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Way2Drug Platform: From Biological Activity Prediction to Systems Pharmacology

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Global chemical space is extremely vast and finding a molecule with the required pharmacotherapeutic properties is a formidable challenge. Starting from analysis of big chemical-biological data obtained in silico, in vitro, in vivo and in clinics it is necessary to finish with one active pharmaceutical ingredient possessing the needed safety and efficacy. Combining information extracted from the curated datasets of active/inactive compounds available through World Wide Web and AI/ML tools, investigators are surfing from global to local scales in pharmaceutical R&D, enabling faster and more efficient development of new therapeutic remedies.

Way2Drug is a quickly expanding web portal focused at integrating of demanded in silico tools for drug discovery. Way2Drug currently hosts services for predicting the biological activities (PHARMA), toxicity (TOX), metabolism (META) and physicochemical characteristics (ADME) of drug-like molecules. All tools are freely available for non-commercial academic research.

In addition to the predictive web-services, several informational resources are available at the Way2Drug portal, including WWAD (World-Wide Approved Drugs), phytocomponents of the Russian officinal medicinal plants Phyto4Health, host gut microbiota metabolism xenobiotics database HGMMX.

Way2Drug is evolving as the basis for development of computational platform for efficient analysis and interpretation of the extensive biomedical and clinical data, comparative analysis of information extracted from this data to differentiate the normal and pathological states, obtaining new knowledge to identify potential pharmacological targets and biomarkers, designing potential pharmacological substances with the required properties, determining the optimal approach to therapy taking into account the individuality of patients.

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