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7th International Conference on

PHARMACEUTICS & ADVANCED DRUG DELIVERY SYSTEMS

March 27-28, 2023 | London, UK

Received date: 14-03-2023 | Accepted date: 16-03-2023 | Published date: 03-04-2023

Bioinformatics and genomic analyses of eight riboswitches and their suitability for antibacterial drug targets

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Antibiotic resistance is a global problem affecting people across the globe, leading to a persistent and debilitating disease. The annual mortality caused by antibiotic resistance is increasing exponentially and causes a pressing need to research novel mechanisms of action, untested target molecules, and novelly designed compounds.

This poster presents in silico analyses of eight bacterial riboswitches - cyclic-di-GMP I, cyclic-di-GMP II, fluoride, glycine, Mg2+, Mn2+, MoCo RNA, and PreQ1, for their suitability as antibacterial drug targets. All of them are located in the 5-untranslated region of messenger RNAs, act as allosteric cis-acting gene control elements, and have not been found in humans yet. Sensing specific metabolites, the riboswitches regulate the synthesis of vital cellular metabolites in various pathogenic bacteria. As regulators of metabolites with an important role for the bacteria, they might be classified by their suitability for antibacterial drug targets.

The complete and informative genome-wide bioinformatics analysis of the adequacy of eight riboswitches as antibacterial drug targets in different pathogenic bacteria is based on four precise, clear, and easy-to-establish criteria. Based on these, I evaluate the possibility for each of the riboswitches to be used as a potential target for the development of an antisense oligonucleotide or other designer compound with an antibacterial effect. Due to the ability of the riboswitch to control specific biosynthetic pathways and/or carrier proteins important for the transport of essential metabolites, and the presence/absence of alternative biosynthetic pathways, we classified them into four groups. The groups are based on riboswitches' suitability as antibacterial drug targets guided by the mentioned in silico analyses. Results from the bioinformatics and genomic-based research concluded that PreQ1, MoCo RNA, cyclic-di-GMP I, and cyclic-di-GMP II riboswitches are promising targets for antibacterial drug discovery.

Acknowledgments: This research is supported by grant KP-06-H63/1/13.12.2022, awarded by the Bulgarian National Science Fund, Bulgaria. The Project's name is: "Comparative analysis of the effectiveness of new antibacterial agents based on different types of antisense oligonucleotides using different molecular mechanisms of RNA inhibition" with project leader Prof. dr. Robert Penchovsky.

Recent Publications

1. Article: Bioinformatics and Genomic Analyses of the Suitability of Eight Riboswitches for Antibacterial Drug Targets, Nikolet Pavlova and Robert Penchovsky, Antibiotics, 2022, DOI:10.3390/antibiotics11091177, IF: 5.22, SJR=0,785, Q1

2. Article: Versatile tools of synthetic biology applied to drug discovery and production, Nikolet Pavlova, Georgi Y Miloshev, Antoniya V Georgieva, Martina Traykovska & Robert Penchovsky, Future Medicinal Chemistry, 2022, DOI:10.4155/fmc-2022-0063, IF: 4,7, SJR=0,649, Q2

3. Book: New Frontiers and Applications of Synthetic Biology; chapter 8. Small RNA-based systems for sensing and therapeutic applications, Robert Penchovsky, Georgi Miloshev, Nikolet Pavlova, Katya Popova, Lozena Otcheva, Martina Traykovska, Elsevier, 2022, https://doi.org/10.1016/B978-0-12-824469-2.00004-X, Q3

Biography

Nikolet Pavlova is a 32 years old scientist from Sofia, Bulgaria, who works in the field of bioinformatics, genetics, and genomics. Most of her interests relate to RNA biology – aptamers and riboswitches as potential drug targets for antibacterial drug discovery. During the last 5 years, she has been developing a method for the selection of suitable targets from the genome of bacteria in the fight against antibiotic resistance, as well as a method for the design of new antibacterial agents based on antisense oligonucleotide technologies and bioinformatics analyses. On 07.03.2023, she won an award for the best young microbiologist for 2022 in Bulgaria, second place, for her contribution to the fight against antibiotic resistance and her work: Bioinformatics and Genomic Analyses of the Suitability of Eight Riboswitches for Antibacterial Drug Targets, Nikolet Pavlova and Robert Penchovsky, Antibiotics, 2022.

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