



北京大學
PEKING UNIVERSITY

当HDAC遇上ABC

Group 5

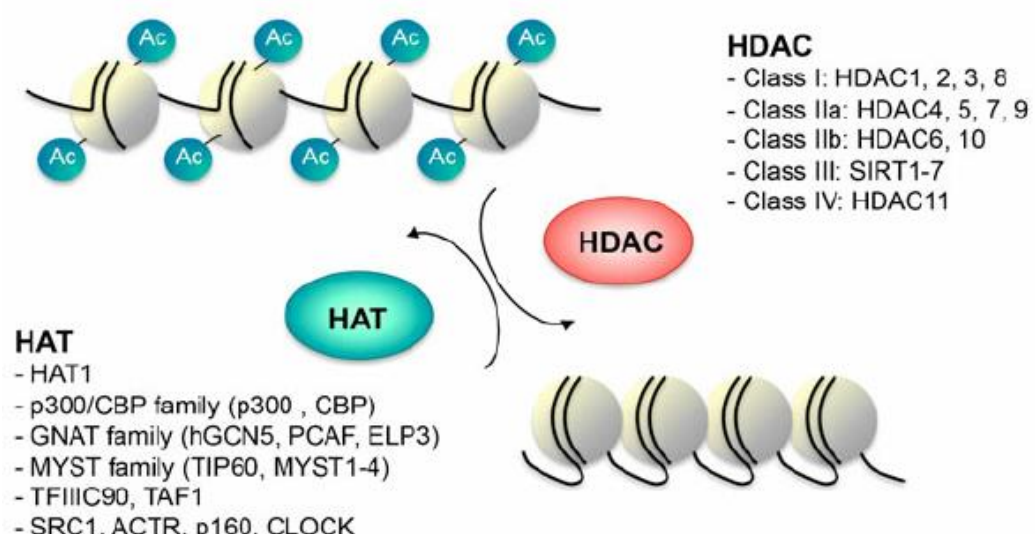
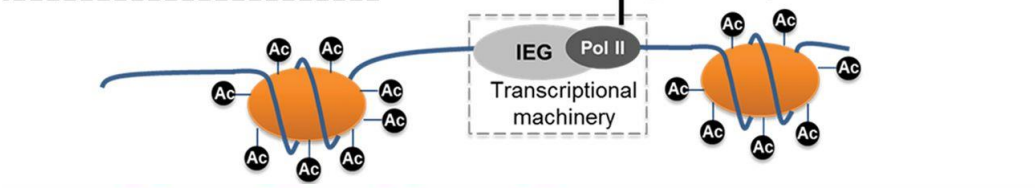
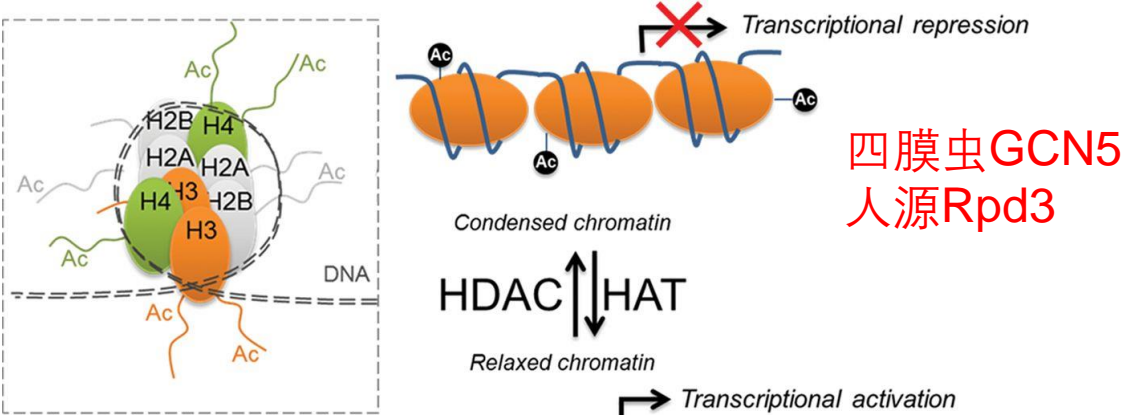
Members: Minqiang Hu (胡敏强)
Dan Cao (曹丹)
Kun Zhang (张坤)
Hailing Chen (陈海灵)

Date: 01/06/2019

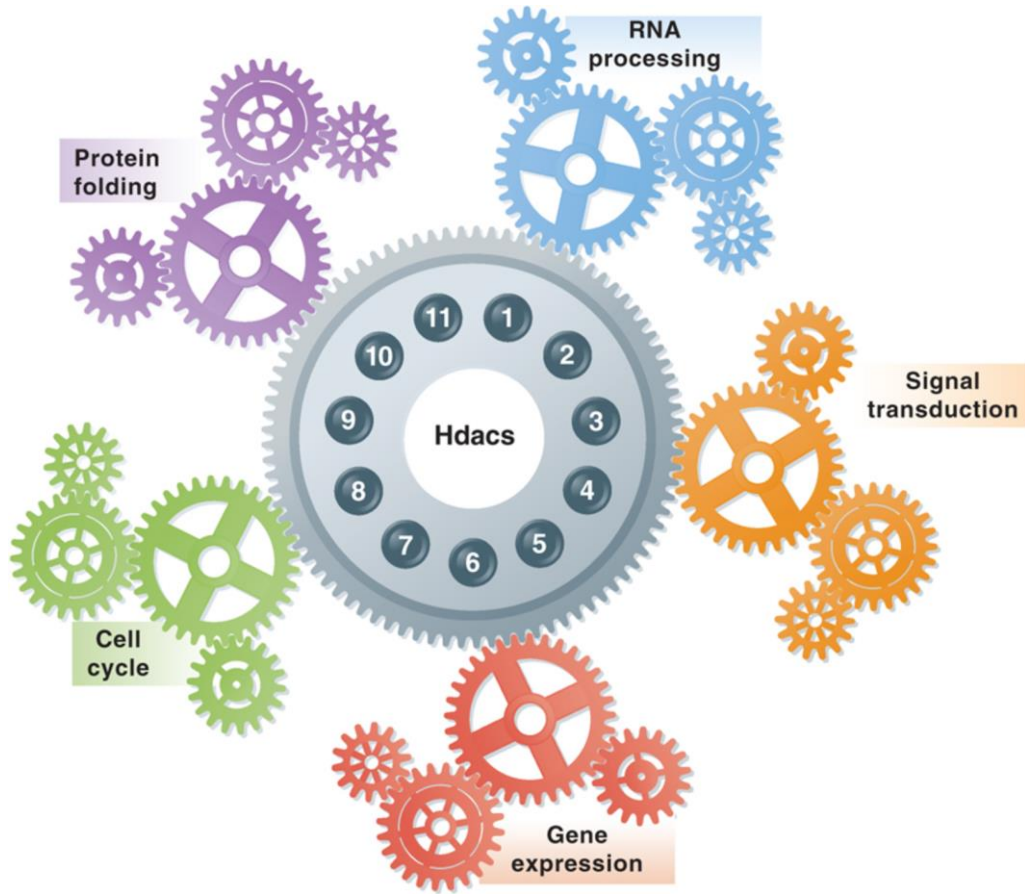
Outline

- Background
- Sequence Alignment
- Structure analysis
- Tools

Histone Deacetylase (HDAC)

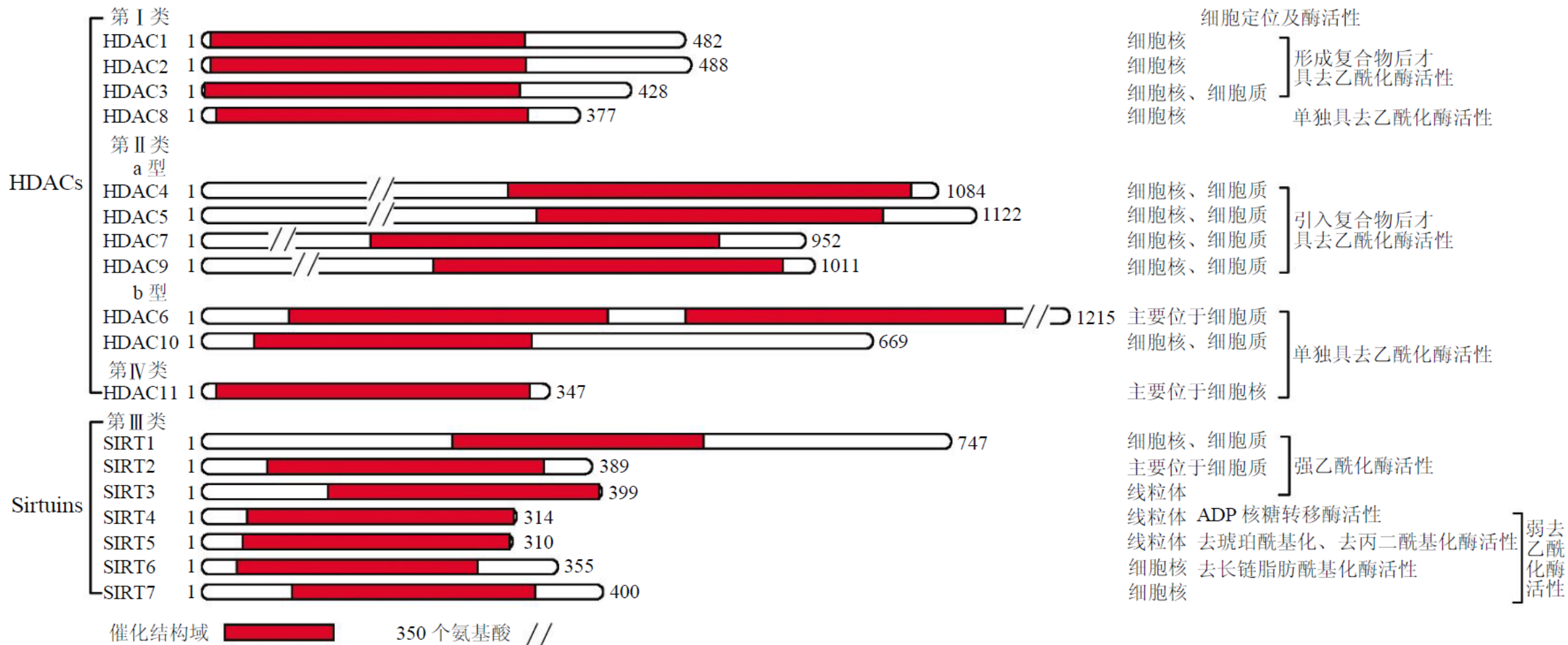


Histone Acetyltransferase (HAT)



Histone Deacetylase (HDAC)

Classification and domain structures of human HDAC



Cancer Research

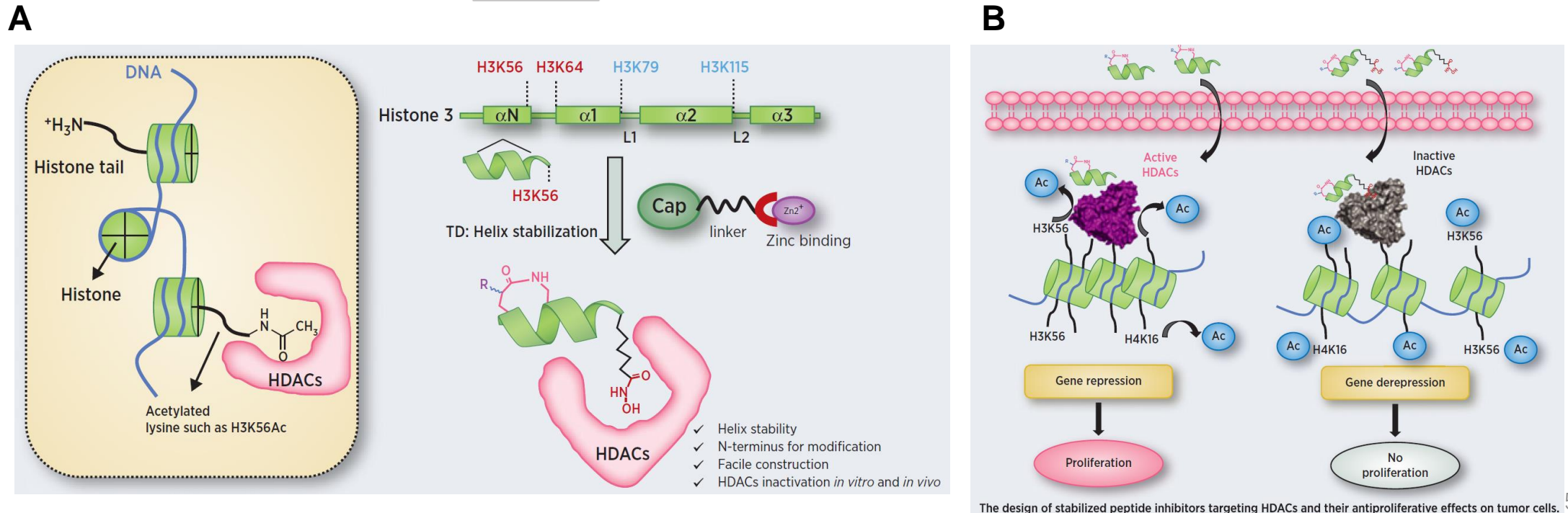
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Research Article

Stabilized peptide HDAC inhibitors derived from HDAC1 substrate H3K56 for the treatment of cancer stem-like cells *in vivo*

Dongyuan Wang, Wenjun Li, Rongtong Zhao, Longjian Chen, Na Liu, Yuan Tian, Hui Zhao, Mingsheng Xie, Fei Lu, Qi Fang, Wei Liang, Feng Yin, and Zigang Li

DOI: 10.1158/0008-5472.CAN-18-1421 [Check for updates](#)



Sequence Alignment

Sequence Alignment

File Edit Select View Annotations Format Colour Calculate Web Service

HDAC1/1-482 1 MAQTQGRTRKVCYYYDGDVGNYYGGGHPMKPHRIRMTNHLNLLNYGLYRKMIEYRPHKANAEEMTKYHSDDYIKFLRIRPDNMSSEYKQMRFNVDGDCPVPFDGLFEFCQLSTGGSVASAVKLNKQQTIDAVNWAGGL 138
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HDAC9/1-1011 1 MHSMISSVDVKSVEPVGLEPIPLDLRLTLRMMMPVDPVYREKQLQQLLELLIQQQQIQKQLLAEFQKQENLTRHQALQHEIKELLAIKQQQELLEKEKLEQQRQEQEVERHRRRQQLPLRKGKDRGRERAVA 138
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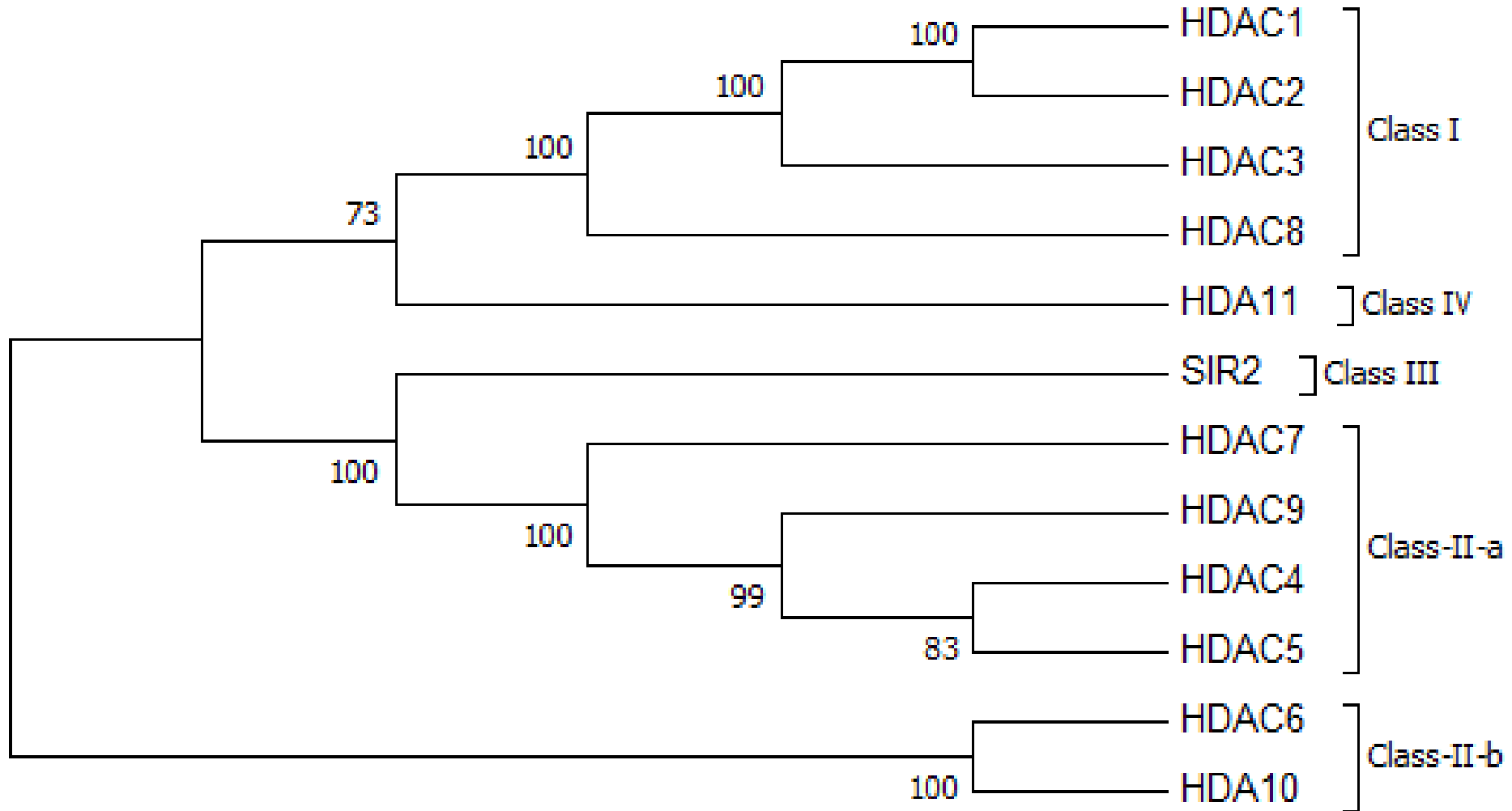
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HDAC3/1-428 139 EASGFCYVNDIVLAILLELLKYHQRVLYIDIDIHGGDVEEAFYTTDRVMTVSFHKYGEYFPGTGLDRDIDGAGKGYAVNYPFRDGDIDDESIEAIFKPYMSKVMEMFQPSAVVLQCGSDLSLSDRLGCFNLT 276
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Phylogenetic tree construction



IIa类HDACs

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HDAC9 YDPLMLKHQCVCGNSTTHPEHAGRIQSIWSRLQETGLLNKCEIRIGRKASLEEIQLVHSE
HDAC4 YDTLMLKHQCTCGSSSSHPEHAGRIQSIWSRLQETGLRGKCECIRGRKATLEELQTVHSE
HDAC7 YDSVMLKHQCSOCDNSRHPEHAGRIQSIWSRLQERGLRSQCCELRGRKASLEELQSVHSE
**.*.***** **.. ***** ** ..** :****:*:* *

HDAC5 YHTLLYGTSPNLRQKLDKSKLLGPISQKMYAVLPCGGIGVSDTVWNEMHSSSAVRMAVG
HDAC9 HHSLLYGTNPLDGQKLDPRILLGDDSQKFFSSLPCGGIGVSDTIWNELHSSGAARMAVG
HDAC4 AHTLLYGTNPLNRQKLDKSKLLGSLAS-VFVRLPCGGVGVSDTIWNEVHSAAGARLAVG
HDAC7 RHVLLYGTNPLSRKLDNGKLAGLLAQRMFVMLPCGGVGVSDTTIWNELHSSNAARWAAG
* ****.*. ** * * . . : *****:**:**:**:**.* * *

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HDAC9 CVIELASKVASGELKNGFAVVRPPGHAEESTAMGFCFFNSVAITAKYLRDQLNISKILI
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HDAC7 SVTDLAFKVASRELKNGFAVVRPPGHADHSTAMGFCFFNSVAITACRQLQKQSKASKILI
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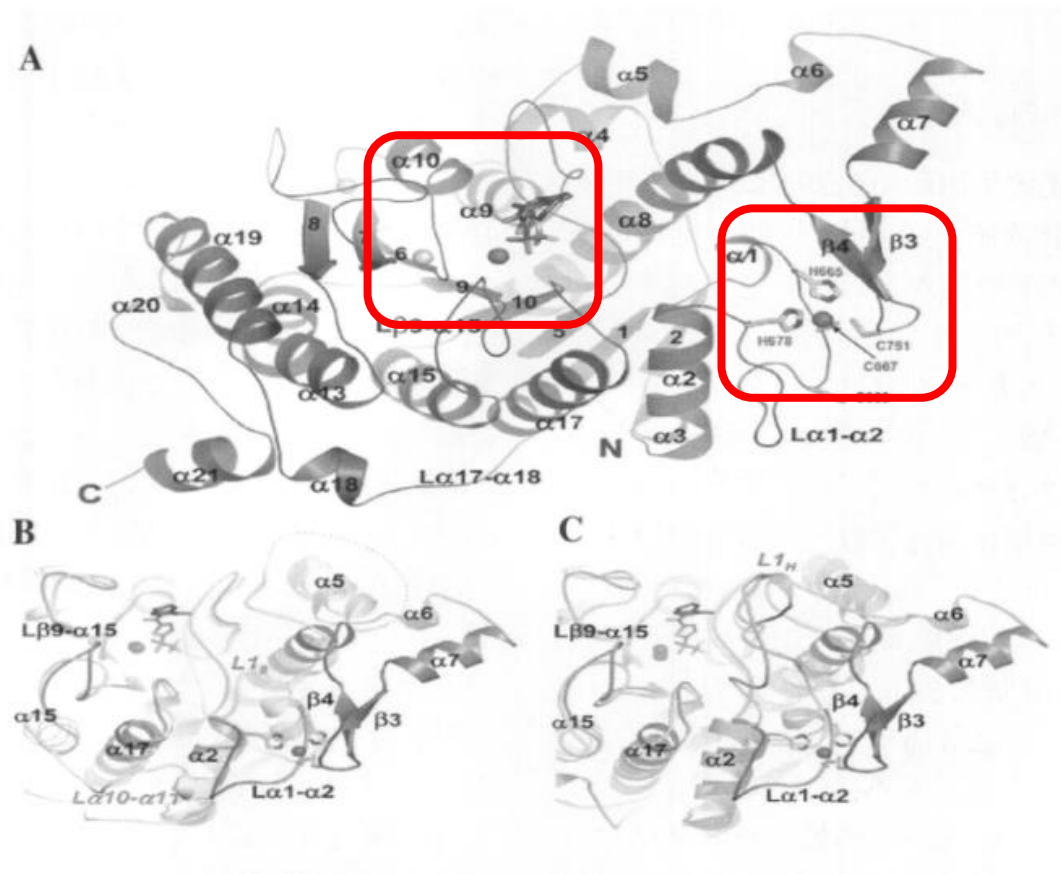
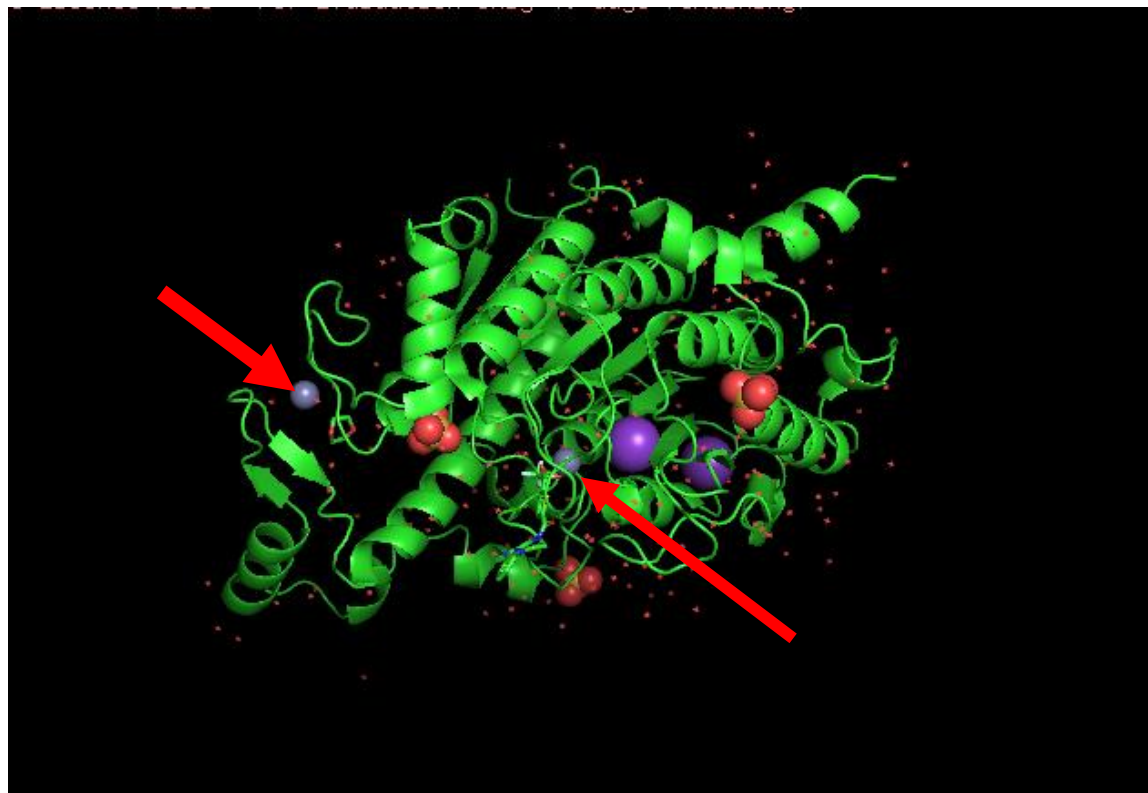
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* :***:** ** * * * * * : * * * * * :*****:** ** * .***** :**:**:**

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* :*** ** * :*****:***** ** * . :*** * * * * * : ** * * : *
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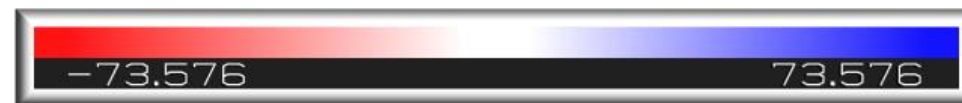
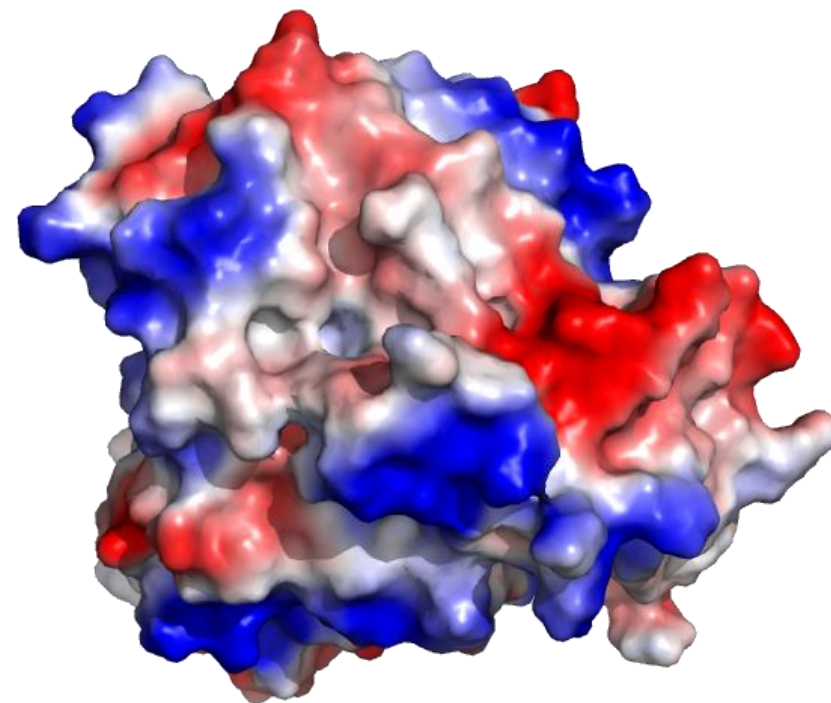


IIa类HDACs



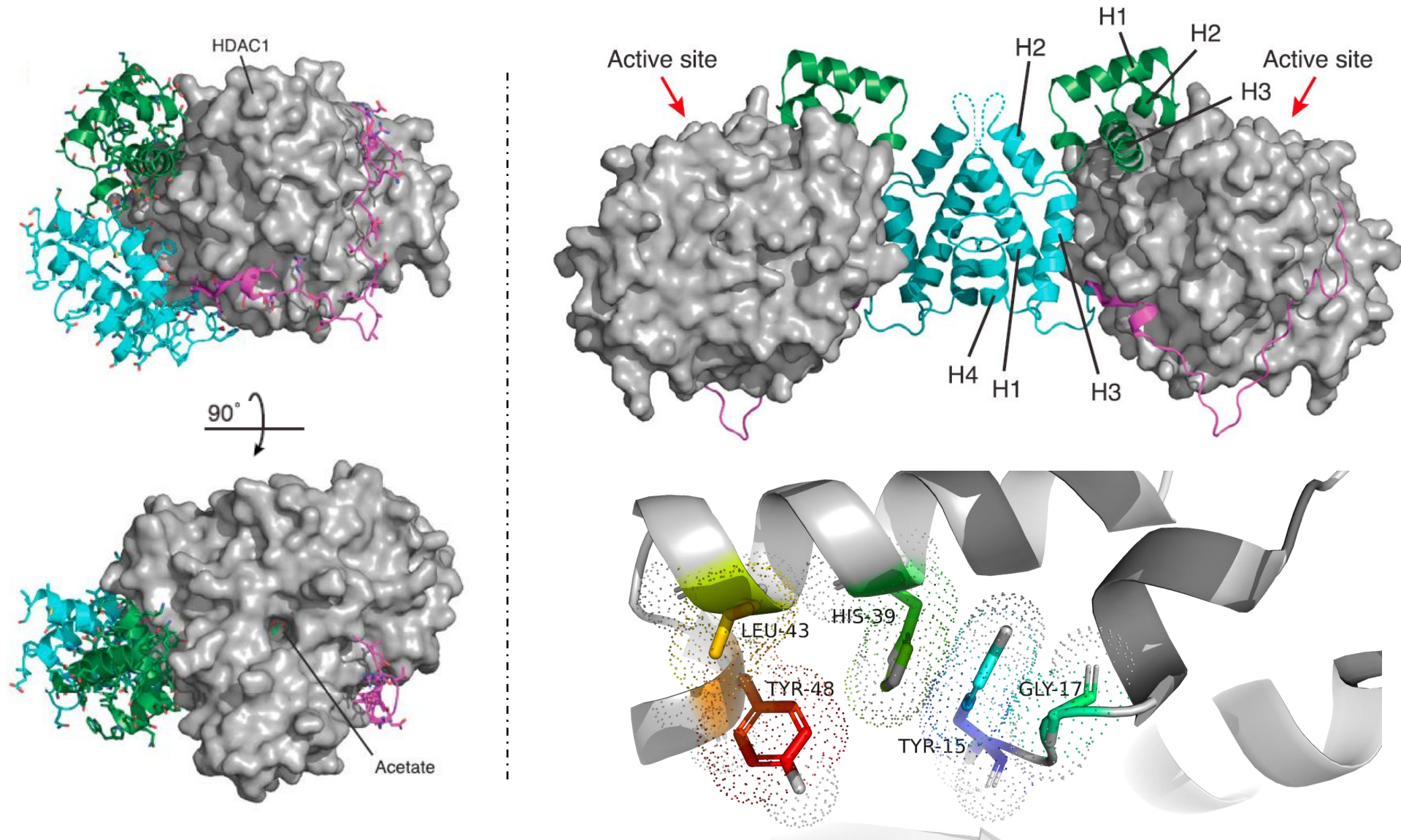
Structure analysis

Predicted model for HDAC1

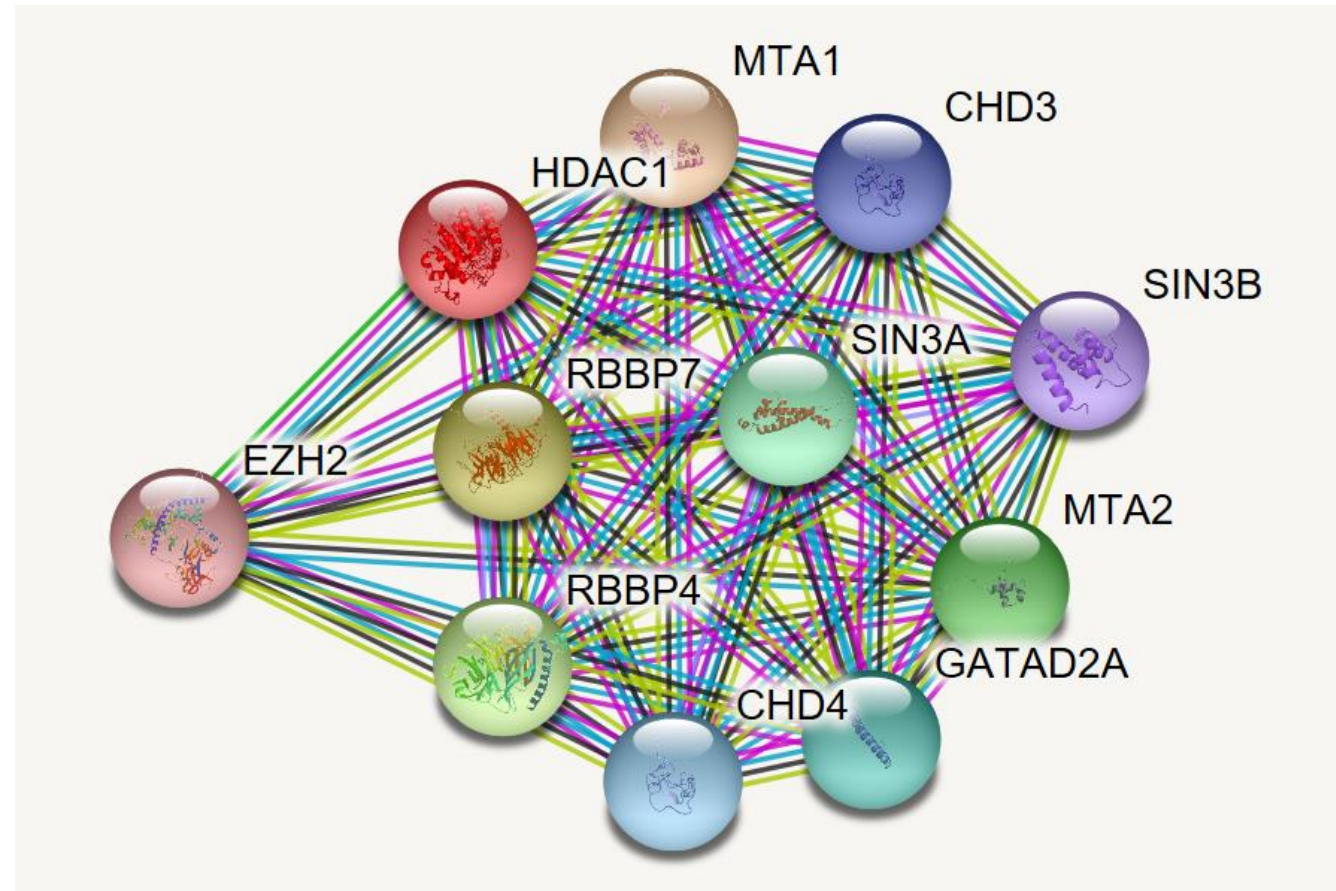


PDB code: 1TYI

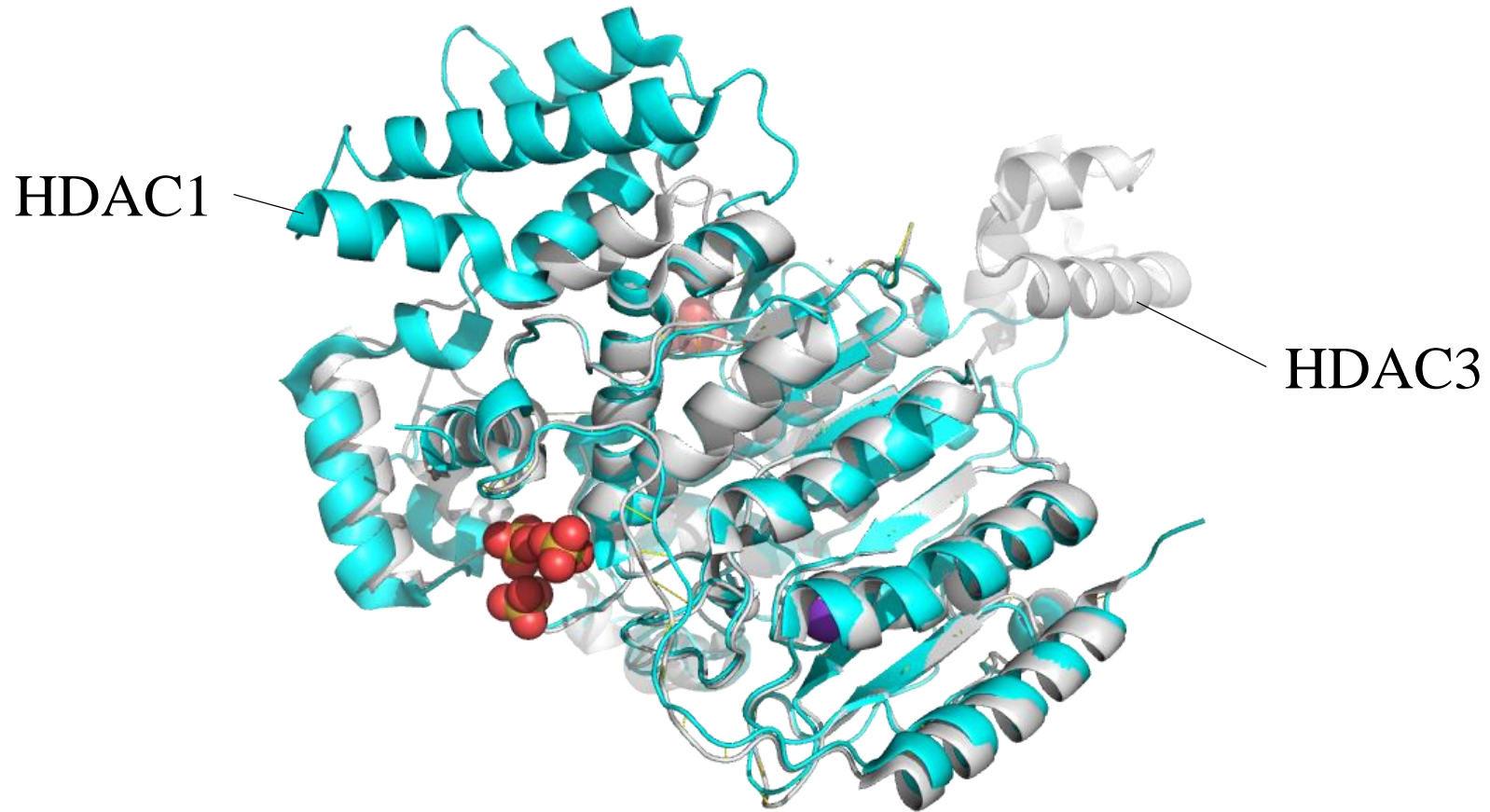
Structure of the HDAC1:MTA1 Complex



The complex interaction of HDAC1

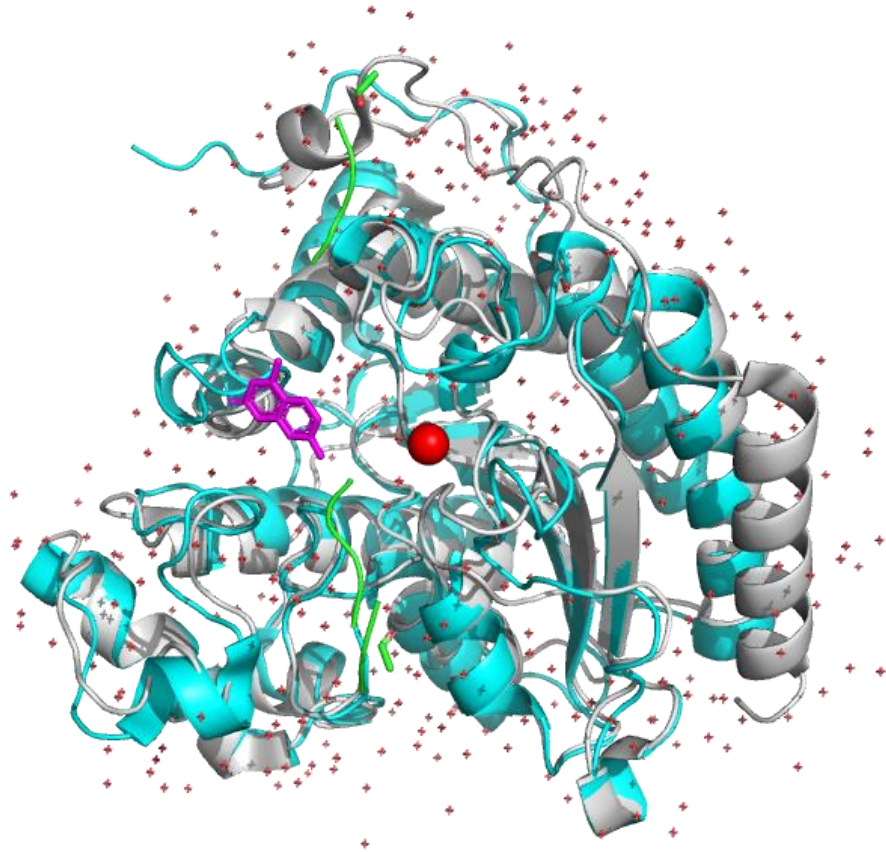
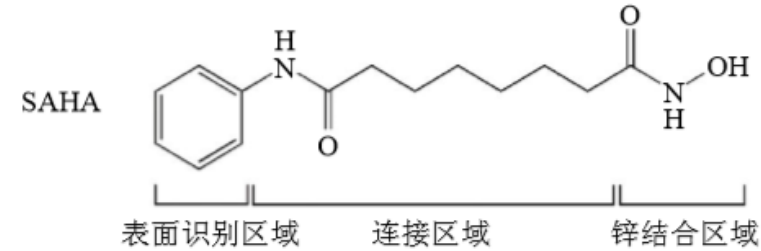


Overlapped structure of HDAC1 and HDAC3

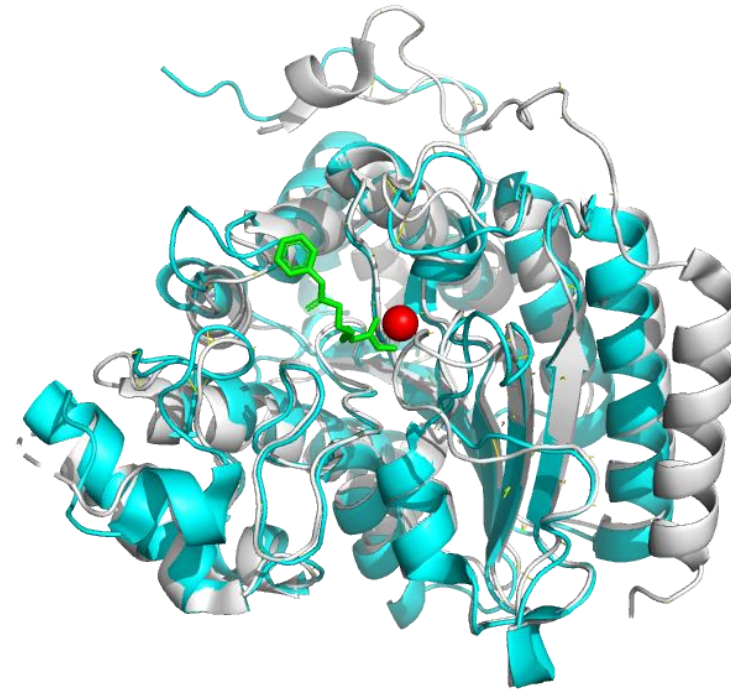


PDB code: 4A69(HDAC3), 4BKX(HDAC1)

Overlapped structure of HDAC1 and HDAC8 binding to substrate and SAHA



HDAC1 & HDAC8 Binding to substrate



HDAC1 & HDAC8 Binding to SAHA

Tools

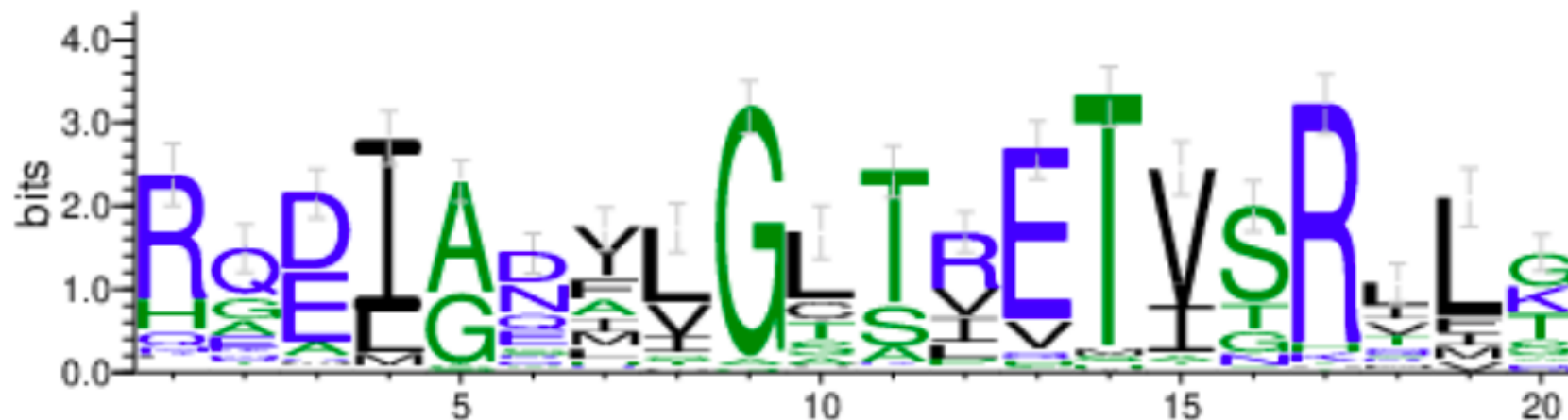


序列标识围(sequence logo)是以图形的方式依次绘出序列比对中各个位置上出现的残基。每个位置上残基的累积可反应出该位置上残基的一致性。每个残基对应图形字符的大小与残基在该位置上出现的频率成正比。但图形字符的大小并不等于频率百分比，而是经过简单统计计算后转化的结果。

Weblogo在线工具

<http://weblogo.threeplusone.com>

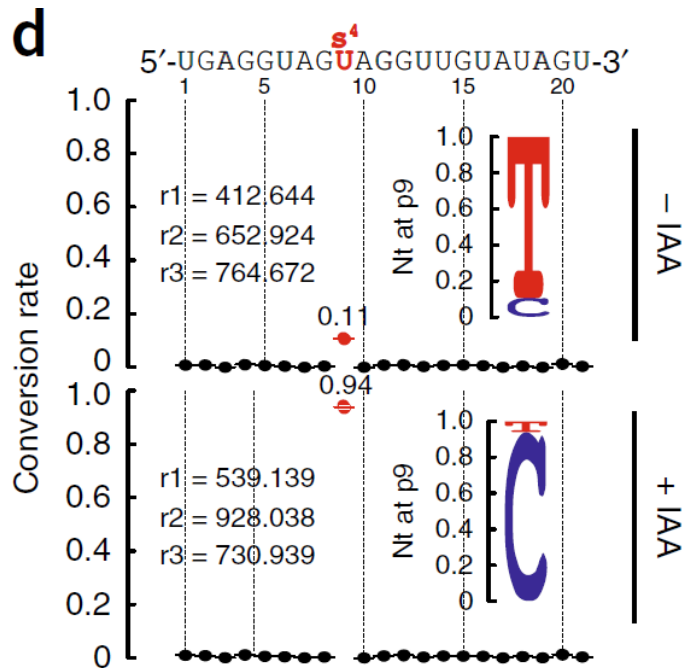
<https://mp.weixin.qq.com/s/R2E5oQwCa1X8QZ81xULopg>



Article | Published: 25 September 2017

Thiol-linked alkylation of RNA to assess expression dynamics

Veronika A Herzog, Brian Reichholf, Tobias Neumann, Philipp Rescheneder, Pooja Bhat, Thomas R Burkard, Wiebke Wlotzka, Arndt von Haeseler, Johannes Zuber & Stefan L Ameres



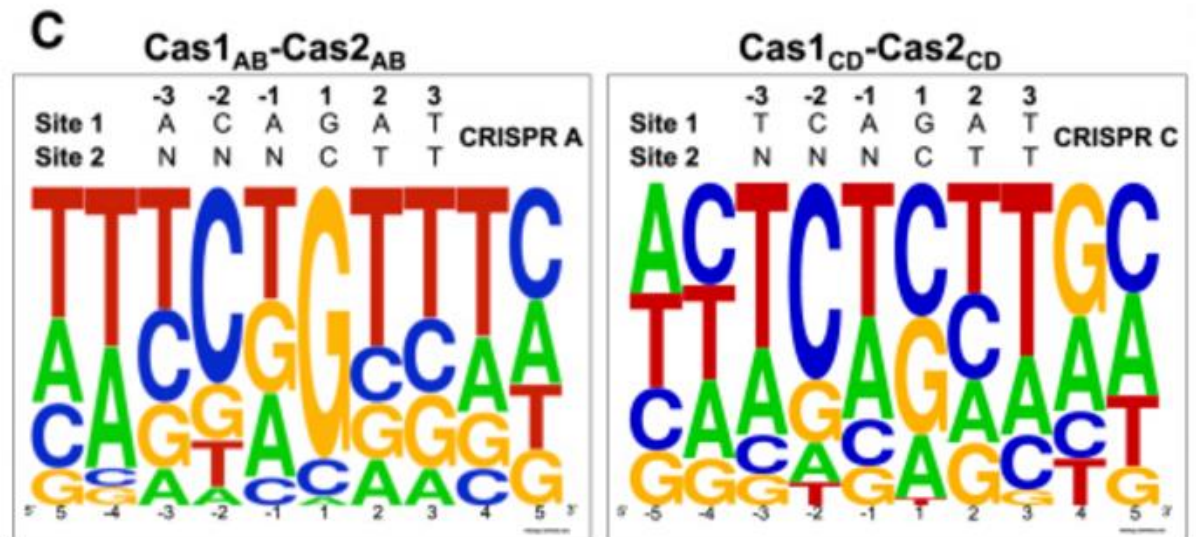
Herzog V A, et al. *Nature Methods*, 2017.

NAR Breakthrough Article

Prespacer processing and specific integration in a Type I-A CRISPR system

Clare Rollie, Shirley Graham, Christophe Rouillon and Malcolm F. White*

Biomedical Sciences Research Complex, School of Biology, University of St Andrews, North Haugh, St Andrews, Fife KY16 9ST, UK



Rollie C, et al. *Nucleic Acids Research*, 2017.

Weblogo的首页

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Introduction

WebLogo is a web-based application designed to make the generation of sequence logos easy and painless. WebLogo has been featured in over 4000 scientific publications.

A [sequence logo](#) is a graphical representation of an amino acid or nucleic acid multiple sequence alignment. Each logo consists of stacks of symbols, one stack for each position in the sequence. The overall height of the stack indicates the sequence conservation at that position, while the height of symbols within the stack indicates the relative frequency of each amino or nucleic acid at that position. In general, a sequence logo provides a richer and more precise description of, for example, a binding site, than would a consensus sequence.

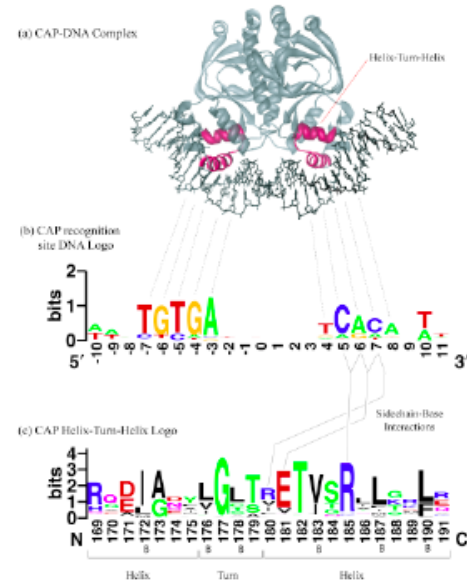
WebLogo is a web-based application designed to make the generation of sequence logos easy and painless. WebLogo has featured in over 4000 scientific publications.

- [Create your own logos](#)
- [View example sequence logos and input data.](#)
- [Read the release notes for latest changes and updates.](#)
- [Read the User's Manual](#)
- [WebLogo source code](#)
- [WebLogo discussion group](#)

References

Crooks GE, Hon G, Chandonia JM, Brenner SE WebLogo: A sequence logo generator, *Genome Research*, 14:1188-1190, (2004) [Full Text]

Schneider TD, Stephens RM. 1990. [Sequence Logos: A New Way to Display Consensus Sequences.](#) *Nucleic Acids Res.* 18:6097-6100



Create——绘制自己的seqlogo

在Create界面选择上传数据文件或者直接输入序列

WebLogo 3: Create

Sequence Data Input:

选取文件 未选择文件

URL:

Or Paste Sequence Data Here

✓ Create WebLogo

Clear

Download to local drive

颜色更改及其它参数

Title: 58 CAP Binding Sites → 输标题入

Output Format: PNG (low res.) → 输出文件格式

Sequence type: auto → 输入数据类型

Logo-size: large → seqlogo规格

Stacks per Line: 40 → 横坐标每行显示的碱基或氨基酸个数超出后自动换行

Ignore lower case:

Units: bits →

First position number: -10 → 横坐标起始位点

Logo range: logo start - logo end → 横坐标的起始和终止位置

Figure label: → 给logo图一个编号, 如“A、B”, 将显示在左上角

Scale stack widths:

Composition: auto → or % CG

Error bars:

Show Sequence Ends labels:

Version fingerprint:

X-axis Label: → 默认参数

Y-axis Label:

Y-axis scale:

Y-axis tic spacing: → 自定义logo颜色

Color scheme: Custom (Specify below) →

Symbols:	Color:
red	#ff0000
yellow	#ffff00
fuchsia	#ff00ff
green	#008000
<input type="text"/>	<input type="text"/>

Reset Defaults

蛋白质修饰位点预测

<https://www.phosphosite.org/homeAction.action>



PhosphoSitePlus® provides comprehensive information and tools for the study of protein post-translational modifications (PTMs) including phosphorylation, acetylation, and more. The web use is free for everyone including commercial.

PhosphoSitePlus

The image shows two search interface components. The top component is titled 'Protein or Substrate Search' and contains a dropdown menu labeled 'Protein Name', a text input field, and a blue 'Search' button. The bottom component is titled 'Alternative Search Options' and lists five search methods, each with an icon and a link: 'Protein, Sequence, or Reference Search' (with a protein structure icon), 'Site Search' (with a 'P' and 'Y' icon), 'Comparative Site Search' (with a 'P' and 'Y' icon), 'Browse MS2 Data by Disease' (with a caduceus icon), and 'Browse MS2 Data by Cell Line' (with a cell line icon).

蛋白质修饰位点预测



CSS-Palm

<http://csspalm.biocuckoo.org/>



任间 (中大)

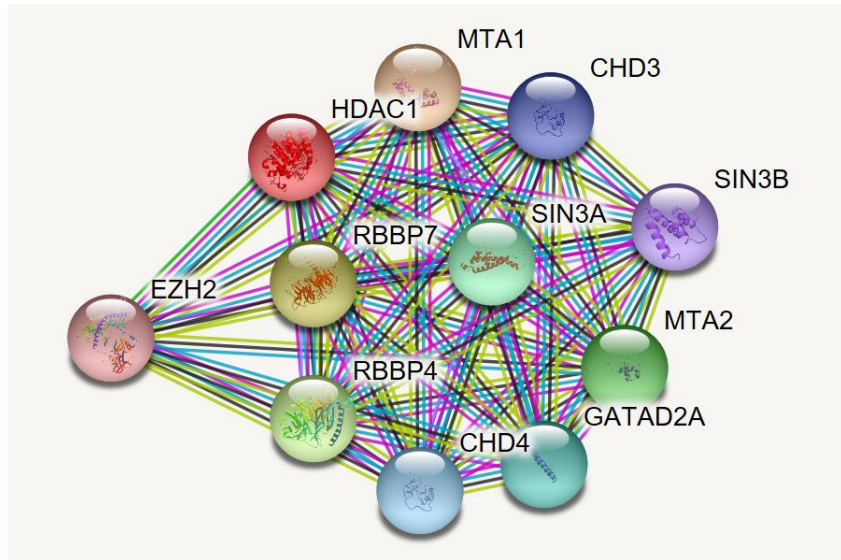


薛宇 (华科)

PTMs Predictor
GPS (Phosphorylation)
iGPS (Phosphorylation)
GPS-MSP (Protein Methylation)
CSS-Palm (Palmitoylation)
GPS-SUMO (Sumoylation)
GPS-SNO (S-nitrosylation)
GPS-YNO2 (Tyrosine Nitration)
GPS-CCD (Calpain Cleavage)
GPS-Polo (Polo-like Kinases)
GPS-PUP (Pupylation)
GPS-MBA (MHC-binding)
GPS-ARM (APC/C)
GPS-TSP (Tyrosine sulfation)
GPS-PAIL (Lysine acetylation)

String 分析

<https://string-db.org/>



STRING数据库(<http://string-db.org/>)是一个搜寻已知蛋白质之间和预测蛋白质之间相互作用的系统。这种相互作用既包括蛋白质之间直接的物理的相互作用，也包括蛋白质之间间接的功能的相关性。

圆圈 (node) 表示蛋白质，点击可以查看蛋白质相关信息；
直线 (edge) 表示蛋白质之间的相互作用关系。点击可以查看两蛋白的互作信息。

String 分析

Protein by name >

Protein by sequence >

Multiple proteins >

Multiple sequences >

Proteins with Values/Ranks **New** >

Organisms >

Protein families ("COGs") >

Examples >

Random entry >

SEARCH

Single Protein by Sequence

Amino Acid Sequence: (examples: [#1](#) [#2](#) [#3](#))

Organism:

auto-detect ▼

- auto-detect
- Homo sapiens
- Saccharomyces cerevisiae
- Escherichia coli K12 MG1655



北京大學
PEKING UNIVERSITY

Thanks for

Jingchu Luo
all the group members
all of you

