

Synthesis of 6b,11b-dihydroxy-12-methylphenyl-11b,12-dihydrobenzo-[g]indeno[1,2-*b*]indole-5,6,7(6*bH*)-triones and 2-(3-hydroxy-4,9-dioxo-4,9-dihydro-1*H*-benzo[*f*]indol-2-yl)benzamides, their structure and antiproliferative activity

Leonid M. Gornostaev^{1*}, Olga I. Fominykh¹, Tatyana A. Rukovets^{1,2},
Tatyana I. Lavrikova¹, Juliya G. Khalyavina¹, Alexander A. Shtil³, Alexei V. Shunaev³,
Sergey F. Dunaev⁴, Elena V. Murashova⁴, Vladimir V. Chernyshev⁴

¹ Krasnoyarsk State Pedagogical University named after V. P. Astafyev,
89 Ady Lebedevoi St., Krasnoyarsk 660049, Russia; e-mail: gornostaev@kspu.ru

² Prof. V. F. Voyno-Yasenetsky Krasnoyarsk State Medical University,
1 Partizana Zheleznyaka St., Krasnoyarsk 660022, Russia; e-mail: tatyana_xim@mail.ru

³ N. N. Blokhin National Medical Research Center of Oncology,
Ministry of Health of the Russian Federation,
Kashirskoe Shosse 23, Moscow 115478, Russia; e-mail: shtilaa@yahoo.com

⁴ Lomonosov Moscow State University,
1, Build. 3 Leninskie Gory, Moscow 119991, Russia;
e-mail: vladimir@struct.chem.msu.ru

SUPPLEMENTARY INFORMATION

TABLE 1. Crystallographic data of compounds **2a** and **2b**

| | 2a | 2b |
|--|---|---|
| Formula | C ₂₆ H ₁₇ NO ₅ | C ₂₆ H ₁₇ NO ₅ ·H ₂ O |
| Singony | Monoclinic | Monoclinic |
| Space group | <i>P2₁/c</i> | <i>C2/c</i> |
| <i>a</i> , Å | 9.8232(9) | 17.2562(12) |
| <i>b</i> , Å | 17.3036(15) | 8.2752(8) |
| <i>c</i> , Å | 11.6672(11) | 29.0593(19) |
| β, ° | 97.691(13) | 99.197(10) |
| <i>V</i> , Å ³ | 1965.3(3) | 4096.3(6) |
| <i>M</i> ₂₀ [*] | 22 | 31 |
| <i>F</i> ₃₀ [*] | 69 (0.008, 53) | 74 (0.007, 57) |
| <i>Z</i> | 4 | 8 |
| <i>D</i> _x (g/cm ³) | 1.431 | 1.432 |
| Diffractometer | Stoe Stadi-P | EMPYREAN |
| Emission, wavelength (Å) | CuK _{α1} , 1.54059 | CuK _α , 1.5418 |
| Diffractogram: 2θ _{min} – 2θ _{max} , measurement step, ° | 7.00–80.00, 0.01 | 4.00 – 80.00, 0.017 |
| <i>R</i> _p / <i>R</i> _{wp} / <i>R</i> _{exp} ^{**} | 0.061/0.075/0/065 | 0.052/0.073/0/020 |
| <i>GOF</i> ^{**} | 1.149 | 3.610 |

* Indication quality indicators *M*₂₀ and *F*₃₀ are defined in [15] and [16], respectively.

** *R*_p, *R*_{wp}, *R*_{exp}, and *GOF* are defined in [17].

Figures 1 and 2 show the experimental and difference curves based on the results of refinement by the Rietveld method.

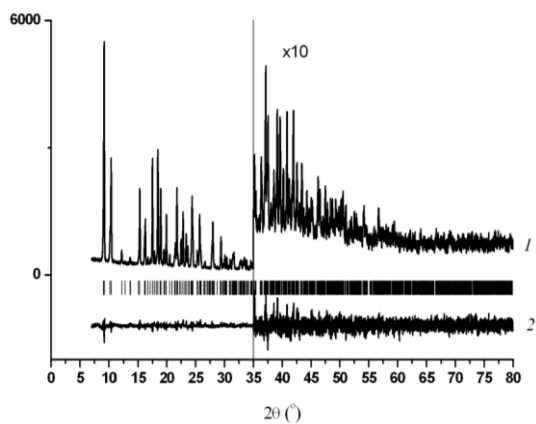


Figure 1. The result of refinement by the Rietveld method of the crystal of structure **2a**. Designations: 1 - experimental curve; 2 - the difference between the experimental and calculated curves according to the refinement; θ the high-angle region ($2 > 35^\circ$) is represented on an enlarged scale. The calculated positions of the reflexes are indicated by vertical segments.

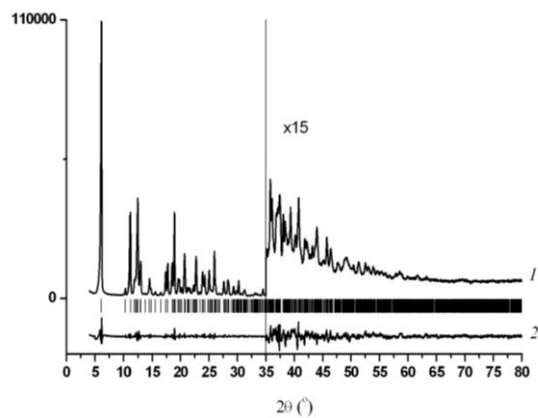


Figure 2. The result of refinement by the Rietveld method of the crystal of structure **2b**.