

# **Pseudoknotted duplexed folds of single-stranded RNA**

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The simplest RNA folds are those induced by Watson-Crick base pair complementarity, inducing double-helices (duplexes), in particular folds formed by a single strand (ss) of RNA. We classify those folds by what we call a "polarised strand graph", whose vertices correspond to duplexes and edges unduplexed regions of the strand. Each vertex is "polarised" along an axis corresponding to the helical twist axis. The construction is in one-to-one correspondence with an algebraic fold label, which is easily deduced from the graph, and vice versa. We can think of the graph as a planar shadow of a knot on the page, with a skeleton related to that formed in the usual checkerboard colouring of the shadow diagram. Those tools give a natural quasi-ranking of folds via the skeletal topology (cyclomatic number) allowing lower topology folds to be enumerated exhaustively [1]. We like to think of these ssRNA folds as (polarised) examples of generic tangles, which can invariably be reduced to duplexed structures winding the edges of skeletons. If the duplexes are identical on each edge, the tangle can be realised with "maximal" symmetry, almost equal to that of the embedding of the skeleton in space. That led us to infinite families of what we call "polyhedral tangles", which are maximally symmetric. The varieties of tangles on any given (Platonic) polyhedral skeleton have been enumerated in detail (earlier results have been published in [2]). (We have generalised that approach to windings on simpler extended infinite 2- and 3-periodic nets, allowing us to systematically explore tangles in that class too.)

*These ideas have been developed joint with Dr. Myfanwy Evans (Potsdam).*

[1] S. T. Hyde, bioRxiv (2021), 10.1101/2021.03.12.435210,  
<https://www.biorxiv.org/content/early/2021/03/14/2021.03.12.435210.full.pdf>.

[2] S. T. Hyde and M. E. Evans, Proceedings of the National Academy of Sciences **119** (2022).