Radical cyclization of 1,6-dienes with azobis(alkylcarbonitriles) on-water under additive-free conditions

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Supporting Information

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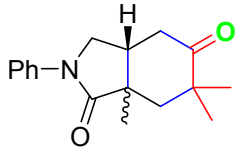
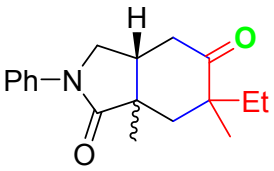
(A) Typical experimental procedure for the radical cyclization

To a Schlenk tube were added 1,6-dienes **1** (0.2 mmol), azobis(alkylcarbonitriles) **2** (0.4 mmol) and H_2O (2.0 mL). Then the tube was stirred at 85 ^oC sealed in air for the indicated time until complete consumption of starting material as monitored by TLC and/or GC-MS analysis. After the reaction was finished, the mixture was extracted three times with EtOAc. The organic layer was dried over Na_2SO_4, filtration and evaporation of the solvent. The mixture was purified by flash column chromatography over silica gel (hexane/ethyl acetate = 8:1) to afford the desired products **3**.

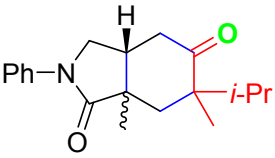
(B) Analytical data



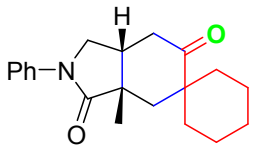
6,6,7a-Trimethyl-2-phenylhexahydro-1H-isoindole-1,5(4H)-dione (3aa), yellow solid (0.0444 g, 82% yield, d.r. = 4:1); ^1H NMR (500 MHz, $CDCl_3$) δ: 7.67-7.61 (m, 2H), 7.38 (t, J = 8.0 Hz, 2H), 7.17 (t, J = 7.5 Hz, 1H), 4.17-4.13 (m, 0.2H), 4.09-4.05 (m, 0.8H), 3.44-3.41 (m, 0.2H), 3.39-3.37 (m, 0.8H), 2.66-2.61 (m, 1H), 2.55-2.50 (m, 1H), 2.38 (t, J = 15.0 Hz, 1H), 1.78 (t, J = 11.5 Hz, 1.2H), 1.56 (t, J = 9.5 Hz, 0.8H), 1.35 (d, J = 1.0 Hz, 2.4H), 1.30 (d, J = 1.0 Hz, 0.6H), 1.19 (s, 0.6H), 1.34 (s, 2.4H), 1.12 (s, 2.4H), 1.09 (s, 0.6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 215.4, 214.2, 177.4, 176.5, 139.4, 139.3, 129.0, 128.9, 124.9, 124.8, 120.0, 119.7, 51.5, 51.2, 45.6, 44.1, 43.9, 43.7, 43.6, 40.3, 38.8, 26.7, 26.1, 25.9, 25.5, 25.0, 23.5; HRMS *m/z* (ESI) calcd for $C_{17}H_{22}NO_2$ ($[M+H]^+$) 272.1645, found 272.1643.



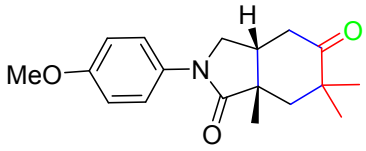
6-Ethyl-6,7a-dimethyl-2-phenylhexahydro-1H-isoindole-1,5(4H)-dione (3ab), yellow solid (0.0410 g, 72% yield, d.r. = 2:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.65-7.60 (m, 2H), 7.41-7.36 (m, 2H), 7.19-7.15 (m, 1H), 4.10-4.03 (m, 1H), 3.40-3.36 (m, 1H), 2.70-2.59 (m, 1H), 2.54-2.43 (m, 2H), 1.69-1.63 (m, 2H), 1.56-1.50 (m, 2H), 1.30 (s, 2H), 1.26 (s, 1H), 1.07 (s, 2H), 1.02 (s, 1H), 0.88 (t, J = 7.5 Hz, 1H), 0.79 (t, J = 7.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 215.8, 215.1, 177.6, 177.4, 139.5, 139.2, 129.0 (2), 124.9 (2), 120.1 (2), 51.6, 51.3, 47.8, 46.9, 44.1, 43.8, 43.3, 42.8, 41.1, 40.8, 39.4, 38.0, 31.4, 31.0, 26.6, 25.4, 22.7, 22.1, 8.4, 8.1; HRMS *m/z* (ESI) calcd for $C_{18}H_{24}NO_2$ ($[M+H]^+$) 286.1802, found 286.1798.



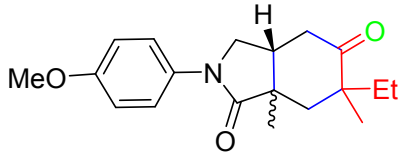
6-Isopropyl-6,7a-dimethyl-2-phenylhexahydro-1H-isoindole-1,5(4H)-dione (3ac), yellow solid (0.0425 g, 71% yield, d.r. = 1.5:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.58-7.52 (m, 2H), 7.35-7.29 (m, 2H), 7.13-7.07 (m, 1H), 4.05-3.94 (m, 1H), 3.33-3.29 (m, 1H), 2.75-2.62 (m, 1H), 2.54-2.47 (m, 1H), 2.41-2.35 (m, 1H), 1.66-1.54 (m, 3H), 1.21 (s, 1.8H), 1.18 (s, 1.2H), 1.05 (s, 1.8H), 0.97 (s, 1.2H), 0.84-0.82 (m, 3.6H), 0.77 (d, J = 6.5 Hz, 1.2H), 0.71 (d, J = 6.0 Hz, 1.2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 215.9, 215.5, 177.6, 177.4, 139.5, 139.1, 129.0 (2), 124.9, 124.8, 120.1, 119.9, 51.6, 51.3, 49.1, 48.0, 47.9, 47.4, 45.4, 44.2 (2), 41.2, 40.9, 40.0, 38.1, 25.1, 24.9, 24.8, 24.7, 24.3, 24.0, 23.6, 23.3; HRMS *m/z* (ESI) calcd for $C_{19}H_{26}NO_2$ ($[M+H]^+$) 300.1958, found 300.1960.



3a'-Methyl-2'-phenylhexahydrospiro[cyclohexane-1,5'-isoindole]-3',6'-dione (3ad), yellow solid (0.0317 g, 51% yield, d.r. > 20:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.61 (d, J = 8.0 Hz, 2H), 7.39 (t, J = 8.0 Hz, 2H), 7.17 (t, J = 7.5 Hz, 1H), 4.07-4.03 (m, 1H), 3.39-3.36 (m, 1H), 2.66-2.61 (m, 1H), 2.58-2.56 (m, 2H), 1.81-1.58 (m, 12H), 1.32 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 215.6, 177.3, 139.4, 129.0, 124.8, 120.0, 51.5, 48.0, 40.4, 39.6, 35.5, 34.8, 25.7, 25.6 (2), 24.8; HRMS *m/z* (ESI) calcd for $C_{20}H_{26}NO_2$ ([M+H]$^+$) 312.1958, found 312.1956.

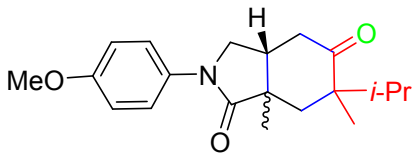


2-(4-Methoxyphenyl)-6,6,7a-trimethylhexahydro-1H-isoindole-1,5(4H)-dione (3ba), yellow solid (0.0512 g, 85% yield, d.r. > 20:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.50 (d, J = 9.0 Hz, 2H), 6.91 (d, J = 9.0 Hz, 2H), 4.05-4.01 (m, 1H), 3.80 (s, 3H), 3.34-3.32 (m, 1H), 2.65-2.62 (m, 1H), 2.54-2.49 (m, 1H), 2.40-2.33 (m, 1H), 1.81-1.70 (m, 2H), 1.34 (s, 3H), 1.13 (s, 3H), 1.11 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 215.5, 177.0, 156.9, 132.5, 121.8, 114.2, 55.5, 51.9, 45.6, 43.9, 43.8, 40.4, 38.7, 26.8, 25.9, 25.4; HRMS *m/z* (ESI) calcd for $C_{18}H_{24}NO_3$ ([M+H]$^+$) 302.1751, found 302.1755.

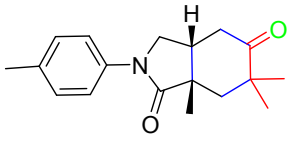


6-Ethyl-2-(4-methoxyphenyl)-6,7a-dimethylhexahydro-1H-isoindole-1,5(4H)-dione (3bb), yellow solid (0.0511 g, 81% yield, d.r. =1.5:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.53-7.48 (m, 2H), 6.91 (t, J = 9.5 Hz, 2H), 4.06-3.98 (m, 1H), 3.80 (s, 3H), 3.34-3.31 (m, 1H), 2.72-2.63 (m, 1H), 2.56-2.43 (m, 2H), 1.92-1.84 (m, 1H), 1.69-1.62 (m, 1H), 1.55-1.50 (m, 2H), 1.38 (s, 1.2H), 1.30 (s,

1.8H), 1.06 (s, 1.8H), 1.01 (s, 1.2H), 0.88 (t, J = 7.5 Hz, 1.8H), 0.79 (t, J = 7.5 Hz, 1.2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 216.0, 215.3, 177.2, 177.1, 156.9, 156.8, 132.6, 132.3, 121.9, 121.7, 114.2 (2), 55.5 (2), 52.0, 51.8, 47.8, 46.9, 43.8, 43.6, 43.1, 42.8, 41.2, 40.9, 39.4, 38.0, 32.7, 30.9, 26.8, 25.4, 22.8, 22.0, 8.4, 8.1; HRMS *m/z* (ESI) calcd for $C_{19}H_{26}NO_3$ ($[M+H]^+$) 316.1907, found 316.1905.

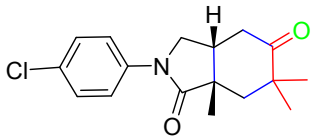


6-Isopropyl-2-(4-methoxyphenyl)-6,7a-dimethylhexahydro-1H-isoindole-1,5(4H)-dione (3bc), yellow solid (0.0527 g, 80% yield, d.r. = 1.5:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.45 (d, J = 9.0 Hz, 1.4H), 7.41 (d, J = 9.5 Hz, 0.6H), 6.87-6.82 (m, 2H), 3.99 (t, J = 9.5 Hz, 0.6H), 3.91 (t, J = 9.5 Hz, 0.4H), 3.74 (s, 1.8H), 3.73 (s, 1.2H), 3.27-3.24 (m, 1H), 2.74-2.62 (m, 1H), 2.51-2.45 (m, 1H), 2.42-2.33 (m, 1H), 1.60-1.52 (m, 3H), 1.32 (s, 1.2H), 1.21 (s, 1.8H), 1.05 (s, 1.8H), 0.96 (s, 1.2H), 0.83-0.82 (m, 3.6H), 0.77 (d, J = 6.0 Hz, 1.2H), 0.72 (d, J = 6.0 Hz, 1.2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 216.0, 215.6, 177.2, 177.1, 156.8 (2), 132.7, 132.3, 121.8, 121.6, 114.2 (2), 55.5 (2) , 52.0, 51.7, 49.2, 48.0, 47.8, 47.3, 45.2, 44.1, 44.0, 43.5, 41.3, 41.0, 40.0, 38.0, 25.1, 24.8 (2), 24.7, 24.3, 24.1, 23.7, 23.2; HRMS *m/z* (ESI) calcd for $C_{20}H_{28}NO_3$ ($[M+H]^+$) 330.2064, found 330.2066.

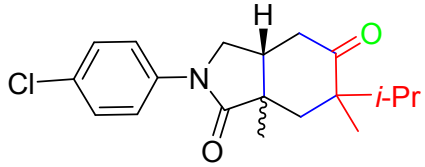


6,6,7a-Trimethyl-2-(*p*-tolyl)hexahydro-1H-isoindole-1,5(4H)-dione (3ca), yellow solid (0.0473 g, 83% yield, d.r. > 20:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.42 (d, J = 8.5 Hz, 2H), 7.11 (d, J = 8.5 Hz, 2H), 3.99-3.96 (m, 1H), 3.29-3.27 (m, 1H), 2.58-2.53 (m, 2H), 2.48-2.44 (m, 1H), 2.26 (s, 3H), 1.72 (d, J = 15.0 Hz, 1H), 1.40-1.34 (m, 1H), 1.27 (s, 3H), 1.06 (s, 3H),

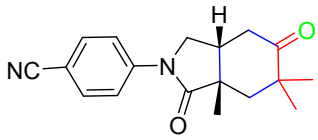
1.04 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 215.6, 177.3, 136.7, 134.7, 129.5, 120.1, 51.6, 45.6, 44.0, 43.9, 40.4, 38.8, 26.8, 25.9, 25.5, 20.9; HRMS *m/z* (ESI) calcd for $C_{18}H_{24}NO_2$ ($[M+H]^+$) 286.1802, found 286.1800.



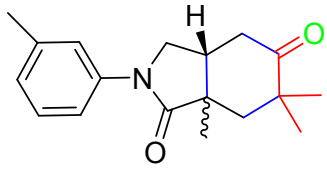
2-(4-Chlorophenyl)-6,6,7a-trimethylhexahydro-1H-isoindole-1,5(4H)-dione (3da), yellow solid (0.0476 g, 78% yield, d.r. > 20:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.59-7.58 (m, 2H), 7.35-7.33 (m, 2H), 4.05-4.02 (m, 1H), 3.36-3.33 (m, 1H), 2.67-2.62 (m, 1H), 2.53-2.47 (m, 1H), 2.34 (d, J = 15.0 Hz, 1H), 1.79 (t, J = 13.5 Hz, 1H), 1.56 (t, J = 9.5 Hz, 1H), 1.35 (s, 3H), 1.14 (s, 3H), 1.09 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 215.2, 177.5, 137.8, 130.0, 129.0, 121.0, 51.4, 45.6, 44.1, 43.9, 40.3, 38.6, 26.8, 25.9, 25.4; HRMS *m/z* (ESI) calcd for $C_{17}H_{21}ClNO_2$ ($[M+H]^+$) 306.1255, found 306.1259.



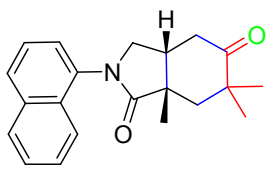
2-(4-Chlorophenyl)-6-isopropyl-6,7a-dimethylhexahydro-1H-isoindole-1,5(4H)-dione (3dc), yellow solid (0.0493 g, 74% yield, d.r. = 2.3:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.54-7.50 (m, 2H), 7.29-7.26 (m, 2H), 4.00-3.94 (m, 1H), 3.29-3.25 (m, 1H), 2.64-2.53 (m, 1H), 2.45-2.38 (m, 2H), 1.65-1.55 (m, 2H), 1.46-1.38 (m, 1H), 1.32 (s, 0.9H), 1.23 (s, 2.1H), 1.00 (s, 2.1H), 0.92 (s, 0.9H), 0.82-0.73 (m, 3H), 0.71 (d, J = 7.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 215.0, 214.9, 177.6, 177.5, 138.0 (2), 129.0 (2), 121.1(2) 120.9 (2), 51.5, 51.4, 47.8, 47.7, 44.1, 44.0, 43.2, 43.1, 40.8, 40.7, 39.2 (2), 37.9, 37.8, 26.7 (2), 25.5, 25.4, 22.7 (2), 22.0 (2); HRMS *m/z* (ESI) calcd for $C_{19}H_{25}ClNO_2$ ($[M+H]^+$) 334.1568, found 334.1564.



4-(6,6,7a-Trimethyl-1,5-dioxooctahydro-2H-isoindol-2-yl)benzonitrile (3ea), yellow solid (0.0426 g, 72% yield, d.r. > 20:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.80 (d, J = 8.5 Hz, 2H), 7.67 (d, J = 9.0 Hz, 2H), 4.09-4.05 (m, 1H), 3.44-3.39 (m, 1H), 2.70-2.64 (m, 1H), 2.52-2.48 (m, 1H), 2.34 (d, J = 15.0 Hz, 1H), 1.84-1.80 (m, 1H), 1.71-1.64 (m, 1H), 1.37 (s, 3H), 1.15 (s, 3H), 1.09 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 214.6, 178.3, 143.0, 133.1, 119.4, 118.6, 107.7, 51.0, 45.6, 44.3, 43.9, 40.1, 38.5, 26.7, 25.9, 25.5; HRMS *m/z* (ESI) calcd for $C_{18}H_{21}N_2O_2$ ([M+H]$^+$) 297.1598, found 297.1596.

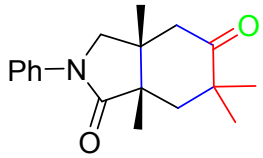


6,6,7a-Trimethyl-2-(m-tolyl)hexahydro-1H-isoindole-1,5(4H)-dione （3fa）, yellow solid (0.0479 g, 84% yield, d.r. = 4:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.44 (s, 1H), 7.32 (d, J = 8.5 Hz, 1H), 7.28 (d, J = 2.0 Hz, 1H), 6.99 (d, J = 7.5 Hz, 1H), 4.32-4.28 (m, 0.2H), 4.06-4.03 (m, 0.8H), 3.27 (d, J = 10.0 Hz, 1H), 2.37 (s, 3H), 2.23-2.19 (m, 1H), 2.11-2.02 (m, 2H), 1.63-1.57 (m, 1H), 1.47-1.41 (m, 1H), 1.34 (s, 0.5H), 1.28 (s, 1H), 1.17 (s, 2.5H), 1.16 (s, 2.5H), 1.14 (s, 2.5H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 215.6, 177.5, 176.7, 139.5, 139.2, 138.9, 128.8 (2), 125.8, 125.7, 120.9, 120.7, 117.2, 117.0, 51.7, 50.9, 46.5, 45.6, 44.1 (2), 43.9, 43.4, 40.3, 38.8, 37.9, 37.6, 26.9, 26.7, 26.4, 25.9, 25.5, 25.1, 21.6; HRMS *m/z* (ESI) calcd for $C_{18}H_{24}NO_2$ ([M+H]$^+$) 286.1802, found 286.1806.

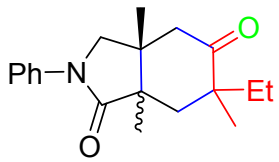


6,6,7a-Trimethyl-2-(naphthalen-1-yl)hexahydro-1H-isoindole-1,5(4H)-dione (3ga), yellow solid (0.0514 g, 80% yield, d.r. > 20:1);^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.90 (d, J =

7.5 Hz, 1H), 7.85 (d, *J* = 8.5 Hz, 1H), 7.71 (d, *J* = 7.5 Hz, 1H), 7.54-7.50 (m, 3H), 7.33 (d, *J* = 7.5 Hz, 1H), 4.09 (t, *J* = 8.5 Hz, 1H), 3.41 (d, *J* = 10.0 Hz, 1H), 2.81-2.75 (m, 2H), 2.71-2.67 (m, 1H), 2.42 (d, *J* = 14.5 Hz, 1H), 1.90 (d, *J* = 14.5 Hz, 1H), 1.53 (s, 3H), 1.20 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) *δ*: 215.6, 178.4, 135.1, 134.6, 129.9, 128.7, 128.6, 126.9, 126.4, 125.7, 124.5, 122.2, 54.7, 45.2, 44.0, 43.3, 40.7, 40.0, 27.1, 26.2, 25.5; HRMS *m/z* (ESI) calcd for $C_{21}H_{24}NO_2$ ($[M+H]^+$) 322.1802, found 322.1804.

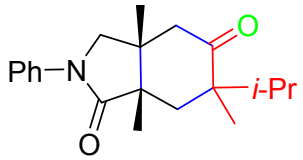


3a,6,6,7a-Tetramethyl-2-phenylhexahydro-1H-isoindole-1,5(4H)-dione (3ia), orange oil (0.0485 g, 85% yield, d.r. > 20:1);^{1}H NMR (500 MHz, $CDCl_3$) *δ*: 7.63 (d, *J* = 7.5 Hz, 2H), 7.39 (t, *J* = 8.0 Hz, 2H), 7.17 (t, *J* = 7.5 Hz, 1H), 3.66 (d, *J* = 10.0 Hz, 1H), 3.37 (d, *J* = 10.0 Hz, 1H), 2.96 (d, *J* = 13.5 Hz, 1H), 2.46 (d, *J* = 15.0 Hz, 1H), 2.15 (d, *J* = 13.5 Hz, 1H), 1.58 (d, *J* = 15.0 Hz, 1H), 1.23 (s, 3H), 1.14 (s, 3H), 1.11 (s, 3H), 1.09 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) *δ*: 214.3, 177.3, 139.6, 129.0, 124.7, 119.8, 57.8, 47.4, 46.7, 45.4, 45.0, 43.7, 26.6, 25.9, 21.2, 19.7; HRMS *m/z* (ESI) calcd for $C_{18}H_{24}NO_2$ ($[M+H]^+$) 286.1802, found 286.1806.

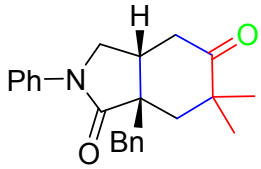


6-Ethyl-3a,6,7a-trimethyl-2-phenylhexahydro-1H-isoindole-1,5(4H)-dione (3ib), yellow solid (0.0491 g, 82% yield, d.r. = 1:1); ^{1}H NMR (500 MHz, $CDCl_3$) *δ*: 7.58-7.54 (m, 2H), 7.34-7.30 (m, 2H), 7.12-7.08 (m, 1H), 3.59-3.54 (m, 1H), 3.33-3.28 (m, 1H), 2.84 (d, *J* = 13.5 Hz, 0.5H), 2.77 (d, *J* = 13.5 Hz, 0.5H), 2.50 (d, *J* = 15.0 Hz, 0.5H), 2.27 (d, *J* = 15.0 Hz, 0.5H), 2.14 (d, *J* = 13.5 Hz, 0.5H), 2.00 (d, *J* = 13.0 Hz, 0.5H),

1.65 (d, J = 21.5 Hz, 0.5H), 1.56 (d, J = 15.0 Hz, 0.5H), 1.47-1.42 (m, 2H), 1.09 (s, 1.5H), 1.08 (s, 1.5H), 1.08 (s, 1.5H), 1.06 (s, 1.5H), 1.01 (s, 1.5H), 0.94 (s, 1.5H), 0.82 (t, J = 7.5 Hz, 1.5H), 0.69 (t, J = 7.5 Hz, 1.5H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 214.7, 214.3, 177.6, 177.4, 139.6, 139.5, 129.0 (2), 124.8, 124.7, 119.8 (2), 57.8 (2), 49.1, 47.8, 47.4, 47.3, 47.2, 47.0, 44.0, 43.7, 43.1, 42.6, 31.7, 31.5, 23.5, 21.6, 21.5, 21.3, 20.5, 19.2, 8.7, 8.2; HRMS m/z (ESI) calcd for $C_{19}H_{26}NO_2$ ($[M+H]^+$) 300.1958, found 300.1954.

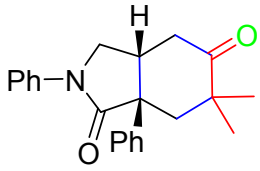


6-Isopropyl-3a,6,7a-trimethyl-2-phenylhexahydro-1H-isoindole-1,5(4H)-dione (3ic), yellow solid (0.0507 g, 81% yield, d.r. > 20:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.57-7.55 (m, 2H), 7.34 (t, J = 8.0 Hz, 2H), 7.12 (t, J = 7.5 Hz, 1H), 3.60 (d, J = 9.5 Hz, 1H), 3.26 (d, J = 10.0 Hz, 1H), 3.02 (d, J = 13.0 Hz, 1H), 2.49 (d, J = 14.5 Hz, 1H), 2.00 (d, J = 13.0 Hz, 1H), 1.81-1.77 (m, 1H), 1.40 (d, J = 35.5 Hz, 1H), 1.06 (s, 3H), 1.01 (s, 3H), 0.99 (s, 3H), 0.84 (d, J = 6.5 Hz, 3H), 0.63 (d, J = 6.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 214.9, 177.4, 139.7, 129.1, 124.7, 119.8, 57.8, 49.4, 48.7, 47.2, 47.1, 44.5, 25.2, 25.1, 23.0, 22.6, 21.5, 19.0; HRMS m/z (ESI) calcd for $C_{20}H_{28}NO_2$ ($[M+H]^+$) 314.2115, found 314.2117.

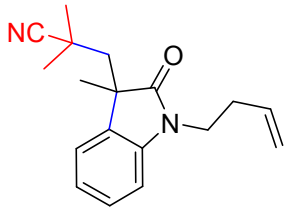


7a-Benzyl-6,6-dimethyl-2-phenylhexahydro-1H-isoindole-1,5(4H)-dione (3ja), white solid (0.0472g, 68% yield, d.r. > 20:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.37-7.33 (m, 4H), 7.23 (t, J = 3.5 Hz, 3H), 7.20-7.18 (m, 2H), 7.15 (t, J = 7.0 Hz, 1H), 3.24 (d, J = 13.0 Hz, 1H), 3.07-3.04 (m, 2H), 2.91-2.87 (m, 1H), 2.76 (d, J = 13.5 Hz, 1H), 2.68-2.63 (m,

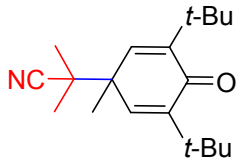
1H), 2.41-2.36 (m, 2H), 2.00 (d, J = 15.0 Hz, 1H), 1.18 (s, 3H), 1.12 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 215.9, 176.3, 138.7, 136.4, 130.1, 128.9, 128.4, 127.2, 125.2, 120.7, 52.2, 49.3, 45.4, 45.1, 43.7, 41.3, 33.8, 27.8, 25.1; HRMS *m/z* (ESI) calcd for $C_{23}H_{26}NO_2$ ([M+H]$^+$) 348.1958, found 348.1954.



6,6-Dimethyl-2,7a-diphenylhexahydro-1H-isoindole-1,5(4H)-dione (3ka), white solid (0.0473 g, 71% yield, d.r. > 20:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.56-7.54 (m, 2H), 7.45-7.43 (m, 2H), 7.32-7.28 (m, 4H), 7.22-7.20 (m, 1H), 7.10 (t, J = 7.5 Hz, 1H), 3.89-3.86 (m, 1H), 3.37-3.33 (m, 2H), 2.74-2.67 (m, 2H), 2.63 (t, J = 14.0 Hz, 1H), 2.17 (d, J = 15.0 Hz, 1H), 1.15 (s, 3H), 0.93 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 214.9, 174.7, 141.3, 139.3, 129.0, 128.9, 127.5, 126.3, 125.0, 120.0, 52.6, 51.4, 47.3, 44.6, 40.0, 38.9, 26.2, 26.1; HRMS *m/z* (ESI) calcd for $C_{22}H_{24}NO_2$ ([M+H]$^+$) 334.1802, found 334.1804.



3-(1-(But-3-en-1-yl)-3-methyl-2-oxoindolin-3-yl)-2,2-dimethylpropanenitrile (4ma), (0.0305 g, 54% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.32 (t, J = 4.8 Hz, 2H), 7.10 (t, J = 5.6 Hz, 1H), 6.91 (t, J = 8.0 Hz, 1H), 5.85-5.79 (m, 1H), 5.06 (t, J = 14.8 Hz, 2H), 3.85-3.76 (m, 2H), 2.48-2.43 (m, 2H), 2.31 (d, J = 7.2 Hz, 1H), 2.19 (d, J = 7.2 Hz, 1H), 1.33 (s, 3H), 1.21 (s, 3H), 1.06 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 179.6, 142.4, 134.5, 131.0, 128.5, 125.0, 124.2, 122.3, 117.5, 108.7, 47.0, 46.1, 39.5, 31.6, 30.8, 29.8, 28.1, 26.3; HRMS *m/z* (ESI) calcd for $C_{18}H_{23}N_2O$ ([M+H]$^+$) 283.1805, found 283.1807.



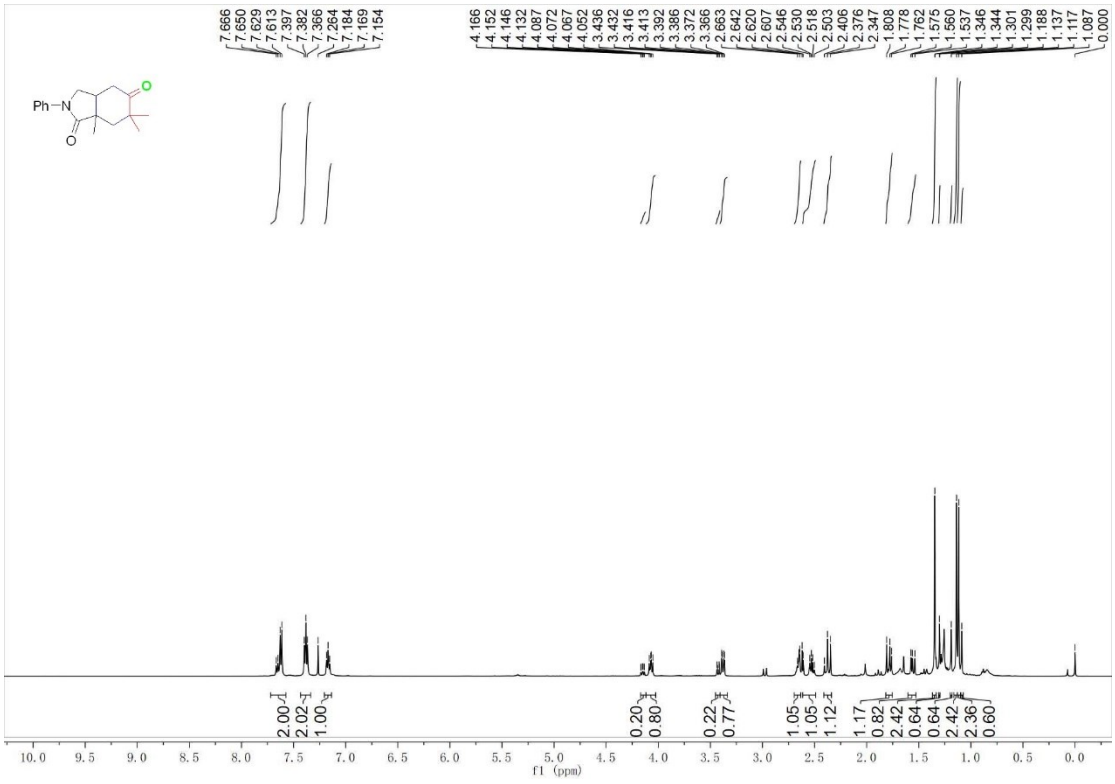
2-(3,5-di-*tert*-Butyl-1-methyl-4-oxocyclohexa-2,5-dien-1-yl)-2-methylpropanenitrile (4a),[1] (0.0838 g, 73% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ: 6.47 (s, 2H), 1.34 (s, 3H), 1.22 (s, 6H), 1.18 (s, 18H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 185.6, 149.3, 140,7, 123.5, 42.7, 39.8, 35.1, 29.4, 22.9, 22.6.

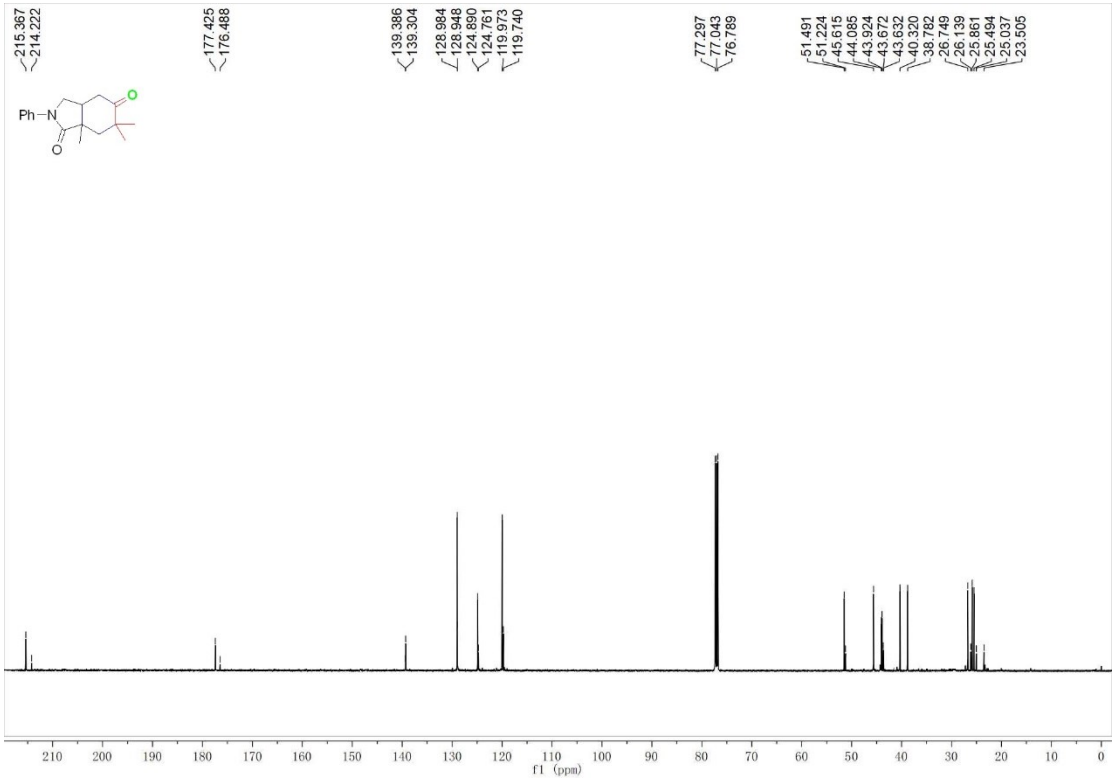
(C) Reference

[1] Y. Li, Y. Chang, Y. Li, C. Cao, J. Yang, B. Wang, D. Liang, *Adv. Synth. Catal.* 2018, **360**, 2488.

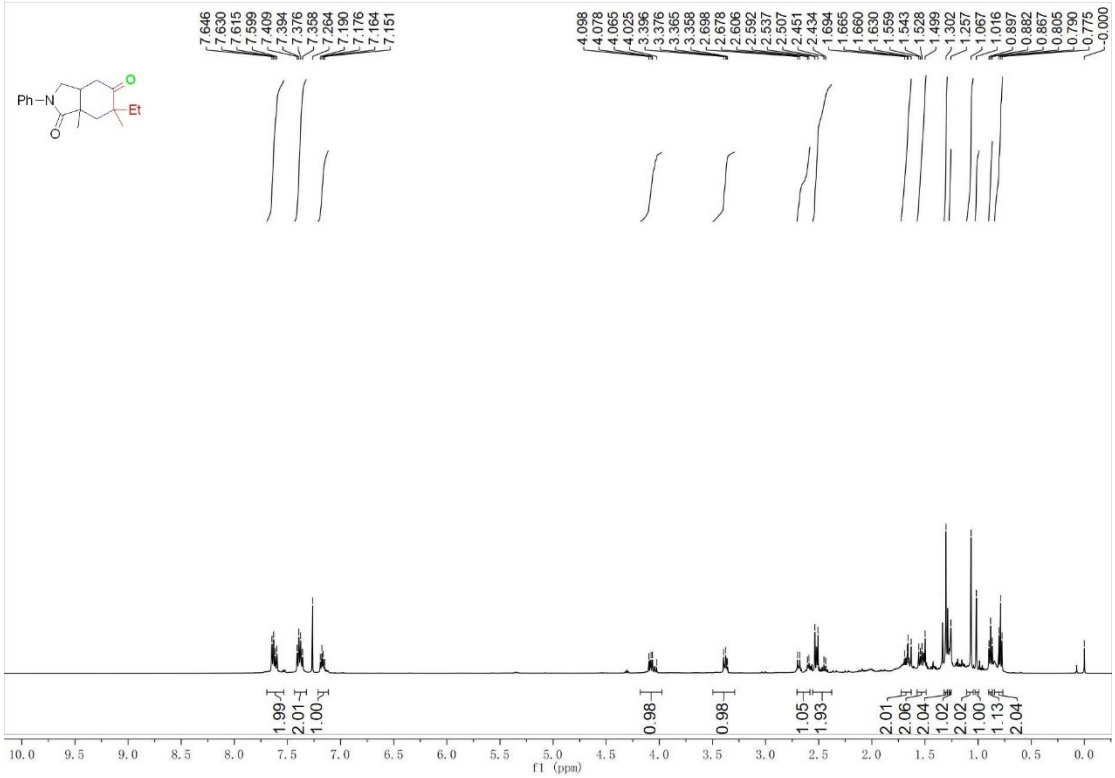
(D) Spectra

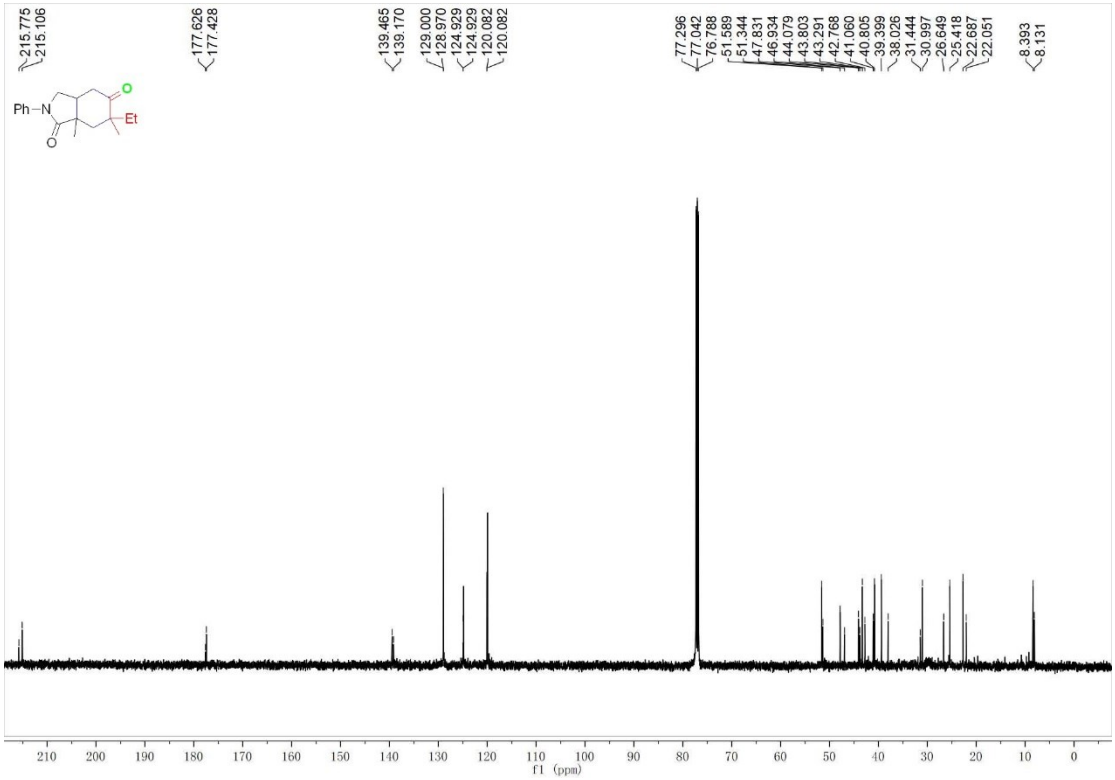
6,6,7a-Trimethyl-2-phenylhexahydro-1H-isoindole-1,5(4H)-dione (3aa)



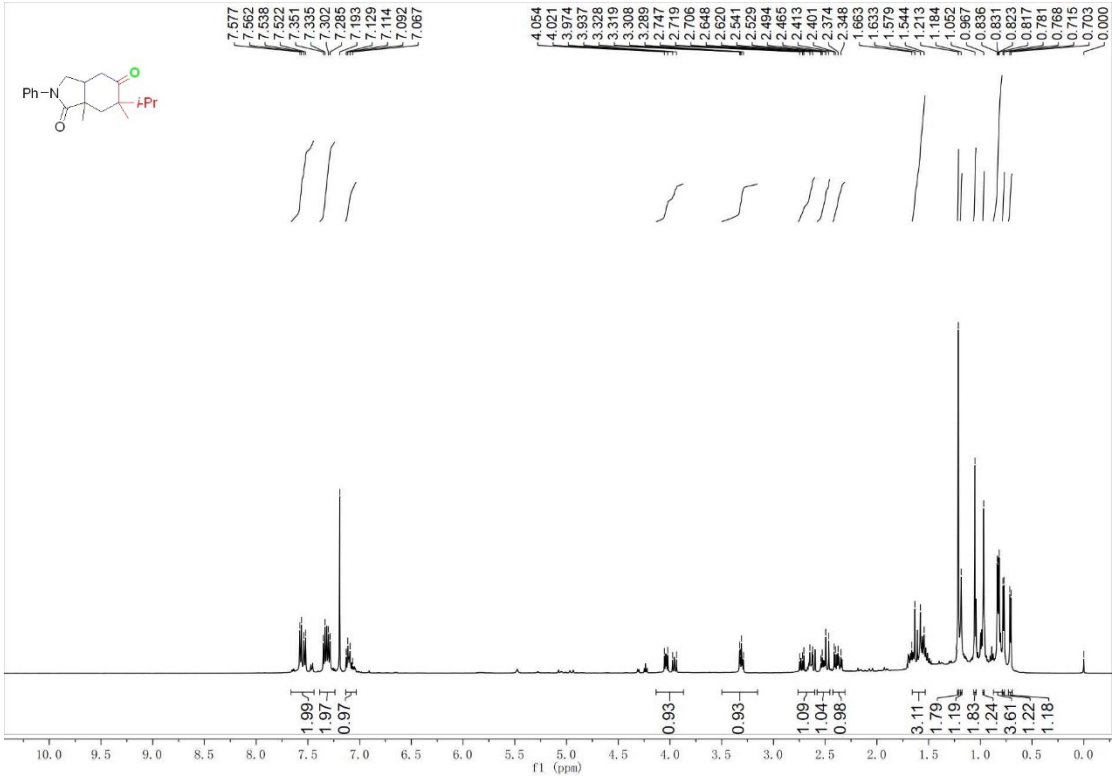


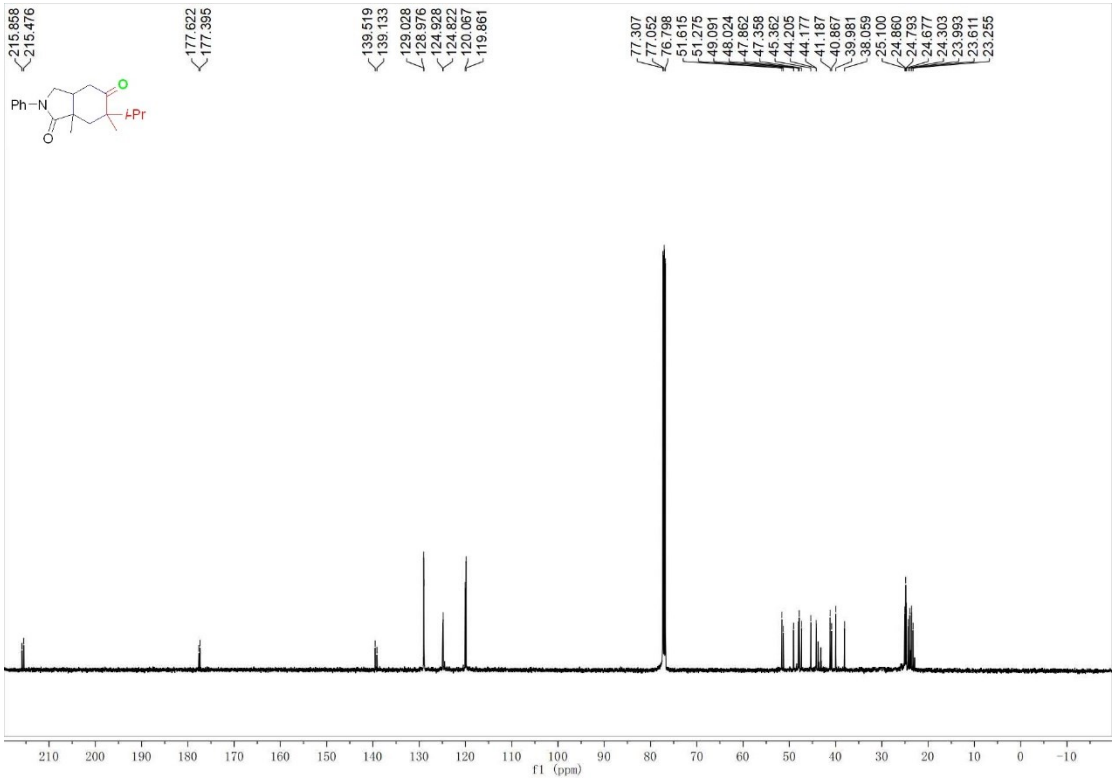
6-Ethyl-6,7a-dimethyl-2-phenylhexahydro-1H-isoindole-1,5(4H)-dione (3ab)



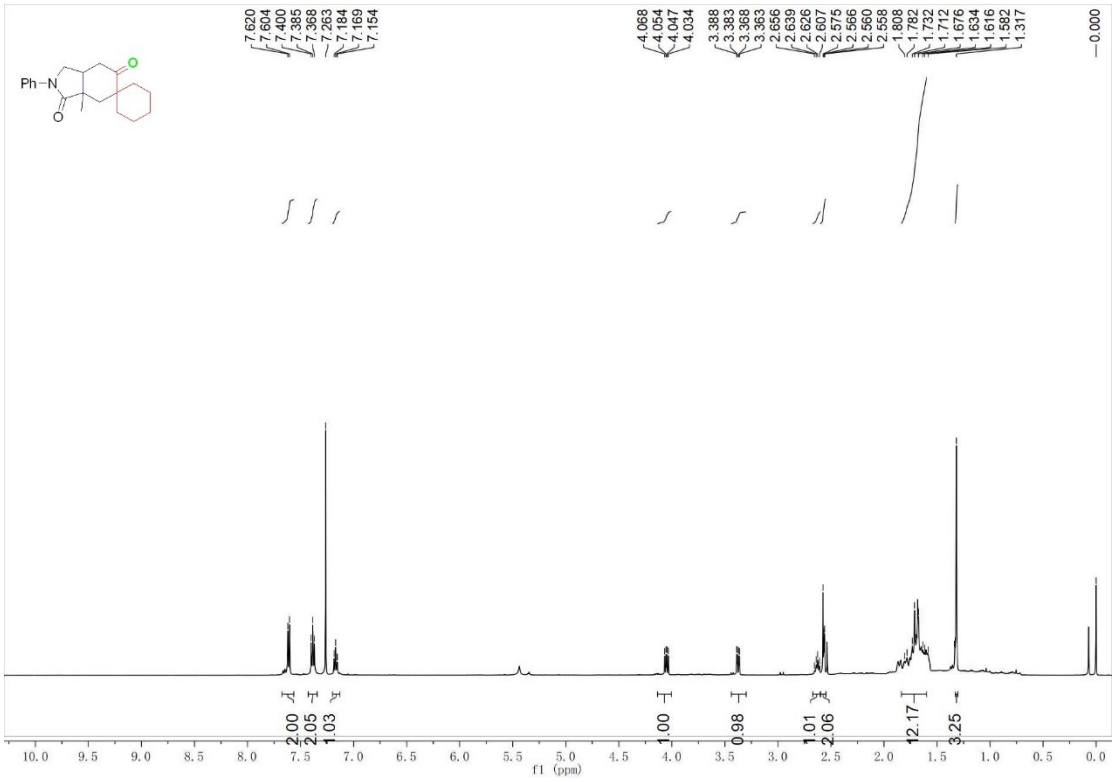


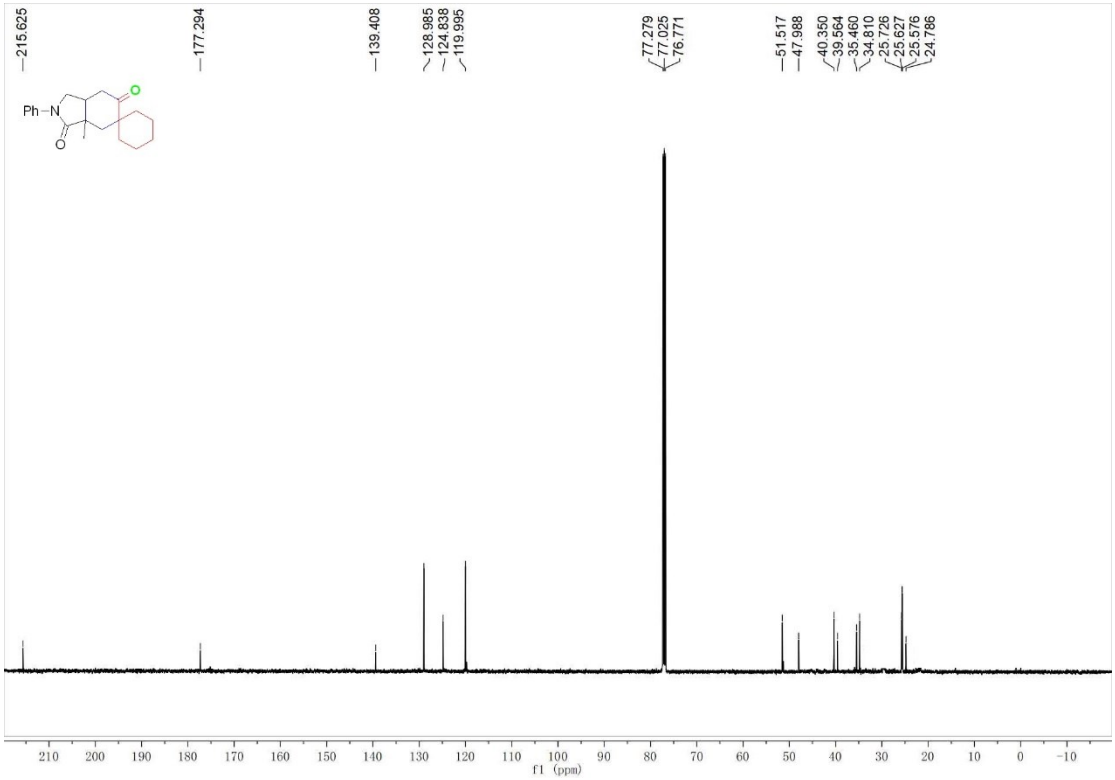
6-Isopropyl-6,7a-dimethyl-2-phenylhexahydro-1H-isoindole-1,5(4H)-dione (3ac)



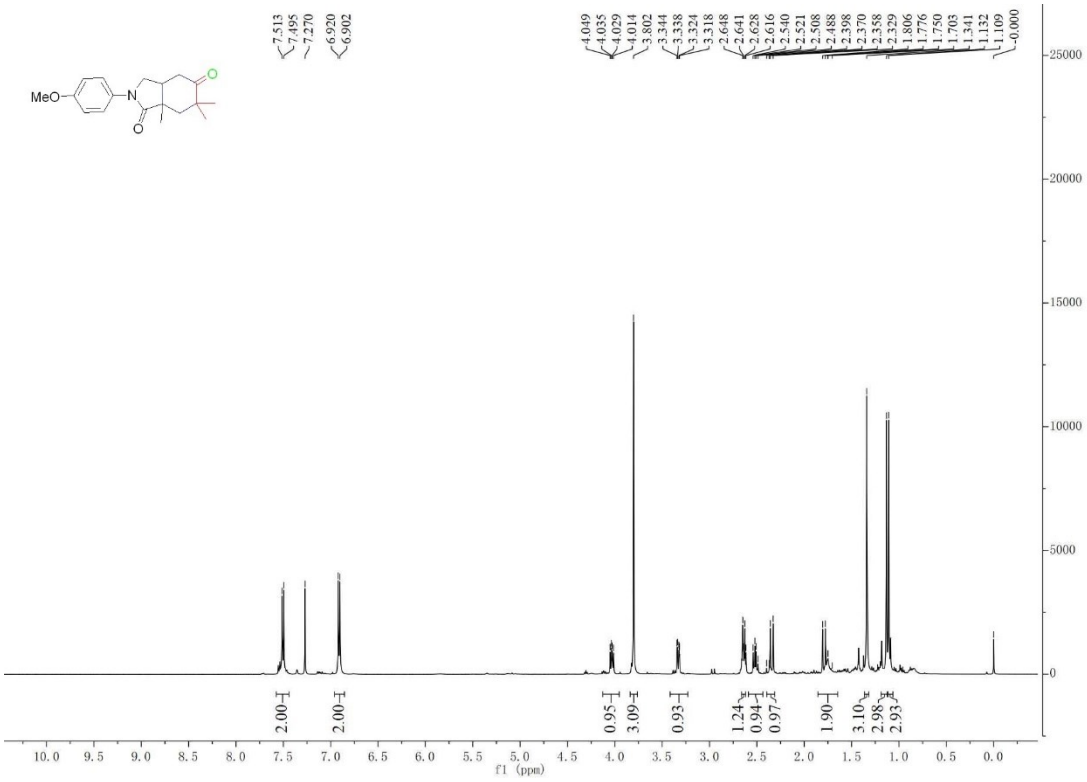


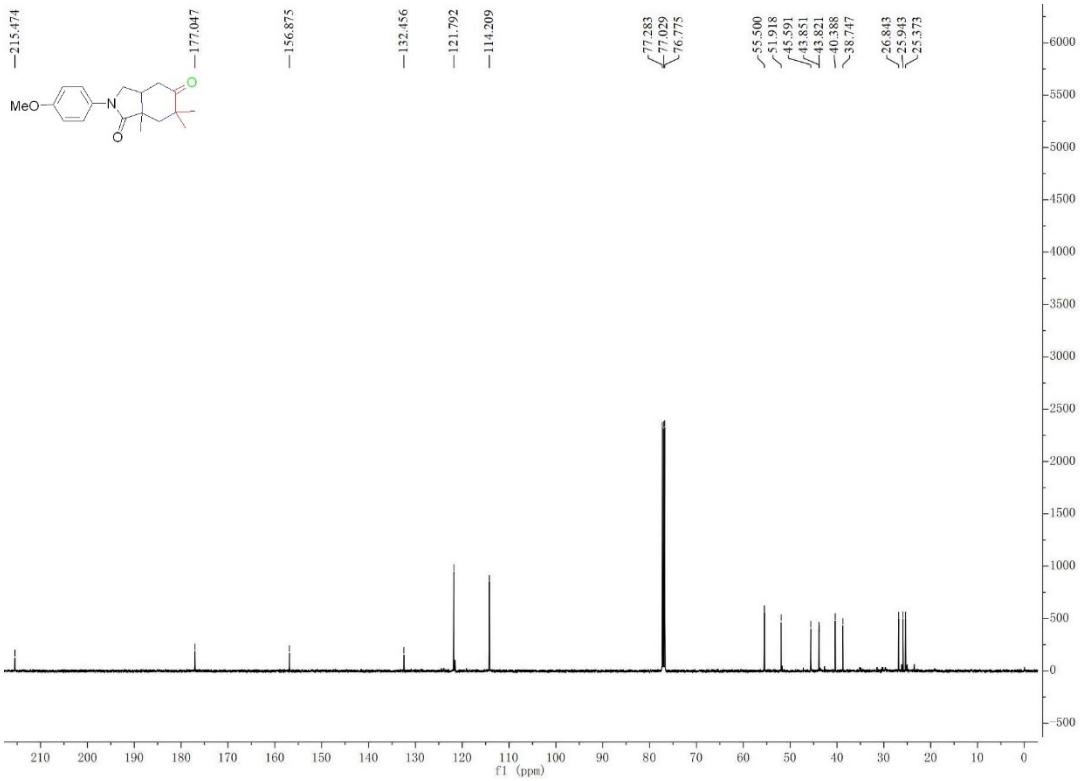
3a'-Methyl-2'-phenylhexahydrospiro[cyclohexane-1,5'-isoindole]-3',6'-dione (3ad)



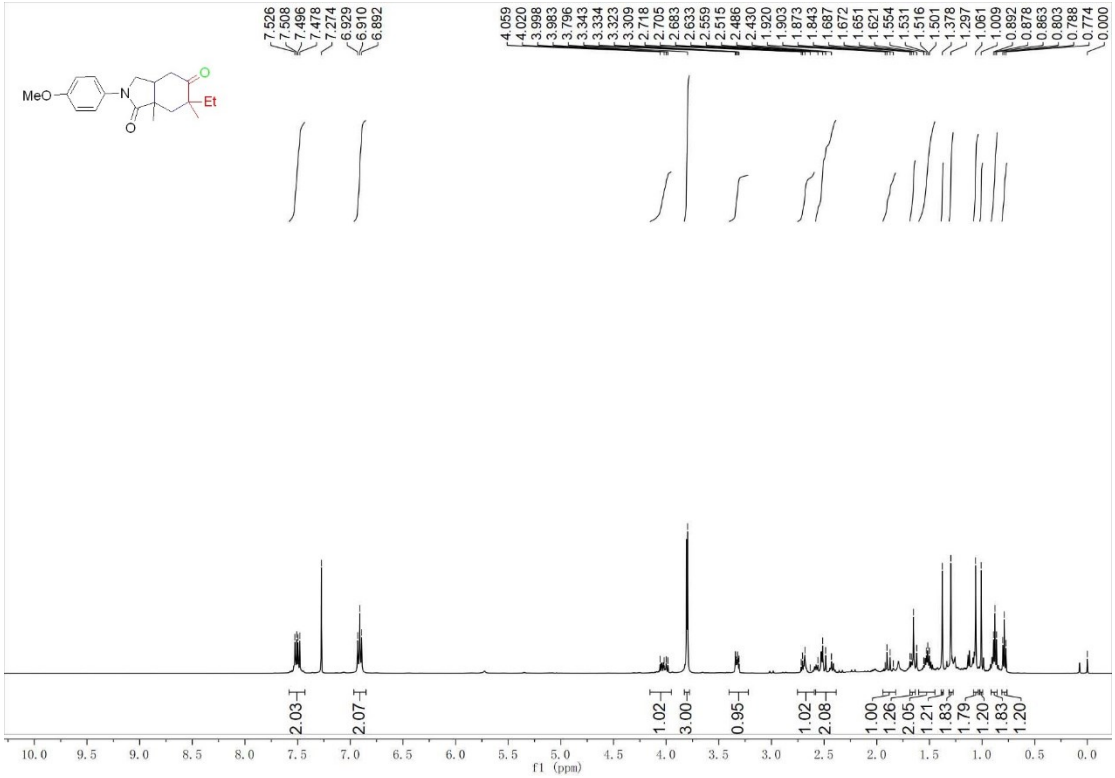


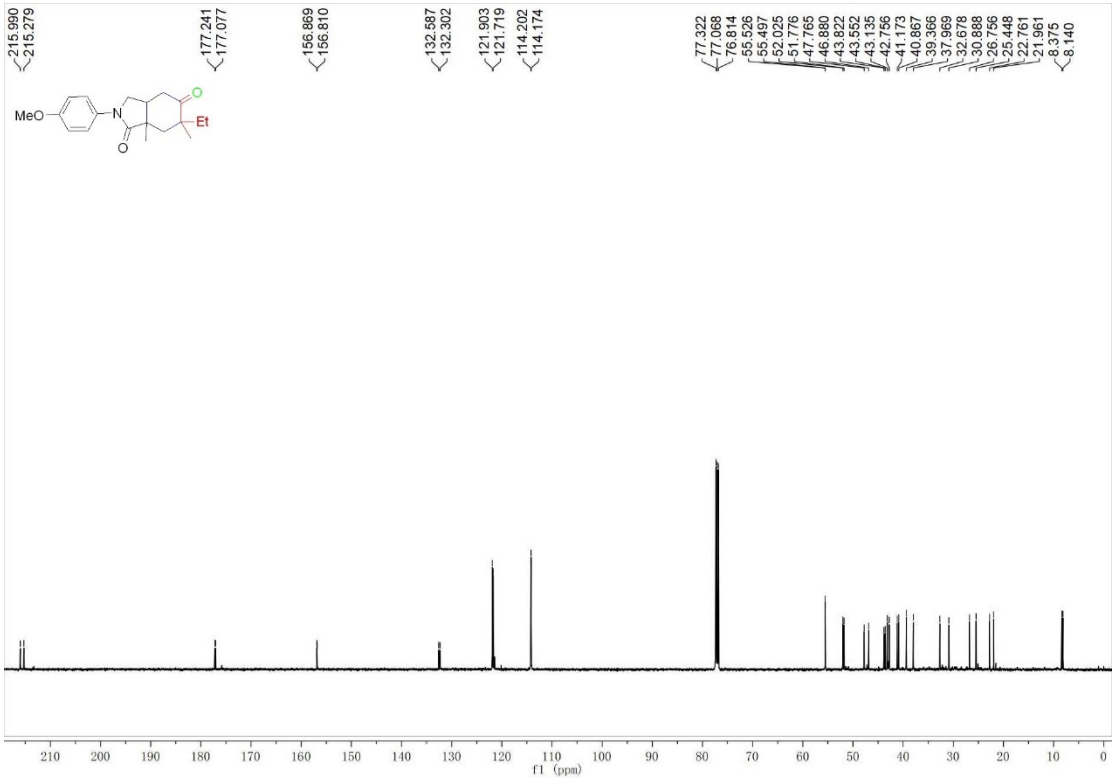
2-(4-Methoxyphenyl)-6,6,7a-trimethylhexahydro-1H-isoindole-1,5(4H)-dione (3ba)



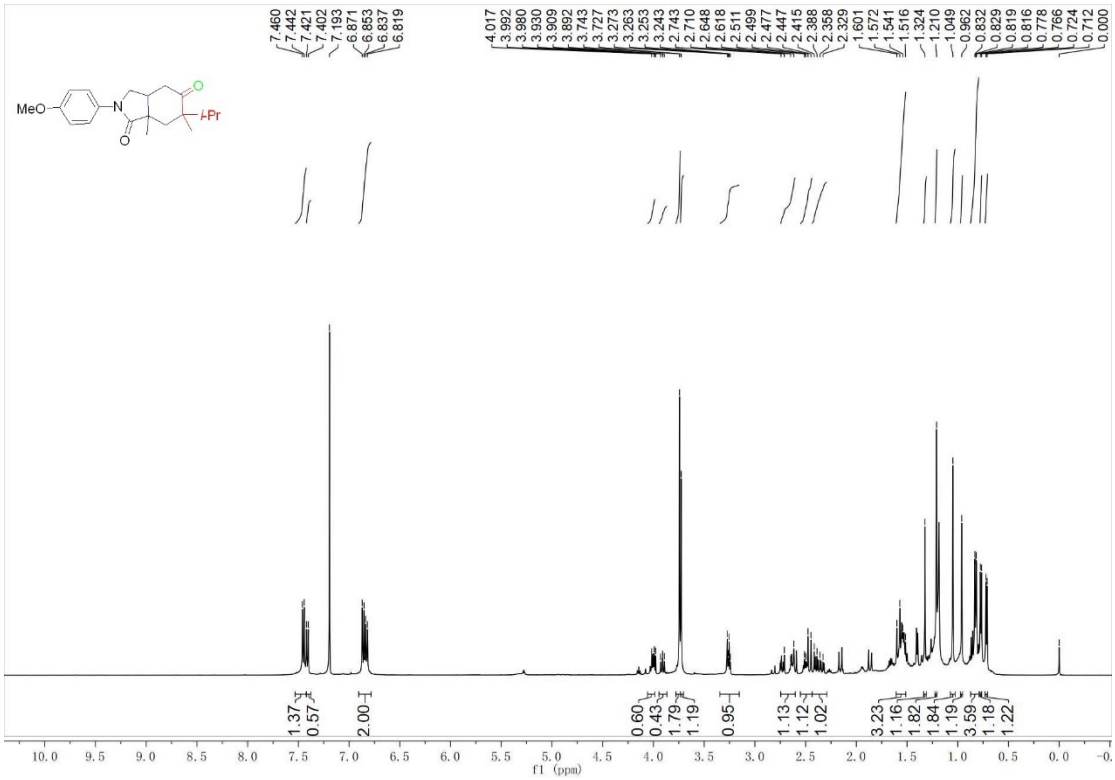


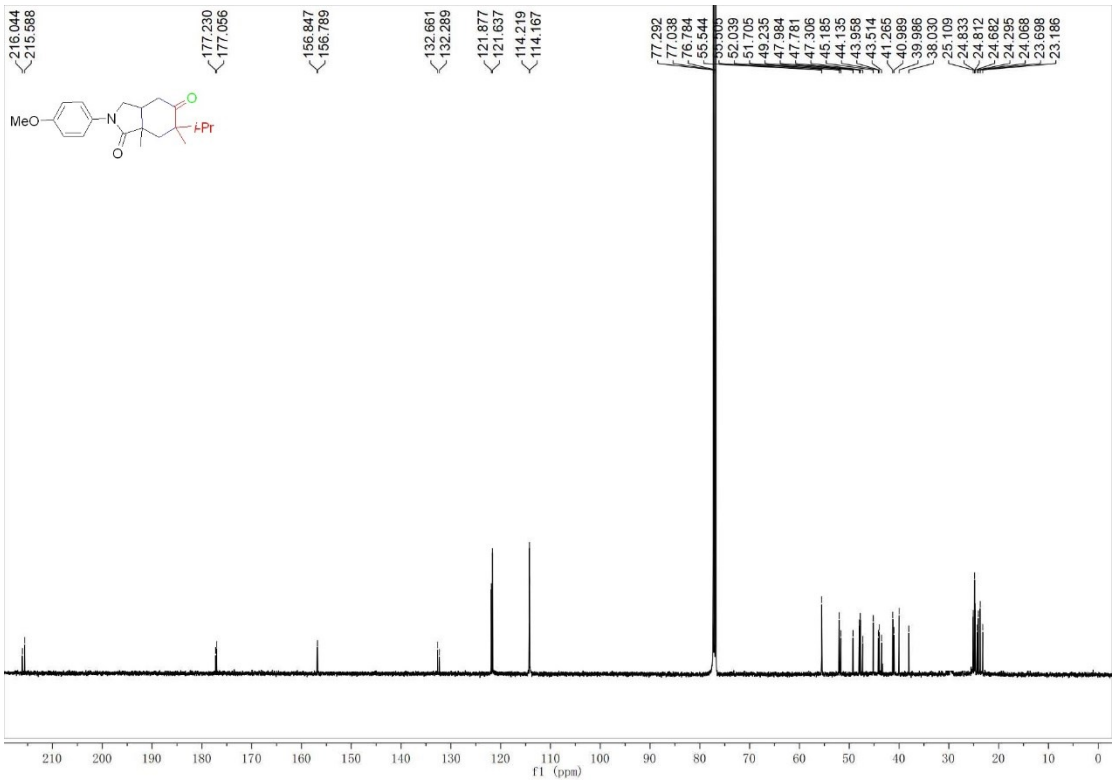
6-Ethyl-2-(4-methoxyphenyl)-6,7a-dimethylhexahydro-1H-isoindole-1,5(4H)-dione (3bb)



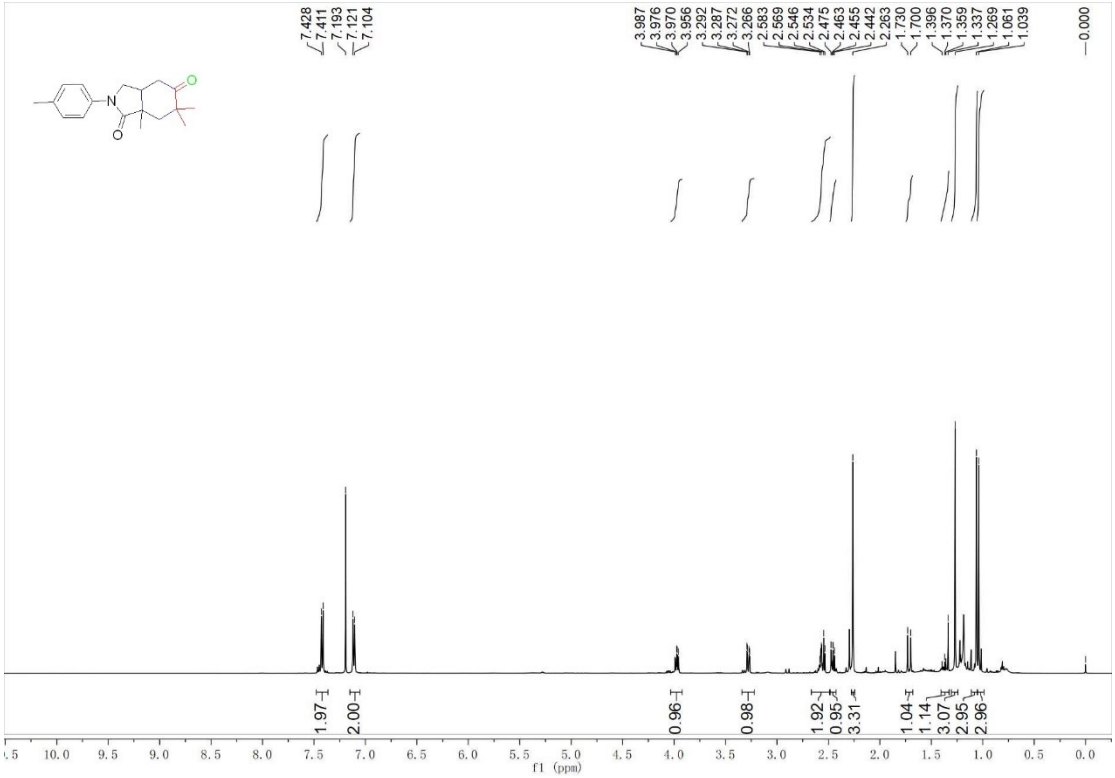


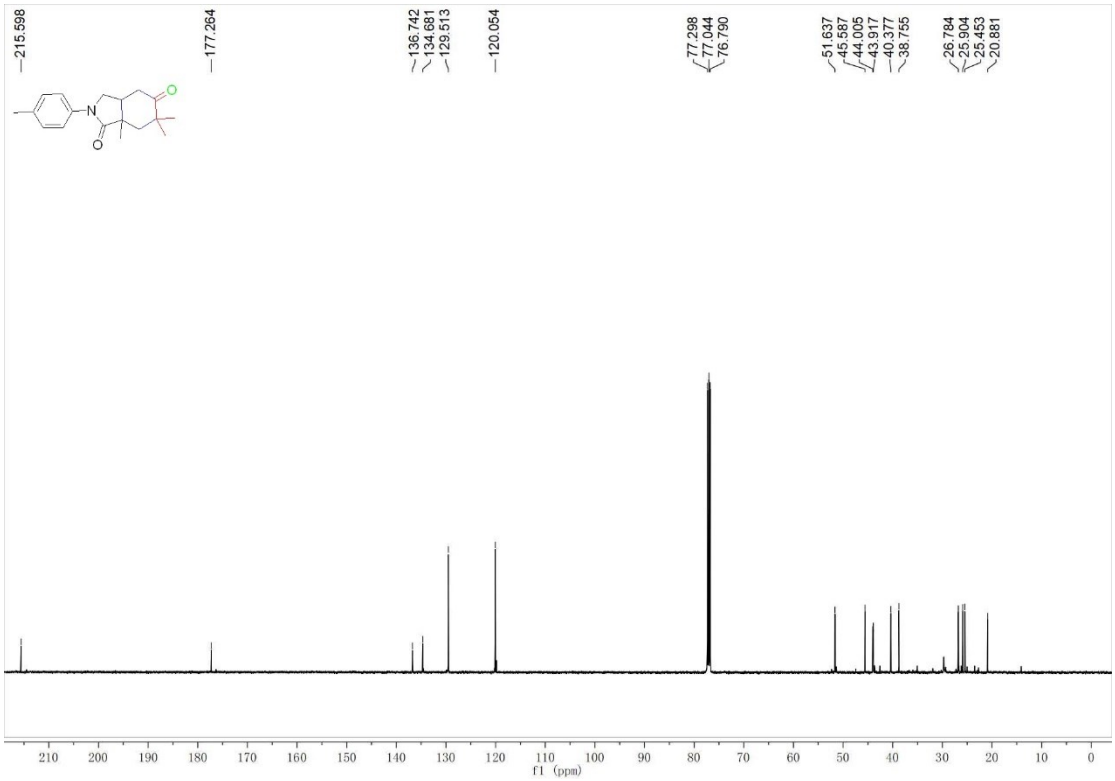
6-Isopropyl-2-(4-methoxyphenyl)-6,7a-dimethylhexahydro-1H-isoindole-1,5(4H)-dione (3bc)



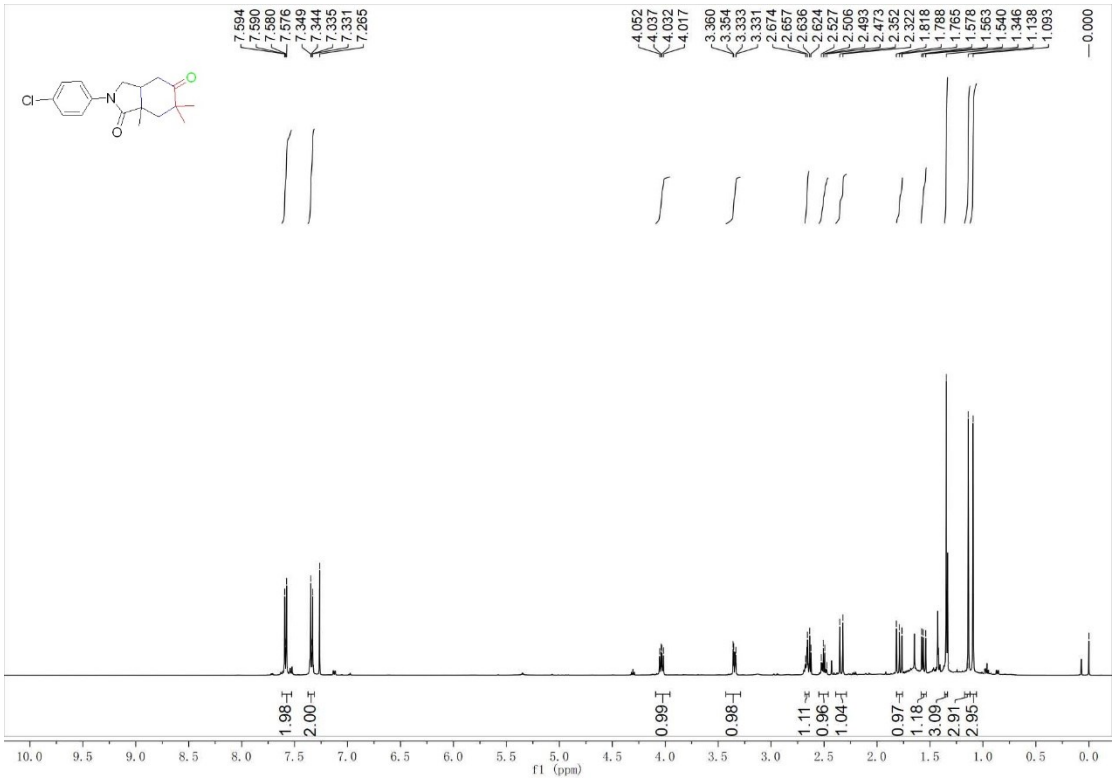


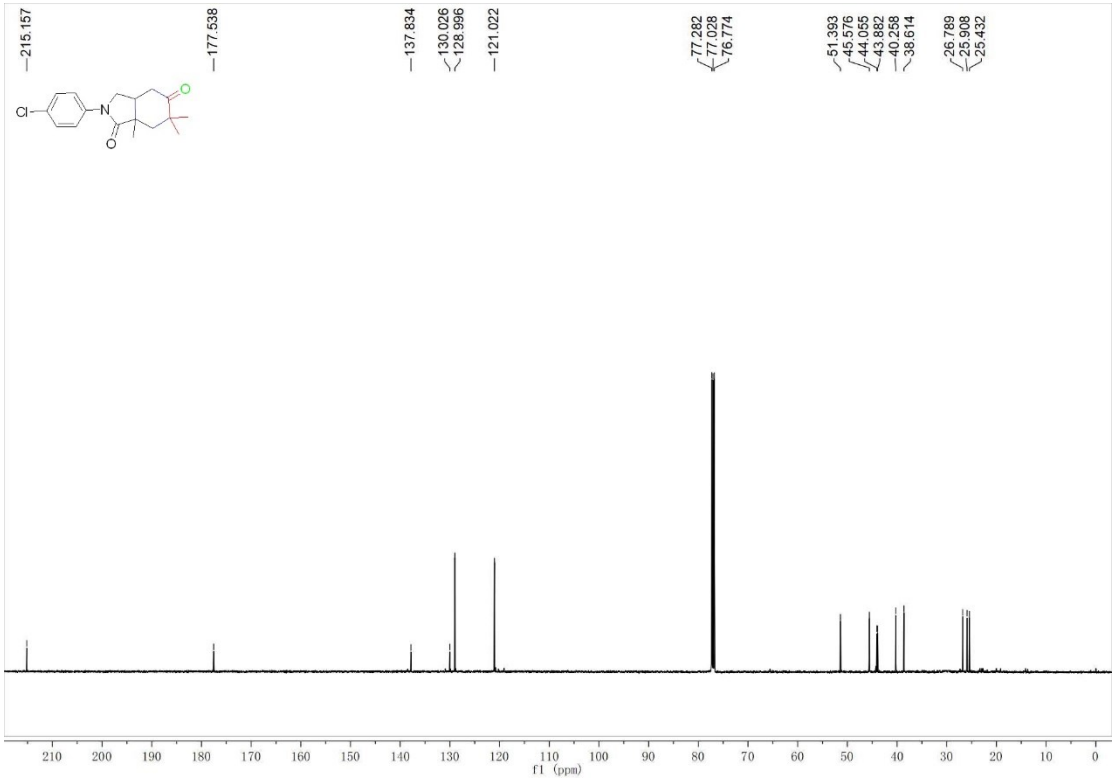
6,6,7a-Trimethyl-2-(*p*-tolyl)hexahydro-1H-isoindole-1,5(4H)-dione (3ca)



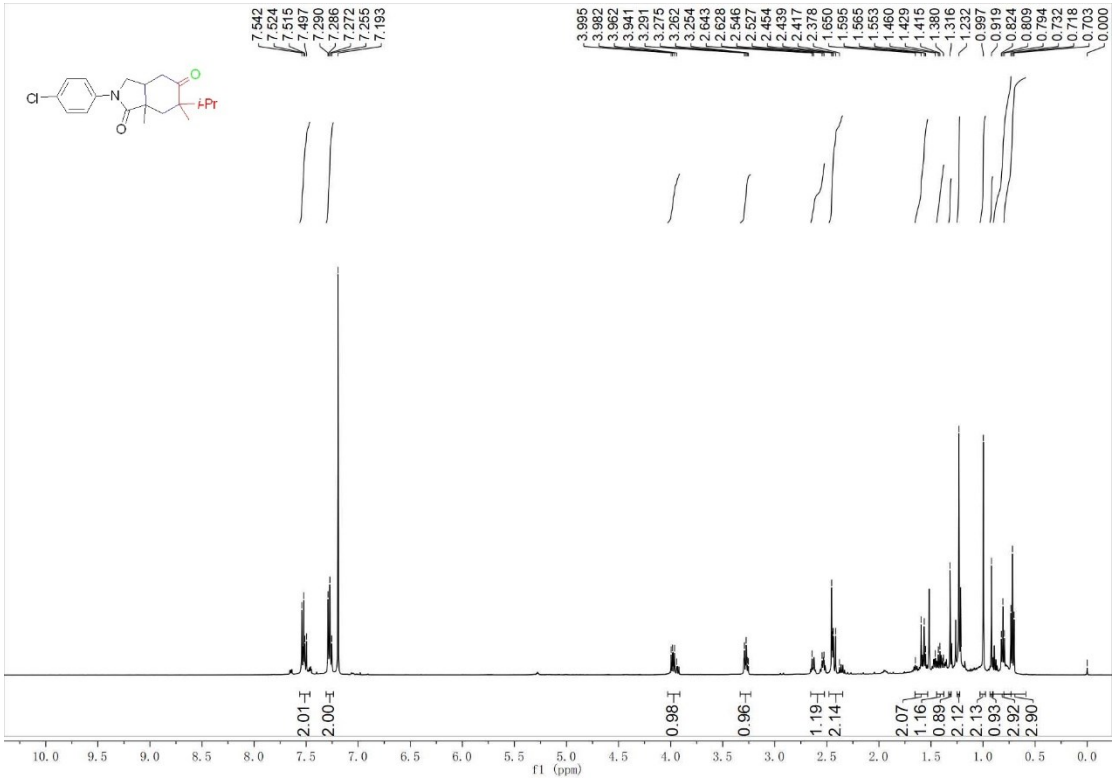


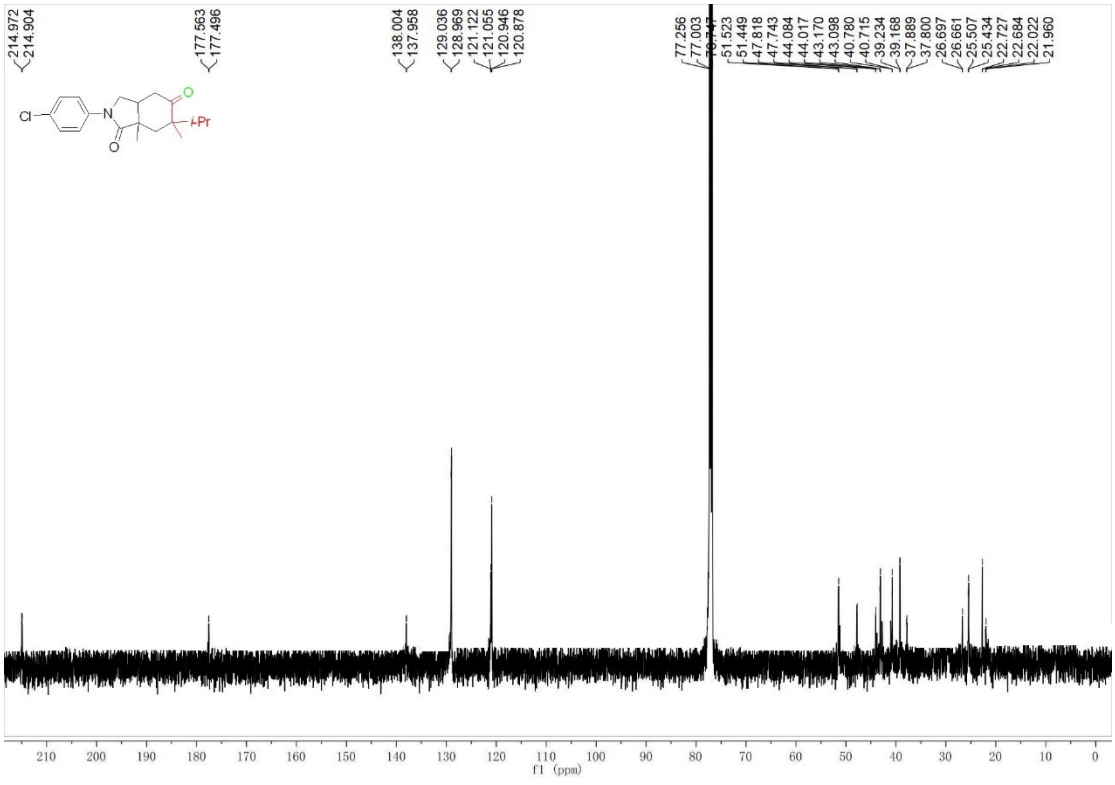
2-(4-Chlorophenyl)-6,6,7a-trimethylhexahydro-1H-isoindole-1,5(4H)-dione (3da)



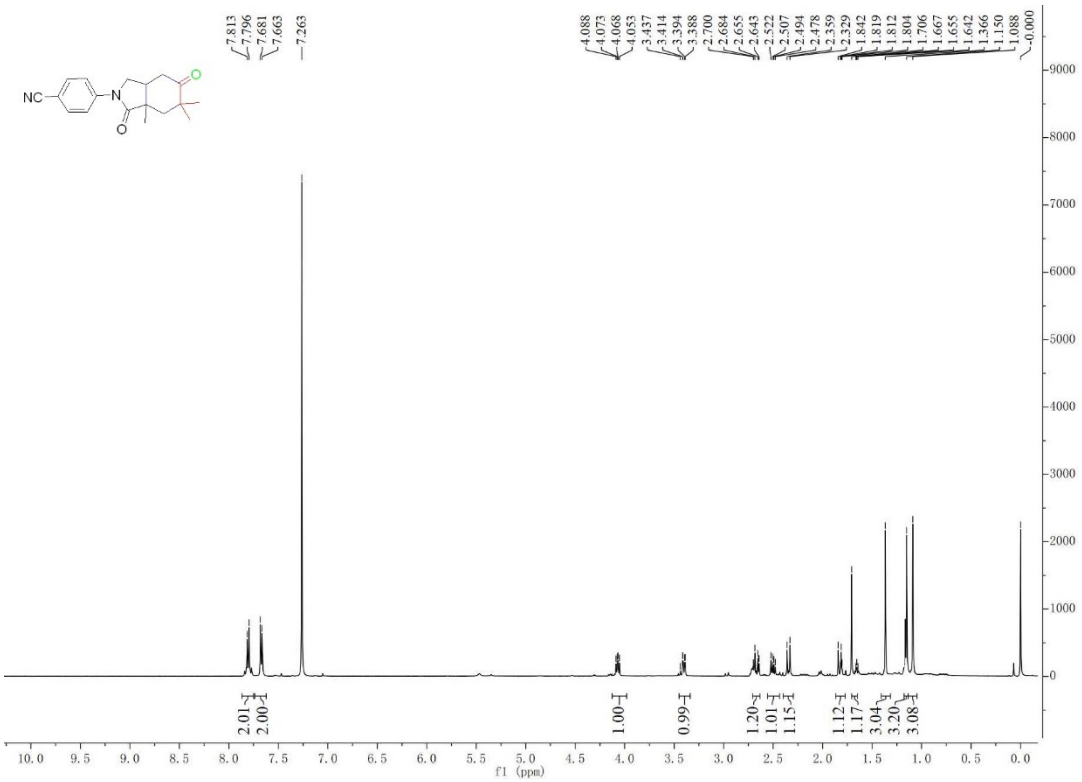


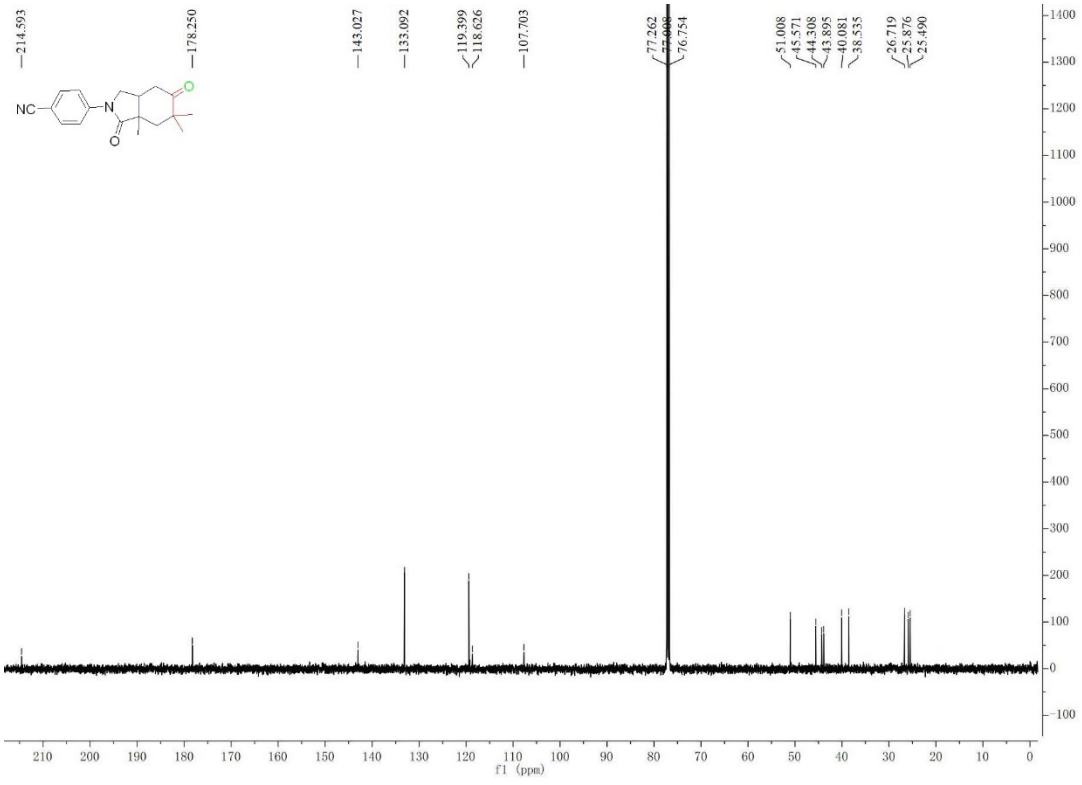
2-(4-Chlorophenyl)-6-isopropyl-6,7a-dimethylhexahydro-1H-isoindole-1,5(4H)-dione (3dc)



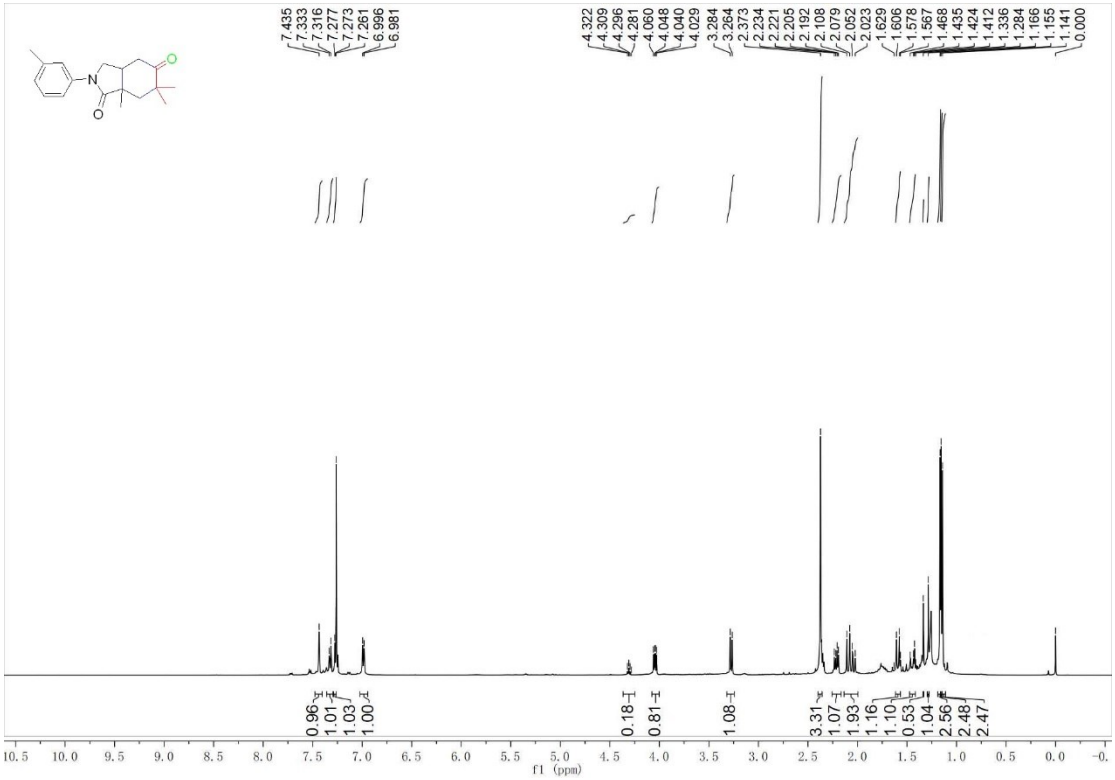


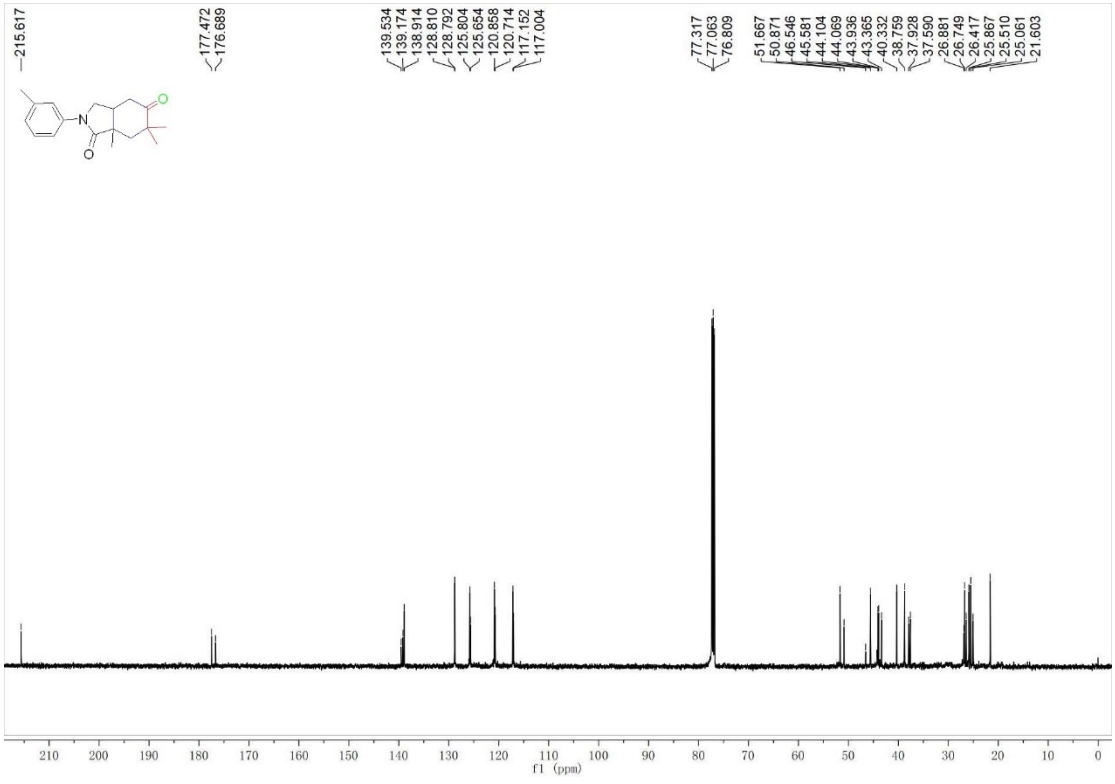
4-(6,6,7a-Trimethyl-1,5-dioxooctahydro-2H-isoindol-2-yl)benzonitrile (3ea)



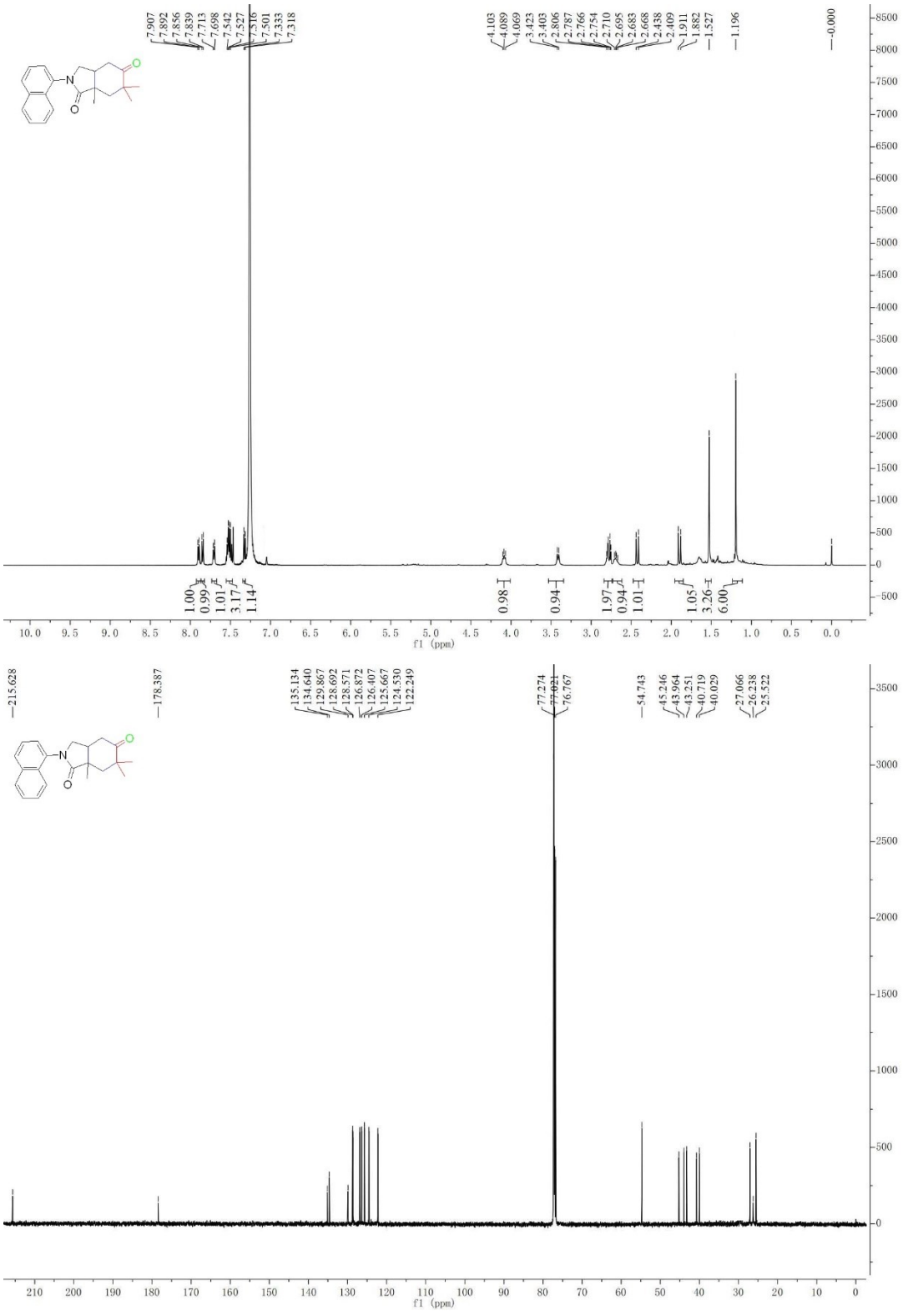


6,6,7a-Trimethyl-2-(*m*-tolyl)hexahydro-1H-isoindole-1,5(4H)-dione （3fa）

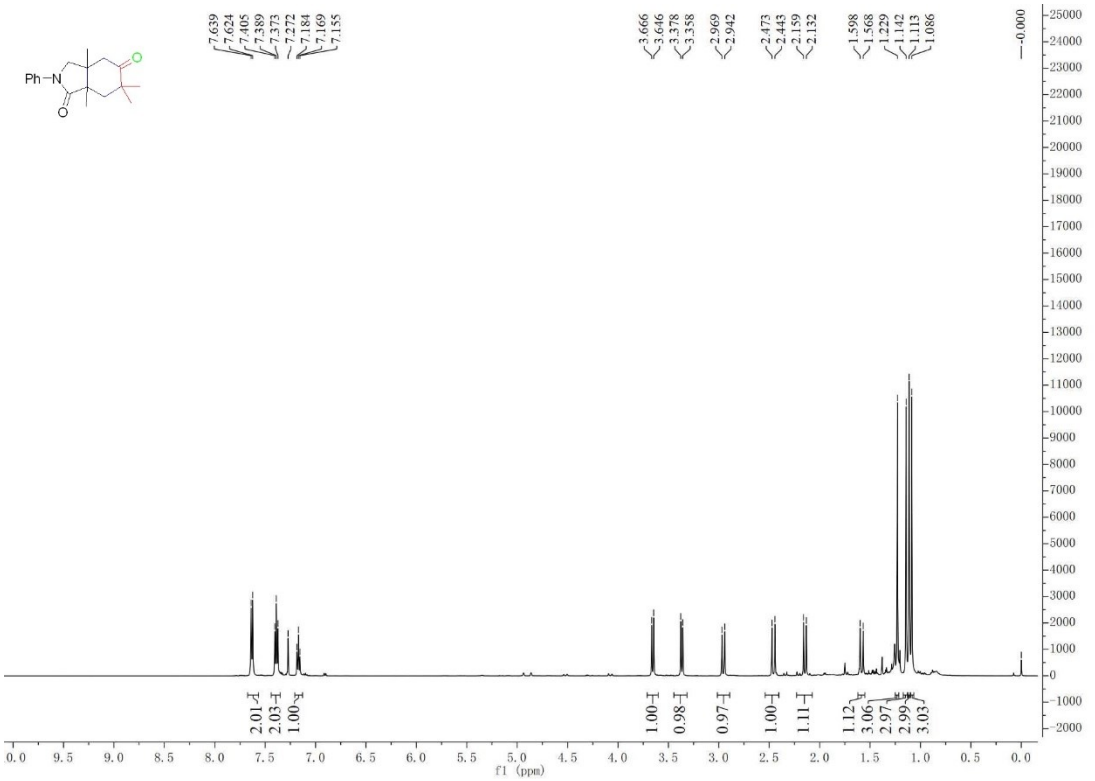


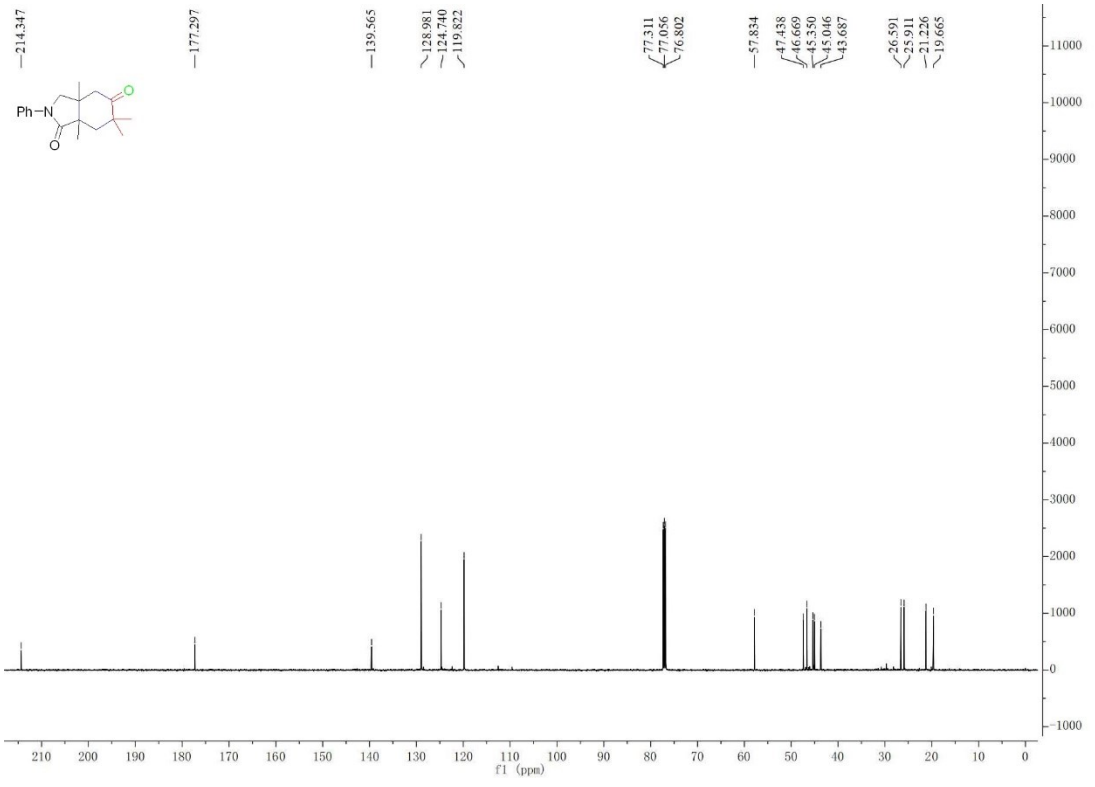


6,6,7a-Trimethyl-2-(naphthalen-1-yl)hexahydro-1H-isoindole-1,5(4H)-dione (3ga)

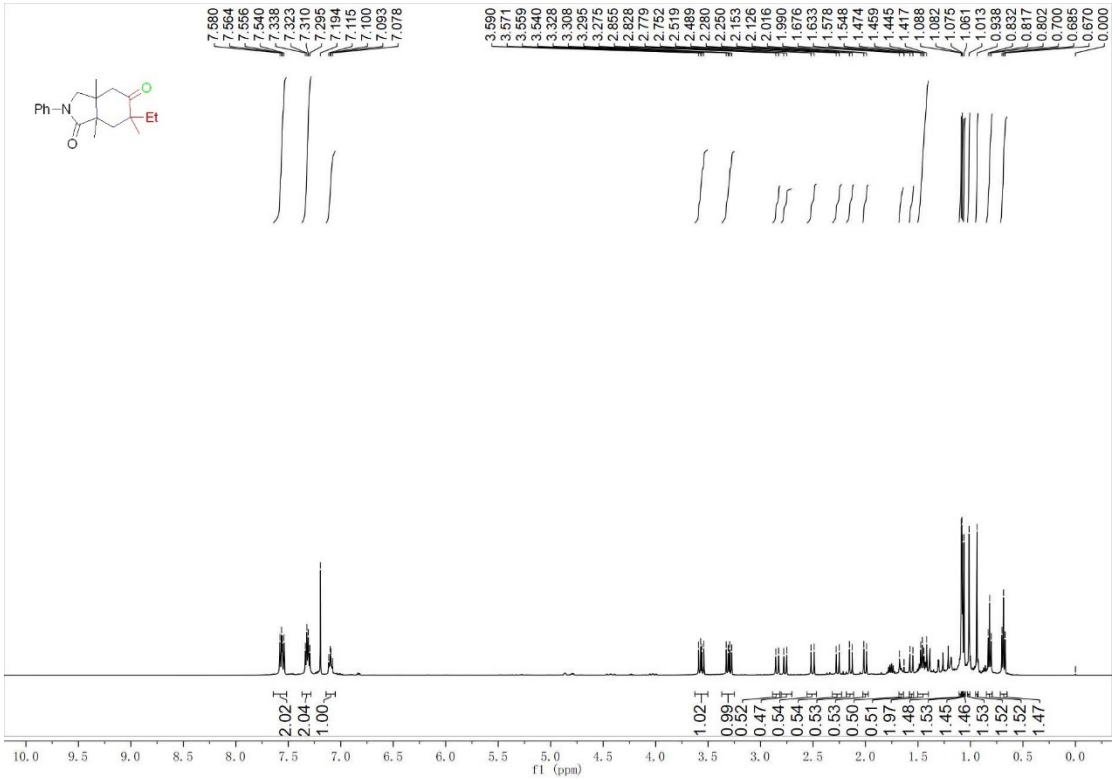


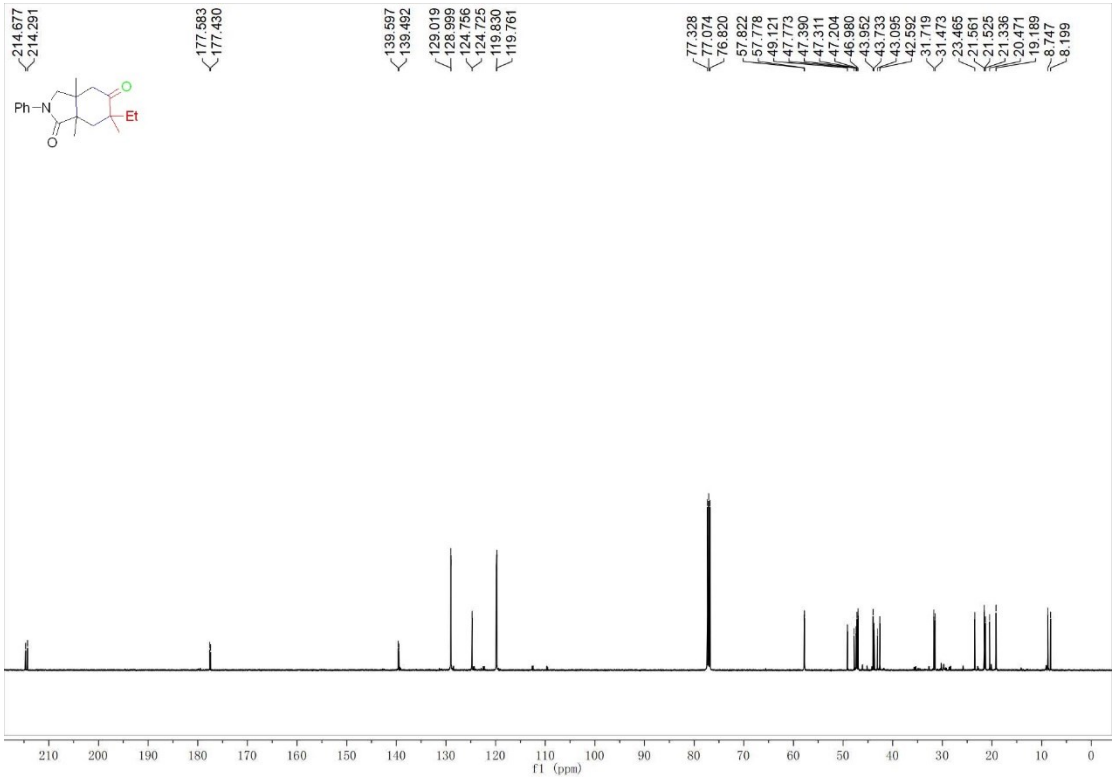
3a,6,6,7a-Tetramethyl-2-phenylhexahydro-1H-isoindole-1,5(4H)-dione (3ia)





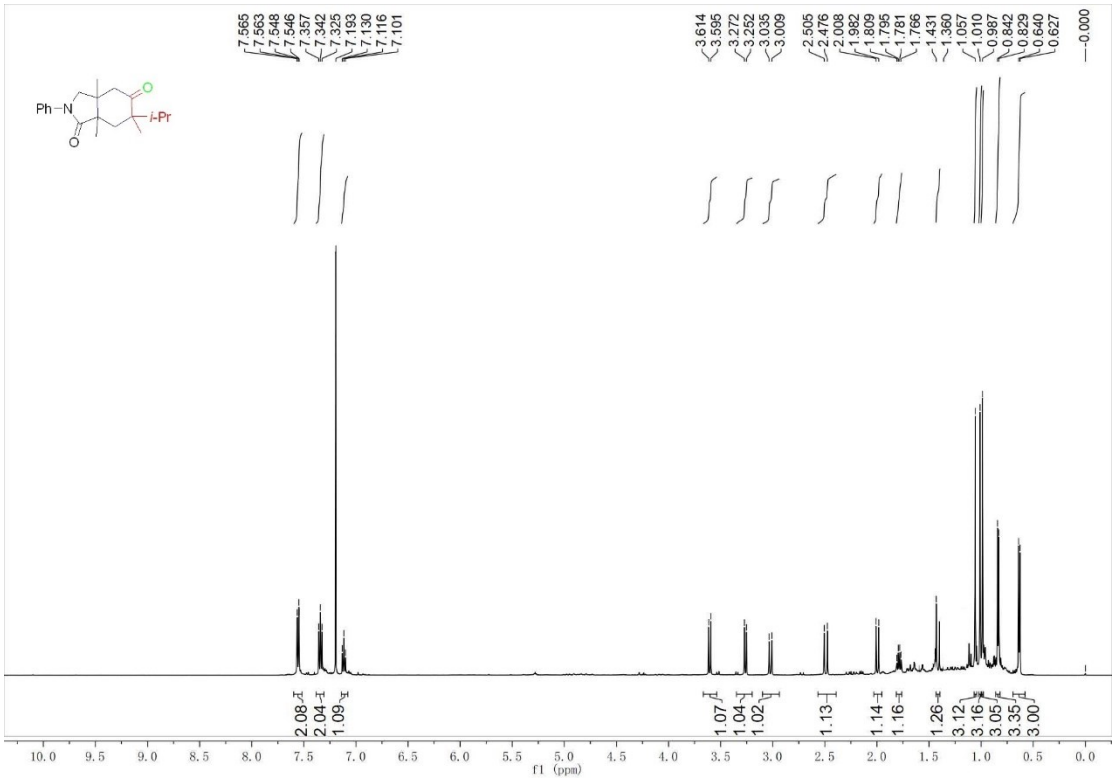
6-Ethyl-3a,6,7a-trimethyl-2-phenylhexahydro-1H-isoindole-1,5(4H)-dione (3ib)

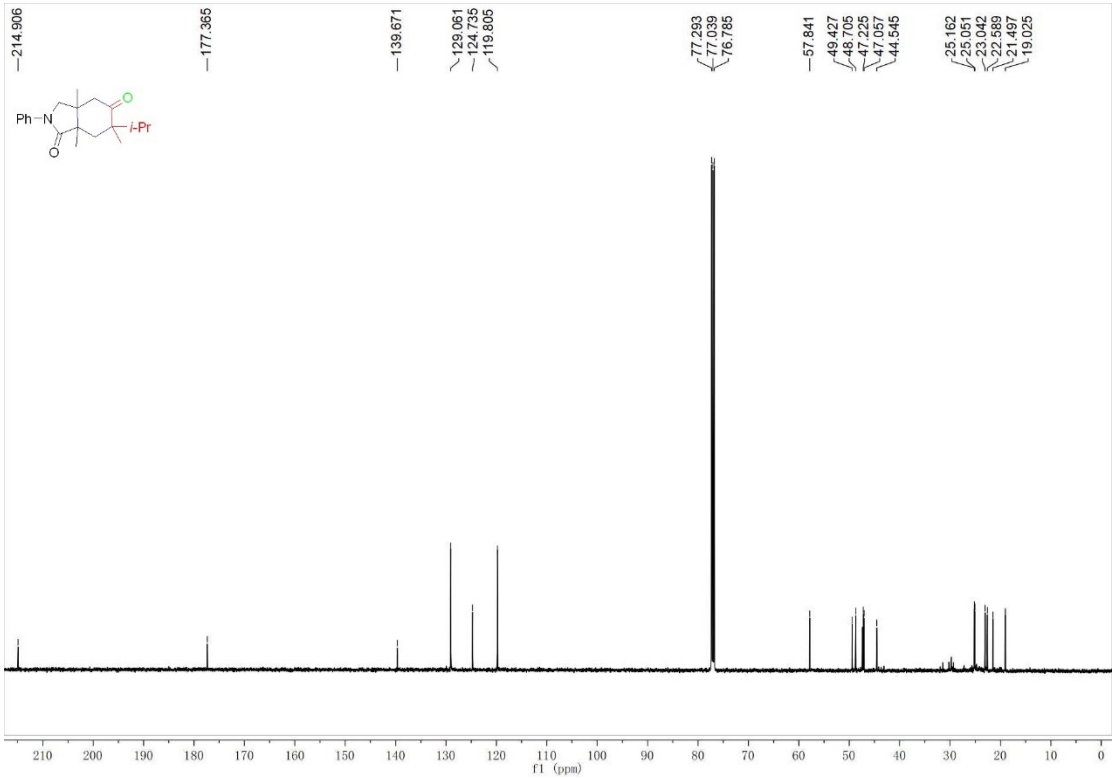




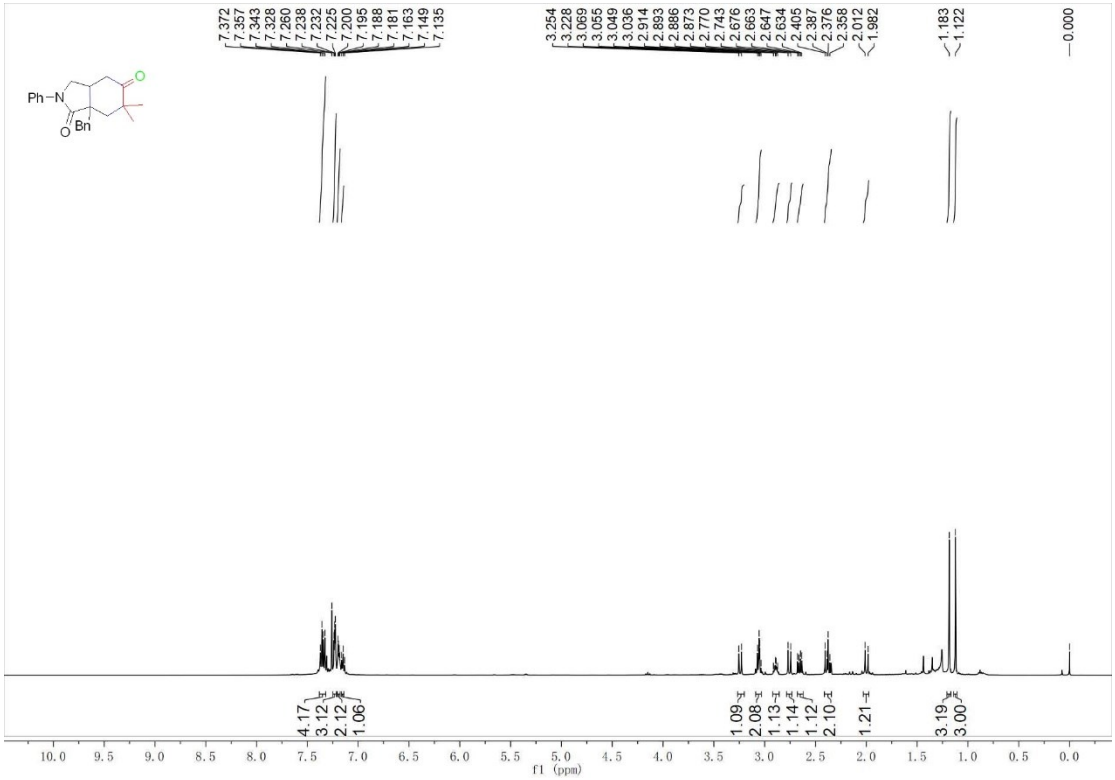
6-Isopropyl-3a,6,7a-trimethyl-2-phenylhexahydro-1H-isoindole-1,5(4H)-dione

(3ic)





7a-Benzyl-6,6-dimethyl-2-phenylhexahydro-1H-isoindole-1,5(4H)-dione (3ja)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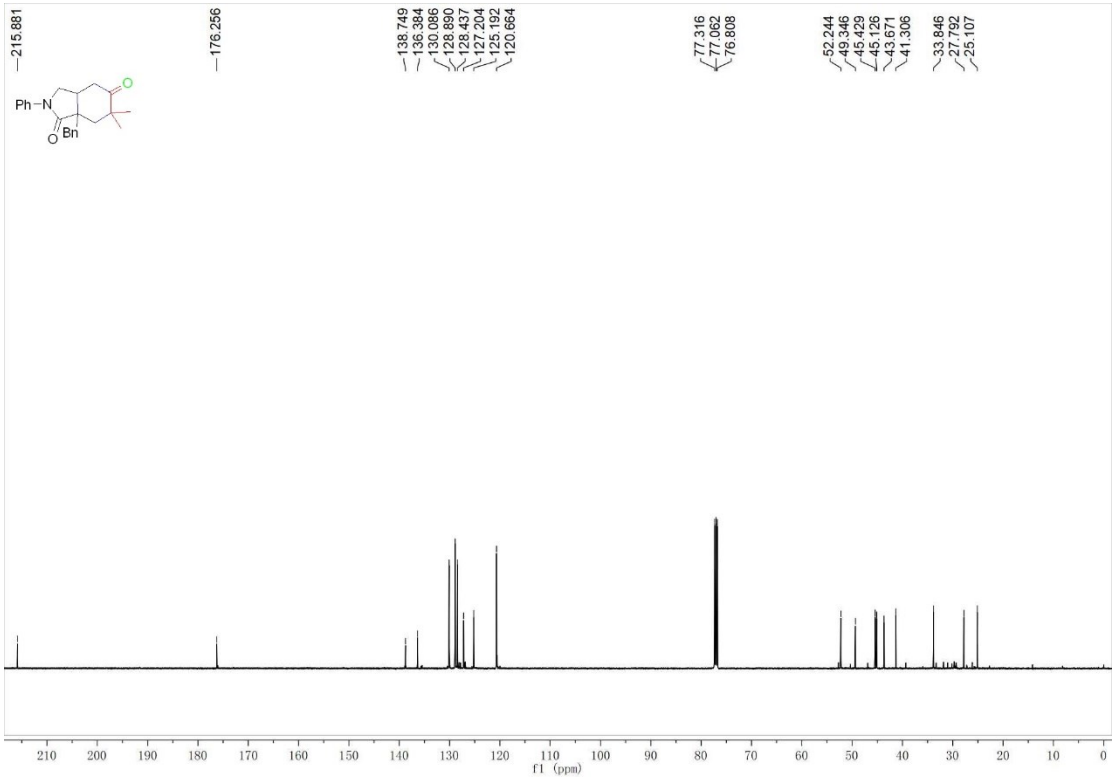
7.357
7.343
7.328
7.260
7.238
7.232
7.225
7.200
7.195
7.188
7.181
7.163
7.149
7.135
3.254
3.228
3.069
3.055
3.049
3.036
2.914
2.893
2.886
2.873
2.770
2.743
2.676
2.663
2.647
2.634
2.405
2.387
2.376
2.358
2.012
1.982
1.183
1.122
0.000
Ph
N
O
Bn
O
4.17
3.12
2.12
1.06
1.09
2.08
1.13
1.14
1.12
2.10
1.21
3.19
3.00
f1 (ppm)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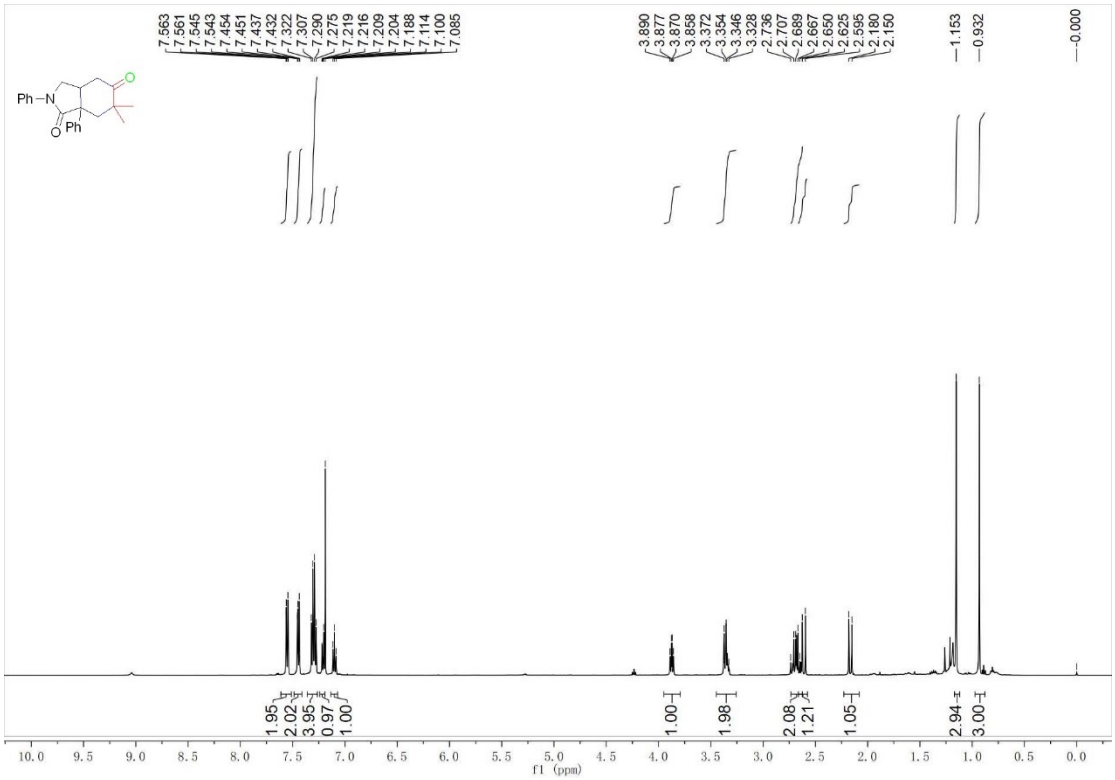
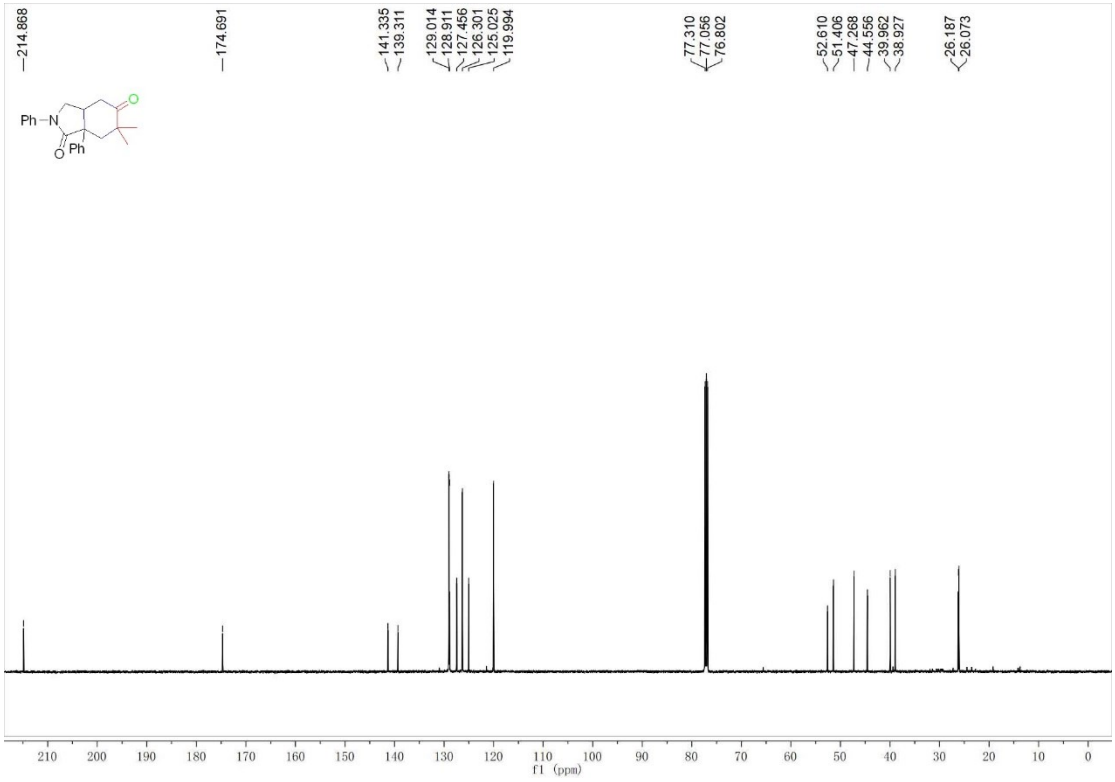
176.256
138.749
136.384
130.086
128.890
128.437
127.204
125.192
120.664
77.316
77.062
76.808
52.244
49.346
45.429
45.126
43.671
41.306
33.846
27.792
25.107
Ph
N
O
Bn
O
f1 (ppm)

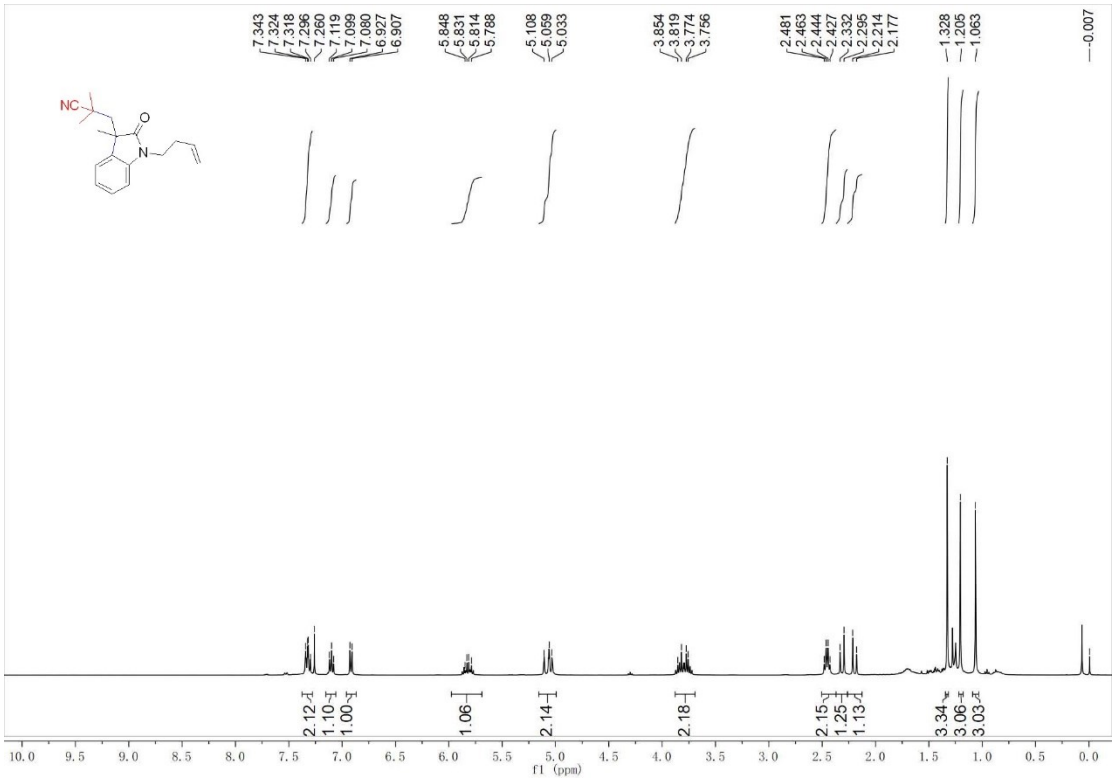
6,6-Dimethyl-2,7a-diphenylhexahydro-1H-isoindole-1,5(4H)-dione (3ka)

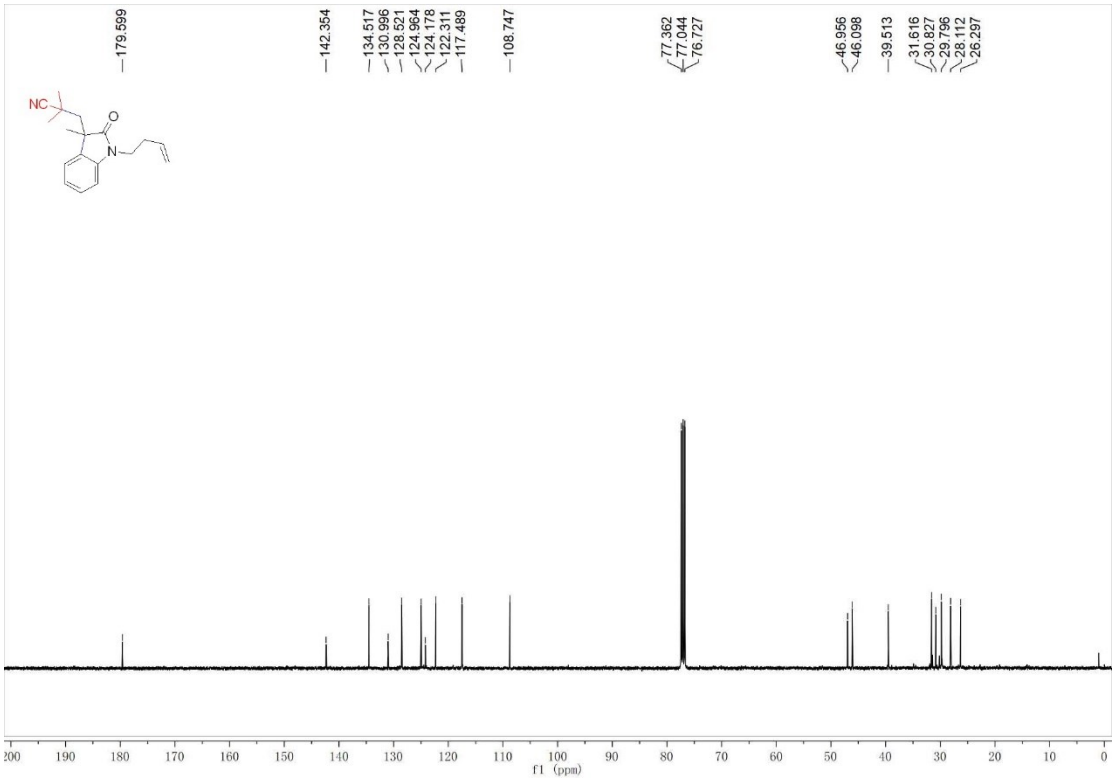




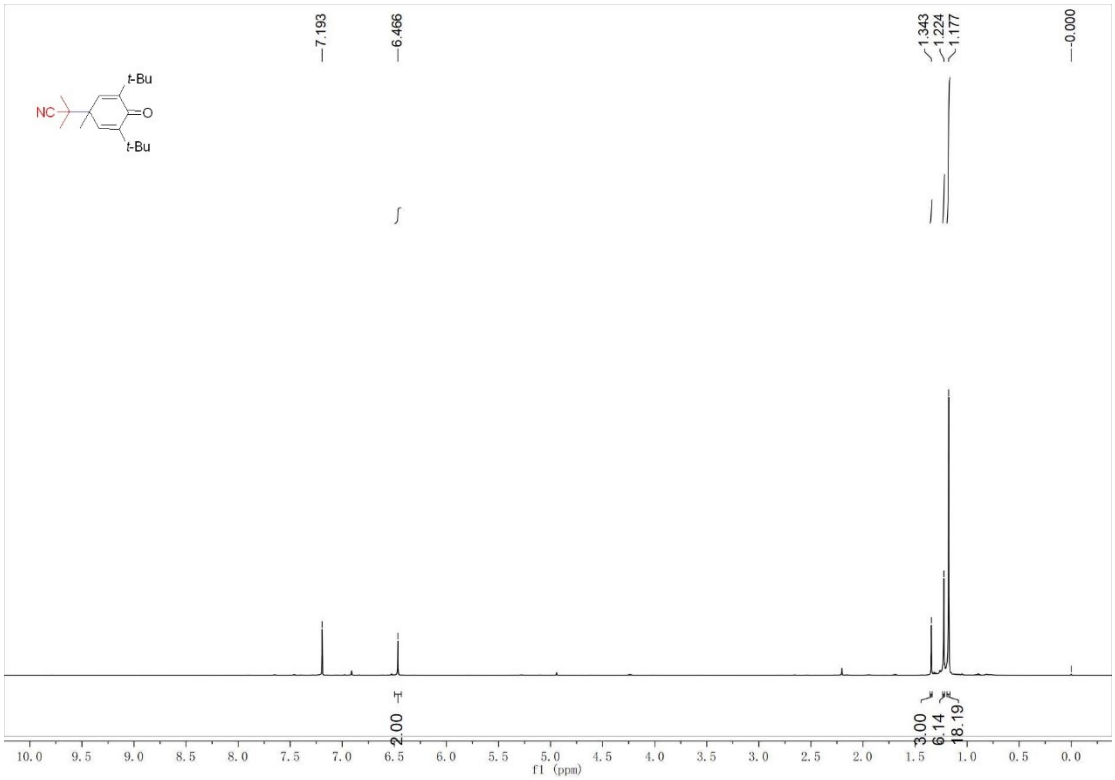
3-(1-(But-3-en-1-yl)-3-methyl-2-oxoindolin-3-yl)-2,2-dimethylpropanenitrile

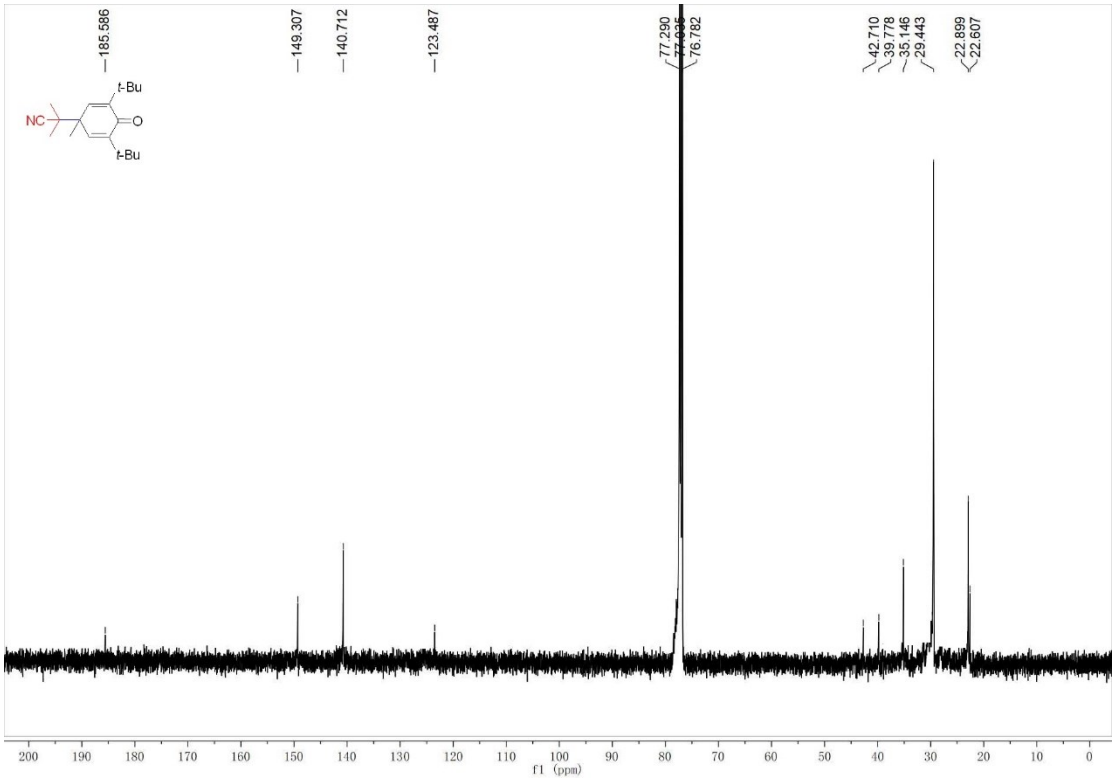
(4ma)



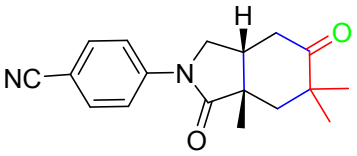


2-(3,5-di-*tert*-Butyl-1-methyl-4-oxocyclohexa-2,5-dien-1-yl)-2-methylpropanenitrile (4a)





(E) The X-ray single-crystal diffraction analysis of product 3ea



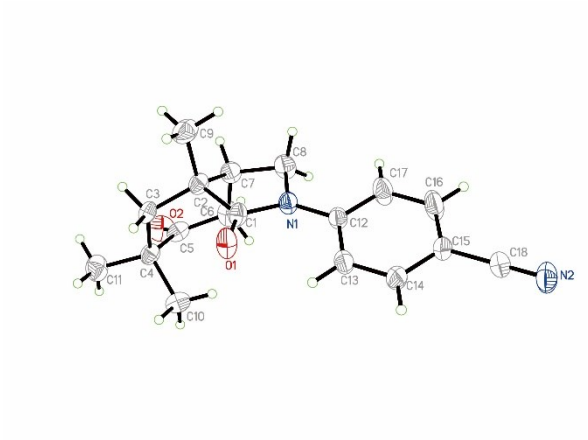


Table 1. Crystal data and structure refinement for 3ea.

Identification code	200513a	
Empirical formula	$C_{18}H_{20}N_2O_2$	
Formula weight	296.36	
Temperature	293(2) K	
Wavelength	1.54178	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 11.8025(4)	a= 90
	b = 6.6554(2)	b= 90.687(2)
	c = 19.9584(8)	g = 90
Volume	$1567.63(9)^3$	
Z	4	
Density (calculated)	1.256 Mg/m^3	
Absorption coefficient	0.660 mm^{-1}	
F(000)	632	
Crystal size	0.180 x 0.070 x 0.040 mm^3	
Theta range for data collection	3.745 to 66.039	
Index ranges	-10<=h<=13, -7<=k<=7, -23<=l<=23	
Reflections collected	9039	
Independent reflections	2724 [R(int) = 0.0378]	

Completeness to theta = 66.039	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9741 and 0.8905
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2724 / 0 / 203
Goodness-of-fit on F^2	1.024
Final R indices [I>2sigma(I)]	R1 = 0.0482, wR2 = 0.1227
R indices (all data)	R1 = 0.0698, wR2 = 0.1363
Extinction coefficient	0.0025(4)
Largest diff. peak and hole	0.155 and -0.140 $e.^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (^{2}x 10^3)

for 3ea. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	7722(2)	6699(2)	2066(1)	48(1)
N(2)	10683(2)	7586(4)	4978(1)	80(1)
O(1)	7081(1)	9933(2)	1907(1)	63(1)
O(2)	4001(2)	4098(3)	781(1)	82(1)
C(1)	7177(2)	8214(3)	1718(1)	45(1)
C(2)	6798(2)	7402(3)	1040(1)	47(1)
C(3)	5677(2)	8267(3)	782(1)	45(1)
C(4)	4576(2)	7437(3)	1083(1)	48(1)
C(5)	4680(2)	5168(3)	1069(1)	53(1)
C(6)	5691(2)	4331(3)	1426(1)	63(1)
C(7)	6807(2)	5120(3)	1154(1)	55(1)
C(8)	7763(2)	4833(3)	1666(1)	62(1)
C(9)	7733(2)	8013(5)	547(1)	74(1)
C(10)	4417(2)	8152(4)	1811(1)	64(1)
C(11)	3574(2)	8159(4)	662(1)	73(1)
C(12)	8327(2)	6891(3)	2676(1)	46(1)
C(13)	8150(2)	8482(4)	3106(1)	65(1)
C(14)	8750(2)	8632(4)	3699(1)	66(1)
C(15)	9531(2)	7205(4)	3878(1)	52(1)
C(16)	9701(2)	5607(4)	3455(1)	82(1)
C(17)	9107(2)	5450(4)	2859(1)	76(1)
C(18)	10171(2)	7396(4)	4496(1)	60(1)

Table 3. Bond lengths [Å] and angles [deg] for 3ea.

N(1)-C(1)	1.379(3)
N(1)-C(12)	1.409(2)
N(1)-C(8)	1.477(2)
N(2)-C(18)	1.136(3)
O(1)-C(1)	1.211(2)
O(2)-C(5)	1.212(2)
C(1)-C(2)	1.518(3)
C(2)-C(3)	1.527(3)
C(2)-C(7)	1.536(3)
C(2)-C(9)	1.543(3)
C(3)-C(4)	1.540(3)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-C(5)	1.516(3)
C(4)-C(11)	1.521(3)
C(4)-C(10)	1.542(3)
C(5)-C(6)	1.491(3)
C(6)-C(7)	1.524(3)
C(6)-H(6A)	0.9700
C(6)-H(6B)	0.9700
C(7)-C(8)	1.525(3)
C(7)-H(7)	0.9800
C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700
C(9)-H(9A)	0.9600
C(9)-H(9B)	0.9600
C(9)-H(9C)	0.9600
C(10)-H(10A)	0.9600
C(10)-H(10B)	0.9600
C(10)-H(10C)	0.9600
C(11)-H(11A)	0.9600
C(11)-H(11B)	0.9600
C(11)-H(11C)	0.9600
C(12)-C(17)	1.376(3)
C(12)-C(13)	1.381(3)
C(13)-C(14)	1.377(3)

C(13)-H(13)	0.9300
C(14)-C(15)	1.367(3)
C(14)-H(14)	0.9300
C(15)-C(16)	1.373(3)
C(15)-C(18)	1.445(3)
C(16)-C(17)	1.377(3)
C(16)-H(16)	0.9300
C(17)-H(17)	0.9300
C(1)-N(1)-C(12)	126.67(17)
C(1)-N(1)-C(8)	111.15(16)
C(12)-N(1)-C(8)	121.53(16)
O(1)-C(1)-N(1)	125.36(18)
O(1)-C(1)-C(2)	125.91(19)
N(1)-C(1)-C(2)	108.59(17)
C(1)-C(2)-C(3)	114.25(18)
C(1)-C(2)-C(7)	102.64(16)
C(3)-C(2)-C(7)	115.25(17)
C(1)-C(2)-C(9)	105.69(17)
C(3)-C(2)-C(9)	107.98(17)
C(7)-C(2)-C(9)	110.6(2)
C(2)-C(3)-C(4)	117.74(17)
C(2)-C(3)-H(3A)	107.9
C(4)-C(3)-H(3A)	107.9
C(2)-C(3)-H(3B)	107.9
C(4)-C(3)-H(3B)	107.9
H(3A)-C(3)-H(3B)	107.2
C(5)-C(4)-C(11)	111.52(19)
C(5)-C(4)-C(3)	106.34(18)
C(11)-C(4)-C(3)	109.02(18)
C(5)-C(4)-C(10)	109.61(18)
C(11)-C(4)-C(10)	108.7(2)
C(3)-C(4)-C(10)	111.67(17)
O(2)-C(5)-C(6)	121.9(2)
O(2)-C(5)-C(4)	122.8(2)
C(6)-C(5)-C(4)	115.33(18)
C(5)-C(6)-C(7)	113.04(19)
C(5)-C(6)-H(6A)	109.0
C(7)-C(6)-H(6A)	109.0

C(5)-C(6)-H(6B)	109.0
C(7)-C(6)-H(6B)	109.0
H(6A)-C(6)-H(6B)	107.8
C(6)-C(7)-C(8)	110.7(2)
C(6)-C(7)-C(2)	112.93(18)
C(8)-C(7)-C(2)	103.11(17)
C(6)-C(7)-H(7)	110.0
C(8)-C(7)-H(7)	110.0
C(2)-C(7)-H(7)	110.0
N(1)-C(8)-C(7)	103.17(17)
N(1)-C(8)-H(8A)	111.1
C(7)-C(8)-H(8A)	111.1
N(1)-C(8)-H(8B)	111.1
C(7)-C(8)-H(8B)	111.1
H(8A)-C(8)-H(8B)	109.1
C(2)-C(9)-H(9A)	109.5
C(2)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(2)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(4)-C(10)-H(10A)	109.5
C(4)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(4)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(4)-C(11)-H(11A)	109.5
C(4)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(4)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(17)-C(12)-C(13)	118.3(2)
C(17)-C(12)-N(1)	119.84(19)
C(13)-C(12)-N(1)	121.82(18)
C(14)-C(13)-C(12)	120.7(2)
C(14)-C(13)-H(13)	119.7

C(12)-C(13)-H(13)	119.7
C(15)-C(14)-C(13)	120.8(2)
C(15)-C(14)-H(14)	119.6
C(13)-C(14)-H(14)	119.6
C(14)-C(15)-C(16)	118.7(2)
C(14)-C(15)-C(18)	120.4(2)
C(16)-C(15)-C(18)	120.9(2)
C(15)-C(16)-C(17)	120.9(2)
C(15)-C(16)-H(16)	119.6
C(17)-C(16)-H(16)	119.6
C(12)-C(17)-C(16)	120.6(2)
C(12)-C(17)-H(17)	119.7
C(16)-C(17)-H(17)	119.7
N(2)-C(18)-C(15)	178.5(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (^{2}x 10^3) for 3ea.

The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	57(1)	41(1)	45(1)	-7(1)	-12(1)	7(1)
N(2)	75(2)	97(2)	66(1)	-7(1)	-29(1)	14(1)
O(1)	86(1)	37(1)	65(1)	-5(1)	-32(1)	2(1)
O(2)	73(1)	77(1)	94(1)	-24(1)	-9(1)	-27(1)
C(1)	52(1)	40(1)	44(1)	1(1)	-10(1)	-5(1)
C(2)	48(1)	53(1)	39(1)	-3(1)	-6(1)	-8(1)
C(3)	55(1)	46(1)	34(1)	2(1)	-8(1)	-8(1)
C(4)	50(1)	53(1)	41(1)	0(1)	-4(1)	-9(1)
C(5)	59(1)	56(1)	45(1)	-7(1)	5(1)	-18(1)
C(6)	80(2)	39(1)	69(2)	1(1)	-9(1)	-9(1)
C(7)	64(1)	50(1)	50(1)	-15(1)	-9(1)	5(1)
C(8)	72(2)	49(1)	66(2)	-20(1)	-16(1)	13(1)
C(9)	56(1)	112(2)	54(2)	4(1)	1(1)	-16(1)
C(10)	70(2)	67(2)	54(1)	-9(1)	10(1)	-4(1)
C(11)	56(1)	90(2)	74(2)	7(1)	-16(1)	-8(1)
C(12)	46(1)	48(1)	45(1)	-1(1)	-7(1)	4(1)
C(13)	72(2)	71(2)	52(1)	-12(1)	-18(1)	31(1)
C(14)	74(2)	78(2)	47(1)	-18(1)	-15(1)	27(1)
C(15)	46(1)	66(1)	45(1)	2(1)	-8(1)	4(1)
C(16)	87(2)	77(2)	81(2)	-14(2)	-38(2)	37(2)
C(17)	88(2)	64(2)	74(2)	-23(1)	-33(1)	34(1)
C(18)	50(1)	72(2)	57(1)	1(1)	-11(1)	6(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (^{2}x 10 ^{3}) for 3ea.

	x	y	z	U(eq)
H(3A)	5641	8057	302	54
H(3B)	5691	9706	858	54
H(6A)	5681	2878	1387	75
H(6B)	5646	4665	1898	75
H(7)	6991	4426	737	66
H(8A)	7630	3662	1944	75
H(8B)	8488	4689	1448	75
H(9A)	7780	9452	525	111
H(9B)	7553	7491	110	111
H(9C)	8447	7477	697	111
H(10A)	3754	7534	1993	95
H(10B)	4331	9586	1817	95
H(10C)	5069	7780	2076	95
H(11A)	3668	7738	206	110
H(11B)	3533	9598	680	110
H(11C)	2887	7595	834	110
H(13)	7620	9463	2993	78
H(14)	8624	9717	3982	80
H(16)	10223	4619	3573	98
H(17)	9235	4360	2579	91

Table 6. Torsion angles for 3ea.

C(12)-N(1)-C(1)-O(1)	-4.6(4)
C(8)-N(1)-C(1)-O(1)	-175.3(2)
C(12)-N(1)-C(1)-C(2)	171.24(19)
C(8)-N(1)-C(1)-C(2)	0.5(2)
O(1)-C(1)-C(2)-C(3)	-38.8(3)
N(1)-C(1)-C(2)-C(3)	145.43(18)
O(1)-C(1)-C(2)-C(7)	-164.3(2)
N(1)-C(1)-C(2)-C(7)	19.9(2)
O(1)-C(1)-C(2)-C(9)	79.8(3)
N(1)-C(1)-C(2)-C(9)	-96.0(2)
C(1)-C(2)-C(3)-C(4)	-77.8(2)
C(7)-C(2)-C(3)-C(4)	40.7(3)
C(9)-C(2)-C(3)-C(4)	164.91(19)
C(2)-C(3)-C(4)-C(5)	-47.9(2)
C(2)-C(3)-C(4)-C(11)	-168.21(18)
C(2)-C(3)-C(4)-C(10)	71.7(3)
C(11)-C(4)-C(5)-O(2)	-3.4(3)
C(3)-C(4)-C(5)-O(2)	-122.2(2)
C(10)-C(4)-C(5)-O(2)	117.0(2)
C(11)-C(4)-C(5)-C(6)	175.6(2)
C(3)-C(4)-C(5)-C(6)	56.8(2)
C(10)-C(4)-C(5)-C(6)	-64.0(3)
O(2)-C(5)-C(6)-C(7)	120.5(2)
C(4)-C(5)-C(6)-C(7)	-58.5(3)
C(5)-C(6)-C(7)-C(8)	160.30(18)
C(5)-C(6)-C(7)-C(2)	45.3(3)
C(1)-C(2)-C(7)-C(6)	87.9(2)
C(3)-C(2)-C(7)-C(6)	-37.0(3)
C(9)-C(2)-C(7)-C(6)	-159.77(19)
C(1)-C(2)-C(7)-C(8)	-31.6(2)
C(3)-C(2)-C(7)-C(8)	-156.47(19)
C(9)-C(2)-C(7)-C(8)	80.7(2)
C(1)-N(1)-C(8)-C(7)	-20.9(3)
C(12)-N(1)-C(8)-C(7)	167.78(19)
C(6)-C(7)-C(8)-N(1)	-89.0(2)
C(2)-C(7)-C(8)-N(1)	32.1(2)

C(1)-N(1)-C(12)-C(17)	-159.8(2)
C(8)-N(1)-C(12)-C(17)	10.0(3)
C(1)-N(1)-C(12)-C(13)	21.1(3)
C(8)-N(1)-C(12)-C(13)	-169.0(2)
C(17)-C(12)-C(13)-C(14)	0.8(4)
N(1)-C(12)-C(13)-C(14)	179.8(2)
C(12)-C(13)-C(14)-C(15)	-0.3(4)
C(13)-C(14)-C(15)-C(16)	-0.4(4)
C(13)-C(14)-C(15)-C(18)	178.8(2)
C(14)-C(15)-C(16)-C(17)	0.7(4)
C(18)-C(15)-C(16)-C(17)	-178.6(3)
C(13)-C(12)-C(17)-C(16)	-0.5(4)
N(1)-C(12)-C(17)-C(16)	-179.6(3)
C(15)-C(16)-C(17)-C(12)	-0.2(5)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for 3ea

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)