Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Copper-Catalyzed 1,2,2-Trifunctionalization of Maleimides with 1,7-Enynes and Oxime Esters *via* Radical Relay/1,5-Hydrogen-atom Transfer

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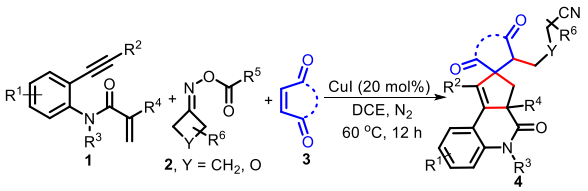
(A) General information

All chemicals were acquired from commercial sources and were employed as received unless otherwise mentioned. 1,7-Enynes[1] and oxime esters[2] were synthesized according to relevant literature reports. The reaction was monitored by TLC with silica gel plates, and the visualization was displayed under UV light (254 nm). ^{1}H NMR, ^{13}C NMR, and ^{19}F NMR spectra were recorded on a Bruker 400 (400, 101, and 376 MHz) or 500 (500, 126, and 471 MHz) advance spectrometer at room temperature in $CDCl_3$ (solvent signals, δ 7.26 and 77.0 ppm) or DMSO-d6 (solvent signals, δ 3.35 and 39.5 ppm) using TMS as internal standard. HRMS spectra were measured on an electrospray ionization quadrupole time-of-flight (ESI-Q-TOF) mass spectrometer.

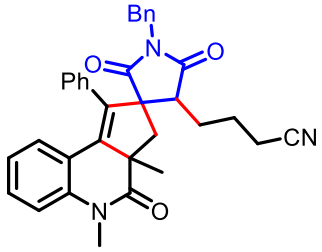
(B) Typical experimental procedures for the synthesis of compounds 4



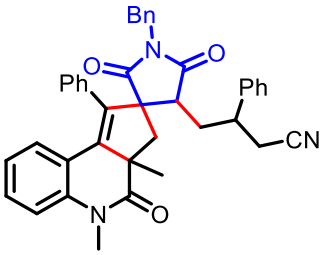
To a Schlenk tube were added 1,7-enynes **1** (0.2 mmol), oxime esters **2** (1.5 equiv), maleimides **3** (1.5 equiv), CuI (20 mol%), and 1,2-dichloroethane (DCE) (1.0 mL). Then the tube was stirred at 60 °C under N_2 atmosphere, and until complete consumption of starting material as monitored by TLC and/or GC-MS analysis. After the reaction was completed, the crude mixture was washed three times with saturated $NaHCO_3$ solution and then extracted three times with EtOAc. The organic layer was dried over Na_2SO_4, filtration and evaporation of the solvent. And the resulting residue

was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 2:1 or 3:1) to acquire the desired products **4**.

(C) Analytical data

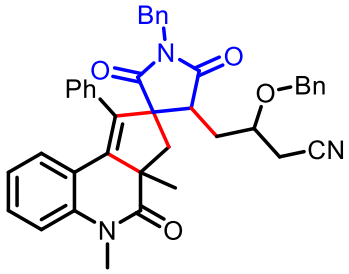


4-(1'-Benzyl-3a,5-dimethyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4a). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (2:1, v/v). Yellow oil (84.7 mg, 80% yield, d.r. = 2:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.29 (t, J = 3.2 Hz, 3H), 7.20-7.16 (m, 3H), 7.13-7.08 (m, 2H), 7.03-6.92 (m, 3H), 6.76-6.69 (m, 3H), 4.74-4.53 (m, 2H), 3.36 (d, J = 4.4 Hz, 3H), 2.88-2.81 (m, 1H), 2.59-2.41 (m, 1H), 2.39-2.25 (m, 1H), 2.21-2.10 (m, 2H), 1.95-1.72 (m, 2H), 1.61-1.52 (m, 2H), 1.43 (s, 2H), 1.30 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 180.2, 178.5, 177.3, 177.2, 174.6, 173.6, 140.0, 139.5, 138.2, 136.8, 135.4, 135.2, 133.7, 133.3, 129.3 (2), 129.1, 128.9, 128.7, 128.6, 128.5, 128.4, 128.3, 128.1 (2), 127.7, 127.1, 122.6, 122.5, 120.2, 120.1, 118.9, 118.8, 115.1, 115.0, 63.8, 63.1, 53.5, 53.1, 46.5, 45.0, 42.8, 42.4, 39.0, 36.9, 30.1, 27.9, 26.9, 26.0, 25.3, 23.4, 22.5, 16.9; HRMS *m/z* (ESI) calcd for $C_{34}H_{31}N_3NaO_3$ ($[M+Na]^+$) 552.2258, found 552.2250.



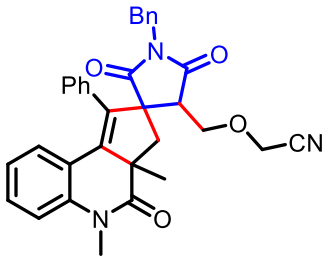
4-(1'-Benzyl-3a,5-dimethyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)-3-phenylbutanenitrile (4b). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (2:1, v/v). Yellow oil (94.4 mg, 78% yield, d.r. = 5:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.74-7.72 (m, 1H), 7.56-7.53 (m, 1H), 7.37-7.30

(m, 5H), 7.24-7.20 (m, 2H), 7.17-7.13 (m, 3H), 7.07-7.01 (m, 3H), 6.96-6.90 (m, 2H), 6.75-6.68 (m, 2H), 4.73 (d, *J* = 17.6 Hz, 1H), 4.62 (d, *J* = 14.0 Hz, 1H), 3.52-3.39 (m, 4H), 2.91-2.87 (m, 1H), 2.55-2.50 (m, 2H), 2.46-2.34 (m, 2H), 2.09-2.05 (m, 2H), 1.50 (s, 0.5H), 1.46 (s, 2.5H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 180.0, 179.8, 177.7, 177.5, 175.3, 174.7, 140.0, 139.9, 136.2, 135.4, 133.1, 131.9, 131.1, 129.3, 129.2, 129.1, 129.0, 128.8, 128.7, 128.5, 128.4, 128.1, 128.0, 127.9, 127.8, 127.7, 127.4, 127.2 (2), 122.6 (2), 120.3, 118.3, 118.0, 115.1, 115.0, 63.3, 53.7, 53.4, 52.6, 42.7, 42.5, 39.6, 39.2, 33.6, 32.8, 30.1 (2), 29.7, 29.3, 26.2, 26.0, 25.1; HRMS *m/z* (ESI) calcd for $C_{40}H_{35}N_3NaO_3$ ([M+Na]$^+$) 628.2571, found 628.2561.

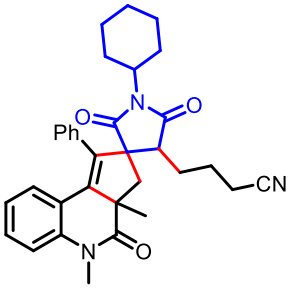


4-(1'-Benzyl-3a,5-dimethyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)-3-(benzyloxy)butanenitrile (4c). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (2:1, v/v). Yellow oil (64.8 mg, 51% yield, d.r. > 20:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.38-7.30 (m, 6H), 7.25-7.14 (m, 5H), 7.10-7.03 (m, 3H), 6.95-6.92 (m, 1H), 6.90-6.86 (m, 2H), 6.76-6.73 (m, 2H), 4.73-4.68 (m, 1H), 4.62-4.59 (m, 1H), 4.47 (d, *J* = 11.6 Hz, 1H), 4.31 (d, *J* = 11.2 Hz, 1H), 3.42 (s, 3H), 2.99-2.95 (m, 1H), 2.83 (d, *J* = 14.4 Hz, 1H), 2.57-2.47 (m, 2H), 2.08 (d, *J* = 14.4 Hz, 2H), 1.84-1.77 (m, 2H), 1.49 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 180.1, 177.8, 174.6, 140.4, 140.0, 136.9, 136.1, 135.5, 133.7, 131.1, 129.3, 129.0, 128.9, 128.7 (2), 128.5, 128.3 (2), 128.0, 127.8, 122.5, 120.3, 117.0, 115.0, 72.3, 71.5, 63.5, 53.5, 42.6, 41.4, 39.5, 32.2, 26.2, 23.4; HRMS *m/z* (ESI) calcd for

$C_{41}H_{37}N_3NaO_4$ ([M+Na]$^+$) 658.2676, found 658.2670.

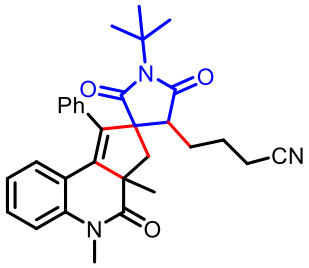


2-((1'-Benzyl-3a,5-dimethyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)methoxy)acetonitrile (4d). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (3:1, v/v). Yellow oil (79.7 mg, 75% yield, d.r. = 2:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.39-7.35 (m, 4H), 7.23-7.21 (m, 2H), 7.20-7.15 (m, 2H), 7.06-7.02 (m, 3H), 6.75-6.69 (m, 3H), 4.83-4.69 (m, 1H), 4.66-4.62 (m, 1H), 4.22-4.15 (m, 2H), 3.94-3.91 (m, 2H), 3.43 (s, 3H), 2.95-2.87 (m, 1H), 2.45-2.34 (m, 1H), 2.18-2.05 (m, 1H), 1.56 (s, 2H), 1.38 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 180.3, 179.8, 175.7, 175.4, 174.9, 173.7, 140.0, 139.9, 139.5, 137.5, 135.1, 135.0, 133.2, 131.1, 129.3, 129.2, 129.1, 129.0, 128.8, 128.7, 128.5, 128.4 (2), 128.3, 128.1, 128.0 (2), 127.5, 127.1, 122.5, 122.4, 120.3, 119.9, 115.0, 114.9, 68.9, 67.9, 61.9, 61.5, 56.4, 53.3, 52.9, 49.5, 47.8, 43.0, 42.6, 39.1, 37.4, 30.0, 29.2, 27.0, 26.1; HRMS *m/z* (ESI) calcd for $C_{33}H_{29}N_3NaO_4$ ([M+Na]$^+$) 554.2050, found 554.2039.

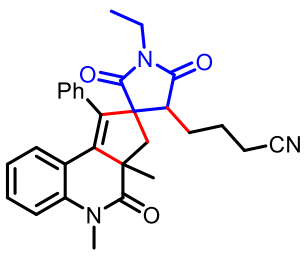


4-(1'-Cyclohexyl-3a,5-dimethyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4e). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (2:1, v/v). Colorless oil (78.2 mg, 75% yield, d.r. > 20:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.37-7.31 (m, 4H), 7.06 (d, J = 8.0 Hz, 1H), 7.02-6.97 (m, 2H), 6.82-6.76 (m, 2H), 3.45 (s, 3H), 3.43-3.40 (m, 1H), 2.91 (t, J = 12.0 Hz, 1H),

2.54 (t, J = 6.8 Hz, 1H), 2.31-2.22 (m, 2H), 2.11-2.07 (m, 1H), 1.88-1.81 (m, 4H), 1.71-1.60 (m, 6H), 1.51 (s, 3H), 1.29-1.24 (m, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 180.6, 177.7, 174.7, 139.9, 136.9, 134.0, 129.4, 129.3 (2), 128.8, 128.5, 128.1, 122.6, 120.3, 119.1, 115.1, 63.0, 53.4, 51.9, 44.7, 39.1, 30.1, 29.0, 28.6, 26.1, 25.8, 25.7, 25.4, 25.0, 23.4, 17.0; HRMS *m/z* (ESI) calcd for $C_{33}H_{35}N_3NaO_3$ ($[M+Na]^+$) 544.2571, found 544.2561.

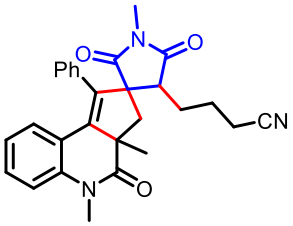


4-(1'-(*tert*-Butyl)-3a,5-dimethyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4f). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (2:1, v/v). Yellow oil (72.3 mg, 73% yield, d.r. = 4:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.41-7.31 (m, 4H), 7.09-7.01 (m, 3H), 6.83-6.72 (m, 2H), 3.45 (s, 3H), 3.41-3.39 (m, 1H), 2.92-2.85 (m, 1H), 2.51-2.47 (m, 1H), 2.28-2.16 (m, 2H), 1.96-1.66 (m, 4H), 1.60 (s, 9H), 1.26 (s, 0.6H), 1.20 (s, 2.4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 181.3 (2), 178.8, 178.5, 174.7, 174.5, 139.9, 139.3, 138.0, 137.1, 134.1, 134.0, 129.3, 129.2, 129.1, 129.0, 128.7, 128.4, 128.1, 127.8, 127.4, 122.6, 122.4, 120.3, 119.1, 118.8, 115.0 (2), 63.5, 63.2, 58.6, 53.3, 52.6, 47.5, 45.1, 39.1, 36.6, 30.1, 30.0, 28.3, 28.2, 27.9, 26.5, 26.0, 25.2, 23.5, 22.1, 17.0; HRMS *m/z* (ESI) calcd for $C_{31}H_{33}N_3NaO_3$ ($[M+Na]^+$) 518.2414, found 518.2423.



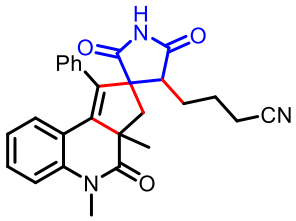
4-(1'-Ethyl-3a,5-dimethyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4g). The product was

purified by silica gel column chromatography with petroleum ether/ethyl acetate (2:1, v/v). Yellow oil (72.9 mg, 78% yield, d.r. = 2:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.37-7.28 (m, 4H), 7.08-7.00 (m, 3H), 6.81-6.74 (m, 2H), 3.68-3.50 (m, 2H), 3.45 (s, 2H), 3.43 (s, 1H), 3.27-3.19 (m, 1H), 3.01-2.90 (m, 1H), 2.61-2.49 (m, 1H), 2.28-2.25 (m, 1H), 2.15-2.09 (m, 1H), 1.89-1.73 (m, 2H), 1.71-1.56 (m, 2H), 1.52 (s, 2H), 1.39 (s, 1H), 1.20 (t, J = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 180.3, 178.3, 177.5, 177.4, 174.6, 173.6, 140.0, 139.9, 139.8, 139.0, 138.7, 136.7, 134.0, 133.6, 129.3, 129.0 (2), 128.5, 128.0, 127.3, 122.6, 122.5, 120.2, 119.8, 119.0, 118.8, 115.1, 115.0, 63.5, 63.3, 53.4, 52.9, 47.1, 45.0, 39.0, 36.5, 34.0, 33.7, 30.1, 30.0, 28.6, 26.6, 26.1, 25.3, 23.5, 22.3, 16.9, 12.9, 12.0; HRMS *m/z* (ESI) calcd for $C_{29}H_{29}N_3NaO_3$ ([M+Na]$^{+}$) 490.2101, found 490.2109.

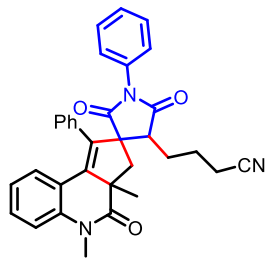


4-(1',3a,5-Trimethyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4h). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (2:1, v/v). Yellow soild (68.9 mg, 76% yield, d.r. = 4:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.36-7.31 (m, 3H), 7.09-7.04 (m, 2H), 7.02-6.99 (m, 2H), 6.80-6.78 (m, 2H), 3.45 (s, 3H), 3.44-3.42 (m, 1H), 3.05 (s, 3H), 2.93-2.89 (m, 1H), 2.63-2.58 (m, 1H), 2.27-2.25 (m, 1H), 2.19-2.13 (m, 1H), 1.85-1.75 (m, 2H), 1.67-1.58 (m, 2H), 1.52 (s, 2.4H), 1.39 (s, 0.6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 180.5, 179.3, 178.7, 177.6, 174.5, 173.6, 140.1, 139.9, 138.3, 136.6, 133.9, 133.4, 129.4, 128.9, 128.5, 128.0, 127.1, 122.6, 122.5, 120.1, 119.9, 119.0, 118.8, 115.1, 64.2, 63.5, 53.4, 53.0, 46.9, 45.1, 38.9, 36.4, 30.1, 28.1,

26.8, 26.1, 25.3 (2), 24.6, 23.4, 22.5, 16.9; HRMS *m/z* (ESI) calcd for $C_{28}H_{27}N_3NaO_3$ ($[M+Na]^+$) 476.1945, found 476.1938.

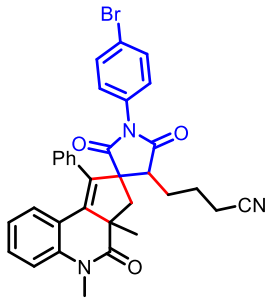


4-(3a,5-Dimethyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4i). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (2:1, v/v). Yellow oil (56.2 mg, 64% yield, d.r. = 2:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.63 (s, 0.7H), 8.37 (s, 0.3H), 7.38-7.34 (m, 3H), 7.25-7.21 (m, 1H), 7.14-7.01 (m, 3H), 6.82-6.73 (m, 2H), 3.45 (s, 2H), 3.43 (s, 1H), 2.99-2.92 (m, 1.3H), 2.70 (t, *J* = 7.2 Hz, 0.7H), 2.52-2.48 (m, 1H), 2.28-2.20 (m, 2H), 1.95-1.84 (m, 2H), 1.76-1.54 (m, 2H), 1.50 (s, 2H), 1.38 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 180.5, 178.8, 177.7, 177.6, 174.6, 173.6, 140.5, 139.9, 139.7, 137.7, 136.0, 133.9, 133.5, 129.4, 129.3, 129.1, 128.6 (2), 128.1, 127.1, 122.7, 122.6, 120.2, 120.1, 119.0, 118.9, 115.1 (2), 65.4, 64.8, 53.5, 53.1, 47.4, 46.0, 39.1, 36.9, 30.2, 30.1, 27.4, 26.9, 26.0, 24.8, 23.4, 22.8, 17.1, 16.9; HRMS *m/z* (ESI) calcd for $C_{27}H_{25}N_3NaO_3$ ($[M+Na]^+$) 462.1788, found 462.1780.

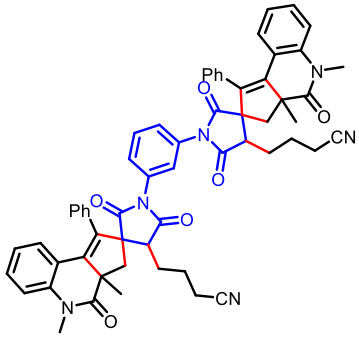


4-(3a,5-Dimethyl-2',4,5'-trioxo-1,1'-diphenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4j). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (2:1, v/v). Yellow oil (63.9 mg, 62% yield, d.r. = 6.5:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.43 (t, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 7.2 Hz, 1H), 7.33-7.31 (m, 3H), 7.22-7.16 (m, 4H), 7.11-7.04 (m, 2H), 6.69 (t, *J* = 18.0 Hz, 2H), 3.39 (s, 2.6H), 3.36 (s,

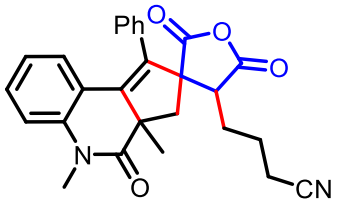
0.4H), 2.96 (d, *J* = 14.4 Hz, 1H), 2.73 (t, *J* = 7.2 Hz, 1H), 2.30-2.25 (m, 1H), 2.24-2.17 (m, 2H), 1.92-1.74 (m, 2H), 1.71-1.57 (m, 2H), 1.47 (s, 2.6H), 1.37 (s, 0.4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 179.4, 177.6, 176.5, 174.6, 173.9, 140.5, 140.0, 139.9, 139.3, 136.5, 134.0, 133.7, 131.8, 131.3, 129.5 (2), 129.3, 129.2, 129.1, 128.9, 128.7, 128.6, 128.1, 126.4, 126.2, 122.7, 122.6, 120.2, 119.0, 118.8, 115.1, 64.0, 63.7, 53.6, 53.0, 47.7, 45.4, 39.1, 36.6, 30.1, 29.3, 26.6, 26.2, 25.6, 23.5, 22.6, 17.0, 14.1; HRMS *m/z* (ESI) calcd for $C_{33}H_{29}N_3NaO_3$ ($[M+Na]^+$) 538.2101, found 538.2108.



4-(1'-(4-Bromophenyl)-3a,5-dimethyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4k). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (2:1, v/v). Yellow oil (75.9 mg, 64% yield, d.r. = 5:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.64-7.59 (m, 2H), 7.39-7.36 (m, 4H), 7.21-7.17 (m, 2H), 7.11-7.06 (m, 3H), 6.81-6.79 (m, 2H), 3.46 (s, 3H), 3.44-3.42 (m, 1H), 3.04-3.00 (m, 1H), 2.80 (t, *J* = 7.2 Hz, 1H), 2.30-2.26 (m, 2H), 1.94-1.83 (m, 2H), 1.68-1.61 (m, 2H), 1.53 (s, 2.5H), 1.43 (s, 0.5H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 179.1, 178.6, 176.3, 176.1, 174.4, 173.4, 140.6, 140.0, 139.9, 139.4, 138.3, 136.2, 133.8, 133.6, 132.3, 132.1, 130.7, 129.7, 129.5, 129.3, 129.0, 128.7, 128.0, 127.9, 127.7 (2), 127.4, 122.7, 122.5, 120.0, 119.5, 118.9, 118.7, 115.1, 64.0, 63.8, 53.5, 52.9, 47.7, 45.4, 39.0, 30.1, 30.0, 26.6, 26.2, 25.5, 23.4, 22.2, 17.0; HRMS *m/z* (ESI) calcd for $C_{33}H_{28}BrN_3NaO_3$ ($[M+Na]^+$) 616.1206, found 616.1215.

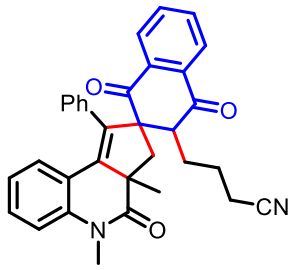


4,4'-(1,3-Phenylenebis(3a,5-dimethyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidine]-1',4'-diyl))dibutanenitrile (4l). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (2:1, v/v). Yellow oil (110.5 mg, 58% yield, d.r. = 9:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.71 (d, J = 8.4 Hz, 1H), 7.61-7.57 (m, 1H), 7.48-7.45 (m, 3H), 7.41-7.35 (m, 7H), 7.15-7.02 (m, 6H), 6.88 (t, J = 4.0 Hz, 2H), 6.81-6.79 (m, 2H), 3.46 (s, 5.4H), 3.43 (s, 0.6H), 3.04-2.99 (m, 2H), 2.82-2.78 (m, 2H), 2.33-2.23 (m, 6H), 1.95-1.78 (m, 4H), 1.72-1.58 (m, 4H), 1.54 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 179.0, 177.3, 176.1, 174.5, 168.9, 140.5, 140.0, 136.5, 134.3, 133.7, 132.3, 132.0, 129.6, 129.5 (2), 129.0, 128.8, 128.0, 127.8, 125.6, 125.5, 125.1, 123.3, 123.1, 122.7, 120.1, 119.0, 115.1, 64.0, 63.7, 53.5, 53.0, 47.6, 45.5, 39.0, 30.1, 29.7, 29.3, 26.1, 25.7, 23.4, 22.6, 17.0, 14.1; HRMS *m/z* (ESI) calcd for $C_{60}H_{52}N_6NaO_6$ ($[M+Na]^+$) 975.3841, found 975.3831.

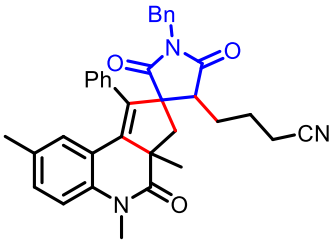


4-(3a,5-Dimethyl-2',4,5'-trioxo-1-phenyl-3,3a,4,4',5,5'-hexahydro-2'*H*-spiro[cyclopenta[*c*]quinoline-2,3'-furan]-4'-yl)butanenitrile (4m). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (2:1, v/v). Yellow oil (51.9 mg, 59% yield, d.r. > 20:1); ^{1}H NMR (500 MHz, DMSO-d_6) δ: 7.38-7.35 (m, 3H), 7.28-7.24 (m, 1H), 7.22-7.16 (m, 1H), 7.07-7.00 (m, 2H), 6.78-6.75 (m, 1H), 6.59-6.54 (m, 1H), 3.35 (s, 3H), 3.00-2.89 (m, 1H), 2.73-2.52 (m, 1H),

2.36-2.31 (m, 2H), 2.29-2.24 (m, 1H), 1.68-1.60 (m, 1H), 1.38-1.34 (m, 1H), 1.31 (s, 3H), 1.20-1.16 (m, 1H), 1.09-1.00 (m, 1H); ^{13}C NMR (126 MHz, DMSO-d_6) δ: 176.1, 175.5, 173.9, 139.9, 139.2, 134.2, 129.0, 128.9, 128.6, 128.4, 128.1, 127.0, 122.0, 120.5, 120.3, 115.5, 64.5, 52.9, 29.8, 26.6, 26.1, 25.0, 23.9, 16.3, 15.9; HRMS *m/z* (ESI) calcd for $C_{27}H_{24}N_2NaO_4$ ([M+Na]$^+$) 463.1628, found 463.1636.

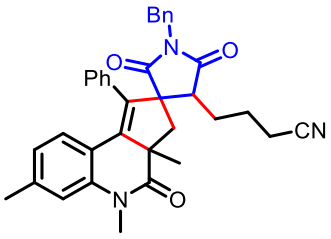


4-(3a,5-Dimethyl-1',4,4'-trioxo-1-phenyl-3,3a,3',4,4',5-hexahydro-1'*H*-spiro[cyclopenta[*c*]quinoline-2,2'-naphthalen]-3'-yl)butanenitrile (4n). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (3:1, v/v). Yellow oil (61.0 mg, 61% yield, d.r. = 2:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.06-7.98 (m, 1H), 7.82-7.67 (m, 2H), 7.31-7.28 (m, 4H), 7.25-7.22 (m, 3H), 7.12-6.93 (m, 2H), 6.86-6.77 (m, 1H), 3.44 (s, 2H), 3.41 (s, 1H), 3.06-2.99 (m, 1H), 2.68-2.53 (m, 1H), 2.08-2.01 (m, 3H), 1.65-1.55 (m, 2H), 1.31 (s, 1H), 1.28-1.24 (m, 2H), 1.21 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 199.9, 197.8, 197.2, 196.2, 174.5, 173.5, 140.9, 140.2, 139.7, 139.5, 138.1, 137.2, 135.2, 135.1, 134.6, 134.4, 134.3 (2), 133.6, 130.2, 129.3, 128.9, 128.6, 128.4, 128.1, 127.9, 127.2, 126.5, 126.1, 122.6, 122.5, 121.4, 120.3, 119.4, 115.1, 114.9, 70.8, 69.8, 53.3, 53.0, 52.9, 40.0, 38.8, 30.4, 30.0, 29.7, 26.4, 24.7, 24.5, 24.4, 17.5, 16.8; HRMS *m/z* (ESI) calcd for $C_{33}H_{28}N_2NaO_3$ ([M+Na]$^+$) 523.1992, found 523.1983.



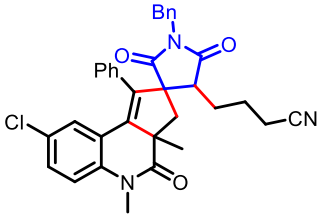
4-(1'-Benzyl-3a,5,8-trimethyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4o). The product was

purified by silica gel column chromatography with petroleum ether/ethyl acetate (2:1, v/v). Yellow oil (88.0 mg, 81% yield, d.r. = 5:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.40-7.33 (m, 5H), 7.26-7.20 (m, 1H), 7.15 (t, J = 7.6 Hz, 2H), 7.07-7.00 (m, 2H), 6.95-6.91 (m, 1H), 6.83-6.80 (m, 1H), 6.59-6.52 (m, 1H), 4.76 (d, J = 14.0 Hz, 1H), 4.66 (d, J = 10.4 Hz, 1H), 3.41 (s, 3H), 3.40-3.37 (m, 1H), 2.87 (t, J = 10.8 Hz, 1H), 2.60 (t, J = 7.2 Hz, 1H), 2.26-2.18 (m, 2H), 2.00 (s, 3H), 1.79-1.71 (m, 2H) 1.60-1.53 (m, 2H), 1.50 (s, 2.5H), 1.47 (s, 0.5H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 180.2, 179.8, 177.2, 176.7, 174.5, 174.3, 140.2, 139.7, 137.6, 137.4, 136.4, 135.4, 135.2, 133.7, 133.3, 132.0, 130.0, 129.9, 129.3, 129.1, 128.9, 128.7, 128.6 (2), 128.5, 128.3 (2), 128.2, 128.0, 120.0, 119.9, 119.0, 118.8, 114.9, 114.8, 63.0, 62.4, 53.5, 53.1, 46.1, 45.0, 42.7, 42.4, 38.9, 30.1, 28.6, 27.9, 26.9, 26.0, 25.3, 23.4, 22.7, 20.4, 17.0, 16.9; HRMS *m/z* (ESI) calcd for $C_{35}H_{33}N_3NaO_3$ ($[M+Na]^+$) 566.2414, found 566.2403.

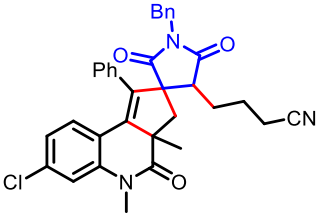


4-(1'-Benzyl-3a,5,7-trimethyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4p). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (2:1, v/v). Yellow oil (85.8 mg, 79% yield, d.r. = 2:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.40-7.34 (m, 5H), 7.23-7.18 (m, 2H), 7.15-7.10 (m, 1H), 7.06-7.00 (m, 1H), 6.87-6.82 (m, 2H), 6.69-6.65 (m, 1H), 6.60-6.56 (m, 1H), 4.74-4.64 (m, 2H), 3.43 (s, 3H), 3.42-3.37 (m, 1H), 2.86 (t, J = 12.4 Hz, 1H), 2.64-2.56 (m, 1H), 2.33 (s, 2H), 2.29 (s, 1H), 2.25-2.17 (m, 2H), 1.81-1.71 (m, 2H), 1.63-1.54 (m, 2H), 1.51 (s, 2H), 1.37 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 180.3, 179.8,

177.4, 177.2, 175.1, 174.7, 140.0, 139.9, 139.6, 139.4, 135.7, 135.4, 133.8, 129.4, 129.2, 129.1, 128.9 (2), 128.7, 128.6, 128.5, 128.3, 128.0, 127.9, 127.8, 127.7, 126.9, 123.4, 123.3, 119.0, 117.4, 115.8, 63.7, 63.0, 53.6, 53.1, 46.7, 45.0, 42.7, 42.4, 38.9, 36.9, 30.1, 28.0, 27.0, 26.1, 25.3, 23.4, 22.7, 22.5, 21.8, 16.9; HRMS *m/z* (ESI) calcd for $C_{35}H_{33}N_3NaO_3$ ($[M+Na]^+$) 566.2414, found 566.2404.

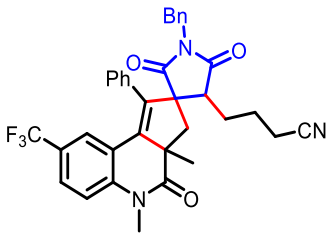


4-(1'-Benzyl-8-chloro-3a,5-dimethyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4q). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (2:1, v/v). Yellow oil (72.1 mg, 64% yield, d.r. > 20:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.38-7.32 (m, 5H), 7.29 (t, J = 7.2 Hz, 1H), 7.22-7.16 (m, 3H), 7.00-6.97 (m, 1H), 6.81-6.75 (m, 2H), 6.69 (d, J = 2.4 Hz, 1H), 4.77-4.64 (m, 2H), 3.42 (s, 3H), 2.88 (d, J = 14.4 Hz, 1H), 2.64-2.57 (m, 1H), 2.27-2.21 (m, 2H), 2.10 (d, J = 14.4 Hz, 1H), 1.91-1.80 (m, 2H), 1.66-1.58 (m, 2H), 1.51 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 179.8, 177.1, 174.3, 138.6 (2), 138.4, 135.3, 132.9, 131.1, 129.4, 129.1, 128.8, 128.7 (2), 128.1, 127.9, 127.7, 121.6, 118.9, 116.3, 63.1, 53.3, 44.6, 42.8, 39.4, 30.2, 26.8, 25.4, 23.4, 17.6; HRMS *m/z* (ESI) calcd for $C_{34}H_{30}ClN_3NaO_3$ ($[M+Na]^+$) 586.1868, found 586.1874.



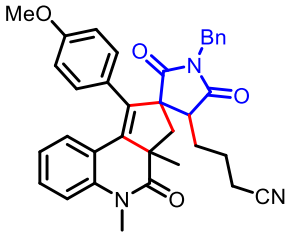
4-(1'-Benzyl-7-chloro-3a,5-dimethyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4r). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (2:1,

v/v). Yellow oil (76.6 mg, 68% yield, d.r. = 1.5:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.68-7.64 (m, 0.4H), 7.51-7.44 (m, 0.6H), 7.21-7.19 (m, 2H), 7.17-7.09 (m, 4H), 7.02-6.98 (m, 1H), 6.95-6.84 (m, 3H), 6.70-6.60 (m, 2H), 4.42-4.19 (m, 2H), 3.34 (s, 1.8H), 3.32 (s, 1.2H), 3.16-3.05 (m, 1H), 2.97-2.76 (m, 1H), 2.70-2.54 (m, 1H), 2.42-2.27 (m, 2H), 1.68-1.53 (m, 2H), 1.35-1.27 (m, 2H), 1.18 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 178.4, 178.0, 177.2, 176.5, 175.7, 173.4, 140.8, 138.9, 138.4, 135.1, 134.9, 134.7, 132.9, 131.8, 131.1, 129.9, 129.2, 129.1, 129.0, 128.9, 128.8 (2), 128.7 (2), 128.6, 128.5, 128.4, 128.3, 128.1, 128.0, 127.7, 122.5, 118.8, 118.5, 115.4, 63.7, 63.0, 53.7, 53.0, 52.6, 46.4, 45.2, 42.4, 36.9, 31.7, 30.2, 29.2, 28.6, 27.9, 27.0, 22.9, 22.5, 17.0; HRMS *m/z* (ESI) calcd for $C_{34}H_{30}ClN_3NaO_3$ ($[M+Na]^+$) 586.1868, found 586.1876.

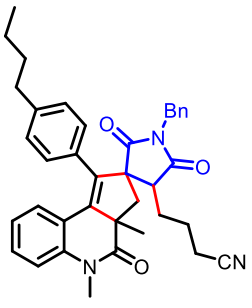


4-(1'-Benzyl-3a,5-dimethyl-2',4,5'-trioxo-1-phenyl-8-(trifluoromethyl)-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4s). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (2:1, v/v). Yellow oil (75.3 mg, 63% yield, d.r. = 2:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.58-7.43 (m, 2H), 7.38-7.34 (m, 3H), 7.30-7.24 (m, 2H), 7.20-7.10 (m, 3H), 7.08-7.03 (m, 1H), 7.00-6.96 (m, 1H), 6.88-6.78 (m, 1H), 4.75-4.65 (m, 1H), 4.51-4.34 (m, 1H), 3.46 (s, 3H), 2.99-2.89 (m, 1H), 2.65-2.61 (m, 1H), 2.50-2.36 (m, 1H), 2.33-2.21 (m, 2H), 1.92-1.77 (m, 2H), 1.56-1.50 (m, 2H), 1.38 (s, 1H), 1.25 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 179.8, 178.3, 177.1, 177.0, 174.6, 173.5, 142.5, 142.2, 140.3, 139.0, 138.4, 138.1, 135.1 (q, $J_{C\text{-}F}$ = 20.3 Hz), 132.6, 132.3, 131.8, 131.1, 129.5, 129.1,

129.0 (2), 128.9, 128.8 (2), 128.7 (2), 128.5, 128.3, 128.1, 127.7, 125.3 (q, $J_{C\text{-}F}$ = 273.5 Hz), 125.2 (q, $J_{C\text{-}F}$ = 3.8 Hz), 120.3, 118.9, 118.8, 115.1, 115.0, 63.7, 63.0, 53.7, 53.3, 52.9, 52.6, 46.3, 45.0, 42.8, 39.0, 36.9, 30.3, 29.2, 27.0, 26.0, 25.4, 23.3, 22.6, 17.0, 16.9; ^{19}F NMR (377 MHz, $CDCl_3$) δ: -62.8; HRMS *m/z* (ESI) calcd for $C_{35}H_{30}F_3N_3NaO_3$ ([M+Na]$^+$) 620.2131, found 620.2121.

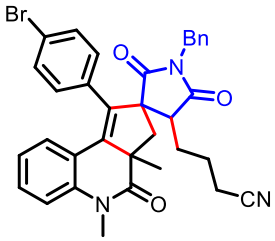


4-(1'-Benzyl-1-(4-methoxyphenyl)-3a,5-dimethyl-2',4,5'-trioxo-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4t). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (2:1, v/v). Yellow soild (79.4 mg, 71% yield, d.r. = 2:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.69-7.64 (m, 2H), 7.50-7.46 (m, 2H), 7.38-7.28 (m, 1H), 7.23-7.16 (m, 2H), 7.15-7.11 (m, 2H), 7.01-6.98 (m, 1H), 6.84-6.61 (m, 3H), 4.71-4.53 (m, 1H), 4.33-4.31 (m, 1H), 3.85 (s, 6H), 3.71-3.70 (m, 1H), 3.36-3.34 (m, 1H), 2.89-2.76 (m, 1H), 2.39-2.29 (m, 2H), 1.79-1.68 (m, 2H), 1.54-1.45 (m, 2H), 1.29 (s, 1H), 1.18 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 178.7, 177.5, 175.5, 173.7, 168.1, 159.4, 139.7, 139.4, 138.2, 135.1, 131.9, 131.1, 130.2, 129.2, 128.8 (2), 128.7, 128.4, 128.0, 127.7, 127.2, 125.1, 122.5, 120.2, 118.8, 115.0, 114.3, 63.7, 55.0, 52.9, 52.7, 46.7, 42.5, 39.0, 36.8, 34.4, 30.5, 30.1, 28.1, 26.9, 22.8, 22.5, 17.0 (2); HRMS *m/z* (ESI) calcd for $C_{35}H_{33}N_3NaO_4$ ([M+Na]$^+$) 582.2363, found 582.2355.



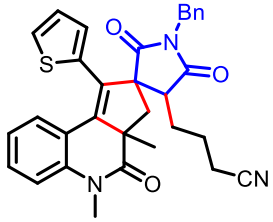
4-(1'-Benzyl-1-(4-butylphenyl)-3a,5-dimethyl-2',4,5'-trioxo-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4u). The product was purified

by silica gel column chromatography with petroleum ether/ethyl acetate (2:1, v/v). Yellow oil (92.5 mg, 79% yield, d.r. = 2:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.30-7.28 (m, 3H), 7.22-7.06 (m, 3H), 7.04-6.94 (m, 2H), 6.89-6.87 (m, 1H), 6.84-6.75 (m, 1H), 6.73-6.63 (m, 3H), 4.70-4.57 (m, 1.4H), 4.31-4.23 (m, 0.7H), 3.36 (s, 3H), 2.87-2.79 (m, 1H), 2.60-2.53 (m, 1H), 2.51-2.46 (m, 2H), 2.33 (t, J = 18.0 Hz, 1H), 2.17-2.10 (m, 2H), 1.92-1.60 (m, 4H), 1.52-1.48 (m, 2H), 1.42 (s, 2H), 1.29-1.26 (m, 2H), 1.18 (s, 1H), 0.87 (t, J = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 180.2, 178.7, 177.4, 177.3, 174.7, 173.6, 143.2, 139.9, 139.5, 138.4, 136.9, 135.4, 135.2, 131.8, 131.1, 130.6, 129.2, 128.9 (2), 128.8, 128.7, 128.6, 128.4, 128.3, 128.1, 128.0, 122.5, 120.3, 119.0, 115.0, 63.8, 63.1, 53.7, 53.4, 53.0, 52.6, 46.5, 44.9, 42.7, 42.3, 38.9, 35.3, 33.2, 30.1, 29.2, 26.9, 26.0, 25.3, 23.3, 22.5, 22.3 (2), 17.0, 16.9, 13.9; HRMS *m/z* (ESI) calcd for $C_{38}H_{39}N_3NaO_3$ ($[M+Na]^+$) 608.2884, found 608.2875.

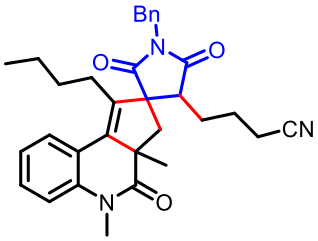


4-(1'-Benzyl-1-(4-bromophenyl)-3a,5-dimethyl-2',4,5'-trioxo-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4v). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (2:1, v/v). Yellow oil (76.5 mg, 63% yield, d.r. = 1:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.37 (s, 2H), 7.31-7.28 (m, 1H), 7.22-7.18 (m, 3H), 7.07-6.97 (m, 4H), 6.84-6.77 (m, 1H), 6.71-6.67 (m, 2H), 4.80-4.63 (m, 1H), 4.41-4.31 (m, 1H), 3.43 (s, 1.5H), 3.41 (s, 1.5H), 3.40-3.37 (m, 1H), 2.95-2.88 (m, 1H), 2.55-2.44 (m, 1H), 2.38-2.21 (m, 2H), 1.95-1.80 (m, 2H), 1.78-1.62 (m, 2H), 1.49 (s, 1.5H), 1.37 (s, 1.5H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 180.0, 178.4, 177.2, 176.9, 174.4, 173.4, 140.8, 140.0, 138.9, 138.5,

135.4, 135.1, 135.0, 132.9, 132.5, 132.1, 130.6, 129.6, 129.0, 128.9, 128.8, 128.7, 128.5, 128.3, 127.7, 122.7, 122.5, 119.8, 118.8, 118.5, 115.4, 115.2, 63.7, 62.9, 53.6, 53.0, 46.4, 45.2, 42.8, 42.4, 38.9, 36.9, 30.1, 27.9, 27.0, 26.0, 25.4, 23.4, 22.5, 17.0; HRMS *m/z* (ESI) calcd for $C_{34}H_{30}BrN_3NaO_3$ ([M+Na]$^+$) 630.1363, found 630.1354.

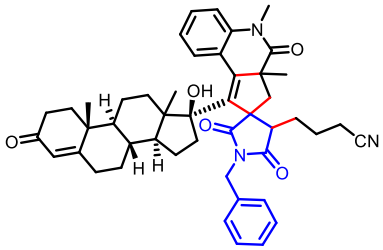


4-(1'-Benzyl-3a,5-dimethyl-2',4,5'-trioxo-1-(thiophen-2-yl)-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4w). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (2:1, v/v). Yellow oil (67.5 mg, 63% yield, d.r. = 9:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.39-7.33 (m, 6H), 7.30-7.28 (m, 2H), 7.06-7.02 (m, 2H), 6.89-6.85 (m, 2H), 4.77-4.65 (m, 2H), 3.43 (s, 2.7H), 3.42 (s, 0.3H), 3.23-3.13 (m, 1H), 2.93-2.88 (m, 1H), 2.72-2.68 (m, 1H), 2.46-2.31 (m, 2H), 1.83-1.77 (m, 2H), 1.64-1.56 (m, 2H), 1.48 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 180.1, 179.7, 177.4, 177.2, 174.3, 174.2, 142.6, 140.0, 135.4, 133.7, 129.8, 129.7, 129.5, 129.3, 128.7 (2), 128.6, 128.5, 128.1, 127.9, 127.7, 127.6, 127.2, 127.1, 122.7, 122.6, 119.9, 119.0, 118.8, 115.2, 115.1, 63.6, 63.4, 53.7, 53.3, 46.7, 45.3, 43.3, 42.8, 39.1, 38.5, 30.1, 29.6, 26.2, 25.4, 23.4, 22.6, 17.0, 14.1; HRMS *m/z* (ESI) calcd for $C_{32}H_{29}N_3NaO_3S$ ([M+Na]$^+$) 558.1822, found 558.1814.



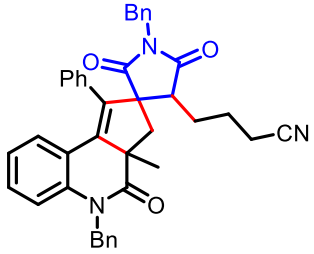
4-(1'-Benzyl-1-butyl-3a,5-dimethyl-2',4,5'-trioxo-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4x). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (3:1, v/v). Yellow oil (71.3 mg, 70% yield, d.r. > 20:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.41-7.36 (m, 4H),

7.33-7.29 (m, 3H), 7.15-7.07 (m, 2H), 4.72-4.65 (m, 2H), 3.38 (s, 3H), 2.87 (t, *J* = 7.2 Hz, 1H), 2.81 (t, *J* = 7.2 Hz, 1H), 2.43-2.36 (m, 3H), 1.95-1.91 (m, 2H), 1.66-1.51 (m, 2H), 1.34 (s, 3H), 1.31-1.08 (m, 6H), 0.79 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) *δ*: 180.4, 177.5, 175.0, 139.6, 138.4, 137.6, 135.4, 129.0, 128.7, 128.1, 127.2, 123.0, 122.0, 121.4, 119.0, 115.1, 61.9, 52.9, 45.1, 42.8, 38.7, 30.8, 30.1, 26.1, 26.0, 25.5, 23.5, 23.0, 17.1, 13.6; HRMS *m/z* (ESI) calcd for $C_{32}H_{35}N_3NaO_3$ ($[M+Na]^+$) 532.2571, found 532.2563.

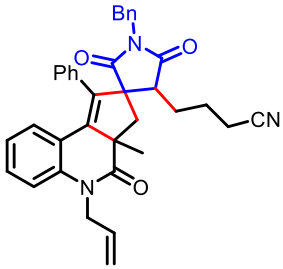


4-(1'-Benzyl-1-((8*R*,9*S*,10*R*,14*S*,17*S*)-17-hydroxy-10,13-dimethyl-3-oxo-2,3,6,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[*a*]phenanthren-17-yl)-3a,5-dimethyl-2',4,5'-trioxo-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4y). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (2:1, v/v). Yellow oil (88.7 mg, 60% yield, d.r. > 20:1); ^{1}H NMR (400 MHz, $CDCl_3$) *δ*: 8.14 (d, *J* = 8.4 Hz, 1H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.51 (d, *J* = 8.0 Hz, 1H), 7.44 (t, *J* = 8.0 Hz, 1H), 7.32 (s, 1H), 7.20-7.15 (m, 4H), 5.70 (s, 1H), 3.71 (s, 2H), 3.16 (s, 3H), 2.43-2.26 (m, 6H), 2.17-2.10 (m, 5H), 1.95-1.80 (m, 4H), 1.70-1.55 (m, 5H), 1.44-1.32 (m, 4H), 1.19 (s, 6H), 1.16 (s, 3H), 1.09-0.98 (m, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) *δ*: 199.7, 171.2, 168.1, 162.7, 160.2, 146.1, 138.8, 130.4, 129.2, 128.8, 127.1, 126.7, 125.5, 125.4, 123.6, 122.1, 120.3, 114.2, 111.0, 60.0, 53.4, 49.0, 39.5, 38.7, 35.4, 34.6, 34.5, 34.3, 33.9, 33.0,

32.8, 31.9, 31.1, 29.9, 29.7 (2), 29.5, 29.3, 27.2, 20.3, 20.0, 18.7, 17.4, 14.8; HRMS *m/z* (ESI) calcd for $C_{47}H_{53}N_3NaO_5$ ([M+Na]$^+$) 762.3877, found 762.3869.

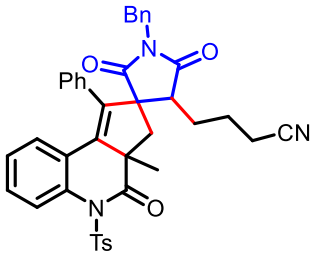


4-(1',5-Dibenzyl-3a-methyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4z). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (2:1, v/v). Yellow oil (75.1 mg, 62% yield, d.r. = 2:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.38-7.32 (m, 7H), 7.21-7.17 (m, 3H), 7.12-7.01 (m, 4H), 6.95-6.77 (m, 4H), 6.74-6.70 (m, 1H), 5.65 (d, *J* = 16.0 Hz, 1H), 4.80 (d, *J* = 8.8 Hz, 1H), 4.76 (d, *J* = 6.4 Hz, 1H), 4.67 (d, *J* = 14.0 Hz, 1H), 2.96 (t, *J* = 6.8 Hz, 1H), 2.67-2.60 (m, 1H), 2.48-2.36 (m, 1H), 2.25-2.17 (m, 2H), 1.85-1.75 (m, 2H), 1.64 (s, 2H), 1.62-1.58 (m, 2H), 1.51 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 180.2, 178.6, 177.4, 177.2, 174.8, 173.8, 139.9, 139.6, 139.5, 139.1, 138.4, 137.0, 136.9, 135.4, 135.2, 133.7, 133.3, 129.4, 129.3, 129.2, 128.9 (2), 128.8, 128.7 (2), 128.6, 128.5, 128.3, 128.2, 128.1, 127.7, 127.2, 127.1, 126.2, 126.0, 122.8, 122.6, 120.4, 118.9, 118.8, 115.9, 115.8, 63.9, 63.1, 53.7, 53.3, 46.7, 46.4, 45.0, 42.8, 42.4, 38.8, 36.9, 29.7, 27.7, 27.0, 26.1, 25.3, 23.4, 22.7, 17.0, 16.9; HRMS *m/z* (ESI) calcd for $C_{40}H_{35}N_3NaO_3$ ([M+Na]$^+$) 628.2571, found 628.2562.



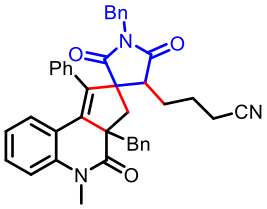
4-(5-Allyl-1'-benzyl-3a-methyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4aa). The product was purified by silica gel column chromatography with petroleum

ether/ethyl acetate (2:1, v/v). Yellow oil (80.0 mg, 72% yield, d.r. = 2:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.38-7.34 (m, 4H), 7.21-7.12 (m, 4H), 7.10-6.98 (m, 3H), 6.84-6.79 (m, 2H), 6.73 (t, J = 8.0 Hz, 1H), 5.96-5.88 (m, 1H), 5.23-5.15 (m, 2H), 5.01-4.93 (m, 1H), 4.79-4.63 (m, 2H), 4.28-4.20 (m, 1H), 2.96-2.91 (m, 1H), 2.66-2.58 (m, 1H), 2.49-2.27 (m, 1H), 2.26-2.17 (m, 2H), 1.80-1.70 (m, 2H), 1.66-1.58 (m, 2H), 1.56 (s, 2H), 1.42 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 180.2, 178.5, 177.3, 177.2, 174.2, 173.2, 139.9, 139.3, 139.0, 138.2, 136.9, 135.4, 135.1, 133.6, 132.3, 132.2, 129.3, 129.1, 128.9, 128.7, 128.6, 128.5, 128.4, 128.3, 128.1 (2), 127.7, 127.1, 122.7, 122.5, 120.3, 120.2, 118.9, 118.8, 116.0, 115.7, 115.6, 63.8, 63.1, 53.5, 53.1, 46.4, 45.3, 45.0, 42.8, 42.4, 38.8, 36.8, 27.7, 26.9, 26.0, 25.3, 23.3, 22.6, 17.0, 16.9; HRMS *m/z* (ESI) calcd for $C_{36}H_{33}N_3NaO_3$ ($[M+Na]^+$) 578.2414, found 578.2406.

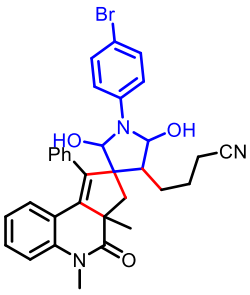


4-(1'-Benzyl-3a-methyl-2',4,5'-trioxo-1-phenyl-5-tosyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4ab). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (2:1, v/v). Yellow oil (76.3 mg, 57% yield, d.r. = 2.3:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.98 (d, J = 8.4 Hz, 1.4H), 7.88 (d, J = 8.4 Hz, 0.6H), 7.78-7.74 (m, 1H), 7.40-7.34 (m, 7H), 7.32-7.30 (m, 2H), 7.22-7.19 (m, 1H), 7.15 (t, J = 7.6 Hz, 1H), 7.02-6.97 (m, 2H), 6.82-6.79 (m, 2H), 4.81-4.66 (m, 0.6H), 4.65-4.55 (m, 1.4H), 2.76-2.71 (m, 1H), 2.47 (s, 3H), 2.40-2.33 (m, 2H), 2.24-2.15 (m, 2H), 1.76-1.58 (m, 2H), 1.49-1.40 (m, 2H), 1.33 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 179.7, 177.4, 176.9, 176.8, 175.3, 145.1, 144.9, 138.7, 138.4, 138.2, 136.9, 136.2,

135.3, 135.2, 135.1, 134.6, 132.5, 130.5, 129.5, 129.3, 129.1, 128.9, 128.8, 128.6, 128.5, 128.4, 128.2 (2), 127.9, 127.5, 127.0, 126.3, 126.1, 125.5, 125.4, 124.4, 123.7 (2), 123.6, 118.8 (2), 64.0, 63.0, 56.7, 55.9, 45.8, 45.1, 42.9, 42.4, 38.7, 37.2, 36.7, 29.7, 27.2, 25.3, 25.0, 24.3, 22.7, 21.7, 17.0, 16.8; HRMS *m/z* (ESI) calcd for $C_{40}H_{35}N_3NaO_5S$ ([M+Na]$^+$) 692.2190, found 692.2181.

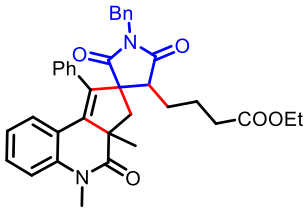


4-(1',3a-Dibenzyl-5-methyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4ac). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (2:1, v/v). Yellow oil (84.7 mg, 70% yield, d.r. = 2:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.41-7.33 (m, 4H), 7.24-7.18 (m, 8H), 7.14-7.09 (m, 4H), 7.02-6.97 (m, 1H), 6.81-6.76 (m, 1H), 6.61 (t, J = 7.6 Hz, 1H), 4.48-4.46 (m, 2H), 3.52-3.48 (m, 2H), 3.44 (s, 1H), 3.43 (s, 2H), 2.76-2.57 (m, 1H), 2.27-2.20 (m, 4H), 1.77-1.72 (m, 2H), 1.30-1.23 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 178.1, 178.0, 177.8 (2), 172.4, 172.2, 139.7, 139.2, 138.9, 138.3 (2), 137.4, 137.2, 135.5, 135.2, 134.0, 133.8, 132.0, 131.9, 131.0, 130.6, 130.3, 129.9, 128.8, 128.7, 128.6, 128.4 (2), 128.2 (2), 127.9, 127.5, 127.0, 126.8, 126.4, 126.3, 122.9, 122.7, 122.5 (2), 118.9, 118.8, 115.1, 114.6 (2), 64.2, 58.6, 46.7, 46.4, 46.3, 45.9, 42.3, 41.9, 36.9, 36.8, 36.3, 30.6, 30.0, 29.4, 27.1, 22.1, 21.9, 17.1, 17.0; HRMS *m/z* (ESI) calcd for $C_{40}H_{35}N_3NaO_3$ ([M+Na]$^+$) 628.2571, found 628.2562.



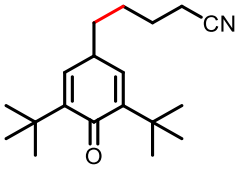
4-(1'-(4-Bromophenyl)-2',5'-dihydroxy-3a,5-dimethyl-4-oxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (5a). The product was

purified by silica gel column chromatography with petroleum ether/ethyl acetate (2:1, v/v). Yellow oil (77.6 mg, 65% yield, d.r. = 4:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.56-7.50 (m, 2H), 7.45-7.38 (m, 3H), 7.18 (d, J = 7.2 Hz, 2H), 7.01-6.92 (m, 3H), 6.79-6.70 (m, 3H), 5.32 (d, J = 5.2 Hz, 1H), 5.29-4.83 (m, 1H), 3.35 (t, J = 2.8 Hz, 1H), 3.32 (d, J = 6.4 Hz, 3H), 3.26-3.20 (m, 1H), 2.85-2.80 (m, 1H), 2.35-2.25 (m, 1H), 2.21 (d, J = 14.4 Hz, 1H), 1.99-1.91 (m, 2H), 1.82-1.76 (m, 1H), 1.64-1.58 (m, 1H), 1.37 (s, 2.4H), 1.33 (s, 0.6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 177.3, 176.0, 139.7 (2), 139.6, 138.8, 138.1, 137.6, 137.3, 135.3, 135.1, 134.7, 134.4, 132.4, 132.0 (2), 131.9, 131.8, 131.5, 129.9, 129.5, 129.1 (2), 129.0, 128.8, 128.6, 128.3 (2), 128.2, 128.0, 125.5, 125.4, 124.9, 123.9, 123.7, 122.8, 120.7 (2), 119.5, 119.4, 118.8, 115.1 (2), 86.1, 83.4, 83.0, 64.4, 63.6, 53.6, 53.4, 46.1, 42.7, 40.2, 38.2, 30.3, 30.1, 27.5, 26.5, 26.2, 26.0, 23.5, 23.0, 17.1, 16.9.

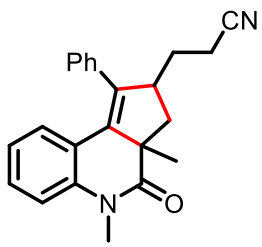


Ethyl 4-(1'-benzyl-3a,5-dimethyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanoate (6a). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (1:1, v/v). White solid (96.8 mg, 84% yield, d.r. = 2:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.56 (s, 4H), 7.51-7.44 (m, 4H), 7.42-7.33 (m, 2H), 7.22 (t, J = 7.6 Hz, 1H), 7.03 (d, J = 7.2 Hz, 1H), 6.98-6.89 (m, 2H), 4.97-4.84 (m, 2H), 4.79-4.31 (m, 2H), 3.64 (s, 2H), 3.62 (s, 1H), 3.42-3.04 (m, 2H), 2.87-2.77 (m, 1H), 2.60-2.39 (m, 2H), 2.34-2.12 (m, 2H), 1.97 (s, 2H), 1.77 (s, 1H), 1.71 (s, 2H), 1.45 (t, J = 6.8 Hz, 1H), 1.05 (t, J = 7.6 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 180.1, 179.7, 178.5, 177.3, 177.1, 175.3, 174.5,

173.5, 139.9, 139.4, 138.2, 136.7, 135.4, 135.1, 133.6, 133.2, 129.4, 129.3, 129.2, 129.0, 128.9 (2), 128.7, 128.6, 128.5, 128.4, 128.3, 128.0 (3), 127.7, 127.1, 122.5, 122.4, 120.1, 118.9, 118.8, 115.0, 114.9, 63.7, 63.1, 62.9, 62.5, 53.5, 53.0, 46.5, 45.0, 42.7, 40.9, 38.9, 36.9, 30.1, 27.9, 26.0, 25.3, 23.3, 22.5, 16.9 (2).



5-(3,5-Di-*tert*-butyl-4-oxocyclohexa-2,5-dien-1-yl)pentanenitrile (7a).[3] The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (10:1, v/v), 29.9 mg, 52% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 6.40 (s, 2H), 2.30 (t, J = 7.2 Hz, 2H), 1.77-1.73 (m, 2H), 1.44-1.25 (m, 5H), 1.23 (s, 18H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 186.2, 147.2, 145.4, 119.2, 39.7, 39.5, 34.6, 29.4, 27.2, 20.8, 17.3.



3-(3a,5-Dimethyl-4-oxo-1-phenyl-3,3a,4,5-tetrahydro-2*H*-cyclopenta[*c*]quinolin-2-yl)propanenitrile (8a).[1] The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (2:1, v/v), 38.3 mg, 56% yield, d.r. = 2:1; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.29 (d, J = 7.6 Hz, 2H), 7.24-7.17 (m, 1H), 7.13 (t, J = 8.4 Hz, 3H), 6.98 (d, J = 8.0 Hz, 1H), 6.93 (t, J = 7.2 Hz, 1H), 6.70 (t, J = 7.6 Hz, 1H), 3.34 (s, 1H), 3.32 (s, 2H), 2.96-2.91 (m, 1H), 2.38-2.32 (m, 1H), 2.28-2.11 (m, 2H), 2.09-2.00 (m, 1H), 1.74-1.60 (m, 2H), 1.26 (s, 2H), 1.17 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 175.1, 174.9, 141.9, 140.3, 140.1, 139.5, 136.7, 135.7, 135.5, 134.8, 128.9, 128.7, 128.6 (3), 128.1, 127.7 (2), 127.6, 127.2, 122.5, 122.4, 121.3, 120.8, 119.4, 119.3, 115.1, 114.8, 53.8, 52.7, 49.8, 45.0, 39.9, 37.6, 31.0, 30.1, 29.9, 29.6, 27.6, 23.5, 16.0, 14.8.

(D) Density functional theory calculations

All data in this study were calculated with the Gaussian 16 software package[4] and were optimized at the B3LYP level of density functional theory (DFT).[5] The basis set 6-31G (d) was selected for C, H, O, N and F atoms. Vibrational frequency analysis was computed to ensure the points that the minimum have no imaginary frequency and the transition states have only one imaginary frequency. In order to consider the solvent effects, the solvation corrected single-point energy calculations (based on the gas-phase optimized geometries) were calculated by using the M06 method in conjunction with the SMD solvation model[6] in solvent (DCE). In the solvation-corrected calculations, 6-311++G (d, p) basis set was chosen for all nonmetal atoms. The single-point energy corrected relative free energies in kcal/mol are used for discussion throughout the text.

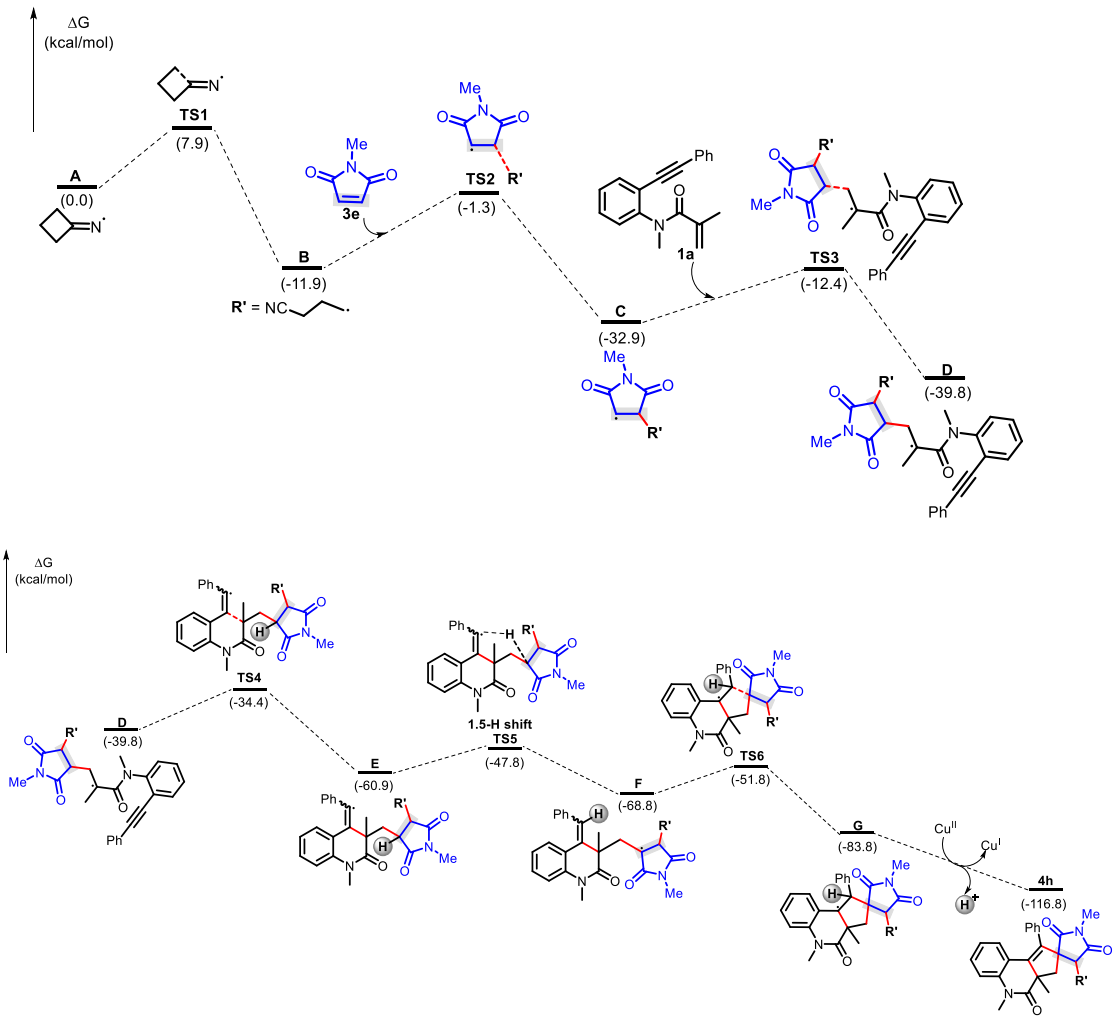


Figure 1. Proposed reaction mechanisms with DFT calculations.

Table 1. XYZ Coordinates.

1a			
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6	-1.137814000	-3.133253000	0.322067000
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6	-3.517282000	-2.767846000	0.136121000
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1	-0.292921000	-3.787433000	0.513002000
1	-2.610004000	-4.673293000	0.593547000
1	-4.535009000	-3.145080000	0.180287000
7	-1.755472000	0.448224000	-0.574541000
6	-2.167364000	1.434282000	0.305304000
8	-2.807217000	1.172204000	1.318888000

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1	-3.288143000	3.713292000	1.300696000
1	-2.493405000	4.899078000	0.228184000
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6	1.602419000	-0.897038000	0.056870000
6	2.953532000	-0.441162000	0.085338000
6	3.254723000	0.889974000	0.438724000
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6	4.575550000	1.330374000	0.463170000
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1	6.645973000	0.803372000	0.159006000
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1	-1.373298000	1.725563000	-2.200003000
1	-0.247835000	0.356142000	-2.068771000

2a

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A			
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B			
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C			
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1	-3.262357000	-0.256904000	1.659676000
7	-5.673607000	0.664757000	-0.153905000
6	-2.220000000	0.050382000	-0.232807000
1	-2.403502000	-0.153697000	-1.294972000
1	-2.154626000	1.139810000	-0.127168000
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1	-0.724595000	-0.403387000	1.271665000
1	4.654948000	-0.128307000	-0.265573000

TS1

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7	2.025192000	0.201105000	-0.096712000

TS2

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6	-1.014419000	1.175566000	1.019679000
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6	1.044416000	-0.867731000	-0.285236000
1	0.906964000	-1.910187000	-0.011708000
1	0.558036000	-0.555354000	-1.206094000
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TS3

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6	-3.407857000	0.305423000	-0.905777000
6	-1.936344000	0.053086000	-1.163216000

6	-1.286373000	1.362044000	-1.299451000
1	-3.919992000	0.250353000	-1.883559000
1	-1.619239000	-0.751431000	-1.813024000
7	-2.194158000	2.325076000	-0.824440000
8	-0.161853000	1.639590000	-1.700197000
8	-4.361885000	2.411753000	-0.021116000
6	-1.857851000	3.732225000	-0.685840000
1	-1.576124000	4.148428000	-1.657355000
1	-2.739085000	4.244754000	-0.297965000
6	-7.901349000	-1.316204000	0.776743000
6	-6.444377000	-1.385960000	0.923993000
1	-6.135576000	-2.431328000	0.791576000
1	-6.186836000	-1.108892000	1.954263000
7	-9.052598000	-1.254407000	0.642933000
6	-5.704044000	-0.472573000	-0.075261000
1	-6.012278000	-0.734173000	-1.095622000
1	-5.992459000	0.568462000	0.092390000
6	-4.181167000	-0.614710000	0.058012000
1	-3.889431000	-1.652574000	-0.145281000
1	-3.882531000	-0.398914000	1.091610000
1	-1.018316000	3.854466000	0.004946000
6	3.430716000	-3.844660000	-0.513593000
6	3.081466000	-2.503271000	-0.349120000
6	4.085279000	-1.528806000	-0.153172000
6	5.434054000	-1.944655000	-0.143257000
6	5.770777000	-3.282890000	-0.310500000
6	4.767381000	-4.238549000	-0.492647000
1	2.641800000	-4.577405000	-0.645665000
1	6.205779000	-1.195520000	0.002518000
1	6.815158000	-3.581698000	-0.296295000
1	5.023900000	-5.286551000	-0.618197000
7	1.700843000	-2.109644000	-0.403132000
6	0.872325000	-2.525092000	0.614487000
8	1.252498000	-3.293006000	1.496958000
6	-0.530969000	-1.981182000	0.738099000
6	-0.794522000	-0.625669000	0.684885000
1	0.022687000	0.067396000	0.513497000
1	-1.628782000	-0.240035000	1.263678000
6	-1.552483000	-2.982383000	1.202420000
1	-1.096149000	-3.656598000	1.932399000
1	-2.421845000	-2.495359000	1.652322000
1	-1.907441000	-3.605992000	0.367943000
6	3.780272000	-0.150135000	0.046368000
6	3.614008000	1.042350000	0.223043000

6	3.465089000	2.443038000	0.454339000
6	2.417518000	3.173313000	-0.142664000
6	4.384967000	3.117712000	1.283408000
6	2.303830000	4.542854000	0.089430000
1	1.704508000	2.665013000	-0.783879000
6	4.257742000	4.485507000	1.510589000
1	5.192212000	2.556137000	1.743633000
6	3.217758000	5.203681000	0.914437000
1	1.498995000	5.099613000	-0.383923000
1	4.972680000	4.992619000	2.152917000
1	3.122392000	6.271841000	1.089963000
6	1.230997000	-1.482491000	-1.645072000
1	1.889990000	-1.800876000	-2.456874000
1	0.223187000	-1.836561000	-1.876031000
1	1.224441000	-0.390252000	-1.602418000

D

6	-3.466150000	-2.627212000	-0.087703000
6	-2.612554000	-1.591333000	0.654286000
6	-1.159015000	-2.123635000	0.472249000
6	-1.273506000	-3.126698000	-0.680392000
1	-2.910623000	-1.600609000	1.708302000
1	-0.927101000	-2.751808000	1.344508000
7	-2.619420000	-3.408314000	-0.874583000
8	-0.366176000	-3.644777000	-1.300727000
8	-4.674979000	-2.748001000	-0.057109000
6	-3.091023000	-4.425474000	-1.802884000
1	-2.620239000	-5.385235000	-1.574582000
1	-4.173316000	-4.497404000	-1.690081000
6	-5.816691000	2.320862000	0.119791000
6	-4.530796000	1.723661000	-0.252073000
1	-3.730947000	2.424432000	0.020937000
1	-4.498146000	1.625871000	-1.344847000
7	-6.834091000	2.787567000	0.427204000
6	-4.297609000	0.349470000	0.411624000
1	-4.408469000	0.449638000	1.498484000
1	-5.063596000	-0.356988000	0.081273000
6	-2.893544000	-0.179738000	0.086064000
1	-2.155115000	0.518246000	0.497088000
1	-2.737934000	-0.185047000	-1.002487000
1	-2.837276000	-4.146820000	-2.829657000
6	5.409538000	-1.285291000	0.100078000
6	4.202273000	-0.575270000	0.082941000
6	4.180092000	0.717417000	-0.513446000
6	5.369748000	1.246031000	-1.046342000

6	6.560033000	0.525964000	-1.017071000
6	6.574538000	-0.745651000	-0.444511000
1	5.447068000	-2.268922000	0.554462000
1	5.335858000	2.234540000	-1.493639000
1	7.464769000	0.952377000	-1.440049000
1	7.494905000	-1.322112000	-0.411014000
7	3.002655000	-1.161862000	0.559694000
6	2.196664000	-0.443451000	1.478750000
8	2.659943000	0.452984000	2.184830000
6	0.760931000	-0.749164000	1.513076000
6	0.022581000	-1.148590000	0.262998000
1	0.709991000	-1.600060000	-0.455322000
1	-0.334976000	-0.231223000	-0.229296000
6	-0.003752000	-0.294189000	2.716707000
1	0.671045000	-0.059928000	3.542097000
1	-0.582517000	0.617657000	2.497414000
1	-0.728398000	-1.050669000	3.047769000
6	2.982892000	1.483575000	-0.599329000
6	1.974241000	2.160411000	-0.656564000
6	0.784362000	2.945511000	-0.583322000
6	0.184501000	3.490447000	-1.735347000
6	0.195071000	3.190999000	0.675636000
6	-0.972648000	4.259729000	-1.629368000
1	0.636848000	3.306743000	-2.705134000
6	-0.961606000	3.962360000	0.771893000
1	0.672040000	2.781592000	1.561160000
6	-1.549414000	4.499806000	-0.378582000
1	-1.422678000	4.679725000	-2.524909000
1	-1.397493000	4.158795000	1.748058000
1	-2.443182000	5.112950000	-0.299049000
6	2.913776000	-2.624271000	0.554936000
1	3.545487000	-3.079081000	1.330999000
1	1.886247000	-2.934972000	0.742150000
1	3.215832000	-3.012736000	-0.421370000

TS4

6	-4.114953000	-0.983826000	0.476397000
6	-2.835905000	-0.166344000	0.693394000
6	-1.705642000	-1.220766000	0.505649000
6	-2.390532000	-2.363653000	-0.254027000
1	-2.849047000	0.227517000	1.714985000
1	-1.494878000	-1.649815000	1.496429000
7	-3.767532000	-2.183094000	-0.137115000
8	-1.860874000	-3.297240000	-0.821248000
8	-5.259822000	-0.659194000	0.726070000

6	-4.753306000	-3.147777000	-0.600828000
1	-5.352680000	-3.505955000	0.240796000
1	-5.421085000	-2.682608000	-1.331145000
6	-4.806298000	4.300378000	-0.719437000
6	-3.832195000	3.242703000	-1.005439000
1	-2.831499000	3.694040000	-1.025365000
1	-4.025107000	2.860608000	-2.016271000
7	-5.578999000	5.132941000	-0.480835000
6	-3.883902000	2.090468000	0.020335000
1	-3.716678000	2.496933000	1.025354000
1	-4.881510000	1.643476000	0.025694000
6	-2.818323000	1.029036000	-0.289042000
1	-1.829763000	1.498817000	-0.246798000
1	-2.943295000	0.660916000	-1.317932000
1	-4.212260000	-3.976155000	-1.059539000
6	2.489120000	-3.816245000	-0.637722000
6	2.350566000	-2.533087000	-0.085122000
6	2.666336000	-1.408432000	-0.890655000
6	3.094033000	-1.613521000	-2.214523000
6	3.228302000	-2.891896000	-2.746370000
6	2.923337000	-3.995518000	-1.949062000
1	2.238218000	-4.683939000	-0.038657000
1	3.328867000	-0.739733000	-2.814185000
1	3.565614000	-3.023210000	-3.770113000
1	3.012658000	-5.002457000	-2.346721000
7	1.960507000	-2.398505000	1.266469000
6	1.309381000	-1.280826000	1.797904000
8	1.238737000	-1.113305000	3.017764000
6	0.663083000	-0.317691000	0.874241000
6	-0.341733000	-0.841242000	-0.132430000
1	0.024407000	-1.752733000	-0.610627000
1	-0.487248000	-0.105732000	-0.931486000
6	0.416007000	1.040750000	1.468424000
1	-0.477028000	1.038408000	2.110386000
1	1.251336000	1.358562000	2.095564000
1	0.266833000	1.789081000	0.682508000
6	2.569298000	-0.057005000	-0.400265000
6	2.925126000	1.127449000	-0.366498000
6	3.221704000	2.500822000	-0.204658000
6	2.804376000	3.448636000	-1.168706000
6	3.955929000	2.953366000	0.917113000
6	3.107079000	4.796714000	-1.008333000
1	2.246762000	3.108633000	-2.036243000
6	4.251166000	4.304305000	1.066086000

1	4.284179000	2.231363000	1.658337000
6	3.829445000	5.231559000	0.107581000
1	2.779571000	5.513284000	-1.756749000
1	4.813535000	4.637427000	1.934069000
1	4.063253000	6.285461000	0.228645000
6	2.353363000	-3.447152000	2.212386000
1	3.371471000	-3.781231000	1.994551000
1	2.307563000	-3.020450000	3.213020000
1	1.676477000	-4.309230000	2.162809000

E

6	-4.026227000	-1.391436000	0.126693000
6	-2.850745000	-0.499337000	0.544277000
6	-1.604920000	-1.401682000	0.291230000
6	-2.130019000	-2.495895000	-0.642714000
1	-2.963104000	-0.271462000	1.609548000
1	-1.396036000	-1.930332000	1.231800000
7	-3.520107000	-2.467030000	-0.599300000
8	-1.484501000	-3.298490000	-1.286765000
8	-5.209441000	-1.199735000	0.332222000
6	-4.353897000	-3.463955000	-1.253237000
1	-4.097882000	-4.462797000	-0.889685000
1	-5.392568000	-3.230607000	-1.016477000
6	-5.194795000	3.929260000	-0.315869000
6	-4.097596000	3.028774000	-0.682821000
1	-3.151214000	3.569736000	-0.551311000
1	-4.183042000	2.799958000	-1.753045000
7	-6.065289000	4.635303000	-0.014327000
6	-4.093700000	1.725025000	0.143602000
1	-4.035504000	1.976000000	1.209835000
1	-5.036588000	1.191501000	-0.000909000
6	-2.904464000	0.832751000	-0.240445000
1	-1.976715000	1.384422000	-0.050405000
1	-2.925318000	0.624086000	-1.320197000
1	-4.197414000	-3.435563000	-2.335359000
6	3.639976000	-3.203587000	-0.635703000
6	2.850051000	-2.225496000	-0.012005000
6	2.847833000	-0.909397000	-0.522480000
6	3.637685000	-0.610135000	-1.638906000
6	4.425436000	-1.580744000	-2.251290000
6	4.419721000	-2.880953000	-1.745134000
1	3.646287000	-4.220835000	-0.264175000
1	3.620959000	0.405967000	-2.022750000
1	5.028921000	-1.327474000	-3.117787000
1	5.019695000	-3.655482000	-2.214465000

7	2.090825000	-2.539412000	1.139971000
6	1.113090000	-1.707775000	1.655563000
8	0.480361000	-2.011406000	2.664268000
6	0.773084000	-0.421922000	0.880247000
6	-0.276857000	-0.809783000	-0.219961000
1	0.173186000	-1.556620000	-0.882542000
1	-0.450373000	0.080549000	-0.833039000
6	0.206839000	0.611446000	1.864235000
1	-0.652704000	0.208283000	2.401706000
1	0.959876000	0.889765000	2.607634000
1	-0.089201000	1.520375000	1.331537000
6	2.019501000	0.117363000	0.155569000
6	2.302242000	1.398468000	0.106669000
6	2.640363000	2.729015000	0.041294000
6	2.154308000	3.569262000	-1.016010000
6	3.486228000	3.331213000	1.031839000
6	2.496683000	4.909828000	-1.066673000
1	1.514266000	3.132600000	-1.776876000
6	3.814167000	4.674048000	0.956899000
1	3.864629000	2.712260000	1.839305000
6	3.326206000	5.476608000	-0.086434000
1	2.118018000	5.527707000	-1.876810000
1	4.457185000	5.109376000	1.717366000
1	3.588855000	6.529117000	-0.134987000
6	2.316882000	-3.815002000	1.821164000
1	3.383384000	-3.945384000	2.027886000
1	1.757469000	-3.792367000	2.753871000
1	1.963110000	-4.653497000	1.210509000

TS5

6	-3.206647000	1.135691000	0.898860000
6	-2.450816000	0.093125000	0.069004000
6	-1.186091000	-0.178311000	0.904926000
6	-1.486820000	0.358626000	2.269105000
1	-2.200823000	0.534208000	-0.904457000
1	-0.309560000	0.619229000	0.451988000
7	-2.622012000	1.174435000	2.158459000
8	-0.877349000	0.210537000	3.316130000
8	-4.175659000	1.791107000	0.562934000
6	-3.128508000	1.972001000	3.262713000
1	-2.356502000	2.662233000	3.614707000
1	-3.992902000	2.527850000	2.897337000
6	-6.480582000	-1.890326000	-2.305806000
6	-5.404468000	-2.103710000	-1.333221000
1	-4.807352000	-2.963525000	-1.664284000

1	-5.856703000	-2.386061000	-0.373801000
7	-7.324672000	-1.708749000	-3.081581000
6	-4.507707000	-0.859931000	-1.155928000
1	-4.095517000	-0.572648000	-2.131223000
1	-5.108483000	-0.015475000	-0.807332000
6	-3.360703000	-1.139523000	-0.174868000
1	-2.745708000	-1.958475000	-0.566446000
1	-3.763276000	-1.488379000	0.786761000
1	-3.419832000	1.324323000	4.094639000
6	5.150398000	-1.536319000	-0.559593000
6	3.770386000	-1.461620000	-0.316500000
6	3.176576000	-0.204420000	-0.056602000
6	3.992132000	0.934452000	-0.026494000
6	5.361522000	0.855728000	-0.266918000
6	5.936693000	-0.385603000	-0.536502000
1	5.618974000	-2.492181000	-0.759235000
1	3.538356000	1.893335000	0.197790000
1	5.971791000	1.753297000	-0.235909000
1	7.003805000	-0.468292000	-0.722992000
7	2.971581000	-2.625189000	-0.362582000
6	1.670411000	-2.666507000	0.114059000
8	0.991121000	-3.682583000	0.030430000
6	1.130600000	-1.409105000	0.828258000
6	-0.425875000	-1.488938000	0.737595000
1	-0.769633000	-2.240430000	1.455564000
1	-0.666552000	-1.888110000	-0.251144000
6	1.618293000	-1.521219000	2.302744000
1	1.317895000	-2.490141000	2.716045000
1	2.707449000	-1.438503000	2.368374000
1	1.158229000	-0.734272000	2.903380000
6	1.715021000	-0.145242000	0.188600000
6	0.965144000	0.927724000	-0.067226000
6	1.063709000	2.220570000	-0.694975000
6	1.203474000	2.332364000	-2.098321000
6	0.939901000	3.407372000	0.064373000
6	1.243516000	3.582343000	-2.708419000
1	1.287981000	1.427430000	-2.692637000
6	0.979615000	4.652928000	-0.555090000
1	0.819526000	3.335037000	1.141900000
6	1.131507000	4.747279000	-1.942399000
1	1.360576000	3.650017000	-3.786704000
1	0.889854000	5.554714000	0.044550000
1	1.157832000	5.721009000	-2.423227000
6	3.525212000	-3.860013000	-0.918095000

1	4.300264000	-4.274913000	-0.263163000
1	2.709397000	-4.575127000	-1.000615000
1	3.956379000	-3.668607000	-1.905572000

F

6	3.431893000	1.635771000	1.095258000
6	2.444502000	0.807835000	0.255387000
6	1.443724000	1.829512000	-0.212613000
6	1.864024000	3.144121000	0.259850000
1	1.977349000	0.066336000	0.921179000
1	0.425380000	-0.801657000	-0.482112000
7	3.029967000	2.958641000	1.034080000
8	1.352203000	4.239411000	0.062212000
8	4.408520000	1.225107000	1.696536000
6	3.727565000	4.054962000	1.682066000
1	3.054381000	4.574124000	2.370372000
1	4.573102000	3.633200000	2.226882000
6	5.536169000	-2.987774000	-1.106432000
6	4.765996000	-1.820537000	-1.546697000
1	4.056199000	-2.148317000	-2.317569000
1	5.452840000	-1.113988000	-2.029953000
7	6.135215000	-3.912820000	-0.742270000
6	4.021399000	-1.131420000	-0.383806000
1	3.375292000	-1.866924000	0.111856000
1	4.738196000	-0.781946000	0.363894000
6	3.173217000	0.044858000	-0.884925000
1	2.421823000	-0.322230000	-1.596295000
1	3.800269000	0.755286000	-1.440222000
1	4.080376000	4.772716000	0.935445000
6	-5.164291000	0.481694000	0.358900000
6	-3.843937000	0.578871000	-0.101763000
6	-2.822520000	-0.164527000	0.530358000
6	-3.145525000	-0.942115000	1.648934000
6	-4.456589000	-1.030029000	2.113533000
6	-5.465014000	-0.323255000	1.457808000
1	-5.956127000	1.042229000	-0.124037000
1	-2.352621000	-1.484512000	2.153060000
1	-4.686363000	-1.641525000	2.980913000
1	-6.492124000	-0.382787000	1.806883000
7	-3.512588000	1.396582000	-1.205131000
6	-2.219525000	1.838868000	-1.443565000
8	-1.958978000	2.556476000	-2.399259000
6	-1.137061000	1.419819000	-0.401959000
6	0.250962000	1.655880000	-1.091011000
1	0.126568000	2.580914000	-1.661251000

1	0.420103000	0.855866000	-1.820910000
6	-1.290155000	2.383651000	0.809685000
1	-1.048960000	3.405997000	0.507630000
1	-2.302725000	2.361686000	1.219299000
1	-0.602061000	2.088515000	1.608962000
6	-1.445495000	-0.023025000	0.004306000
6	-0.577288000	-1.046372000	-0.146169000
6	-0.786087000	-2.498394000	0.048709000
6	-1.943892000	-3.164717000	-0.391901000
6	0.244773000	-3.268036000	0.617054000
6	-2.070923000	-4.544766000	-0.246674000
1	-2.739193000	-2.596266000	-0.862535000
6	0.115269000	-4.648084000	0.770265000
1	1.153805000	-2.774504000	0.954450000
6	-1.045984000	-5.292270000	0.339675000
1	-2.971326000	-5.040049000	-0.600463000
1	0.923209000	-5.218954000	1.219813000
1	-1.147625000	-6.368360000	0.450108000
6	-4.568520000	1.870375000	-2.099369000
1	-5.183801000	2.639611000	-1.617291000
1	-4.089847000	2.302013000	-2.976156000
1	-5.208348000	1.033370000	-2.394022000

TS6

6	-0.890405000	2.780854000	-0.197026000
6	-1.242533000	1.308211000	0.060028000
6	-0.056832000	0.811284000	0.868465000
6	0.689907000	1.987588000	1.319766000
1	-1.349431000	0.790644000	-0.901288000
1	0.764477000	0.201859000	-1.755332000
7	0.177295000	3.102810000	0.622656000
8	1.598799000	2.069547000	2.134371000
8	-1.456222000	3.554874000	-0.950276000
6	0.745785000	4.433454000	0.743847000
1	0.655158000	4.790300000	1.774077000
1	1.805438000	4.411801000	0.474670000
6	-6.297227000	1.788037000	-0.164635000
6	-5.129650000	1.522572000	0.681446000
1	-5.262428000	0.538313000	1.149712000
1	-5.117200000	2.258780000	1.495342000
7	-7.212759000	1.993353000	-0.847942000
6	-3.802189000	1.571980000	-0.104502000
1	-3.853299000	0.864294000	-0.941237000
1	-3.664891000	2.565660000	-0.539789000
6	-2.610084000	1.218699000	0.795551000

1	-2.737037000	0.196953000	1.175160000
1	-2.590248000	1.876241000	1.675741000
1	0.195685000	5.090964000	0.069106000
6	-1.197126000	-4.221458000	-1.205028000
6	-0.375743000	-3.366464000	-0.452390000
6	0.244253000	-2.244714000	-1.082906000
6	0.077153000	-2.117667000	-2.485972000
6	-0.730307000	-2.971545000	-3.220224000
6	-1.385507000	-4.020606000	-2.569703000
1	-1.693484000	-5.056350000	-0.728050000
1	0.619739000	-1.337702000	-3.007306000
1	-0.836299000	-2.832687000	-4.291790000
1	-2.024598000	-4.701128000	-3.124829000
7	-0.147197000	-3.639376000	0.905028000
6	0.655436000	-2.845522000	1.717584000
8	0.918793000	-3.188137000	2.862638000
6	1.099210000	-1.473982000	1.190156000
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1	0.114310000	-0.260578000	2.728162000
1	-1.007051000	-0.968241000	1.559526000
6	2.420199000	-1.118256000	1.897163000
1	2.292192000	-1.286140000	2.967444000
1	3.231638000	-1.769347000	1.557189000
1	2.690902000	-0.075984000	1.741146000
6	1.055491000	-1.313308000	-0.326663000
6	1.373630000	-0.058209000	-0.890203000
6	2.622499000	0.727769000	-0.895769000
6	3.882753000	0.187134000	-0.577992000
6	2.588586000	2.039824000	-1.415044000
6	5.044740000	0.946414000	-0.706674000
1	3.955248000	-0.846513000	-0.263138000
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1	1.638133000	2.462370000	-1.730465000
6	4.984550000	2.259268000	-1.175952000
1	6.003346000	0.501449000	-0.453777000
1	3.689703000	3.807497000	-1.942713000
1	5.892074000	2.847403000	-1.279355000
6	-0.677015000	-4.871062000	1.494602000
1	-0.323479000	-5.746024000	0.939429000
1	-0.317317000	-4.919314000	2.519658000
1	-1.772232000	-4.861596000	1.489971000
G			
6	3.194234000	0.540323000	-1.229387000
6	2.245574000	-0.055325000	-0.193362000

6	0.817476000	0.209442000	-0.765097000
6	1.078401000	1.336830000	-1.780848000
1	2.357249000	0.599939000	0.684643000
1	0.113219000	-0.043340000	1.242933000
7	2.445785000	1.404618000	-2.023022000
8	0.273415000	2.029571000	-2.375244000
8	4.388858000	0.351331000	-1.352589000
6	3.019892000	2.264671000	-3.047310000
1	2.835576000	3.314304000	-2.802400000
1	4.091796000	2.066667000	-3.079066000
6	5.346381000	-3.083135000	2.424208000
6	4.195719000	-2.998770000	1.519680000
1	3.337141000	-3.475966000	2.010387000
1	4.415168000	-3.591591000	0.622598000
7	6.254524000	-3.131558000	3.145462000
6	3.855471000	-1.545516000	1.127798000
1	3.687389000	-0.958712000	2.040025000
1	4.704430000	-1.096225000	0.606245000
6	2.607763000	-1.485306000	0.234016000
1	1.756972000	-1.918547000	0.778273000
1	2.761870000	-2.111673000	-0.653642000
1	2.565111000	2.046820000	-4.017316000
6	-4.865967000	-1.366539000	0.972375000
6	-3.634538000	-1.269248000	0.317971000
6	-2.727920000	-0.203519000	0.657713000
6	-3.092655000	0.648078000	1.736064000
6	-4.309738000	0.521045000	2.387288000
6	-5.209968000	-0.473501000	1.990553000
1	-5.562217000	-2.153532000	0.709421000
1	-2.408738000	1.436178000	2.026474000
1	-4.564649000	1.201542000	3.194601000
1	-6.174379000	-0.571154000	2.480459000
7	-3.231622000	-2.272268000	-0.592295000
6	-2.032884000	-2.219572000	-1.292233000
8	-1.579649000	-3.188038000	-1.890287000
6	-1.362135000	-0.848759000	-1.360831000
6	0.170140000	-0.988163000	-1.531619000
1	0.468535000	-1.024218000	-2.583594000
1	0.486670000	-1.934082000	-1.086765000
6	-2.041983000	-0.128412000	-2.568305000
1	-1.914589000	-0.733270000	-3.473540000
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1	-1.589160000	0.851373000	-2.726022000
6	-1.525862000	-0.078656000	-0.078994000

6	-0.223572000	0.548419000	0.373600000
6	-0.222600000	1.999128000	0.848856000
6	-0.948539000	3.004859000	0.191815000
6	0.529451000	2.352137000	1.979531000
6	-0.908082000	4.322241000	0.646493000
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1	1.166866000	3.920705000	3.311028000
1	-0.113925000	5.691288000	2.115790000
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1	-3.457080000	-4.187689000	-1.337686000
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TS7

6	-4.575570000	-1.842847000	-1.516377000
6	-3.591181000	-2.893637000	-1.240003000
1	-3.218602000	-3.286600000	-2.193421000
1	-4.092112000	-3.722287000	-0.725770000
7	-5.324467000	-0.977174000	-1.711918000
6	-2.408173000	-2.358050000	-0.376538000
1	-1.962482000	-1.505724000	-0.901408000
1	-2.822364000	-1.968274000	0.561134000
6	-1.370484000	-3.403081000	-0.102716000
1	-0.704889000	-3.689088000	-0.913688000
1	-1.638664000	-4.222221000	0.561487000
6	4.252886000	0.279955000	-0.806315000
6	2.892839000	0.411962000	-0.517840000
6	2.301722000	1.696879000	-0.480367000
6	3.107538000	2.822012000	-0.750834000
6	4.460679000	2.677751000	-1.036609000
6	5.036181000	1.404752000	-1.060623000
1	4.692586000	-0.710484000	-0.811687000
1	2.650168000	3.806079000	-0.725333000
1	5.066459000	3.556844000	-1.237758000
1	6.093808000	1.286005000	-1.278482000
7	2.077462000	-0.743999000	-0.281549000
6	2.396807000	-1.580125000	0.780713000
8	3.444794000	-1.454485000	1.409697000
6	1.398695000	-2.598332000	1.258981000
6	0.071389000	-2.295521000	1.403287000
1	-0.299832000	-1.310766000	1.135418000

1	-0.522620000	-2.851058000	2.122319000
6	1.992689000	-3.868951000	1.805843000
1	2.822971000	-3.635272000	2.479418000
1	1.244066000	-4.458139000	2.344478000
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6	-0.249032000	2.093195000	0.092963000
6	-1.618797000	2.344210000	0.412748000
6	-2.654098000	1.689893000	-0.284397000
6	-1.957691000	3.253085000	1.435250000
6	-3.988584000	1.929409000	0.036151000
1	-2.403284000	1.000833000	-1.085113000
6	-3.293691000	3.491116000	1.748980000
1	-1.164958000	3.760823000	1.976045000
6	-4.311029000	2.830786000	1.054312000
1	-4.769550000	1.406668000	-0.508796000
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1	-5.351625000	3.018485000	1.304511000
6	1.164937000	-1.110594000	-1.364625000
1	1.712909000	-1.142479000	-2.314597000
1	0.749288000	-2.096659000	-1.168658000
1	0.347460000	-0.388004000	-1.458438000

TS8

6	-4.399066000	-1.059413000	-0.061606000
6	-3.149604000	-0.342471000	0.456182000
6	-2.009019000	-1.373340000	0.201596000
6	-2.610543000	-2.337187000	-0.825604000
1	-3.282265000	-0.155573000	1.526837000
1	-1.897690000	-1.981886000	1.109672000
7	-3.987061000	-2.144363000	-0.837356000
8	-2.030361000	-3.168960000	-1.495676000
8	-5.560092000	-0.739917000	0.104900000
6	-4.898760000	-2.985809000	-1.596354000
1	-4.775134000	-4.031894000	-1.303215000
1	-5.913302000	-2.649661000	-1.378953000
6	-4.627948000	4.494511000	-0.058765000
6	-3.734606000	3.421827000	-0.504906000
1	-2.696862000	3.714809000	-0.296466000
1	-3.822430000	3.331228000	-1.595446000
7	-5.336987000	5.337847000	0.307374000
6	-4.037957000	2.066478000	0.170975000
1	-3.995004000	2.195436000	1.259723000
1	-5.054260000	1.740023000	-0.067044000
6	-3.000971000	1.020745000	-0.260092000

1	-2.009759000	1.430929000	-0.047507000
1	-3.050625000	0.871967000	-1.349141000
1	-4.693535000	-2.896765000	-2.667147000
6	3.461300000	-3.226362000	-0.549782000
6	2.603661000	-2.310165000	0.079565000
6	2.566659000	-0.965540000	-0.365581000
6	3.345083000	-0.612666000	-1.483245000
6	4.184484000	-1.525507000	-2.109344000
6	4.247957000	-2.835018000	-1.629657000
1	3.502404000	-4.254281000	-0.212551000
1	3.271932000	0.397746000	-1.867910000
1	4.771859000	-1.222431000	-2.970605000
1	4.895232000	-3.565076000	-2.107229000
7	1.797275000	-2.719003000	1.158416000
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8	-0.020041000	-2.412775000	2.485881000
6	0.413751000	-0.616975000	0.941630000
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1	-0.186603000	-1.666802000	-0.878009000
1	-0.677886000	0.014779000	-0.823408000
6	-0.179809000	0.282299000	2.045583000
1	-0.987454000	-0.240275000	2.558546000
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1	-0.551220000	1.220706000	1.635082000
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6	1.832882000	1.341402000	0.225423000
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6	4.281242000	1.779977000	0.547023000
6	4.009855000	4.241991000	-0.753242000
1	1.910798000	3.752197000	-0.905934000
6	5.389061000	2.600766000	0.375372000
1	4.379248000	0.831589000	1.065267000
6	5.260533000	3.831102000	-0.281092000
1	3.903709000	5.204759000	-1.245414000
1	6.355587000	2.289489000	0.762074000
1	6.128281000	4.472646000	-0.407546000
6	2.012021000	-4.032721000	1.768337000
1	3.066074000	-4.150261000	2.035716000
1	1.392222000	-4.085455000	2.660490000
1	1.719756000	-4.837993000	1.084676000
1	0.854132000	2.017607000	0.266963000
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1	0.032242000	3.480833000	1.107304000

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1	-0.762745000	-0.477450000	0.000000000

8a

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6	-3.175905000	-0.119707000	0.513127000
6	-1.948791000	-1.056270000	0.294343000
6	-2.467768000	-2.113156000	-0.685348000
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1	-1.801676000	-1.613945000	1.230006000
7	-3.857103000	-2.042397000	-0.697352000
8	-1.820815000	-2.921908000	-1.320015000
8	-5.544040000	-0.744557000	0.195881000
6	-4.693091000	-2.999595000	-1.405661000
1	-4.474195000	-4.013876000	-1.061291000
1	-5.733013000	-2.745731000	-1.197195000
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6	-4.271642000	3.458780000	-0.712983000
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7	-6.206181000	5.120903000	-0.084933000
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1	-4.308683000	2.385658000	1.169218000
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6	-3.157582000	1.225166000	-0.251314000
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6	2.423147000	-0.766475000	-0.421667000
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1	2.876944000	-4.158058000	-0.427855000
1	3.099577000	0.537792000	-1.983553000
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6	0.444041000	-0.210671000	1.015381000
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1	-0.693234000	0.426957000	-0.715746000
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1	-1.023760000	0.322944000	2.522600000
1	0.564376000	1.015081000	2.819169000
1	-0.465310000	1.698858000	1.545723000
6	1.764050000	0.269797000	0.402689000
6	2.240810000	1.517173000	0.615971000
6	3.537150000	2.120436000	0.241962000
6	3.572380000	3.480563000	-0.115543000
6	4.757462000	1.423479000	0.313643000
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1	2.642029000	4.043035000	-0.152289000
6	5.959982000	2.058146000	0.010309000
1	4.760077000	0.383310000	0.621777000
6	5.974932000	3.403251000	-0.369480000
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8	0.000000000	0.000000000	0.109254000
1	0.000000000	0.000000000	-0.874036000

(E) References

[1] Yu, J.-X.; Teng, F.; Xiang, J.-N.; Deng, W.; Li, J.-H. One-Carbon Incorporation Using Cyclobutanone Oxime Ester Enabled [2+2+1] Carboannulation of 1,7-Enynes by C−C/N−O Bond Cleavage and C−H Functionalization. *Org. Lett.* **2019**, *21*, 9434−9437.

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B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A. Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian Inc Wallingford CT, **2016**.

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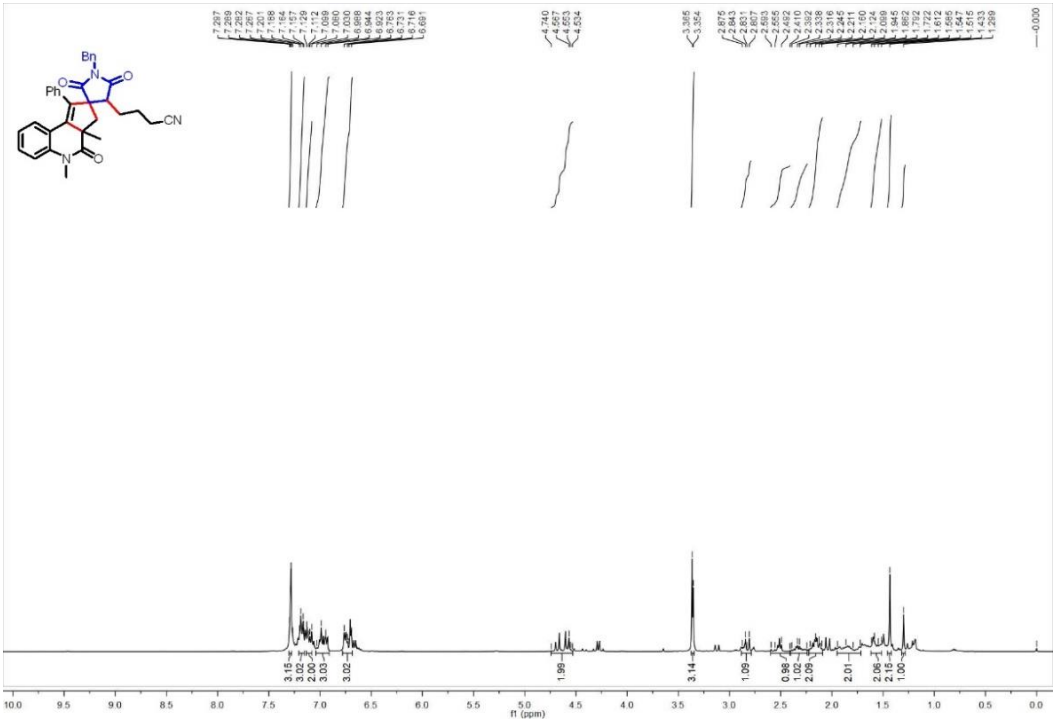
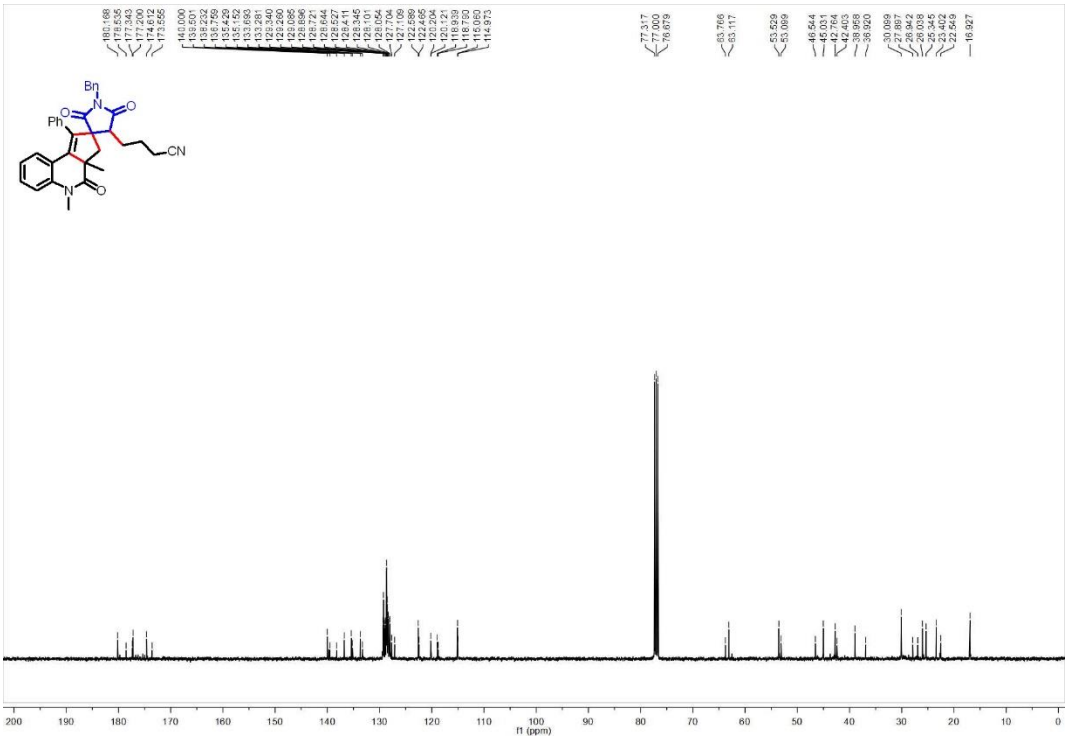
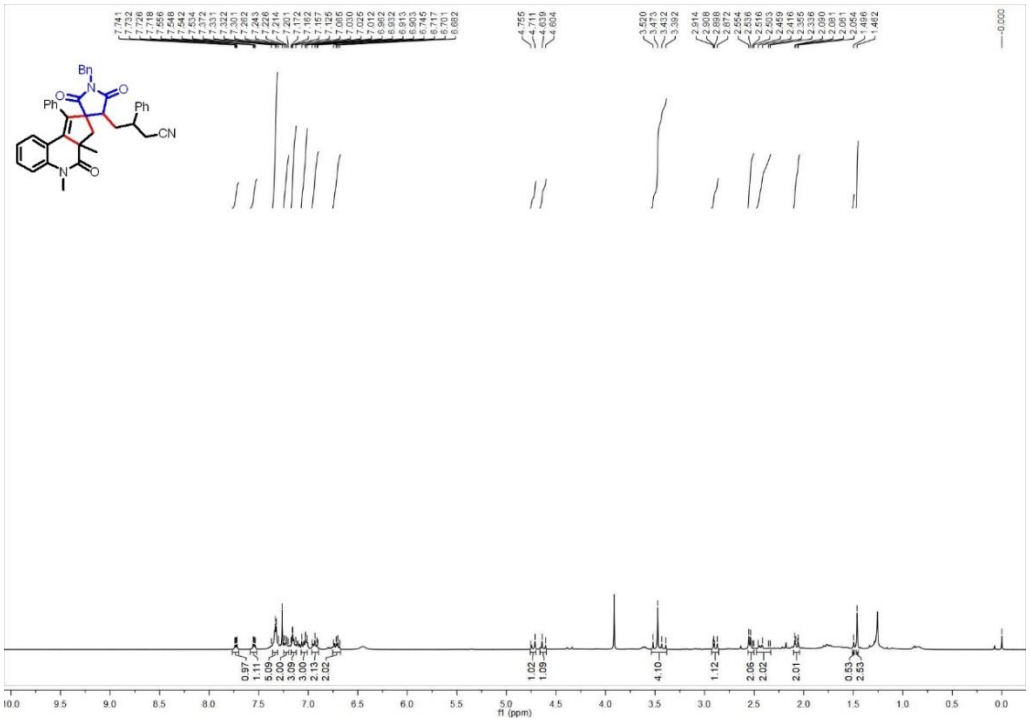
(F) Spectra

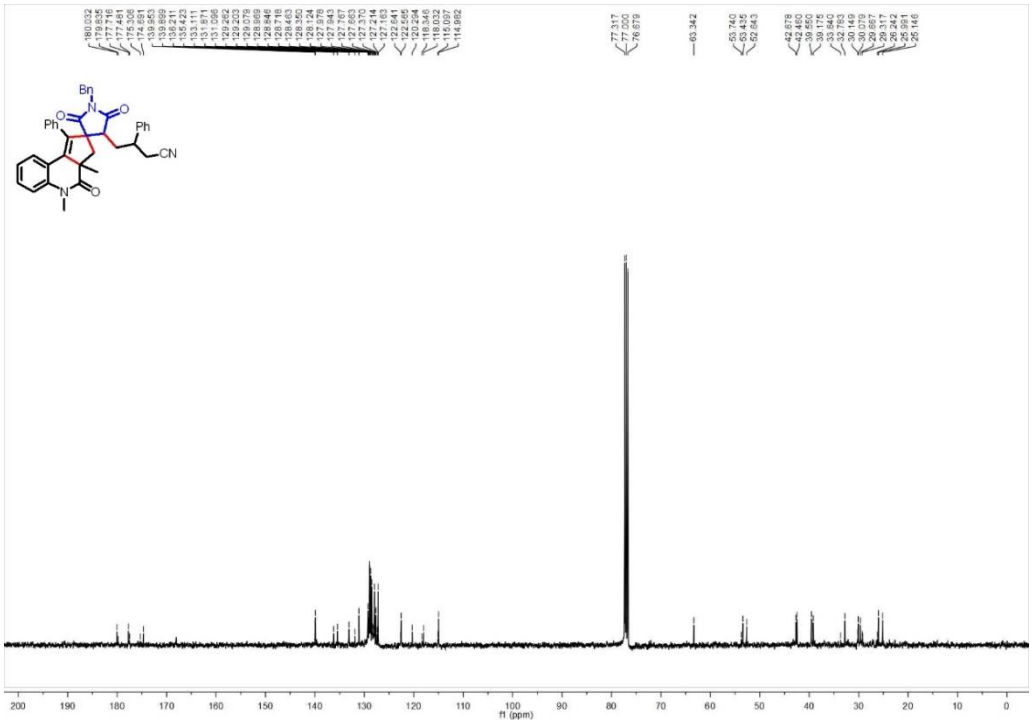
4-(1'-Benzyl-3a,5-dimethyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4a)



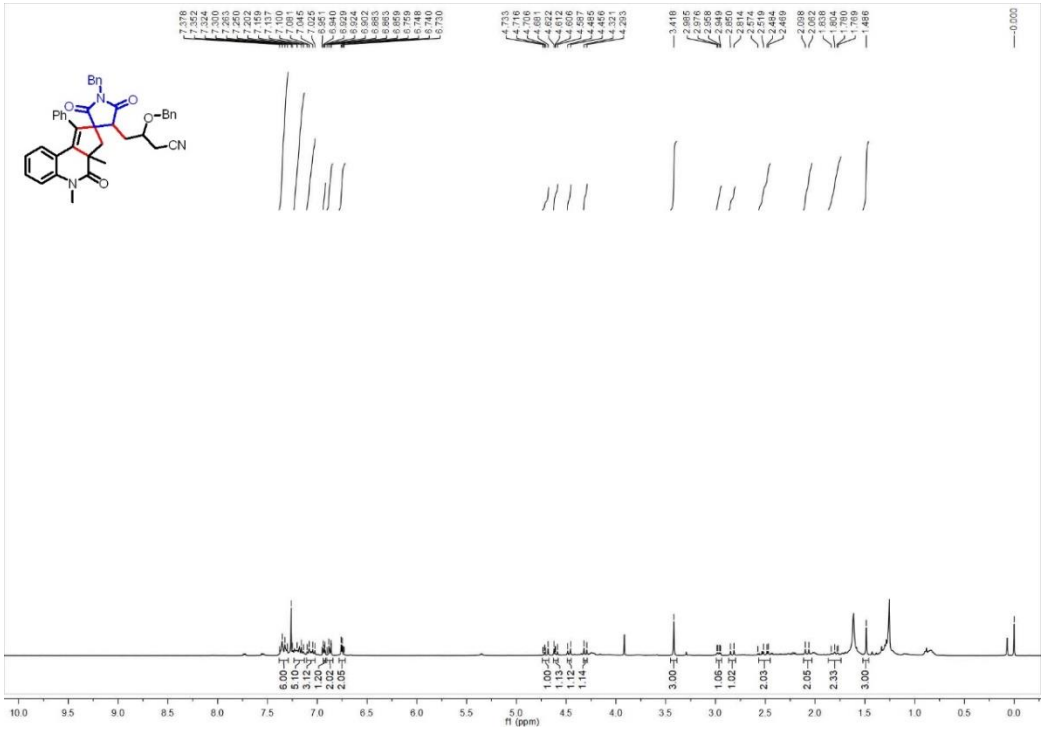


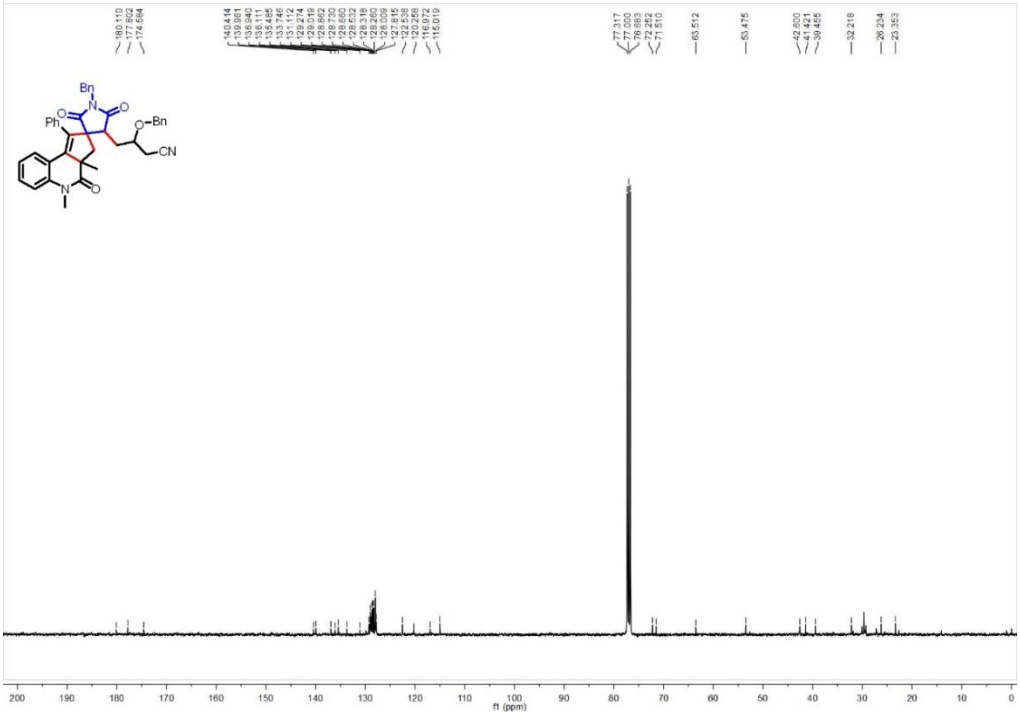
4-(1'-Benzyl-3a,5-dimethyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)-3-phenylbutanenitrile (4b)



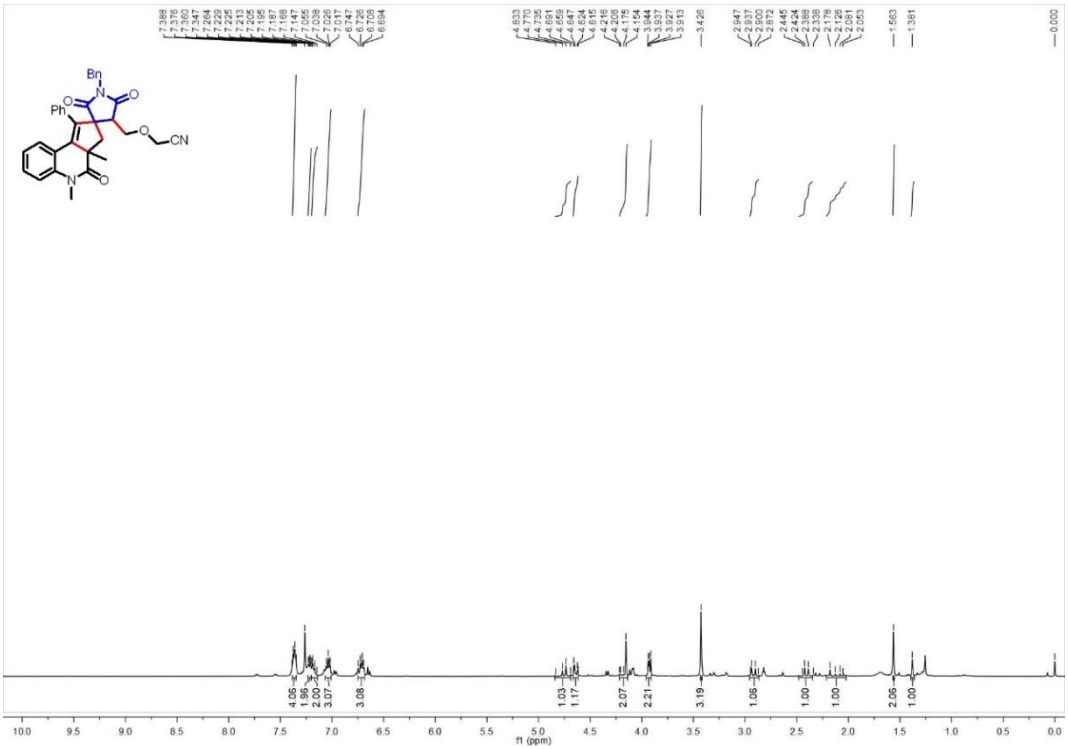


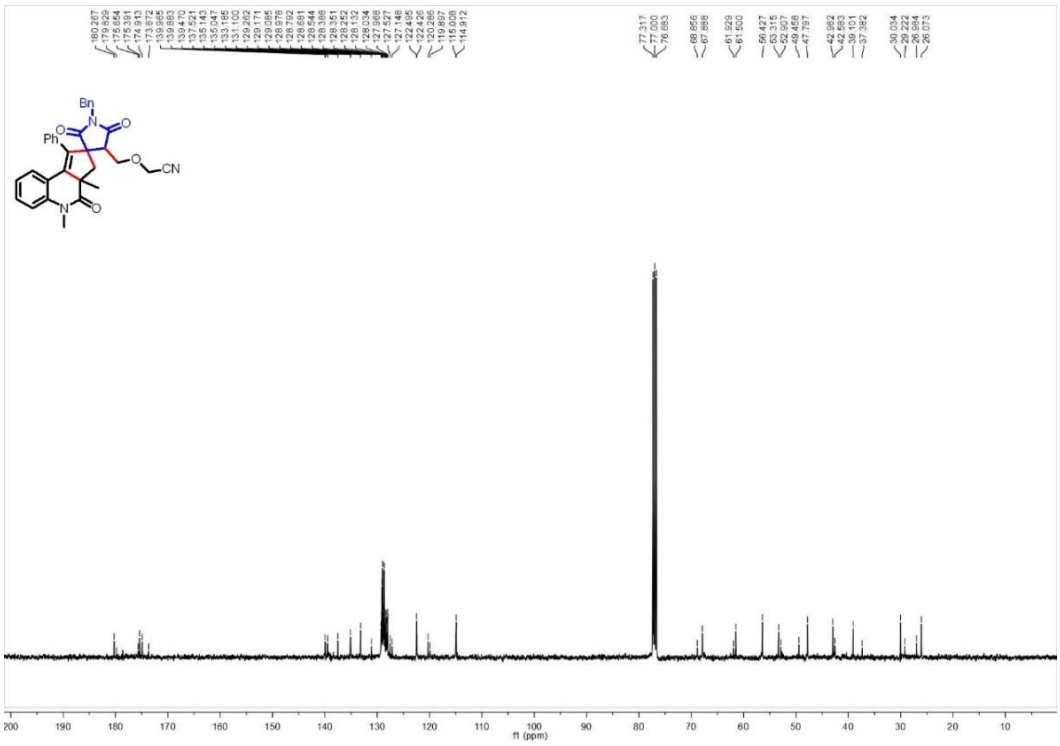
4-(1'-Benzyl-3a,5-dimethyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)-3-(benzyloxy)butanenitrile (**4c**)



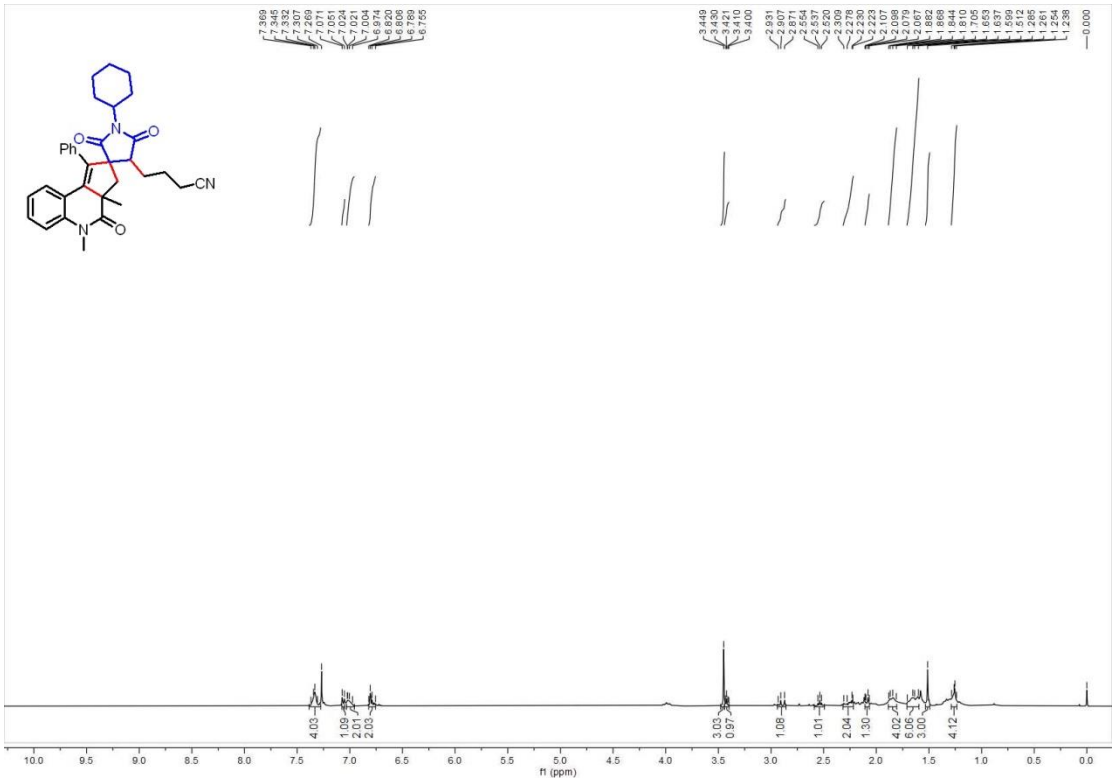


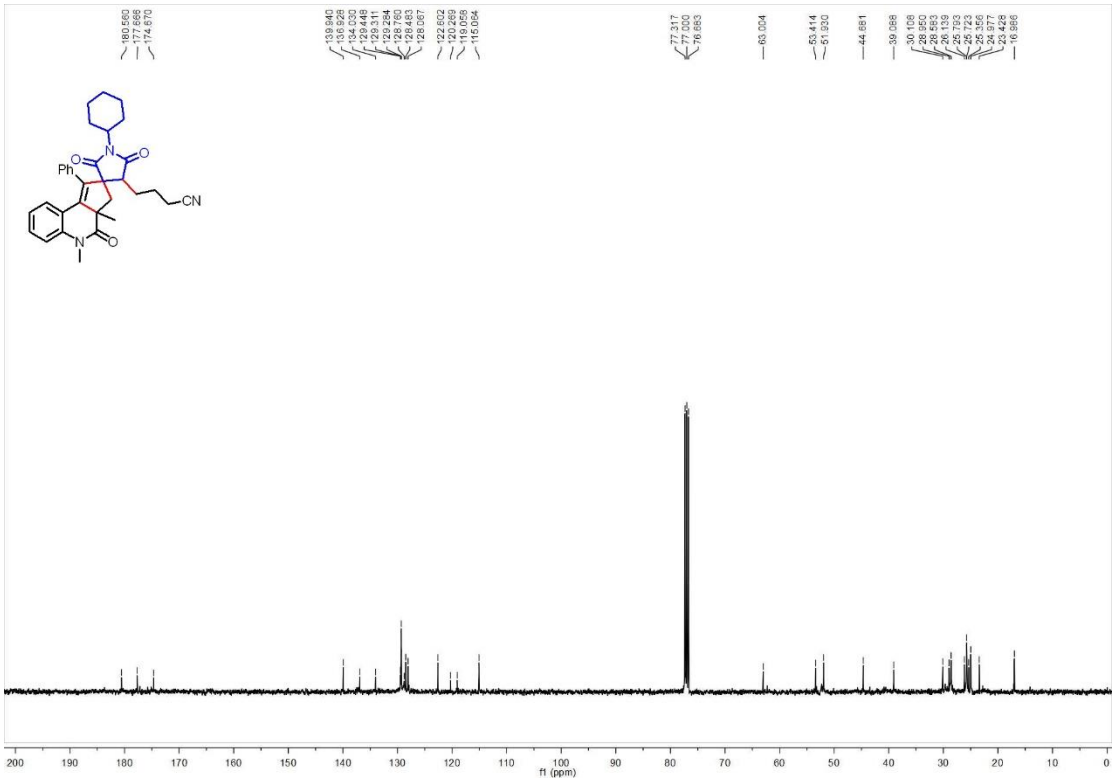
2-((1'-Benzyl-3a,5-dimethyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)methoxy)acetonitrile (4d)



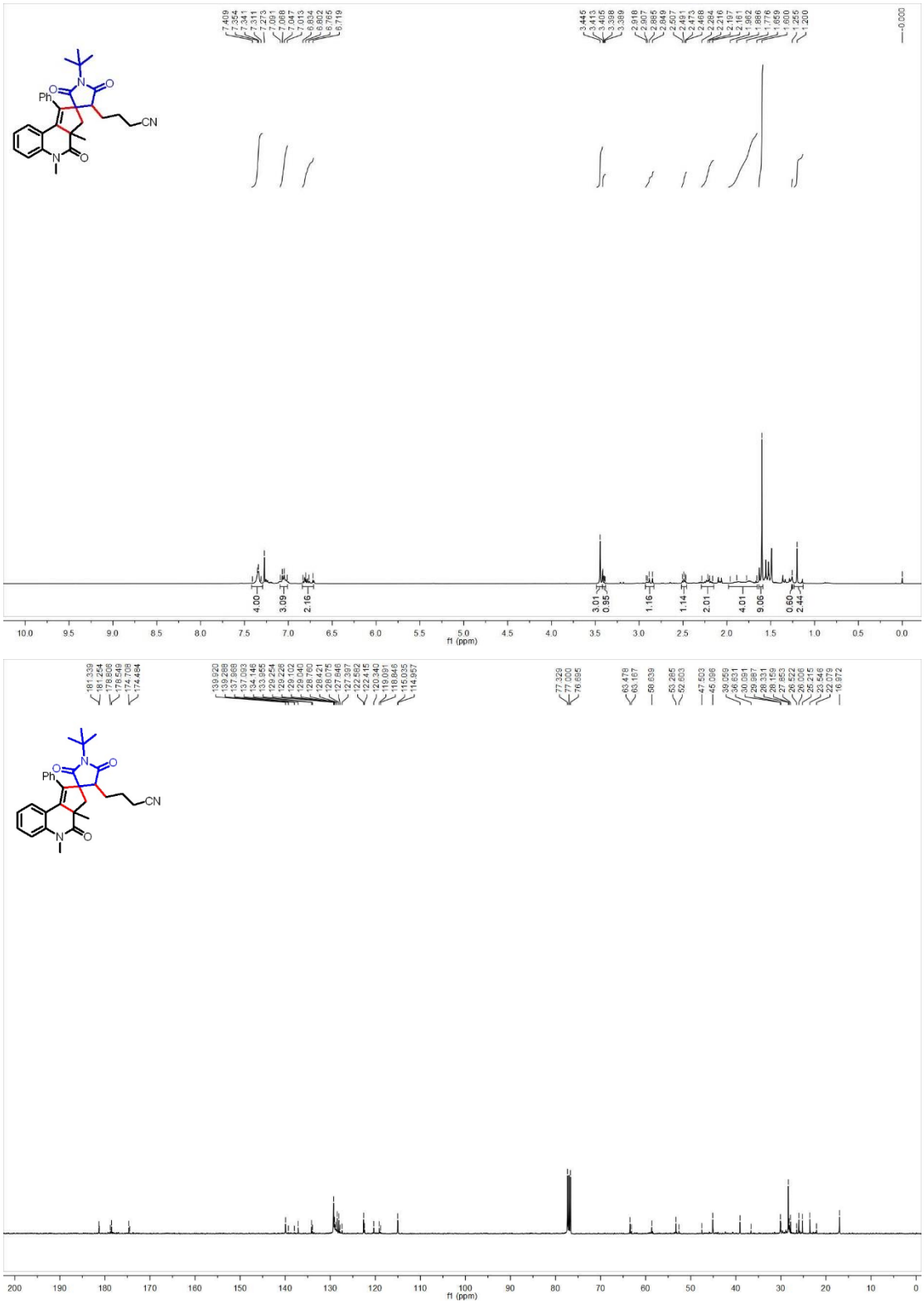


4-(1'-Cyclohexyl-3a,5-dimethyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4e)





4-(1'-(*tert*-Butyl)-3a,5-dimethyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4f)



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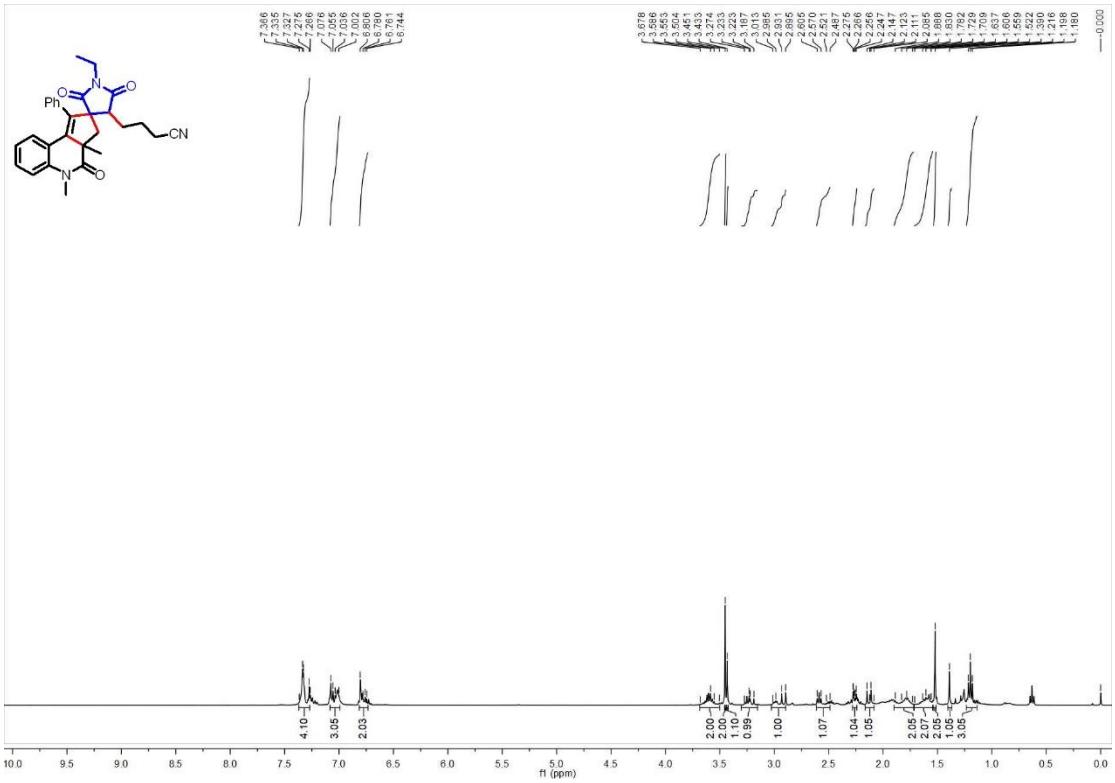
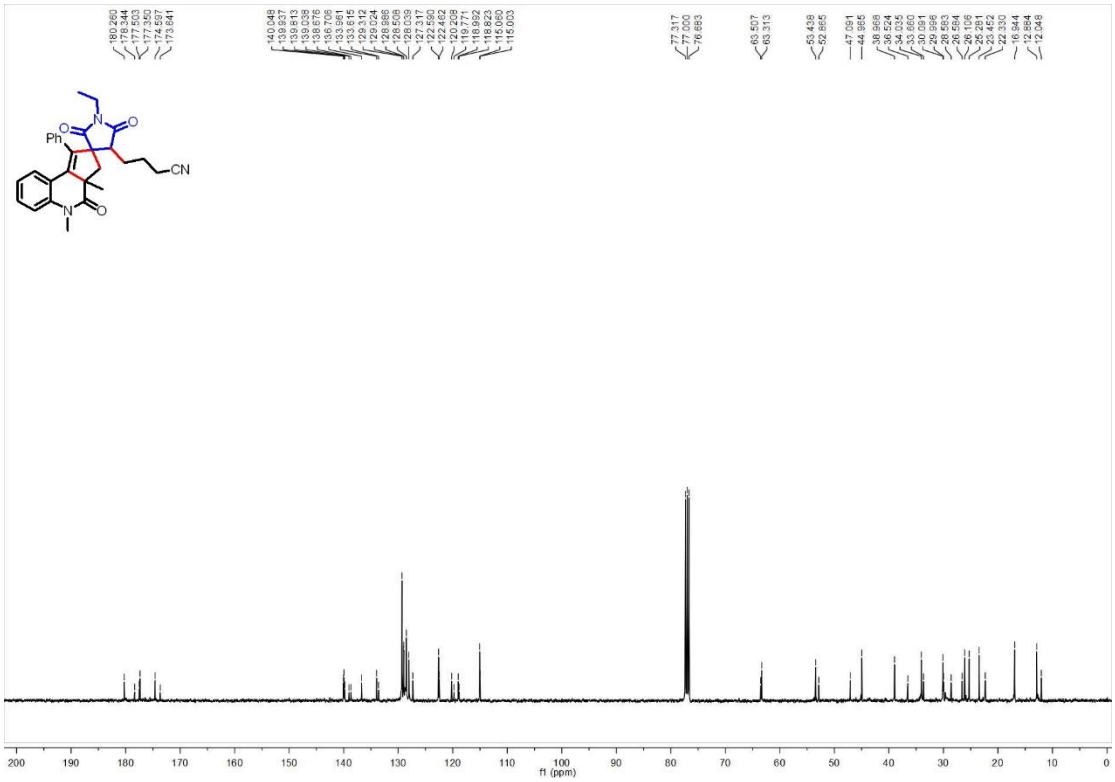
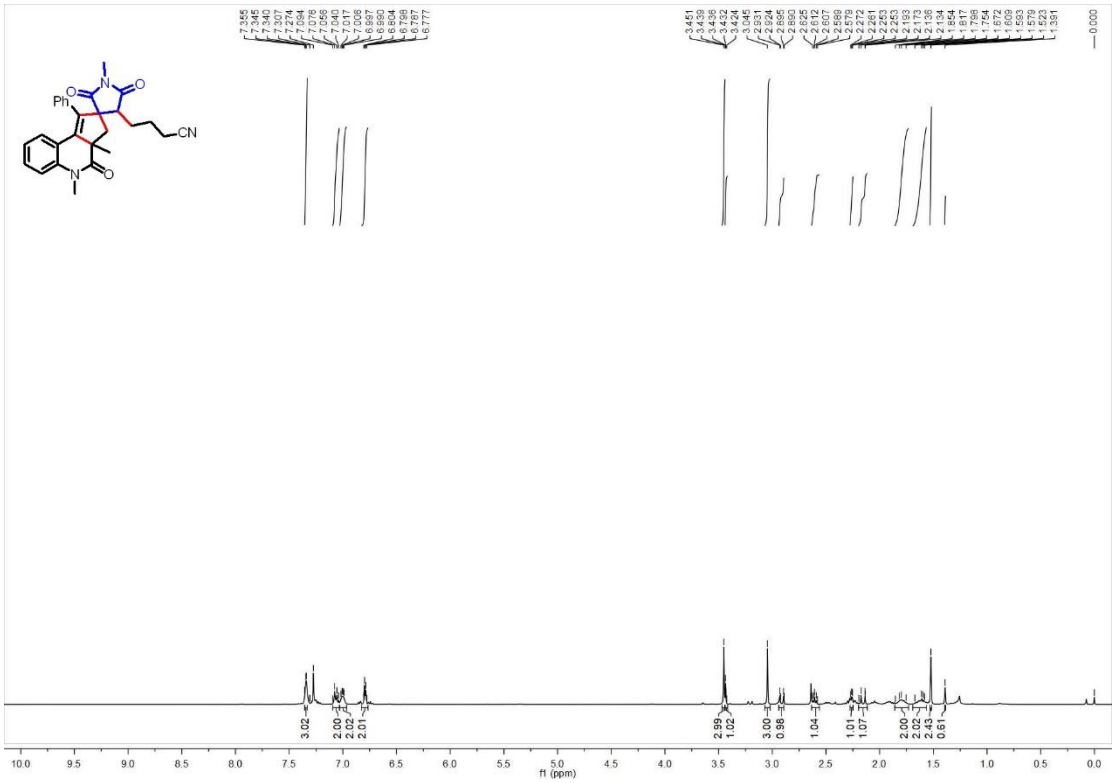
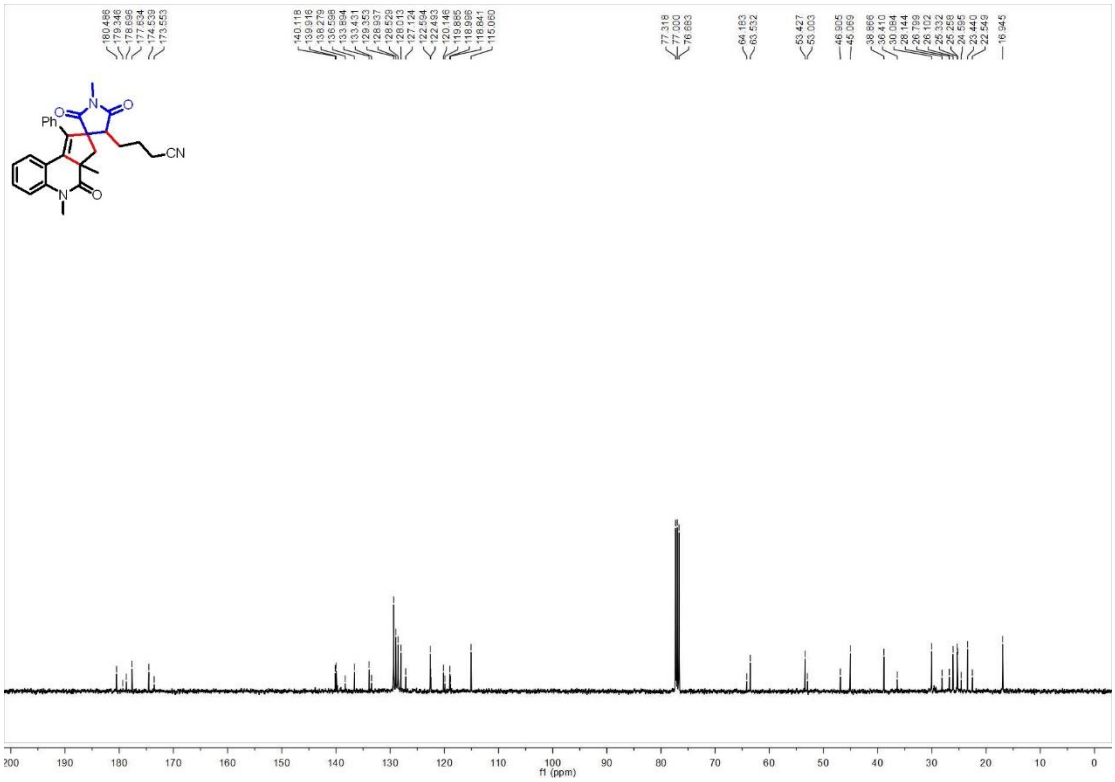


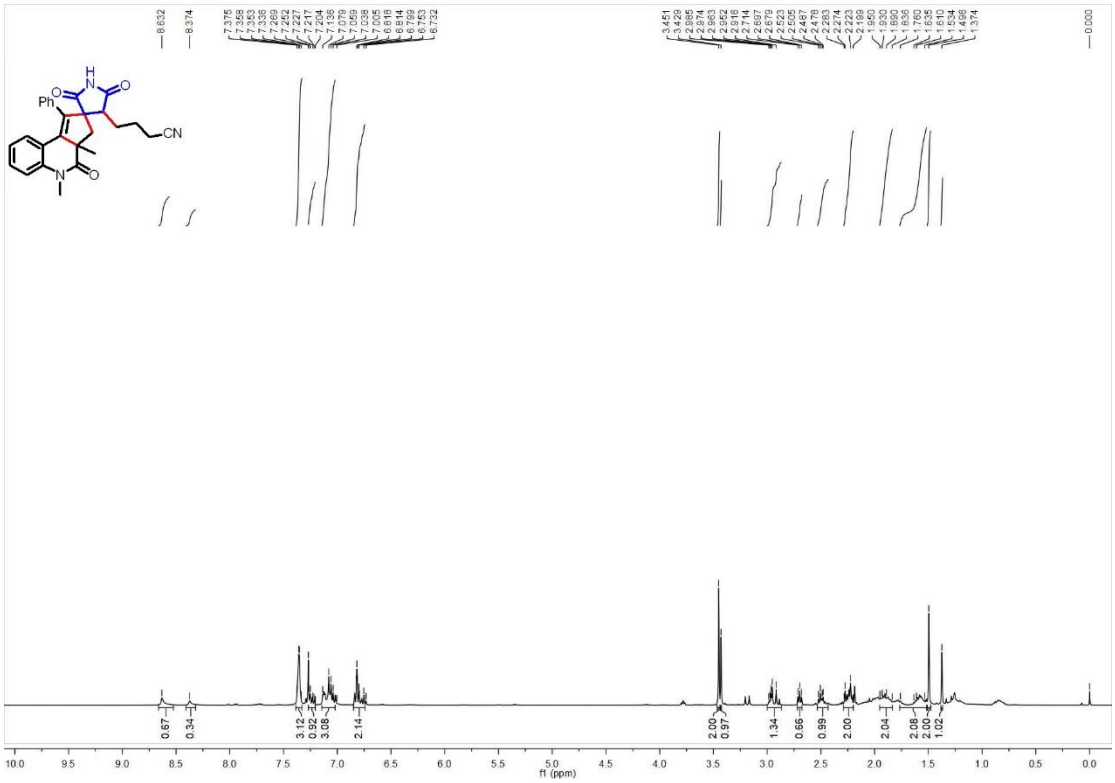


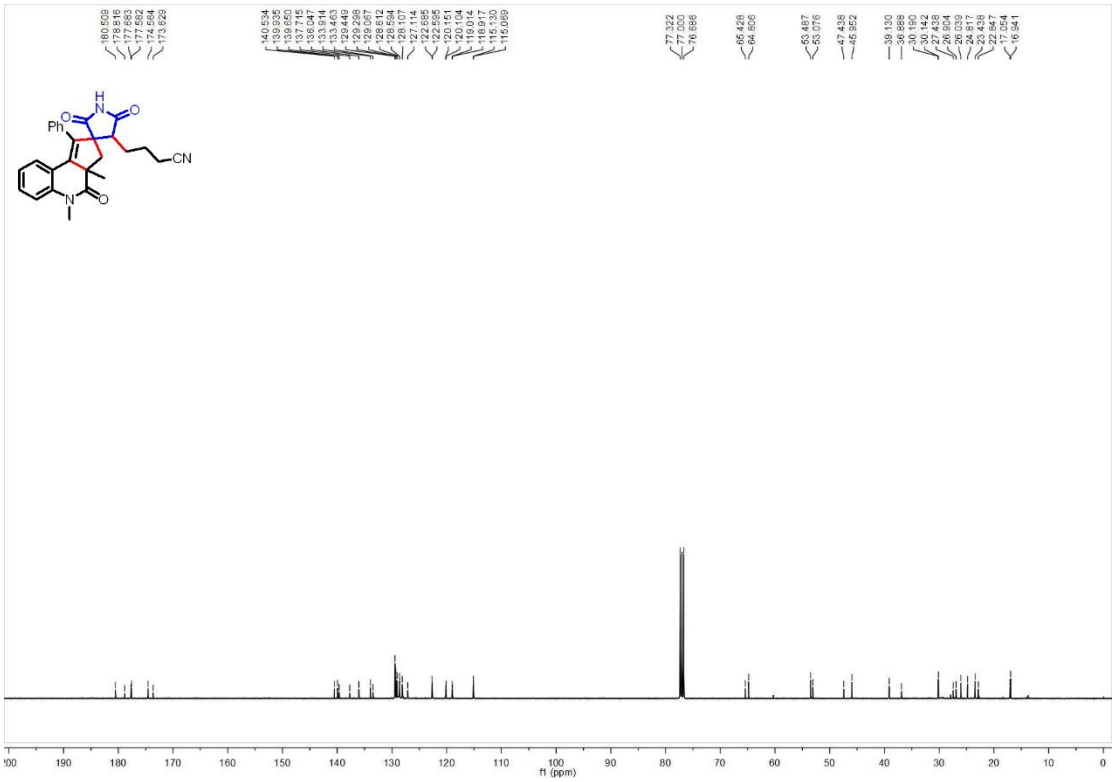
4-(1',3a,5-Trimethyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4h)



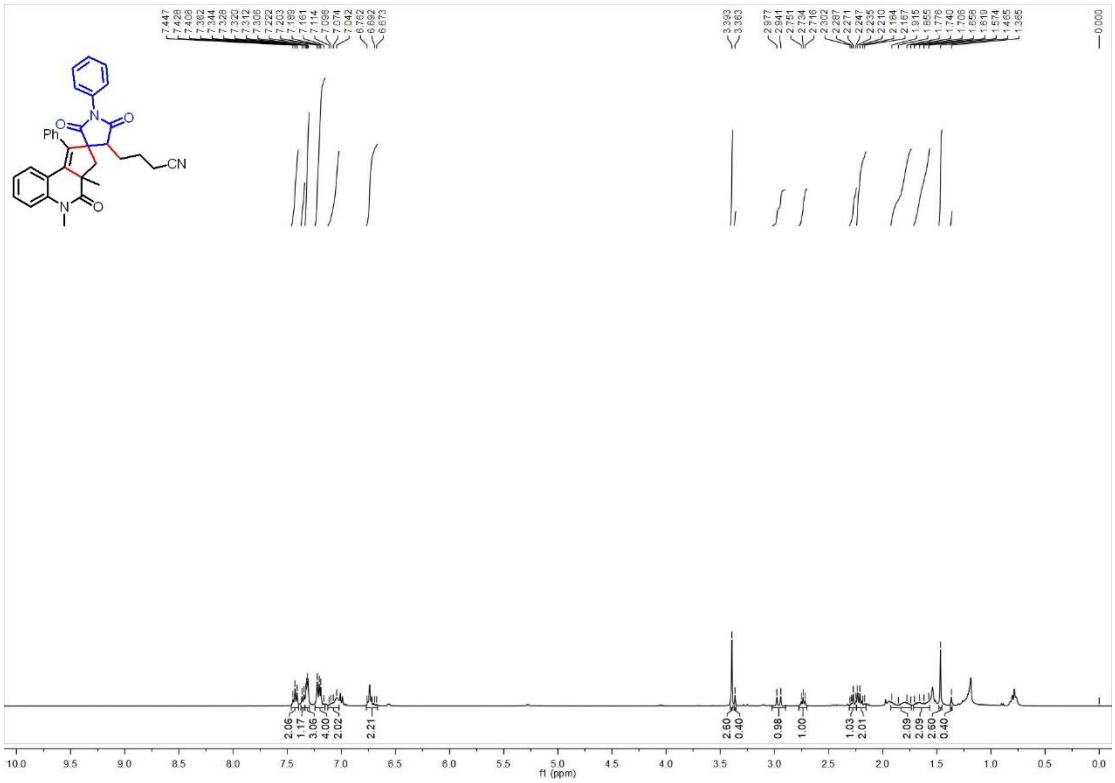


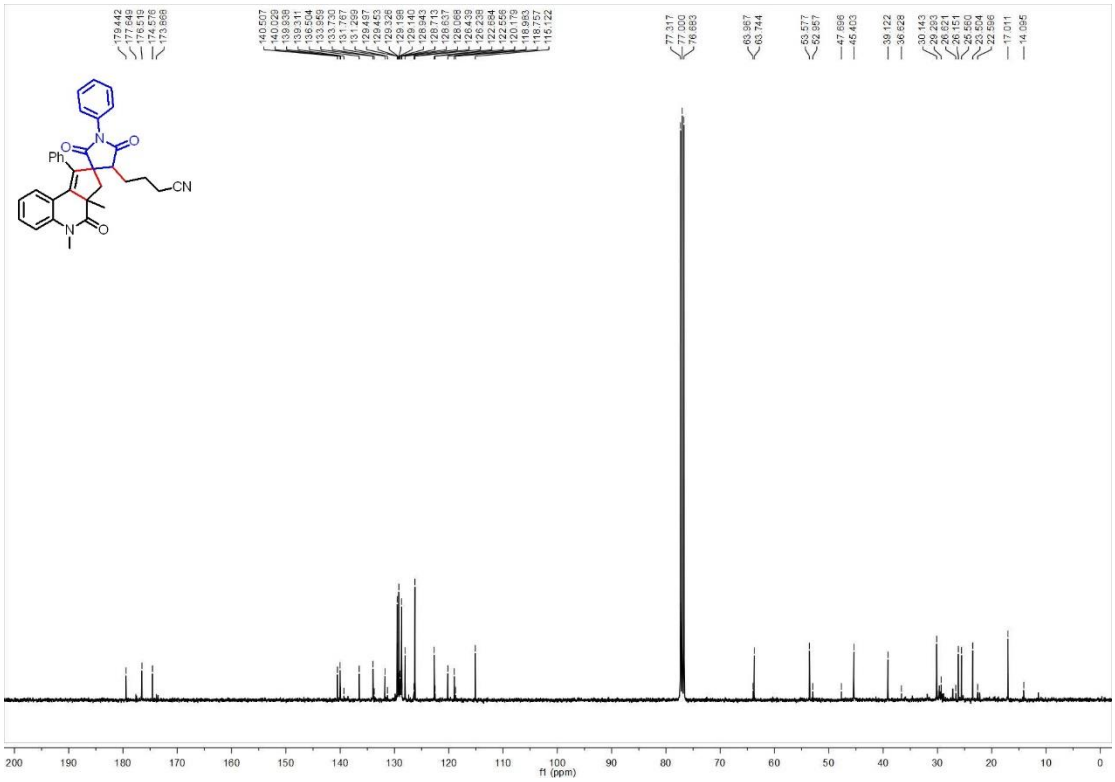
4-(3a,5-Dimethyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4i)



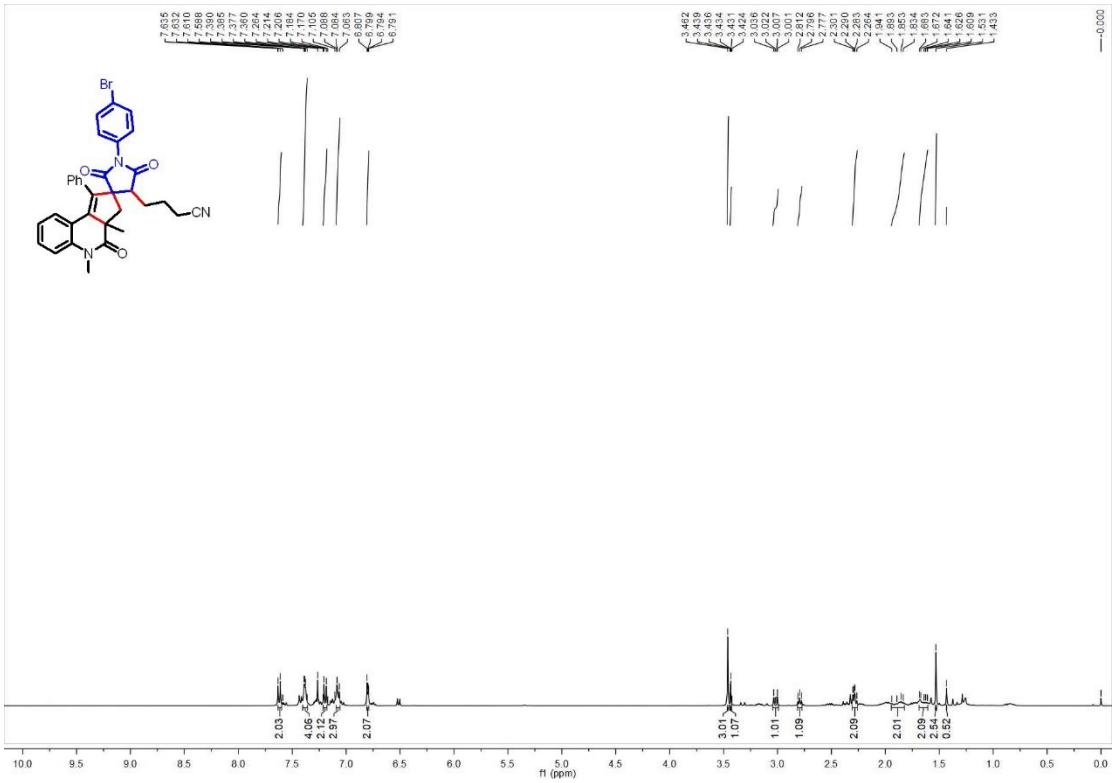


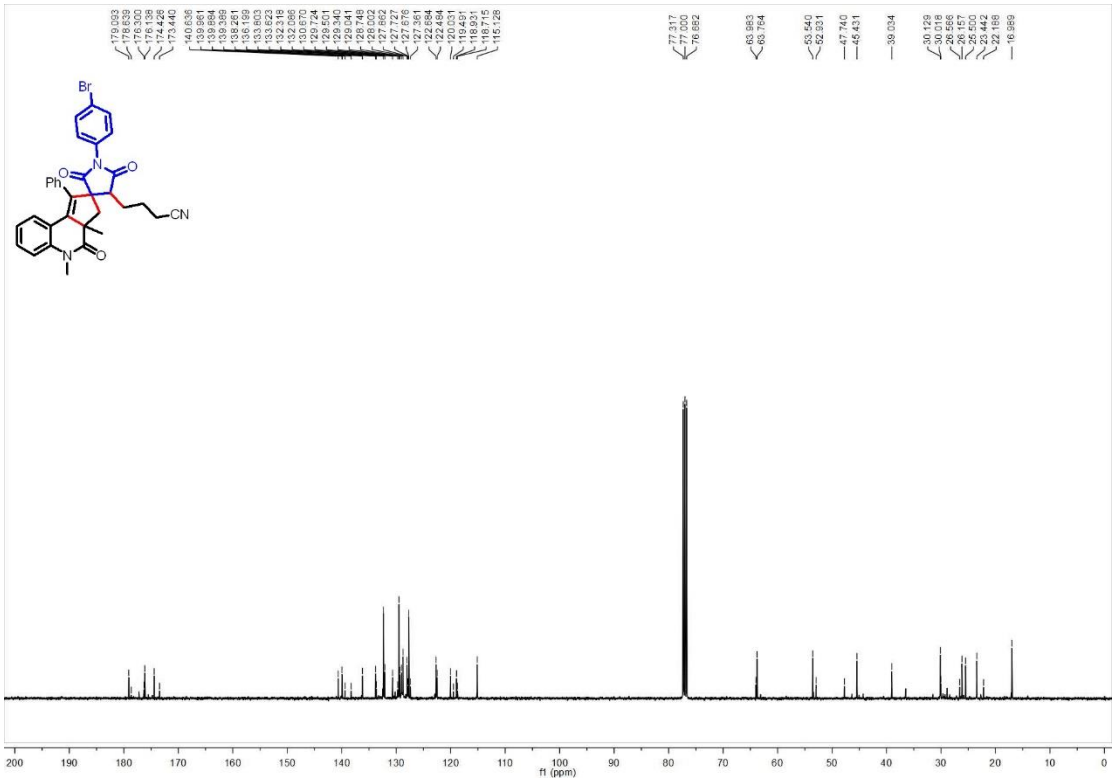
4-(3a,5-Dimethyl-2',4,5'-trioxo-1,1'-diphenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4j)



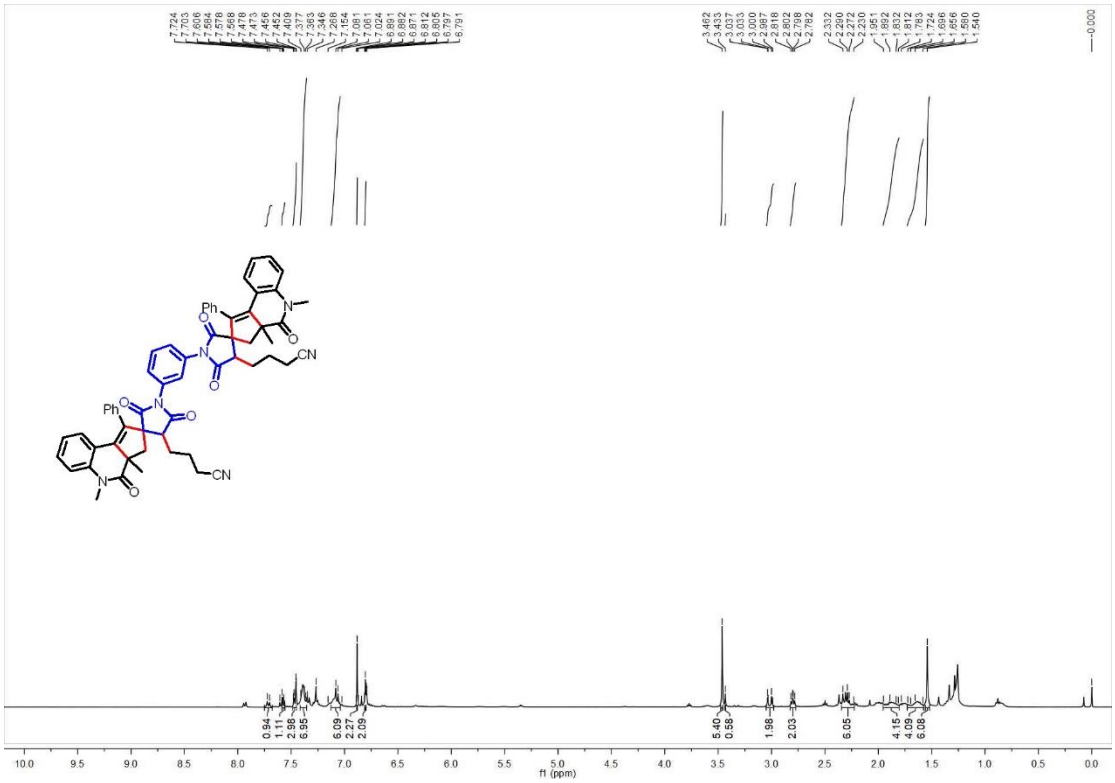


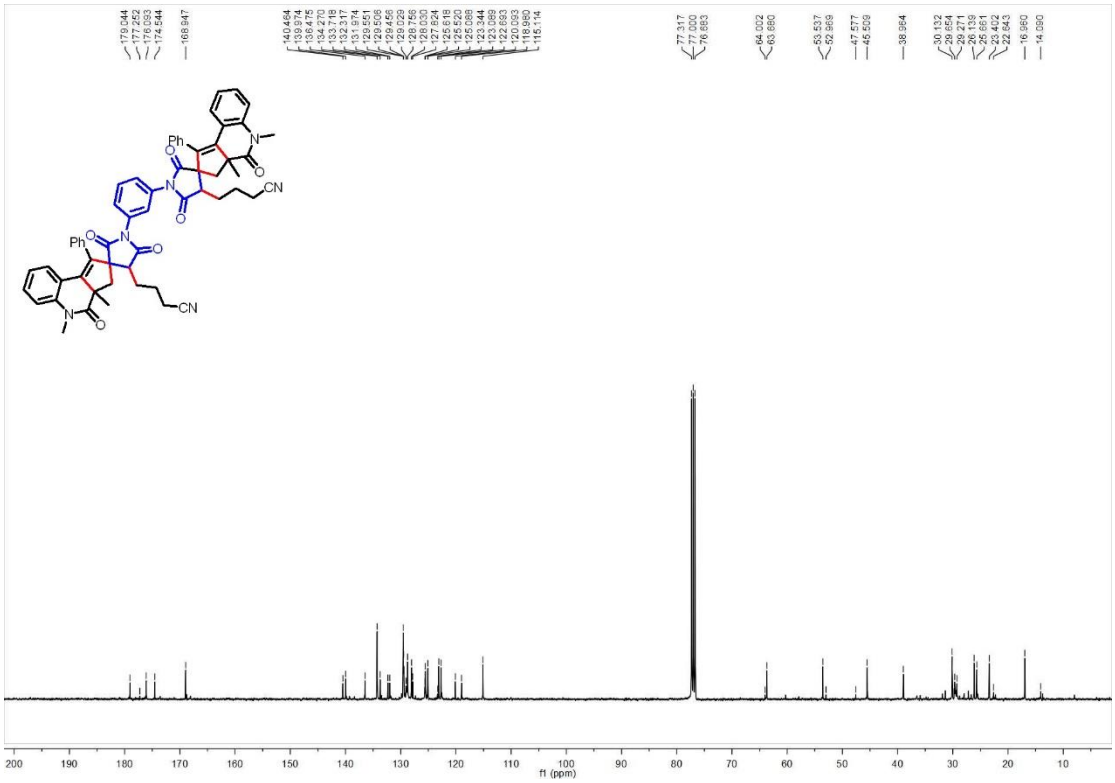
4-(1'-(4-Bromophenyl)-3a,5-dimethyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4k)



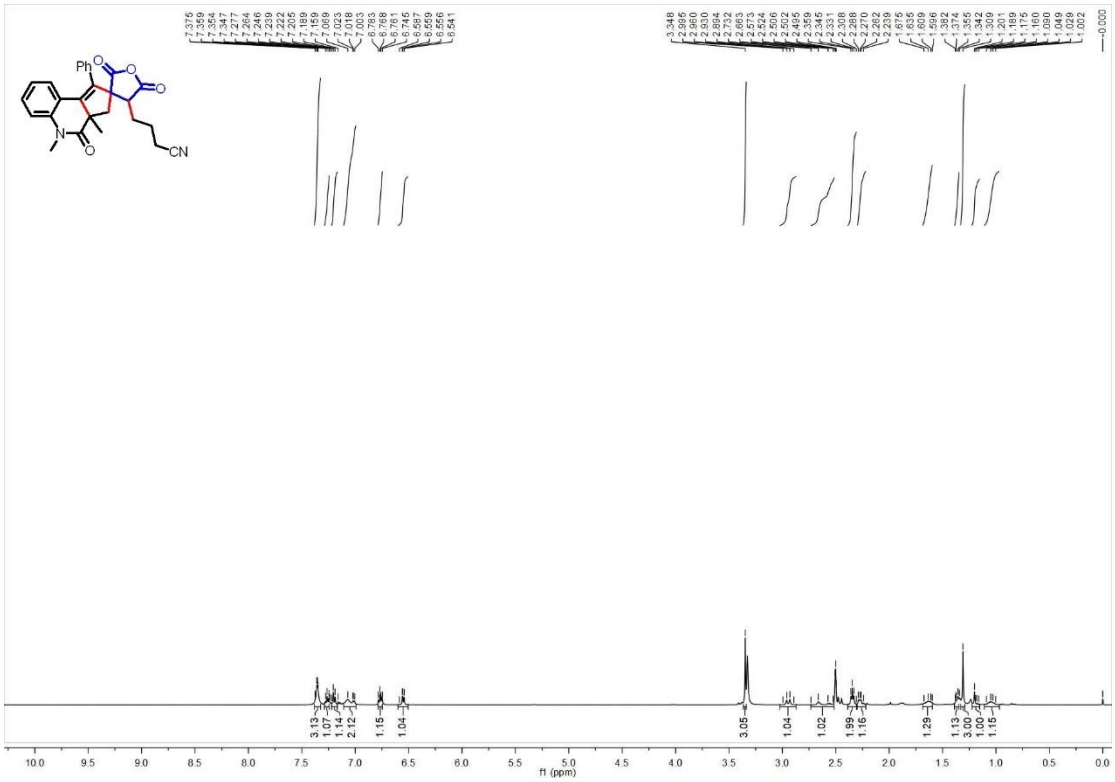


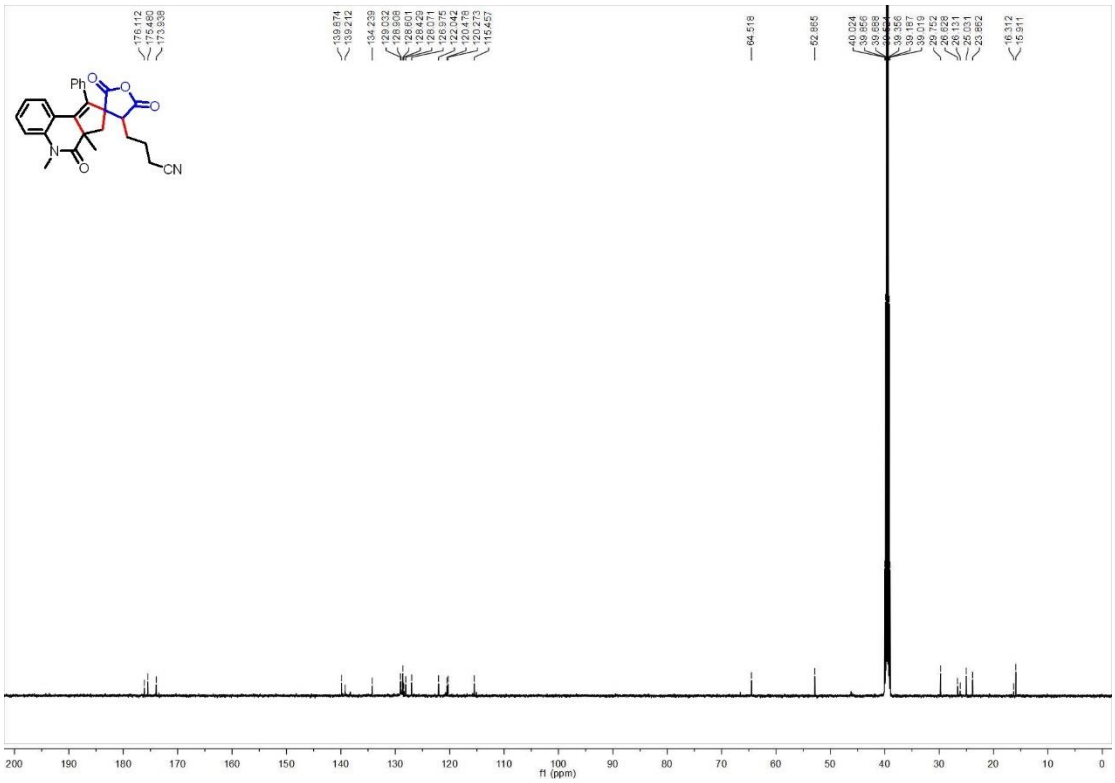
4,4'-(1,3-Phenylenebis(3a,5-dimethyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidine]-1',4'-diyl))dibutanenitrile (4l)



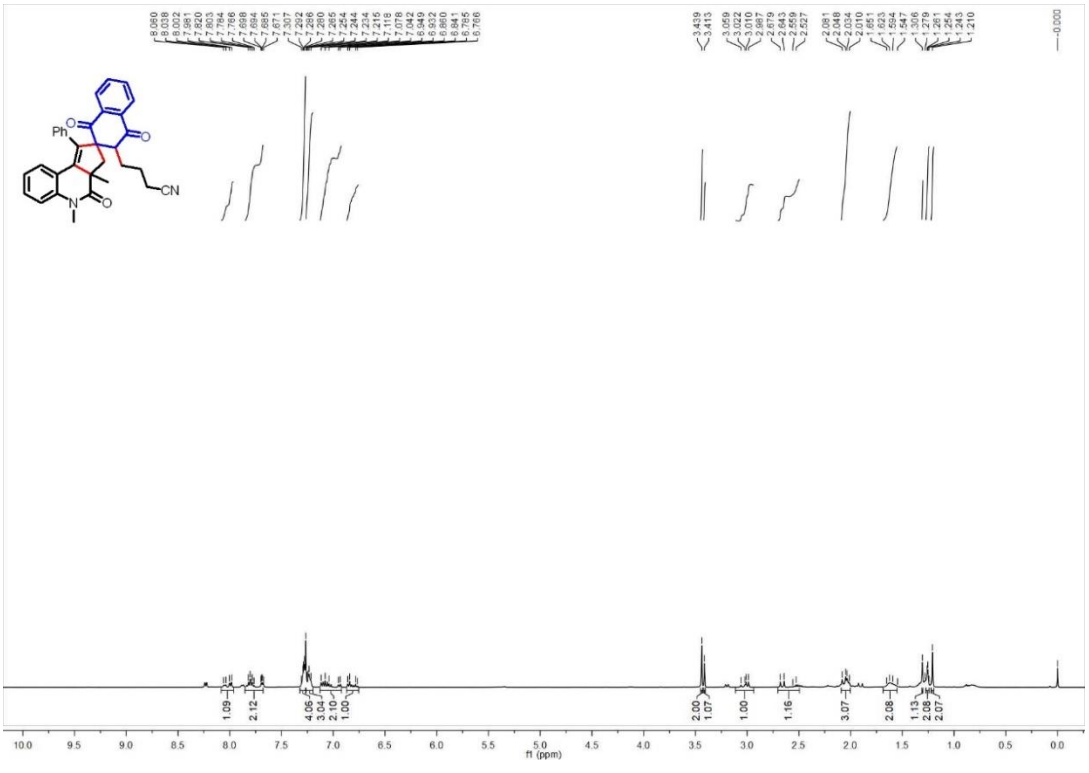


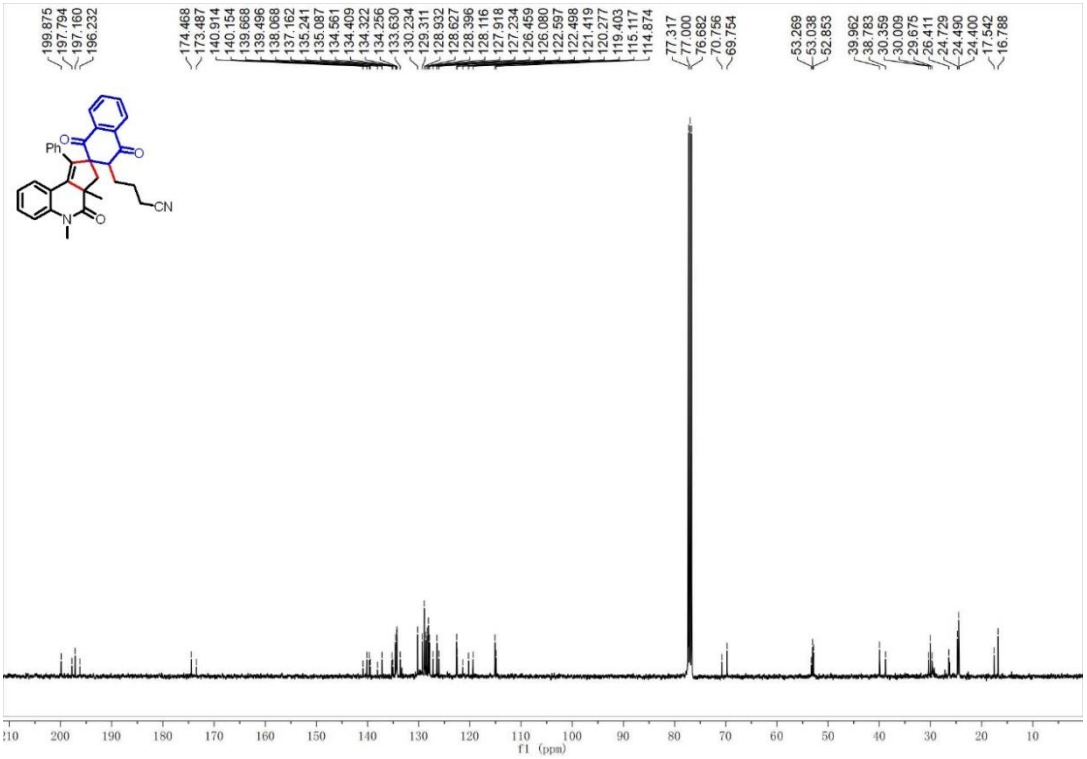
4-(3a,5-Dimethyl-2',4,5'-trioxo-1-phenyl-3,3a,4,4',5,5'-hexahydro-2'*H*-spiro[cyclopenta[*c*]quinoline-2,3'-furan]-4'-yl)butanenitrile (4m)



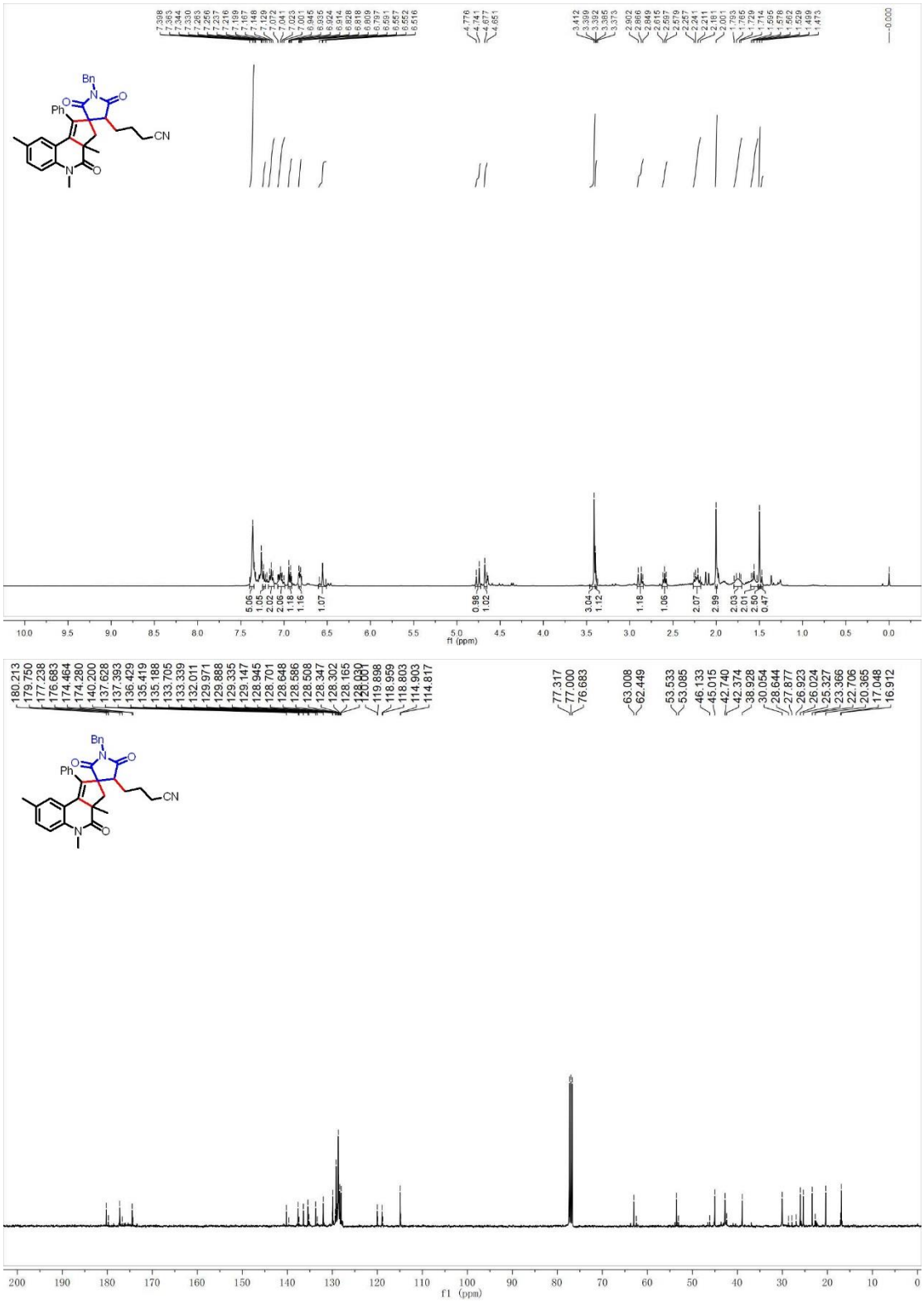


4-(3a,5-Dimethyl-1',4,4'-trioxo-1-phenyl-3,3a,3',4,4',5-hexahydro-1'*H*-spiro[cyclopenta[*c*]quinoline-2,2'-naphthalen]-3'-yl)butanenitrile (4n)





4-(1'-Benzyl-3a,5,8-trimethyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4o)



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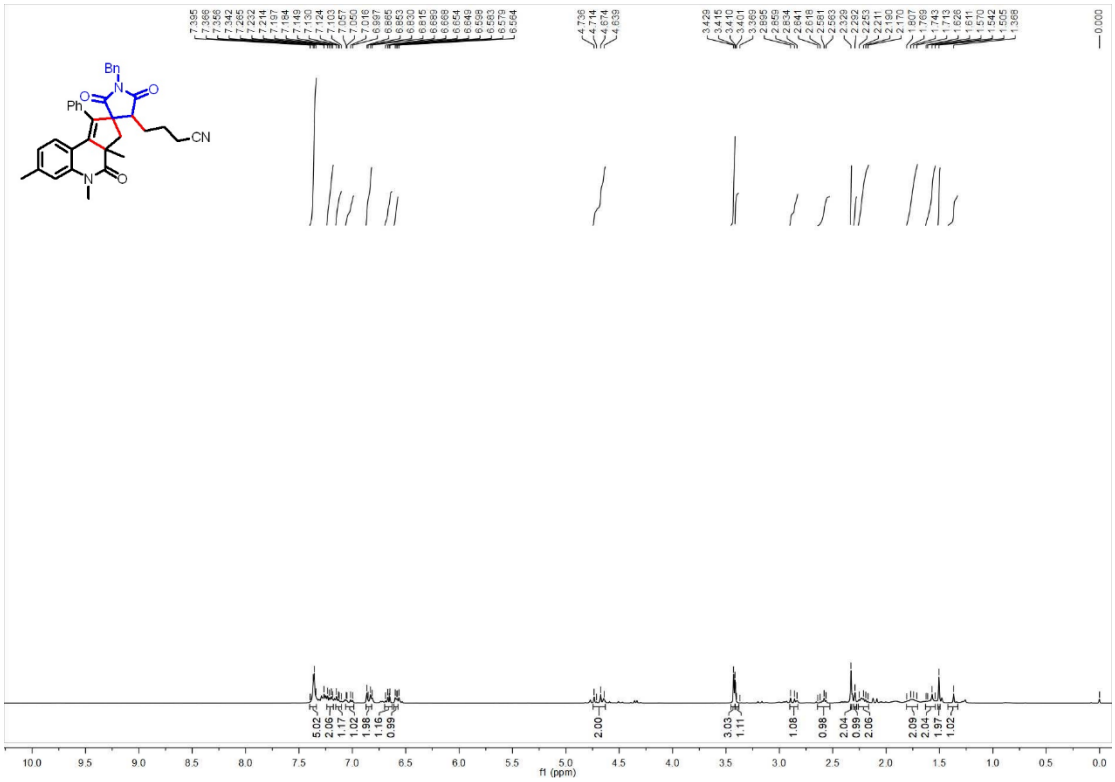

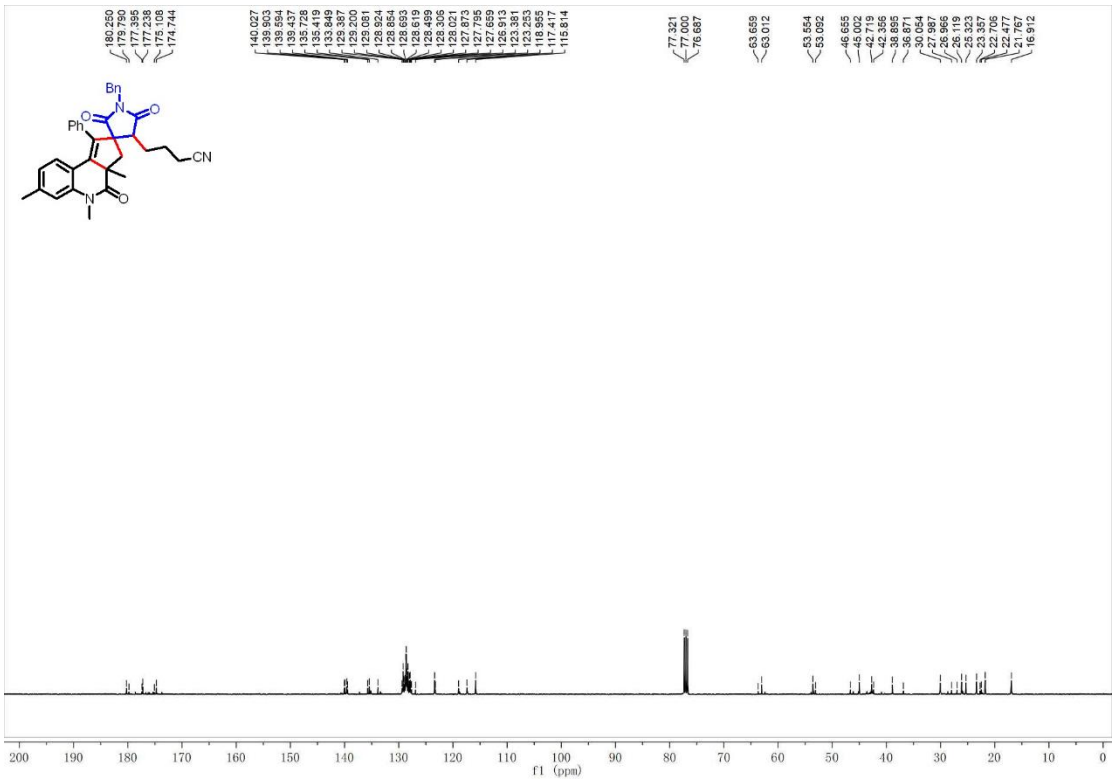

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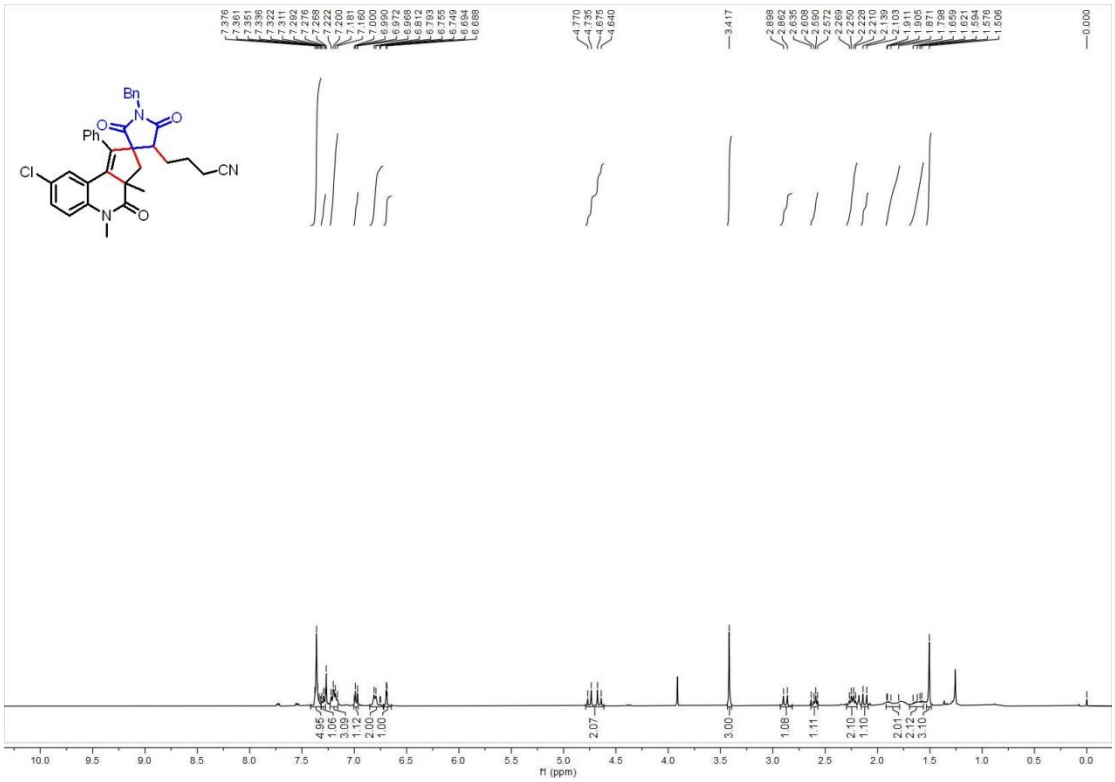

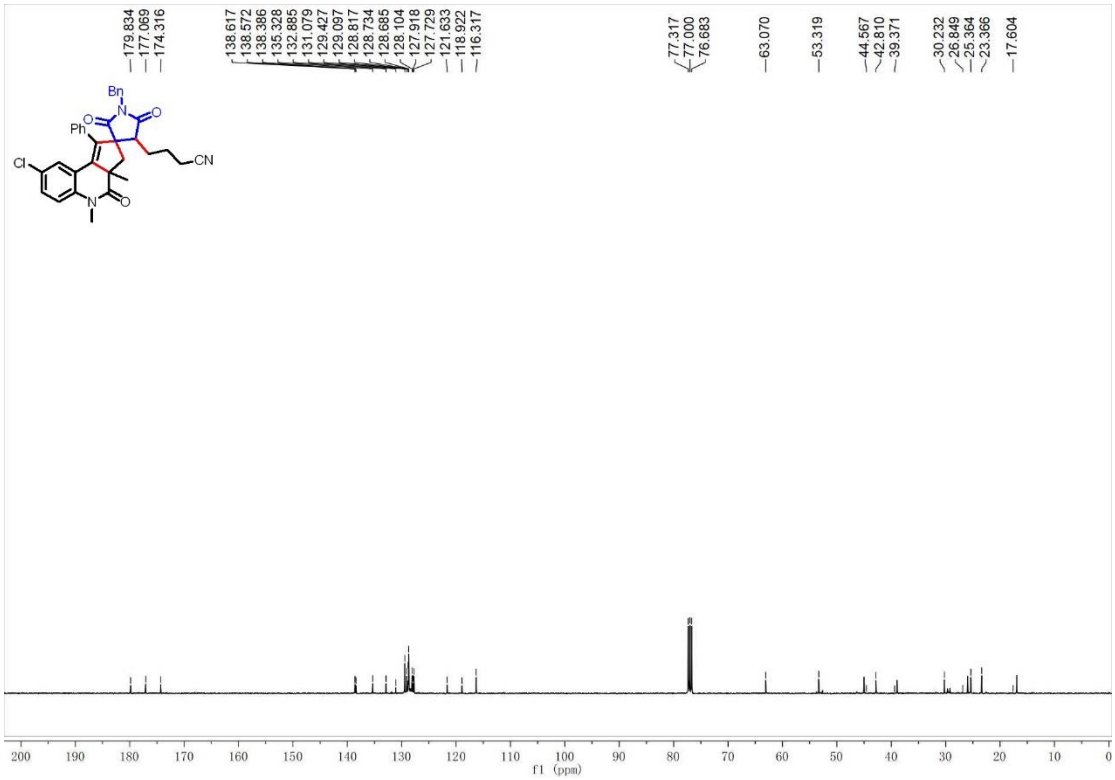

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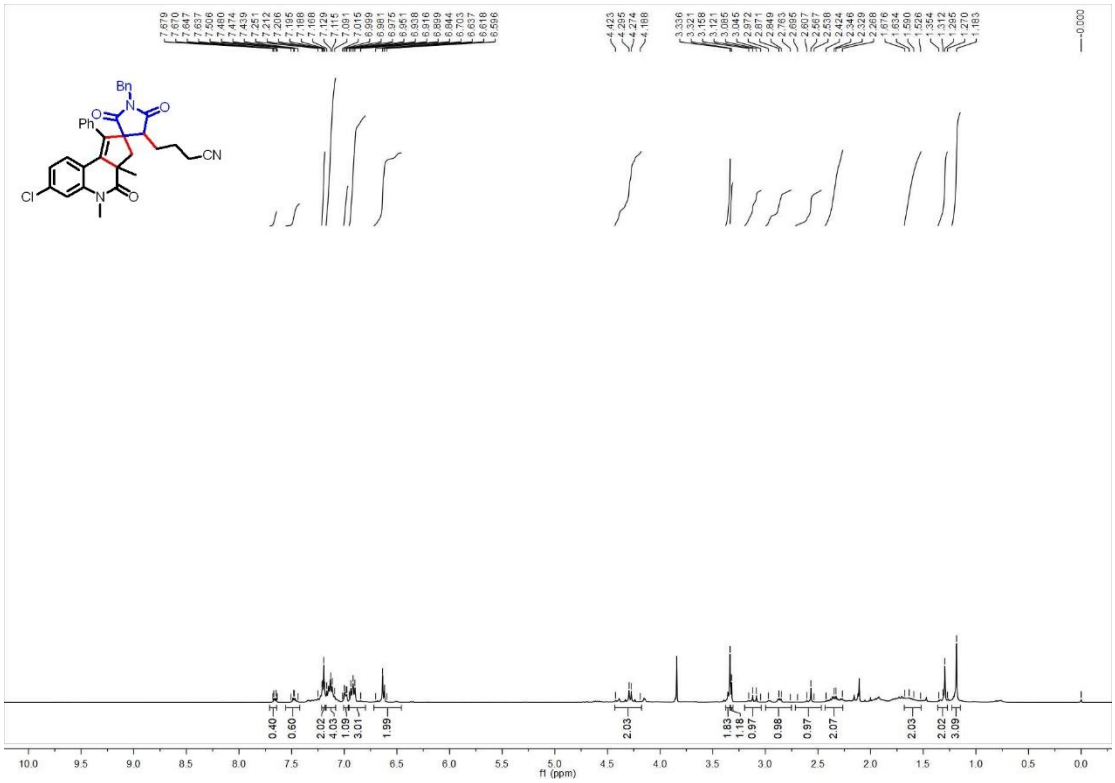

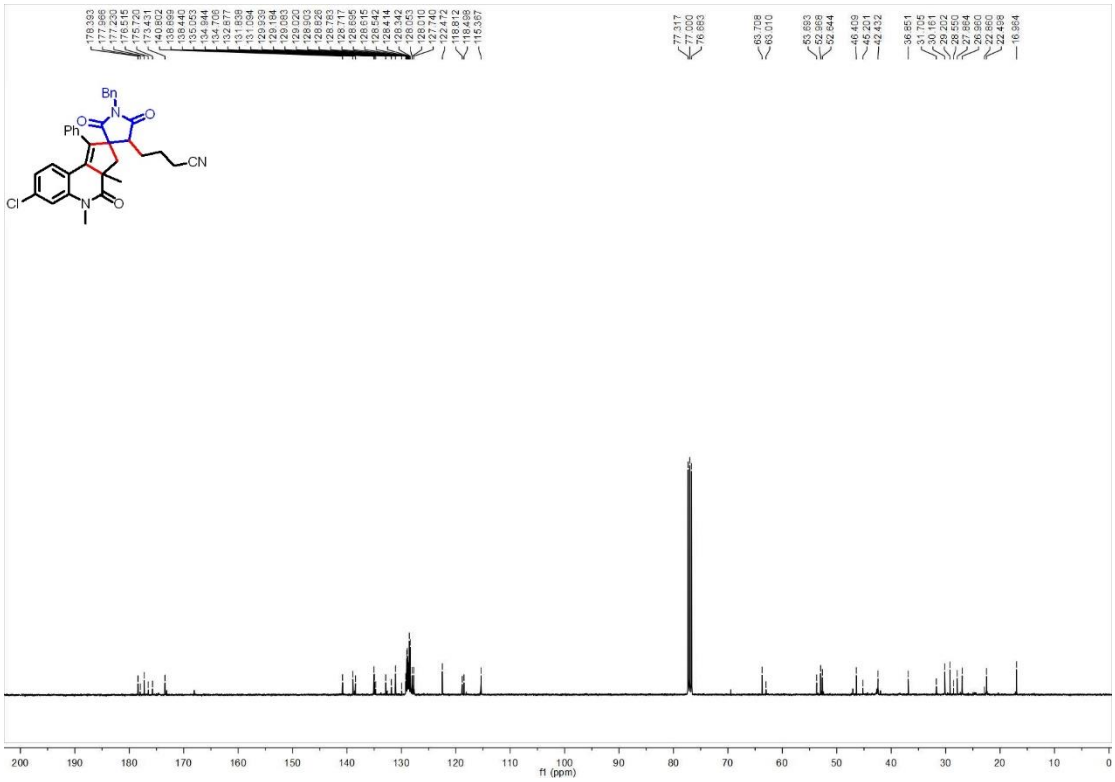

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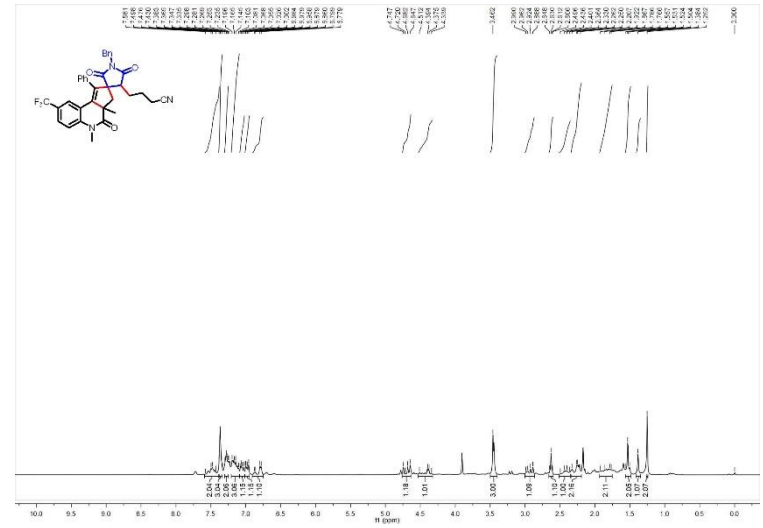

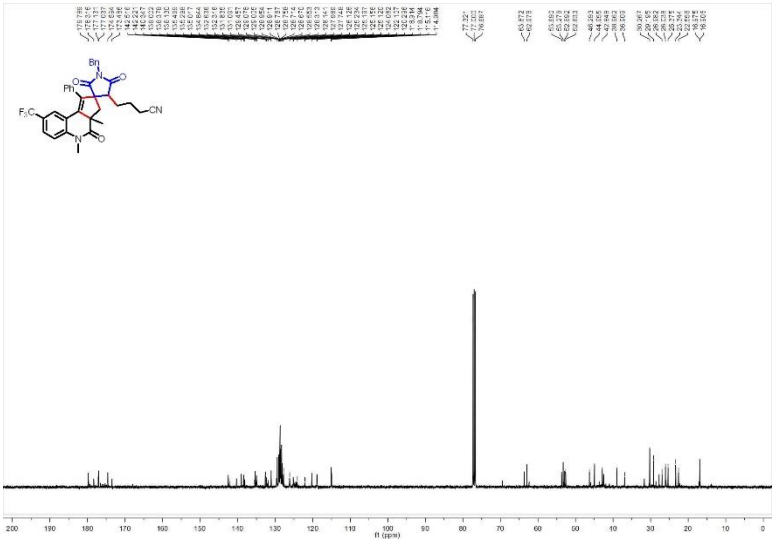

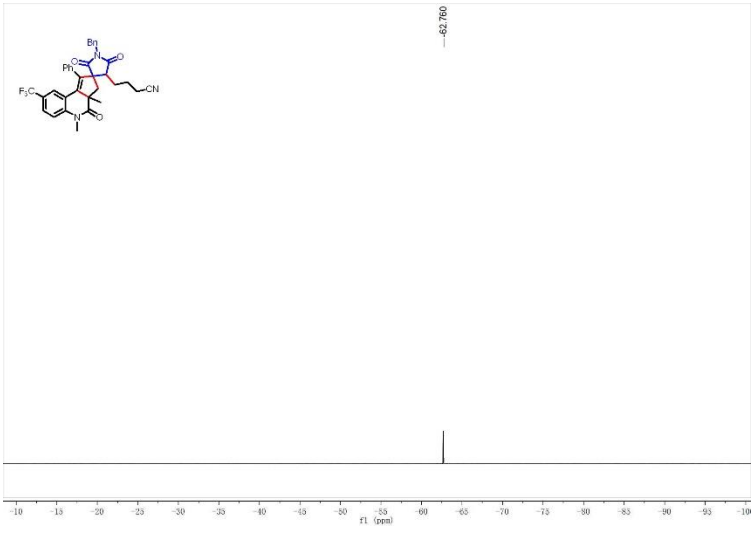

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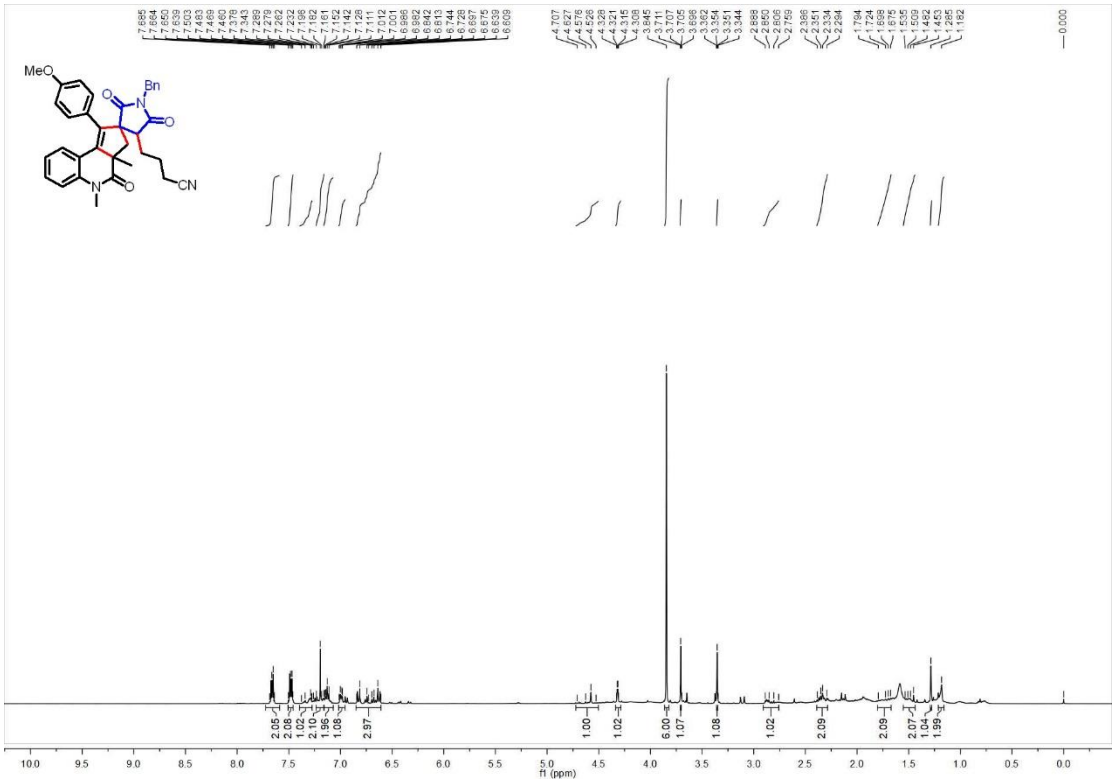

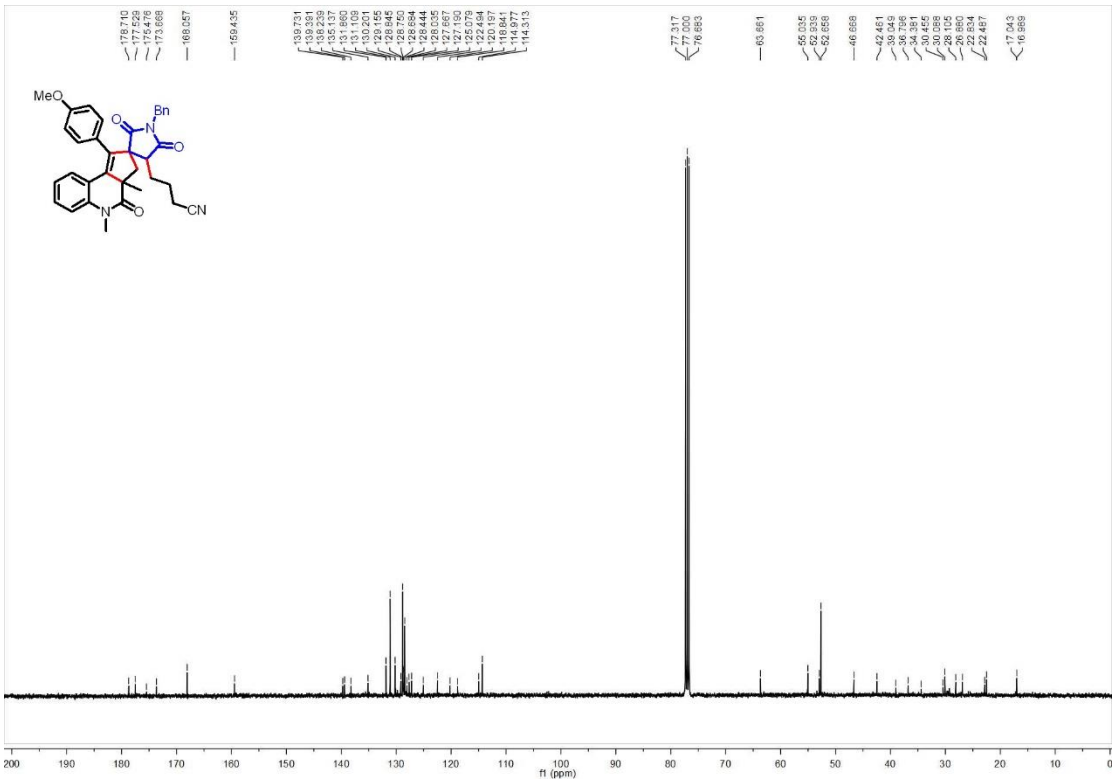

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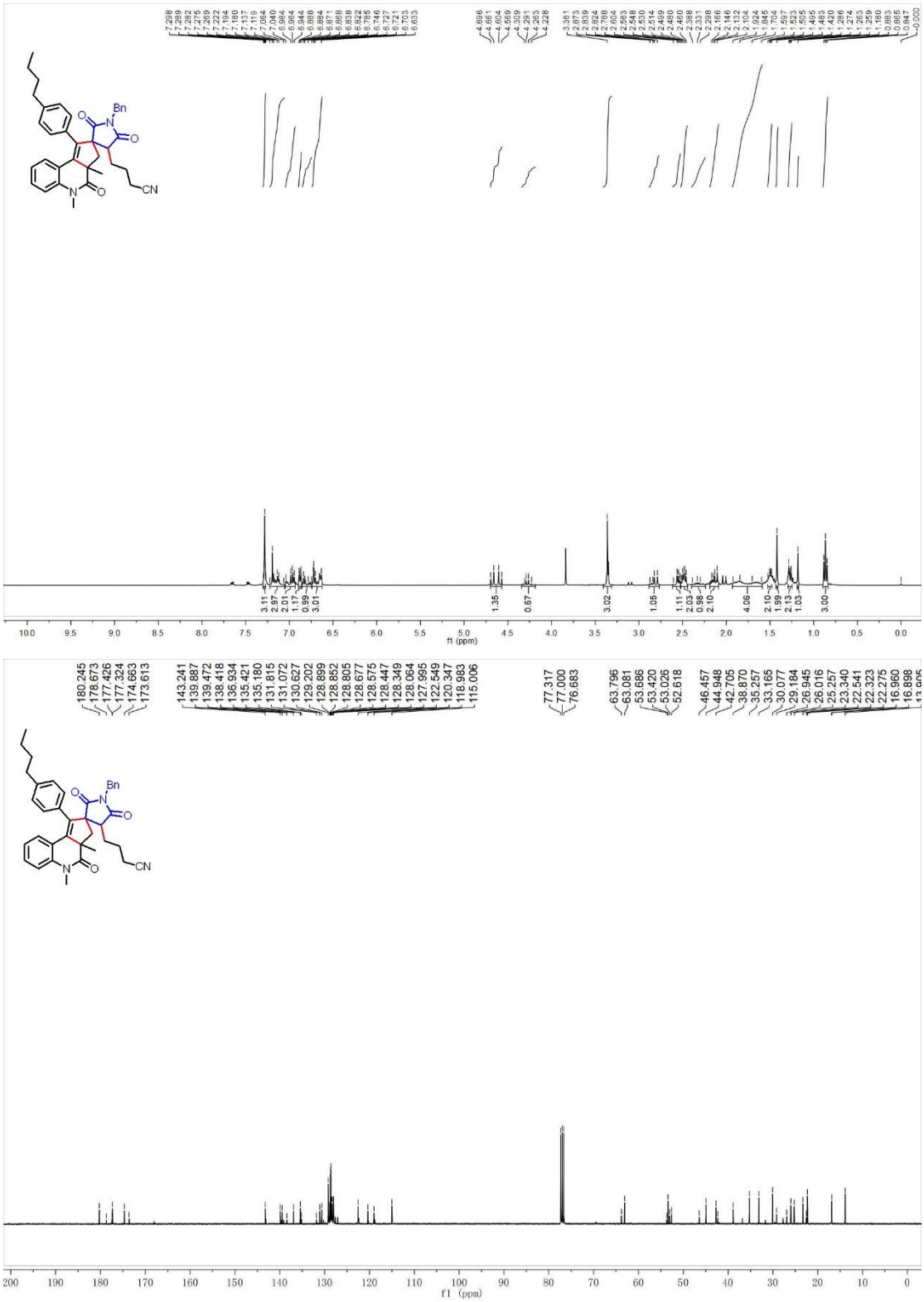
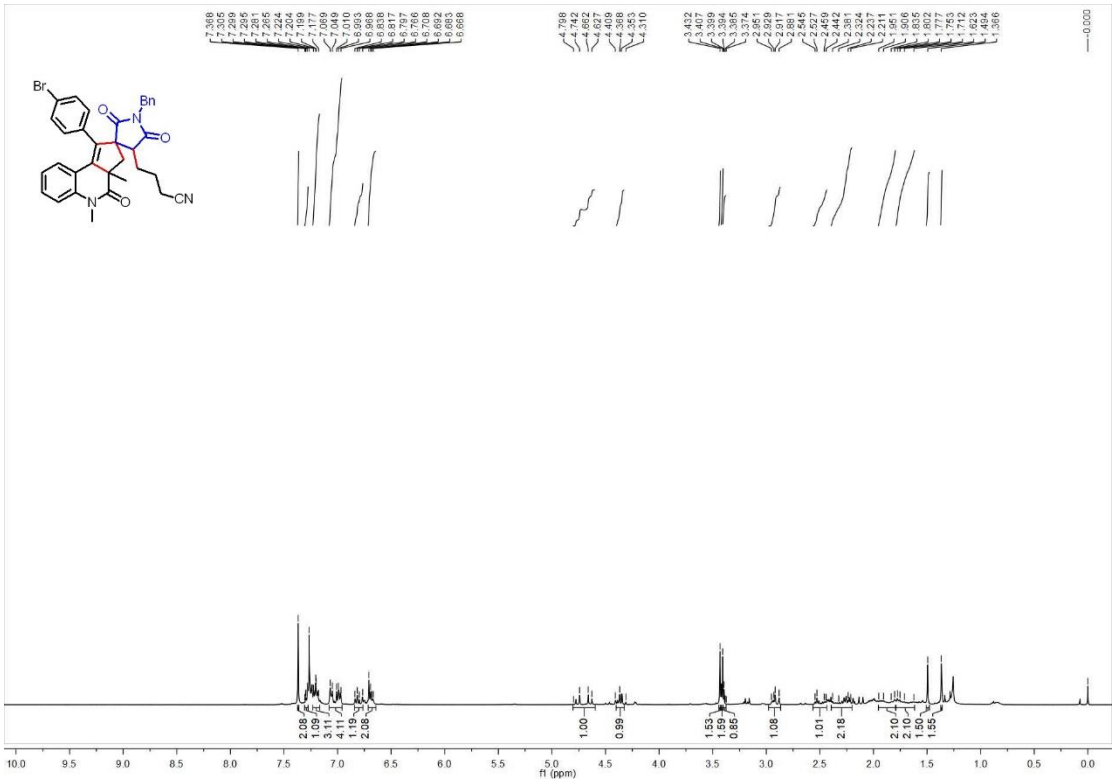
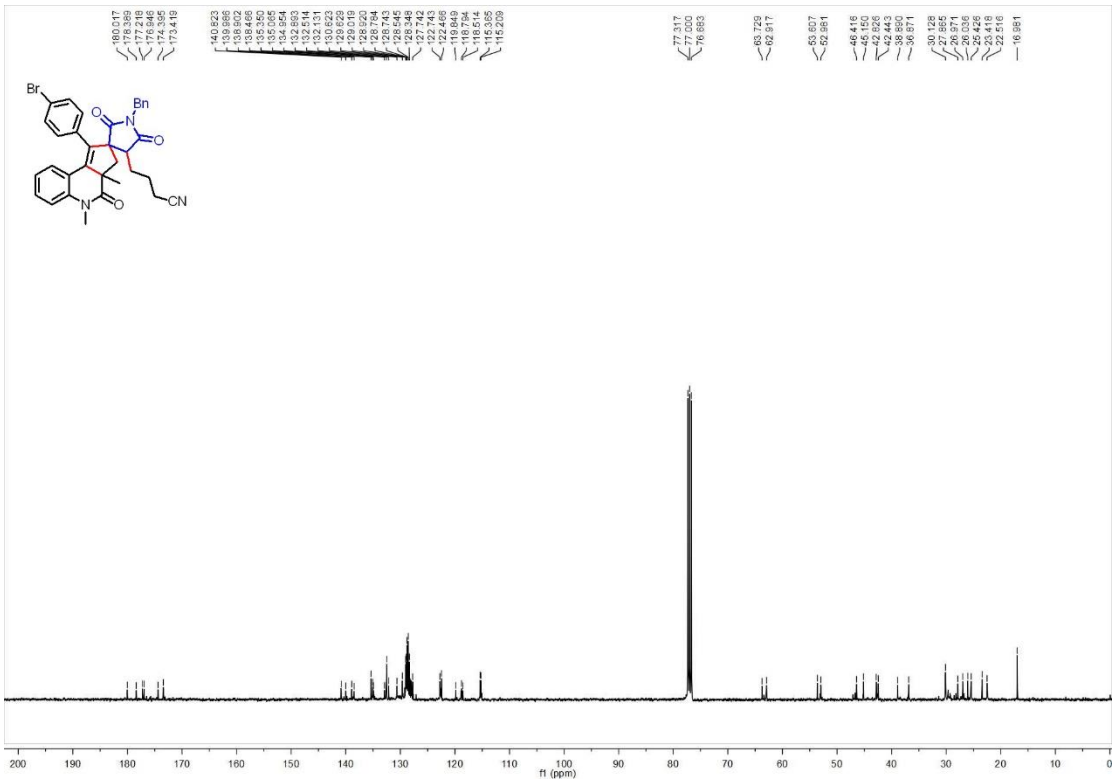
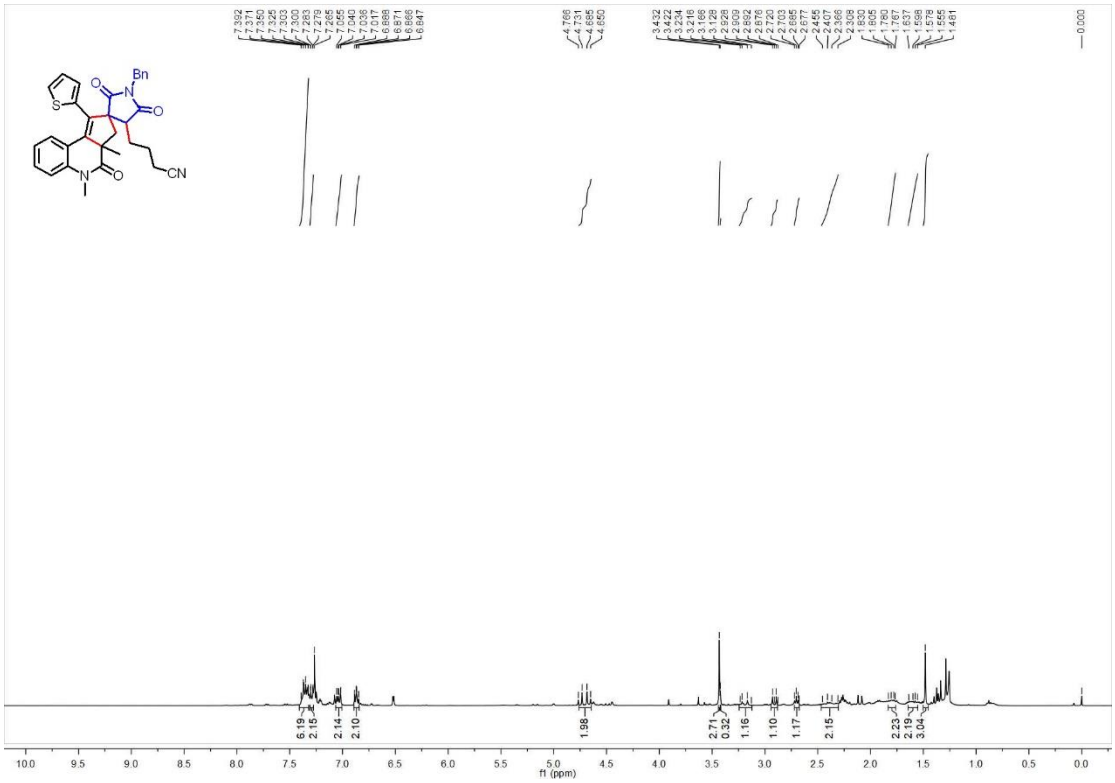


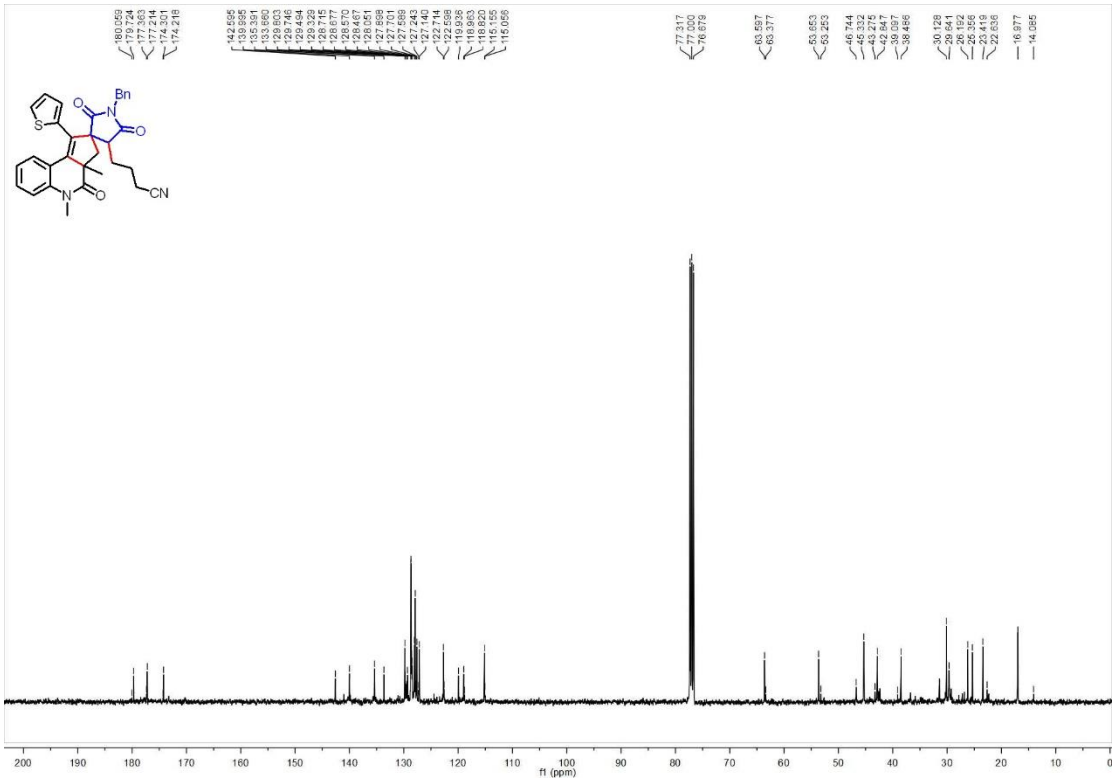
4-(1'-Benzyl-1-(4-bromophenyl)-3a,5-dimethyl-2',4,5'-trioxo-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4v)



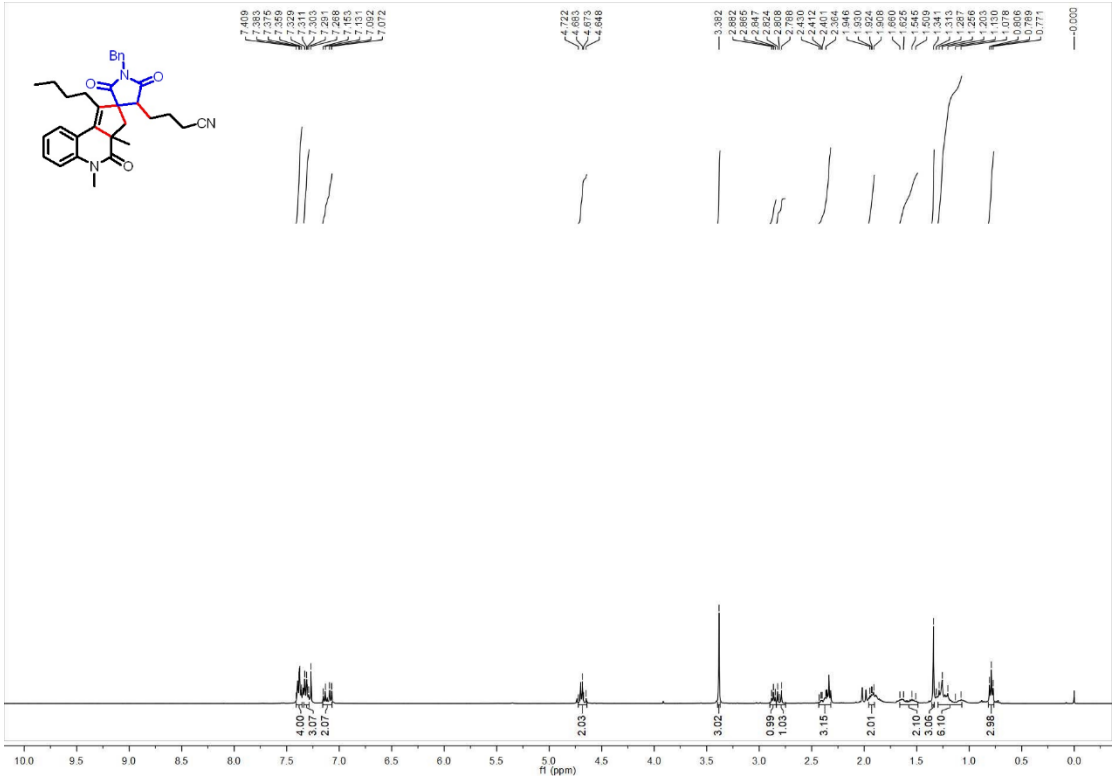


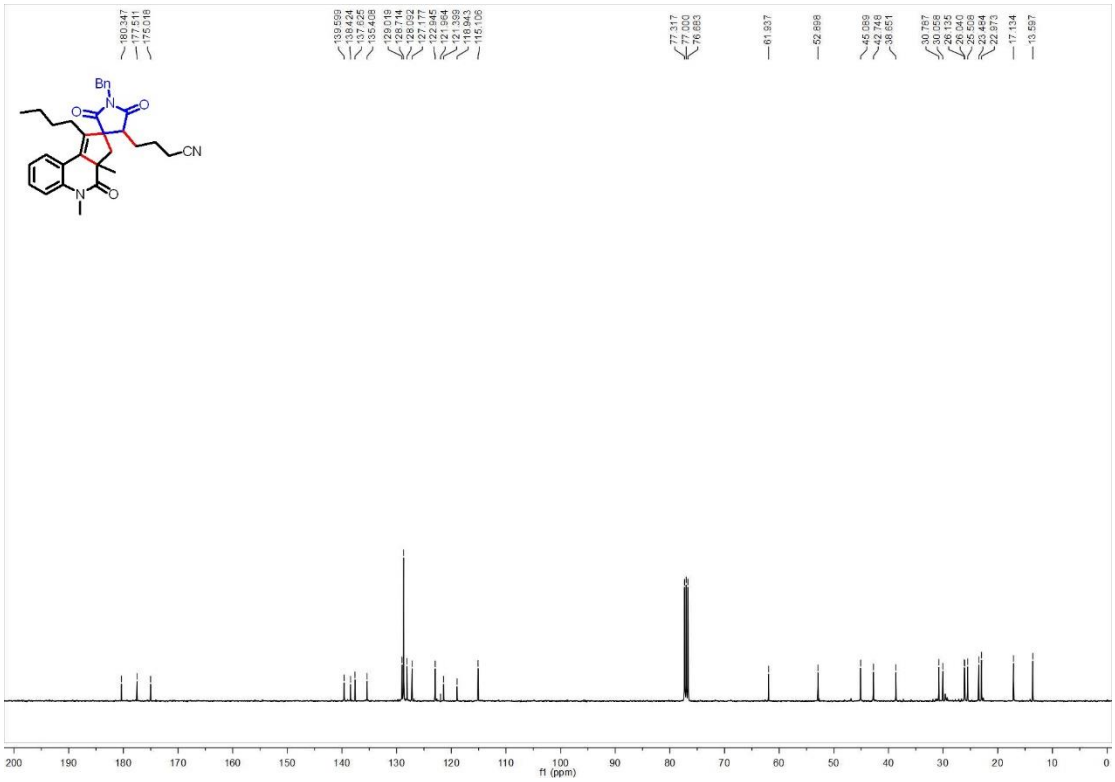
4-(1'-Benzyl-3a,5-dimethyl-2',4,5'-trioxo-1-(thiophen-2-yl)-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4w)



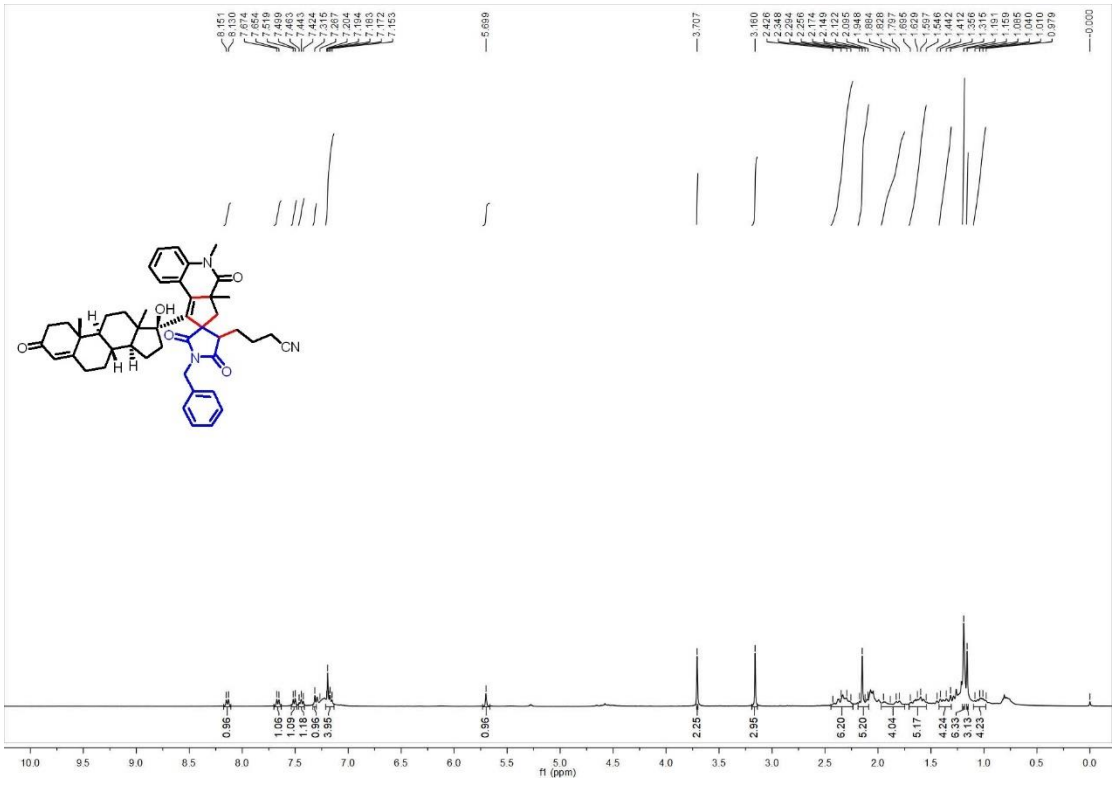


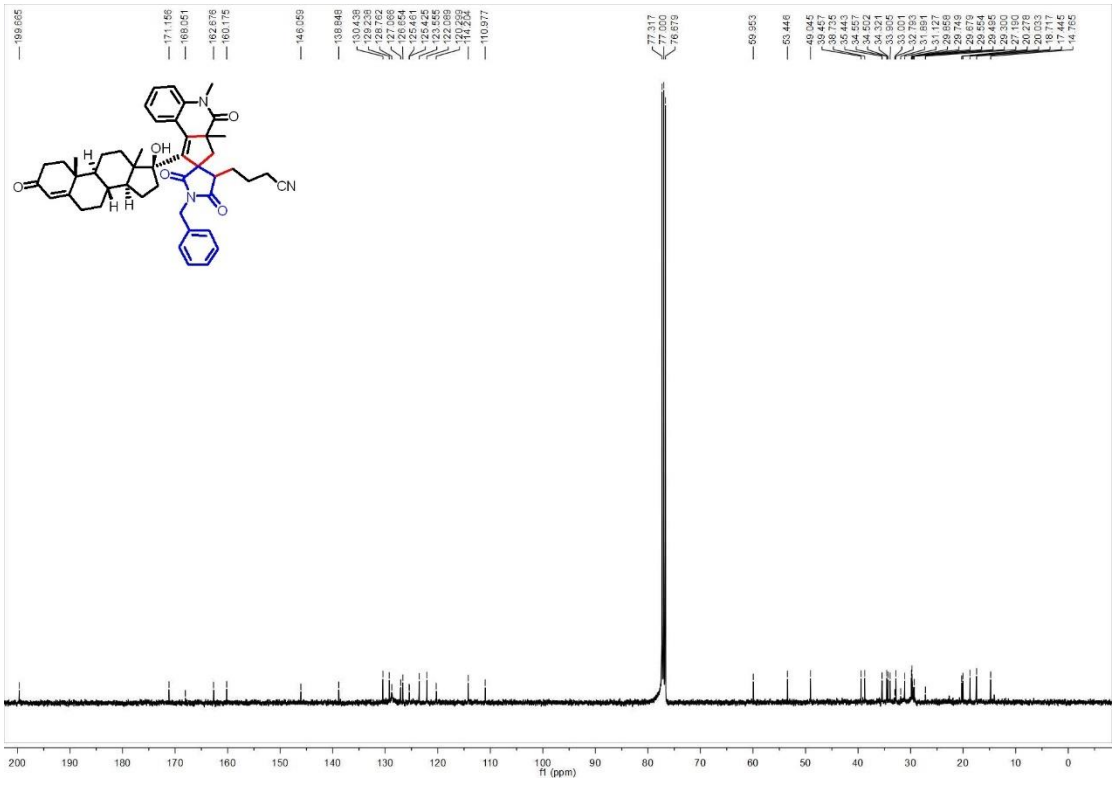
4-(1'-Benzyl-1-butyl-3a,5-dimethyl-2',4,5'-trioxo-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4x)



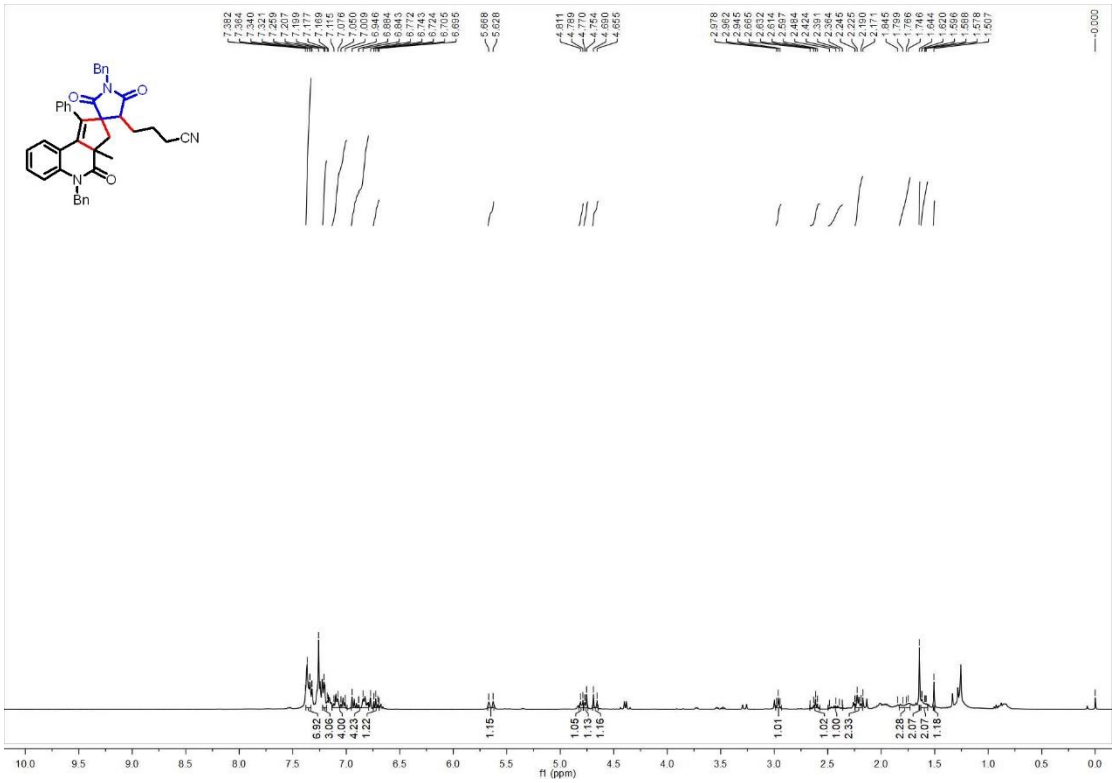


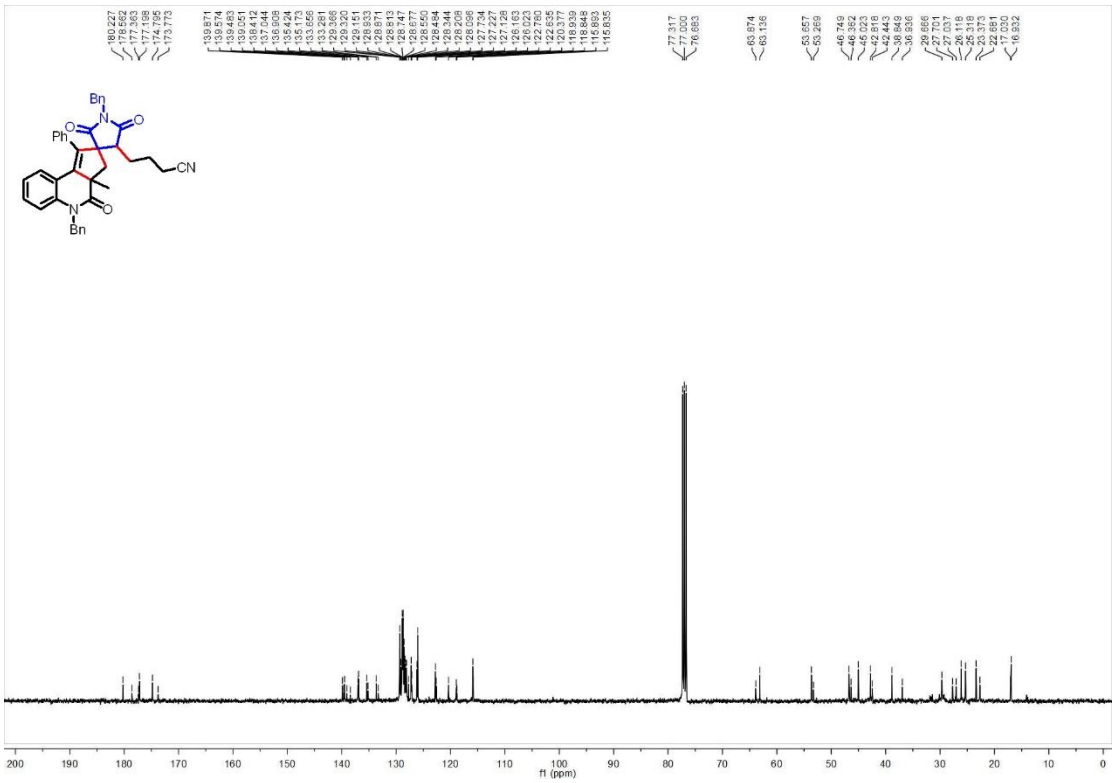
4-(1'-Benzyl-1-((8*R*,9*S*,10*R*,14*S*,17*S*)-17-hydroxy-10,13-dimethyl-3-oxo-2,3,6,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[a]phenanthren-17-yl)-3a,5-dimethyl-2',4,5'-trioxo-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4y)



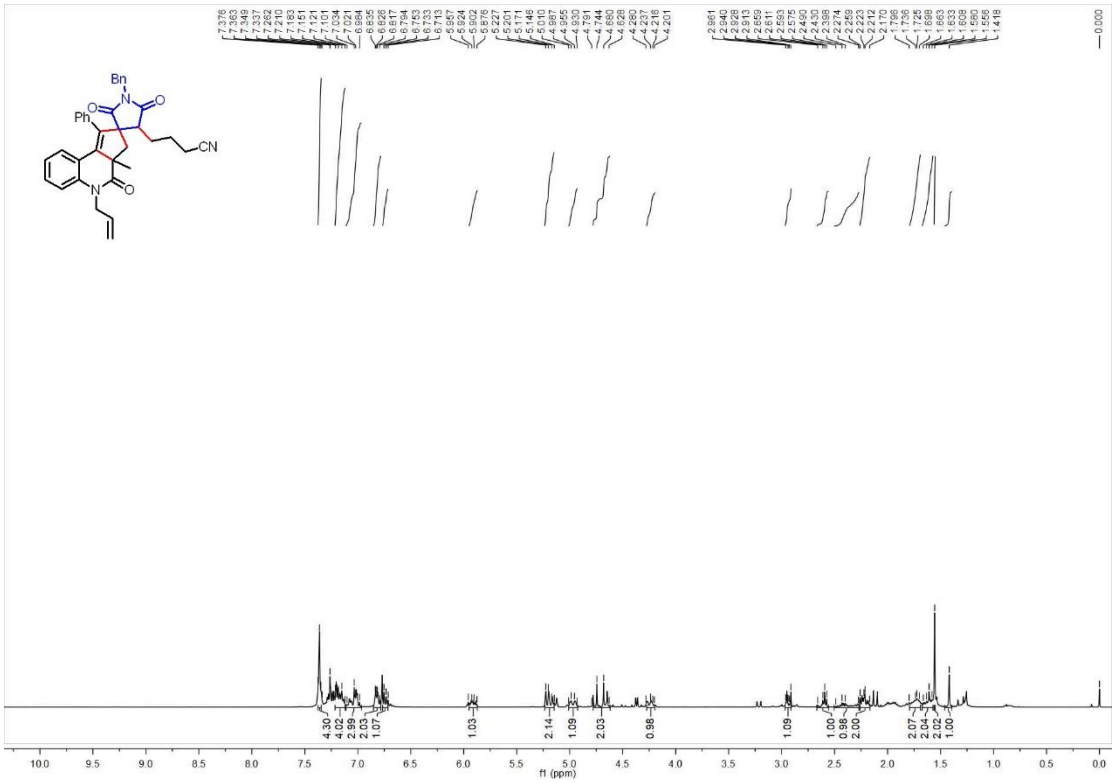


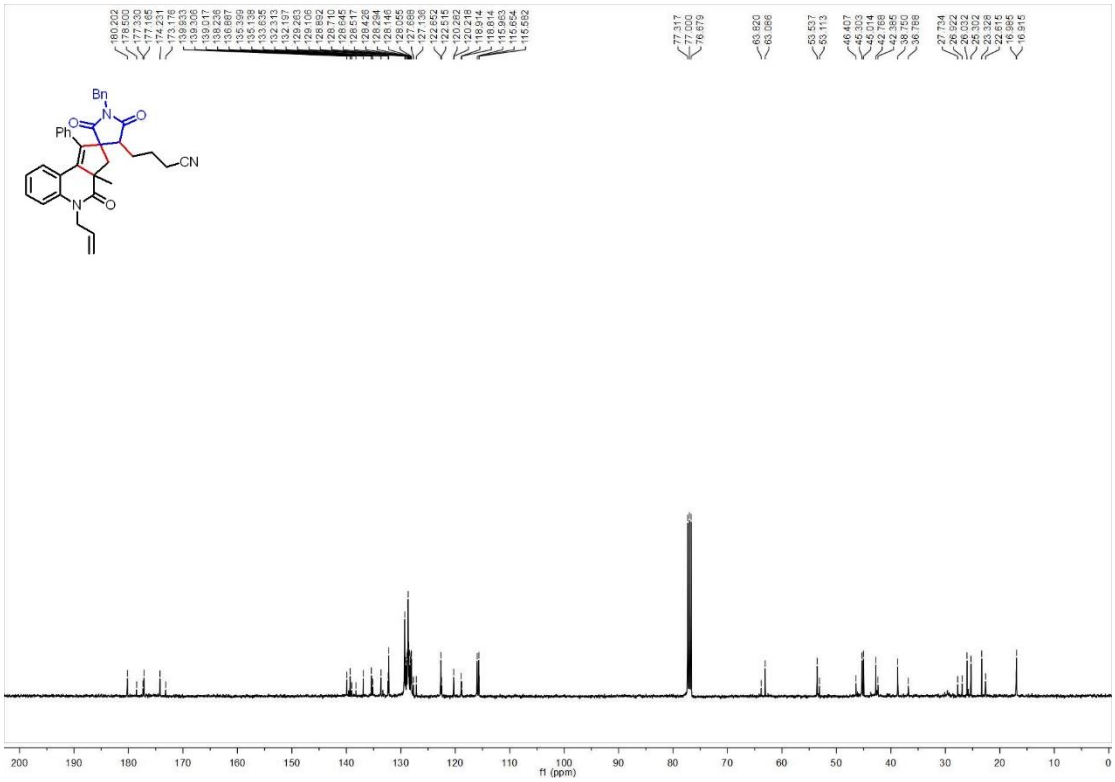
4-(1',5-Dibenzyl-3a-methyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4z)



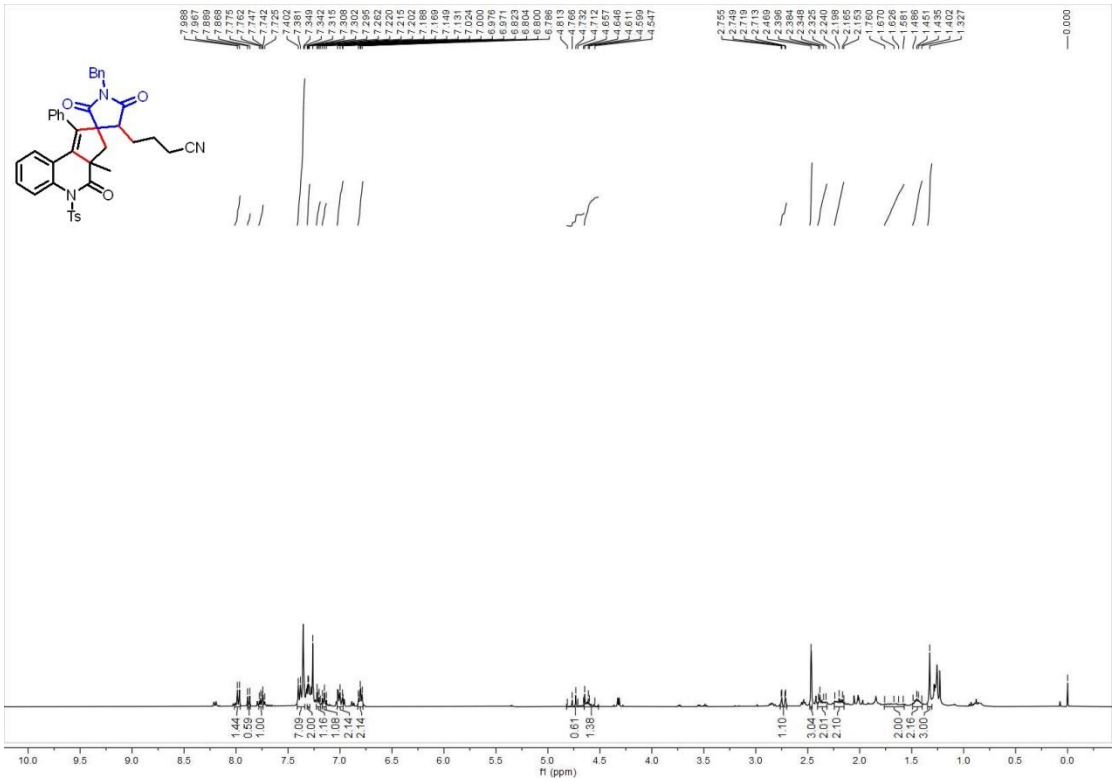


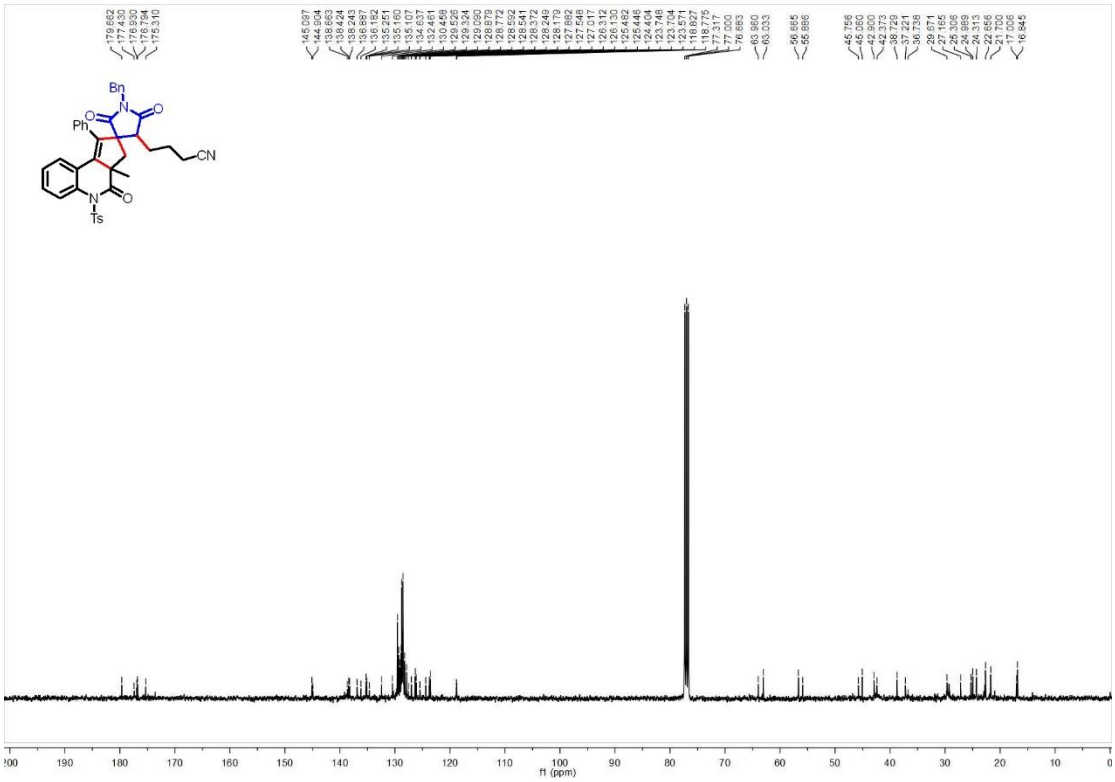
4-(5-Allyl-1'-benzyl-3a-methyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4aa)



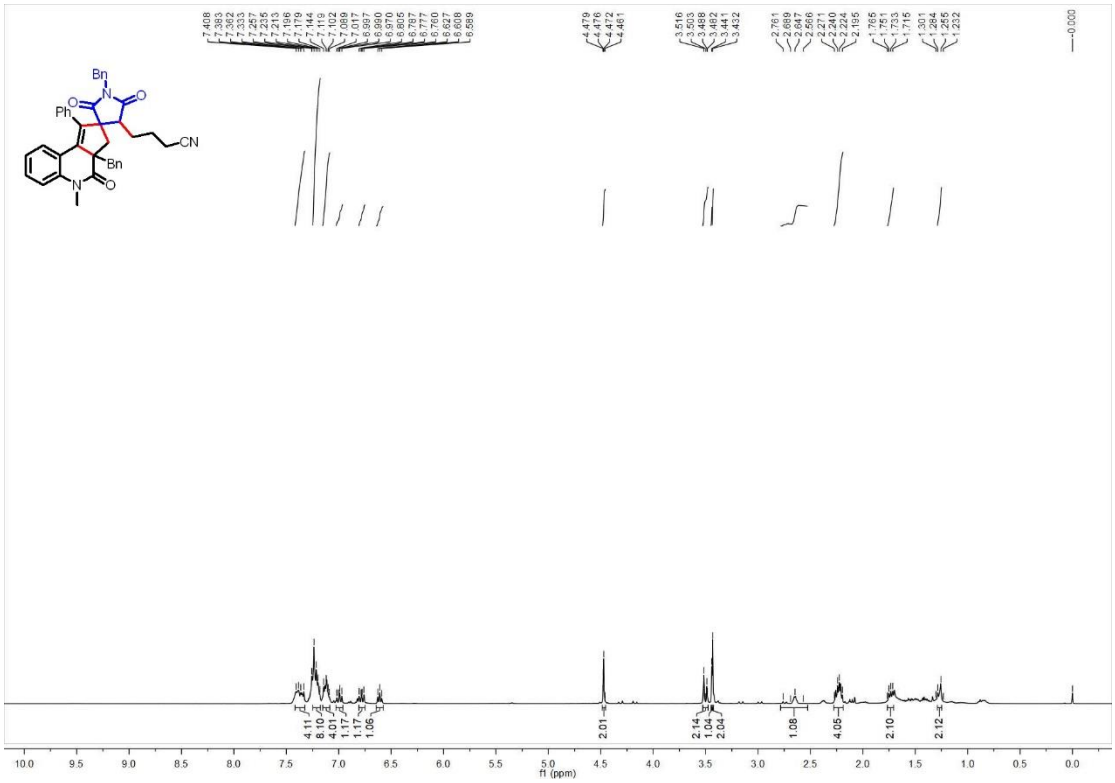


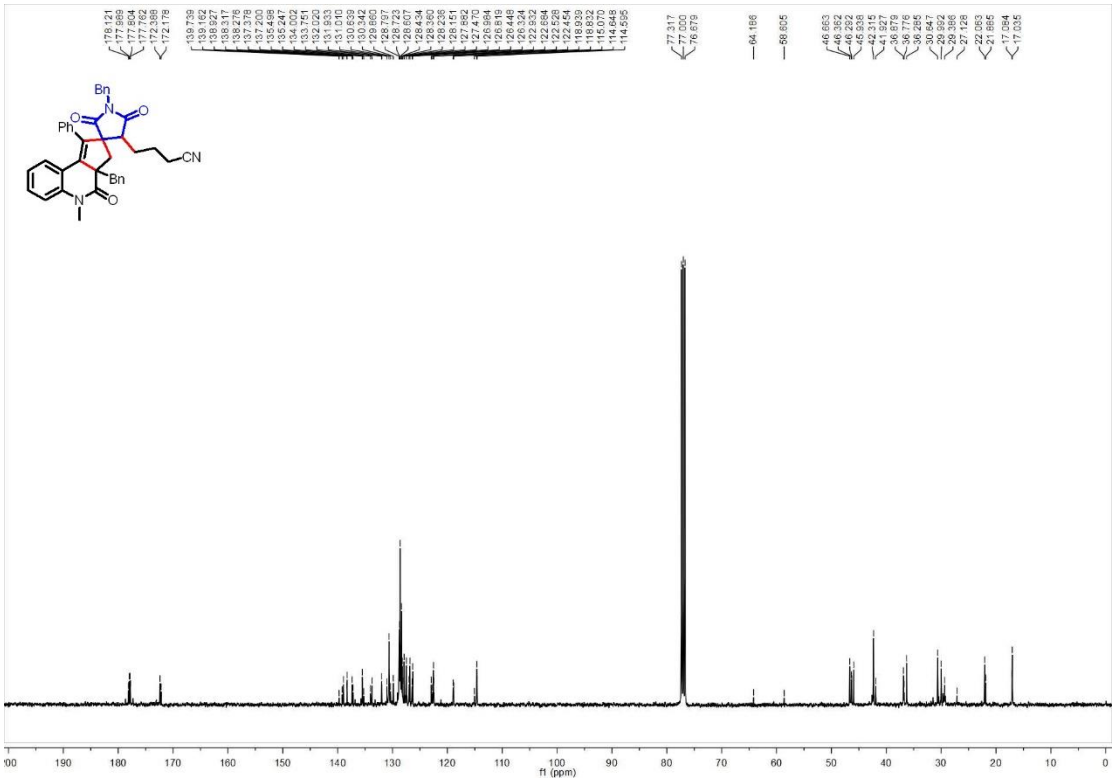
4-(1'-Benzyl-3a-methyl-2',4,5'-trioxo-1-phenyl-5-tosyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4ab)



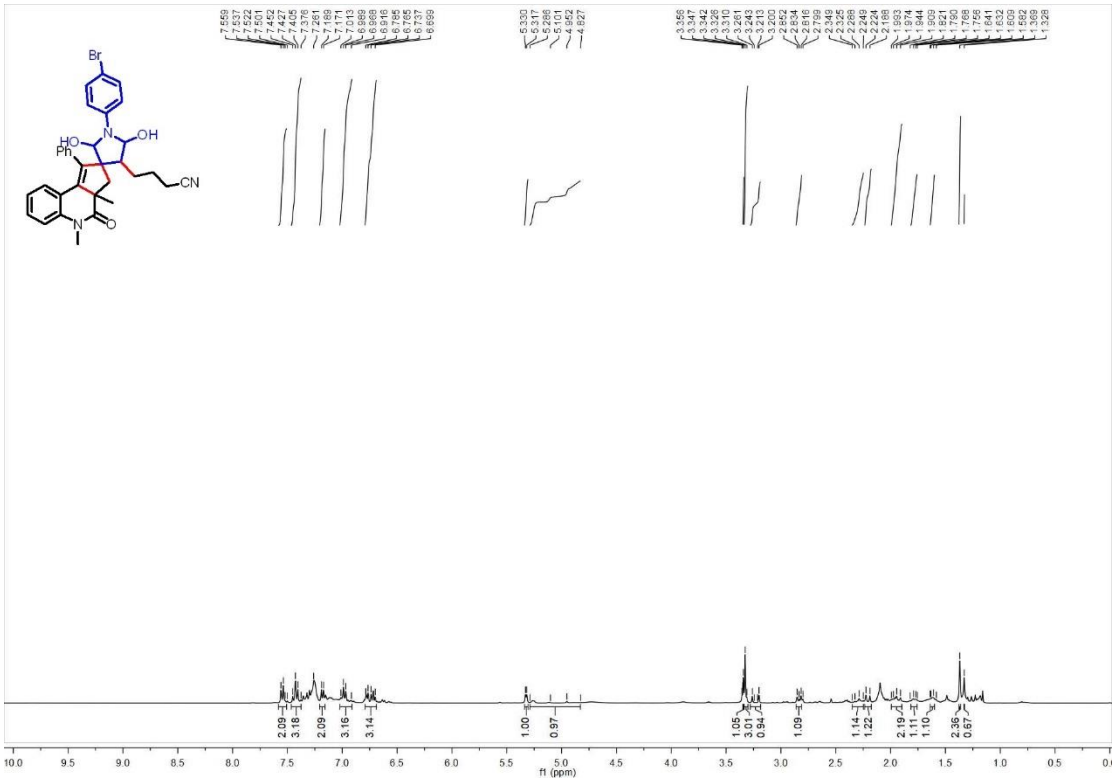


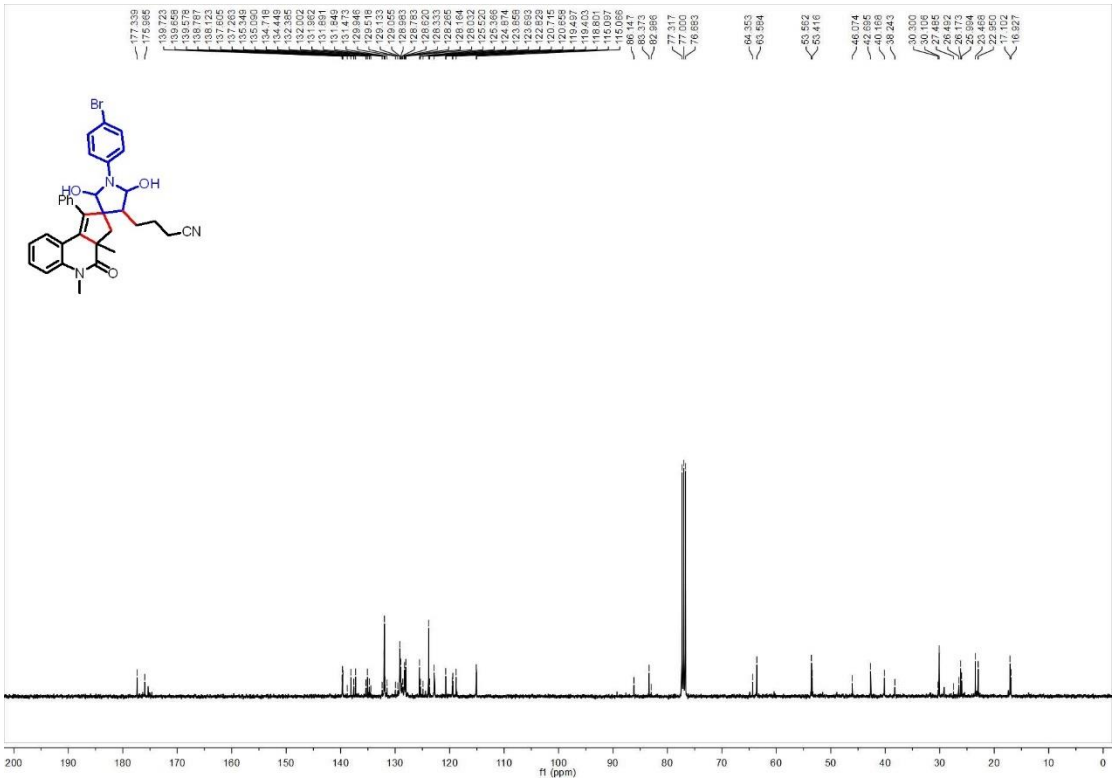
4-(1',3a-Dibenzyl-5-methyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (4ac)



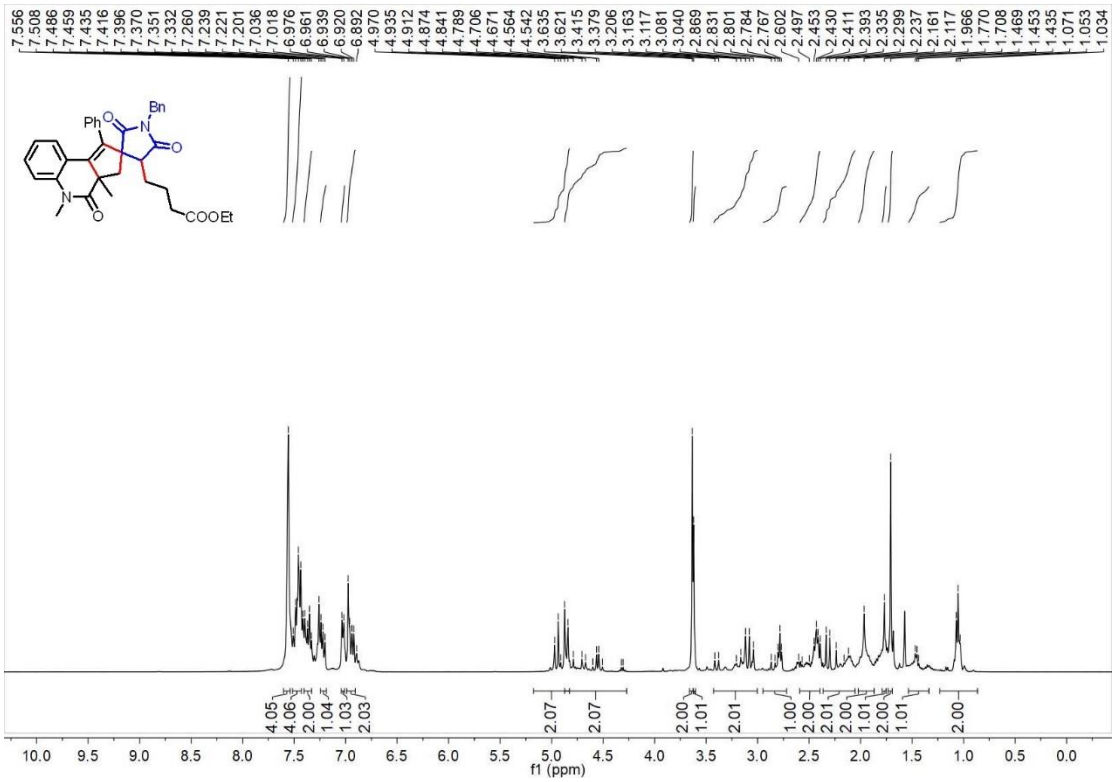


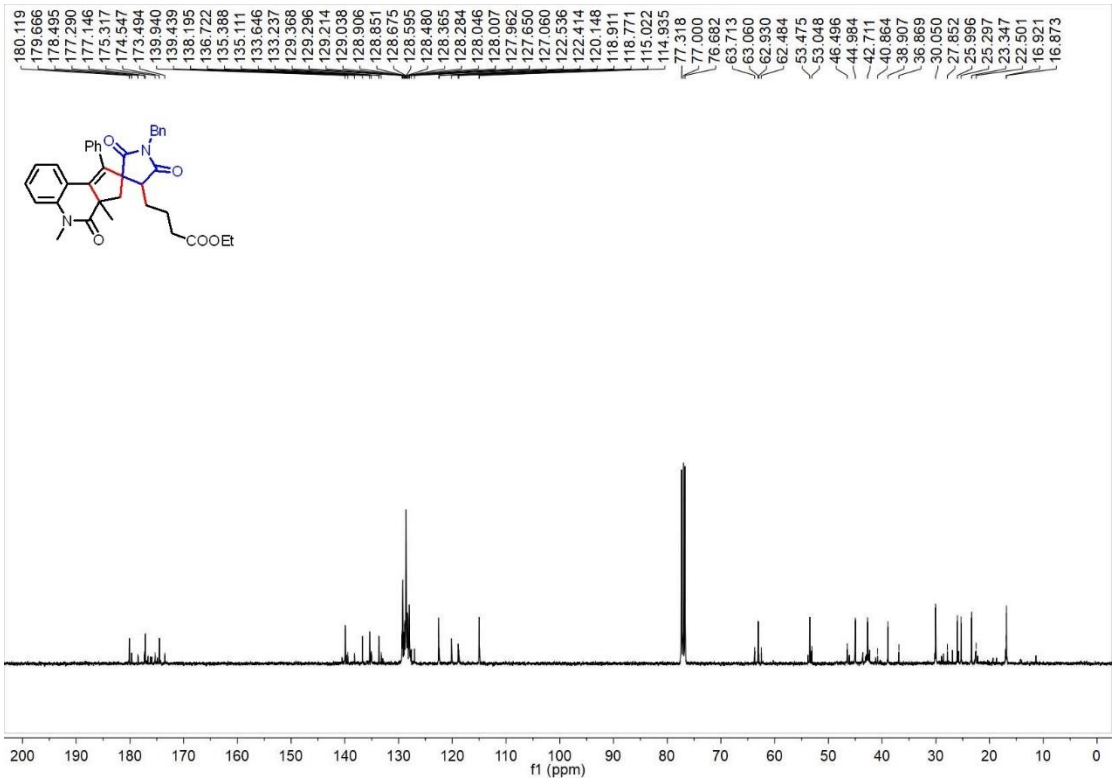
4-(1'-(4-Bromophenyl)-2',5'-dihydroxy-3a,5-dimethyl-4-oxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanenitrile (5a)



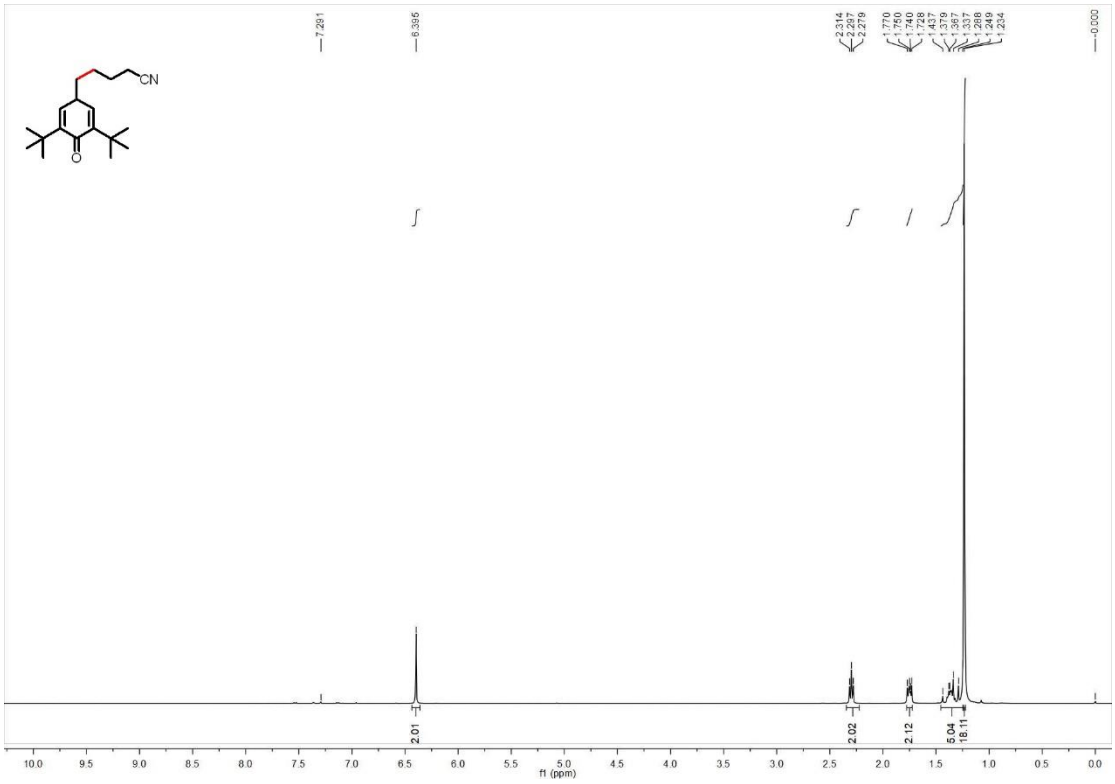


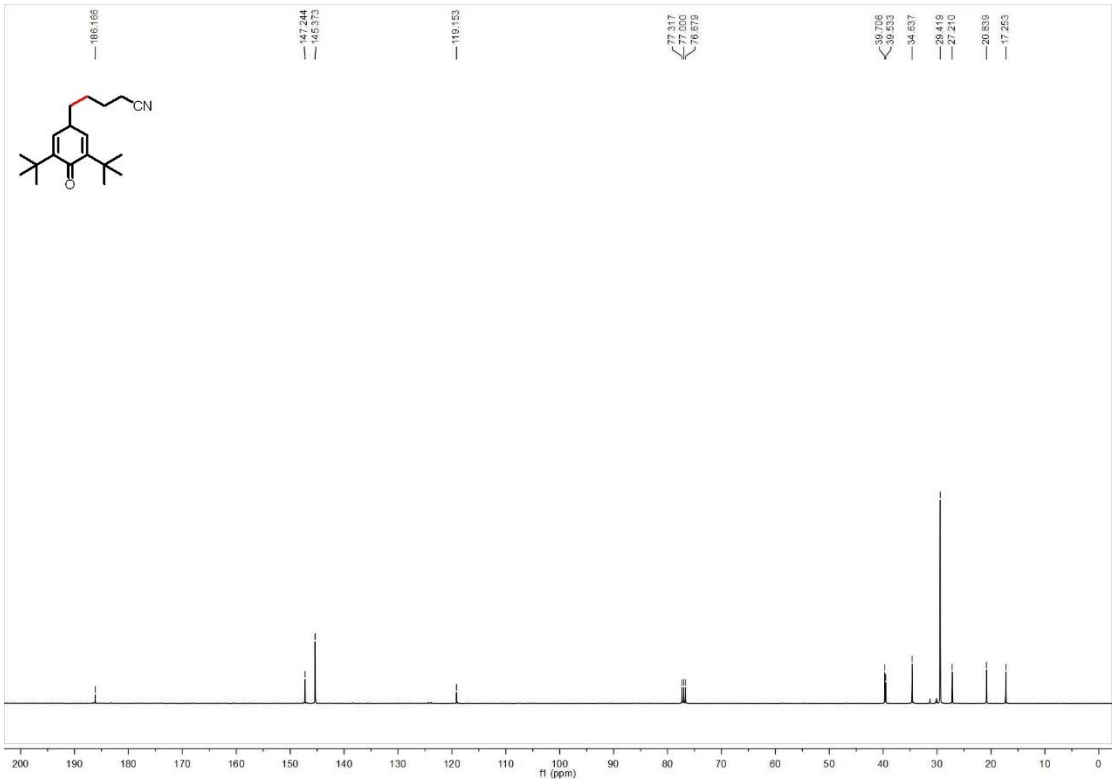
Ethyl 4-(1'-benzyl-3a,5-dimethyl-2',4,5'-trioxo-1-phenyl-3,3a,4,5-tetrahydrospiro[cyclopenta[*c*]quinoline-2,3'-pyrrolidin]-4'-yl)butanoate (6a)



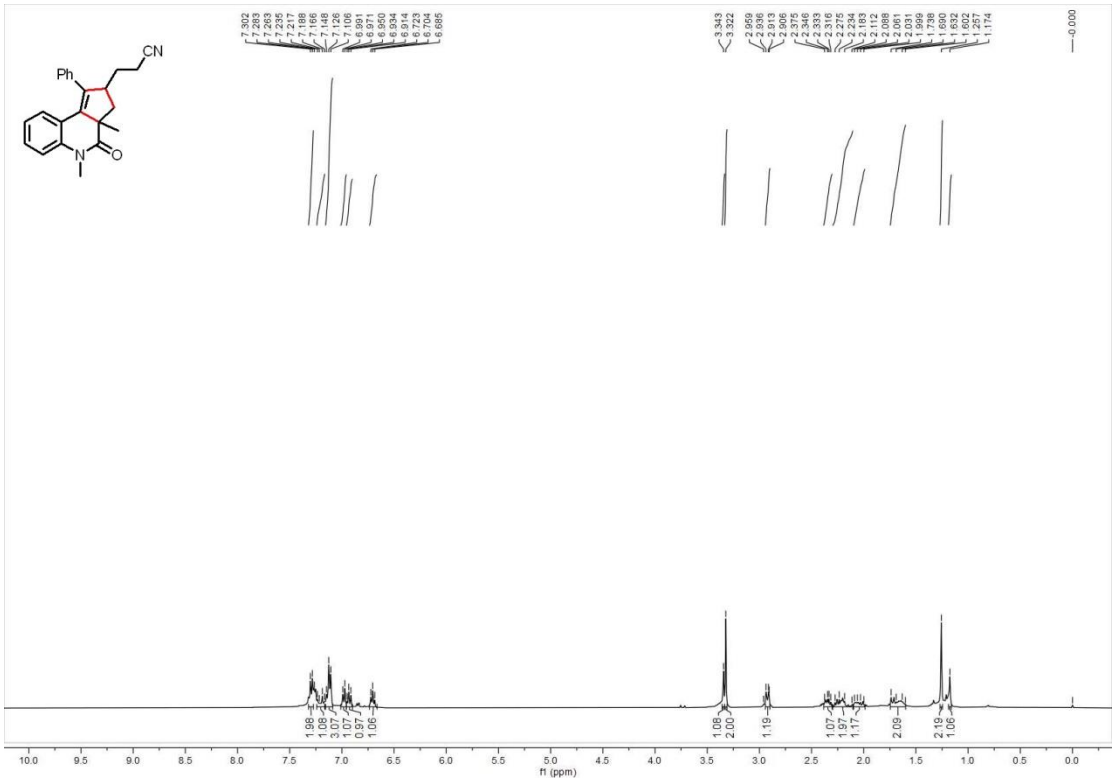


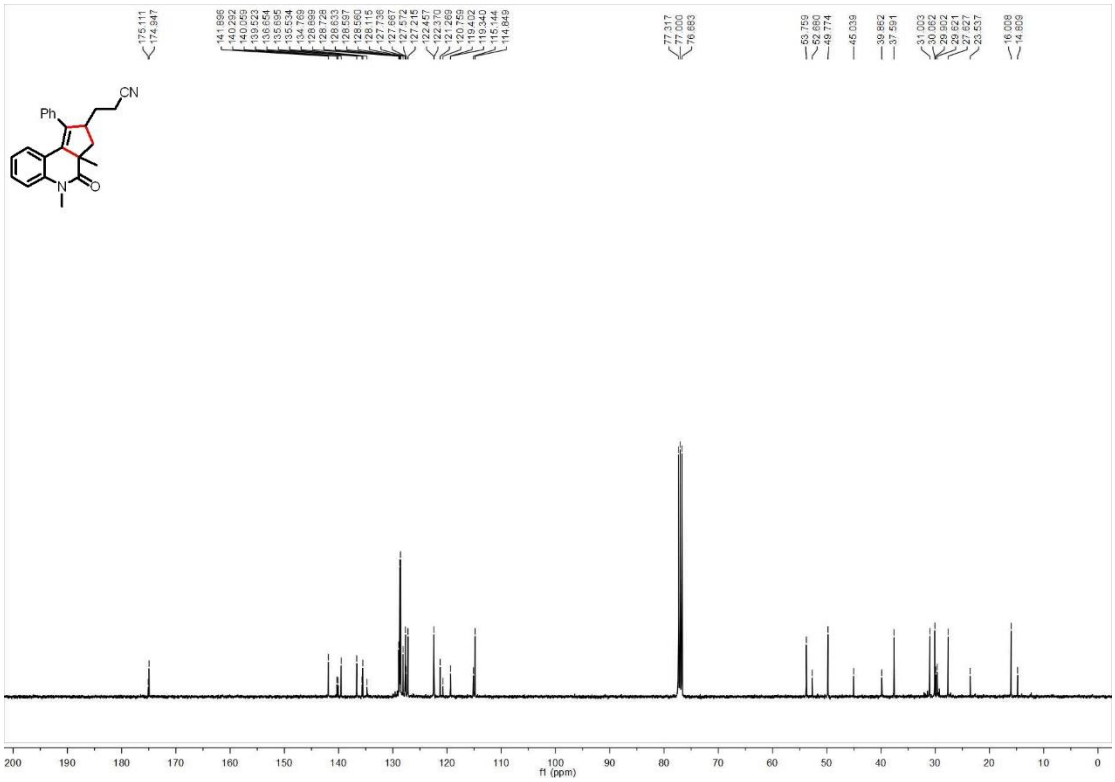
5-(3,5-Di-*tert*-butyl-4-oxocyclohexa-2,5-dien-1-yl)pentanenitrile (7a)



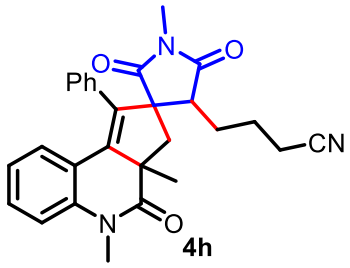


3-(3a,5-Dimethyl-4-oxo-1-phenyl-3,3a,4,5-tetrahydro-2*H*-cyclopenta[*c*]quinolin-2-yl)propanenitrile (8a)





(G) The *X*-ray single-crystal diffraction analysis of product 4h



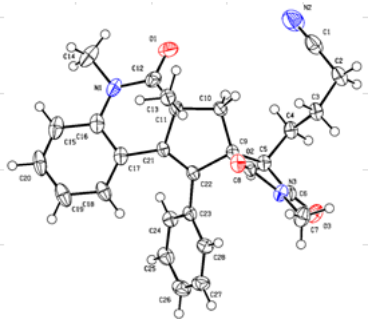


Table 2 Crystal data and structure refinement for **4h**.

Identification code	**4h**
Empirical formula	$C_{28}H_{27}N_3O_3$
Formula weight	453.52
Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	8.6308(9)
b/Å	9.4001(9)
c/Å	28.739(3)
α/°	90
β/°	98.326(3)
γ/°	90
Volume/Å^3	2307.0(4)
Z	4
ρ_{calc}g/cm^3	1.306
μ/mm^{-1}	0.086
F(000)	960.0
Crystal size/mm^3	0.15 × 0.08 × 0.05
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.564 to 52.8
Index ranges	$-10 \leq h \leq 10$, $-11 \leq k \leq 10$, $-35 \leq l \leq 35$
Reflections collected	16976
Independent reflections	4654 [R_{int} = 0.0665, R_{sigma} = 0.0691]
Data/restraints/parameters	4654/0/310
Goodness-of-fit on F^2	1.059
Final R indexes [I>=2σ (I)]	R_1 = 0.0533, wR_2 = 0.1013
Final R indexes [all data]	R_1 = 0.1071, wR_2 = 0.1281
Largest diff. peak/hole / e Å^{-3}	0.20/-0.27

Table 3 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **4h**.

U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
O(2)	5990.6(17)	5722.4(17)	5514.8(6)	30.7(4)
O(3)	1110.8(18)	6661.7(19)	5856.8(6)	35.8(4)
O(1)	8295.1(19)	3687(2)	7316.8(6)	39.1(4)
N(3)	3474(2)	6351(2)	5595.1(7)	27.6(5)
N(1)	8297(2)	1564(2)	6935.2(7)	33.2(5)
C(22)	4754(2)	3320(2)	6082.7(7)	22.2(5)
C(23)	3304(2)	2595(2)	5859.7(8)	23.5(5)
C(21)	6142(2)	2699(2)	6222.2(8)	22.7(5)
C(8)	4897(3)	5703(2)	5737.5(8)	25.4(5)
C(10)	6352(2)	5034(2)	6550.0(8)	25.9(5)
C(9)	4821(2)	4912(2)	6200.5(8)	23.0(5)
C(11)	7321(2)	3688(2)	6487.2(8)	25.3(5)
C(17)	6670(3)	1233(2)	6171.8(8)	27.4(5)
C(5)	3287(2)	5502(2)	6355.8(8)	25.1(5)
C(6)	2441(3)	6204(2)	5918.9(8)	27.2(5)
C(28)	2548(3)	2936(3)	5413.0(8)	28.5(5)
C(4)	3465(3)	6605(2)	6751.6(8)	28.3(5)
C(12)	7983(3)	2998(3)	6952.8(9)	29.8(6)
C(24)	2683(3)	1518(2)	6111.1(8)	28.0(5)
C(3)	4279(3)	7984(2)	6640.1(8)	29.1(6)
C(25)	1352(3)	789(3)	5916.8(9)	33.0(6)
C(13)	8734(3)	3998(3)	6229.0(9)	31.1(6)
C(26)	600(3)	1149(3)	5477.6(9)	36.2(6)
C(16)	7811(3)	720(3)	6532.0(9)	31.7(6)
C(7)	3070(3)	7082(3)	5146.1(9)	37.1(6)
N(2)	6426(3)	7842(3)	7753.3(9)	62.4(8)
C(2)	4571(3)	8996(3)	7061.7(8)	35.2(6)
C(18)	6187(3)	383(2)	5782.8(9)	31.7(6)
C(27)	1194(3)	2214(3)	5222.8(9)	34.2(6)
C(15)	8419(3)	-649(3)	6490.3(10)	39.6(7)
C(20)	7942(3)	-1456(3)	6092.5(11)	43.1(7)
C(1)	5619(4)	8361(3)	7452.5(10)	42.3(7)
C(19)	6825(3)	-954(3)	5739.4(10)	41.0(7)
C(14)	9287(3)	928(3)	7340.0(10)	48.6(8)

Table 4 Anisotropic Displacement Parameters ($Å^2×10^3$) for **4h**.

The Anisotropic displacement factor exponent takes the form:
$-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
O(2)	29.5(9)	26.4(9)	38.4(10)	2.3(7)	12.6(8)	0.5(7)
O(3)	26.1(9)	41.4(11)	40.4(10)	4.6(8)	6.0(8)	8.2(8)
O(1)	29.9(9)	49.5(12)	35.7(10)	-3.6(9)	-3.2(8)	-1.2(8)
N(3)	27.0(10)	27.0(11)	29.2(11)	5.7(9)	5.7(9)	4.7(8)
N(1)	26.8(11)	31.9(13)	40.3(13)	11.0(10)	3.1(9)	7.2(9)
C(22)	25.2(12)	19.2(12)	23.2(12)	-0.8(9)	7.1(10)	-1.7(9)
C(23)	24.3(12)	21.0(13)	26.4(13)	-2.8(10)	7.3(10)	-0.7(9)
C(21)	25.5(12)	18.0(12)	25.7(12)	0.2(9)	7.3(10)	-0.2(9)
C(8)	27.4(12)	18.4(12)	30.8(13)	-1.9(10)	5.8(11)	-1.2(10)
C(10)	24.7(12)	22.5(13)	30.3(13)	-4.7(10)	3.6(10)	-0.6(10)
C(9)	22.8(11)	18.8(12)	28.1(13)	-0.1(10)	6.2(10)	1.2(9)
C(11)	20.4(11)	22.5(13)	32.6(13)	0.8(10)	2.7(10)	1.0(9)
C(17)	24.9(12)	22.6(13)	37.0(14)	3.4(11)	12.6(11)	0.9(10)
C(5)	23.8(12)	23.2(13)	29.5(13)	1.5(10)	8.2(10)	0.0(10)
C(6)	25.4(12)	23.8(13)	33.3(14)	-1.7(10)	7.1(11)	1.0(10)
C(28)	30.4(13)	29.7(14)	25.8(13)	-2.3(10)	5.3(11)	-2.8(11)
C(4)	32.1(13)	24.5(13)	29.9(13)	0.0(10)	10.3(11)	3.2(10)
C(12)	19.3(12)	33.6(15)	36.3(15)	2.1(12)	3.9(11)	1.0(10)
C(24)	28.3(13)	27.0(14)	29.5(13)	0.0(11)	6.5(10)	-0.8(10)
C(3)	36.2(13)	21.4(13)	31.1(14)	0.7(10)	9.7(11)	2.2(10)
C(25)	31.5(13)	27.0(14)	42.6(16)	-2.3(12)	12.5(12)	-6.6(11)
C(13)	24.3(12)	28.0(14)	42.2(15)	-2.2(11)	8.5(11)	-1.1(10)
C(26)	27.5(13)	39.0(16)	43.0(16)	-13.1(12)	8.4(12)	-6.2(11)
C(16)	27.4(13)	24.5(14)	46.4(16)	4.1(12)	15.9(12)	0.5(10)
C(7)	41.1(15)	37.9(16)	33.8(14)	8.8(12)	9.8(12)	8.4(12)
N(2)	97(2)	46.9(17)	38.8(15)	0.1(13)	-4.5(15)	-1.9(15)
C(2)	47.6(15)	25.4(14)	34.7(14)	-4.3(11)	13.3(13)	-1.0(11)
C(18)	36.9(14)	20.9(13)	41.4(15)	-3.7(11)	19.9(12)	-5.2(10)
C(27)	31.2(14)	43.7(16)	26.9(13)	-8.3(12)	1.7(11)	1.2(12)
C(15)	28.4(13)	30.0(15)	64.6(19)	14.3(14)	20.4(13)	5.3(11)
C(20)	41.9(16)	18.3(14)	77(2)	3.0(14)	34.9(16)	0.8(12)
C(1)	64.4(19)	30.7(16)	32.9(15)	-6.1(13)	10.4(15)	-2.1(14)
C(19)	47.0(16)	24.5(15)	59.0(19)	-6.9(13)	32.6(15)	-5.6(12)
C(14)	37.0(15)	56(2)	51.4(18)	21.0(15)	1.8(14)	14.1(14)

Table 5 Bond Lengths for **4h**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O(2)	C(8)	1.215(2)	C(9)	C(5)	1.558(3)
O(3)	C(6)	1.214(3)	C(11)	C(12)	1.522(3)
O(1)	C(12)	1.227(3)	C(11)	C(13)	1.544(3)
N(3)	C(8)	1.379(3)	C(17)	C(16)	1.407(3)
N(3)	C(6)	1.386(3)	C(17)	C(18)	1.388(3)
N(3)	C(7)	1.459(3)	C(5)	C(6)	1.510(3)
N(1)	C(12)	1.378(3)	C(5)	C(4)	1.531(3)
N(1)	C(16)	1.417(3)	C(28)	C(27)	1.393(3)
N(1)	C(14)	1.467(3)	C(4)	C(3)	1.531(3)
C(22)	C(23)	1.485(3)	C(24)	C(25)	1.385(3)
C(22)	C(21)	1.341(3)	C(3)	C(2)	1.532(3)
C(22)	C(9)	1.534(3)	C(25)	C(26)	1.376(3)
C(23)	C(28)	1.391(3)	C(26)	C(27)	1.382(3)
C(23)	C(24)	1.395(3)	C(16)	C(15)	1.401(3)
C(21)	C(11)	1.502(3)	N(2)	C(1)	1.138(4)
C(21)	C(17)	1.465(3)	C(2)	C(1)	1.463(4)
C(8)	C(9)	1.534(3)	C(18)	C(19)	1.385(3)
C(10)	C(9)	1.544(3)	C(15)	C(20)	1.384(4)
C(10)	C(11)	1.541(3)	C(20)	C(19)	1.378(4)

Table 6 Bond Angles for **4h**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C(8)	N(3)	C(6)	112.89(19)	C(12)	C(11)	C(13)	106.29(18)
C(8)	N(3)	C(7)	123.99(19)	C(16)	C(17)	C(21)	116.4(2)
C(6)	N(3)	C(7)	123.10(19)	C(18)	C(17)	C(21)	124.0(2)
C(12)	N(1)	C(16)	122.8(2)	C(18)	C(17)	C(16)	119.5(2)
C(12)	N(1)	C(14)	117.7(2)	C(6)	C(5)	C(9)	104.25(17)
C(16)	N(1)	C(14)	119.3(2)	C(6)	C(5)	C(4)	107.80(19)
C(23)	C(22)	C(9)	123.02(19)	C(4)	C(5)	C(9)	117.12(18)
C(21)	C(22)	C(23)	126.2(2)	O(3)	C(6)	N(3)	123.5(2)
C(21)	C(22)	C(9)	110.80(19)	O(3)	C(6)	C(5)	127.6(2)
C(28)	C(23)	C(22)	123.1(2)	N(3)	C(6)	C(5)	108.71(18)
C(28)	C(23)	C(24)	118.7(2)	C(23)	C(28)	C(27)	120.3(2)
C(24)	C(23)	C(22)	118.2(2)	C(5)	C(4)	C(3)	114.72(18)
C(22)	C(21)	C(11)	113.1(2)	O(1)	C(12)	N(1)	121.9(2)
C(22)	C(21)	C(17)	131.1(2)	O(1)	C(12)	C(11)	122.2(2)
C(17)	C(21)	C(11)	115.78(19)	N(1)	C(12)	C(11)	115.8(2)
O(2)	C(8)	N(3)	124.3(2)	C(25)	C(24)	C(23)	120.6(2)
O(2)	C(8)	C(9)	126.8(2)	C(4)	C(3)	C(2)	112.83(19)
N(3)	C(8)	C(9)	108.85(18)	C(26)	C(25)	C(24)	120.1(2)
C(11)	C(10)	C(9)	106.89(18)	C(25)	C(26)	C(27)	120.2(2)
C(22)	C(9)	C(8)	106.64(18)	C(17)	C(16)	N(1)	120.2(2)
C(22)	C(9)	C(10)	102.56(17)	C(15)	C(16)	N(1)	120.9(2)
C(22)	C(9)	C(5)	113.82(17)	C(15)	C(16)	C(17)	118.9(2)
C(8)	C(9)	C(10)	112.81(18)	C(1)	C(2)	C(3)	111.5(2)
C(8)	C(9)	C(5)	102.78(17)	C(19)	C(18)	C(17)	121.2(3)
C(10)	C(9)	C(5)	118.02(18)	C(26)	C(27)	C(28)	120.0(2)
C(21)	C(11)	C(10)	103.21(17)	C(20)	C(15)	C(16)	120.2(3)
C(21)	C(11)	C(12)	108.83(19)	C(19)	C(20)	C(15)	120.9(2)
C(21)	C(11)	C(13)	113.40(18)	N(2)	C(1)	C(2)	178.7(3)
C(10)	C(11)	C(13)	112.40(18)	C(20)	C(19)	C(18)	119.3(3)
C(12)	C(11)	C(10)	112.83(19)				

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **4h**.

Atom	x	y	z	U(eq)
H(10A)	6939.27	5896.58	6482.51	31
H(10B)	6117.63	5095.59	6876.54	31
H(5)	2643.89	4688.01	6444.91	30
H(28)	2957.23	3664.36	5236.65	34
H(4A)	4067.93	6172	7035.78	34
H(4B)	2411.95	6842.25	6826.92	34
H(24)	3178.18	1283.45	6418.49	34
H(3A)	3624.8	8474.63	6376.81	35
H(3B)	5293.6	7748.45	6536.31	35
H(25)	956.51	37.56	6087.1	40
H(13A)	9251.97	3101.45	6169.96	47
H(13B)	9475.75	4617.63	6424.08	47
H(13C)	8369.89	4469.91	5929.04	47
H(26)	-330.57	665.19	5349.05	43
H(7A)	2885.87	8092.07	5202.72	56
H(7B)	2120.03	6659.14	4972.89	56
H(7C)	3933.56	6986.63	4961.19	56
H(2A)	5039.37	9889.92	6964.6	42
H(2B)	3560.17	9233.51	7167.22	42
H(18)	5403.79	724.5	5542.1	38
H(27)	679.4	2452.99	4917.97	41
H(15)	9162.4	-1024.01	6735.81	48
H(20)	8389.8	-2368.35	6062.58	52
H(19)	6496.66	-1518.75	5468.97	49
H(14A)	10303.15	669.58	7250.49	73
H(14B)	8775.54	73.96	7441.11	73
H(14C)	9442.16	1615.57	7598.9	73