Supporting Information

Cp*Co^{III}-Catalyzed Alkylation of Primary and Secondary C(sp³)-H Bonds of 8-Alkylquinolines with Maleimides

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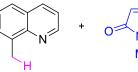
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1. Reaction of 8-methyl quinoline with N-methyl maleimide

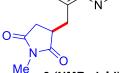
1.1 Table S1. Optimization details





[Catalyst] (mol%) [Ag] (mol%), Additive (mol%) Solvent, Argon

1, 0.1 mmol **2**, 0.15 mmol



^{le} 3 (NMR yield)

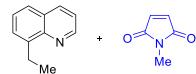
| Entry | Catalyst (mol%) | [Ag] (mol%) | Additive (mol%) | Solvent | Temp. (°C) | NMR Yield (%) ^b |
|-------|------------------------------|-------------------------|-----------------|---------|------------|----------------------------|
| 1 | Cp*Co(CO)I ₂ (10) | $AgSbF_6(20)$ | - | TFE | 100 | 10 |
| 2 | Cp*Co(CO)I ₂ (10) | - | AdCOOH (20) | TFE | 100 | 25 |
| 3 | Cp*Co(CO)I ₂ (10) | - | - | TFE | 100 | n.d. |
| 4 | - | AgOTf (20) | AdCOOH (20) | TFE | 100 | n.d. |
| 5 | Cp*Co(CO)I ₂ (10) | AgOTf (20) | NaOAc (20) | TFE | 100 | 40 |
| 6 | Cp*Co(CO)I ₂ (10) | AgOTf (20) | PivOH (20) | TFE | 100 | 22 |
| 7 | Cp*Co(CO)I ₂ (10) | AgOTf (20) | AcOH (20) | TFE | 100 | 25 |
| 8 | $Cp*Co(CO)I_2(10)$ | AgNTf ₂ (20) | AdCOOH (20) | TFE | 100 | 98 |
| 9 | Cp*Co(CO)I ₂ (10) | $AgSbF_6(20)$ | AdCOOH (20) | TFE | 100 | 85 |
| 10 | $Cp*Co(CO)I_2(10)$ | AgOTf (20) | NaOPiv (20) | TFE | 100 | 95 |
| 11 | $Cp*Co(CO)I_2(10)$ | AgOTf (20) | AdCOOH (20) | TFE | 100 | 98 |
| 12 | $Cp*Co(CO)I_2(5)$ | AgOTf (10) | AdCOOH (10) | TFE | 100 | 95 (92) ^c |
| 13 | Cp*Co(CO)I ₂ (10) | AgOTf (20) | AdCOOH (20) | TFE | Rt | 15 |
| 14 | Cp*Co(CO)I ₂ (10) | AgOTf (20) | AdCOOH (20) | TFE | 50 | 30 |
| 15 | Cp*Co(CO)I ₂ (10) | AgOTf (20) | AdCOOH (20) | TFE | 80 | 75 |
| 16 | Cp*Co(CO)I ₂ (10) | AgOTf (20) | AdCOOH (20) | TFE | 70 | 70 |
| 17 | Cp*Co(CO)I ₂ (10) | AgOTf (20) | AdCOOH (20) | TFE | 90 | 90 |
| 18 | $[Ru(p-cymene)Cl_2]_2(5)$ | AgOTf (20) | AdCOOH (20) | TFE | 100 | 40 |
| 19 | $[Cp*RhCl_2]_2(5)$ | AgOTf (20) | AdCOOH (20) | TFE | 100 | 40 |
| 20 | $[Cp*IrCl_2]_2(5)$ | AgOTf (20) | AdCOOH (20) | TFE | 100 | n.d. |
| 21 | Cp*Co(CO)I ₂ (10) | AgOTf (20) | AdCOOH (20) | DCE | 100 | 46 |
| 22 | Cp*Co(CO)I ₂ (10) | AgOTf (20) | AdCOOH (20) | toluene | 100 | n.d. |
| 23 | Cp*Co(CO)I ₂ (10) | AgOTf (20) | AdCOOH (20) | ACN | 100 | n.d. |
| 24 | Cp*Co(CO)I ₂ (10) | AgOTf (20) | AdCOOH (20) | H_2O | 100 | n.d. |
| 25° | Cp*Co(CO)I ₂ (10) | AgOTf (20) | AdCOOH (20) | TFE | 100 | 46 |

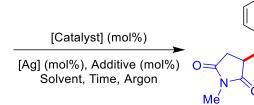
^{*a*}reaction conditions: 1a (0.1 mmol), 2a (0.15 mmol), solvent (0.5 ml), under argon. ^{*b*}NMR yield of crude reaction mixture was calculated by using tetrachloroethane (TCE) as internal standard, ^{*c*}isolated yield, ^{*d*}2a (2 equiv.).

2. Reaction of 8-ethyl quinoline with N-methyl maleimide

2a, 0.15 mmol

2.1 Table S2. Optimization details





`Me

5aa (NMR yield)

4a, 0.1 mmol

| Entry | Catalyst (mol%) | [Ag] (mol%) | Additive (mol%) | Solvent | Time | Temp. (°C) | NMR Yield (%) ^b |
|-------|------------------------------|-------------|--------------------|----------------|------|------------|----------------------------|
| 1 | $Cp*Co(CO)I_2(5)$ | AgOTf (10) | AdCOOH (10) | TFE | 48h | 100 | 33 (30) ^c |
| 2 | $Cp*Co(CO)I_2(10)$ | AgOTf (20) | AdCOOH (20) | TFE | 24h | 100 | 48 (44) ^c |
| 3 | $Cp*Co(CO)I_2(10)$ | AgOTf (20) | AdCOOH (20) | TFE | 48h | 100 | 45 |
| 4 | $Cp*Co(CO)I_2(2.5)$ | AgOTf (10) | AdCOOH (10) | TFE | 24h | 100 | <5 |
| 5 | $Cp*Co(CO)I_2(10)$ | AgOTf (20) | AdCOOH (10) | TFE | 24h | 100 | 42 |
| 6 | $Cp*Co(CO)I_2(10)$ | AgOTf (10) | AdCOOH (20) | TFE | 24h | 100 | <5 |
| 7 | $Cp*Co(CO)I_2(10)$ | AgOTf (20) | AdCOOH (100) | TFE | 24h | 100 | <5 |
| 8 | $Cp*Co(CO)I_2(10)$ | AgOTf (100) | AdCOOH (20) | TFE | 24h | 100 | <5 |
| 9^d | $Cp*Co(CO)I_2(20)$ | AgOTf (30) | AdCOOH (30) | TFE | 24h | 100 | 31 |
| 10 | $Cp*Co(CO)I_2(10)$ | AgOTf (40) | AdCOOH (20) | TFE | 24h | 100 | <5 |
| 11 | $Cp*Co(CO)I_2(10)$ | AgOTf (20) | AdCOOH (20) | HFIP | 24h | 100 | n.d. |
| 12 | $Cp*Co(CO)I_2(10)$ | AgOTf (20) | AdCOOH (20) | DCE | 24h | 100 | <5 |
| 13 | $Cp*Co(CO)I_2(10)$ | AgOTf (20) | AdCOOH (20) | toluene | 24h | 100 | n.d. |
| 14 | Cp*Co(CO)I ₂ (10) | AgOTf (20) | AdCOOH (20) | 1,4 dioxane | 24h | 100 | n.d. |
| 15 | $Cp*Co(CO)I_2(10)$ | AgOTf (20) | AdCOOH (20) | DMF | 24 h | 100 | n.d. |
| 16 | $Cp*Co(CO)I_2(10)$ | AgOTf (20) | AdCOOH (20) | DME | 24h | 100 | n.d. |
| 17 | $Cp*Co(CO)I_2(10)$ | AgOTf (20) | NaOPiv (20) | TFE | 24h | 100 | >5 |
| 18 | $Cp*Co(CO)I_2(10)$ | AgOTf (20) | AcOH (20) | TFE | 24h | 100 | 15 |

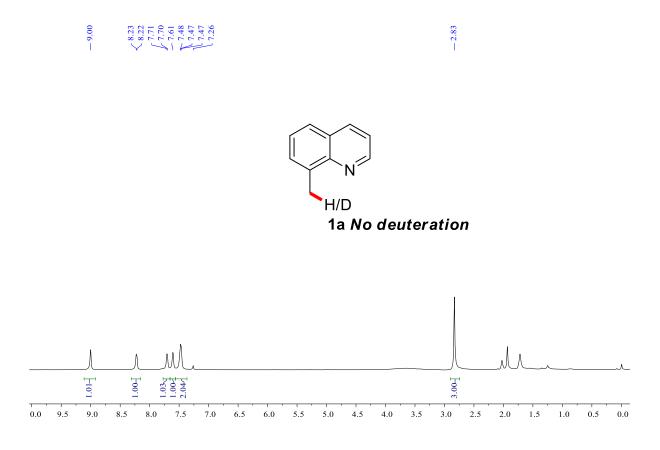
^{*a*}reaction conditions: 1a (0.1 mmol), 2a (0.15 mmol), solvent (0.5 ml), under argon. ^{*b*}NMR yield of crude reaction mixture was calculated by using tetrachloroethane (TCE) as internal standard, ^{*c*}isolated yield, ^{*d*}**2a** (2 equiv.).

3. Mechanistic study

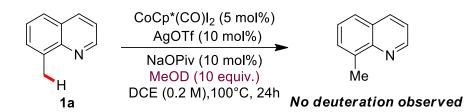
3.1 Scheme S1. Deuterium lebling experiments



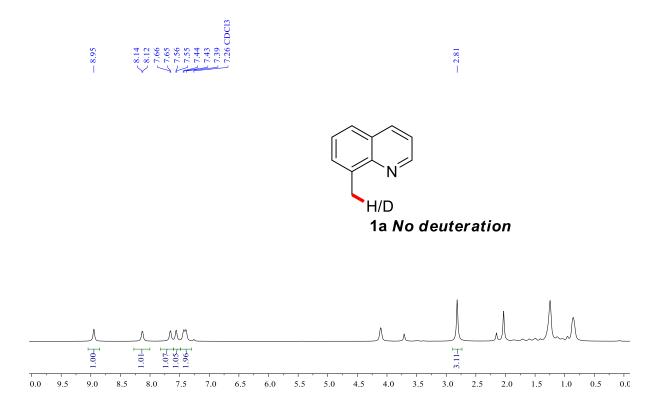
To an oven-dried screw cap reaction vial charged with a spin vane magnetic stir-bar, $[Cp*Co(CO)I_2]$ (5 mol%), AgOTf (10 mol%), AdCOOH (10 mol%) were added under argon atmosphere followed by addition of 8-methyl quinoline (0.1 mmol), CD₃OD (5 equiv.), and 2,2,2-Trifluoroethanol (0.5 mL) subsequent reaction mixture was stir at 100 °C for 24 h. The solvent was evaporated under reduced pressure and the crude mixture was purified by flash chromatography using silica gel (230-400 mesh size) and *n*-hexane: EtOAc as eluent. No deuteration was observed in the ¹H NMR analysis.



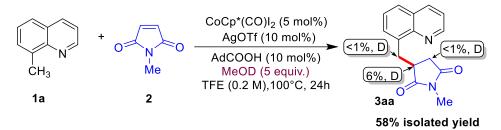
3.2 Scheme S2. Deuterium lebling experiments



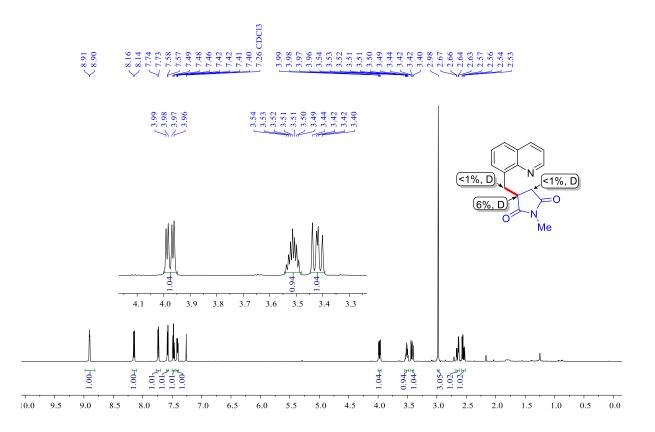
To an oven-dried screw cap reaction vial charged with a spin vane magnetic stir-bar, $[Cp*Co(CO)I_2]$ (5 mol%), AgOTf (10 mol%), NaOPiv (10 mol%) were added under argon atmosphere followed by addition of 8-methyl quinoline (0.1 mmol), CD₃OD (10 equiv.), and DCE (0.5 mL) subsequent reaction mixture was stir at 100 °C for 24 h. Solvent was evaporated under reduced pressure and the crude mixture was purified by flash chromatography using silica gel (230-400 mesh size) and *n*-hexane: EtOAc as eluent. No deuteration was observed in the ¹H NMR analysis.



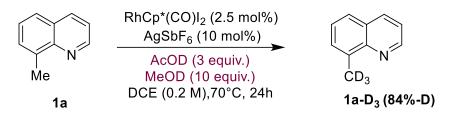
3.3 Scheme S3. Deuterium lebling experiments



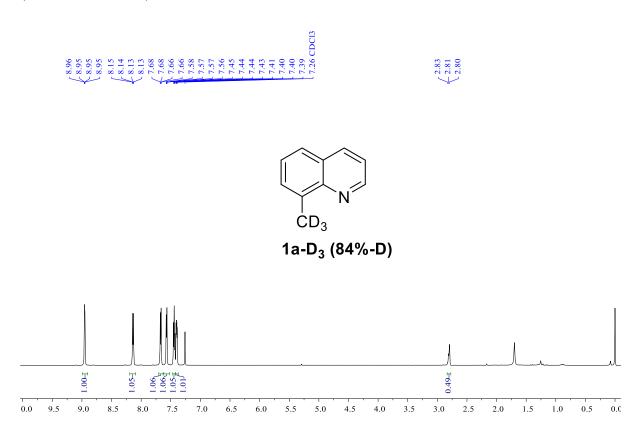
To an oven-dried screw cap reaction vial charged with a spin vane magnetic stir-bar, *N*-methyl maleimide (0.3 mmol), $[Cp*Co(CO)I_2]$ (5 mol%), AgOTf (10 mol%), AdCOOH (10 mol%) were added under argon atmosphere followed by addition of 8-methyl quinoline (0.2 mmol), CD_3OD (5 equiv.), and 2,2,2-Trifluoroethanol (1.0 mL) subsequent reaction mixture was stir at 100 °C for 24 h. The solvent was evaporated under reduced pressure and the crude mixture was purified by flash chromatography using silica gel (230-400 mesh size) and *n*-hexane: EtOAc as eluent. No deuteration was observed in the ¹H NMR analysis.

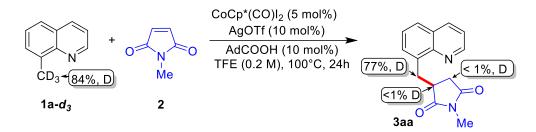


3.4 Scheme S4. Synthesis of 1a-D3

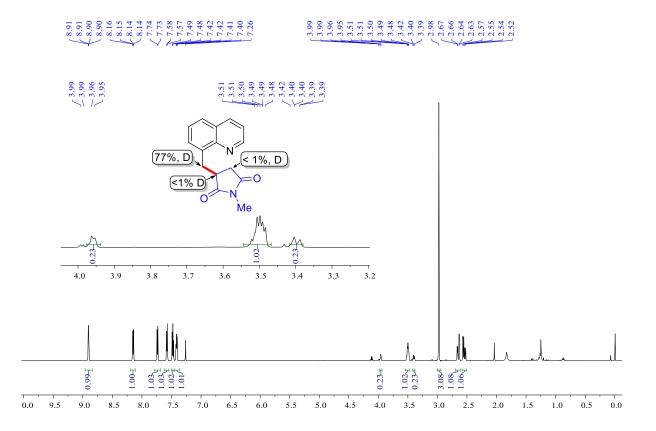


To an oven-dried screw cap reaction vial charged with a spin vane magnetic stir-bar, 8methylquinoline (**1a**) (0.2 mmol), [RhCp*Cl₂]₂ (2.5 mol %), AcOD (3 equiv.) and MeOD (20.0 equiv.) and AgSbF6 (10 mol %) were added in DCE (1 mL) under air at room temperature subsequent reaction mixture was stir at 70°C for 24 h. The solvent was evaporated under reduced pressure and the crude mixture was purified by flash chromatography using silica gel (230-400 mesh size) and n-hexane: EtOAc as eluent.

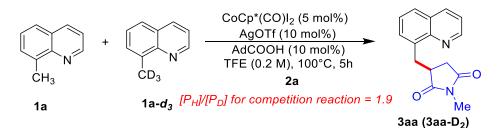




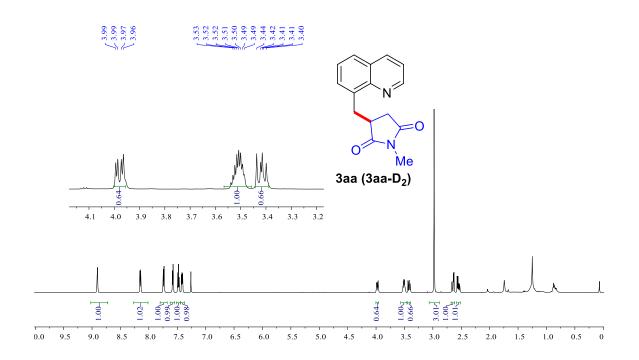
To an oven-dried screw cap reaction vial charged with a spin vane magnetic stir-bar, *N*-methyl maleimide (0.3 mmol), $[Cp*Co(CO)I_2]$ (5 mol%), AgOTf (10 mol%), AdCOOH (10 mol%) were added under argon atmosphere followed by addition of 8-methyl quinoline-D₃ (0.2 mmol), and 2,2,2-Trifluoroethanol (1.0 mL) subsequent reaction mixture was stir at 100 °C for 24 h. The solvent was evaporated under reduced pressure and the crude mixture was purified by flash chromatography using silica gel (230-400 mesh size) and *n*-hexane: EtOAc as eluent. No deuterium exchange was observed in the ¹H NMR analysis.



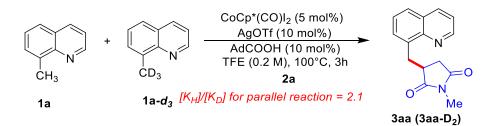
3.6 Scheme S6. Competition experiment Kinetic isotopic effect



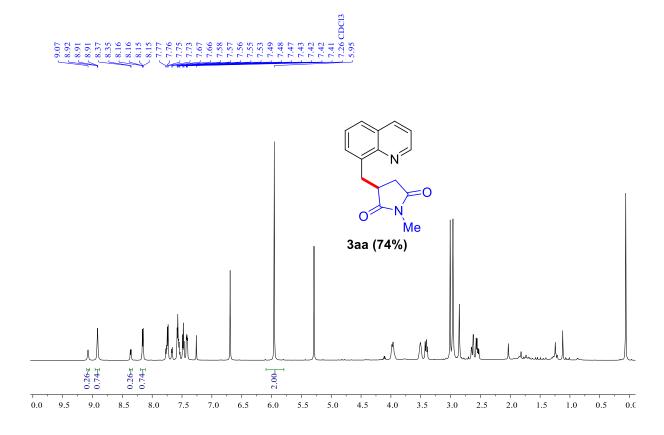
To an oven-dried screw cap reaction vial charged with a spin vane magnetic stir-bar, *N*-methyl maleimide (0.3 mmol), [Cp*Co(CO)I₂] (5 mol%), AgOTf (10 mol%), AdCOOH (10 mol%) were added under argon atmosphere followed by addition of 8-methyl quinoline (0.1 mmol), 8-methyl quinoline-D₃ (0.1 mmol), and 2,2,2-Trifluoroethanol (1.0 mL) subsequent reaction mixture was stir at 100 °C for 24 h. The solvent was evaporated under reduced pressure and the crude mixture was purified by flash chromatography using silica gel (230-400 mesh size) and *n*-hexane: EtOAc as eluent. The kinetic isotopic effect value ($k_{\rm H}/k_{\rm D}$) was calculated from ¹H NMR analysis and found 1.9.

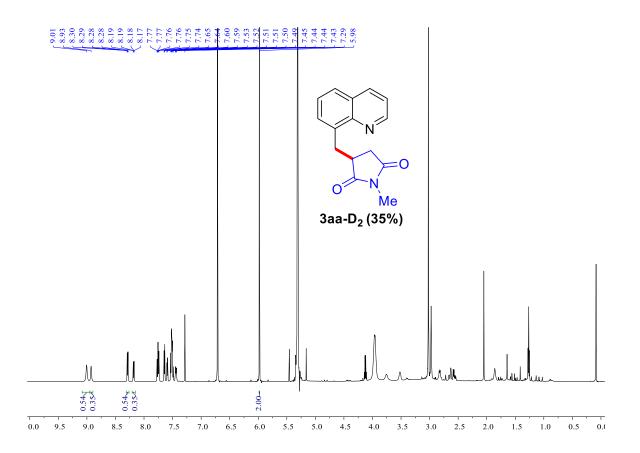


3.7 Scheme S7. Parallel experiment Kinetic isotopic effect



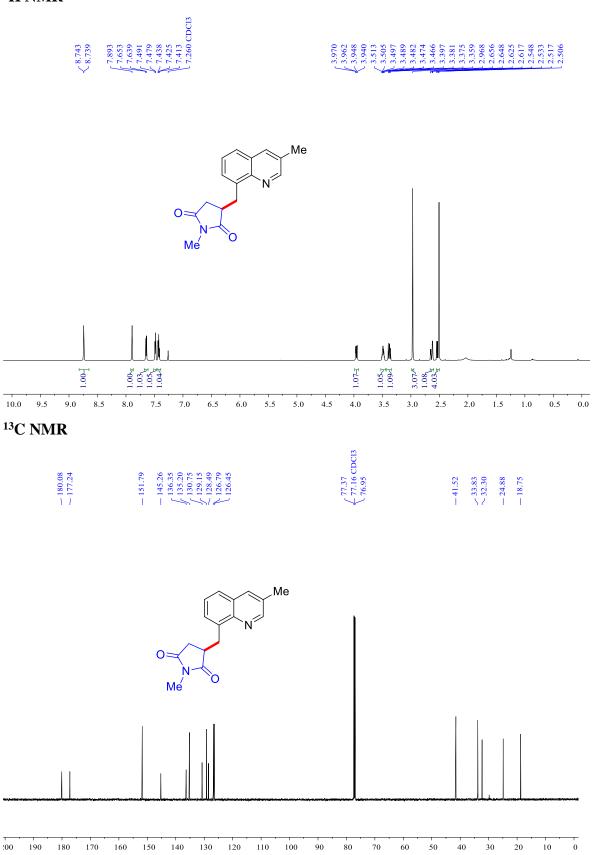
To an oven-dried screw cap reaction vial charged with a spin vane magnetic stir-bar, *N*-methyl maleimide (0.15 mmol), $[Cp*Co(CO)I_2]$ (5 mol%), AgOTf (10 mol%), AdCOOH (10 mol%) were added under argon atmosphere followed by addition of 8-methyl quinoline (0.1 mmol), and 2,2,2-Trifluoroethanol (1.0 mL). In another reaction tube 8-methyl quinoline-*d*₃ (0.1 mmol) was used instead of 8-methyl quinoline. The two-reaction mixtures were allowed to stir at 100 °C for 3h. Both reaction mixtures were analysed through 1HNMR using TCE as an internal standard and the calculated NMR yields of products **3aa** and **3aa-D**₂ was 74% and 35% respectively. The kinetic isotope effect value (*k*H/*k*D) was found 2.1.



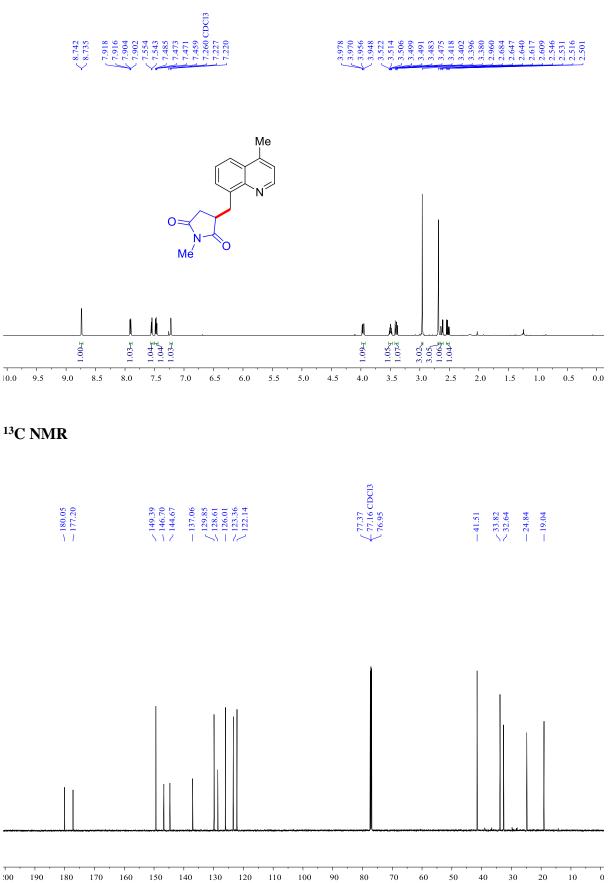


4. ¹H and ¹³C Spectral Data

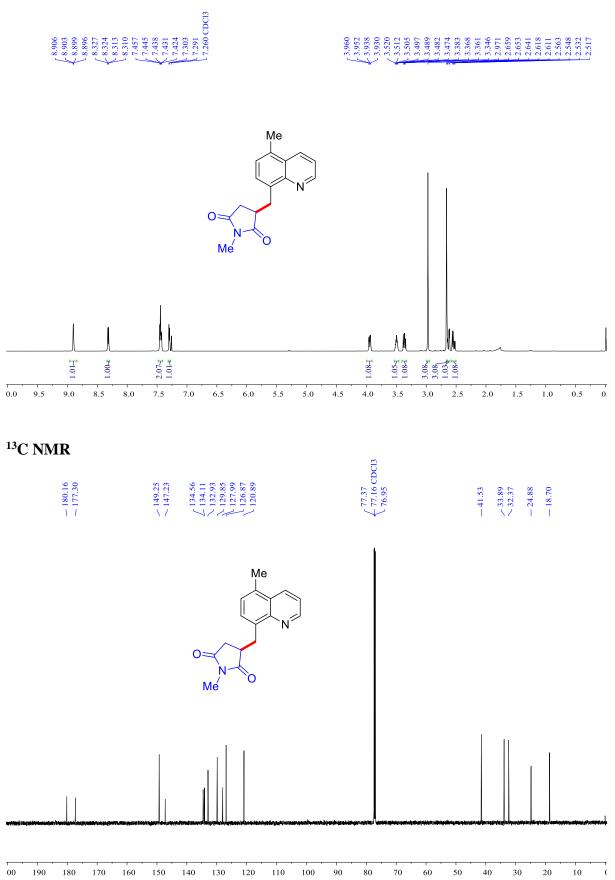
1-Methyl-3-((3-methylquinolin-8-yl)methyl)pyrrolidine-2,5-dione (Table 2, entry 3ba): ¹H NMR



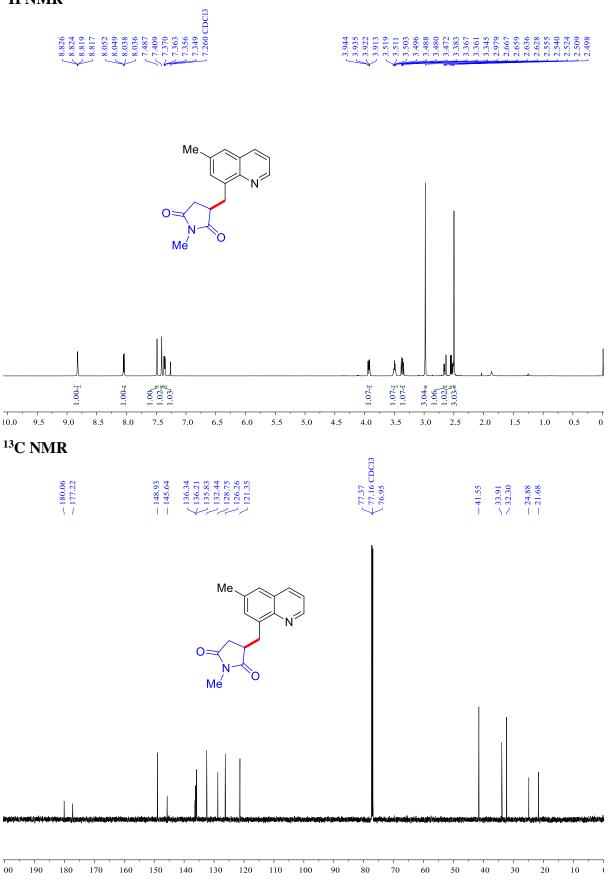
1-Methyl-3-((4-methylquinolin-8-yl)methyl)pyrrolidine-2,5-dione (Table 2, entry 3ca): ¹H NMR



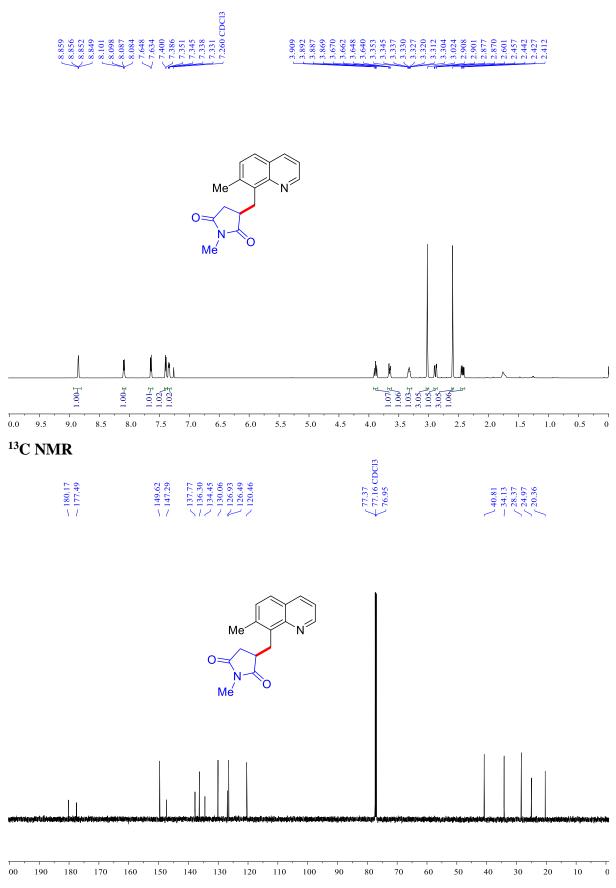
1-Methyl-3-((5-methylquinolin-8-yl)methyl)pyrrolidine-2,5-dione (*Table 2, entry 3da*): ¹H NMR



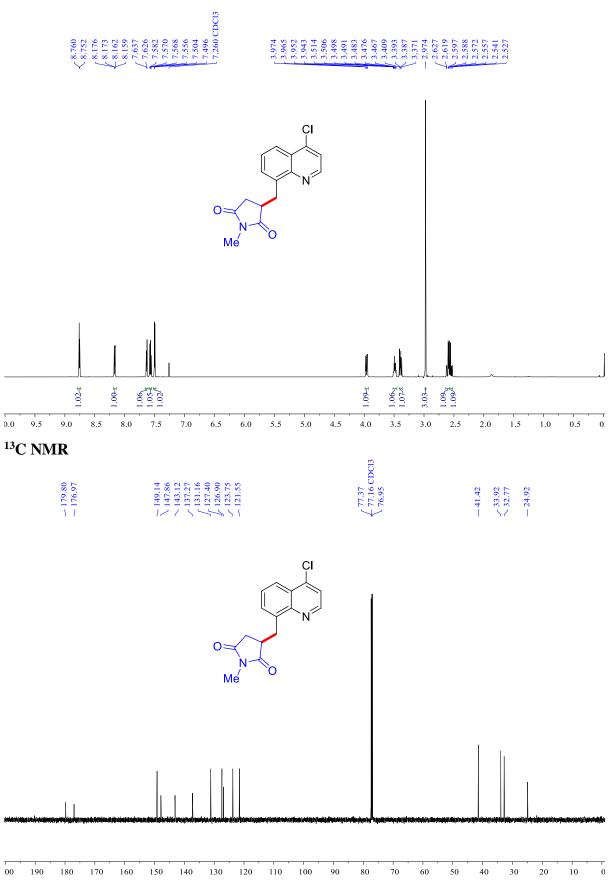
1-Methyl-3-((6-methylquinolin-8-yl)methyl)pyrrolidine-2,5-dione (Table 2, entry 3ea): ¹H NMR



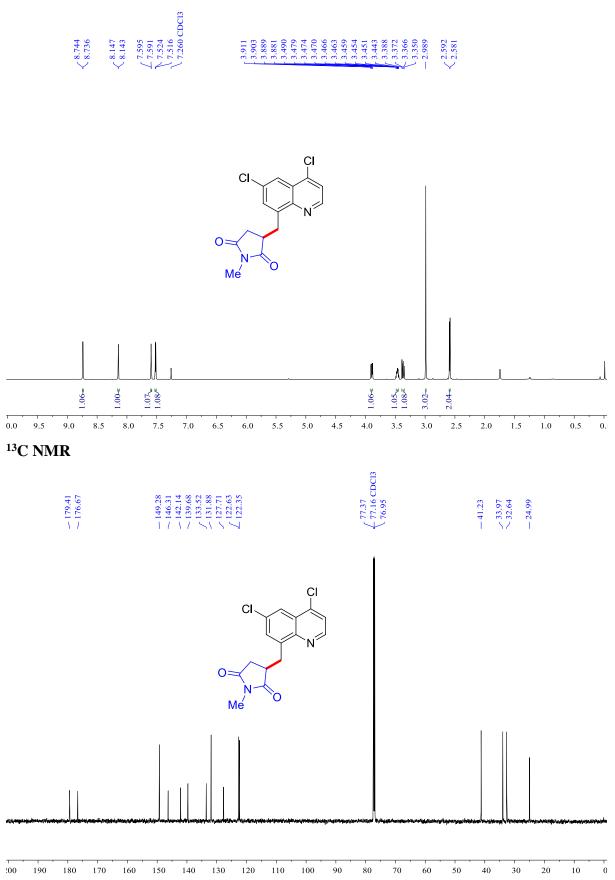
1-Methyl-3-((7-methylquinolin-8-yl)methyl)pyrrolidine-2,5-dione (*Table 2, entry 3fa*): ¹H NMR

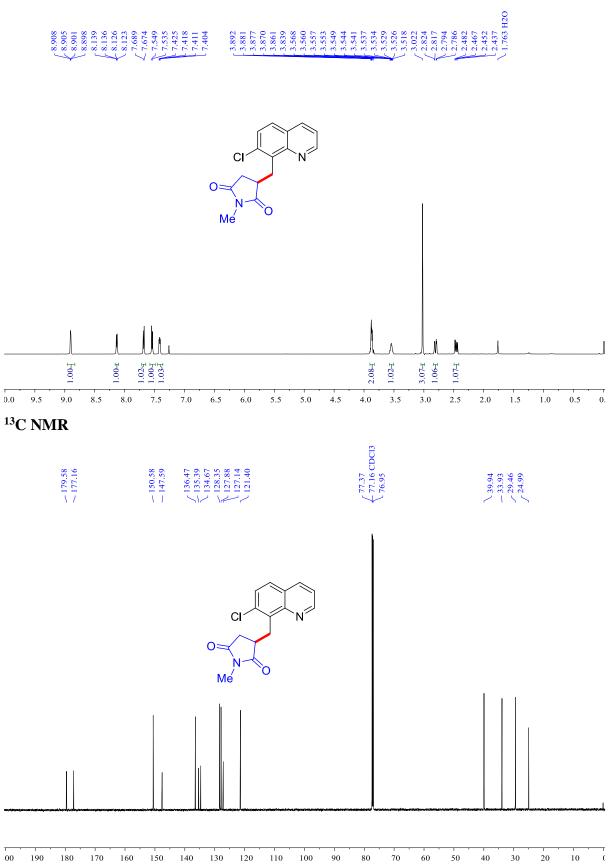


3-((4-Chloroquinolin-8-yl)methyl)-1-methylpyrrolidine-2,5-dione (*Table 2, entry 3ga*): ¹H NMR



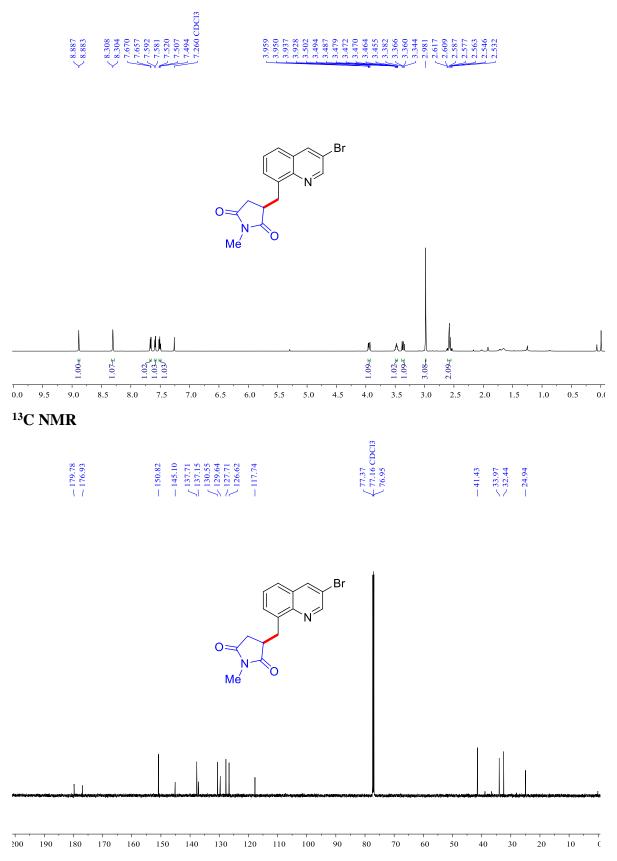
3-((4,6-Dichloroquinolin-8-yl)methyl)-1-methylpyrrolidine-2,5-dione (Table 2, entry ha): ¹H NMR



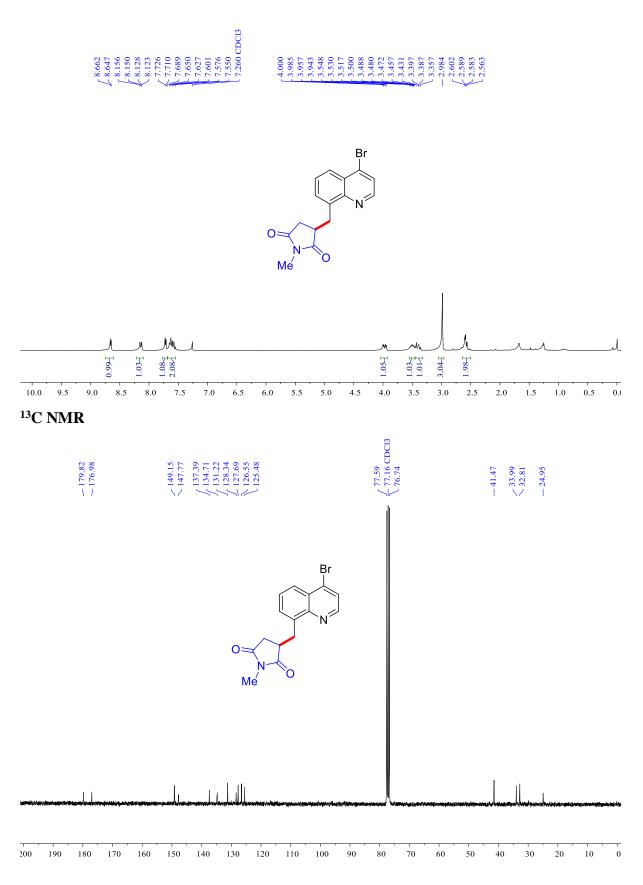


3-((7-Chloroquinolin-8-yl)methyl)-1-methylpyrrolidine-2,5-dione (Table 2, entry ia): ¹H NMR

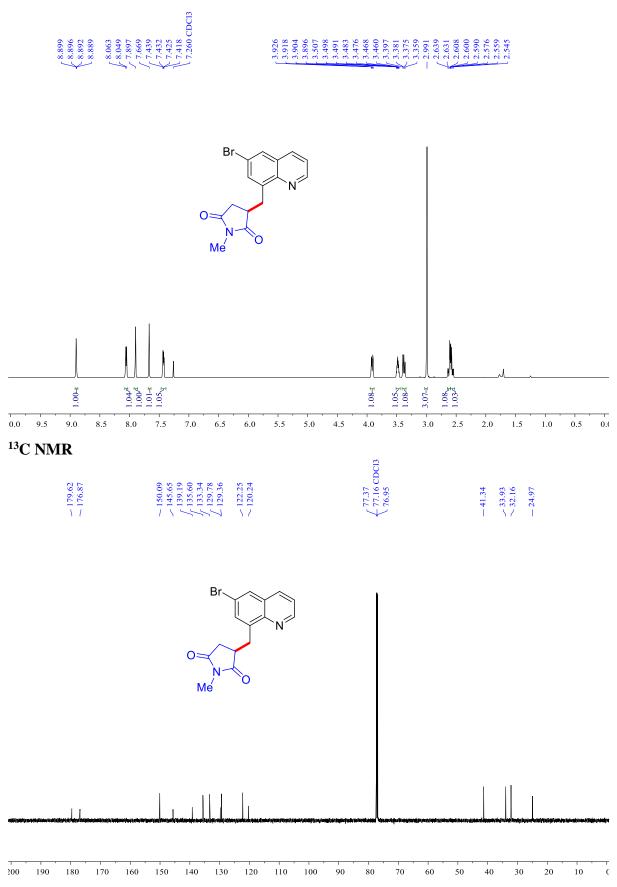
3-((3-Bromoquinolin-8-yl)methyl)-1-methylpyrrolidine-2,5-dione (*Table 2, entry 3ja*): ¹H NMR



3-((4-bromoquinolin-8-yl)methyl)-1-methylpyrrolidine-2,5-dione (Table 2, entry 3ka): ¹H NMR

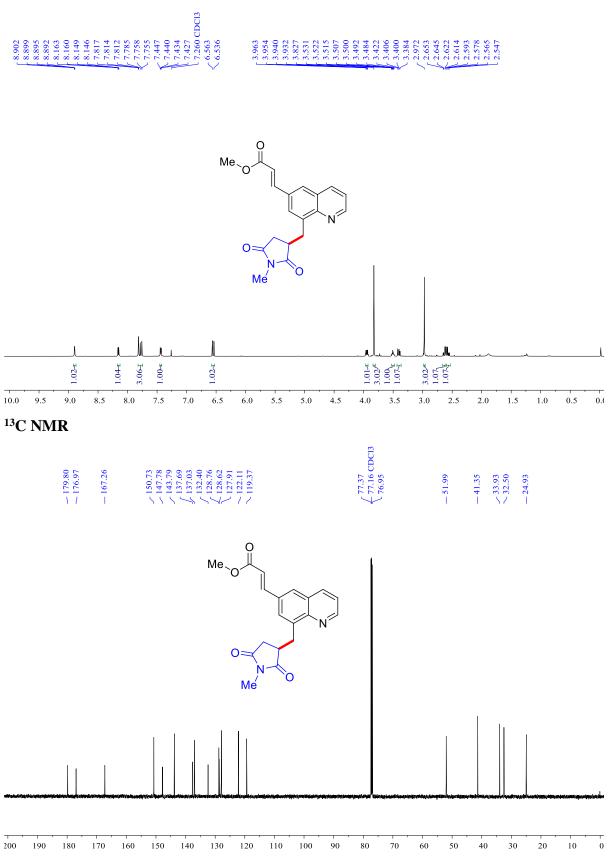


3-((6-Bromoquinolin-8-yl)methyl)-1-methylpyrrolidine-2,5-dione (Table 2, entry 3la): ¹H NMR

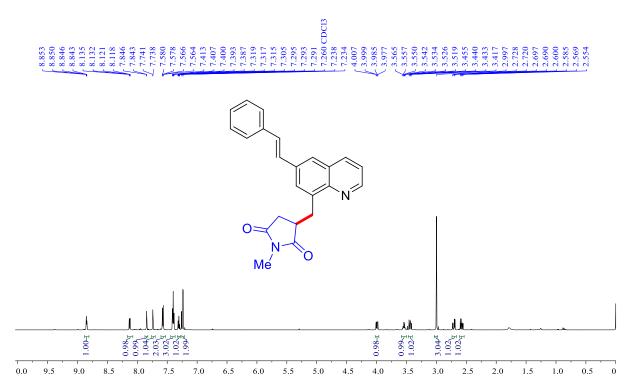


(E)-Methyl 3-(8-((1-methyl-2,5-dioxopyrrolidin-3-yl)methyl)quinolin-6-yl)acrylate (Table 2, entry 3ma):

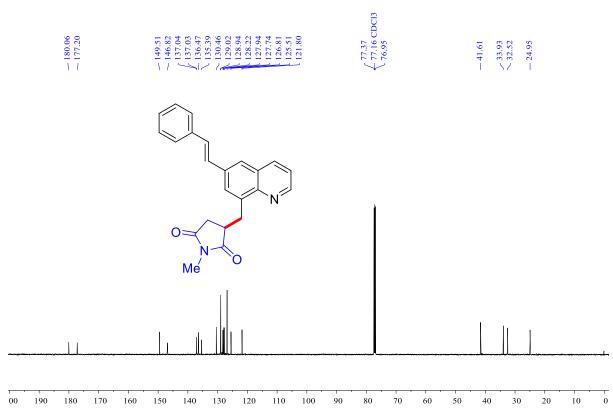
¹H NMR

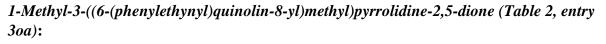


(*E*)-1-methyl-3-((6-styrylquinolin-8-yl)methyl)pyrrolidine-2,5-dione (*Table 2, entry 3na*): ¹H NMR

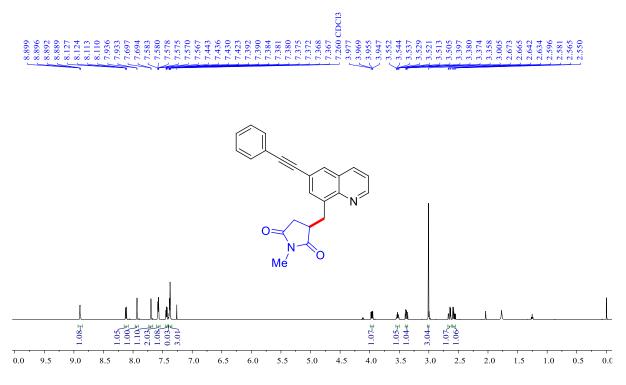


¹³C NMR



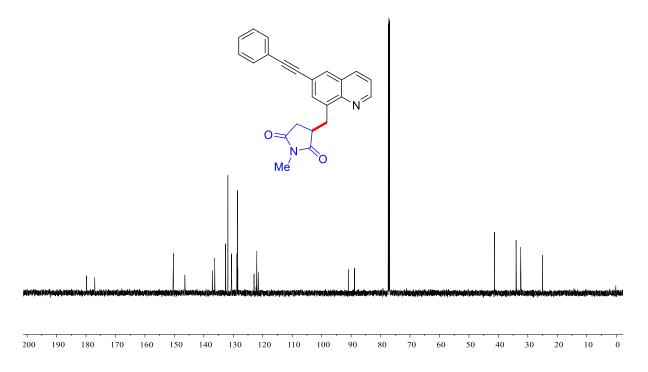


¹H NMR

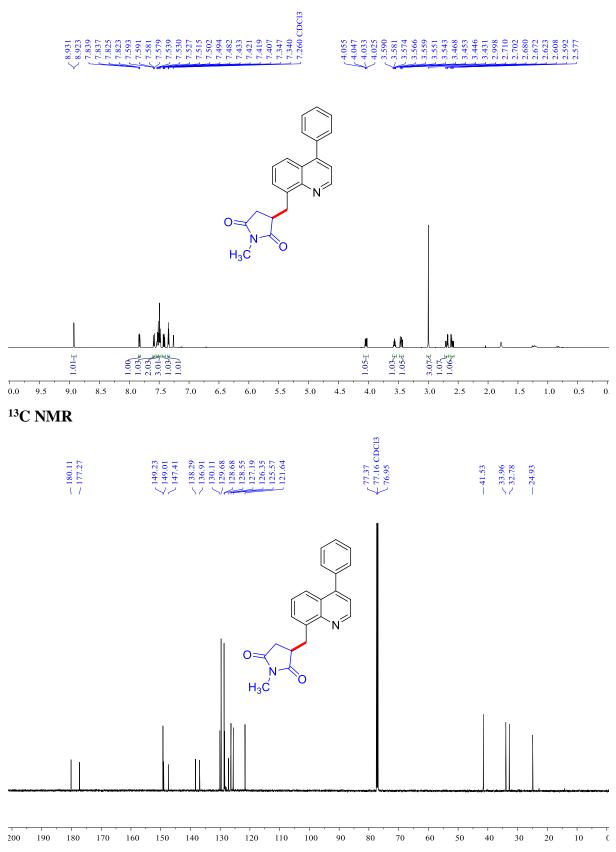


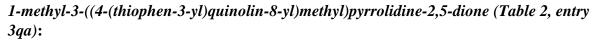
¹³C NMR



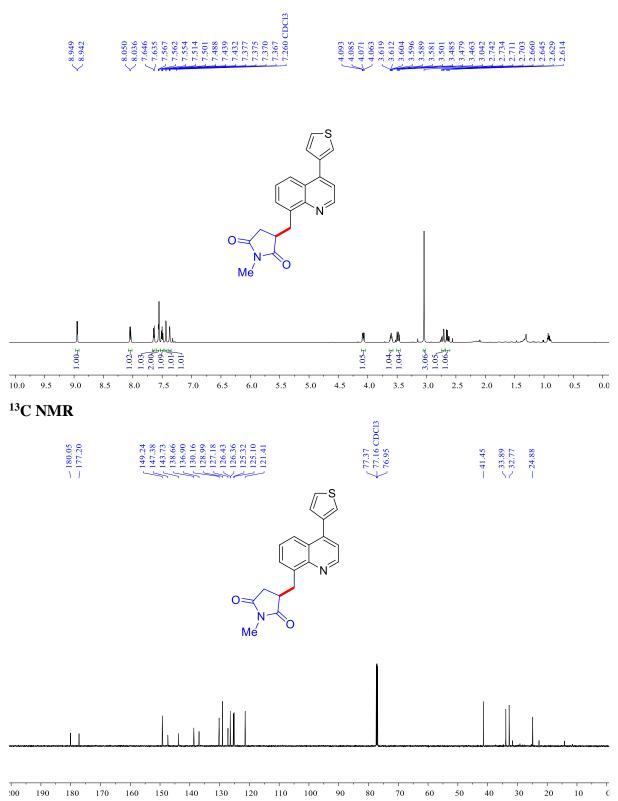


1-Methyl-3-((4-phenylquinolin-8-yl)methyl)pyrrolidine-2,5-dione (Table 2, entry 3pa): ¹H NMR



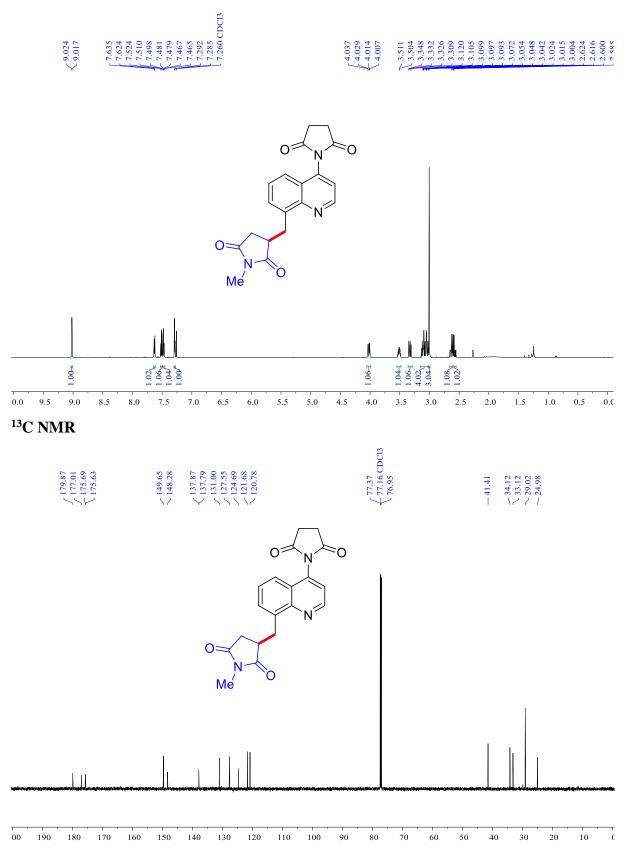


¹H NMR

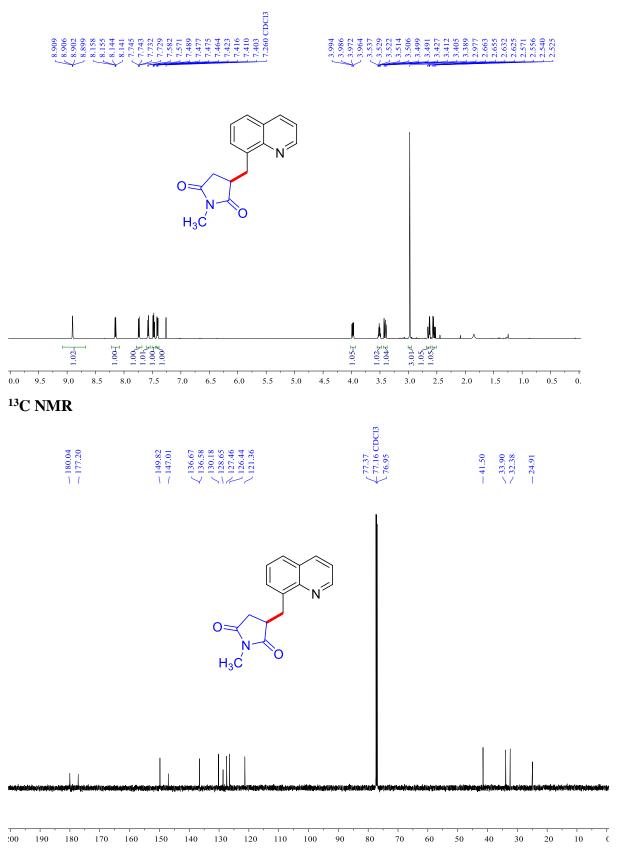


3-((4-(2,5-Dioxopyrrolidin-1-yl)quinolin-8-yl)methyl)-1-methylpyrrolidine-2,5-dione (Table 2, entry 3ra):

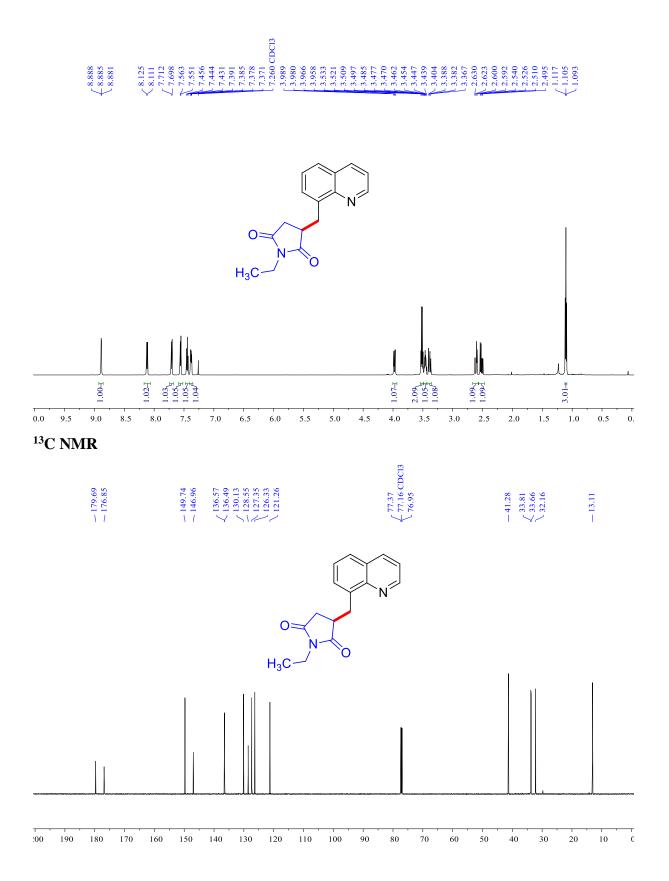
¹H NMR



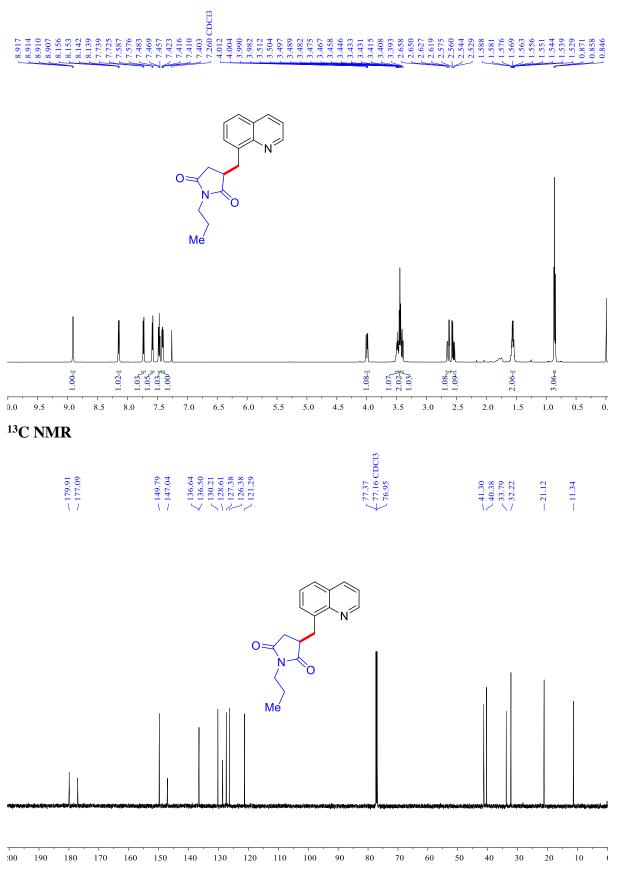
1-Methyl-3-(quinolin-8-ylmethyl)pyrrolidine-2,5-dione (Table 3, entry 3aa): ¹H NMR



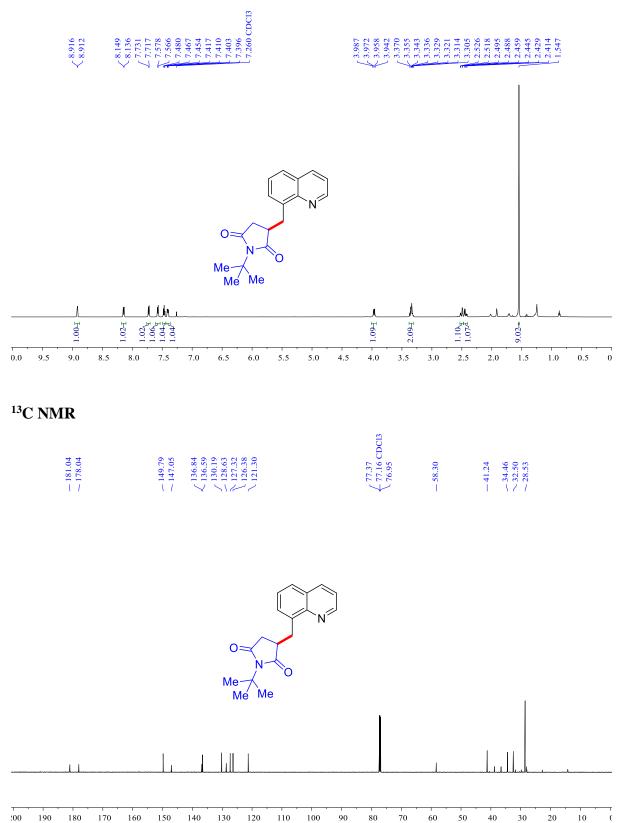
1-Ethyl-3-(quinolin-8-ylmethyl)pyrrolidine-2,5-dione (Table 3, entry 3ab): ¹H NMR



1-Propyl-3-(quinolin-8-ylmethyl)pyrrolidine-2,5-dione (Table 3, entry 3ac): ¹H NMR

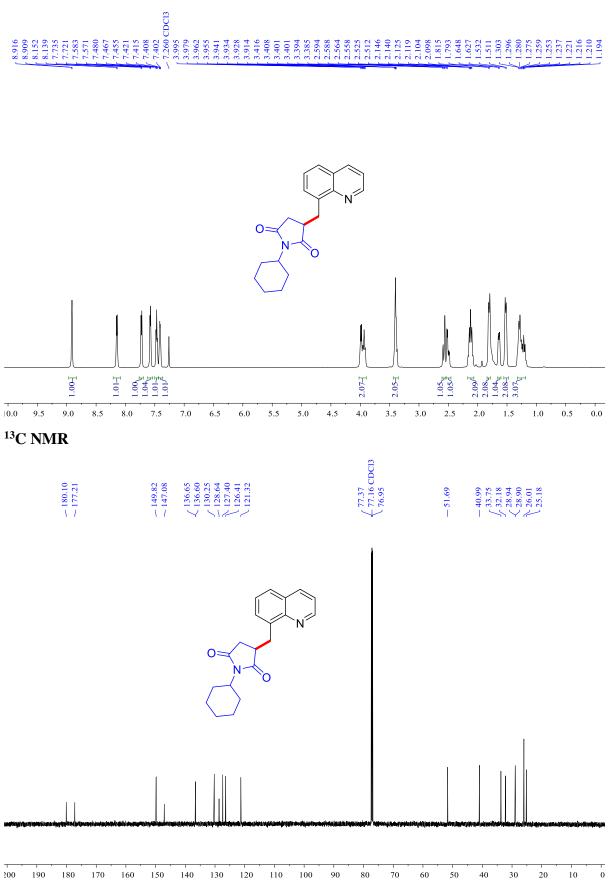


1-(tert-Butyl)-3-(quinolin-8-ylmethyl)pyrrolidine-2,5-dione (Table 3, entry 3ad): ¹H NMR

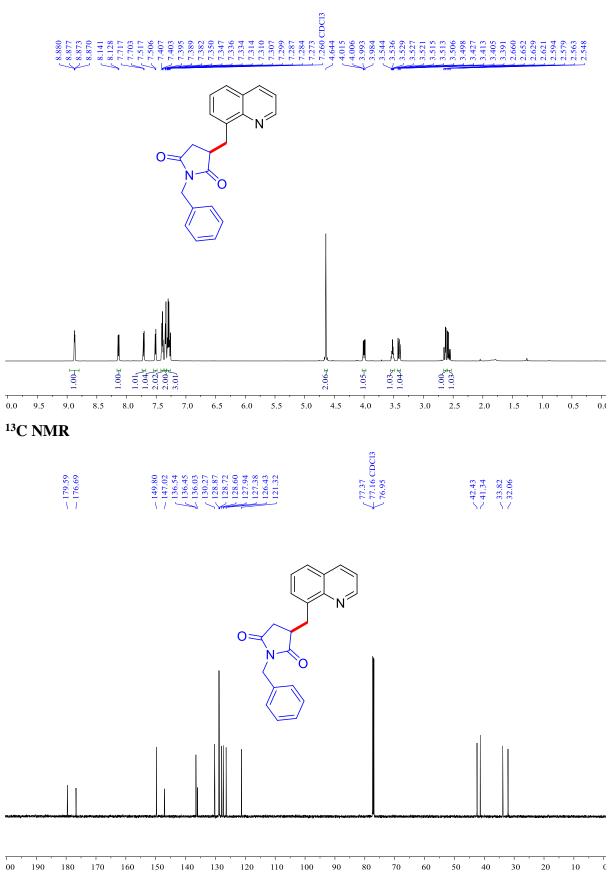


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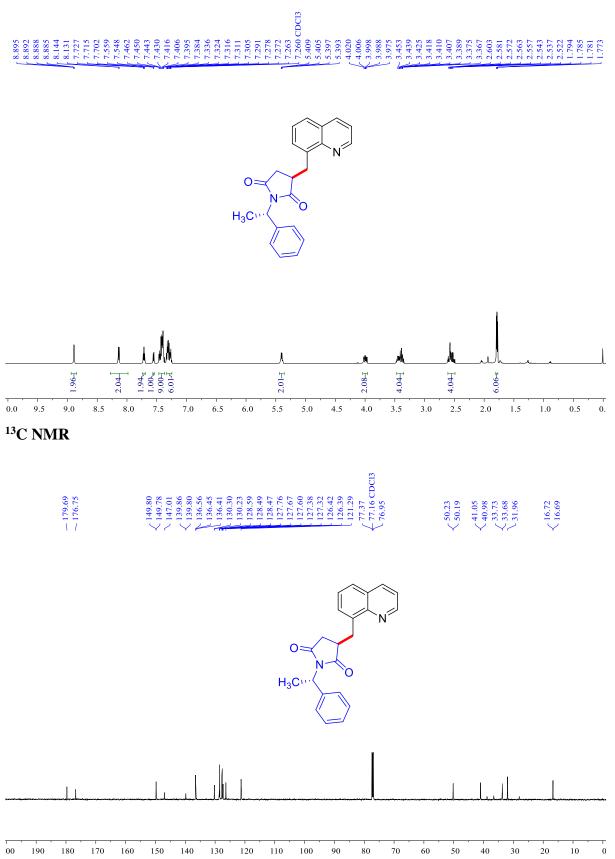
1-Cyclohexyl-3-(quinolin-8-ylmethyl)pyrrolidine-2,5-dione (Table 3, entry 3ae): ¹H NMR



1-Benzyl-3-(quinolin-8-ylmethyl)pyrrolidine-2,5-dione (Table 3, entry 3af): ¹H NMR

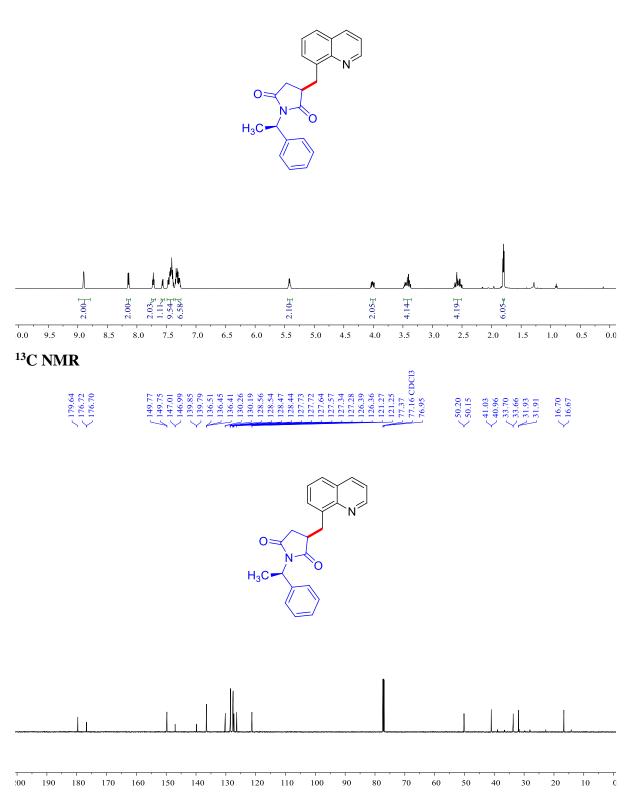


1-Phenylethyl)-3-(quinolin-8-ylmethyl)pyrrolidine-2,5-dione (Table 3, entry 3ag): ¹H NMR

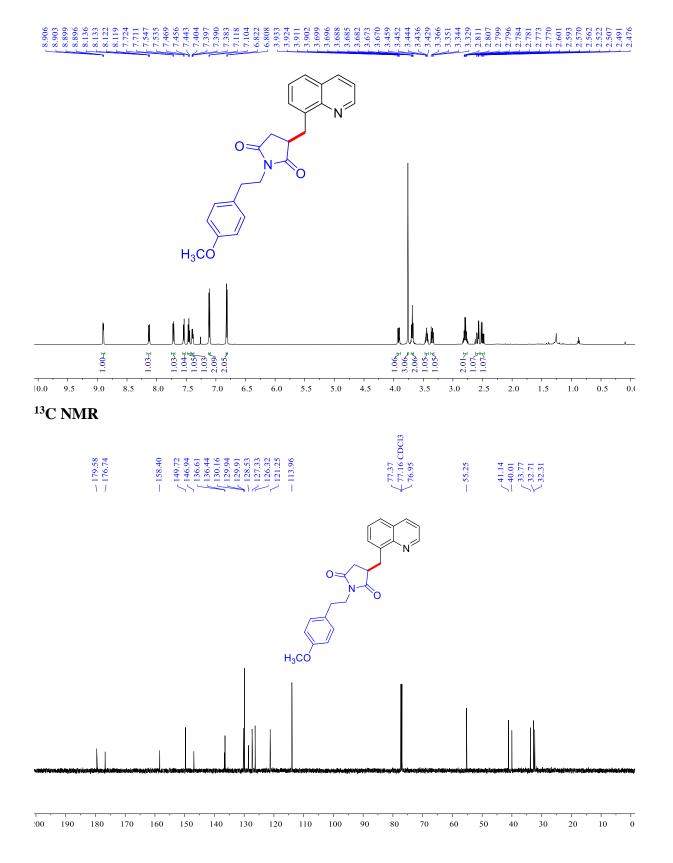


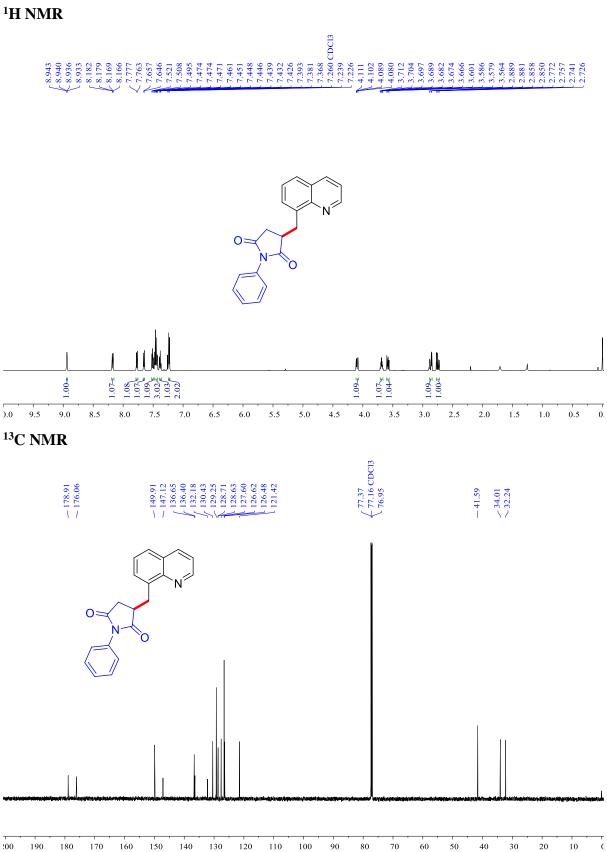
1-(1-Phenylethyl)-3-(quinolin-8-ylmethyl)pyrrolidine-2,5-dione (Table 3, entry 3ah): ¹H NMR

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1-(4-Methoxyphenethyl)-3-(quinolin-8-ylmethyl)pyrrolidine-2,5-dione (Table 3, entry 3ai): ¹H NMR

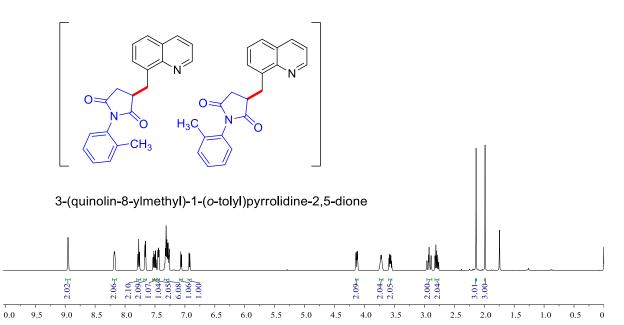




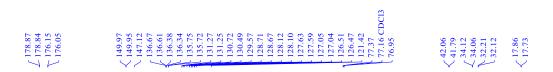
1-Phenyl-3-(quinolin-8-ylmethyl)pyrrolidine-2,5-dione (Table 3, entry 3aj): ¹H NMR

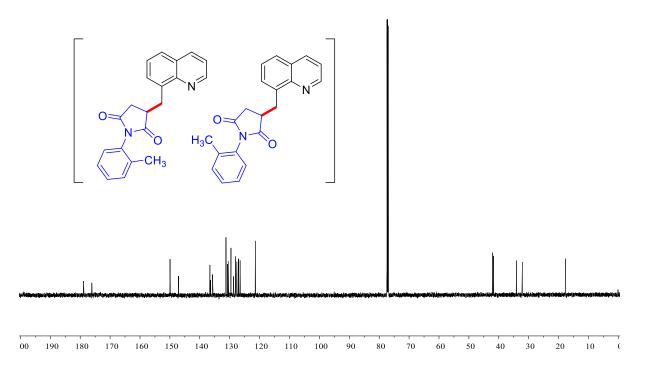
3-(Quinolin-8-ylmethyl)-1-(o-tolyl)pyrrolidine-2,5-dione (Table 3, entry 3ak): ¹H NMR

7.278 7.260 CDCl3 7.070 4.146 4.138 4.138 4.123 4.123 4.115 1.115 7.728 7.728 7.721 7.718 7.718 ٨.186 6.918 8.958 8.955 8.951 8.948 8.944 8.944 8.189 7.057 .567 .560 .929 .181 175 172 168 165 165 787 670 520 439 .432 7.326 .313 570 757 658 533 504 578 507 <u>9</u> .291 6

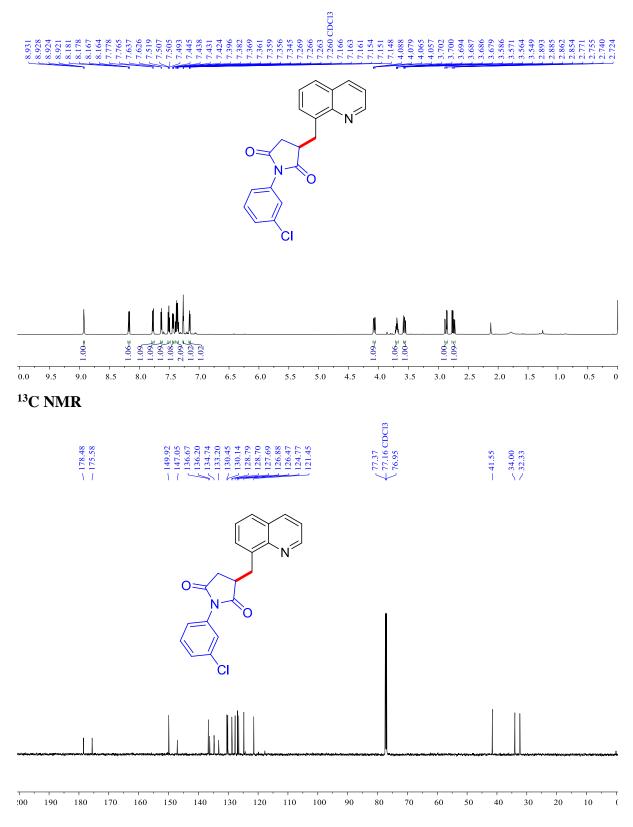


¹³C NMR

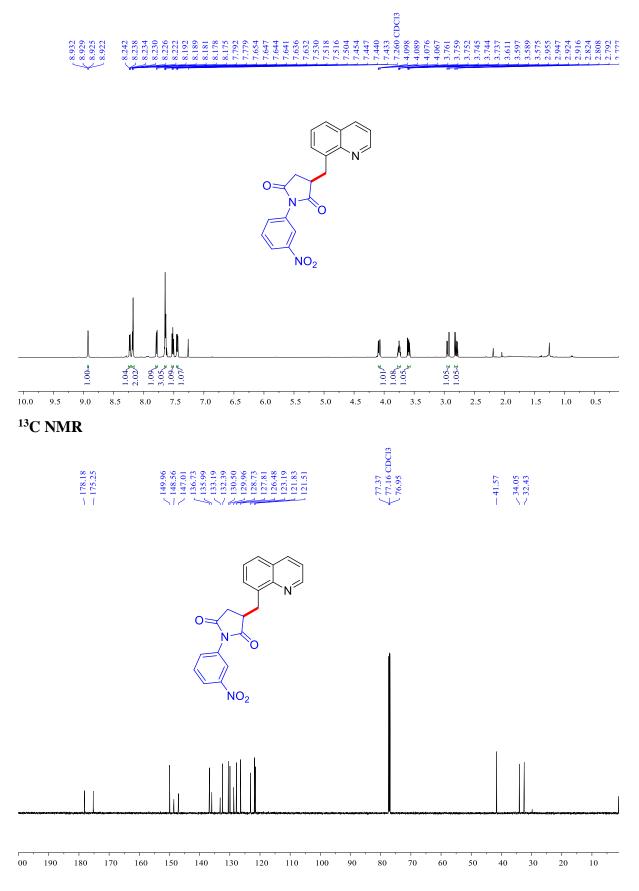




1-(3-Chlorophenyl)-3-(quinolin-8-ylmethyl)pyrrolidine-2,5-dione (Table 3, entry 3al): ¹H NMR

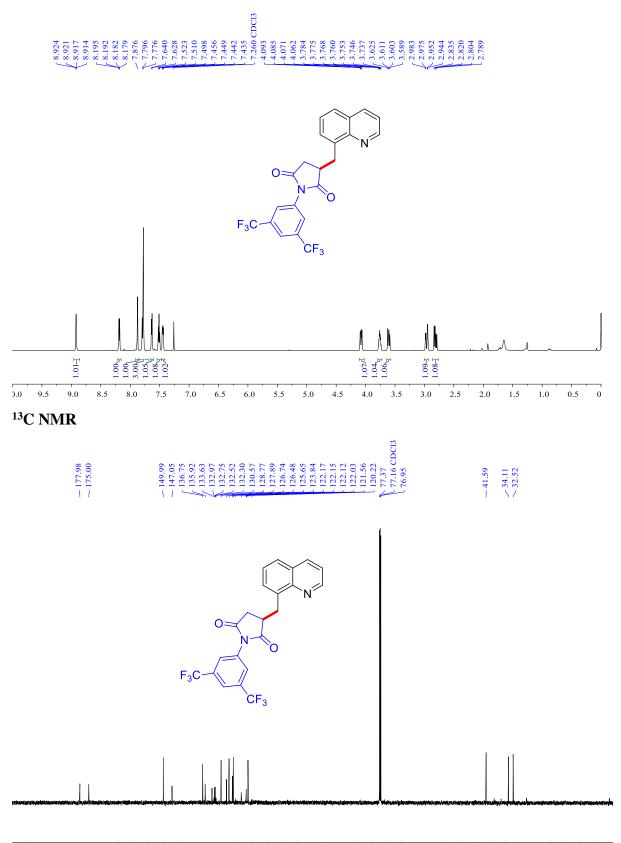


1-(3-Nitrophenyl)-3-(quinolin-8-ylmethyl)pyrrolidine-2,5-dione (*Table 3, entry 3am*): ¹H NMR



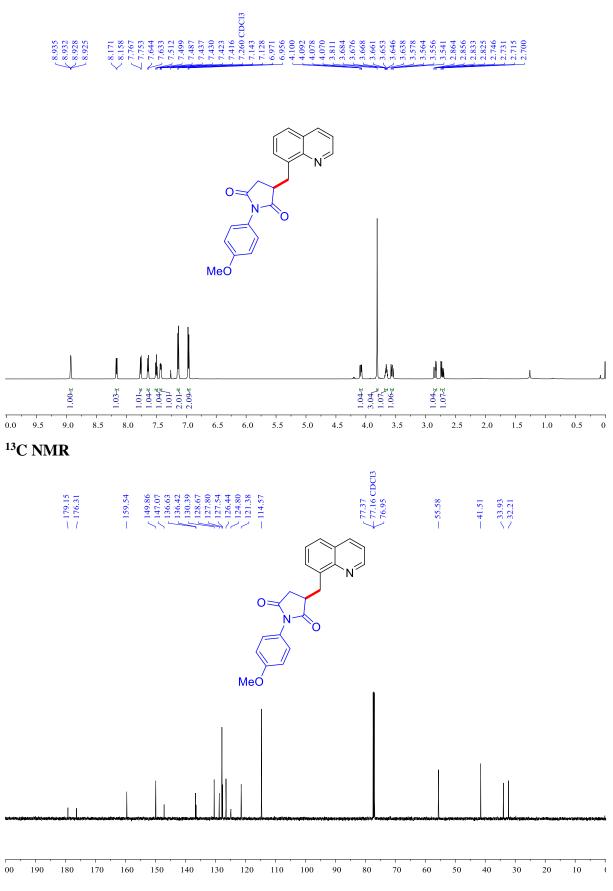
1-(3,5-Bis(trifluoromethyl)phenyl)-3-(quinolin-8-ylmethyl)pyrrolidine-2,5-dione (Table 3, entry 3an):

¹H NMR

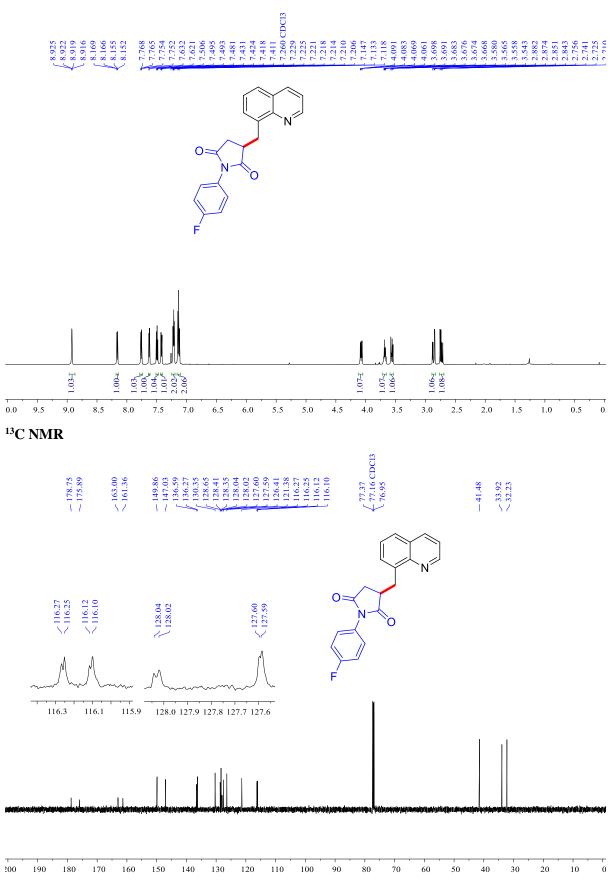


. 160 . 90

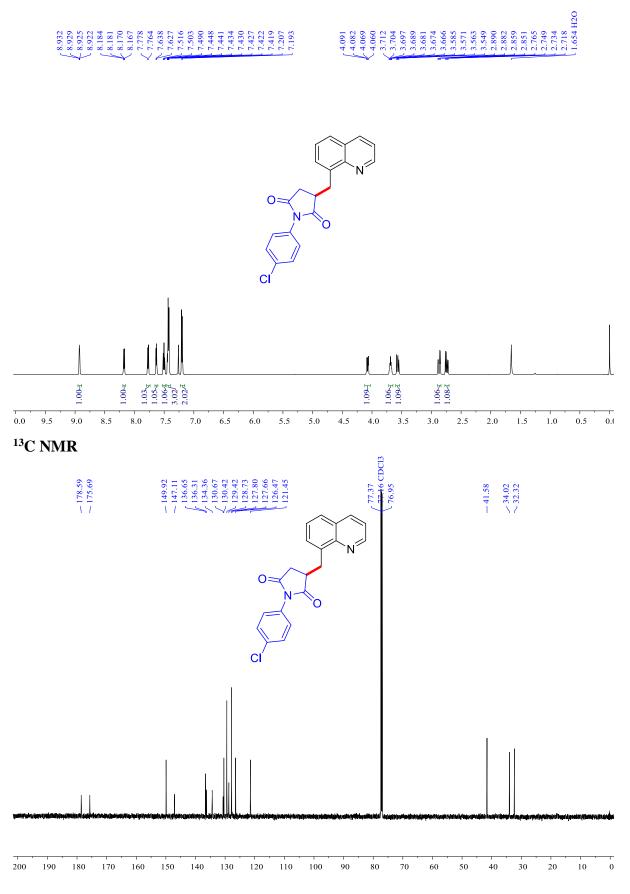
1-(4-Methoxyphenyl)-3-(quinolin-8-ylmethyl)pyrrolidine-2,5-dione (Table 3, entry 3ao): ¹H NMR



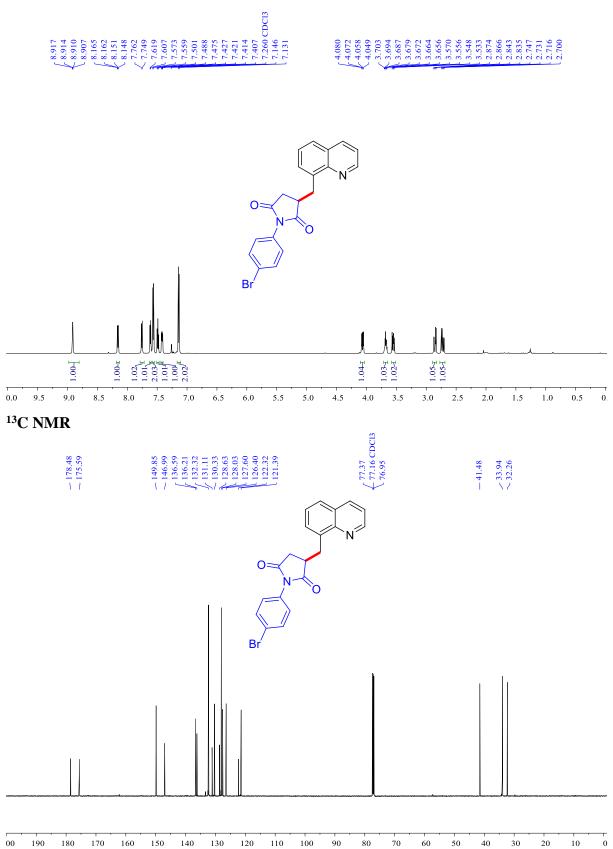
1-(4-Fluorophenyl)-3-(quinolin-8-ylmethyl)pyrrolidine-2,5-dione (Table 3, entry 3ap): ¹H NMR



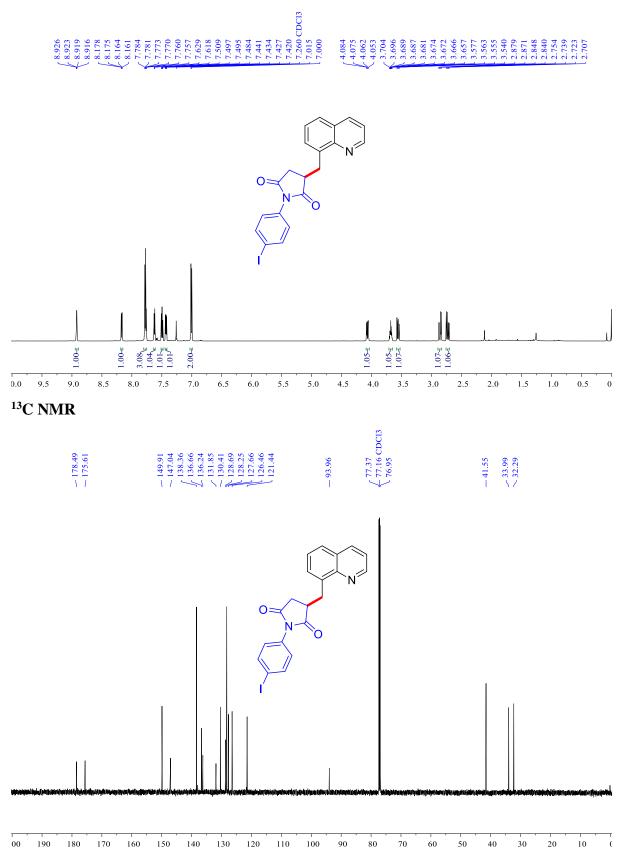
1-(4-Chlorophenyl)-3-(quinolin-8-ylmethyl)pyrrolidine-2,5-dione (*Table 3, entry 3aq*): ¹H NMR



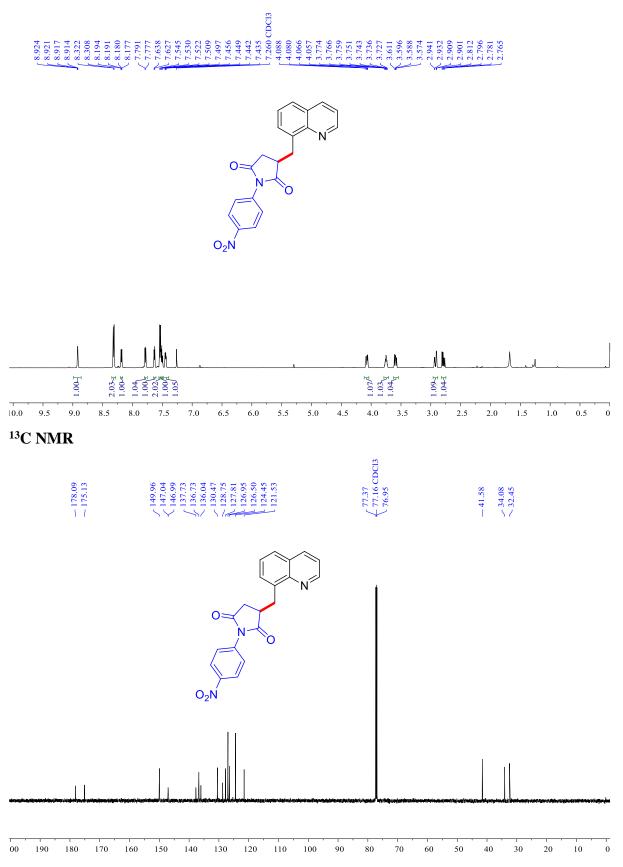
1-(4-Bromophenyl)-3-(quinolin-8-ylmethyl)pyrrolidine-2,5-dione (*Table 3, entry 3ar*): ¹H NMR

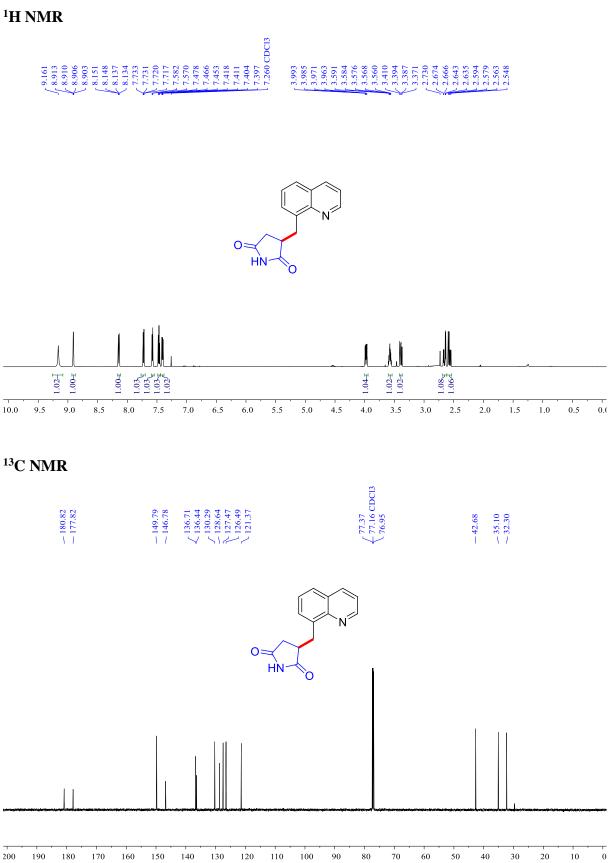


1-(4-Iodophenyl)-3-(quinolin-8-ylmethyl)pyrrolidine-2,5-dione (Table 3, entry 3as): ¹H NMR



1-(4-Nitrophenyl)-3-(quinolin-8-ylmethyl)pyrrolidine-2,5-dione (*Table 3, entry 3at*): ¹H NMR

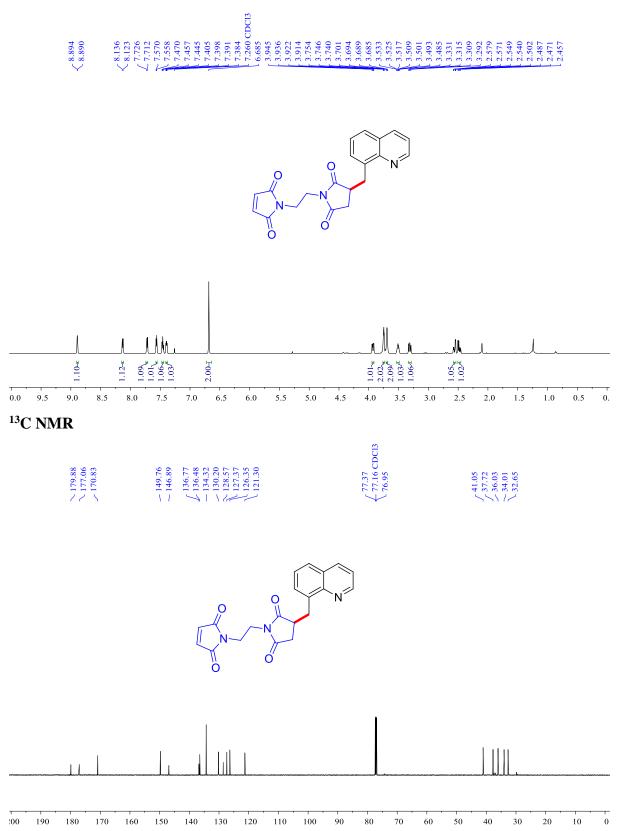




3-(quinolin-8-ylmethyl)pyrrolidine-2,5-dione (Table 3, entry 3au): ¹H NMR

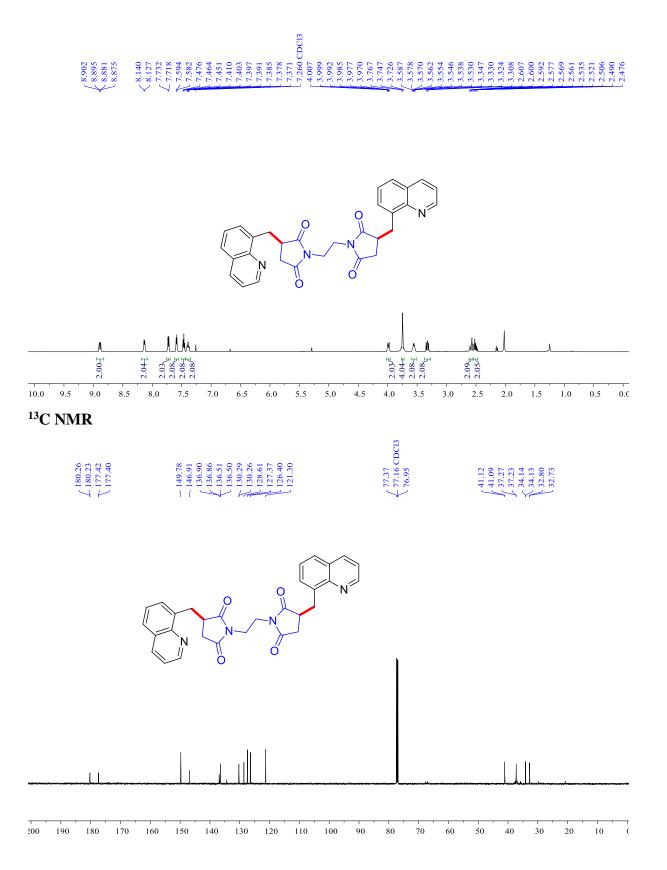
1-(2-(2,5-Dioxo-3-(quinolin-8-ylmethyl)pyrrolidin-1-yl)ethyl)-1H-pyrrole-2,5-dione (Table 3, entry 3av₁):

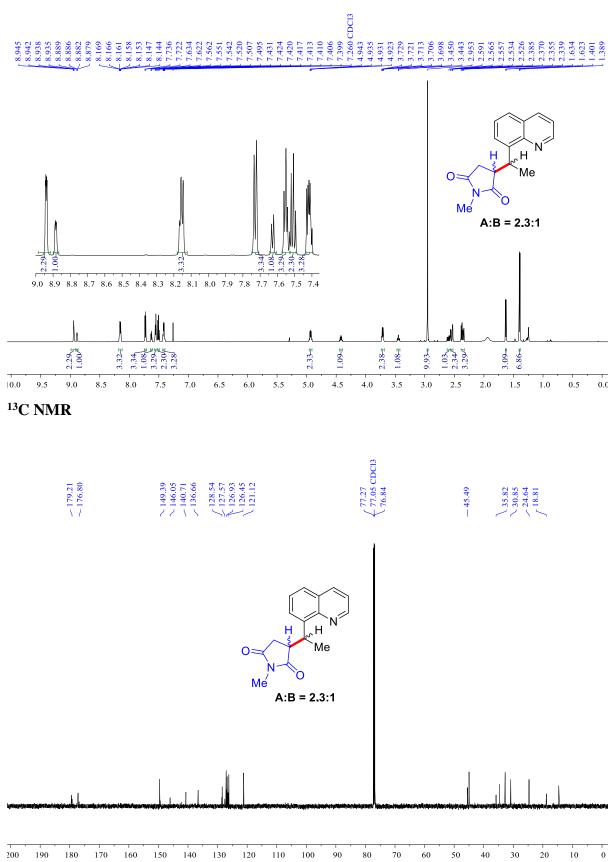
¹H NMR



1,1'-(ethane-1,2-diyl)bis(3-(quinolin-8-ylmethyl)pyrrolidine-2,5-dione) (Table 3, entry 3av₂):

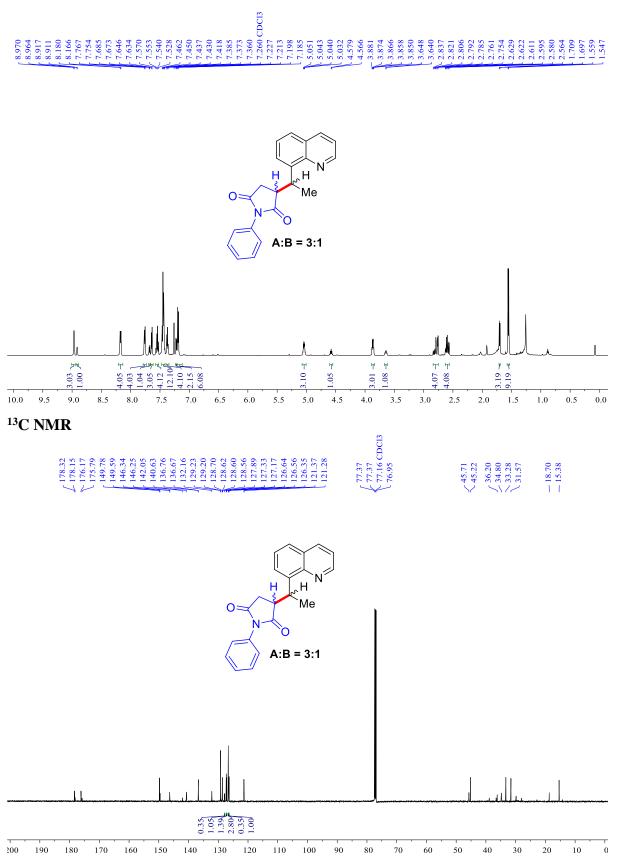
¹H NMR





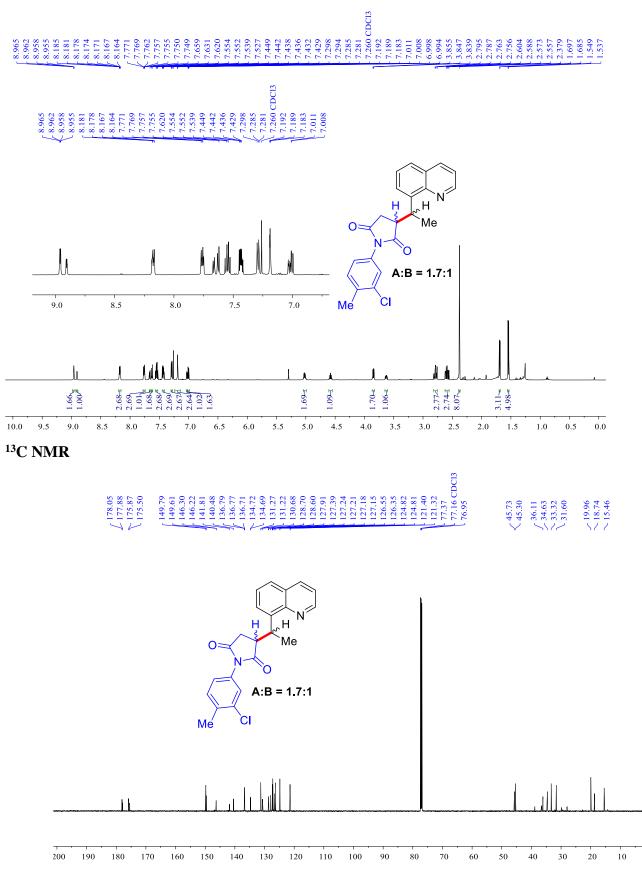
1-methyl-3-(1-(quinolin-8-yl)ethyl)pyrrolidine-2,5-dione (Table 2, entry 3sa): ¹H NMR

1-phenyl-3-(1-(quinolin-8-yl)ethyl)pyrrolidine-2,5-dione (Table 4, entry 5aj) ¹H NMR



1-(3-Chloro-4-methylphenyl)-3-(1-(quinolin-8-yl)ethyl)pyrrolidine-2,5-dione (Table 4, entry 5ay):

¹H NMR



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