

4.3 Preparing for REACH implementation: CODES: A topological method to encode chemical structures based on neural computing. Application in biokinetic parameters prediction.

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Dr. Campillo addressed CODES, which is a topological method to encode chemical structures based on neural computing. The method is used to predict biokinetic parameters. QSAR (quantitative structure-activity/properties) relationships can be solved using multilinear regression, principal component analysis, comparative field analysis or artificial neural networks. Dr. Campillo's presentation dealt exclusively with self learning artificial neural networks (ANN).

An ANN is an information processing paradigm inspired by biological nervous systems, such as the brain processes information. It is a self modelling method with great ability to adapt to a new situation, or control an unknown system, using data acquired in previous experiments. The learning can be supervised (each output unit is told which should be the desired response to input signals) or unsupervised (it self organises data and is able to detect emergent collective properties).

CODES generates numeric topological descriptors taking into account atomic number, type of bond, connectivity with the rest of the molecule and chiral centres. It can be applied successfully to QSAR and QSPR studies.