

White, W. Timothy J.; Beyer, Stephan; Dührkop, Kai; Chimani, Markus; Böcker, Sebastian
Speedy colorful subtrees. (English) [\[Zbl 1467.92078\]](#)

Xu, Dachuan (ed.) et al., Computing and combinatorics. 21st international conference, COCOON 2015, Beijing, China, August 4–6, 2015. Proceedings. Cham: Springer. Lect. Notes Comput. Sci. 9198, 310-322 (2015).

Summary: Fragmentation trees are a technique for identifying molecular formulas and deriving some chemical properties of metabolites – small organic molecules – solely from mass spectral data. Computing these trees involves finding exact solutions to the NP-hard MAXIMUM COLORFUL SUBTREE problem. Existing solvers struggle to solve the large instances involved fast enough to keep up with instrument throughput, and their performance remains a hindrance to adoption in practice.

We attack this problem on two fronts: by combining fast and effective reduction algorithms with a strong integer linear program (ILP) formulation of the problem, we achieve overall speedups of 9.4 fold and 8.8 fold on two sets of real-world problems – without sacrificing optimality. Both approaches are, to our knowledge, the first of their kind for this problem. We also evaluate the strategy of solving *global* problem instances, instead of first subdividing them into many *candidate* instances as has been done in the past. Software (C++ source for our reduction program and our CPLEX/Gurobi driver program) available under LGPL at https://github.com/wtwhite/speedy_colorful_subtrees/.

For the entire collection see [\[Zbl 1316.68028\]](#).

MSC:

[92C40](#) Biochemistry, molecular biology

[90C10](#) Integer programming

Cited in **3** Documents

Software:

[SIRIUS](#); [CPLEX](#); [speedy_colorful_subtrees](#); [MolFind](#); [Gurobi](#); [GitHub](#)

Full Text: [DOI](#)