Supplementary Materials for:

Multiclass Classifier for P-glycoprotein Substrates, Inhibitors, and Non-Active Compounds

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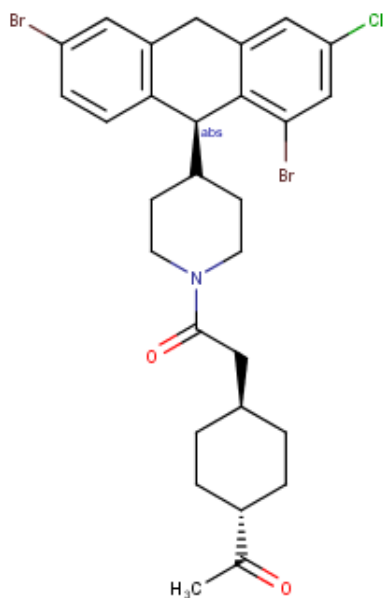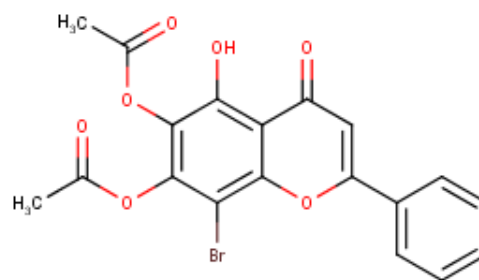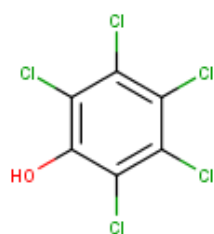[*] Correspondence: marjana.novic@ki.si; Tel.: +386-01-476-0253
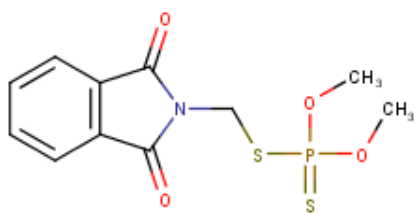
(a)
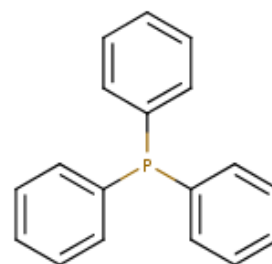
(b)

Figure S1. Structures of the compound with largest ED to the central neuron in the TE set: (**a**) Phosmed; (**b**) Triphenylphosphane.
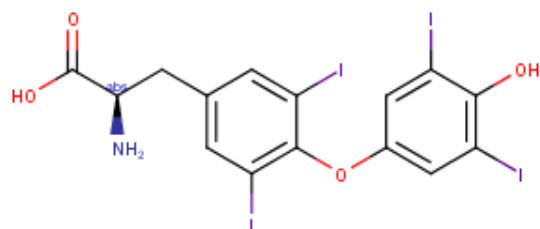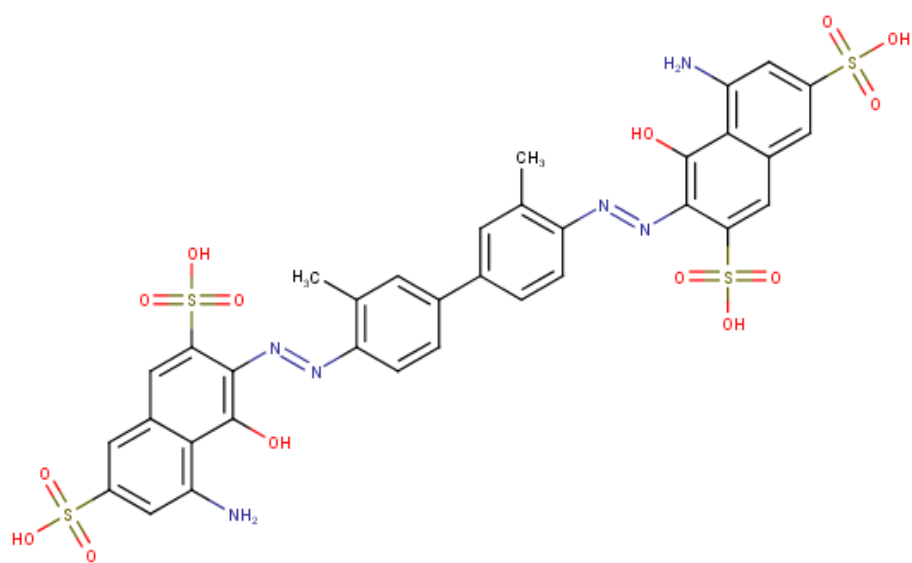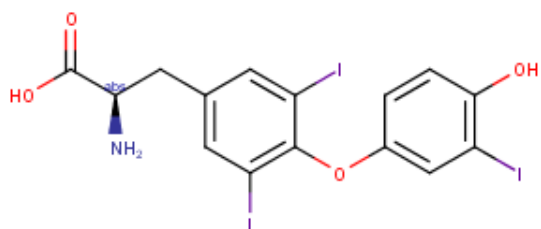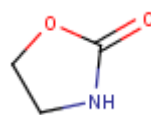

(a)

(b)

(c)

(d)

(**e**)

(**f**)

(**g**)
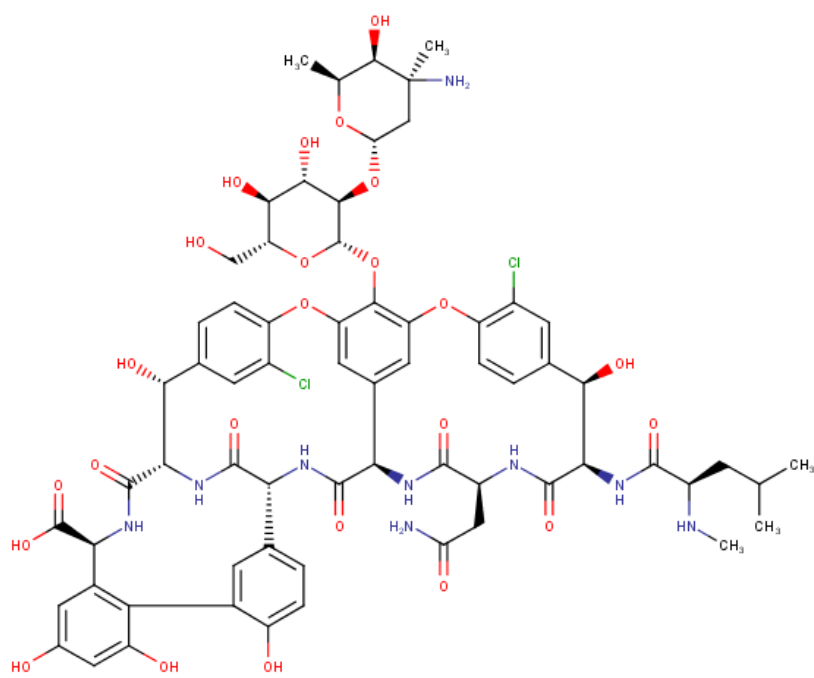
(**h**)
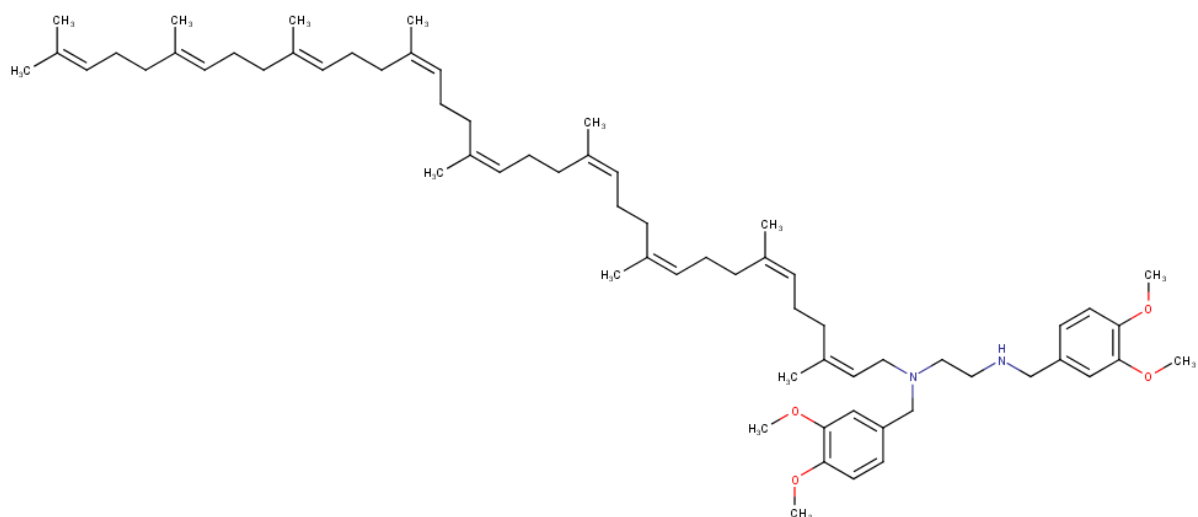
(**i**)
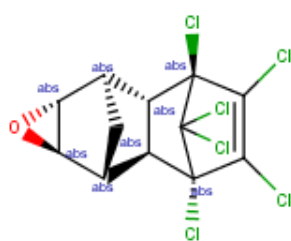
(**j**)

(**k**)
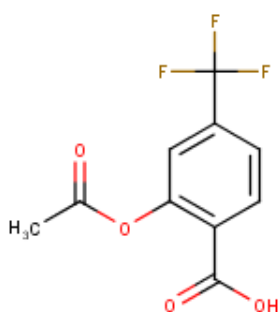
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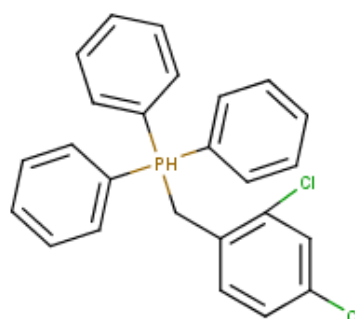
(**m**)

Figure S1. Structures of the compound with largest ED to the central neuron in the V set: (**a**) 2-(4-acetylcyclohexyl)-1-[4-[(9S)-1,6-dibromo-3-chloro-9,10-dihydroanthracen-9-yl]piperidin-1-yl]ethanone; (**b**) (7-acetyloxy-8-bromo-5-hydroxy-4-oxo-2-phenylchromen-6-yl) acetate; (**c**) Pentachlorophenol; (**d**) Thyroxine; (**e**) Trypan blue; (**f**) Triiodothyronine; (**g**) 2-Oxazolidinone; (**h**) Vancomycin; (**i**)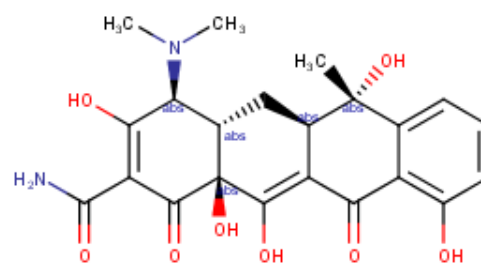 Sdb-ethylenediamine; (**j**) Dieldrin; (**k**) Tetracycline; (**l**) Triflusal; (**m**) (2,4-dichlorophenyl)methyl-triphenylphosphanium.
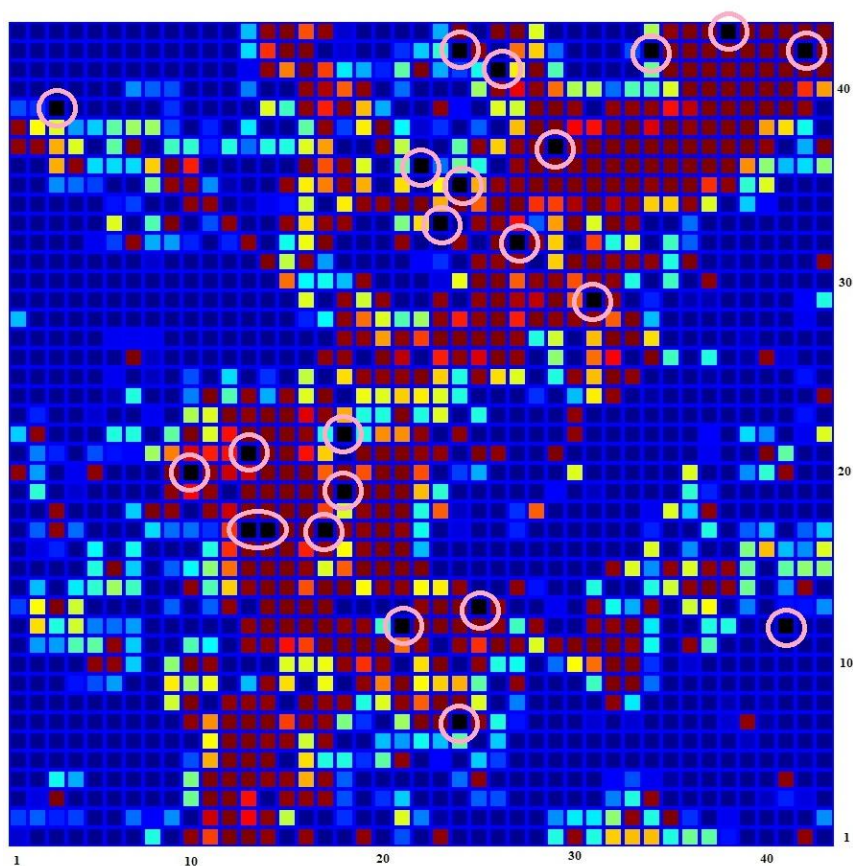
Figure S3. Distribution of the 24 overlapping negative compounds (P-gp non-inhibitor (NI) and P-gp non-substrate (NS)) in the response map of the non-active class. These are the only absolutely certain non-active compounds. The position of the neurons where these compounds are located were coloured black and highlighted with a pink circle. They are well spread over the whole area occupied by the all non-active compounds meaning that structural similarity (which is the only influencing factor for forming clusters in the Counter-Propagation Artificial Neural Network output layer) with other non-actives, tested with only one assay, is significant. The only area of non-active compounds that does not include any of the double-tested non-actives, is around the neuron at the position (13, 5) in lower left part of the map, so we may consider the predictions associated with this area less reliable.