

“The Emergence of DNA Splicing in Industrial Applications”

International Conference on Progress in Mathematics Towards Industrial Applications

Organized by

Department of Mathematics, SRMIST,
Ramapuram, Chennai,
TN, India

27 October 2023

Innovating Solutions



PROF DR NOR HANIZA SARMIN

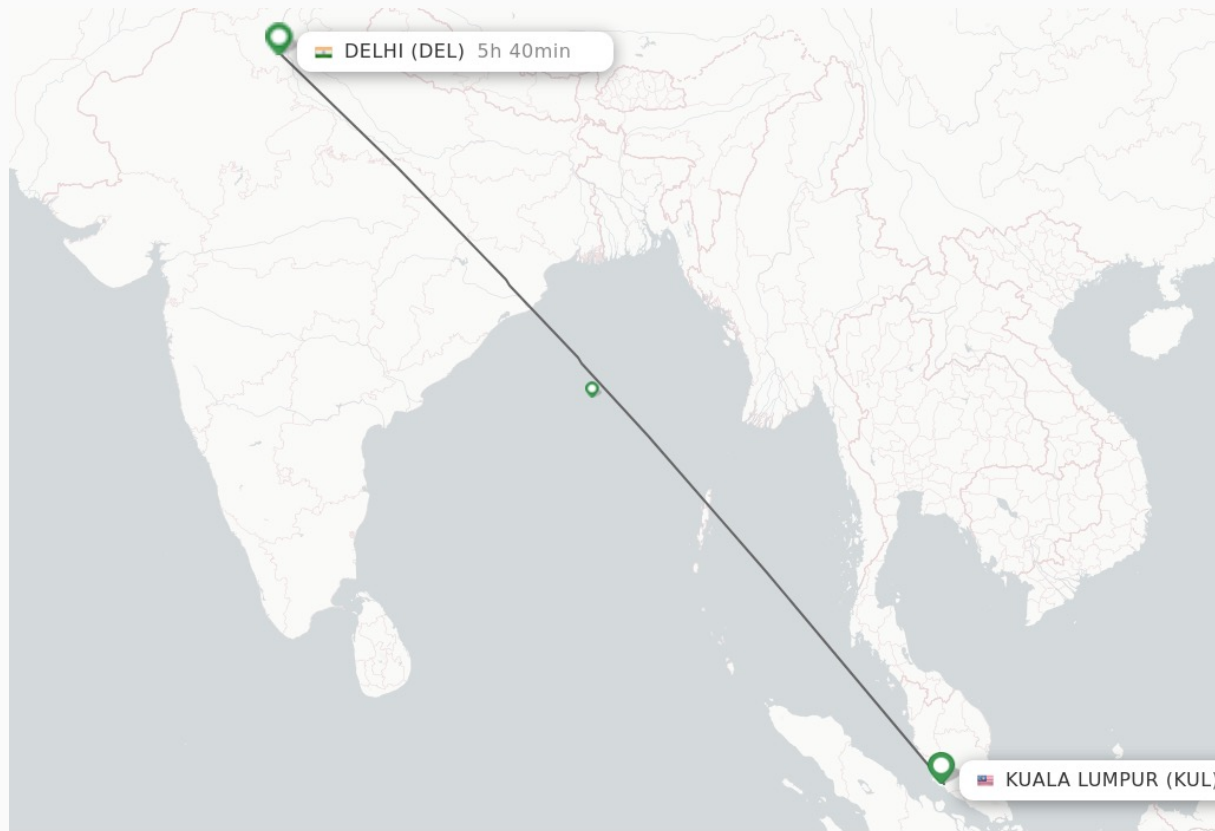
Department of Mathematical Sciences,
Faculty of Science, Universiti Teknologi Malaysia

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Malaysia in the World Map



From India to Malaysia



- The distance between India and Malaysia is estimated at 4,218 km or 2621 miles.
- A typical flight would have a flying time of about 4 – 5 hours.
- Time difference between India and Malaysia is 2:30 hours.



Faculties in UTM

12

Faculties

Civil Engineering <ul style="list-style-type: none"> Structure Materials Geotechnics and Transportation Water and Environmental Engineering 	Mechanical Engineering <ul style="list-style-type: none"> Applied Mechanics & Design Thermo Fluids Aeronautics, Automotive & Ocean Engineering Materials, Manufacturing & Industrial Engineering 	Chemical & Energy Engineering <ul style="list-style-type: none"> Chemical Engineering Petroleum Engineering Bioprocess & Polymer Energy Engineering <p>Petroleum Engineering #44 & 2 in MAS</p>	Electrical Engineering <ul style="list-style-type: none"> Communication Engineering Control and Mechatronics Engineering Electronic and Computing Engineering Electrical Power Engineering 	Computing <ul style="list-style-type: none"> Computer Science Applied Computing Software Engineering 	Built Environment & Surveying <ul style="list-style-type: none"> Architecture Quantity Surveying Urban and Regional Planning Landscape Architecture Geoinformation Real Estate <p>Architecture/ Built Environment TOP 100 & #3 in MAS</p>
Management <ul style="list-style-type: none"> Management Accounting Marketing Technology Management Information Technology Information Systems 	Science <p>Environmental Sciences TOP 200 & #3 in MAS</p> <ul style="list-style-type: none"> Biosciences Physics Chemistry Mathematical Sciences 	Social Sciences & Humanities <p>Education TOP 200 & #3 in MAS</p> <ul style="list-style-type: none"> School of Education School of Human Resource Development & Psychology Academy of Islamic Civilisation Language Academy Centre for Advanced Studies on Islam, Science, and Civilisation FSSH KL 	Razak Faculty of Technology & Informatics <ul style="list-style-type: none"> Engineering & Technology Science, Management & Design Advanced Informatics Perdana Centre 	Azman Hashim International Business School <ul style="list-style-type: none"> Business Administration Accounting and Finance Information System <p>Accounting & Finance TOP 250 & #7 in MAS</p>	Malaysia-Japan International Institute of Technology <ul style="list-style-type: none"> Electronic System Engineering Mechanical Precision Engineering Chemical and Environmental Engineering Management of Technology Software Engineering

50

ACADEMIC STAFF

456

UG STUDENTS

195

PG STUDENTS

8

**RESEARCH CENTRE &
GROUPS**

POSTGRADUATE PROGRAMMES

We offer Masters and Doctoral Programmes in Mathematics.

UNDERGRADUATE PROGRAMS

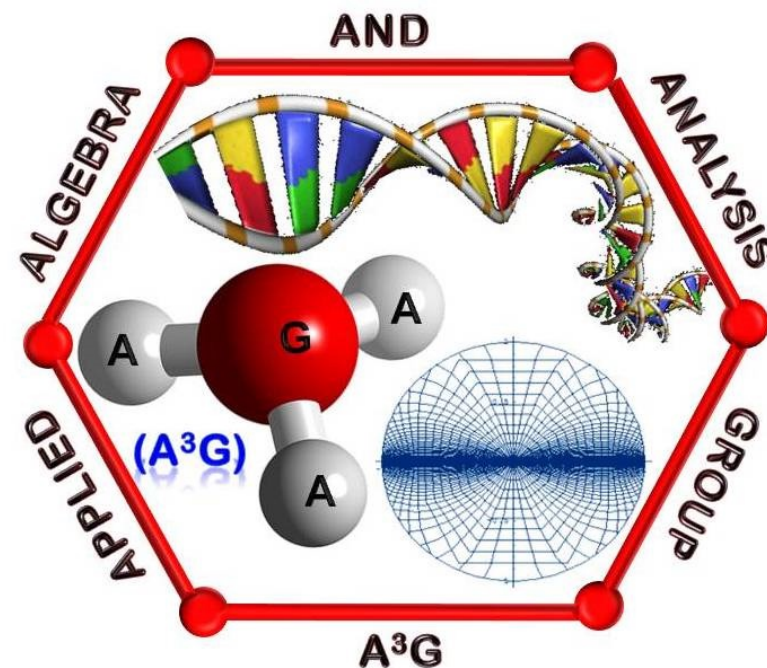
Bachelor of Science
(Mathematics) with Honours

Bachelor of Science (Industrial
Mathematics) with Honours

The department is divided into 5 broad research areas/**academic panels**:

1. Algebra & Analysis
2. Applied Mathematics
3. Numerical & Computational
4. Operations Research
5. Statistics

Members belong to specific **research groups** focused on diverse studies.



**Joined Department of Mathematics,
Faculty of Science, UTM on
2 May 1991**

MY BACKGROUND



State University of New York at Binghamton
(now known as Binghamton University), New York, USA

1986 – 1989

B.Sc (Hons) Mathematics
(Minor in Economics)

1989 – 1990

MA Mathematics

1995 – 1998

PhD Mathematics

“The Emergence of DNA Splicing in Industrial Applications”

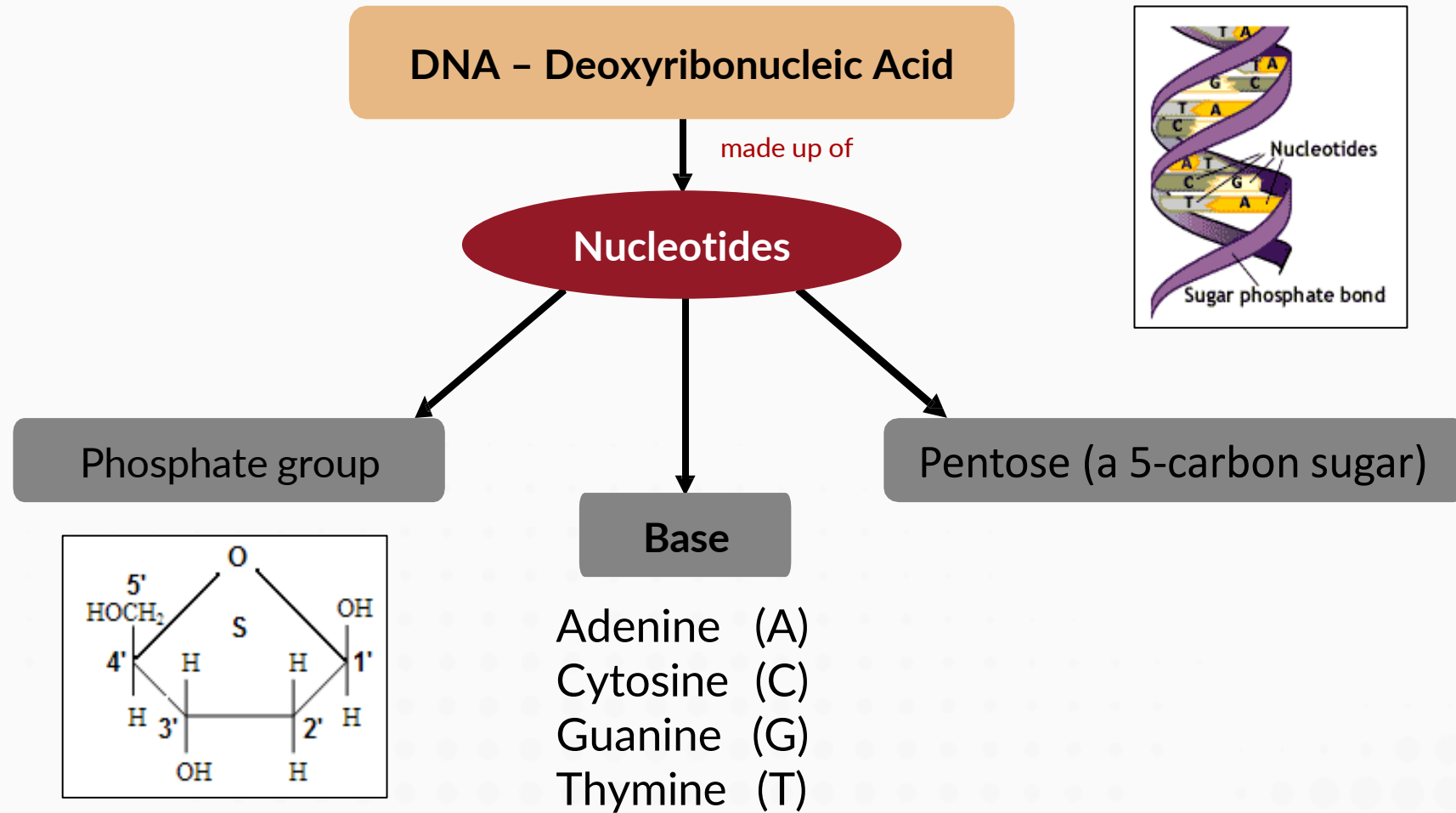
Abstract

The **diversity of mathematical applications** in various scientific concepts has led to significant advancements in understanding complex biological processes. One area where this interdisciplinary collaboration thrives is **DNA splicing**, a basic biological process in manipulating genetic information and simulated by the technique of **recombinant DNA** molecules that relies on **restriction enzymes**. This presentation explores the idea of DNA splicing in various concepts. Firstly, the **fundamental mathematical framework** behind DNA splicing is presented. Also, the **interplay between mathematical models and wet lab experiments** is shared to validate the theoretical findings. The emergence of DNA splicing in industrial applications, particularly in **computer science** where some computational models such as **graphical user interface** (GUI) are discussed. Finally, the **graphical approach in mathematics** to studying DNA splicing is presented to emphasize the role of **visual representation** in comprehending complex biological processes.

DNA Structure

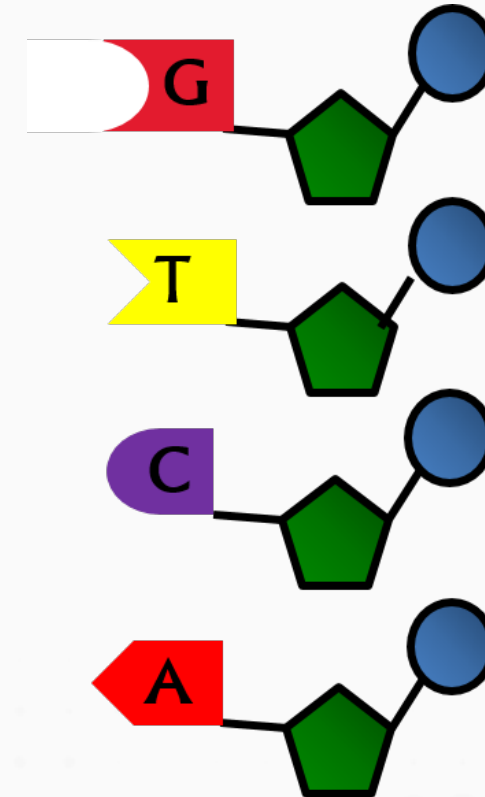
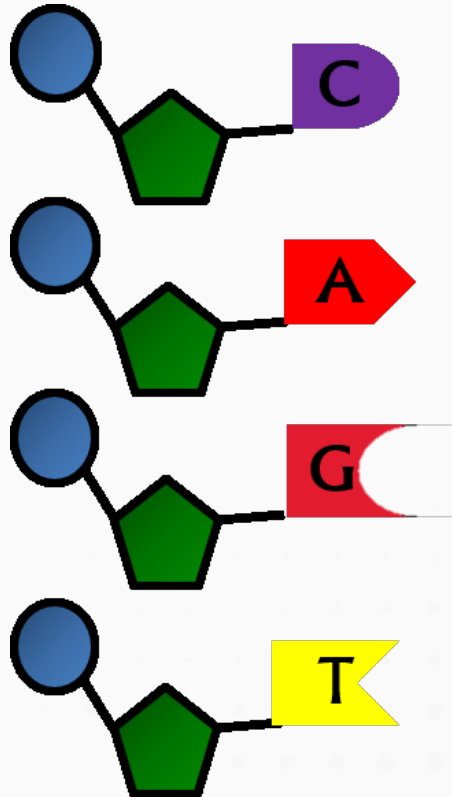


Structure of DNA

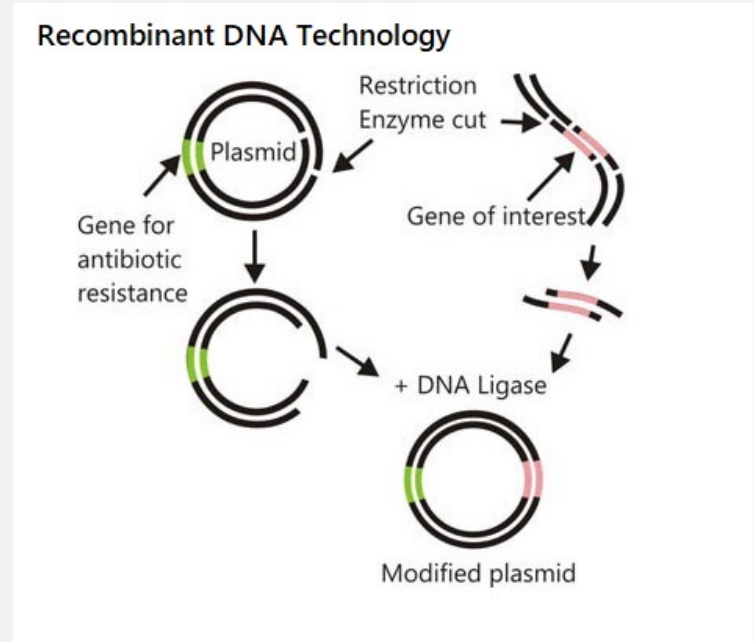


Structure of DNA (Cont.)

Watson-Crick Complementary



Recombinant DNA



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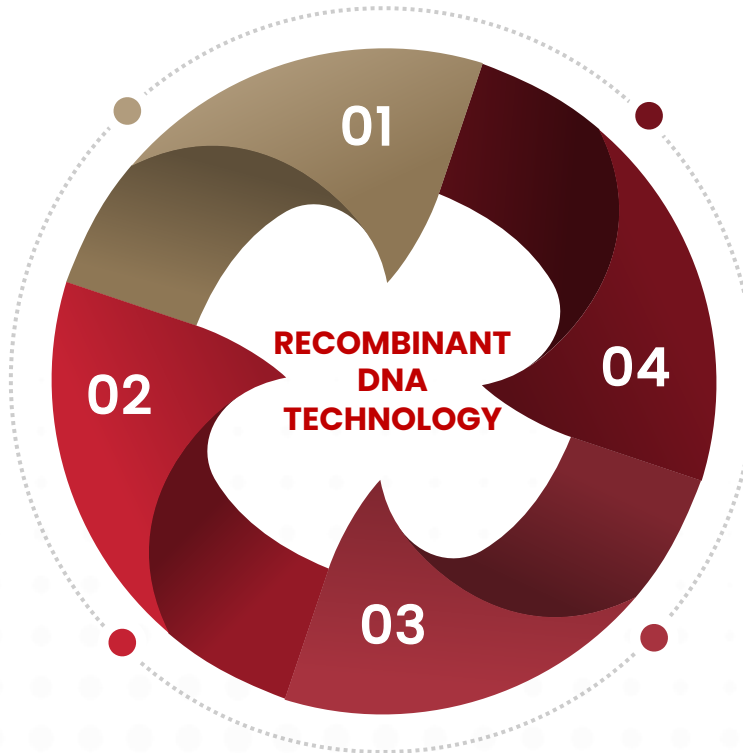
VARIOUS APPLICATIONS OF RECOMBINANT DNA TECHNOLOGY

2. THERAPEUTIC PRODUCTS

Vaccines
Growth hormones
Antibodies
Anticancer drugs
Recombinant protein

3. DIAGNOSIS

Gene therapy
Monitoring device
Therapeutic strategies
CRISPR



1. GENETICALLY MODIFIED PRODUCTS

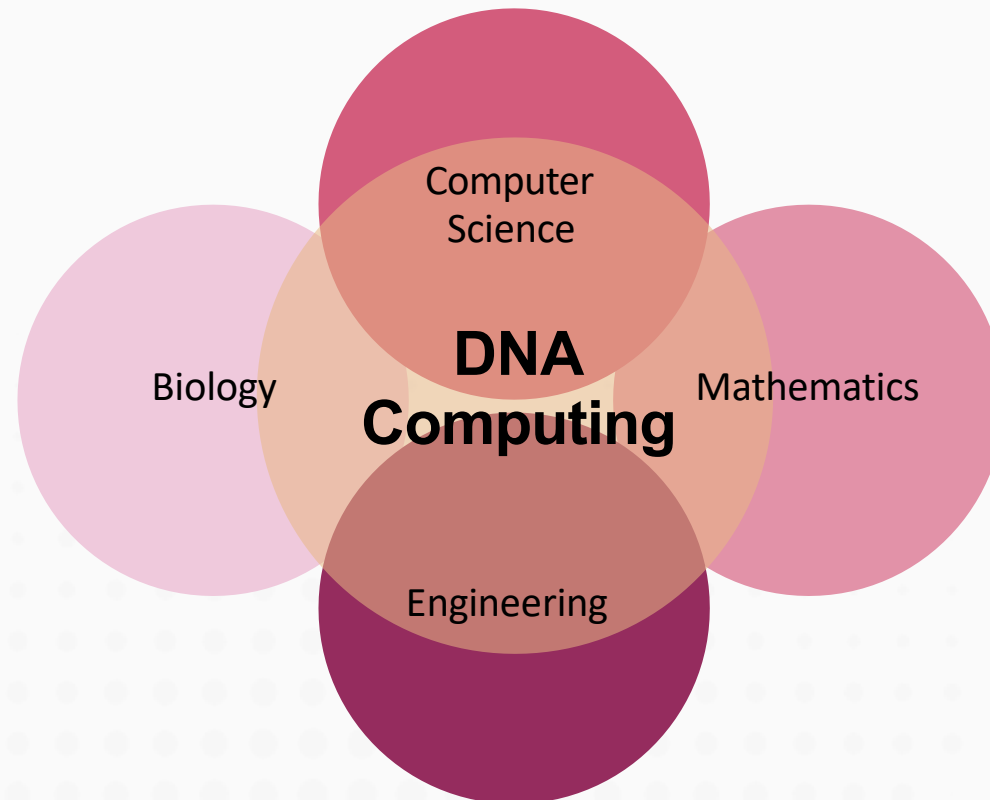
Fruits
Vegetables
Crops
Microbs
Animals

4. ENERGY APPLICATIONS

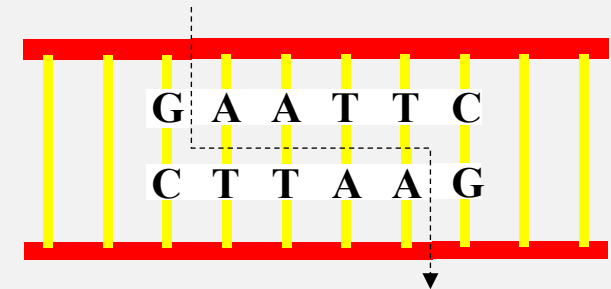
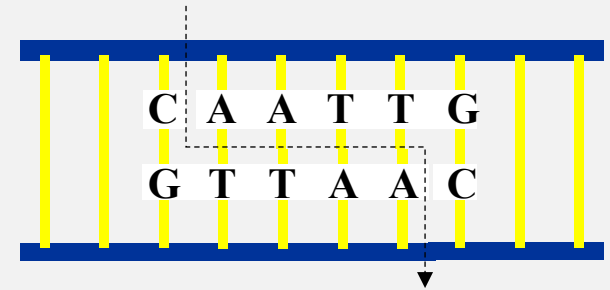
Biohydrogen
Bioethanol
Biomethanol
Biobutanol

DNA Computing

- **DNA computing** has emerged in the last twenty years as an exciting new research field at the intersection of Biology, Computer Science, Mathematics and Engineering.



DNA Splicing System



...



Mathematics and DNA Splicing System

- The mathematical modelling of splicing system was first defined by **Tom Head** in 1987.
- It was introduced as a **mathematical model** of the generative capacity of a **biological system** containing **DNA molecules** in the presence of appropriate **enzymes**.



Prof Head's visit to UTM, 2004

Mathematical Modelling of DNA Splicing System

How do we model it?

Mathematics and Formal Language

Alphabets

h, n, i, z, a, s, m, r, o

Strings

nor & haniza & sarmin

Grammar

Nor + Haniza
Haniza + Sarmin

Language

Nor Haniza
Haniza Sarmin

DNA in Mathematical Model

DNA bases

a, c, g, t

DNA Sequence

acgttgat & gcgttga

DNA Splicing

acgt- -tgat & gcgt- -tga

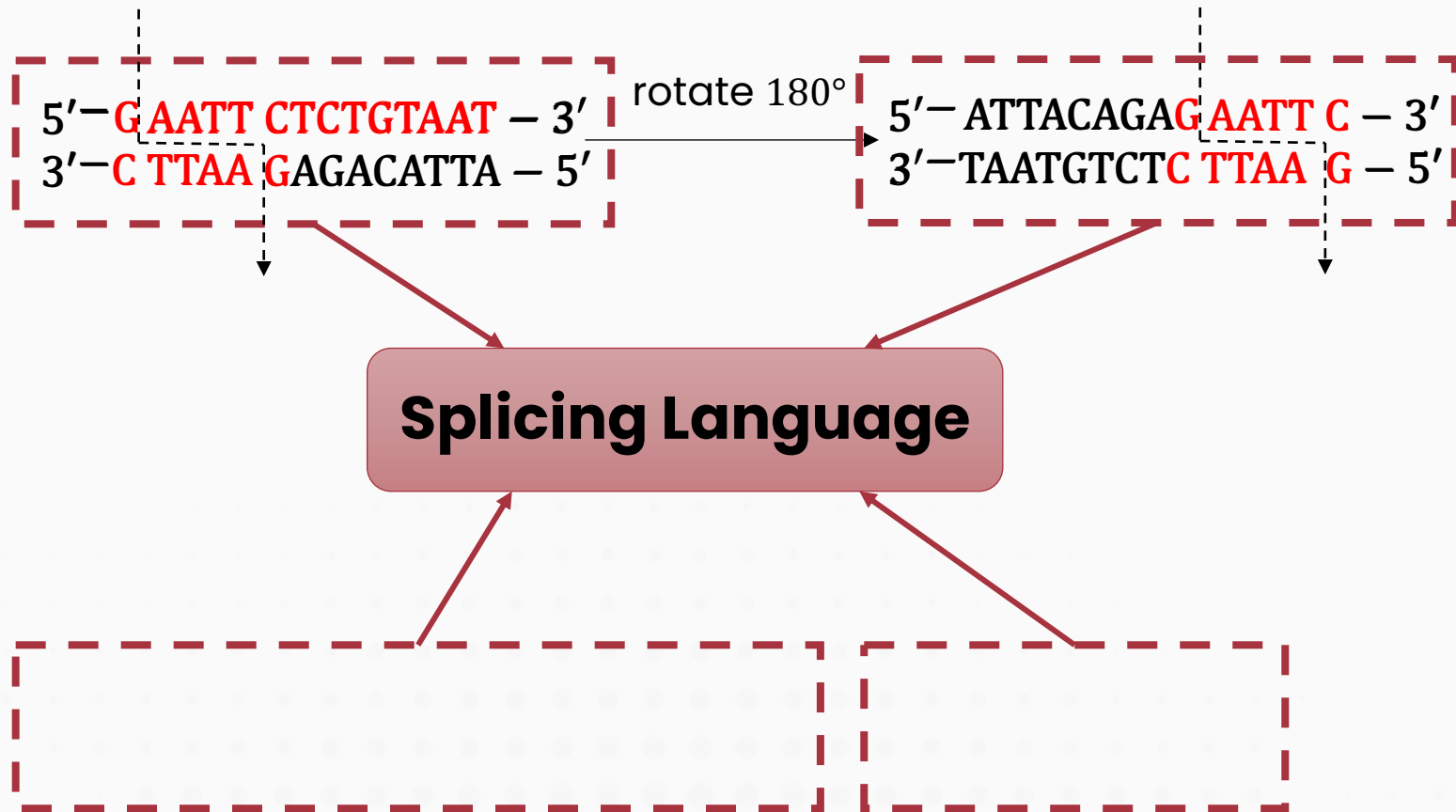
Grammar

Watson-Crick

Language

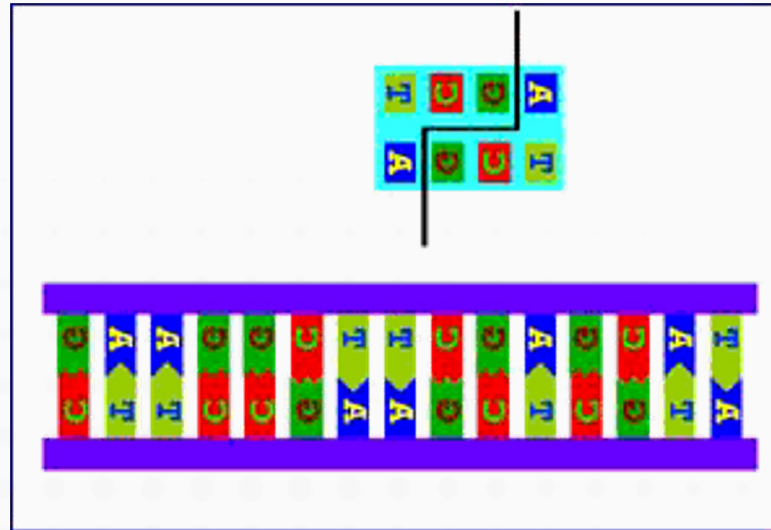
acgttga & gcgttgat

Mathematical Modelling of DNA Splicing System (Cont.)



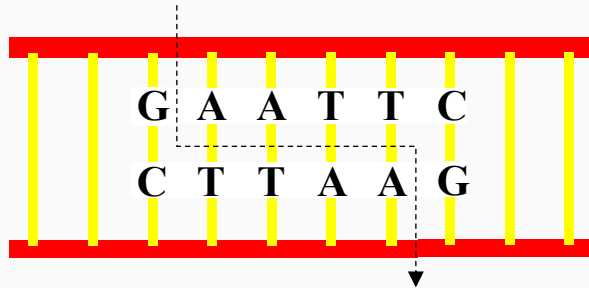
Restriction Enzymes

- A restriction enzyme is an enzyme that **cuts** double-stranded or single stranded DNA at **specific recognized nucleotide sequences**, known as **restriction sites**.

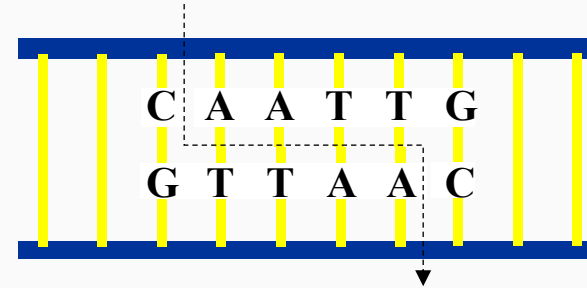


Restriction Enzymes (Cont.)

EcoRI: ([G/C],[A/T],[A/T],[T/A],[T/A],[C/G])



MfeI: ([C/G],[A/T],[A/T],[T/A],[T/A],[G/C])



Types of DNA Splicing Systems



- Head, T. (1987). **Formal Language Theory and DNA: An Analysis of the Generative Capacity of Specific Recombinant Behaviors.** *Bulletin of Mathematical Biology*, 49(6), 737-759. doi:<https://doi.org/10.1007/BF0248177>
- Păun, G. (1996). **On the Splicing Operation.** *Discrete Applied Mathematics*, 70(1), 57-79. doi:[https://doi.org/10.1016/0166-218X\(96\)00101-1](https://doi.org/10.1016/0166-218X(96)00101-1)
- Pixton, D. (1996). **Regularity of Splicing Languages.** *Discrete Applied Mathematics*, 69(1-2), 101-124. doi:[https://doi.org/10.1016/0166-218X\(95\)00079-7](https://doi.org/10.1016/0166-218X(95)00079-7)
- Goode, E., & Pixton, D. (2004). **Splicing to the Limit.** In N. Jonoska, G. Păun, & G. Rozenberg (Eds.), *Aspects of Molecular Computing, Lecture Notes in Computer Science* (pp. 189-201). Germany: Springer-Verlag.
- Yusof, Y., Sarmin, N. H., Fong, W. H., Goode, T. E., & Ahmad, M. A. (2013). **An Analysis of Four Variants of Splicing System.** Paper presented at the 20th National Symposium on Mathematical Sciences - Research in Mathematical Sciences: A Catalyst for Creativity and Innovation (SKSM 2012).
- Karimi, F., Turaev, S., Sarmin, N. H., & Fong, W. H. (2014). **Fuzzy Splicing Systems.** In D. Hwang, J. J. Jung, & N. T. Nguyen (Eds.), *Computational Collective Intelligence. Technologies and Applications, ICCCI 2014, Lecture Notes in Computer Science* (pp. 20-29). Cham, Switzerland: Springer International Publishing.

Types of DNA Splicing Systems (Cont.)

Splicing System	Head $S = (A, I, B, C)$	Paun $\sigma = (A, R)$	Pixton $\zeta = (R, I)$	Goode-Pixton $(w, w') \vdash_r z$	Yusof-Goode $S = (A, I, R)$	Fuzzy $S = (A, T, I, R, \odot)$
Initial String	$ucxdv$ $pexfq$	uu_1u_2v $u'u_3u_4v'$	$\xi\alpha\eta$ $\xi'\alpha'\eta'$	$w = xuvy$ $w' = x'u'v'y'$	$\alpha uxv\beta$ $\gamma yz\delta$	(ua, x) (bv, y) $x, y \in [0, 1]$
Rule	(c, x, d) (e, x, f)	$u_1\#u_2\$u_3$ $\#u_4$	$(\alpha, \alpha': \beta)$	$r = (u, v; u'; v')$	$(u, x, v: y, x, z)$	$u\#a\$b\#v$
Splicing Language	$ucxfq$ $pexdv$	uu_1u_4v'	$\xi\beta\eta'$	$z = xuv'y'$	$\alpha uxz\delta$ $\gamma yxv\beta$	$(uv, x \odot y)$ \odot is fuzzy operation

- S : splicing system
- σ and ζ : splicing schemes
- A : finite alphabet
- $T \subseteq A$: terminal alphabet
- I : set of initial strings
- B : set of rules with left pattern
- C : set of rules with right pattern
- $R = B \cup C$: set of rules

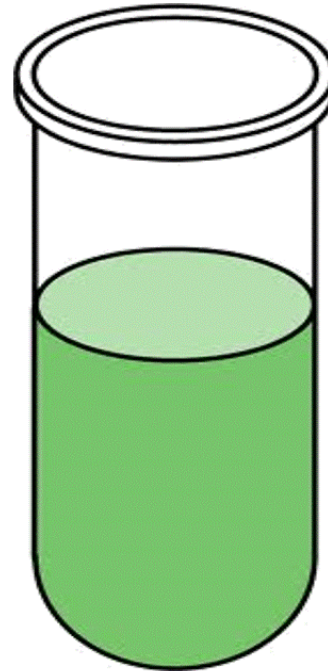
Theoretical vs Wet Lab



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Wet Experiment on Splicing System

$$S = (A, I, B, C)$$



Theoretical vs Lab Results

Wet Splicing System involving *Cvi*QI and *Ac*II

- An initial DNA molecule I used in this splicing model is a small segment taken from bacteriophage lambda between 42958 and 43117 with the length of 160 base pairs (bp).
- The initial molecule contains one cutting site each of the restriction enzymes *Cvi*QI and *Ac*II where the genome locations for the cutting sites are found at 42992-42995 and 43036-43039 respectively.
- Five sticky ends of molecules α , β , γ , $\alpha - \beta$ and $\beta - \gamma$ are produced by the restriction enzymes when cutting the initial molecule. The lengths of fragments for the sticky ends are given in the following.

Fragment: $\alpha \xrightarrow{\text{CviQI site}} \beta \xrightarrow{\text{AcII site}} \gamma$

$$|\alpha| = 35 \text{ bp}$$

$$|\beta| = 44 \text{ bp}$$

$$|\gamma| = 81 \text{ bp}$$

$$|\alpha - \beta| = 79 \text{ bp}$$

$$|\beta - \gamma| = 125 \text{ bp}$$

Theoretical vs Lab Results (Cont.)

Wet Splicing System involving CviQI and Acil

- Initial Molecule (42958 and 43117 from bacteriophage lambda)

*ggactatcgaagagtgcaaggcgatcaaggcagaggtaccaacagaaactcaaagacctgcgaaatagcagaa
gtgaggccgcatgacggttctcagtaaaaaccattccagacatgctcgttgaaacatacggaaatcagacagaagt
agcacgcagactg* (160 bp)

- Enzyme CviQI (palindromic)

5'...G▼TAC...3'

3'...CAT▲G...5'

- Enzyme Acil (non-palindromic)

5'...C▼CGC...3'

3'...CGC▲C...5'

Theoretical vs Lab Results (Cont.)

Wet Splicing System involving CviQI and Acil

The splicing language from this splicing system S involving **one cutting site** each of **palindromic** restriction enzyme CviQI (g, ta, c) and **non-palindromic** restriction enzyme Acil (c, cg, c) with different palindromic crossings is shown in the following:

$$L(S) = \{\alpha gtac(\beta ccgg\beta' gtac)^{n-1}(\alpha' + \beta ccgc\gamma)\} \\ + \{\gamma' gcg(g\beta' gtac\beta ccg)^{n-1}(c\gamma + g\beta' gtac\alpha')\}.$$

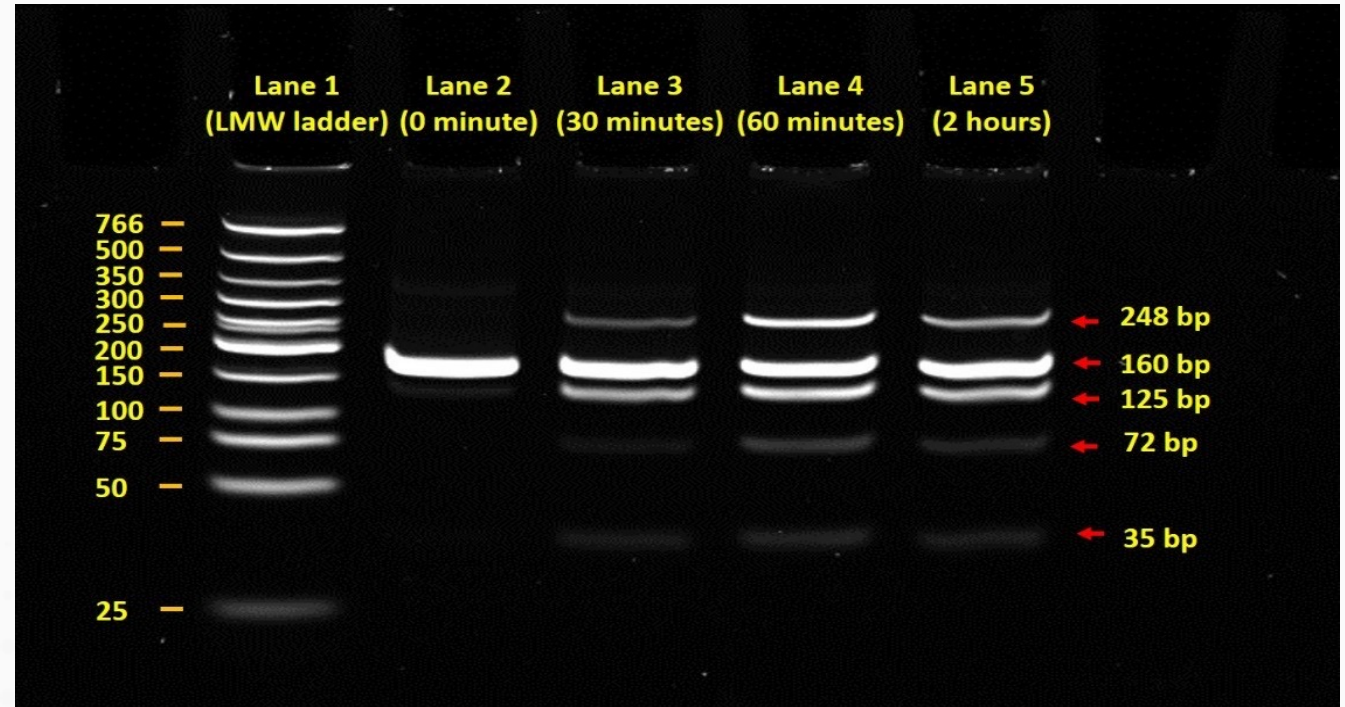
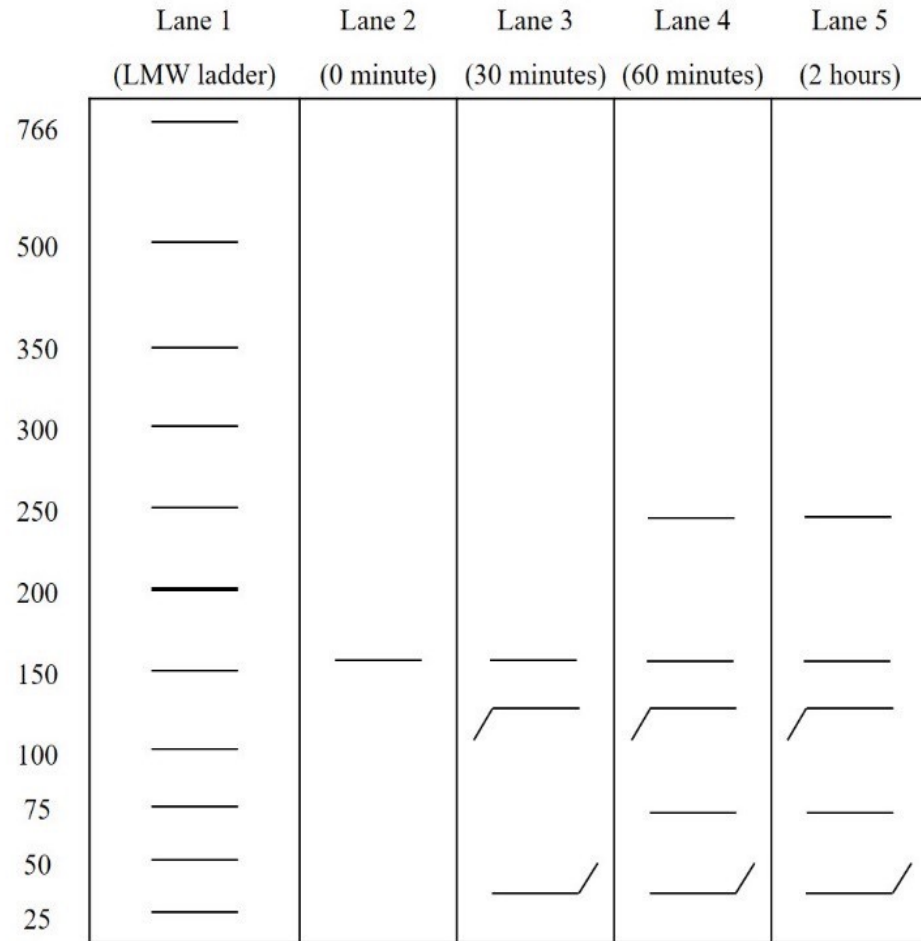
where $n \in \mathbb{Z}^+$. The fragments of DNA strings in the splicing language $L(S)$ are stated as follows:

$$\alpha \underline{gtac} \left(\beta \underline{ccgg} \beta' \underline{gtac} \right)^{n-1} \alpha', \\ \alpha \underline{gtac} \left(\beta \underline{ccgg} \beta' \underline{gtac} \right)^{n-1} \beta \underline{ccgc} \gamma, \\ \gamma' \underline{gcg} \left(\underline{g} \beta' \underline{gtac} \beta \underline{ccg} \right)^{n-1} \underline{c} \gamma \text{ and} \\ \gamma' \underline{gcg} \left(\underline{g} \beta' \underline{gtac} \beta \underline{ccg} \right)^{n-1} \underline{g} \beta' \underline{gtac} \alpha'$$

where $n \in \mathbb{Z}^+$ represents multiple copies of the specific strings.

Theoretical vs Lab Results (Cont.)

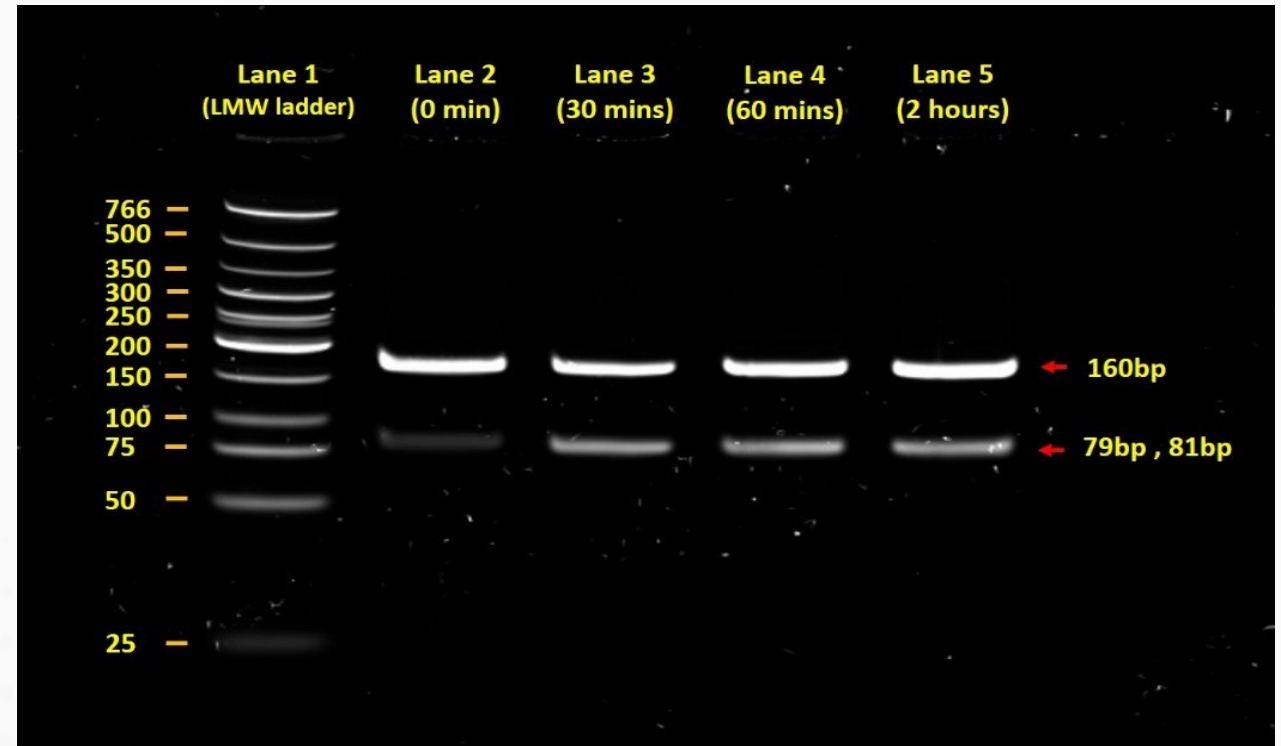
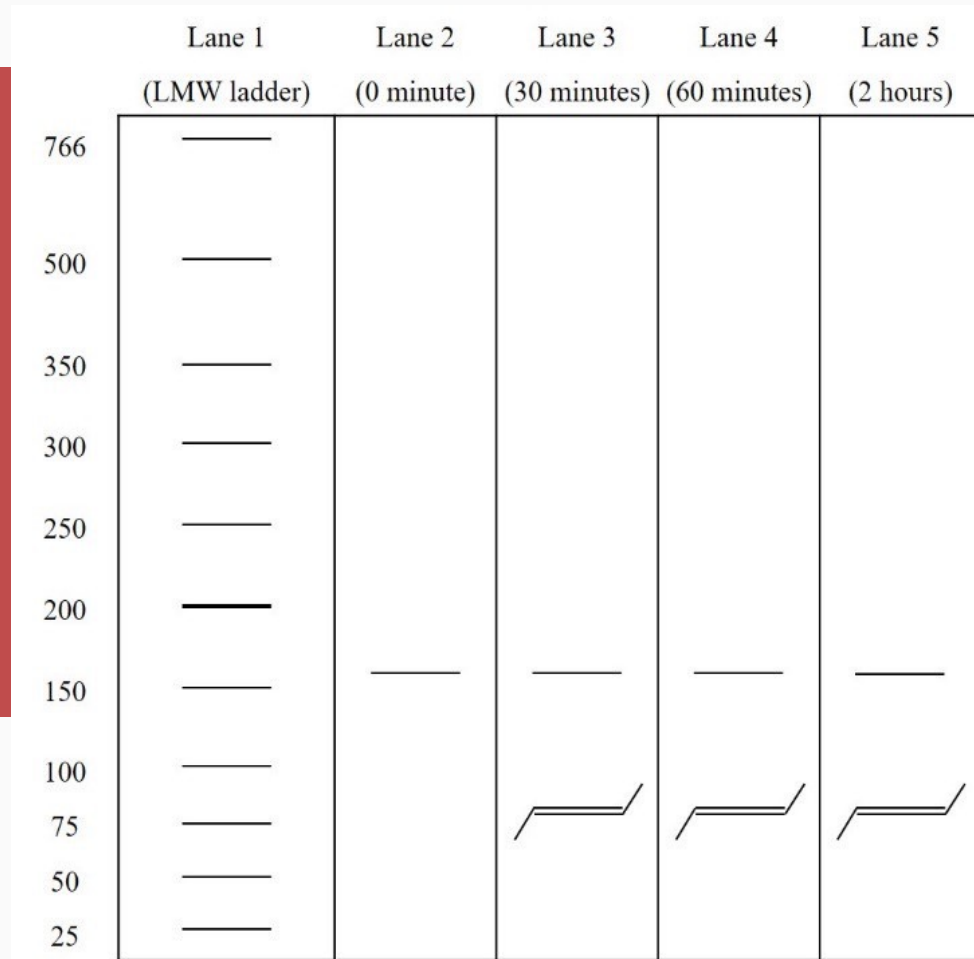
Wet Splicing System involving CviQI



- Lane 1: LMW ladder
- Lane 2 (0 minute): 160 bp
- Lane 3 (30 minutes): 35 bp, 72 bp, 125 bp, 160 bp and 248 bp
- Lane 4 (60 minutes): 35 bp, 72 bp, 125 bp, 160 bp and 248 bp
- Lane 5 (2 hours): 35 bp, 72 bp, 125 bp, 160 bp and 248 bp

Theoretical vs Lab Results (Cont.)

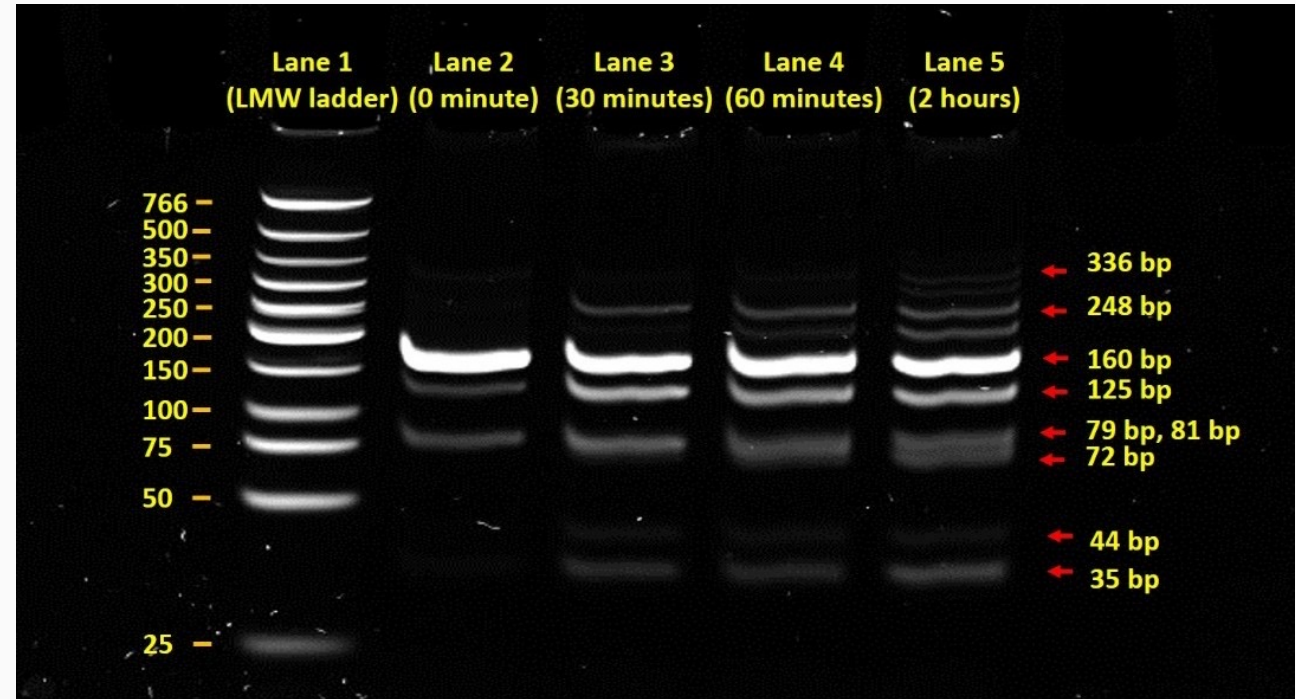
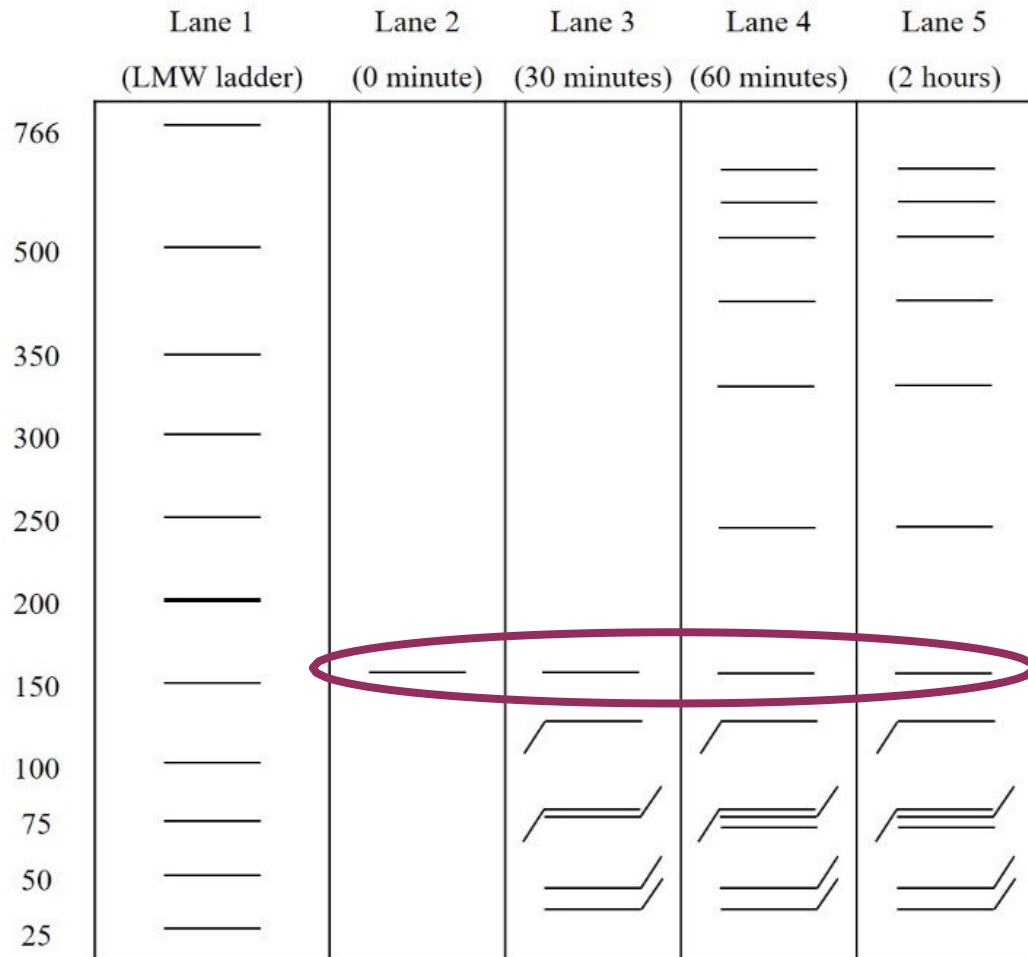
Wet Splicing System involving *Acil*



- Lane 1: LMW ladder
- Lane 2 (0 minute): 79 bp (or 81 bp) and 160 bp
- Lane 3 (30 minutes): 79 bp, 81 bp and 160 bp
- Lane 4 (60 minutes): 79 bp, 81 bp and 160 bp
- Lane 5 (2 hours): 79 bp, 81 bp and 160 bp

Theoretical vs Lab Results (Cont.)

Wet Splicing System involving CviQI and Acil



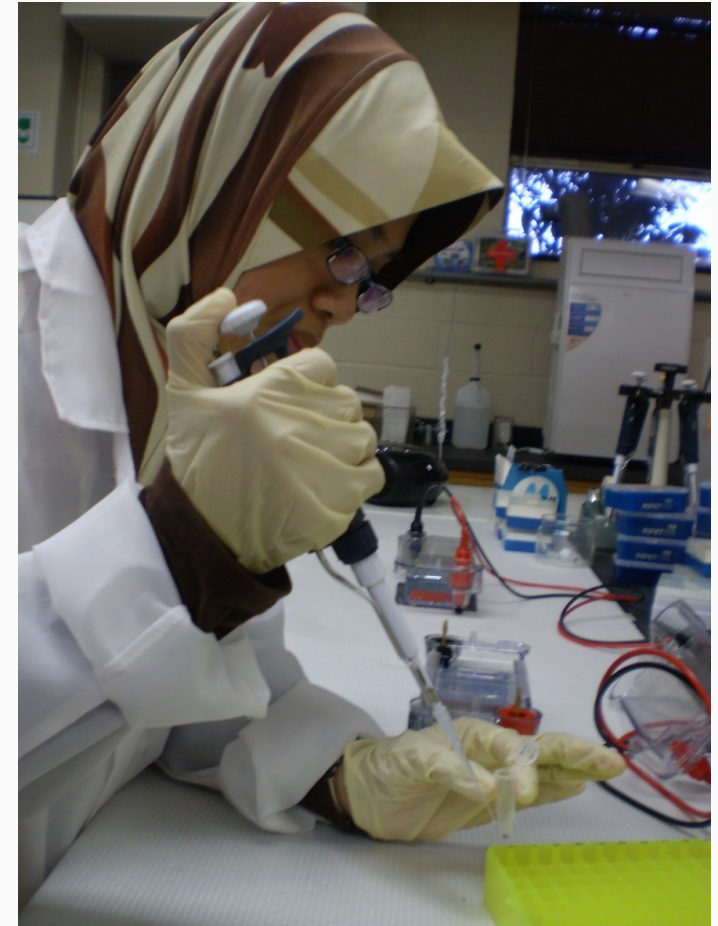
- Lane 1: LMW ladder
- Lane 2 (0 minute): 79 bp (or 81 bp), 125 bp and 160 bp
- Lane 3 (30 minutes): 35 bp, 44 bp, 79 bp, 81 bp, 125 bp, 160 bp, 248 bp
- Lane 4 (60 minutes): 35 bp, 44 bp, 79 bp, 81 bp, 125 bp, 160 bp, 248 bp
- Lane 5 (2 hours): 35 bp, 44 bp, 72 bp, 79 bp, 81 bp, 125 bp, 160 bp, 248 bp, 336 bp

Wet-lab Experiment on Splicing System



Universiti Teknologi Malaysia, 2007

Wet-lab Experiment on Splicing System



State University of New York, Binghamton, New York, and Towson University, USA, 2010

Wet-lab Experiment on Splicing System



Universiti Teknologi Malaysia, 2012

Wet-lab Experiment on Splicing System



Universiti Teknologi Malaysia, 2015

Wet-lab Experiment on Splicing System



Universiti Teknologi Malaysia, 2020

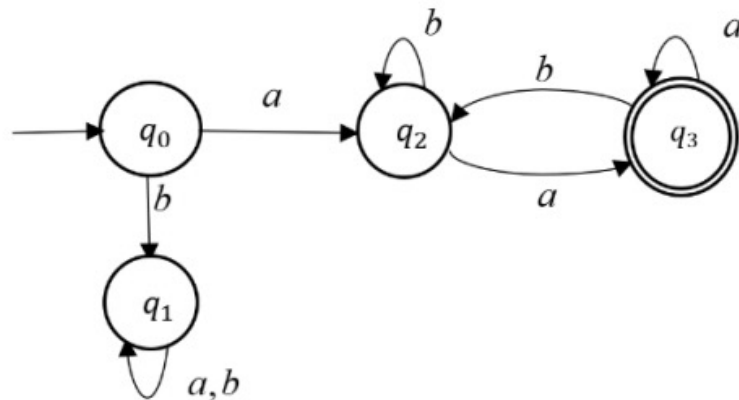
DNA Splicing in Computer Science



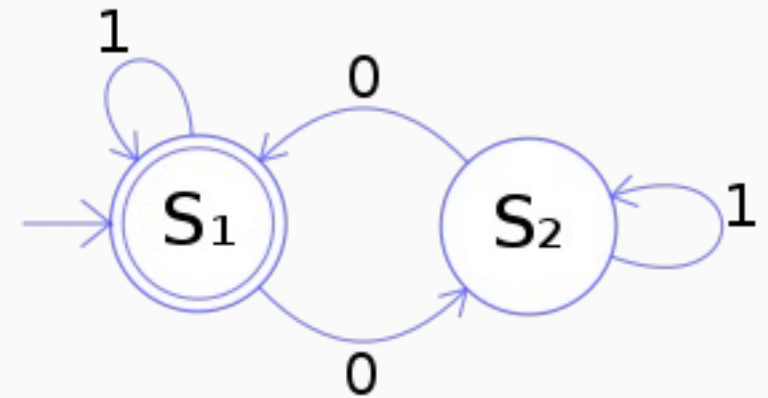


Automata of Splicing System

Automata theory is the study of abstract machines, as well as the computational problems that can be solved using them. It is a theory in theoretical computer science.



The automaton diagram for regular language



The automaton described by this state diagram starts in state S_1 , and changes states following the arrows marked 0 or 1 according to the input symbols as they arrive. The double circle marks S_1 as an accepting state. Since all paths from S_1 to itself contain an even number of arrows marked 0, this automaton accepts strings containing even numbers of 0s.

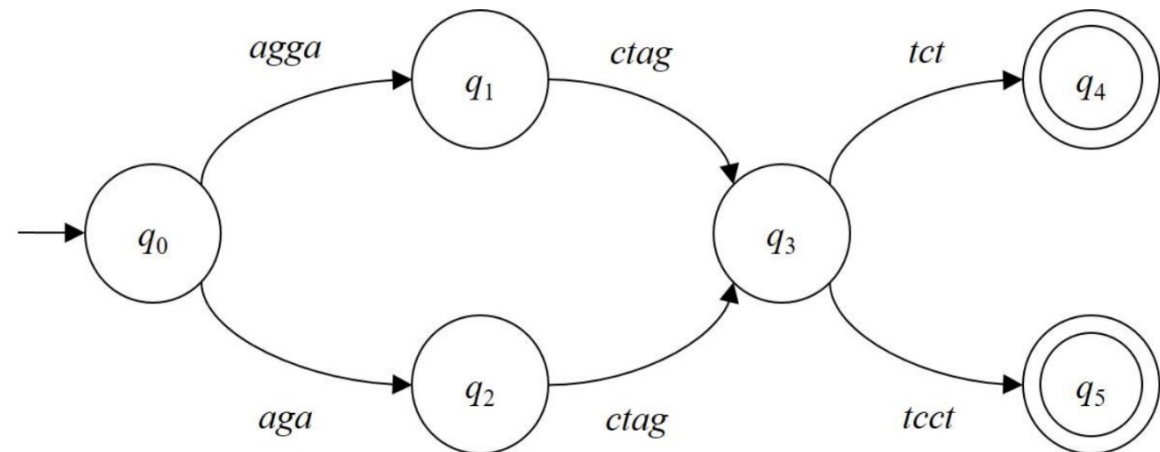


Example

Given a splicing system $S = (A, I, B, C)$ where $I = \{ \text{AGGACTAGTCT} \}$ is the set of initial string, set $B = \left\{ \begin{pmatrix} \text{C} & \text{TA} & \text{G} \\ \text{G} & \text{AT} & \text{C} \end{pmatrix} \right\}$ is the set of cleavage pattern for the enzyme *BfaI*, and set C is the empty set.

The enzyme *BfaI*, $5' - \text{CTAG} - 3'$ is a palindromic rule since the base sequence of enzyme *BfaI* reads the same forwards and backwards.

The automata for the splicing system S



Graphical User Interface (GUI) for DNA Splicing System

DNA Splicing Language Generator (DNASpliceGen)

A C++ program that is created in **Microsoft Visual Studio** to **develop the Graphical User Interface (GUI)** for DNA splicing systems involving palindromic and non-palindromic rules.

The screenshot shows a window titled "DNA Splicing System with Palindromic and Non-Palindromic Rules". Inside the window, there is an instruction box that says "Instruction: Insert the initial string and the cleavage pattern of the enzyme(s).". Below this, there are input fields for "Initial string", "Enzyme 1", and "Enzyme 2". The "Enzyme 1" and "Enzyme 2" fields are each divided into three sub-fields by commas. At the bottom of the input area are two buttons: "Compute" and "Clear".

Annotations with arrows point to the following elements:

- An arrow points to the "Initial string" input field with the text: "Insert the initial DNA string".
- An arrow points to the "Enzyme 1" and "Enzyme 2" input fields with the text: "Insert the cleavage pattern of the enzyme(s)".
- An arrow points to the "Compute" button with the text: "Click 'Compute' button to generate the results".
- An arrow points to the "Clear" button with the text: "Click 'Clear' button to reset the interface".

DNA Splicing Language Generator (DNASpliceGen)

DNA Splicing System with Palindromic and Non-Palindromic Rules

Instruction: Insert the initial string and the cleavage pattern of the enzyme[s].

Initial string:

Enzyme 1: , ,

Enzyme 2: , ,

The initial molecule:

5'-A G G A C T A G T C T -3'
3'-T C C T G A T C A G A -5'

Restriction site of the enzyme :

The enzyme 5'-C T A G -3'
3'-G A T C -5' is a palindromic rule with palindromic crossing.

The number of cutting sites found: 1

The resulting molecules: Case 1

5'- A G G A + A G A C T A G T C T + T C C T -3'
3'- (T C C T + T C T) G A T C (A G A + A G G A) -5'

One restriction enzyme is inserted by user

The boxes indicate the cutting site of the restriction enzyme found in the initial string

The algorithm determines if the restriction enzyme is a palindrome or not a palindrome including crossing

The algorithm states the number of cutting sites

The algorithm generates all the splicing languages

DNA Splicing Language Generator (DNASpliceGen)

Output of GUI for DNA Splicing System involving Two Rules

DNA Splicing System with Palindromic and Non-Palindromic Rules

Instruction: Insert the initial string and the cleavage pattern of the enzyme(s).

Initial string:

Enzyme 1: , ,

Enzyme 2: , ,

The initial molecule:

```
5'-A T T C G A C T G C G C A G A -3'
3'-T A A G C T G A C G C G T C T -5'
```

Restriction site of the enzyme :

The enzyme 5'-T C G A -3' is a palindromic rule with palindromic crossing.
3'-A G C T -5'

The enzyme 5'-G C G C -3' is a palindromic rule with palindromic crossing.
3'-C G C G -5'

The enzymes 1 and 2 have the same crossing.

The number of cutting sites found: 2

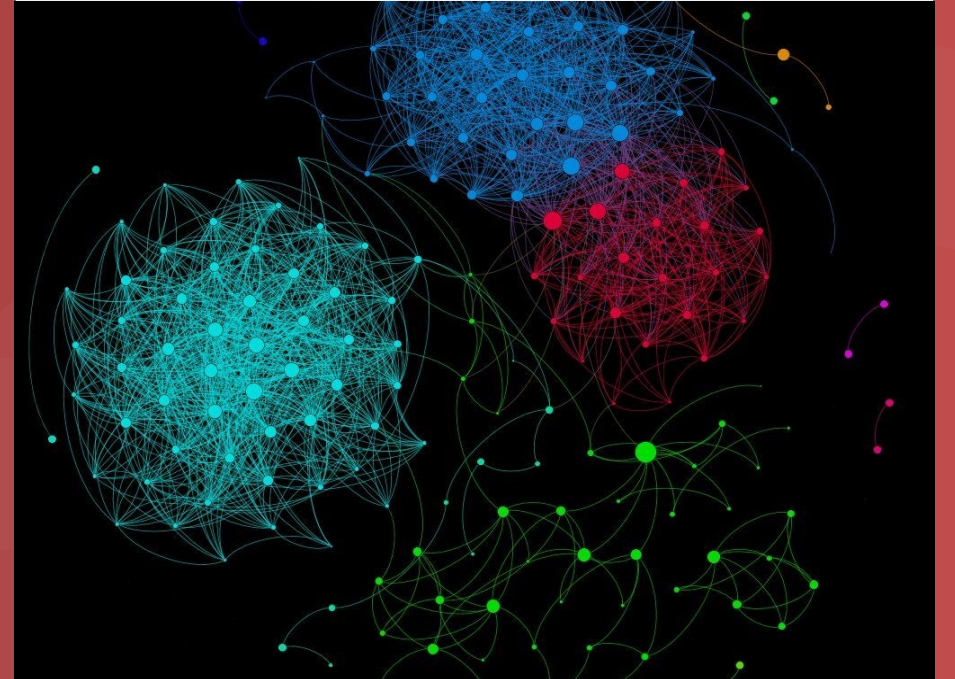
The resulting molecules: Case 3

```
5'- A T T T C T G { C G A C T G C A G T } * C G C A G A A A T -3'
3'- T A A + A G A C { G C T G A C + G T C A } G C G T C T + T T A -5'
```

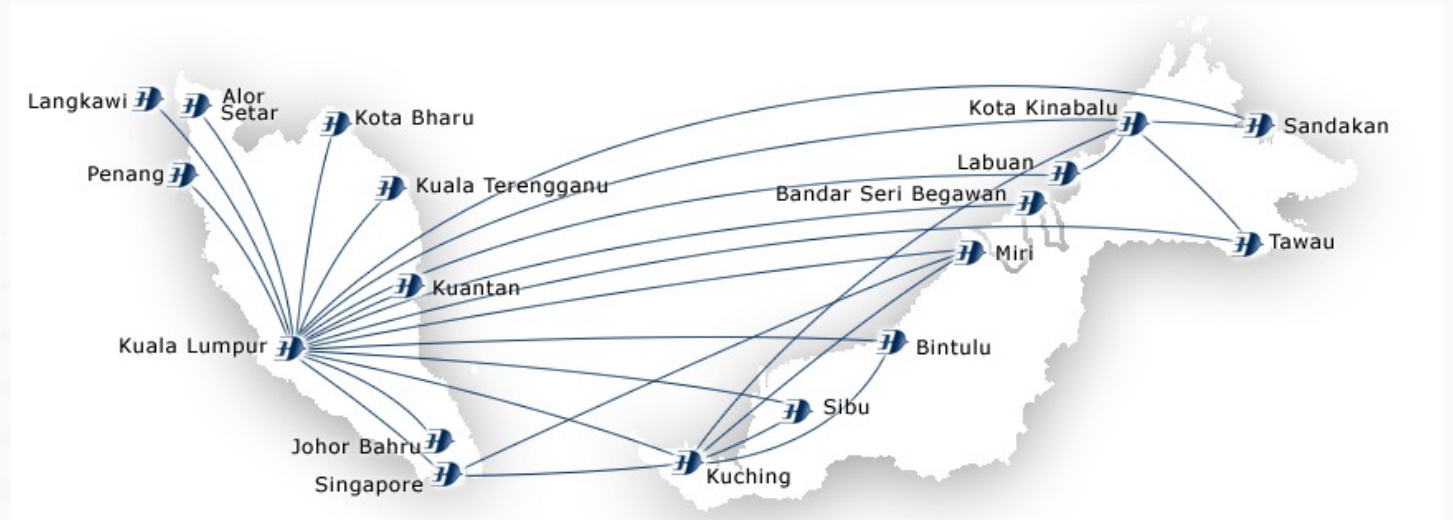
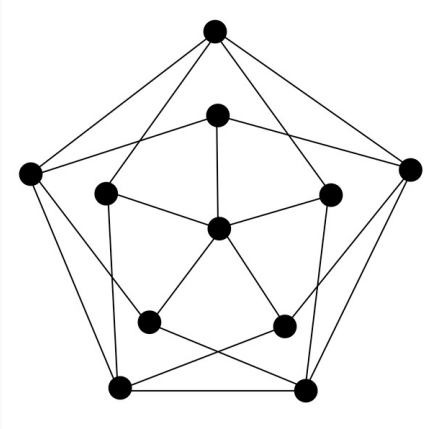
Additional features:

- Certain messages are displayed on the interface if the number of cutting sites found exceeds two
- The interface prompts the users if the cutting sites of restriction enzyme overlap
- The users will be notified if the inputs are incorrect.

DNA Splicing on Graph Theory

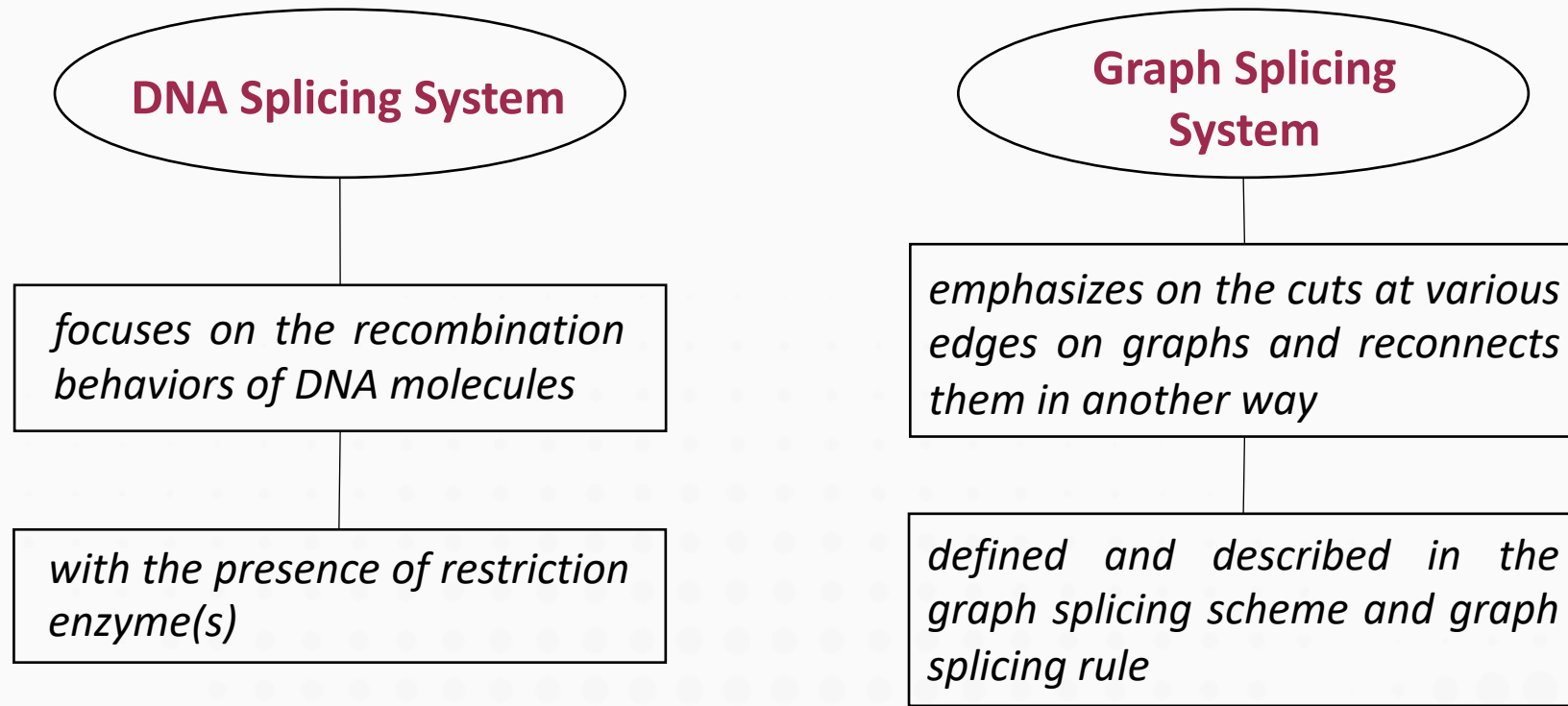


A graph is a **mathematical structure** consists of two finite sets called the set of **vertices, V** and **edges, E** .



Splicing System in Graph Theory

Graph splicing system is originally introduced by Freund in 1995 to describe the DNA splicing system in the form of graphs instead of one-dimensional strings.



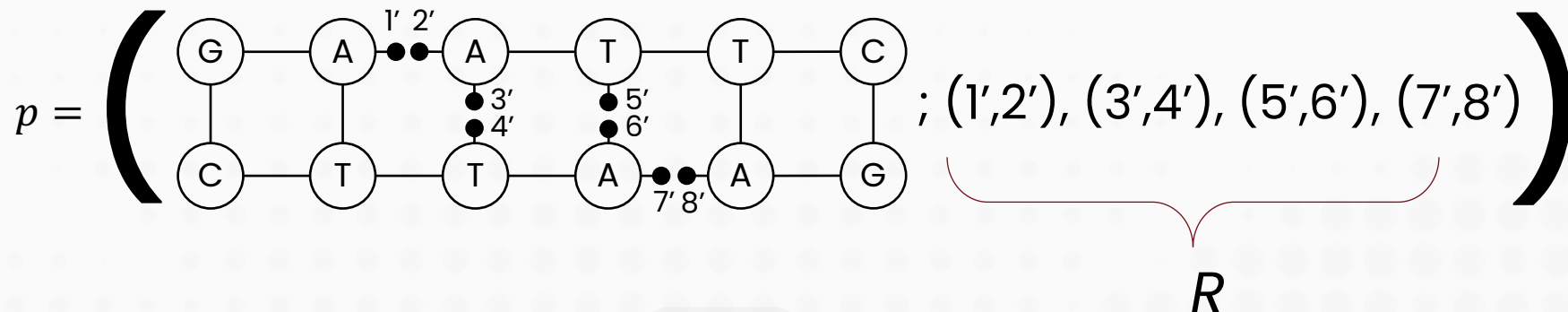
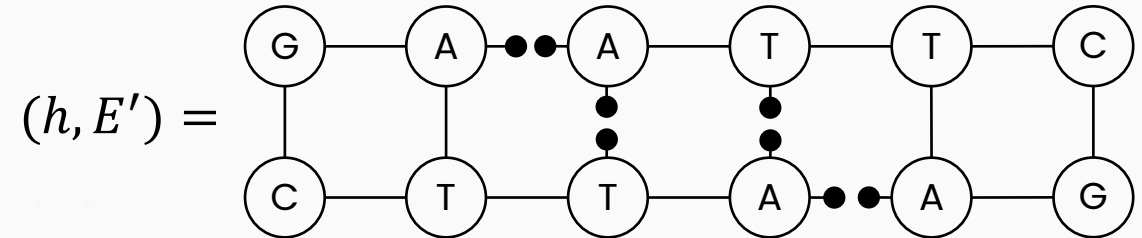
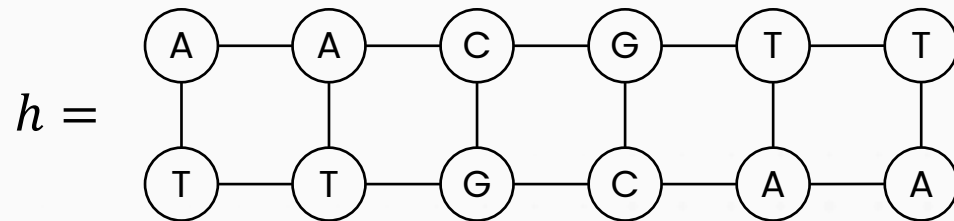
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Graph Splicing Rule

- A graph splicing rule consisting the enzyme *AcI* can be written as follows.

$$p = ((h, E'); R)$$

$$EcoRI: \begin{Bmatrix} AA & CG & TT \\ TT' & GC' & AA \end{Bmatrix}$$

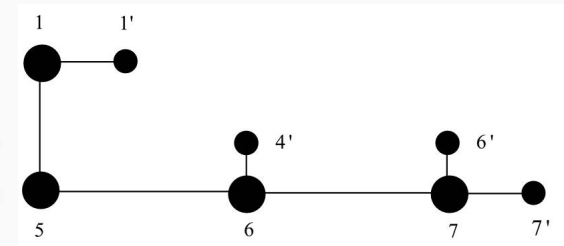
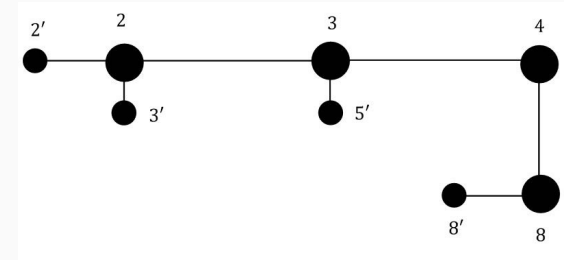
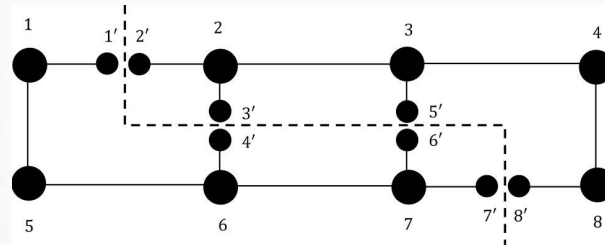
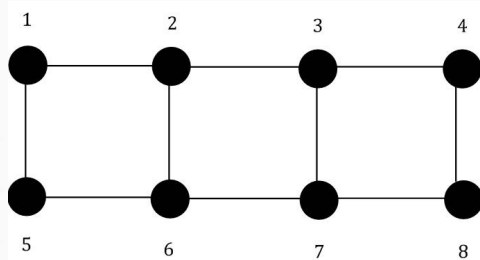


n -Cut Splicing (Cont.)

Semigraph representation of DNA molecule

An n -cut splicing is applied

Two components of n -cut spliced semigraphs are generated



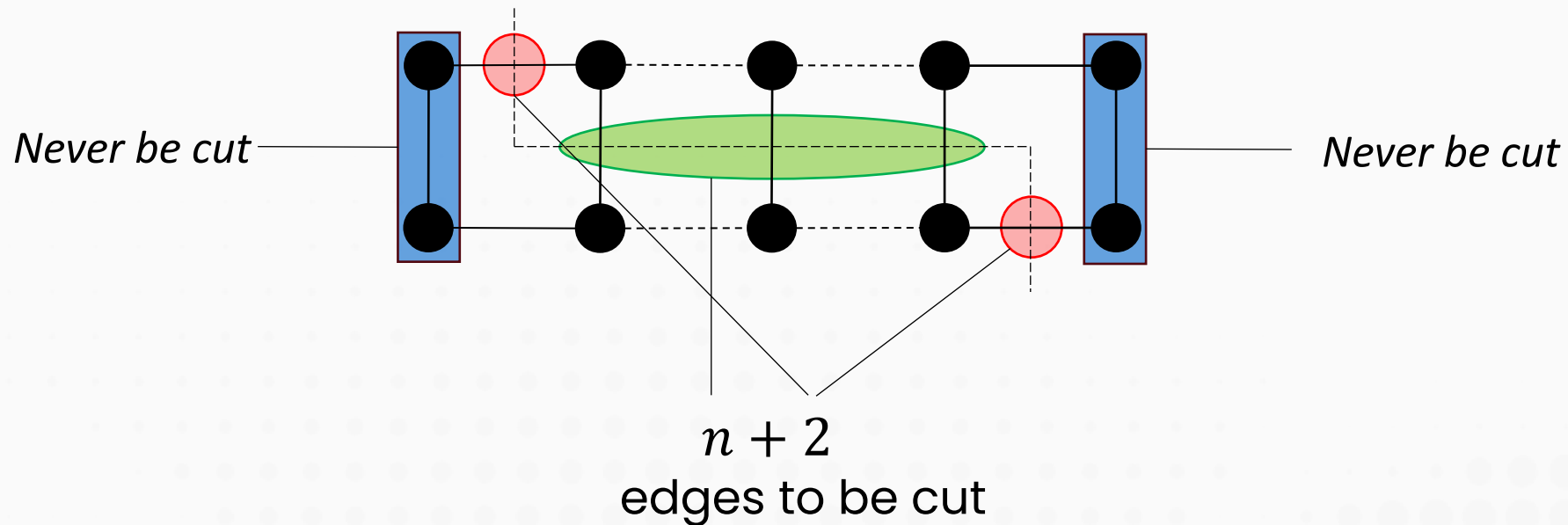
n -Cut Splicing (Cont.)

Example of n -cut splicing & n -cut spliced semigraph

n	n -cut splicing
1	<p>1-cut splicing</p>
2	<p>2-cut splicing</p>
3	<p>3-cut splicing</p>

n -Cut Splicing (Cont.)

An n -cut splicing will cut $n+2$ number of edges and the two vertices from the left most of the graphs as well as the two vertices from the right most of the graphs will never be cut.



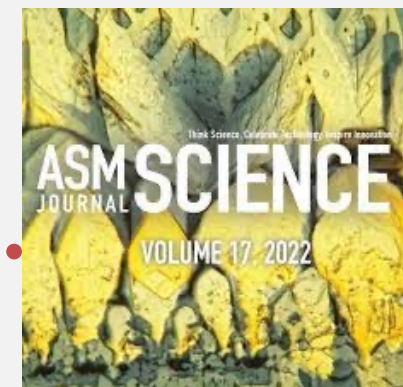
Future Research?

A Theoretical DNA Based Computer Model for Food Authentication Process

The authentication of food is an urgent concern owing to the increasing population and direct consequences of food on public health. Food authentication using DNA and omics-based methods is gaining ground due to critical advantages notably in the areas of food adulteration in plant and animal-based food and feed products and in determining the quality of food and food spoilage. Besides, there is greater demand for the detection of genetically modified foods (GMOs) and the detection of allergens, toxins, and carcinogens like tobacco in the food. Advanced DNA and omics-based methods (genomics, metabolomics, and proteomics) have been used in the food industry including DNA-based methods that rely on specific markers known as reference genes for food authentication. Novel methods like CRISPR-Cas have been recently introduced for the management of beneficial micro-organisms relevant to food like probiotics.

Publication

<https://people.utm.my/nizasarmin/journal-papers/>





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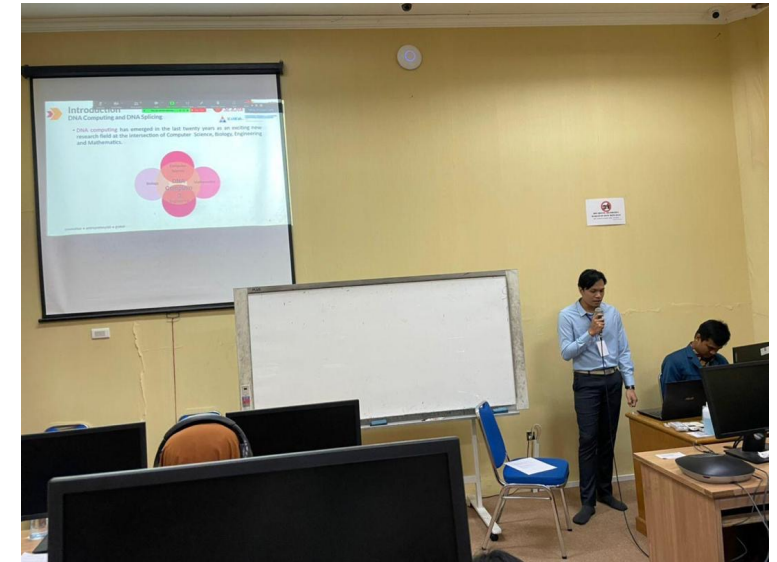
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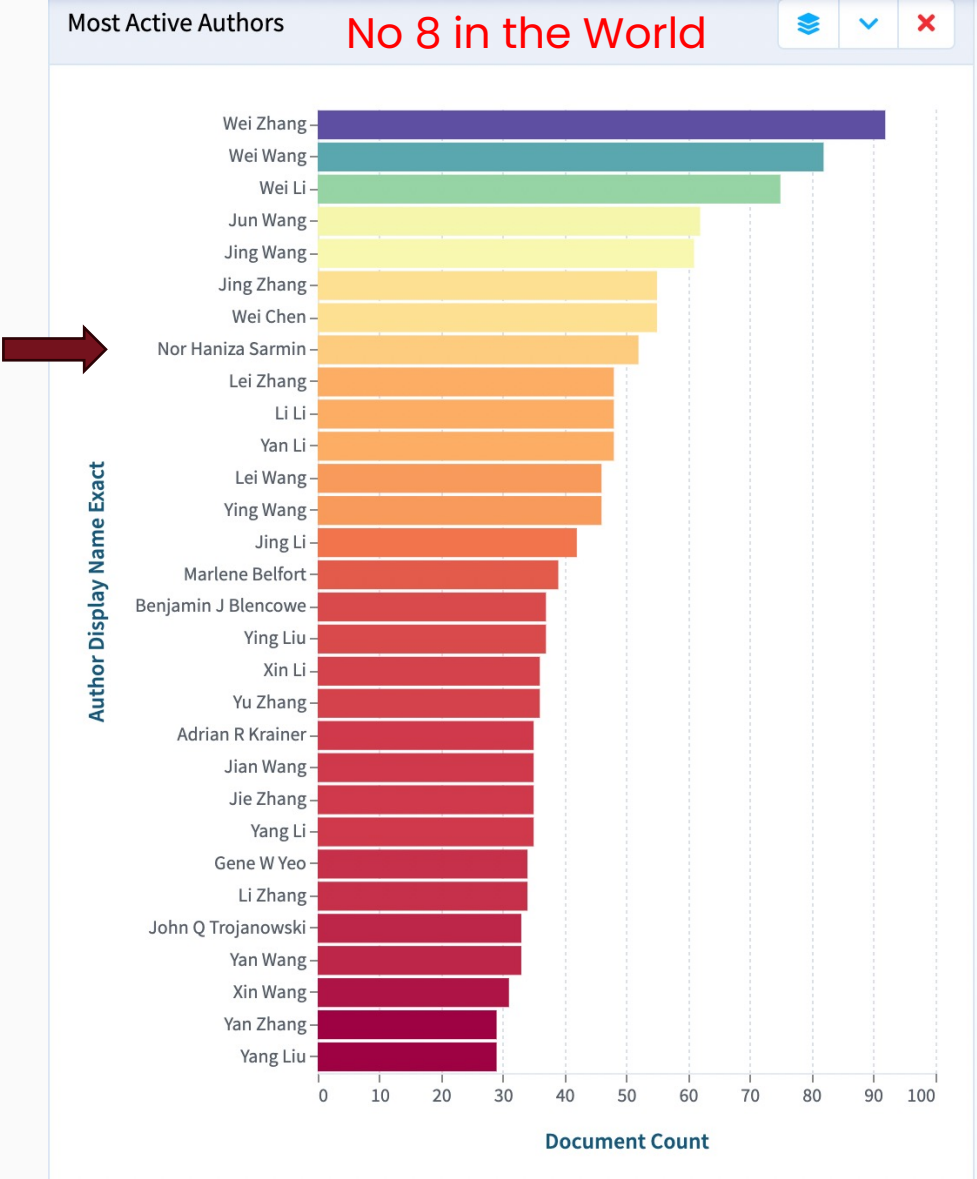
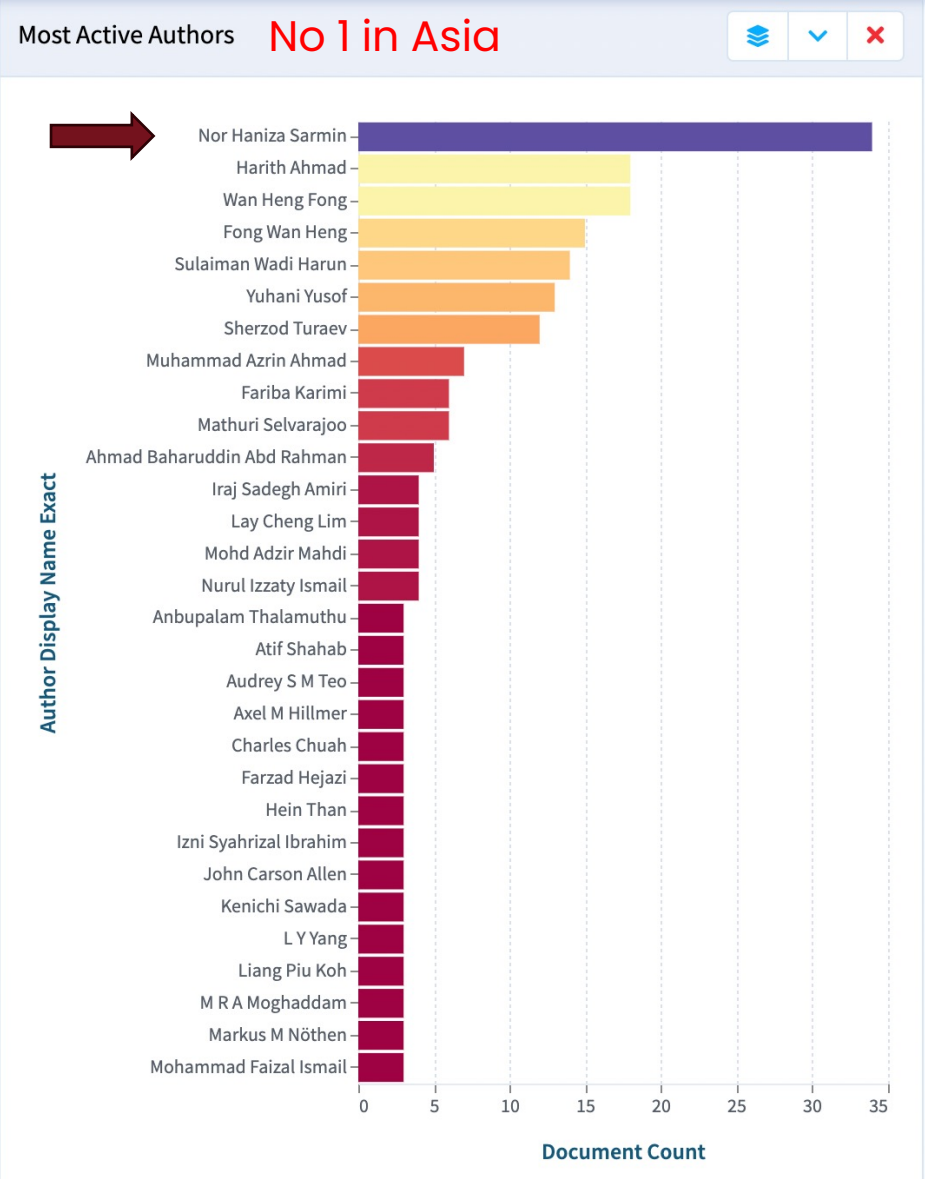
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Ranking in Splicing Systems (Lens.org)



Active Collaborator on DNA Splicing System



Specialization:

1. Formal Languages and Automata
2. DNA Computing
3. Artificial Intelligence
4. Cryptography

Ass. Prof. Dr. Sherzod Turaev

College of Information Technology, United Arab Emirates University

Co-supervisor for some PhD students

Active Collaborator on DNA Splicing System



Specialization:

1. Spectral of Laplacian Hypergraph and Graph
2. Distance Matrices and Quadratic Embedding of Graphs
3. Machine Learning
4. DNA Sequencing

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My Collaborators Around the World



ISMI 2024

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Mathematics for Sustainable Industry

9-11 September 2024  |  Kuala Lumpur
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THANK YOU



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Niza Sarmin



Niza Sarmin

In the Name of God for Mankind