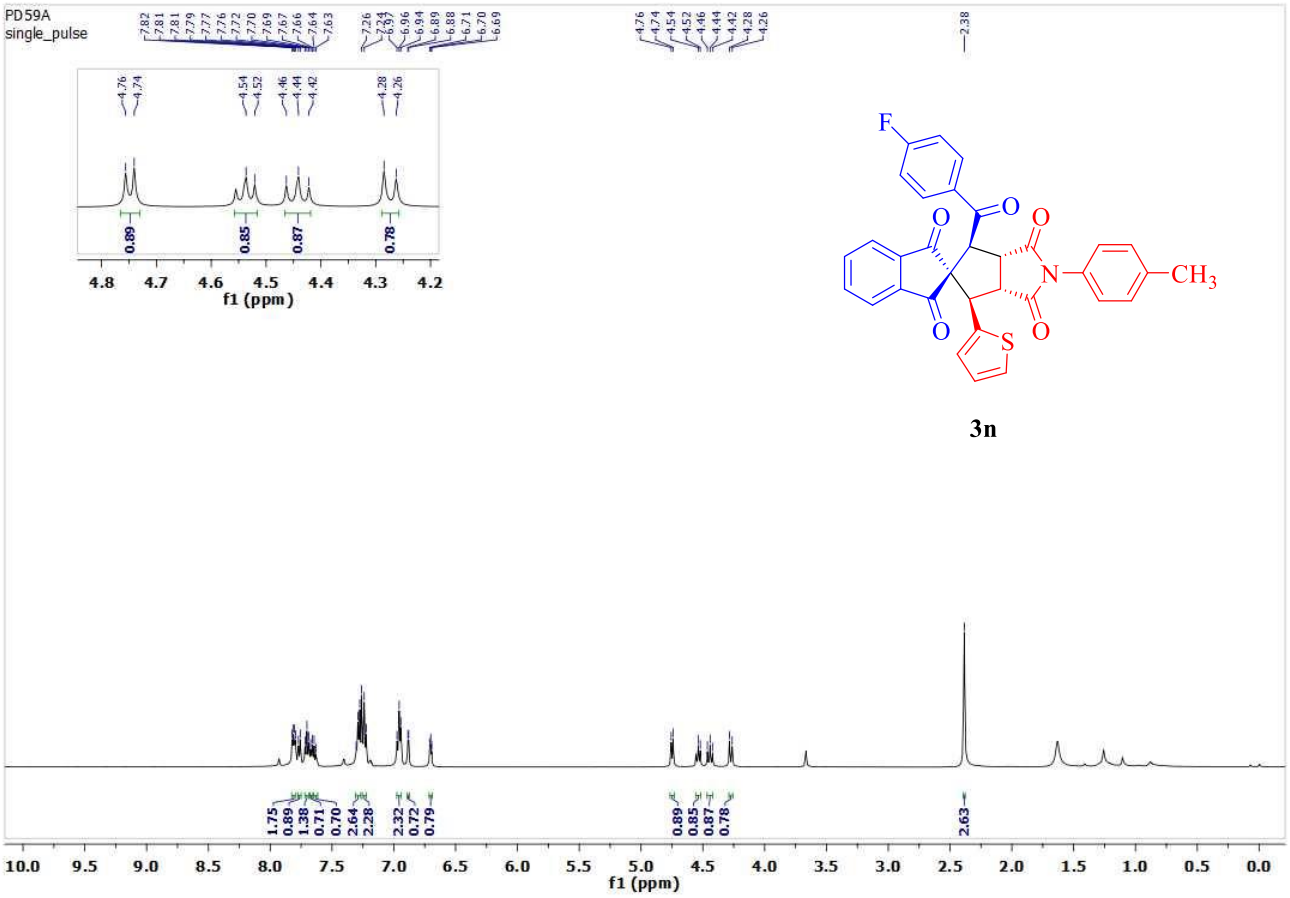
3m


PD58A
single pulse decoupled gated NOE
f1 (ppm)

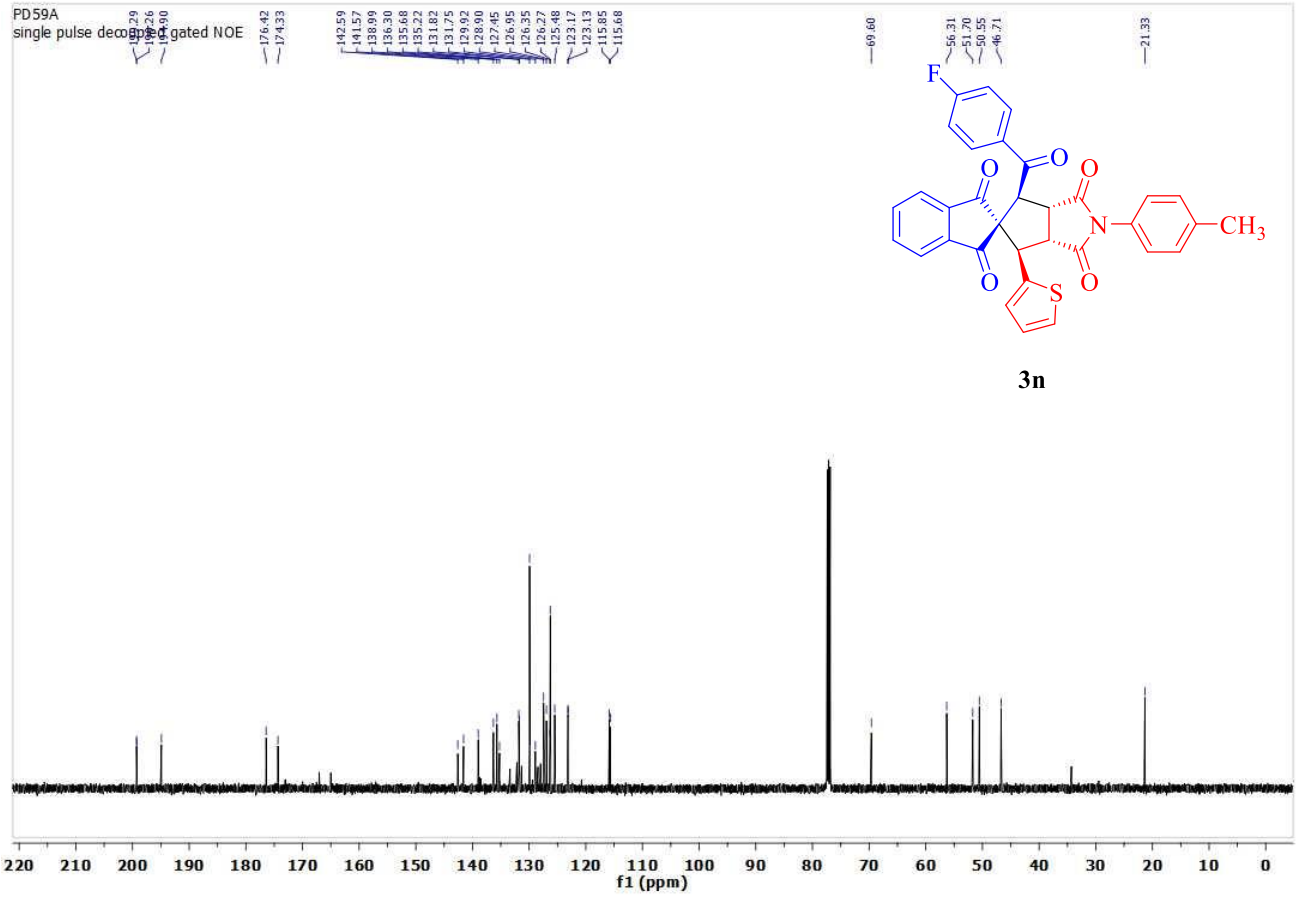
3m


PD59
-19F
-103.40
F
O
O
O
O
N
O
O
CH3
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-220
-230
-240
f1 (ppm)

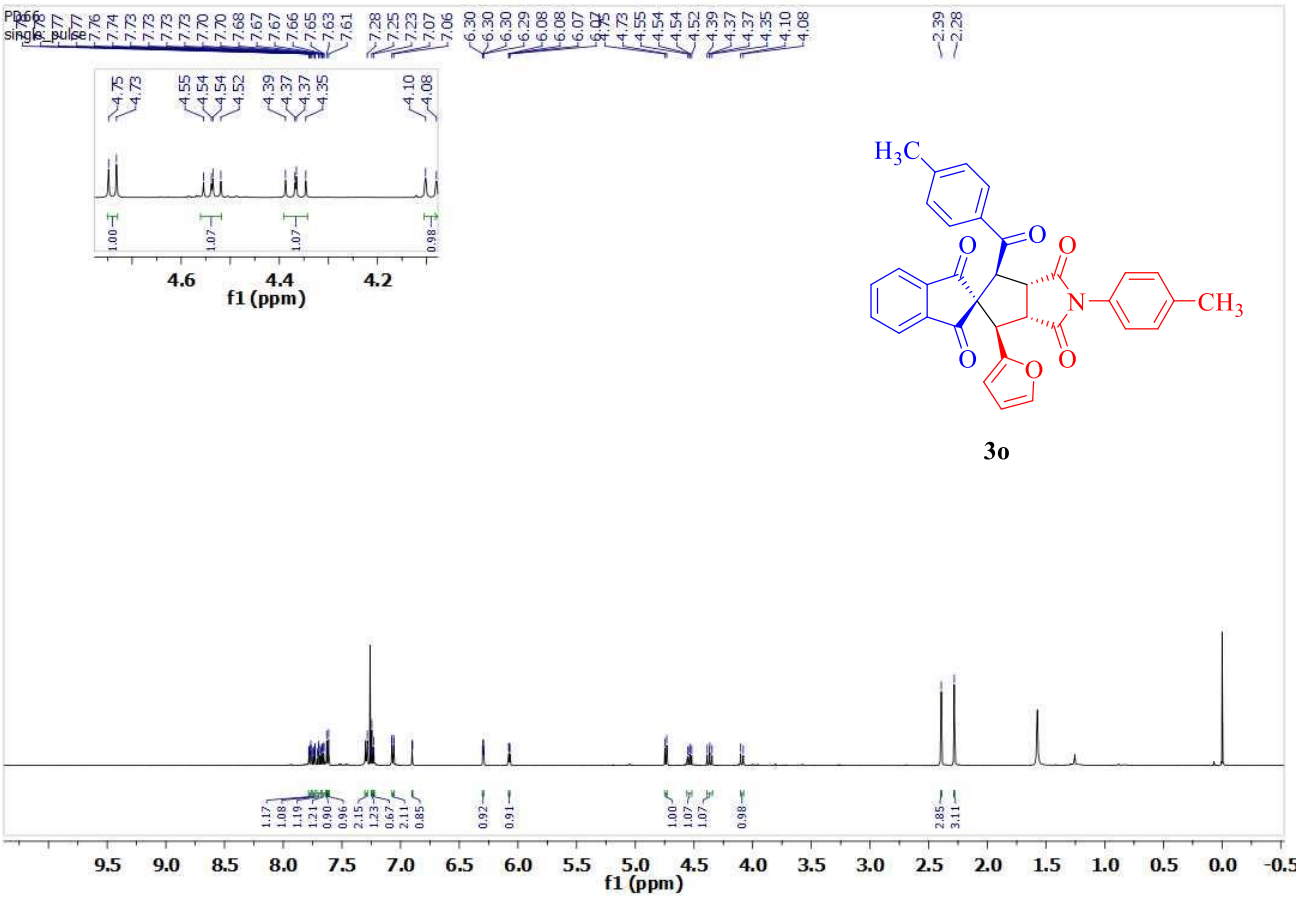
3m


PD59A
single_pulse
f1 (ppm)

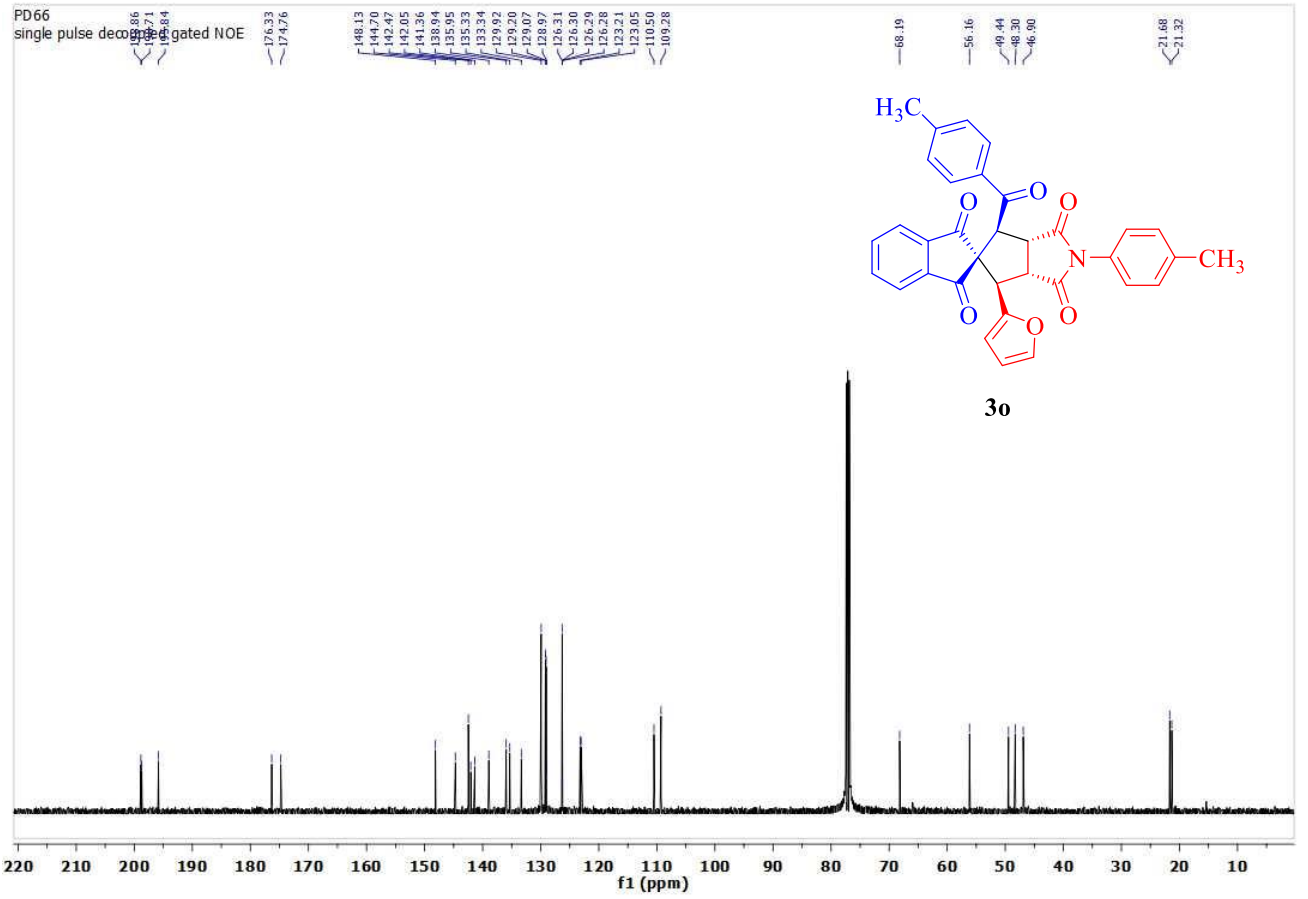
3n


PD59A
single pulse decoupled gated NOE
f1 (ppm)

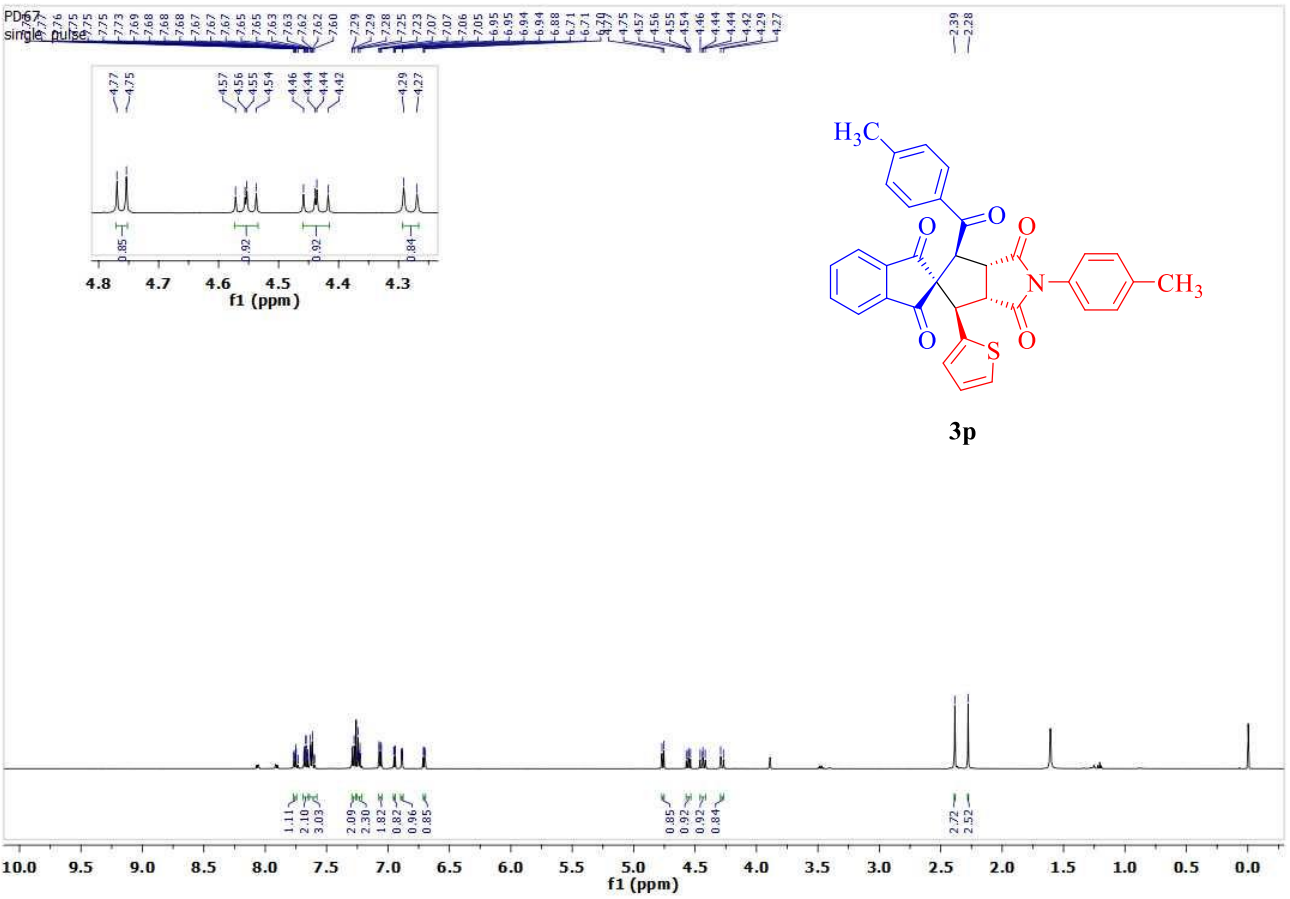
3n


PD66
single_pulse
f1 (ppm)

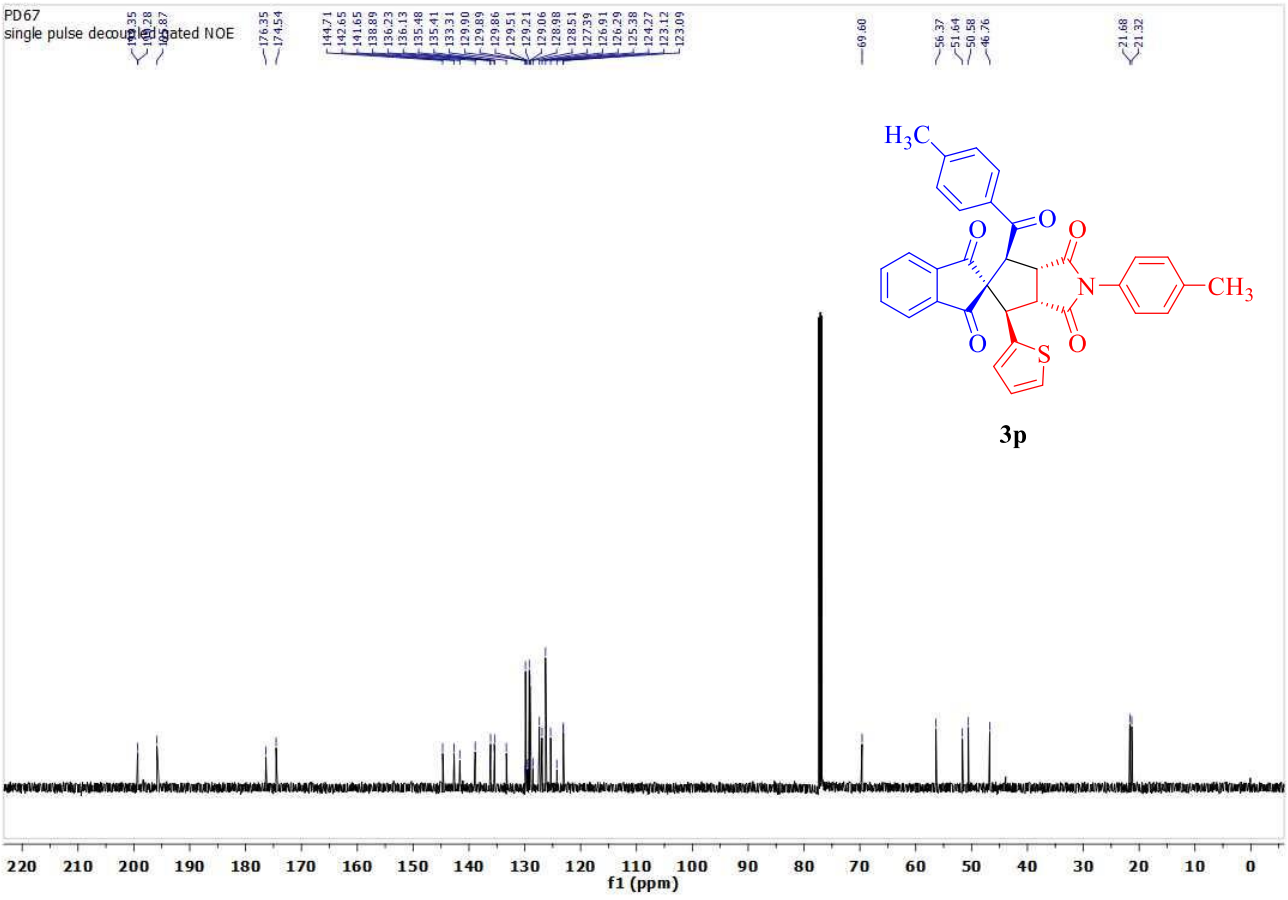
3o


PD66
single pulse decoupled gated NOE
f1 (ppm)

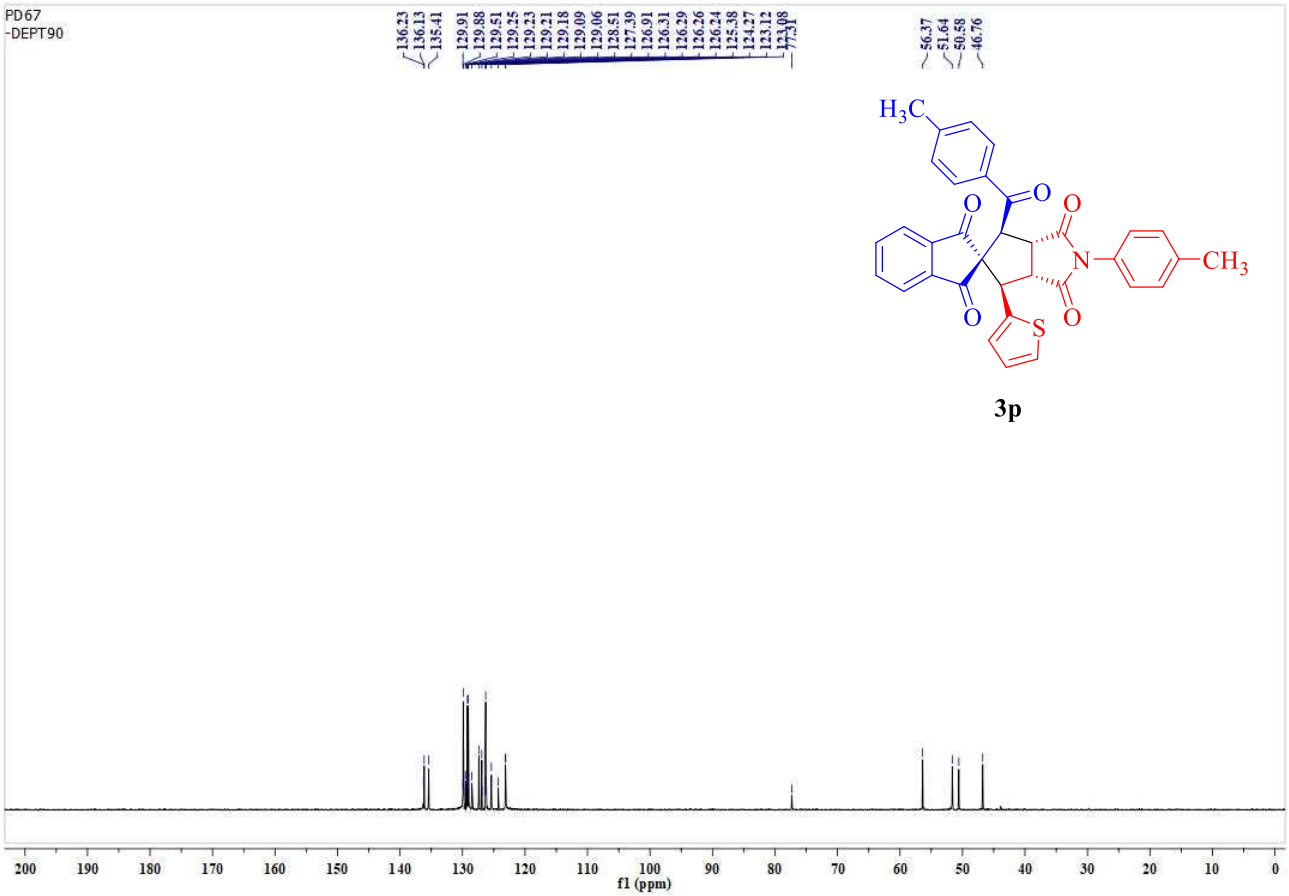
3o


PD67
single pulse
f1 (ppm)

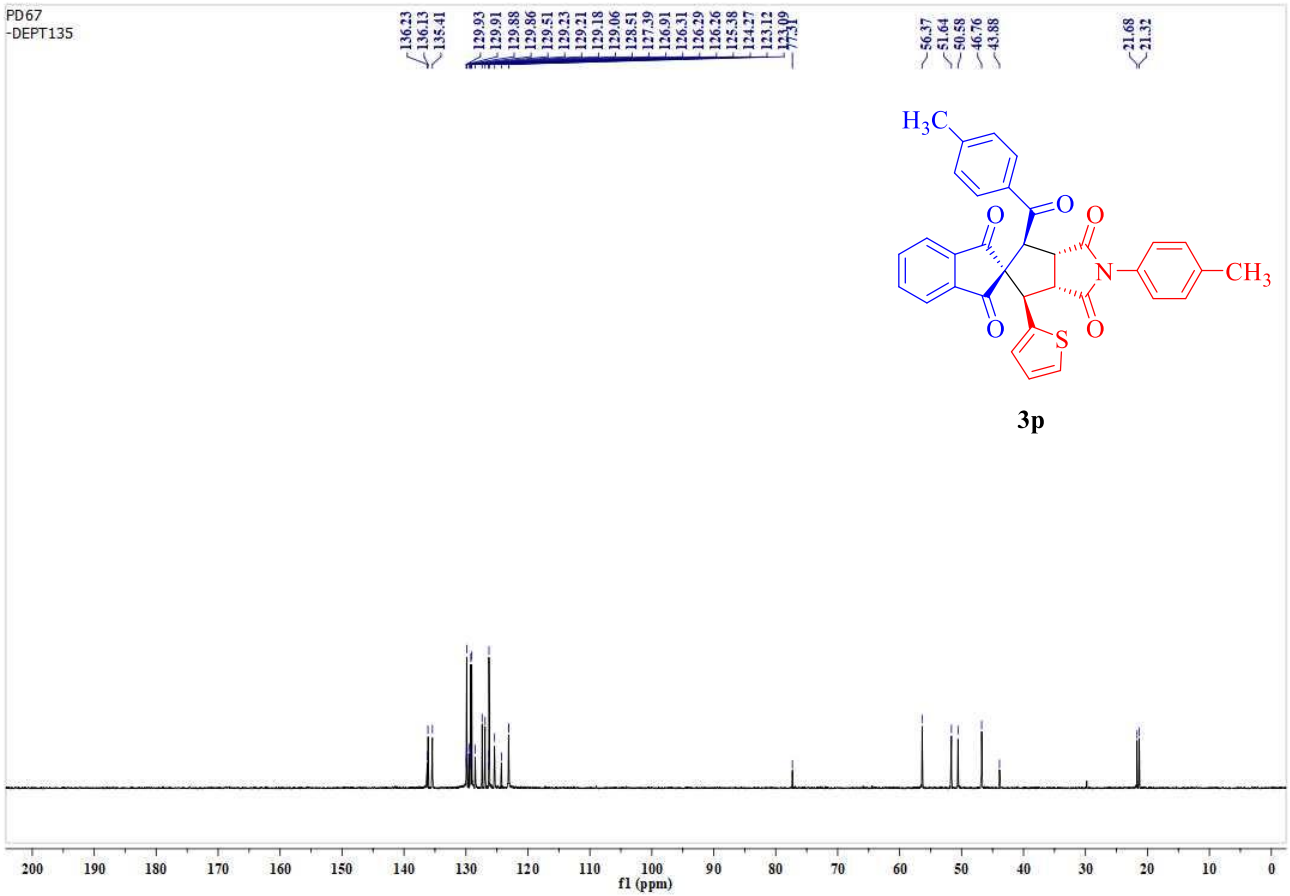
3p


PD67
single pulse decoupled gated NOE
f1 (ppm)

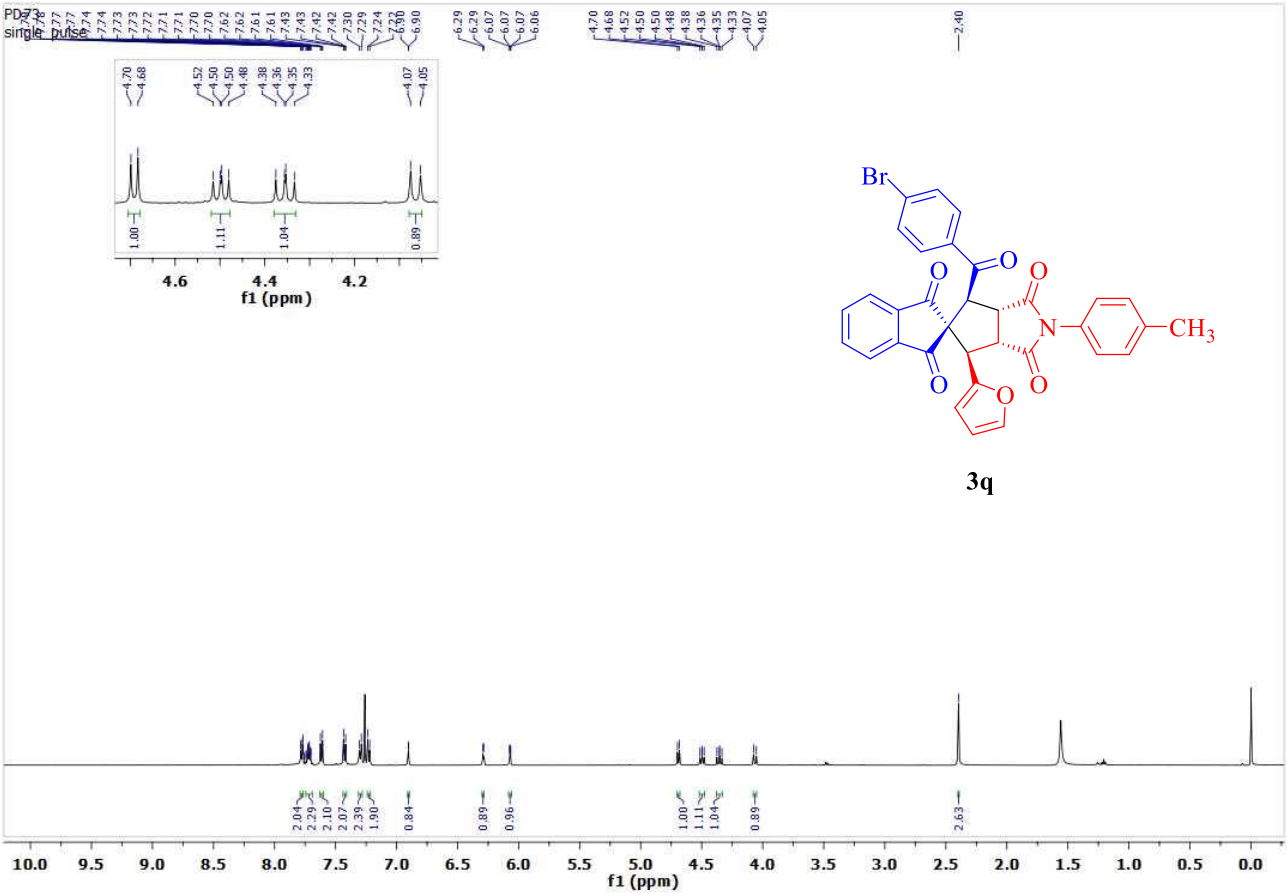
3p


PD67
-DEPT90
136.23
136.13
135.41
129.91
129.88
129.51
129.25
129.23
129.21
129.18
129.09
129.06
128.51
127.39
126.91
126.31
126.29
126.26
126.24
125.38
124.27
123.12
123.08
77.31
56.37
51.64
50.58
46.76
H3C
O
O
O
O
N
CH3
O
S
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

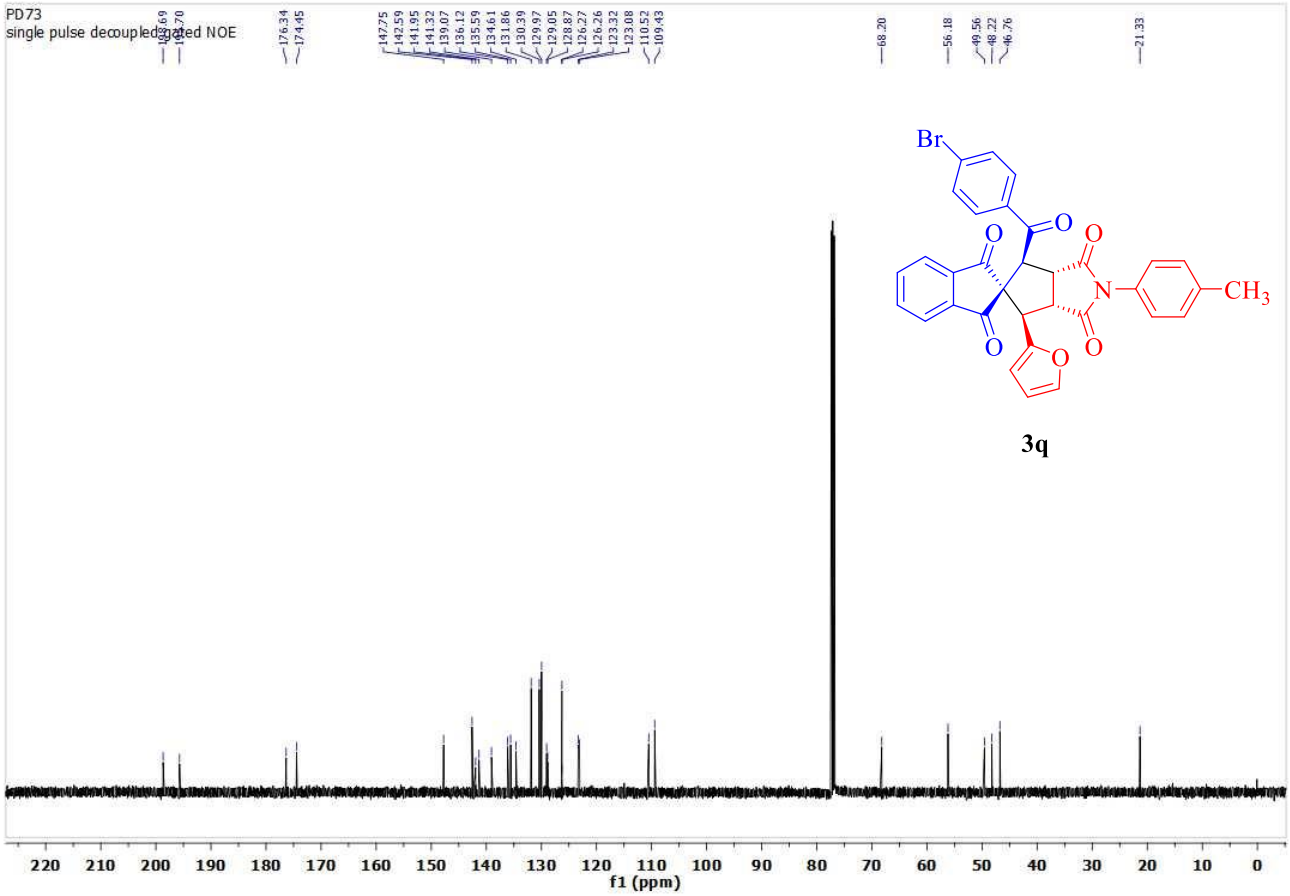
3p


PD67
-DEPT135
136.23
136.13
135.41
129.93
129.91
129.88
129.86
129.51
129.23
129.21
129.18
129.06
128.51
127.39
126.91
126.31
126.29
126.26
125.38
124.27
123.12
123.09
77.31
56.37
51.64
50.58
46.76
43.88
21.68
21.32
H3C
O
O
O
O
N
CH3
O
S
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

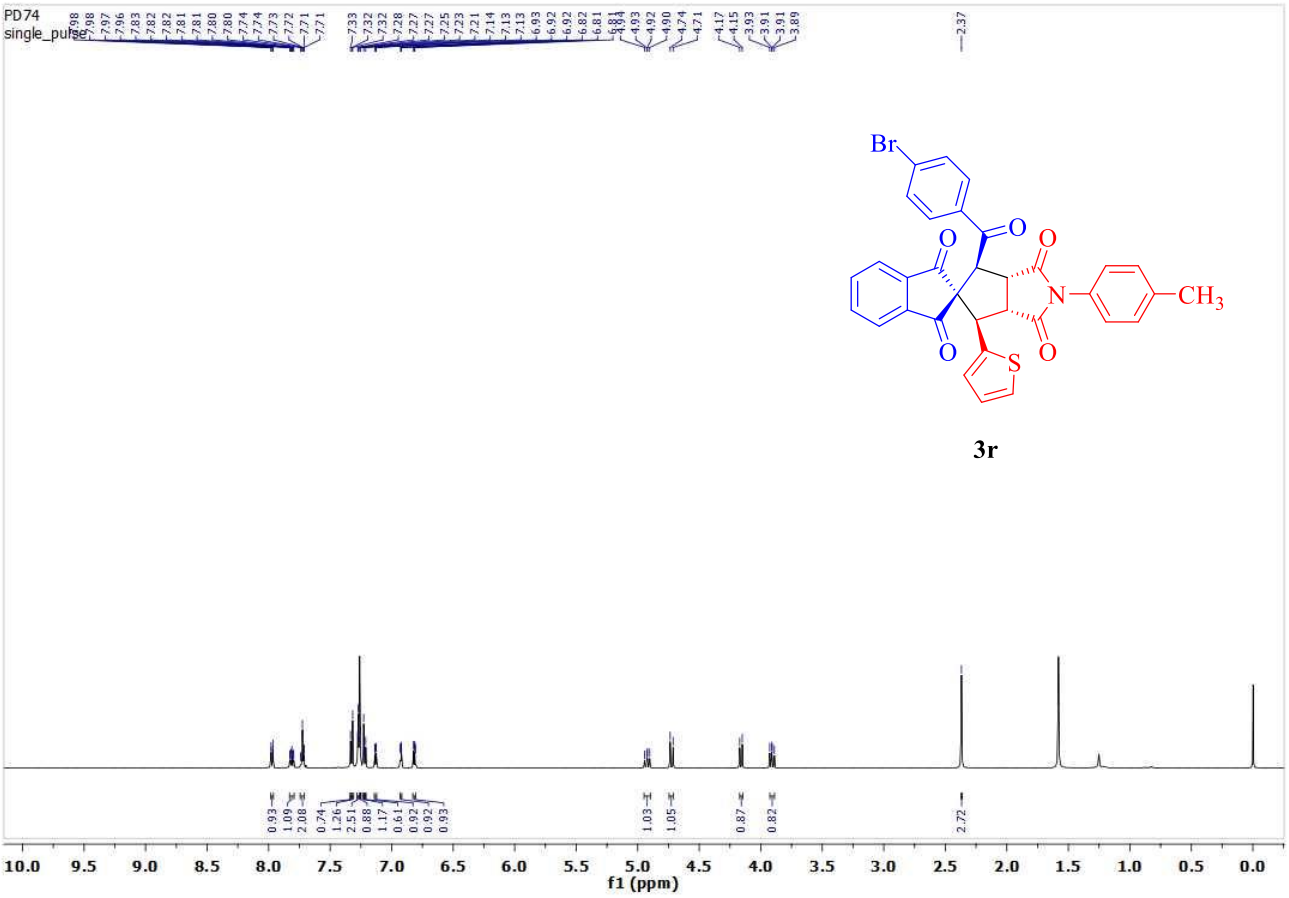
3p


PD73
single pulse
f1 (ppm)
Br
O
N
CH3

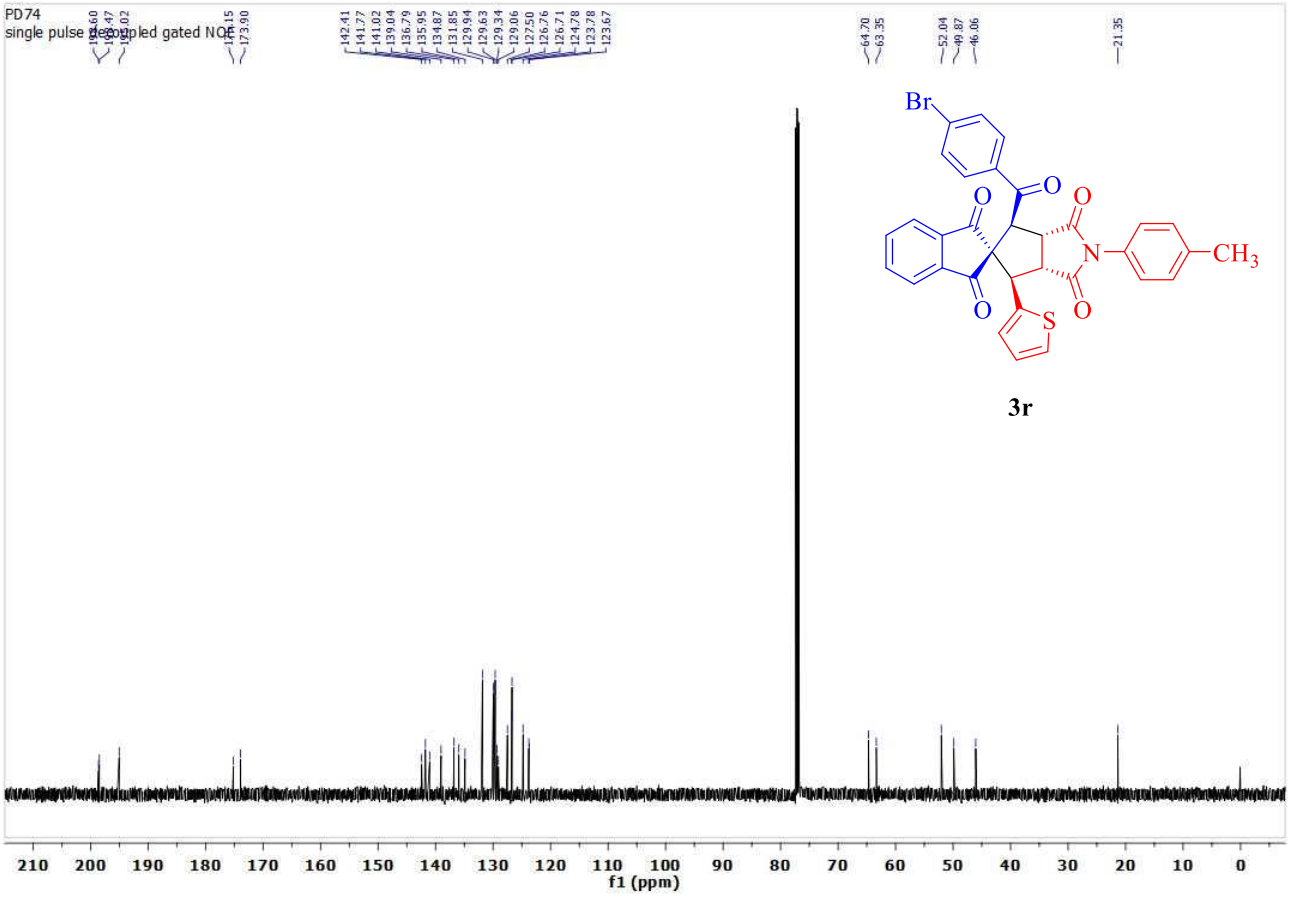
3q


PD73
single pulse decoupled gated NOE
f1 (ppm)
Br
O
N
CH3

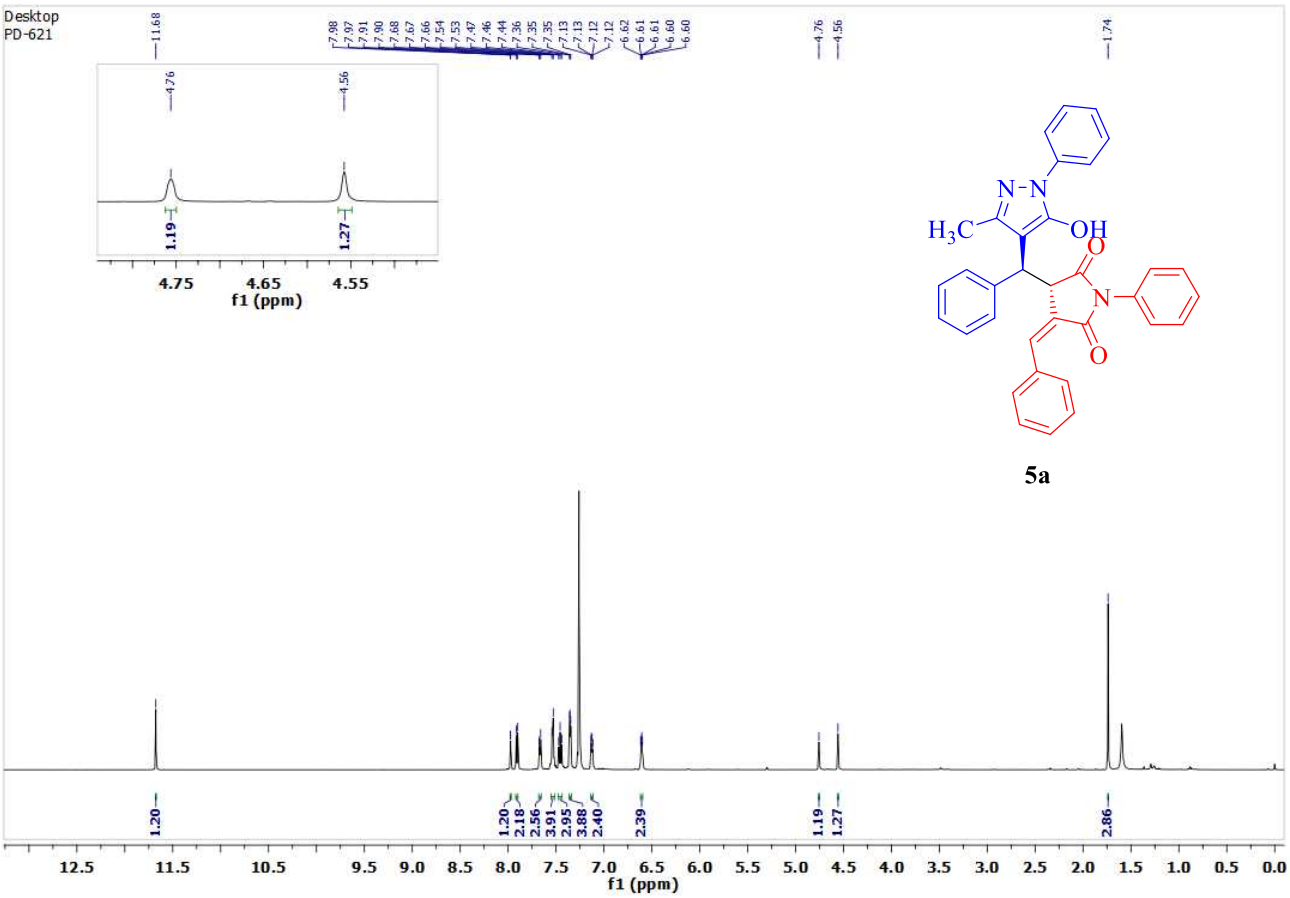
3q


PD74
single_pulse
Br
O
O
O
O
O
N
CH3
S
O
f1 (ppm)

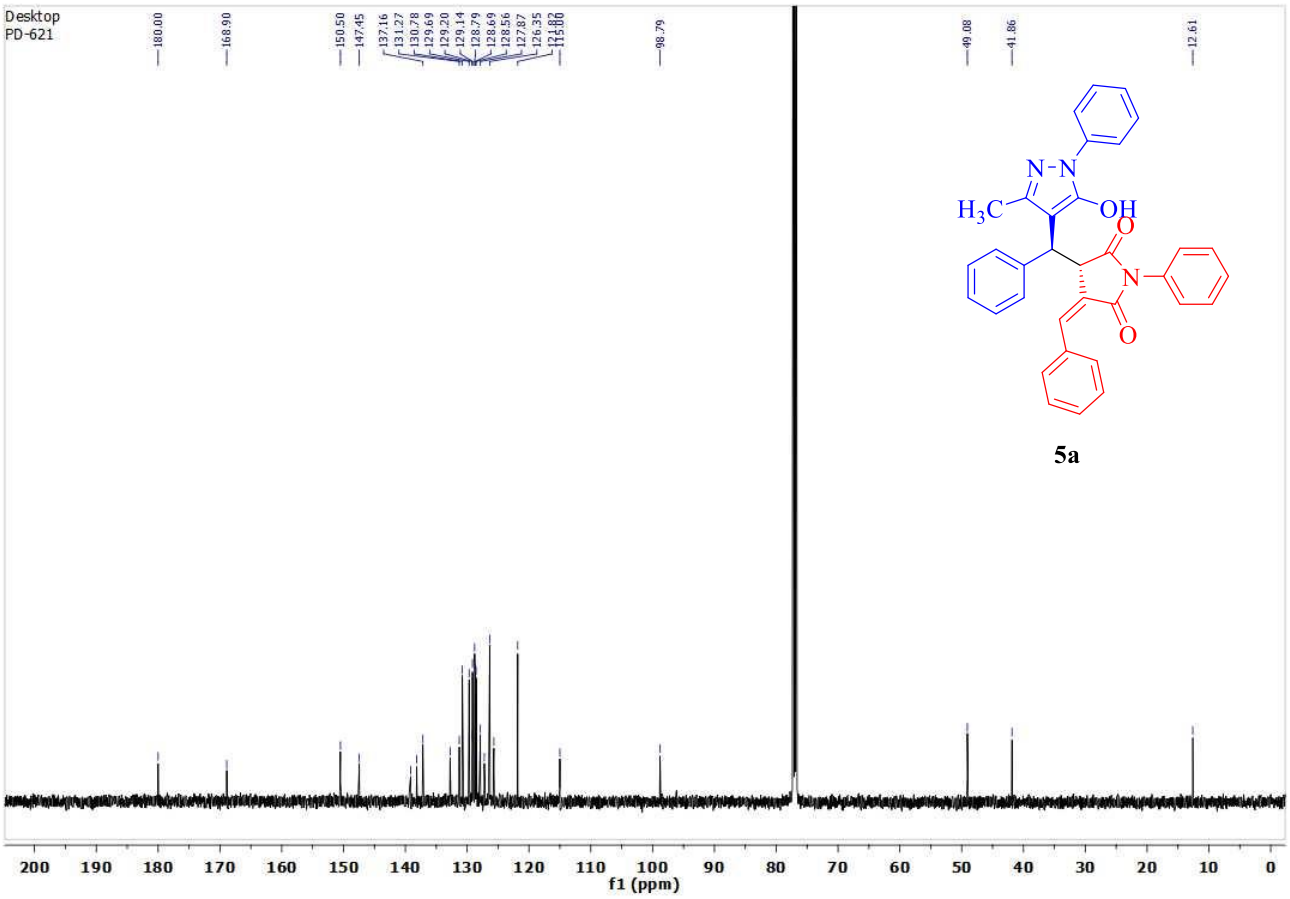
3r


PD74
single pulse decoupled gated NOE
Br
O
O
O
O
O
N
CH3
S
O
f1 (ppm)

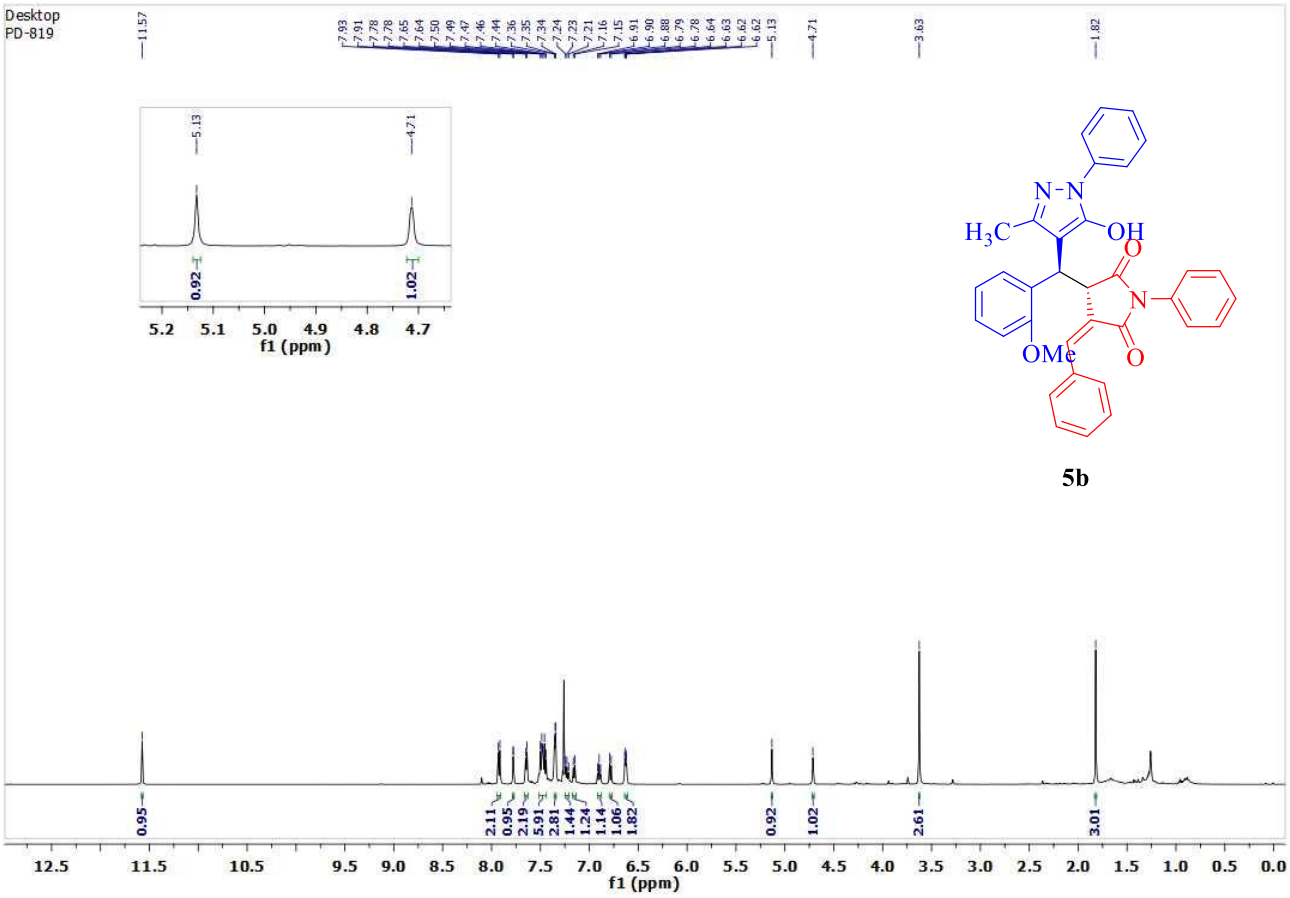
3r


Desktop
PD-621
11.68
7.98
7.97
7.91
7.90
7.68
7.67
7.66
7.54
7.53
7.47
7.46
7.44
7.36
7.35
7.35
7.13
7.12
7.12
6.62
6.61
6.61
6.60
6.60
4.76
4.56
1.74
4.76
4.56
1.19
1.27
4.75
4.65
4.55
f1 (ppm)
N-N
H3C
OH
O
N
O
1.20
1.20
2.18
2.56
3.91
2.95
3.88
2.40
2.39
1.19
1.27
2.86
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

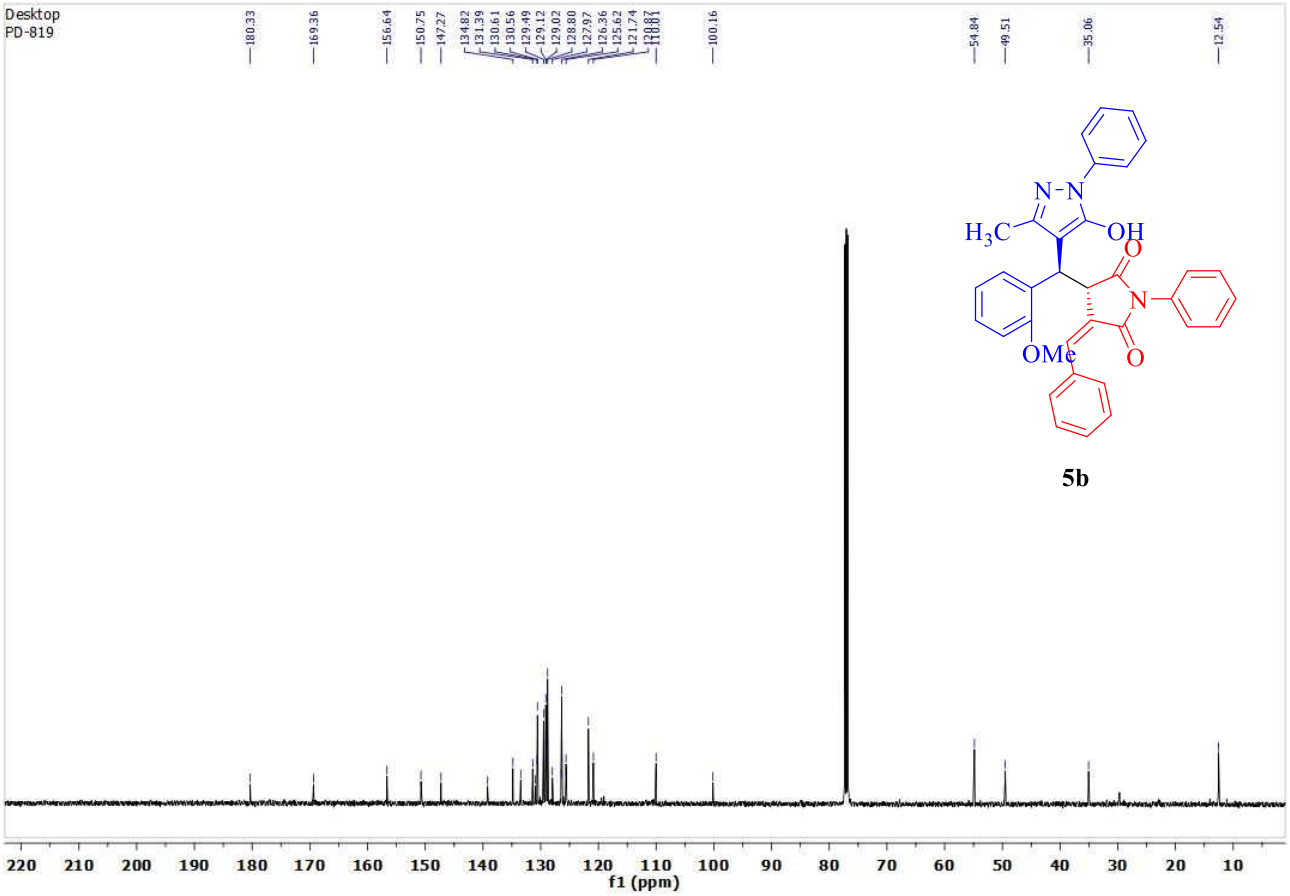
5a


Desktop
PD-621
180.00
168.90
150.50
147.45
137.16
131.27
130.78
129.69
129.20
129.14
128.79
128.69
128.56
127.87
126.35
98.79
49.08
41.86
12.61
N-N
H3C
OH
O
N
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

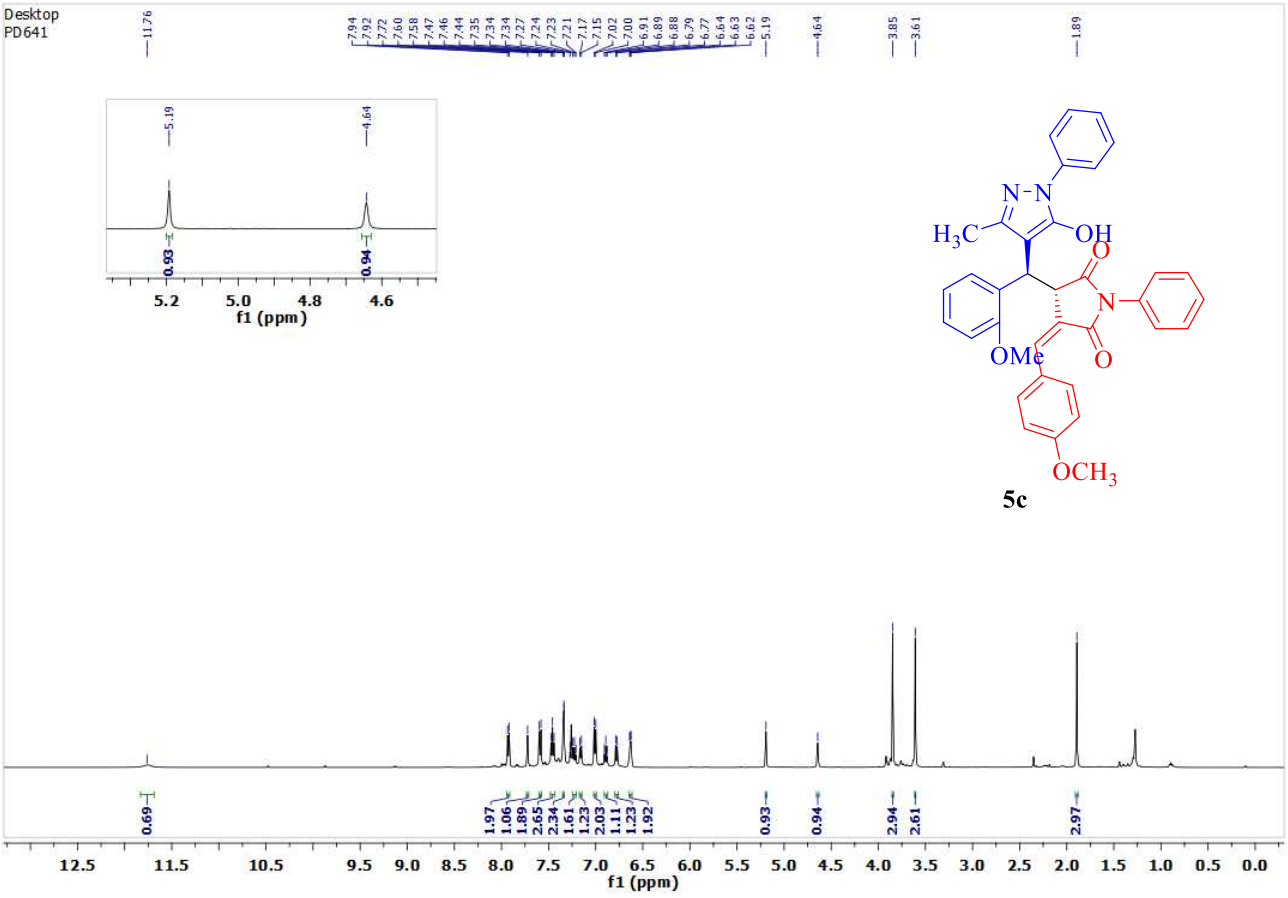
5a

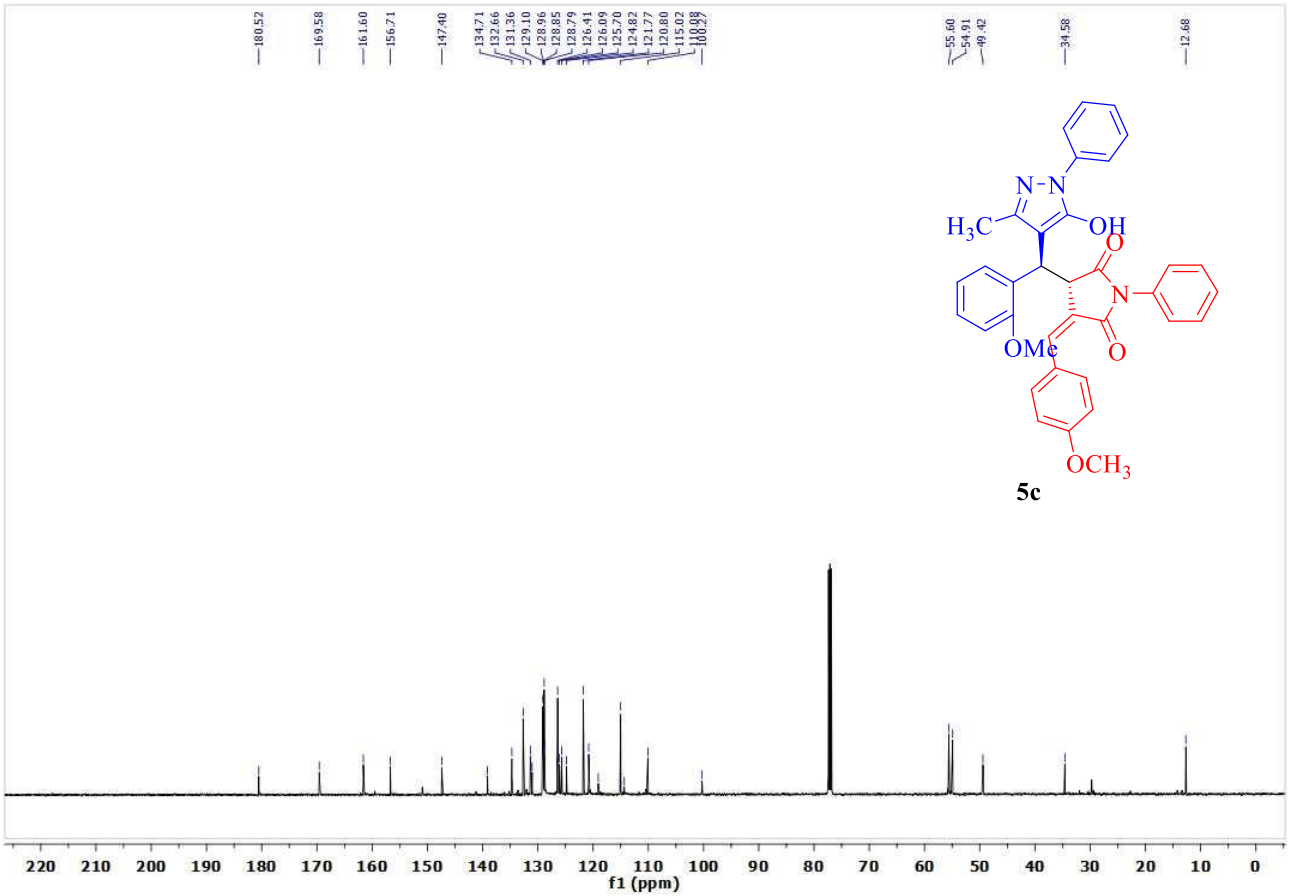


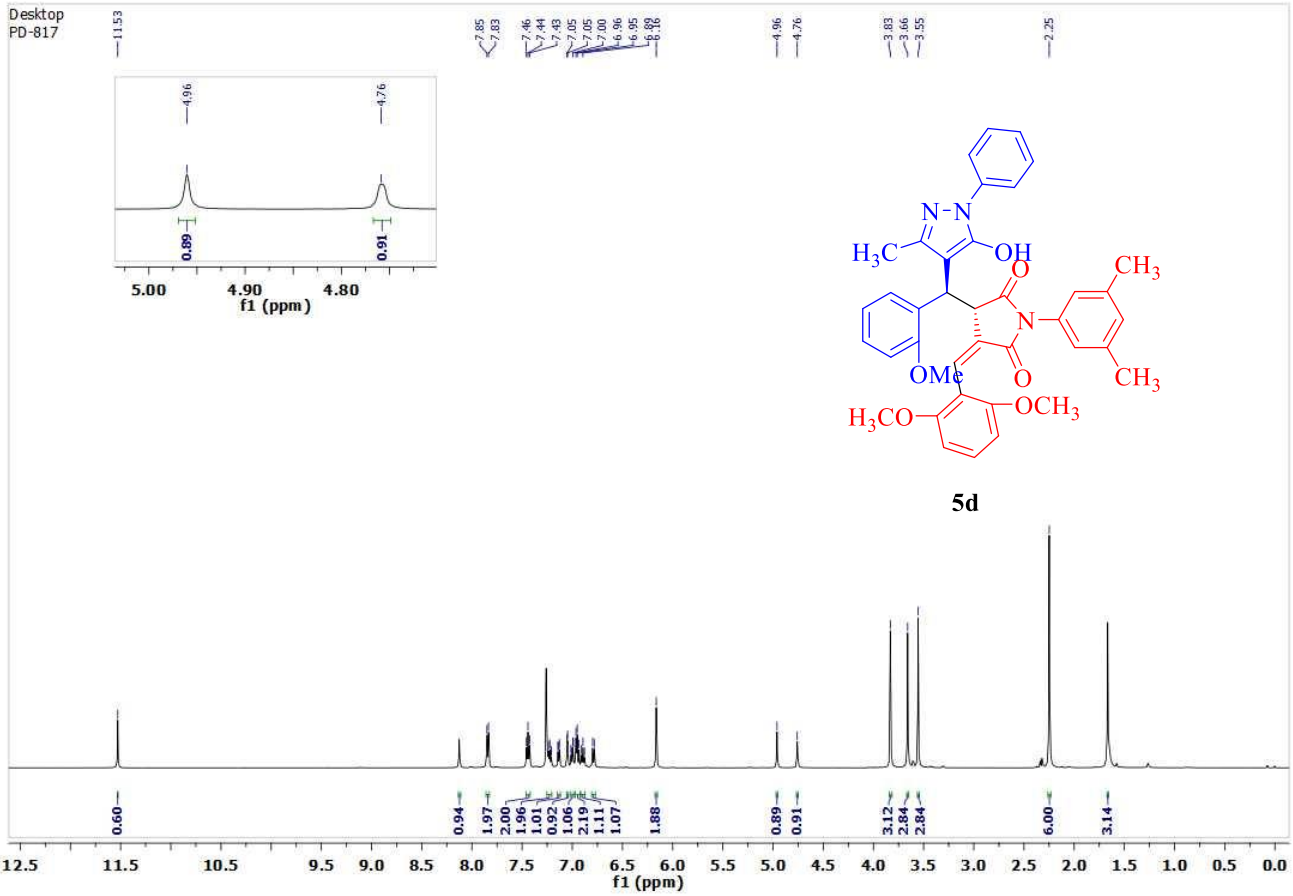
5b



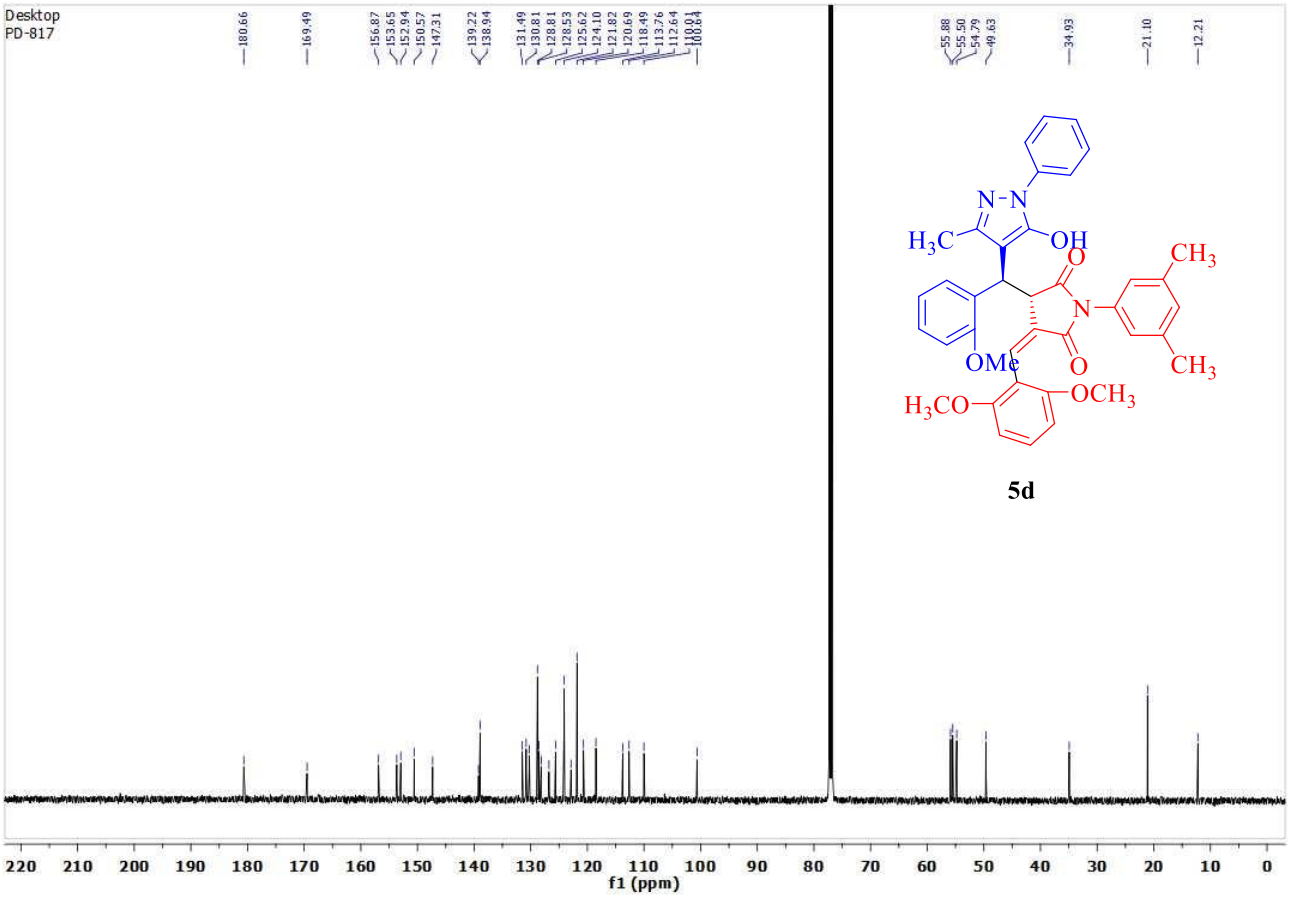
5b


Desktop
PD641
f1 (ppm)
5c

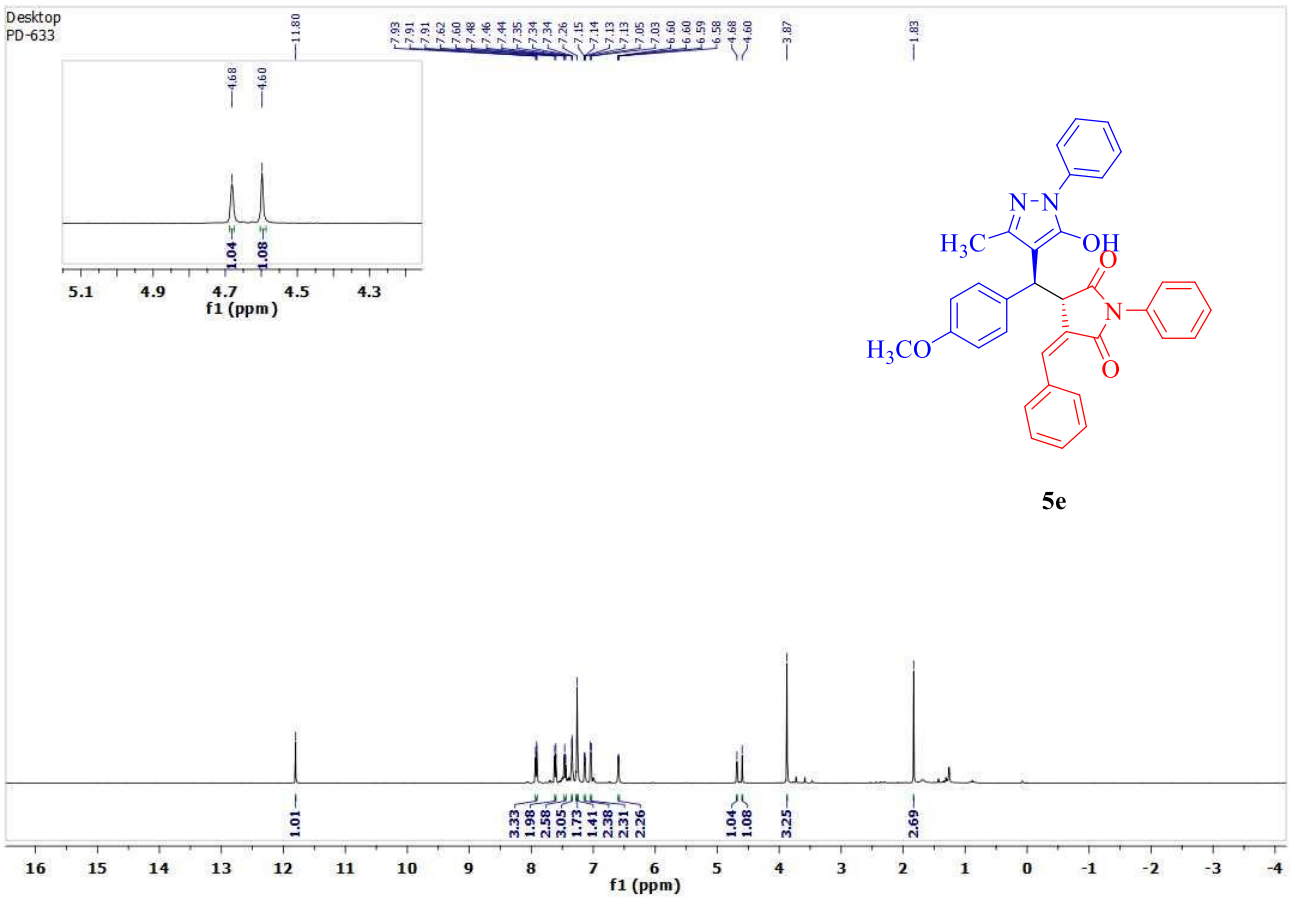

f1 (ppm)
5c


Desktop
PD-817
11.53
7.85
7.83
7.46
7.44
7.43
7.05
7.05
7.00
6.96
6.95
6.88
6.86
4.96
4.76
3.83
3.66
3.55
2.25
4.96
4.76
0.89
0.91
5.00
4.90
4.80
f1 (ppm)
N-N
H3C
OH
O
CH3
N
OMe
O
CH3
H3CO
OCH3
0.60
0.94
1.97
2.00
1.96
1.01
0.92
1.06
2.19
1.11
1.07
1.88
0.89
0.91
3.12
2.84
2.84
6.00
3.14
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

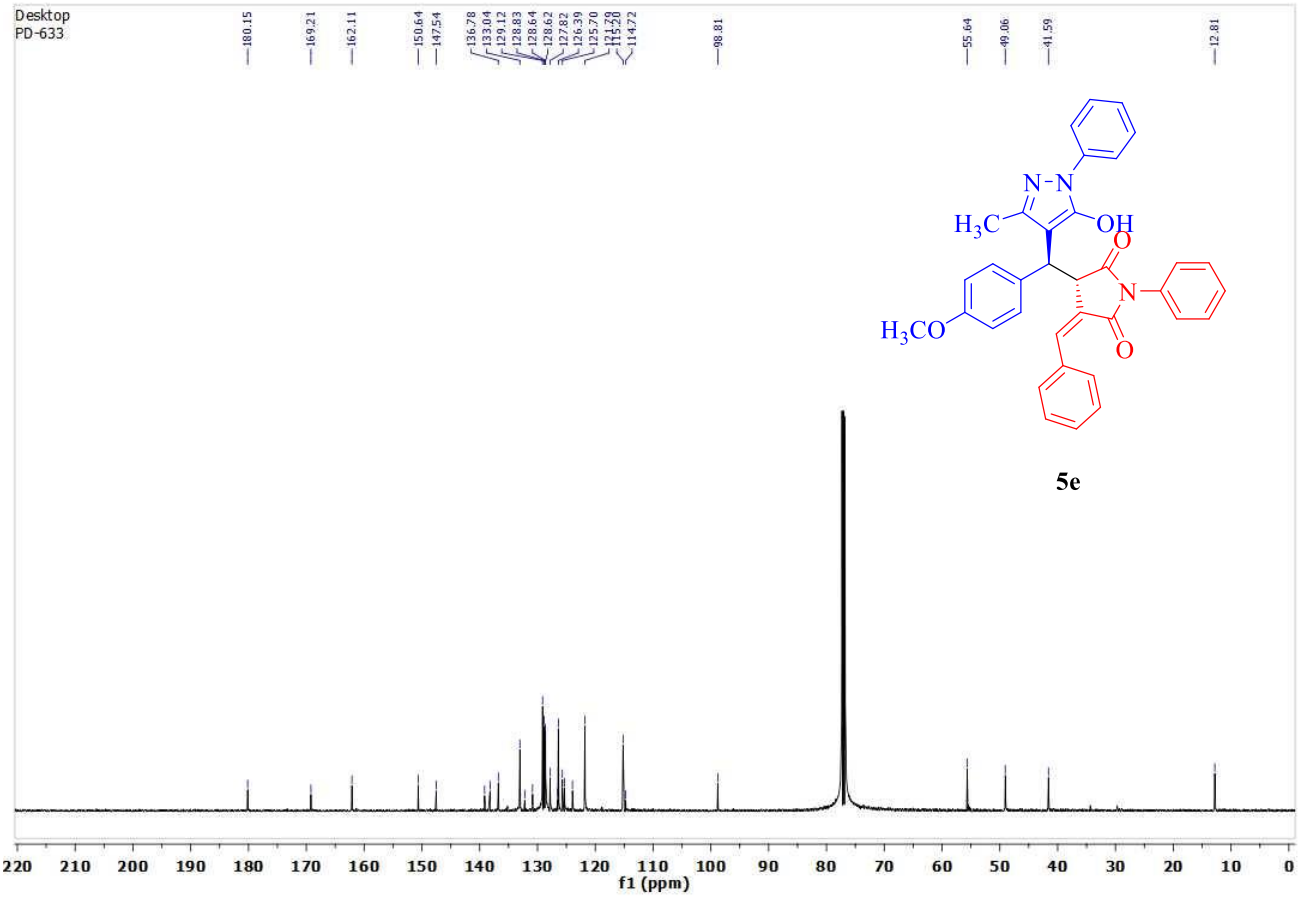
5d


Desktop
PD-817
180.66
169.49
156.87
153.65
152.94
150.57
147.31
139.22
138.94
131.49
130.81
128.81
128.53
125.62
124.10
121.82
120.69
118.49
113.76
112.64
100.81
100.64
55.88
55.50
54.79
49.63
34.93
21.10
12.21
N-N
H3C
OH
O
CH3
N
OMe
O
CH3
H3CO
OCH3
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

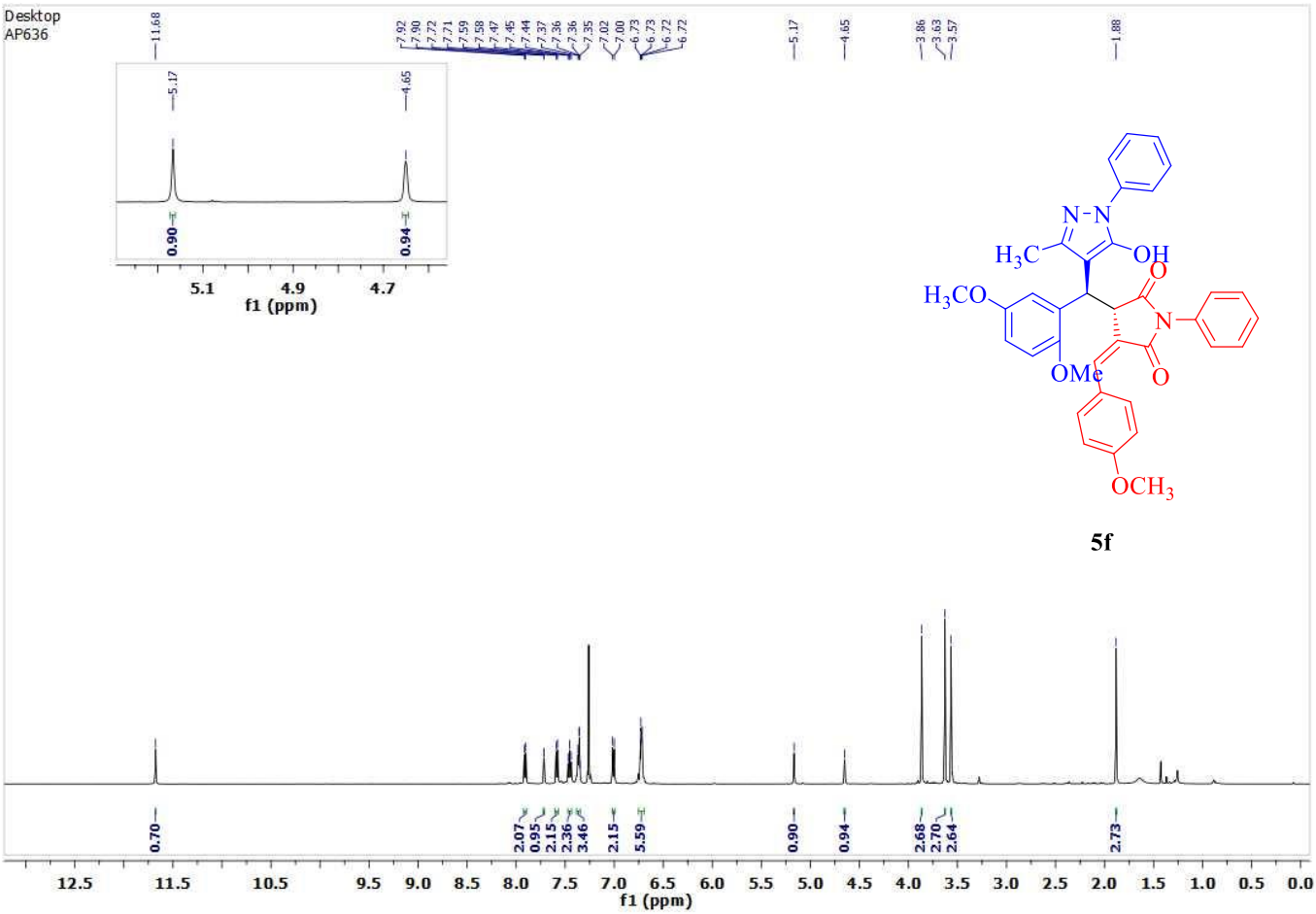
5d


Desktop
PD-633
11.80
7.93
7.91
7.91
7.62
7.60
7.48
7.46
7.44
7.35
7.34
7.34
7.26
7.15
7.14
7.13
7.13
7.05
7.03
6.60
6.60
6.59
6.58
4.68
4.60
3.87
1.83
4.68
4.60
1.04
1.08
5.1
4.9
4.7
4.5
4.3
f1 (ppm)
N-N
H3C
OH
O
N
O
H3CO
O
1.01
3.33
1.98
2.58
3.05
1.73
1.41
2.38
2.31
2.26
1.04
1.08
3.25
2.69
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
f1 (ppm)

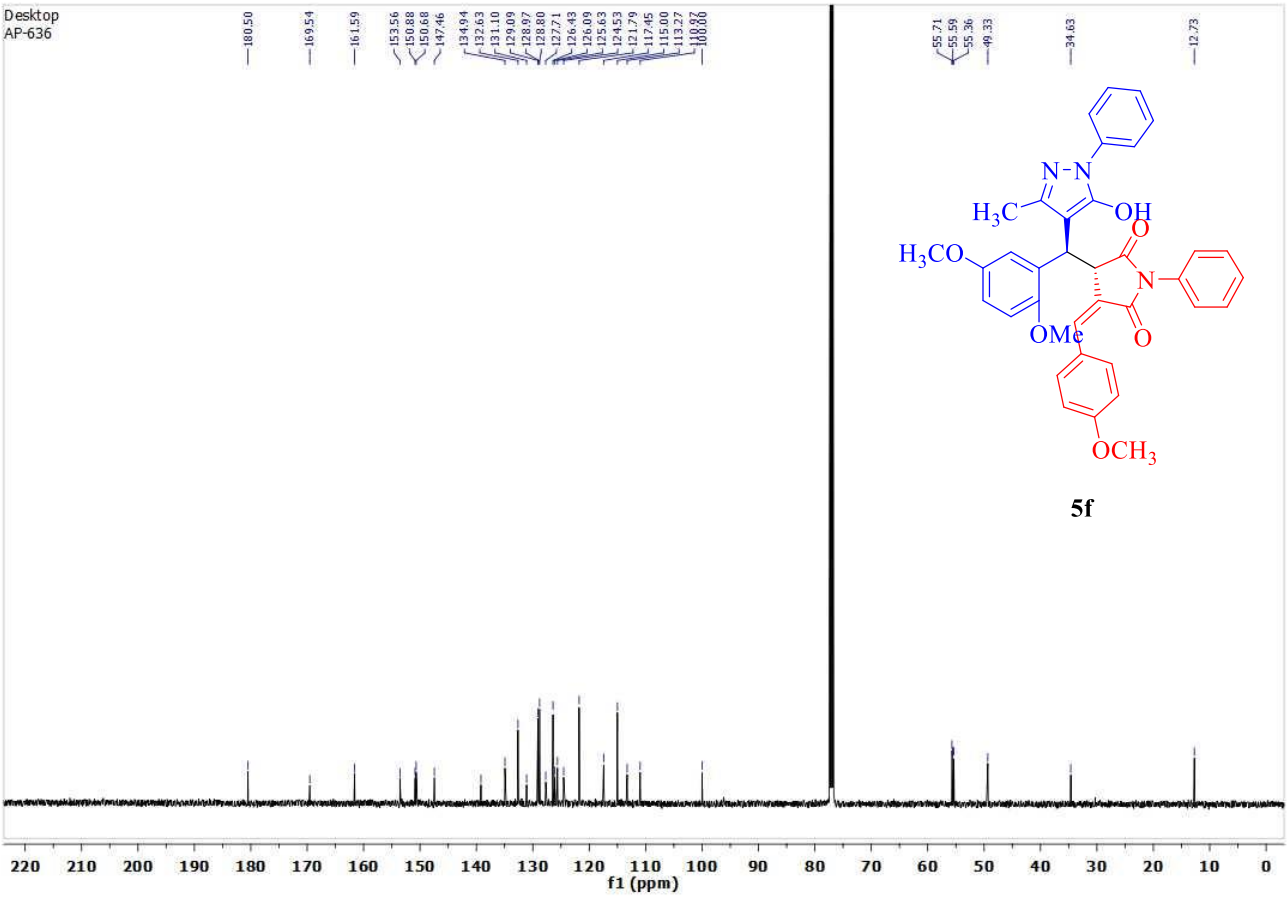
5e


Desktop
PD-633
180.15
169.21
162.11
150.64
147.54
136.78
133.04
129.12
128.83
128.64
128.62
127.82
126.39
125.70
121.28
115.20
114.72
98.81
55.64
49.06
41.59
12.81
N-N
H3C
OH
O
N
O
H3CO
O
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

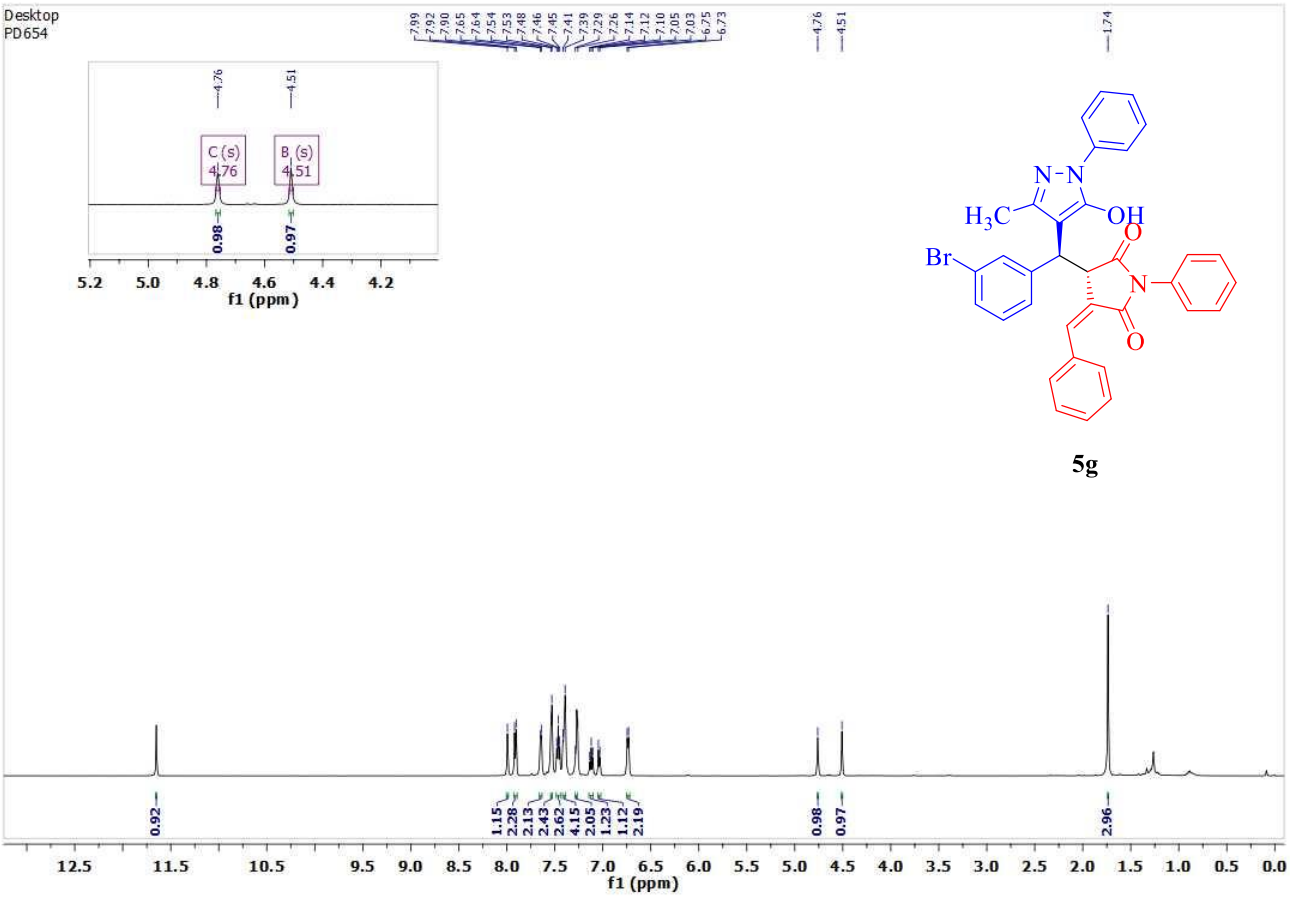
5e

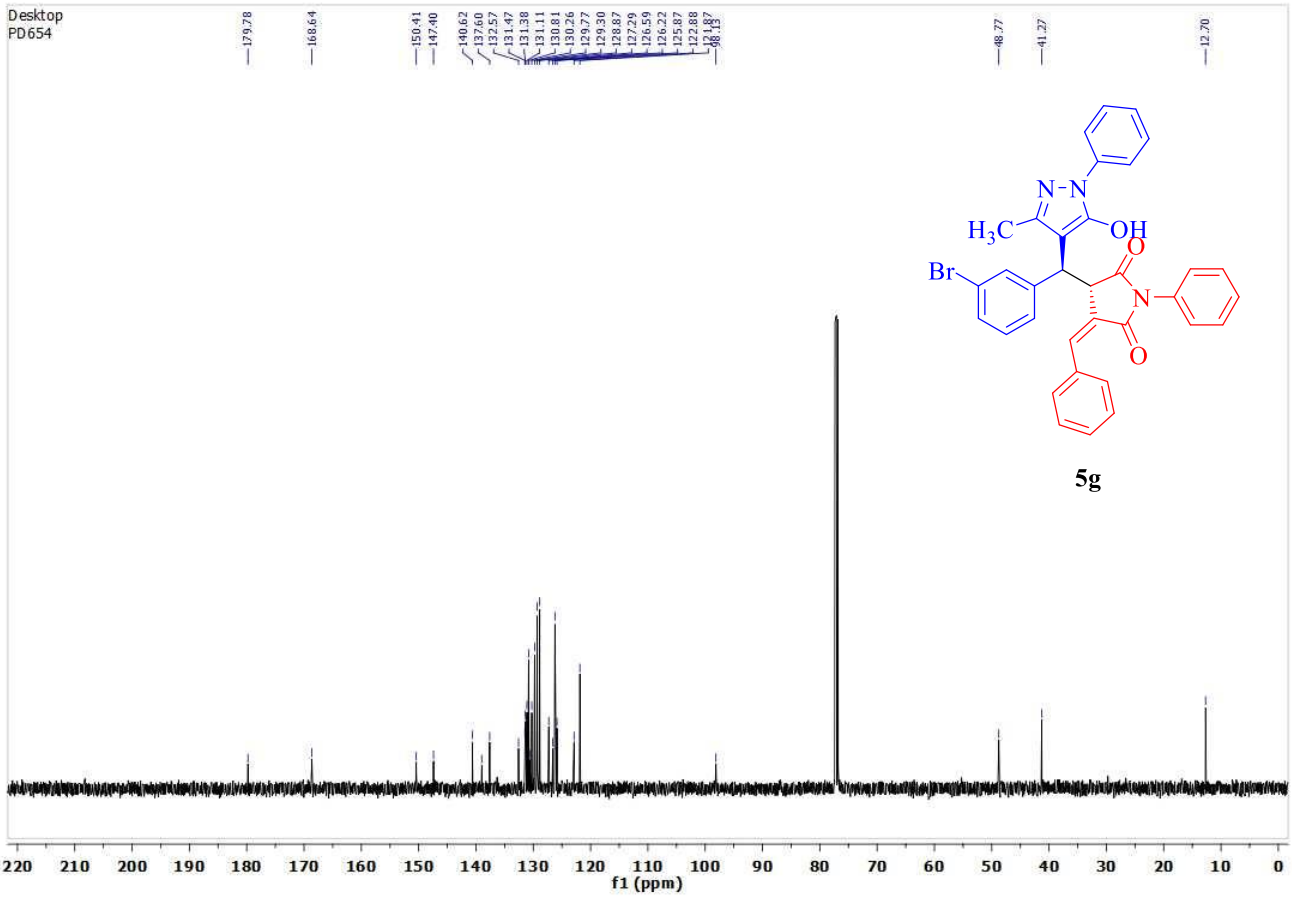

Desktop
AP636
11.68
7.92
7.90
7.72
7.71
7.59
7.58
7.47
7.45
7.44
7.37
7.36
7.36
7.35
7.02
7.00
6.73
6.73
6.72
6.72
5.17
4.65
3.86
3.63
3.57
1.88
5.17
4.65
0.90
0.94
5.1
4.9
4.7
f1 (ppm)
N-N
H3C
OH
H3CO
O
N
OMe
O
OCH3
0.70
2.07
0.95
2.15
2.36
3.46
2.15
5.59
0.90
0.94
2.68
2.70
2.64
2.73
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

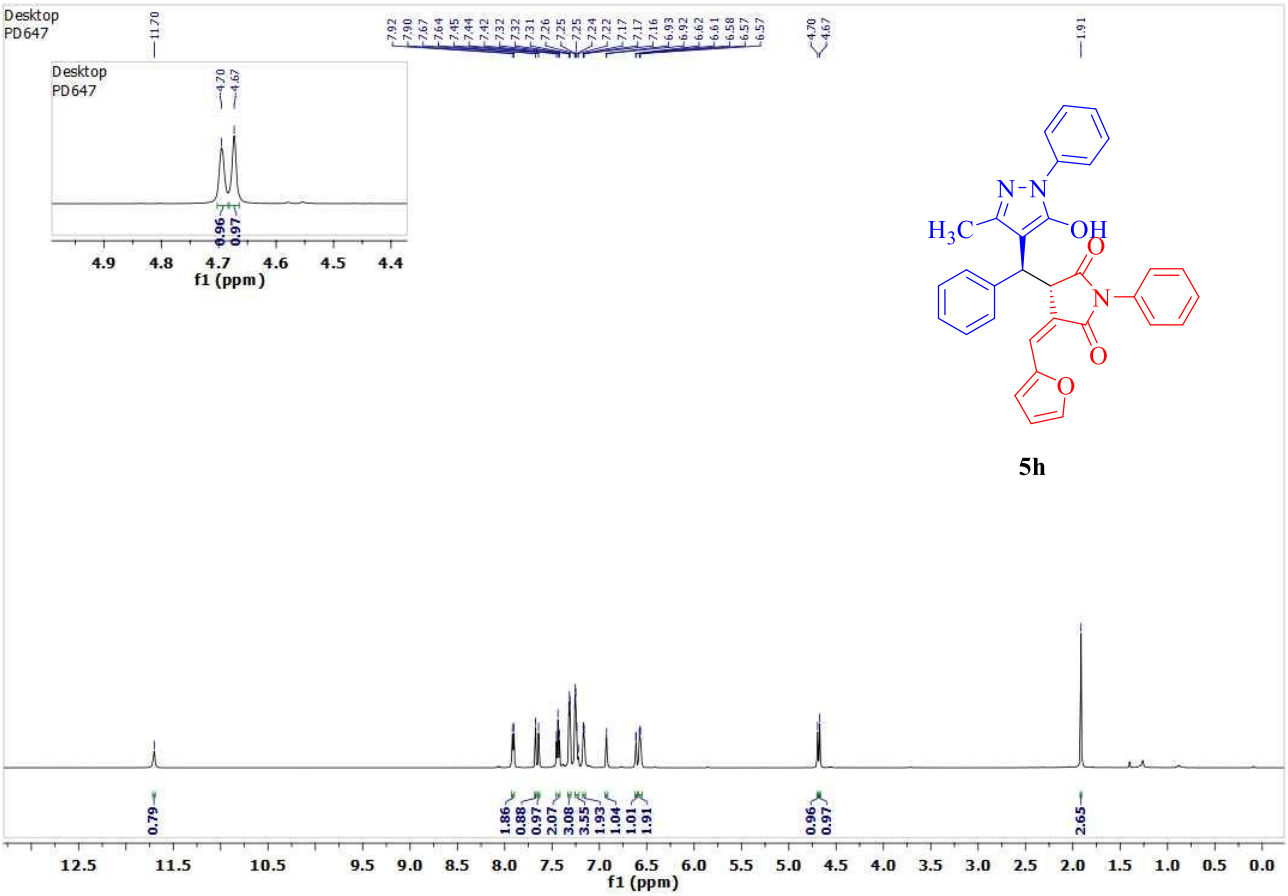
5f


Desktop
AP-636
180.50
169.54
161.59
153.56
150.88
150.68
147.46
134.94
132.63
131.10
129.09
128.97
128.80
127.71
126.43
126.09
125.63
124.53
121.79
117.45
115.00
113.27
55.71
55.59
55.36
49.33
34.63
12.73
N-N
H3C
OH
H3CO
O
N
OMe
O
OCH3
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

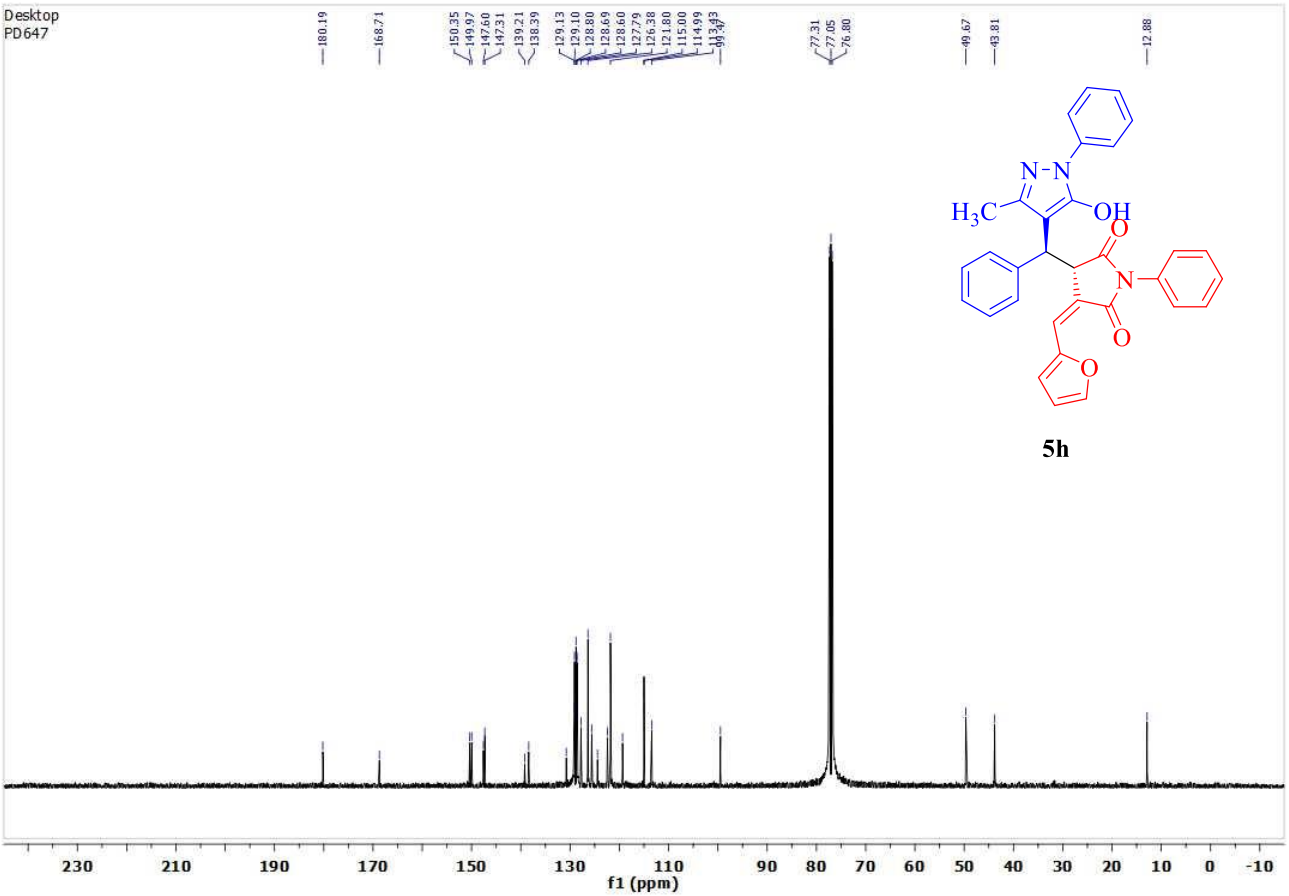
5f


Desktop
PD654
C (s)
4.76
B (s)
4.51
0.98
0.97
f1 (ppm)
Br
OH
O
N
5g
0.92
1.15
2.28
2.13
2.43
2.62
4.15
2.05
1.23
1.12
2.19
0.98
0.97
2.96
f1 (ppm)

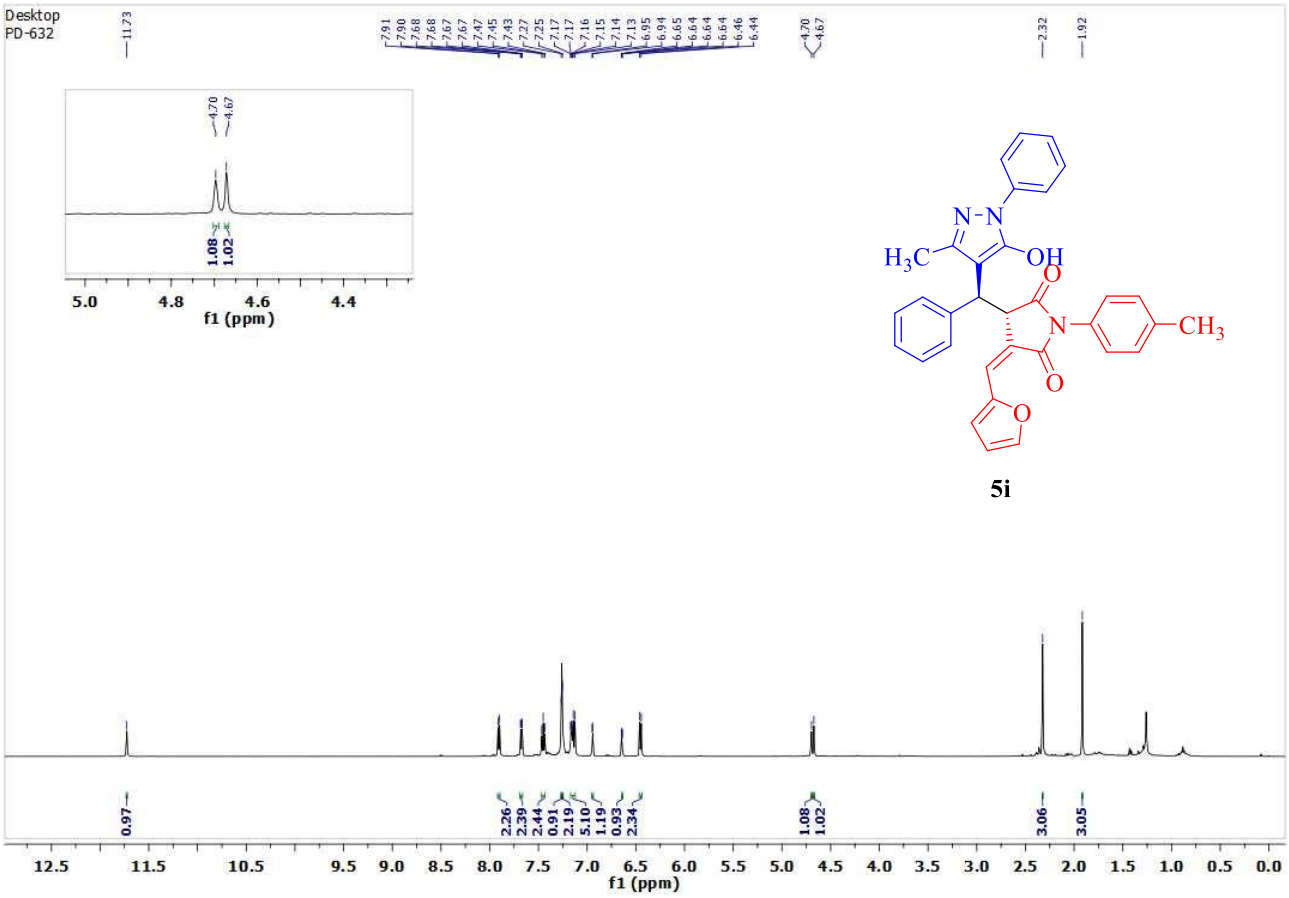

Desktop
PD654
Br
OH
O
N
5g
f1 (ppm)


Desktop
PD647
11.70
7.92
7.90
7.67
7.64
7.45
7.44
7.42
7.32
7.31
7.26
7.25
7.25
7.24
7.22
7.17
7.17
7.16
6.93
6.92
6.62
6.61
6.58
6.57
6.57
4.70
4.67
1.91
Desktop
PD647
4.70
4.67
0.96
0.97
4.9
4.8
4.7
4.6
4.5
4.4
f1 (ppm)
N-N
H3C
OH
O
N
O
O
0.79
1.86
0.88
0.97
2.07
3.08
3.55
1.93
1.04
1.01
1.91
0.96
0.97
2.65
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

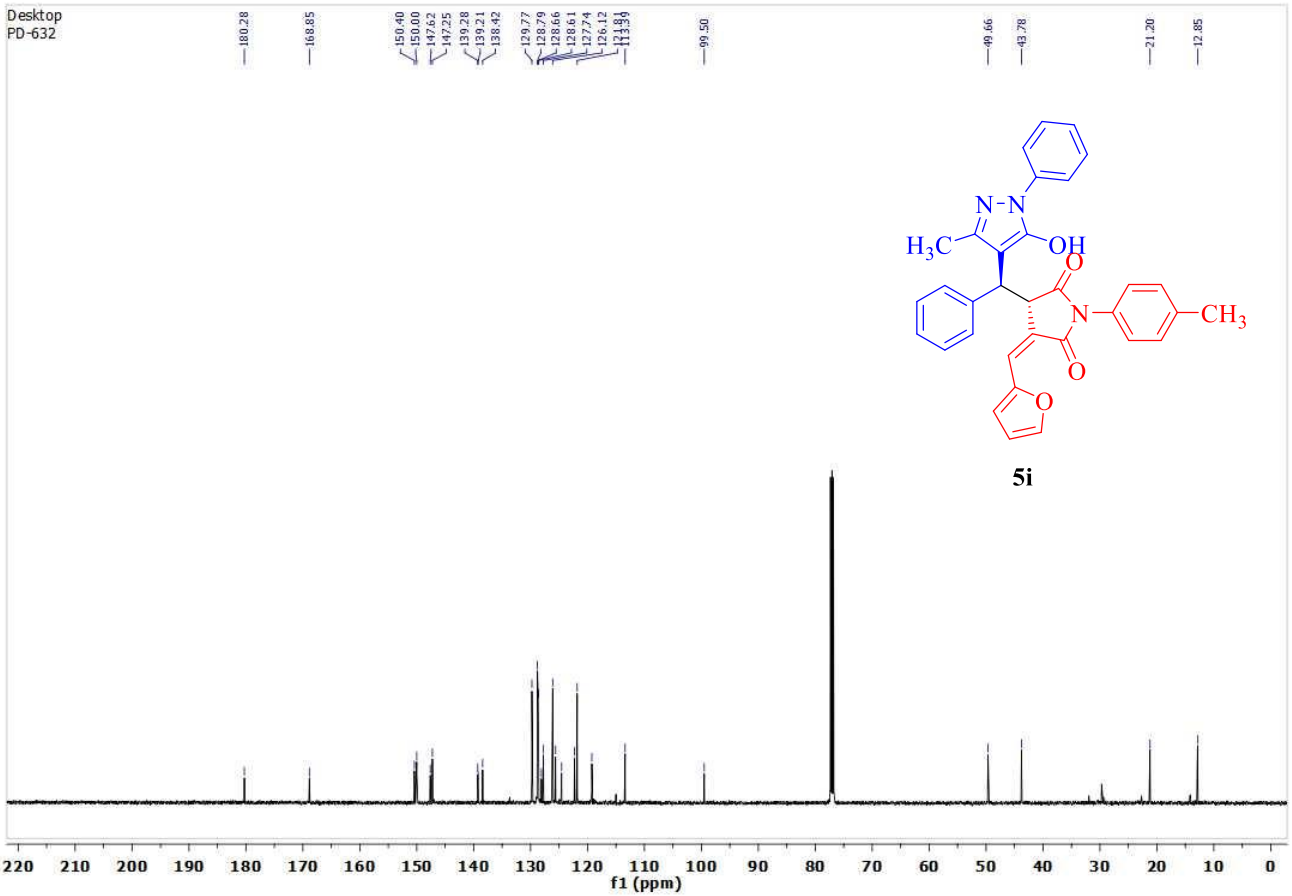
5h


Desktop
PD647
180.19
168.71
150.35
149.97
147.60
147.31
139.21
138.39
129.13
129.10
128.80
128.69
128.60
127.79
126.38
121.80
115.00
114.99
113.43
99.47
77.31
77.05
76.80
49.67
43.81
12.88
N-N
H3C
OH
O
N
O
O
230
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

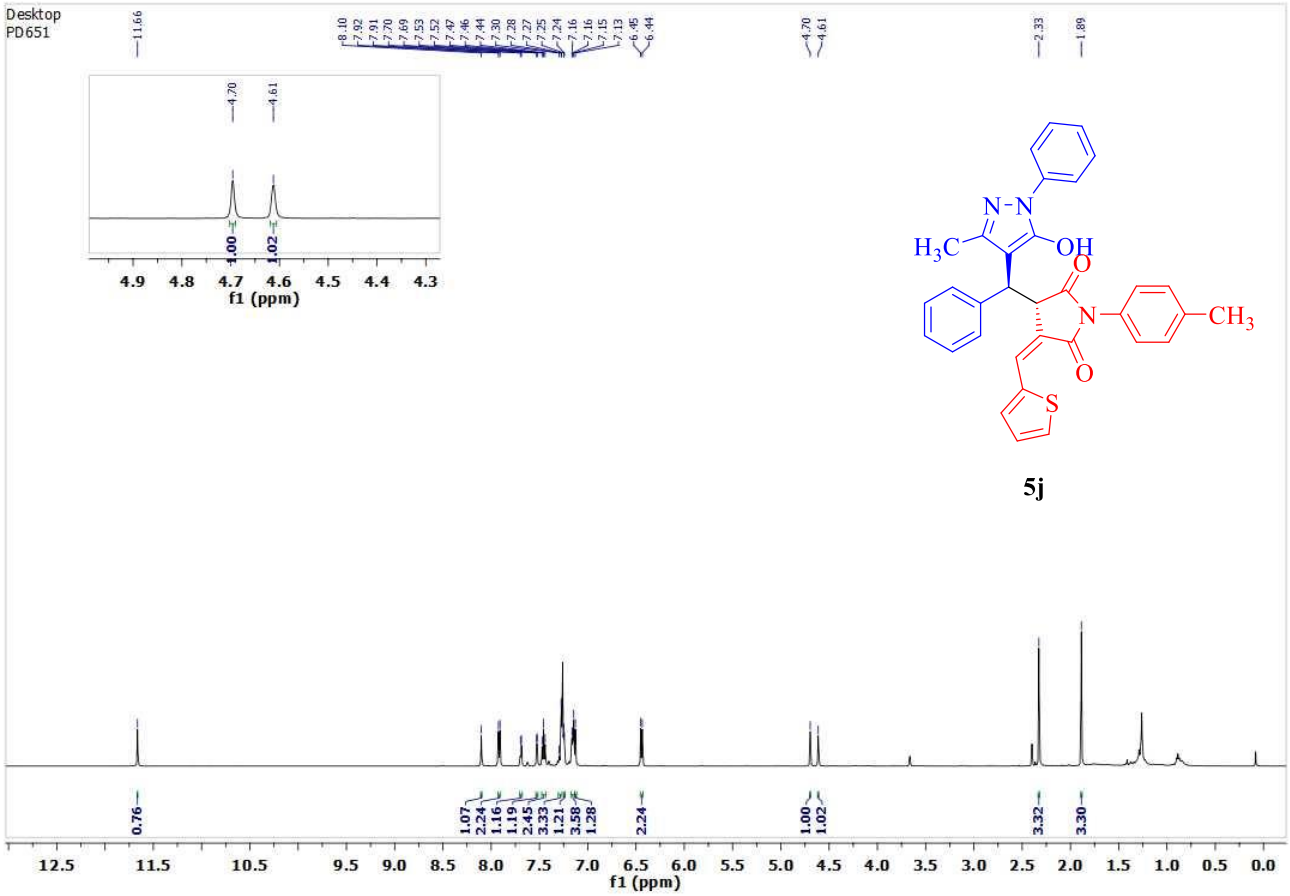
5h


Desktop
PD-632
11.73
7.91
7.90
7.68
7.68
7.67
7.67
7.47
7.45
7.43
7.27
7.25
7.17
7.17
7.16
7.15
7.14
7.13
6.95
6.94
6.65
6.64
6.64
6.64
6.46
6.44
4.70
4.67
2.32
1.92
4.70
4.67
1.08
1.02
5.0
4.8
4.6
4.4
f1 (ppm)
N-N
H3C
OH
O
N
CH3
O
O
O
0.97
2.26
2.39
2.44
0.91
2.19
5.10
1.19
0.93
2.34
1.08
1.02
3.06
3.05
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

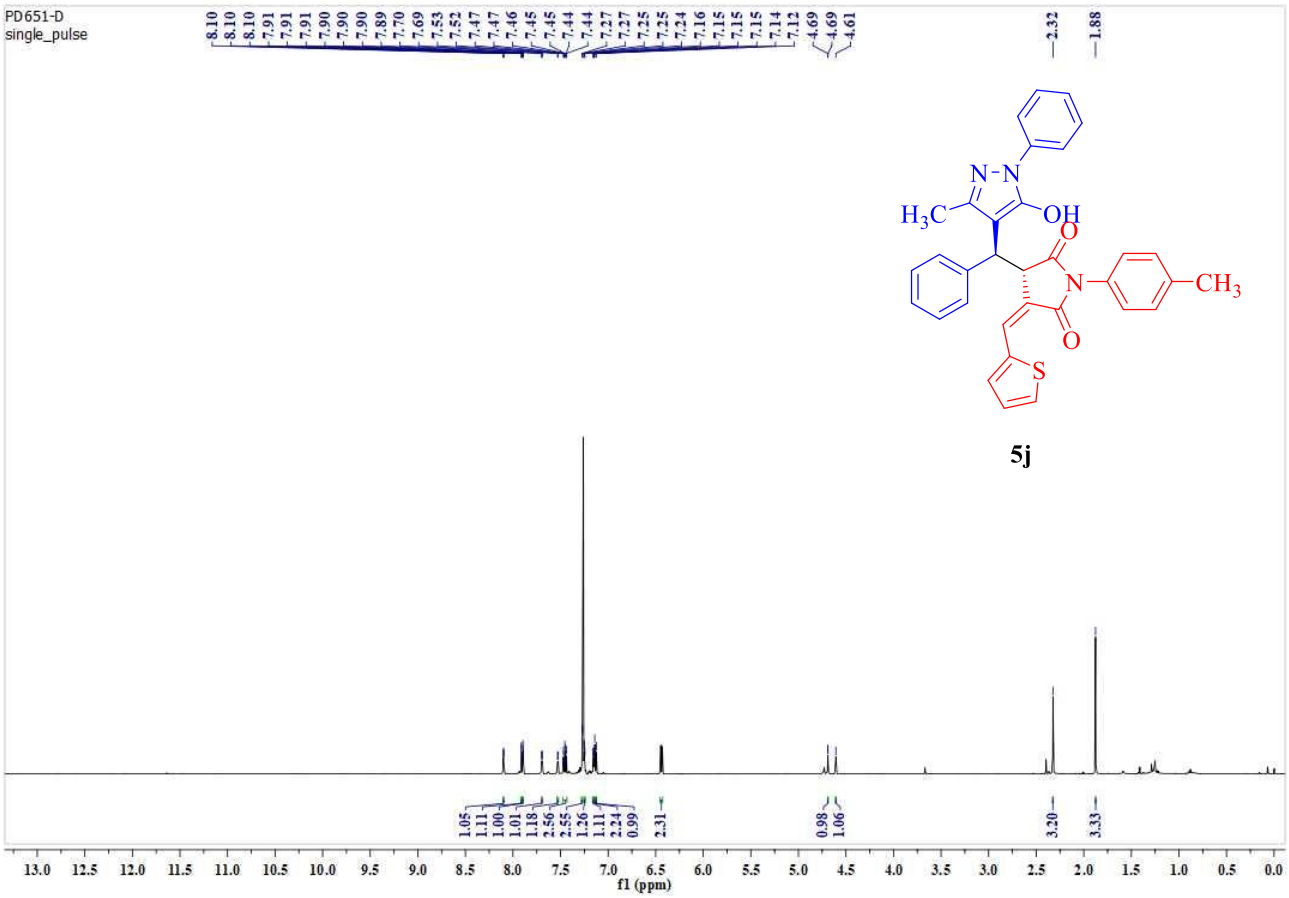
5i


Desktop
PD-632
180.28
168.85
150.40
150.00
147.62
147.25
139.28
139.21
138.42
129.77
128.79
128.66
128.61
127.74
126.12
99.50
49.66
43.78
21.20
12.85
N-N
H3C
OH
O
N
CH3
O
O
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

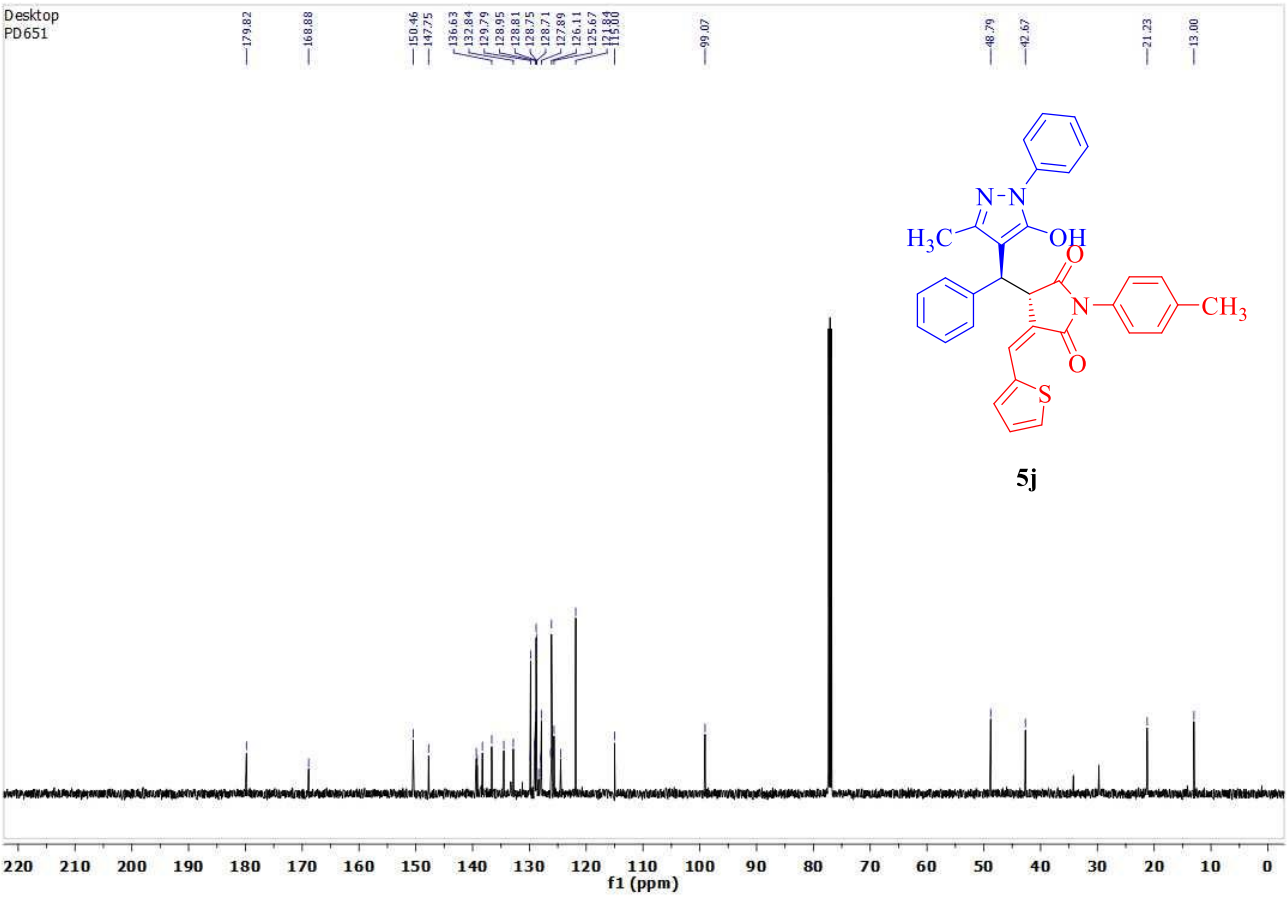
5i



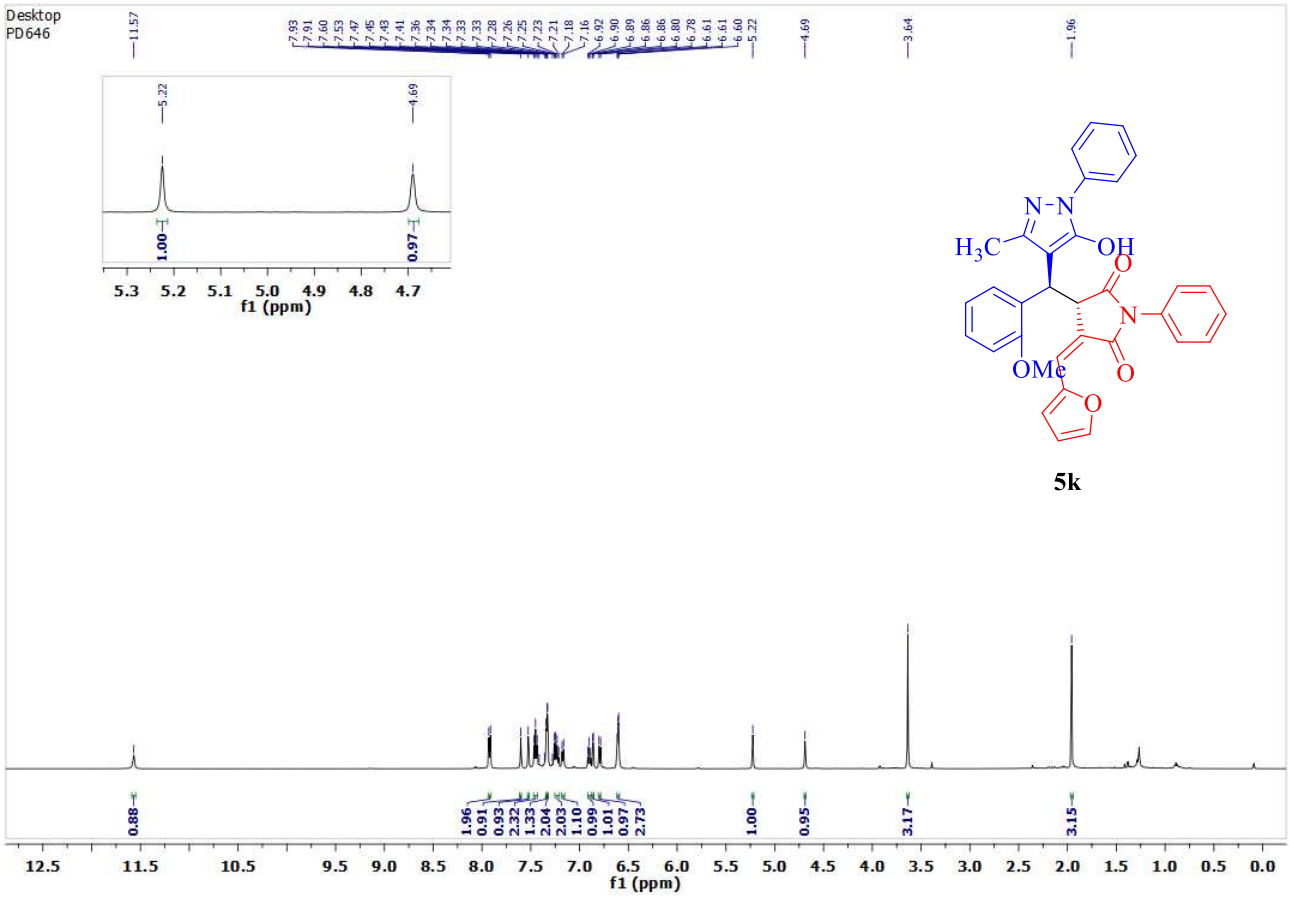
5j



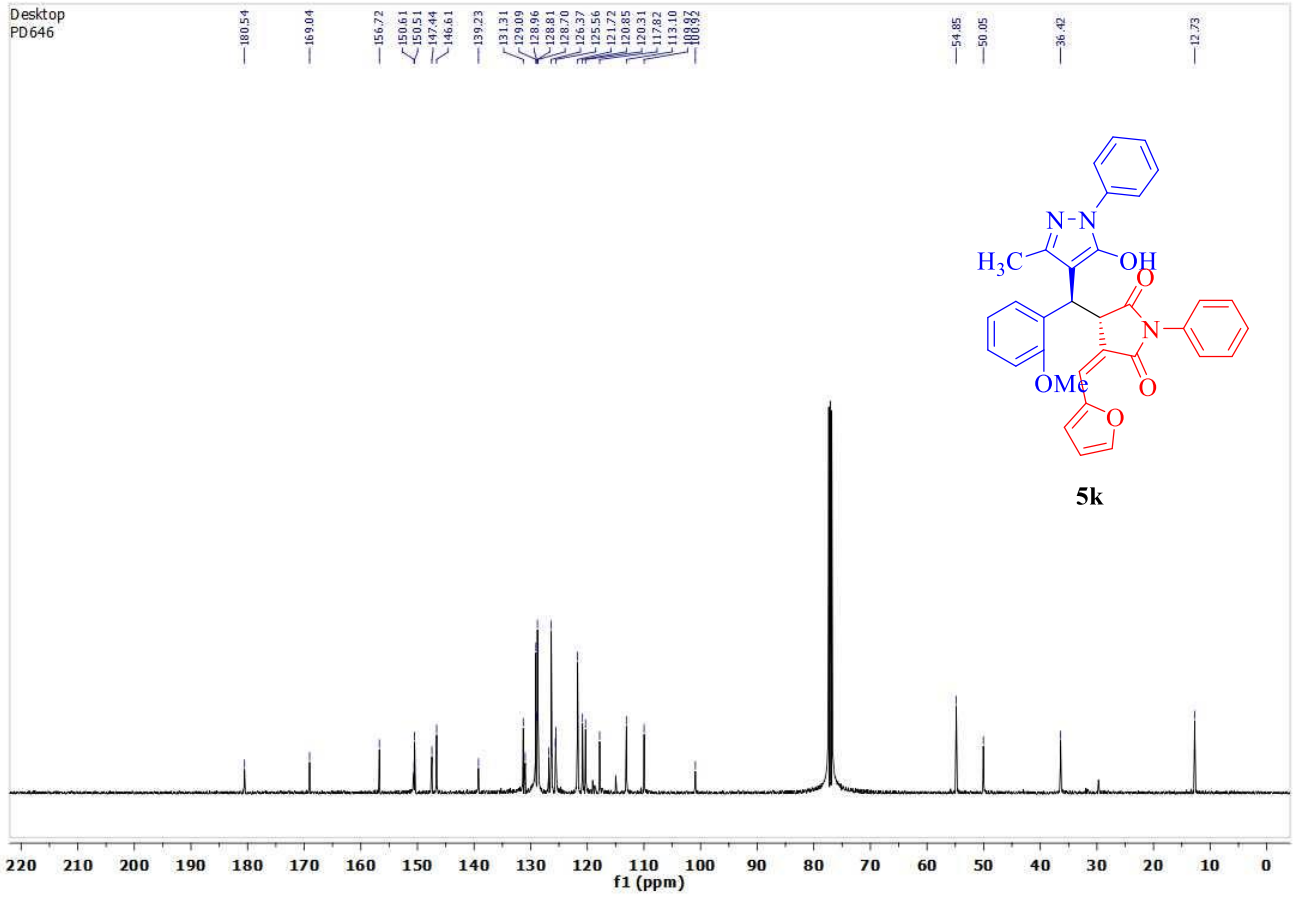
5j


Desktop
PD651
179.82
168.88
150.46
147.75
136.63
132.84
129.79
128.95
128.81
128.75
128.71
127.89
126.11
125.67
99.07
48.79
42.67
21.23
13.00
N-N
H3C
OH
O
N
CH3
O
S
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

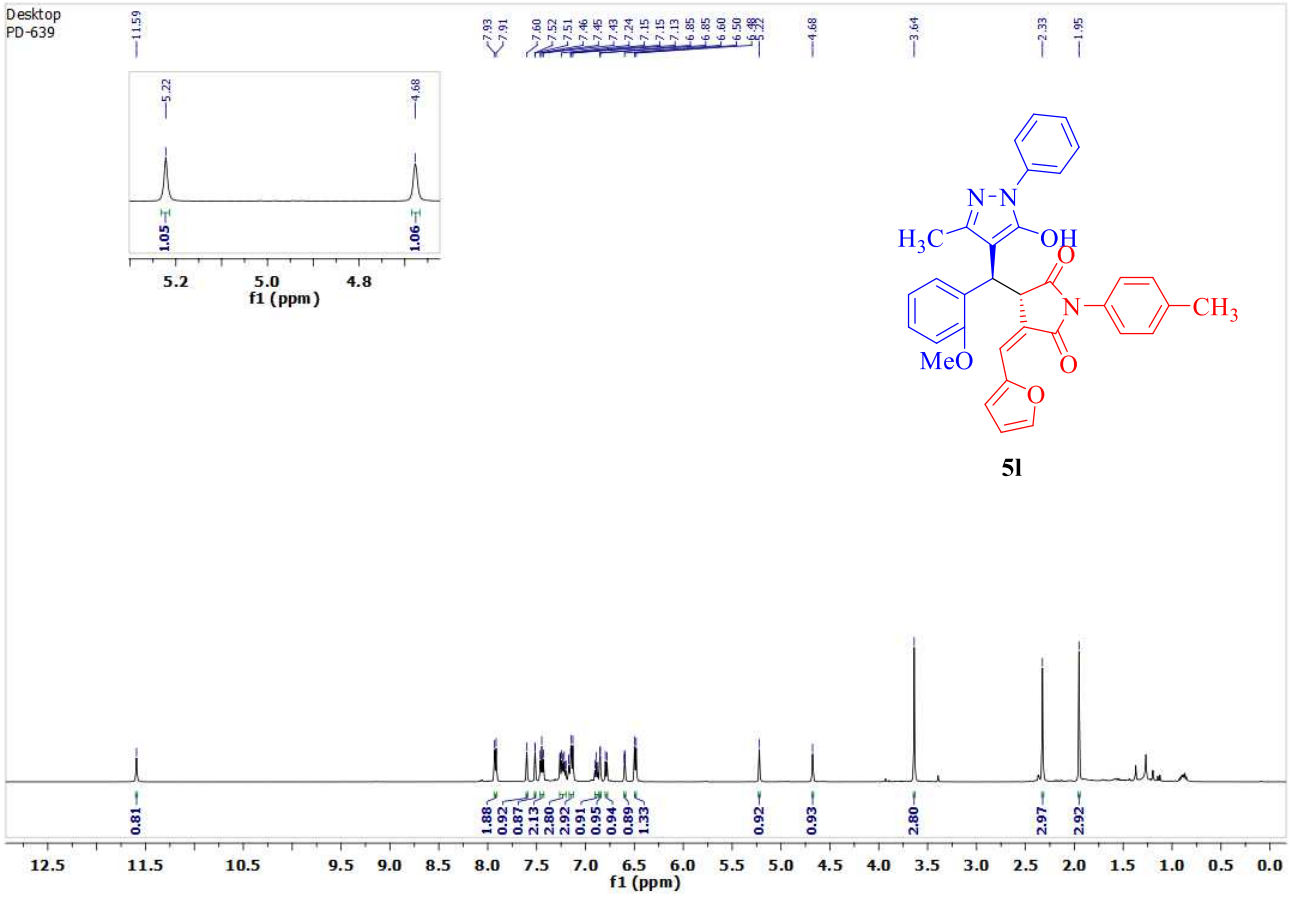
5j



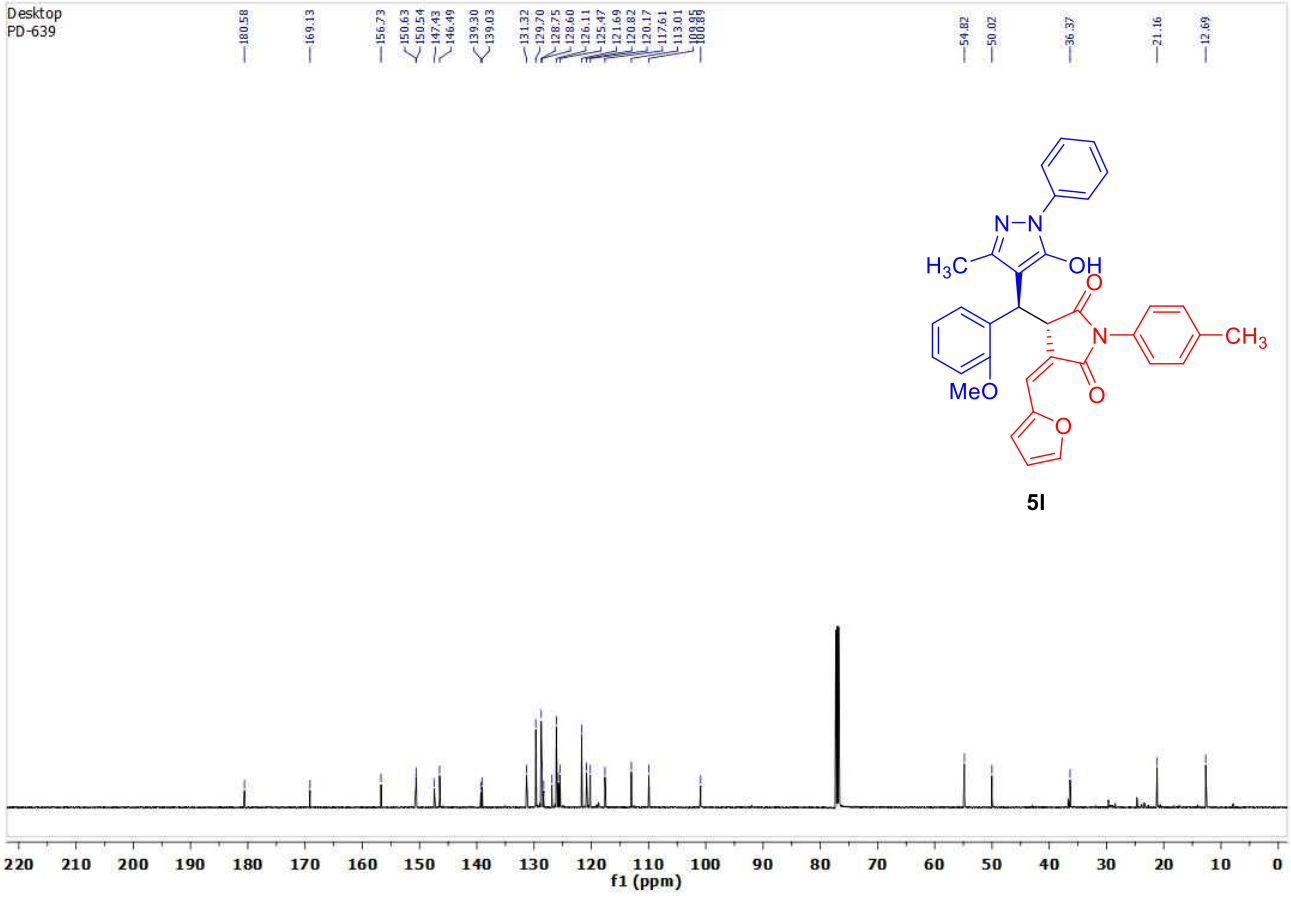
5k



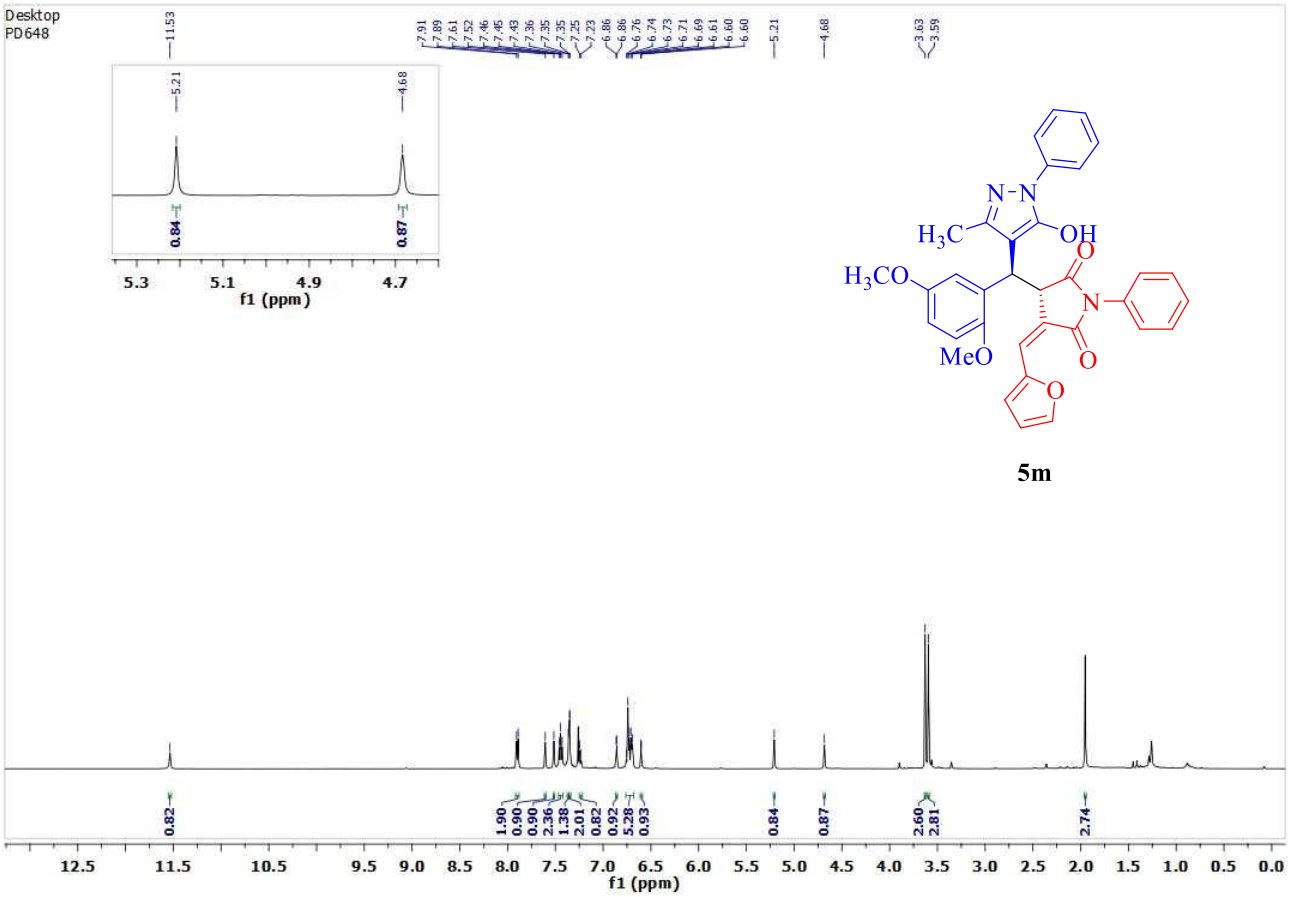
5k


Desktop
PD-639
11.59
7.93
7.91
7.60
7.52
7.51
7.46
7.45
7.43
7.24
7.15
7.15
7.13
6.85
6.85
6.60
6.50
5.22
4.68
3.64
2.33
1.95
5.22
4.68
1.05
1.06
5.2
5.0
4.8
f1 (ppm)
N-N
H3C
OH
O
N
CH3
MeO
O
O
O
0.81
1.88
0.92
0.87
2.13
2.80
2.92
0.91
0.95
0.94
0.89
1.33
0.92
0.93
2.80
2.97
2.92
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

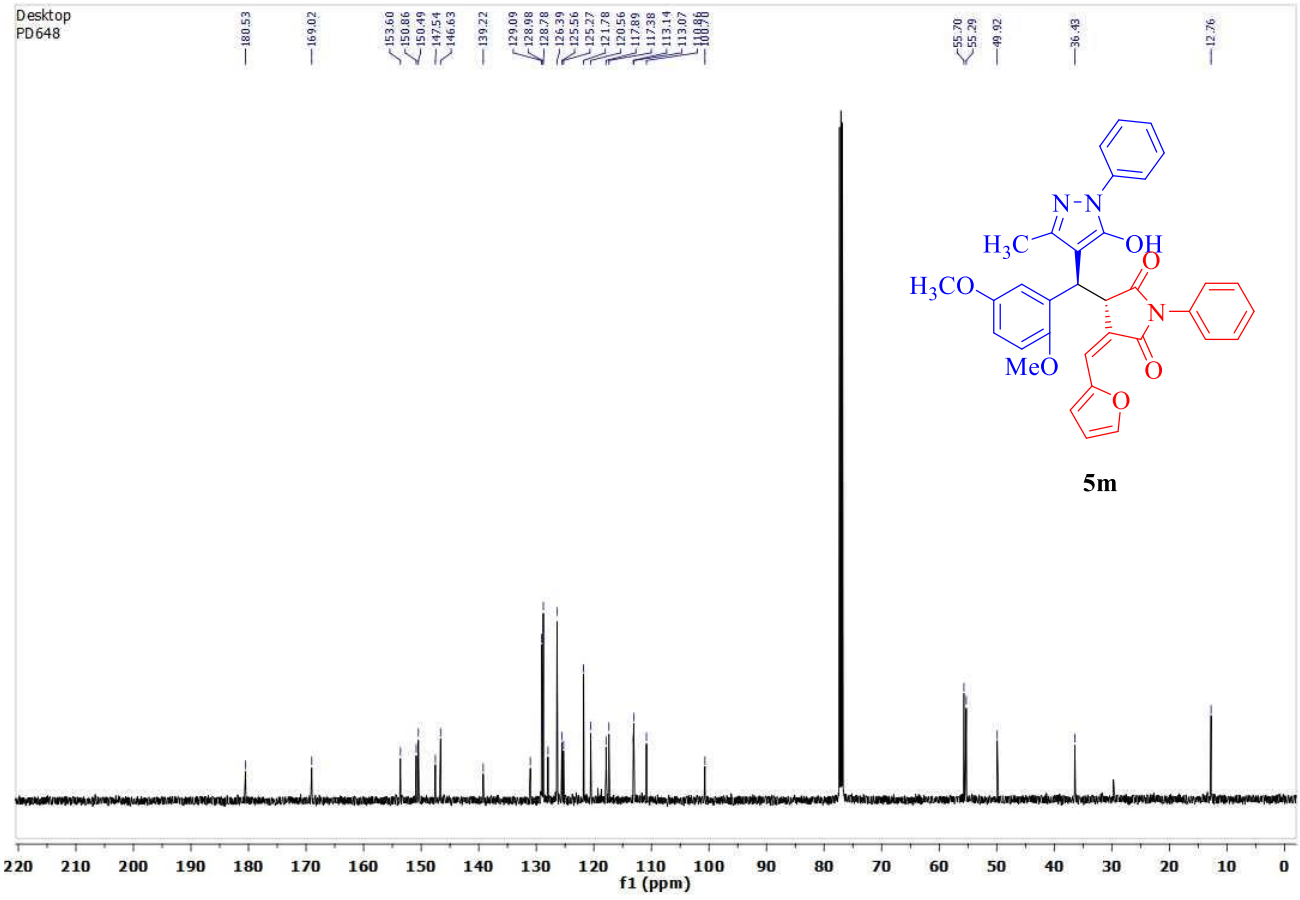
5l


Desktop
PD-639
180.58
169.13
156.73
150.63
150.54
147.43
146.49
139.30
139.03
131.32
129.70
128.75
128.60
126.11
125.47
121.69
120.82
120.17
117.61
113.01
54.82
50.02
36.37
21.16
12.69
N-N
H3C
OH
O
N
CH3
MeO
O
O
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

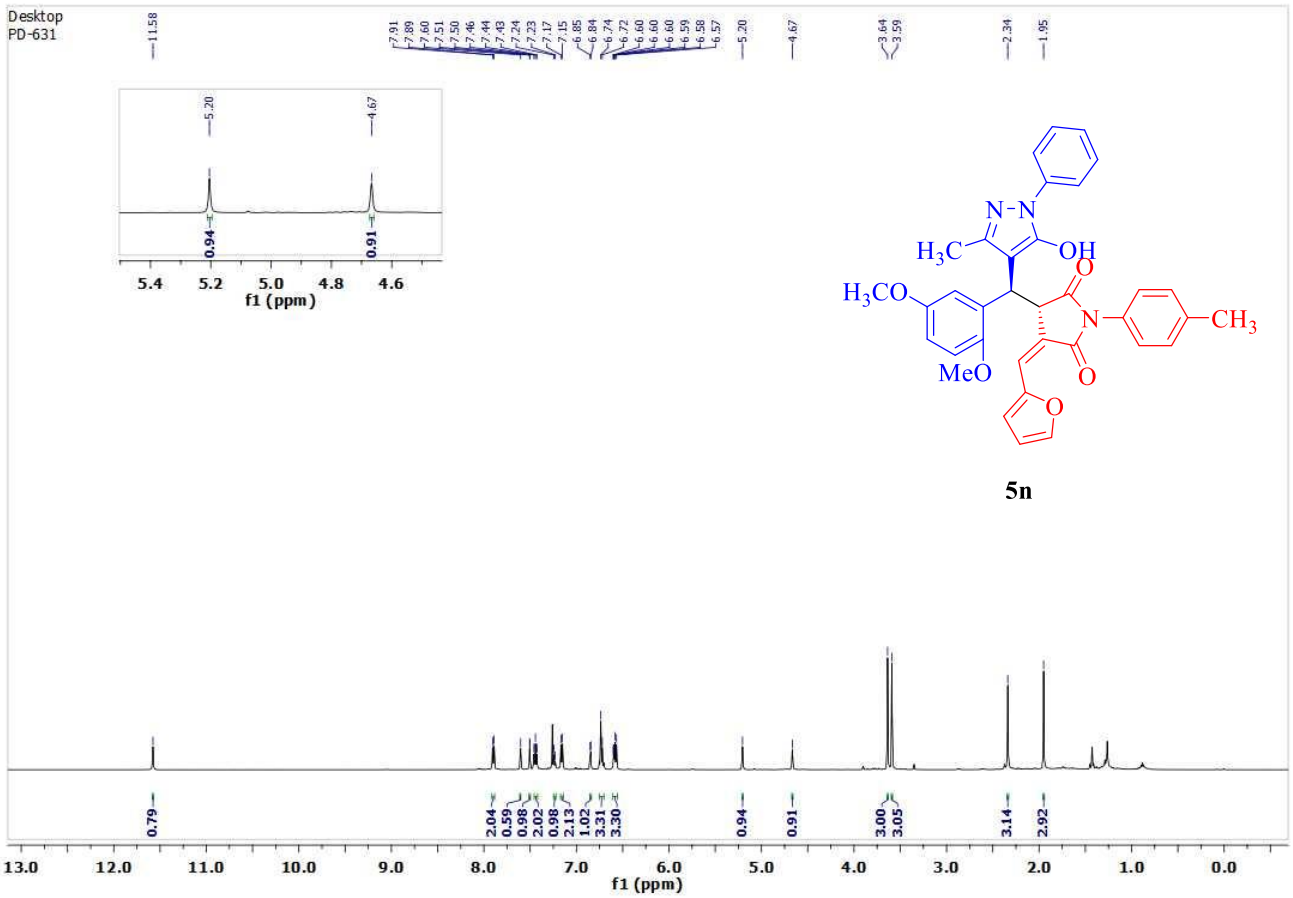
5l



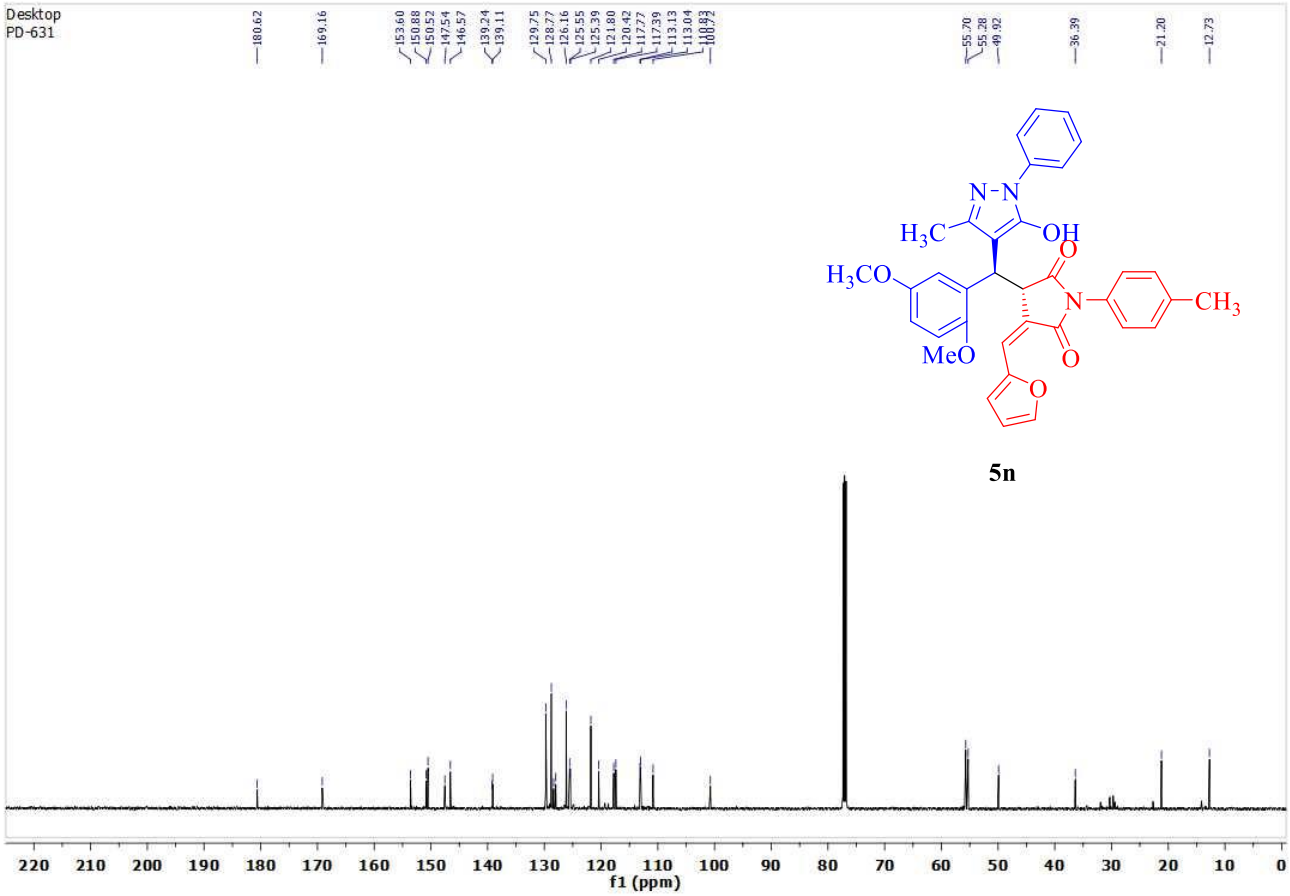
5m



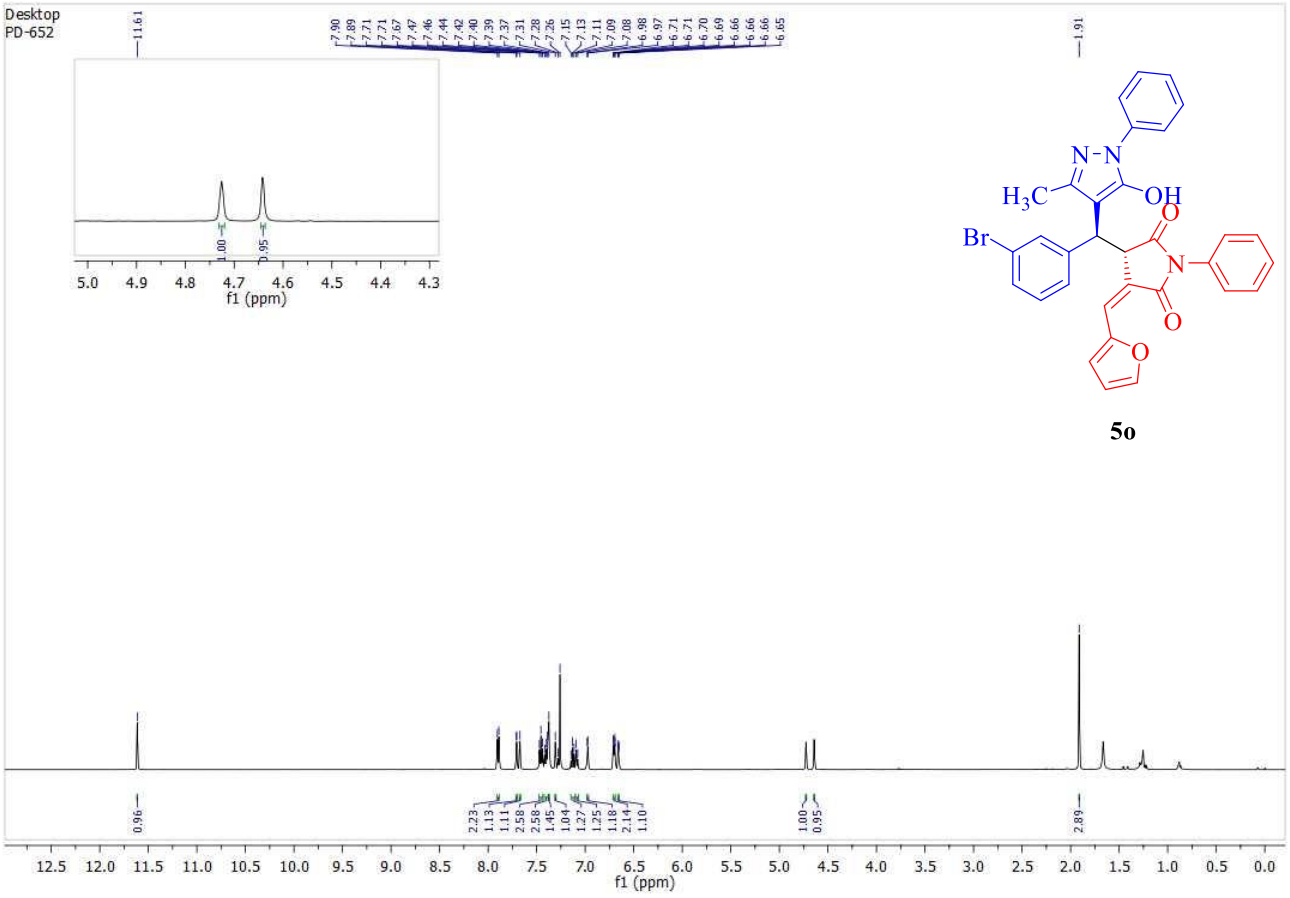
5m


Desktop
PD-631
11.58
7.91
7.89
7.60
7.51
7.50
7.46
7.44
7.43
7.24
7.23
7.17
7.15
6.85
6.84
6.74
6.72
6.60
6.60
6.59
6.58
6.57
5.20
4.67
3.64
3.59
2.34
1.95
5.20
4.67
0.94
0.91
5.4
5.2
5.0
4.8
4.6
f1 (ppm)
N-N
H3C
OH
H3CO
O
N
CH3
O
MeO
O
0.79
2.04
0.59
0.98
2.02
0.98
2.13
1.02
3.31
3.30
0.94
0.91
3.00
3.05
3.14
2.92
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

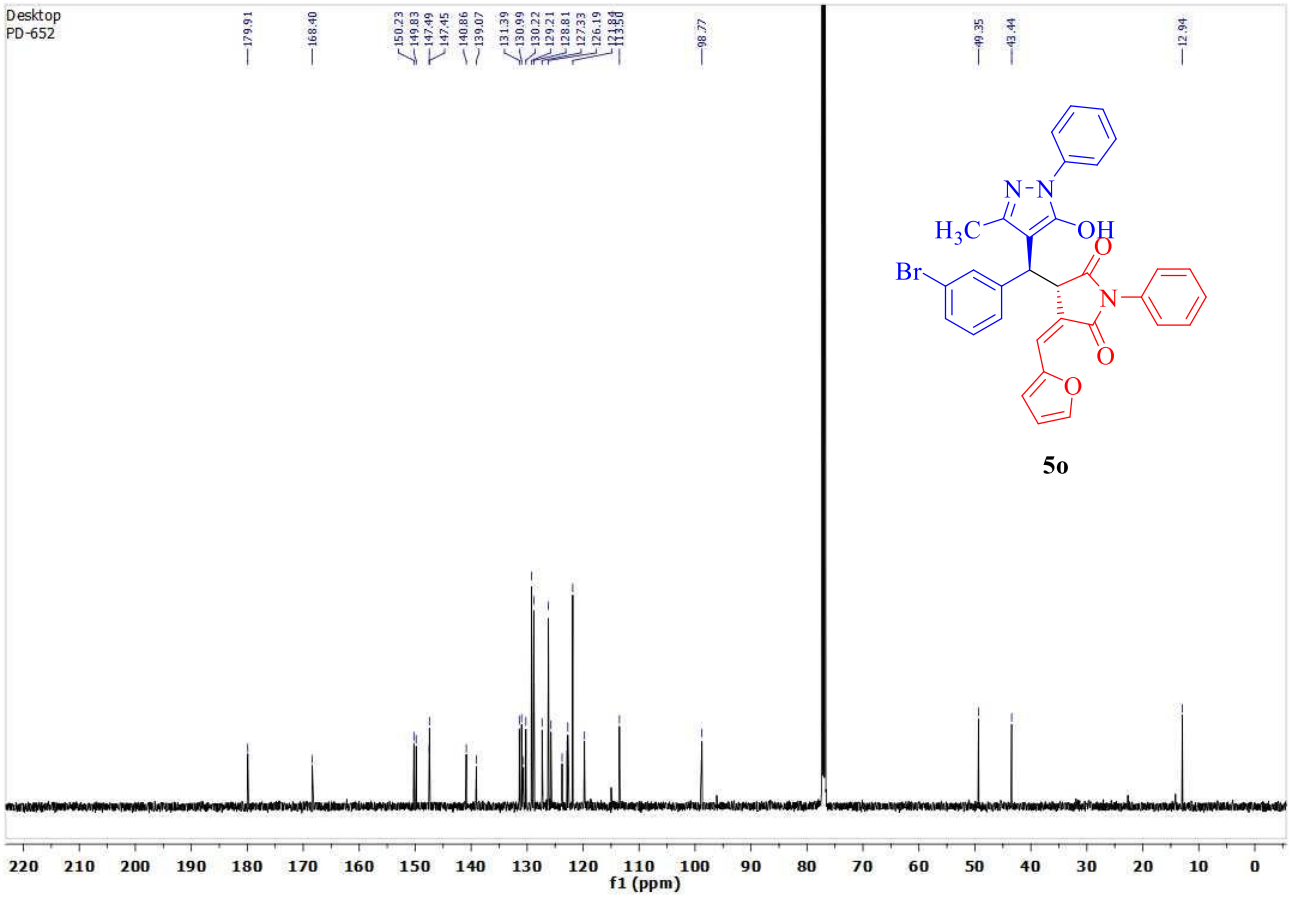
5n


Desktop
PD-631
180.62
169.16
153.60
150.88
150.52
147.54
146.57
139.24
139.11
129.75
128.77
126.16
125.55
125.39
121.80
120.42
117.77
117.39
113.13
113.04
55.70
55.28
49.92
36.39
21.20
12.73
N-N
H3C
OH
H3CO
O
N
CH3
O
MeO
O
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

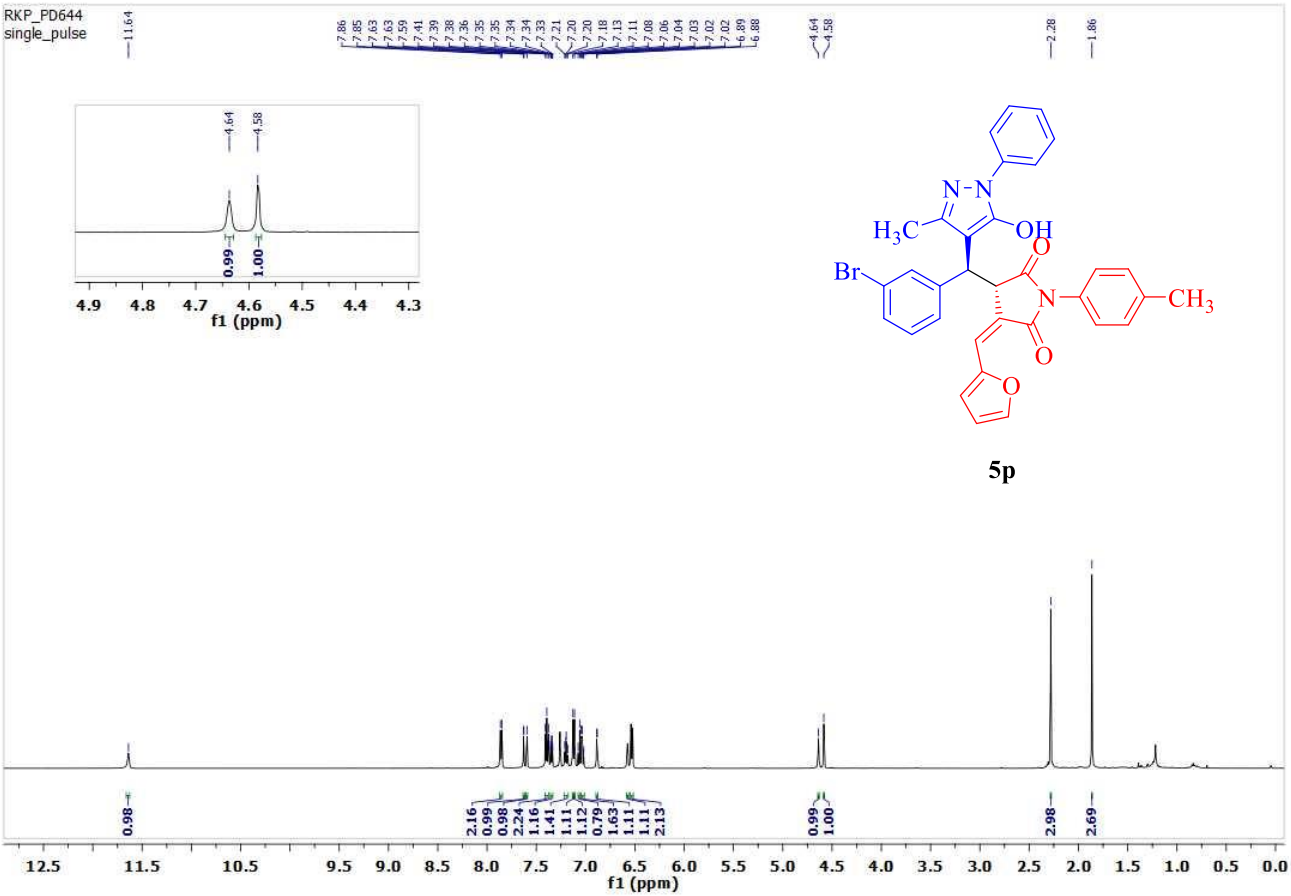
5n


Desktop
PD-652
11.61
7.90
7.89
7.71
7.71
7.67
7.47
7.46
7.44
7.42
7.40
7.39
7.37
7.31
7.28
7.26
7.15
7.13
7.11
7.09
7.08
6.98
6.97
6.71
6.71
6.70
6.69
6.66
6.66
6.66
6.65
1.91
1.00
0.95
5.0 4.9 4.8 4.7 4.6 4.5 4.4 4.3
f1 (ppm)
N-N
H3C
OH
Br
O
N
O
O
0.96
2.23
1.13
1.11
2.58
2.58
1.45
1.04
1.27
1.25
1.18
2.14
1.10
1.00
0.95
2.89
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

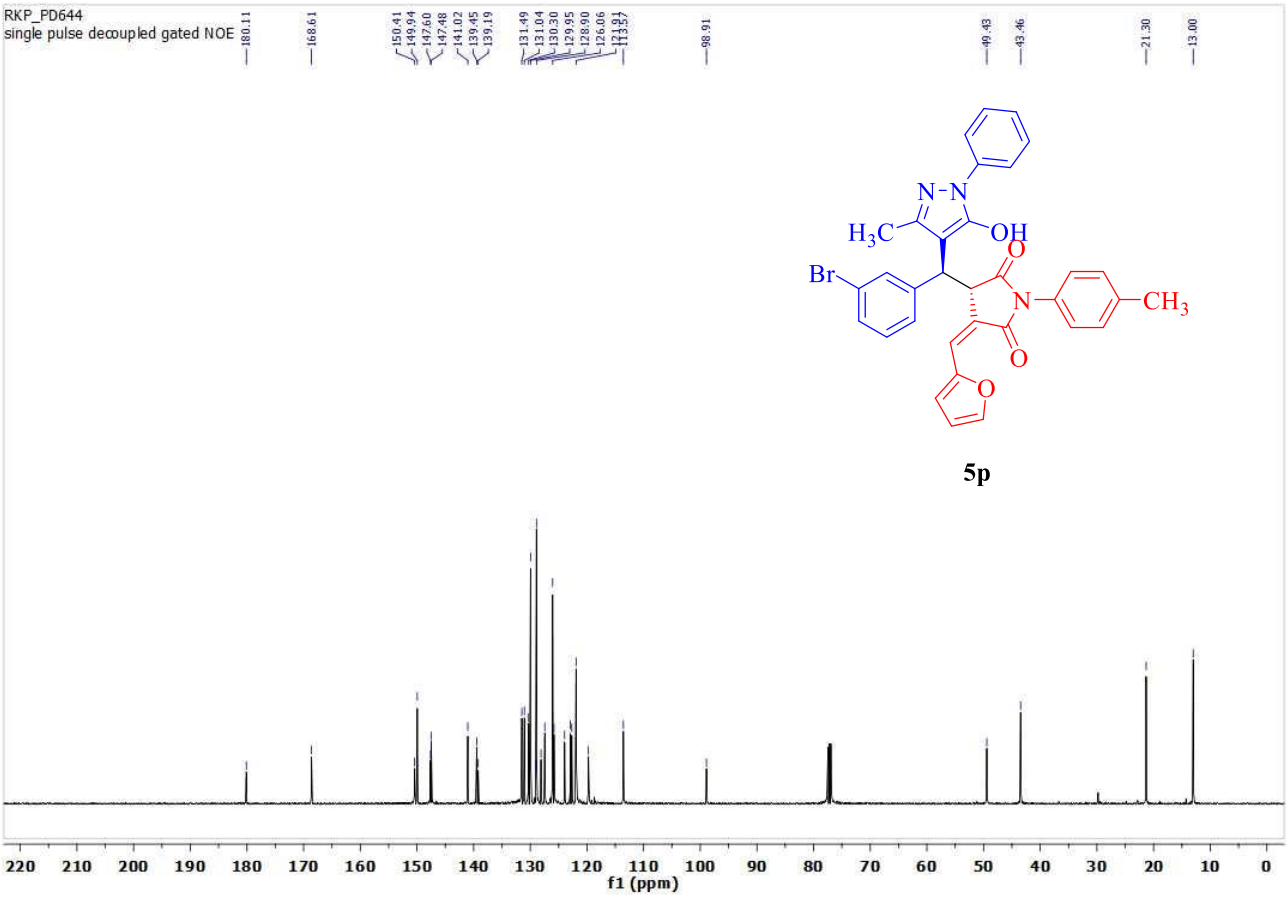
5o


Desktop
PD-652
179.91
168.40
150.23
149.83
147.49
147.45
140.86
139.07
131.39
130.99
130.22
129.21
128.81
127.33
126.19
98.77
49.35
43.44
12.94
N-N
H3C
OH
Br
O
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

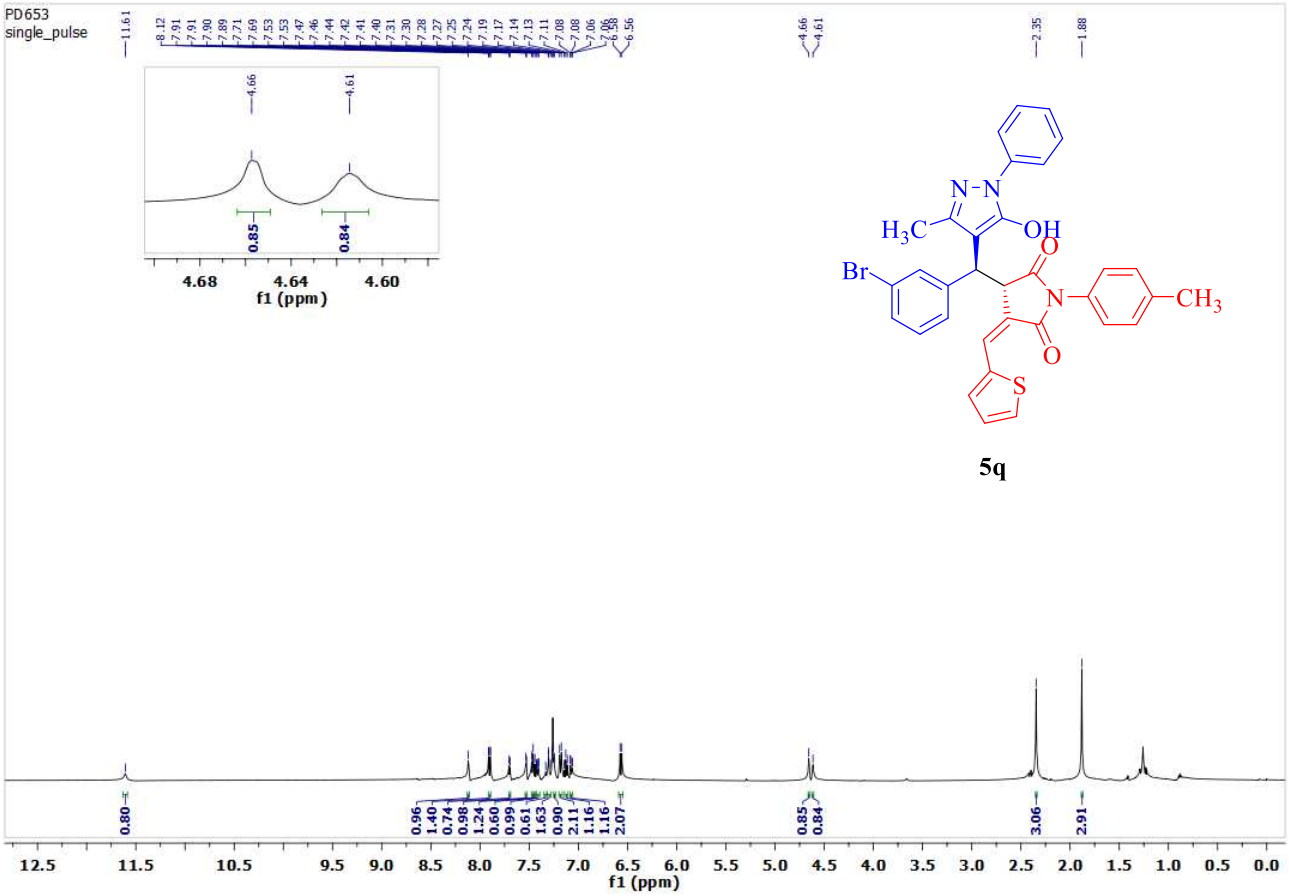
5o


RKP_PD644
single_pulse
11.64
7.86
7.85
7.63
7.63
7.59
7.41
7.39
7.38
7.36
7.35
7.35
7.34
7.34
7.33
7.21
7.20
7.20
7.18
7.13
7.11
7.08
7.06
7.04
7.03
7.02
7.02
6.89
6.88
4.64
4.58
2.28
1.86
4.64
4.58
0.99
1.00
4.9 4.8 4.7 4.6 4.5 4.4 4.3
f1 (ppm)
N-N
H3C
OH
Br
O
N
CH3
O
O
0.98
2.16
0.99
0.98
2.24
1.16
1.41
1.11
1.12
0.79
1.63
1.11
1.11
2.13
0.99
1.00
2.98
2.69
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

5p

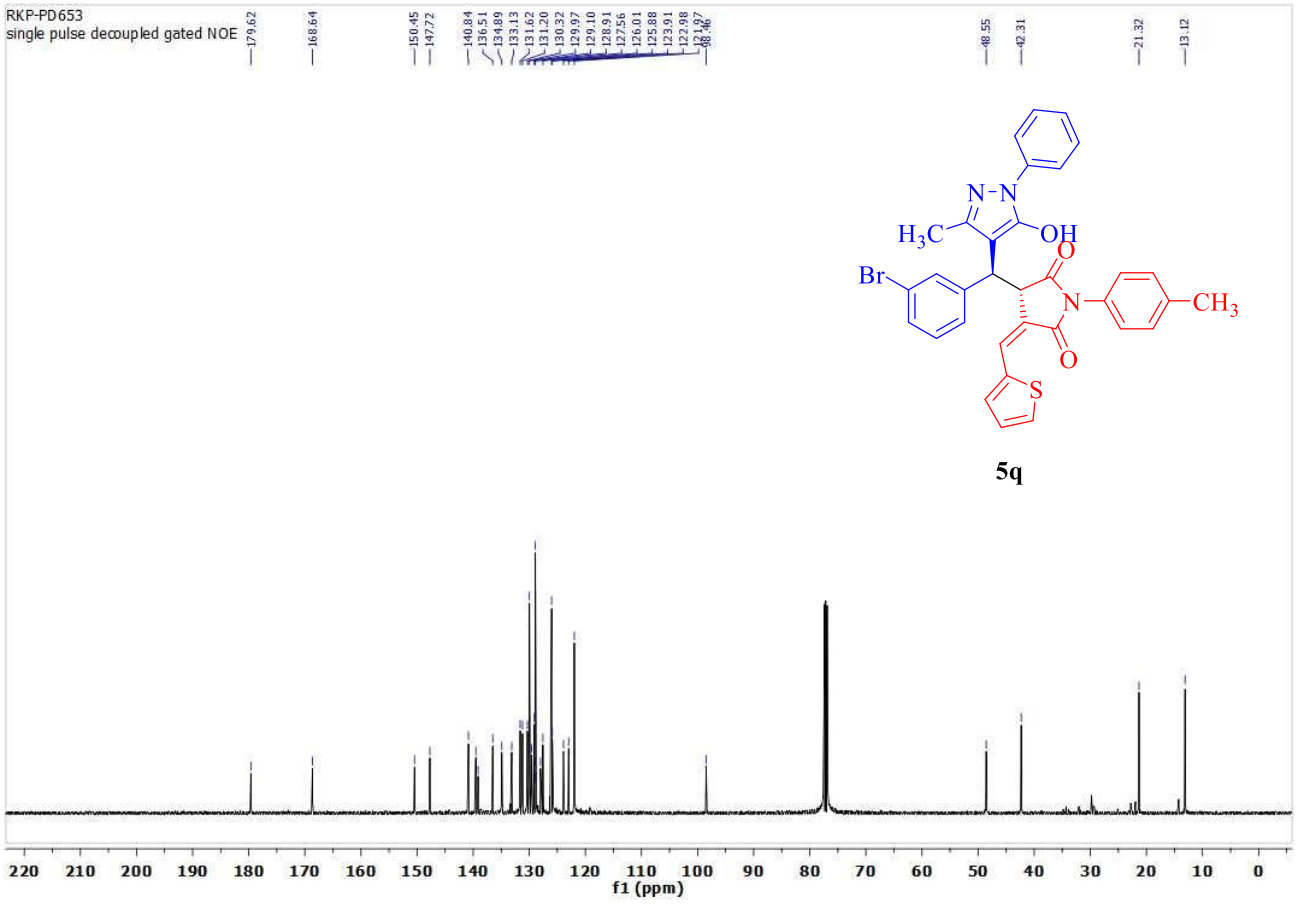

RKP_PD644
single pulse decoupled gated NOE
180.11
168.61
150.41
149.94
147.60
147.48
141.02
139.45
139.19
131.49
131.04
130.30
129.95
128.90
126.06
121.91
113.57
98.91
49.43
43.46
21.30
13.00
N-N
H3C
OH
Br
O
N
CH3
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

5p


PD653
single_pulse
f1 (ppm)

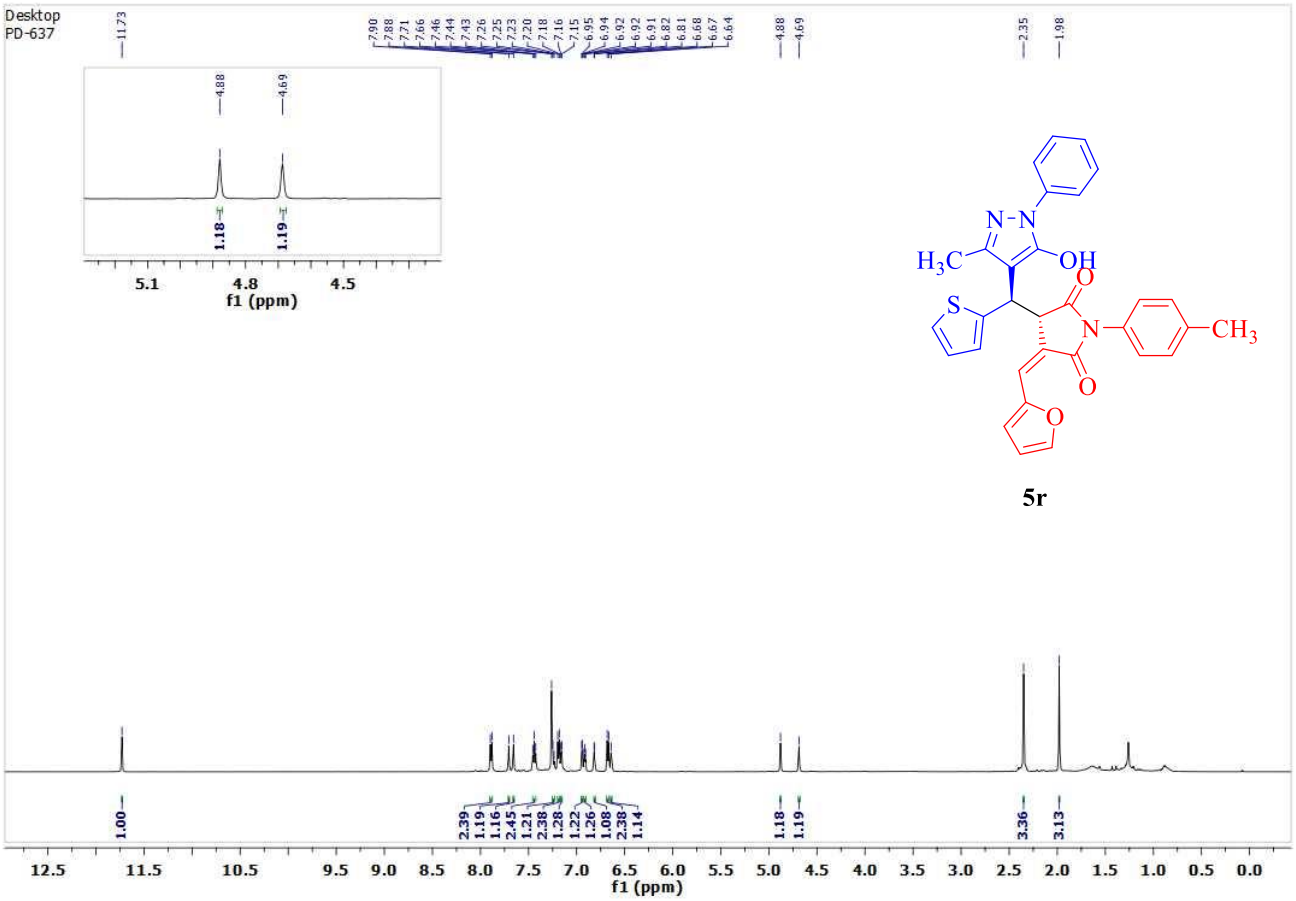
N-N
H3C
OH
Br
O
N
CH3
O
S

5q

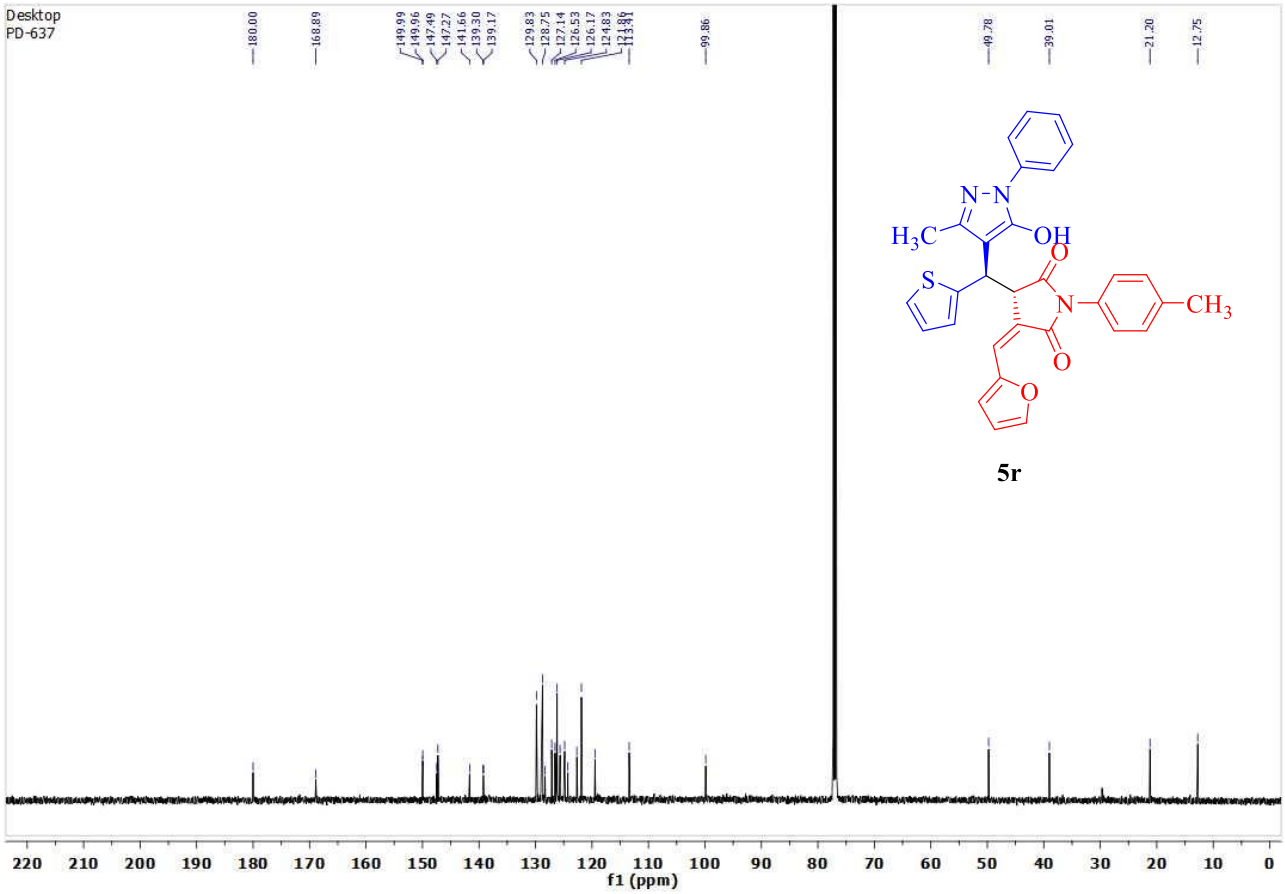

RKP-PD653
single pulse decoupled gated NOE
f1 (ppm)

N-N
H3C
OH
Br
O
N
CH3
O
S

5q


Desktop
PD-637
11.73
7.90
7.88
7.71
7.66
7.46
7.44
7.43
7.26
7.25
7.23
7.20
7.18
7.16
7.15
6.95
6.94
6.92
6.92
6.91
6.82
6.81
6.68
6.67
6.64
4.88
4.69
2.35
1.98
1.18
1.19
5.1
4.8
4.5
f1 (ppm)
N-N
H3C
OH
S
O
N
CH3
O
O
1.00
2.39
1.19
1.16
2.45
1.21
2.38
1.28
1.22
1.26
1.08
2.38
1.14
1.18
1.19
3.36
3.13
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

5r


Desktop
PD-637
180.00
168.89
149.99
149.96
147.49
147.27
141.66
139.30
139.17
129.83
128.75
127.14
126.53
126.17
124.83
123.86
113.91
99.86
49.78
39.01
21.20
12.75
N-N
H3C
OH
S
O
N
CH3
O
O
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

5r

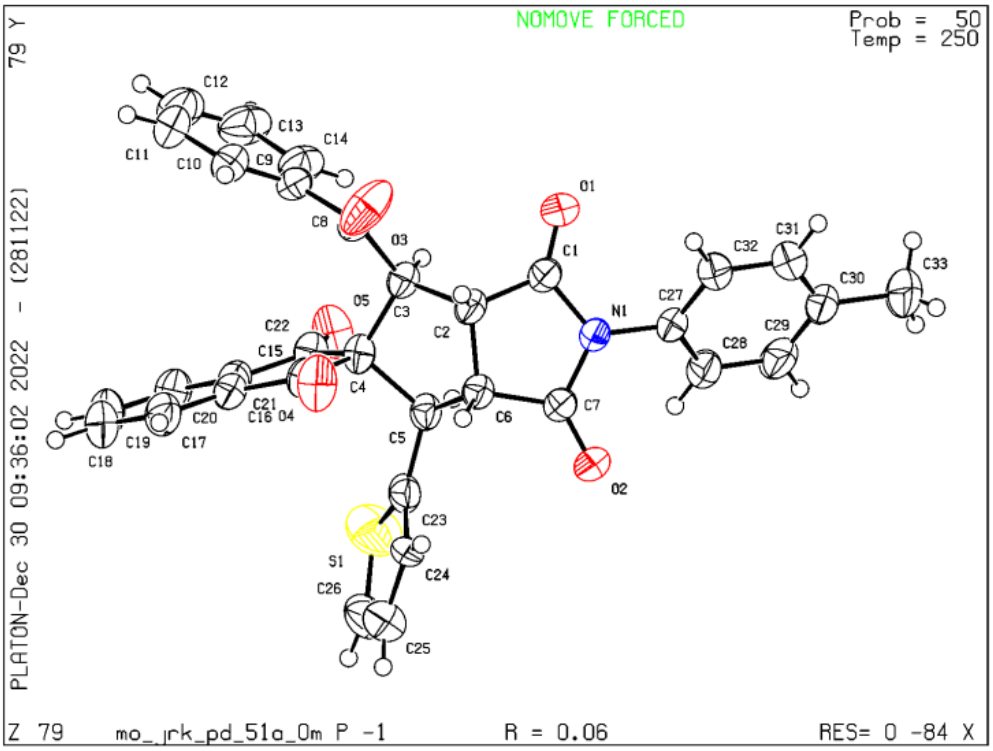
Table S1: ^{1}H NMR data table for characteristic protons of **3a-3r**

Compound	H_a	H_b	H_c	H_d
3a	4.84	3.99	4.65	4.55
3b	4.83	3.97	4.64	4.51
3c	4.81–4.78	3.99–3.95	4.58	4.56
3d	4.76	3.60	4.54	4.52–4.40
3e	4.82	3.98	4.62–4.58	4.55
3f	4.79	3.95	4.58	4.50
3g	4.75	3.93	4.54	4.17
3h	4.75	3.93	4.54	4.48
3i	4.79	3.93	4.59	4.46
3j	4.73	3.91	4.50	4.45
3k	4.76	4.10	4.58	4.36
3l	4.77	4.27	4.58	4.41
3m	4.72	4.08	4.54–4.50	4.37
3n	4.75	4.27	4.53	4.47–4.42
3o	4.74	4.09	4.54	4.37
3p	4.76	4.09	4.55	4.44
3q	4.69	4.06	4.50	4.35
3r	4.92	3.93–3.89	4.72	4.16

Table S2: ^{1}H NMR data table for characteristic protons of **5a-5r**

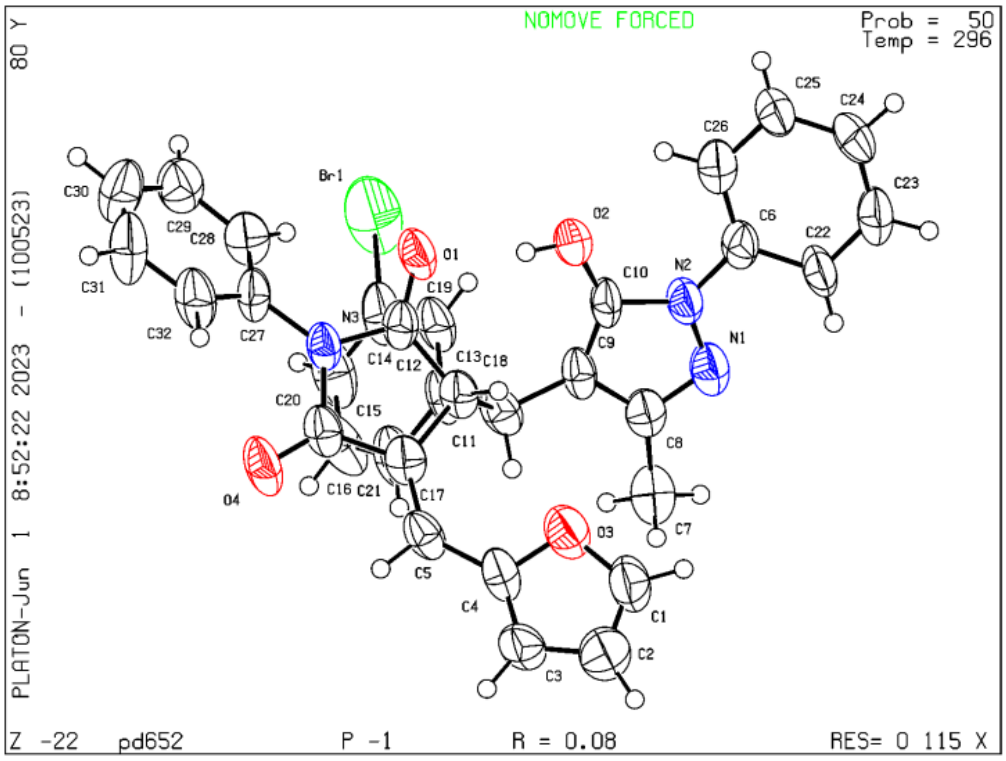
Compound	H_a	H_b	OH
5a	4.76	4.56	11.68
5b	5.13	4.71	11.57
5c	5.19	4.64	11.76
5d	4.96	4.76	11.53
5e	4.68	4.60	11.80
5f	5.17	4.65	11.68
5g	4.76	4.57	11.65
5h	4.70	4.67	11.70
5i	4.70	4.67	11.73
5j	4.70	4.61	11.66
5k	5.22	4.69	11.57
5l	5.22	4.68	11.59
5m	5.21	4.68	11.53
5n	5.20	4.67	11.58
5o	4.73	4.64	11.61
5p	4.64	4.58	11.64
5q	4.66	4.61	11.61
5r	4.88	4.69	11.73

Note: The chemical shift values are in ppm.



Formula	$C_{33}H_{22}NO_5S$
Formula Wt.	544.6010
Crystal color	Colorless
Crystal system	Triclinic
Space group	P –1
a(Å)	10.988(2)
b(Å)	11.648(2)
c(Å)	12.588(3)
α(deg)	114.144(6)
β(deg)	108.931(7)
c(deg)	92.315(7)

Figure S9: ORTEP plot of the crystal structure of **3l**



Formula	$C_{32}H_{24}N_3O_4Br$
Formula Wt.	594.44
Crystal color	Colorless
Crystal system	Triclinic
Space group	P –1
a(Å)	12.80(14)
b(Å)	12.93(15)
c(Å)	18.3(2)
α(deg)	101.19(14)
β(deg)	94.84(15)
c(deg)	107.4(2)
V(Å^3)	2802(54)

Figure S10: ORTEP plot of the crystal structure of **5o**