Volgograd State Medical University, Volgograd, Russia
Research Center for Innovative Medicines
Department of Pharmacology and Bioinformatics

DEEP LEARNING CONVOLUTIONAL CORRELATION NEURAL NETWORK BASED ON MULTIPLE DOCKING FOR IDENTIFYING PHARMACOLOGICALLY ACTIVE COMPOUNDS

M.A. Perfilev,
P.M. Vassiliev, A.V. Golubeva, A.N. Kochetkov

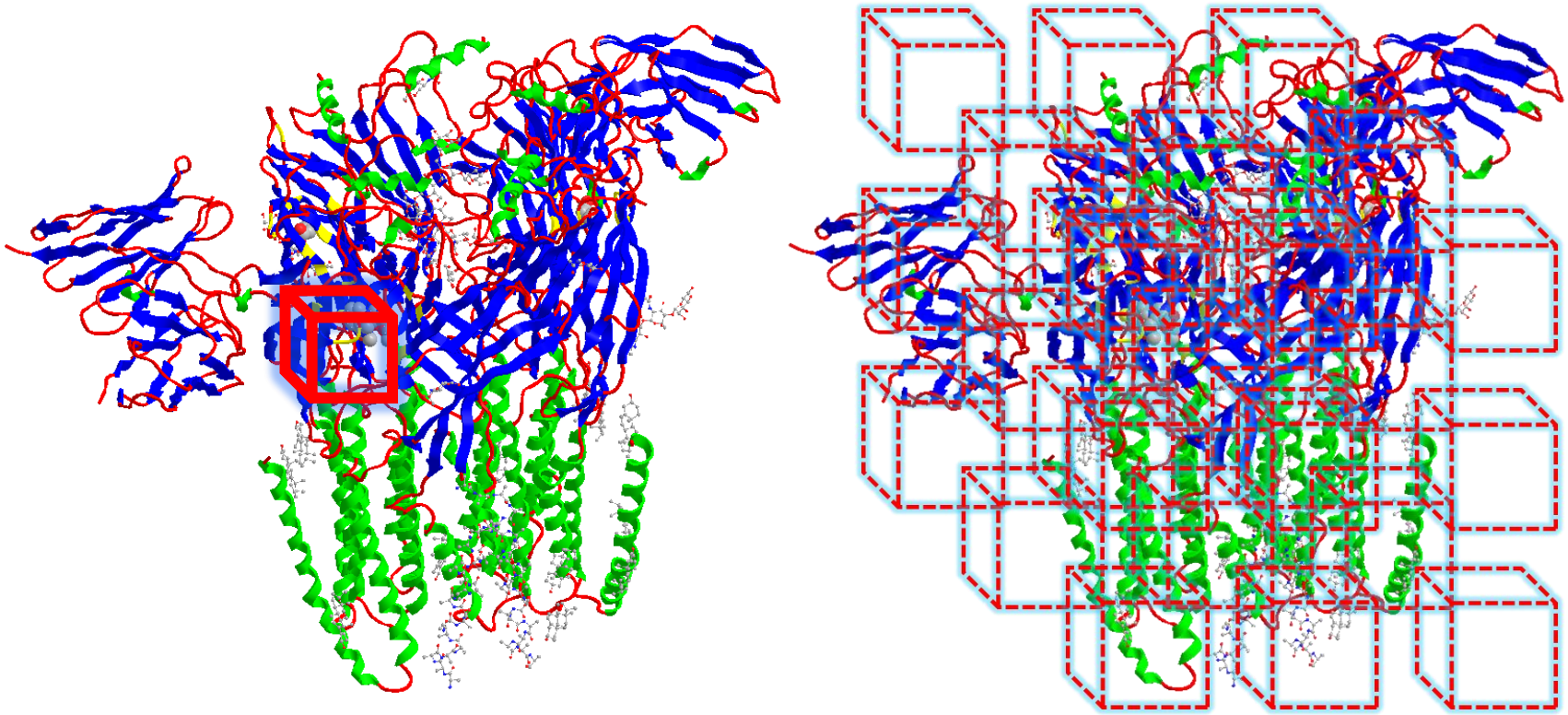
The aim of the study

The aim of this study is to compare neural network models for predicting pharmacological activity based on correlation networks with one hidden layer and those with two hidden layers.

Tasks

1. Prepare main training sample for neural network modeling.
2. Train neural network models to predict two types of pharmacological activity.
3. Compare the resulting models with previously constructed models.

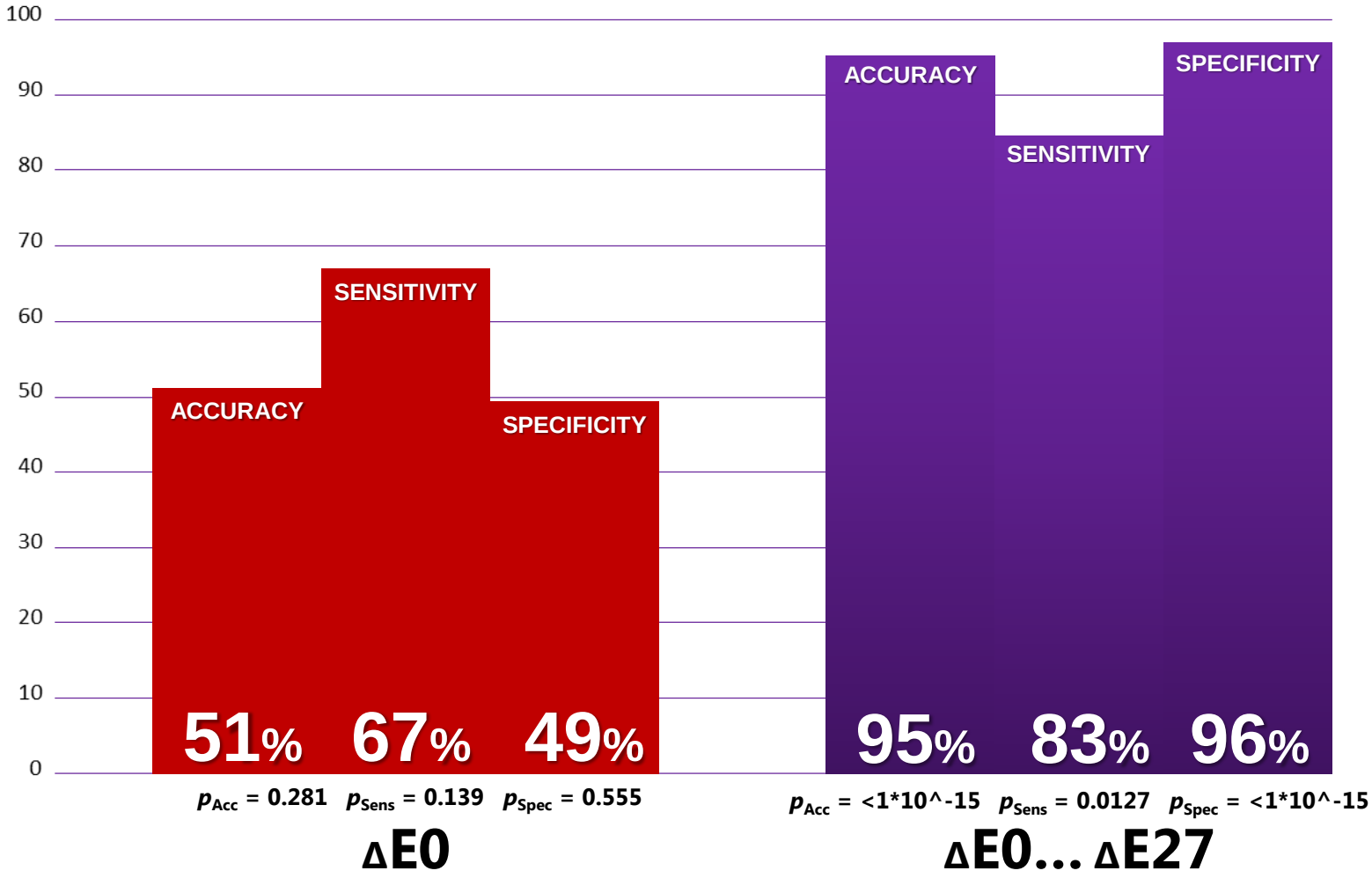
Classic and Multiple Docking



3D-model of GABAAR, 6d6t, α1-β2-γ2

Vassiliev, P.M., Kochetkov, A.N., Spasov, A.A., Perfilev, M.A. (2021) Volgograd scientific and medical journal, 3, 57-61.

GABA-ergic activity



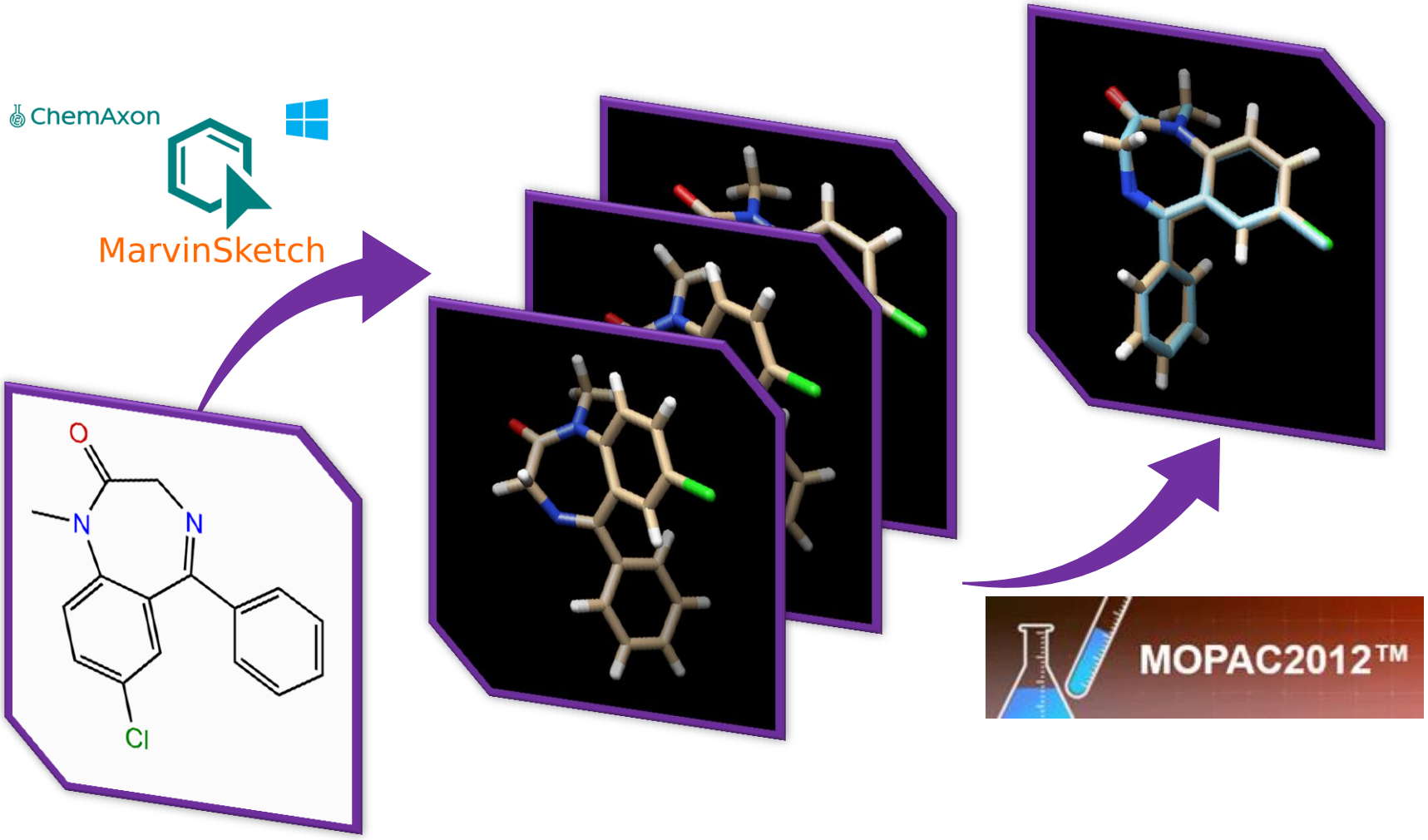
p_{Acc} = 0.281 p_{Sens} = 0.139 p_{Spec} = 0.555

p_{Acc} = <1*10^-15 p_{Sens} = 0.0127 p_{Spec} = <1*10^-15

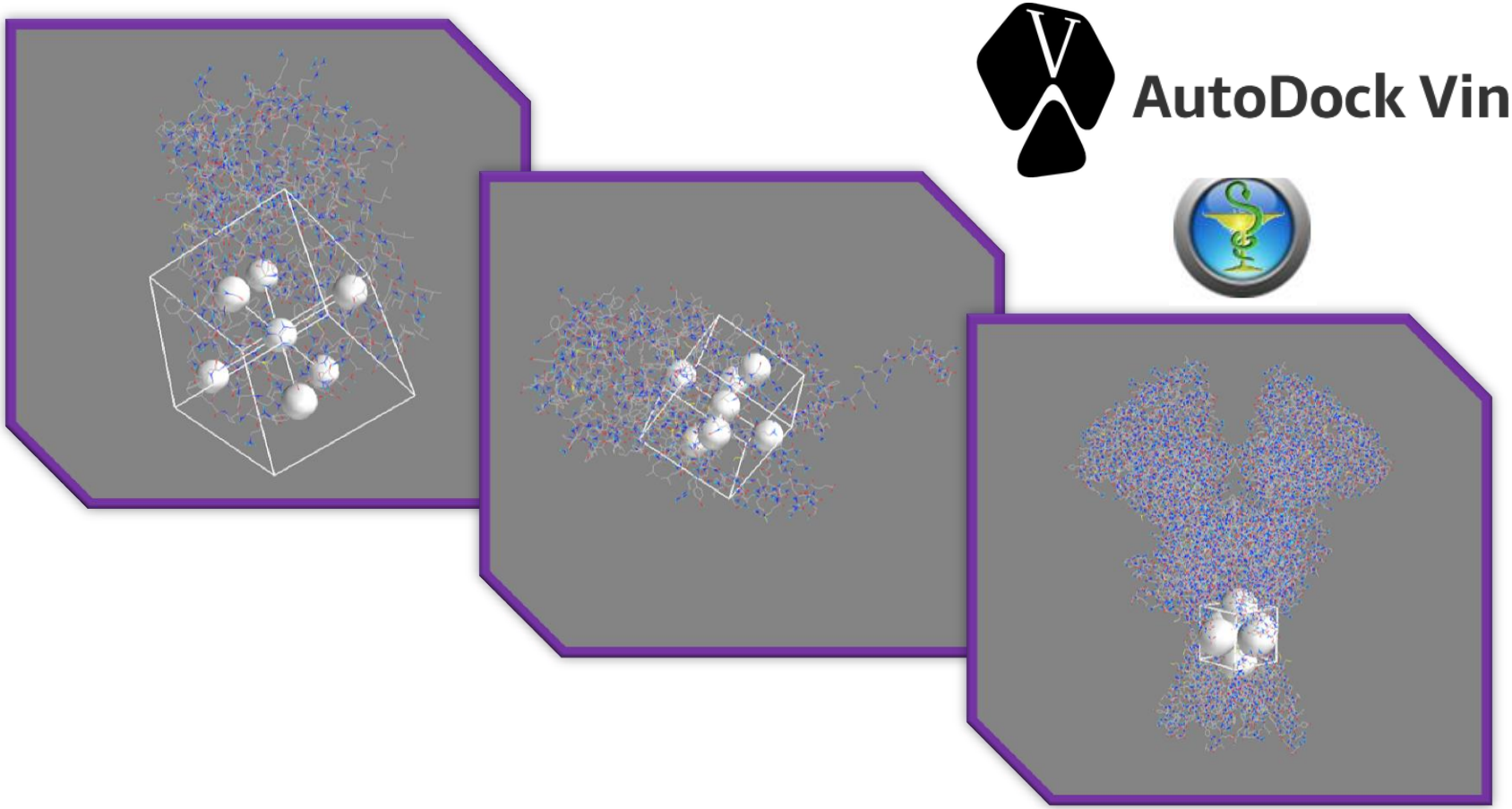
ΔE0 **ΔE0… ΔE27**

Vassiliev, P.M., Kochetkov, A.N., Perfilev, M.A. (2022) Journal of Volgograd State Medical University, 19(4), 88-93.

Ligand optimization



Docking



AutoDock Vina

ANN with one hidden layer

РОССИЙСКАЯ ФЕДЕРАЦИЯ

СВИДЕТЕЛЬСТВО

о государственной регистрации программы для ЭВМ

№ 2025682291

Формирование пространств для множественного докинга MSite

Правообладатель: *Федеральное государственное бюджетное образовательное учреждение высшего образования "Волгоградский государственный медицинский университет "Министерства здравоохранения Российской Федерации (RU)*

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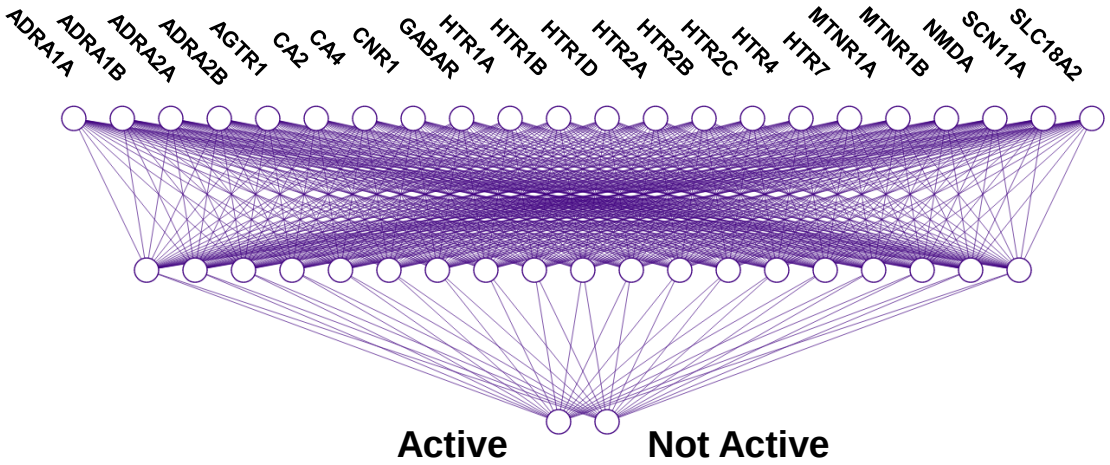
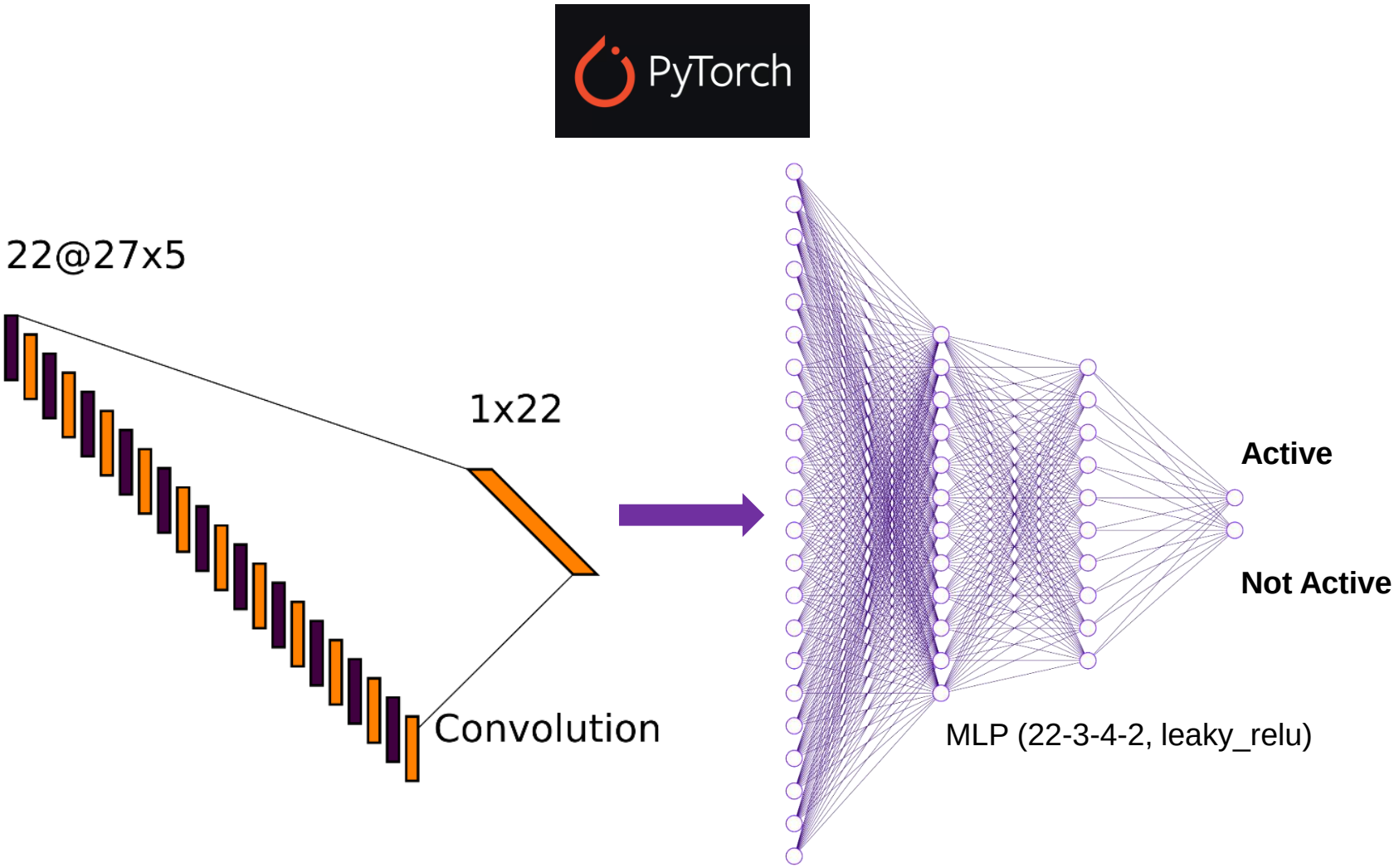
Руководитель Федеральной службы по интеллектуальной собственности

Ю.С. Зубов

StatSoft®
STATISTICA

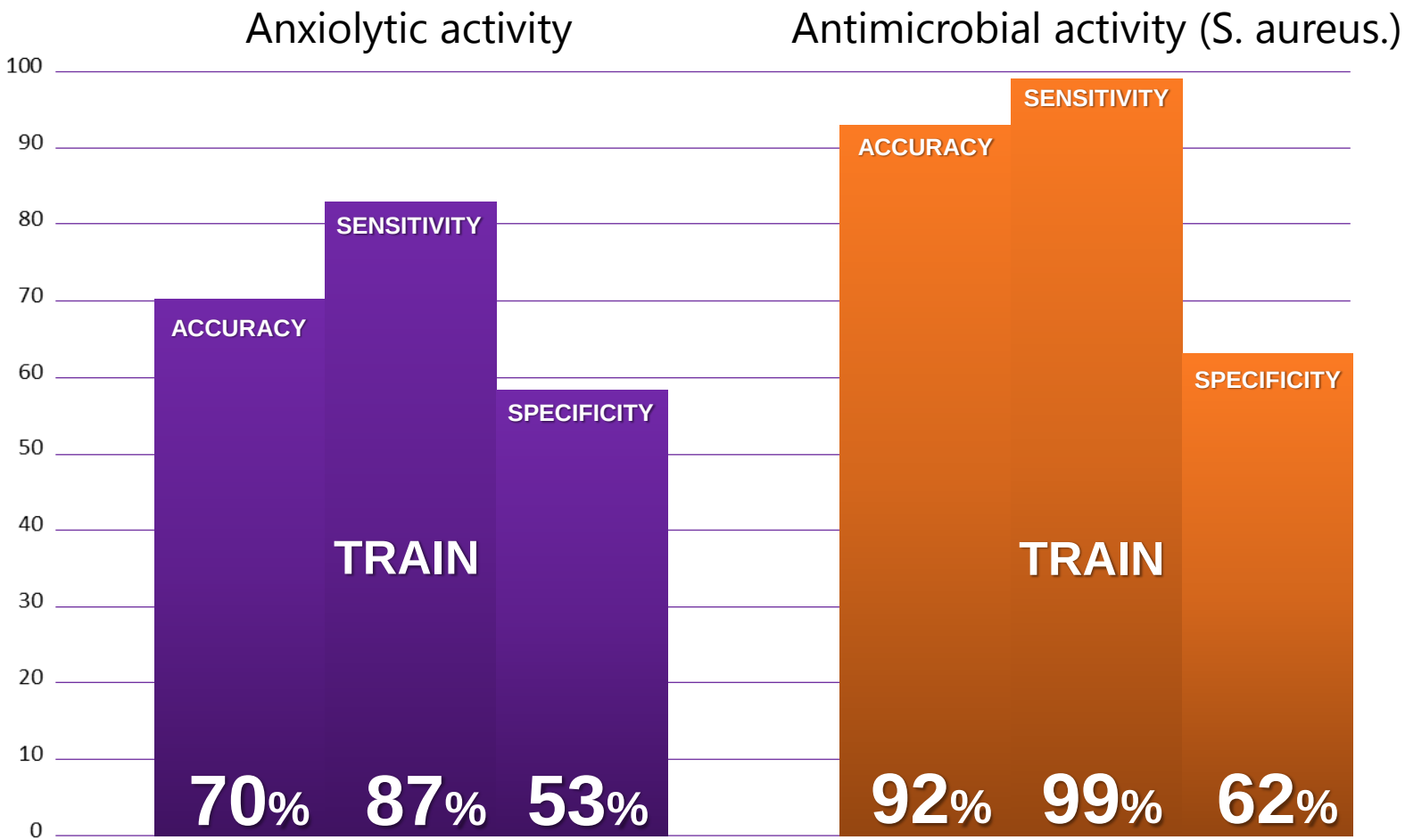


CNN with two hidden layers



Paszke, A., Gross, S., Massa, F., Lerer, A. et al. (2019) Advances in neural information processing systems, 32.

Training accuracy



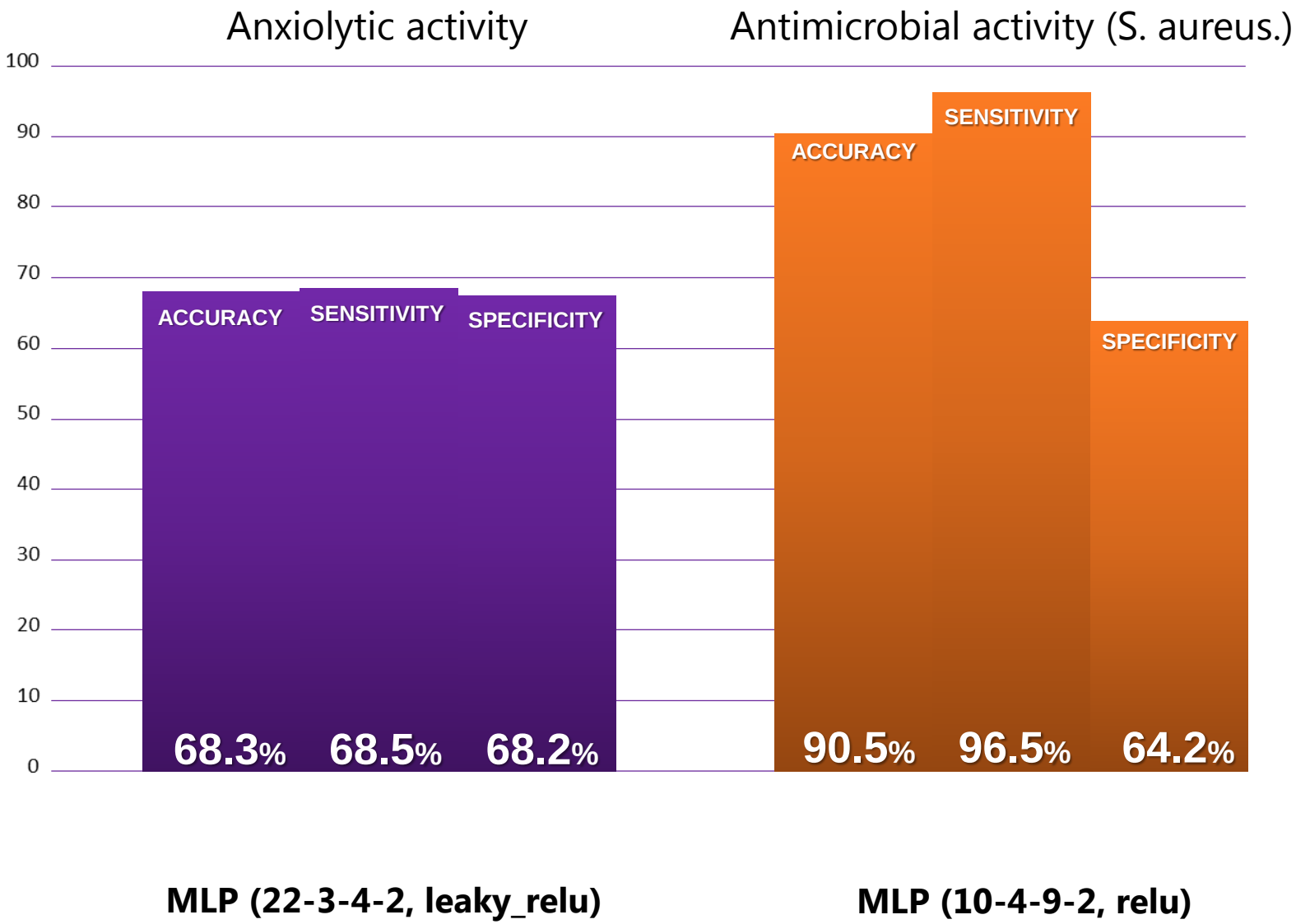
Test: Acc = 62%, Sens = 81%, Spec = 43%; Validation: Acc = 68%, Sens = 95%, Spec = 40%; AUC_{ROC} = 68%

MLP (22-3-4-2, leaky_relu)

Test: Acc = 84%, Sens = 94%, Spec = 38%; Validation: Acc = 93%, Sens = 100%, Spec = 63%; AUC_{ROC} = 98%

MLP (10-4-9-2, relu)

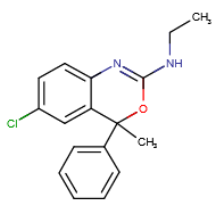
Autotest accuracy



DRUGBANK Online

Etifoxine

Structure



Description

A medication used to treat anxiety.

DrugBank ID	Type
DB08986	**Small Molecule**

US Approved	Other Approved	Patents	Indicated Conditions
NO	YES	0	1

Clinical Trials

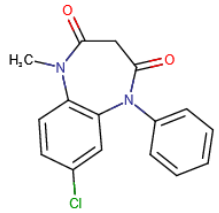
Phase 0	Phase 1	Phase 2	Phase 3	Phase 4
0	0	0	2	0

Drug Categories

- Anti-Anxiety Agents
- Central Nervous System Agents

Clobazam

Structure



Description

A medication used to control different types of dangerous seizures.

DrugBank ID	Type
DB00349	**Small Molecule**

US Approved	Other Approved	Patents	Indicated Conditions
YES	YES	3	5

Clinical Trials

Phase 0	Phase 1	Phase 2	Phase 3	Phase 4
0	1	5	10	9

Therapeutic Categories

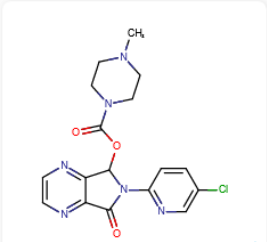
Benzodiazepines and benzodiazepine derivatives

Drug Categories

- Anti-Anxiety Agents

Zopiclone

Structure



Description

A medication used for insomnia or sleeplessness.

DrugBank ID	Type
DB01198	**Small Molecule**

US Approved	Other Approved	Patents	Indicated Conditions
NO	YES	0	1

Clinical Trials

Phase 0	Phase 1	Phase 2	Phase 3	Phase 4
1	12	1	9	4

Therapeutic Categories

Hypnotics (Nonbenzodiazepine)

Miscellaneous Anxiolytics Sedatives and Hypnotics

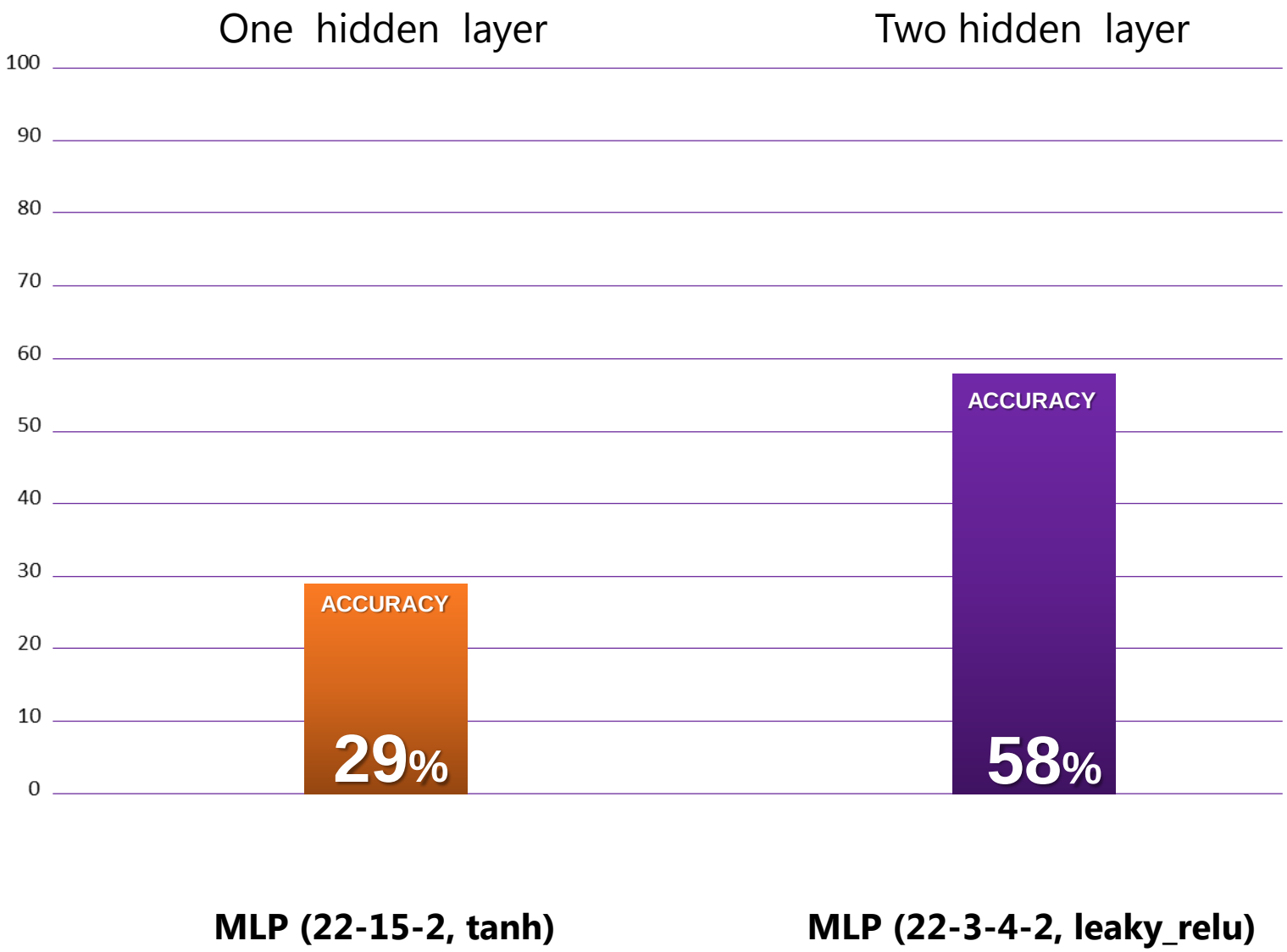
Mechanism of Action

Gamma-aminobutyric acid receptor subunit alpha-1 Potentiator

Gamma-aminobutyric acid receptor subunit alpha-2 Potentiator

Gamma-aminobutyric acid receptor subunit alpha-3 Potentiator

Reference drugs accuracy



The work was carried out within the framework of the state assignment of the Ministry of Health of the Russian Federation No. 23022400009-9.

Thank you for your attention

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