Structure-activity rules in suramin analogues

Suramin analogues act as anti-cancer agents by interfering with the formation of blood vessels for the tumour. Using the atomic structure and bond relationships present in such compounds, the task for an ILP system is to discover structural features that can be used to improve such compounds. The data here are described in [1]. In collaboration with Professor Harris (Institute of Molecular Medicine, University of Oxford), the ILP system *Progol* [2] was used to suggest several novel structural ideas that will be incorporated in the synthesis of new compounds.

All data is as used in the *Progol* experiments, and contained in a single compressed file with a ".pl.Z" suffix. Each compound has associated "atm" and "bond" predicates describing its atomic and bond structure. These were obtained using the QUANTA molecular modelling package. There are 7 positive examples and 4 negative examples (expressed as negative ground clauses).

References

[1] Braddock, P. S., D.-E. Hu, et al. (1994). A structure-activity analysis of the growth factor and angiogenic activity of basic fibrobalst growth factor by suramin and related polyanions. *Br. J. Cancer.* 69: 890-898.

[2] Muggleton S.H. (1995) Inverse Entailment and Progol. *New Gen. Comput.* (to appear).