Computer Based Aided Enzyme Selectivity by Enzyme Channel Engineering

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Received: August 01, 2022, Manuscript No. TOSOCIAL-22-75850; **Editor assigned:** August 03, 2022, PreQC No. TOSOCIAL-22-75850 (PQ); **Reviewed:** August 17, 2022, QC No. TOSOCIAL-22-75850; **Revised:** August 22, 2022, Manuscript No. TOSOCIAL-22-75850 (R); **Published:** August 29, 2022

Description

Enzymes with chemo-selectivity, region-selectivity, and stereo-selectivity enable the asymmetric synthesis of high-quality chiral molecules. Unfortunately, the drawback that naturally occurring enzymes are often inefficient or exhibit undesired selectivity towards unnatural substrates hinders the expansion of biocatalytic applications. To meet specific selectivity needs in asymmetric synthesis, biochemists have implemented different computational strategies to understand and develop enzymatic selectivity, diversifying the collection of available engineered enzymes. . As the entire asymmetric catalytic cycle with precise interactions within the active site and substrate transport within the enzyme channel can affect enzyme efficiency and selectivity, here we provide a comprehensive computational workflow for enzyme selectivity. I gave you an overview. This review describes a mechanistic understanding of enzyme selectivity based on quantum mechanics calculations, rational design of enzyme selectivity controlled by enzyme-substrate interactions, and regulation of enzyme selectivity by enzyme channel engineering. . Finally, we described a computational paradigm for in silico enzyme selectivity design to facilitate further development of asymmetric biosynthesis.

The ability to measure microtissue contraction *in vitro* can provide important information when modeling heart, cardiovascular, respiratory, gastrointestinal, skin, and skeletal tissues. However, measuring tissue contraction *in vitro* often requires the use of large numbers of cells per tissue construct, in addition to time-consuming microscopy and image analysis. Here, we present a low-cost, versatile, high-throughput platform for measuring microtissue contraction in a 96-well plate configuration using one-step batch imaging. More specifically, a fiber optic microprobe is implanted in the micro tissue and contraction is measured as a function of the deflection of the optical signal emitted from the end of the fiber. A digital camera allows simultaneous measurement of signals from all filled wells on the plate. The algorithm uses pixel-based image analysis and computer vision techniques for precise multiwell quantification of optical microprobe positional changes induced by micro-tissue contraction.

A motivational framework of engagement and its relationship with three contemporary theories (self-determination theory, expected value theory, and social cognitive theory of self-regulation) was presented. To understand how engagement is influenced by intrinsic and extrinsic motivations, child and parent values and expectations, and the characteristics of technology and intervention design that influence self-regulatory processes. A coping review was conducted. We extracted data from 26 articles reviewed by several reviewers and describing home clinical trials of computer game-based interactive exercise interventions for children with cerebral palsy. A narrative synthesis framework was used for the analysis.

Conclusion

Recent advances in the classification of electroencephalogram (EEG) signals have mainly focused on domain-specific approaches that hinder the cross-cutting capabilities of algorithms. This study presents a new computer-aided diagnosis (CAD) system for classifying two different EEG domains under a unified sequential framework. The main motivation for considering two neurological disorders in one framework is to develop a unified algorithm for EEG classification. The main contribution of this study is 5-fold. First, decompose the EEG signal into 10 eigenmode functions (IMFs) using an empirical wavelet transform. Second, a new two-dimensional (2D) modeling of the IMF is drawn to visualize the complexity of the EEG signal. Third, some new geometric features are extracted to analyze the dynamic and chaotic nature. Fourth, the important features are selected by a binary particle swarm optimization (B-PSO) algorithm. Fifth, the selected features are fed to a k-nearest neighbor classifier to classify the EEG signal. All experiments are performed on one depression and two epilepsy EEG datasets with a leak-free cross-validation strategy.

Acknowledgement

None.

Conflict of Interest

The author has declared no conflict of interest.