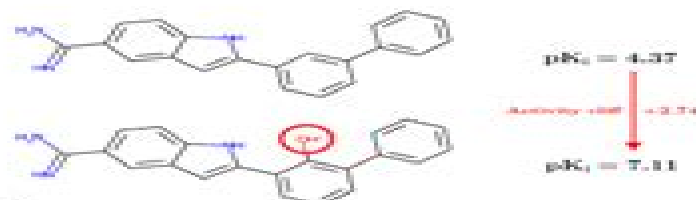


# Exploring Molecular Machine Learning Models for Activity-Cliff Prediction

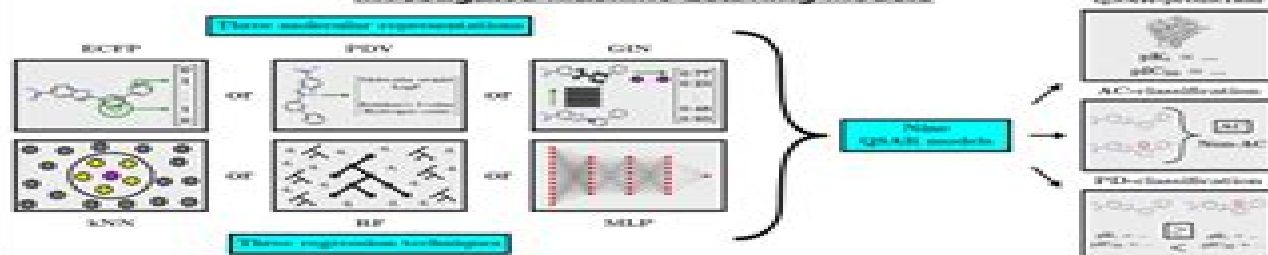
Markus Dablander, Thierry Hanzer, Renaud Lambiotte, Garrett M. Morris

## Activity Cliffs (ACs)

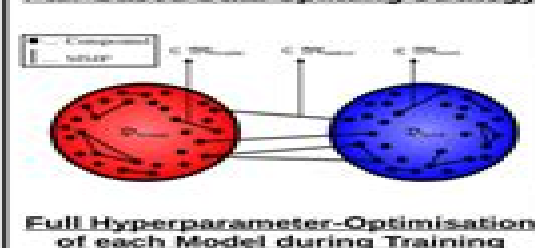
- **Matched molecular pair (MMP):** structural core + small structural change.
- **Large difference in binding affinity (= activity)** for a protein target of at least two orders of magnitude.
- **Importance of ACs in drug discovery:** compound-optimisation, elucidation of structure-activity relationships (SARs), ...
- **Computational study:** prediction of ACs via machine learning models trained to predict binding affinities of individual compounds (QSAR-prediction).
- **Questions:** Can molecular machine learning models predict the existence and direction of ACs? What is the relationship between QSAR- and AC-prediction performance for such models? Do state-of-the-art graph neural networks outperform classical molecular representation methods for QSAR- and/or AC-prediction?



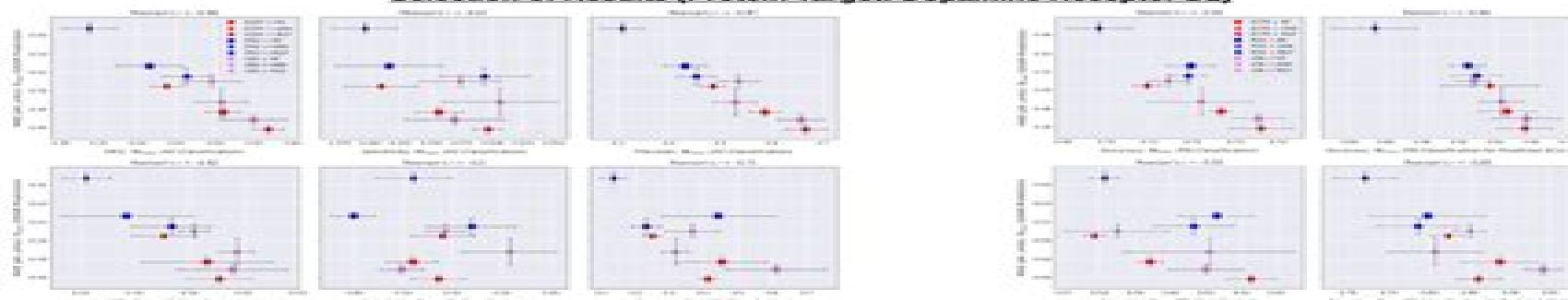
## Investigated Machine Learning Models



## Pair-Based Data-Splitting Strategy



## Selection of Results (Protein Target: Dopamine Receptor D2)



## Conclusions

- If the activities of both molecules are unknown, then the models show low AC-sensitivity. In this case, ACs form a major source of prediction error.
- However, if the activity of one molecule is a priori given, then the models show drastically increased AC-sensitivity and become useful for compound optimisation and SAR-elucidation.
- The accuracy of the predicted potency direction tends to be low for general MMPs, but high when restricted to predicted ACs.
- **Molecular representations:** At QSAR-prediction, classical precomputed ECFPs still tend to beat trainable GINs. At AC-classification, however, GINs tend to beat ECFPs.
- **Potential future research:** development of techniques to boost the AC-sensitivity of molecular machine learning models (twin network training, contrastive learning, ...).

## Full Analysis: Journal Paper

Dablander, M., Hanzer, T., Lambiotte, R., & Morris, G. M. (2023). Exploring QSAR models for activity-cliff prediction. *Journal of Cheminformatics*, 15(1), 47.

## Acknowledgements



# Molecular Approaches To Learning Memor

**Guillaume Favre**



## **Molecular Approaches To Learning Memor:**

*Molecular Approaches to learning and memory*, 1967      **Neurobiology of Learning and Memory** Joe L. Martinez Jr., Raymond P. Kesner, 1998-06-29 Neurobiology of Learning and Memory provides an excellent overview of current information on this fast growing field of neurobiology The contents have been structured for use as a course text or as a handy resource for researchers in neuro and cognitive psychology It discusses learning and memory from developmental pharmacological and psychobiological perspectives as well as changes in learning and memory with age Neurobiology of Learning and Memory also includes research on invertebrates and vertebrates presenting basics in anatomy and development along with computational models It is written in an easy to follow format with summaries at the end of each chapter Key Features Provides an overview of information on the neurobiology of learning and memory Discusses learning and memory from developmental pharmacological and psychobiological perspectives and changes in learning and memory with age Includes research on invertebrates and vertebrates Gives basics on anatomy and development Written for easy comprehension with chapter summaries      Physics and Mathematics of the Nervous System M. Conrad, W. Güttinger, M. Dal Cin, 2013-03-08 This volume is the record and product of the Summer School on the Physics and Mathematics of the Nervous System held at the International Centre for Theoretical Physics in Trieste from August 21 31 1973 and jointly organized by the Institute for Information Sciences University of Tübingen and by the Centre The school served to bring biologists physicists and mathematicians together to exchange ideas about the nervous system and brain and also to introduce young scientists to the field The program attended by more than a hundred scientists was interdisciplinary both in character and participation The primary support for the school was provided by the Volkswagen Foundation of West Germany We are particularly indebted to Drs G Gambke M L Zarnitz and H Penschuck of the Foundation for their interest in and help with the project The school also received major support from the International Centre for Theoretical Physics in Trieste and its sponsoring agencies including the use of its excellent facilities We are deeply indebted to Professor A Salam for his kind cooperation and also to Professor P Budini Dr A M Hamende and to the many members of the Centre staff whose hospitality and efficiency contributed so much to the success of the school We are pleased to acknowledge the generous aid and cooperation of the University of Tübingen and would like to thank its President A      Processes of Animal Memory (PLE: Memory) Douglas Medin, William Roberts, Roger Davis, 2014-05-09 Originally published in 1976 this volume contains new and original contributions of the time addressed to a related set of ideas concerning processes of memory in animals The theme is that animals remember and that theories of animal learning must take this into account as well as the coding processes that have been assumed to be specific to human beings The focus of the book is on processes and some progress is reported in differentiating types of memory The emphasis in applying animal work to studies of human memory is made not in terms of paradigms but in terms of processes implicated via performance in a variety of tasks Also many of the chapters reflect the

usefulness of applying a memory framework to a variety of nonmemory paradigms This work will be essential reading for all those interested in animal as well as human memory and provided the most up to date and broadest examination of animal memory processes at the time from both a theoretical and conceptual framework

**Alterations of Chemical Equilibrium in the Nervous System** Abel Lajtha, 2013-11-21 It has been recognized for more than a thousand years that the function of the brain like the function of the other organs of the body is determined by its physical chemical and biological properties Evidence that even its highest functions could be explained by these properties was gathered only in recent years however these findings which clearly have to be confirmed by a great deal of further experimental evidence indicate that most if not all of the functions of the brain are based on its bio chemical and biophysical mechanisms This at first hearing may sound rather simple but the ability to understand learning emotion perhaps even creativity on biological terms may well be the most important scientific discovery of all time Few pieces of knowledge can influence our future health and well being to the degree that understanding of mental mechanisms will It has been clearly shown in many ways in the previous volumes of this Handbook that from the biochemical or neurochemical point of view the brain is one of the most active organs The brain seems stable and in some respects permanent this is evidence not of inactivity but of carefully controlled homeostasis of dynamic rather than static equilibrium with most components undergoing metabolic alterations

*Psychopharmacology Bulletin* ,1966

Biochemistry of Brain Sudhir Kumar, 2013-10-22 Biochemistry of Brain is a collection of articles dealing with the developments in the biochemistry of the brain This book gives a comprehensive and critical discussion of important developments in studies concerning the above subject This text discusses the structure function and metabolism of glycosphingolipids which are related to the study of sphingolipid storage diseases Inborn defects of metabolism are found in Gaucher s and Fabry s disease which are characterized by lipid accumulation in the brain Another paper reviews the chemical and genetics of critically lysosomal hydrolase deficiencies that can cause the storage of sphingolipids This book then explains the role of myelin basic protein in lipids in vivo that the weak bonding of the protein is not a major component of myelin stability Another paper discusses the procedures for isolating subfractions of myelin and myelin related membranes with some attention given on the alterations in the subfractionation of myelin in pathological hypomyelinating and demyelinating conditions Another article discusses the biochemical and enzymatic composition of lysosomes and the biosynthesis intracellular transport storage and the degradation of lysosomal constituents This collection of papers will benefit scientists doing research in microbiology microchemistry molecular genetics and neurochemistry

**The Structure and Function of Nervous Tissue V2** Geoffrey Bourne, 2012-12-02 The Structure and Function of Nervous Tissue Volume IV Physiology II and Biochemistry II focuses on the structure and function of nervous tissue It investigates the plasticity of synapses their degeneration and regeneration neuronal inclusions RNA of nervous tissue and molecular organization of neural information processing Furthermore it covers topics on gamma aminobutyric acid GABA in the nervous system the

blood brain barrier and the extracellular space ECS in the vertebrate central nervous system CNS Organized into 10 chapters this volume begins with an overview of synapses with emphasis on changes in both the efficacy of individual synapses and the numbers of synapses made by axons upon neurons It then discusses the orthograde terminal degeneration of synapses and the use of light and electron microscopy in studying synapse degeneration and regeneration It also explains the synthesis storage and release of acetylcholine from nerve terminals inclusions associated with viral infections metabolism of RNA in nervous tissue chemical correlates of information processing metabolism of GABA in mammalian CNS electrical activity of the normal brain and chemistry of the cerebrospinal fluid The book concludes with a chapter on the mechanism by which vertebrate central nervous tissue alters the magnitude of the ECS This book will be of interest to anatomists embryologists biochemists pathologists clinicians and molecular biologists This will be invaluable as well to graduate students in a variety of disciplines and those specializing in particular aspects of nervous tissue study

**Behavioral Neuroscience** Carl W. Cotman, James L McGaugh, 2014-04-24 Behavioral Neuroscience An Introduction provides a basic understanding of what is known about the means by which neurons communicate and about the nervous system which interprets integrates and transmits signals into meaningful and appropriate behaviors The book starts with an overview of the nervous system The text then describes the general operation and organization of the nervous system and some of the major types of neurons in the context of their systems The basic characteristics of neurons and how they communicate the processes and the basic integrative properties of defined groups of neurons and complex learning and memory are also considered The book further tackles the auditory somesthetic olfactory gustatory visual and motor systems the functions of the autonomic nervous system and the neuroendocrine system and the neural basis of two types of motivated behavior drinking and feeding The text also encompasses sleep and activity rhythms the development of the neural circuitry and its plasticity throughout life and the development of behavior Behavioral disorders and the aspects of the human nervous system which make man unique among all living creatures are also looked into Behavioral psychologists behavioral neuroscientists and psychobiologists will find the book invaluable

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National Library of Medicine Current Catalog National Library of Medicine (U.S.), 1970 First multi year cumulation covers six years 1965 70

*International Review of Neurobiology*, 1975-05-30 Published since 1959 this serial presents in depth reviews of key topics in neuroscience from molecules to behavior The

serial stays keenly attuned to recent developments through the contributions of first class experts in the many fields of neuroscience. Neuroscientists as well as clinicians, psychologists, physiologists and pharmacologists will find this serial an indispensable addition to their library. **Planaria: A Model for Drug Action and Abuse** Robert B. Raffa, 2008-12-03. The study of drug action has benefitted greatly from the development and use of in vivo model systems. In model systems, manipulations and observations can be more rigorously controlled and screens of novel therapeutic agents can be more safely conducted. No single model system provides all of the possible advantages. At one end, mammalian models al

*Advances in Insect Physiology*, 1972-10-27. *Advances in Insect Physiology*. *The Memory System Of The Brain* Jean Delacour, 1994-04-22. The purpose of this book is to describe the memory system of the brain taking into account all the levels of neural organization: molecule, cell, small network and anatomical circuit. This synthetic approach is necessary for determining the real mechanisms among the potential ones that is the neural bases of learning and memory in intact organisms functioning under normal conditions. For this purpose, data from molecular, cellular and behavioral neurobiology, neuropsychology, animal and human psychology and neural modelling are comprehensively reviewed by leading specialists and brought together in an original synthesis. **Memory and Transfer of Information** H. Zippel, 2012-12-06. The contents of this book are the presentations of a Symposium on Memory and Transfer of Information held at Gottingen May 24-26, 1972. One of the main reasons for organizing this Symposium was to stimulate interdisciplinary discussion between scientists working in the field as a whole. Most of the previous meetings dealing with memory and transfer of information have tended to be rather limited in scope. The present Symposium covered a wide range of topics including neurophysiological, neuropharmacological, neurochemical, behavioral and clinical aspects of learning and chemical transfer of information presented by specialists in these areas. The Proceedings of the meeting present a large number of previously unpublished results, e.g. recent experiments in neurophysiology and neurochemistry, new approaches to chemical transfer of learned information, experiments using synthetic scotophobin and drugs influencing learning and behavior. The importance of interdisciplinary discussion is perhaps most clearly emphasized by the advances in neurochemical micromethods which are of particular interest to scientists working on the chemical transfer of information. Only such interdisciplinary collaboration between highly specialized scientists guarantees further progress and deeper insight into the complex and until now little understood mechanisms of that most intricate of organs, the brain. Hans Peter ZIPPEL, vii. CONTRIBUTORS: BRADLEY P. B. Department of Pharmacology, Medical School, Birmingham B15 2TJ, England. BYRNE W. L. Department of Biochemistry, University of Tennessee College of Basic Medical Sciences, Memphis, Tennessee 38103, U.S.A. CREUTZFELDT O. D. Neural Plasticity and Memory Federico Bermudez-Rattoni, 2007-04-17. A comprehensive multidisciplinary review. Neural Plasticity and Memory. From Genes to Brain Imaging provides an in-depth up-to-date analysis of the study of the neurobiology of memory. Leading specialists share their scientific experience in the field covering a wide range of topics where molecular

genetic behavioral and brain imaging techniq

**Function** Mary Agnes Burniston Brazier, 1963

**Biomedical Index to PHS-supported Research**, 1991

**Brain**

Fundamental Neuroscience Larry Squire, James L. Roberts, Nicholas C.

Spitzer, Michael J. Zigmond, Darwin Berg, Floyd E. Bloom, Sascha du Lac, Anirvan Ghosh, Larry R. Squire, Susan K.

McConnell, 2002-11-19 With over 300 training programs in neuroscience currently in existence demand is great for a comprehensive textbook that both introduces graduate students to the full range of neuroscience from molecular biology to clinical science but also assists instructors in offering an in depth course in neuroscience to advanced undergraduates The second edition of Fundamental Neuroscience accomplishes all this and more The thoroughly revised text features over 25% new material including completely new chapters illustrations and a CD ROM containing all the figures from the text More concise and manageable than the previous edition this book has been retooled to better serve its audience in the neuroscience and medical communities Key Features Logically organized into 7 sections with uniform editing of the content for a one voice feel throughout all 54 chapters Includes numerous text boxes with concise detailed descriptions of specific experiments disorders methodological approaches and concepts Well illustrated with over 850 full color figures also included on the accompanying CD ROM

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