Supporting information

# Synthesis, Single Crystal X-ray Analysis, Prediction and Study of Pharmacological Activity of 4-(1*H*-Benzo[d]imidazol-2-yl)-1-phenyl-1*H*-1,2,3-triazol-5-amine and Its Solvates

**Alexandre V. Ivachtchenko [1], Oleg D. Mitkin [1]*, Dmitry V. Kravchenko [2], Sergiy M. Kovalenko [1,3,6], Svitlana V. Shishkina [3,5,6], Natalya D. Bunyatyan [3,4], Irina S. Konovalova [5], Vladimir V. Ivanov [6], Olena D. Konovalova [6], Thierry Langer [7]**

[1] ChemRar Research and Development Institute, 7 Nobel st., Innovation Center Skolkovo territory, Moscow, 143026, Russia; e-mail: mod@chemrar.ru, av@chemrar.ru
[2] Chemical Diversity Research Institute, 2A Rabochaya st., Khimki, Moscow Region, 141400, Russia; e-mail: dk@chemrar.ru, ivk@iihr.ru
[3] Federal State Autonomous Educational Institution of Higher Education I.M. Sechenov First Moscow State Medical University of the Ministry of Healthcare of the Russian Federation (Sechenov University). 8 Trubetskaya st., Moscow, 119991, Russia; e-mail: ndbun@mail.ru
[4] Federal State Budgetary Institution "Scientific Centre for Expert Evaluation of Medicinal Products" of the Ministry of Health of the Russian Federation, Petrovsky boulevard 8, bld. 2, Moscow, 127051, Russia, e-mail: ndbun@mail.ru
[5] State Scientific Institution “Institute for Single Crystals” of the National Academy of Sciences of Ukraine, 61001, Kharkov, Ukraine.
[6] V.N. Karazin Kharkiv National University, 4 Svobody sq., Kharkiv, 61077, Ukraine; e-mail: kovalenko.sergiy.m@gmail.com
[7] Department of Pharmaceutical Chemistry, University of Vienna, Althanstraße 14, A-1090, Vienna, Austria; e-mail: thierry.langer@univie.ac.at

* Correspondence: mod.chemdiv@gmail.com; Tel.: +7-495-995-4941 (O.D.M.)

SUPPLEMENTARY MATERIAL

## Table of Contents

**Figure S1.** UV/Vis spectrum of the title compound **3** (acetonitrile)

**Figure S2**. IR spectrum of the title compound **3** (KBr pellet)

**Figure S3**. $^{13}C$ NMR (100 MHz, DMSO-d6) spectrum of the title compound **3**

**Figure S4**. $^{1}H$ NMR (400 MHz, DMSO-d6) spectrum of the title compound **3**

**Figure S5**. LC/MS Data for Structural Determination of of the title compound **3**

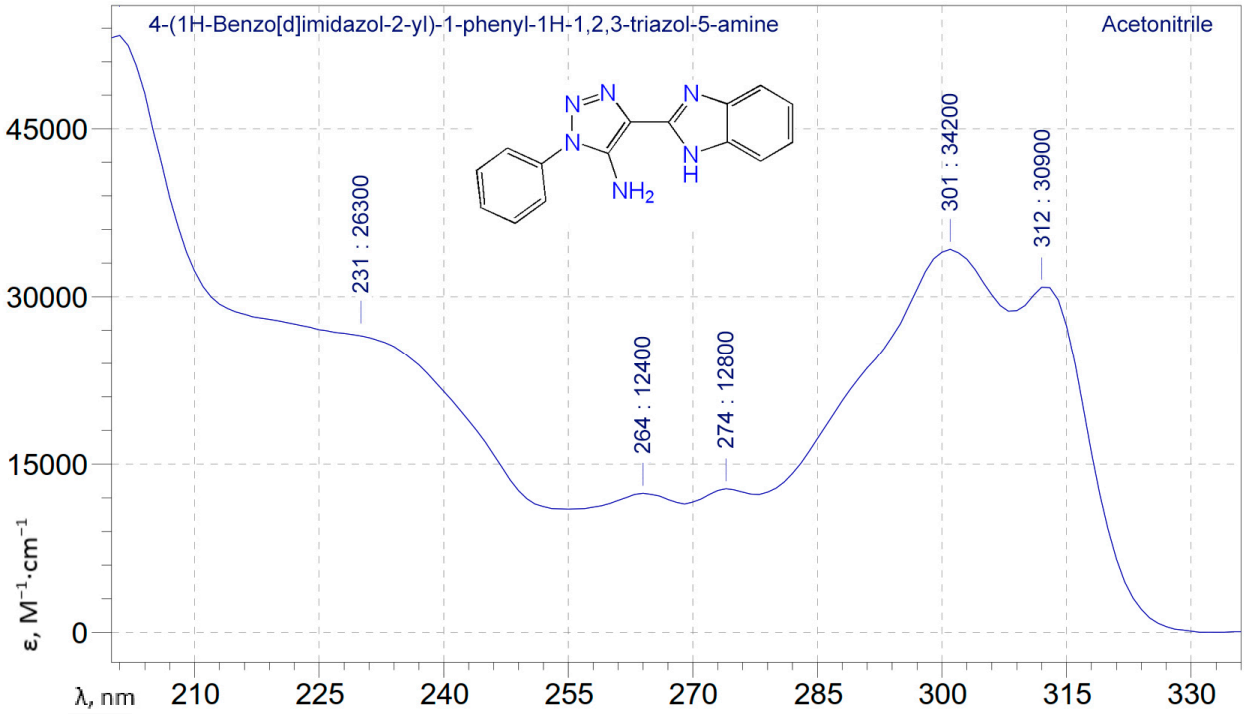



**Figure S1**. UV/Vis spectrum of the title compound **3** (acetonitrile).

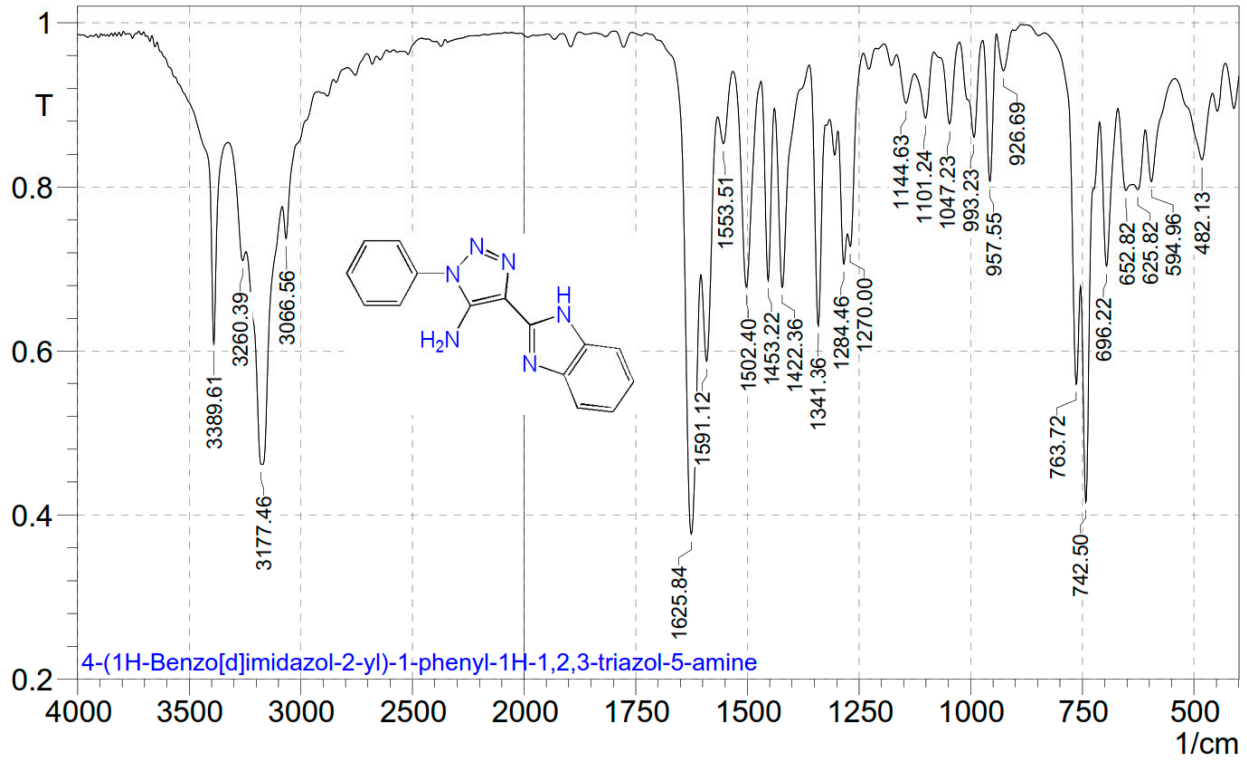



**Figure S2**. IR spectrum of the title compound **3** (KBr pellet).

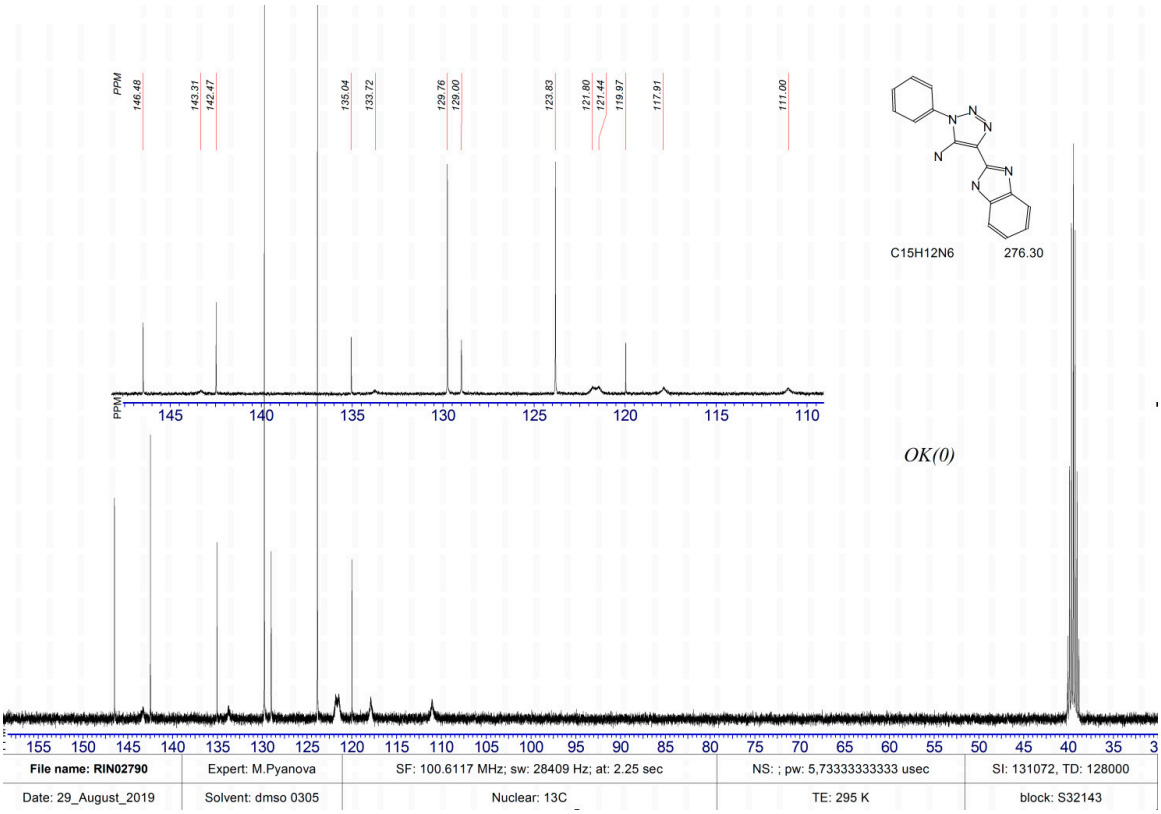



**Figure S3**. [13]C NMR spectrum (100 MHz, DMSO-d6) of the title compound **3**.

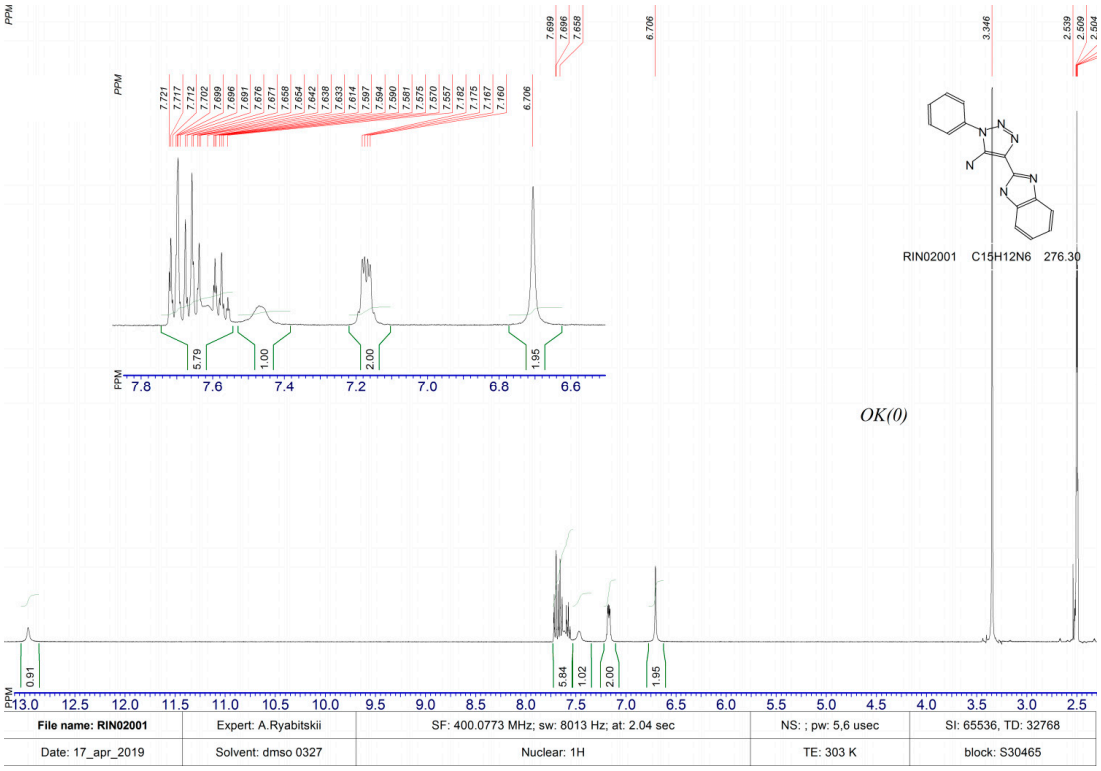


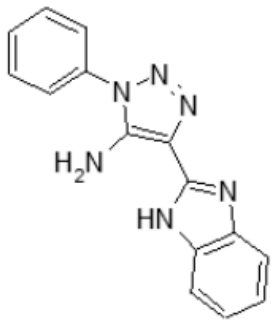

**Figure S4**. [1]H NMR spectrum (400 MHz, DMSO-d6) of the title compound **3**.

X:\OUTPUT\2019\19_04\190418\M30781\RIN02001.D Sample Name: RIN02001 Page 1 of 1

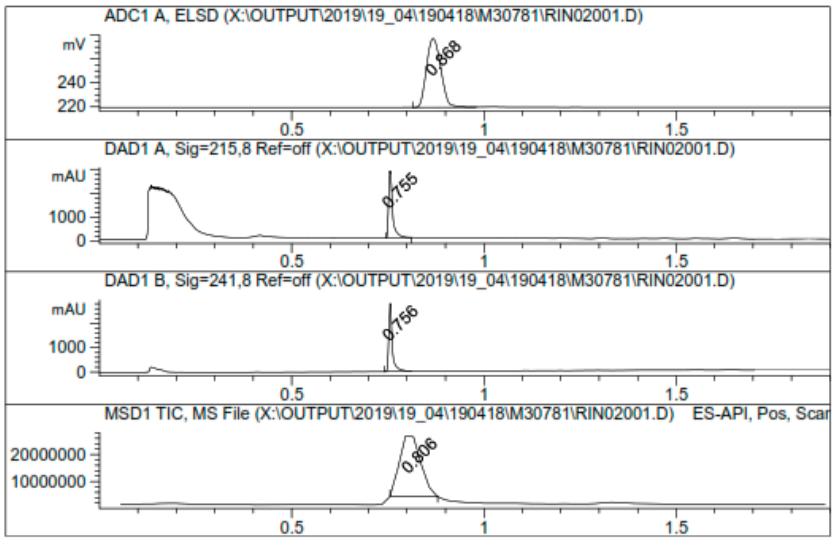
-.o.-Syntez Purity Report -.o.-

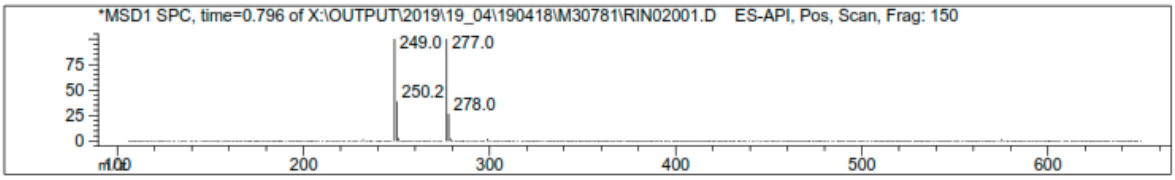
Agilent 1100 LC/MSD
Diodearrey G1315B (DAD1A-215nm; DAD1B-241nm)
Mass Quad G1956B (MSD1-Pos, MSD2-Neg)
ELSD Altech 3300 (ADC1 A, ELSD)

Mobile Phase:A-H2O+0.1HCOOH;B-MeCN+0.1HCOOH
Separation column: **100%**
Rapid Resolutionn HT Cartige 4.6x30mm,
1.8-Micron, Zorbax SB-C18



Mw 276,30




| # | Signal | R.Time | Area % |
|---|---|---|---|
| 1 | ADC1 A, ELSD | 0.868 | 100.000 |

| # | Signal | R.Time | Area % |
|---|---|---|---|
| 1 | DAD1 A, Sig=215,8 Ref=off | 0.755 | 100.000 |

| # | Signal | R.Time | Area % |
|---|---|---|---|
| 1 | DAD1 B, Sig=241,8 Ref=off | 0.756 | 100.000 |

| # | Signal | R.Time | Area % |
|---|---|---|---|
| 1 | MSD1 TIC, MS File | 0.806 | 100.000 |

**Figure S5**. LC/MS LC/MS data for the title compound **3**.