

Supplementary Information

Metal-free direct cyanoisopropylation/arylation of *N*-arylacrylamides or *N*-alkyl-*N*- (arylsulfonyl)acrylamides with AIBN: a simple and mild approach to cyano-containing oxindoles

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General remarks

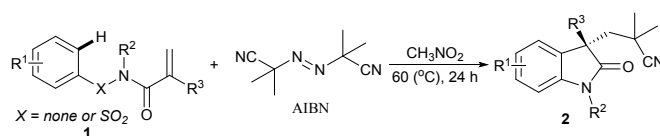
Reagents were purchased from commercial sources and were used as received unless mentioned otherwise. All solvents were dried and distilled prior to use according to the standard protocols. ^1H and ^{13}C NMR spectra were obtained in CDCl_3 with TMS as internal standard (400 MHz ^1H , 100 MHz ^{13}C) at room temperature. Multiplicities are indicated as s (singlet), d (doublet), t (triplet), q (quintet), m (multiplet) and coupling constants (J) are reported in hertz. HRMS was measured on an electrospray ionization (ESI) apparatus using time-of-flight (TOF) mass spectrometry. IR measurements were performed with a FTIR SHIMADZU DR-8000 spectrometer that was fitted with a Pike Technologies MIRacle Single Reflection ATR adapter. Melting points were determined using XT-4 apparatus and are uncorrected.

Typical experimental procedure

(1) Synthesis of substrates

N-Arylacrylamides **1a-q** and **4**^[S1] and *N*-alkyl-*N*-(arylsulfonyl) acrylamides **1t-v**^[S2] were prepared according to literature procedures.

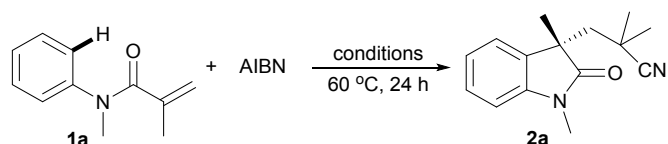
(2) General procedure for the synthesis of cyano-containing oxindoles through metal-free direct cyanoisopropylation/arylation of alkenes with AIBN



To an oven-dried Schlenk tube was added substrate **1** (0.2 mmol), AIBN (0.6 mmol), and CH_3NO_2 (1 mL). The tube was then charged with nitrogen, and the mixture was stirred at $60\text{ }^\circ\text{C}$ for 24 h. The reaction mixture was then allowed to cool

to room temperature, after which the crude reaction mixture was loaded directly onto a column of silica gel and purified by column chromatography (petroleum ether-ethyl acetate = 6:1) to give the desired product **2**.

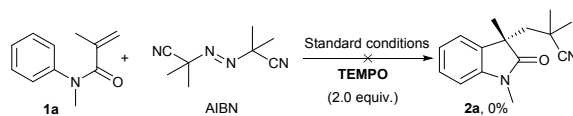
Table S1. Screening of Reaction Conditions.^a



Entry	AIBN (equiv.)	Oxidant (equiv.)	Solvent	Conv ^b (%)	Yield ^c (%)
1	1.5	none	CH ₃ NO ₂	63	61
2	1.5	O ₂ (balloon)	CH ₃ NO ₂	10	trace
3	1.5	K ₂ S ₂ O ₈ (2.0)	CH ₃ NO ₂	86	58
4	1.5	(NH ₄) ₂ S ₂ O ₈ (2.0)	CH ₃ NO ₂	85	54
5 ^d	1.5	none	CH ₃ NO ₂	52	49
6 ^e	1.5	none	CH ₃ NO ₂	68	64
7	3.0	none	CH ₃ NO ₂	95	89
8	4.0	none	CH ₃ NO ₂	>95	86
9	3.0	none	DMSO	>95	31
10	3.0	none	DMF	32	trace
11	3.0	none	toluene	60	15
12	3.0	none	CH ₃ CN	67	12
13	3.0	none	CH ₃ NO ₂	>95	87
14	3.0	none	CH ₃ NO ₂	93	85
15	3.0	none	CH ₃ NO ₂	>95	88

^aReaction conditions: *N*-arylacrylamide **1a** (0.2 mmol), solvent (1.0 mL), 60 °C, under N₂ atmosphere. ^bConversion based on TLC analysis and amount of recovered starting material. ^cYield of isolated product. ^dTemperature: 80 °C. ^eReaction time: 48h.

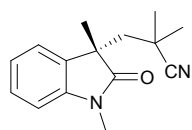
Preliminary mechanistic studies with TEMPO



To an oven-dried Schlenk tube was added *N*-arylacrylamide **1a** (0.2 mmol), AIBN (0.6 mmol), TEMPO (0.4 mmol), and CH₃NO₂ (1 mL). The tube was then charged with nitrogen, and the mixture was stirred at 60 °C for 24 h. When the reaction mixture was investigated by GC-MS, no desired product was observed.

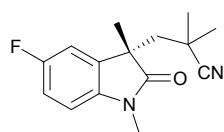
Characterization data of products

3-(1,3-Dimethyl-2-oxindolin-3-yl)-2,2-dimethylpropanenitrile (**2a**):



White solid (43.1 mg, 89%); mp 117-118 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.35-7.31 (m, 2H), 7.11 (t, *J* = 7.5 Hz, 1H), 6.90 (d, *J* = 7.6 Hz, 1H), 3.24 (s, 3H), 2.33 (d, *J* = 14.4 Hz, 1H), 2.16 (d, *J* = 14.4 Hz, 1H), 1.35 (s, 3H), 1.16 (s, 3H), 1.08 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 179.5, 143.0, 130.8, 128.5, 124.6, 123.8, 122.4, 108.4, 46.9, 46.4, 30.6, 29.5, 27.3, 26.6, 26.3; IR (KBr): $\tilde{\nu}$ = 2242, 1718, 1613, 1436, 1379, 1339 cm⁻¹; HRMS *m/z* (ESI) calcd for C₁₅H₁₈N₂O⁺ [M⁺], 242.1419; found, 242.1417.

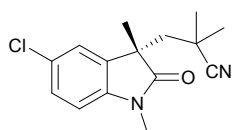
3-(5-Fluoro-1,3-dimethyl-2-oxindolin-3-yl)-2,2-dimethylpropanenitrile (**2b**):



Yellow oil (27 mg, 52%); ¹H NMR (400 MHz, CDCl₃) δ 7.07-7.00 (m, 2H), 6.84-6.80 (m, 1H), 3.23 (s, 3H), 2.33 (d, *J* = 14.6 Hz, 1H), 2.11 (d, *J* = 14.6

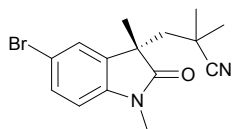
Hz, 1H), 1.35 (s, 3H), 1.17 (s, 3H), 1.11 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 179.1, 160.4, 158.0, 139.0, 132.7, 132.6, 123.7, 115.0, 114.7, 112.8, 112.6, 109.0, 108.9, 47.4, 47.4, 46.5, 30.6, 29.6, 27.3, 26.8, 26.5; IR (KBr): $\tilde{\nu}$ = 2236, 1717, 1621, 1435, 1376, 1338 cm^{-1} ; HRMS m/z (ESI) calcd for $\text{C}_{15}\text{H}_{17}\text{FN}_2\text{O}^+$ [M^+], 260.1325; found, 260.1324.

3-(5-Chloro-1,3-dimethyl-2-oxoindolin-3-yl)-2,2-dimethylpropanenitrile (2c):



White solid (37.6 mg, 68%); mp 135-136 $^{\circ}\text{C}$; ^1H NMR (400 MHz, CDCl_3) δ 7.31-7.28 (m, 2H), 6.82 (d, J = 8.4 Hz, 1H), 3.22 (s, 3H), 2.32 (d, J = 14.6 Hz, 1H), 2.11 (d, J = 14.6 Hz, 1H), 1.35 (s, 3H), 1.16 (s, 3H), 1.11 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 179.0, 141.7, 132.7, 128.5, 127.9, 125.0, 123.6, 109.4, 47.2, 46.5, 30.6, 29.6, 27.2, 27.0, 26.5; IR (KBr): $\tilde{\nu}$ = 2242, 1715, 1614, 1436, 1378, 1334 cm^{-1} ; HRMS m/z (ESI) calcd for $\text{C}_{15}\text{H}_{17}\text{ClN}_2\text{O}^+$ [M^+], 276.1028; found, 276.1027; HRMS m/z (ESI) calcd for $\text{C}_{15}\text{H}_{17}^{37}\text{ClN}_2\text{O}^+$ [M^+], 278.1001; found, 278.1003.

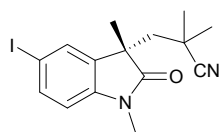
3-(5-Bromo-1,3-dimethyl-2-oxoindolin-3-yl)-2,2-dimethylpropanenitrile (2d):



White solid (48.2 mg, 75%); mp 141-143 $^{\circ}\text{C}$; ^1H NMR (400 MHz, CDCl_3) δ 7.46-7.41 (m, 2H), 6.78 (d, J = 8.2 Hz, 1H), 3.22 (s, 3H), 2.32 (d, J = 14.6 Hz, 1H), 2.10 (d, J = 14.6 Hz, 1H), 1.34 (s, 3H), 1.15 (s, 3H), 1.11 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 178.9, 142.2, 133.1, 131.4, 127.7, 123.6, 115.1, 109.9, 47.2, 46.5, 30.6, 29.5, 27.2, 27.1, 26.4; IR (KBr): $\tilde{\nu}$ = 2235, 1716, 1621, 1431, 1380, 1329 cm^{-1} ; HRMS m/z (ESI) calcd for $\text{C}_{15}\text{H}_{17}\text{BrN}_2\text{O}^+$ [M^+], 320.0524; found, 320.0525; HRMS

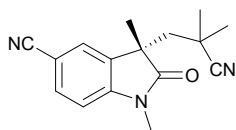
m/z (ESI) calcd for $C_{15}H_{17}^{81}BrN_2O^+$ [M^+], 322.0504; found, 322.0502.

3-(5-Iodo-1,3-dimethyl-2-oxoindolin-3-yl)-2,2-dimethylpropanenitrile (2e):



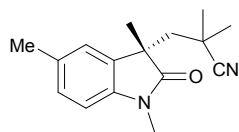
White solid (60 mg, 80%); mp 138-139 °C; 1H NMR (400 MHz, $CDCl_3$) δ 7.64-7.57 (m, 2H), 6.68 (d, $J = 8.2$ Hz, 1H), 3.20 (s, 3H), 2.31 (d, $J = 14.6$ Hz, 1H), 2.09 (d, $J = 14.6$ Hz, 1H), 1.33 (s, 3H), 1.14 (s, 3H), 1.10 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 178.7, 142.9, 137.3, 133.4, 133.3, 123.6, 110.5, 84.9, 47.0, 46.5, 30.5, 29.5, 27.2, 27.1, 26.4; IR (KBr): $\tilde{\nu} = 2237, 1718, 1625, 1437, 1381, 1341$ cm^{-1} ; HRMS m/z (ESI) calcd for $C_{15}H_{17}IN_2O^+$ [M^+], 368.0386; found, 368.0389.

3-(2-Cyano-2-methylpropyl)-1,3-dimethyl-2-oxoindoline-5-carbonitrile (2f):



White solid (32 mg, 60%); mp 123-125 °C; 1H NMR (400 MHz, $CDCl_3$) δ 7.66-7.63 (m, 1H), 7.54 (d, $J = 1.2$ Hz, 1H), 6.97 (d, $J = 8.0$ Hz, 1H), 3.26 (s, 3H), 2.33 (d, $J = 14.8$ Hz, 1H), 2.14 (d, $J = 14.8$ Hz, 1H), 1.36 (s, 3H), 1.13 (d, $J = 3.4$ Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.1, 147.0, 133.8, 132.1, 127.7, 123.7, 119.0, 109.0, 105.6, 46.8, 46.4, 30.4, 29.5, 27.3, 27.0, 26.5; IR (KBr): $\tilde{\nu} = 2218, 1719, 1611, 1448, 1359, 1318$ cm^{-1} ; HRMS m/z (ESI) calcd for $C_{16}H_{17}N_3O^+$ [M^+], 267.1372; found, 267.1370.

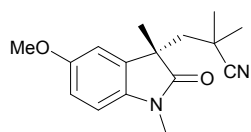
2,2-Dimethyl-3-(1,3,5-trimethyl-2-oxoindolin-3-yl)propanenitrile (2h):



White solid (41.5 mg, 81%); mp 100-102 °C; 1H NMR (400 MHz, $CDCl_3$) δ 7.11 (d, $J = 8.8$ Hz, 2H), 6.77 (d, $J = 7.6$ Hz, 1H), 3.20 (s, 3H), 2.34 (s, 3H),

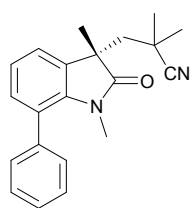
2.29 (d, $J = 14.6$ Hz, 1H), 2.13 (d, $J = 14.6$ Hz, 1H), 1.32 (s, 3H), 1.15 (s, 3H), 1.05 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 179.5, 140.6, 131.9, 130.8, 128.7, 125.5, 124.0, 108.1, 46.9, 46.3, 30.6, 29.6, 27.3, 26.4, 26.3, 21.1; IR (KBr): $\tilde{\nu} = 2232, 1720, 1619, 1431, 1377, 1320$ cm^{-1} ; HRMS m/z (ESI) calcd for $\text{C}_{16}\text{H}_{20}\text{N}_2\text{O}^+$ [M^+], 256.1576; found, 256.1577.

3-(5-Methoxy-1,3-dimethyl-2-oxindolin-3-yl)-2,2-dimethylpropanenitrile (2i):



White solid (50.7 mg, 93%); mp 108-109 °C; ^1H NMR (400 MHz, CDCl_3) δ 6.94 (d, $J = 2.4$ Hz, 1H), 6.87-6.84 (m, 1H), 6.80 (d, $J = 8.4$ Hz, 1H), 3.81 (s, 3H), 3.21 (s, 3H), 2.32 (d, $J = 14.6$ Hz, 1H), 2.14 (d, $J = 14.6$ Hz, 1H), 1.34 (s, 3H), 1.19 (s, 3H), 1.07 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 179.2, 155.8, 136.5, 132.1, 124.0, 113.1, 112.1, 108.7, 55.8, 47.3, 46.3, 30.6, 29.6, 27.4, 26.4, 26.3; IR (KBr): $\tilde{\nu} = 2238, 1718, 1625, 1432, 1372, 1314$ cm^{-1} ; HRMS m/z (ESI) calcd for $\text{C}_{16}\text{H}_{20}\text{N}_2\text{O}_2^+$ [M^+], 272.1525; found, 272.1526.

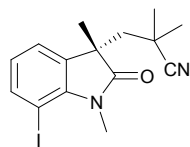
3-(1,3-Dimethyl-2-oxo-7-phenylindolin-3-yl)-2,2-dimethylpropanenitrile (2j):



White solid (52.2 mg, 82%); mp 130-132 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.42-7.35 (m, 5H), 7.31-7.29 (m, 1H), 7.17-7.09 (m, 2H), 2.75 (s, 3H), 2.36 (d, $J = 14.4$ Hz, 1H), 2.18 (d, $J = 14.4$ Hz, 1H), 1.40 (s, 3H), 1.20 (s, 3H), 1.15 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 180.5, 140.1, 138.8, 131.5, 130.1, 129.5, 127.7, 127.6, 125.9, 123.8, 123.4, 121.6, 46.8, 46.2, 30.6, 30.3, 29.7, 27.6, 26.9; IR (KBr): $\tilde{\nu} = 2238,$

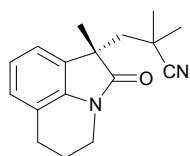
1719, 1622, 1427, 1377, 1330 cm^{-1} ; HRMS m/z (ESI) calcd for $\text{C}_{21}\text{H}_{22}\text{N}_2\text{O}^+$ [M^+], 318.1732; found, 318.1731.

3-(7-Iodo-1,3-dimethyl-2-oxoindolin-3-yl)-2,2-dimethylpropanenitrile (2k):



White solid (46.4 mg, 63%); mp 136-138 $^{\circ}\text{C}$; ^1H NMR (400 MHz, CDCl_3) δ 7.75-7.73 (m, 1H), 7.27 (d, $J = 7.8$ Hz, 1H), 6.82 (t, $J = 7.7$ Hz, 1H), 3.64 (s, 3H), 2.32 (d, $J = 14.6$ Hz, 1H), 2.16 (d, $J = 14.6$ Hz, 1H), 1.34 (s, 3H), 1.20 (s, 3H), 1.09 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 180.3, 143.4, 141.2, 133.8, 124.4, 124.1, 123.8, 71.9, 46.5, 46.5, 30.6, 30.3, 29.7, 27.8, 26.4; IR (KBr): $\tilde{\nu} = 2236, 1719, 1625, 1435, 1380, 1338$ cm^{-1} ; HRMS m/z (ESI) calcd for $\text{C}_{15}\text{H}_{17}\text{IN}_2\text{O}^+$ [M^+], 368.0386; found, 368.0385.

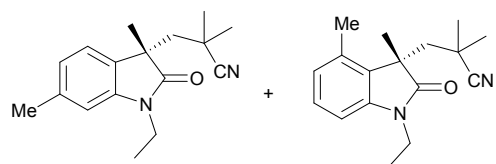
2,2-Dimethyl-3-(1-methyl-2-oxo-1,2,5,6-tetrahydro-4H-pyrrolo[3,2,1-ij] quinolin-1-yl)propanenitrile (2l):



Colorless oil (45.6 mg, 85%); ^1H NMR (400 MHz, CDCl_3) δ 7.12 (d, $J = 7.6$ Hz, 1H), 7.05 (d, $J = 7.6$ Hz, 1H), 6.96 (t, $J = 7.5$ Hz, 1H), 3.76-3.67 (m, 2H), 2.81-2.76 (m, 2H), 2.30 (d, $J = 14.4$ Hz, 1H), 2.11 (d, $J = 14.4$ Hz, 1H), 2.05-1.96 (m, 2H), 1.33 (s, 3H), 1.14 (s, 3H), 1.10 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 178.3, 138.8, 129.3, 127.2, 123.9, 122.4, 121.7, 120.5, 48.2, 46.3, 38.8, 30.6, 29.4, 27.0, 26.8, 24.5, 20.9; IR (KBr): $\tilde{\nu} = 2237, 1717, 1615, 1470, 1379, 1345$ cm^{-1} ; HRMS m/z (ESI) calcd for $\text{C}_{17}\text{H}_{20}\text{N}_2\text{O}^+$ [M^+], 268.1576; found, 268.1578.

3-(1-Ethyl-3,6-dimethyl-2-oxoindolin-3-yl)-2,2-dimethylpropanenitrile and 3-(1-

Ethyl-3,4-dimethyl-2-oxoindolin-3-yl)-2,2-dimethylpropanenitrile (2m + 2m'):

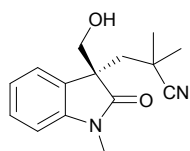


Colorless oil (48.7 mg, 90%); ¹H NMR (400

MHz, CDCl₃) δ 7.21 (t, *J* = 7.7 Hz, 1.31H), 6.90 (d, *J* = 7.3 Hz, 0.35H), 6.85 (d, *J* = 7.8 Hz, 1H), 6.77 -6.73 (m, 1.32H), 3.84-3.69 (m, 2.8H), 2.44 (s, 3H), 2.41-2.37 (m, 2.11H), 2.31-2.15 (m, 1.8H), 1.61 (s, 1H), 1.39 (s, 3H), 1.29-1.20 (m, 9.37H), 1.07 (s, 3H), 1.04 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 179.5, 179.1, 142.2, 142.0, 138.5, 136.1, 128.3, 128.2, 125.0, 124.7, 124.2, 123.5, 122.7, 109.4, 106.2, 47.5, 46.6, 46.0, 44.7, 34.7, 34.6, 30.9, 30.7, 29.6, 29.4, 27.9, 25.9, 25.7, 24.8, 21.8, 19.0, 12.2, 12.1; IR (KBr): $\tilde{\nu}$ = 2244, 1728, 1627, 1476, 1369, 1349 cm⁻¹; HRMS *m/z* (ESI) calcd for C₁₇H₂₂N₂O⁺ [M⁺], 270.1732; found, 270.1729.

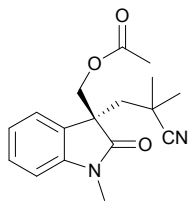
3-(3-(Hydroxymethyl)-1-methyl-2-oxoindolin-3-yl)-2,2-dimethylpropanenitrile (2o):

(2o):



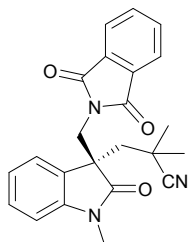
White solid (25.8 mg, 50%); mp 141-142 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.9-7.34 (m, 2H), 7.12 (t, *J* = 7.5 Hz, 1H), 6.93 (d, *J* = 7.8 Hz, 1H), 3.70 (d, *J* = 10.8 Hz, 1H), 3.60 (d, *J* = 10.8 Hz, 1H), 3.24 (s, 3H), 2.47 (d, *J* = 14.7 Hz, 1H), 2.25 (d, *J* = 14.7 Hz, 1H), 1.18 (s, 3H), 1.11 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 178.2, 143.9, 129.2, 127.0, 125.1, 123.9, 122.6, 108.7, 68.9, 52.7, 41.6, 30.3, 29.7, 26.9, 26.3; IR (KBr): $\tilde{\nu}$ = 3569, 2228, 1723, 1630, 1473, 1495, 1385, 1350 cm⁻¹; HRMS *m/z* (ESI) calcd for C₁₅H₁₈N₂O₂⁺ [M⁺], 258.1368; found, 258.1365.

(3-(2-Cyano-2-methylpropyl)-1-methyl-2-oxoindolin-3-yl)methyl acetate (2p):



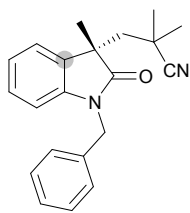
White solid (46.3 mg, 77%); mp 159-162 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.37-7.33 (m, 2H), 7.08 (t, *J* = 7.6 Hz, 1H), 6.91-6.89 (m, 1H), 4.34 (d, *J* = 10.7 Hz, 1H), 3.99 (d, *J* = 10.7 Hz, 1H), 3.23 (s, 3H), 2.28 (s, 2H), 1.89 (s, 3H), 1.17 (s, 3H), 1.10 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 176.3, 170.1, 143.9, 129.3, 126.3, 125.8, 123.6, 122.4, 108.5, 68.4, 50.9, 41.5, 30.2, 29.7, 26.7, 26.4, 20.4; IR (KBr): $\tilde{\nu}$ = 2241, 1745, 1713, 1617, 1488, 1377, 1341 cm⁻¹; HRMS *m/z* (ESI) calcd for C₁₇H₂₀N₂O₃⁺ [M⁺], 300.1474; found, 300.1473.

3-(3-((1,3-Dioxoisindolin-2-yl)methyl)-1-methyl-2-oxoindolin-3-yl)-2,2-dimethylpropanenitrile (2q):



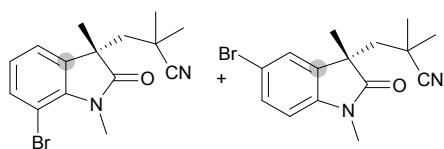
White solid (43.4 mg, 56%); mp 188-189 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.83-7.79 (m, 2H), 7.72-7.69 (m, 2H), 7.34-7.31 (m, 2H), 7.07-7.03 (m, 1H), 6.90-6.88 (m, 1H), 3.98 (d, *J* = 14.0 Hz, 1H), 3.84 (d, *J* = 14.0 Hz, 1H), 3.24 (s, 3H), 2.51-2.42 (m, 2H), 1.21 (s, 3H), 1.07 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 176.7, 168.0, 143.8, 134.1, 131.6, 129.5, 126.4, 125.9, 123.9, 123.5, 122.2, 108.7, 51.3, 45.4, 43.2, 30.5, 30.1, 26.6, 26.5; IR (KBr): $\tilde{\nu}$ = 2240, 1728, 1721, 1690, 1617, 1538, 1472, 1379, 1344 cm⁻¹; HRMS *m/z* (ESI) calcd for C₂₃H₂₁N₃O₃⁺ [M⁺], 387.1583; found, 387.1583.

3-(1-Benzyl-3-methyl-2-oxoindolin-3-yl)-2,2-dimethylpropanenitrile (2u):



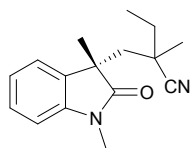
Colorless oil (41.3 mg, 65%); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.35-7.20 (m, 7H), 7.08 (t, $J = 7.5$ Hz, 1H), 6.84 (d, $J = 7.6$ Hz, 1H), 5.13 (d, $J = 15.6$ Hz, 1H), 4.74 (d, $J = 15.6$ Hz, 1H), 2.37 (d, $J = 14.8$ Hz, 1H), 2.23 (d, $J = 14.8$ Hz, 1H), 1.41 (s, 3H), 1.19 (s, 3H), 1.04 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 179.6, 142.2, 135.7, 130.8, 128.8, 128.6, 128.4, 127.6, 127.5, 124.8, 124.0, 122.4, 109.4, 46.9, 46.1, 44.0, 30.7, 29.6, 28.0, 26.3; IR (KBr): $\tilde{\nu} = 2239, 1717, 1616, 1471, 1377, 1348$ cm^{-1} ; HRMS m/z (ESI) calcd for $\text{C}_{21}\text{H}_{22}\text{N}_2\text{O}^+$ [M^+], 318.1732; found, 318.1729.

3-(7-Bromo-1,3-dimethyl-2-oxoindolin-3-yl)-2,2-dimethylpropanenitrile and 3-(5-Bromo-1,3-dimethyl-2-oxoindolin-3-yl)-2,2-dimethylpropanenitrile (2v + 2v'):



Colorless oil (40.5 mg, 63%); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.467.41 (m, 2.5H), 7.23 (d, $J = 7.3$ Hz, 0.5H), 6.94 (t, $J = 7.8$ Hz, 0.5H), 6.78 (d, $J = 8.2$ Hz, 1H), 3.62 (s, 1.5H), 3.22 (s, 3H), 2.34-2.29 (m, 1.56H), 2.17-2.08 (m, 1.65H), 1.34 (d, $J = 4.3$ Hz, 4.5H), 1.19 (s, 1.5H), 1.15 (s, 3H), 1.11 (s, 3H), 1.08 (s, 1.5H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 180, 178.9, 142.2, 140.4, 134.3, 133.9, 133.1, 131.4, 127.7, 123.8, 123.7, 123.6, 115.2, 109.9, 102.8, 47.2, 46.7, 46.5, 46.5, 30.6, 30.0, 29.8, 29.5, 27.8, 27.2, 27.1, 26.4, 26.3, 25.1; IR (KBr): $\tilde{\nu} = 2236, 1723, 1614, 1477, 1378, 1339$ cm^{-1} ; HRMS m/z (ESI) calcd for $\text{C}_{15}\text{H}_{17}\text{BrN}_2\text{O}^+$ [M^+], 320.0525; found, 320.0528; HRMS m/z (ESI) calcd for $\text{C}_{15}\text{H}_{17}^{81}\text{BrN}_2\text{O}^+$ [M^+], 322.0505; found, 322.0504.

2-((1,3-Dimethyl-2-oxindolin-3-yl)methyl)-2-methylbutanenitrile (3):



White solid (43.6 mg, 85%); mp 124-125 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.37-7.28 (m, 2H), 7.15-7.07 (m, 1H), 6.91 (d, *J* = 7.8 Hz, 1H), 3.25 (s, 3H), 2.43 (d, *J* = 14.6 Hz, 1H), 2.25 (q, *J* = 14.7 Hz, 1H), 2.04 (d, *J* = 14.6 Hz, 1H), 1.56-1.49 (m, 1H), 1.45-1.33 (m, 4H), 1.01-0.93 (m, 6H); ¹³C NMR (100 MHz, CDCl₃) δ 179.9, 179.4, 143.2, 142.9, 131.3, 130.7, 128.5, 128.4, 124.8, 124.1, 123.1, 122.6, 122.4, 122.1, 108.5, 108.3, 46.8, 46.7, 45.2, 44.3, 35.5, 35.3, 35.1, 33.1, 27.7, 27.4, 26.3, 26.2, 25.7, 22.6, 9.0, 8.9; IR (KBr): $\tilde{\nu}$ = 2233, 1719, 1608, 1467, 1370, 1337 cm⁻¹; HRMS *m/z* (ESI) calcd for C₁₆H₂₀N₂O⁺ [M⁺], 256.1576; found, 256.1578.

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NMR Spectra

