Commercial QSAR modeling? Sorry, already patented…

Egon Willighagen ⬤

Published July 23, 2008

Citation

Willighagen, E. (2008, July 23). Commercial QSAR modeling? Sorry, already patented… *Chem-bla-ics*. https://doi.org/10.59350/ejb9x-yf544

Keywords

Qsar

Abstract

QSAR has been patented in 2001 (US patent 20010049585).

chem-bla-ics

[QSAR has been patented](#) in 2001 (US patent 20010049585).

Claim 1:

> *A method for predicting a set of chemical, physical or biological features related to chemical substances or related to interactions of chemical substances using a system comprising a plurality of prediction means, the method comprising using at least 16 different individual prediction means, thereby providing an individual prediction of the set of features for each of the individual prediction means and predicting the set of features on the basis of combining the individual predictions, the combining being performed in such a manner that the combined prediction is more accurate on a test set than substantially any of the predictions of the individual prediction means.*

They use averaging or weighted averaging of the individual predictions (claim 2). Oh, and just in case you think you are clever and you use 17, 32, etc individual predictions. Sorry, no luck either; you have to use way beyond 1M individual predictions according to the following claim ;)

Claim 2:

> *A method according to claim 1, wherein the number of different predictions means is at least 20, such as at least 30, such as at least 40, 50, 75, 100, 200, 400, 600, 800, 1000, 1200, 1400, 1600, 1800, 2000, 2500, 3000, 4000, 5000, 6000, 7000, 8000, 9000, 10,000, 15,000, 20,000, 30,000, 40,000, 50,000, 100,000, 200,000, 500,000, 1,000,000.*

What can I say about this? Please leave your opinion in the comments...