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Synthesis of novel cytotoxic 3-azolylsteroids *via* Cu-catalyzed C–N coupling

Mikhail J. Parulava, Yury N. Kotovshchikov, Gennadij V. Latyshev, Darina V. Sokolova, Irina P. Beletskaya and Nikolay V. Lukashev

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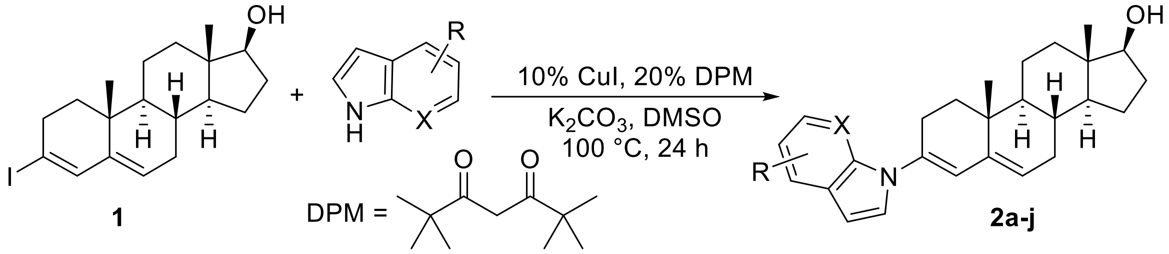
General information

NMR spectra were recorded with Bruker Avance 400, Agilent 400MR (^{1}H 400 MHz, ^{13}C 100 MHz), and Bruker Avance 600 (^{1}H 600 MHz, ^{13}C 150 MHz) spectrometers at ambient temperature. Chemical shifts are presented in ppm (δ scale) and referenced to tetramethylsilane (δ = 0 ppm) in the ^{1}H NMR spectra and to the solvent signal in the ^{13}C NMR spectra. ESI-TOF spectra were recorded with a Thermo Scientific Orbitrap Elite instrument. Column chromatography was carried out on Macherey–Nagel silica gel 60 (0.040–0.063 mm).

Iodosteroid **1** was prepared from testosterone as reported [Kotovshchikov Y. N., Latyshev G. V., Lukashev N. V., Beletskaya I. P. *Eur. J. Org. Chem.* 2013, 7823].

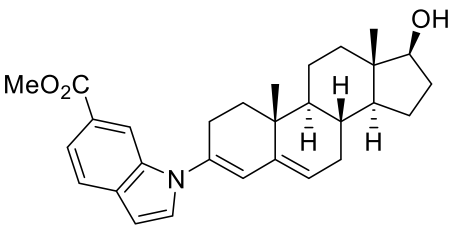
Experimental procedures and analysis data for new compounds

Synthesis of 3-azolylsubstituted steroids 2



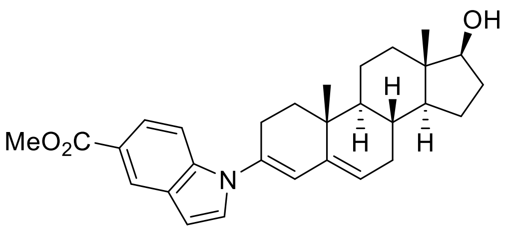
General procedure. In a vial with a screw cap, iodosteroid **1** (59.7 mg, 0.150 mmol), azole (0.180 mmol, 1.2 equiv), anhydrous K_2CO_3 (41.5 mg, 0.300 mmol, 2 equiv), CuI (2.9 mg, 15 μmol, 10 mol%), and dipivaloylmethane (6.3 μl, 30 μmol, 20 mol%) were loaded under an Ar atmosphere in DMSO (0.5 ml). The mixture was stirred at 100 °C for 24 h, then diluted with CH_2Cl_2 (25 ml), and washed with water (5 × 25 ml). The organic layer was dried with anhydrous Na_2SO_4, and the solvents were evaporated *in vacuo*. The residue was purified by column chromatography.

3-[6-(Methoxycarbonyl)-1*H*-indol-1-yl]androsta-3,5-dien-17β-ol (2a)



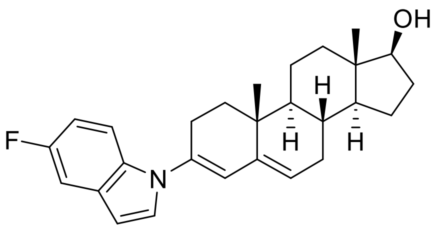
Eluent: hexanes–EtOAc = 2:1. Yield 47.0 mg (70%). Brown solid; mp 123–125 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 [br s, 1H, 7-CH(indole)], 7.80 [dd, J = 8.3, 1.0 Hz, 1H, 5-CH(indole)], 7.63 [d, J = 8.3 Hz, 1H, 4-CH(indole)], 7.35 [d, J = 3.2 Hz, 1H, 2-CH(indole)], 6.60 [d, J = 3.2 Hz, 1H, 3-CH(indole)], 6.21 (m, 1H, 4-CH), 5.56 (m, 1H, 6-CH), 3.93 (s, 3H, CH_3O), 3.68 (t, J = 8.5 Hz, 1H, 17-C*H*OH), 2.69 (m, 1H), 2.54 (m, 1H), 2.26 (m, 1H), 2.09 (m, 1H), 2.01 (m, 1H), 1.89 (m, 1H), 1.82–1.58 (m, 5H), 1.55–1.42 (m, 3H), 1.34 (m, 1H), 1.21–1.00 (m, 3H), 1.12 (s, 3H, 19-CH_3), 0.82 (s, 3H, 18-CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.2 (C=O), 139.9 (quat), 135.0 (quat), 132.6 (2C, quat), 129.7, 125.3, 123.5 (quat), 123.1, 120.9, 120.5, 113.7 [7-CH(indole)], 102.8 [3-CH(indole)], 81.7 (17-CHOH), 52.0 (CH_3O), 51.4, 48.2, 42.8 (quat), 36.5, 34.9 (quat), 33.9, 31.8, 31.5, 30.4, 26.5, 23.3, 20.7, 19.1, 11.1; HRMS (ESI) calcd for $C_{29}H_{36}NO_3$ $[M+H]^+$ 446.2690; found 446.2686.

3-[5-(Methoxycarbonyl)-1*H*-indol-1-yl]androsta-3,5-dien-17β-ol (2b)



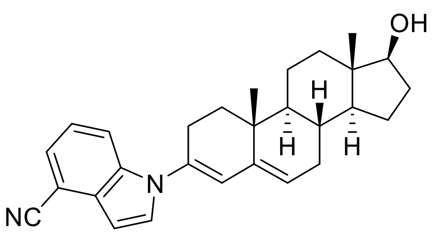
Eluent: hexanes–EtOAc = 2:1. Yield 53.0 mg (79%). Orange solid; mp 141–143 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 [d, J = 1.4 Hz, 1H, 4-CH(indole)], 7.89 [dd, J = 8.8, 1.4 Hz, 1H, 6-CH(indole)], 7.51 [d, J = 8.8 Hz, 1H, 7-CH(indole)], 7.26 [d, J = 3.2 Hz, 1H, 2-CH(indole)], 6.65 [d, J = 3.2 Hz, 1H, 3-CH(indole)], 6.20 (m, 1H, 4-CH), 5.55 (m, 1H, 6-CH), 3.93 (s, 3H, CH_3O), 3.68 (t, J = 8.5 Hz, 1H, 17-C*H*OH), 2.66 (m, 1H), 2.53 (m, 1H), 2.27 (m, 1H), 2.10 (m, 1H), 2.01 (m, 1H), 1.89 (m, 1H), 1.81–1.59 (m, 5H), 1.55–1.41 (m, 3H), 1.33 (m, 1H), 1.20–1.00 (m, 3H), 1.11 (s, 3H, 19-CH_3), 0.82 (s, 3H, 18-CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.0 (C=O), 139.9 (quat), 138.0 (quat), 132.6 (quat), 128.4 (quat), 127.8, 125.2, 123.9, 123.2, 123.0, 121.8 (quat), 110.9 [7-CH(indole)], 104.0 [3-CH(indole)], 81.7 (17-CHOH), 51.8 (CH_3O), 51.4, 48.1, 42.8 (quat), 36.4, 34.9 (quat), 33.8, 31.8, 31.5, 30.4, 26.3, 23.3, 20.7, 19.1, 11.1; HRMS (ESI) calcd for $C_{29}H_{36}NO_3$ $[M+H]^+$ 446.2690; found 446.2690.

3-(5-Fluoro-1*H*-indol-1-yl)androsta-3,5-dien-17β-ol (2c)



Eluent: hexanes–EtOAc = 2:1. Yield 55 mg (90%). Grey solid; mp 148–150 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 [dd, J = 9.0, 4.4 Hz, 1H, 7-CH(indole)], 7.27–7.22 [m, 2H, 2,4-CH(indole)], 6.94 [td, J = 9.1, 2.5 Hz, 1H, 6-CH(indole)], 6.51 [d, J = 3.2 Hz, 1H, 3-CH(indole)], 6.17 (m, 1H, 4-CH), 5.51 (m, 1H, 6-CH), 3.68 (t, J = 8.4 Hz, 1H, 17-C*H*OH), 2.65 (m, 1H), 2.53 (m, 1H), 2.25 (m, 1H), 2.10 (m, 1H), 2.01 (m, 1H), 1.88 (m, 1H), 1.79–1.40 (m, 8H), 1.33 (m, 1H), 1.20–1.00 (m, 3H), 1.10 (s, 3H, 19-CH_3), 0.82 (s, 3H, 18-CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.9 [d, J_{CF} = 235 Hz, CF], 140.1 (quat), 132.9 (quat), 132.2 (quat), 129.3 [d, J_{CF} = 10.1 Hz, 3a-C(indole)], 127.8, 124.6, 122.0, 112.0 [d, J_{CF} = 10.1 Hz, 7-CH(indole)], 110.1 [d, J_{CF} = 26.1 Hz, 4- or 6-CH(indole)], 105.6 [d, J_{CF} = 22.8 Hz, 4- or 6-CH(indole)], 102.5 [d, J_{CF} = 4.2 Hz, 3-CH(indole)], 81.8 (17-CHOH), 51.4, 48.2, 42.9 (quat), 36.5, 34.9 (quat), 33.9, 31.8, 31.5, 30.5, 26.3, 23.3, 20.7, 19.1, 11.1; HRMS (ESI) calcd for $C_{27}H_{33}FNO$ $[M+H]^+$ 406.2541; found 406.2537.

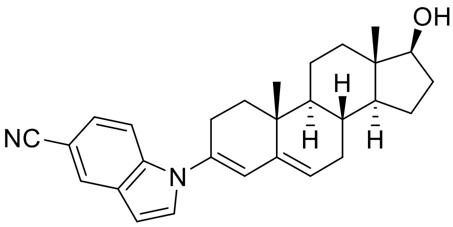
3-(4-Cyano-1*H*-indol-1-yl)androsta-3,5-dien-17β-ol (2d)



Eluent: CH_2Cl_2–MeOH = 20:1. Yield 58.5 mg (95%). Orange solid; mp 167–169 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.71 [dt, J = 8.4, 0.8 Hz, 1H, 5-CH(indole)], 7.46 [dd, J = 7.4, 0.8 Hz, 1H, 7-CH(indole)], 7.37 [d, J = 3.3 Hz, 1H, 2-CH(indole)], 7.22 [dd, J = 8.4, 7.4 Hz, 1H, 6-CH(indole)], 6.78 [dd, J = 3.3, 0.8 Hz, 1H, 3-CH(indole)], 6.17 (m, 1H, 4-CH), 5.56 (m, 1H, 6-CH), 3.69 (t, J = 8.5 Hz, 1H, 17-

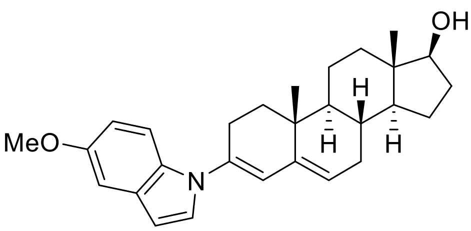
C*H*OH), 2.66 (m, 1H), 2.52 (m, 1H), 2.27 (m, 1H), 2.10 (m, 1H), 2.03 (m, 1H), 1.90 (m, 1H), 1.80–1.43 (m, 8H), 1.34 (m, 1H), 1.21–1.01 (m, 3H), 1.11 (s, 3H, 19-CH_3), 0.82 (s, 3H, 18-CH_3); ^{13}C NMR (150 MHz, $CDCl_3$) δ 139.8 (quat), 135.4 (quat), 132.2 (quat), 130.1 (quat), 129.1, 125.7, 125.3, 123.8, 121.5, 118.6 (quat), 116.0, 103.2 (C≡N), 101.5 [3-CH(indole)], 81.7 (17-CHOH), 51.4, 48.1, 42.9 (quat), 36.5, 34.9 (quat), 33.8, 31.8, 31.5, 30.4, 26.5, 23.3, 20.7, 19.1, 11.1; HRMS (ESI) calcd for $C_{28}H_{33}N_2O$ $[M+H]^+$ 413.2587; found 413.2595.

3-(5-Cyano-1*H*-indol-1-yl)androsta-3,5-dien-17β-ol (2e)



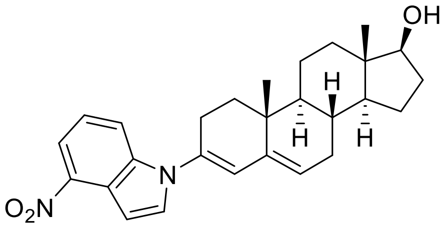
Eluent: CH_2Cl_2–MeOH = 20:1. Yield 54.4 mg (88%). Orange solid; mp 226–228 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.96 [m, 1H, 4-CH(indole)], 7.53 [m, 1H, 7-CH(indole)], 7.42 [dd, *J* = 8.6, 1.6 Hz, 1H, 6-CH(indole)], 7.31 [d, *J* = 3.3 Hz, 1H, 2-CH(indole)], 6.64 [dd, *J* = 3.3, 0.7 Hz, 1H, 3-CH(indole)], 6.18 (m, 1H, 4-CH), 5.57 (m, 1H, 6-CH), 3.69 (t, *J* = 8.5 Hz, 1H, 17-C*H*OH), 2.66 (m, 1H), 2.51 (m, 1H), 2.28 (m, 1H), 2.11 (m, 1H), 2.03 (m, 1H), 1.90 (m, 1H), 1.80–1.43 (m, 8H), 1.35 (m, 1H), 1.20–1.02 (m, 3H), 1.11 (s, 3H, 19-CH_3), 0.83 (s, 3H, 18-CH_3); ^{13}C NMR (150 MHz, $CDCl_3$) δ 139.8 (quat), 137.2 (quat), 132.2 (quat), 128.8, 128.6 (quat), 126.5, 125.9, 124.8, 124.0, 120.6 (quat), 112.0 [7-CH(indole)], 103.4 [3-CH(indole)], 102.9 (C≡N), 81.7 (17-CHOH), 51.4, 48.2, 42.9 (quat), 36.5, 34.9 (quat), 33.8, 31.8, 31.5, 30.5, 26.4, 23.3, 20.8, 19.1, 11.1; HRMS (ESI) calcd for $C_{28}H_{33}N_2O$ $[M+H]^+$ 413.2587; found 413.2589.

3-(5-Methoxy-1*H*-indol-1-yl)androsta-3,5-dien-17β-ol (2f)



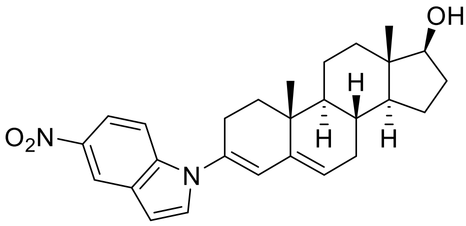
Eluent: hexanes–EtOAc = 2:1. Yield 39.0 mg (62%). Yellow solid; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.44 [d, *J* = 9.0 Hz, 1H, 7-CH(indole)], 7.19 [d, *J* = 3.2 Hz, 1H, 2-CH(indole)], 7.07 [d, *J* = 2.5 Hz, 1H, 4-CH(indole)], 6.85 [dd, *J* = 9.0, 2.5 Hz, 1H, 6-CH(indole)], 6.48 [d, *J* = 3.2 Hz, 1H, 3-CH(indole)], 6.18 (m, 1H, 4-CH), 5.50 (m, 1H, 6-CH), 3.85 (s, 3H, CH_3O), 3.68 (t, *J* = 8.4 Hz, 1H, 17-C*H*OH), 2.64 (m, 1H), 2.56 (m, 1H), 2.25 (m, 1H), 2.10 (m, 1H), 2.00 (m, 1H), 1.88 (m, 1H), 1.79–1.39 (m, 8H), 1.33 (m, 1H), 1.20–1.01 (m, 3H), 1.10 (s, 3H, 19-CH_3), 0.82 (s, 3H, 18-CH_3); ^{13}C NMR (150 MHz, $CDCl_3$) δ 154.2 [5-C(indole)], 140.3 (quat), 133.3 (quat), 130.9 (quat), 129.6 (quat), 126.7, 124.0, 121.1, 112.3, 112.0, 102.6, 102.4, 81.8 (17-CHOH), 55.8 (CH_3O), 51.5, 48.3, 42.9 (quat), 36.5, 35.0 (quat), 34.0, 31.9, 31.5, 30.5, 26.3, 23.4, 20.8, 19.1, 11.1; HRMS (ESI) calcd for $C_{28}H_{36}NO_2$ $[M+H]^+$ 418.2741; found 418.2737.

3-(4-Nitro-1*H*-indol-1-yl)androsta-3,5-dien-17β-ol (2g)



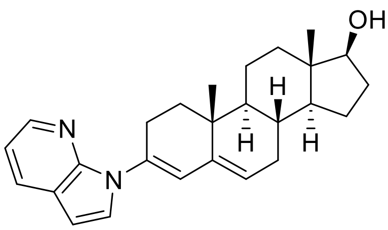
Eluent: CH_2Cl_2–MeOH = 20:1. Yield 61.0 mg (94%). Yellow solid; mp 242–244 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.13 [d, J = 8.1 Hz, 1H, 5-CH(indole)], 7.79 [d, J = 8.1 Hz, 1H, 7-CH(indole)], 7.43 [d, J = 3.2 Hz, 1H, 2- or 3-CH(indole)], 7.31 [d, J = 3.2 Hz, 1H, 2- or 3-CH(indole)], 7.26 [t, J = 8.1 Hz, 1H, 6-CH(indole)], 6.18 (m, 1H, 4-CH), 5.58 (m, 1H, 6-CH), 3.69 (t, J = 8.5 Hz, 1H, 17-C*H*OH), 2.67 (m, 1H), 2.52 (m, 1H), 2.27 (m, 1H), 2.11 (m, 1H), 2.03 (m, 1H), 1.90 (m, 1H), 1.89–1.60 (m, 5H), 1.54–1.44 (m, 3H), 1.35 (m, 1H), 1.20–1.02 (m, 3H), 1.12 (s, 3H, 19-CH_3), 0.83 (s, 3H, 18-CH_3); ^{13}C NMR (150 MHz, $CDCl_3$) δ 140.4 (quat), 139.7 (quat), 137.9 (quat), 132.1 (quat), 130.9, 126.2, 124.7, 122.9 (quat), 120.7, 117.88, 117.85, 103.0 [3-CH(indole)], 81.7 (17-CHOH), 51.4, 48.2, 42.9 (quat), 36.5, 34.9 (quat), 33.8, 31.8, 31.5, 30.5, 26.7, 23.3, 20.8, 19.1, 11.1; HRMS (ESI) calcd for $C_{27}H_{33}N_2O_3$ $[M+H]^+$ 433.2486; found 433.2485.

3-(5-Nitro-1*H*-indol-1-yl)androsta-3,5-dien-17β-ol (2h)



Eluent: CH_2Cl_2–MeOH = 20:1. Yield 62.5 mg (96%). Yellow solid; mp 227–229 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.57 [d, J = 2.2 Hz, 1H, 4-CH(indole)], 8.08 [dd, J = 9.1, 2.2 Hz, 1H, 6-CH(indole)], 7.50 [d, J = 9.1 Hz, 1H, 7-CH(indole)], 7.34 [d, J = 3.3 Hz, 1H, 2-CH(indole)], 6.74 [d, J = 3.3 Hz, 1H, 3-CH(indole)], 6.20 (m, 1H, 4-CH), 5.59 (m, 1H, 6-CH), 3.69 (t, J = 8.5 Hz, 1H, 17-C*H*OH), 2.68 (m, 1H), 2.52 (m, 1H), 2.28 (m, 1H), 2.11 (m, 1H), 2.04 (m, 1H), 1.90 (m, 1H), 1.81–1.43 (m, 8H), 1.35 (m, 1H), 1.21–1.02 (m, 3H), 1.12 (s, 3H, 19-CH_3), 0.83 (s, 3H, 18-CH_3); ^{13}C NMR (150 MHz, $CDCl_3$) δ 141.8 (quat), 139.7 (quat), 138.4 (quat), 132.2 (quat), 129.7, 128.1 (quat), 126.2, 124.2, 118.1, 117.5, 111.1 [7-CH(indole)], 104.9 [3-CH(indole)], 81.7 (17-CHOH), 51.4, 48.2, 42.9 (quat), 36.5, 34.9 (quat), 33.8, 31.8, 31.6, 30.5, 26.4, 23.3, 20.8, 19.1, 11.1; HRMS (ESI) calcd for $C_{27}H_{33}N_2O_3$ $[M+H]^+$ 433.2486; found 433.2470.

3-(1*H*-Pyrrolo[2,3-*b*]pyridin-1-yl)androsta-3,5-dien-17β-ol (2j)



Eluent: CH_2Cl_2–MeOH = 20:1. Yield 31.1 mg (53%). White solid; mp 161–163 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.34 [dd, J = 4.7, 1.6 Hz, 1H, 6-CH(azaindole)], 7.88 [dd, J = 7.8, 1.6 Hz, 1H, 4-CH(azaindole)], 7.33 [d, J = 3.6 Hz, 1H, 2-CH(azaindole)], 7.06 [dd, J = 7.8, 4.7 Hz, 1H, 5-CH(azaindole)], 6.57 (m, 1H, 4-CH), 6.48 [d, J = 3.6 Hz, 1H, 3-CH(azaindole)], 5.57 (m, 1H, 6-CH), 3.68 (t, J = 8.5 Hz, 1H, 17-C*H*OH), 2.93 (m, 1H), 2.83 (m, 1H), 2.25 (m, 1H), 2.09 (m, 1H), 2.01 (m, 1H), 1.88 (m, 1H), 1.78–1.59 (m, 5H), 1.54–1.44 (m, 3H), 1.33 (m, 1H), 1.19–1.01 (m, 3H), 1.11 (s, 3H, 19-CH_3), 0.81 (s, 3H, 18-CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.7 (quat), 143.0 [6-CH(azaindole)], 140.3 (quat), 133.0 (quat), 128.7, 127.1, 124.3, 121.7 (quat), 121.0, 116.1, 100.5 [3-CH(azaindole)], 81.8 (17-CHOH), 51.4, 48.2, 42.9 (quat), 36.5, 34.9 (quat), 33.9, 31.8, 31.6, 30.5, 25.7, 23.3, 20.7, 19.2, 11.1; HRMS (ESI) calcd for $C_{26}H_{33}N_2O$ $[M+H]^+$ 389.2587; found 389.2593.

Cell lines and cell viability assay

We used the methyl thiazolyl tetrazolium (MTT) method to measure the cytotoxic activity of the compounds against human ovarian (SKOV-3), breast (MCF-7), and prostate (DU-145 and PC-3) cancer cell lines. Cell lines were obtained from the ATCC. The cells were trypsinized, counted and seeded at the density of 5×10^4 cells per ml in 96-well plates. After 24 h, the cells were treated with serial dilutions of the samples. Each sample was initially dissolved in DMSO and further diluted in medium to produce different concentrations (0.1–50 μM). The final mixture used for treating the cells contained not more than 0.5% of the solvent (DMSO), the same as in the solvent-control wells. Cells not treated with compounds served as negative control. After 72 h exposition with compounds, MTT (5 mg ml^{-1}) was added to the cells, and the cells were incubated at 37 °C for 3-4 h in the dark. Subsequently, DMSO was added and was incubated for 10 min. The absorbance was measured at 540 nm using microplate reader *Tirerteck Multiscan MCC/340* (Flow Lab., USA). Cell survival in the control was considered 100% and all other groups were normalized to this value using formula:

$$\text{\% live cells} = \frac{\text{treated absorbance} - \text{control media absorbance}}{\text{control absorbance} - \text{control media absorbance}} \times 100\%$$

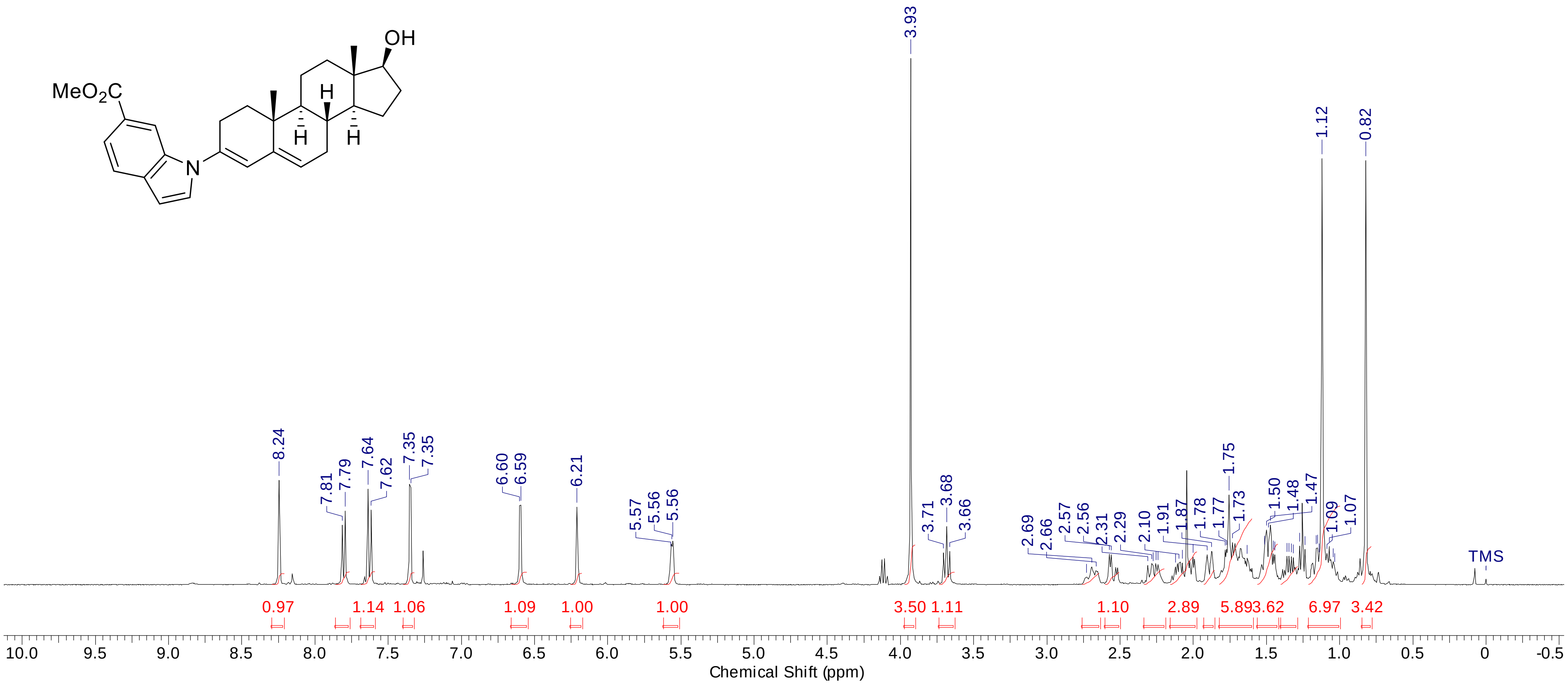
Results expressed as (IC_{50}), the drug concentration that inhibited 50% cell growth.

Statistical analysis. All experiments were carried out in triplicate. The inhibitory concentration 50% (IC_{50}) was calculated by nonlinear regression curve with the use of *Prism Graphpad* version 4.0 for Windows.

Copies of NMR spectra

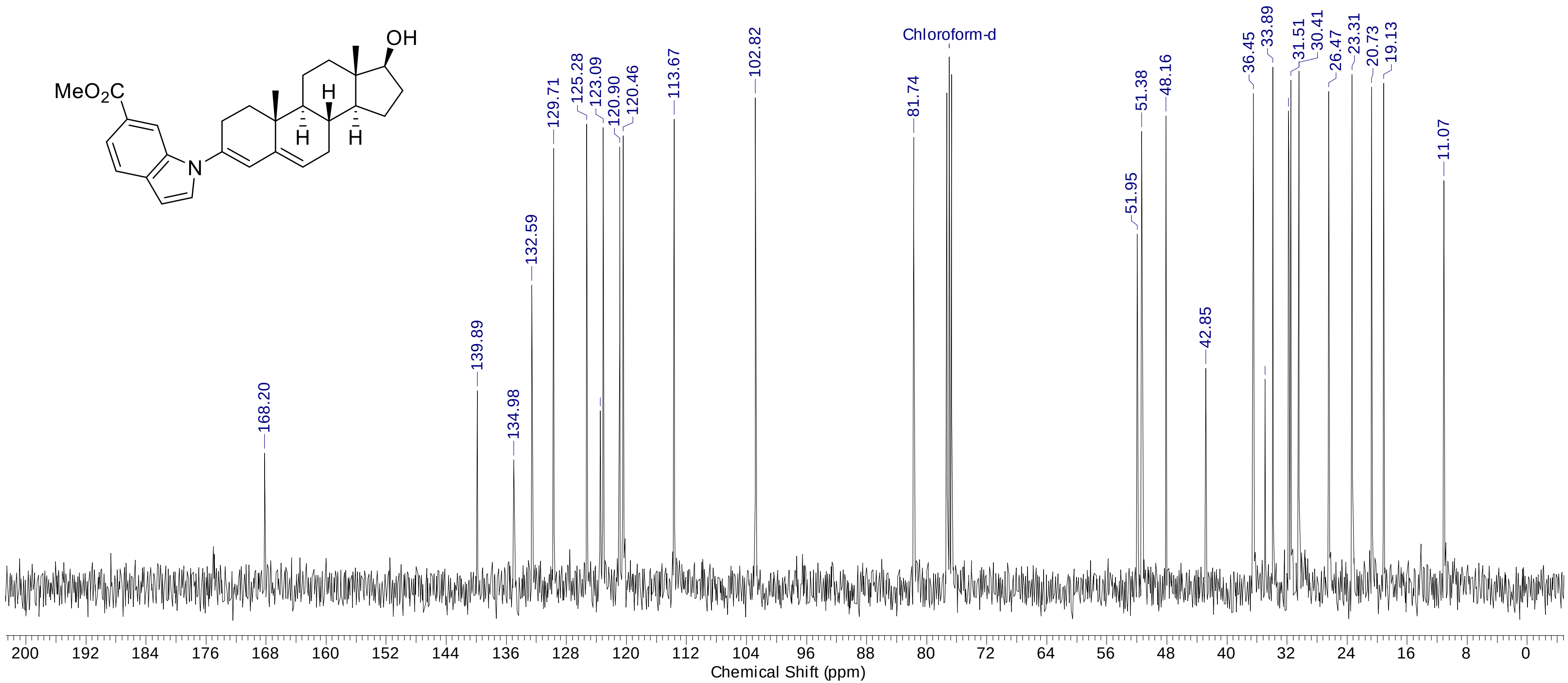
3-[6-(Methoxycarbonyl)-1*H*-indol-1-yl]androsta-3,5-dien-17β-ol (2a)

^{1}H NMR (400 MHz, $CDCl_3$)



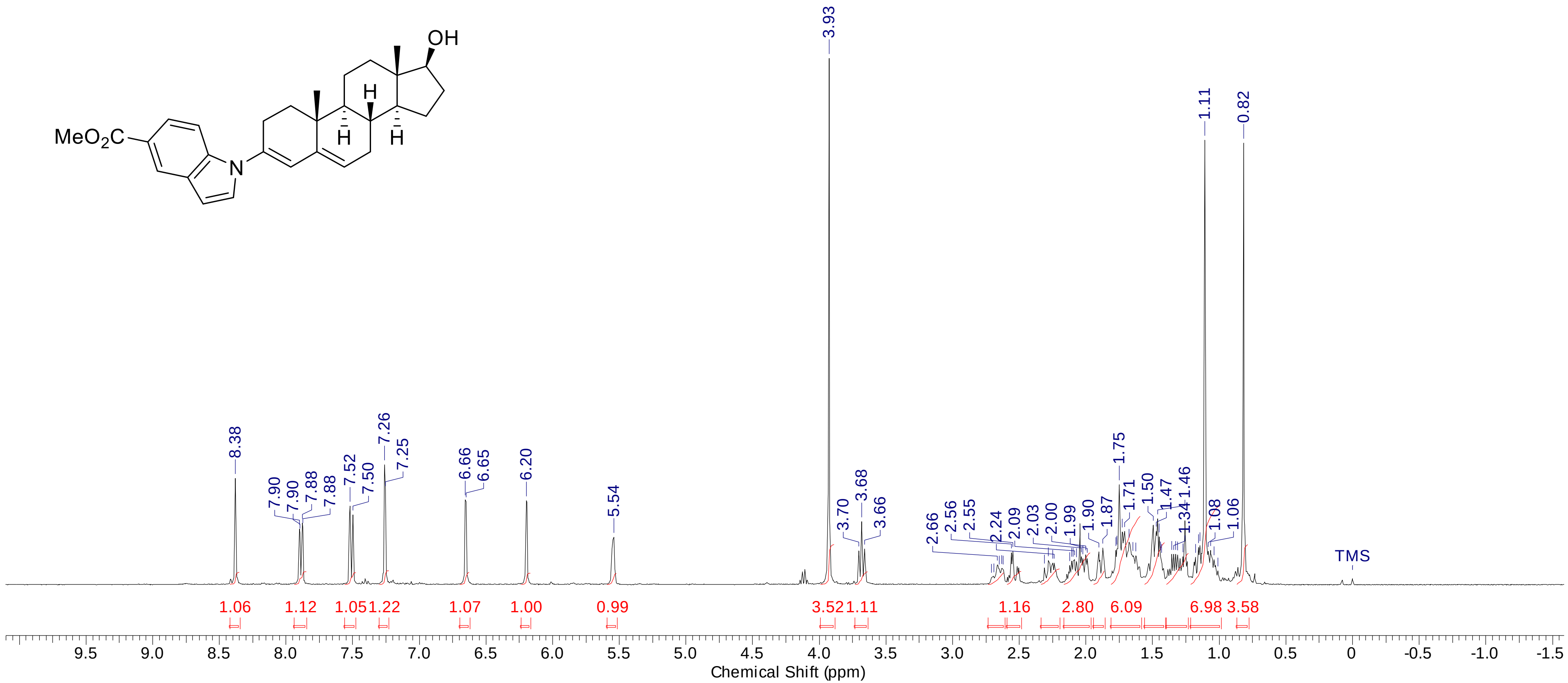
3-[6-(Methoxycarbonyl)-1*H*-indol-1-yl]androsta-3,5-dien-17β-ol (2a)

^{13}C NMR (100 MHz, $CDCl_3$)



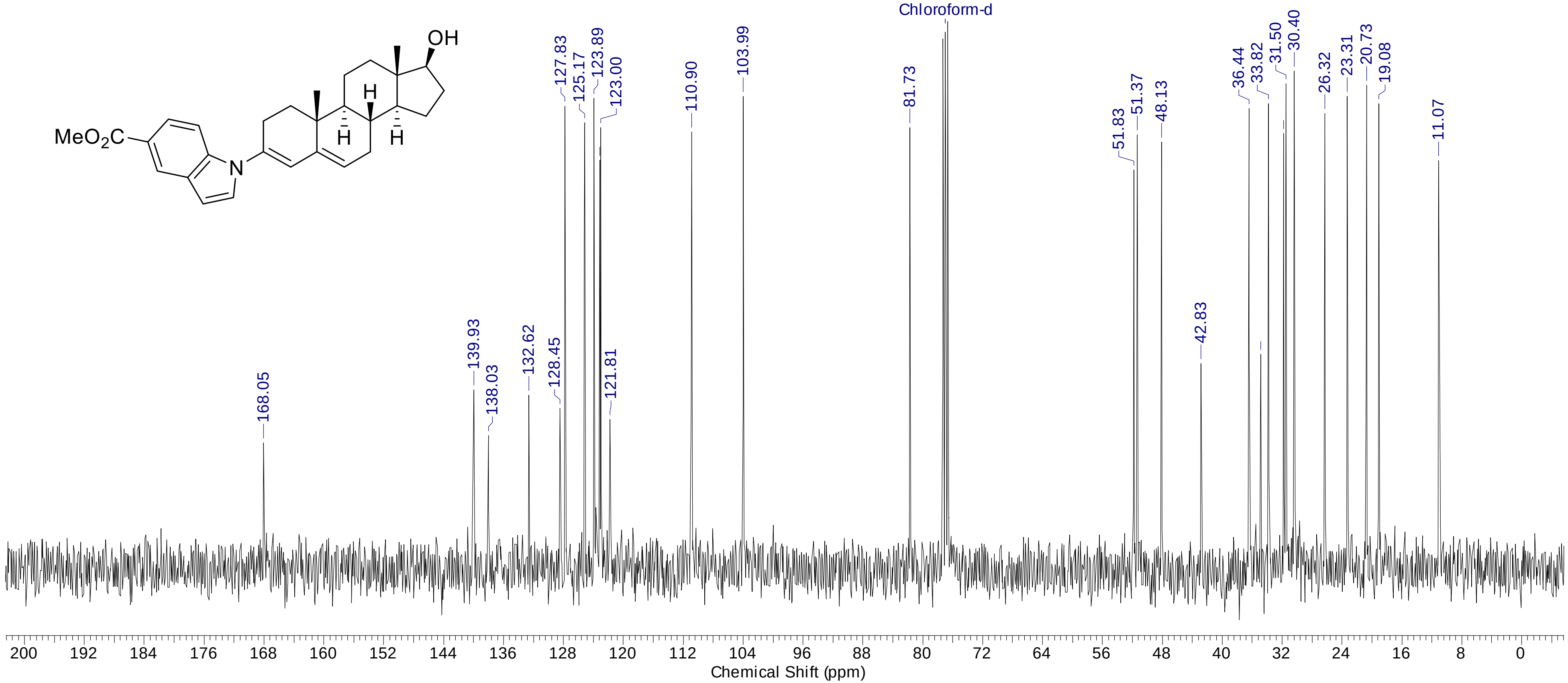
3-[5-(Methoxycarbonyl)-1*H*-indol-1-yl]androsta-3,5-dien-17β-ol (2b)

^{1}H NMR (400 MHz, $CDCl_3$)



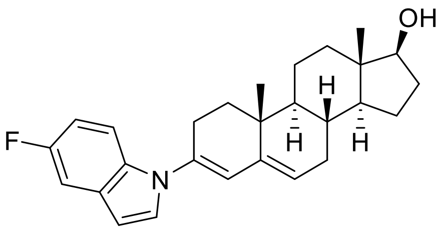
3-[5-(Methoxycarbonyl)-1*H*-indol-1-yl]androsta-3,5-dien-17β-ol (2b)

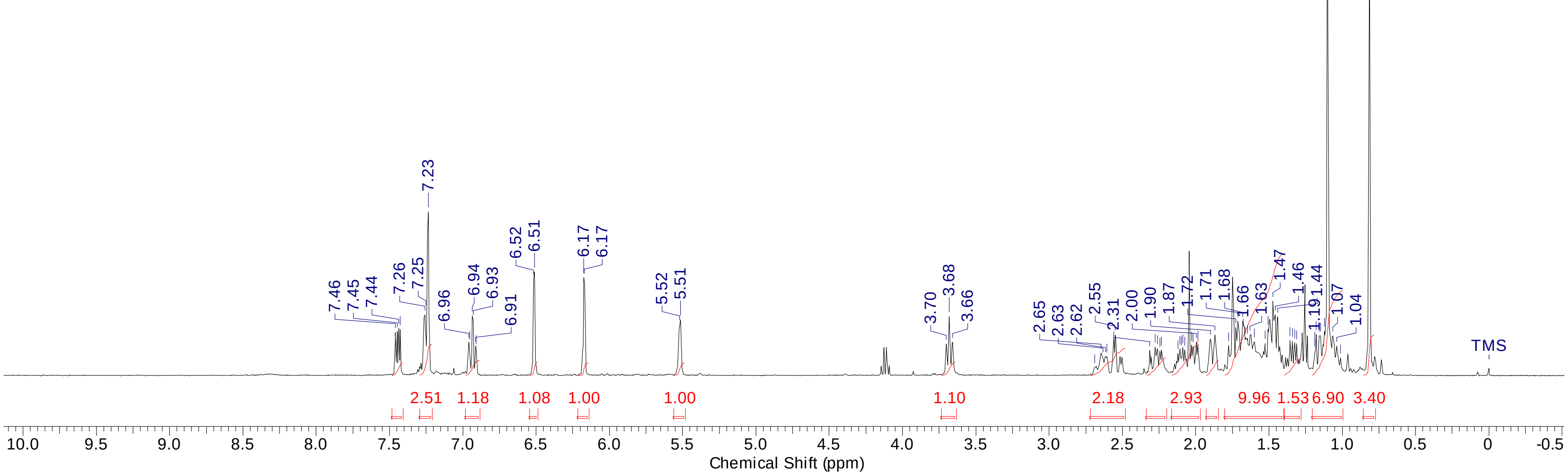
^{13}C NMR (100 MHz, $CDCl_3$)



3-(5-Fluoro-1*H*-indol-1-yl)androsta-3,5-dien-17β-ol (2c)

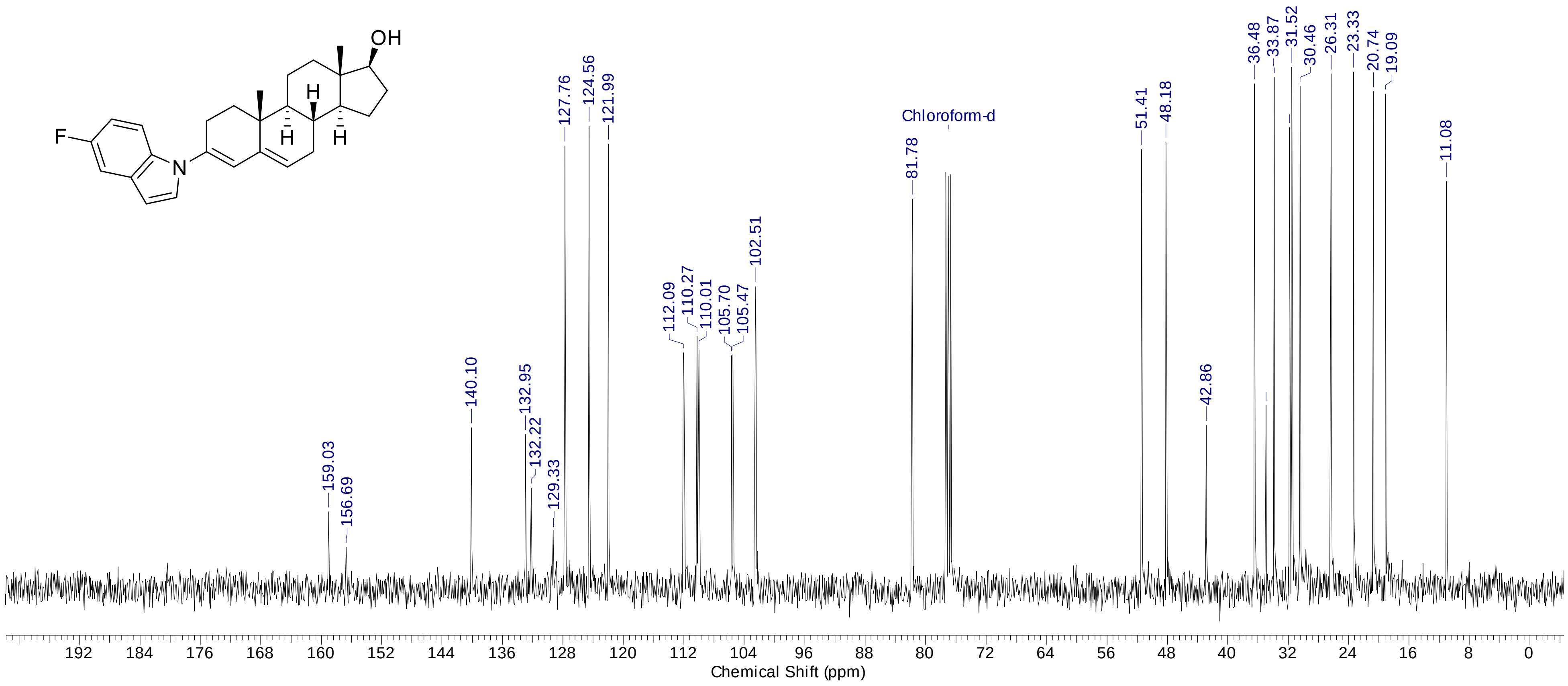
^{1}H NMR (400 MHz, $CDCl_3$)





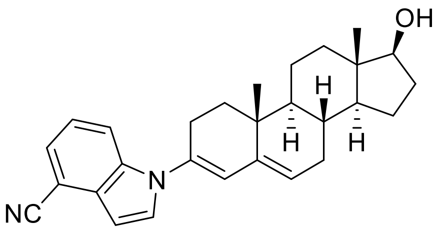
3-(5-Fluoro-1*H*-indol-1-yl)androsta-3,5-dien-17β-ol (2c)

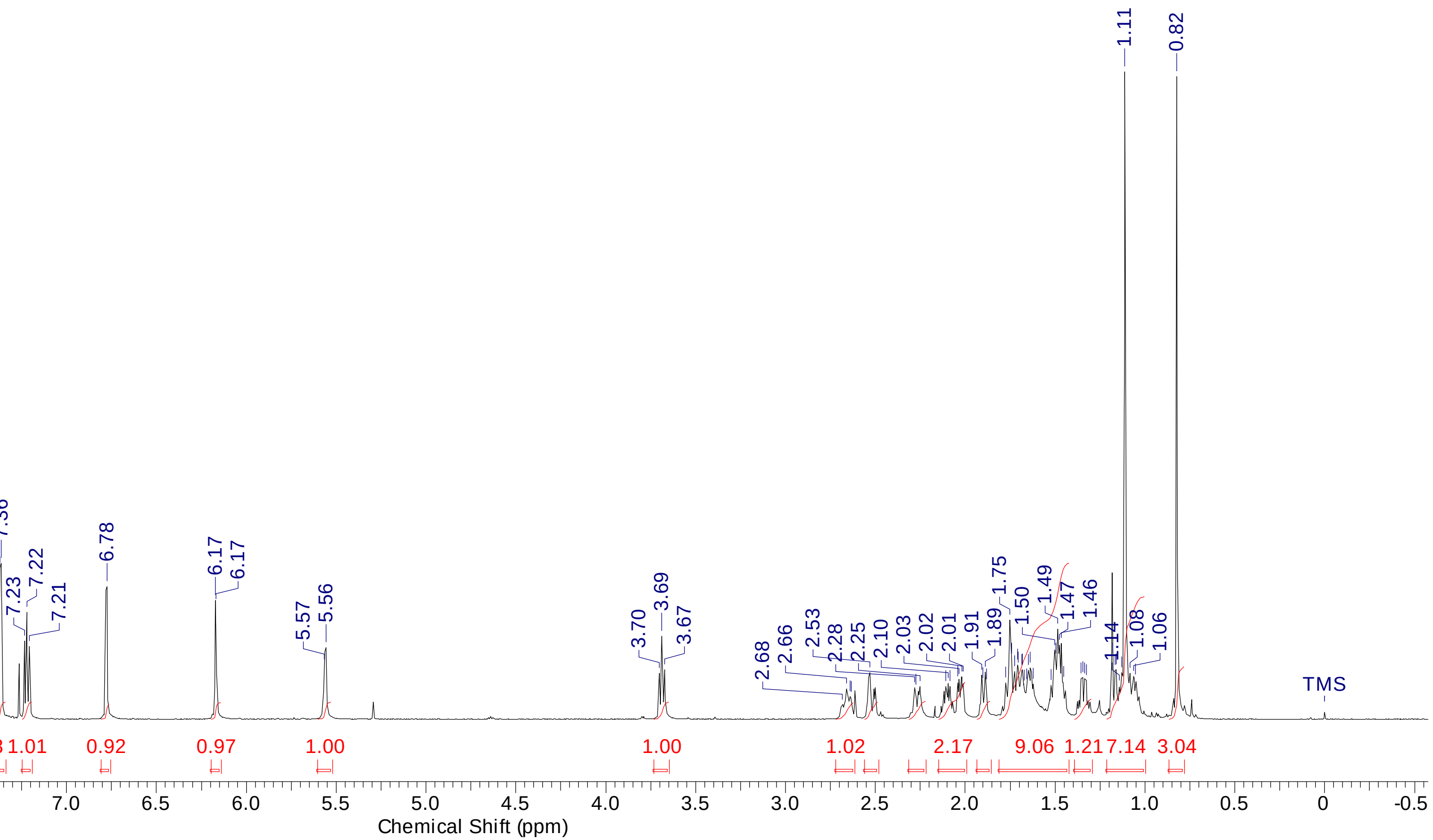
^{13}C NMR (100 MHz, $CDCl_3$)



3-(4-Cyano-1*H*-indol-1-yl)androsta-3,5-dien-17β-ol (2d)

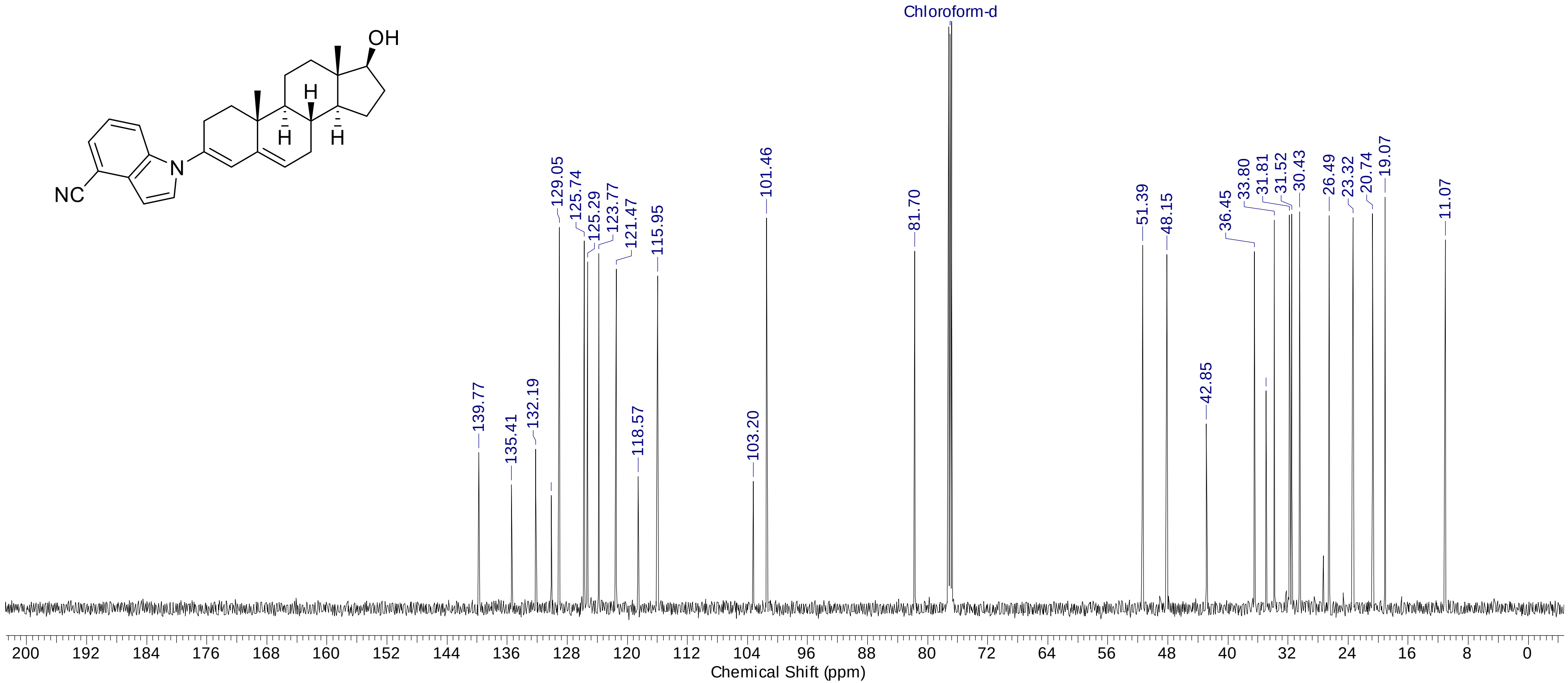
^{1}H NMR (600 MHz, $CDCl_3$)





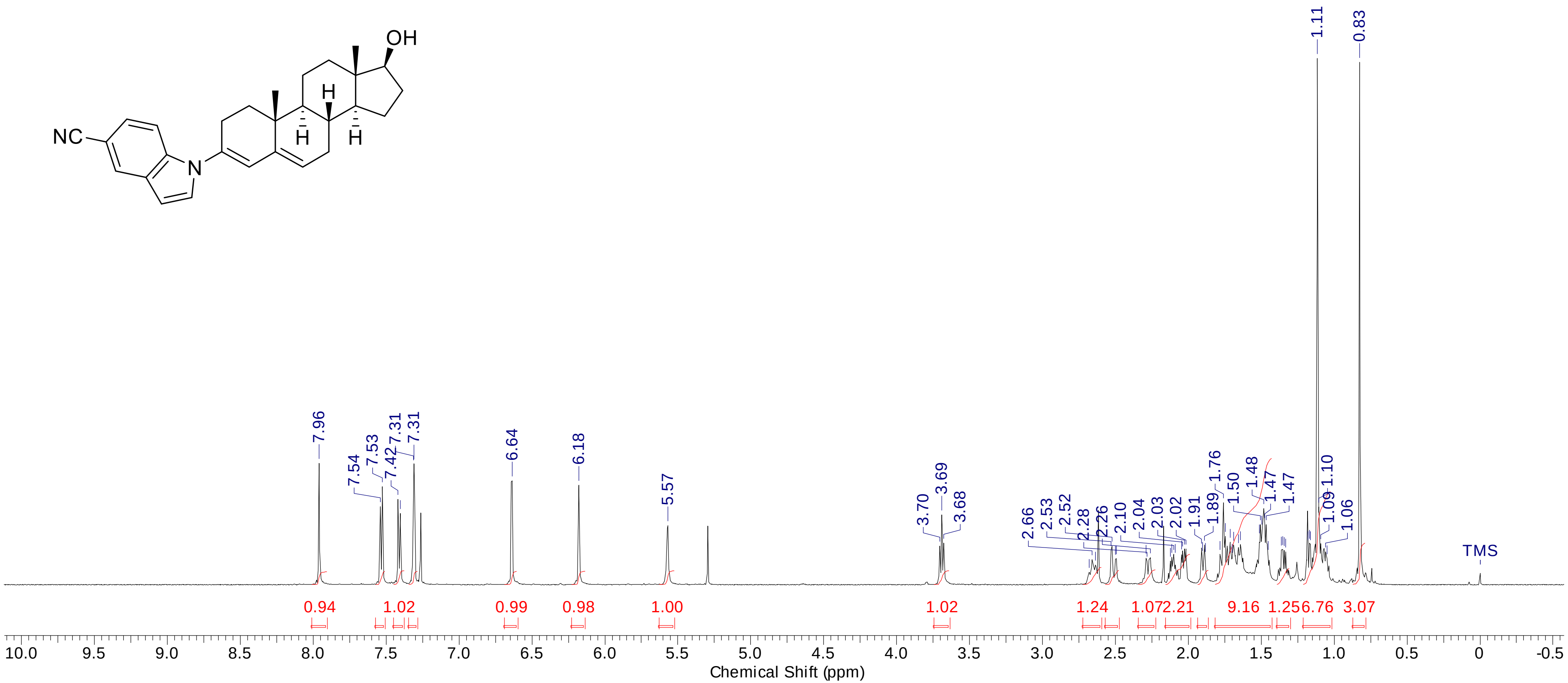
3-(4-Cyano-1*H*-indol-1-yl)androsta-3,5-dien-17β-ol (2d)

^{13}C NMR (150 MHz, $CDCl_3$)



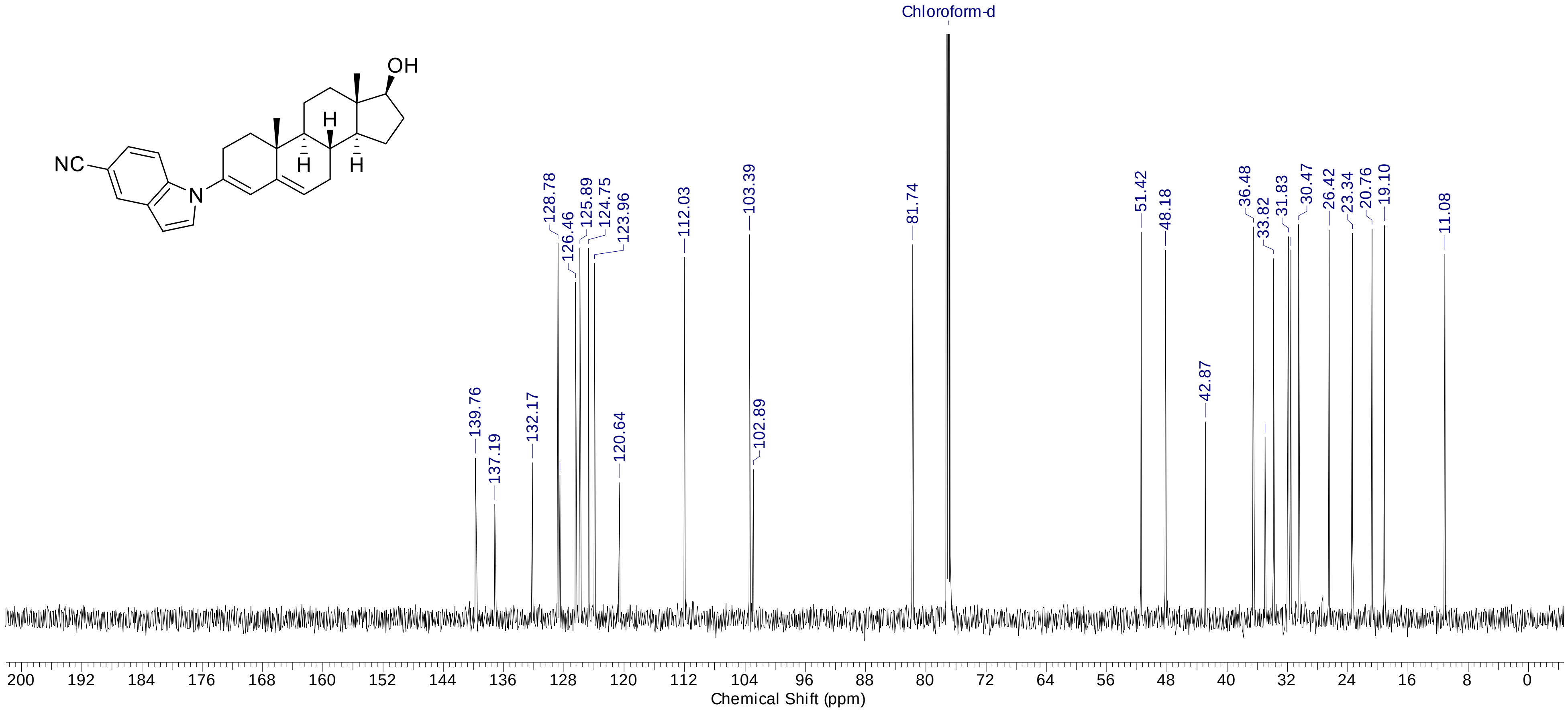
3-(5-Cyano-1*H*-indol-1-yl)androsta-3,5-dien-17β-ol (2e)

^{1}H NMR (600 MHz, $CDCl_3$)



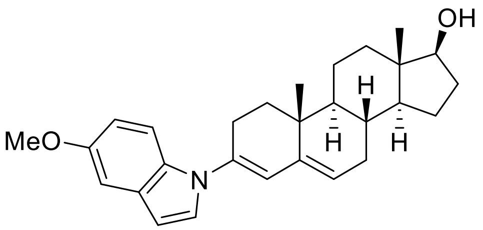
3-(5-Cyano-1*H*-indol-1-yl)androsta-3,5-dien-17β-ol (2e)

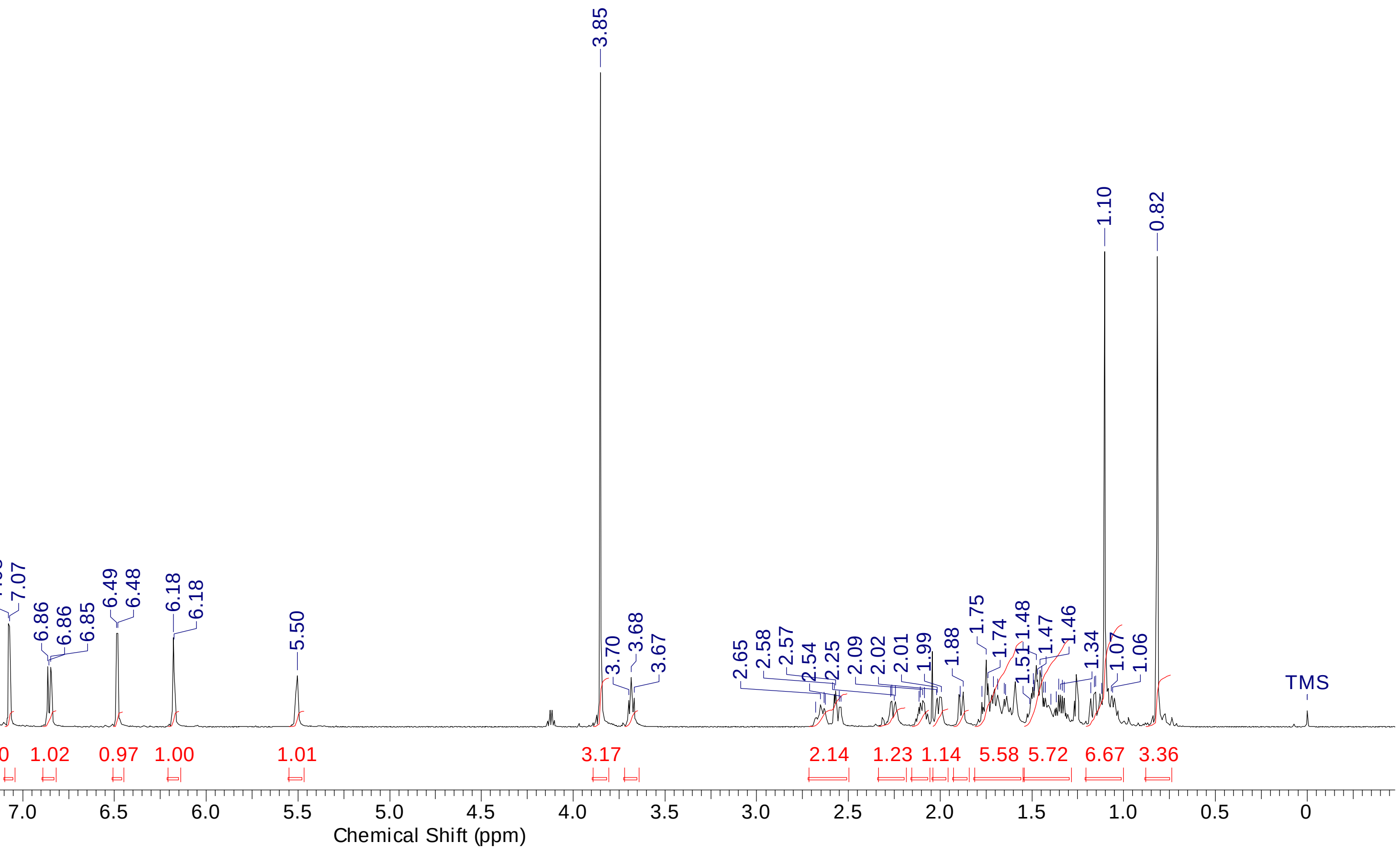
^{13}C NMR (150 MHz, $CDCl_3$)



3-(5-Methoxy-1*H*-indol-1-yl)androsta-3,5-dien-17β-ol (2f)

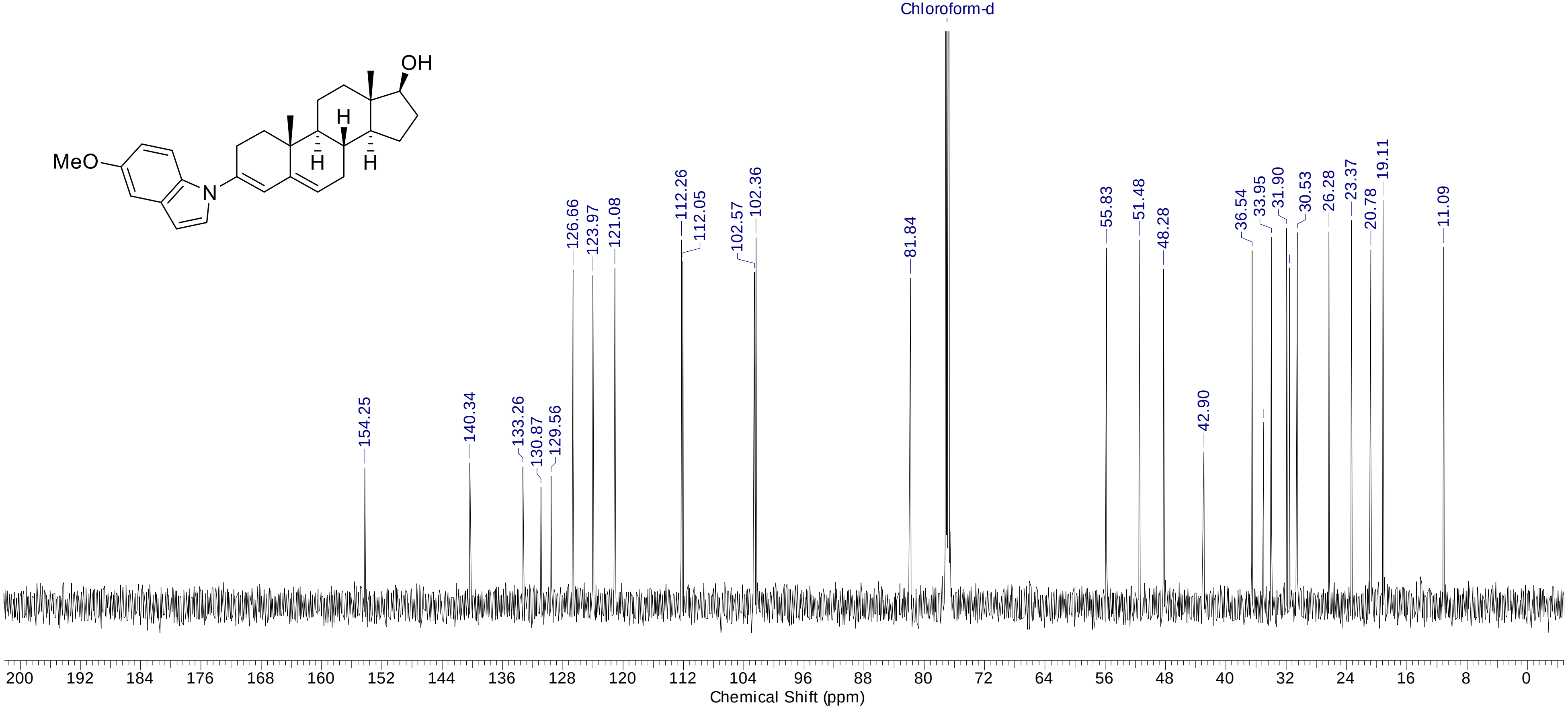
^{1}H NMR (600 MHz, $CDCl_3$)





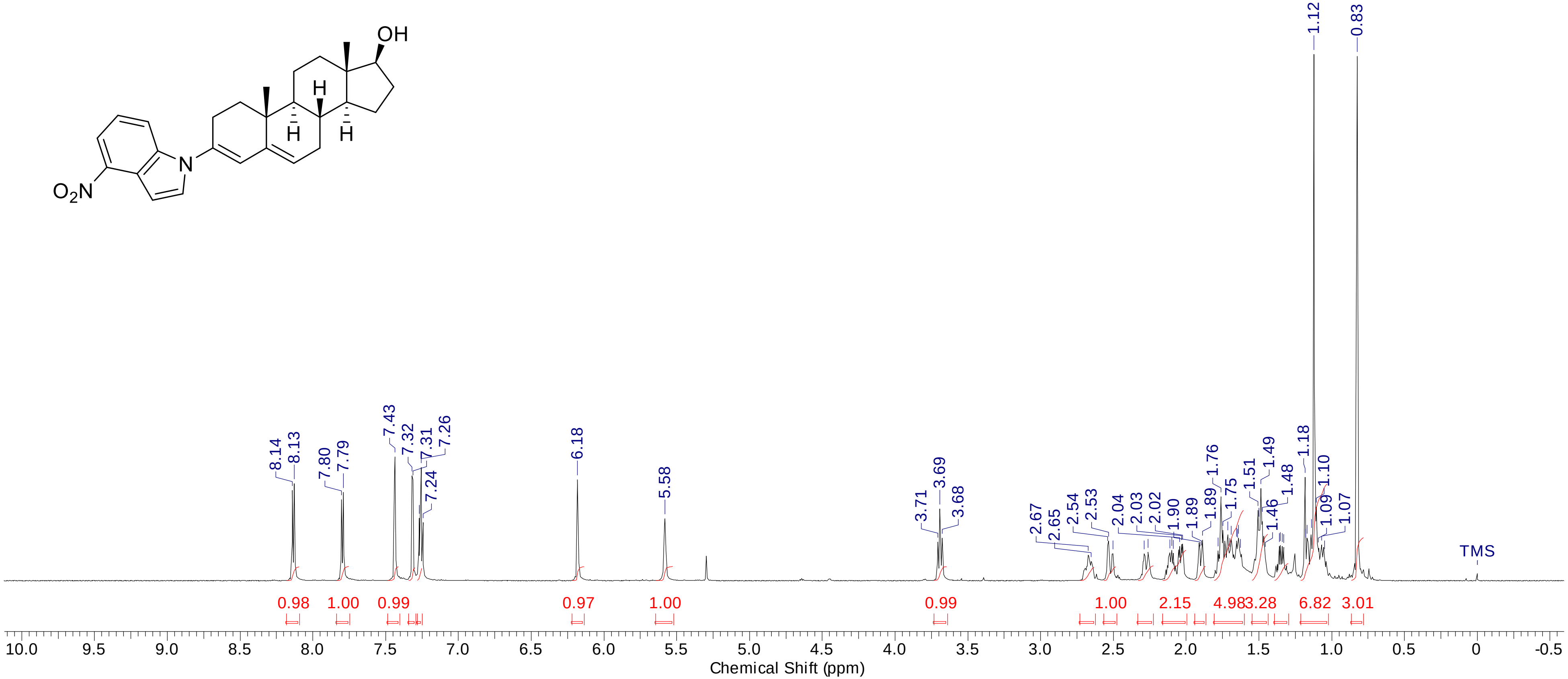
3-(5-Methoxy-1*H*-indol-1-yl)androsta-3,5-dien-17β-ol (2f)

^{13}C NMR (150 MHz, $CDCl_3$)



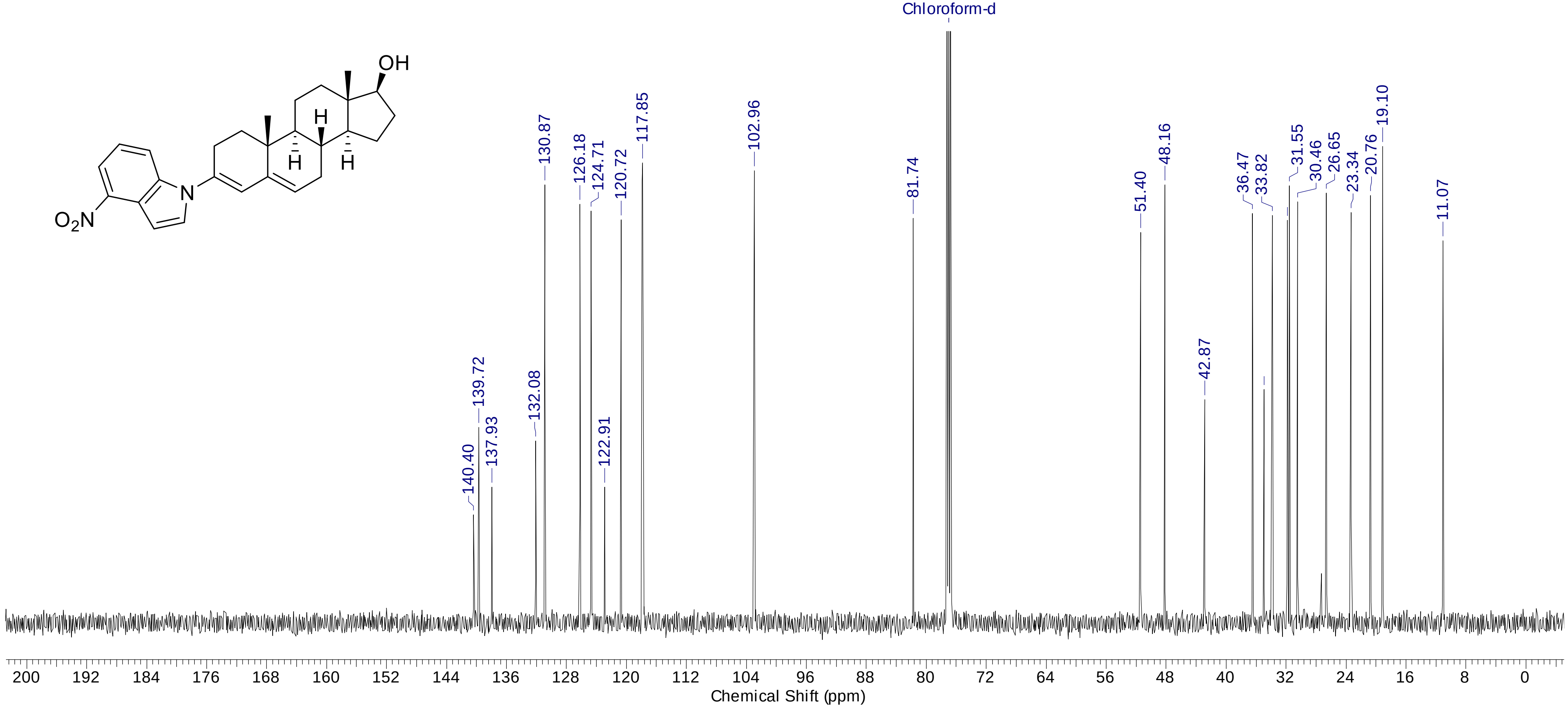
3-(4-Nitro-1*H*-indol-1-yl)androsta-3,5-dien-17β-ol (2g)

[1]H NMR (600 MHz, $CDCl_3$)



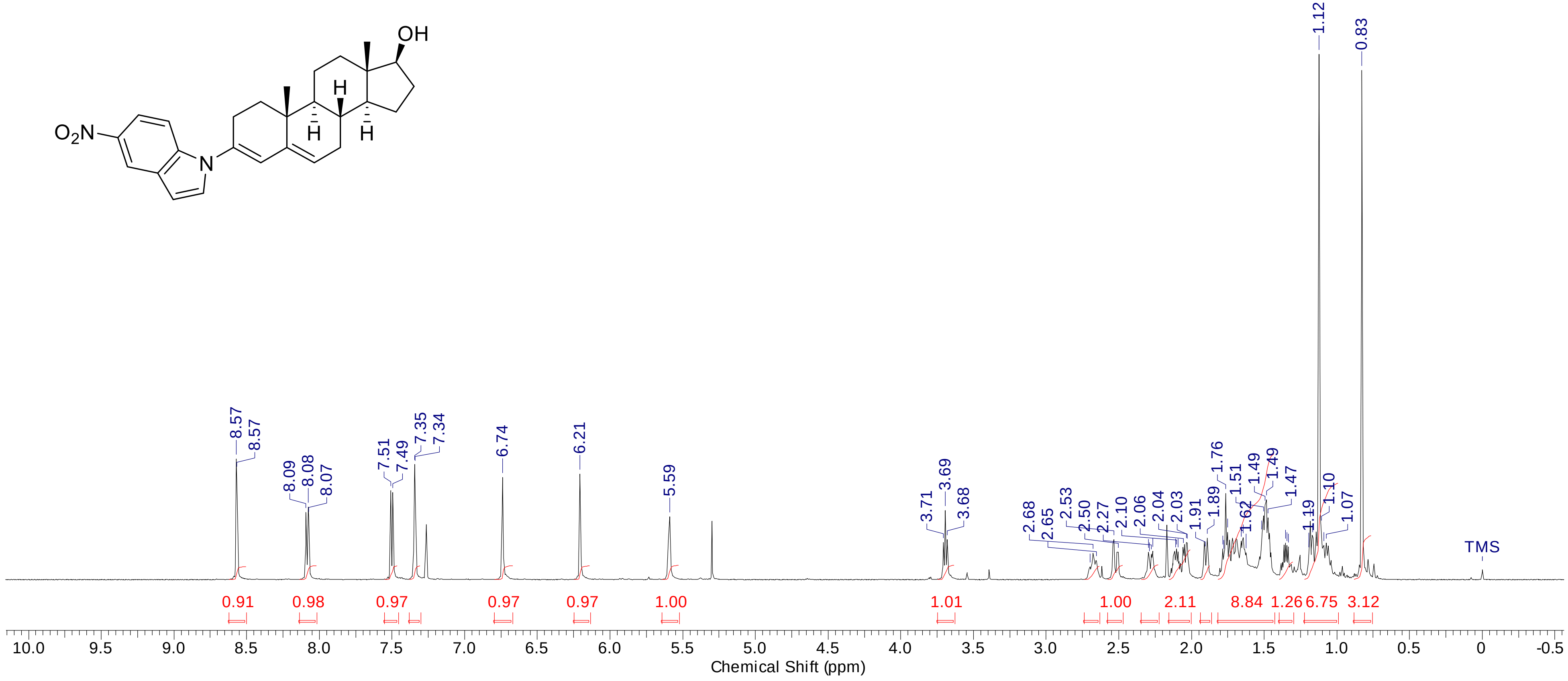
3-(4-Nitro-1*H*-indol-1-yl)androsta-3,5-dien-17β-ol (2g)

^{13}C NMR (150 MHz, $CDCl_3$)



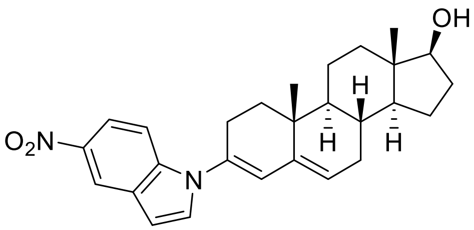
3-(5-Nitro-1*H*-indol-1-yl)androsta-3,5-dien-17β-ol (2h)

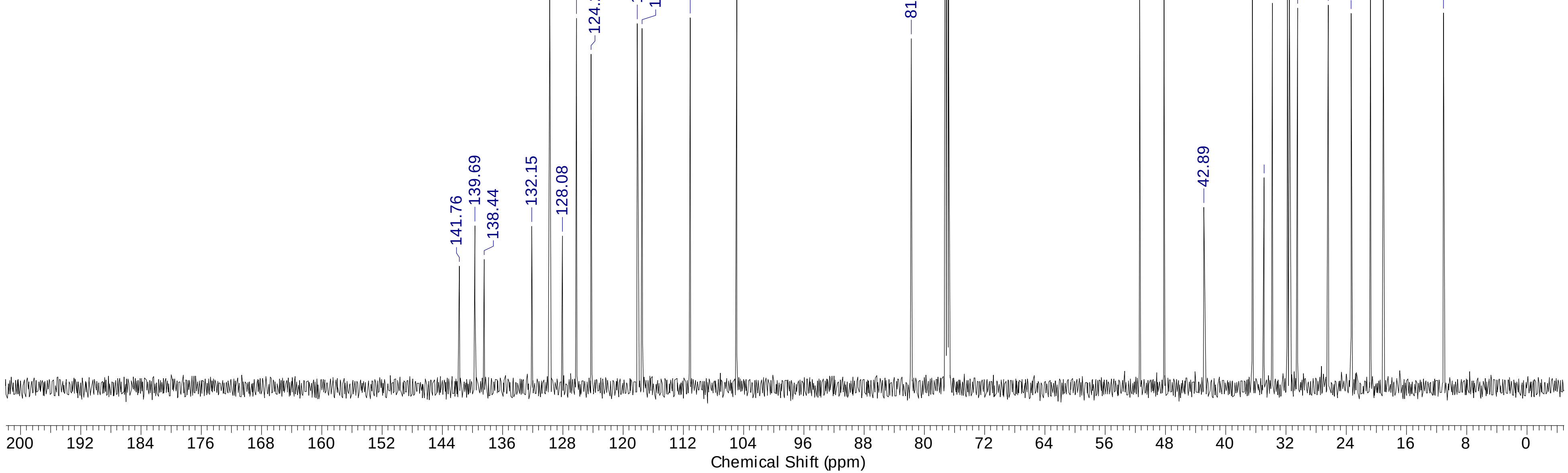
^{1}H NMR (600 MHz, $CDCl_3$)



3-(5-Nitro-1*H*-indol-1-yl)androsta-3,5-dien-17β-ol (2h)

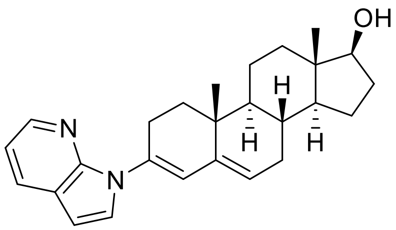
^{13}C NMR (150 MHz, $CDCl_3$)

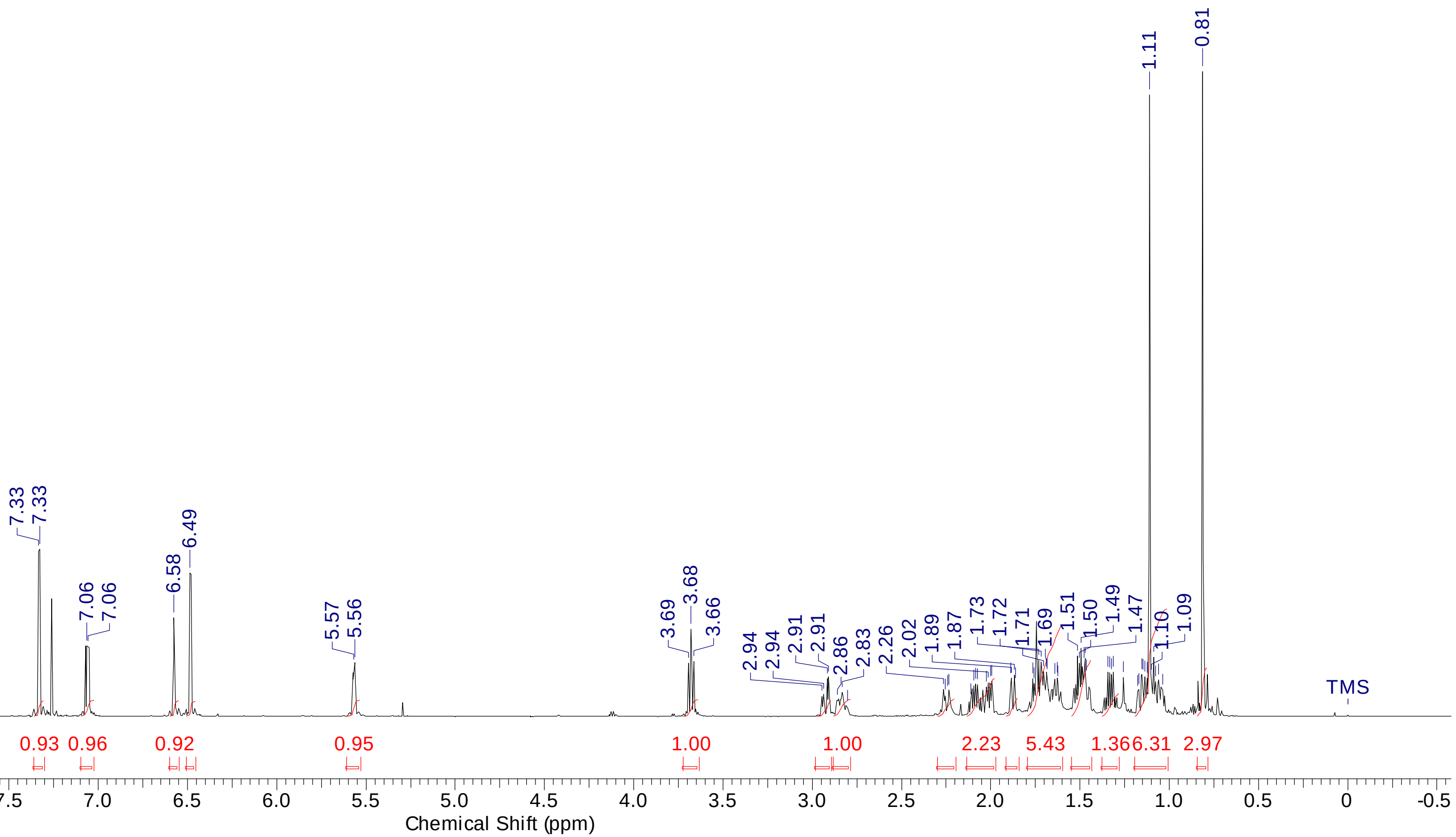




3-(1*H*-Pyrrolo[2,3-*b*]pyridin-1-yl)androsta-3,5-dien-17β-ol (2j)

^{1}H NMR (600 MHz, $CDCl_3$)





3-(1*H*-Pyrrolo[2,3-*b*]pyridin-1-yl)androsta-3,5-dien-17β-ol (2j)

^{13}C NMR (100 MHz, $CDCl_3$)