Supporting Information

Facile Synthesis of 11-aryl-6H-isoindolo[2,1-a]indol-6-ones via Hypervalent Iodine (III)-Promoted Cascade Cyclization

Kapil Dev and RakeshMaurya*

Medicinal and Process Chemistry Division, CSIR- Central Drug Research Institute, Lucknow 226031, India; Academy of Scientific and Innovative Research, New Delhi 110001, India
E-mail: mauryarakesh@rediffmail.com

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1. General information

All reagents and solvents were purchased from commercial suppliers and used without further purification. Thin layer chromatography (TLC) was performed on silica gel 60 F_{254} coated on aluminium sheet and UV light (254 nm & 365 nm) as well as iodine, adsorbed on silica gel were used for visualization of TLC plate. IR spectra of the compounds were recorded on Perkin-Elmer spectrometer using KBr pellets or neat and the infrared frequencies were reported in cm\(^{-1}\). \(^1\)H-NMR spectra were recorded on Bruker Advance DPX 300 MHz & 400 MHz spectrometers in CDCl\(_3\) or as stated deuterated solvent and \(^13\)C-NMR spectra were recorded on 75.4 MHz & 100.6 MHz and DEPT, HSQC, HMBC & \(^1\)H-\(^1\)H COSY were also recorded on same NMR instrument. The calibration of the NMR spectra was done by using residual undeuterated solvent as an internal reference. Chemical shifts and coupling constants are reported in parts per million (ppm) relative to residual signal of TMS in deuterated solvents and Hertz, respectively. High resolution mass spectra were acquired on Electro spray ionization mass spectrometer in positive ionization mode. Melting points are uncorrected and were determined in capillary tubes on a melting point apparatus containing silicon oil. Silica gel 100-200 and 230-400 mesh were used as stationary phase to isolate the compounds.

2. Experimental procedures and compounds characterization
2.1. Synthesis and characterization of 2-iodobenzamides\(^1\)

2-iodo-\(N\)-phenylbenzamide (S1a)

\[
\begin{array}{c}
\text{R}^1 \quad \text{I} \\
\text{OH} \\
(1) (\text{COCl})_2, \text{DMF}, \text{CH}_2\text{Cl}_2 \\
(2) \text{R}^2\text{NH}_2, \text{Et}_3\text{N}, \text{CH}_2\text{Cl}_2
\end{array}
\]

To a solution of 2-iodobenzoic acid (10.1 mmol, 1.00 equiv) and oxalyl chloride (20.2 mmol) in CH\(_2\)Cl\(_2\) 50 mL were added the catalytic amount of \(N,N'\)-dimethylformamide (50 µL). The resulting mixture was then stirred at room temperature continuously till the solid disappeared. The solution was concentrated under reduced pressure and another 50 mL of CH\(_2\)Cl\(_2\) was added followed by addition of aniline (11.1 mmol) and triethylamine (24.4 mmol). The corresponding reaction mixture was stirred at room temperature for 6 h. The reaction mixture was quenched with water and the aqueous phase was extracted with CH\(_2\)Cl\(_2\) (3 X 50 mL). The organic phases
were combined and washed with 10 % HCl (aq.), water, saturated NaHCO₃ (aq.), and brine respectively, and dried over anhy. Na₂SO₄. The solvent was removed at reduced pressure and residue was purified by column chromatography on silica gel (100-200 mesh) eluting with hexane/EtOAc (95: 05), afforded white solid product in 90 %. The compound was characterized by comprehensive analysis of ¹H NMR and ¹³C NMR.

**N-(phenyl)-2-iodobenzamide (S1a)**

![Chemical Structure](image)

White solid, Yield 90%; FT-IR (KBr): 3436, 2143, 1658, 1601, 1538, 1498, 1440, 1324,1219, 1015, 691, 667 cm⁻¹;¹H NMR (300 MHz, CDCl₃): δ (ppm) 7.93 (d, J = 7.9 Hz, 1H), 7.68 (d, J = 7.8 Hz, 3H), 7.55–7.52 (m, 1H), 7.47–7.39 (m, 3H), 7.24–7.15 (m, 2H);¹³C NMR (75.4 MHz, CDCl₃): δ (ppm) 167.3, 142.1, 140.0, 137.5, 131.5, 129.1(2C), 128.5, 128.3, 124.9, 120.1(2C), 92.4;HRMS (ESI): m/z calculated for C₁₃H₁₁INO [M+H]⁺= 323.9879, found [M+H]⁺= 323.9876.

**N-(4-ethylphenyl)-2-iodobenzamide (S1b)**

The compound S1b was synthesized from commercially available 2-iodobenzoic acid and 4-ethylaniline. The compound was purified by column chromatography on silica gel (100-200 mesh) eluting with hexane/EtOAc (95: 05) and product was afforded as a white solid (91 % yield);FT-IR (KBr): 3418, 3019, 2960, 2400, 1653, 1599, 1516, 1462, 1409, 1328, 1215, 1015, 924, 669 cm⁻¹;¹H NMR (400 MHz, CDCl₃): δ 7.88 (d, J = 8.0 Hz, 1H), 7.54–7.47 (m, 4H), 7.39 (t, J = 7.6 Hz, 1H), 7.19 (d, J = 8.4 Hz, 2H), 7.12 (td, J = 7.6, 1.6 Hz, 1H), 2.64 (q, J = 7.6 Hz, 2H), 1.23 (t, J = 7.6 Hz, 3H);¹³C NMR (75.4 MHz, CDCl₃): δ 167.1, 142.2, 142.0, 140.0, 135.1, 131.4, 128.5, 128.4(2C), 128.3, 120.2(2C), 92.4, 28.3, 15.6;HRMS (ESI): m/z calculated for C₁₅H₁₅INO [M+H]⁺= 352.0192, found [M+H]⁺= 352.0188.

**N-(3,4-dimethylphenyl)-2-iodobenzamide (S1c)**

The compound S1c was synthesized from commercially available 2-iodobenzoic acid and 3,4-dimethylaniline. The compound was purified by column chromatography on silica gel (100-200 mesh) eluting with hexane/EtOAc (95: 05) and product was afforded as a white solid (88 % yield);FT-IR (KBr): 3436, 3417, 3019, 2400, 1671, 1617, 1520, 1449, 1404, 1311, 1215, 1043, 1017, 669 cm⁻¹;¹H
NMR (400 MHz, CDCl$_3$): $\delta$ (ppm) 7.89 (d, $J = 8.0$ Hz, 1H), 7.50 (dd, $J = 7.6$, 1.6 Hz, 1H), 7.45–7.39 (m, 3H), 7.34 (dd, $J = 8.0$, 2.0 Hz, 1H), 7.15–7.11 (m, 2H), 2.25 (s, 3H), 2.25 (s, 3H); $^{13}$C NMR (75.4 MHz, CDCl$_3$): $\delta$ (ppm) 167.1, 142.3, 139.9, 137.3, 135.2, 133.3, 131.3, 130.0, 128.5, 128.3, 121.4, 117.6, 92.4, 19.9, 19.2; HRMS (ESI): $m/z$ calculated for C$_{15}$H$_{15}$INO [M+H]$^+$ = 352.0192, found [M+H]$^+$ = 352.0189.

**N-(2,4-dimethylphenyl)-2-iodobenzamide (S1d)**

The compound **S1d** was synthesized from commercially available 2-iodobenzoic acid and 2,4-dimethylaniline. The compound was purified by column chromatography on silica gel (100-200 mesh) eluting with hexane/EtOAc (95: 05) and product was afforded as a white solid (90 % yield); FT-IR (KBr): 3418, 3019, 2400, 1646, 1522, 1405, 1215, 929, 669 cm$^{-1}$. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ (ppm) 7.92 (d, $J = 8.0$ Hz, 1H), 7.81 (d, $J = 8.0$Hz, 1H), 7.54 (dd, $J = 7.6$, 1.2 Hz, 1H), 7.44 (t, $J = 7.6$ Hz, 1H), 7.19 (brs, 1H), 7.14 (td, $J = 7.5$, 1.6 Hz, 1H), 7.09–7.05 (m, 2H), 2.324 (s, 3H), 2.320 (s, 3H); $^{13}$C NMR (100.6MHz, CDCl$_3$ + CD$_3$OD): $\delta$ (ppm) 169.4, 142.3, 139.4, 136.1, 132.6, 131.9, 131.0, 130.7, 127.8, 127.6, 126.6, 125.3, 91.9, 20.2, 17.4; HRMS (ESI): $m/z$ calculated for C$_{15}$H$_{15}$INO [M+H]$^+$ = 352.0192, found [M+H]$^+$ = 352.0188.

**N-(2,5-dimethylphenyl)-2-iodobenzamide (S1e)**

The compound **S1e** was synthesized from commercially available 2-iodobenzoic acid and 2,5-dimethylaniline. The compound was purified by column chromatography on silica gel (100-200 mesh) eluting with hexane/EtOAc (95: 05) and product was afforded as a white solid (90 % yield); FT-IR (KBr): 3431, 3019, 2400, 1636, 1528, 1481, 1446, 1405, 1292, 1043, 928, 669, 626 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ (ppm) 7.90 (d, $J = 8.0$ Hz, 1H), 7.81 (s, 1H), 7.53–7.51 (m, 1H), 7.44–7.40 (m, 1H), 7.26 (brs, 1H), 7.16–7.12 (m, 1H), 7.10 (d, $J = 7.6$ Hz, 1H), 6.94 (d, $J = 7.6$ Hz, 1H), 2.35 (s, 3H), 2.28 (s, 3H); $^{13}$C NMR (75.4MHz, CDCl$_3$): $\delta$ (ppm) 167.3, 140.0, 136.6, 135.0, 131.4, 130.4(2C), 128.4(2C), 128.3, 126.5, 123.6, 92.3, 21.1, 17.6; HRMS (ESI): $m/z$ calculated for C$_{15}$H$_{15}$INO [M+H]$^+$ = 352.0192, found [M+H]$^+$ = 352.0198.
**N-(p-tolyl)-2-iodobenzamide (S1f)**

The compound **S1f** was synthesized from commercially available 2-iodobenzoic acid and 4-methylaniline. The compound was purified by column chromatography on silica gel (100-200 mesh) eluting with hexane/EtOAc (96: 04) and product was afforded as a white solid (94 % yield); FT-IR (KBr): 3417, 3019, 2399, 1671, 1517, 1403, 1318, 1215, 1120, 1017, 928, 669 cm⁻¹;¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.91 (dd, J = 8.0, 1.2 Hz, 1H), 7.55–7.51 (m, 3H), 7.49 (brs, 1H), 7.43 (dt, J = 7.6, 0.8 Hz, 1H), 7.20 (d, J = 8.0 Hz, 2H), 7.15 (td, J = 7.6, 1.6 Hz, 1H), 2.37 (s, 3H);¹³C NMR (100.6 MHz, CDCl₃): δ (ppm) 167.1, 142.2, 139.9, 135.0, 134.6, 131.4, 129.6 (2C), 128.5, 128.3, 120.2 (2C), 92.4, 20.9; HRMS (ESI): m/z calculated for C₁₄H₁₃INO [M+H]⁺ = 338.0036, found [M+H]⁺ = 338.0041.

**N-(m-tolyl)-2-iodobenzamide (S1g)**

The compound **S1g** was synthesized from commercially available 2-iodobenzoic acid and 3-methylaniline. The compound was purified by column chromatography on silica gel (100-200 mesh) eluting with hexane/EtOAc (96: 04) and product was afforded as a white solid (89 % yield); FT-IR (KBr): 3415, 3290, 3018, 1663, 1613, 1537, 1489, 1430, 1312, 1216, 1017, 876, 669 cm⁻¹;¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.90 (d, J = 8.0 Hz, 1H), 7.51 (brs 2H), 7.44–7.38 (m, 3H), 7.28–7.24 (m, 2H), 7.14 (t, J = 7.2 Hz, 1H), 6.99(d, J = 7.2 Hz, 1H), 2.38 (s, 3H);¹³C NMR (100.6 MHz, CDCl₃): δ (ppm) 167.2, 142.1, 140.0, 139.0, 137.5, 131.4, 128.9, 128.5, 128.3, 125.7, 120.7, 117.2, 92.4, 21.5; HRMS (ESI): m/z calculated for C₁₄H₁₃INO [M+H]⁺ = 338.0036, found [M+H]⁺ = 338.0041.

**N-(4-methoxyphenyl)-2-iodobenzamide (S1h)**

The compound **S1h** was synthesized from commercially available 2-iodobenzoic acid and 4-methoxyaniline. The compound was purified by column chromatography on silica gel (100-200 mesh) eluting with hexane/EtOAc (95: 05) and product was afforded as a white solid (90 % yield); FT-IR (KBr): 3419, 3303, 3019, 2402, 1649, 1514, 1460, 1409, 1216, 1114, 1023, 670 cm⁻¹;¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.90 (dd, J = 8.0, 1.2 Hz, 1H), 7.55 (dd, J = 6.8, 2.0
Hz, 2H), 7.51 (dd, \( J = 7.6, 1.6 \) Hz, 1H), 7.49 (brs, 1H), 7.42 (dt, \( J = 7.6, 0.8 \) Hz, 1H), 7.14 (td, \( J = 7.6, 1.6 \) Hz, 1H), 6.92 (d, \( J = 9.2 \) Hz, 2H), 3.82 (s, 3H); \(^{13}\)C NMR (100.6 MHz, CDCl\(_3\)): \( \delta \) (ppm) 167.2, 156.8, 142.2, 139.9, 131.3, 130.6, 128.5, 128.3, 122.0 (2C), 114.2 (2C), 92.4, 55.5; HRMS (ESI): \( m/z \) calculated for C\(_{14}\)H\(_{13}\)INO \([M+H]^+\) = 353.9985, found \([M+H]^+\) = 353.9989.

**N-(3-methoxyphenyl)-2-iodobenzamide (S1i)**

The compound S1i was synthesized from commercially available 2-iodobenzoic acid and 3-methoxyaniline. The compound was purified by column chromatography on silica gel (100-200 mesh) eluting with hexane/EtOAc (95: 05) and product was afforded as a white solid (90% yield); FT-IR (KBr): 3419, 3303, 3019, 2402, 1650, 1514, 1460, 1409, 1216, 1112, 923, 670 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)): \( \delta \) (ppm) 7.90 (d, \( J = 7.6 \) Hz, 1H), 7.51–7.50 (m, 2H), 7.43–7.40 (m, 2H), 7.26–7.24 (m, 1H), 7.16–7.09 (m, 2H), 6.73 (d, \( J = 8.0 \) Hz, 1H), 3.83 (s, 3H); \(^{13}\)C NMR (100.6 MHz, CDCl\(_3\) + CD\(_3\)OD): \( \delta \) (ppm) 168.2, 159.9, 142.4, 139.6, 139.0, 131.0, 129.5, 128.1, 128.0, 112.5, 110.4, 105.9, 92.2, 55.2; HRESIMS: \( m/z \) calculated for C\(_{14}\)H\(_{13}\)INO \([M+H]^+\) = 353.9985, found \([M+H]^+\) = 353.9985.

**N-(naphthalen-2-yl)-2-iodobenzamide (S1j)**

The compound S1j was synthesized from commercially available 2-iodobenzoic acid and 2-naphthylamine. The compound was purified by column chromatography on silica gel (100-200 mesh) eluting with hexane/EtOAc (92: 08) and product was afforded as a white solid (92% yield); FT-IR (KBr): 3416, 3019, 2399, 1625, 1530, 1497, 1405, 1215, 928, 848, 669 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)): \( \delta \) (ppm) 8.35 (d, \( J = 1.2 \) Hz, 1H), 7.91 (d, \( J = 8.0 \) Hz, 1H), 7.85–7.80 (m, 3H), 7.76 (s, 1H), 7.58–7.54 (m, 2H), 7.51–7.41 (m, 3H), 7.15 (dt, \( J = 7.6, 1.6 \) Hz, 1H); \(^{13}\)C NMR (75.4 MHz, CDCl\(_3\) + CD\(_3\)OD): \( \delta \) (ppm) 168.5, 142.2, 139.4, 135.2, 133.5, 130.8, 130.6, 128.3, 127.8 (2C), 127.4, 127.2, 126.1, 124.8, 119.9, 117.0, 92.4; HRMS (ESI): \( m/z \) calculated for C\(_{17}\)H\(_{13}\)INO \([M+H]^+\) = 374.0036, found \([M+H]^+\) = 374.0038.

**N-(4-chlorophenyl)-2-iodobenzamide (S1k)**
The compound S1k was synthesized from commercially available 2-iodobenzoic acid and 4-chloroaniline. The compound was purified by column chromatography on silica gel (100-200 mesh) eluting with hexane/EtOAc (94: 06) and product was afforded as a white solid (84 % yield); FT-IR (KBr): 3414, 3022, 2401, 1622, 1524, 1444, 1319, 1215, 928, 670 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) (ppm) 7.89 (d, \(J = 7.8\) Hz, 1H), 7.76 (brs, 1H), 7.58 (d, \(J = 8.7\) Hz, 2H), 7.40 (t, \(J = 7.3\) Hz, 1H), 7.14 (dt, \(J = 7.7, 1.4\) Hz, 1H); \(^{13}\)C NMR (100.6 MHz, CDCl\(_3\)): \(\delta\) (ppm) 167.3, 141.7, 140.0, 136.1, 131.6, 129.9, 129.1 (2C), 128.5, 128.3, 121.4 (2C), 92.3; HRMS (ESI): \(m/z\) calculated for C\(_{13}\)H\(_{10}\)ClINO \([\text{M+H}]^+\) = 357.9490, found \([\text{M+H}]^+\) = 357.9490.

2-iodo-5-nitro-N-phenylbenzamide (S1l)

The compound S1l was synthesized 2-iodo-5-nitro-benzoic acid\(^2\) and aniline. The compound was purified by column chromatography on silica gel (100-200 mesh) eluting with hexane/acetone (94: 06) and product was afforded as a yellow solid (85 % yield); FT-IR (KBr): 3389, 3021, 2401, 1626, 1525, 1410, 1322, 1215, 928, 758 cm\(^{-1}\); \(^1\)H NMR (400 MHz, Acetone-\(d_6\)): \(\delta\) (ppm) 9.79 (s, 1H), 8.35 (d, \(J = 2.6\) Hz, 1H), 8.27 (d, \(J = 8.6\) Hz, 1H), 8.04 (dd, \(J = 8.6, 2.6\) Hz, 1H), 7.80–7.77 (m, 2H), 7.41–7.36 (m, 2H), 7.19–7.14 (m, 1H); \(^{13}\)C NMR (100.6 MHz, Acetone-\(d_6\)): \(\delta\) (ppm) 166.5, 148.8, 145.4, 142.2, 139.7, 129.7 (2C), 125.8, 125.2, 123.2, 120.8, 120.7, 102.2; HRMS (ESI): \(m/z\) calculated for C\(_{13}\)H\(_{10}\)N\(_2\)O\(_3\) \([\text{M+H}]^+\) = 368.9731, found \([\text{M+H}]^+\) = 368.9732.

5-bromo-2-iodo-N-phenylbenzamide (S1m)

The compound S1m was synthesized from 5-bromo-2-iodo-benzoic acid\(^2\) and aniline. The compound was purified by column chromatography on silica gel (100-200 mesh) eluting with hexane/EtOAc (93: 07) and product was afforded as a white solid (80 % yield); FT-IR (KBr): 3410, 3019, 2399, 1630, 1403, 1318, 1215, 1120, 928, 669 cm\(^{-1}\); \(^1\)H NMR (400 MHz, Acetone-\(d_6\)): \(\delta\) (ppm) 9.60 (brs, 1H), 7.88 (d, \(J = 8.4\) Hz, 1H), 7.82–7.79 (m, 2H), 7.72 (d, \(J = 2.3\) Hz, 1H), 7.43–7.37 (m, 3H), 7.18 (t, \(J = 1.1\) Hz, 1H); \(^{13}\)C NMR (100.6 MHz, Acetone-\(d_6\)): \(\delta\) (ppm)
165.8, 145.1, 141.1, 139.0, 133.8, 130.8, 128.7 (2C), 124.1, 121.8, 119.7 (2C), 90.8; HRMS (ESI): m/z calculated for C$_{13}$H$_{10}$BrINO [M+H]$^+$ = 401.8990, found [M+H]$^+$ = 401.8985.

**N-(4-acetylphenyl)-2-iodobenzamide (S1n)**

The compound **S1n** was synthesized from commercially available 2-iodobenzoic acid and 4-acetylaniline. The compound was purified by column chromatography on silica gel (100-200 mesh) eluting with hexane/EtOAc (93: 07) and product was afforded as a white solid (70% yield); FT-IR (KBr): 3375, 3019, 1670, 1539, 1318, 1215, 1120, 765, 669 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$): 6 (ppm) 7.97 (d, $J = 8.5$ Hz, 2H), 7.90 (d, $J = 8.2$ Hz, 2H), 7.75 (d, $J = 8.2$ Hz, 2H), 7.52 (d, $J = 7.2$ Hz, 1H), 7.43 (t, $J = 7.3$ Hz, 1H), 7.16 (dt, $J = 7.8$, 1.2 Hz, 1H), 2.58 (s, 3H); $^{13}$C NMR (100.6 MHz, CDCl$_3$): 6 (ppm) 197.0, 167.4, 141.9, 141.5, 140.1, 133.3, 131.7, 129.7 (2C), 128.5 (2C), 128.3, 119.3, 92.3, 26.4; HRMS (ESI): m/z calculated for C$_{15}$H$_{13}$INO$_2$ [M+H]$^+$ = 365.9985, found [M+H]$^+$ = 365.9982.

**Methyl-4-(2-iodobenzamido)benzoate (S1o)**

The compound **S1o** was synthesized from commercially available 2-iodo-benzoic acid and methyl-4-aminobenzoate. The compound was purified by column chromatography on silica gel (100-200 mesh) eluting with hexane/EtOAc (90: 10) and product was afforded as a white solid (75% yield); FT-IR (KBr): 3147, 3019, 1742, 1670, 1403, 1318, 1215, 1017, 928, 669 cm$^{-1}$; $^1$H NMR (400 MHz, CD$_3$OD + CDCl$_3$): 6 (ppm) 7.90 (d, $J = 8.4$ Hz, 2H), 7.78 (d, $J = 7.8$ Hz, 1H), 7.64 (d, $J = 8.0$ Hz, 2H), 7.36-7.28 (m, 2H), 7.05-7.01 (m, 1H), 3.79 (s, 3H); $^{13}$C NMR (100.6 MHz, CD$_3$OD + CDCl$_3$): 6 (ppm) 168.4, 166.8, 142.2, 141.8, 139.4, 131.0, 130.4 (2C), 127.8 (2C), 125.3, 119.2 (2C), 92.1, 51.8; HRMS (ESI): m/z calculated for C$_{15}$H$_{13}$INO$_3$ [M+H]$^+$ = 381.9935, found [M+H]$^+$ = 381.9938.
2.2 General procedure for the synthesis of o-(1-Alkynyl)benzamides

To a solution of N-phenyl-2-iodobenzamide (S1a) (323 mg, 1 mmol) in DMF (6 mL) were added Pd(PPh₃)Cl₂ (24.5 mg, 3.5 mol%), CuI (30.4 mg, 16 mol%) and triethylamine (0.55 mL, 4.0 mmol), consecutively, under inert atmosphere. After 10 min stirring phenylacetylene (0.22 mL, 2.0 mmol) was added and the reaction mixture was heated with stirring at 85°C till the disappearance of starting material. The progress of reaction was monitored by TLC. The reaction mixture was cooled down, quenched with saturated aqueous solution of NH₄Cl and extracted with ethyl acetate (3 x 25 mL). The organic layers were combined and washed with brine and dried over anhy. Na₂SO₄. The solvent were removed under vacuum and obtained residue was purified by column chromatography on silica gel (230-400 mesh) eluting with hexane/EtOAc (96: 04) to afford the product 1a (88% yield).

N-phenyl-2- (phenylethynyl)benzamide (1a)

FT-IR (KBr): 3416, 3019, 2400, 1668, 1600, 1537, 1498, 1445, 1322, 1215, 1044, 928, 690,669 cm⁻¹;¹H NMR (300 MHz, CDCl₃): δ (ppm) 9.23 (s, 1H), 8.18–8.15 (m, 1H), 7.71–7.68 (m, 3H), 7.53–7.51 (m, 4H), 7.40–7.34 (m, 5H), 7.17 (t, J = 7.5 Hz, 1H);¹³C NMR (100.6 MHz, CDCl₃): δ (ppm) 164.4, 137.9, 135.9, 133.5, 131.7(2C), 130.9, 130.3, 129.3, 129.1(3C), 128.6(2C), 124.5, 121.8, 120.0 (2C), 119.5, 96.6, 87.2;HRMS (ESI): m/z calculated for C₂₁H₁₆NO [M+H]⁺ = 298.1226, found [M+H]⁺ = 298.1234.

N-(p-ethylphenyl)-2-(phenylethynyl)benzamide (1b)

The compound 1b was prepared by using starting materials S1b and phenylacetylene as above described general procedure. The compound 1b was purified by column chromatography on silica gel (230-400 mesh) eluting with hexane/EtOAc (96: 04) to afford the product 1b (88% yield).
mesh) by eluting with hexane/EtOAc (96: 04) to afford white solid product in 83% yield; FT-IR (KBr): 3413, 3019, 2970, 2930, 2400, 1662, 1599, 1529, 1493, 1409, 1321, 1215, 1125, 1046, 928, 690, 626, 542 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) (ppm) 9.16 (s, 1H), 8.14–8.12 (m, 1H), 7.65–7.63 (m, 1H), 7.56 (d, \(J = 8.4\) Hz, 2H), 7.50–7.46 (m, 4H), 7.38–7.33 (m, 3H), 7.15 (d, \(J = 8.0\) Hz, 2H), 2.62 (q, \(J = 7.6\) Hz, 2H), 1.22 (t, \(J = 7.6\) Hz, 3H); \(^13\)C NMR (100.6 MHz, CDCl\(_3\)): \(\delta\) (ppm) 164.2, 140.5, 136.0, 135.6, 133.5, 131.7 (2C), 130.8, 130.3 129.2, 129.0, 128.6 (2C), 128.4(2C), 121.9, 120.1(2C), 119.5, 96.5, 87.3, 28.3, 15.6; HRMS (ESI): \(m/z\) calculated for C\(_{23}\)H\(_{20}\)NO [M+H]\(^+\) = 326.1539, found [M+H]\(^+\) = 326.1546.

\(N\)-(3,4-dimethylphenyl)-2-(phenylethynyl)benzamide (1c)

The compound 1c was synthesized by using starting materials S1c and phenylacetylene as above described general procedure. The compound 1c was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (96: 04) to afford viscous brown oily product in 80% yield; FT-IR (neat): 3376, 3019, 2401, 1663, 1600, 1531, 1445, 1404, 1316, 1215, 1029, 927, 670 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) (ppm)9.14 (s, 1H), 8.15–8.13 (m, 1H), 7.65–7.63 (m, 1H), 7.53–7.49 (m, 4H), 7.38–7.33 (m, 3H), 2.23(s, 3H), 2.20(s, 3H); \(^13\)C NMR (100.6 MHz, CDCl\(_3\)): \(\delta\) (ppm) 164.7, 137.2, 136.0, 135.7, 133.4, 132.8, 131.7 (2C), 130.8, 130.3, 130.0, 129.3, 129.1, 128.6 (2C), 121.9, 121.3, 119.5, 117.5, 96.5, 87.4, 19.8, 19.2; HRMS (ESI): \(m/z\) calculated for C\(_{23}\)H\(_{20}\)NO [M+H]\(^+\) = 326.1539, found [M+H]\(^+\) = 326.1546.

\(N\)-(2,4-dimethylphenyl)-2-(phenylethynyl)benzamide (1d)

The compound 1d was synthesized by using starting materials S1d and phenylacetylene as above described general procedure. The compound 1d was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (96: 04) to afford white solid product in 82% yield; FT-IR (KBr): 3407, 3018, 2855, 2402, 1662, 1518, 1459, 1305, 1216, 1037, 927, 670 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) (ppm) 8.80 (s, 1H),8.14–8.12 (m, 1H), 7.83 (d, \(J = 8.0\) Hz, 1H), 7.69–7.67 (m, 1H), 7.51–7.49 (m, 2H), 7.45–7.43 (m, 2H), 7.37–7.33 (m, 3H), 7.07 (d, \(J = 8.0\) Hz, 1H), 7.02 (s, 1H), 2.32(s, 3H), 2.24(s, 3H); \(^13\)C NMR (100.6 MHz, CDCl\(_3\)): \(\delta\) (ppm) 164.7, 136.3, 135.2, 133.6, 133.2, 131.6 (2C), 131.2, 130.7, 130.2, 130.0,
N-(2,5-dimethylphenyl)-2-(phenylethynyl)benzamide (1e)

The compound 1e was prepared by using starting materials S1e and phenylacetylene as above described general procedure. The compound 1e was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (96: 04) to afford white solid product in 80% yield; FT-IR (KBr): 3417, 3019, 2927, 2400, 1662, 1534, 1492, 1405, 1291, 928, 691, 668, 519 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ (ppm) 8.78 (s, 1H), 8.12–8.09 (m, 1H), 7.85 (s, 1H), 7.67–7.65 (m, 1H), 7.50–7.48 (m, 2H), 7.41 (d, $J$ = 6.8 Hz, 2H), 7.35–7.31 (m, 3H), 7.06 (d, $J$ = 7.6 Hz, 1H), 6.92 (d, $J$ = 7.6 Hz, 1H), 2.34 (s, 3H), 2.21 (s, 3H); $^{13}$C NMR (100.6 MHz, CDCl$_3$): $\delta$ (ppm) 164.8, 136.4, 136.4, 135.6, 133.6, 131.6 (2C), 130.7, 130.3, 130.2, 129.1, 129.0, 128.5 (2C), 126.6, 126.2, 124.0, 122.0, 119.6, 96.2, 87.4, 21.1, 17.5; HRMS (ESI): $m/z$ calculated for $C_{23}H_{20}NO$ [M+H]$^+$ = 326.1539, found [M+H]$^+$ = 326.1543.

N-($p$-tolyl)-2-(phenylethynyl)benzamide (1f)

The compound 1f was prepared by using starting materials S1f and phenylacetylene as above described general procedure. The compound 1f was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (96: 04) afforded viscous brown oily product in 82% yield; FT-IR (neat): 3415, 3019, 2926, 2398, 1662, 1534, 1491, 1404, 1291, 928, 668 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ (ppm) 9.15 (s, 1H), 8.14–8.12 (m, 1H), 7.65–7.63 (m, 1H), 7.54 (d, $J$ = 8.4 Hz, 2H), 7.50–7.46 (m, 4H), 7.38–7.34 (m, 3H), 7.13 (d, $J$ = 8.4 Hz, 2H), 2.33 (s, 3H); $^{13}$C NMR (100.6 MHz, CDCl$_3$): $\delta$ (ppm) 164.3, 136.0, 135.4, 134.1, 133.5, 131.7 (2C), 130.8, 130.3, 129.2, 129.0, 128.6 (2C), 121.9, 120.0 (2C), 119.5, 96.5, 87.3, 20.9; HRMS (ESI): $m/z$ calculated for $C_{22}H_{18}NO$ [M+H]$^+$ = 312.1382, found [M+H]$^+$ = 312.1386.

N-($m$-tolyl)-2-(phenylethynyl)benzamide (1g)

The compound 1g was prepared by using starting materials S1g and phenylacetylene as above described general procedure. The compound 1g was purified by column chromatography on
silica gel (230-400 mesh) by eluting with hexane/EtOAc (96: 04) afforded viscous brown oily product in 81% yield; FT-IR (neat): 3349, 3027, 2956, 2400, 1725, 1620, 1532, 1381, 1216, 1045, 928 cm⁻¹; H NMR (400 MHz, CDCl₃): δ (ppm) 9.20 (s, 1H), 8.18–8.16 (m, 1H), 7.69–7.67 (m, 1H), 7.55–7.48 (m, 6H), 7.42–7.36 (m, 3H), 7.24 (t, J = 7.6 Hz, 1H), 6.98 (d, J = 7.6 Hz, 1H), 2.33 (s, 3H); ¹³C NMR (100.6 MHz, CDCl₃): δ (ppm) 164.3, 138.9, 137.8, 136.0, 133.4, 131.7 (2C), 130.8, 130.3, 129.3, 129.1, 128.9, 128.6 (2C), 125.3, 121.9, 120.6, 119.5, 117.1, 96.6, 87.3, 21.4; HRMS (ESI): m/z calculated for C₂₂H₁₈NO [M+H]+ = 312.1382, found [M+H]+ = 312.1386.

N-(p-methoxyphenyl)-2-(phenylethynyl)benzamide (1h)

The compound 1h was prepared by using starting materials S1h and phenylacetylene as above described general procedure. The compound 1h was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (94: 06) afforded viscous yellow oily product in 75% yield; FT-IR (neat): 3416, 3019, 2400, 1668, 1537, 1498, 1445, 1322, 1215, 1044, 928, 669 cm⁻¹; H NMR (400 MHz, CDCl₃): δ (ppm) 9.13 (s, 1H), 8.13–8.11 (m, 1H), 7.67–7.65 (m, 1H), 7.59 (d, J = 9.0 Hz, 2H), 7.52–7.48 (m, 4H), 7.41–7.35 (m, 3H), 6.89 (d, J = 8.9 Hz, 2H), 3.82 (s, 3H); ¹³C NMR (100.6 MHz, CDCl₃): δ (ppm) 164.3, 156.5, 136.0, 133.4, 131.6 (2C), 131.1, 130.7, 130.2, 129.2, 129.0, 128.6 (2C), 121.9, 121.7 (2C), 119.5, 114.2 (2C), 96.4, 87.3, 55.5; HRMS (ESI): m/z calculated for C₂₂H₁₈NO₂ [M+H]+ = 328.1332, found [M+H]+ = 328.1333.

N-(m-methoxyphenyl)-2-(phenylethynyl)benzamide (1i)

The compound 1i was prepared by using starting materials S1i and phenylacetylene as above described general procedure. The compound 1i was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (94: 06) afforded viscous yellow oily product in 70% yield; FT-IR (neat): 3416, 3019, 2399, 1665, 1537, 1498, 1445, 1322, 1215, 1044, 928, 669 cm⁻¹; H NMR (400 MHz, CDCl₃): δ (ppm) 9.23 (s, 1H), 8.15–8.13 (m, 1H), 7.66–7.64 (m, 1H), 7.52–7.48 (m, 4H), 7.41–7.33 (m, 4H), 7.20 (t, J = 8.0
Hz, 1H), 7.13 (d, J = 8.0 Hz, 1H), 6.70–6.67 (m, 1H), 3.73 (s, 3H);\textsuperscript{13}C NMR (100.6 MHz, CDCl\textsubscript{3}): δ (ppm) 164.3, 160.2, 139.1, 135.8, 133.5, 131.7 (2C), 130.9, 130.3, 129.7, 129.3, 129.1, 128.6 (2C), 121.8, 119.5, 112.1, 110.9, 105.2, 96.6, 87.2, 55.2; HRMS (ESI): m/z calculated for C\textsubscript{22}H\textsubscript{18}NO\textsubscript{2} [M+H]\textsuperscript{+} = 328.1332, found [M+H]\textsuperscript{+} = 328.1333.

\textit{N-(naphthalen-2-yl)-2-(phenylethynyl)benzamide (1j)}

The compound \textbf{1j} was prepared by using starting materials S\textbf{1j} and phenylacetylene as above described general procedure. The compound \textbf{1j} was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (94: 06) afforded white solid product in 90% yield; FT-IR (KBr): 3436, 3019, 2400, 1661, 1543, 1503, 1474, 1431, 1358, 1215, 1045, 928, 669 cm\textsuperscript{-1}; \textsuperscript{1}H NMR (400 MHz, CDCl\textsubscript{3}): δ (ppm) 9.42 (s, 1H), 8.38 (d, J = 1.2 Hz, 1H), 8.20–8.17 (m, 1H), 7.78–7.74 (m, 3H), 7.68–7.57 (m, 1H), 7.56 (dd, J = 8.8, 2.0 Hz, 1H), 7.53–7.49 (m, 4H), 7.45–7.32 (m, 5H); \textsuperscript{13}C NMR (100.6 MHz, CDCl\textsubscript{3}): δ (ppm) 164.6, 135.9, 135.4, 133.9, 133.5, 131.7 (2C), 130.9, 130.8, 130.3, 129.3, 129.1, 128.8, 128.7 (2C), 127.7, 127.6, 126.5, 125.0, 121.8, 120.0, 119.6, 116.9, 96.7, 87.4; HRMS (ESI): m/z calculated for C\textsubscript{25}H\textsubscript{18}ClNO [M+H]\textsuperscript{+} = 348.1382, found [M+H]\textsuperscript{+} = 348.1381.

\textit{N-(4-chlorophenyl)-2-(phenylethynyl)benzamide (1k)}

The compound \textbf{1k} was prepared by using starting materials S\textbf{1k} and phenylacetylene as above described general procedure. The compound \textbf{1k} was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (93: 07) afforded white solid product in 78% yield; FT-IR (KBr): 3416, 3019, 2399, 1655, 1530, 1497, 1405, 1215, 928, 669 cm\textsuperscript{-1}; \textsuperscript{1}H NMR (400 MHz, CDCl\textsubscript{3}): δ (ppm) 9.27 (s, 1H), 8.17–8.14 (m, 1H), 7.69–7.67 (m, 1H), 7.63 (d, J = 8.8 Hz, 2H), 7.54–7.50 (m, 4H), 7.45–7.37 (m, 3H), 7.31 (dd, J = 6.8, 2.0 Hz, 2H); \textsuperscript{13}C NMR (100.6 MHz, CDCl\textsubscript{3}): δ (ppm) 164.3, 136.5, 135.5, 133.5, 131.6 (2C), 131.0, 130.3, 129.4, 129.1 (4C), 128.7 (2C), 121.7, 121.1 (2C), 119.5, 96.7, 87.2; HRMS (ESI): m/z calculated for C\textsubscript{21}H\textsubscript{15}ClNO [M+H]\textsuperscript{+} = 332.0836, found [M+H]\textsuperscript{+} = 332.0836.
5-nitro-N-phenyl-2-(phenylethynyl)benzamide (1I)

The compound 1I was prepared by using starting materials S11 and phenylacetylene as above described general procedure. The compound 1I was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (92:08) afforded yellow solid product in 75% yield; FT-IR (KBr): 3853, 3019, 2400, 2345, 1655, 1524, 1404, 1385, 1345, 1104, 929, 626 cm⁻¹;¹H NMR (400 MHz, CDCl₃): δ (ppm) 9.10 (s, 1H), 8.99 (d, J = 1.8 Hz, 1H), 8.34 (dd, J = 8.4, 2.4 Hz, 1H), 7.83 (d, J = 8.5 Hz, 1H), 7.68 (d, J = 7.8 Hz, 2H), 7.54 (d, J = 7.1 Hz, 2H), 7.50–7.46 (m, 1H), 7.43–7.37 (m, 4H), 7.21 (t, J = 7.3 Hz, 1H);¹³C NMR (100.6 MHz, CDCl₃ + CD₃OD): δ (ppm) 163.8, 146.6, 138.6, 137.3, 133.7, 131.6 (2C), 129.5, 128.7 (2C), 128.3 (2C), 126.8, 124.7, 124.5, 123.7, 121.0, 120.0 (2C), 99.9, 85.3; HRMS (ESI): m/z calculated for C₂₁H₁₅N₂O₃ [M+H]+ = 343.1077, found [M+H]+ = 343.1077.

N-phenyl-2,5-bis(phenylethynyl)benzamide (1m)

The compound 1m was prepared by using starting materials S1m and phenylacetylene as above described general procedure. The compound 1m was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (96:04) afforded white solid product in 60% yield; FT-IR (KBr): 3414, 3021, 2399, 1665, 1535, 1497, 1405, 1215, 928, 669 cm⁻¹;¹H NMR (400 MHz, CDCl₃): δ (ppm) 9.15 (s, 1H), 8.32 (s, 1H), 7.69 (d, J = 7.7 Hz, 2H), 7.65 (d, J = 1.3 Hz, 2H), 7.58–7.56 (m, 2H), 7.53–7.51 (m, 2H), 7.42–7.35 (m, 8H), 7.20–7.16 (m, 1H); HRMS (ESI): m/z calculated for C₂₉H₂₀N₀ [M+H]+ = 398.1539, found [M+H]+ = 398.1520.

N-(3-acetylphenyl)-2-(phenylethynyl)benzamide (1n)

The compound 1n was prepared by using starting materials S1n and phenylacetylene as above described general procedure. The compound 1n was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (95:05) afforded white solid product in 77% yield; FT-IR (KBr): 3380, 3019, 2399,
1704, 1530, 1497, 1404, 1215, 928, 669 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$): δ (ppm) 9.48 (s, 1H), 8.16–8.14 (m, 1H), 7.94 (d, $J = 8.6$ Hz, 2H), 7.75 (d, $J = 8.6$ Hz, 2H), 7.68–7.66 (m, 1H), 7.53–7.48 (m, 4H), 7.41–7.35 (m, 3H) 2.58 (s, 3H); $^{13}$C NMR (100.6 MHz, CDCl$_3$): δ (ppm) 196.9, 164.5, 142.2, 135.2, 133.6, 133.0, 131.6 (2C), 131.3, 130.4, 129.8 (2C), 129.5, 129.2, 128.7 (2C), 121.5, 119.6, 119.1 (2C), 97.0, 87.0, 26.4; HRMS (ESI): m/z calculated for C$_{23}$H$_{18}$NO$_2$ [M+H]$^+$ = 340.1332, found [M+H]$^+$ = 340.1332.

Methyl 4-(2-(phenylethynyl)benzamido)benzoate (1o)

The compound 1o was prepared by using starting materials S1o and phenylacetylene as above described general procedure. The compound 1o was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (92: 08) afforded white solid product in 85% yield; FT-IR (KBr): 3415, 3020, 1740, 1664, 1644, 1403, 1318, 1215, 1017, 928, 669 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$): δ (ppm) 9.43 (s, 1H), 8.16–8.13 (m, 1H), 8.01 (d, $J = 8.4$, 2H), 7.73 (d, $J = 8.8$ Hz, 2H), 7.68–7.65 (m, 1H), 7.52–7.48 (m, 4H), 7.41–7.35 (m, 3H), 3.90 (s, 3H); $^{13}$C NMR (100.6 MHz, CDCl$_3$): δ (ppm) 166.6, 164.6, 142.1, 135.4, 133.5, 131.6 (2C), 131.2, 130.9 (2C), 130.3, 129.4, 129.1, 128.7 (2C), 125.7, 121.6, 119.6, 119.1 (2C), 96.8, 87.1, 52.0; HRMS (ESI): m/z calculated for C$_{23}$H$_{18}$NO$_3$ [M+H]$^+$ = 356.1281, found [M+H]$^+$ = 356.1282.

2-((4-ethylphenyl)ethynyl)-N-phenylbenzamide (1p)

The compound 1p was prepared by using starting materials S1a and p-ethylphenylacetylene as above described general procedure. The compound 1p was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (97: 03) afforded white solid product in 80% yield; FT-IR (KBr): 3382, 3029, 2958, 2391, 1729, 1629, 1532, 1380, 1318, 1215, 1045, 918 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$): δ (ppm) 9.31 (s, 1H), 8.19–8.17 (m, 1H), 7.70–7.66 (m, 3H), 7.53–7.50 (m, 2H), 7.45 (dd, $J = 6.4$, 1.7 Hz, 2H), 7.38–7.34 (m, 2H), 7.21 (d, $J = 8.3$ Hz, 2H), 7.18–7.14 (m, 1H), 2.70 (q, $J = 7.6$ Hz, 2H), 1.27 (t, $J = 6.4$ Hz, 3H); $^{13}$C NMR (100.6 MHz, CDCl$_3$): δ (ppm) 164.4, 145.9, 137.9, 135.6, 133.5, 131.7 (2C), 130.9, 130.4, 129.1 (2C), 128.9, 128.2 (2C), 124.2, 120.0 (2C), 119.7, 118.9, 97.0,
The compound 1q was prepared by using starting materials S1a and p-methylphenylacetylene as above described general procedure. The compound 1q was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (96: 03) afforded viscous brown oily product in 83% yield; FT-IR (neat): 3379, 3027, 2956, 2390, 1729, 1628, 1532, 1381, 1318, 1216, 1045, 928. cm\(^{-1}\);\(^{1}\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) (ppm) 9.27 (s, 1H), 8.16–8.14 (m, 1H), 7.67–7.63 (m, 3H), 7.51–7.45 (m, 2H), 7.38 (d, \(J = 8.0\) Hz, 2H), 7.33 (t, \(J = 7.5\) Hz, 2H), 7.17–7.11 (m, 3H), 2.37 (s, 3H);\(^{13}\)C NMR (100.6 MHz, CDCl\(_3\)): \(\delta\) (ppm) 164.3, 139.7, 138.0, 135.6, 133.4, 131.6 (2C), 130.9, 130.4, 129.4 (2C), 129.0 (2C), 128.9, 124.4, 120.0 (2C), 119.7, 118.7, 97.0, 86.7, 21.5; HRMS (ESI): \(m/z\) calculated for C\(_{22}\)H\(_{18}\)NO [M+H]\(^+\)=312.1383, found [M+H]\(^+\)= 312.1380.

The compound 1r was prepared by using starting materials S1a and m-methylphenylacetylene as above described general procedure. The compound 1r was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (96: 03) afforded white solid product in 86% yield; FT-IR (KBr):3349, 3027, 2956, 2400, 1725, 1620, 1532, 1381, 1216, 1045, 928 cm\(^{-1}\);\(^{1}\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) (ppm) 9.20 (s, 1H), 8.15–8.12 (m, 1H), 7.68–7.63 (m, 3H), 7.49–7.47 (m, 2H), 7.35–7.29 (m, 4H), 7.23–7.11 (m, 3H), 2.30 (s, 3H);\(^{13}\)C NMR (100.6MHz, CDCl\(_3\)): \(\delta\) (ppm) 164.4, 138.4, 138.0, 135.9, 133.4, 132.3, 130.8, 130.3, 130.2, 129.0 (3C), 128.7, 128.5, 124.4, 121.6, 120.0 (2C), 119.7, 96.9, 86.9, 21.1; HRMS (ESI): \(m/z\) calculated for C\(_{22}\)H\(_{18}\)NO [M+H]\(^+\)=312.1383, found [M+H]\(^+\)= 312.1382.

The compound 1s was prepared by using starting materials S1a and p-tert-butylphenylacetylene as above described general procedure. The compound 1s was purified by column
chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (96: 04) afforded viscous yellow oily product in 85% yield; IR (neat): 3416, 3020, 2970, 2401, 1625, 1531, 1397, 1218, 928, 669 cm⁻¹;¹H NMR (400 MHz, CDCl₃): δ (ppm) 9.32 (s, 1H), 8.19–8.17 (m, 1H), 7.71 (d, J = 7.6 Hz, 2H), 7.68–7.66 (m, 1H), 7.51–7.48 (m, 2H), 7.47–7.45 (m, 2H), 7.41–7.35 (m, 4H) 7.19–7.15 (m, 1H), 1.36 (s, 9H);¹³C NMR (100.6 MHz, CDCl₃): δ (ppm) 164.4, 152.8, 138.0, 135.6, 133.5, 131.4 (2C), 130.9, 130.4, 129.1 (2C), 128.9, 125.6 (2C), 124.4, 120.1 (2C), 119.8, 118.7, 97.0, 86.7, 34.9, 31.1 (3C); HRMS (ESI): m/z calculated for C₂₅H₂₄NO [M+H]⁺ =354.1852, found [M+H]⁺ = 354.1856.

N-phenyl-2-((trimethylsilyl)ethynyl)benzamide (1t)

The compound 1t was prepared by using starting materials S1a and trimethylsilylacetylene as above described general procedure. The compound 1t was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (96: 04) afforded viscous yellow oily product in 80% yield; IR (neat): 3440, 3120, 2960, 2401, 1625, 1531, 1397, 1218, 928, 669 cm⁻¹;¹H NMR (400 MHz, CDCl₃): δ (ppm) 9.33 (s, 1H), 8.18–8.15 (m, 1H), 7.70–7.68(m, 2H), 7.63–7.61 (m, 1H), 7.53–7.45 (m, 2H), 7.42–7.39 (m, 2H), 7.20–7.16 (m, 1H), 0.26 (s, 9H);¹³C NMR (100.6 MHz, CDCl₃): δ (ppm) 164.0, 137.8, 135.8, 134.0, 130.7, 130.3, 129.3, 128.9 (2C), 124.5, 120.1 (2C), 119.3, 103.0, 102.7, -0.2 (3C); HRMS (ESI): m/z calculated for C₁₈H₂₀NOSi [M+H]⁺ =294.1309, found [M+H]⁺ = 294.1312.
2.3 General procedure for the synthesis of 11-aryl-6H-isoindolo[2,1-a]indol-6-ones

To a stirred solution of 1a (100 mg, 0.34 mmol, 1.0 eq.) in trifluoroethanol (1.5 mL) was added phenyliodidediacetate (PIDA) (184 mg, 0.57 mmol, 1.7 eq.) in a oven dried round bottom flask at room temperature. The resultant solution was stirred and the progress of reaction was monitored by TLC analysis by visualizing starting material in short wavelength (254 nm) UV-light and product in long wavelength (365 nm) UV-light. The solid product was filtered off and washed with HPLC grade hexane and methanol.

![Chemical structure of 1a-t and 2a-t](image)

11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2a)

Yellow solid; TLC Rf 0.6 Hexane/EtOAc (98:02); Yield 89%; m.p. = 221–222 °C; FT-IR (KBr): 3436, 3021, 2401, 1721, 1636, 1446, 1386, 1215, 1031, 757, 669 cm⁻¹;¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.95 (d, J = 8.0 Hz, 1H), 7.76 (d, J = 7.2 Hz, 1H), 7.69 (d, J = 7.2 Hz, 2H), 7.57–7.52 (m, 4H), 7.47–7.44 (m, 1H), 7.39 (t, J = 7.2 Hz, 1H), 7.31 (q, J = 8.0 Hz, 2H), 7.17 (t, J = 7.2 Hz, 1H);¹³C NMR (75.4 MHz, CDCl₃): δ (ppm) 162.5, 134.6, 134.1, 133.9, 133.8, 133.7, 133.6, 132.2, 129.0(2C), 128.9(2C), 128.7, 128.3, 126.8, 125.3, 124.0, 121.2, 121.2, 120.5, 113.3; HRMS (ESI): m/z calculated for C₂₁H₁₄NO [M+H]⁺ = 296.1069, found [M+H]⁺ = 296.1064.

2-ethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2b)

The compound (2b) was prepared by using 1b as a starting material under the same reaction conditions and procedure as stated above. The product was afforded as yellow solid in 70% yield; TLC Rf 0.5 Hexane/EtOAc (98:02); m.p. = 185–187 °C; FT-IR (KBr): 3433, 3019,
1721, 1625, 1467, 1447, 1399, 1215, 1138, 1093, 701, 669 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.84 (d, J = 8.0 Hz, 1H), 7.74 (d, J = 7.2 Hz, 1H), 7.68 (d, J = 6.8 Hz, 2H), 7.57–7.52 (m, 3H), 7.45 (t, J = 7.6 Hz, 1H), 7.38–7.33 (m, 2H), 7.29–7.25 (m, 1H), 7.16 (d, J = 7.6 Hz, 1H), 2.67 (q, J = 7.6 Hz, 2H), 1.24 (t, J = 7.6 Hz, 3H); ¹³C NMR (75.4 MHz, CDCl₃): δ (ppm) 162.4, 140.3, 134.6, 134.3, 134.1, 133.9, 133.4, 132.3, 132.0, 129.0(3C), 128.6, 128.2, 128.3, 126.8, 125.2, 121.0, 120.5, 120.1, 113.2, 29.0, 16.1; HRMS (ESI): m/z calculated for C₂₃H₁₈NO [M+H]^⁺ = 324.1382, found [M+H]^⁺ = 324.1382.

1,2-dimethyl-11-phenyl-6H-isouindolo[2,1-a]indol-6-one (2c)

The compound (2c) was prepared under the same reaction conditions and procedure as abovestated, by using 1c as a starting material to afford the product, as yellow solid. The mixture of compound (2c) and compound (2c'), the regioisomer of 2c was purified by column chromatography on silica gel (230–400 mesh) and hexane: ethyl acetate (99.5: 0.5) as eluting solvent. Yield 67%; m.p. = 192–194 °C; FT-IR (KBr): 3434, 3019, 1731, 1622, 1467, 1495, 1215, 1127, 752, 699, 669 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.77–7.73 (m, 2H), 7.54–7.50 (m, 5H), 7.30–7.29 (m, 1H), 7.27 (d, J = 1.2 Hz, 1H), 7.15 (d, J = 8.0 Hz, 1H), 7.02–6.99 (m, 1H), 2.29 (s, 3H), 2.02 (s, 3H); ¹³C NMR (100.6 MHz, CDCl₃): δ (ppm) 162.5, 135.2, 134.6, 134.2, 133.8, 133.3, 132.8, 132.6, 132.3, 131.4, 129.9 (2C), 128.9, 128.7, 128.4 (2C), 128.3, 128.1, 125.1, 120.8, 110.6, 19.8, 15.7; HRMS (ESI): m/z calculated for C₂₃H₁₈NO [M+H]^⁺ = 324.1382, found [M+H]^⁺ = 324.1385.

2,3-dimethyl-11-phenyl-6H-isouindolo[2,1-a]indol-6-one (2c')

Yellow solid; yield 24%; m.p. = 163–165°C; FT-IR (KBr): 3436, 3020, 1734, 1620, 1465, 1495, 1215, 1127, 752, 699, 669 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.79–7.78 (m, 2H), 7.73 (d, J = 1.3 Hz, 1H), 7.71 (s, 1H), 7.60–7.56 (m, 3H), 7.50–7.46 (m, 1H), 7.40 (dt, J = 7.5, 1.1 Hz, 1H), 7.33–7.29 (m, 2H), 2.39 (s, 3H), 2.32 (s, 3H); ¹³C NMR (100.6 MHz, CDCl₃): δ (ppm) 162.5, 136.2, 134.8, 133.9, 133.5, 133.4, 132.7, 132.5, 132.4, 132.0, 128.9 (4C), 128.4, 128.2, 125.2, 121.6, 120.8, 120.6, 114.3, 20.3, 20.1; HRMS (ESI): m/z calculated for C₂₃H₁₈NO [M+H]^⁺ = 324.1382, found [M+H]^⁺ = 324.1385.
2.4-dimethyl-11-phenyl-6H-isooindolo[2,1-a]indol-6-one (2d)

The compound (2d) was prepared by using 1d as a starting material under the same reaction conditions and procedure, as yellow solid product in 45% yield; R f 0.5 Hexane/EtOAc (98: 02); m.p. = 148–149 °C; FT-IR (KBr): 3437, 3019, 2926, 2854, 2399, 1731, 1664, 1522, 1467, 1403, 1215, 1093, 1027, 924, 668 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.74 (d, J = 7.2 Hz, 1H), 7.65 (d, J = 7.2 Hz, 2H), 7.55 (t, J = 7.2 Hz, 2H), 7.45 (d, J = 7.2 Hz, 2H), 7.37 (t, J = 7.2 Hz, 1H), 7.29 (t, J = 7.2 Hz, 1H), 7.08 (s, 1H), 6.92 (s, 1H), 2.89 (s, 3H), 2.33 (s, 3H); ¹³C NMR (100.6 MHz, CDCl₃): δ (ppm) 162.1, 135.6, 135.2, 134.2, 133.9, 133.6, 133.4, 132.5, 132.3, 130.5, 129.2 (2C), 128.9 (2C), 128.5, 128.2, 125.2, 124.7, 120.6 (2C) 118.3, 21.2, 21.1; HRMS (ESI): m/z calculated for C₂₃H₁₈NO [M + H]^+ = 324.1382, found [M + H]^+ = 324.1389.

1,4-dimethyl-11-phenyl-6H-isooindolo[2,1-a]indol-6-one (2e)

The compound (2e) was prepared by using 1e as a starting material under the same reaction conditions and procedure, as yellow solid product in 75% yield; m.p. = 152–154 °C; FT-IR (KBr): 3434, 3021, 1731, 1625, 1402, 1338, 1215, 1137, 899, 669 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.74 (d, J = 6.4 Hz, 1H), 7.51 (brs 5H), 7.31–7.25 (m, 2H), 6.98 (d, J = 7.6 Hz, 1H), 6.91 (d, J = 7.6 Hz, 1H), 6.81 (d, J = 7.6 Hz, 1H), 2.91 (s, 3H), 2.02 (s, 3H); ¹³C NMR (75.4 MHz, CDCl₃): δ (ppm) 162.3, 136.3, 134.4, 134.2, 134.0, 133.4, 133.4, 133.1, 129.9(2C), 129.1, 128.3 (2C), 128.3, 128.1, 126.4, 125.2, 122.6, 121.0, 120.5, 21.2, 19.6; HRMS (ESI): m/z calculated for C₂₃H₁₈NO [M+H]^+ = 324.1382, found [M+H]^+ = 324.1384.

2-methyl-11-phenyl-6H-isooindolo[2,1-a]indol-6-one (2f)

The compound (2f) was prepared by using 1f as a starting material under the same reaction conditions and procedure, as yellow crystalline solid product in 71% yield; m.p. = 176–177 °C; FT-IR (KBr): 3434, 3019, 1730, 1621, 1410, 1335, 1215, 1130, 669 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.82 (d, J = 8.4 Hz, 1H), 7.75 (d, J = 7.2 Hz, 1H), 7.68 (d, J = 7.2 Hz, 2H), 7.55 (t, J = 7.2 Hz, 3H), 7.46 (t, J = 7.2 Hz, 1H), 7.38 (t, J = 7.2 Hz, 1H), 7.37 (t, J = 7.2 Hz, 1H), 7.29 (t, J = 7.2 Hz, 1H), 6.91 (d, J = 7.6 Hz, 1H), 6.81 (d, J = 7.6 Hz, 1H), 2.91 (s, 3H), 2.02 (s, 3H); ¹³C NMR (75.4 MHz, CDCl₃): δ (ppm) 162.3, 136.3, 134.4, 134.2, 134.0, 133.4, 133.4, 133.1, 129.9(2C), 129.1, 128.3 (2C), 128.3, 128.1, 126.4, 125.2, 122.6, 121.0, 120.5, 21.2, 19.6; HRMS (ESI): m/z calculated for C₂₃H₁₈NO [M+H]^+ = 324.1382, found [M+H]^+ = 324.1384.
7.31 (brs, 1H), 7.28 (d, J = 7.6 Hz, 1H), 7.13 (d, J = 8.0 Hz, 1H), 2.38 (s, 3H);\(^{13}\)C NMR (100.6 MHz, CDCl\(_3\)): δ (ppm) 162.4, 134.6, 134.3, 134.1, 133.9, 133.7, 133.4, 132.3, 131.9, 129.0 (4C), 128.6, 128.2, 127.9, 125.2, 121.3, 121.0, 120.4, 113.1, 21.5; HRMS (ESI): m/z calculated for C\(_{22}\)H\(_{16}\)NO [M+H]\(^+\) = 310.1226, found [M+H]\(^+\) = 310.1225.

3-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2g)

The compound (2g) was prepared under the same reaction conditions and procedure as above stated, by using 1g as a starting material to afford the product, as yellow solid. The mixture of compound (2g) and compound (2g\(^'*\)), the regioisomer of 2g was purified by column chromatography on silica gel (230-400 mesh) and hexane: ethyl acetate (99.4: 0.6) as eluting solvent. Yield 64%; m.p. = 181–183 °C; FT-IR (KBr): 3432, 3018, 1725, 1620, 1410, 1332, 1213, 1130, 669 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)): δ (ppm) 7.83 (t, J = 0.7 Hz, 1H), 7.81 (dt, J = 7.5, 0.8 Hz, 1H), 7.73–7.71 (m, 2H), 7.61–7.55 (m, 3H), 7.50–7.45 (m, 1H), 7.44–7.40 (m, 2H), 7.35–7.31 (m, 1H), 7.04–7.02 (m, 1H), 2.49 (s, 3H); \(^{13}\)C NMR (100.6 MHz, CDCl\(_3\)): δ (ppm) 162.6, 137.4, 134.8, 134.1, 133.8, 133.5, 132.3, 131.6, 129.0 (2C), 128.9 (2C), 128.5, 128.2, 125.3 (2C), 121.0, 120.9, 120.8, 120.7, 113.9, 21.7; HRMS (ESI): m/z calculated for C\(_{22}\)H\(_{16}\)NO [M+H]\(^+\) = 310.1226, found [M+H]\(^+\) = 310.1225.

1-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2g\(^'*\))

Yield 24%; m.p. = 150–152 °C; FT-IR (KBr): 3434, 3019, 1724, 1621, 1410, 1335, 1214, 1130, 669 cm\(^{-1}\); \(^1\)H NMR (400 MHz, CDCl\(_3\)): δ (ppm) 7.85 (d, J = 7.9 Hz, 1H), 7.77 (dd, J = 6.6, 1.4 Hz, 1H), 7.57–7.49 (m, 5H), 7.35–7.30 (m, 2H), 7.23 (t, J = 7.6 Hz, 1H), 7.06 (dd, J = 6.5, 0.7 Hz, 1H), 6.92 (d, J = 7.4 Hz, 1H), 2.12 (s, 3H); \(^{13}\)C NMR (100.6 MHz, CDCl\(_3\)): δ (ppm) 162.6, 135.0, 134.6, 133.7 (2C), 133.4, 133.1, 132.5, 132.4, 129.9 (2C), 128.5, 128.3 (2C), 128.1, 126.6, 126.1, 125.2, 121.1, 121.0, 111.2, 19.9; HRMS (ESI): m/z calculated for C\(_{22}\)H\(_{16}\)NO [M+H]\(^+\) = 310.1226, found [M+H]\(^+\) = 310.1225.
2-methoxy-11-phenyl-6H-isoiindolo[2,1-a]indol-6-one (2h)

The compound (2h) was prepared by using 1h as a starting material under the same reaction conditions and procedure as yellow solid product in 60% yield; TLC Rf 0.6 Hexane/EtOAc (97: 03); m.p. = 193–195 °C; FT-IR (KBr): 3434, 3019, 1735, 1620, 1467, 1495, 1215, 1127, 669 cm⁻¹;¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.87 (d, J = 8.6 Hz, 1H), 7.78 (d, J = 7.3 Hz, 1H), 7.71 (d, J = 7.0 Hz, 2H), 7.60–7.55 (m, 3H), 7.49 (t, J = 7.4 Hz, 1H), 7.41 (t, J = 7.4 Hz, 1H), 7.33 (d, J = 7.6 Hz, 1H), 7.05 (d, J = 2.2 Hz, 1H), 6.95 (dd, J = 8.6, 2.4 Hz, 1H), 3.85 (s, 3H);¹³C NMR (100.6 MHz, CDCl₃): δ (ppm) 162.2, 157.0, 135.1, 135.0, 134.6, 133.9, 133.4, 132.2, 129.0 (2C), 128.9 (2C), 128.7, 128.4, 128.3, 125.2, 121.0, 120.3, 114.3, 114.0, 105.1, 55.8; HRMS (ESI): m/z calculated for C₂₂H₁₆NO₂ [M+H]⁺ = 326.1176, found [M+H]⁺ = 326.1182.

3-methoxy-11-phenyl-6H-isoiindolo[2,1-a]indol-6-one (2i)

The compound (2i) was prepared under the same reaction conditions and procedure as above stated, by using 1i as a starting material to afford the product, as yellow solid. The mixture of compound (2i) and compound (2i’), the regioisomer of 2i was purified by column chromatography on silica gel (230-400 mesh) and hexane: ethyl acetate (99: 01) as eluting solvent. Yield 70%; m.p. = 189–191°C; FT-IR (KBr): 3434, 3019, 1731, 1622, 1467, 1495, 1215, 1127, 752, 699, 669 cm⁻¹;¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.79 (td, J = 7.6, 0.8 Hz, 1H), 7.73–7.70 (m, 2H), 7.59–7.55 (m, 3H), 7.53 (d, J = 2.4Hz, 1H), 7.50–7.45 (m, 1H), 7.44–7.40 (m, 2H), 7.31 (dd, J = 7.6, 1.2 Hz, 1H), 6.80 (dd, J = 8.8, 2.8 Hz, 1H), 3.93 (s, 3H);¹³C NMR (100.6 MHz, CDCl₃): δ (ppm) 162.7, 159.9, 134.9, 134.9, 133.6, 133.4, 132.8, 132.3, 129.0 (2C), 128.8 (2C), 128.2, 128.1, 127.3, 125.3, 121.9, 120.9, 120.7, 112.7, 97.9, 55.8; HRMS (ESI): m/z calculated for C₂₂H₁₆NO₂ [M+H]⁺ = 326.1175, found [M+H]⁺ = 326.1176.
1-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2i’)

The compound (2i’) is the regioisomer of compound (2i) which were isolated by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (99:01) in very slight (2i’/2i = 13.6/1) impurity of compound (2i) in 11% yield as yellowsolid; m.p. = 157–159 °C, FT-IR (KBr): 3434, 3019, 1730, 1467, 1495, 1215, 1127, 752, 699, 669 cm⁻¹;¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.78 (d, J = 7.4 Hz, 1H), 7.68 (dd, J = 8.2, 1.5 Hz, 2H), 7.64 (d, J = 7.9 Hz, 1H), 7.51–7.44 (m, 3H), 7.39–7.35 (m, 2H), 7.31–7.27 (m, 2H), 6.66 (d, J = 8.1 Hz, 1H), 3.75 (s, 3H);¹³C NMR (100.6 MHz, CDCl₃): δ (ppm) 162.8, 155.1, 135.1, 133.6, 133.4, 133.0, 130.1 (2C), 129.0, 128.3, 128.1, 127.8, 127.6 (2C), 125.3, 122.2, 120.9, 120.8, 106.6, 105.7, 55.2; HRMS (ESI): m/z calculated for C₂₂H₁₆NO₂ [M+H]⁺= 326.1175, found [M+H]⁺= 326.1176.


The compound (2j) was prepared by using 1j as a starting material under the same reaction conditions and procedure, as yellow solid product in 86% yield; TLC Rₜ 0.6 Hexane/EtOAc (97: 03); m.p. = 209–210 °C; FT-IR (KBr): 3431, 3021, 1732, 1621, 1526, 1400, 1215, 758, 670 cm⁻¹;¹H NMR (400 MHz, CDCl₃): δ (ppm) 8.12 (d, J = 8.8 Hz, 1H), 7.85–7.83 (m 1H), 7.76–7.71 (m, 3H), 7.67–7.64 (m, 2H), 7.59–7.54 (m, 3H), 7.37–7.26 (m, 3H), 7.23–7.20 (m, 1H), 7.04 (d, J = 7.6 Hz, 1H);¹³C NMR (100.6 MHz, CDCl₃): δ (ppm) 163.1, 135.3, 134.4, 133.8 (2C), 133.1, 131.4, 131.1, 129.8 (2C), 129.1, 128.8 (2C), 128.7, 128.4, 128.1, 127.9, 127.2, 126.3, 125.4, 124.4, 123.1, 121.6, 120.5, 113.2; HRMS (ESI): m/z calculated for C₂₅H₂₆NO [M+H]⁺= 346.1226, found [M+H]⁺= 346.1226.

2-chloro-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2k)

The compound (2k) was prepared by using 1k as a starting material under the same condition and procedure as yellow solid product in 81% yield; TLC Rₜ 0.6 Hxane/EtOAc (96: 04); m.p. = 193–194°C; FT-IR (KBr): 3409, 3021, 2401, 1726, 1622, 1524, 1444, 1319, 1215, 928, 670 cm⁻¹;¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.87 (d, J = 8.4 Hz,
1H), 7.78 (d, J = 7.4 Hz, 1H), 7.68–7.65 (m, 2H), 7.58–7.54 (m, 3H), 7.49 (dd, J = 8.1, 1.8 Hz, 2H), 7.42 (td, J = 7.5, 1.0 Hz, 1H), 7.34 (td, J = 7.5, 0.8 Hz, 1H), 7.28 (dd, J = 8.4, 1.9 Hz, 1H); 13C NMR (100.6 MHz, CDCl₃): δ (ppm) 162.2, 135.2, 135.1, 134.3, 133.7, 133.5, 131.9, 131.5, 129.6, 129.1 (3C), 128.8 (2C), 128.5, 126.7, 125.4, 121.3, 120.9, 119.5, 114.2; HRMS (ESI): m/z calculated for C₂₁H₁₃ClNO [M+H]^+ = 330.0680, found [M+H]^+ = 330.0675.

8-nitro-11-phenyl-6H-isoirindo[2,1-a]indol-6-one (2l)

The compound (2l) was prepared by using 1l as a starting material under the same condition and procedure as orange yellow colored solid product in 78% yield; TLC R_f 0.5 Hexane/EtOAc (94:06); m.p. = 246–248°C; FT-IR (KBr): 3434, 3019, 1724, 1655, 1524, 1404, 1345, 1215, 1104, 929 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ (ppm) 8.60 (d, J = 1.8 Hz, 1H), 8.31 (dd, J = 8.4, 2.0 Hz, 1H), 8.01 (d, J = 8.0 Hz, 1H), 7.73–7.69 (m, 3H), 7.64–7.60 (m, 3H), 7.56 (t, J = 7.2 Hz, 1H), 7.43 (t, J = 7.7 Hz, 1H), 7.27 (t, J = 7.6 Hz, 1H); ¹³C NMR (100.6 MHz, CDCl₃): δ (ppm) 160.1, 147.8, 139.5, 134.7, 134.2, 133.6, 132.0, 131.2, 129.3 (2C), 129.1, 128.9 (3C), 128.2, 124.9, 124.5, 122.1, 121.3, 120.8, 113.9; HRMS (ESI): m/z calculated for C₂₁H₁₃N₂O₃ [M+H]^+ = 341.0921, found [M+H]^+ = 341.0912.

11-phenyl-8-(phenylethynyl)-6H-isoirindo[2,1-a]indol-6-one (2m)

The compound (2m) was prepared by using 1m as a starting material under the same condition and procedure as yellow solid product in 80% yield; TLC R_f 0.6, Hexane/EtOAc (96:04); mp = 194–195°C; FT-IR (KBr): 3434, 3019, 2401, 1722, 1622, 1467, 1355, 1215, 1127, 752, 699, 669 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.99 (d, J = 7.9 Hz, 1H), 7.95 (s, 1H), 7.73 (d, J = 7.0 Hz, 2H), 7.62–7.55 (m, 7H), 7.51 (t, J = 7.3 Hz, 1H), 7.40–7.38 (m, 4H), 7.22 (t, J = 7.8 Hz, 1H); ¹³C NMR (100.6 MHz, CDCl₃): δ (ppm) 161.7, 136.5, 134.0, 133.9, 133.8, 133.7 (2C), 132.0, 131.7 (2C), 129.1 (2C), 128.9 (2C), 128.7, 128.5, 128.4 (2C), 128.3, 127.1, 124.2, 123.9, 122.7, 121.3, 121.2, 121.0, 113.5, 91.7, 88.4; HRMS (ESI): m/z calculated for C₂₉H₁₈NO [M+H]^+ = 396.1383, found [M+H]^+ = 396.1376.
11-(4-ethylphenyl)-6H-isoindolo[2,1-a]indol-6-one (2p)

The compound (2p) was prepared by using 1p as a starting material under the same condition and procedure as yellow crystalline solid product in 61% yield; TLC Rf 0.7 (hexane/EtOAc 98:02); m.p. = 140–142°C; FT-IR (KBr): 3433, 3019, 1721, 1625, 1467, 1447, 1399, 1361, 1215, 1138, 1093, 669 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.99 (d, J = 7.9 Hz, 1H), 7.81 (d, J = 7.4 Hz, 1H), 7.66–7.63 (m, 3H), 7.58 (d, J = 7.8 Hz, 1H), 7.45 (dd, J = 7.5, 1.0 Hz, 1H), 7.41 (d, J = 8.0 Hz, 2H), 7.38–7.36 (m, 1H), 7.31 (dd, J = 7.4, 0.9 Hz, 1H), 7.23–7.18 (m, 1H), 2.79 (q, J = 7.6 Hz, 2H), 1.36 (t, J = 7.6 Hz, 3H); ¹³C NMR (100.6 MHz, CDCl₃): δ (ppm) 162.5, 144.5, 134.7, 134.1, 133.9, 133.8 (2C), 133.5, 129.4, 128.9 (2C), 128.6, 128.5 (2C), 126.7, 125.3, 123.9, 121.3, 121.2, 120.7, 113.5, 28.7, 15.4; HRMS (ESI): m/z calculated for C₂₃H₁₈NO [M+H]+ = 324.1382, found [M+H]+ = 324.1388.

11-(p-tolyl)-6H-isoindolo[2,1-a]indol-6-one (2q)

The compound (2q) was prepared by using 1q as a starting material under the same condition and procedure as yellow crystalline solid product in 65% yield; TLC Rf 0.6 Hexane/EtOAc (98: 02); m.p. = 169–170°C; FT-IR (KBr): 3433, 3019, 1721, 1625, 1467, 1447, 1399, 1361, 1215, 1138, 1093, 669 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.98 (d, J = 7.9 Hz, 1H), 7.80 (d, J = 7.4 Hz, 1H), 7.63–7.61 (m, 3H), 7.56 (d, J = 7.8 Hz, 1H), 7.45–7.43 (m, 1H), 7.43-7.31 (m, 4H), 7.20 (t, J = 7.8 Hz, 1H), 2.49 (s, 3H); ¹³C NMR (100.6 MHz, CDCl₃): δ (ppm) 162.5, 138.2, 134.7, 134.1, 133.9, 133.8 (2C), 133.5, 129.7 (2C), 129.1, 128.8 (2C), 128.6, 126.7, 125.3, 123.9, 121.3, 121.2, 120.6, 113.5, 21.4; HRMS (ESI): m/z calculated for C₂₂H₁₆NO [M+H]+ = 310.1226, found [M+H]+ = 310.1225.

11-(m-tolyl)-6H-isoindolo[2,1-a]indol-6-one (2r)

The compound (2r) was prepared by using 1r as a starting material under the same condition and procedure as yellow crystalline solid product in 77% yield; TLC Rf 0.6 Hexane/EtOAc (98: 02); m.p. = 217–219°C; FT-IR (KBr): 3433, 3019, 1721, 1625, 1467, 1447, 1399, 1361, 1215, 1138, 1093, 669 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.96 (d, J = 8.0 Hz, 1H),
7.78 (d, J = 7.4 Hz, 1H), 7.59–7.53 (m, 2H), 7.52–7.49 (m, 2H), 7.45 (d, J = 7.4 Hz, 1H), 7.43–7.39 (m, 1H), 7.35–7.31 (m, 2H), 7.29–7.27 (m, 1H), 7.20–7.16 (m, 1H), 2.47 (s, 3H); \(^{13}\)C NMR (100.6 MHz, CDCl\(_3\)): δ (ppm) 162.5, 138.7, 134.7, 134.1, 134.0, 133.8, 133.7, 133.6, 132.1, 129.5, 129.1, 128.9, 128.7, 126.7, 126.0, 125.3, 124.0, 121.3, 121.2, 120.7, 113.5, 21.5; HRMS (ESI): \(m/z\) calculated for C\(_{22}\)H\(_{16}\)NO [M+H]\(^{+}\) = 310.1226, found [M+H]\(^{+}\) = 310.1222.

11-(4-tert-butylphenyl)-6H-isoindolo[2,1-a]indol-6-one (2s)

The compound (2s) was prepared by using 1s as a starting material under the same condition and procedure as yellow crystalline solid product in 59% yield; TLC R\(_f\) 0.6, Hexane/EtOAc (98:02); m.p. = 172–175°C; FT-IR (KBr): 3433, 3019, 1721, 1625, 1467, 1447, 1399, 1361, 1215, 1138, 1093, 669 cm\(^{-1}\); \(^{1}\)H NMR (400 MHz, CDCl\(_3\)): δ (ppm) 7.99 (d, J = 7.5 Hz, 1H), 7.80 (d, J = 6.9 Hz, 1H), 7.67–7.59 (m, 6H), 7.46–7.43 (m, 1H), 7.34 (d, J = 6.9 Hz, 2H), 7.22–7.19 (m, 1H), 1.45 (s, 9H); \(^{13}\)C NMR (100.6 MHz, CDCl\(_3\)): δ (ppm) 162.5, 151.4, 134.7, 134.1, 133.9, 133.8 (2C), 133.5, 129.1, 128.6 (3C), 126.7, 125.9 (2C), 125.3, 123.9, 121.4, 121.3, 120.6, 113.4, 34.8, 31.3 (3C); HRMS (ESI): \(m/z\) calculated for C\(_{25}\)H\(_{22}\)NO [M+H]\(^{+}\) = 352.1696, found [M+H]\(^{+}\) = 352.1696.

3. Procedure for control experiments.

(A) Experiment with TEMPO:

To a stirred solution of 1a (100 mg, 0.34 mmol, 1.0 eq.) and TEMPO (2.0 eq.) in trifluoroethanol (TFE) (1.5 mL) was added phenyliodidediacetate (PIDA) (184 mg, 0.57 mmol, 1.7 eq.) in an oven dried round bottom flask at room temperature. The resultant solution was stirred and the progress of reaction was monitored by TLC analysis. After the completion of reaction, the reaction mixture was evaporated under vacuum at 45°C and extracted with dichloromethane (30 mL X 3). The organic layers were combined and dried over anhydrous Na\(_2\)SO\(_4\) followed by the filtration and then condensed. The obtained solid product was washed with HPLC grade hexane and then methanol. The obtained solid product was characterized as compound 2a with the yield 85%.
(B) Experiment with 2,6-di-tert-butyl-4-methylphenol (BHT):

To a stirred solution of 1a (100 mg, 0.34 mmol, 1.0 eq.) and 2,6-di-tert-butyl-4-methylphenol (BHT) (2.0 eq.) in trifluoroethanol (TFE) (1.5 mL) was added phenyliodidediacetate (PIDA) (184 mg, 0.57 mmol, 1.7 eq.) in an oven dried round bottom flask at room temperature. The resultant solution was stirred and the progress of reaction was monitored by TLC analysis. After the completion of reaction, the reaction mixture was evaporated under vacuum at 45°C and extracted with dichloromethane (30 mL X 3). The organic layers were combined and dried over anhydrous Na₂SO₄ followed by the filtration and then condensed. The obtained solid product was washed with HPLC grade hexane and then methanol. The obtained solid product was characterized as compound 2a with the yield 82%.

(C) Experiment with 1,1-Diphenylethylene (DPE):

To a stirred solution of 1a (100 mg, 0.34 mmol, 1.0 eq.) and 1,1-diphenylethylene (DPE) (2.0 eq.) in trifluoroethanol (TFE) (1.5 mL) was added phenyliodidediacetate (PIDA) (184 mg, 0.57 mmol, 1.7 eq.) in an oven dried round bottom flask at room temperature. The resultant solution was stirred and the progress of reaction was monitored by TLC analysis. After the completion of reaction, the reaction mixture was evaporated under vacuum at 45°C and extracted with dichloromethane (30 mL X 3). The organic layers were combined and dried over anhydrous Na₂SO₄ followed by the filtration and then condensed. The obtained solid product was washed
with HPLC grade hexane and then methanol. The obtained solid product was characterized as compound 2a with the yield 86%.

4. Discussion of Proposed Mechanism by Time Dependent Mass Spectra (ESI-MS):

The mechanism and role of solvent were investigated by mass spectra (ESI-MS) of reaction mixture. The mass spectra was recorded after 3 and 10 min of addition of hypervalent iodine reagent, showed peaks at 500.0494 \([C_{27}H_{19}INO_2]^+\), 396.1196 \([C_{23}H_{17}F_3NO_2]^+\) and 298.1217 \([C_{21}H_{16}NO_2]^+\), and peaks at 500.0508 \([C_{27}H_{19}INO_2]^+\), 396.1207 \([C_{23}H_{17}F_3NO_2]^+\) and 296.1067 \([C_{21}H_{14}NO_2]^+\) respectively. In both mass spectra there were peaks at 500.05 and 396.1207 indicated that the formation of intermediates, nitrenium ion \(B\) and carbonium ion \(C\), which was stabilized by iodine and solvent (TFE), respectively.
ESI-MS Spectrum of Reaction Mixture after 3 min of Addition of Hypervalent Iodine Reagent
ESI-MS Spectrum of Reaction Mixture after 10 min of Addition of Hypervalent Iodine Reagent

5. References:
$^1$H NMR Spectrum of N-(phenyl)-2-iodobenzenamide (S1a) (300 MHz, CDCl$_3$)

$^{13}$C NMR Spectrum of N-(phenyl)-2-iodobenzenamide (S1a) (75 MHz, CDCl$_3$)
$^1$H NMR Spectrum of N-(4-ethylphenyl)-2-iodobenzamide (S1b) (400 MHz, CDCl$_3$)

$^{13}$C NMR Spectrum of N-(4-ethylphenyl)-2-iodobenzamide (S1b) (75 MHz, CDCl$_3$)
$^1$H NMR Spectrum of N-(3,4-dimethylphenyl)-2-iodobenzamide (S1c) (400 MHz, CDCl$_3$)

$^{13}$C NMR Spectrum of N-(3,4-dimethylphenyl)-2-iodobenzamide (S1c) (75 MHz, CDCl$_3$)
$^1$H NMR Spectrum of N-(2,4-dimethylphenyl)-2-iodobenzamide (S1d) (400 MHz, CDCl$_3$)

$^{13}$C NMR Spectrum of N-(2,4-dimethylphenyl)-2-iodobenzamide (S1d) (100 MHz, CDCl$_3$ + CD$_3$OD)
$^1$H NMR Spectrum of N-(2,5-dimethylphenyl)-2-iodobenzamide (S1e) (400 MHz, CDCl$_3$)

$^{13}$C NMR Spectrum of N-(2,5-dimethylphenyl)-2-iodobenzamide (S1e) (75 MHz, CDCl$_3$)
\[ ^{1}H \text{ NMR Spectrum of } N-(4\text{-methylphenyl})-2\text{-iodobenzamide (S1f) (400 MHz, CDCl}_3) \]

\[ ^{13}C \text{ NMR Spectrum of } N-(4\text{-methylphenyl})-2\text{-iodobenzamide (S1f) (100 MHz, CDCl}_3) \]
$^1$H NMR Spectrum of N-(3-methylphenyl)-2-iodobenzamide (S1g) (400 MHz, CDCl$_3$)

$^{13}$C NMR Spectrum of N-(3-methylphenyl)-2-iodobenzamide (S1g) (100 MHz, CDCl$_3$)
$^1$H NMR Spectrum of N-(4-methoxyphenyl)-2-iodobenzamide (S1h) (400 MHz, CDCl$_3$)

$^{13}$C NMR Spectrum of N-(4-methoxyphenyl)-2-iodobenzamide (S1h) (100 MHz, CDCl$_3$)
^1^H NMR Spectrum of N-(3-methoxyphenyl)-2-iodobenzamide (S1i) (400 MHz, CDCl_3)

^1^3^C NMR Spectrum of N-(3-methoxyphenyl)-2-iodobenzamide (S1i) (100 MHz, CDCl_3 + CD_3OD)
$^1$H NMR Spectrum of N-(naphthalen-2-yl)-2-iodobenzamide (S1j) (400 MHz, CDCl$_3$)

$^{13}$C NMR Spectrum of N-(naphthalen-2-yl)-2-iodobenzamide (S1j) (75 MHz, CDCl$_3$ + CD$_3$OD)
$^1$H NMR Spectrum of N-(4-chlorophenyl)-2-iodobenzamide (S1k) (400 MHz, CDCl$_3$)

$^{13}$C NMR Spectrum of N-(4-chlorophenyl)-2-iodobenzamide (S1k) (100 MHz, CDCl$_3$)
**1H NMR Spectrum of 2-iodo-5-nitro-N-phenylbenzamide (S1I) (400 MHz, Acetone-d$_6$)**

![1H NMR Spectrum](image)

**13C NMR Spectrum of 2-iodo-5-nitro-N-phenylbenzamide (S1I) (100 MHz, Acetone-d$_6$)**

![13C NMR Spectrum](image)
$^1$H NMR Spectrum of 5-bromo-2-iodo-N-phenylbenzamide (S1m) (400 MHz, Acetone-d$_6$)

$^{13}$C NMR Spectrum of 5-bromo-2-iodo-N-phenylbenzamide (S1m) (100 MHz, Acetone-d$_6$)
$^1$H NMR Spectrum of $N$-$(4$-acetylphenyl$)$-$2$-iodobenzamide (S1n) (400 MHz, CDCl$_3$)

$^{13}$C NMR Spectrum of $N$-$(4$-acetylphenyl$)$-$2$-iodobenzamide (S1n) (100 MHz, CDCl$_3$)
$^1$H NMR Spectrum of methyl 4-(2-iodobenzamido)benzoate (S1o) (400 MHz, CD$_3$OD + CDCl$_3$)

$^{13}$C NMR Spectrum of methyl 4-(2-iodobenzamido)benzoate (S1o) (100 MHz, CD$_3$OD + CDCl$_3$)
$^1$H NMR Spectrum of N-phenyl-2-(phenylethynyl)benzamide (1a) (300 MHz, CDCl$_3$)

$^{13}$C NMR Spectrum of N-phenyl-2-(phenylethynyl)benzamide (1a) (100 MHz, CDCl$_3$)
$^1$H NMR Spectrum of N-(4-ethylphenyl)-2-(phenylethynyl)benzamide (1b) (400 MHz, CDCl$_3$)

$^{13}$C NMR Spectrum of N-(4-ethylphenyl)-2-(phenylethynyl)benzamide (1b) (100 MHz, CDCl$_3$)
$^1$H NMR Spectrum of $N$-(3,4-dimethylphenyl)-2-(phenylethynyl)benzamide (1c) (400 MHz, CDCl$_3$)

$^{13}$C NMR Spectrum of $N$-(3,4-dimethylphenyl)-2-(phenylethynyl)benzamide (1c) (100 MHz, CDCl$_3$)
$^1$H NMR Spectrum of N-(2,4-dimethylphenyl)-2-(phenylethynyl)benzamide (1d) (400 MHz, CDCl$_3$)

$^{13}$C NMR Spectrum of N-(2,4-dimethylphenyl)-2-(phenylethynyl)benzamide (1d) (100 MHz, CDCl$_3$)
$^1$H NMR Spectrum of $N$-(2,5-dimethylphenyl)-2-(phenylethynyl)benzamide(1e) (400 MHz, CDCl$_3$)

$^{13}$C NMR Spectrum of $N$-(2,5-dimethylphenyl)-2-(phenylethynyl)benzamide(1e) (100 MHz, CDCl$_3$)
$^1$H NMR Spectrum of $N$-\((4\text{-methylphenyl})\)-2-(phenylethynyl)benzamide\((1f)\) (400 MHz, CDCl$_3$)

$^{13}$C NMR Spectrum of $N$-\((4\text{-methylphenyl})\)-2-(phenylethynyl)benzamide\((1f)\) (100 MHz, CDCl$_3$)
$^1$H NMR Spectrum of $N$-(3-methylphenyl)-2-(phenylethynyl)benzamide (1g) (400 MHz, CDCl$_3$)

$^{13}$C NMR Spectrum of $N$-(3-methylphenyl)-2-(phenylethynyl)benzamide (1g) (100 MHz, CDCl$_3$)
$^1$H NMR Spectrum of $N$-(4-methoxyphenyl)-2-(phenylethynyl)benzamide (1h) (400 MHz, CDCl$_3$)

$^{13}$C NMR Spectrum of $N$-(4-methoxyphenyl)-2-(phenylethynyl)benzamide (1h) (100 MHz, CDCl$_3$)
$^1$H NMR Spectrum of $N$-(3-methoxyphenyl)-2-(phenylethynyl)benzamide (1i) (400 MHz, CDCl$_3$)

$^{13}$C NMR Spectrum of $N$-(3-methoxyphenyl)-2-(phenylethynyl)benzamide (1i) (100 MHz, CDCl$_3$)
$^1\text{H}$ NMR Spectrum of $N$-(naphthalen-2-yl)-2-(phenylethynyl)benzamide (1j) (400 MHz, CDCl$_3$)

$^{13}\text{C}$ NMR Spectrum of $N$-(naphthalen-2-yl)-2-(phenylethynyl)benzamide (1j) (100 MHz, CDCl$_3$)
$^1$H NMR Spectrum of $N$-(4-chlorophenyl)-2-(phenylethynyl)benzamide(1k) (400 MHz, CDCl$_3$)

$^{13}$C NMR Spectrum of $N$-(4-chlorophenyl)-2-(phenylethynyl)benzamide(1k) (100 MHz, CDCl$_3$)
$^1$H NMR Spectrum of 5-nitro-N-phenyl-2-(phenylethynyl)benzamide (II) (400 MHz, CDCl$_3$)

$^{13}$C NMR Spectrum of 5-nitro-N-phenyl-2-(phenylethynyl)benzamide (II) (100 MHz, CDCl$_3$ + CD$_3$OD)
$^1$H NMR Spectrum of 5-bromo-N-phenyl-2-(phenylethynyl)benzamide(1m) (400 MHz, CDCl$_3$)

$^1$H NMR Spectrum of N-(4-acetylphenyl)-2-(phenylethynyl)benzamide(1n) (400 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of $N$-(4-acetylphenyl)-2-(phenylethynyl)benzamide (1n) (100 MHz, CDCl$_3$)

$^1$H NMR Spectrum of methyl 4-(2-(phenylethynyl)benzamido)benzoate (1o) (400 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of methyl 4-(2-(phenylethynyl)benzamido)benzoate (1o) (100 MHz, CDCl$_3$)

$^1$H NMR Spectrum of 2-((4-ethylphenyl)ethynyl)-N-phenylbenzamide (1p) (400 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 2-((4-ethylphenyl)ethynyl)-N-phenylbenzamide (1p) (100 MHz, CDCl$_3$)

$^1$H NMR Spectrum of N-phenyl-2-(p-tolylethynyl)benzamide (1q) (400 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of N-phenyl-2-(p-tolylethynyl)benzamide (1q) (100 MHz, CDCl$_3$)

$^1$H NMR Spectrum of N-phenyl-2-(m-tolylethynyl)benzamide (1r) (400 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of $N$-phenyl-2-(m-tolylethynyl)benzamide (1r) (100 MHz, CDCl$_3$)

$^1$H NMR Spectrum of 2-((4-tert-butylphenyl)ethynyl)-$N$-phenylbenzamide (1s) (400 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 2-((4-tert-butylphenyl)ethynyl)-N-phenylbenzamide(1s) (100 MHz, CDCl$_3$)

$^1$H NMR Spectrum of N-phenyl-2-((trimethylsilyl)ethynyl)benzamide(1t) (400 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of $N$-phenyl-2-((trimethylsilyl)ethynyl)benzamide (1t) (100 MHz, CDCl$_3$)
$^1$H NMR Spectrum of 11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2a) (400 MHz, CDCl$_3$)

$^{13}$C NMR Spectrum of 11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2a) (75 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum (expansion) of 11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2a) (75 MHz, CDCl$_3$)

DEPT 135 NMR Spectrum of 11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2a)
HSQC Spectrum of 11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2a)
HSQC Spectrum (expansion) of 11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2a)
HMBC Spectrum of 11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2a)
HMBC Spectrum (expansion) of 11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2a)
$^1\text{H}-^1\text{H}$ COSY Spectrum of 11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2a)
$^1$H-$^1$H COSY Spectrum (expansion) of 11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2a)
$^1$H NMR Spectrum of 2-ethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2b) (400 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 2-ethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2b) (75 MHz, CDCl$_3$)
$^1$H NMR Spectrum of 1,2-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one(2c) (400 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 1,2-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2c) (100 MHz, CDCl$_3$)
HMBC Spectrum of 1,2-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2c)
HMBC Spectrum (expansion) of 1,2-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2c)
$^1$H-$^1$H COSY Spectrum of 1,2-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2c)
$^1$H-$^1$H COSY Spectrum (expansion) of 1,2-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2c)
\(^1\)H NMR Spectrum of 2,3-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one(2c') (400 MHz, CDCl\(_3\))
$^{13}$C NMR Spectrum of 2,3-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one(2c') (100 MHz, CDCl$_3$)
HSQC Spectrum of 2,3-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2c')
HSQC Spectrum (expansion) of 2,3-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one(2c')
HMBC Spectrum of 2,3-dimethyl-11-phenyl-6H-isooindolo[2,1-a]indol-6-one(2c')

HMBC Spectrum(expansion) of 2,3-dimethyl-11-phenyl-6H-isooindolo[2,1-a]indol-6-one(2c')
$^1$H-$^1$H COSY Spectrum of 2,3-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2c')
$^1$H-$^1$H COSY Spectrum (expansion) of 2,3-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one(2c')
$^1$H NMR Spectrum of 2,4-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one(2d) (400 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of $2,4$-dimethyl-$11$-phenyl-$6$H-isoindolo[2,1-$a$]indol-6-one (2d) (100 MHz, CDCl$_3$)

$^1$H NMR Spectrum of $1,4$-dimethyl-$11$-phenyl-$6$H-isoindolo[2,1-$a$]indol-6-one (2e) (400 MHz, CDCl$_3$)
\[ ^{13}C \text{ NMR Spectrum of 1,4-dimethyl-11-phenyl-6H-isooindolo[2,1-a]indol-6-one (2e) (75 MHz, CDCl}_3 \]
$^1$H NMR Spectrum of 2-methyl-11-phenyl-6H-isoindolo[2,1-ajindol-6-one (2f) (400 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 2-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2f) (100 MHz, CDCl$_3$)
$^1$H NMR Spectrum of 3-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2g) (400 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 3-methyl-11-phenyl-6H-isodolo[2,1-a]indol-6-one (2g) (100 MHz, CDCl$_3$)
HSQC Spectrum of 3-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one(2g)
HSQC Spectrum (expansion) of 3-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one(2g)
HMBC Spectrum of 3-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2g)
HMBC Spectrum (expansion) of 3-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one(2g)
$^1$H-$^1$H COSY Spectrum of 3-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one(2g)
$^1$H-$^1$H COSY Spectrum (expansion) of 3-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one(2g)
$^1$H NMR Spectrum of 1-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one(2g') (400 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 1-methyl-11-phenyl-6H-isoindolo[2,1-α]indol-6-one(2g') (100 MHz, CDCl$_3$)
HSQC Spectrum of 1-methyl-11-phenyl-6H-isoindolo[2,1-f]indol-6-one(2\textsuperscript{g}')
HSQC Spectrum (expansion) of 1-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one(2g')
HMBC Spectrum of 1-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one(2g')
HMBC Spectrum (expansion) of 1-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one(2g')
$^{1}$H-$^{1}$H COSY Spectrum of 1-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one(2g')
$^{1}$H-$^{1}$H COSYSpectrum (expansion) of 1-methyl-11-phenyl-6H-isoiindolo[2,1-ajindol-6-one(2g')
$^1$H NMR Spectrum of 2-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2h) (400 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 2-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2h) (100 MHz, CDCl$_3$)
$^1$H NMR Spectrum of 3-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2i) (400 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 3-methoxy-11-phenyl-6H-isoirido[2,1-a]indol-6-one(2i) (100 MHz, CDCl$_3$)
HSQC Spectrum of 3-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one(2i)
 HSQC Spectrum (expansion) of 3-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one(2i)
HMBC Spectrum of 3-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one(2i)
HMBC Spectrum (expansion) of 3-methoxy-11-phenyl-6H-isooindolo[2,1-a]indol-6-one(2i)
$^{1}H-{^1}H$ COSY Spectrum of 3-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one(2i)
$^1$H-$^1$H COSYSpectrum (expansion) of 3-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2i)
\(^1\)H NMR Spectrum of 1-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2i') (400 MHz, CDCl\(_3\))
$^{13}$C NMR Spectrum of 1-methoxy-11-phenyl-6H-isoinol[2,1-a]indol-6-one (2i') (100 MHz, CDCl$_3$)
HSQC Spectrum of 1-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2i')
HSQC Spectrum (expansion) of 1-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2i')
HMBC Spectrum of 1-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2i')
HMBC Spectrum (expansion) of 1-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2i')
$^1$H-$^1$H COSY NMR Spectrum of 1-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2i')
$^1$H-$^1$H COSY Spectrum (expansion) of 1-methoxy-11-phenyl-6H-isindolo[2,1-a]indol-6-one (2i')
$^1$H NMR Spectrum of 13-phenyl-8H-benzo[e]isoindolo[2,1-a]indol-8-one (2j) (400 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 13-phenyl-8H-benzo[e]isoindolo[2,1-a]indol-8-one (2j) (100 MHz, CDCl$_3$)
$^{1}$H NMR Spectrum of 2-chloro-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2k) (400 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 2-chloro-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2k) (100 MHz, CDCl$_3$)
$^1$H NMR Spectrum of 8-nitro-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2l) (400 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 8-nitro-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2l) (100 MHz, CDCl$_3$)
$^1$H NMR Spectrum of 11-phenyl-8-(phenylethynyl)-6H-isoindolo[2,1-a]indol-6-one (2m) (400 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 11-phenyl-8-(phenylethynyl)-6H-isoindolo[2,1-a]indol-6-one (2m) 
(100 MHz, CDCl$_3$)
$^1$H NMR Spectrum of $11$-(4-ethylphenyl)-6H-isoindolo[2,1-a]indol-6-one (2p) (400 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 11-(4-ethylphenyl)-6H-isoindolo[2,1-a]indol-6-one (2p) (100 MHz, CDCl$_3$)
$^{1}H$ NMR Spectrum of 11-p-tolyl-6H-isoindolo[2,1-a]indol-6-one (2q) (400 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 11-p-tolyl-6H-isoindolo[2,1-a]indol-6-one (2q) (100 MHz, CDCl$_3$)
$^1$H NMR Spectrum of 11-m-tolyl-6H-isoindolo[2,1-a]indol-6-one (2r) (400 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 11-m-tolyl-6H-isoinodo[2,1-ajindol-6-one (2r) (100 MHz, CDCl$_3$)
$^1$H NMR Spectrum of 11-(4-tert-butylphenyl)-6H-isoindolo[2,1-a]indol-6-one(2s) (400 MHz, CDCl$_3$)
$^{13}$C NMR Spectrum of 11-(4-tert-butylphenyl)-6H-isooindolo[2,1-a]indol-6-one(2s) (100 MHz, CDCl$_3$)