



# Modeling Self Assembling DNA Structures for Lollipop Graphs

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## Background

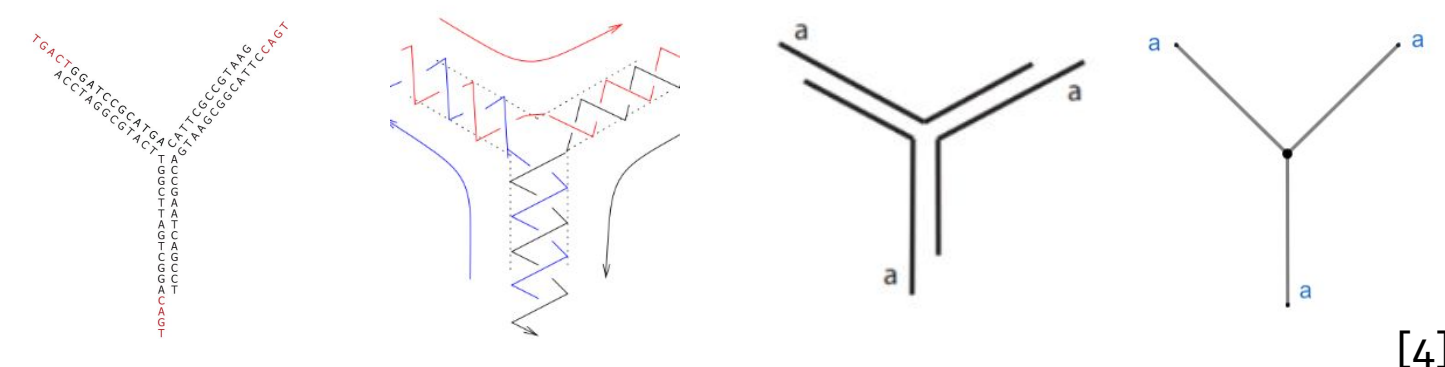
The ability of DNA strands to self-assemble into nanostructures has prompted researchers to develop new techniques to guide the self-assembly process.



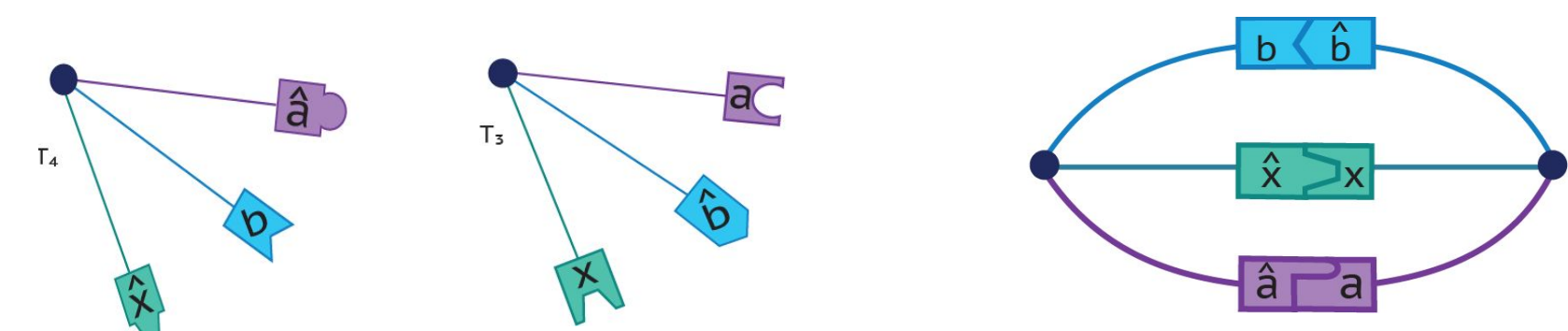
Self-assembling DNA molecules have extended arms that can bond through the pairing of complementary Watson-Crick base pairs. A complete nanostructure can be formed from a collection of these molecules.



DNA structures can be represented by discrete graphs. A **graph** is a set of edges and vertices. The **size of a graph** is the number vertices in the graph. The number of edges emanating from a vertex is called the **degree**. [3]



A **K-Armed Branched Junction Molecule** (above left) that combines to form a complete DNA structure is represented by a **tile** (above right) which is a vertex with extending half-edges. [3]



Each half edge is labeled by a hatted or unhatted letter, called its **bond-edge type**, to represent specific cohesive ends of the DNA sequence. A collection of tiles is called a **pot**. [3]

## General Methods

A minimal labeling of a graph  $G$  can be found using the following inequality:

$$av(G) \leq T_1(G) \leq ev(G) + 2ov(G)$$

Number of different degrees in  $G$       Number of different even degrees in  $G$       Number of different odd degrees in  $G$

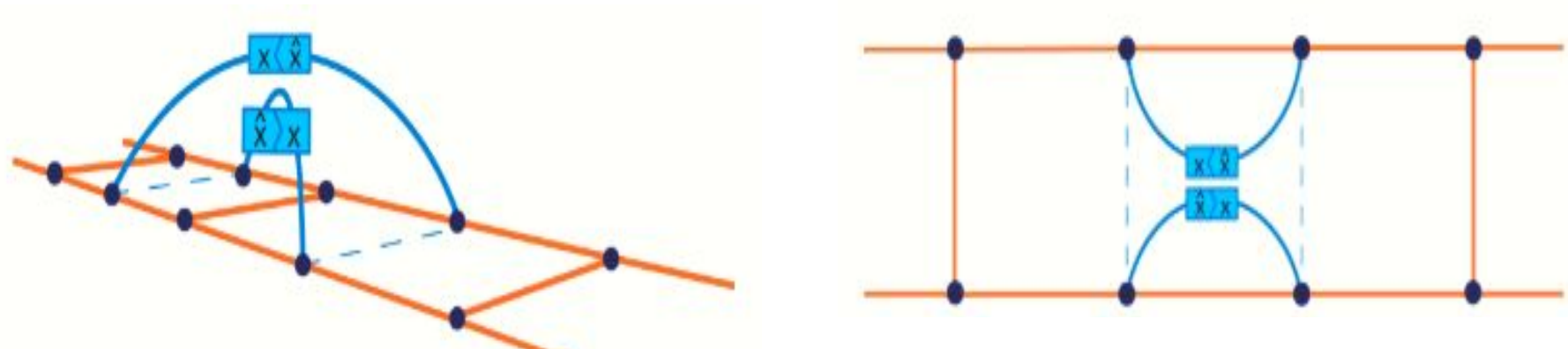
The **construction matrix** organizes tile type and bond-edge type information about a collection of tiles. Solutions to the matrix help determine if a graph of smaller size than the target graph can be formed from the proposed collection of tiles.<sup>1</sup>

$$M(G) = \begin{bmatrix} t_1 & t_2 & t_3 \\ a & -1 & -1 & 0 \\ 0 & 1 & -1 & 0 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

Solution Set:

Tile 1	1/5
Tile 2	1/5
Tile 3	2/5

Finally, graph edges of the same bond type can be broken apart and re-joined to determine if a graph non-isomorphic to the target graph can be created.



In all cases, we begin with the minimal labeling and must justify any additional tile or bond types until determining the most efficient labeling.

## Research Findings

### Specific Goals

Determine the minimum numbers of tile and bond-edge types

#### Scenario 1

Allowing the possibility that any other structure could be created from the pot, giving the minimum labeling.

#### Scenario 2

Allowing the possibility that structures of the same size as, but not smaller than, the pot could be created.

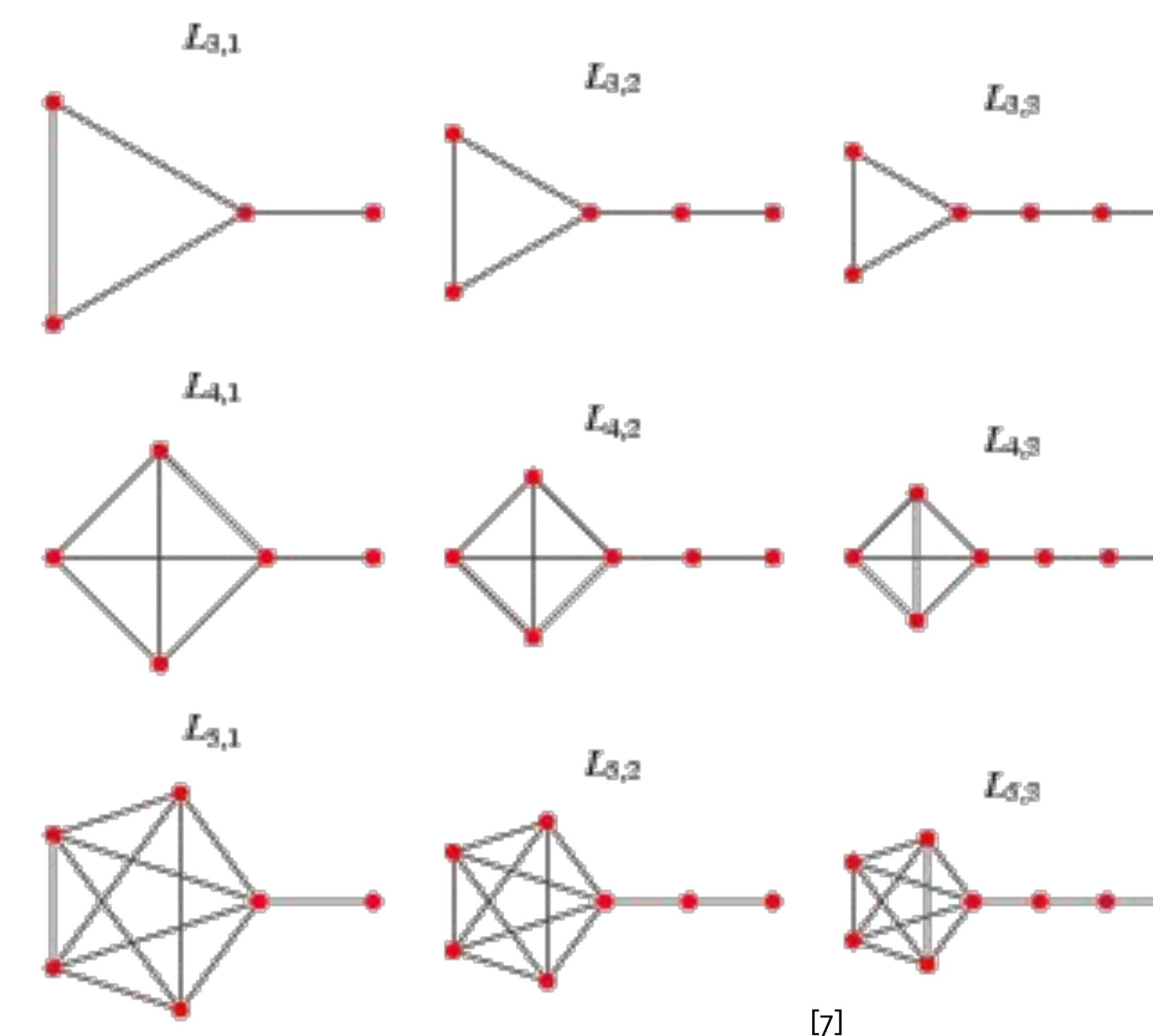
#### Scenario 3

Requiring that no structures other than precisely the target graph are built from the pot.

### Lollipop Graphs

A **Lollipop Graph**  $L_{m,n}$  is a  $K_m$  Complete Graph connected to a  $P_n$  path by a single vertex.

A **complete graph** is a fully connected graph, in which every vertex is attached to every other vertex.

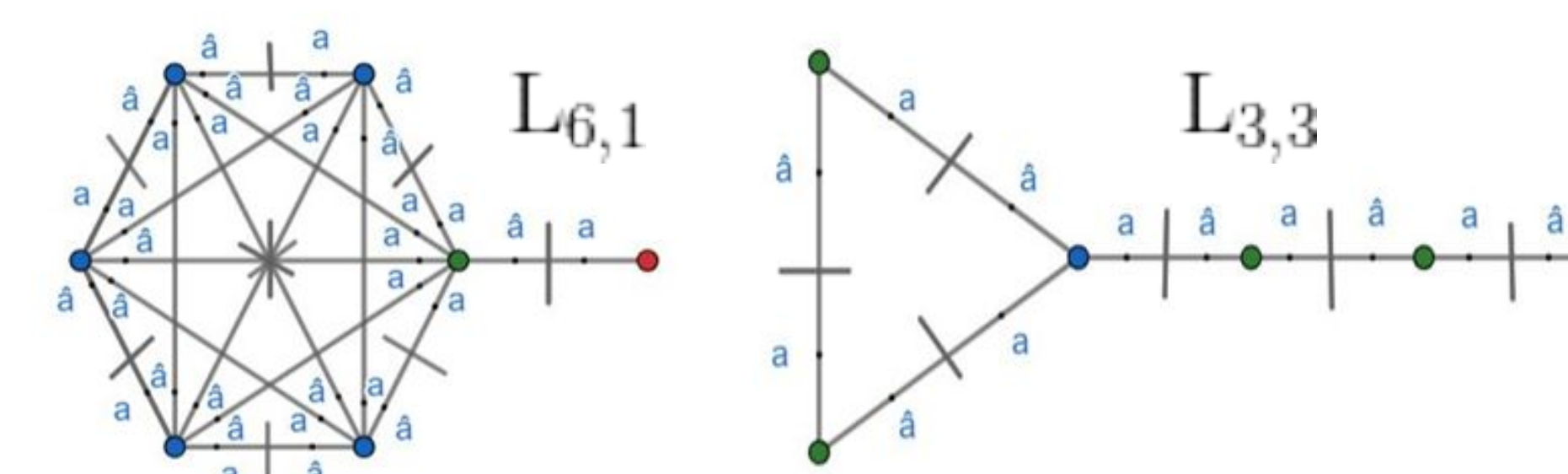


## Results for Lollipop Graphs

### Scenarios 1, 2, and 3

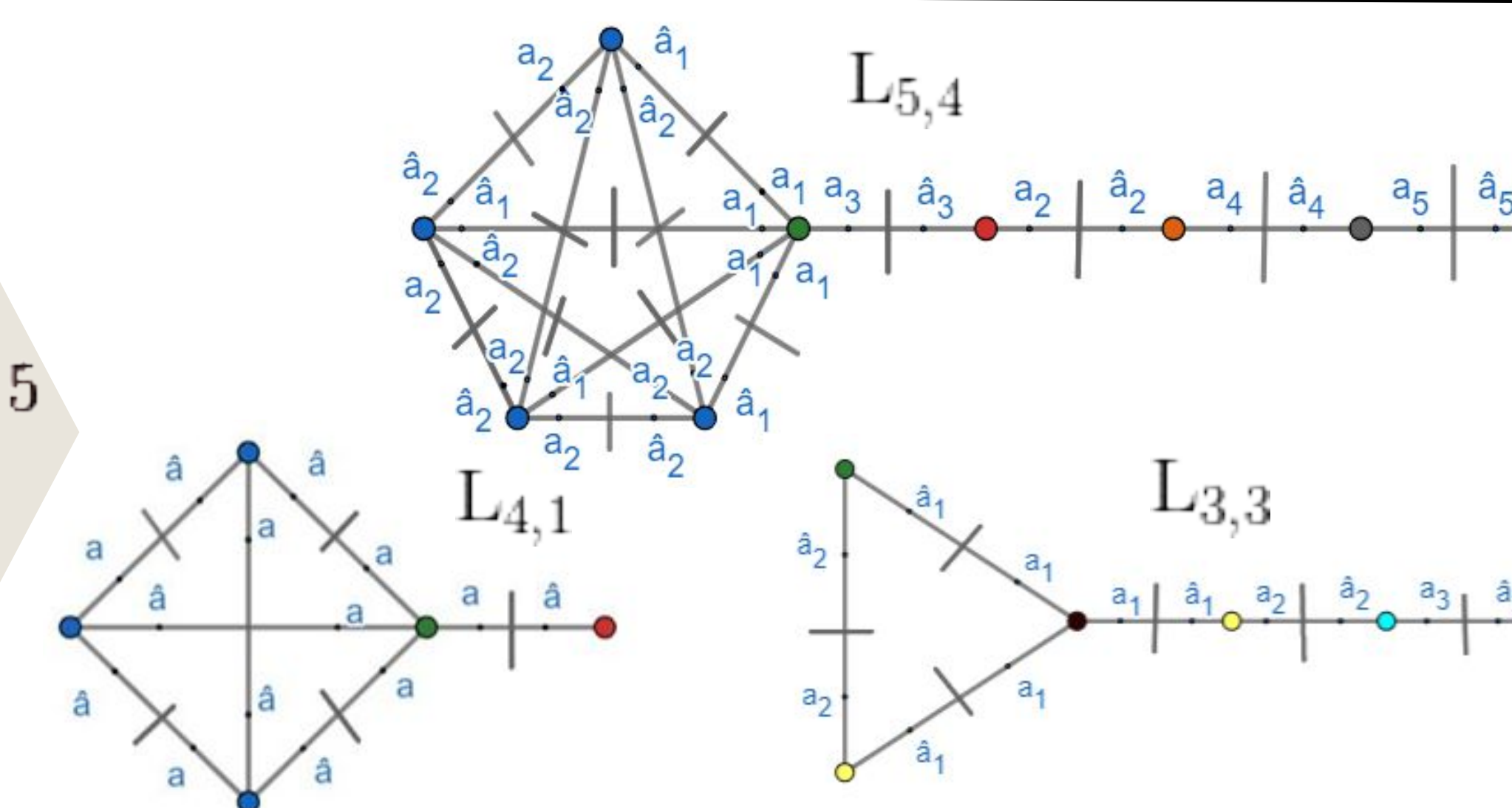
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$$T_1(L_{m,n}) = \begin{cases} 3 & \text{for } m = 3 \text{ or } n = 1 \\ 4 & \text{for } m > 3 \text{ and } n > 1 \end{cases}$$



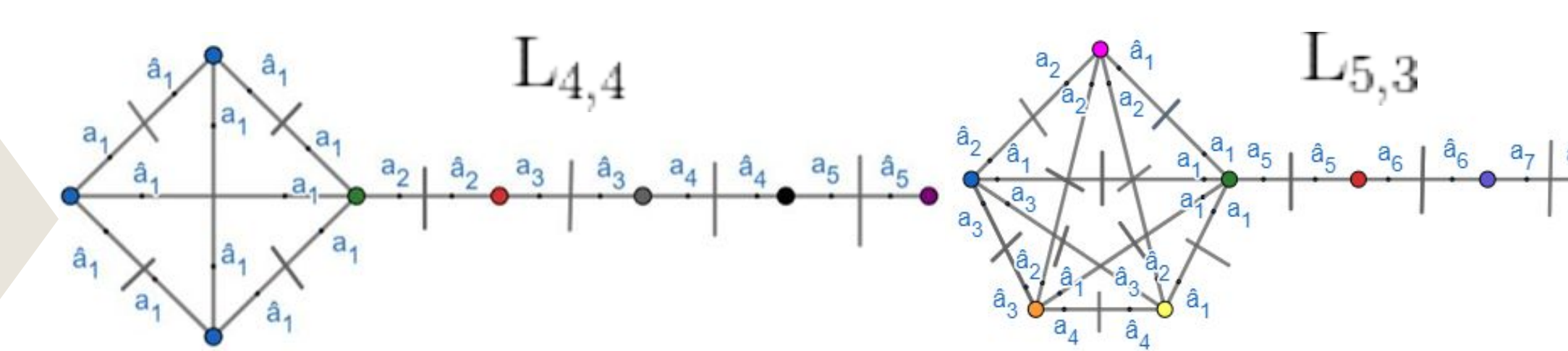
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$$\begin{aligned} T_2(L_{2k,1}) &= 3 \text{ and } B_2(L_{2k,1}) = 2 \\ T_2(L_{2k+1,1}) &= 4 \text{ and } B_2(L_{2k+1,1}) = 2 \\ T_2(L_{3,n}) &= n + 2 \text{ and } B_2(L_{3,n}) = n \text{ for } 2 \leq n \leq 5 \\ T_2(L_{2k+1,n}) &= n + 3 \text{ and } B_2(L_{2k+1,n}) = n + 1 \\ T_2(L_{2k,n}) &= n + 2 \text{ and } B_2(L_{2k,1}) = n + 1 \end{aligned}$$



03

$$T_3(L_{m,n}) = m + n \text{ and } B_3(L_{m,n}) = m + n - 1$$

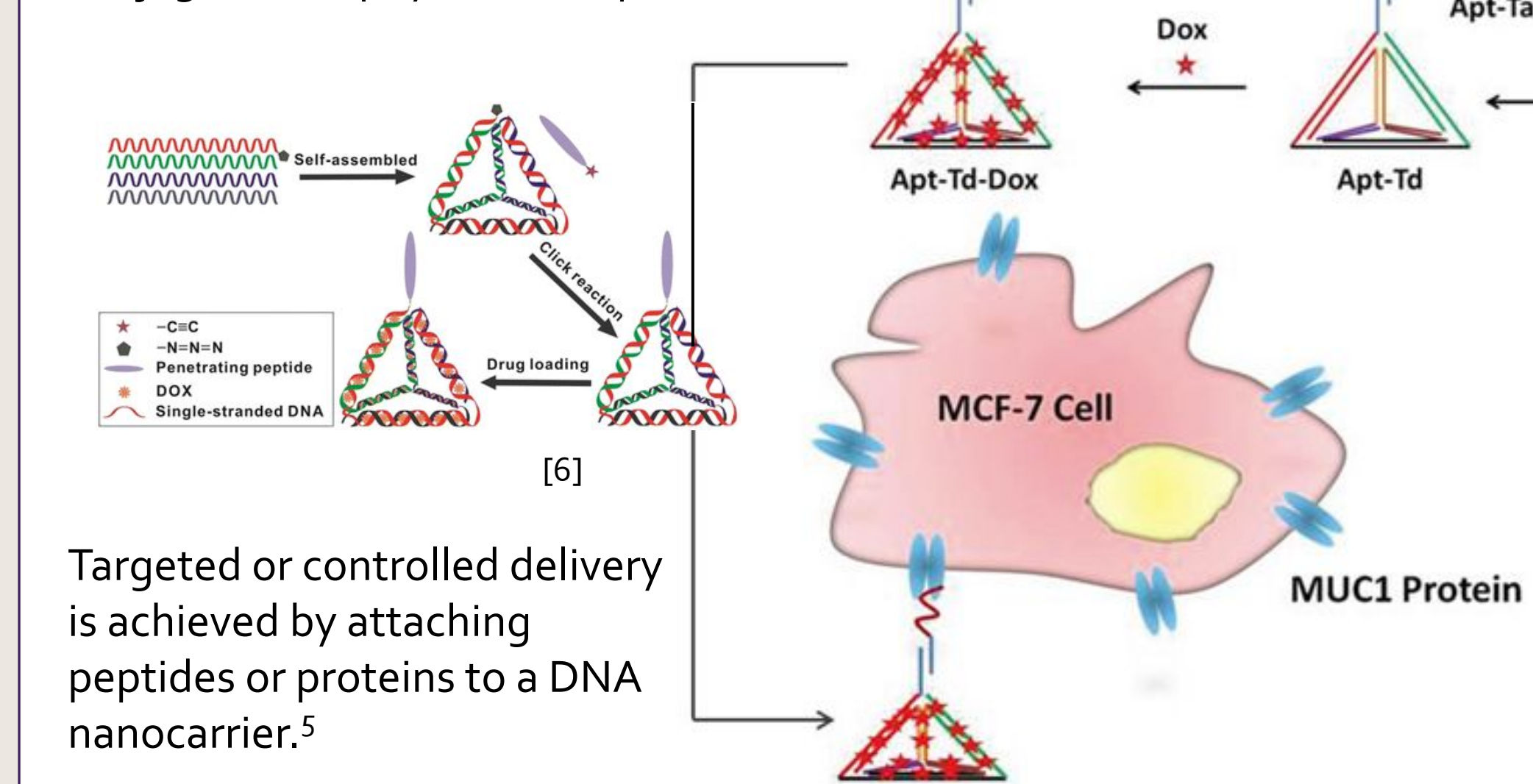


## Application

DNA Nanostructures are helpful in **drug delivery**. Nanostructures improve

- Solubility,
- Absorption, and
- Targeted release

Self-Assembled DNA Structures are loaded with a drug through chemical conjugation or physical encapsulation.



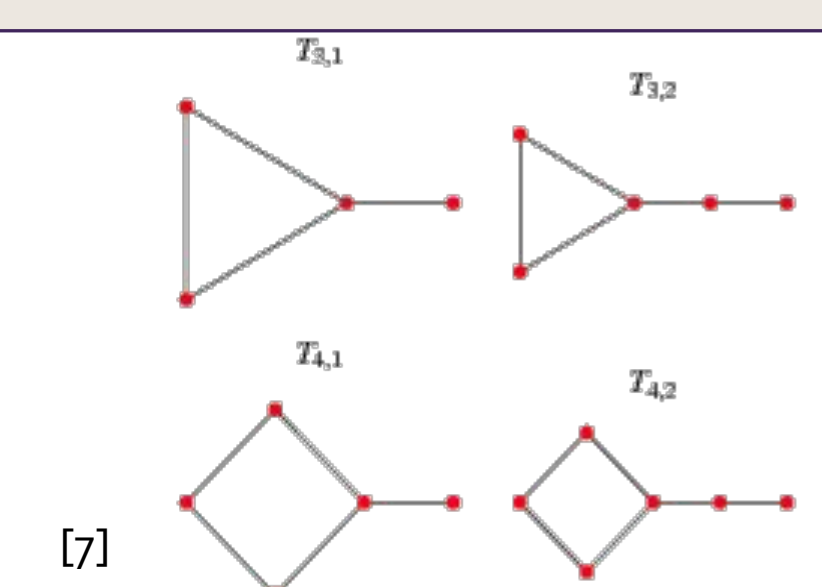
Targeted or controlled delivery is achieved by attaching peptides or proteins to a DNA nanocarrier.<sup>5</sup>

## Conclusions

- Constant solution independent of path length in Scenario 1
- There are several cases in Scenario 2 since the path can bond with the complete subgraph to form non-isomorphic structures.
- Scenario 3 results were less complex than expected, but required maximum numbers of tile and bond-edge types.

## Future Work

- Tadpole Graph Family (pictured right)
- Determine the relationship between a graph and its covering
- Find general rules for appending a path onto a graph.



## Acknowledgements

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### References

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