IDENTIFICATION OF NERVE AGENTS USING NEURAL NETWORKS
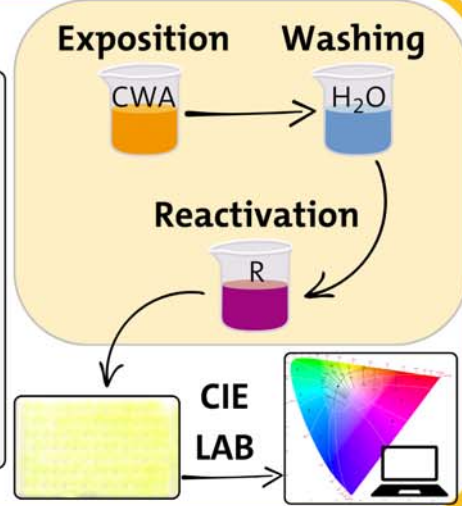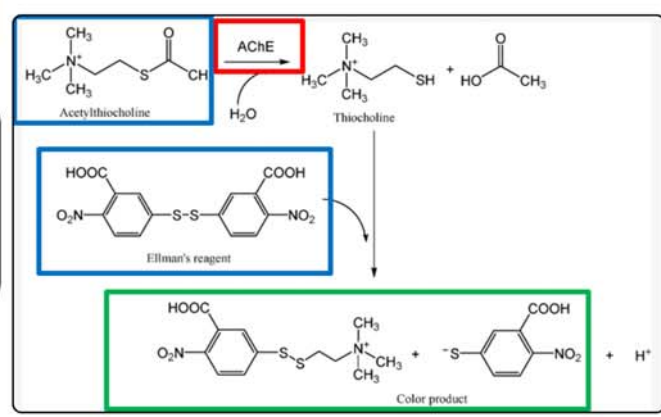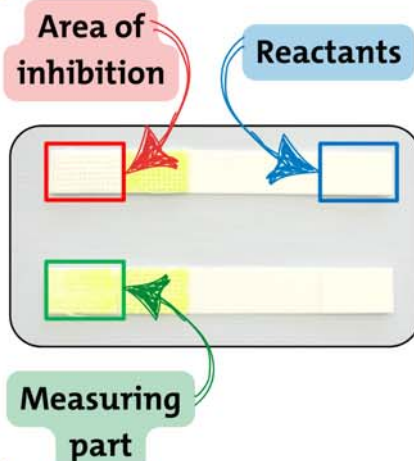
Monika Hoskovcová, Dušan Trefilík, Jiří Žeravík
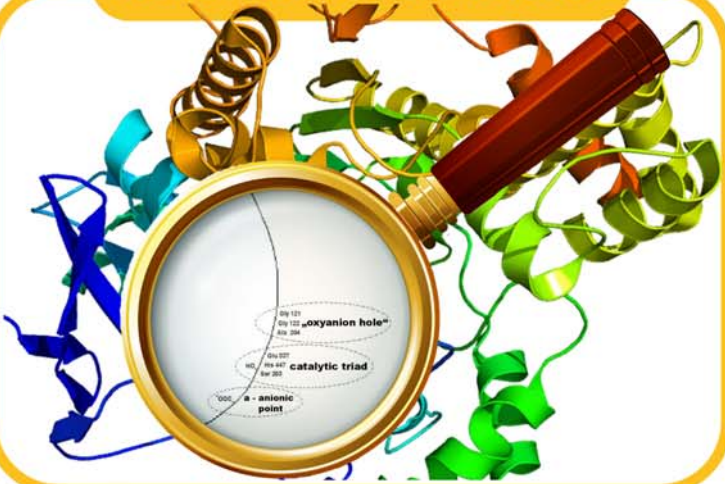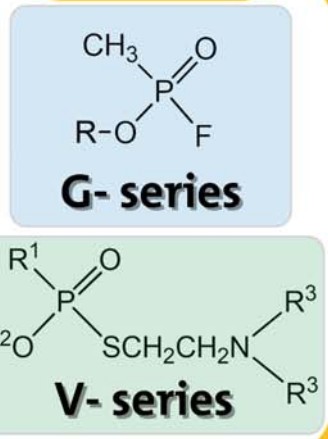
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NBC Defence Institute

INTRODUCTION

Area of inhibition

Reactants

Measuring part

AChE

Acetylthiocholine

Thiocholine

Ellman's reagent

Color product

Exposition

Washing

CWA

H₂O

Reactivation

R

CIE LAB

ACETYLCHOLINESTERASE

"oxyanion hole"

catalytic triad

a - anionic point

INHIBITORS

$$CH_3 - P(=O)(O-R)(F)$$

G- series

$$R^1 - P(=O)(O-R^2)(SCH_2CH_2N(R^3)(R^3))$$

V- series

REACTIVATORS

CH=NOH   CH=NOH

(CH₂)ₙ

n=1 MMB-4
n=2 DMB-4
n=3 TMB-4
n=4 TeMB-4
n=5 PMB-4
n=6 HMB-4
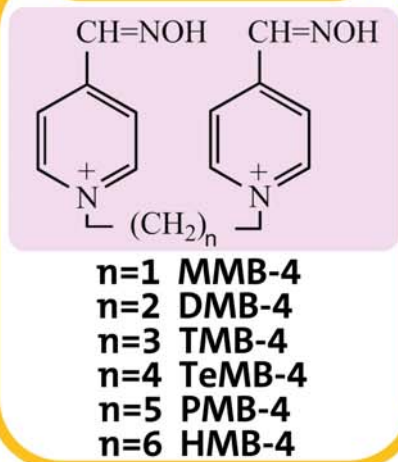
NEURAL NETWORK ANALYSIS

CWA cCWA
R   cR   tR
time

6

Skrytá vrstva

b
w
+

10

Výstupní vrstva

b
w
+

1

L
a
b

Differences in the efficacy of reactivators

$v = f(s,t)$

START

END
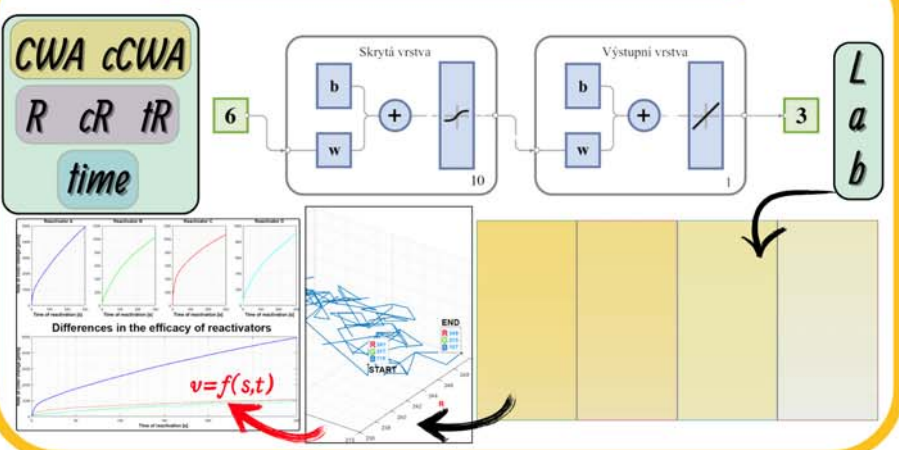
CONCLUSIONS

- Extending the capability of the Ellman method for selective identification of inhibitors.
- Modification of this reaction by bispyridinium aldoximes.
- Utilization of the change in trichromatic values of the biosensor's colored surface.
- Determining the correlations between the different chemical structures of reactivators and their ability to reactivate the inhibited enzyme.
- Evaluation of a large dataset using neural analysis.

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