

Supporting Information

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

Diego R. Merchán-Arenas,^{a*} Felipe Sojo,^{b,c} Francisco Arvelo,^{b,c} Vladimir V. Kouznetsov^a

^a*Laboratorio de Química Orgánica y Biomolecular, Universidad Industrial de Santander, Parque Tecnológico Guatiguará, km 2 vía refugio, Piedecuesta, A.A. 681011, Colombia. Tel: +57 76 344000-Ext. 3593*

^b*Centro de Biociencias Fundación Instituto de Estudios Avanzados-IDEA, Caracas Venezuela.*

^c*Laboratorio de Cultivo de Tejidos y Biología de Tumores, Instituto de Biología Experimental, Universidad Central de Venezuela, código postal 1041, Caracas, Venezuela.*

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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. ^1H NMR spectra were recorded on Bruker AM-400 or AC-300 spectrometers. Chemical shifts are reported in ppm (δ) 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 $\text{K}\alpha$ radiation ($\lambda = 0.71073 \text{ \AA}$). 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(5*H*)-ones 4a-m

Aryl amines **1** (1 mmol), *o*-phthaldehydic acid (**2**) (1.1 mmol) and AMCell-SO₃H (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(5*H*)-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 N₂ atmosphere. After 5 min 0.026 g (0.18 mmol) of BF₃·OEt₂ 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 Na₂CO₃ saturated solution and extracted with ethyl acetate (2x20 mL). The organic layer was separated, and dried with Na₂SO₄. 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(5*H*)-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, =CH₂ and =CH (Figure S1).

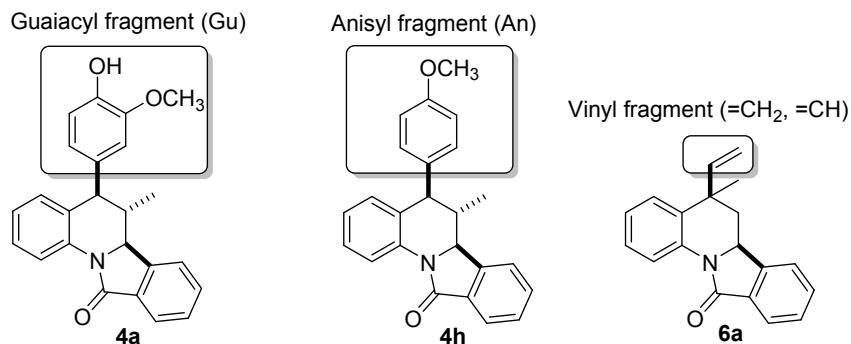


Figure S1. C-5 Aromatic protons fragments.

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

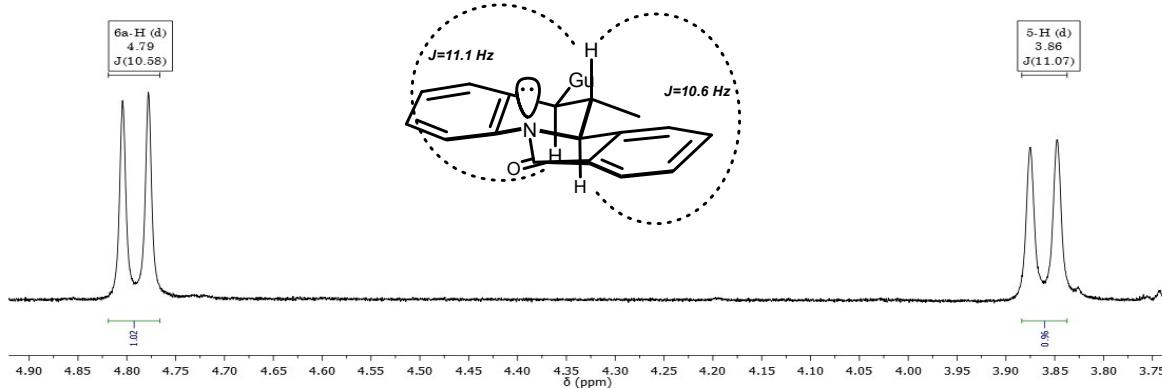


Figure S2. Expansion of the spectrum ¹H NMR (400 MHz, DMSO-d6) for compound **4a**.

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

3.1. Crystal preparation

The crystallization of *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.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 α radiation ($\lambda = 0.71073 \text{ \AA}$). 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 software² was used to correct absorption effects using a redundancy algorithm. Crystal structure was determined by direct methods using the SIR92 program³ and refined by full-matrix least-squares calculation of F2.

Using the Crystals software⁴ 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 \AA (aromatic) and 0.97 \AA (methyl), while a 0.89 \AA 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.

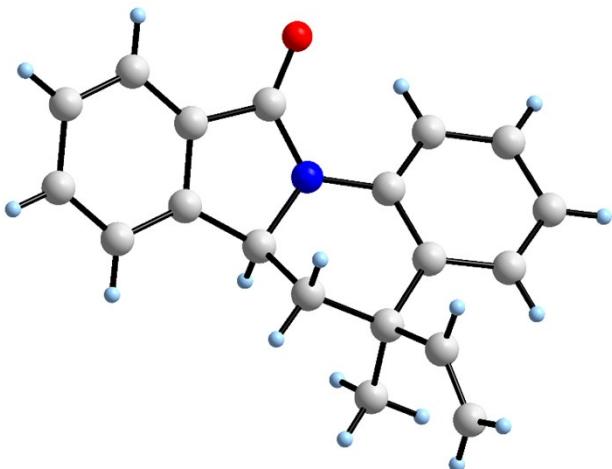


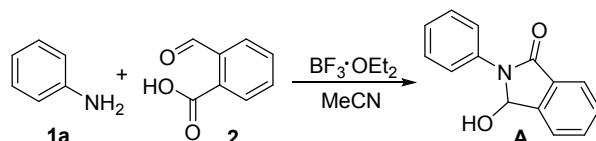
Figure S3. Stick-ball model of **6a** asymmetric unit from monocrystal X-ray diffraction.

Table S1. Crystal data details of the **6a** structure determination

Chemical formula	C ₁₉ H ₁₇ NO
Formula weight (g/mol)	275.33
Crystal system	<i>Monoclinic</i>
Space group	<i>Pc</i> (No 7)
<i>a</i> (Å)	5.8738(2)
<i>b</i> (Å)	9.4468(4)
<i>c</i> (Å)	13.2892(5)
V (Å ³)	737.39(5)
<i>Z</i>	2
d _x (g cm ⁻³)	1.240
F (000)	292
μ (mm ⁻¹)	0.596
θ range (°)	4.7-74.2
<i>hkl</i> range	-13≤ <i>h</i> ≤13 -14≤ <i>k</i> ≤14 -31≤ <i>l</i> ≤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) <i>T</i> _{min} = 0.87, <i>T</i> _{max} = 0.98
<i>Reflections</i>	
Collected	52522
Unique (R _{int})	3132 (0.036)
With I > 2σ(I)	2706
Refinement method	Full-matrix least-squares on <i>F</i> ²
Number of parameters	192
R(<i>F</i>) [I > 2σ(I)]	0.0447
wR(<i>F</i>) [I > 2σ(I)]	0.1230
Goodness of fit on <i>F</i> ²	1.017
Max/Min Δρ (e Å ⁻³)	-0.15/0.16

4. Analysis of *N*-aryl-3-hydroxyisoindolinone 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.** 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).⁵ Its ¹H NMR spectrum (Figure S4) was found to be identical to the literature report.⁵

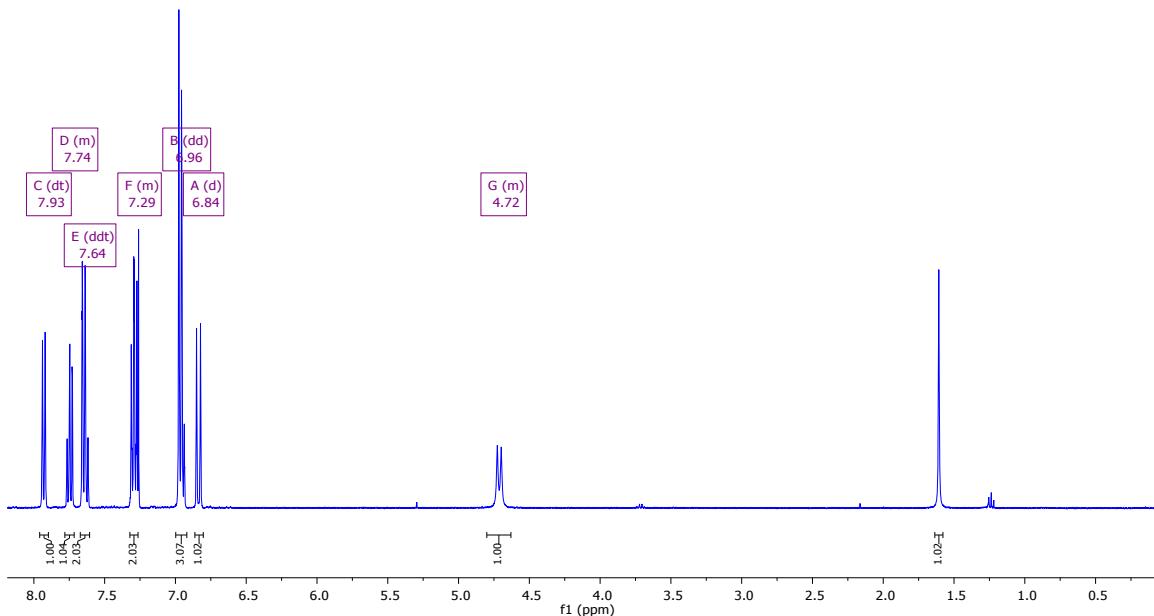


Figure S4. ¹H NMR spectrum (400 MHz, CDCl₃) of isoindolinone **A**.

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.¹⁴ 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% CO₂. 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.⁶

5.2. Selectivity Index (SI)

The selectivity index was calculated as the IC₅₀ (control cells)/IC₅₀ (tumoral cell line) ratio. A selectivity index >1 indicates that the cytotoxicity on tumoral cells surpassed that on healthy non-tumoral cells.⁷

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 (IC₅₀) 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).⁸

6. Theoretical considerations

Calculation of electronic density for the coefficient orbital was performed using the methodology proposed by Cao and co-workers.⁹ Each coefficient contribution was introduced in the follow formula where C_i 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				
	C-1	C-4	C-5	C-9	C-11
ORBITALES					
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	-0.00001	-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	0.00003	0.00002	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
pi-HOMO	44.1948	14.93425	0.004327	8.880632	31.98617

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

ISOPRENE	LUMO				
	C-1	C-4	C-5	C-9	C-11
ORBITALES					
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	0.00002
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	0.00004	-0.00003	0.00000	-0.00003	0.00004
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
pi-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-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, 135.5, 143.5, 145.3, 147.8, 165.0. GC/MS (70 eV), *t*_R = 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-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), *t*_R = 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-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), *t*_R = 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-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-H_{Gu}), 6.68 (1H, d, *J* = 1.5 Hz, 2-H_{Gu}), 6.72 (1H, d, *J* = 8.0 Hz, 4-H_{Gu}), 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, 135.8, 145.2, 145.5, 147.8, 153.3, 155.9, 163.9. GC/MS (70 eV), *t*_R = 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 °C; 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 H_{Gu} 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), *t*_R = 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 °C; 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-H_{Gu}), 6.68 (1H, d, *J* = 1.5 Hz, 2-H_{Gu}), 6.72 (1H, d, *J* = 8.0 Hz, 4-H_{Gu}), 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 (d, *J*_{C,F} = 10.8 Hz), 123.2, 123.9, 124.9 (d, *J*_{C,F} = 11.2 Hz), 125.1, 125.7, 128.8, 131.3, 131.9, 133.8, 135.8, 145.5 (d, *J*_{C,F} = 24.2 Hz), 147.8, 153.3 (d, *J*_{C,F} = 23.0 Hz), 155.9, 163.9 (d, *J*_{C,F} = 245.1 Hz). GC/MS (70 eV), *t*_R = 37.71 min., m/z 389 (M⁺, 70), 250 (50), 151 (100). Anal. calcd for C₂₄H₂₀FNO₃: C, 74.02; H, 5.18; F, 4.88; N, 3.60. Found: C, 74.21; H, 5.29; N, 3.73.

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

mp: 262-264 °C. IR (KBr): 3450, 3300, 2945 cm⁻¹; ¹H NMR (400 MHz, DMSO-d₆) δ (ppm) 1.15 (3H, d, *J* = 6.0 Hz, CH₃), 1.84 (1H, m, 3-H), 3.76 (1H, d, *J* = 10.9 Hz, 4-H), 3.67 (3H, s, OCH₃), 4.72 (1H, d, *J* = 10.6 Hz, 2-H), 5.96 (2H, s, CH₂), 6.17 (1H, s, 5-H), 6.59 (1H, d, *J* = 7.7 Hz, 6-H_{Gu}), 6.65 (1H, s, 2-H_{Gu}), 6.72 (1H, d, *J* = 7.7 Hz, 5-H_{Gu}), 7.50 (1H, *J* = 7.2 Hz, 7-H), 7.56 (1H, ‘t’, *J* = 7.2 Hz, 9-H), 7.67 (1H, ‘t’, *J* = 7.3 Hz, 10-H), 7.74 (1H, *J* = 7.2 Hz, 8-H), 7.92 (1H, s, 1-H), 8.89 (1H, s, OH); ¹³C NMR (100 MHz, DMSO-d₆) δ (ppm) 15.6, 51.4, 55.5, 63.2, 100.4, 100.9, 108.7, 109.4, 112.5, 115.2, 121.8, 123.3, 124.3, 124.5, 128.5, 129.2, 131.6, 132.1, 134.2, 143.1, 143.3, 145.1, 145.2, 147.7, 164.5, GC/MS (70 eV), t_R = 80.4 min., 415 (50, M⁺), 276 (30), 149 (100). Anal. Calcd. for C₂₅H₂₁NO₅: C, 72.28; H, 5.10; N, 3.37. Found: C, 72.37; H, 5.34; N, 3.23.

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, 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, 128.7, 129.9, 130.4, 131.1, 131.9, 132.2, 135.6, 143.4, 157.9, 164.9. GC/MS (70 eV), t_R = 62.64 min., m/z 355 (M⁺, 100), 340 (10), 326 (10), 232 (60), 135 (80). Anal. calcd for C₂₄H₂₁NO₂: 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(5-H)-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, 135.6, 143.3, 157.9, 164.7. GC/MS (70 eV), t_R = 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_{An} and 3-H_{An}), 7.13 – 7.05 (3H, m, 2-H, 2-H_{An} and 3-H_{An}), 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). ¹³C NMR (101 MHz, DMSO-d₆) 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_R = 73.47 min., m/z 383 (M⁺, 100), 368 (30), 260 (35). Anal. calcd for C₂₆H₂₅NO₂: 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-6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (4k). Were obtained 340 mg (0.88 mmol, 68 %), yellow solid; mp: 190–192 °C; FTIR (KBr disk): 1682, 1150 cm⁻¹; ¹H NMR (400 MHz, DMSO-d₆) δ (ppm) 1.17 (3H, d, J = 6.4 Hz, CH₃), 2.05 – 1.96 (1H, m, 6-H), 3.74 (3H, d, J = 14.5 Hz, OCH₃), 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_{An} and 3-H_{An}), 7.18 (2H, d, J = 8.7 Hz, 2-H_{An} and 3-H_{An}), 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). ¹³C NMR (101 MHz, DMSO-d₆) 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_R = 83.66 min., m/z 385 (M⁺, 100), 370 (10), 262 (15). Anal. calcd for C₂₄H₂₀N₂O₄: 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-6a-dihydro-[1,3]dioxolo[4,5-g]isoindolo[2,1-a]quinolin-11(5H)-one (4l). Were obtained 455 mg (1.1 mmol, 91 %), white solid; mp 250–252 °C. IR (KBr): 3300, 1146 cm⁻¹; ¹H NMR (400 MHz, DMSO-d₆) δ (ppm) 1.15 (3H, d, J = 6.4 Hz, CH₃) 1.75 (1H, dd, J = 16.9, 10.6 Hz, 6-H), 3.73 (3H, s, OCH₃), 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, CH₂), 6.09 (1H, s, 4-H), 6.89 (2H, d, J = 8.4 Hz, 2-H_{An} and 3-H_{An}), 7.08 (2H, d, J = 8.4 Hz, 2-H_{An} and 3-H_{An}), 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). ¹³C NMR (101 MHz, DMSO-d₆) 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_R = 83.66 min., m/z 415 (50, M⁺), 276 (30), 149 (100). Anal. Calcd. for C₂₅H₂₁NO₄: 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-8a-dihydrobenzo[h]isoindolo[2,1-a]quinolin-13(7H)-one (4m). Were obtained 365 mg (0.90 mmol, 73 %), white solid; mp: > 300 °C; FTIR (KBr disk): 1682, 1212 cm⁻¹; ¹H NMR (400 MHz, DMSO-d₆) δ (ppm) 1.22 (3H, d, J = 8.9 Hz, CH₃), 1.69 – 1.59 (1H, m, 8-H), 3.71 (3H, d, J = 8.9 Hz, OCH₃), 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_{An} and 3-H_{An}), 6.91 (1H, d, J = 8.8 Hz, 6-H), 7.10 (2H, d, J = 8.5 Hz, 2-H_{An} and 3-H_{An}), 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). ¹³C NMR (100 MHz, DMSO-d₆)

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), t_R = 111.67 min., m/z 405 (M^{+} , 100), 376 (10), 270 (70). Anal. calcd for $C_{28}H_{23}NO_2$: 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, dd, J = 7.3, 1.6 Hz, 10-H). ^{13}C 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), t_R = 24.117 min., m/z (%) 275 (M^{+} , 70), 260 (100), 232 (10); Anal. Calc. for $C_{19}H_{17}NO$: 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, dd, 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). ^{13}C NMR (100 MHz, DMSO-d₆) δ (ppm) 20.7, 22.1, 27.2, 40.0, 40.5, 54.9, 112.5, 119.7, 122.8, 123.4, 127.4, 128.6, 128.9, 131.9, 132.3, 132.5, 132.8, 145.0, 146.7, 165.1; GC/MS (70 eV): t_R = 25.042 min., m/z (%) 289 (M^{+} , 80), 274 (100), 246 (5); Anal. Calc. for $C_{20}H_{19}NO$: 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, CH₃ 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, 10H); ^{13}C 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, 132.8, 145.0, 146.7, 165.1; GC/MS (70 eV): t_R = 25.014 min., m/z (%) 303 (M^{+} , 70), 274 (100), 246 (5); Anal. Calc. for $C_{21}H_{21}NO$: 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), t_R = 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), t_R = 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, 125.5, 129.5, 129.7, 129.8, 131.3, 136.1, 136.6, 142.0, 146.8, 163.7; GC/MS (70 eV), t_R = 25.855 min., m/z (%) 309 (M⁺, 80), 294 (100), 259 (20); Anal. Calc. for C₁₉H₁₆ClNO: C, 73.66; H, 5.21; Cl, 11.44; N, 4.52. Found: C, 73.71; 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-d₆) δ (ppm) 25.1, 40.0, 41.0, 42.4, 58.7, 112.0, 116.6, 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 C₁₉H₁₆FNO: 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; ^1H NMR (400 MHz, DMSO-d₆) δ (ppm) 1.34 (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), 4.94 – 4.90 (1H, m, CH), 4.97 (1H, dd, J = 10.0, 2.5 Hz, =CH₂), 5.04 (1H, dd, J = 16.9, 2.4 Hz, =CH₂), 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-d₆) 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 C₂₀H₁₆NO: 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; ^1H NMR (400 MHz, DMSO-d₆) δ (ppm) 1.27 (1H, 't', J = 12.6 Hz, CH₂), 1.56 (3H, s, CH₃), 2.28 (1H, dd, J = 13.2, 2.6 Hz, CH₂), 3.69 (3H, s, OCH₃), 3.77 (3H, s, OCH₃), 5.06 – 4.81 (3H, m, =CH₂, 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-d₆) 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 C₂₁H₂₁NO₃: C, 75.20; H, 6.31; N, 4.18. Found: C, 75.29; H, 6.40; N, 4.08.

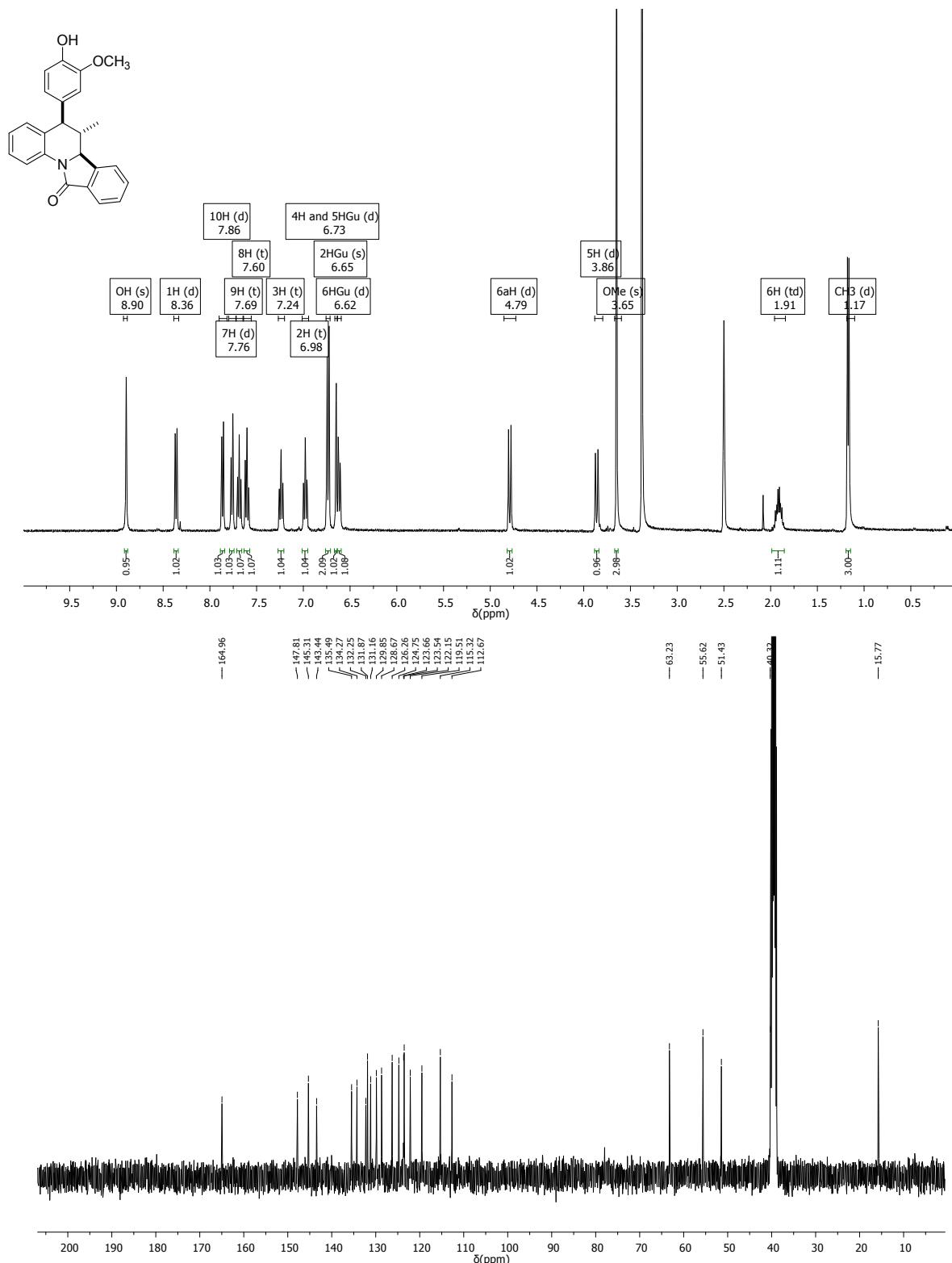
Trans-5-hydroxy-5-vinyl-6,6a-dihydro-[1,3]dioxolo[4,5-g]isoindolo[2,1-a]-quinolin-11(5H)-one (6j). Were obtained 390 mg (1.34 mmol, 78 %), white solid; mp: 150–152 °C; IR (KBr): 3435, 2890, 1682 cm⁻¹; ^1H NMR (400 MHz, DMSO-d₆) δ (ppm) 1.54 (4H, d, J = 8.5 Hz, CH₃ and CH₂), 2.41 – 2.23 (1H, m, CH₂), 5.02 (1H, d, J = 11.9 Hz, 6a-H), 5.15 (1H, d, J = 10.6 Hz, =CH₂), 5.29 (1H, d, J = 17.3 Hz, =CH₂), 5.91 (1H, dd, J = 17.3, 10.5 Hz, =CH₂), 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-d₆) 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 C₁₉H₁₇NO₂: 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), *t*_R = 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.

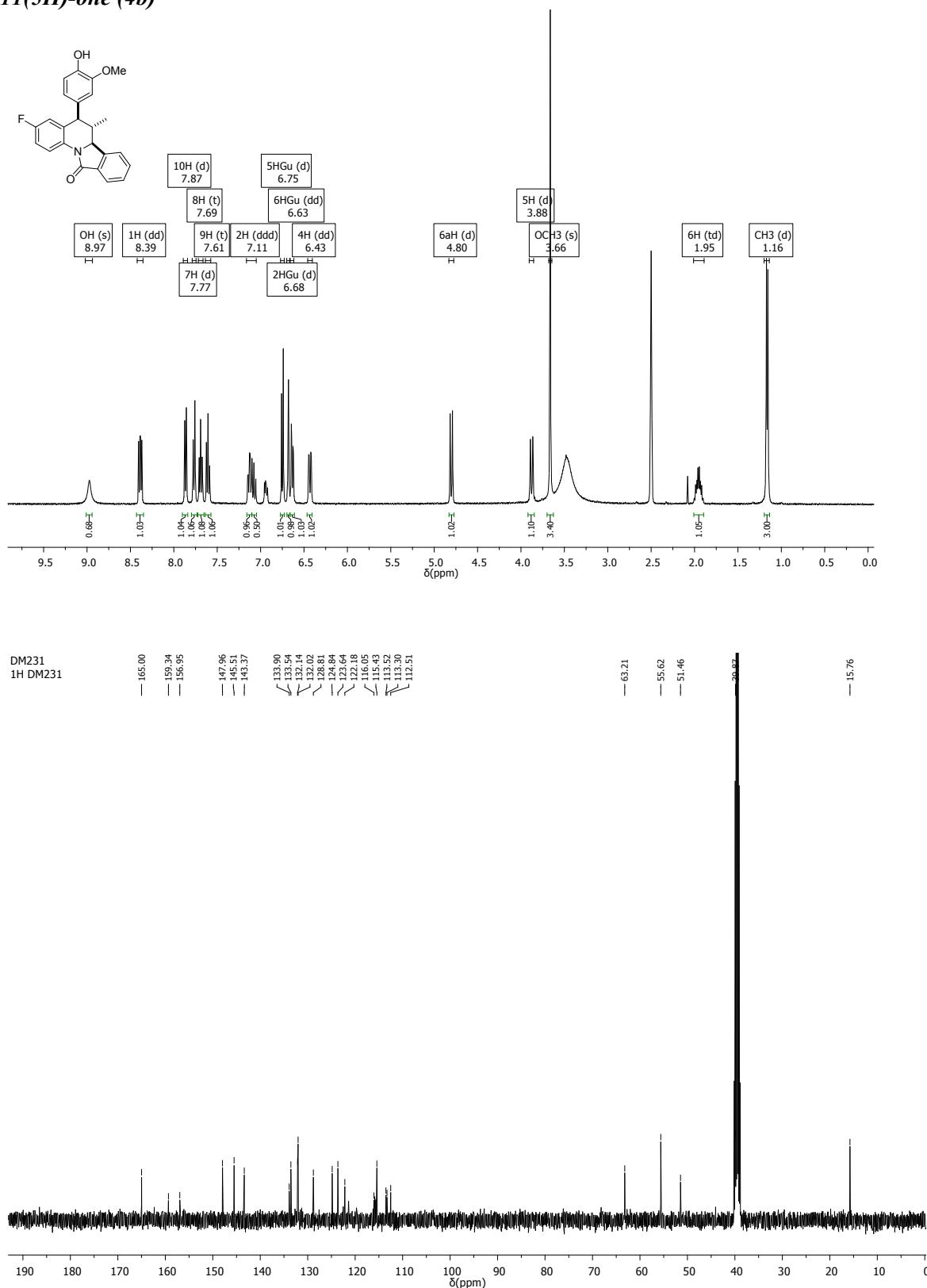
Trans-5-methyl-5-vinyl-6,6a-dihydro-[1,3]dioxolo[4,5-g]isoindolo[2,1-a]-quinolin-11(5H)-one (6l). Were obtained 350 mg (1.10 mmol, 70 %), white solid; mp: 193-194 °C; IR (KBr): 2890, 1682 cm⁻¹; ¹H NMR (400 MHz, DMSO-d₆) δ (ppm) 1.55–1.47 (4H, m, CH₃ and CH₂), 2.40–2.34 (1H, dd, *J* = 13.4, 2.28 Hz, CH₂), 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), *t*_R = 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.

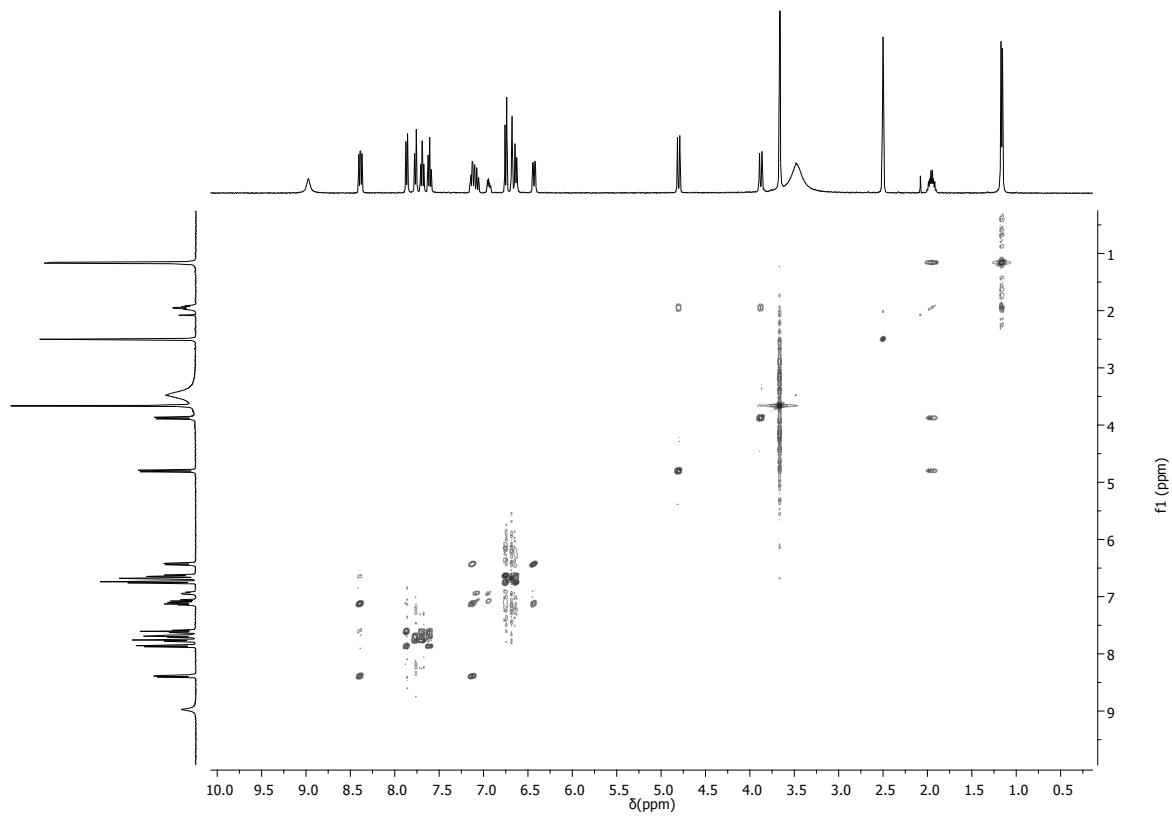
10. Spectral Characterization of Products 4a-m, 6a-l

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

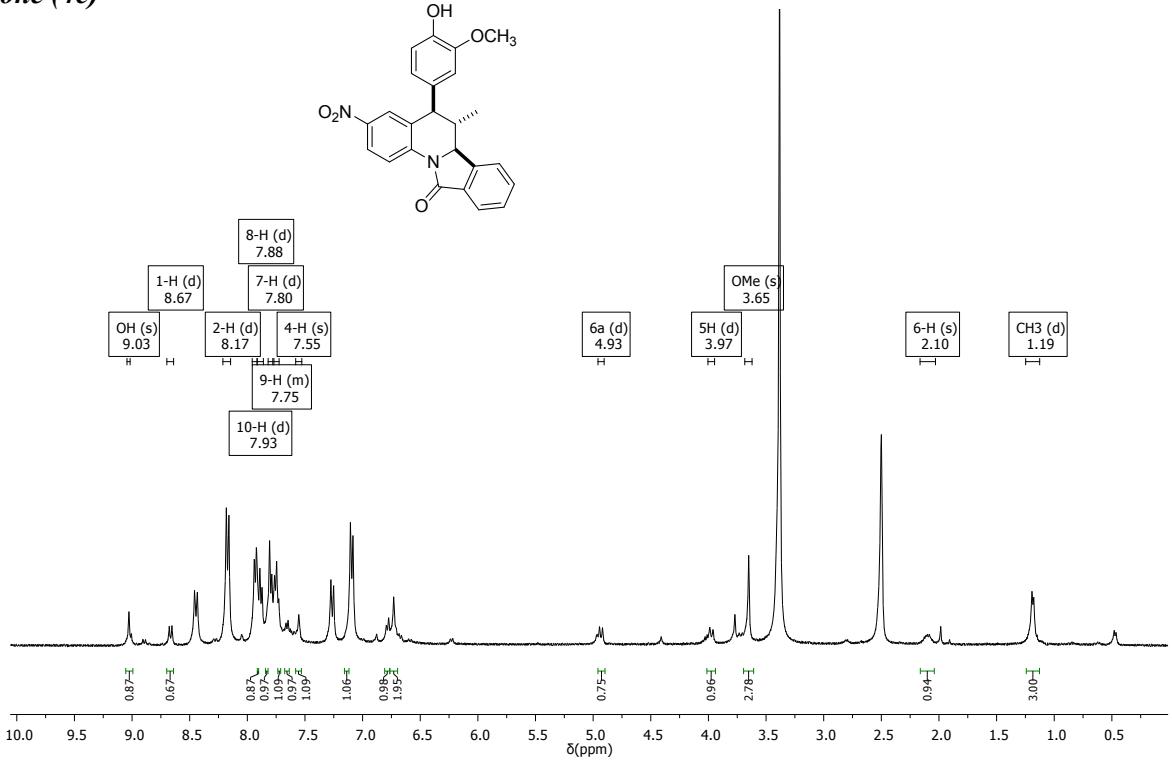


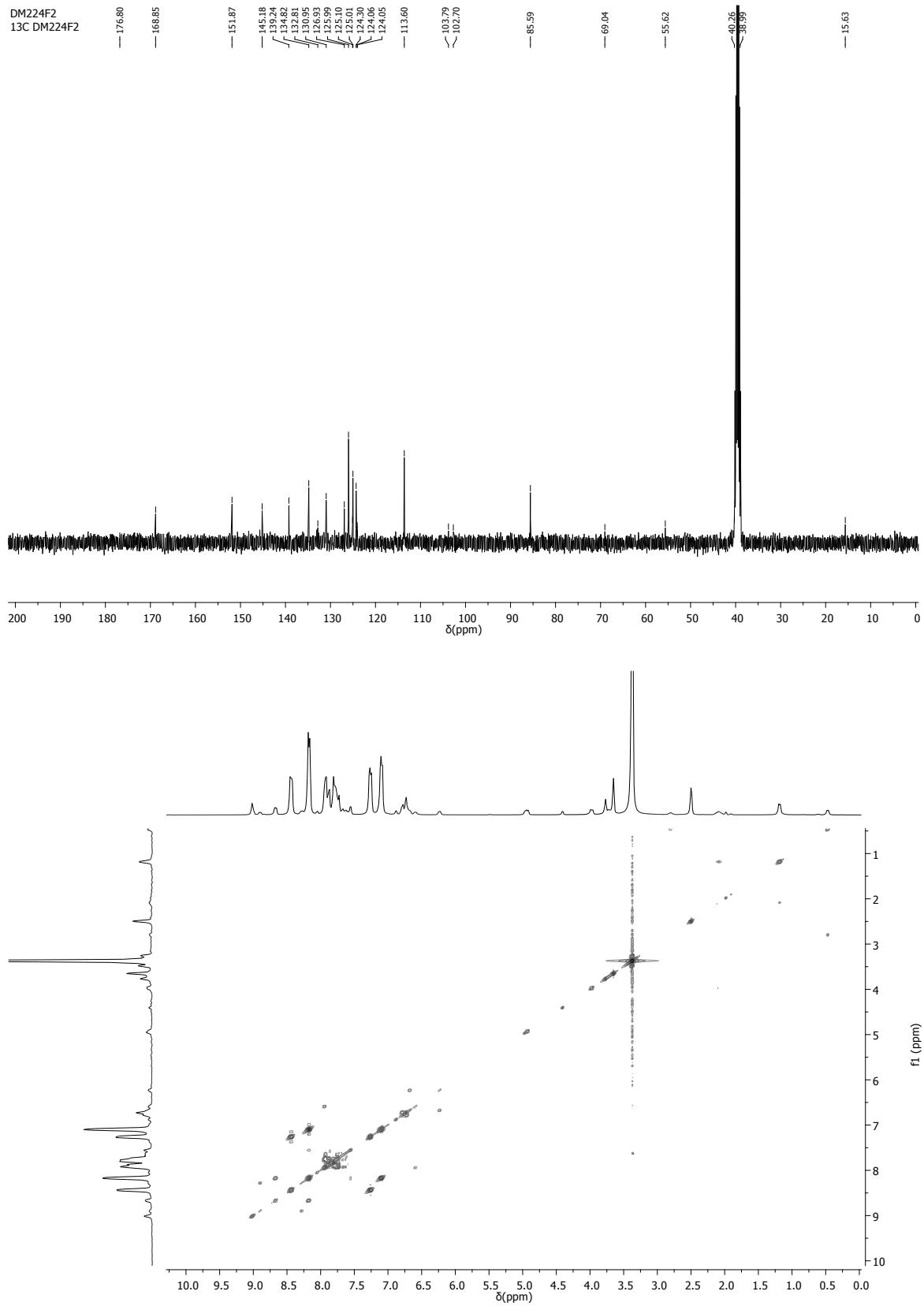
Trans-3-fluoro-5-(4-hydroxy-3-methoxyphenyl)-6-methyl-6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (4b)



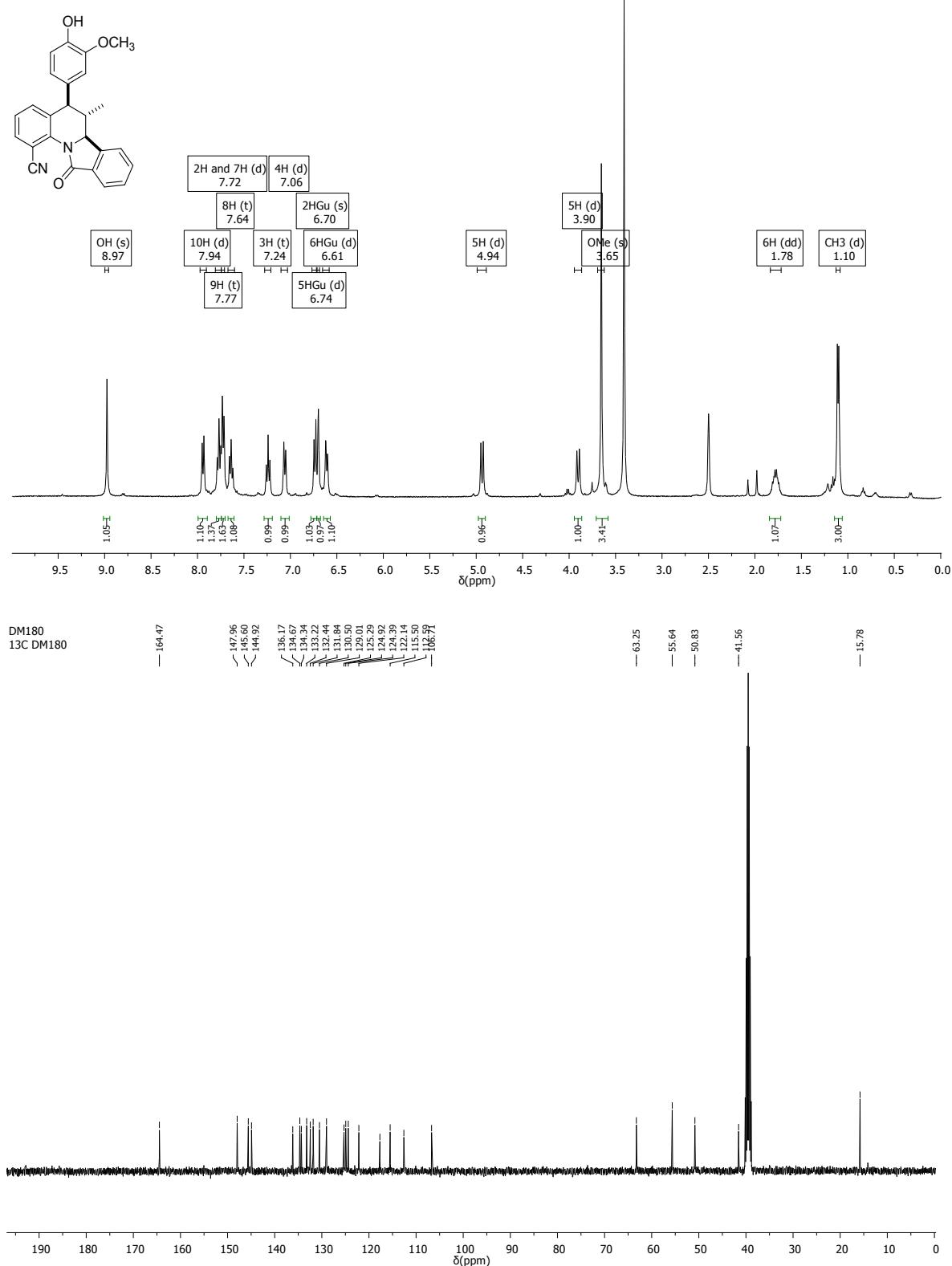


Trans-5-(4-hydroxy-3-methoxyphenyl)-6-methyl-3-nitro-6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (4c)

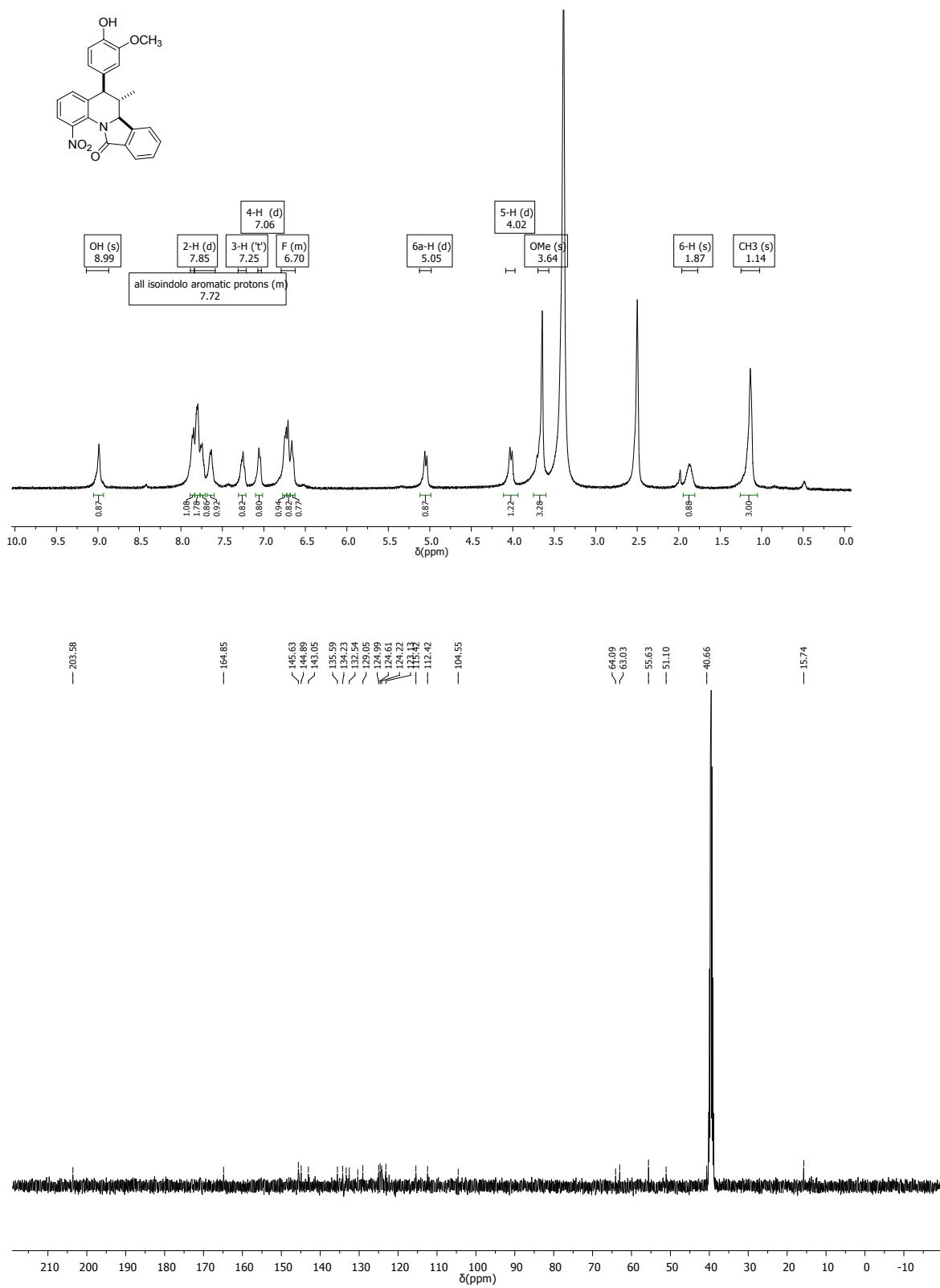


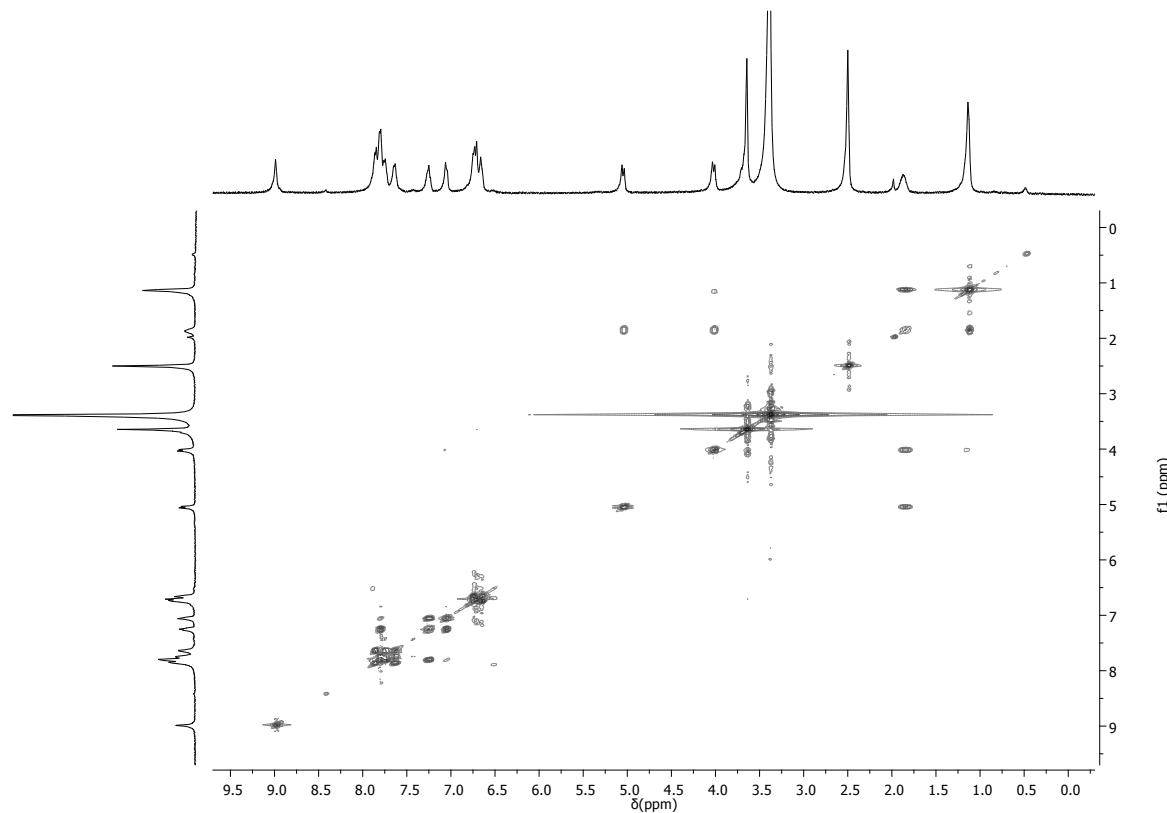


Trans-1-ciano-5-(4-hydroxy-3-methoxyphenyl)-6-methyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (4d)

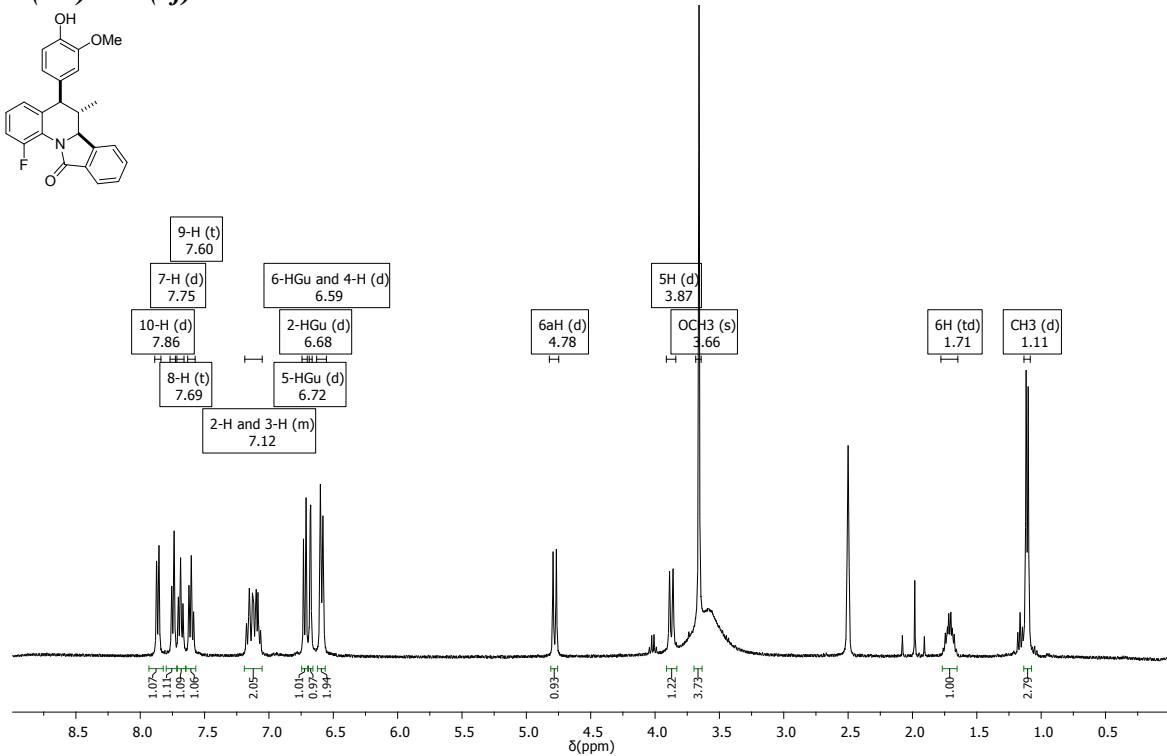


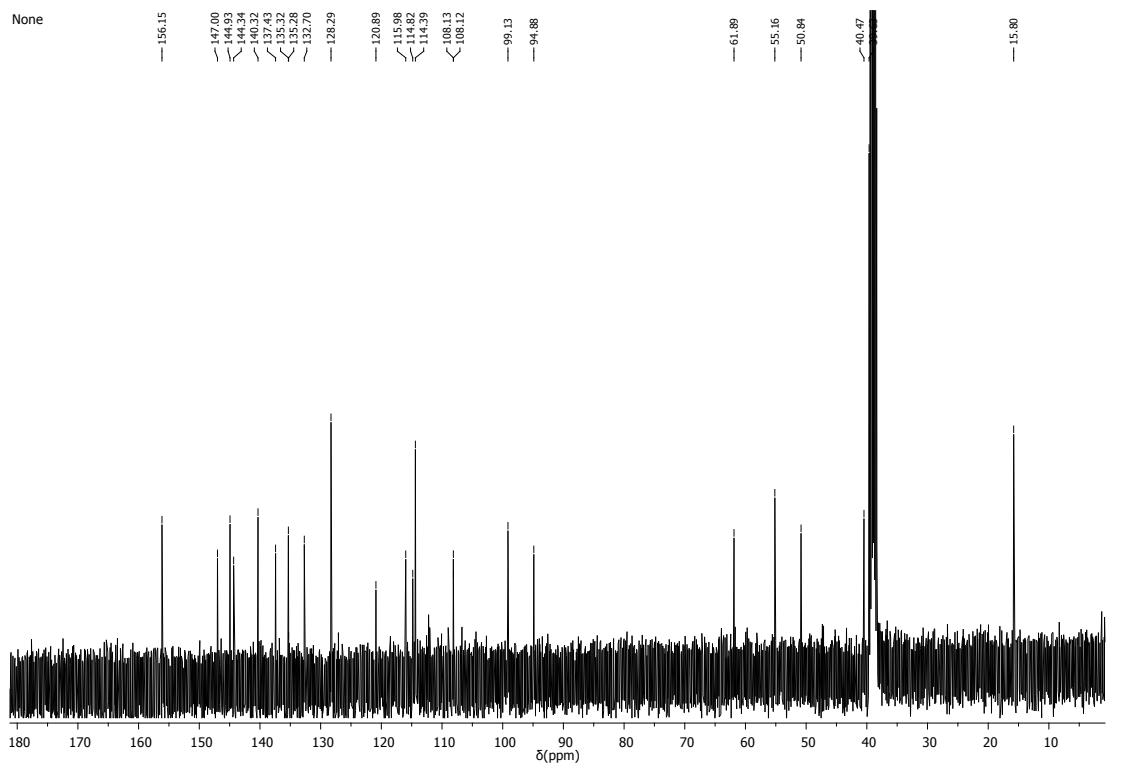
Trans-5-(4-hydroxy-3-methoxyphenyl)-6-methyl-1-nitro-6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (4e)



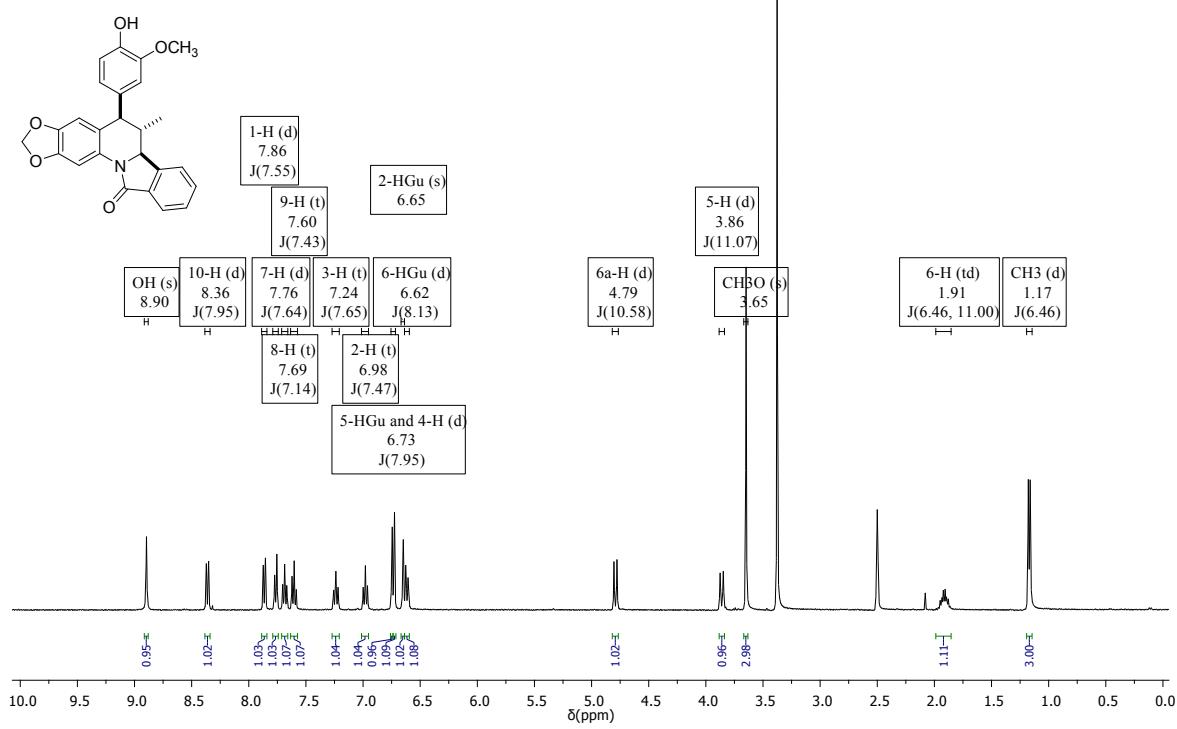


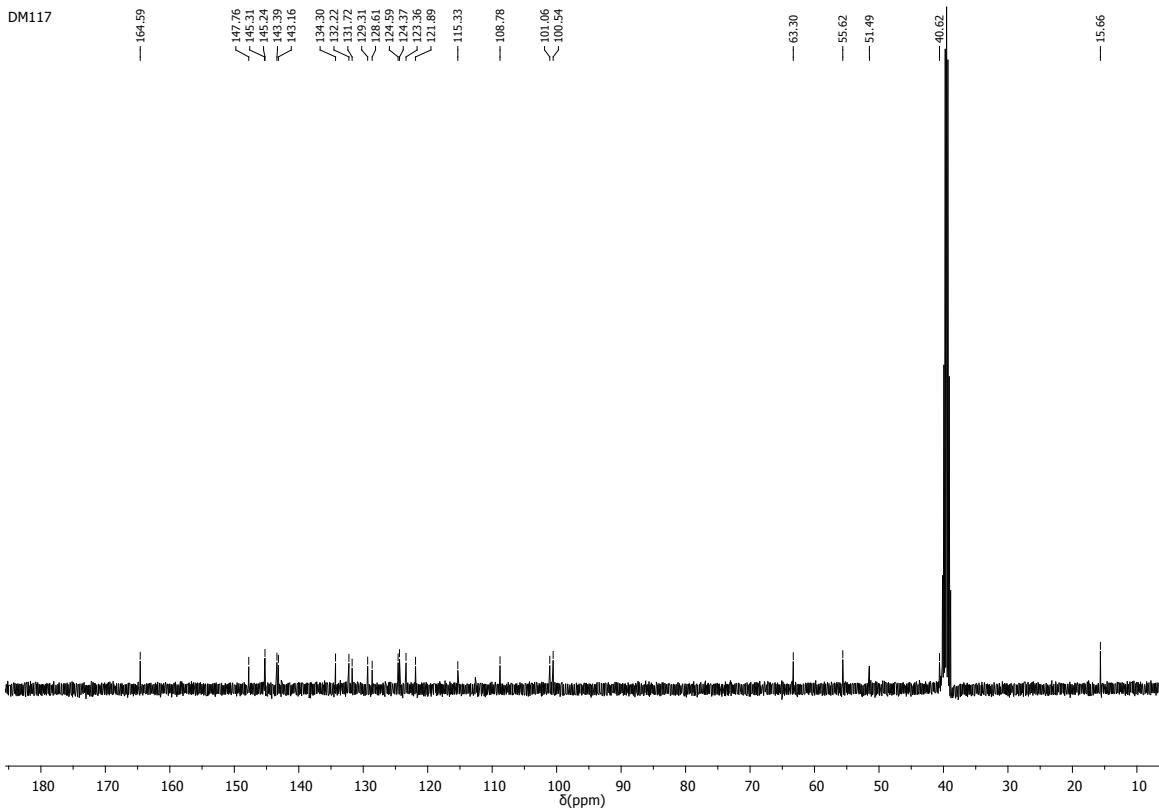
Trans-1-fluoro-5-(4-hydroxy-3-methoxyphenyl)-6-methyl-6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (4f)



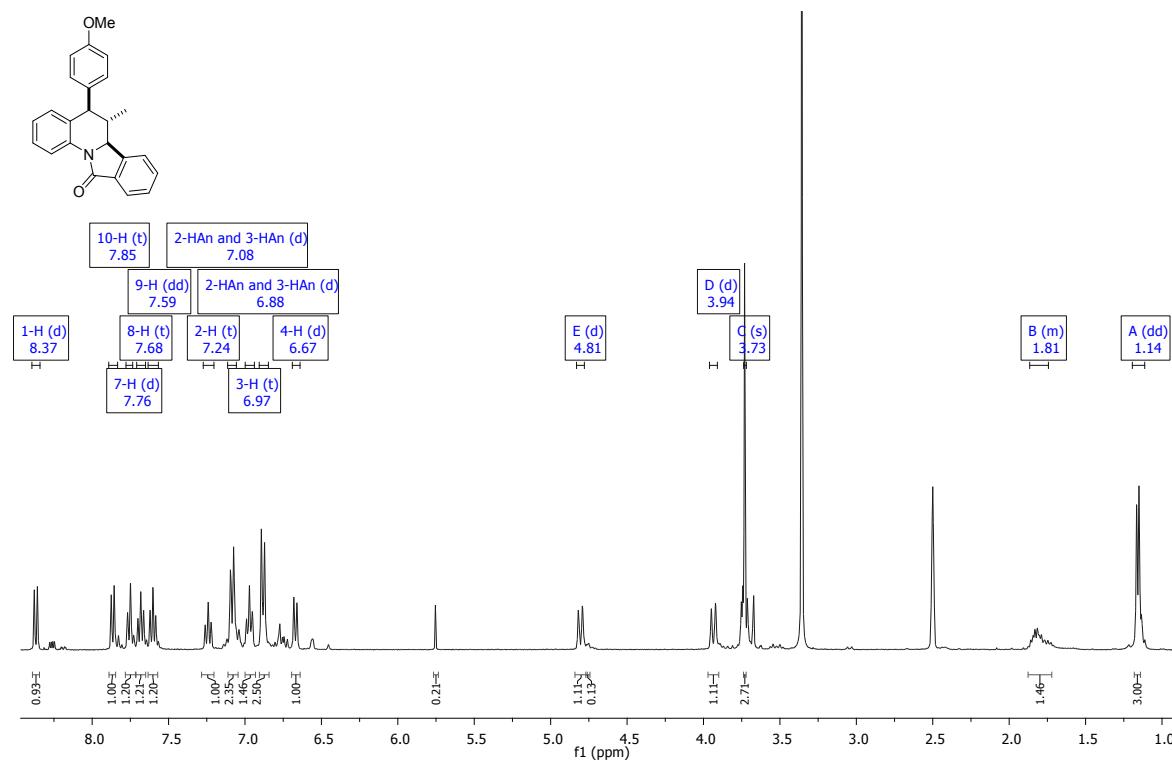


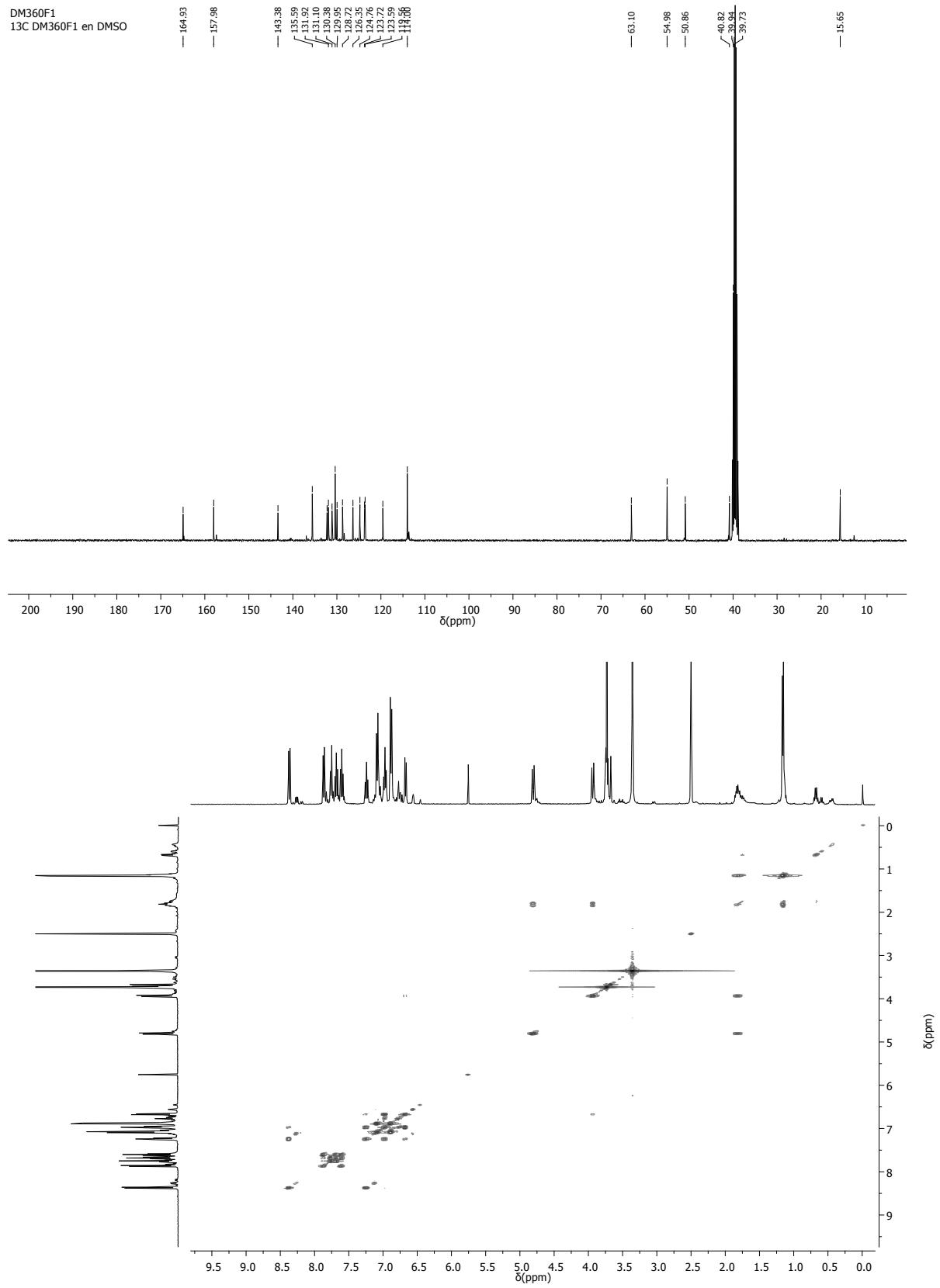
Trans-5-(4-hydroxy-3-methoxyphenyl)-6-methyl-6a-dihydro-[1,3]dioxolo[4,5-g]isoindolo[2,1-a]quino-lin-11(5H)-one (4g)



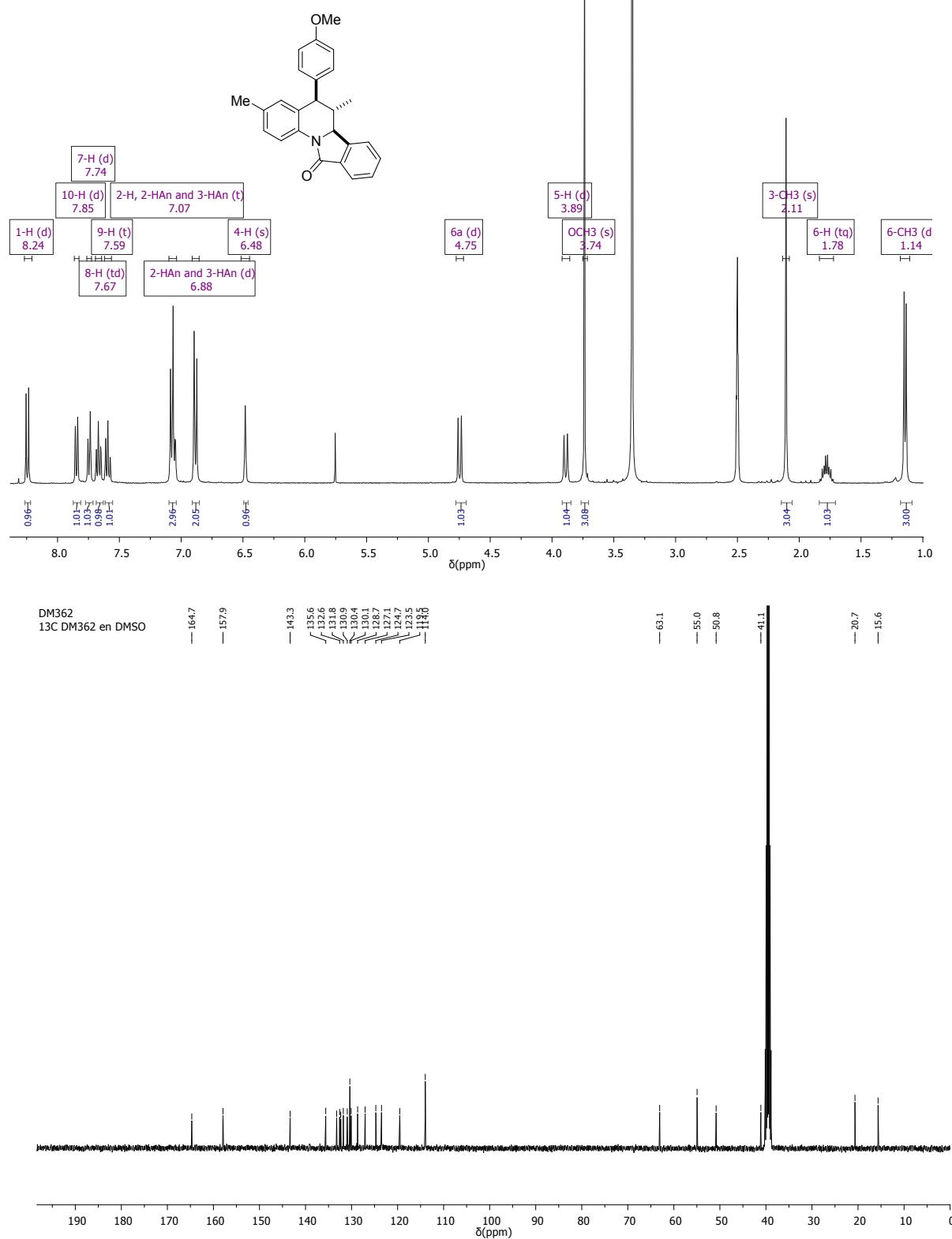


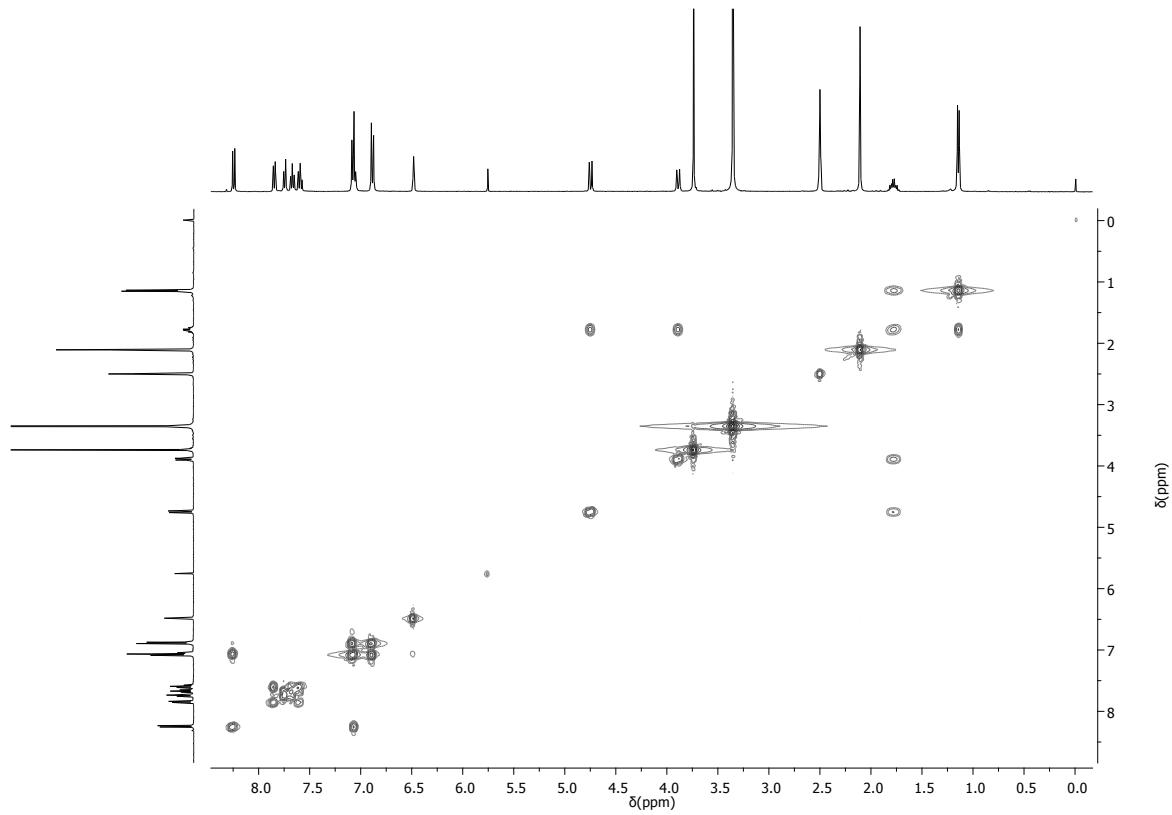
Trans-5-(4-methoxyphenyl)-6-methyl-6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (4h)



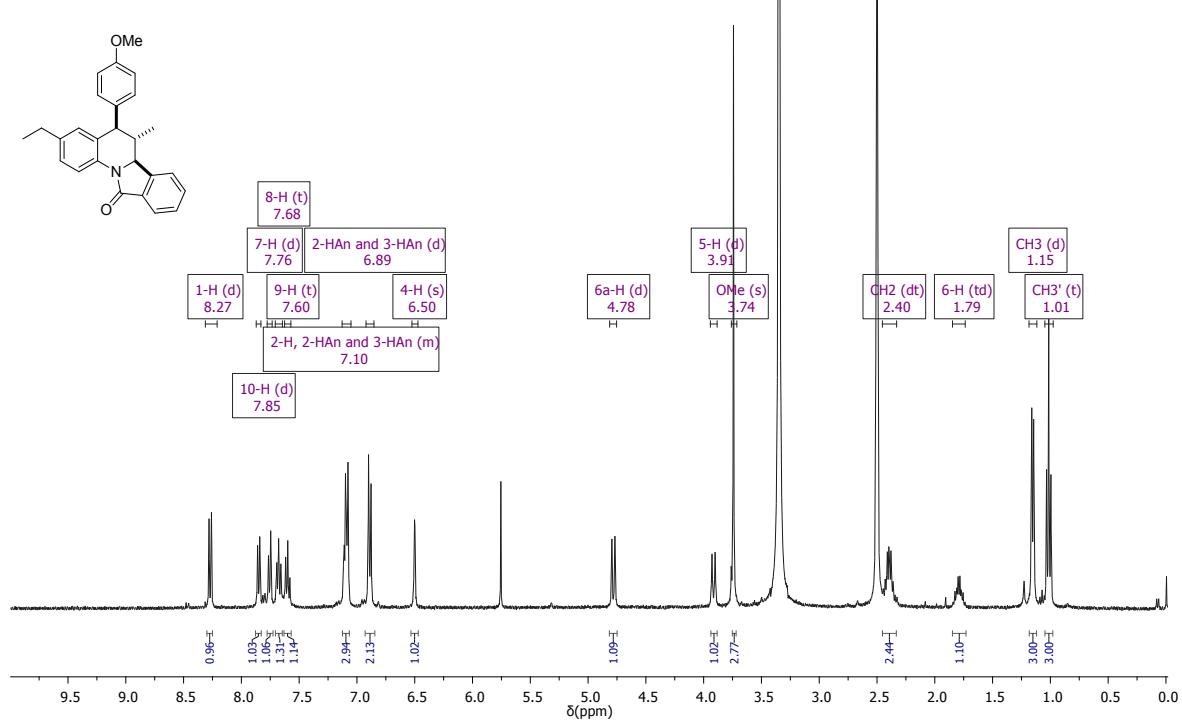


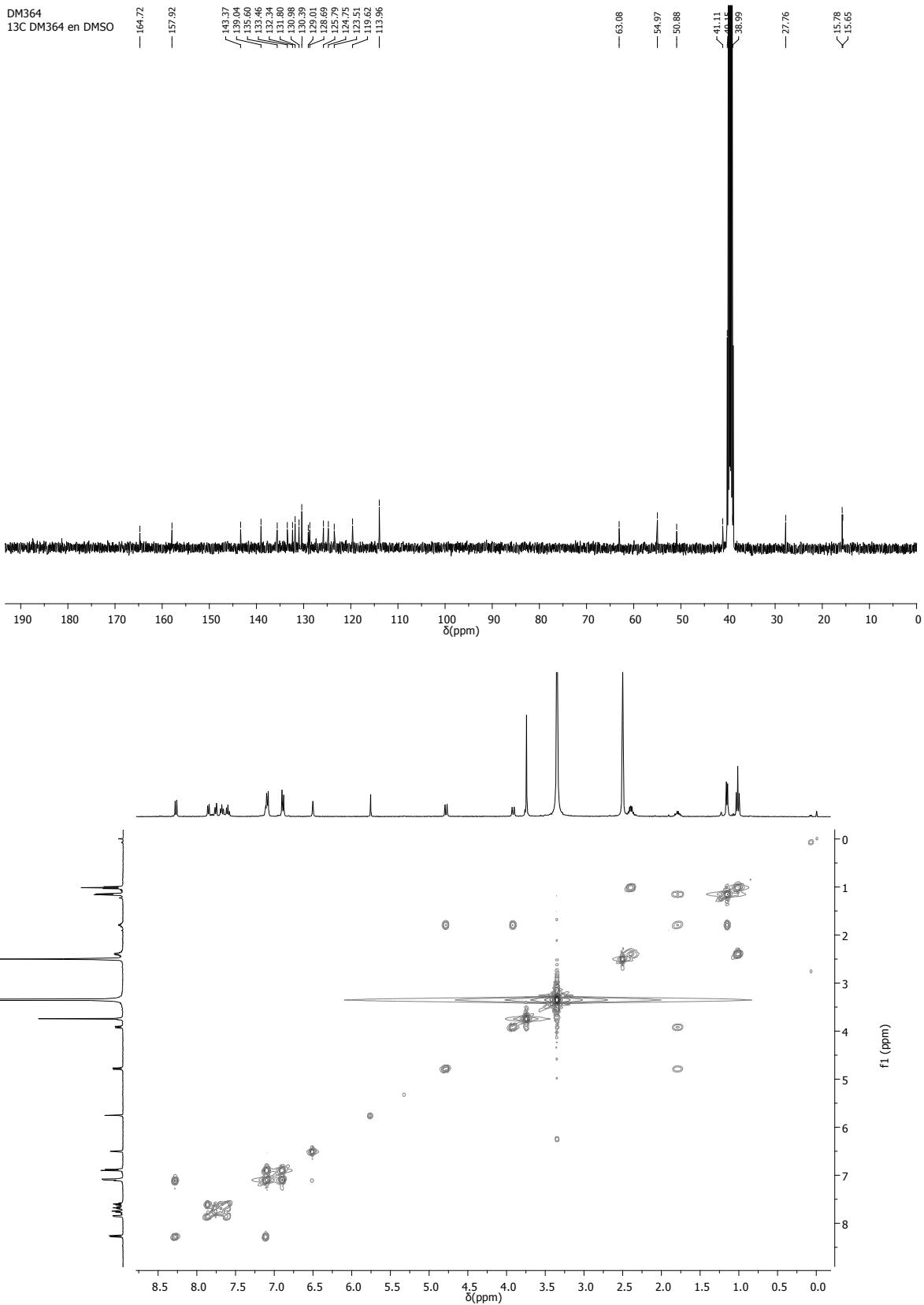
Trans-3,6-dimethyl-5-(4-methoxyphenyl)-6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (4i)



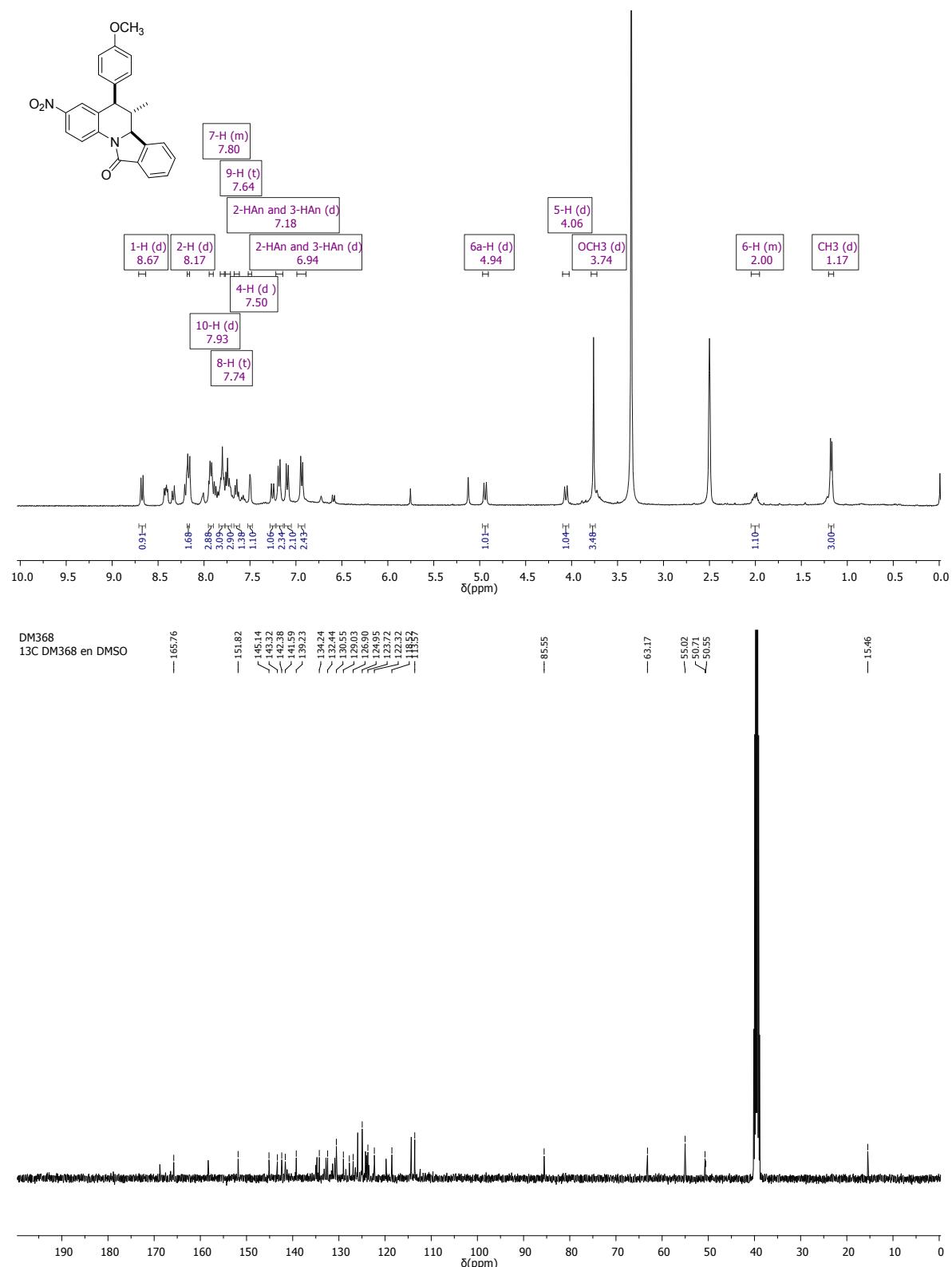


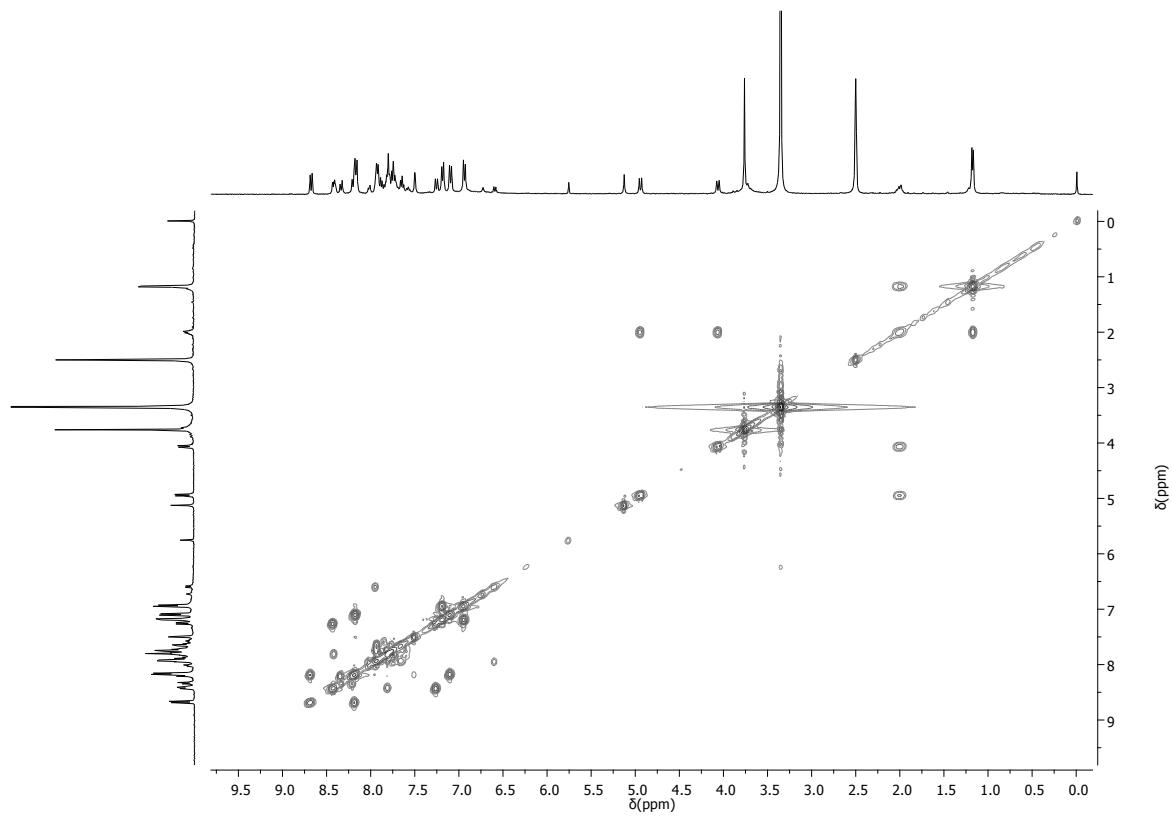
Trans-3-ethyl-5-(4-methoxyphenyl)-6-dimethyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (4j)



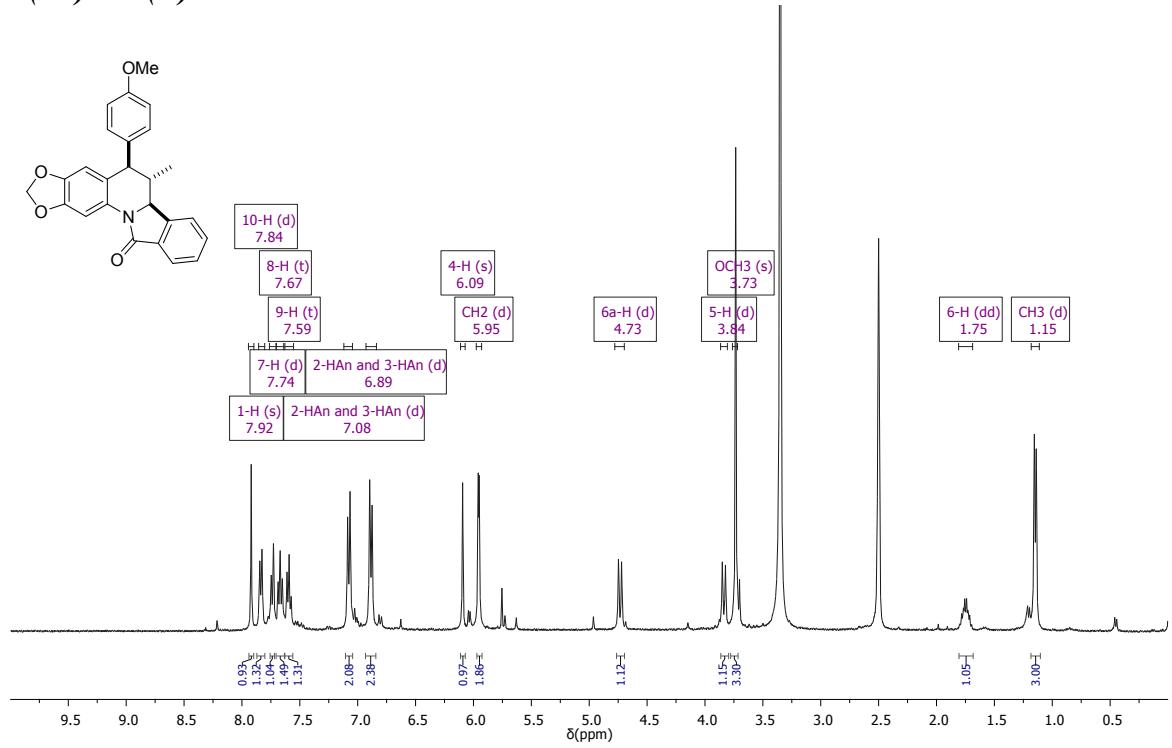


Trans-3-nitro-5-(4-methoxyphenyl)-6-dimethyl-6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (4k)

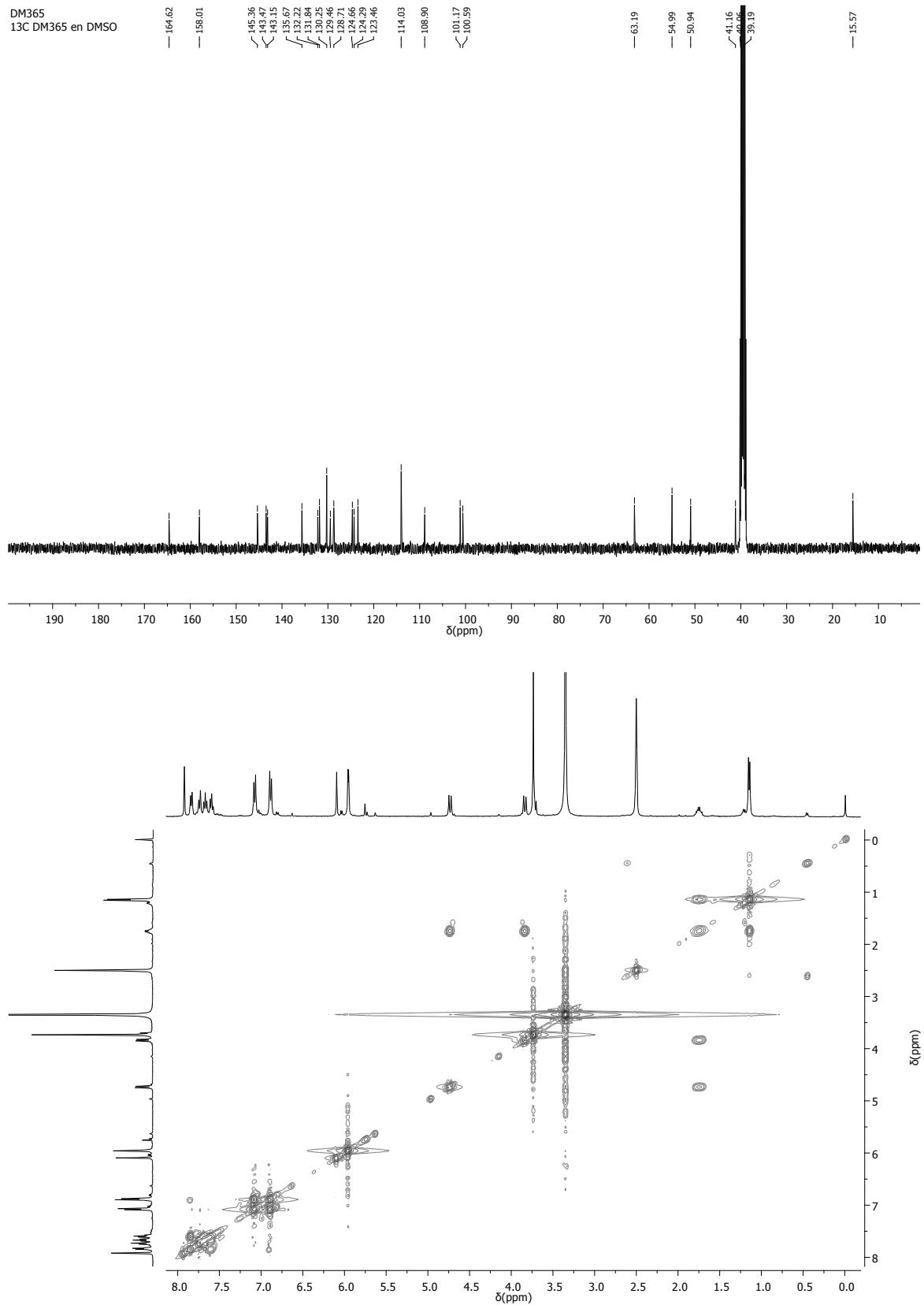




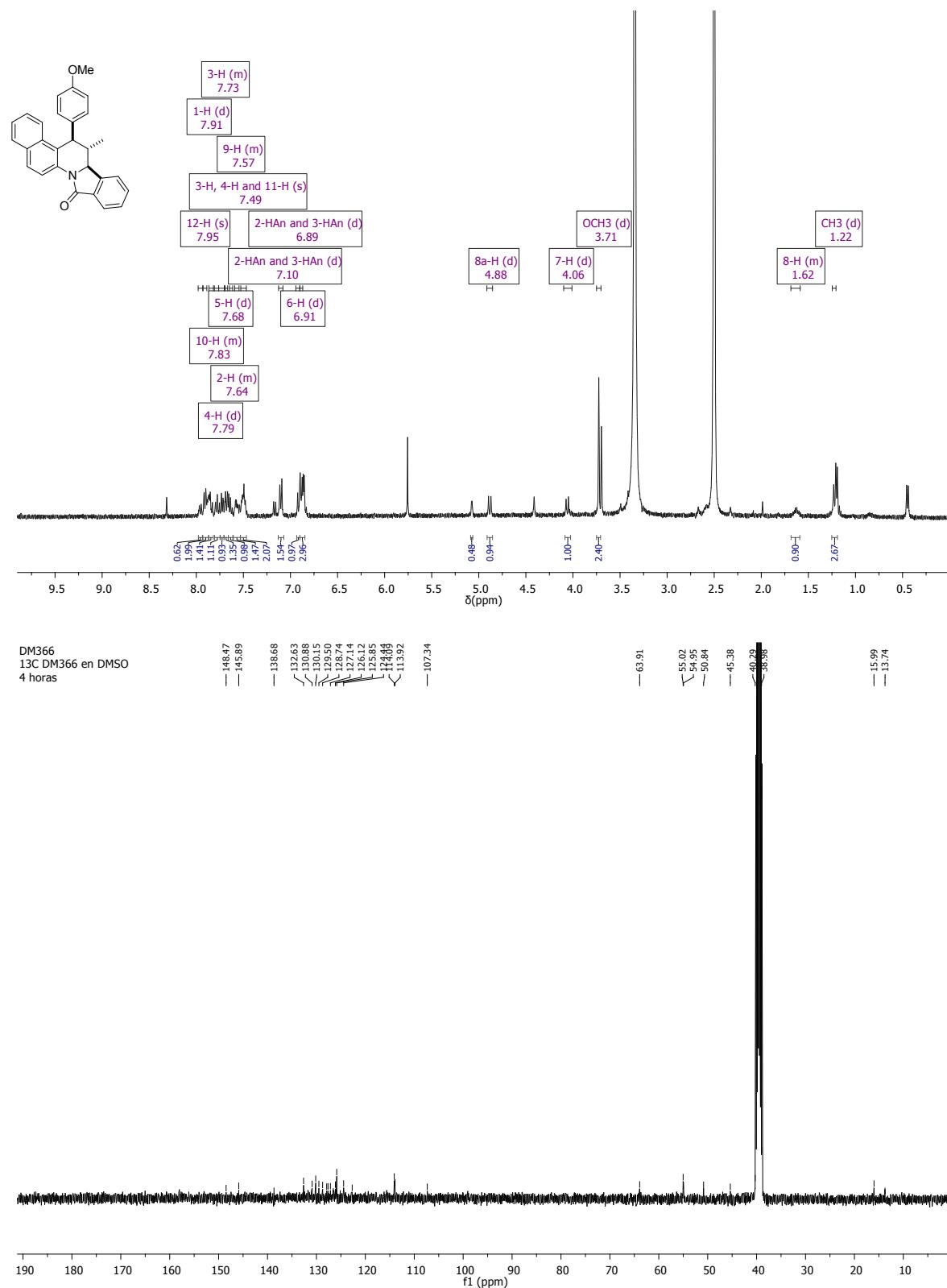
Trans-5-(4-methoxyphenyl)-6-methyl-6a-dihydro-[1,3]dioxolo[4,5-g]isoindolo[2,1-a]qui-nolin-11(5H)-one (4l)

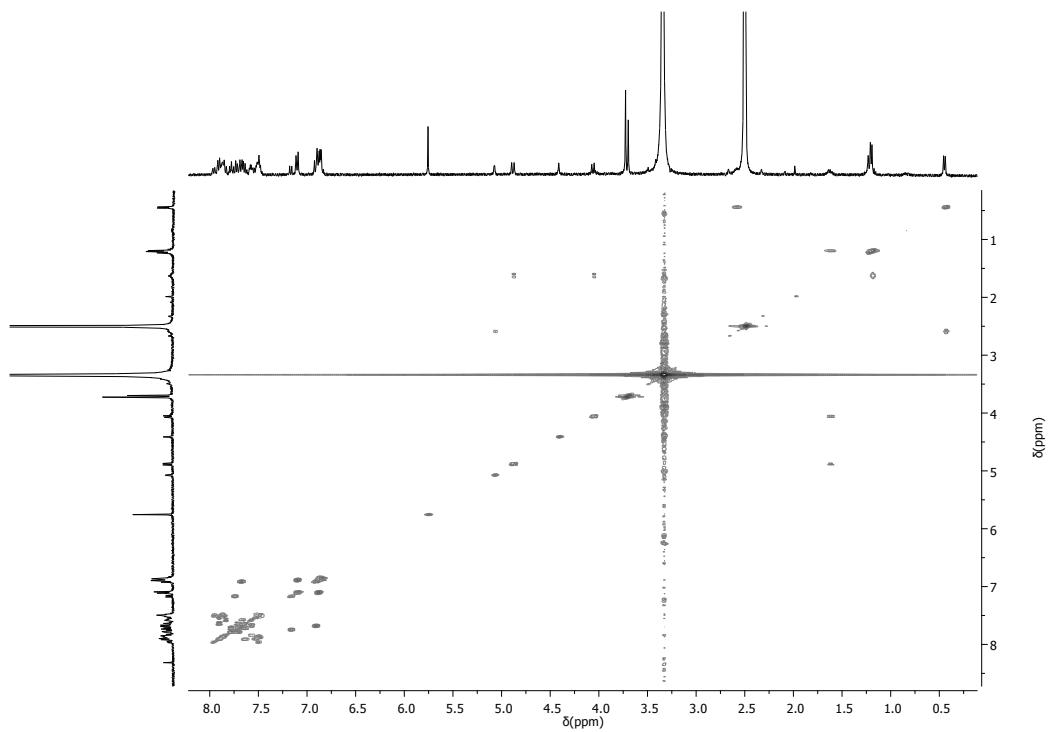


DM365
13C DM365 en DMSO

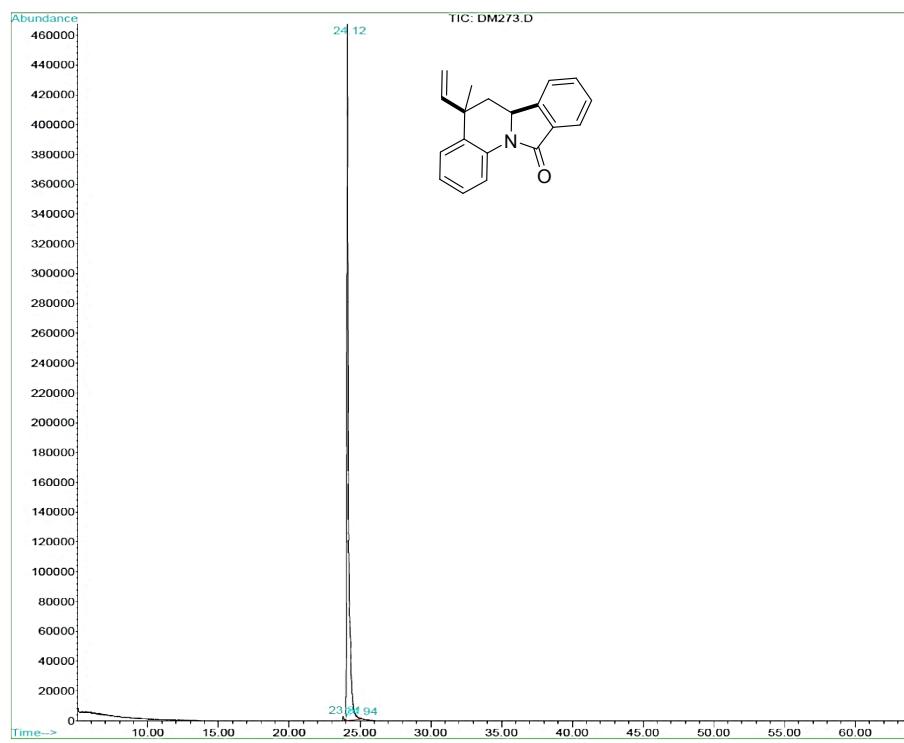


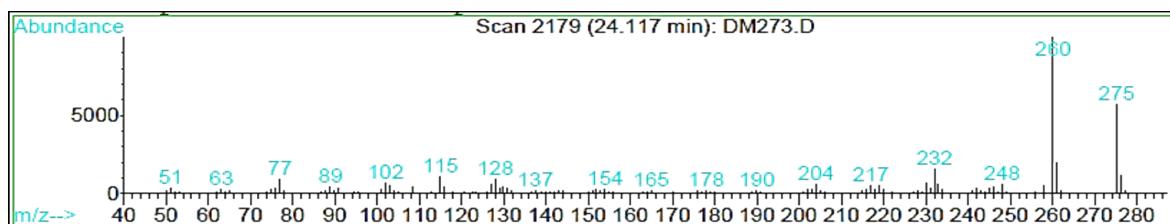
*Trans-7-(4-methoxyphenyl)-8-methyl-8a-dihydrobenzo[*h*]isoindolo[2,1-*a*]quinolin-13(7*H*)-one (4m)*



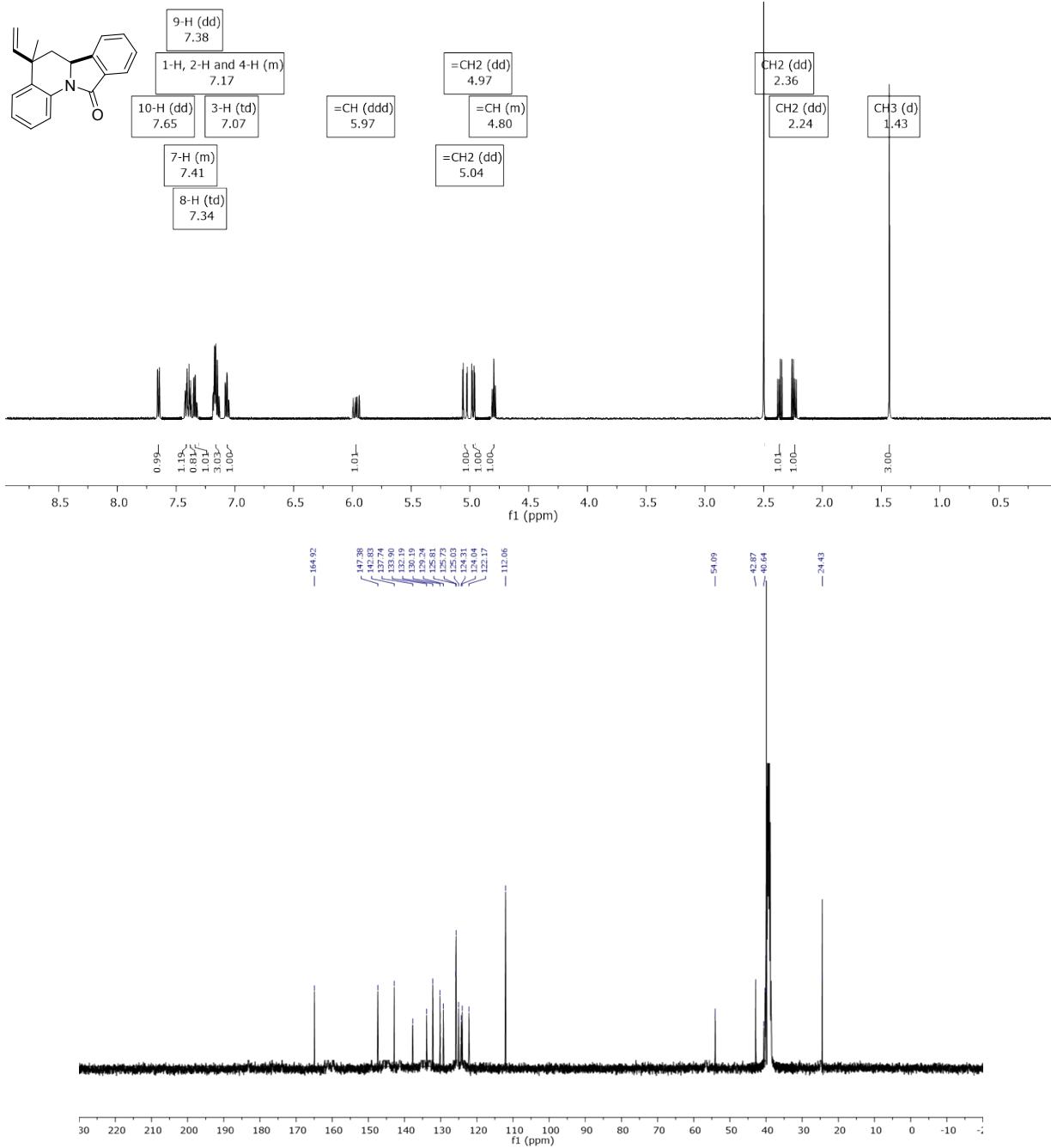


GC-MS Trans-5-methyl-5-vinyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6a)

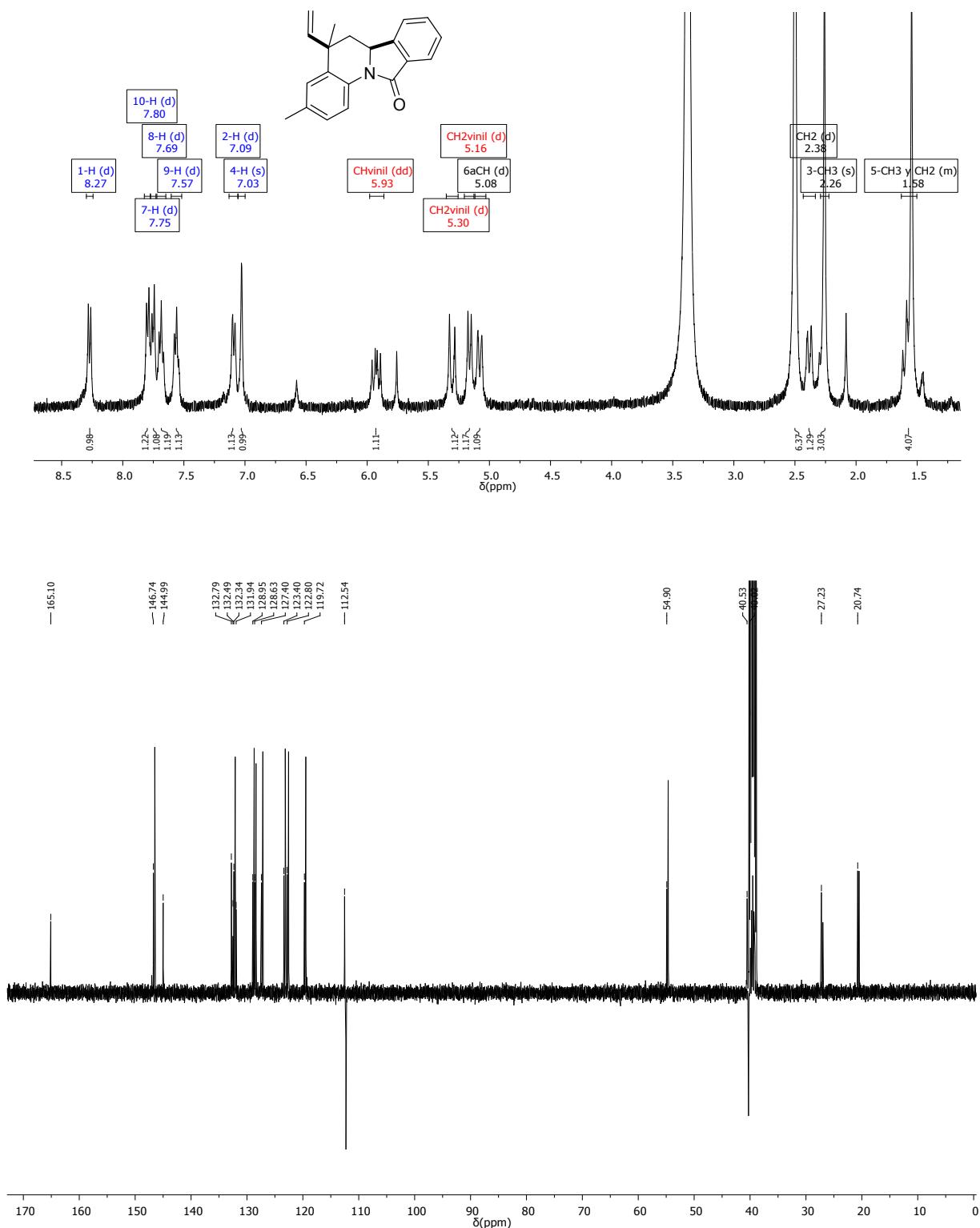




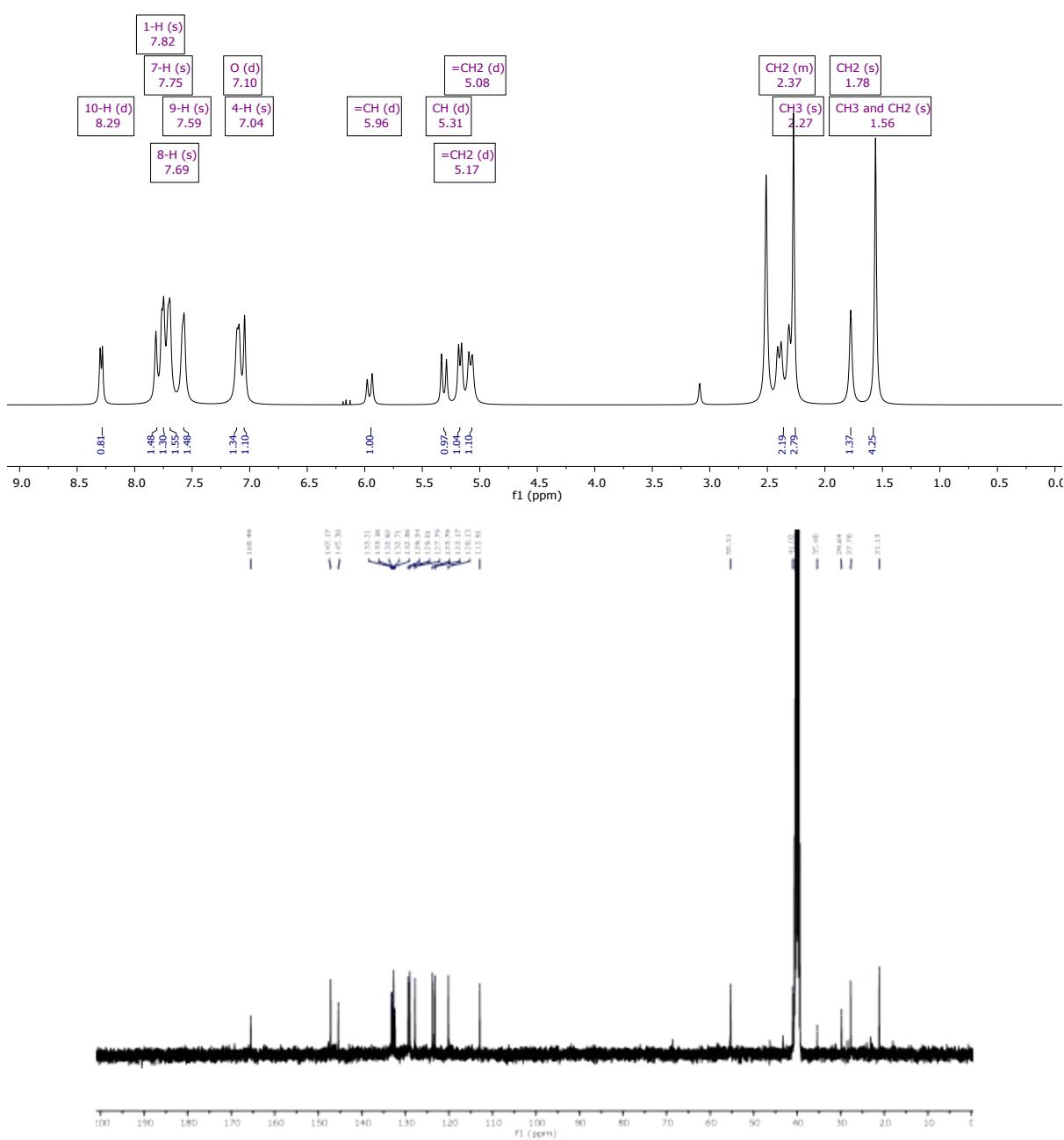
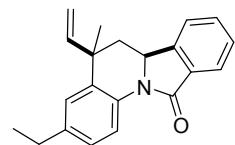
***Trans*-5-methyl-5-vinyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6a)**



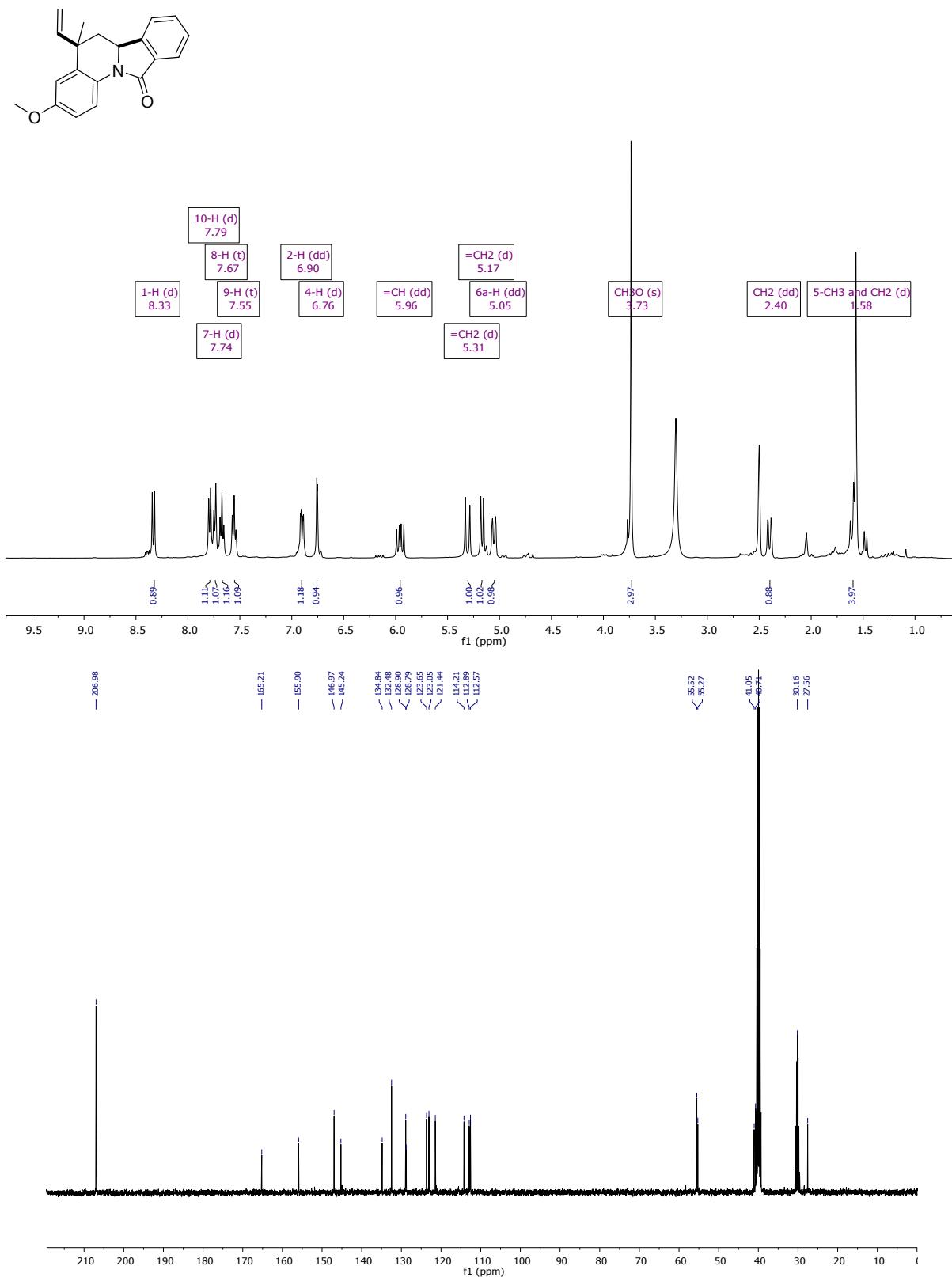
Trans-3,5-dimethyl-5-vinyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6b)



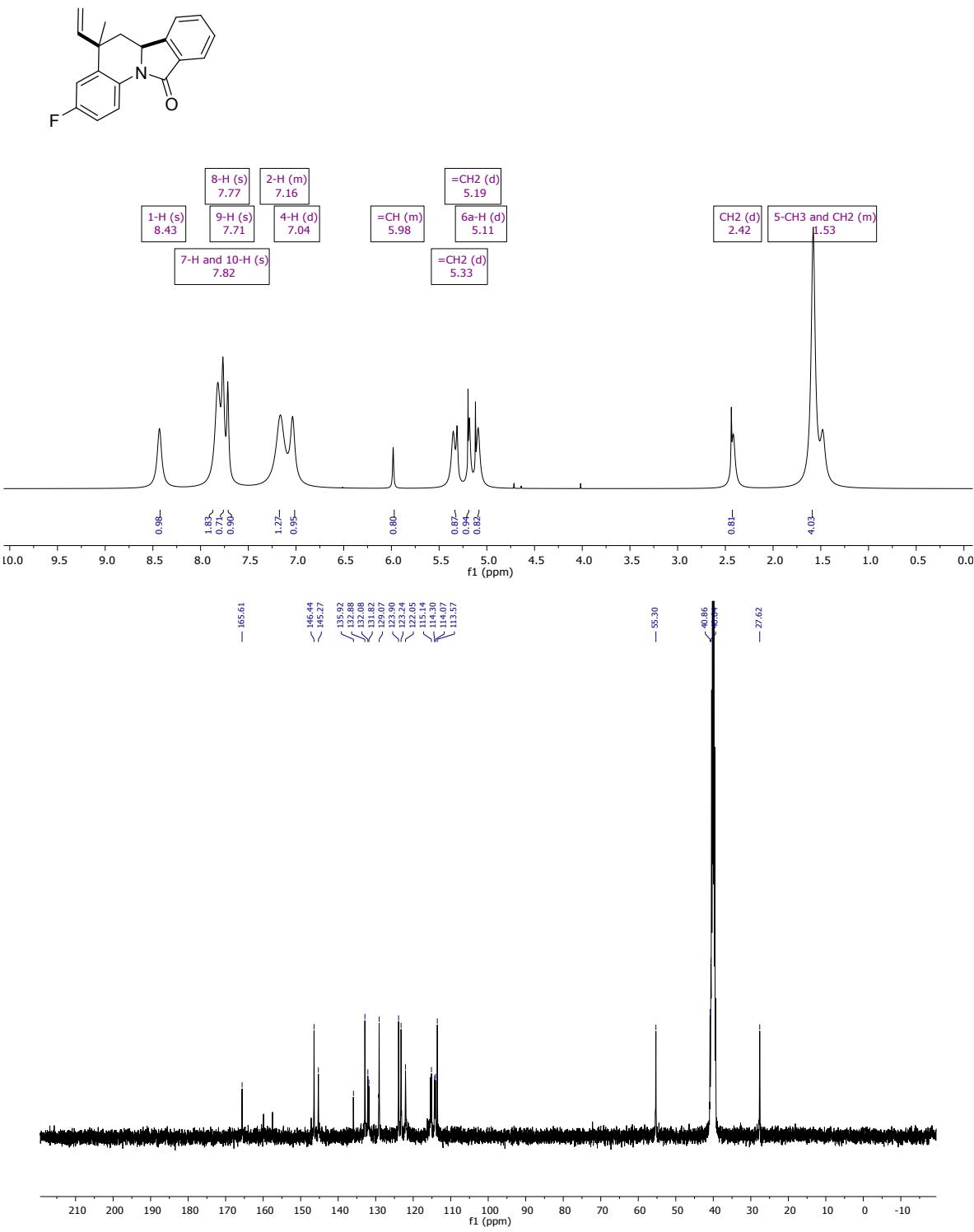
Trans-3-ethyl-5-methyl-5-vinyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6c)



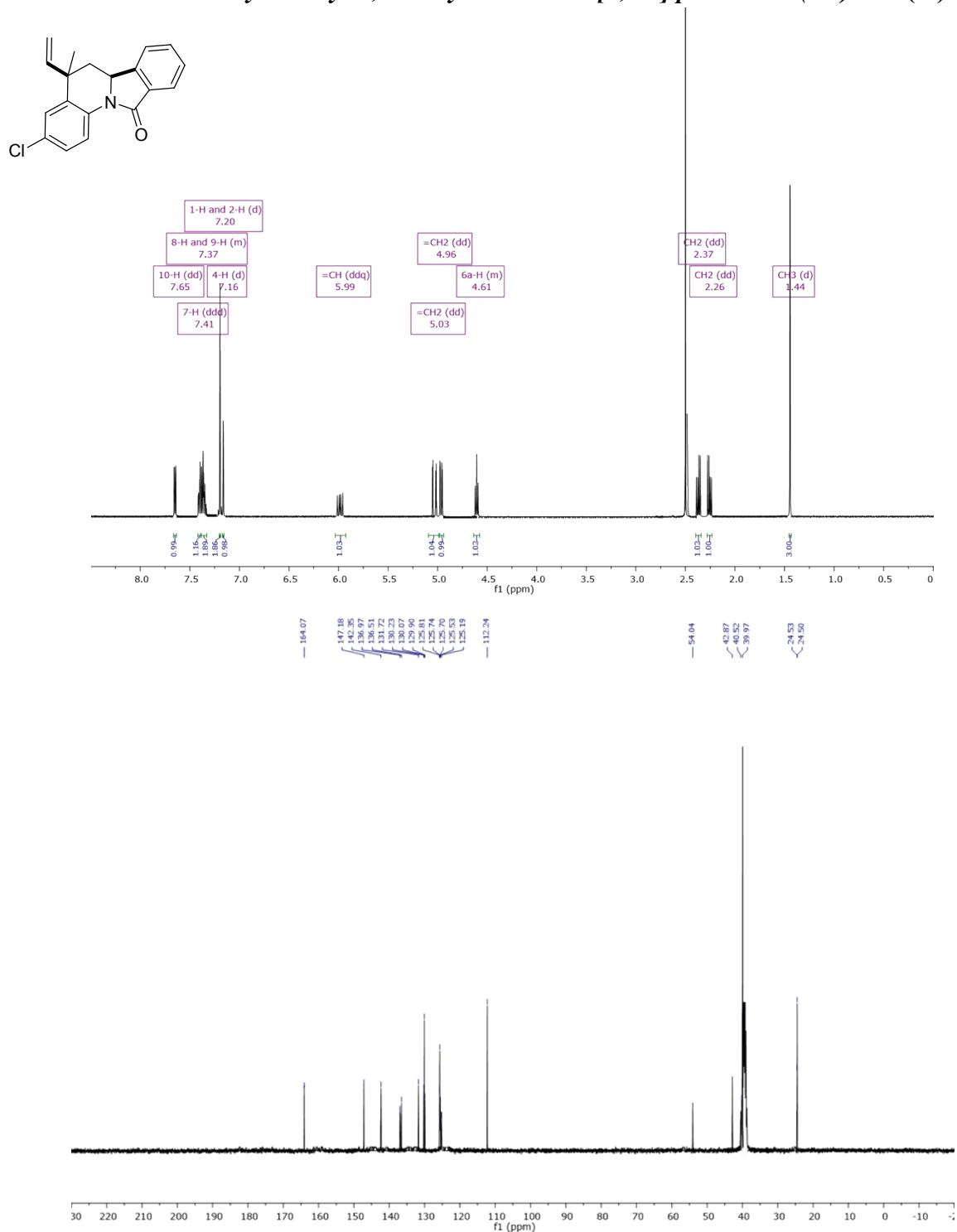
Trans-5-methyl-3-methoxy-5-vinyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6d)



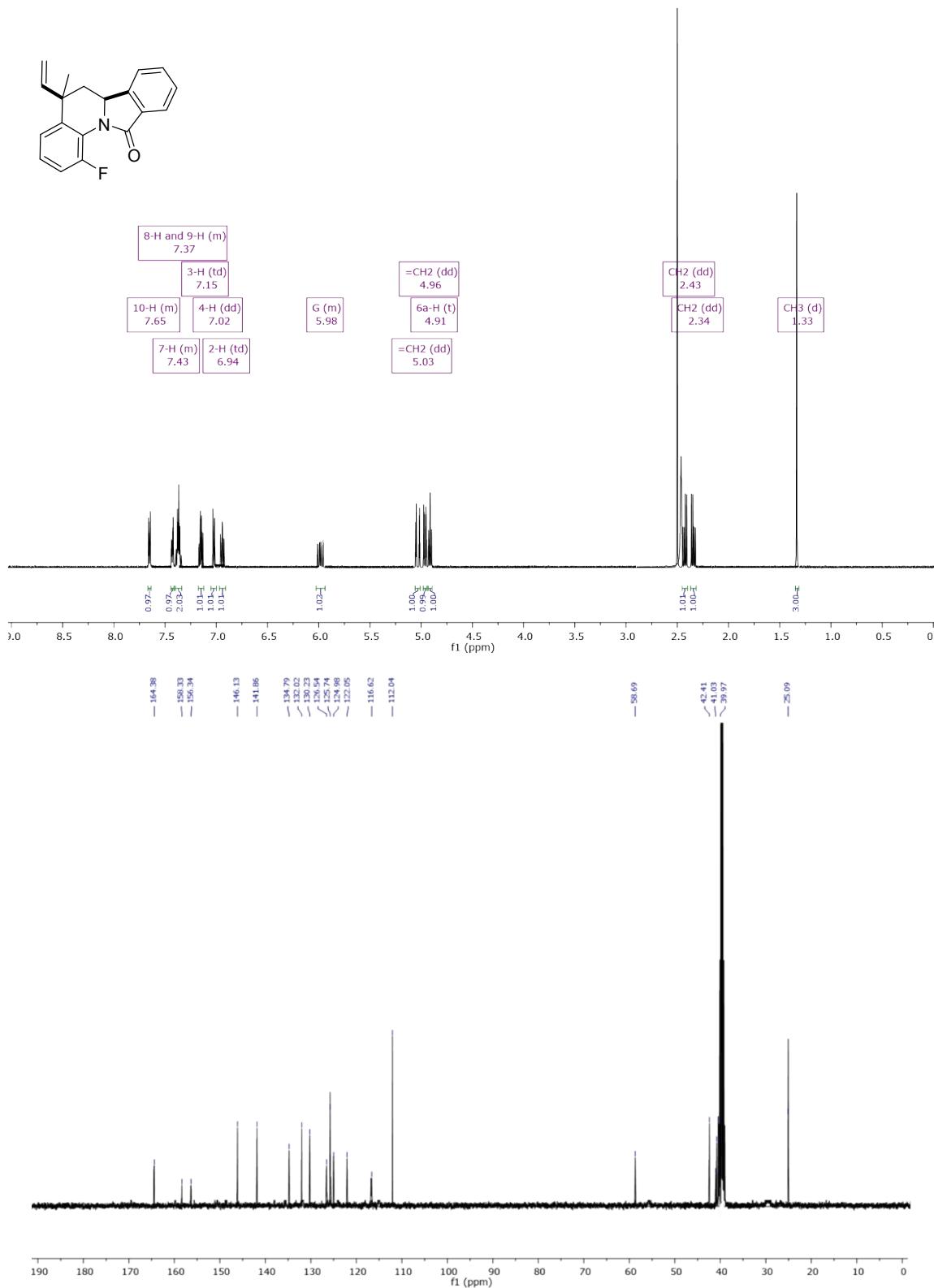
Trans-3-fluor-5-methyl-5-vinyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6e)



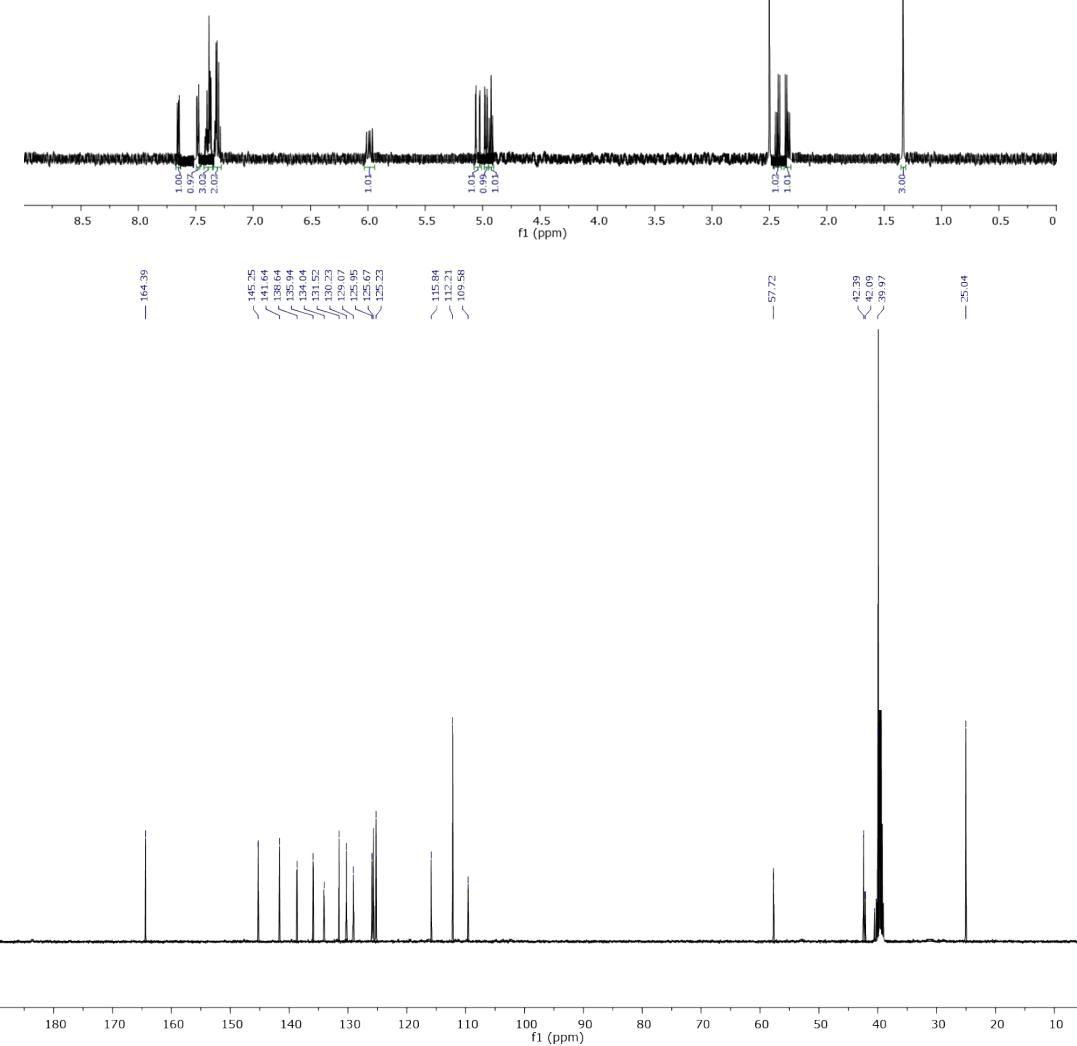
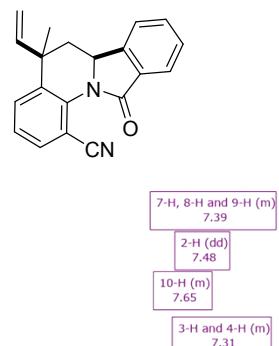
Trans-3-chloro-5-methyl-5-vinyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6f)



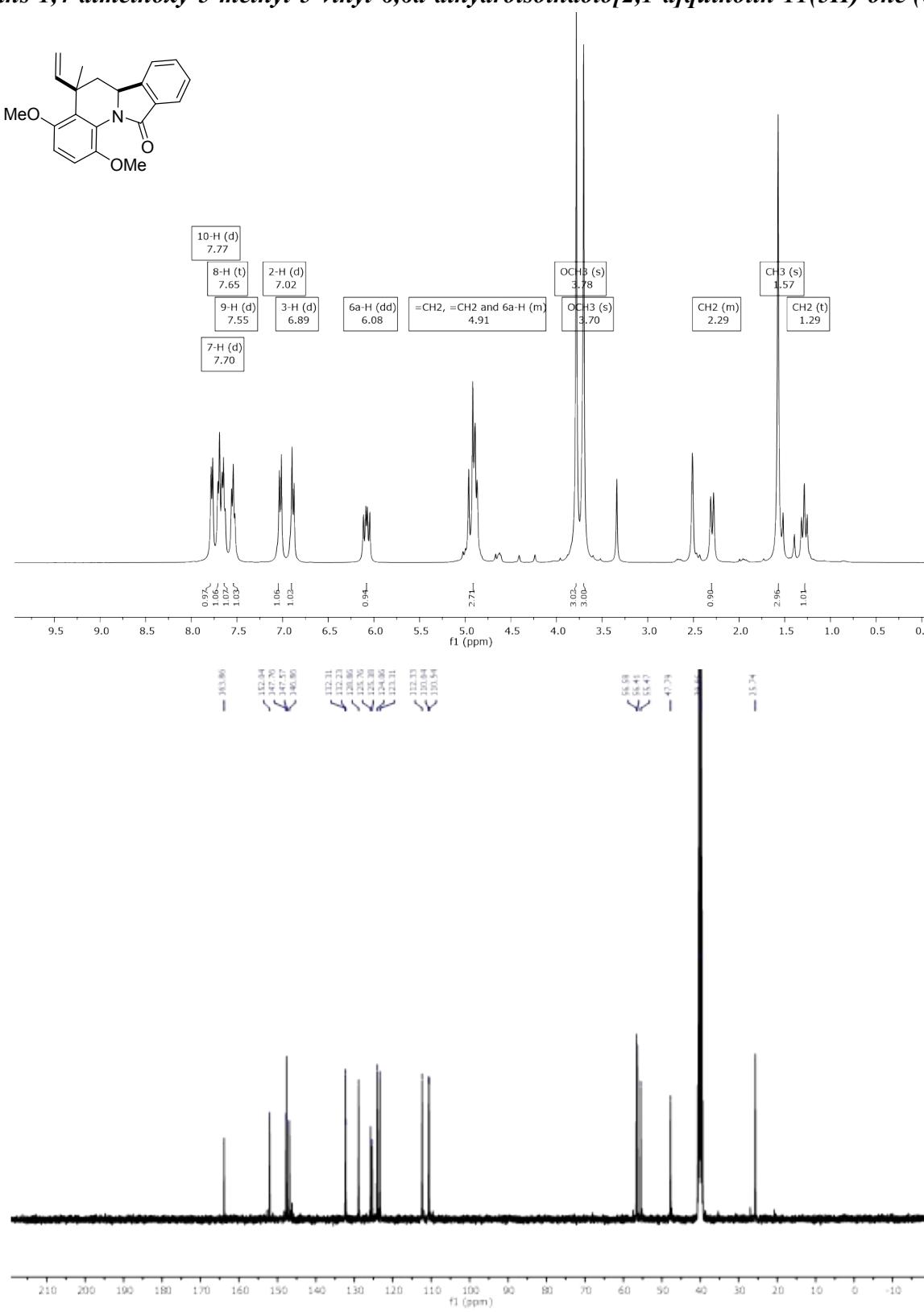
¹H NMR for *trans*-1-fluor-5-methyl-5-vinyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6g)



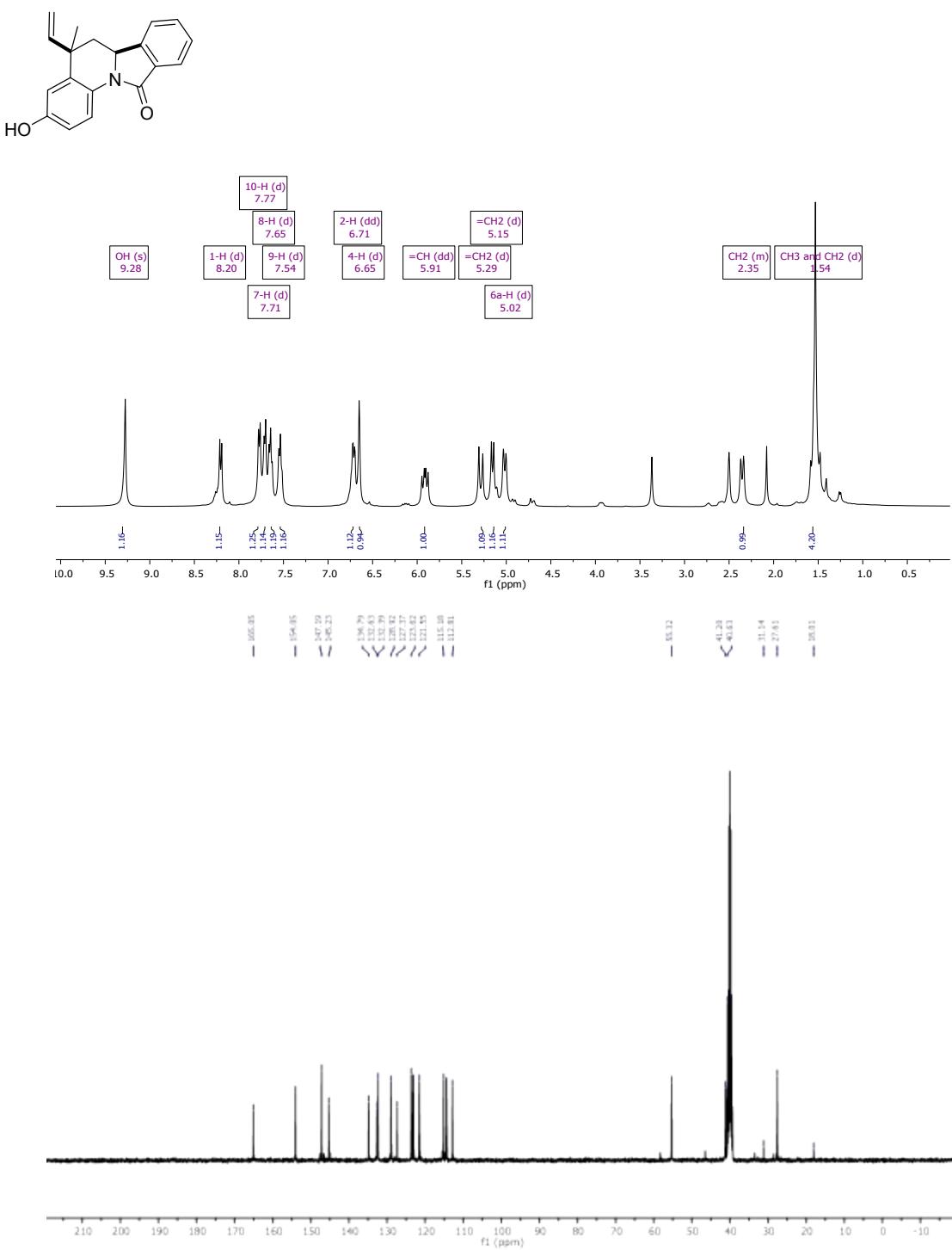
Trans-1-ciano-5-methyl-5-vinyl-6,6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6h)



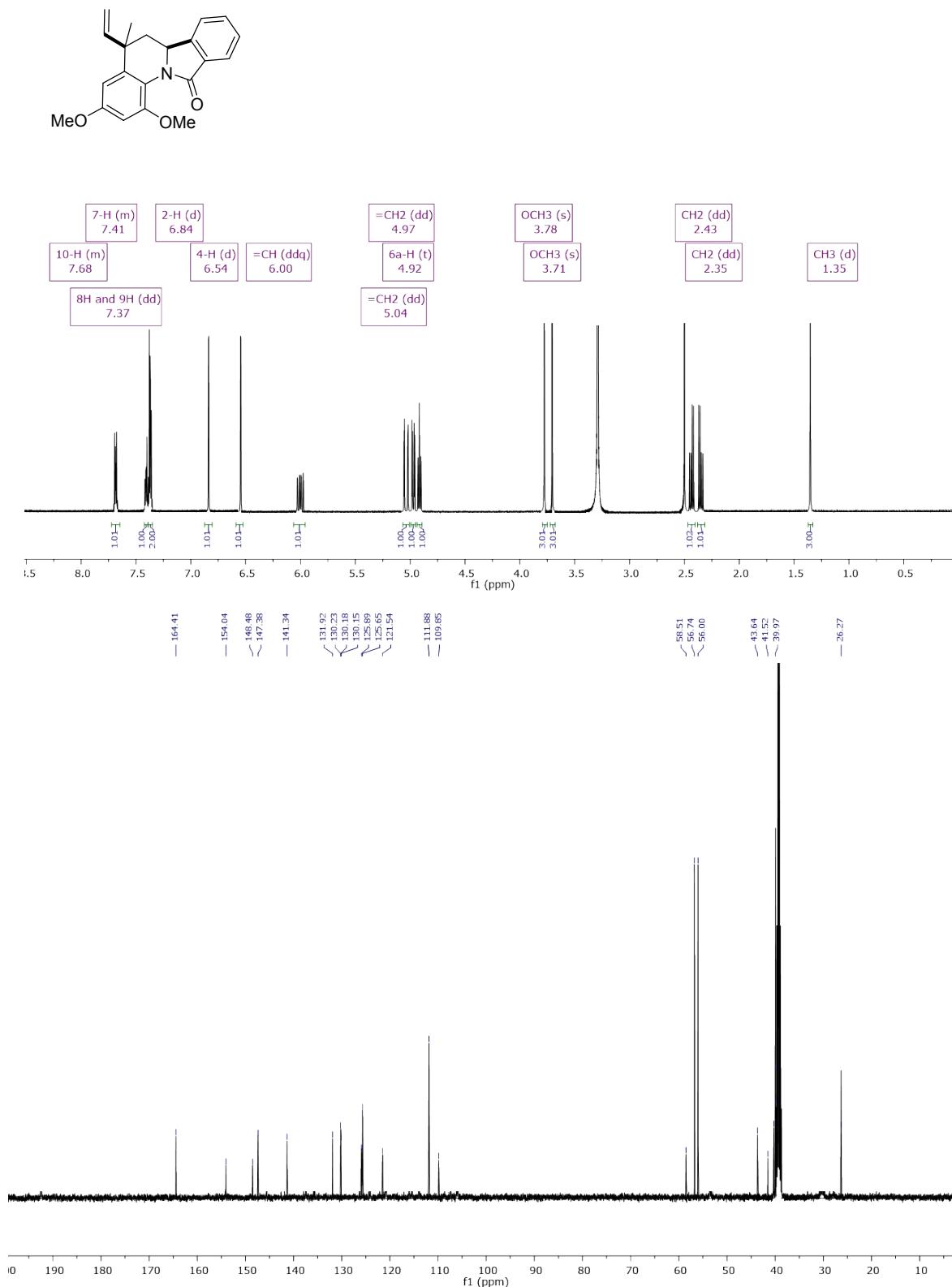
Trans-1,4-dimethoxy-5-methyl-5-vinyl-6a-dihydroisoindolo[2,1-a]quinolin-11(5H)-one (6i)



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-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)

