Supplementary Material (ESI)

Synthesis and conversion of primary and secondary 2-aminoestradiols into A-ring-integrated benzoxazolone hybrids and the investigation of their anticancer

activity in vitro

Ferenc Kovács¹, Mohana K. Gopisetty², Dóra I. Adamecz², Mónika Kiricsi², Éva Anna Enyedy^{3,4}, Éva Frank^{1,*}

¹Department of Organic Chemistry, University of Szeged, Dóm tér 8, H-6720 Szeged, Hungary

²Department of Biochemistry and Molecular Biology, Doctoral School of Biology, University of Szeged, Közép fasor 52., H-6726 Szeged, Hungary

³Department of Inorganic and Analytical Chemistry, Interdisciplinary Excellence Centre, University of Szeged, Dóm tér 7, H-6720 Szeged, Hungary

⁴MTA-SZTE Lendület Functional Metal Complexes Research Group, University of Szeged, Dóm tér 7, H-6720 Szeged, Hungary

*Corresponding author: frank@chem.u-szeged.hu; Tel.: +36-62-544-275

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¹H NMR spectrum of compound **2** (CDCl₃, 500 MHz)

¹³C spectrum of compound **2** (CDCl₃, 125 MHz)





¹H NMR spectrum of compound **3** (DMSO-*d*₆, 500 MHz)

¹³C NMR spectrum of compound **3** (DMSO-*d*₆, 125 MHz)





¹H NMR spectrum of compound **4** (DMSO-*d*₆, 500 MHz)







¹H NMR spectrum of compound **5** (DMSO-*d*₆, 500 MHz)

¹³C NMR spectrum of compound **5** (DMSO-*d*₆, 125 MHz)



¹H NMR spectrum of compound **7** (DMSO-*d*₆, 500 MHz)

¹³C NMR spectrum of compound 7 (DMSO-*d*₆, 125 MHz)

¹H NMR spectrum of compound **8a** (DMSO-*d*₆, 500 MHz)

¹³C NMR spectrum of compound **8a** (DMSO-*d*₆, 125 MHz)

¹H NMR spectrum of compound **8b** (DMSO-*d*₆, 500 MHz)

¹³C NMR spectrum of compound **8b** (DMSO-*d*₆, 125 MHz)

¹H NMR spectrum of compound **8c** (DMSO-*d*₆, 500 MHz)

¹³C NMR spectrum of compound **8c** (DMSO-*d*₆, 125 MHz)

¹H NMR spectrum of compound **8d** (DMSO-*d*₆, 500 MHz)

¹³C NMR spectrum of compound **8d** (DMSO-*d*₆, 125 MHz)

¹H NMR spectrum of compound **8e** (DMSO-*d*₆, 500 MHz)

¹³C NMR spectrum of compound **8e** (DMSO-*d*₆, 125 MHz)

¹H NMR spectrum of compound **8g** (DMSO-*d*₆, 500 MHz)

¹³C NMR spectrum of compound **8g** (DMSO-*d*₆, 125 MHz)

¹H NMR spectrum of compound **8h** (DMSO-*d*₆, 500 MHz)

¹³C NMR spectrum of compound **8h** (DMSO-*d*₆, 125 MHz)

¹H NMR spectrum of compound **9a** (CDCl₃, 500 MHz)

¹³C NMR spectrum of compound **9a** (CDCl₃, 125 MHz)

¹³C NMR spectrum of compound **9b** (CDCl₃, 125 MHz)

¹H NMR spectrum of compound **9c** (DMSO- d_6 , 500 MHz)

¹³C NMR spectrum of compound **9c** (DMSO-*d*₆, 125 MHz)

¹H NMR spectrum of compound **9d** (CDCl₃, 500 MHz)

¹³C NMR spectrum of compound **9d** (CDCl₃, 125 MHz)

¹H NMR spectrum of compound **9e** (DMSO-*d*₆, 500 MHz)

¹³C NMR spectrum of compound **9e** (DMSO-*d*₆, 125 MHz)

¹H NMR spectrum of compound **9f** (DMSO-*d*₆, 500 MHz)

¹³C NMR spectrum of compound **9f** (DMSO-*d*₆, 125 MHz)

¹H NMR spectrum of compound **9g** (DMSO- d_6 , 500 MHz)

¹³C NMR spectrum of compound **9g** (DMSO-*d*₆, 125 MHz)

¹H NMR spectrum of compound **9h** (DMSO-*d*₆, 500 MHz)

¹³C NMR spectrum of compound **9h** (DMSO-*d*₆, 125 MHz)

	MRC-5	PC-3	HeLa	DU145	MCF-7
control	100 ± 1.9	100 ± 4.0	100.0 ± 3.4	100 ± 3.7	$100{\pm}1.7$
2	100 ± 2.0	$100{\pm}12.5$	83.7±2.5	100 ± 1.5	$100{\pm}5.5$
4	100 ± 2.7	94.8±3.1	99.4±3.5	100 ± 4.2	$100{\pm}3.0$
5	100±3.9	99.0±6.7	1.1 ± 0.4	68.7 ± 2.0	$100{\pm}1.8$
7	100±5.3	90.7 ± 2.8	57.2±0.3	82.3±3.6	$100{\pm}1.8$
8 a	100 ± 3.1	100 ± 4.9	98.0±4.8	100 ± 0.2	$100{\pm}0.9$
8b	100±0.3	92.8±6.8	99.8±2.4	94.3±8.6	$100{\pm}4.1$
8c	100±5.3	86.2±4.1	99.4±1.0	71.2±19.3	$100{\pm}3.0$
8d	99.8±16.6	99.9±6.5	96.7±2.8	89.9±6.6	$100{\pm}1.4$
8e	100±0.3	$100{\pm}7.5$	99.2±6.0	100 ± 6.2	$100{\pm}0.2$
8g	100 ± 0.7	89.4±17.5	99.4±1.6	86.0±12.0	100 ± 2.6
8h	100±2.6	100 ± 13.4	$96.8 {\pm} 5.0$	$100{\pm}1.8$	$100{\pm}1.5$
9a	100±3.3	100 ± 4.1	100 ± 5.5	99.6±2.5	$100{\pm}3.5$
9b	100±6.4	$100{\pm}7.5$	$100{\pm}1.0$	75.6±13.0	100 ± 2.4
9c	100 ± 2.4	93.2±6.8	96.9±1.6	88.3±6.0	$100{\pm}1.5$
9d	100 ± 5.0	94.3±3.0	97.9±3.9	90.4±4.3	$100{\pm}7.2$
9e	100 ± 5.8	90.3±2.0	89.9±7.3	99.8±1.6	$100{\pm}1.0$
9f	100 ± 2.2	91.6±5.6	91.3±1.5	87.9±14.4	$100{\pm}1.5$
9g	100±3.4	100±12.9	92.1±3.6	96.3±1.4	100 ± 4.1
9h	$100{\pm}0.7$	$100{\pm}11.8$	98.6±4.5	100 ± 3.8	100 ± 2.2

Table S1. Mean \pm SD values of primary growth inhibitory screen (given as cell viability) used for heat map construction. Compounds were tested in 1.5 μ M concentration for 72 h. Control represents viability of cells receiving no treatment.

Figure S1. Representative cell viability curves to determine growth inhibition and IC_{50} values following treatments with compounds **2**, **5**, **7**, **8c** and **9b** on different cell lines. On X-axis logarithm of applied concentrations represented in nM. Based on the viability data, IC_{50} values were obtained in nM concentration, then were converted and represented in μ M in Table 3.

Figure S2. Representative cell viability curves to determine growth inhibition and IC₅₀ values following treatments with cisplatin on non-cancerous and cancerous cell lines. On the X-axis logarithm of applied concentrations represented in μ M, the title of the axis is Log (μ M Concentration). Based on the viability data, IC₅₀ values were obtained in μ M concentration, which are represented in Table 3.