Supporting Information

Synthesis of 5- Aryl (Vinyl) Dihydroisoindolo[2,1-a]quinolin-11-ones, their in silico ADMET properties and in vitro antitumor activities

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1. Materials and Methods

1.1. Chemistry
The melting points (uncorrected) were determined on a Fisher-Johns melting point apparatus. The IR spectra were recorded using a Infralum FT-02 spectrophotometer in KBr. $^1$H NMR spectra were recorded on Bruker AM-400 or AC-300 spectrometers. Chemical shifts are reported in ppm ($\delta$) relative to the solvent peak (CHCl$_3$ in CDCl$_3$ at 7.24 ppm for protons). Signals are designated as follows: s, singlet; d, doublet; dd, doublet of doublets; m, multiplet. A Hewlett Packard 5890a series II Gas Chromatograph interfaced to an HP 5972 Mass Selective Detector (MSD) with an HP MS Chemstation Data system was used for MS identification at 70 eV using a 60 m capillary column coated with HP-5 [5%-phenyl-poly(dimethyl-siloxane)]. Elemental analyses were performed on a Perkin Elmer 2400 Series II analyzer and were within ±0.4 of theoretical values. The reaction progress was monitored using thin layer chromatography on a silufol UV254 TLC aluminum sheet. The data were collected on a Bruker APEX2 diffractometer using a graphite-monochromatized Mo K$\alpha$ radiation ($\lambda = 0.71073$ Å). After data collection, the intensity data were integrated and corrected for Lorentz, polarization and background effects using the SAINT V7.34A software.

1.2. General procedure for synthesis of the 5-aryl-5-methylisoindolo[2,1-a]quinolin-11(5H)-ones 4a-m
Aryl amines 1 (1 mmol), o-phthaldehydic acid (2) (1.1 mmol) and AMCell-SO$_3$H (0.06 g) were mixed at room temperature. After stirring for 5 min, corresponding alkenes 3a,b (1.2 mmol) were added. The reaction mixture was strongly stirred to 90 °C during 4-8 h. After reaction completion, as indicated by TLC or an appropriate time, the reaction mixture was washed with acetone (3 x 20 mL). The catalyst was filtered and dried for the next cycle. The acetone was evaporated to give the crude product that were purified by column chromatography on silica gel using a mixture of petroleum ether and ethyl acetate (2:1) as eluent to give the isoindolo[2,1-a]quinolines derivatives 4a-m.

1.3. General procedure for synthesis of the 5-vinyl-5-methylisoindole[2,1-a]quinolin-11(5H)-ones 6a-l
In a 100 mL Schlenk reactor, 0.17 g (1.8 mmol) of aryl amines 1, 0.3 g (2.0 mmol) o-phthalaldehyde (2) were dissolved in 20 mL of dry MeCN and N$_2$ atmosphere. After 5 min 0.026 g (0.18 mmol) of BF$_3$·OEt$_2$ were added. Then, after 20 min 0.37 g (5.4 mmol) of isoprene (5) were added and the reaction mix was stirred at room temperature for over 8-12 h according to TLC controls. Afterwards, the reaction mass was treated with a Na$_2$CO$_3$ saturated solution and extracted with ethyl acetate (2x20 mL). The organic layer was separated, and dried with Na$_2$SO$_4$. The organic solvent was removed in vacuum to afford the respective 5-vinyl-5-methyl-isoindolo[2,1-a]quinolines 6a-l, which were purified by column chromatography (silica gel, petroleum ether/EtOAc) to afford pure substances.
2. NMR overview of dihydroisoindolo[2,1-a]quinolin-11(5H)-one 4a-m

The NMR spectra were recorded using DMSO-d6 as solvent. In most cases almost pure products were achieved after purification process and the cis isomer was not obtained after chromatographic purification.

For the assignation of C-5 aromatic protons we followed corresponding nomenclature, according to the C-5 group. For the 2-methoxyphenol (guaiacol), the protons are called H_{Gu}, for the anisole the protons are called, H_{An} and for the vinyl group, from isoprene, the protons are called, =CH\textsubscript{2} and =CH (Figure S1).

![Figure S1. C-5 Aromatic protons fragments.](image)

The endo-trans favored transition state was proposed consistently with the coupling constants $J$ observed in all $^1$H NMR spectra. The coupling constants values $J_{5\text{-}H}$$-$$J_{6\text{-}H}$ = 11.1 Hz and $J_{6\text{a}\text{-}H}$$-$$J_{6\text{-}H}$ = 10.6 Hz for compound 4a (Figure S2).

![Figure S2. Expansion of the spectrum $^1$H NMR (400 MHz, DMSO-d6) for compound 4a.](image)

3. X-ray diffraction analysis of dihydroisoindolo[2,1-\(a\)]quinolin-11(5\(H\))-one derivative 6a

3.1. Crystal preparation
The crystallization of \textit{trans}-5-methyl-5-vinyl-6,6\(a\)-dihydroisoindolo[2,1-\(a\)]quinolin-11(5\(H\))-one (6a) was obtained according to the procedure reported by Spingler et al.\textsuperscript{1}, where ethanol was used as solvent and a mixture of cyclohexane:diethyl-ether in a 1:5 ratio as antisolvent. This method gave single crystals suitable for X-ray diffraction analysis.

3.2. Crystal structure determination
The data were collected on a Bruker APEX2 diffractometer using a graphite-monochromatized Mo K\(\alpha\) radiation (\(\lambda = 0.71073\) Å). After data collection, the intensity data were integrated and corrected for Lorentz, polarization and background effects using the SAINT V7.34A software. The SADABS-2012/1 software\textsuperscript{2} was used to correct absorption effects using a redundancy algorithm. Crystal structure was determined by direct methods using the SIR92 program\textsuperscript{3} and refined by full-matrix least-squares calculation of F².

Using the Crystals software\textsuperscript{4} the anisotropic displacement parameters were refined for C, N and O atoms. All H atoms (constrained to ride on their parent atoms) were placed in geometrically idealized positions which were corroborated by difference-Fourier map calculations. The used C-H mean distances were 0.95 Å (aromatic) and 0.97 Å (methyl), while a 0.89 Å value was used for the N-H distances.

Molecule 6a crystallizes in the monoclinic space group P\(c\) (No. 7), crystallographic information and structure refinement parameters (Table S1). Additionally, a structure representation of the asymmetric unit is shown in Figure S3.

\textbf{Figure S3.} Stick-ball model of 6a asymmetric unit from monocrystal X-ray diffraction.
Table S1. Crystal data details of the 6a structure determination

| Parameter                        | Value                  |
|----------------------------------|------------------------|
| Chemical formula                 | C₁₉H₁₇NO               |
| Formula weight (g/mol)           | 275.33                 |
| Crystal system                   | Monoclinic             |
| Space group                      | Pc (No 7)              |
| a (Å)                            | 5.8738(2)              |
| b (Å)                            | 9.4468(4)              |
| c (Å)                            | 13.2892(5)             |
| V (Å³)                           | 737.39(5)              |
| Z                                | 2                      |
| dₛ (g cm⁻³)                      | 1.240                  |
| F (000)                          | 292                    |
| μ (mm⁻¹)                         | 0.596                  |
| θ range (°)                      | 4.7-74.2               |
| hkl range                        | -13 ≤ h ≤ 13           |
|                                 | -14 ≤ k ≤ 14           |
|                                 | -31 ≤ l ≤ 31           |
| T (K)                            | 293                    |
| Crystal dimensions (mm)          | 0.00 x 0.00 x 0.00     |
| Diffractometer                   | Bruker Kappa Apex 2    |
| Absorption correction           | Multi-scan             |
|                                 | (SADABS 2012/1)        |
|                                 | T_min = 0.87, T_max = 0.98 |
| Refinements                      |                        |
| Collected                        | 52522                  |
| Unique (R(int))                  | 3132 (0.036)           |
| With I > 2σ(I)                   | 2706                   |
| Refinement method                | Full-matrix least-squares on F² |
| Number of parameters             | 192                    |
| R(F) [I > 2σ(I)]                 | 0.0447                 |
| wR(F) [I > 2σ(I)]                | 0.1230                 |
| Goodness of fit on F²            | 1.017                  |
| Max/Min Δρ (e Å⁻³)               | -0.15/0.16             |

4. **Analysis of N-aryl-3-hydroxyisoindolone intermediate**

In order to clarify mechanistic details of Povarov multicomponent reaction, reaction of 1a and 2 was realized in acetonitrile at room temperature. The main isolated and purified product was 2,3-dihydro-3-hydroxy-2-phenyl-isoindol-1-one (A) (Scheme S1).

![Scheme S1](image)

**Scheme S1.** An additional experiment to prove mechanism: Formation of 2,3-dihydro-3-hydroxy-2-phenyl-isoindol-1-one
**Procedure isoindolinone isolation**: In a 10 mL vial, 46.5 mg (0.5 mmol) of aniline 1a and 90 mg (0.6 mmol) of o-phthalaldehyde (2) were mixed in MeCN (2 mL). The mixture was stirred by 1 h, extracted with ethyl acetate and recrystallized in methanol to obtain a white solid in 90 % yield. Mp:166-168 °C (lit. mp: 167-168 °C). Its 1H NMR spectrum (Figure S4) was found to be identical to the literature report.

**Figure S4.** 1H NMR spectrum (400 MHz,CDCl3) of isoindolone A.

**5. Biology**

Human tumor cell lines and culture media: PC3 (Prostate carcinoma), HeLa (Cervical epithelial carcinoma) were grown in RPMI 1640 medium (Invitrogen) supplemented with 10% heat inactivated fetal bovine serum (FBS), 1 % of L-glutamine, 1 % streptomycin, 100 units/mL penicillin (all obtained from Sigma Aldrich USA). MCF-7 (breast carcinoma, no overexpresses the HER2/c-erb-2 gene), SK-BR-3 (breast carcinoma, overexpresses the HER2/c-erb-2 gene) and primary culture of normal human dermis fibroblast used as control cells were grown in DMEM medium (Invitrogen). Cells were grown in a humidified incubator with 5% CO2 and 95% air at 37°C until they reach the exponential growth phase. For treatments exponentially growing cells were collected, counted, re-suspended in fresh culture medium and incubated in 96 sterile well plates.

**5.1. Cytotoxicity evaluation by MTT assay**

Cell viability was assessed using the MTT assay, which is based on the ability of viable cells to metabolically reduce a yellow tetrazolium salt (MTT; Sigma) to a purple formazan product. This
reaction takes place when mitochondrial reductases are active. Cells were grown in 96-well plates (5×10^3 cells/well) for 24 hours. Cultures were carried out at 37°C in a humidified atmosphere with 5% CO_2. cells were incubated with the synthetic products or chemotherapeutic drugs in 100 μL of complete culture medium containing 0, 1, 5, 10, 25, 100 μg/mL concentrations each one compounds for 72 hours. After incubation, the medium was removed, and the cells were treated with 100 μL 0.4mg/mL MTT for 3 hours at 37 °C. Subsequently, 100 μL DMSO was added to the mixture. The solubilized formazan product was quantified with the help of a microtiter plate reader TECAN-sunrise at 570 nm. Adriamycin was used as a positive control in the assay. In all cases the compounds were dissolved in DMSO, at the final concentration in the culture medium was lower than 1%, a concentration that had neither cytotoxic effect nor caused any interference with the colorimetric detection method.

5.2. Selectivity Index (SI)
The selectivity index was calculated as the IC_{50} (control cells)/IC_{50} (tumoral cell line) ratio. A selectivity index >1 indicates that the cytotoxicity on tumoral cells surpassed that on healthy non-tumoral cells.

5.3. Statistical Analysis
All experiments were performed at least three times. The results are expressed as mean ± SD. Anova test were performed. Only post hoc Dunnet test p < 0.01 was considered to be statistically significant. The dose–response curves were plotted with the OriginPro ver.8.0 programs, and 50% growth inhibitory concentrations (IC_{50}) of synthetics products or chemotherapeutic drugs were determined by a non-linear regression of individual experiments calculated through computation with GraphPad prism v.5.02 software program (Intuitive Software for Science, San Diego, CA, USA).

6. Theoretical considerations
Calculation of electronic density for the coefficient orbital was performed using the methodology proposed by Cao and co-workers. Each coefficient contribution was introduced in the follow formula where Ci is the contribution to the frontier orbital (HOMO or LUMO) of atom i, which is the sum of squares of all the orbital coefficients of atom i contributed to the frontier orbital. O in the formulas indicates all the carbon atoms of isoprene molecule.

\[ \rho_{i,HOMO} = C_i^2 / \sum_{i\in O} C_{i,HOMO}^2 \times 100\% \]

\[ \rho_{i,LUMO} = C_i^2 / \sum_{i\in O} C_{i,LUMO}^2 \times 100\% \]
Table S2. HOMO Coefficient orbitals for isoprene (5).

| ISOPRENE | HOMO     |
|----------|----------|
| ORBITALES| C-1 | C-4 | C-5 | C-9 | C-11 |
| 1s       | 0.00000 | 0.00000 | 0.00000 | 0.00000 | 0.00000 |
| 2s       | 0.00000 | 0.00000 | 0.00000 | 0.00000 | 0.00000 |
| 2px      | 0.00002 | 0.00000 | 0.00000 | -0.00001 | -0.00002 |
| 2py      | 0.00000 | 0.00000 | 0.00000 | 0.00000 | 0.00000 |
| 2pz      | 0.27101 | 0.20708 | -0.03726 | -0.18088 | -0.24801 |
| 3s       | 0.00000 | 0.00000 | 0.00000 | 0.00000 | 0.00000 |
| 3px      | 0.00000 | 0.00000 | 0.00000 | -0.00002 | -0.00003 |
| 3py      | 0.00000 | 0.00000 | 0.00000 | 0.00000 | 0.00000 |
| 3pz      | 0.34561 | 0.26315 | -0.02281 | -0.23184 | -0.32030 |
| Ci       | 0.19289 | 0.11213 | 0.00191 | 0.08647 | 0.16410 |
| Ci^2     | 0.03721 | 0.01257 | 0.00000 | 0.00748 | 0.02693 |
| ρi-HOMO  | 44.1948 | 14.93425 | 0.004327 | 8.880632 | 31.98617 |

Table S3. LUMO Coefficient orbitals for isoprene (5).

| ISOPRENE | LUMO     |
|----------|----------|
| ORBITALES| C-1 | C-4 | C-5 | C-9 | C-11 |
| 1s       | 0.00000 | 0.00000 | 0.00000 | 0.00000 | 0.00000 |
| 2s       | 0.00000 | 0.00000 | 0.00000 | 0.00000 | 0.00000 |
| 2px      | 0.00002 | -0.00002 | 0.00000 | -0.00002 | 0.00000 |
| 2py      | 0.00000 | 0.00000 | 0.00000 | 0.00000 | 0.00000 |
| 2pz      | 0.25246 | -0.19233 | -0.00418 | -0.19749 | 0.24780 |
| 3s       | 0.00000 | 0.00000 | 0.00000 | 0.00000 | 0.00000 |
| 3px      | 0.00000 | 0.00000 | 0.00000 | 0.00000 | 0.00000 |
| 3py      | -0.00001 | 0.00000 | 0.00000 | 0.00000 | 0.00000 |
| 3pz      | 0.53066 | -0.37969 | -0.02716 | -0.39816 | 0.53371 |
| Ci       | 0.34534 | 0.18116 | 0.00076 | 0.19753 | 0.34625 |
| Ci^2     | 0.11926 | 0.03282 | 0.00000 | 0.03902 | 0.11989 |
| ρi-LUMO  | 38.3488 | 10.5528 | 0.0002 | 12.5473 | 38.5523 |
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9. Spectroscopic information of compounds 4a-m and 6a-l

Trans-5-(4-hydroxy-3-methoxyphenyl)-6-methyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H-)one (4a). Were obtained 405 mg (1.1 mmol, 81 %), white solid; mp: 238-241 °C; FTIR (KBr disk): 3271, 1682, 1126 cm⁻¹; ¹H NMR (400 MHz, DMSO-d₆) δ (ppm) 1.17 (3H, d, J = 6.5 Hz, CH₃), 1.91 (1H, td, J = 11.0, 6.5 Hz, 6-H), 3.65 (3H, s, OCH₃), 3.86 (1H, d, J = 11.1 Hz, 5-H), 4.79 (1H, d, J = 10.6 Hz, 6a-H), 6.62 (1H, d, J = 8.1 Hz, 6-H_Gu), 6.65 (1H, br. s, 2-H_Gu), 6.73 (2H, m, 4-H and 5-H_Gu), 6.98 (1H, t, J = 7.5 Hz, 2-H), 7.24 (1H, t, J = 7.6 Hz, 3-H), 7.60 (1H, t, J = 7.4 Hz, 8-H), 7.69 (1H, t, J = 7.1 Hz, 9-H), 7.76 (1H, d, J = 7.6 Hz, 7-H), 7.86 (1H, d, J = 7.5 Hz, 1-H), 8.36 (1H, d, J = 8.0 Hz, 10-H), 8.90 (1H, s, OH). ¹³C NMR (100 MHz, DMSO-d₆) δ (ppm) 15.8, 40.3, 51.4, 55.6, 63.3, 112.6, 115.3, 119.5, 122.2, 123.6, 123.7, 124.8, 126.3, 128.7, 129.9, 131.2, 131.9, 132.3, 134.3, 134.5, 143.5, 143.7, 147.8, 165.0. GC/MS (70 eV), tᵣ = 43.43 min., m/z 371 (M⁺⁺, 80), 342 (20), 246 (22), 232 (100), 220 (50), 151 (91). Anal. calcd for C₂₄H₂₁NO₃: C, 77.61; H, 5.70; N, 3.77. Found: C, 76.52; H, 5.83; N, 3.61.

Trans-3-fluoro-5-(4-hydroxy-3-methoxyphenyl)-6-methyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H-)one (4b). Were obtained 380 mg (0.98 mmol, 76 %), white solid; mp: 252-254 °C; FTIR (KBr disk): 3410, 1666, 1487, 1157 cm⁻¹; ¹H NMR (400 MHz, DMSO-d₆) δ (ppm) 1.16 (3H, d, J = 6.5 Hz, CH₃), 1.95 (1H, td, J = 10.8, 6.4 Hz, 6-H), 3.66 (3H, s, OCH₃), 3.88 (1H, d, J = 10.9 Hz, 5-H), 4.80 (1H, d, J = 10.6 Hz, 6a-H), 6.43 (1H, dd, J = 9.9, 2.4 Hz, 4-H), 6.63 (1H, dd, J = 8.0, 1.7 Hz, 6-H_Gu), 6.68 (1H, d, J = 1.7 Hz, 2-H_Gu), 6.75 (1H, d, J = 8.0 Hz, 5-H_Gu), 7.11 (1H, ddd, J = 20.5, 13.2, 5.9 Hz, 2-H), 7.61 (1H, t, J = 7.3 Hz, 9-H), 7.69 (1H, t, J = 6.9 Hz, 8-H), 7.77 (1H, d, J = 7.7 Hz, 7-H), 7.87 (1H, d, J = 7.4 Hz, 10-H), 8.39 (1H, dd, J = 9.1, 5.5 Hz, 1-H), 8.97 (1H, s, OH). ¹³C NMR (100 MHz, DMSO-d₆) δ (ppm) 15.7, 39.9, 51.5, 55.6, 63.2, 112.5, 113.41 (d, J_C,F = 22.2 Hz), 115.4, 115.8 (d, J_C,F = 22.9 Hz), 121.4, 122.2, 123.6, 124.8, 128.8, 132.0, 132.1 (d, J_C,F = 11.2 Hz), 133.5, 133.9 (d, J_C,F = 6.6 Hz), 143.4, 145.5, 148.0, 158.1 (d, J_C,F = 240.5 Hz), 164.8, 165.0. GC/MS (70 eV), tᵣ = 46.16 min., m/z 389 (M⁺⁺, 70), 250 (50), 151 (100). Anal. calcd for C₂₄H₂₀FNO₃: C, 74.02; H, 5.18; N, 3.60. Found: C, 74.19; H, 5.31; N, 3.51.

Trans-5-(4-hydroxy-3-methoxyphenyl)-6-methyl-3-nitro-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H-)one (4c). Were obtained 345 mg (0.89 mmol, 69 %), yellow solid; mp: 228-230 °C; FTIR (KBr disk): 3425, 3332, 1759, 1512 cm⁻¹; ¹H NMR (400 MHz, DMSO-d₆) δ (ppm) 1.19 (3H, d, J = 6.3 Hz, CH₃), 2.10 (1H, m, 6-H), 3.65 (3H, s, OMe), 3.97 (1H, d, J = 11.0 Hz, 5-H), 4.93 (1H, d, J = 10.4 Hz, 6a-H), 6.65-6.80 (3H, m, all H_Gu), 7.55 (1H, s, 4-H), 7.77 - 7.72 (1H, ‘t’, J = 7.26, 9-H), 7.80 (1H, d, J = 7.6 Hz, 7-H), 7.88 (1H, ‘t’, J = 7.6 Hz, 8-H), 7.93 (1H, d, J = 7.3 Hz, 10-H), 8.17 (1H, d, J = 9.0 Hz, 2-H), 8.67 (1H, d, J = 9.3 Hz, 1-H), 9.03 (1H, s, OH). ¹³C NMR (101 MHz, DMSO-d₆) δ (ppm) 15.6, 39.0, 40.3, 55.6, 69.0, 85.6, 102.7, 103.8, 113.6, 124.0, 124.1, 124.3, 125.0, 125.1, 126.0, 126.9, 130.9, 132.8, 134.8, 139.2, 145.2, 151.9, 168.8, 176.8. GC/MS (70 eV), tᵣ = 46.16 min., m/z 389 (M⁺⁺, 70), 250 (50), 151 (100). Anal. calcd for C₂₄H₂₀N₂O₅: C, 69.22; H, 4.84; N, 6.73. Found: C, 69.35; H, 4.98; N, 6.61.
Trans-1-ciano-5-(4-hydroxy-3-methoxyphenyl)-6-methyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (4d). Were obtained 360 mg (0.92 mmol, 72%), white solid; mp: 242-244 °C; FTIR (KBr disk): 3533, 2978, 2222, 1713 cm⁻¹; ¹H NMR (400 MHz, DMSO-d₆) δ (ppm) 1.11 (3H, d, J = 6.4 Hz, CH₃), 1.71 (1H, td, J = 10.5, 6.4 Hz, 6-H), 3.66 (3H, s, OMe), 3.87 (1H, d, J = 10.9 Hz, 5-H), 4.78 (1H, d, J = 10.3 Hz, 6a-H), 6.59 (2H, d, J = 7.9 Hz, 4-H and 6-HGu), 6.68 (1H, d, J = 1.5 Hz, 2-HGu), 6.72 (1H, d, J = 8.0 Hz, 4-HGu), 7.09 (1H, dt, J = 13.7, 6.8 Hz, 2-H), 7.14 (1H, dd, J = 15.8, 6.0 Hz, 3-H), 7.60 (1H, t, J = 7.3 Hz, 9-H), 7.69 (1H, t, J = 7.1 Hz, 8-H), 7.75 (1H, d, J = 7.6 Hz, 7-H), 7.86 (1H, d, J = 7.6 Hz, 10-H), 8.90 (1H, s, OH). ¹³C NMR (101 MHz, DMSO-d₆) δ (ppm) 15.9, 42.4, 50.9, 55.6, 62.9, 112.6, 114.2, 115.5, 122.0, 123.2, 123.9, 124.9, 125.1, 125.7, 128.8, 131.3, 131.9, 133.8, 135.4, 145.2, 145.5, 147.8, 153.3, 155.9, 163.9. GC/MS (70 eV), tᵣ = 46.16 min., m/z 389 (M⁺•, 70), 250 (50), 151 (100). Anal. calcd for C₂₅H₂₀N₂O₃: C, 75.74; H, 5.08; N, 7.07. Found: C, 75.51; H, 5.19; N, 7.14.

Trans-5-(4-hydroxy-3-methoxyphenyl)-6-methyl-1-nitro-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (4e). Were obtained 330 mg (0.84 mmol, 66%), yellow solid; mp: 250-254 ºC; FTIR (KBr disk): 3425, 3332, 1759, 1512 cm⁻¹; ¹H NMR (400 MHz, DMSO-d₆) δ (ppm) 1.14 (3H, d, J = 7.5 Hz, CH₃), 1.87 (1H, m, 6-H), 3.64 (3H, s, OMe), 4.02 (1H, d, J = 10.9 Hz, 5-H), 5.05 (1H, d, J = 10.1 Hz, 6a-H), 6.79 - 6.62 (3H, m, all HGu protons), 7.06 (1H, d, 4-H), 7.25 (1H, 't', 3-H), 7.84 - 7.59 (4H, m, all isondolo aromatic protons), 7.85 (1H, d, J = 7.8 Hz, 2-H), 8.99 (1H, s, OH). ¹³C NMR (101 MHz, DMSO-d₆) δ (ppm) 15.7, 40.7, 51.1, 55.6, 63.0, 64.1, 104.5, 112.4, 115.4, 123.1, 124.2, 124.6, 124.9, 129.1, 130.8, 132.5, 133.3, 134.2, 135.3, 143.0, 144.9, 145.6, 164.8, 203.6. GC/MS (70 eV), tᵣ = 46.16 min., m/z 389 (M⁺•, 70), 250 (50), 151 (100). Anal. calcd for C₂₄H₂₀N₂O₅: C, 69.22; H, 4.84; N, 6.73. Found: C, 69.05; H, 4.94; N, 6.58.

Trans-1-fluoro-5-(4-hydroxy-3-methoxyphenyl)-6-methyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (4f). Were obtained 350 mg (0.89 mmol, 70%), white solid; mp: 245-246 ºC; FTIR (KBr disk): 3410, 1660, 1520, 1157 cm⁻¹; ¹H NMR (400 MHz, DMSO-d₆) δ (ppm) 1.11 (3H, d, J = 6.4 Hz, CH₃), 1.71 (1H, td, J = 10.5, 6.4 Hz, 6-H), 3.66 (3H, s, OMe), 3.87 (1H, d, J = 10.9 Hz, 5-H), 4.78 (1H, d, J = 10.3 Hz, 6a-H), 6.59 (2H, d, J = 7.9 Hz, 4-H and 6-HGu), 6.68 (1H, d, J = 1.5 Hz, 2-HGu), 6.72 (1H, d, J = 8.0 Hz, 4-HGu), 7.09 (1H, dt, J = 13.7, 6.8 Hz, 2-H), 7.14 (1H, dd, J = 15.8, 6.0 Hz, 3-H), 7.60 (1H, t, J = 7.3 Hz, 9-H), 7.69 (1H, t, J = 7.1 Hz, 8-H), 7.75 (1H, d, J = 7.6 Hz, 7-H), 7.86 (1H, d, J = 7.6 Hz, 10-H), 8.90 (1H, s, OH). ¹³C NMR (101 MHz, DMSO-d₆) δ (ppm) 15.9, 42.4, 50.9, 55.6, 62.9, 112.6, 114.2, 115.5, 122.0, 123.2, 123.9, 124.9 (d, JₐC,F = 10.8 Hz), 125.1, 125.7, 128.8, 131.3, 131.9, 133.8, 135.8, 145.5 (d, JₐC,F = 11.2 Hz), 147.8, 153.3 (d, JₐC,F = 23.0 Hz), 155.9, 163.9 (d, JₐC,F = 245.1 Hz). GC/MS (70 eV), tᵣ = 37.71 min., m/z 389 (M⁺•, 70), 250 (50), 151 (100). Anal. calcd for C₂₄H₂₀FNO₃: C, 74.02; H, 4.94; F, 4.88; N, 6.73. Found: C, 74.21; H, 5.29; N, 3.73.

Trans-5-(4-hydroxy-3-methoxyphenyl)-6-methyl-6,6a-dihydroisoindolo[1,3]dioxolo[4,5-gjisoindolo[2,1-a]quinolin-11(5H)-one (4g). Were obtained 400 mg (0.96 mmol, 80%), white solid;
**Trans-5-(4-methoxyphenyl)-6-methyl-6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (4h)**

Were obtained 395 mg (1.11 mmol, 79 %), white solid; mp: 165-167 °C; FTIR (KBr disk): 3220, 1660, 1100 cm⁻¹; ¹H NMR (400 MHz, DMSO-d₆) δ (ppm) 1.16 (3H, d, J = 6.4 Hz, CH₃), 1.87 - 1.74 (1H, m, 6-H), 3.73 (3H, s, OCH₃), 3.94 (1H, d, J = 10.9 Hz, 5-H), 4.81 (1H, d, J = 10.6 Hz, 6a-H), 6.67 (1H, d, J = 7.9 Hz, 4-H). 6.88 (2H, d, J = 8.2 Hz, 2-H_An and 3-H_An). 6.97 (1H, t, J = 7.5 Hz, 3-H), 7.08 (2H, d, J = 8.3 Hz, 2-H_An and 3-H_An), 7.24 (1H, t, J = 7.7 Hz, 2-H), 7.59 (1H, dd, J = 14.4, 7.0 Hz, 9-H), 7.68 (1H, t, J = 7.5 Hz, 8-H), 7.76 (1H, d, J = 7.7 Hz, 7-H), 7.85 (1H, t, J = 8.2 Hz, 10-H), 8.37 (1H, d, J = 8.2 Hz, 1-H). ¹³C NMR (101 MHz, DMSO-d₆) δ (ppm) 12.5, 12.5, 15.6, 40.8, 50.9, 54.9, 55.0, 63.1, 114.0, 119.6, 123.6, 123.7, 124.8, 126.3, 129.9, 130.4, 131.1, 131.9, 132.2, 135.6, 143.4, 157.9, 164.9. GC/MS (70 eV), tᵣ = 62.64 min., m/z 355 (M⁺, 100), 340 (10), 326 (10), 232 (60), 135 (80). Anal. calcd for C₂₅H₂₁NO₅: C, 81.10; H, 5.96; N, 3.94. Found: C, 81.23; H, 5.85; N, 3.76.

**Trans-3,6-dimethyl-5-(4-methoxyphenyl)-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (4i)**

Were obtained 390 mg (0.97 mmol, 78 %), white solid; mp: 198-200 °C; FTIR (KBr disk): 3189, 1680, 1150 cm⁻¹; ¹H NMR (400 MHz, DMSO-d₆) δ (ppm) 1.14 (3H, d, J = 6.5 Hz, 6-CH₃), 1.78 (1H, tq, J = 12.9, 6.4 Hz, 6-H), 2.11 (3H, s, 3-CH₃), 3.74 (3H, s, OCH₃), 3.89 (1H, d, J = 11.1 Hz, 5-H), 4.75 (1H, d, J = 10.6 Hz, 6a-H), 6.48 (1H, s, 4-H), 6.88 (2H, d, J = 8.7 Hz, 2-H_An and 3-H_An), 7.07 (3H, m, 2-H, 2-H_An and 3-H_An), 7.59 (1H, t, J = 7.4 Hz, 9-H), 7.67 (1H, td, J = 7.5, 1.2 Hz, 8-H), 7.74 (1H, d, J = 7.5 Hz, 7-H), 7.85 (1H, d, J = 7.4 Hz, 10-H), 8.24 (1H, d, J = 8.3 Hz, 1-H). ¹³C NMR (101 MHz, DMSO-d₆) δ (ppm) 10.3, 15.6, 20.7, 41.1, 50.8, 54.9, 63.1, 114.0, 116.2, 119.5, 123.5, 124.7, 127.1, 128.7, 130.1, 130.4, 130.9, 131.8, 132.3, 132.6, 133.2, 143.3, 157.9, 164.7. GC/MS (70 eV), tᵣ = 94.04 min., m/z 401 (M⁺⁺, 100), 262 (10), 151 (5). Anal. calcd for C₂₅H₂₃NO₂: C, 81.27; H, 6.27; N, 3.79. Found: C, 81.12; H, 6.44; N, 3.61.

**Trans-3-ethyl-5-(4-methoxyphenyl)-6-dimethyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (4j)**

Were obtained 355 mg (0.93 mmol, 71 %), beige solid; mp: 213-214 °C; FTIR (KBr disk): 1682, 1130 cm⁻¹; ¹H NMR (400 MHz, DMSO-d₆) δ (ppm) 1.01 (3H, t, J = 7.6 Hz, CH₃), 1.15 (3H, d, J = 6.5 Hz, CH₃), 1.79 (1H, td, J = 11.0, 6.5 Hz, 6-H), 2.40 (2H, dt, J = 11.9, 7.3 Hz, CH₂), 3.74 (3H, s, OCH₃), 3.91 (1H, d, J = 10.7 Hz, 5-H), 4.78 (1H, d, J = 10.5 Hz, 6a-H), 6.50
(1H, s, 4-H), 6.89 (2H, d, J = 8.7 Hz, 2-H<sub>A</sub> and 3-H<sub>A</sub>), 7.13 – 7.05 (3H, m, 2-H, 2-H<sub>A</sub> and 3-H<sub>A</sub>), 7.60 (1H, t, J = 7.3 Hz, 9-H), 7.68 (1H, t, J = 7.0 Hz, 8-H), 7.76 (1H, d, J = 7.6 Hz, 7-H), 7.85 (1H, d, J = 7.4 Hz, 10-H), 8.27 (1H, d, J = 8.4 Hz, 1-H).<sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>) δ (ppm) 15.6, 15.8, 27.7, 39.0, 40.1, 41.1, 50.9, 55.0, 63.1, 114.0, 119.6, 123.5, 124.7, 125.8, 128.7, 129.0, 130.4, 131.0, 131.8, 132.3, 133.5, 135.6, 139.0, 143.4, 157.9, 164.7. GC/MS (70 eV), t<sub>r</sub> = 73.47 min., m/z 383 (M<sup>+</sup>*, 100), 368 (30), 260 (35). Anal. calcd for C<sub>26</sub>H<sub>25</sub>NO<sub>2</sub>: C, 81.43; H, 6.57; N, 3.65. Found: C, 81.27; H, 6.76; N, 3.51.

**Trans-3-nitro-5-(4-methoxyphenyl)-6-dimethyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one**<sup>4k</sup>. Were obtained 340 mg (0.88 mmol, 68 %), yellow solid; mp: 190-192 °C; FTIR (KBr disk): 1682, 1150 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ (ppm) 1.17 (3H, d, J = 6.4 Hz, CH<sub>3</sub>), 2.05 – 1.96 (1H, m, 6-H), 3.74 (3H, d, J = 14.5 Hz, OCH<sub>3</sub>), 4.06 (1H, d, J = 10.9 Hz, 5-H), 4.94 (1H, d, J = 10.5 Hz, 6a-H), 6.94 (2H, d, J = 8.7 Hz, 2-H<sub>A</sub> and 3-H<sub>A</sub>), 7.18 (2H, d, J = 8.7 Hz, 2-H<sub>A</sub> and 3-H<sub>A</sub>), 7.50 (1H, m, 4-H), 7.64 (1H, t, J = 7.3 Hz, 9-H), 7.74 (1H, t, J = 7.3 Hz, 8-H), 7.82 – 7.78 (1H, m, 7-H), 7.93 (1H, d, J = 7.1 Hz, 10-H), 8.17 (1H, d, J = 8.0 Hz, 2-H), 8.67 (1H, d, J = 9.2 Hz, 1-H).<sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>) δ (ppm) 15.5, 50.7, 55.0, 63.2, 85.5, 113.6, 114.3, 118.5, 122.3, 123.7, 124.9, 126.9, 126.9, 129.0, 130.5, 132.4, 134.2, 139.2, 142.4, 143.3, 145.1, 151.8, 158.3, 165.8. GC/MS (70 eV), t<sub>r</sub> = 83.66 min., m/z 385 (M<sup>+</sup>*, 100), 370 (10), 262 (15). Anal. calcd for C<sub>26</sub>H<sub>20</sub>N<sub>2</sub>O<sub>4</sub>: C, 71.99; H, 5.03; N, 7.00. Found: C, 71.83; H, 5.15; N, 7.17.

**Trans-5-(4-methoxyphenyl)-6-methyl-6,6a-dihydro-[1,3]dioxolo[4,5-g]isoindolo[2,1-a]quinolin-11(5H)-one**<sup>4l</sup>. Were obtained 455 mg (1.1 mmol, 91 %), white solid; mp 250-252 °C. IR (KBr): 3300, 1146 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ (ppm) 1.15 (3H, d, J = 6.4 Hz, CH<sub>3</sub>), 1.75 (1H, dd, J = 16.9, 10.6 Hz, 6-H), 3.73 (3H, s, OCH<sub>3</sub>), 3.84 (1H, d, J = 10.8 Hz, 5-H), 4.73 (1H, d, J = 10.7 Hz, 6a-H), 5.95 (2H, d, J = 3.2 Hz, CH<sub>2</sub>), 6.09 (1H, s, 4-H), 6.89 (2H, d, J = 8.4 Hz, 2-H<sub>A</sub> and 3-H<sub>A</sub>), 7.08 (2H, d, J = 8.4 Hz, 2-H<sub>A</sub> and 3-H<sub>A</sub>), 7.59 (1H, t, J = 7.2 Hz, 9-H), 7.67 (1H, t, J = 7.3 Hz, 8-H), 7.74 (1H, d, J = 7.6 Hz, 7-H), 7.84 (1H, d, J = 7.4 Hz, 10-H), 7.92 (1H, s, 1-H).<sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>) δ (ppm) 15.6, 39.2, 40.1, 41.2, 50.9, 55.0, 63.2, 100.6, 101.2, 109.0, 114.0, 123.5, 124.3, 124.7, 128.7, 129.5, 130.2, 131.8, 132.2, 135.7, 143.1, 143.5, 145.4, 158.0, 164.6. GC/MS (70 eV), t<sub>r</sub> = 83.66 min., m/z 415 (50, M<sup>+</sup>), 276 (30), 149 (100). Anal. Calcd. for C<sub>32</sub>H<sub>23</sub>N<sub>2</sub>O<sub>6</sub>: C, 75.17; H, 5.30; N, 3.51. Found: C, 75.37; H, 5.34; N, 3.23.

**Trans-7-(4-methoxyphenyl)-8-methyl-8,8a-dihydrobenzo[hh]isoindolo[2,1-a]quinolin-13(7H)-one**<sup>4m</sup>. Were obtained 365 mg (0.90 mmol, 73 %), white solid; mp > 300 °C; FTIR (KBr disk): 1682, 1212 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ (ppm) 1.22 (3H, d, J = 8.9 Hz, CH<sub>3</sub>), 1.69 – 1.59 (1H, m, 8-H), 3.71 (3H, d, J = 8.9 Hz, OCH<sub>3</sub>), 4.06 (1H, d, J = 9.9 Hz, 7-H), 4.88 (1H, d, J = 10.1 Hz, 8a-H), 6.89 (2H, d, J = 8.5 Hz, 2-H<sub>A</sub> and 3-H<sub>A</sub>), 6.91 (1H, d, J = 8.8 Hz, 6-H), 7.10 (2H, d, J = 8.5 Hz, 2-H<sub>A</sub> and 3-H<sub>A</sub>), 7.49 (2H, m, 4-H and 5-H), 7.65 – 7.61 (1H, m, 9-H), 7.68 (2H, d, J = 9.0 Hz, 3-H and 6-H), 7.76 – 7.70 (1H, m, 11-H), 7.79 (1H, d, J = 7.6 Hz, 2-H), 7.87 - 7.82 (1H, m, 10-H), 7.91 (1H, d, J = 7.2 Hz, 12-H), 7.95 (1H, s, 1-H).<sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>)
δ (ppm) 13.7, 15.9, 38.9, 40.3, 45.3, 50.8, 54.9, 55.0, 63.9, 107.3, 113.9, 114.1, 122.6, 124.4, 125.8, 126.1, 126.5, 127.1, 127.6, 127.9, 128.7, 129.5, 130.1, 130.8, 132.6, 138.6, 145.8, 148.4. GC/MS (70 eV), tR = 111.67 min., m/z 405 (M+, 100), 376 (10), 270 (70). Anal. calcd for C28H23NO2: C, 82.94; H, 5.72; N, 3.45. Found: C, 82.85; H, 5.93; N, 3.29.

Trans-5-methyl-5-vinyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6a). Were obtained 400 mg (1.45 mmol, 80 %), white solid; mp: 182-183 °C; IR (KBr): 2947, 1682 cm⁻¹; ¹H NMR (400 MHz, DMSO-d₆) δ (ppm) 1.43 (3H, d, J = 1.0 Hz, CH₃), 2.24 (1H, dd, J = 12.4, 7.1 Hz, CH₂), 2.36 (1H, dd, J = 12.4, 7.0 Hz, CH₂), 4.86 – 4.66 (1H, m, CH), 4.97 (1H, dd, J = 10.0, 2.5 Hz, =CH₂), 5.03 (1H, d, J = 2.6 Hz, =CH₂), 5.97 (1H, ddd, J = 16.7, 9.9, 0.9 Hz, =CH), 7.07 (1H, td, J = 7.2, 1.7 Hz, 3-H), 7.21 – 7.12 (3H, m, 1-H and 2-H), 7.34 (1H, td, J = 7.4, 1.6 Hz, 8-H), 7.38 (1H, dd, J = 7.4, 1.8 Hz, 9-H), 7.44 – 7.39 (1H, m, 7-H), 7.65 (1H, m, 7-H), 7.67 (1H, m, 7-H). 13C NMR (400 MHz, DMSO-d₆) δ (ppm) 24.4, 40.6, 42.9, 54.1 112.1, 122.2, 124.0, 124.3, 125.0, 125.7, 125.8, 129.2, 130.2, 132.2, 133.9, 137.7, 142.8, 147.4, 164.9; GC/MS (70 eV), tR = 24.117 min., m/z (%) 275 (M+, 70), 260 (100), 232 (10); Anal. Calc. for C₁₉H₁₇NO: C, 82.88; H, 6.22; N, 5.09. Found: C, 82.80; H, 6.12; N, 5.19.

Trans-3,5-dimethyl-5-vinyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6b). Were obtained 410 mg (1.41 mmol, 82 %), white solid; mp: 193-195 °C; IR (KBr): 2940, 1660 cm⁻¹; ¹H NMR (400 MHz, DMSO-d₆) δ (ppm) 1.63-1.50 (4H, m, CH₃ and CH₂), 2.26 (3H, s, 3-CH₃), 2.38 (1H, d, J = 12.3 Hz, CH₂), 5.08 (1H, d, J = 12.2 Hz, 6a-H), 5.16 (1H, d, J = 10.9 Hz, =CH₂), 5.30 (1H, d, J = 17.3 Hz, =CH₂), 5.93 (1H, ddd, J = 17.0, 10.5 Hz, =CH), 7.03 (1H, s, 4-H), 7.09 (1H, d, J = 8.1 Hz, 2-H), 7.57 (1H, d, J = 7.3 Hz, 9-H), 7.69 (1H, d, J = 7.4 Hz, 8-H), 7.75 (1H, d, J = 7.4 Hz, 7-H), 7.80 (1H, d, J = 7.8 Hz, 10-H), 8.27 (1H, d, J = 8.0 Hz, 1-H). ¹³C NMR (100 MHz, DMSO-d₆) δ (ppm) 20.7, 22.1, 27.2, 40.0, 40.5, 54.9,112.5, 119.7, 122.4, 124.0, 124.3, 125.0, 125.7, 125.8, 129.2, 130.2, 132.2, 133.9, 137.7, 142.8, 147.4, 164.9; GC/MS (70 eV), tR = 25.042 min., m/z (%) 289 (M+, 80), 274 (100), 246 (5); Anal. Calc. for C₂₀H₁₉NO: C, 83.01; H, 6.62; N, 4.84. Found: C, 82.95; H, 6.59; N, 4.75.

Trans-3-ethyl-5-methyl-5-vinyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6c). Were obtained 375 mg (1.23 mmol, 75 %) white solid; mp: 187-188 °C; IR (KBr): 2809, 1666 cm⁻¹; ¹H NMR (400 MHz, DMSO-d₆) δ (ppm) 1.56 (4H, br. s, CH₂ and CH₂), 1.78 (1H, s, CH₂), 2.27 (3H, s, CH₃), 2.43 – 2.28 (2H, m, CH₂), 5.1 (1H, d, J = 10.1, =CH₂), 5.17 (1H, d, J = 10.2 Hz, =CH₂), 5.31 (1H, d, J = 17.4 Hz, 6a-H), 5.96 (1H, br. d, J = 17.1 Hz, =CH), 7.04 (1H, s, 4-H), 7.10 (1H, d, J = 8.2 Hz, 2-H), 7.59 (1H, br. s, 9-H), 7.69 (1H, br. s, 8-H), 7.75 (1H, s, 7-H), 7.82 (1H, s, 1-H), 8.29 (1H, d, J = 8.2 Hz, 10-H); ¹³C NMR (100 MHz, DMSO-d₆) δ (ppm) 20.7, 27.2, 29.4, 40.0, 40.5, 54.9, 68.2, 112.5, 119.7, 122.8, 123.4, 127.4, 128.6, 128.9, 131.9, 132.3, 132.5, 134.5, 145.0, 146.7, 165.1; GC/MS (70 eV), tR = 25.042 min., m/z (%) 303 (M+, 70), 274 (100), 246 (5); Anal. Calc. for C₂₁H₂₁NO: C, 83.13; H, 6.98; N, 4.62. Found: C, 83.08; H, 7.06; N, 4.55.
Trans-5-methyl-3-methoxy-5-vinyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6d). Were obtained 425 mg (1.39 mmol, 85 %), white solid; mp: 178-179 °C; IR (KBr): 2947, 1680 cm⁻¹; ¹H NMR (400 MHz, DMSO-d₆) δ (ppm) 1.56 (4H, m, 5-CH₃ and CH₂), 2.44 – 2.29 (1H, m, CH₂), 3.72 (3H, s, CH₃O), 5.05 (1H, d, J = 12.5, 2.6 Hz, 6a-H), 5.17 (1H, J = 10.1, =CH₂) 5.31 (1H, d, J = 17.4, =CH₂), 5.96 (1H, dd, J = 17.4, 10.6 Hz, =CH), 6.76 (1H, d, J = 3.0, 4-H), 6.90 (1H, dd, J = 9.0, 3.0 Hz, 2-H), 7.55 (1H, ‘t’, J = 7.4 Hz, 9-H), 7.67 (1H, ‘t’, J = 7.4 Hz, 8-H), 7.74 (1H, br. d, J = 7.6 Hz, 7-H), 7.79 (1H, br. d, J = 7.5 Hz, 10-H), 8.33 (1H, d, J = 9.0 Hz, 1-H); ¹³C NMR (100 MHz, DMSO-d₆) δ (ppm) 27.6, 40.7, 40.9, 55.3, 55.6, 112.6, 113.1, 114.2, 121.4, 123.2, 123.7, 128.8, 129.0, 132.4, 132.6, 134.9, 145.3, 147.0, 155.9, 165.2; GC/MS (70 eV), tᵣ = 26.638 min., m/z (%) 305 (M⁺, 90), 290 (100), 262 (10); Anal. Calc. for C₂₀H₁₉NO₂: C, 78.66; H, 6.27; N, 4.59. Found: C, 78.59; H, 6.19; N, 4.67.

Trans-3-fluor-5-methyl-5-vinyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6e). Were obtained 390 mg (1.33 mmol, 78 %), white solid; mp: 163-165 °C; IR (KBr): 2979, 1660 cm⁻¹; ¹H NMR (400 MHz, DMSO-d₆) δ (ppm) 1.72 - 1.50 (4H, m, 5-CH₃ and CH₂), 2.41 (1H, d, J = 12.4 Hz, CH₂), 5.10 (1H, d, J = 12.5 Hz, 6a-H), 5.19 (1H, d, J = 10.1 Hz, =CH₂), 5.33 (1H, d, J = 17.1 Hz, =CH₂), 6.01 - 5.98 (1H, m, =CH), 7.04 (1H, d, J = 8.3 Hz, 4-H), 7.16 (1H, m, 2-H), 7.71 (1H, br. s, 9-H), 7.77 (1H, s, 8-H), 7.82 (2H, br. s, 7-H and 10-H), 8.41 (1H, br. s, 1-H); ¹³C NMR (100 MHz, DMSO-d₆) δ (ppm) 27.1, 39.9, 40.4, 54.9, 113.2, 113.7, 113.9, 114.8, 121.6, 122.8, 123.5, 128.7, 131.4, 131.6, 132.5, 135.6, 144.8, 146.0, 165.2; GC/MS (70 eV), tᵣ = 24.055 min., m/z (%) 293 (M⁺, 80), 278 (100), 250 (5); Anal. Calc. for C₁₉H₁₆FNO: C, 77.80; H, 5.50; F, 6.48, N, 4.77. Found: C, 77.86; H, 5.42; N, 4.66.

Trans-3-chloro-5-methyl-5-vinyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6f). Were obtained 400 mg (1.29 mmol, 80 %), white solid; mp: 225-226 °C; IR (KBr): 2948, 1682 cm⁻¹; ¹H NMR (400 MHz, DMSO-d₆) δ (ppm) 1.44 (3H, d, J = 1.1 Hz, CH₃), 2.26 (1H, dd, J = 12.4, 7.1 Hz, CH₂), 2.37 (1H, dd, J = 12.5, 7.0 Hz, CH₂), 4.77 – 4.53 (1H, m, 6a-H), 4.96 (1H, dd, J = 10.0, 2.5 Hz, =CH₂), 5.03 (1H, d, J = 2.6 Hz, =CH₂), 5.99 (1H, ddq, J = 16.8, 10.1, 1.1 Hz, =CH), 7.16 (1H, d, J = 1.1 Hz, 4-H), 7.20 (2H, d, J = 1.1 Hz, 1-H and 2-H), 7.39 – 7.33 (2H, m, 8-H and 9-H), 7.41 (1H, ddd, J = 6.9, 2.1, 0.7 Hz, 7-H), 7.65 (1H, dd, J = 7.1, 1.8 Hz, 10-H); ¹³C NMR (100 MHz, DMSO-d₆) δ (ppm) 24.1, 39.6, 40.1, 42.5, 53.6, 111.5, 124.8, 125.1, 125.3, 125.9, 129.7, 129.8, 131.3, 131.6, 136.1, 142.0, 146.8, 163.7; GC/MS (70 eV), tᵣ = 25.855 min., m/z (%) 309 (M⁺, 80), 294 (100), 259 (20); Anal. Calc. for C₁₉H₁₆ClNO: C, 76.66; H, 5.50; Cl, 11.44; N, 4.52. Found: C, 76.71; H, 5.29; N, 4.59.

Trans-1-fluor-5-methyl-5-vinyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6g). Were obtained 320 mg (1.1 mmol, 64 %); white solid; mp: 150-152 °C; ¹H NMR (400 MHz, DMSO-d₆) δ (ppm) 1.33 (3H, d, J = 1.1 Hz, CH₃), 2.34 (1H, dd, J = 12.5, 7.0 Hz, CH₂), 2.43 (1H, dd, J = 12.5, 7.0 Hz, CH₂), 4.91 (1H, t, J = 6.9 Hz, 6a-H), 4.96 (1H, dd, J = 10.0, 2.5 Hz, =CH₂), 5.03 (1H, dd, J = 16.9, 2.4 Hz, =CH₂), 6.05 – 5.93 (1H, m, =CH), 6.94 (1H, td, J = 7.8, 1.5 Hz, 2-H),
7.02 (1H, dd, J = 7.5, 1.6 Hz, 4-H), 7.15 (1H, td, J = 7.5, 5.0 Hz, 3H), 7.40 – 7.31 (2H, m, 8-H and 9-H), 7.45 – 7.40 (1H, m, 7-H), 7.70–7.60 (1H, m, 10-H); $^{13}$C NMR (100 MHz, DMSO-d$_6$) δ (ppm) 25.1, 40.0, 41.0, 42.4, 58.7, 112.0, 116.0, 122.1, 125.0, 125.7, 126.5, 130.2, 132.0, 134.8, 141.9, 146.1, 156.3, 158.3, 164.4; GC/MS (70 eV), t$_R$ = 10.9 min., m/z (%) 293 (M$^{+}$, 100), 278 (80), 250 (30); Anal. Calc. for C$_{19}$H$_{16}$FNO: C, 77.80; H, 5.50; F, 6.48, N, 4.77. Found: C, 77.85; H, 5.45; N, 4.85.

**Trans-1-ciano-5-methyl-5-vinyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6h).** Were obtained 340 mg (1.13 mmol, 68 %), white solid; mp: 198-199 °C; IR (KBr): 2950, 1660 cm$^{-1}$; $^1$H NMR (400 MHz, DMSO-d$_6$) δ (ppm) 1.34 (3H, d, J = 1.1 Hz, CH$_3$), 2.34 (1H, dd, J = 12.5, 7.0 Hz, CH$_3$), 2.43 (1H, dd, J = 12.5, 7.0 Hz, CH$_2$), 4.94 – 4.90 (1H, m, CH), 4.97 (1H, dd, J = 10.0, 2.5 Hz, =CH$_2$), 5.04 (1H, dd, J = 16.9, 2.4 Hz, =CH$_2$), 5.99 (1H, ddd, J = 16.7, 9.9, 0.9 Hz, CH), 7.35 – 7.27 (2H, m, 3-H and 4-H), 7.44 – 7.35 (3H, m, 7-H, 8-H and 9-H), 7.48 (1H, dd, J = 7.0, 2.0 Hz, 2-H), 7.68 – 7.62 (1H, m, 10-H); $^{13}$C NMR (100 MHz, DMSO-d$_6$) δ (ppm) 25.0, 40.0, 42.1, 42.4, 57.7, 109.6, 112.2, 115.8, 125.2, 125.7, 125.9, 129.1, 130.2, 131.5, 134.0, 135.9, 138.6, 141.6, 145.2, 164.4; GC/MS (70 eV), t$_R$ = 25.1 min., m/z (%) 300 (M$^{+}$, 100), 285 (80), 254 (30); Anal. Calc. for C$_{20}$H$_{16}$NO: C, 79.98; H, 5.37; N, 9.33. Found: C, 80.01; H, 5.42; N, 9.29.

**Trans-1,4-dimethoxy-5-methyl-5-vinyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6i).** Were obtained 450 mg (1.34 mmol, 90 %), white solid; mp: 180-181 °C; IR (KBr): 2948, 1660 cm$^{-1}$; $^1$H NMR (400 MHz, DMSO-d$_6$) δ (ppm) 1.27 (1H, t', J = 12.6 Hz, CH$_2$), 1.56 (3H, s, CH$_3$), 2.28 (1H, dd, J = 13.2, 2.6 Hz, CH$_3$), 3.69 (3H, s, OCH$_3$), 3.77 (3H, s, OCH$_3$), 5.06 - 4.81 (3H, m, =CH$_2$ and 6a-H), 6.07 (1H, dd, J = 17.5, 10.6 Hz, =CH), 6.89 (1H, d, J = 9.1 Hz, 3-H), 7.01 (1H, d, J = 9.1 Hz, 2-H), 7.55 (1H, t, J = 7.0 Hz, 9-H), 7.65 (1H, m, 8-H), 7.70 (1H, d, J = 7.5 Hz, 7-H), 7.77 (1H, d, J = 7.5 Hz, 10-H); $^{13}$C NMR (100 MHz, DMSO-d$_6$) δ (ppm) 25.2, 41.1, 47.3, 55.0, 55.9, 56.1, 110.1, 110.2, 111.8, 122.9, 123.6, 124.9, 125.3, 128.4, 131.8, 131.9, 146.4, 147.1, 147.3, 151.6, 163.4; GC/MS (70 eV), t$_R$ = 26.678 min., m/z (%) 335 (M$^{+}$, 100), 320 (30), 306 (10), 361 (25); Anal. Calc. for C$_{21}$H$_{23}$NO$_3$: C, 75.20; H, 6.31; N, 4.18. Found: C, 75.29; H, 6.40; N, 4.08.

**Trans-5-hydroxy-5-vinyl-6,6a-dihydro-[1,3]dioxolo[4,5-g]isoindolo[2,1-a]quinolin-11(5H)-one (6j).** Were obtained 390 mg (1.34 mmol, 78 %), white solid; mp: 150-152 °C; IR (KBr): 3435, 2890, 1682 cm$^{-1}$; $^1$H NMR (400 MHz, DMSO-d$_6$) δ (ppm) 1.54 (4H, d, J = 8.5 Hz, CH$_3$ and CH$_2$), 2.41 – 2.23 (1H, m, CH$_2$), 5.02 (1H, d, J = 11.9 Hz, 6a-H), 5.15 (1H, d, J = 10.6 Hz, =CH$_2$), 5.29 (1H, d, J = 17.3 Hz, =CH$_2$), 5.91 (1H, dd, J = 17.3, 10.5 Hz, =CH$_2$), 6.65 (1H, d, J = 2.9 Hz, 4-H), 6.71 (1H, dd, J = 8.8, 2.8 Hz, 2-H), 7.54 (1H, d, J = 7.5 Hz, 9-H), 7.65 (1H, d, J = 7.4 Hz, 8-H), 7.71 (1H, d, J = 7.2 Hz, 7-H), 7.77 (1H, d, J = 7.3 Hz, 10-H), 8.20 (1H, d, J = 8.7 Hz, 1-H), 9.28 (1H, s, OH); $^{13}$C NMR (100 MHz, DMSO-d$_6$) δ (ppm) 18.0, 27.6, 31.1, 40.6, 41.2, 55.3, 112.8, 115.2, 121.5, 123.6, 127.4, 128.9, 132.4, 132.6, 134.8, 145.2, 147.2, 154.1, 165.1 GC/MS (70 eV), t$_R$ = 35.56 min., m/z (%) 291 (M$^{+}$, 100), 276 (55), 246 (90); Anal. Calc. For C$_{19}$H$_{17}$NO$_2$: C, 78.33; H, 5.88; N, 4.81. Found: C, 78.44; H, 5.97; N, 4.75.
Trans-1,3-dimethoxy-5-methyl-5-vinyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6k).

Were obtained 400 mg (1.19 mmol, 80 %), white solid; mp: 160-161 °C; IR (KBr): 2948, 1660 cm⁻¹; ¹H NMR (400 MHz, DMSO-d₆) δ (ppm) 1.35 (3H, d, J = 0.9 Hz, CH₃), 2.35 (1H, dd, J = 12.4, 7.1 Hz, CH₂), 2.43 (1H, dd, J = 12.4, 7.0 Hz, CH₂), 3.71 (3H, s, OCH₃), 3.78 (3H, s, OCH₃), 4.92 (1H, t, J = 6.9 Hz, 6a-H), 4.97 (1H, dd, J = 10.1, 2.4 Hz, =CH₂), 5.04 (1H, dd, J = 16.9, 2.4 Hz, =CH₂), 6.00 (1H, ddq, J = 16.8, 10.1, 1.0 Hz, =CH), 6.54 (1H, d, J = 1.4 Hz, 4-H), 6.84 (1H, d, J = 1.4 Hz, 2-H), 7.37 (2H, dd, J = 5.4, 3.6 Hz, 8H and 9H), 7.43 – 7.39 (1H, m, 7-H), 7.75 – 7.63 (1H, m, 10H); ¹³C NMR (100 MHz, DMSO-d₆) δ (ppm) 25.1, 39.4, 42.4, 42.7, 55.7, 57.3, 58.5, 100.1, 107.1, 111.9, 122.5, 125.6, 125.7, 130.2, 131.9, 135.8, 141.3, 145.0, 155.1, 157.0, 164.5; GC/MS (70 eV), tᵣ = 25.138 min., m/z (%) 335 (M⁺, 70), 320 (100), 288 (50), 256 (50); Anal. Calc. For C₂₁H₂₁NO₃: C, 75.20; H, 6.31; N, 4.18. Found: C, 75.27; H, 6.38; N, 4.27.

Trans-5-methyl-5-vinyl-6,6a-dihydro-[1,3]dioxolo[4,5-g]isoindolo[2,1-a]-quinolin-11(5H)-one (6l).

Were obtained 350 mg (1.10 mmol, 70 %), white solid; mp: 193-194 °C; IR (KBr): 2890, 1682 cm⁻¹; ¹H NMR (400 MHz, DMSO-d₆) δ (ppm) 1.55–1.47 (4H, m, CH₃ and CH₂), 2.40–2.34 (1H, dd, J = 13.4, 2.28 Hz, CH₂), 5.02 (1H d, J = 11.0 Hz, 6a-H), 5.13 (1H, d, J = 10.6 Hz, =CH₂), 5.26 (1H, d, J = 17.5 Hz, =CH₂), 5.88 (2H, dd, J = 17.3, 10.5 Hz, =CH), 6.02–5.96 (2H, m, CH₂'), 6.72 (1H, s, 4-H), 7.54 (1H, t, J = 7.2 Hz, 9-H), 7.67 (1H, t, J = 7.1 Hz, 8-H), 7.73 (1H, d, J = 7.3 Hz, 7-H), 7.77 (1H, d, J = 7.3 Hz, 10-H), 7.94 (1H, s, 1-H); ¹³C NMR (100 MHz, DMSO-d₆) δ (ppm) 27.7, 40.3, 40.5, 55.1, 100.8, 101.2, 107.9, 112.6, 122.7, 123.3, 126.2, 128.6, 128.9, 131.8, 132.3, 143.6, 144.7, 145.6, 146.7, 165.0; GC/MS (70 eV), tᵣ = 28.88 min., m/z (%) 319 (M⁺, 100), 304 (55), 274 (55), 246 (90); Anal. Calc. For C₂₀H₁₇NO₃: C, 75.22; H, 5.37; N, 4.39. Found: C, 75.30; H, 5.43; N, 4.46.
10. Spectral Characterization of Products 4a-m, 6a-l

*Trans-5-(4-hydroxy-3-methoxyphenyl)-6-methyl-6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (4a)*
Trans-3-fluoro-5-(4-hydroxy-3-methoxyphenyl)-6-methyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (4b)
Trans-5-(4-hydroxy-3-methoxyphenyl)-6-methyl-3-nitro-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (4c)
Trans-1-ciano-5-(4-hydroxy-3-methoxyphenyl)-6-methyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (4d)
Trans-5-(4-hydroxy-3-methoxyphenyl)-6-methyl-1-nitro-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (4e)
Trans-1-fluoro-5-(4-hydroxy-3-methoxyphenyl)-6-methyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (4f)
Trans-5-(4-hydroxy-3-methoxyphenyl)-6-methyl-6,6a-dihydro-[1,3]dioxolo[4,5-g]isoindolo[2,1-a]quino-lin-11(5H)-one (4g)
Trans-5-(4-methoxyphenyl)-6-methyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (4h)
Trans-3,6-dimethyl-5-(4-methoxyphenyl)-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (4i)

![Chemical structure](image)

**NMR Spectra**

- δ (ppm)
  - 7-H (d) 7.26
  - 10-H (d) 7.85
  - 1-H (d) 8.24
  - 9-H (d) 7.59
  - 2-H, 2-HAn and 3-HAn (t) 7.07
  - 4-H (s) 6.48
  - 8-H (d) 7.67
  - 2-HAn and 3-HAn (d) 6.88
  - 6-H (d) 3.89
  - 5-H (d) 3.99
  - 1-H (d) 8.44
  - 2-HAn and 3-HAn (t) 7.07
  - 6a (d) 4.75
  - OCH3 (s) 3.74

**13C NMR**

- δ (ppm)
  - 15.6
  - 20.7
  - 41.1
  - 50.8
  - 55.0
  - 63.1
  - 114.0
  - 119.5
  - 123.5
  - 124.7
  - 127.1
  - 128.7
  - 130.1
  - 130.4
  - 130.9
  - 131.8
  - 132.6
  - 135.6
  - 143.3
  - 157.9
  - 164.7

**Assignments**

- 2-HAn and 3-HAn (d) 6.88
- 6-H (d) 3.89
- OCH3 (s) 3.74
- 1-H (d) 8.44
- 2-HAn and 3-HAn (t) 7.07
- 6a (d) 4.75
- OCH3 (s) 3.74
- 6-H (d) 3.89
- 5-H (d) 3.99
- 1-H (d) 8.44
- 2-HAn and 3-HAn (t) 7.07
- 6a (d) 4.75
- OCH3 (s) 3.74
**Trans-3-ethyl-5-(4-methoxyphenyl)-6-dimethyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (4j)**

Chemical shifts in ppm:
- δ = 0.96
- δ = 1.01
- δ = 1.02
- δ = 1.02
- δ = 1.03
- δ = 1.07
- δ = 1.09
- δ = 1.10
- δ = 1.14
- δ = 1.31
- δ = 1.46
- δ = 1.79
- δ = 2.13
- δ = 2.44
- δ = 2.77
- δ = 3.00
- δ = 3.00
- δ = 3.74
- δ = 5.00
- δ = 7.60
- δ = 7.68
- δ = 7.75
- δ = 7.85
- δ = 7.86
- δ = 7.89
- δ = 8.27
- δ = 8.50
- δ = 8.75

NMR peaks with assignments:
- 1H (d) 8.27, 6.50
- 4-H (s) 7.68
- 5-H (d) 3.74
- 6a-H (d) 4.78
- 2-H, 2-HAn and 3-HAn (d) 6.89
- 7-H (d) 7.75
- 7-H (d) 5.00
- 8-H (d) 7.68
- 9-H (d) 7.66
- 6-H (s) 2.44
- 5-H (d) 3.74
- 3-HAn (d) 6.89
- 6-H (s) 1.79
- 5-H (d) 6.50
- 1-H (d) 8.27
- 4-H (s) 7.68
- 5-H (d) 3.74
- 6-H (s) 2.44
- 5-H (d) 6.50
- 1-H (d) 8.27

Chemical structures and peak integrations are shown in the diagram.
Trans-3-nitro-5-(4-methoxyphenyl)-6-dimethyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (4k)
Trans-5-(4-methoxyphenyl)-6-methyl-6a-dihydro-[1,3]dioxolo[4,5-g]isoindolo[2,1-a]quinolin-11(5H)-one (4l)
Trans-7-(4-methoxyphenyl)-8-methyl-8,8a-dihydrobenzo[h]isindolo[2,1-a]quinolin-13(7H)-one (4m)

\[
\begin{array}{c}
\text{OMe} \\
\end{array}
\]
GC-MS Trans-5-methyl-5-vinyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6a)
Trans-5-methyl-5-vinyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6a)
Trans-3,5-dimethyl-5-vinyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6b)
Trans-3-ethyl-5-methyl-5-vinyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6c)
Trans-5-methyl-3-methoxy-5-vinyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6d)
Trans-3-fluor-5-methyl-5-vinyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6e)
Trans-3-chloro-5-methyl-5-vinyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6f)
$^1$H NMR for trans-1-fluor-5-methyl-5-vinyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6g)
Trans-1-ciano-5-methyl-5-vinyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6h)
Trans-1,4-dimethoxy-5-methyl-5-vinyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6i)
Trans-5-hydroxy-5-vinyl-6,6a-dihydro-[1,3]dioxolo[4,5-g]isoindolo[2,1-a]-quinolin-11(5H)-one (6j)
Trans-1,3-dimethoxy-5-methyl-5-vinyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6k)
Trans-5-methyl-5-vinyl-6,6a-dihydro-[1,3]dioxolo[4,5-g]isoindolo[2,1-a]-quinolin-11(5H)-one (6l)