DNA Tangles

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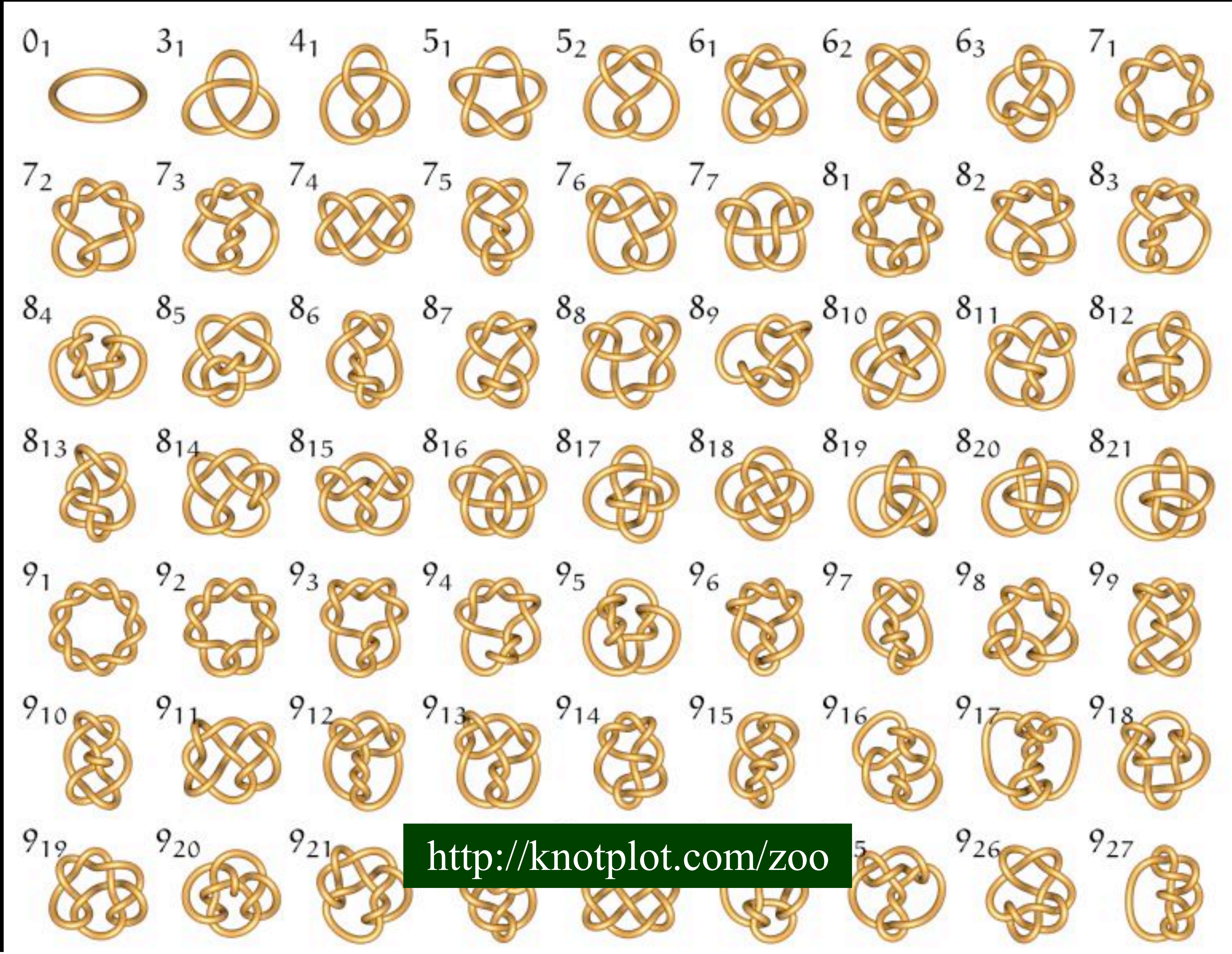
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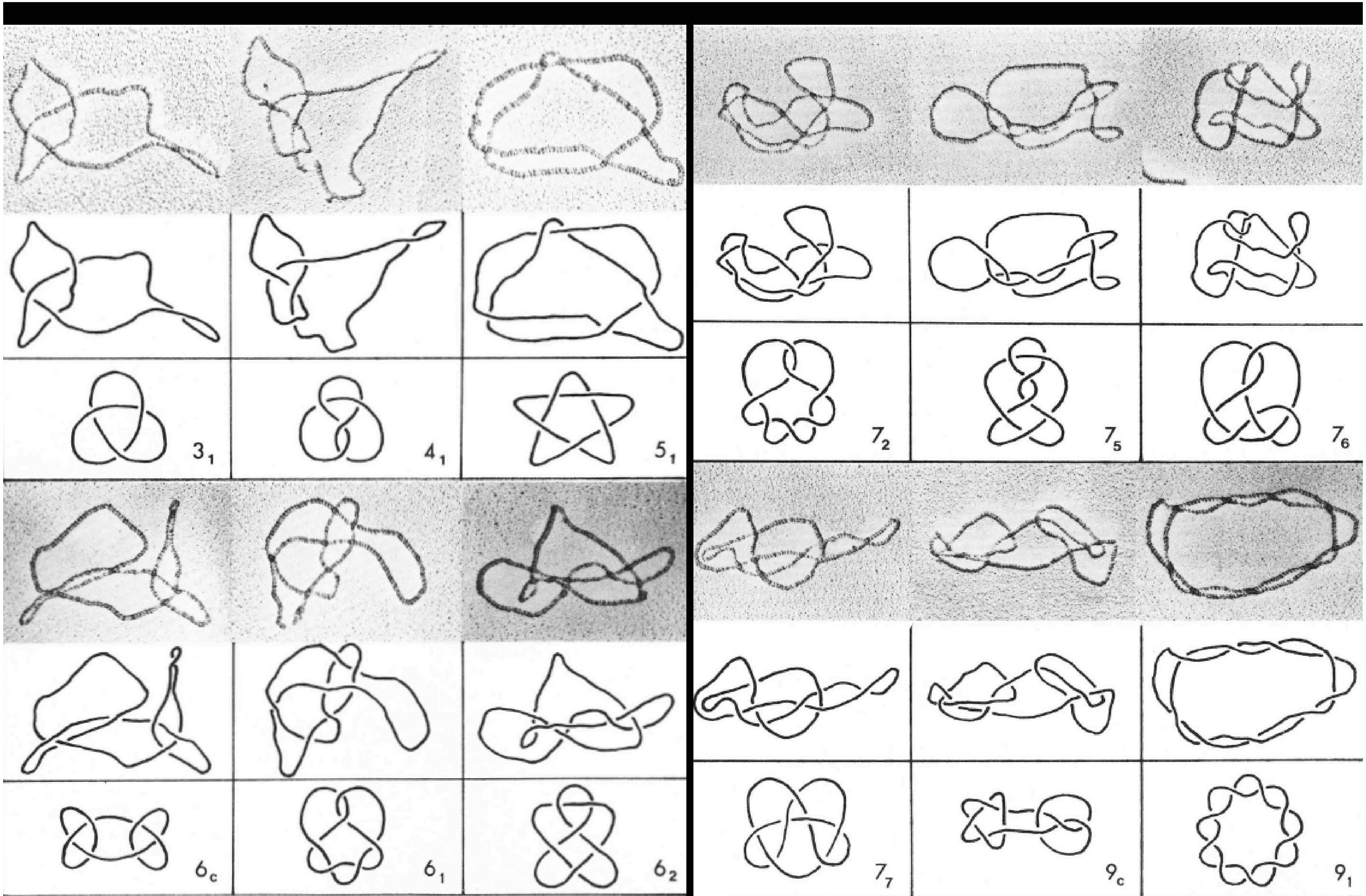
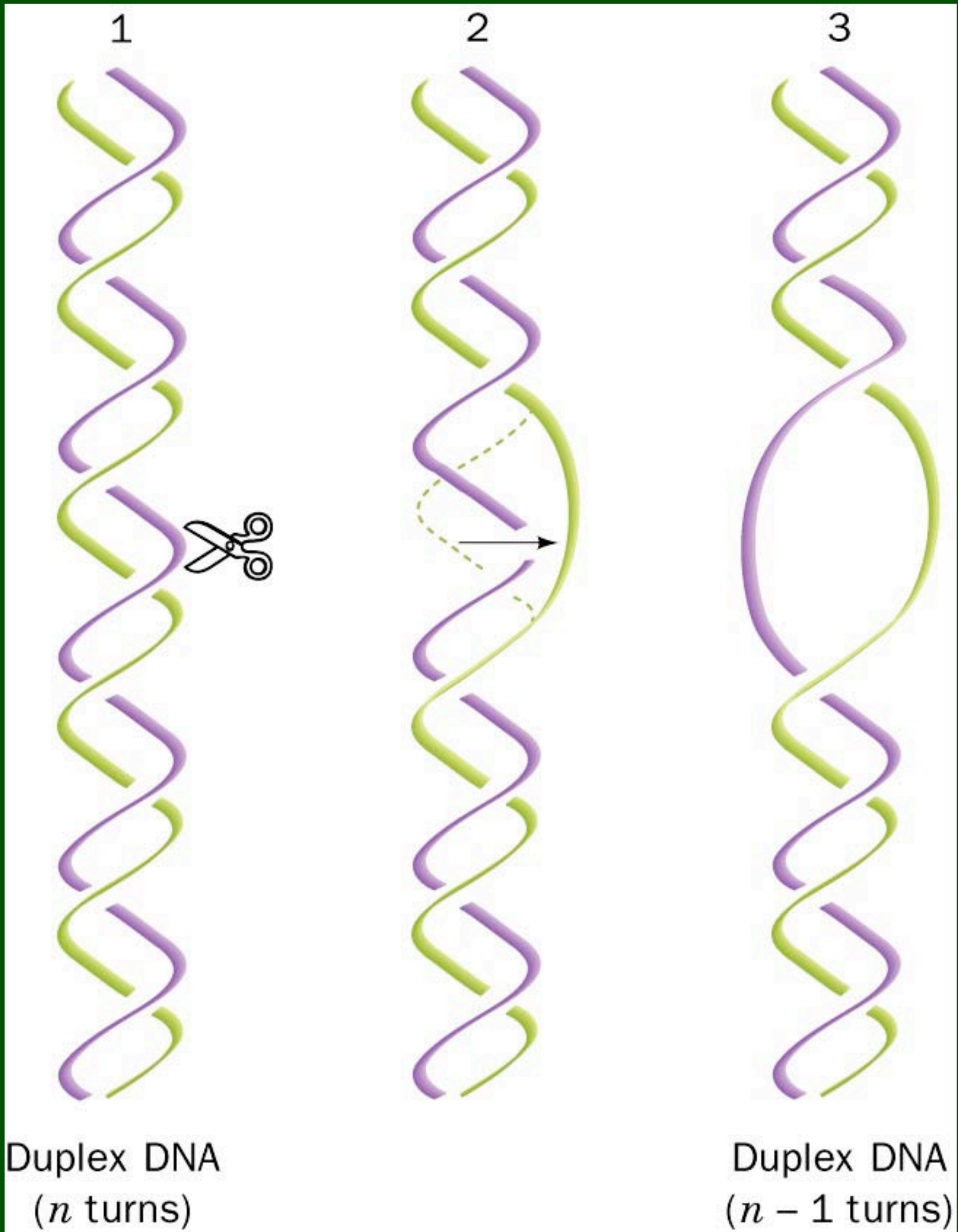
7_2 7_3 7_4 7_5 7_6 7_7 8_1 8_2 8_3
8_4 8_5 8_6 8_7 8_8 8_9 8_{10} 8_{11} 8_{12}
8_{13} 8_{14} 8_{15} 8_{16} 8_{17} 8_{18} 8_{19} 8_{20} 8_{21}
9_1 9_2 9_3 9_4 9_5 9_6 9_7 9_8 9_9
9_{10} 9_{11} 9_{12} 9_{13} 9_{14} 9_{15} 9_{16} 9_{17} 9_{18}
9_{19} 9_{20} 9_{21} 9_{26} 9_{27}
http://knotplot.com/zoo

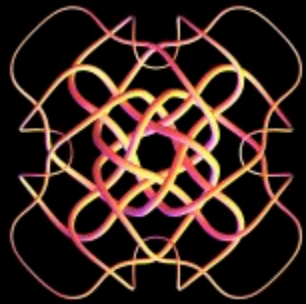


Duplex DNA knots produced by Escherichia coli topoisomerase I. Dean FB, Stasiak A, Koller T, Cozzarelli NR., J Biol Chem. 1985 Apr 25;260(8):4975-83.



From:

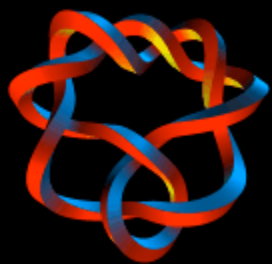
http://web.siumed.edu/~bbartholomew/images/chapter29/F29-25b.jpg

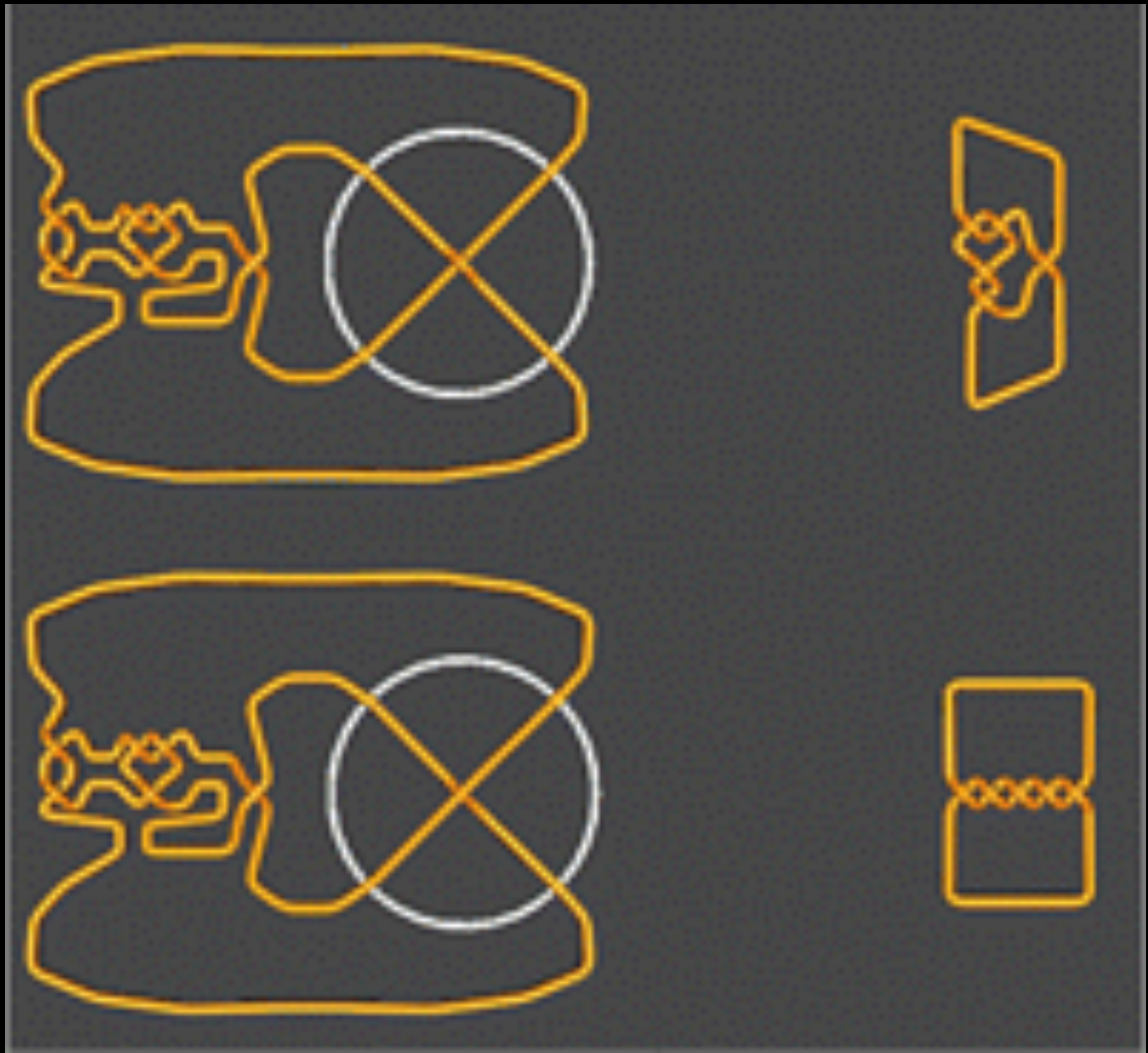



TopoICE in

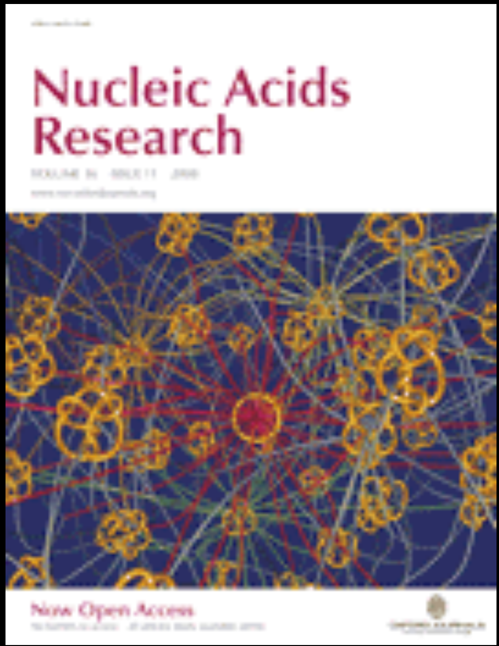
Rob Scharein’s

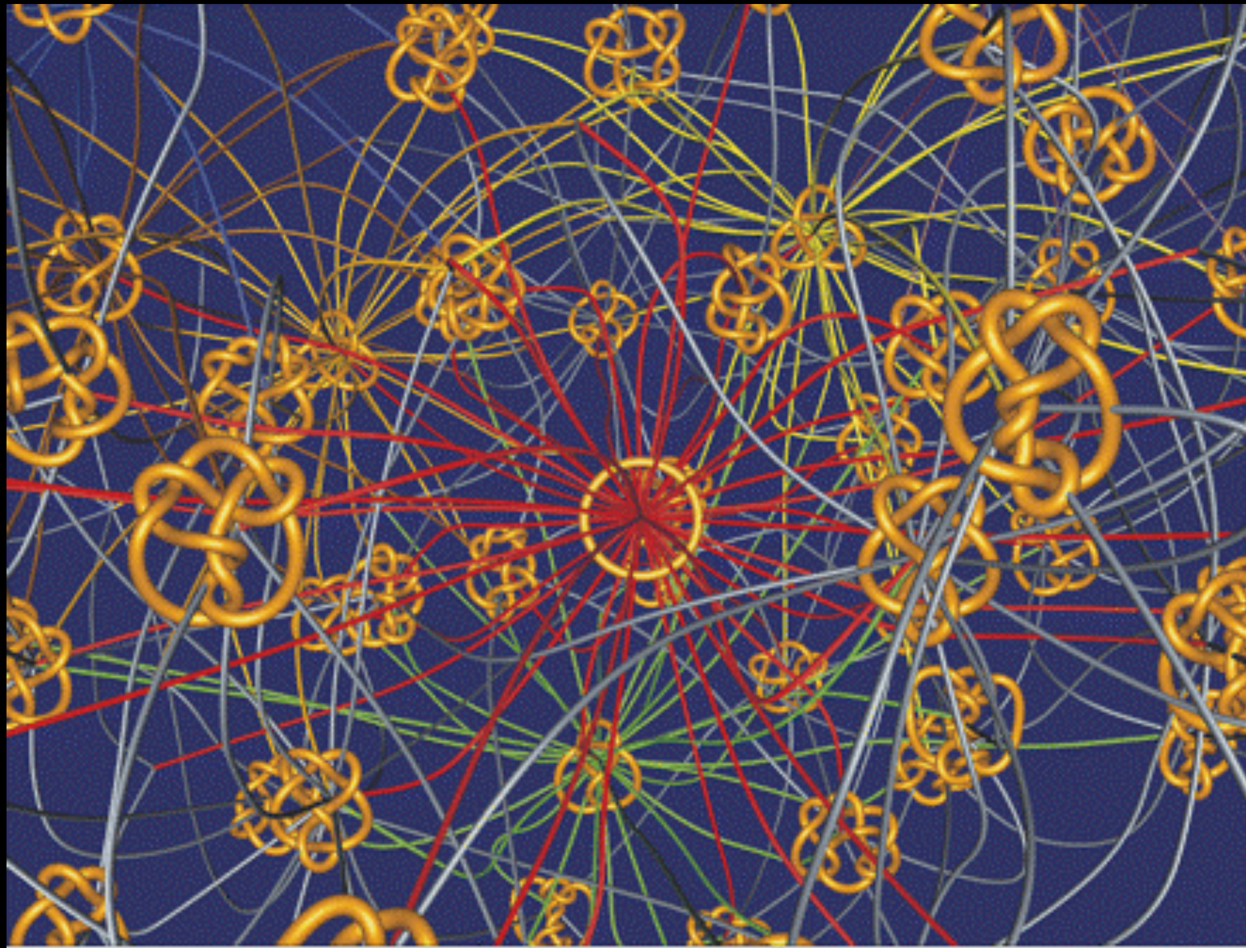
KnotPlot.com



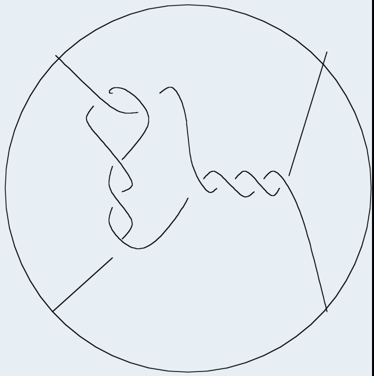
3D visualization software to analyze topological outcomes of topoisomerase reactions
I. K. Darcy, R. G. Scharein and A. Stasiak
Nucleic Acids Research 2008 36(11):3515-3521





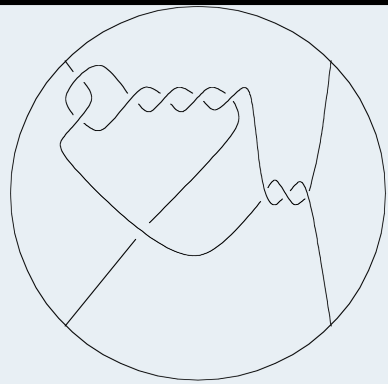
Visual presentation of knot distance metric created using the software TopoICE-X within KnotPlot. A pair of knots in this graph is connected by an edge if they can be converted into one another via a single intersegmental passage. This graph shows all mathematically possible topoisomerase reaction pathways involving small crossing knots. Darcy, Scharein, Stasiak (*Nucleic Acids Res*., 2008; **36**: 3515–3521).

Some tangles (but not all) can be classified using fractions.



(2, 3, 4)

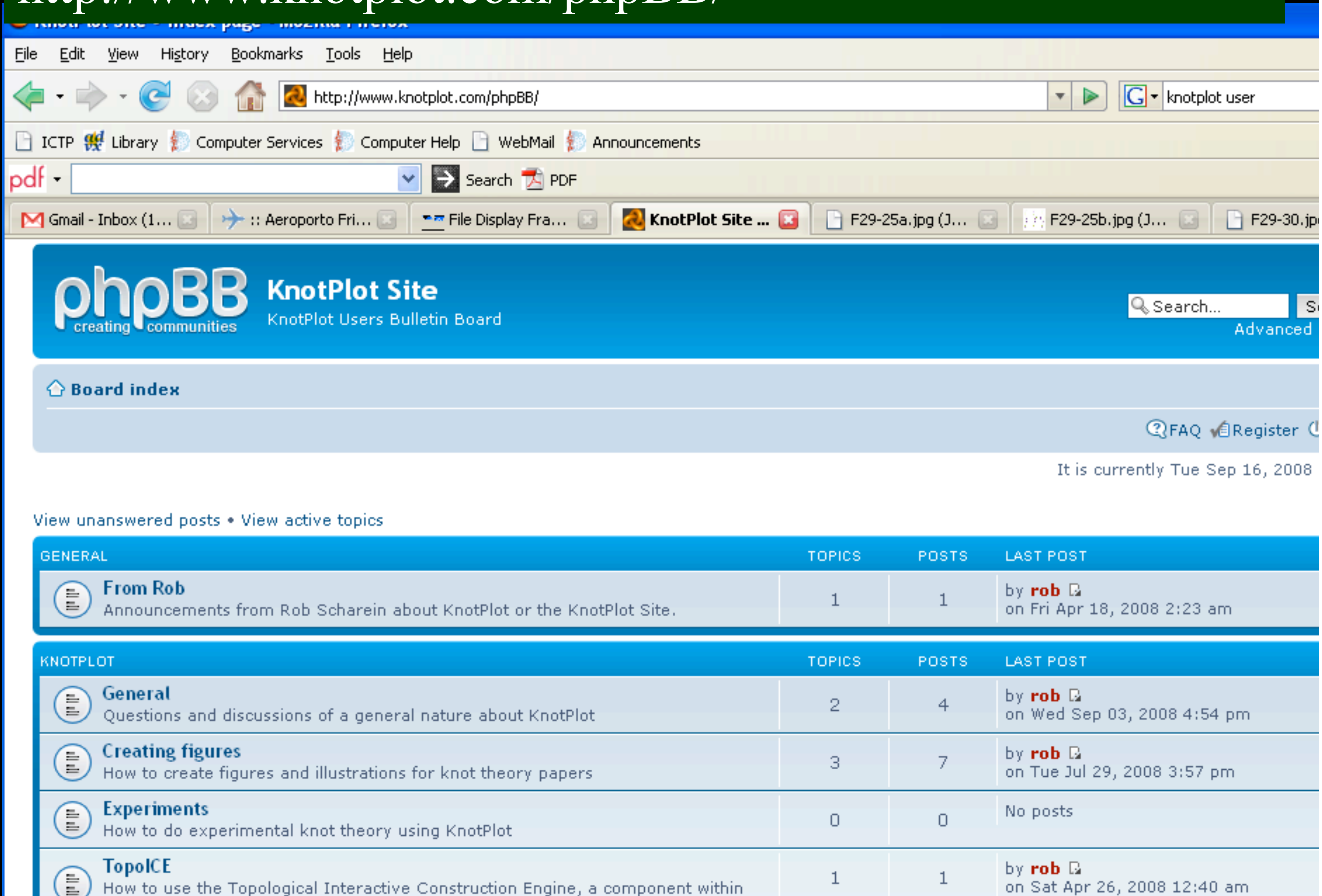
=



(-1, -1, -4, 1, 3)

$$4+\frac{1}{3+\frac{1}{2}}=\frac{30}{7}=3+\frac{1}{1+\frac{1}{-4+\frac{1}{-1+\frac{1}{-1}}}}$$

http://www.knotplot.com/phpBB/



Topoisomerase distance table (joint with H. Moon, M. Devries, A. Stasiak, A. Flammini)

- $d(K_1, K_2) = 1$ if K_2 can be obtained from K_1 by changing exactly one crossing.
- Upper bounds found by
  - –Mathematical formula for rational knots.
  - –Performing crossing changes on diagrams
    - •Small crossing (using table of small crossing tangles)
    - •Large crossing (Flammini and Stasiak simulation)
- Knot invariants used to find lower bounds

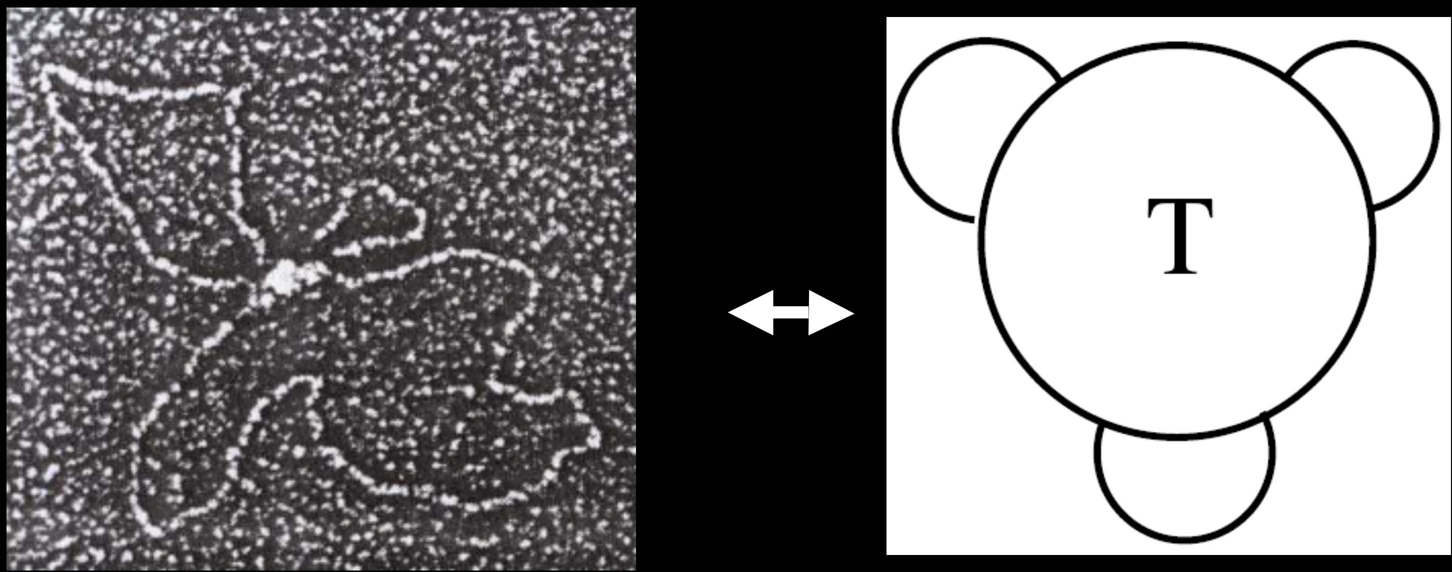
http://math.uiowa.edu/~hmoon/table.html

	0_1	3_1	4_1	5_1	5_2	6_1	6_2	6_3	3_1 \#3_1	3_1 \#3^*_1	7_1	7_2	7_3	7_4	7_5	7_6	7_7	3_1 \#4_1	8_1	8
0_1	0	1	1	2	1	1	1	1	2	2	3	1	2	2	2	1	1	2	1	2
3_1	1	0	2	1	1	2	1	1	1	1	2	2	3	2-3	1	1	2	1	2	1
3^*_1	1	2	2	3	2	2	2	1	3	1	4	2	2	1	3	2	1	2-3	2	3
4_1	1	2	0	2-3	2	1	1	2	2-3	2-3	3-4	2	2-3	2-3	2-3	1	1	1	2	2
5_1	2	1	2-3	0	1	2-3	2	2	2	2	1	2	4	3-4	1	2	2-3	1-2	2-3	1
5^*_1	2	3	2-3	4	3	2-3	3	2	4	2	5	3	1	2	4	3	2	3-4	2-3	4
5_2	1	1	2	1	0	2	2	2	2	2	2	1	3	2-3	1	1	2	1-2	2	2
5^*_2	1	2	2	3	2	2	2	2	3	2	4	2	1	1	3	2	2	2-3	2	3
6_1	1	2	1	2-3	2	0	1	2	2-3	1-3	3-4	2	2-3	2-3	2-3	2	2	2	1	2
6^*_1	1	2	1	2-3	2	1	2	2	2-3	1-3	3-4	2	2-3	2-3	2-3	2	2	2	2	2-

1	8_1	8_2	8_3	8_4	8_5		8_6	8_7	8_8	8_9	8_{10}	8_{11}	8_{12}	8_{13}	8_{14}	8_{15}	8_{16}	8_{17}	8_{18}	8_1
3	2	2	2-3	1-2	4	8_5^*	1	3	2-3	2	3-4	2	2-3	2-3	1-2	1-2	1-3	2-3	2-3	5
2	1	1	2	1	3-4	8_6	0	2-3	2	2	2-3	2	2	2-3	2	1-3	1-2	1-2	1-2	4-
3	2-3	3-4	2	2	1	8_6^*	2-3	2	2	2	1-3	2-3	2	2-3	2-3	3-4	2-3	1-2	1-2	2-
3	2	3	2-3	2-3	1-3	8_7	2-3	0	1	2	1-2	2	2-3	2	2	3	2	1-2	1-2	2
2	2	2	2-3	2-3	3	8_7^*	2	2	2	2	2	2	2-3	1	2	1-2	1-2	1-2	1-2	4
	2-3	2	2-3	2-3	2-3	8_8	2	1	0	2-3	1	2-3	2-3	2	2	2-3	2	1-2	2	3
	2-3	2	2-3	2-3	2-3	8^*_8	2	2	1	2-3	1-2	2	2-3	2	2	2	2	1-2	2	3
3	2	2	2	1	2	8_9	2	2	2-3	0	2-3	2	2-3	2	2	2-3	2-3	2	2-3	3-
3	1-3	3	2-4	2-4	1-3	8_{10}	2-3	1-2	1	2-3	0	2-3	2-4	2	2-3	3-4	2	1-3	1-3	2
3	1-3	1-2	2-4	1-4	3-4	8_{10}^*	1-3	2	1-2	2-3	2	1-2	2-4	2	1-2	1-2	1-2	1-3	1-3	4
3	1	1	2	2	3	8_{11}	2	2	2-3	2	2-3	0	2	2	2	2	1-2	1-2	1-3	4
3	2	3	2	2	2	8^*_{11}	2-3	2	2	2	1-2	2	2	2	2	3	2-3	1-2	1-3	2-

C. Ernst, D. W. Sumners, A calculus for rational tangles: applications to DNA recombination, *Math. Proc. Camb. Phil. Soc.* 108 (1990), 489-515.

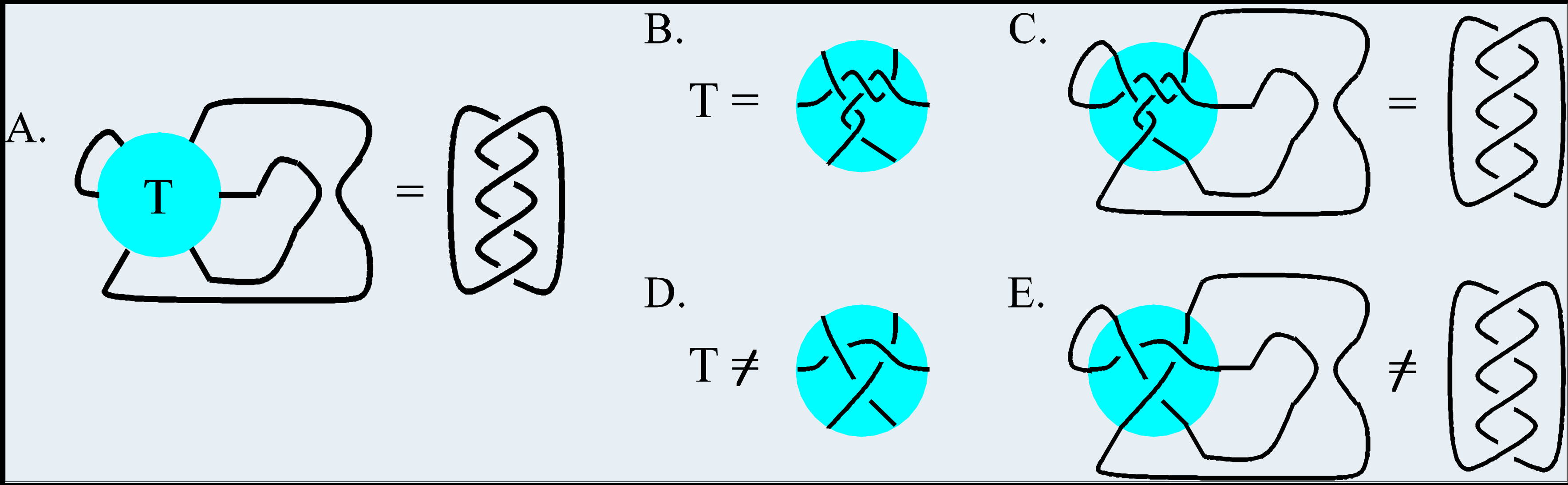
protein = three dimensional ball
protein-bound DNA = strings.

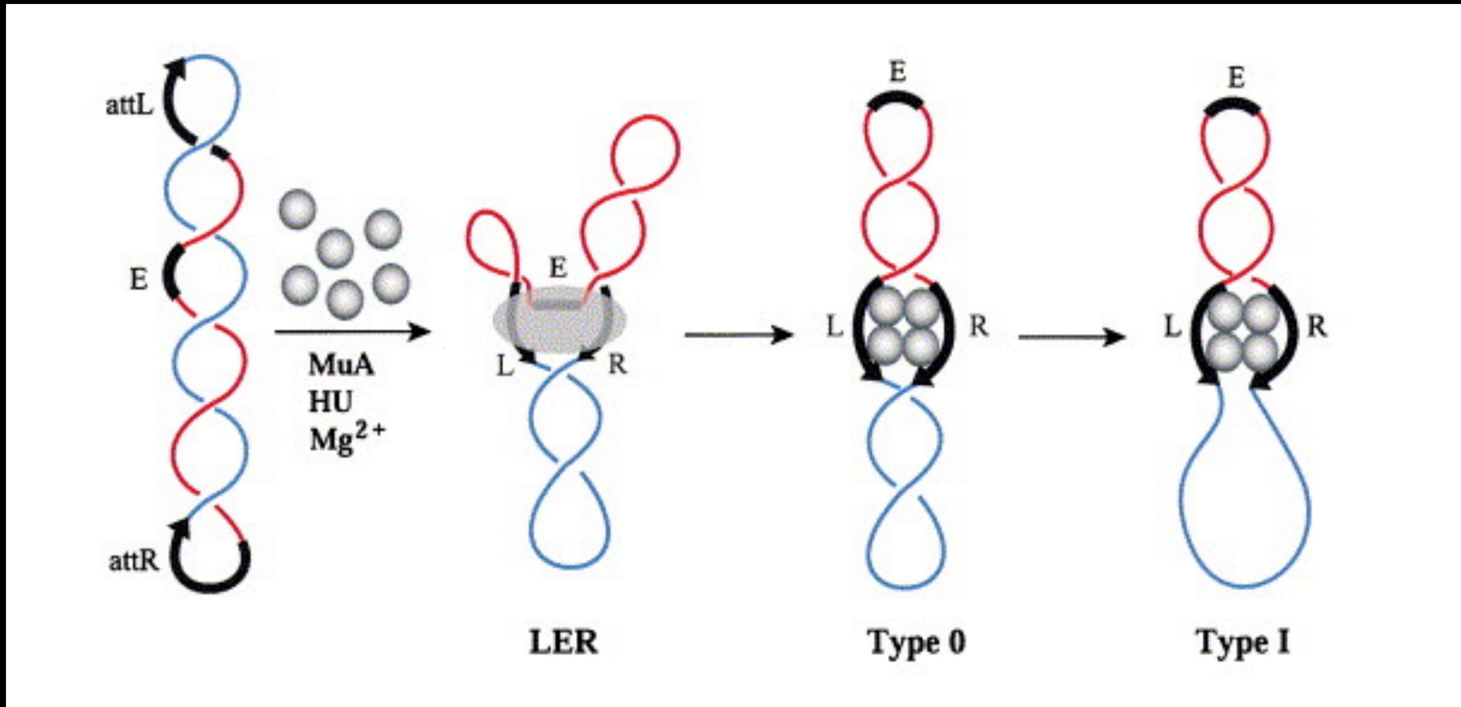


Protein-DNA complex
Heichman and Johnson

Courtesy S. Kim

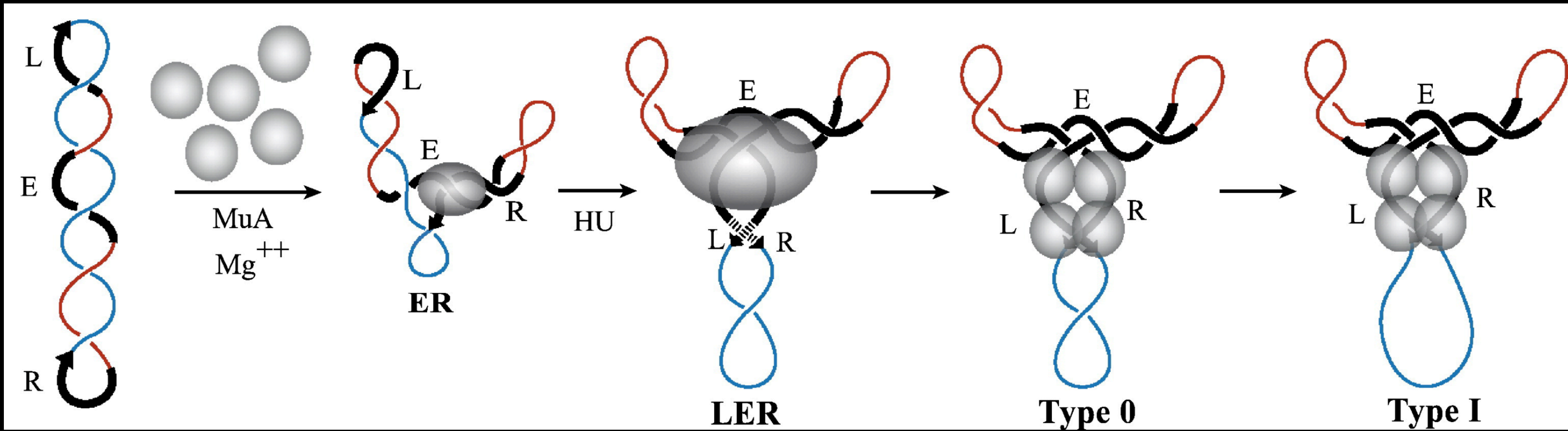
Solving tangle equations





Path of DNA within the Mu Transpososome Transposase Interactions Bridging Two Mu Ends and the Enhancer Trap Five DNA Supercoils, 2002, Cell, 109: 425-436.

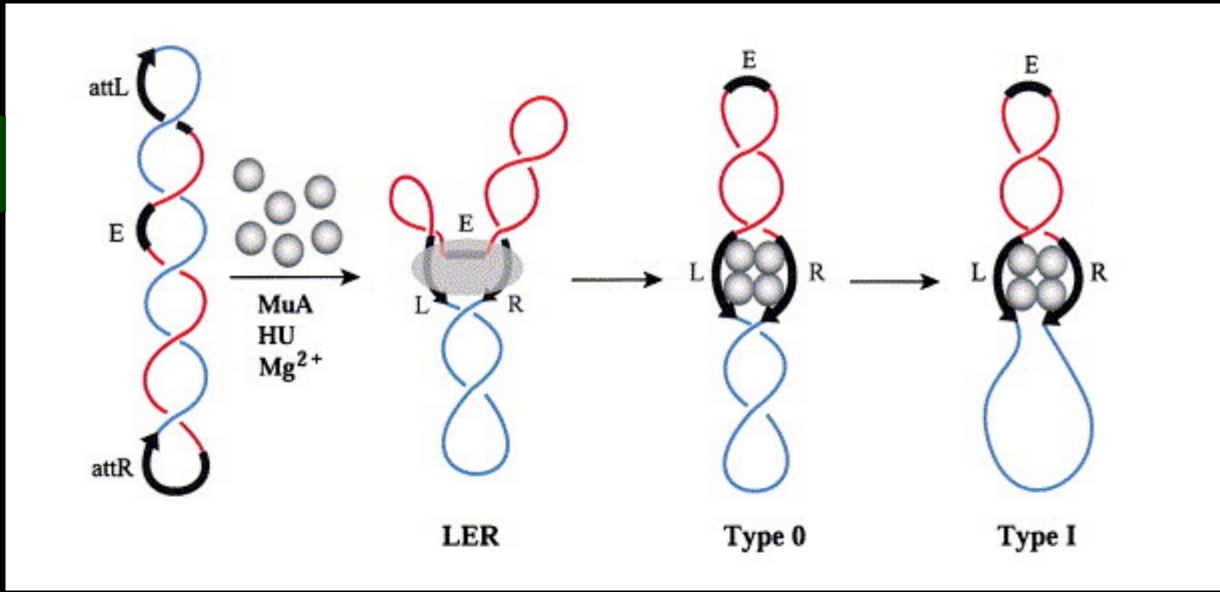
Shailja Pathania, Makkuni Jayaram and Rasika M Harshey



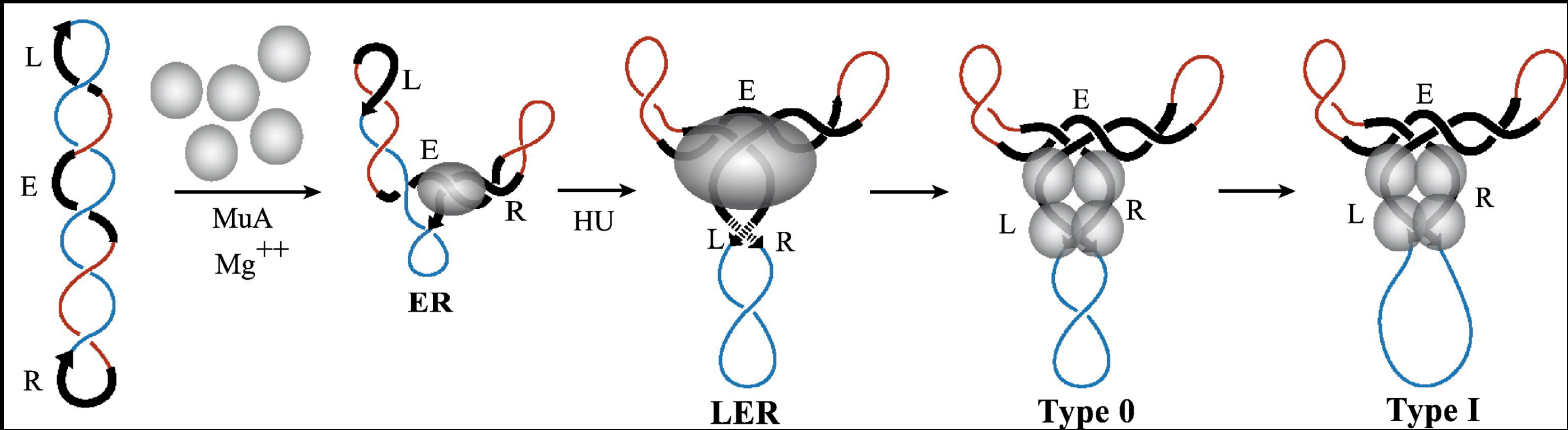
Interactions of Phage Mu Enhancer and Termini that Specify the Assembly of a Topologically Unique Interwrapped Transpososome

Zhiqi Yin, Asaka Suzuki, Zheng Lou,
Makkuni Jayaram and Rasika M. Harshey

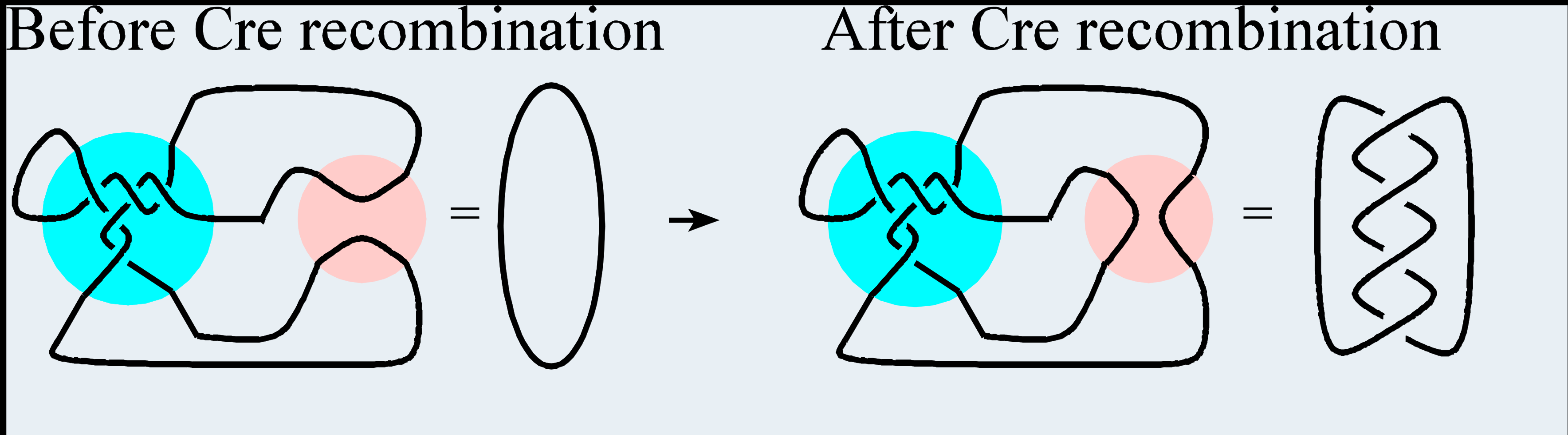
Older Model:

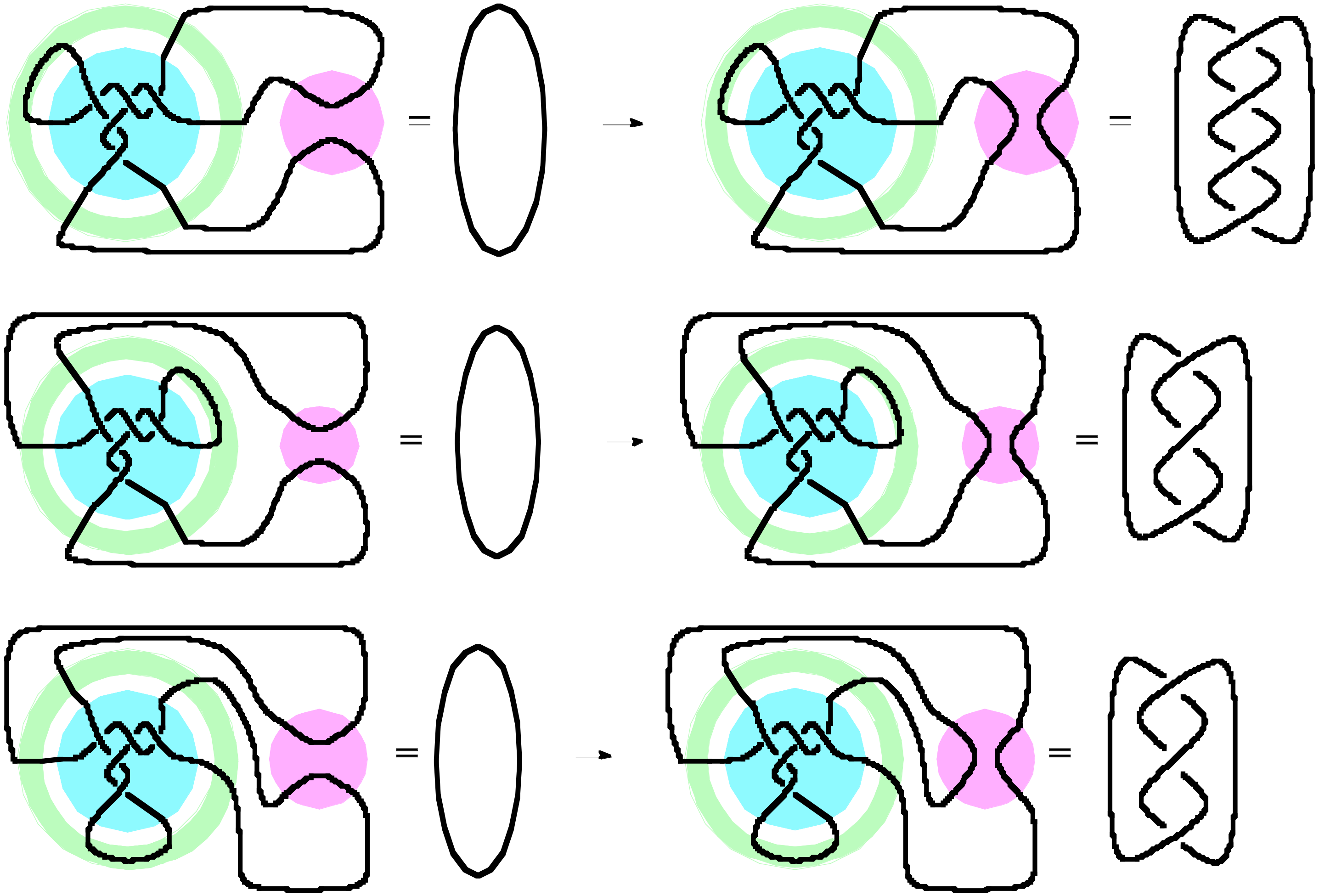


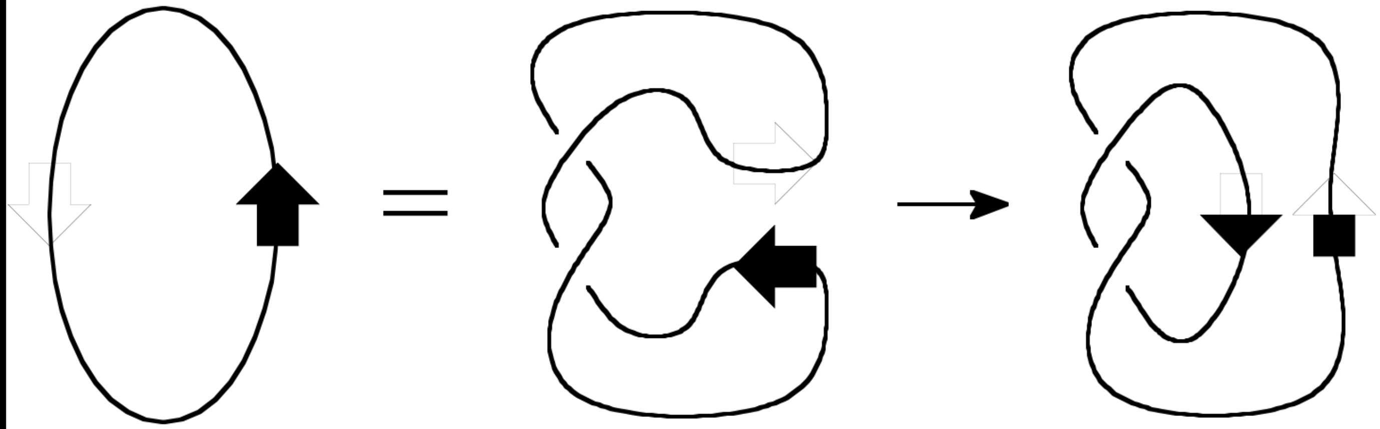
Newer Model:



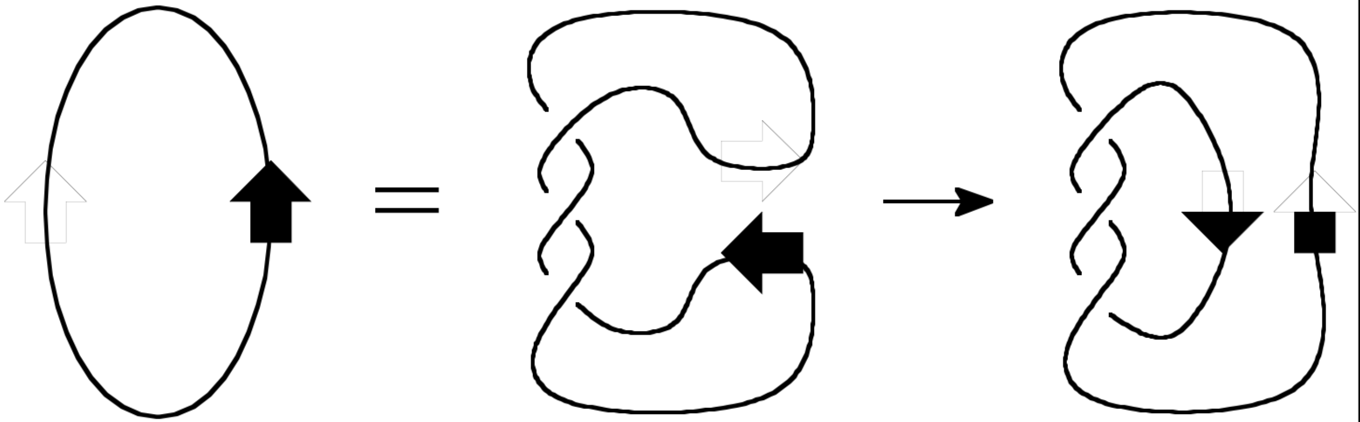
A difference topology experiment:



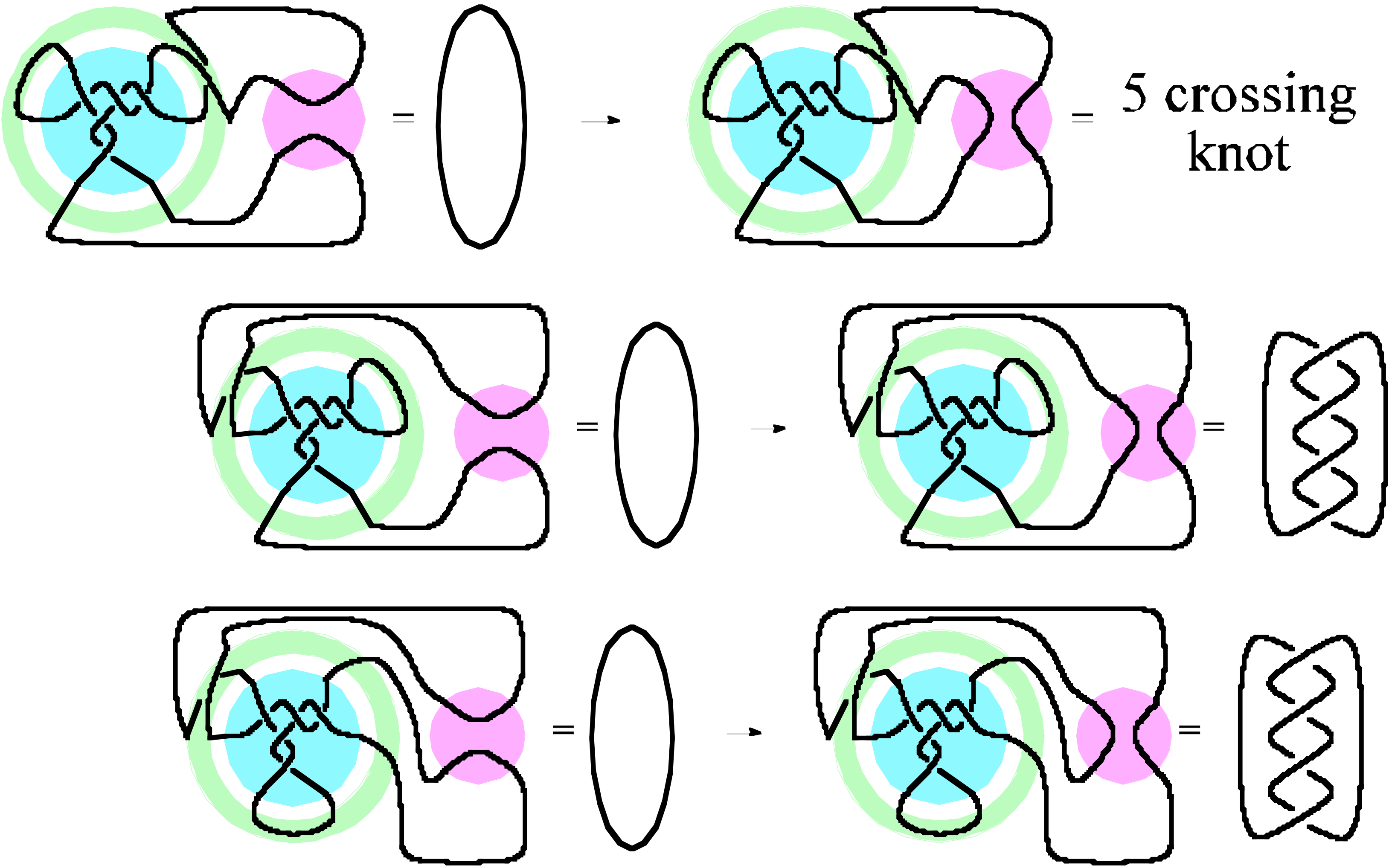


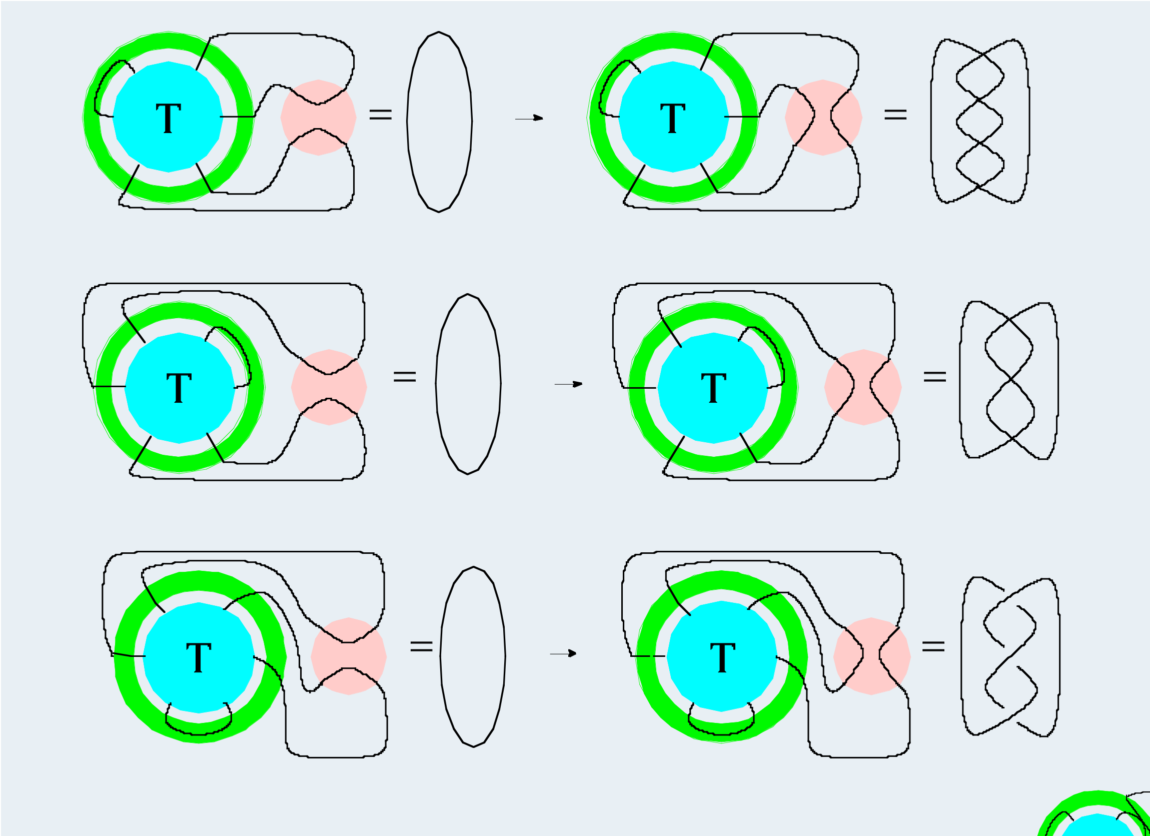


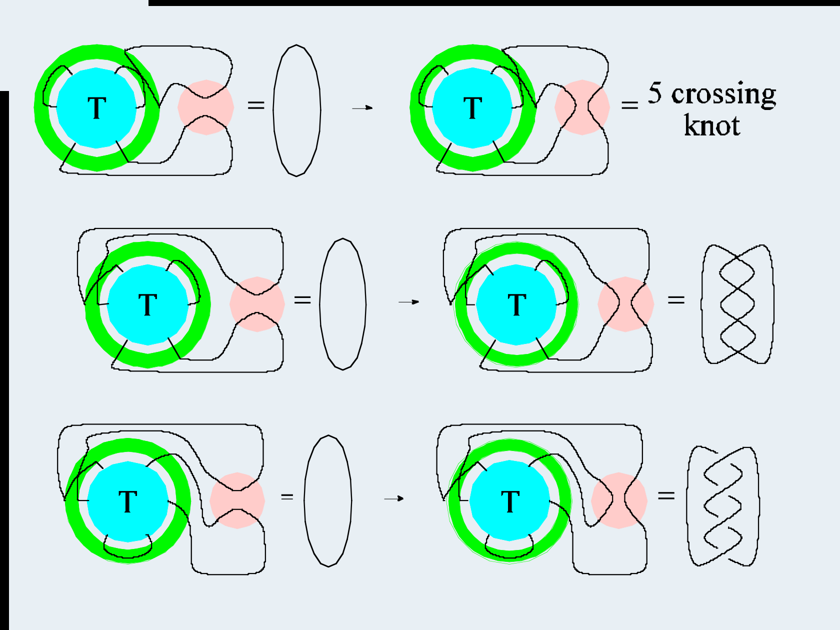
Direct Repeats

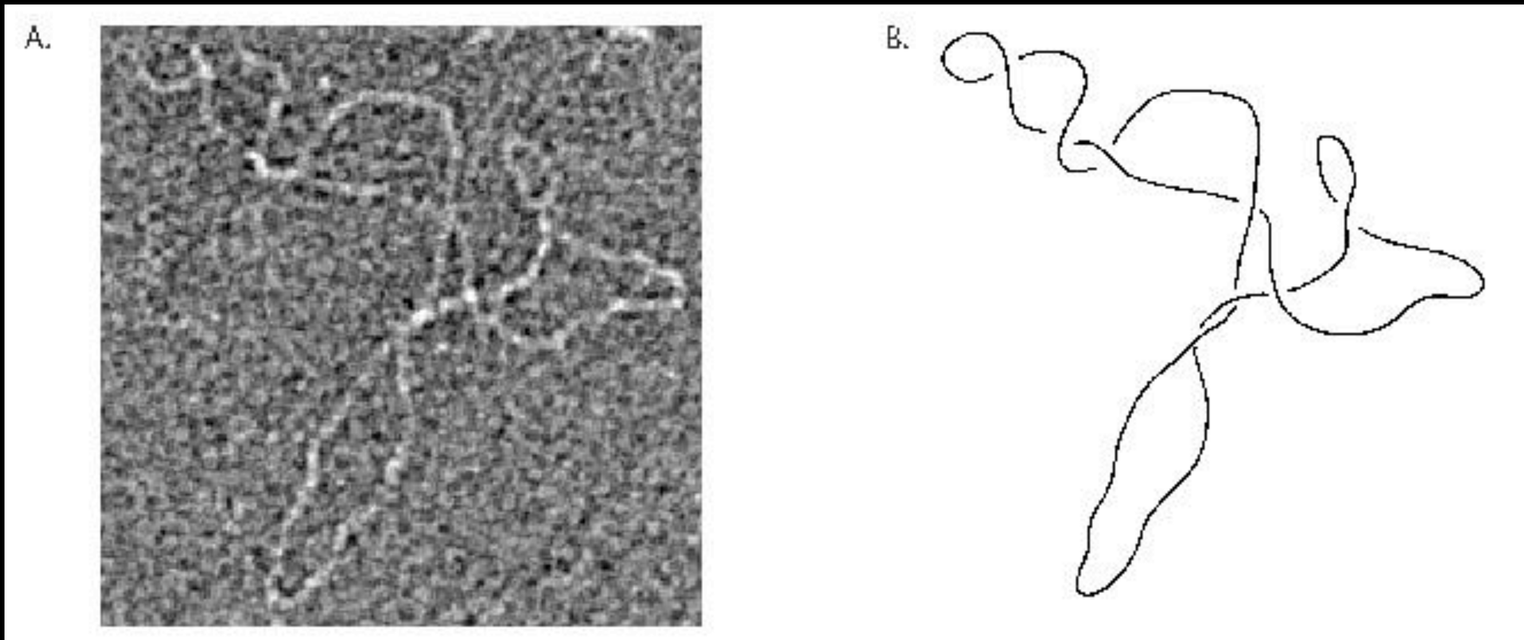


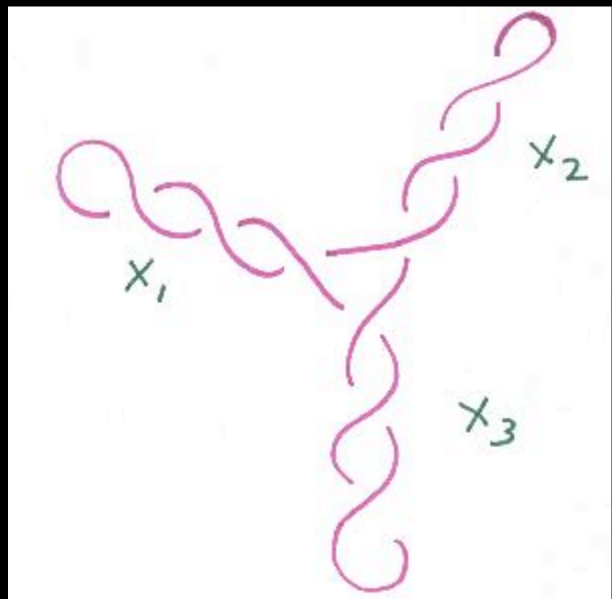
Inverted Repeats

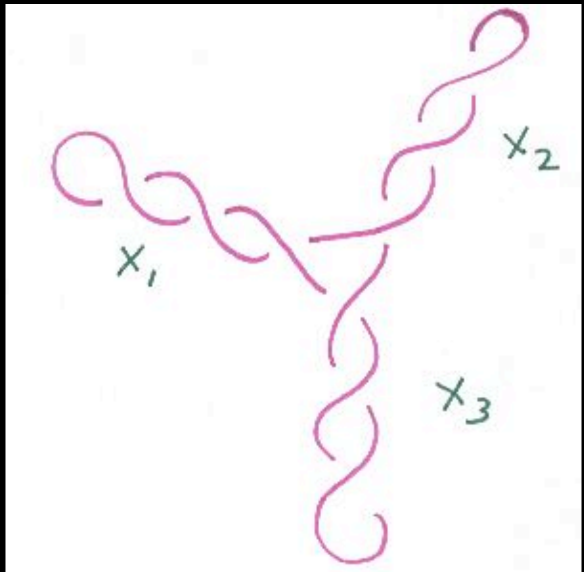

5 crossing knot


T

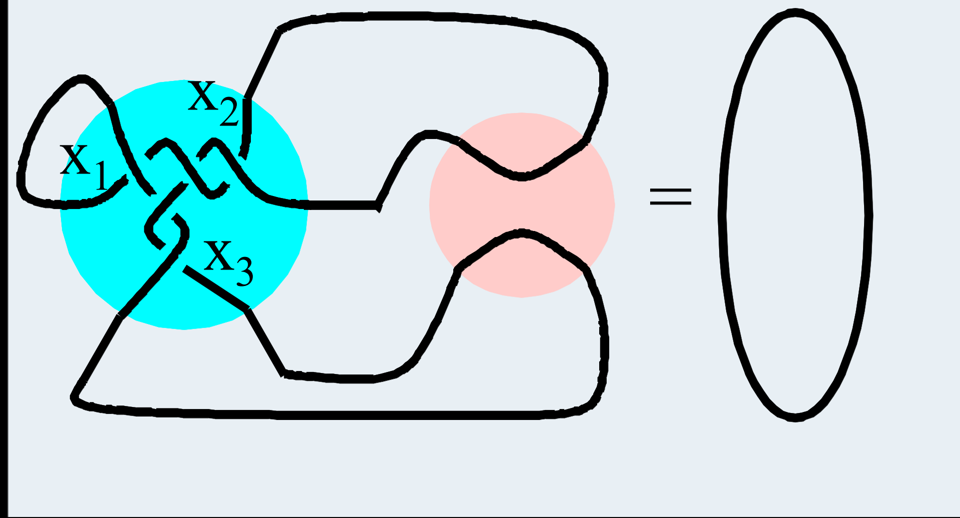

T
5 crossing
knot


A.
B.

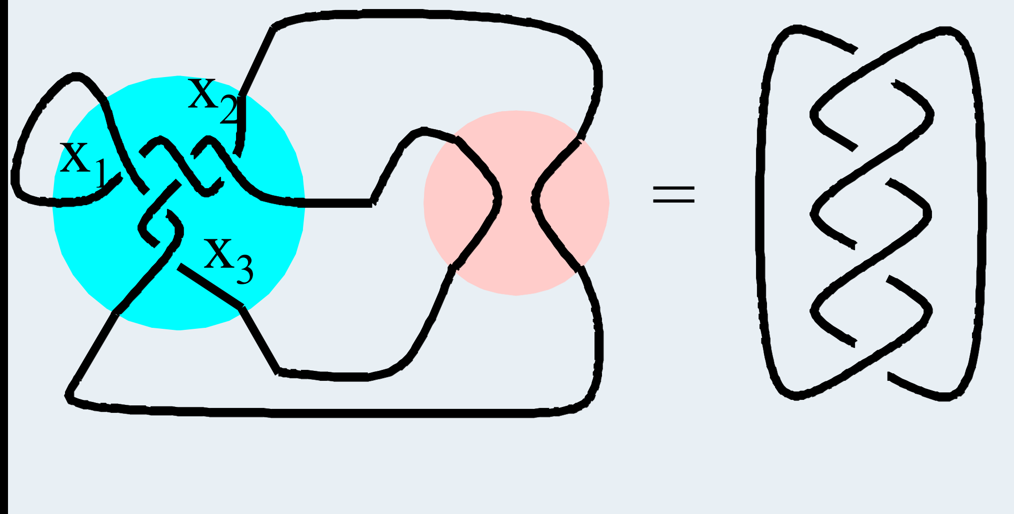

X1
X2
X3



Before Cre recombination



After Cre recombination



$$x_2 + x_3 = 4$$

$x_2 + x_3 = 4$

$x_1 + x_3 = 3$

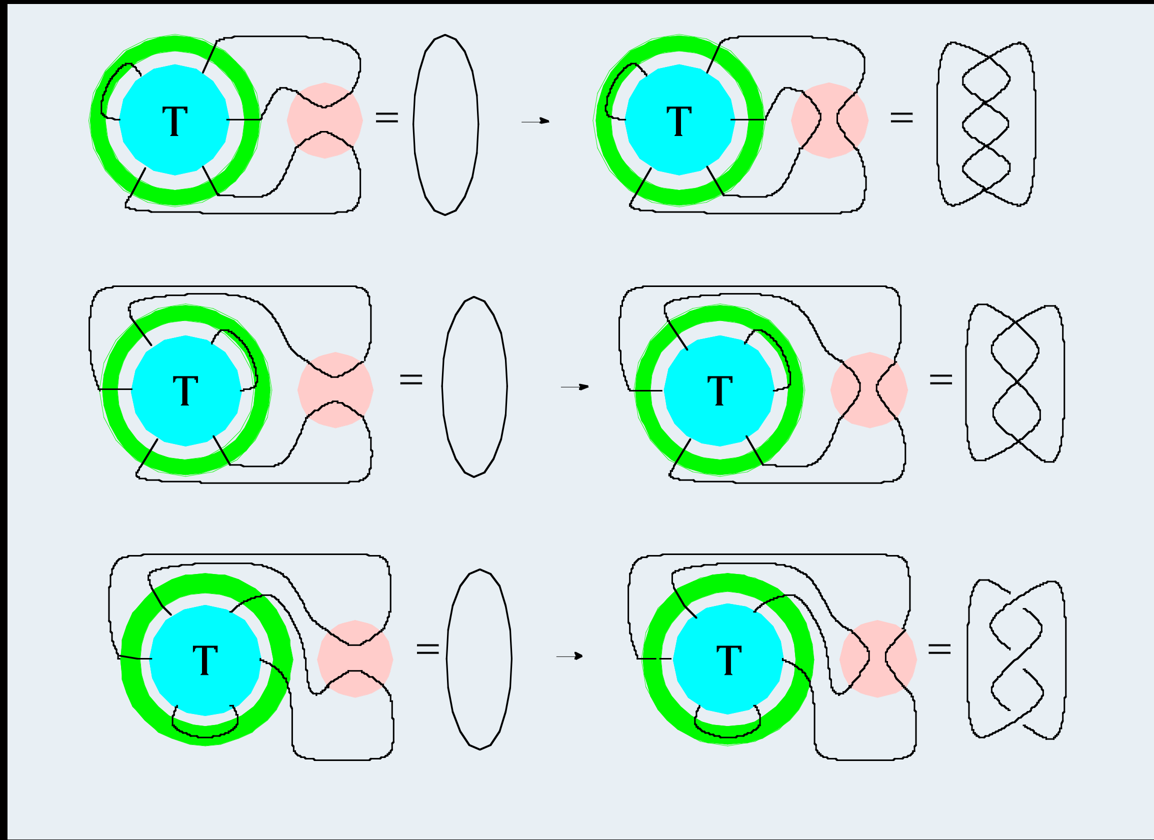
$x_1 + x_2 = 3$

implies

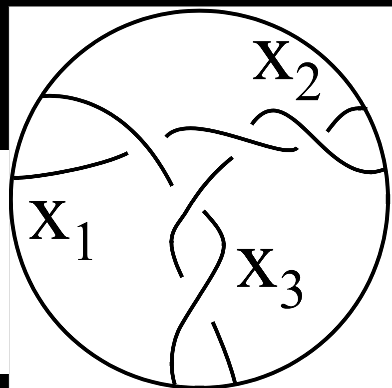
$x_1 = 1,$

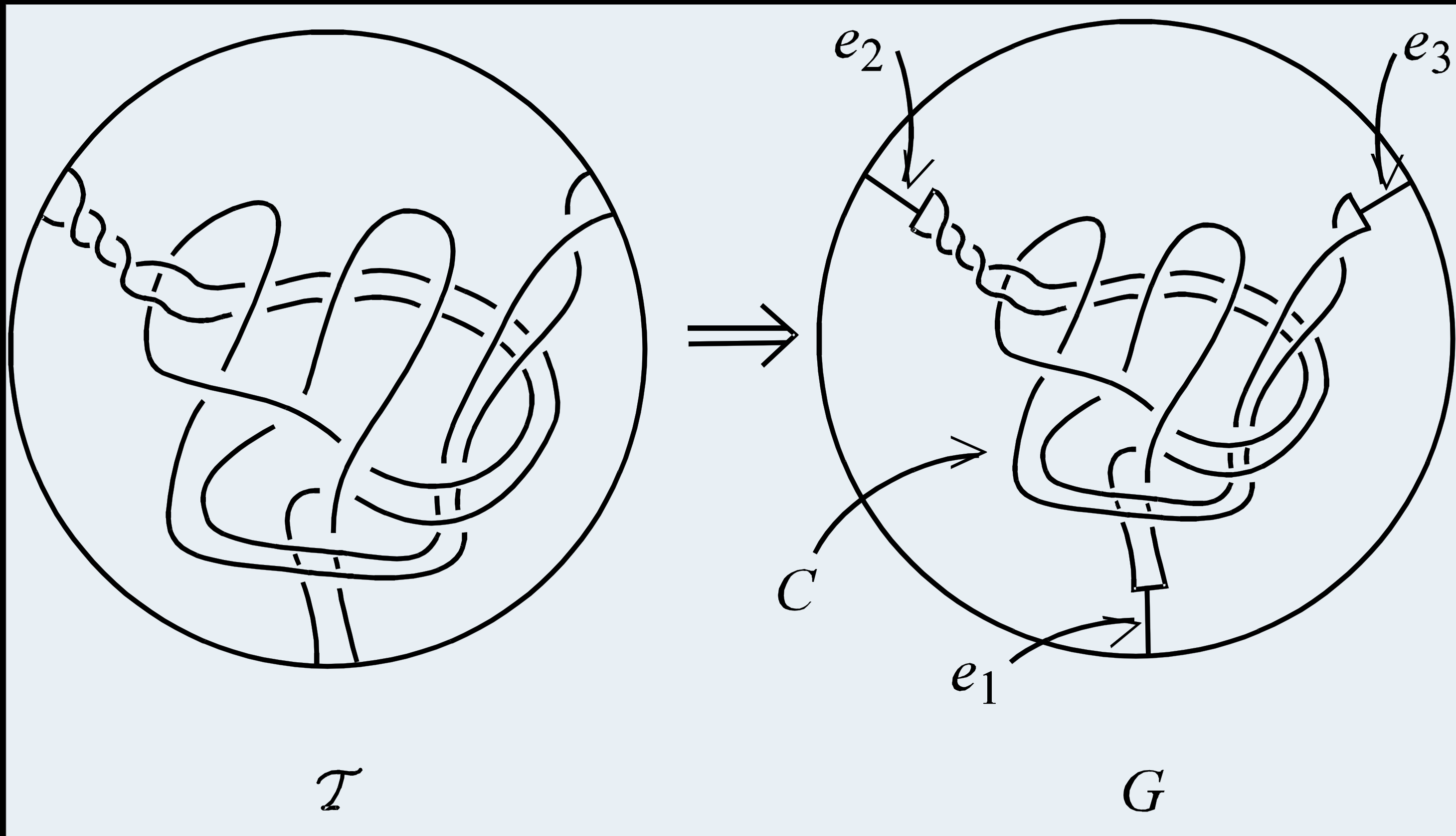
$x_2 = 2,$

$x_3 = 2$



Thus T =





e_2
e_3
C
e_1
$\mathcal{T}$
G

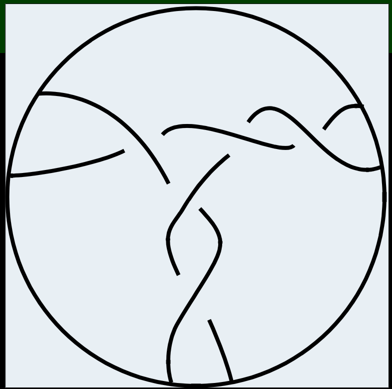
Theorem [D, Luecke, J., Vazquez, M., Tangle analysis of difference topology experiments: applications to a Mu protein-DNA complex]: If **T** is a solution to the Mu-Cre equations, and if either

1.) **T** is rational or split or has parallel strands or

2.) If **T** has fewer than 9 crossings,

Then

T =



(assuming a particular handedness of the products)

Darcy, I. K., Bhutra, A., Chang, J., Druivenga, N., McKinney, C., Medikonduri, R. K., Mills, S., Navarra Madsen, J., Ponnusamy, A., Sweet, J., Thompson, T., Coloring the Mu Transpososome, BMC Bioinformatics. 2006 Oct 5;7:435.

Theorem [Kim, D]: Suppose

1.) T is a 4-string tangle which models a protein-DNA complex where 4 DNA segments are bound by the protein complex.

2.) T satisfies difference topology equations where the products are $(2, p_i)$ torus links.

3.) T is a biologically reasonable solution (can be isotoped to a tangle with less than 8 crossings).

Then T is R-standard.

I.e, we can determine T.