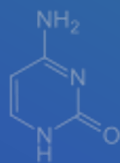


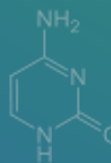
Cytosine



G

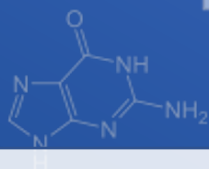
Nucleobases

Cytosine



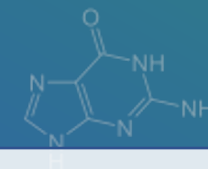
C

Guanine



G

Guanine



G

# Ribocentre

## Databases for functional RNAs

Zhichao (Chichau) Miao

Guangzhou Laboratory

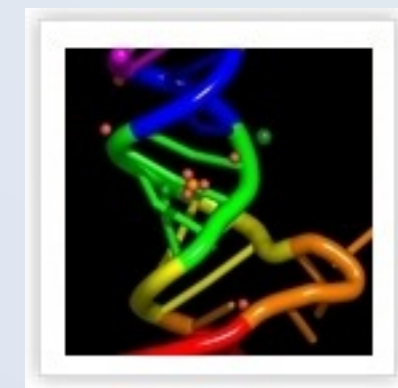
Guangzhou Medical University

[www.rnacentre.org](http://www.rnacentre.org)

Computational Approaches to RNA Structure and Function

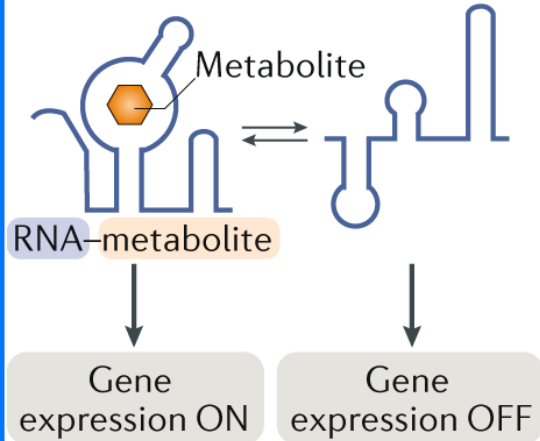
Benasque, Spain

26 July 2024

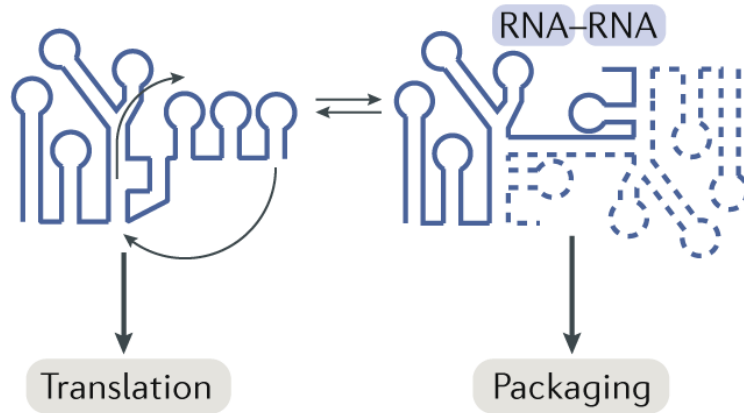


# Understanding RNA: structure - function

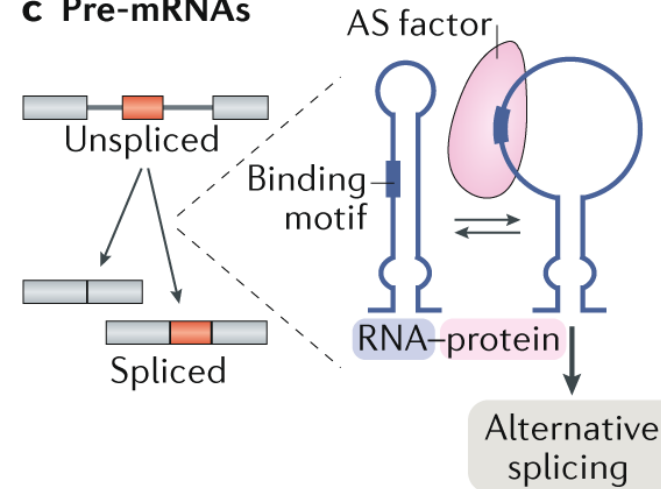
**a Riboswitches**



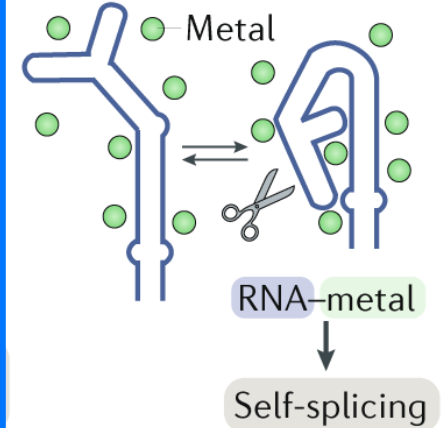
**b HIV-1 genome**



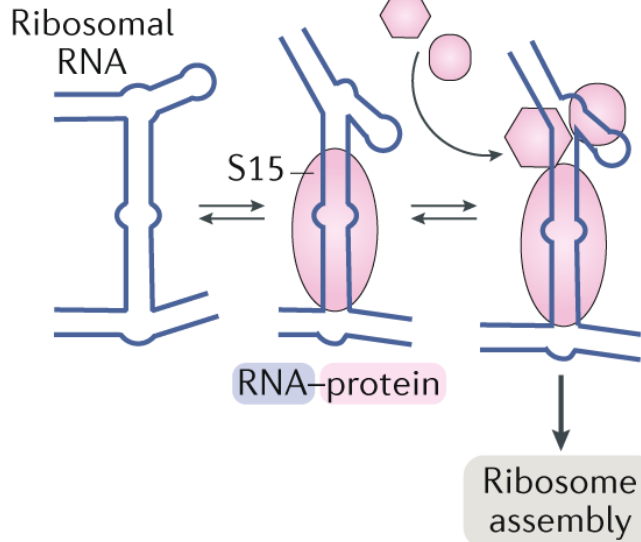
**c Pre-mRNAs**



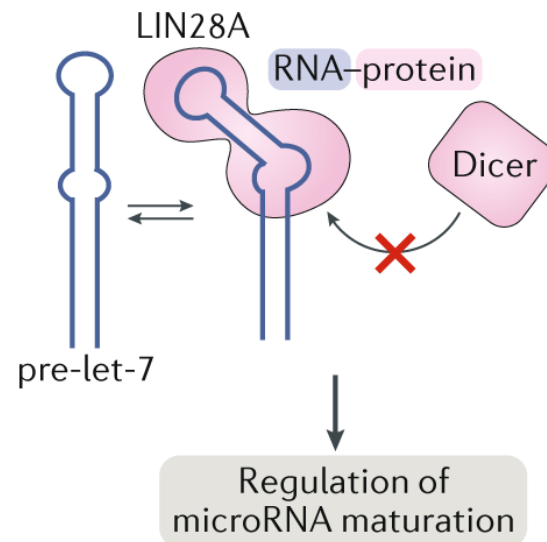
**d Ribozymes**



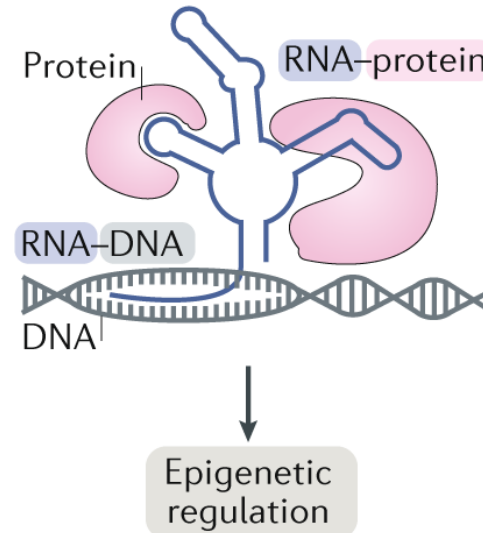
**e RNP assembly**



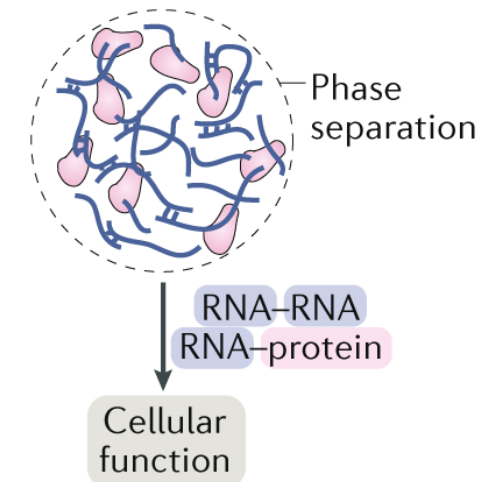
**f MicroRNAs**

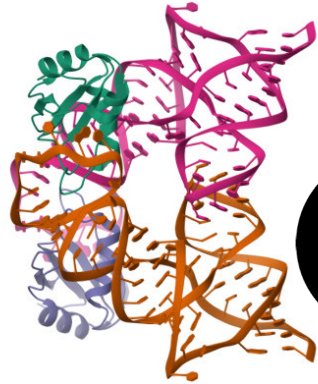


**g Long non-coding RNAs**



**h RNA granules**





**R**ibo  
centre

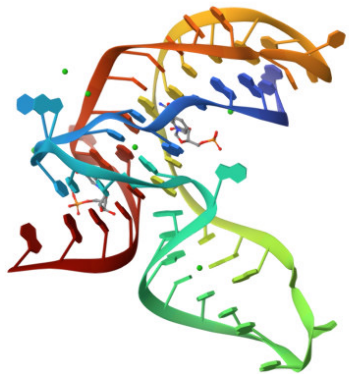
7qr4 HDV-like **ribozyme**



**R**ibo  
aptamer

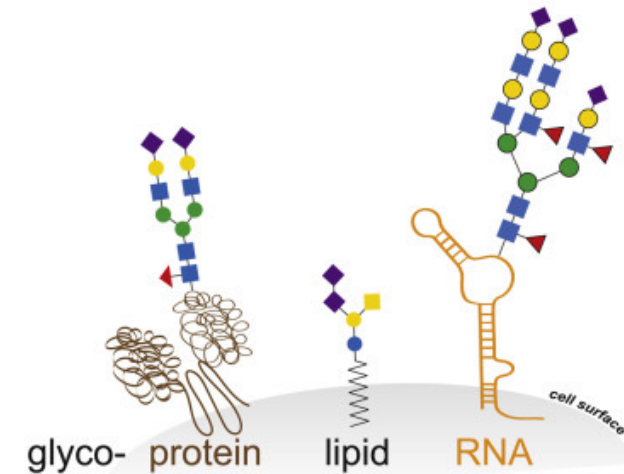
7eoj Pepper **Aptamer**

**R**ibo  
centre



**R**ibo  
switch

8hb8 NAD-II **riboswitch**

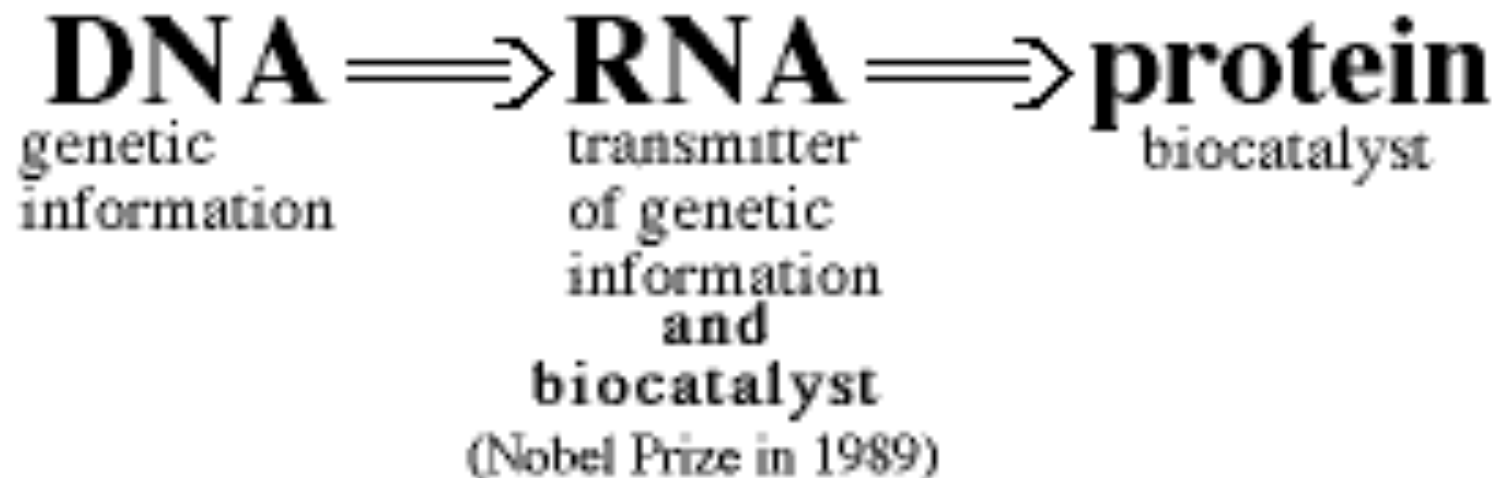


**GlycoRNA**

Cell 184,12, p3109-3124.E22, 2021

[www.ribocentre.org](http://www.ribocentre.org)

## The Nobel Prize in Chemistry 1989



**15** ribozymes



Photo from the Nobel Foundation archive.  
Sidney Altman  
Prize share: 1/2

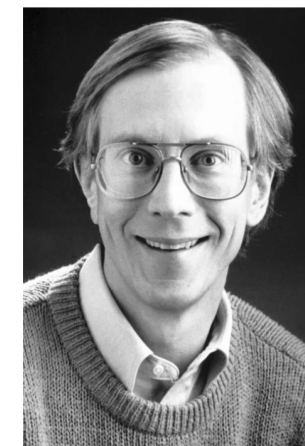
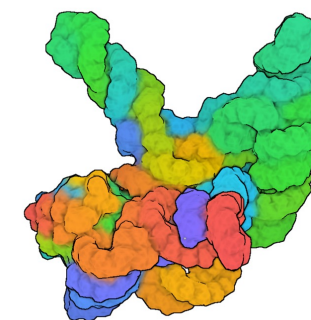
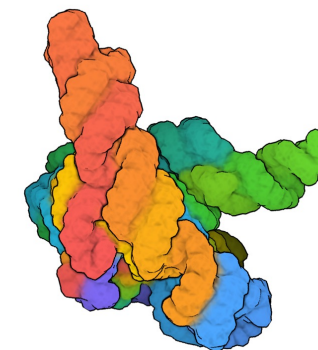


Photo from the Nobel Foundation archive.  
Thomas R. Cech  
Prize share: 1/2



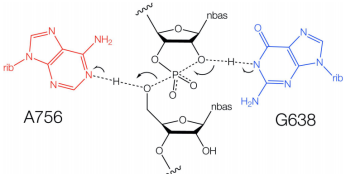
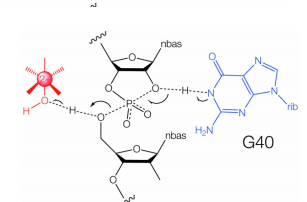
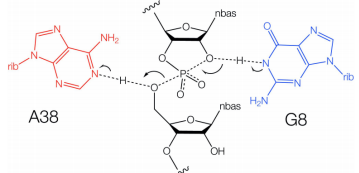
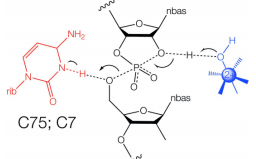
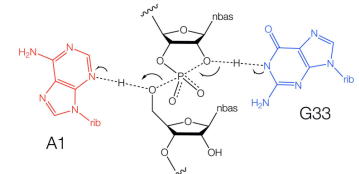
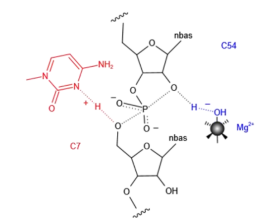
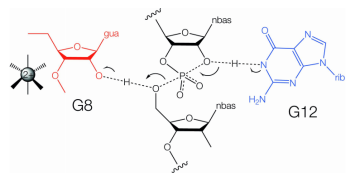
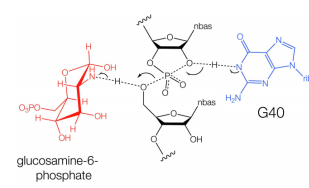
RNase P

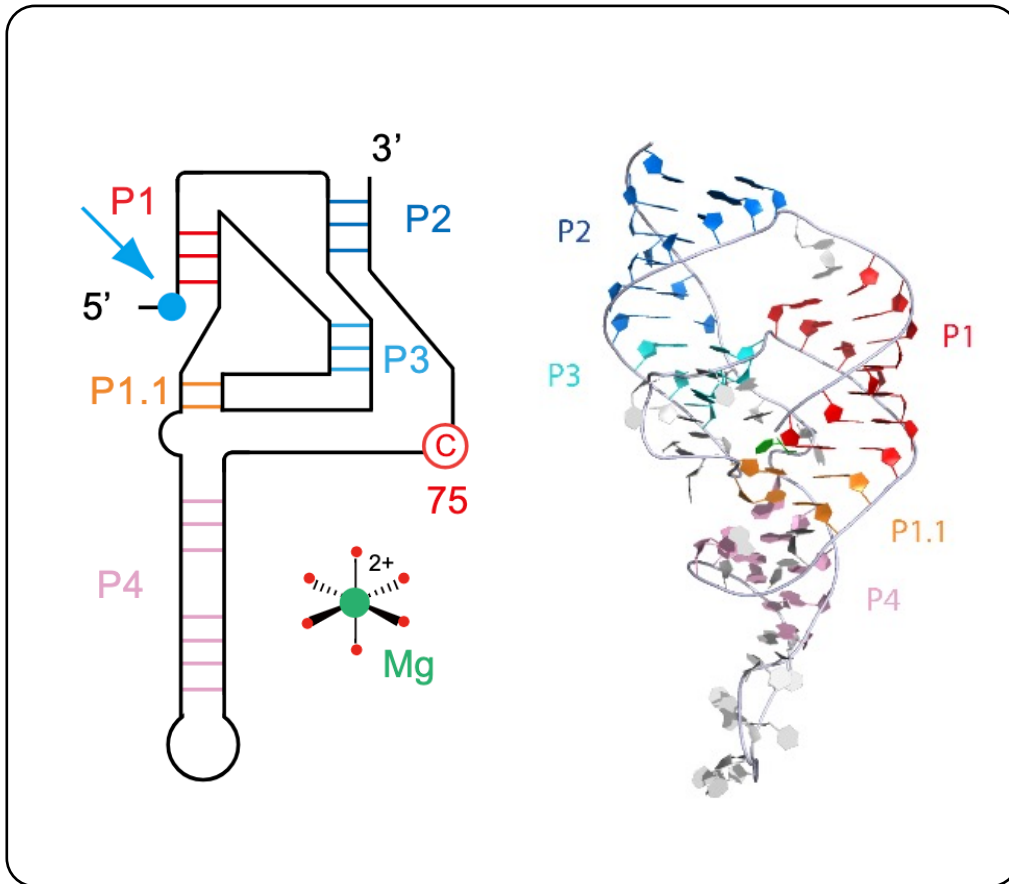


Self-splicing

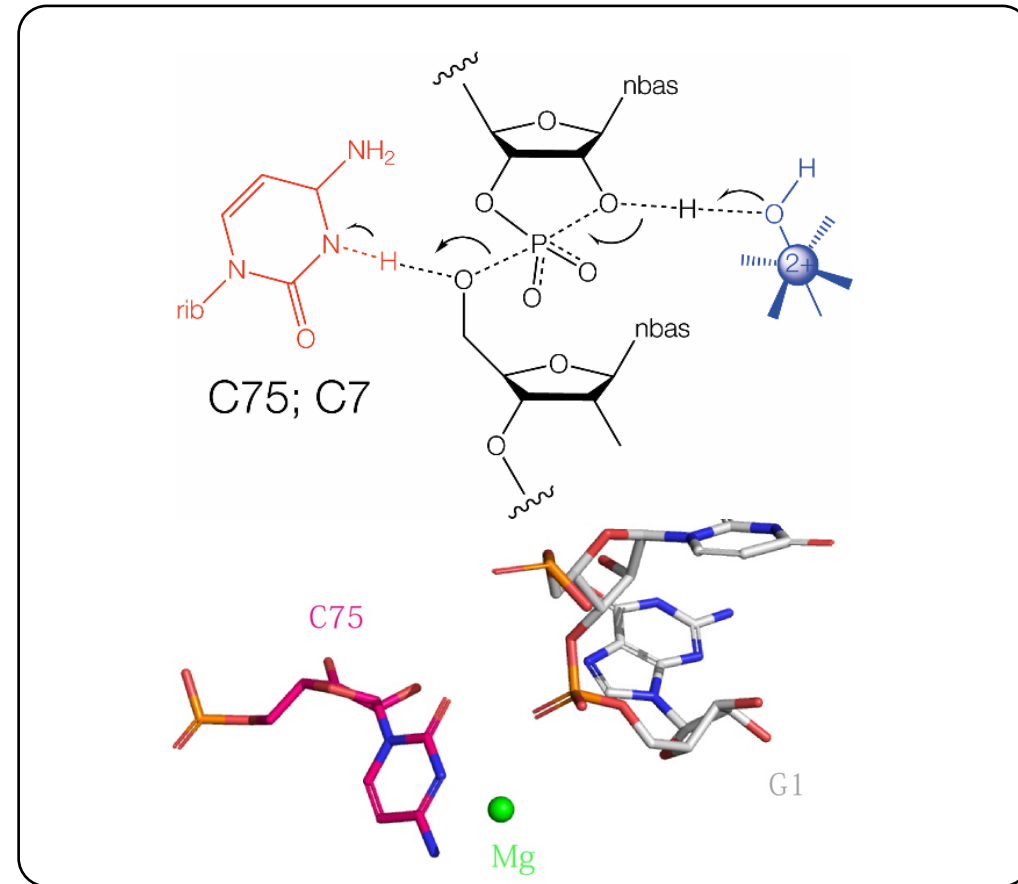


# Summary of the catalysis

Ribozyme	Acid	Base	Catalytic centre	Notes	Ribozyme	Acid	Base	Catalytic centre	Notes
VS	A N1	G N1			Pistol	$Mg^{2+} + H_2O$	G N1		
Hairpin	A N1	G N1			HDV	C N3	$Mg^{2+} + OH^-$		
Twister	A N3	G N1		Acid adjacent to scissile P	Twister-sister	C N3?	$Mg^{2+} + OH^-$		
Hammerhead	O 2'	G N1		O2' activated by $Mg^{2+}$	Glms	Glc6p amine	G N1		Use of a coenzyme



Structure



Function

# The research history of each RNA

1988 Discovery<sup>[1]</sup>

1989 Discovery<sup>[3]</sup>

1991 Pseudoknot-like secondary structure<sup>[6]</sup>

1993 Nonspecific divalent cations are required for self-cleavage<sup>[8]</sup>

1997 NMR structure of the isolated central hairpin(Stem Loop III)<sup>[10]</sup>

2000 C75 acts as the general acid and ribozyme-bound hydrated metal hydroxide as the general base<sup>[12]</sup>

2005 It is proved that C75 acts as the general acid<sup>[14]</sup>

2015 The HDV ribozyme variants were discovered<sup>[16]</sup>

2016 Dynamic reaction mechanism model with two Mg<sup>2+</sup> ions<sup>[18]</sup>

1988 Discovery<sup>[2]</sup>

1990 84 nucleotides are required for rapid and efficient self-cleavage<sup>[4]</sup>

1992 The P4 duplex can reduce the minimum size to about 65 nucleotides<sup>[7]</sup>

1996 Use of cis-delta ribozyme generated 3'homogeneous RNA ends<sup>[9]</sup>

1998 Crystal structure<sup>[11]</sup>

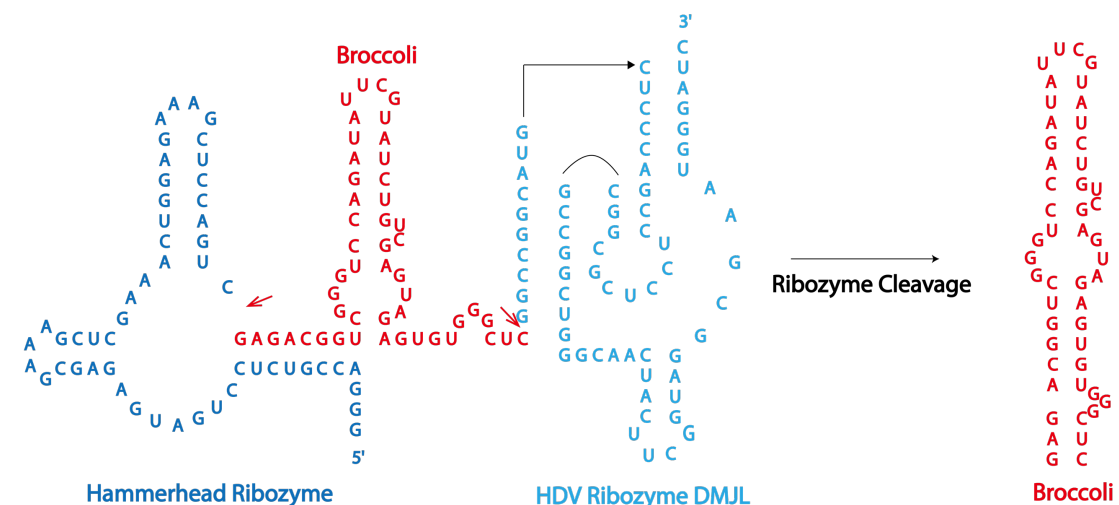
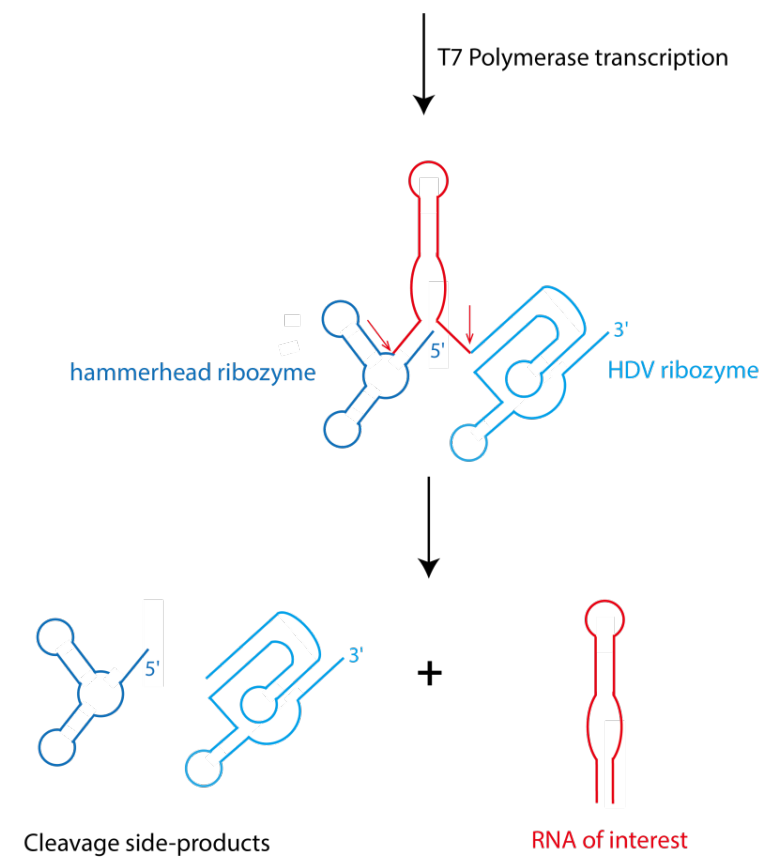
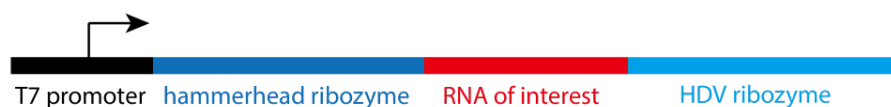
2004 Precursor structures<sup>[13]</sup>

2010 Precleavage structures<sup>[15]</sup>

2015 Transition state features<sup>[17]</sup>

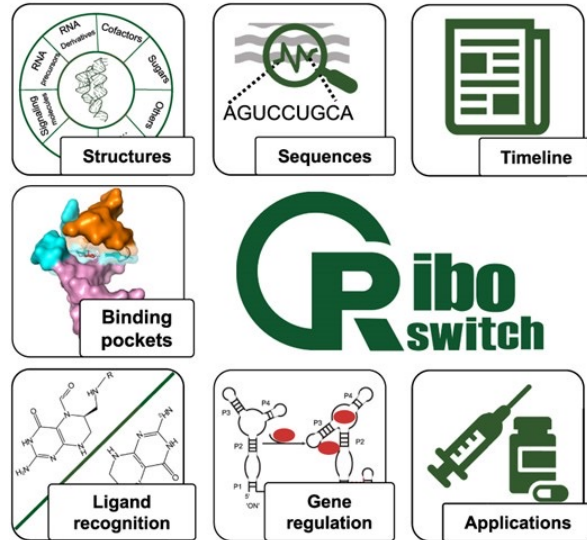
2019 Double-pseudoknot HDV can self-cleave with the same mechanism as the WT ribozyme<sup>[20]</sup>

## HDV as a showcase as a tool for designed RNA

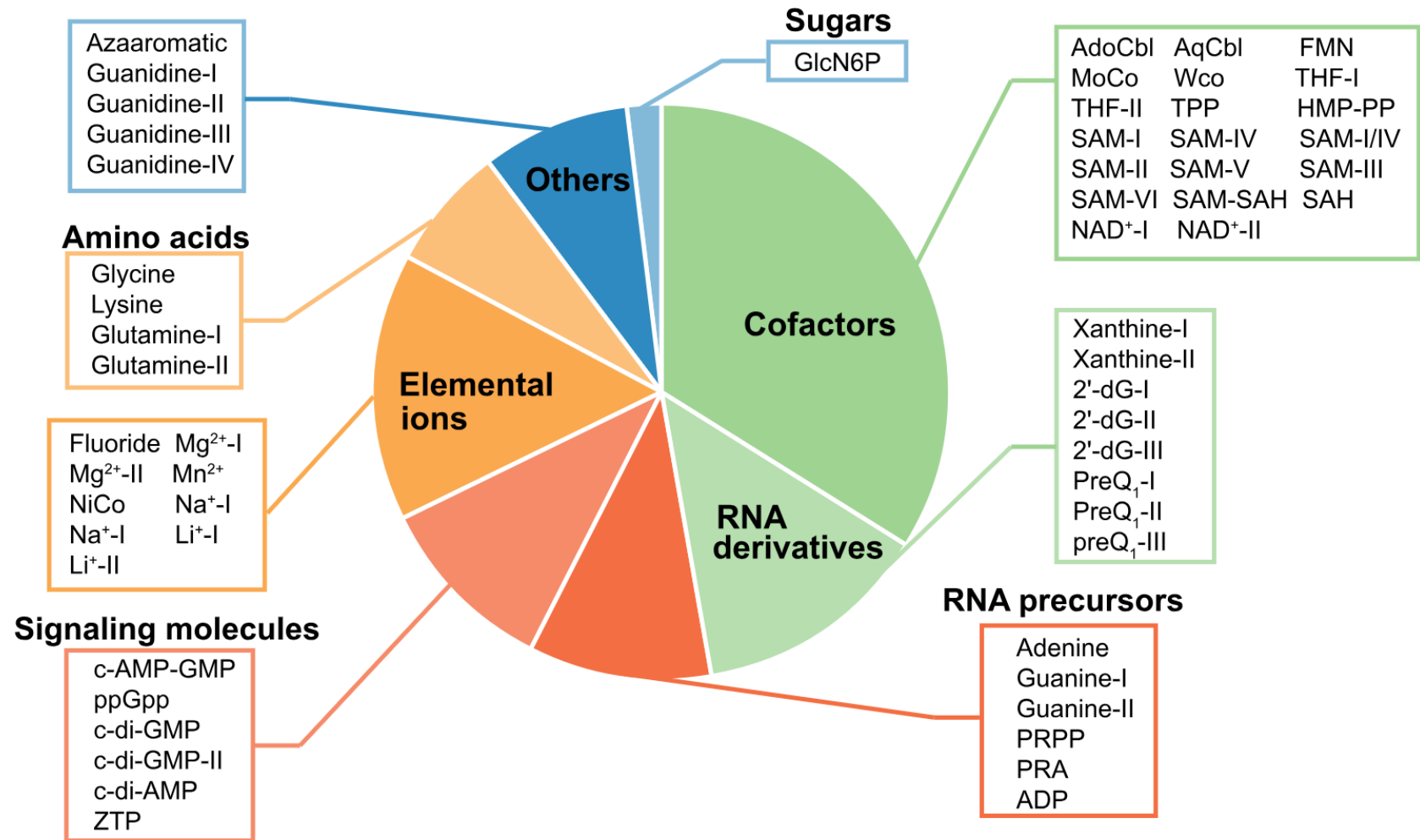




[riboswitch.ribocentre.org](http://riboswitch.ribocentre.org)

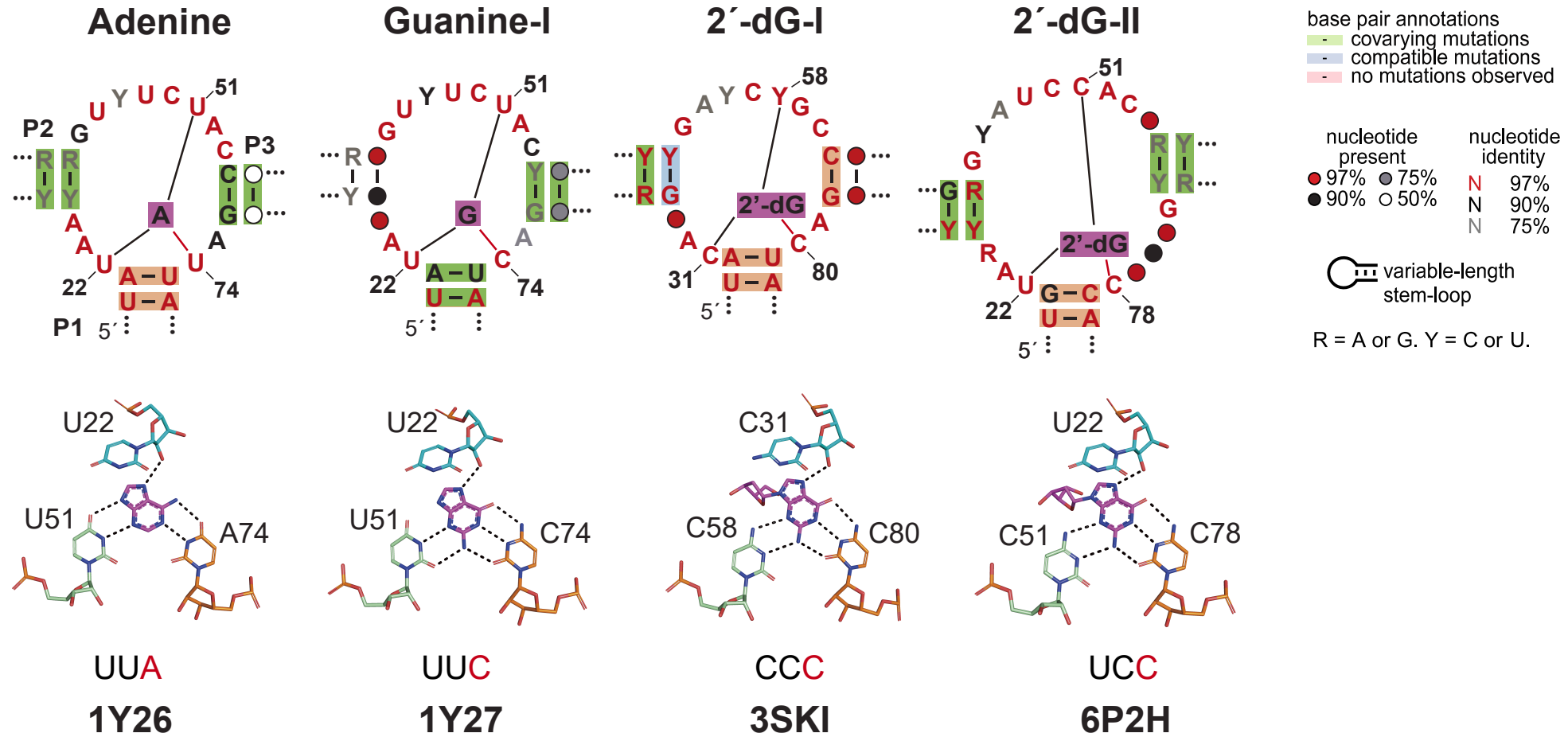


**51** riboswitches

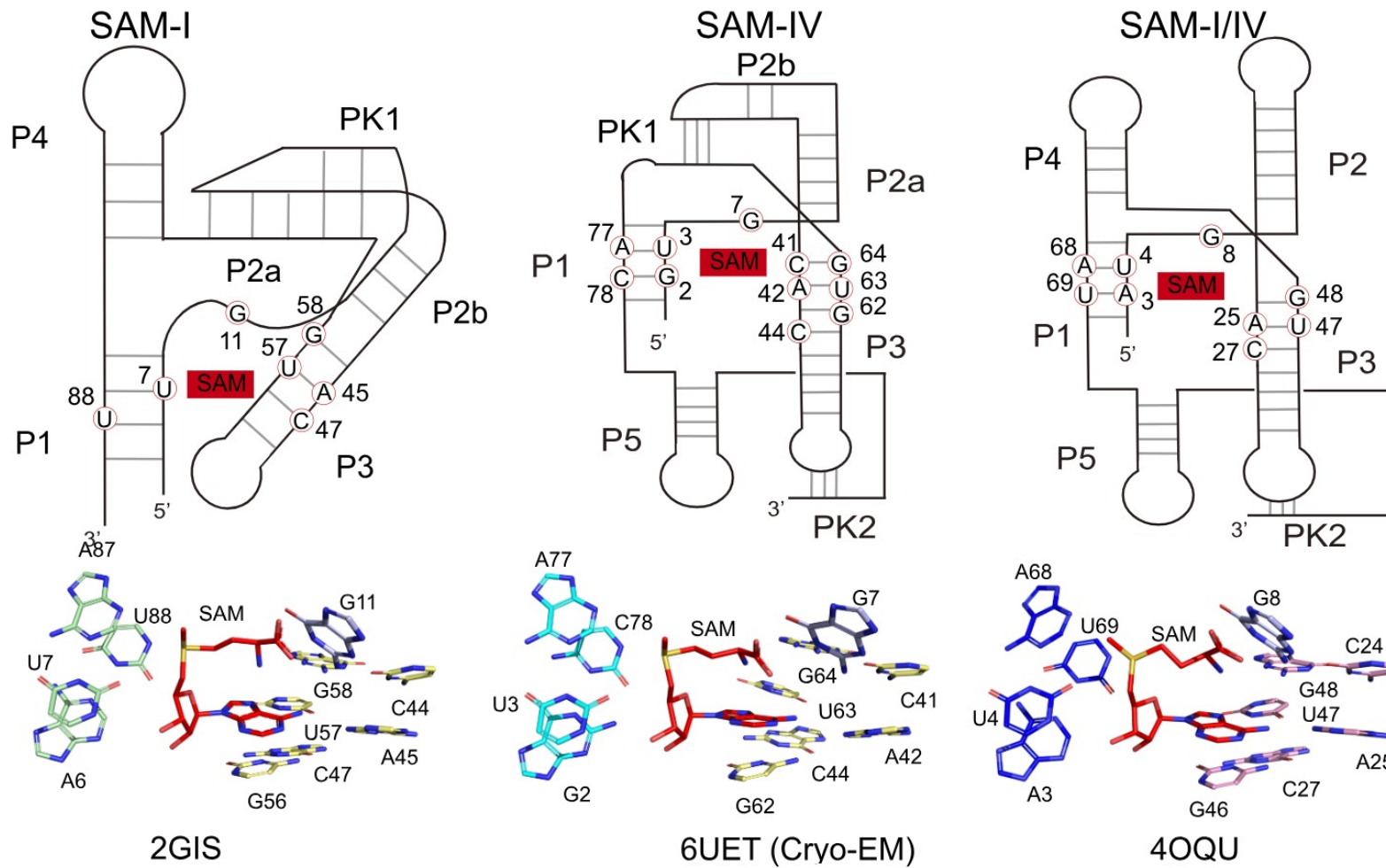


**Experimentally validated riboswitch classes**





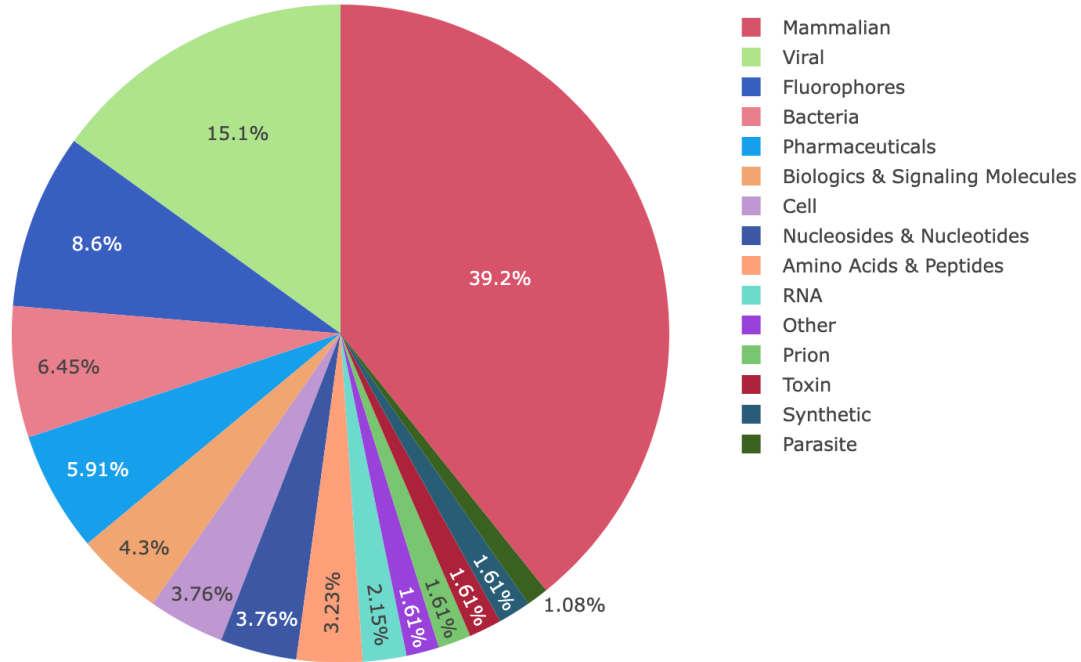
## Summary of the binding pockets in purine riboswitch family



**Comparison of the binding site of SAM-I family riboswitches**



**aptamer.ribocentre.org**

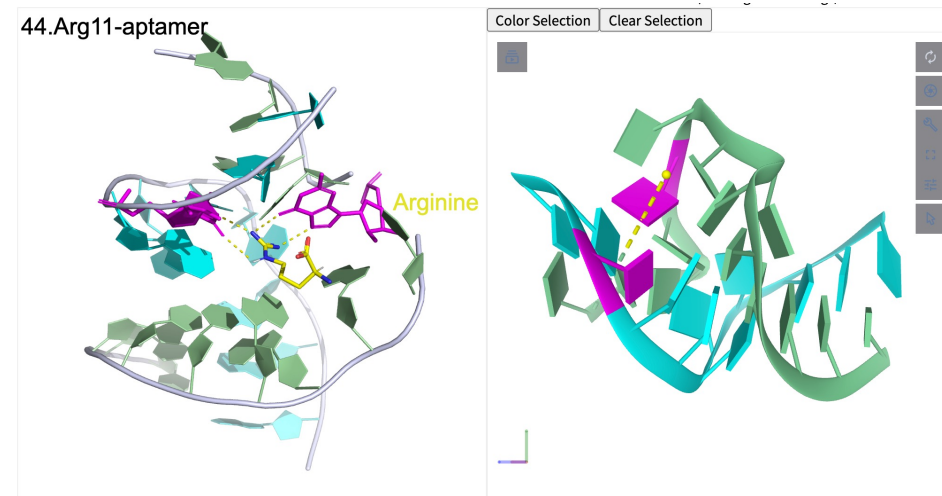


Citrulline	Arginine	Chili	TMR	Mango	Mango III	Spinach	Corn	DIR2s
Pepper	MG	Clivias	Beetroot	FMN	VITAMIN B12	5HTP	Riboflavin	Biotin
AML1	GCPII	eIF4A	GRK2	Human IgG	NF-kappaB	Thrombin	lysozyme	GlnRs
Factor Xa	ATP	GTP	Tetracycline	Neomycin B	Streptomycin	Theophylline	Tobramycin	Hfq
ribosomal protein S8	TetR	RNA polymerase (Pol II)	HIV-1 REV peptide	Tat peptides	HTLV-1 arginine-rich Rex peptide	HIV-1 TAR RNA	Bacteriophage MS2 coat protein	Bovine prion

**183** aptamers

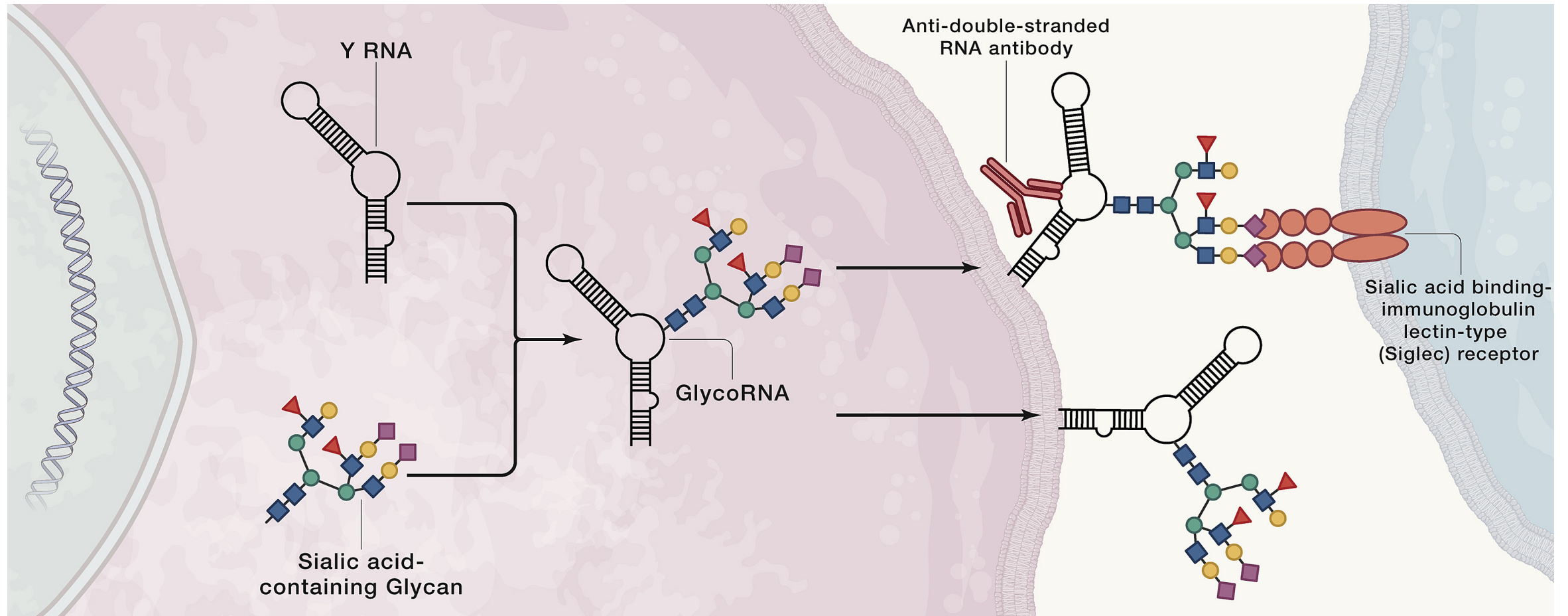
**15** categories

**51** w. structures



## glycorna.ribocentre.org

- GlycoRNAs are present on the **cell surface**, influencing **molecular recognition** and being associated with autoimmune **diseases**.



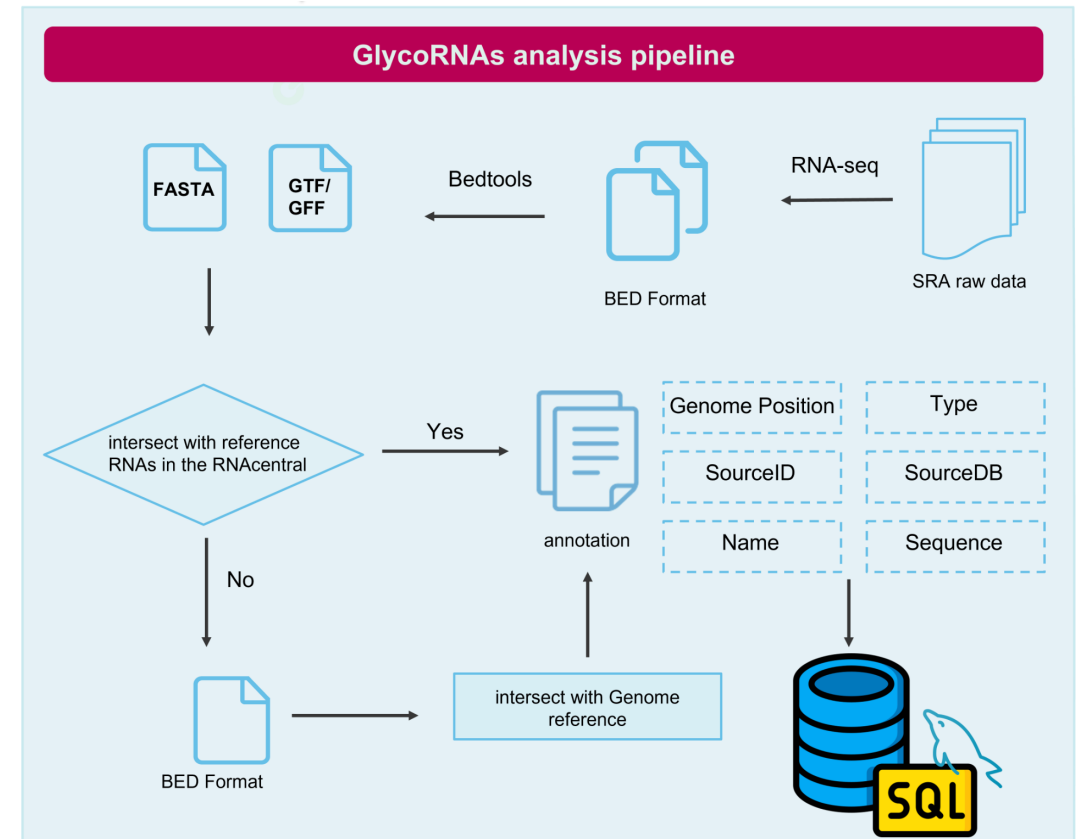
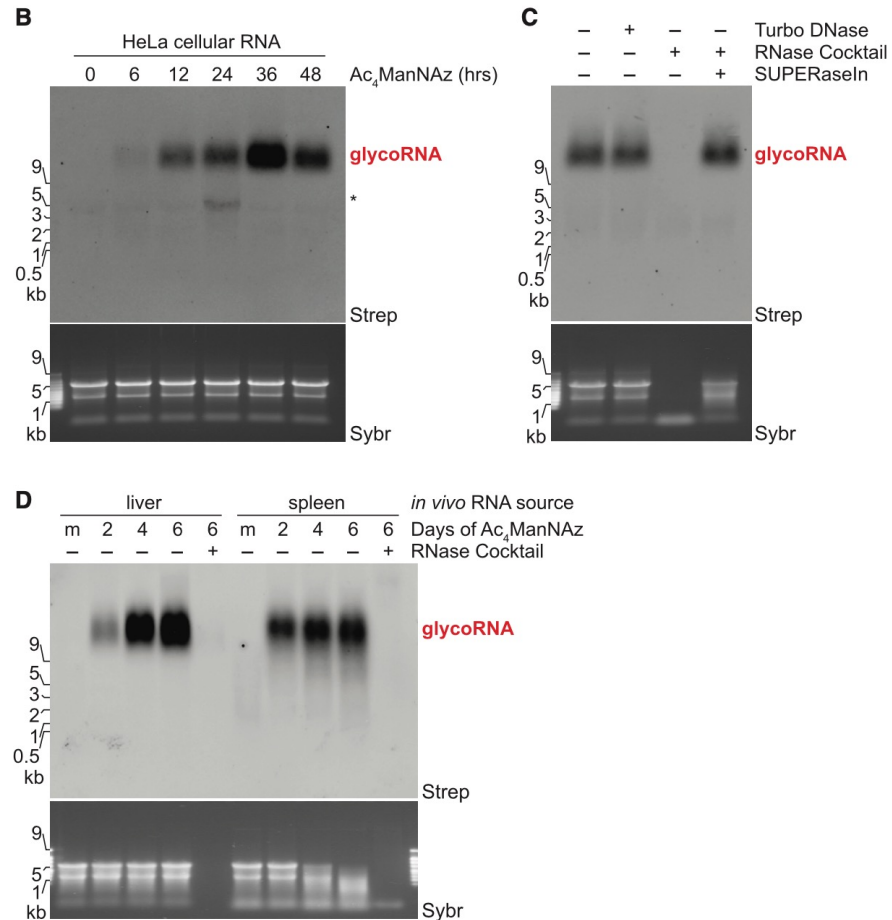
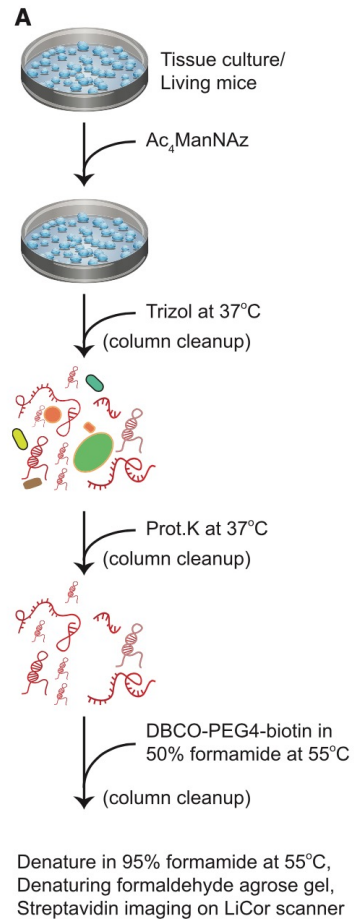


Figure 1. Ac<sub>4</sub>ManNAz, a glycan reporter, incorporates into mammalian cellular RNA

## Reporter system for GlycoRNA detection

## A standardized analysis pipeline

# GlycoRNAdb: A GlycoRNA database



Fat



Brain



Colon



Heart



Intestine



Kidney



Liver



Lung



Muscle



Spleen



Stomach



Testis

GSE id	Samples	Title	Organism	Summary	Reference
<a href="#">GSE136967</a>	4	Ac4ManNAz enriched small RNAs	Homo sapiens	Ac4ManNAz enriched small RNAs in HeLa and H9 ES cells	PMID:34004145 <a href="#">DETAILS</a>

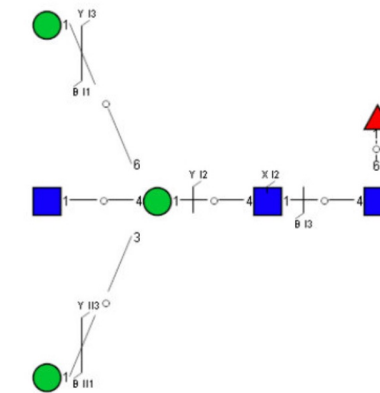
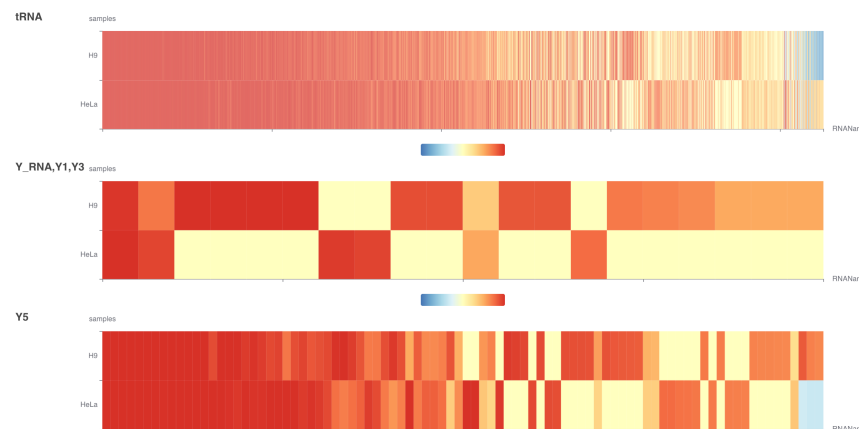
  

GSM ID	Cell Line	Condition/Treatment	Title	Sample type	Library strategy
GSM4064120	HeLa	Input	HeLa_SmallRNA_Input	Input small RNAs	ncRNA-Seq
GSM4064121	HeLa	ManNAz enriched	HeLa_SmallRNA_ManNAz-enrich	ManNAz enriched small RNAs	ncRNA-Seq
GSM4064122	H9 embryonic stem cells	Input	HeLa_SmallRNA_Input	Input small RNAs	ncRNA-Seq
GSM4064123	H9 embryonic stem cells	ManNAz enriched	HeLa_SmallRNA_ManNAz-enrich	ManNAz enriched small RNAs	ncRNA-Seq

Records per page: 5 | 1-4 of 4

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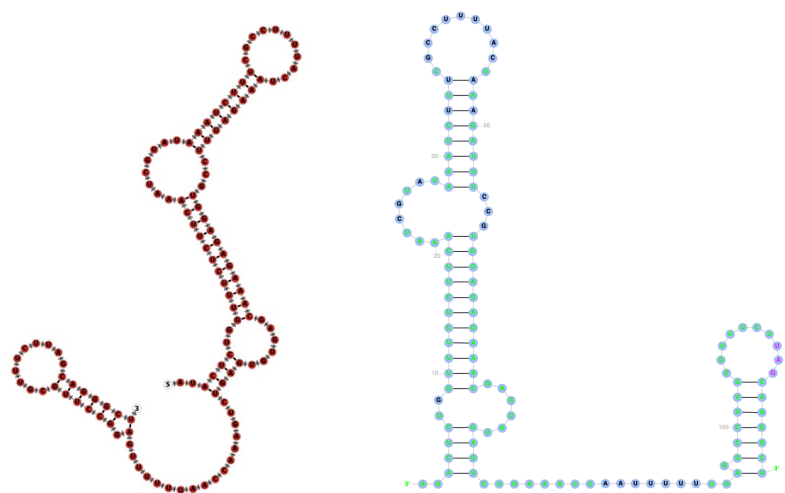
## Study information



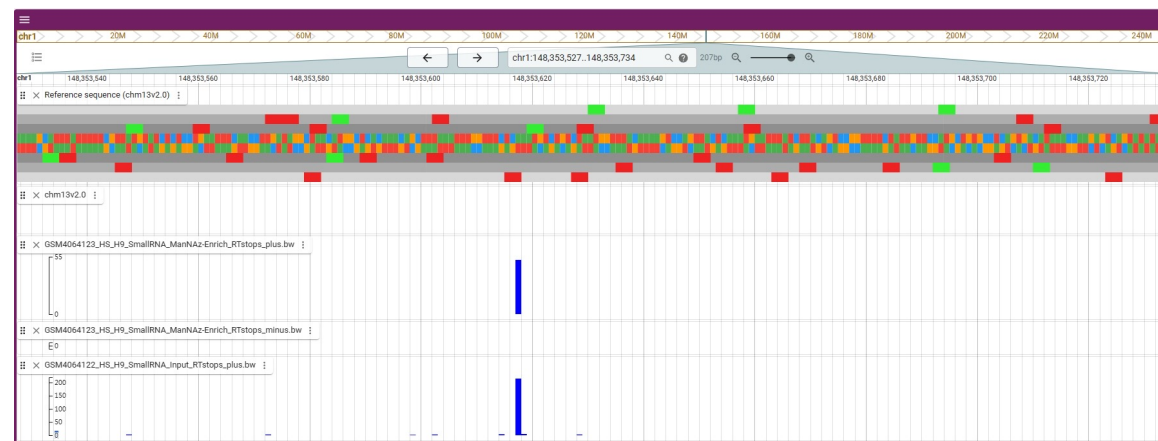
- ▲ Fucose
- Glc
- Man
- GalNAc
- GlcNAc
- ◆ Neu5Ac
- Gal

## Expression level

## Glycan topology

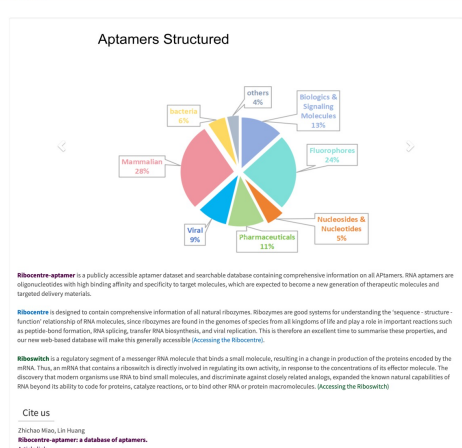
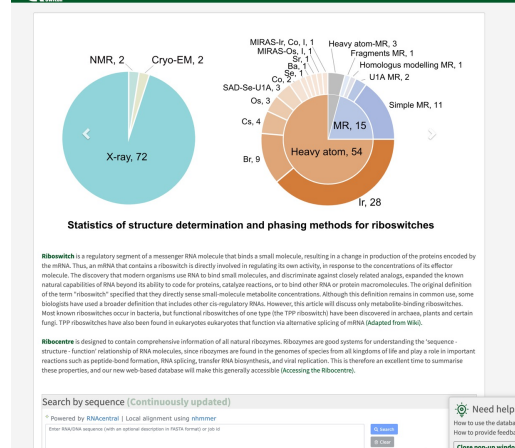
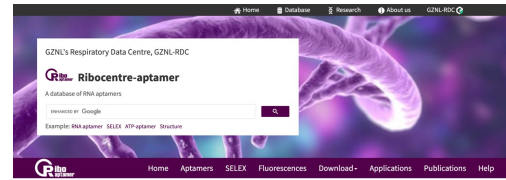
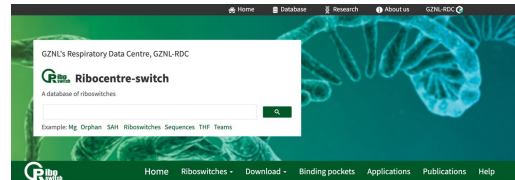
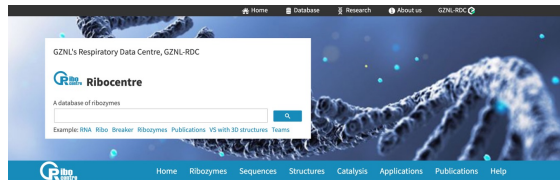


## 2D Structure



## Genome location





**Ribocentre** is designed to contain comprehensive information of all natural ribozymes. Ribozymes are good systems for understanding the 'sequence-structure-function' relationship of RNA molecules, since ribozymes are found in the genomes of species from all kingdoms of life and play a role in important reactions such as peptide bond formation, RNA splicing, transfer RNA biosynthesis, and viral replication. This is therefore an excellent time to summarise these properties, and our new web-based database will make this generally accessible.

In addition to a brief introduction to ribozymes, on each **ribozyme** page, you'll see a timeline of vital breakthroughs in ribozyme research, representative structures and the chemical mechanisms of this ribozyme. Besides, we provide multiple indexing and searching methods, you can index/search about the **publications, structures, catalysis and applications** of ribozymes that interest you. Users are welcomed to submit new ribozyme cases or related comments through the submission portal to help us improve our database.

**Riboswitch** is a regulatory segment of a messenger RNA molecule that binds a small molecule, resulting in a change in the production of the protein encoded by the mRNA, welcome to the Ribocentre switch database!

**Cite us!**  
Jin Deng, Bochang Shi, Kuamei Peng, Xuanlin He, Xiaohu Chen, Mengxiao Li, Xiaowen Lin, Wenjian Luo, Yuanxin Huang, Fajiao Jiang, David M. J. Lilley, Zhihao Miao, and Lin Huang  
**Ribocentre: a database of ribozymes**  
Nucleic Acids Research, gka491, https://doi.org/10.1093/nar/gkz440

The following content of ribozymes information is adapted from Wikipedia.

**Discovery**   **Structure**   **Activities**   **And More...**

**Structure and mechanism**

**Visualization:**

**.ribocentre.org :**

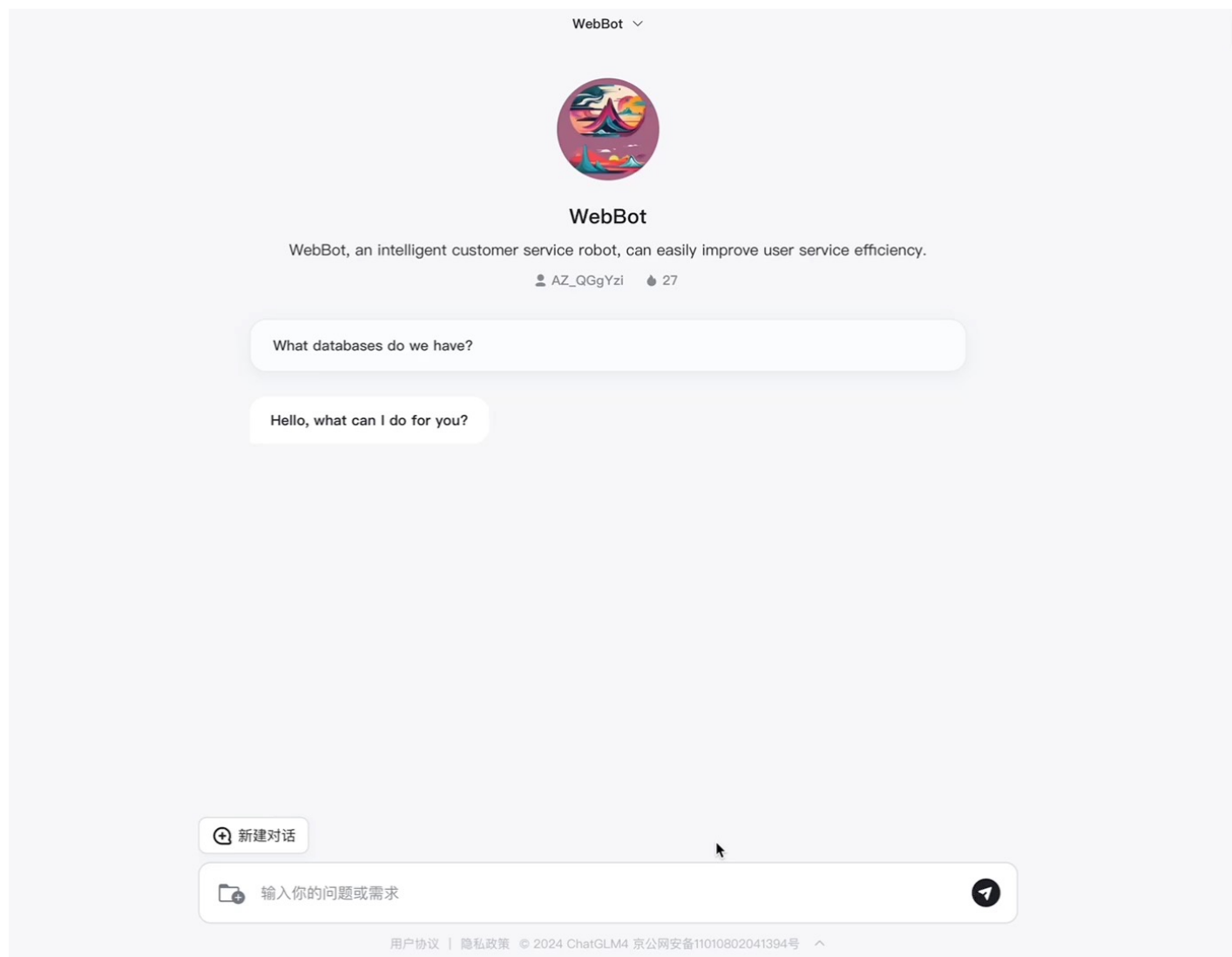
**WWW**  
**ribozyme**  
**riboswitch**  
**aptamer**  
**glycoRNA**

**riboswitch**  
**aptamer**  
**glycoRNA**

Deng et al. NAR 2022

Bu et al. NAR 2023

# Mega-database copilot search



Contact me if interested.

## Miao lab:

- Yaohuang Shi (PhD) Ribocentre
- Fan Bu(PhD) Ribocentre-switch
- Ying Ao (Master)
  - Ribocentre-aptamer & GlycoRNAdb
- Linyan Hu (PhD) Copilot search

## Blake Sweeney (search engine)

## Lin Huang (SYSU)

- Ribocentre
- Ribocentre-switch
- Ribocentre-aptamer



## Ling-ling Zheng (SYSU)

- GlycoRNAdb



## Fundings

### R&D Programs of Guangzhou Laboratory

- GZNL2024A01002
- GZNL2023A01006
- SRPG22-003
- SRPG22-006
- SRPG22-007
- HWYQ23-003

### Natural Science Foundation of China

- 32270707

### National Key R&D Programs of China

- 2021YFF1200903
- 2023YFF1204701



RNA Society



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ACADEMIC SALON

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简介

我们是一群对RNA感兴趣的科学家。我们致力于推动华南地区的RNA研究，促进与其他地区研究人员的交流，旨在将华南地区的RNA研究与国际RNA学会联系起来。同时促进合作交流，培养青年科学家（博士、博士后）。我们期待更多的RNA领域的研究人员加入我们，共同推动RNA领域的研究。

活动介绍

1. 每月研讨会：一到两小时，包括两次演讲：一位高级PI（约30-40分钟），另一位来自初级PI、博士后或学生（约20分钟），然后是问题和讨论部分（约20-30分钟）。
2. 年度座谈会：每年7月中的一整天，将有8到10位国内国外的高级PI参加，展示与讨论RNA领域最前沿的学术问题，研究进展。
3. 不定期的学术交流会



B站视频号



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根据前期会议参与同学申请情况，13位同学已免费获得了2023年国际RNA学会学生会员资格（36 USD/year）！欢迎大家加入我们。关注我们的微信公众号和B站账号，回顾往期精彩视频，及时获取讲座资讯，观看直播，线上提问，与RNA领域知名学者面对面！

往期嘉宾（部分）

 Eric Westhof 法德、欧科学院 院士	 David Lilley 英国皇家学会 院士	 陈润生 中国科学院 院士	 Matthias Hentze 澳德、欧科学院 院士	 屈良鹤 长江学者
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主持人

 苗智超 广州国家实验室 广州医科大学	 黄林 中山大学	 杨建华 中山大学	 王金凯 中山大学
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Sponsors







## Openings:

### Computational Biology

- 2025 PhD students (3)
- Co-PI (2)
- Postdocs (3)
- RA (3)
- Interns

### Biochemistry

- Postdocs (2)

Please email:

[miao\\_zhichao@gzlab.ac.cn](mailto:miao_zhichao@gzlab.ac.cn)



# Thanks!

