Supporting Information

for

A concise synthesis of 3-(1-alkenyl)isoindolin-1-ones and 5-(1-alkenyl)pyrrol-2-ones by the intermolecular coupling reactions of *N*-acyliminium ions with unactivated olefins

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Characterization data of title compounds, ¹H NMR and ¹³C NMR spectra

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General remarks

All reagents were purchased from commercial suppliers and used without further purification. Flash chromatography was carried out with silica gel (200–300 mesh). Analytical TLC was performed with silica gel GF254 plates, and the products were visualized by UV detection. ¹H NMR and ¹³C NMR (400 MHz and 100 MHz, respectively) spectra were recorded in CDCl₃. Chemical shifts (δ) are reported in ppm with TMS as internal standard, and spin–spin coupling constants (*J*) are given in Hz. EIMS were recorded with a HP 5988 A mass spectrometer. HRMS (ESI) were measured on a Bruker Dattonics APEX 47e mass spectrometer.

Experimental procedures

1. General procedure for the preparation of *N*-benzylphthalimide, *N*-methylphthalimide and *N*-benzyl-1*H*-pyrrol-2,5-dione [1]

To a solution of the corresponding anhydride (10 mmol) in glacial acetic acid (4 mL) was added slowly the primary amine (12 mmol). The mixture was heated under reflux for a given time until the corresponding anhydride disappeared (monitored by TLC). The reaction was quenched with ice water. The mixture was filtered and the colorless solid was washed with distilled water. The solid was dried under vacuum (70 mbar) at 80 °C and then recrystallized from ethanol to give *N*-benzylphthalimide (*N*-methylphthalimide and *N*-benzyl-1*H*-pyrrole-2,5-dione) as colorless crystals (80–98%).

2. General procedure for the preparation of N-substituted

3-hydroxy-isoindolin-1-one (1a-c) [2]

1.0 mmol of *N*-substituted phthalimides were stirred at 0 °C in anhydrous MeOH (5 mL) and THF (10 mL) for 10 min. NaBH₄ (1.0 mmol) was added slowly over 5–10 min, the mixture was stirred at 0 °C until the *N*-substituted phthalimides disappeared (monitored by TLC). The reaction was quenched with water, and the mixture was extracted with ethyl acetate. The combined organic layers were dried with anhydrous Na₂SO₄, and concentrated in vacuo. The residue was separated by silica-gel column chromatography to obtain the corresponding products (70–85%).

3. General procedure for the preparation of *N*-substituted **5-hydroxy-1***H*-pyrrol-2(5*H*)-one (5a,b) [2]

1.0 mmol of *N*-substituted-1*H*-pyrrol-2,5-dione and 1.0 mmol of CeCl₃·7H₂O were stirred at 0 °C in anhydrous MeOH (5 mL) and THF (10 mL) for 10 min. NaBH₄ (1.0 mmol) was added slowly over 5–10 min, the mixture was stirred at 0 °C until the 1-substitued-1*H*-pyrrole-2,5-dione disappeared (monitored by TLC). The reaction was quenched with water, and the mixture was extracted with ethyl acetate. The combined organic layers were dried with anhydrous Na₂SO₄, and concentrated in vacuo. The residue was separated by silica-gel column chromatography to obtain the corresponding products **5a** and **5b** (70–85% and 40–50%, respectively).

4. General procedure for the coupling reactions

To a solution of **1a–c** or **5a,b** (1.0 mmol) and olefins (2.0 mmol) in 15 mL of processed methylene dichloride was added BF₃·OEt₂ (2.0 mmol) in one portion under stirring at 25 °C. Stirring was continued for a given time until the **1a–c** or **5a,b** disappeared (monitored by TLC). The reaction was quenched with water, and the mixture was separated. The aqueous phase was extracted with methylene dichloride (10×2 mL). The combined organic layer was dried with anhydrous Na₂SO₄, and concentrated in vacuo. The residue was separated by silica-gel column chromatography to obtain the corresponding products **3a–o**, **4a–d**, **6a–c** and **7a,b** as summarized in Table 2–Table 4 in the main article.

References

- (1) Godt, A.; Sajid, M.; Jeschke, G. Chem. Eur J. 2009, 15(47), 12961;
- (2) (a)Wei Zhang; Airong Zheng; Zhenang Liu. Tetrahedron Lett. 2005, 46, 5693;
 - (b) Wei Zhang; Liming Huang; Junpu Wang. Synthesis. 2006, 12, 2056;
 - (c) Wei Zhang; Yuehua Zhou; Lingfeng Qiang. Synlett. 2009, 5, 846;
 - (d) Wei Zhang; Lingfeng Qiang; Yuehua Zhou. Chin. Chem. Lett. 2009, 20, 807.

Analytical data of products

(E)-2-Benzyl-3-(2-phenylethenyl)isoindolin-1-one (3a)

Colorless syrup. ¹H NMR (400 MHz, CDCl₃) δ ppm 4.22 (d, *J* = 14.8 Hz, 1H), 4.90 (d, *J* = 9,2 Hz, 1H), 5.33 (d, *J* = 14.8 Hz, 1H), 5.82 (dd, *J* = 9.2 Hz, 15.6 Hz, 1H), 6.77 (d, *J* = 15.6 Hz, 1H), 7.28–7.37 (m, 11H), 7.50–7.55 (m, 2H), 7.92 (dd, *J* = 1.6 Hz, 6.4 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃): δ ppm 44.1, 62.7, 123.2, 123.8, 125.6, 126.7 (2C), 127.5, 128.4 (2C), 128.5 (2C), 128.6 (2C), 128.7, 128.7, 131.7, 131.8, 135.7, 135.9, 137.4, 144.5, 168.0 (CO). EIMS *m*/*z* (relative intensity, %): 325 (56), 310 (29), 234 (89), 220 (31), 149 (46), 91 (45), 57 (53), 44 (100); HRMS–ESI (*m*/*z*) calcd for C₂₃H₁₉NO+H⁺, 326.1540; found, 326.1536.

2-Benzyl-3-(2-phenyl-2-propenyl)isoindolin-1-one (4a)

Colorless solid; mp 69–72 °C; ¹H NMR (400 MHz, CDCl₃) δ ppm 2.54 (dd, J = 9.2 Hz, 14.0 Hz, 1H), 3.40 (dd, J = 4.0 Hz, 14.0 Hz, 1H), 4.24 (d, J = 15.6 Hz, 1H), 4.39 (dd, J = 4.0 Hz, 9.2 Hz, 1H), 5.00 (s, 1H), 5.38 (s, 1H), 5.40 (d, J = 15.6 Hz, 1H), 7.20–7.31 (m, 11H), 7.41 (t, J = 4.0 Hz, 2H), 7.86 (t, J = 4.0 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ ppm 38.1, 44.1, 56.9, 116.9, 123.2, 123.7, 126.1 (2C), 127.6, 127.8, 128.1, 128.1 (2C), 128.5 (2C), 128.8 (2C), 130.9, 131.8, 137.0, 139.8, 143.6, 145.2, 168.4 (CO); EIMS *m*/*z* (relative intensity, %): 339 (1), 253 (4), 237 (6), 222 (100), 197 (5), 149 (13), 91 (71); HRMS–ESI (*m*/*z*) calcd for C₂₄H₂₁NO+H⁺, 340.1696; found, 340.1699.

2-Benzyl-3-(2,2-diphenylethenyl)isoindolin-1-one (3b)

Colorless solid; mp 134–136 °C; ¹H NMR (400 MHz, CDCl₃) δ ppm 4.39 (d, J = 15.2 Hz, 1H), 5.10 (d, J = 15.2 Hz, 1H), 5.12 (d, J = 10.0 Hz, 1H), 5.64 (d, J = 10.0 Hz, 1H), 7.07–7.30 (m, 15H), 7.41–7.53 (m, 3H), 7.89 (d, J = 7.6 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ ppm 44.4, 59.4, 123.1, 123.8, 124.5, 127.2, 127.3 (2C), 127.7, 127.8 (2C), 128.0, 128.2 (2C), 128.4, 128.5 (4C), 129.5 (2C), 131.6, 132.0, 137.5, 138.2, 140.8, 144.8, 147.8, 168.2 (CO); EIMS *m*/*z* (relative intensity, %): 401 (2), 223 (6), 205 (7), 178 (8), 149 (91), 97 (36), 57 (47), 43 (68) 40 (100); HRMS–ESI (*m*/*z*) calcd for C₂₉H₂₃NO+H⁺, 402.1853; found, 402.1851.

2-Benzyl-3-(1*H*-inden-2-yl)isoindolin-1-one (3c)

Pale yellow syrup; ¹H NMR (400 MHz, CDCl₃) δ ppm 2.79 (d, J = 22.8 Hz, 1H), 3.06 (d, J = 22.8 Hz, 1H), 3.95 (d, J = 14.8 Hz, 1H), 5.34 (s, 1H), 5.38 (d, J = 14.8 Hz, 1H), 7.03 (s, 1H), 7.16–7.20 (m, 1H), 7.25–7.32 (m, 8H), 7.42 (d, J = 7.6 Hz, 1H), 7.47–7.49 (m, 2H), 7.93–7.95 (m, 1H); ¹³C NMR (100 MHz, CDCl₃) δ ppm 36.1, 44.1, 60.1, 121.2, 122.9, 123.9, 124.0, 125.4, 126.6, 127.6, 128.4 (2C), 128.5 (2C), 128.7, 131.7, 131.8, 133.5, 137.1, 143.4, 143.6, 144.0, 144.9, 168.1 (CO); EIMS *m*/*z* (relative intensity, %): 337 (17), 258 (12), 246 (23), 228 (46), 178 (23), 155 (65), 149 (84), 139 (63), 129 (65), 111 (51), 97 (32), 91 (39), 86 (50), 71 (63), 57 (100), 43 (87); HRMS–ESI (*m*/*z*) calcd for C₂₄H₁₉NO+H⁺, 338.1540; found, 338.1537.

2-Benzyl-3-cyclohexenylisoindolin-1-one (3d)

Colorless solid; mp 109–112 °C; ¹H NMR (400 MHz, CDCl₃) δ ppm 1.15–1.19 (m, 1H), 1.38–1.43 (m, 3H), 1.50–1.59 (m, 2H), 2.13 (t, J = 2.4 Hz, 2H), 4.06 (d, J = 14.8 Hz, 1H), 4.71 (s, 1H), 5.19 (d, J = 14.8 Hz, 1H), 5.93 (s, 1H), 7.26–7.30 (m, 5H), 7.41–7.50 (m, 3H), 7.87 (d, J = 7.2 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ ppm 21.8, 22.0, 22.2, 25.4, 43.9, 66.7, 122.4, 123.4, 127.3, 128.1, 128.4 (4C), 130.2, 131.4, 132.3, 133.4, 137.4, 144.4, 168.3 (CO); EIMS *m*/*z* (relative intensity, %): 303 (64), 222 (27), 199 (70), 183 (6), 170 (12), 157 (15), 129 (27), 91 (100), 40 (37); HRMS–ESI (*m*/*z*) calcd for C₂₁H₂₁NO+H⁺, 304.1696; found, 304.1691.

2-Benzyl-3-(3,4-dihydro-2*H*-pyran-5-yl)isoindolin-1-one (3e)

Colorless solid; mp 96–98 °C; ¹H NMR (400 MHz, CDCl₃) δ ppm 1.20–125 (m, 1H), 1.35–1.43 (m, 1H), 1.67 (t, J = 5.6 Hz, 2H), 3.88–4.00 (m, 2H), 4.13 (d, J = 14.4 Hz, 1H), 4.62 (s, 1H), 5.18 (d, J = 14.4 Hz, 1H), 6.62 (s, 1H), 7.26–7.32 (m, 5H), 7.44–7.54 (m, 3H), 7.88 (d, J = 7.2 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ ppm 17.3, 21.6, 43.8, 63.0, 66.2, 108.1, 122.5, 123.6, 127.4, 128.3, 128.5 (2C), 128.6 (2C), 131.6, 132.6, 137.6, 144.5, 145.1, 168.3 (CO); EIMS *m*/*z* (relative intensity, %): 305 (60), 237 (15), 221 (28), 214 (35), 200 (93), 186 (24), 172 (40), 149 (79), 129 (27), 91 (100), 71 (40), 57 (53); HRMS–ESI (*m*/*z*) calcd for C₂₀H₁₉NO₂+H⁺, 306.1489; found, 306.1492.

2-Benzyl-3-(4,5-dihydrofuran-3-yl)isoindolin-1-one (3f)

Pale yellow syrup; ¹H NMR (400 MHz, CDCl₃) δ ppm 1.88–1.97 (m, 1H), 2.01–2.10 (m, 1H), 4.17 (d, *J* = 14.8 Hz, 1H), 4.26–4.33 (m, 2H), 5.08 (s, 1H), 5.22 (d, *J* = 14.8 Hz, 1H), 6.58 (s, 1H), 7.30–7.32 (m, 6H), 7.48–7.53 (m, 2H), 7.90 (d, *J* = 7.2 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ ppm 26.9, 43.9, 56.8, 70.9, 110.1, 122.5, 123.8, 127.5, 128.5 (2C), 128.7 (2C), 131.7, 132.3, 136.9, 137.4, 144.0, 146.8, 168.1 (CO); EIMS *m*/*z* (relative intensity, %): 291 (56), 222 (15), 208 (36), 200 (47), 198 (88), 174 (37), 160 (29), 151 (67), 91 (100), 57 (47); HRMS–ESI (*m*/*z*) calcd for C₁₉H₁₇NO₂+H⁺, 292.1332; found, 292.1335.

(E)-2-Benzyl-3-(hex-2-enyl)isoindolin-1-one (4b)

Colorless syrup; ¹H NMR (400 MHz, CDCl₃) δ ppm 0.74 (t, *J* = 7.2 Hz, 3H), 1.87–1.25 (m, 2H), 1.79–1.86 (m, 2H), 2.55–2.70 (m, 2H), 4.17 (d, *J* = 15.2 Hz, 1H), 4.39 (dd, *J* = 4.0 Hz, 5.6 Hz, 1H), 4.91–4.98 (m, 1H), 5.42 (d, *J* = 15.2 Hz, 1H), 5.36–5.42 (m, 1H), 7.28–7.32 (m, 5H), 7.37 (d, *J* = 7.2 Hz, 1H), 7.43–7.53 (m, 2H), 7.88 (d, *J* = 7.6 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ ppm 13.4, 22.3, 34.1, 34.5, 43.9, 58.4, 122.4 (2C), 123.7, 127.5, 128.0, 128.1 (2C), 128.7 (2C), 131.2, 132.4, 135.4, 137.2, 145.1, 168.5 (CO); EIMS *m*/*z* (relative intensity, %): 305 (4), 223 (18), 222 (100), 186 (6), 172 (6), 132 (8), 104 (5), 91 (89); HRMS–ESI (*m*/*z*) calcd for C₂₁H₂₃NO+H⁺, 306.1853; found, 306.1851.

(E)-2-Methyl-3-(2-phenylethenyl)isoindolin-1-one (3g)

Colorless syrup; ¹H NMR (400 MHz, CDCl₃) δ ppm 3.12 (s, 3H), 4.94 (d, *J* = 8.8 Hz, 1H), 5.86 (dd, *J* = 8.8 Hz, 15.6 Hz, 1H), 6.91 (d, *J* = 15.6 Hz, 1H), 7.30–7.43 (m, 6H), 7.48 (t, *J* = 7.2 Hz, 1H), 7.53 (t, *J* = 7.2 Hz, 1H), 7.86 (d, *J* = 7.2 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ ppm 27.5, 65.4, 123.0, 123.5, 125.6, 126.7 (2C), 128.5, 128.5, 128.7 (2C), 131.5, 132.1,

135.7, 135.7, 144.3, 168.2 (CO); EIMS *m*/*z* (relative intensity, %): 249 (100), 248 (23), 234 (12), 220 (19), 172 (14), 158 (65) 146 (60), 117 (14), 91 (35), 77 (11), 40 (35); HRMS–ESI (*m*/*z*) calcd for C₁₇H₁₅NO+H⁺, 250.1227; found, 250.1229.

2-Methyl-3-(2-phenyl-2-propenyl)isoindolin-1-one (4c)

Pale yellow syrup; ¹H NMR (400 MHz, CDCl₃) δ 2.76 ppm (dd, J = 7.6 Hz, 14.4 Hz, 1H), 3.08 (s, 3H), 3.25 (dd, J = 4.4 Hz, 14.4 Hz, 1H), 4.42 (dd, J = 4.4 Hz, 7.6 Hz, 1H), 5.08 (d, J =0.8 Hz, 1H), 5.37 (d, J = 0.8 Hz, 1H), 7.28–7.41 (m, 8H), 7.78 (dd, J = 1.6 Hz, 6.4 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ ppm 27.8, 38.7, 60.0, 116.8, 122.7, 123.2, 126.1 (2C), 127.8, 127.9, 128.6 (2C), 130.7, 132.0, 140.3, 143.9, 145.0, 168.2 (CO); EIMS *m/z* (relative intensity, %): 263 (2), 147 (10), 146 (100), 91 (13), 40 (3); HRMS–ESI (*m/z*) calcd for C₁₈H₁₇NO+H⁺, 264.1383; found, 264.1380.

3-(2,2-Diphenylethenyl)-2-methylisoindolin-1-one (3h)

Colorless solid, mp 146–148 °C; ¹H NMR (400 MHz, CDCl₃) δ ppm 3.08 (s, 3H), 5.01 (d, J = 10.0 Hz, 1H), 5.71 (d, J = 10.0 Hz, 1H), 7.25–7.27 (m, 5H), 7.38–7.46 (m, 5H), 7.47–7.52 (m, 3H), 7.83 (d, J = 7.6 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ ppm 27.5, 61.3, 122.8, 123.4, 124.3, 127.2 (2C), 127.9, 128.1, 128.3 (3C), 128.8 (2C), 129.5 (2C), 131.3, 132.3, 138.5, 140.4, 144.5, 148.1, 168.0 (CO); EIMS m/z (relative intensity, %): 325 (28), 310 (15), 294 (9), 265 (5), 248 (11), 220 (18), 188 (10), 178 (11), 165 (13), 149 (37), 91 (30), 57 (63), 43 (100); HRMS–ESI (m/z) calcd for C₂₃H₁₉NO+H⁺, 326.1540; found, 326.1545.

Crystal data for compound **3h** (recrystallized from ethanol): C₂₃H₁₉NO, $M_r = 325.39$. Monoclinic, a = 17.373(11) Å, b = 17.241(11) Å, c = 24.421(16) Å, $\beta = 91.219(9)$, V = 7313(8) Å³, colorless plates, $\rho = 1.182$ g cm⁻³, T = 296(2) K, space group P2(1)/c, Z = 4, μ (Mo K α) = 0.084 mm⁻¹, $2\theta_{max} = 51^{\circ}$, 9126 reflections measured, 3995 unique ($R_{int} = 0.0696$), which were used in all calculations. The final w $R(F^2)$ was 0.1427 (for all data), $R_1 = 0.0764$. CCDC file No. 835330.

3-(2,3-Dihydro-1*H*-inden-2-yl)-2-methylisoindolin-1-one (3i)

Pale yellow solid; mp 132–134 °C; ¹H NMR (400 MHz, CDCl₃) δ ppm 2.81 (d, *J* = 22.8 Hz, 1H), 3.05 (s, 3H), 3.07 (d, *J* = 22.8 Hz, 1H), 5.40 (s, 1H), 7.14 (s, 1H), 7.18 (dt, *J* = 0.8 Hz, 7.2 Hz, 1H), 7.26–7.32 (m, 3H), 7.41 (d, *J* = 7.6 Hz, 1H), 7.47–7.50 (m, 2H), 7.88 (dd, *J* = 2.4 Hz, 6.0 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ ppm 27.6, 36.1, 63.1, 121.1, 122.7, 123.6, 124.0, 125.4, 126.6, 128.5, 131.6, 132.0, 133.1, 143.3, 143.6, 144.1, 144.6, 168.4 (CO). EIMS *m/z* (relative intensity, %): 261 (100), 246 (15), 232 (31), 202 (20), 189 (5), 146 (92), 129 (6), 117 (14), 115 (15), 109 (6), 101 (15), 91 (14), 57 (4), 40 (27); HRMS–ESI (*m/z*) calcd for C₁₈H₁₅NO+H⁺, 264.1383; found, 264.1385.

3-Cyclohexenyl-2-methylisoindolin-1-one (3j)

Colorless solid; mp 91–94 °C; ¹H NMR (400 MHz, CDCl₃) δ ppm 1.16–1.21 (m, 1H), 1.43–1.62 (m, 5H), 2.16 (d, J = 2.8 Hz, 2H), 3.00 (s, 3H), 4.74 (s, 1H), 6.07 (s, 1H), 7.32 (d, J = 7.6 Hz, 1H), 7.44 (t, J = 7.6 Hz, 1H), 7.51 (t, J = 6.8 Hz, 1H), 7.82 (d, J = 7.6 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ ppm 21.7, 22.2, 22.4, 25.4, 27.0, 69.3, 122.3, 123.2, 128.1, 129.7, 131.3, 132.7, 133.9, 144.3, 168.6 (CO); EIMS *m/z* (relative intensity, %): 227 (76), 226 (23),

198 (20), 170 (12), 159 (7), 146 (100), 128 (6), 91 (20), 77 (5), 40 (12); HRMS–ESI (m/z) calcd for C₁₅H₁₇NO+H⁺, 228.1383; found, 228.1379.

3-(3,4-Dihydro-2*H*-pyran-5-yl)-2-methylisoindolin-1-one (3k)

Colorless solid; mp 94–97 °C; ¹H NMR (400 MHz, CDCl₃) δ ppm 1.20–1.27 (m, 1H), 1.40–1.47 (m, 1H), 1.71–1.79 (m, 2H), 3.00 (s, 3H), 3.92–4.04 (m, 2H), 4.65 (s, 1H), 6.79 (s, 1H), 7.36 (d, *J* = 7.2 Hz, 1H), 7.44 (t, *J* = 7.2 Hz, 1H), 7.53 (t, *J* = 7.2 Hz, 1H), 7.81 (d, *J* = 7.2 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ ppm 17.0, 21.5, 26.6, 65.2, 66.0, 108.2, 122.2, 123.0, 128.1, 131.3, 132.7, 144.2, 144.6, 168.2 (CO); EIMS *m*/*z* (relative intensity, %): 229 (100), 200 (47), 186 (35), 172 (54), 146 (51), 128 (20), 115 (17), 91 (24); HRMS–ESI (*m*/*z*) calcd for C₁₄H₁₅NO₂+H⁺, 230.1176; found, 230.1175.

3-(4,5-Dihydrofuran-3-yl)-2-methylisoindolin-1-one (3l)

Pale yellow syrup; ¹H NMR (400 MHz, CDCl₃) δ ppm 1.91–2.00 (m, 1H), 2.12–2.20 (m, 1H), 3.05 (s, 3H), 4.34–4.40 (m, 2H), 5.11 (s, 1H), 6.71 (s, 1H), 7.37 (d, *J* = 7.6 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.54 (t, *J* = 7.6 Hz, 1H), 7.84 (d, *J* = 7.6 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ ppm 27.0, 30.9, 59.2, 70.9, 110.3, 122.4, 123.4, 128.4, 131.5, 132.5, 143.8, 146.5, 168.2 (CO); EIMS *m*/*z* (relative intensity, %): 215 (64), 214 (40), 187 (63), 186 (100), 170 (57), 159 (43), 146 (51), 128 (21), 91 (21); HRMS–ESI (*m*/*z*) calcd for C₁₃H₁₃NO₂+H⁺, 216.1019; found, 216.1017.

(E)-3-(2-Phenylethenyl)isoindolin-1-one (3m)

Colorless syrup; ¹H NMR (400 MHz, CDCl₃) δ ppm 5.21 (d, *J* = 8.8 Hz, 1H), 6.00 (dd, *J* = 8.8 Hz, 15.6 Hz, 1H), 6.83 (s, 1H), 6.84 (s, 1H), 7.31 (d, *J* = 7.2 Hz, 1H), 7.34–7.40 (m, 4H), 7.44 (d, *J* = 7.6 Hz, 1H), 7.51 (t, *J* = 7.2 Hz, 1H), 7.59 (dt, *J* = 1.2 Hz, 7.2 Hz, 1H), 7.89 (d, *J* = 7.6 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ ppm 59.6, 123.4, 123.9, 126.1, 126.6 (2C), 128.4, 128.6 (2C), 128.7, 131.3, 132.3, 133.9, 135.8, 146.4, 170.8 (CO); EIMS *m/z* (relative intensity, %): 235 (30), 206 (15), 182 (15), 168 (19), 144 (64) 44 (100); HRMS–ESI (*m/z*) calcd for C₁₆H₁₃NO+H⁺, 236.1070; found, 236.1068.

3-(2-Phenyl-2-propenyl)isoindolin-1-one (4d)

Pale yellow syrup; ¹H NMR (400 MHz, CDCl₃) δ ppm 2.68 (dd, J = 9.2 Hz, 14.0 Hz, 1H), 3.17 (dd, J = 4.8 Hz, 14.0 Hz, 1H), 4.63 (dd, J = 4.8 Hz, 9.2 Hz, 1H), 5.19 (s, 1H), 5.45 (s, 1H), 7.00 (s, 1H), 7.31 (d, J = 7.6 Hz, 1H), 7.37 (dt, J = 0.8 Hz, 7.6 Hz, 2H), 7.46 (t, J = 6.8 Hz. 4H), 7.54 (t, J = 7.6 Hz, 1H), 7.84 (d, J = 7.6 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ ppm 41.3, 55.0, 116.1, 122.6, 123.7, 126.2 (2C), 128.0, 128.2, 128.6 (2C), 131.6, 131.8, 139.8, 144.5, 147.0, 170.3 (CO); EIMS *m/z* (relative intensity, %): 249 (4), 201 (2), 174 (2), 149 (6), 132 (100), 115 (7), 104 (10), 77 (10), 44 (23); HRMS–ESI (*m/z*) calcd for C₁₇H₁₅NO+H⁺, 250.1227; found, 250.1223.

3-(2,2-Diphenylethenyl)isoindolin-1-one (3n)

Colorless solid; mp 205–207 °C; ¹H NMR (400 MHz, CDCl₃) δ ppm 5.22 (d, *J* = 9,6 Hz, 1H), 5.82 (d, *J* = 9,6 Hz, 1H), 6.97 (s, 1H), 7.21–7.27 (m, 4H), 7.38–7.49 (m, 8H), 7.57 (dt, *J* = 0.8 Hz, 7.6 Hz, 1H), 7.86 (d, *J* = 7.6 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ ppm 56.0, 123.3,

123.8, 124.9, 127.4 (2C), 127.9, 128.1, 128.3 (2C), 128.4, 128.8 (2C), 129.7 (2C), 131.6, 132.0, 138.6, 140.8, 146.7, 146.9, 170.7 (CO); EIMS m/z (relative intensity, %): 311 (6), 306 (2), 276 (3), 215 (18), 200 (40), 172 (51), 149 (68), 129 (16), 97 (27) 44 (100); HRMS–ESI (m/z) calcd for C₂₂H₁₇NO+H⁺, 312.1383; found, 312.1386.

3-(1*H*-Inden-2-yl)isoindolin-1-one (30)

Pale yellow solid; mp 201–204 °C; ¹H NMR (400 MHz, CDCl₃) δ ppm 2.96 (d, *J* = 22.8 Hz, 1H), 3.35 (d, *J* = 22.8 Hz, 1H), 5.66 (s, 1H), 6.66 (s, 1H), 7.03 (s, 1H), 7.17 (dt, *J* = 1.2 Hz, 7.6 Hz, 1H), 7.27 (t, *J* = 7.2 Hz, 1H), 7.33 (d, *J* = 7.6 Hz, 2H), 7.37 (t, *J* = 7.6 Hz, 1H), 7.49 (d, *J* = 7.2 Hz, 1H), 7.51–7.57 (m, 1H), 7.90 (d, *J* = 7.6 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ ppm 36.5, 57.4, 121.1, 123.2, 123.9, 124.0, 125.3, 126.6, 128.6, 131.0, 131.1, 132.3, 143.2, 143.7, 145.1, 146.6, 170.6 (CO); EIMS *m*/*z* (relative intensity, %): 247 (25), 218 (12), 194 (8), 180 (10), 165 (9), 149 (20), 132 (23), 129 (31), 111 (18), 83 (24), 57 (36), 44 (100); HRMS–ESI (*m*/*z*) calcd for C₁₇H₁₃NO+H⁺, 248.1070; found, 248.1073.

(E)-1-Benzyl-5-(2-phenylethenyl)-1H-pyrrol-2(5H)-one (6a)

Colorless syrup; ¹H NMR (400 MHz, CDCl₃) δ ppm 4.08 (d, *J* = 14.8 Hz, 1H), 4.54 (d, *J* = 9.2 Hz, 1H), 5.12 (d, *J* = 14.8 Hz, 1H), 5.69 (dd, *J* = 9.2 Hz, 15.6 Hz, 1H), 6.26 (dd, *J* = 1.6 Hz, 5.6 Hz, 1H), 6.59 (d, *J* = 15.6 Hz, 1H), 6.96 (dd, *J* = 1.6 Hz, 6.0 Hz, 1H), 7.23–7.35 (m, 8H), 7.40 (dd, *J* = 1.6 Hz, 8.0 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ ppm 42.4, 64.8, 126.1, 126.6, 127.4, 128.0, 128.2, 128.6 (2C), 128.7 (2C), 128.7 (2C), 128.9 (2C), 135.7, 137.6, 146.6, 170.9 (CO); EIMS *m*/*z* (relative intensity, %): 275 (22), 190 (11), 189 (100), 184 (30), 161 (29), 160 (39), 132 (37), 119 (22), 104 (48), 91 (21); HRMS–ESI (*m*/*z*) calcd for C₁₉H₁₇NO+H⁺, 276.1383; found, 276.1385.

1-Benzyl-5-(2-phenyl-2-propenyl)-1H-pyrrol-2(5H)-one (7a)

Brown syrup; ¹H NMR (400 MHz, CDCl₃) δ ppm 2.34 (dd, J = 10.4 Hz, 13.6 Hz, 1H), 3.20 (dd, J = 4.4 Hz, 13.6 Hz, 1H), 3.96–4.00 (m, 1H), 4.16 (d, J = 15.2 Hz, 1H), 5.08 (s, 1H), 5.15 (d, J = 15.2 Hz, 1H), 5.38 (s, 1H), 6.12 (dd, J = 1.6 Hz, 6.0 Hz, 1H), 6.91 (dd, J = 1.6 Hz, 6.0 Hz, 1H), 7.19–7.26 (m, 7H), 7.28–7.31 (m, 3H); ¹³C NMR (100 MHz, CDCl₃) δ ppm 37.0, 43.7, 60.5, 115.9, 125.8 (2C), 126.5, 127.5, 127.8 (2C), 127.9 (2C), 128.5, 128.7 (2C), 137.2, 139.6, 143.4, 147.8, 171.0 (CO); EIMS *m*/*z* (relative intensity, %): 289 (17), 274 (6), 220 (17), 172 (48), 171 (35), 91 (100), 40 (58); HRMS–ESI (*m*/*z*) calcd for C₂₀H₁₉NO+H⁺, 290.1540; found, 290.1508.

1-Benzyl-5-(2,2-diphenylethenyl)-1*H*-pyrrol-2(5*H*)-one (6b)

Brown syrup; ¹H NMR (400 MHz, CDCl₃) δ ppm 4.25 (d, J = 14.8 Hz, 1H), 4.64–4.67 (m, 1H), 4.88 (d, J = 14.8 Hz, 1H), 5.49 (d, J = 9.6 Hz, 1H), 6.23 (dd, J = 1.6 Hz, 6.0 Hz, 1H), 6.94 (dd, J = 1.6 Hz, 6.0 Hz, 1H), 7.03–7.10 (m, 6H), 7.20–7.21 (m, 3H), 7.25–7.26 (m, 3H), 7.28–7.30 (m, 3H); ¹³C NMR (100 MHz, CDCl₃) δ ppm 44.2, 62.0, 122.8, 127.2, 127.3, 127.4 (2C), 127.9, 128.0 (2C), 128.1 (2C), 128.2 (2C), 128.4 (2C), 128.5, 129.3 (2C), 137.5, 138.3, 140.7, 146.9, 147.7, 171.0 (CO); EIMS *m*/*z* (relative intensity, %): 351 (2), 190 (12), 189 (100), 182 (8), 161 (28), 160 (43), 132 (37), 129 (18), 119 (22), 104 (46), 91 (21), 77 (17); HRMS–ESI (*m*/*z*) calcd for C₂₅H₂₁NO+H⁺, 352.4476; found, 352.4473.

1-Methyl-5-(2-phenyl-2-propenyl)-1*H*-pyrrol-2(5*H*)-one (7b)

Brown syrup; ¹H NMR (400 MHz, CDCl₃) δ ppm 2.51 (dd, J = 9.2 Hz, 14.0 Hz, 1H), 2.97 (s, 3H), 3.17 (dd, J = 4.8 Hz, 14.0 Hz, 1H), 4.04–4.07 (m, 1H), 5.17 (s, 1H), 5.51 (s, 1H), 6.08 (dd, J = 1.6 Hz, 6.0 Hz, 1H), 6.91 (dd, J = 1.6 Hz, 6.0 Hz, 1H), 7.34–7.40 (m, 5H); ¹³C NMR (100 MHz, CDCl₃) δ ppm 27.2, 37.3, 63.3, 116.2, 126.1 (2C), 127.1, 128.0, 128.7 (2C), 140.2, 143.8, 147.2, 171.2 (CO); EIMS *m*/*z* (relative intensity, %): 213 (41), 198 (11), 154 (4), 115 (11), 96 (100), 91 (3), 77 (5); HRMS–ESI (*m*/*z*) calcd for C₁₄H₁₅NO+H⁺, 214.1227; found, 214.1228.

5-(2,2-Diphenylethenyl)-1-methyl-1*H*-pyrrol-2(5*H*)-one (6c)

Brown syrup; ¹H NMR (400 MHz, CDCl₃) δ ppm 2.92 (s, 3H), 4.63 (d, J = 10.0 Hz, 1H), 5.57 (d, J = 10.0 Hz, 1H), 6.19 (dd, J = 1.6 Hz, 6.0 Hz, 1H), 6.94 (dd, J = 1.6 Hz, 6.0 Hz, 1H), 7.22–7.31 (m, 7H), 7.40–7.45 (m, 3H); ¹³C NMR (100 MHz, CDCl₃) δ ppm 27.1, 63.8, 122.7, 127.2 (2C), 127.8, 128.0, 128.2 (2C), 128.4, 128.7 (2C), 129.4 (2C), 138.5, 140.5, 146.1, 148.1, 171.0 (CO); EIMS *m*/*z* (relative intensity, %): 275 (34), 260 (19), 114 (14), 113 (100), 161 (21), 91 (8); HRMS–ESI (*m*/*z*) calcd for C₁₉H₁₇NO+H⁺, 276.1383; found, 276.1379.





¹H NMR and ¹³C NMR spectra of **3b**











































