

Online Headspace-Solid Phase Microextraction-Gas Chromatography-Mass Spectrometry-based untargeted volatile metabolomics for studying emerging complex biopesticides: a proof of concept

Appendix C

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Summary

Plots shown below belong to the results of the Multivariate Empirical Bayes Analysis of Variance (MEBA). These analyses were applied on the automatically preprocessed GC-MS data. The plots were performed using the R-based MetaboAnalyst platform^{1,2,3}.

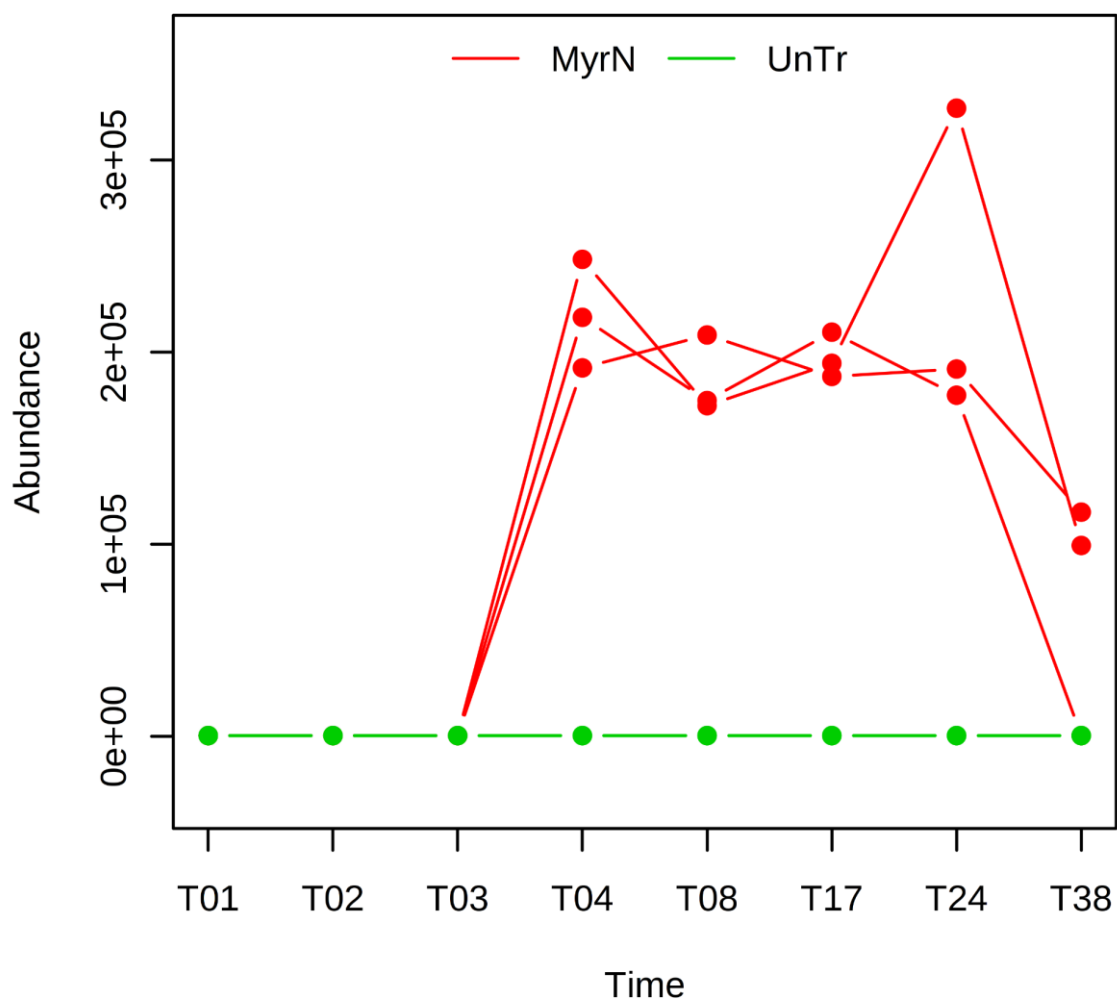
It should be noted that the time scale in those plots is not reliable (*i.e.* each time point is considered as a factor, and the points are separated with the same distance). In addition, in certain of those MEBA plots, the kinetics profiles are not identical to the profiles that were obtained after performing the manual integrations of peaks. This difference can be explained by the recurrent data integration errors that can take place when the automated preprocessing is being performed, and demonstrates the importance of the manual crosscheck of raw GC-MS data.

¹ Chong, J. *et al.* *Curr. Protoc. Bioinformatics* (2019), 68(1):e86. [doi:10.1002/cpbi.86](https://doi.org/10.1002/cpbi.86)

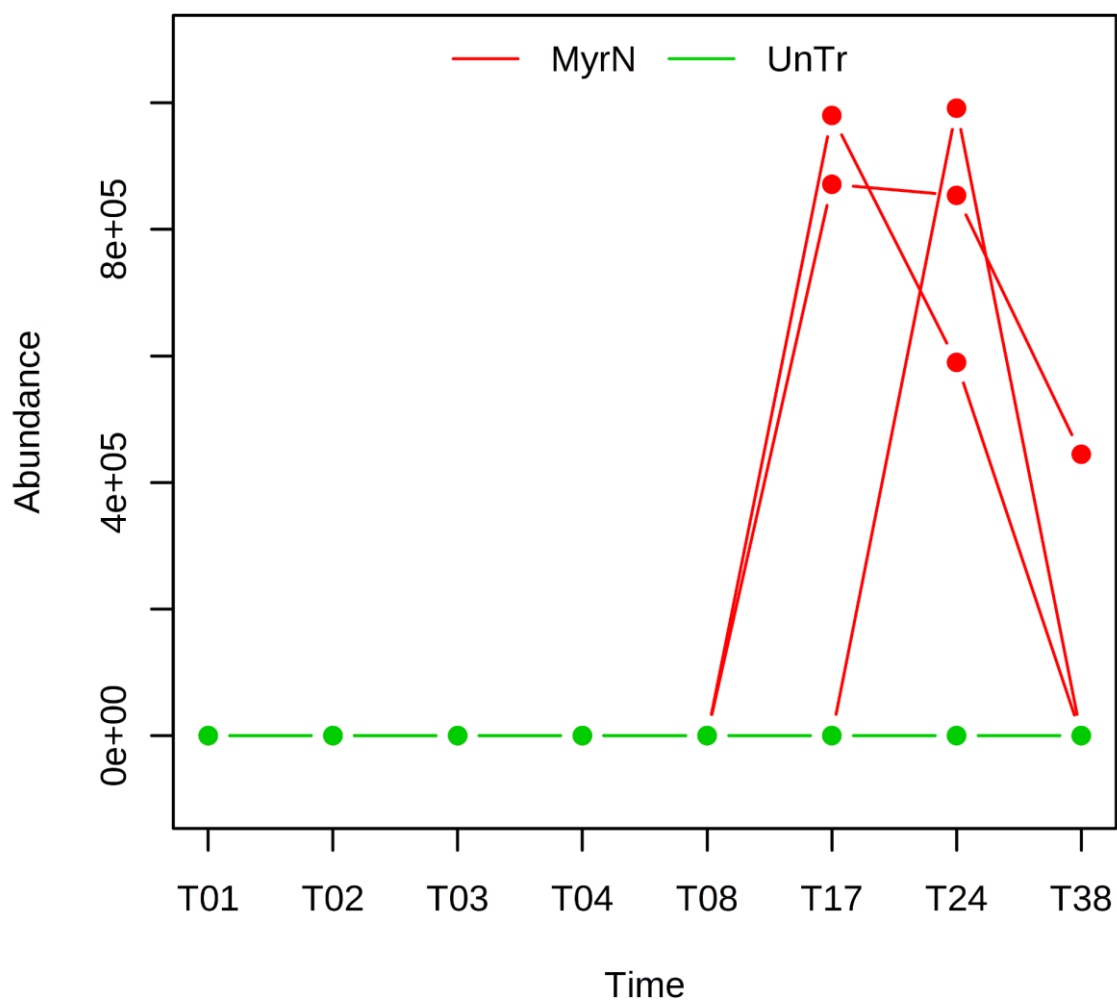
² Chong, J. *et al.* *Nucleic Acids Res.* (2018), 46(W1):W486–W494. [doi:10.1093/nar/gky310](https://doi.org/10.1093/nar/gky310)

³ <https://www.metaboanalyst.ca/>, accessed February 28, 2020.

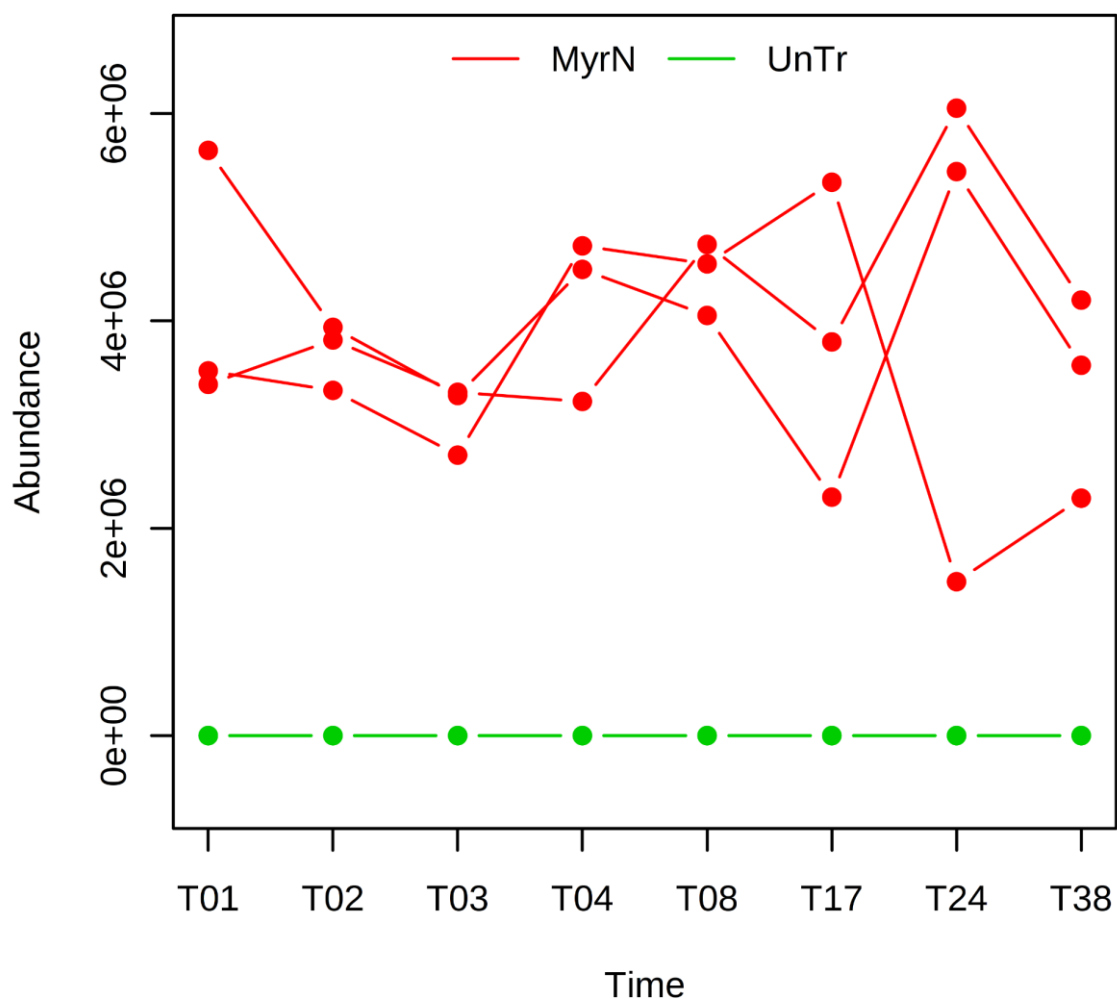
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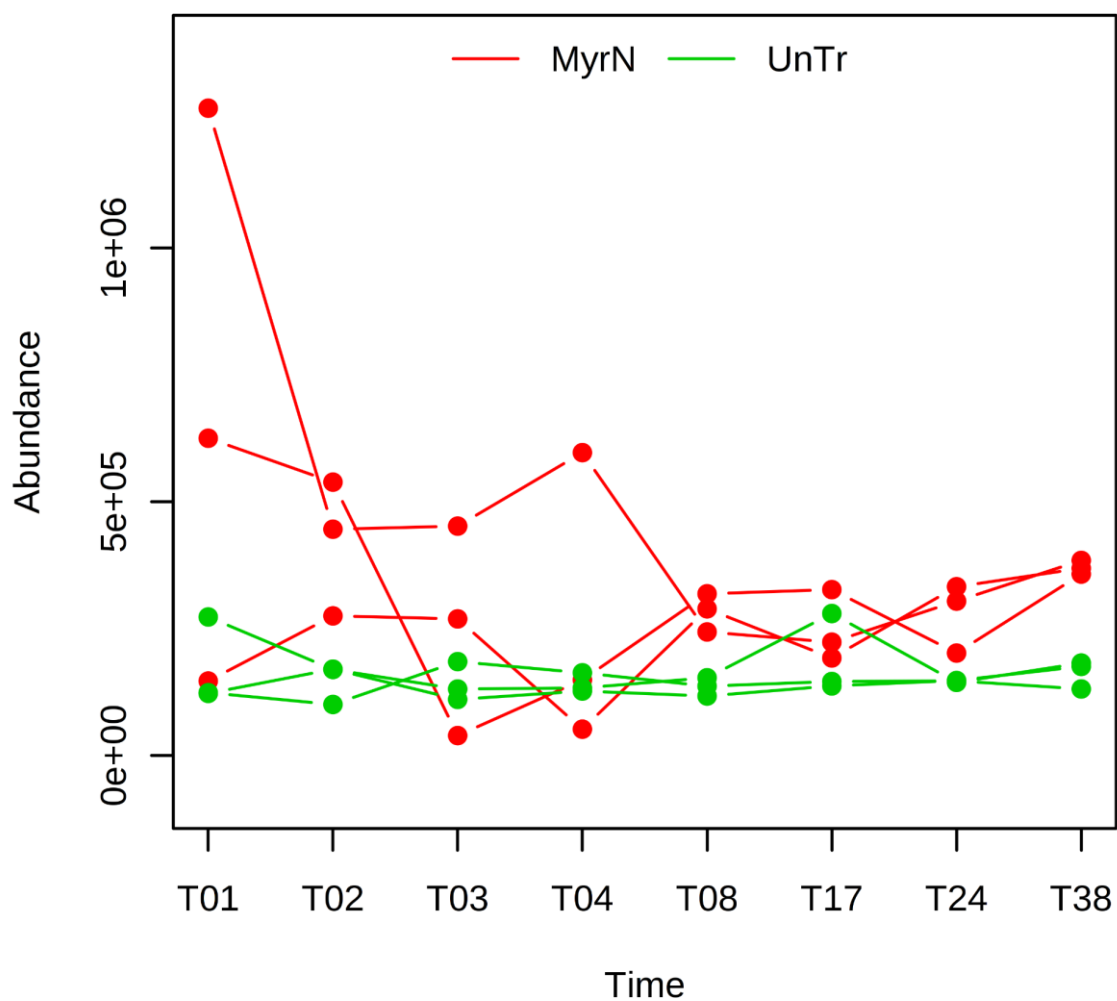
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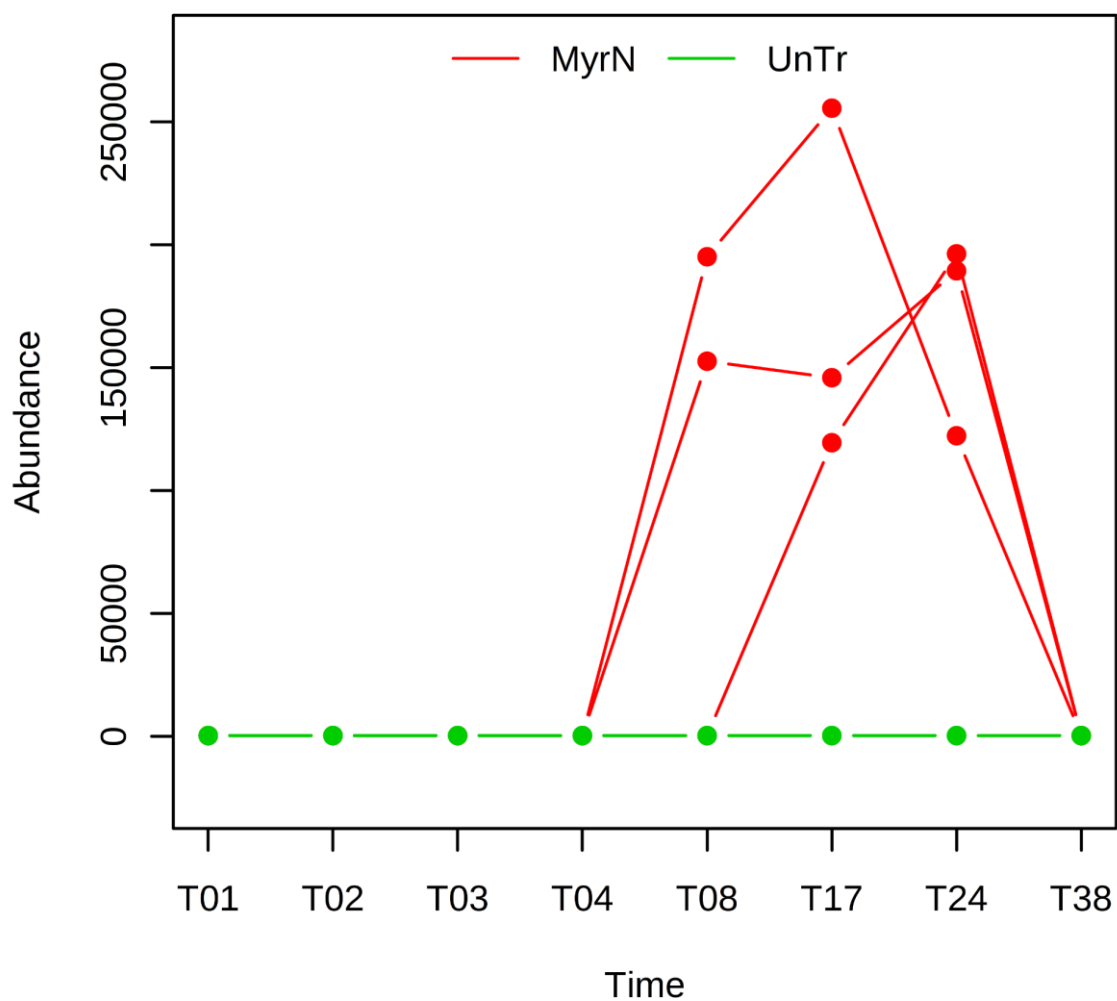
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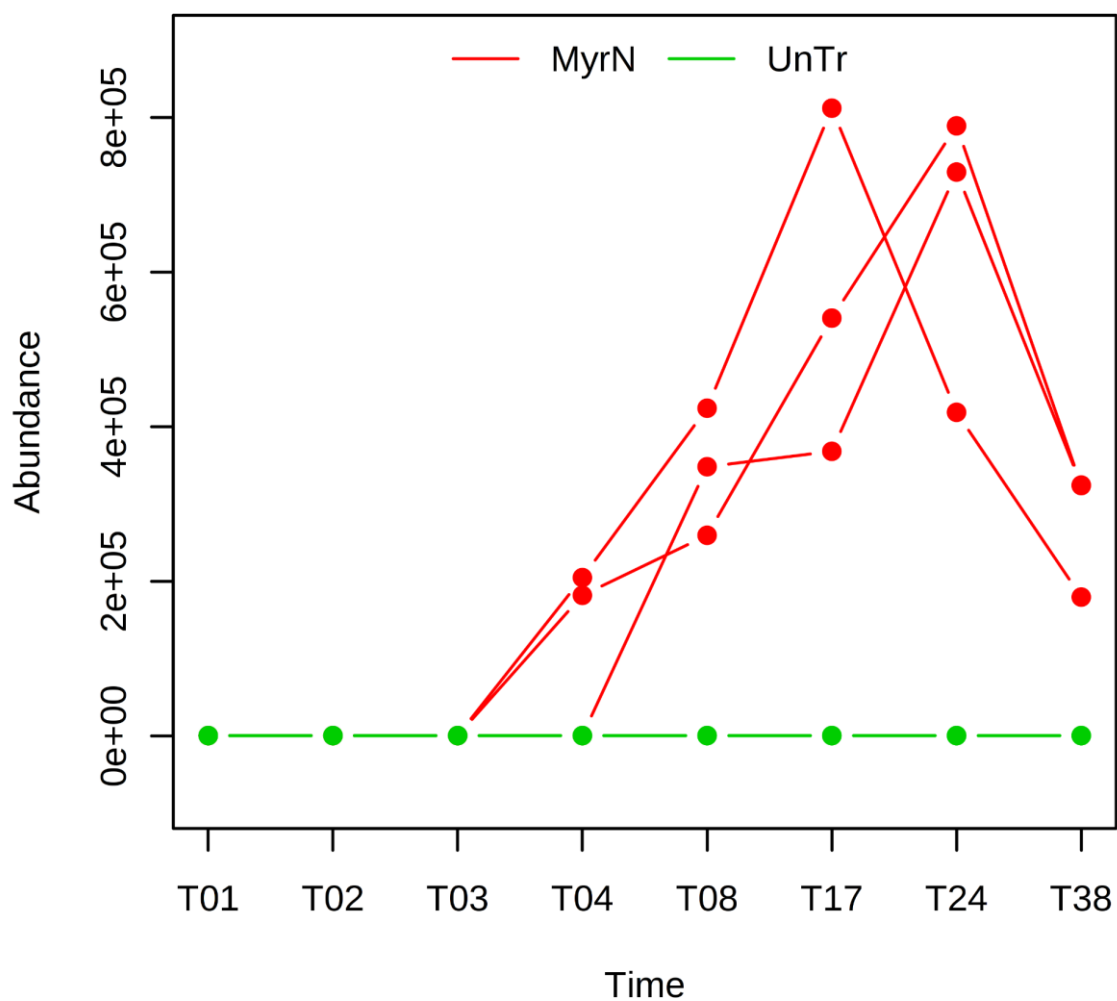
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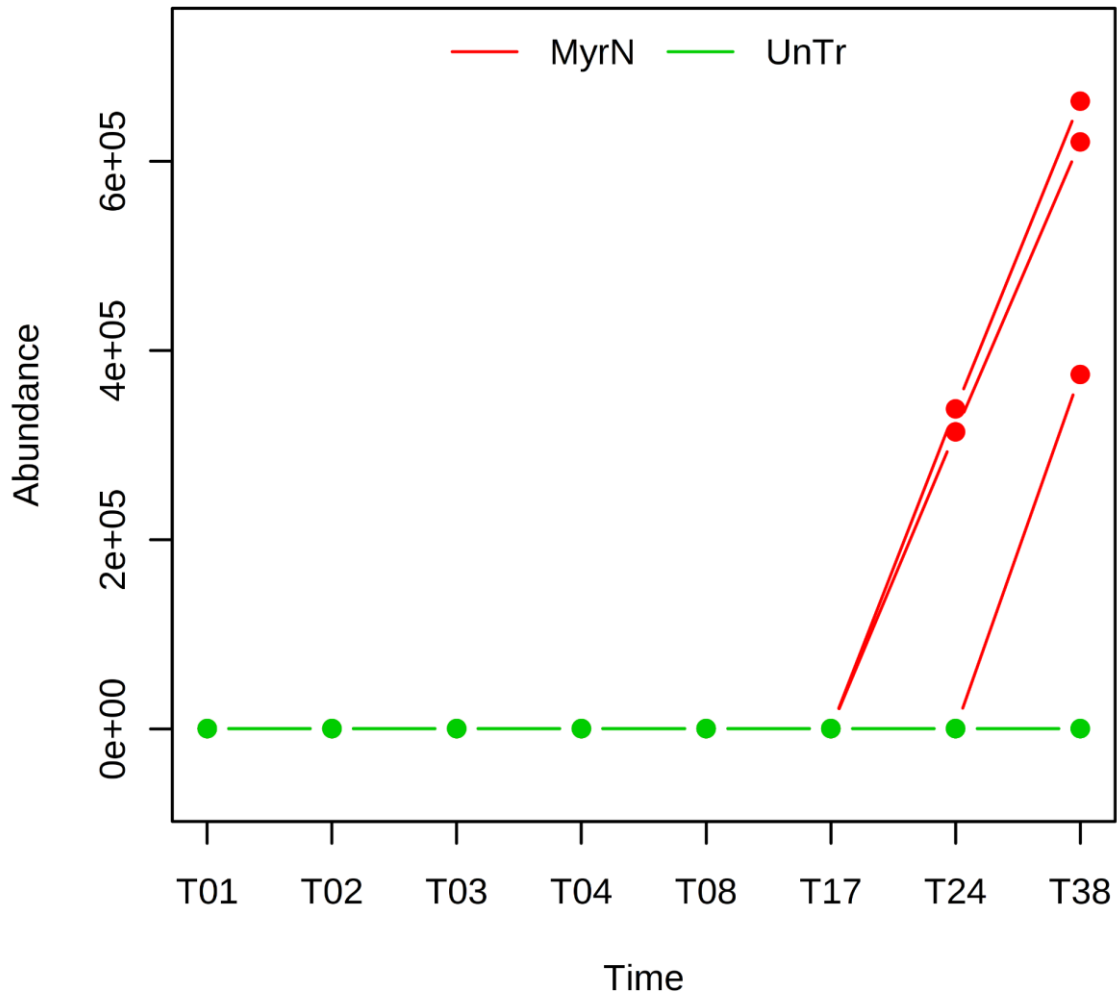
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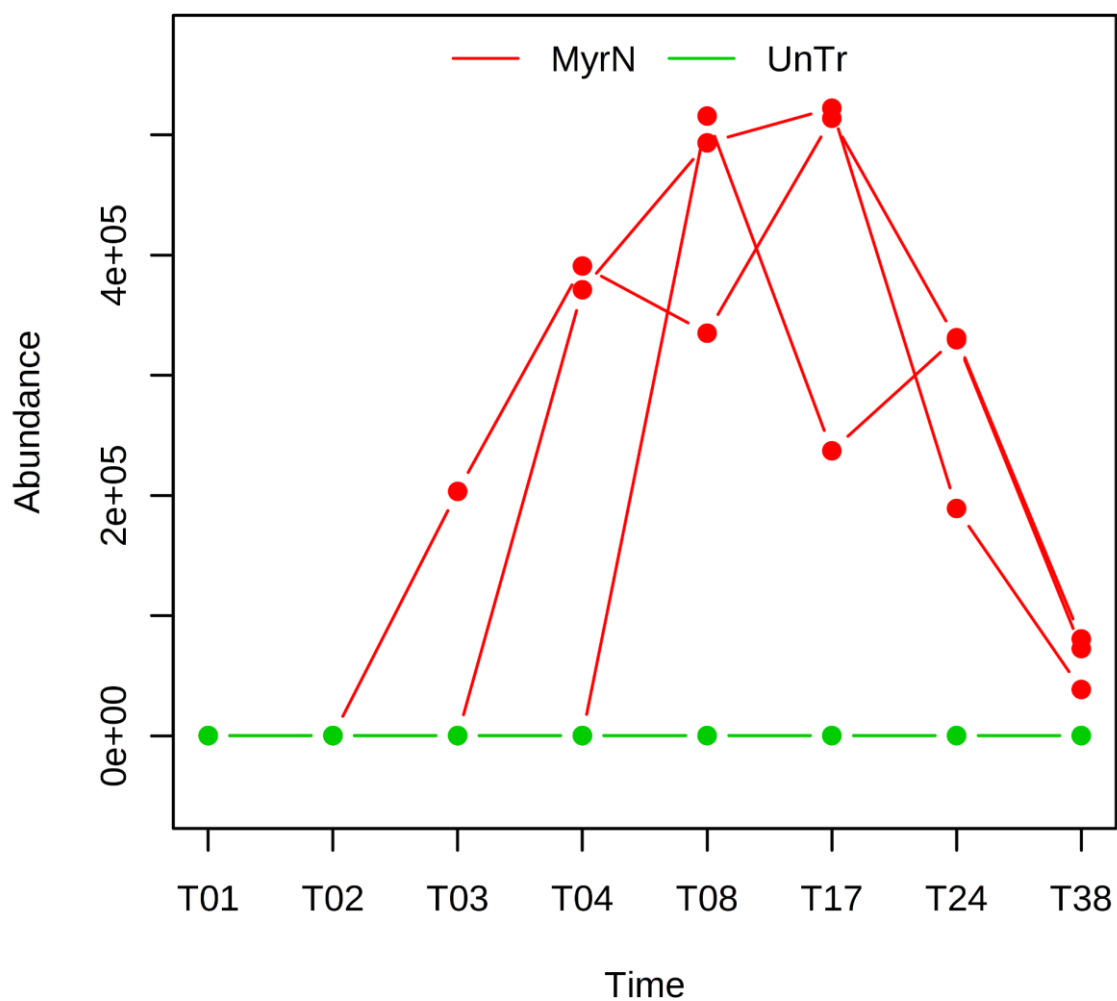
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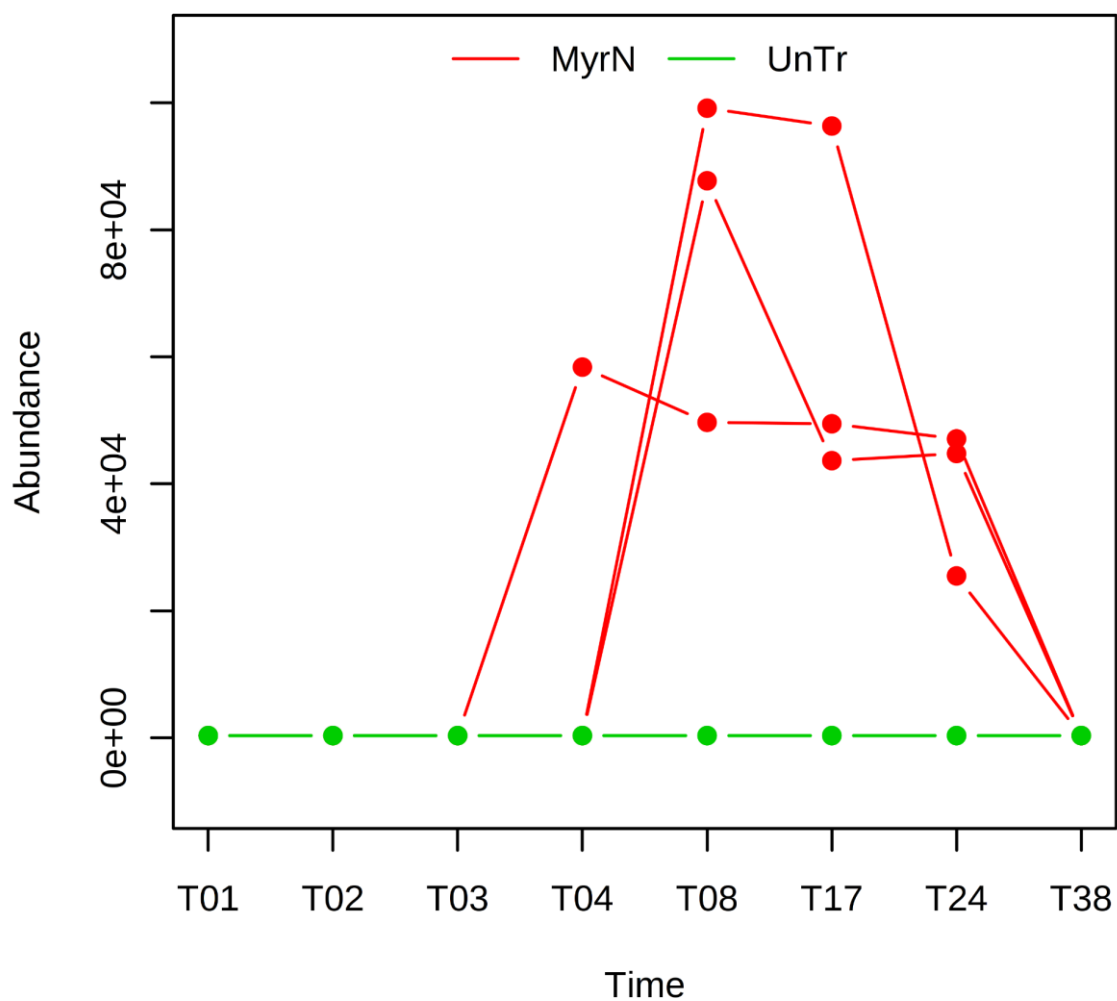
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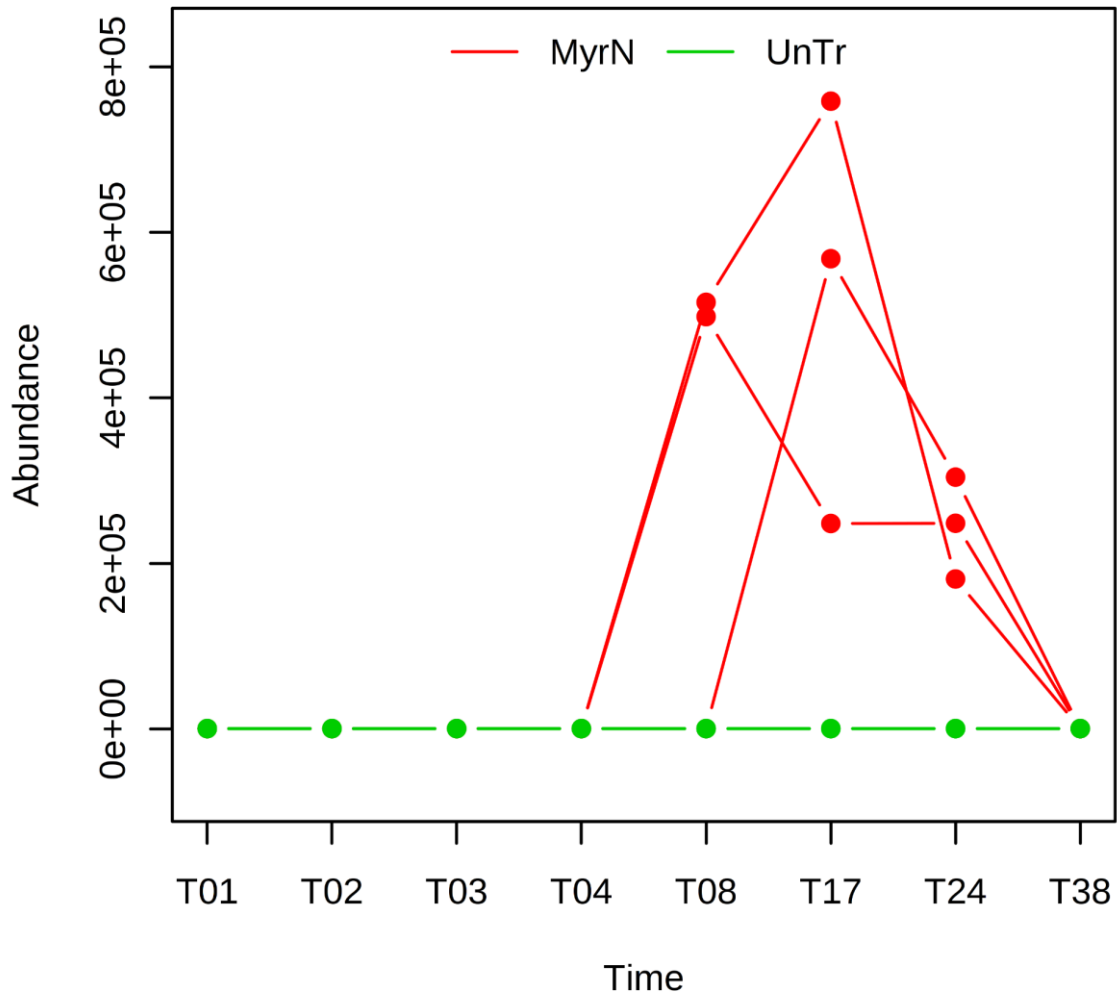
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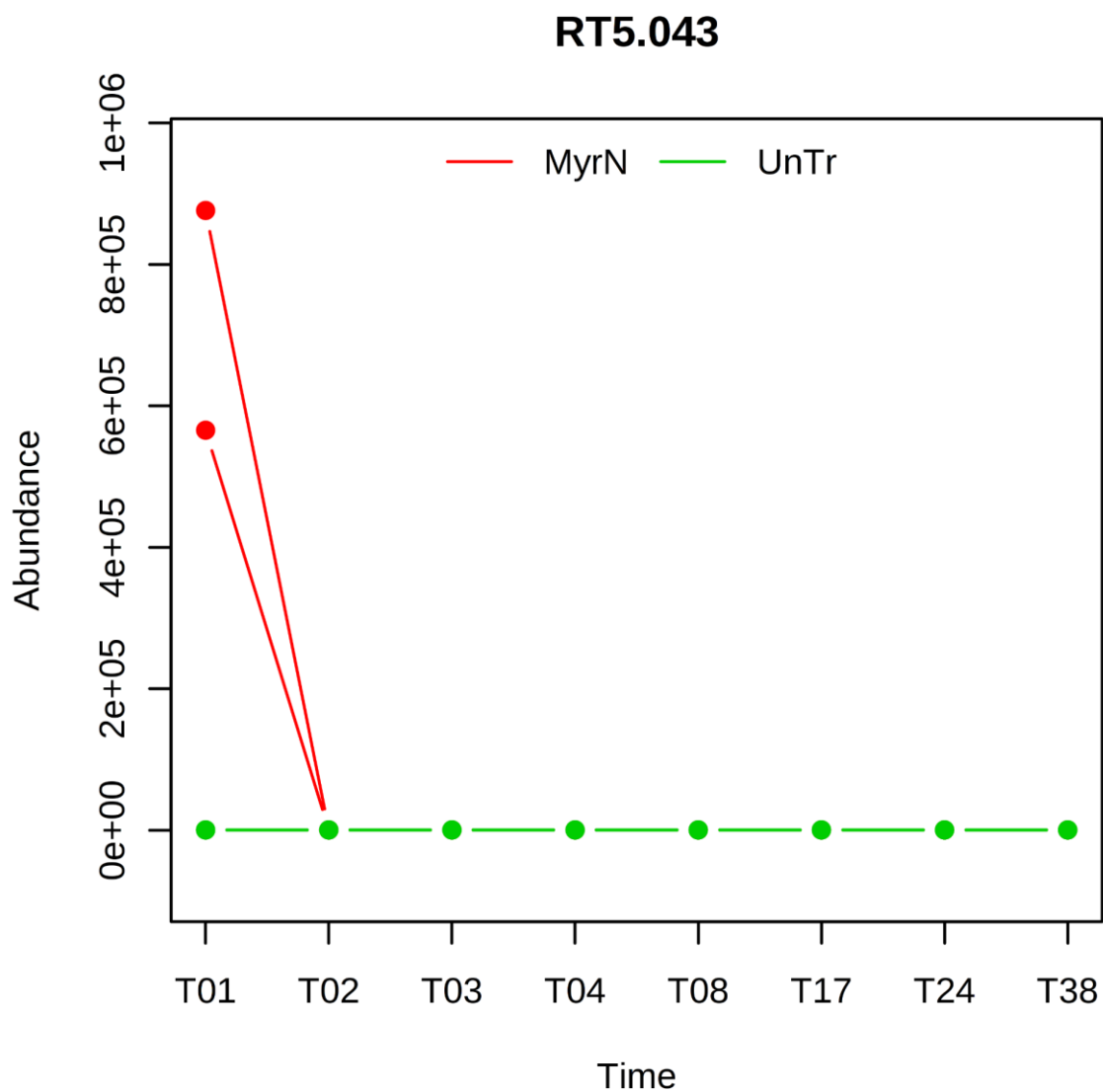


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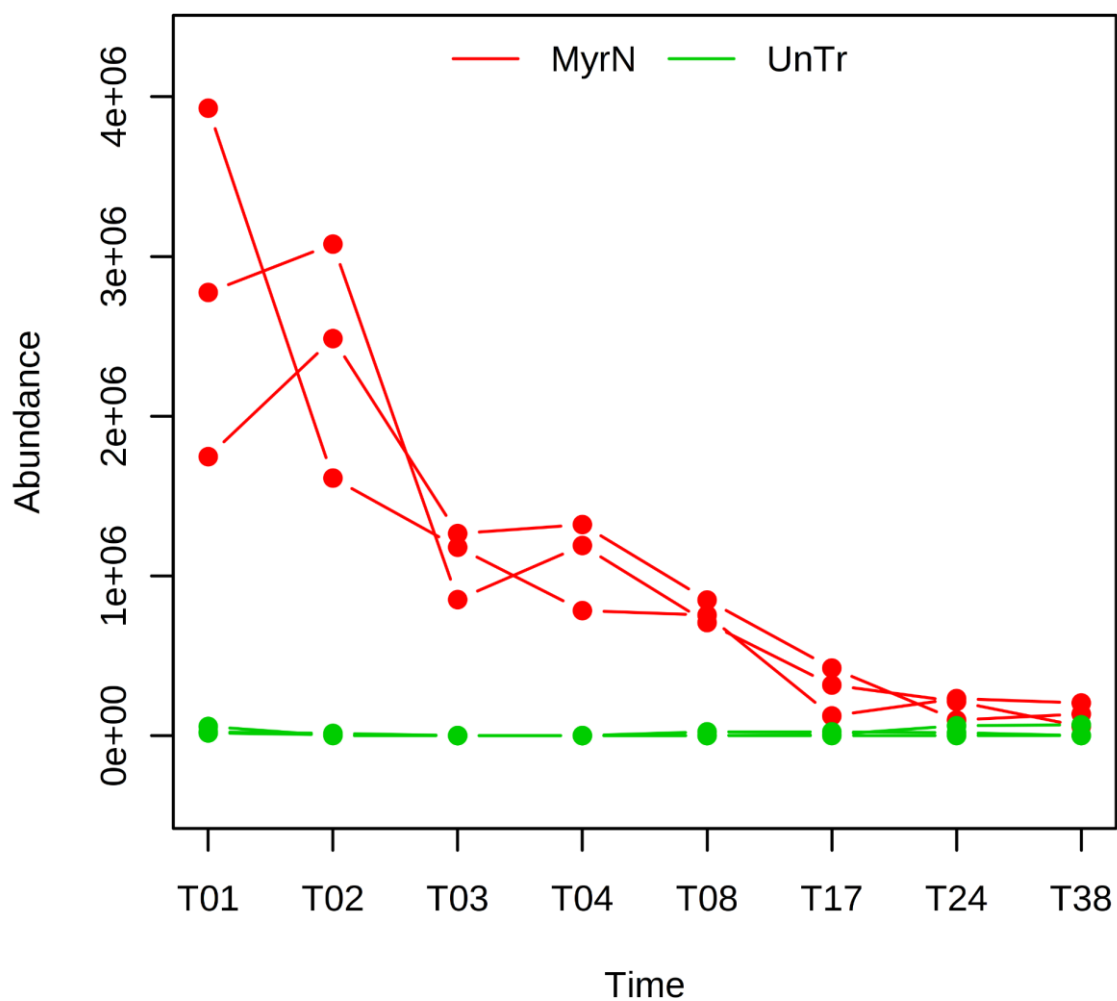


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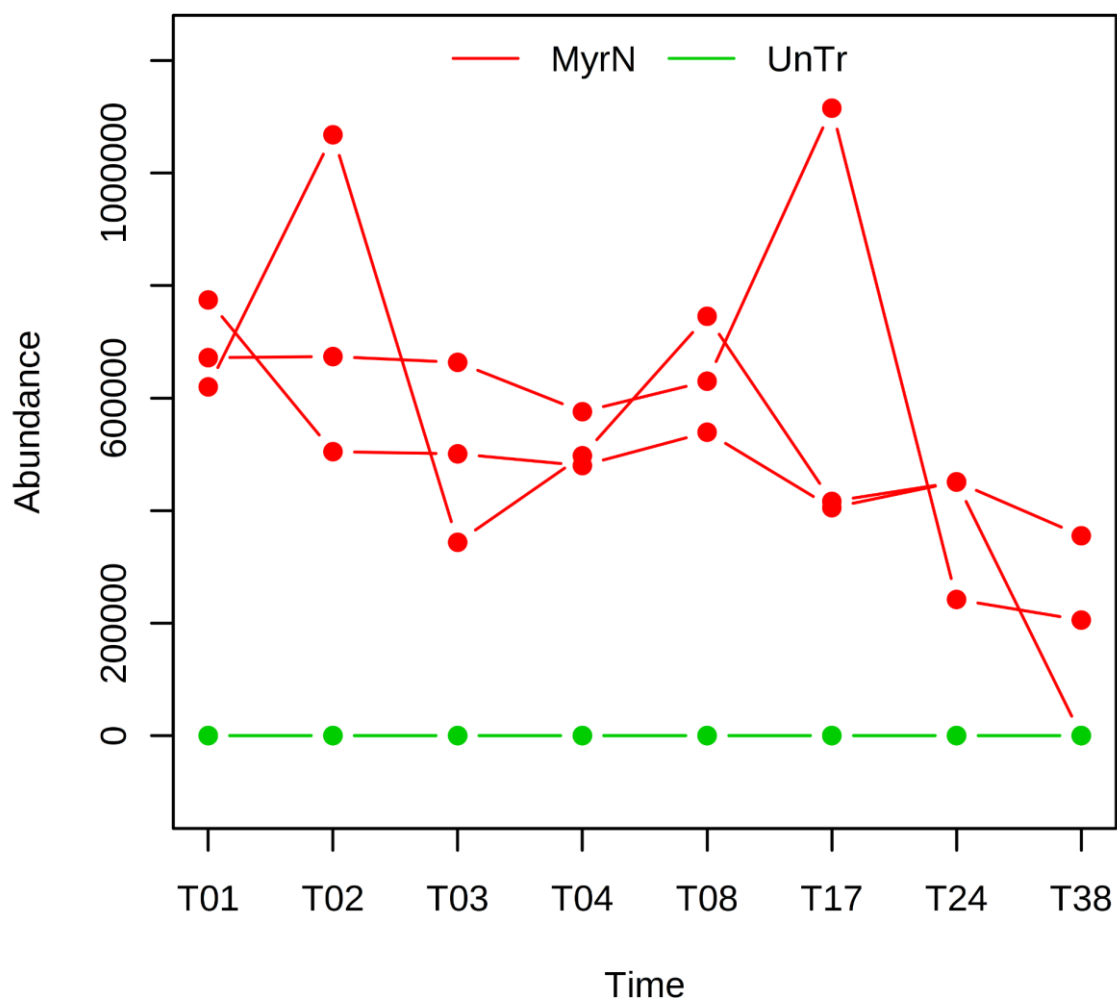




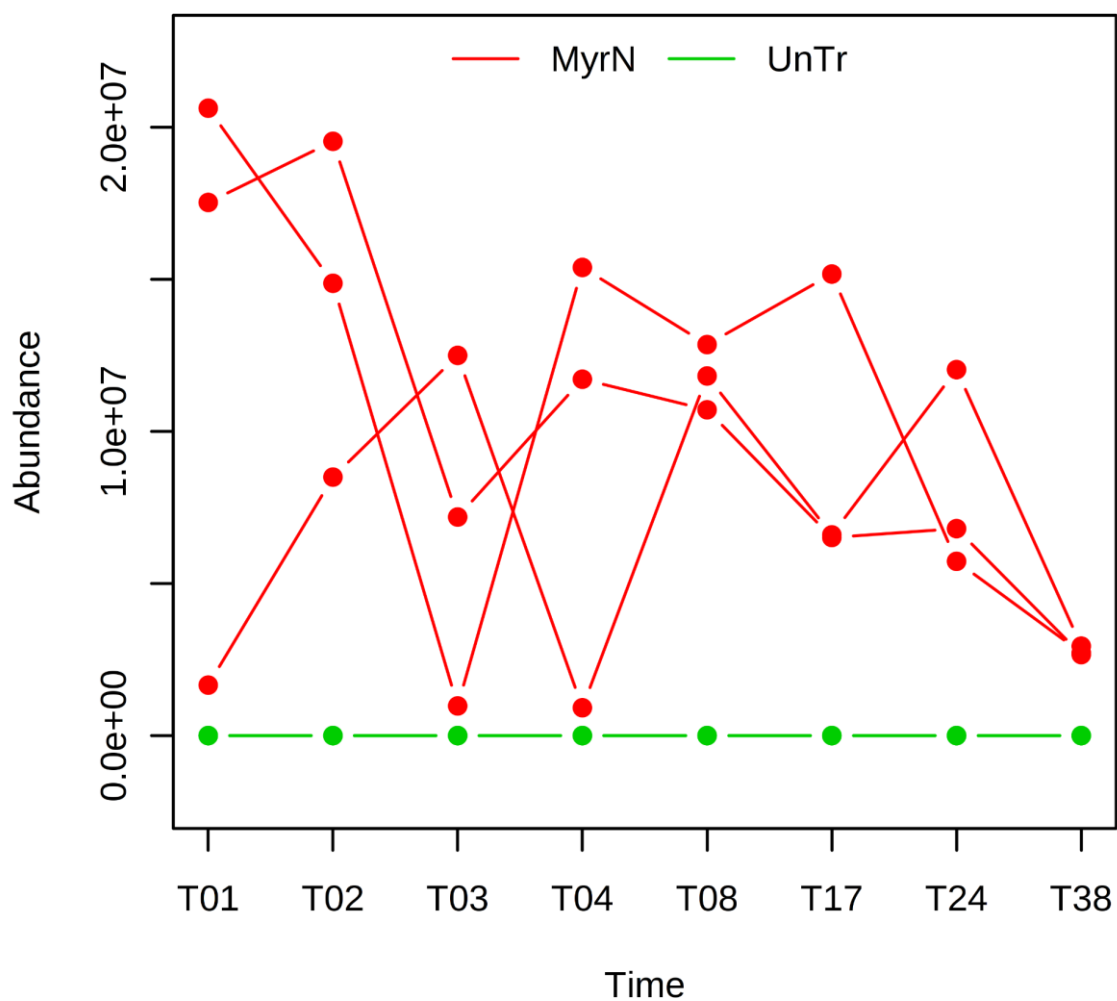
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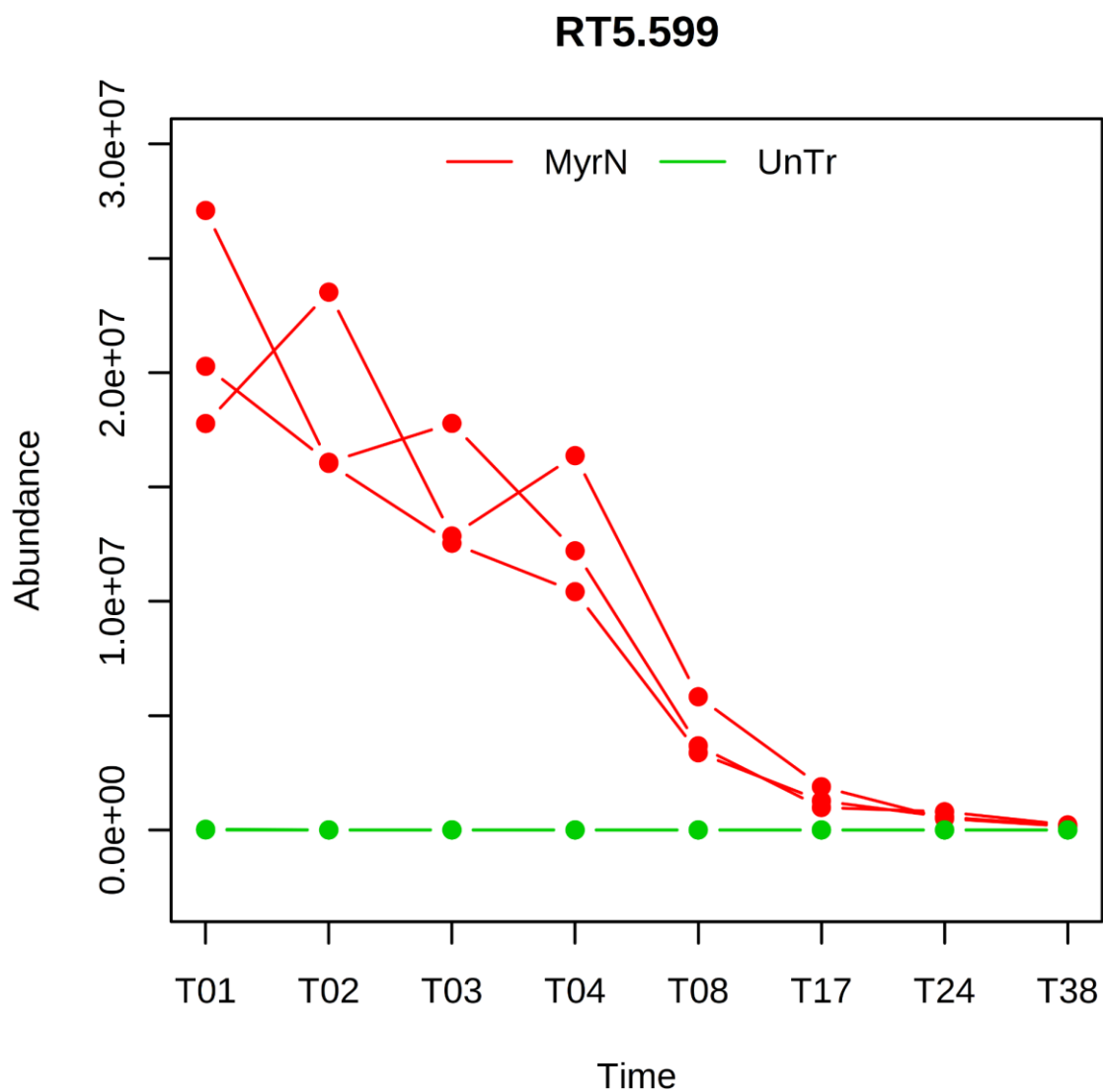


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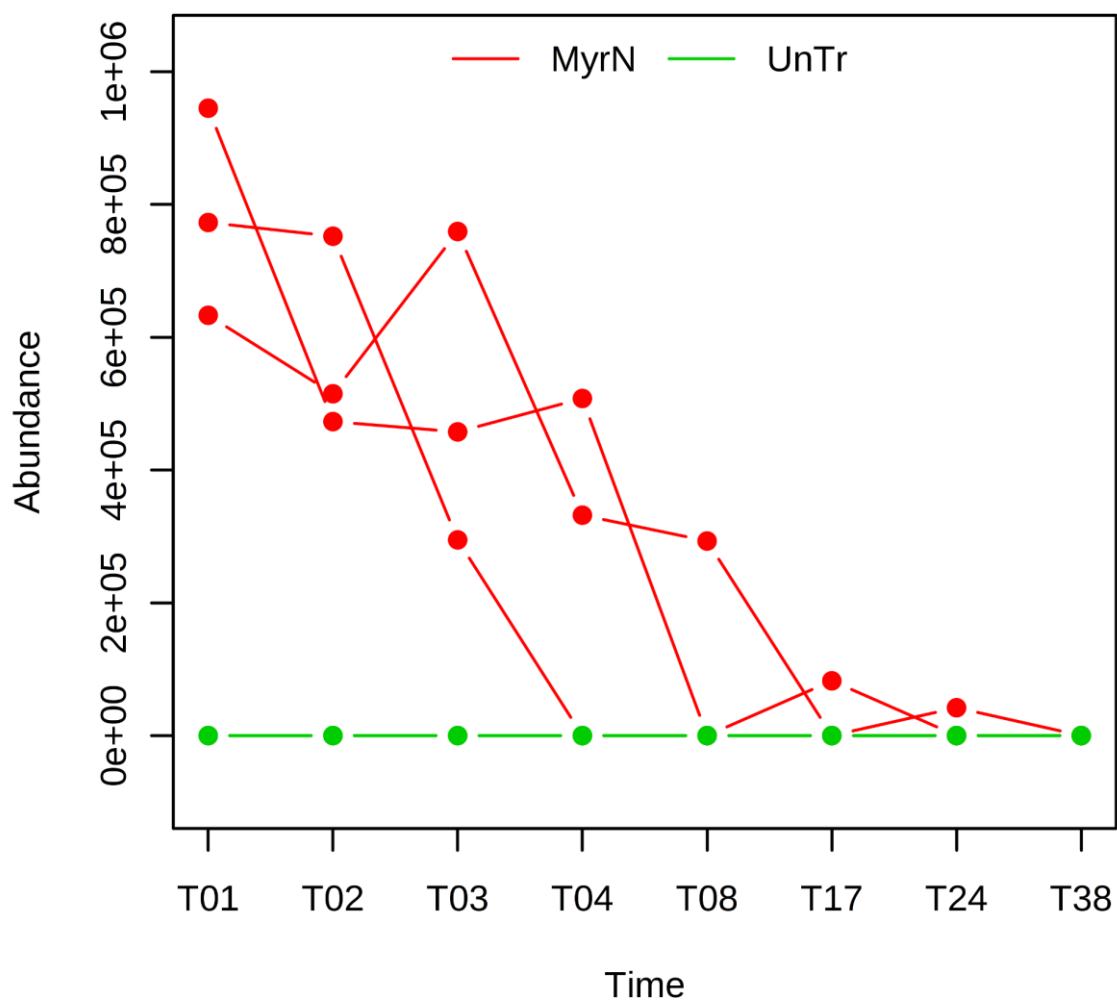


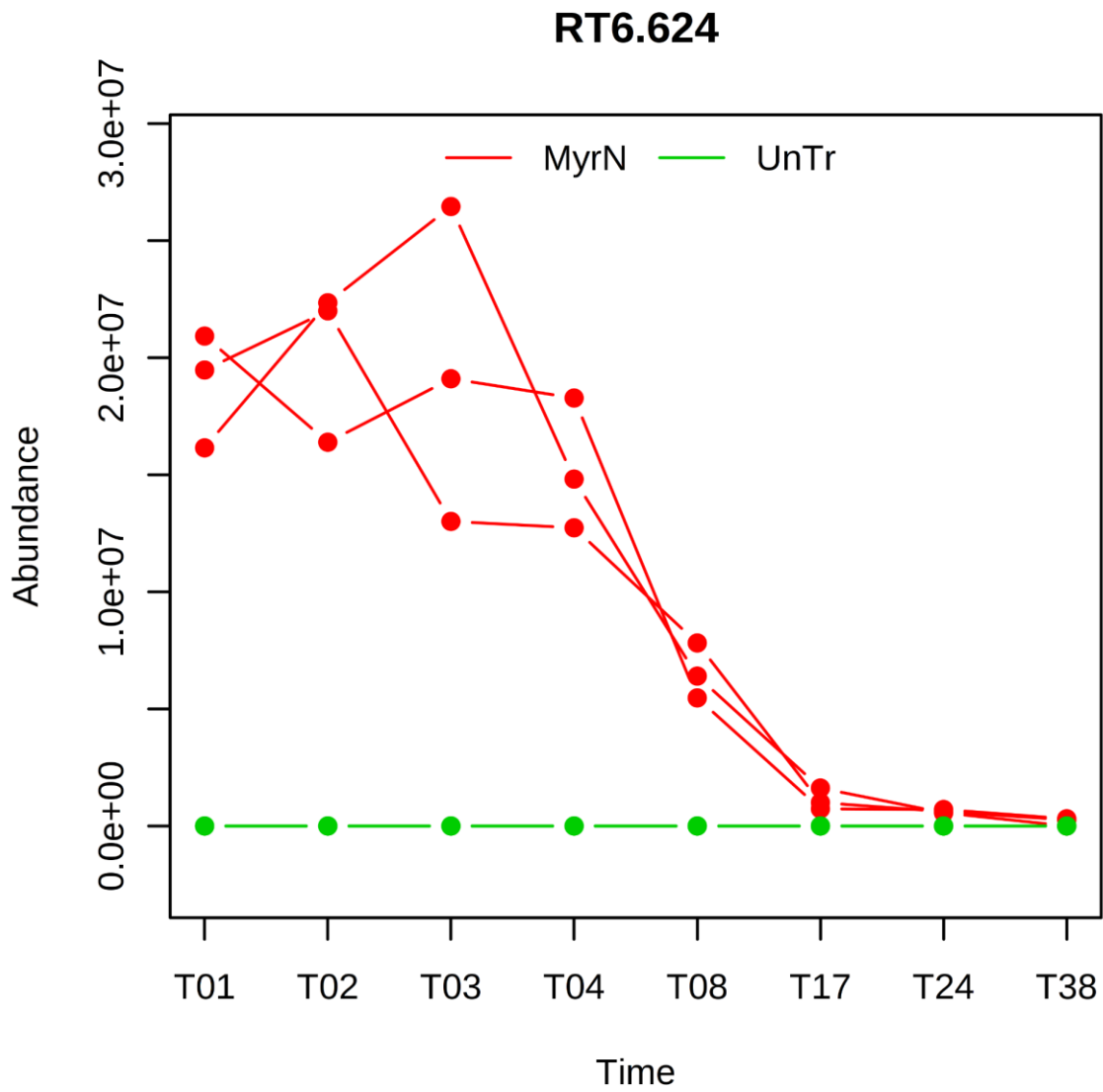
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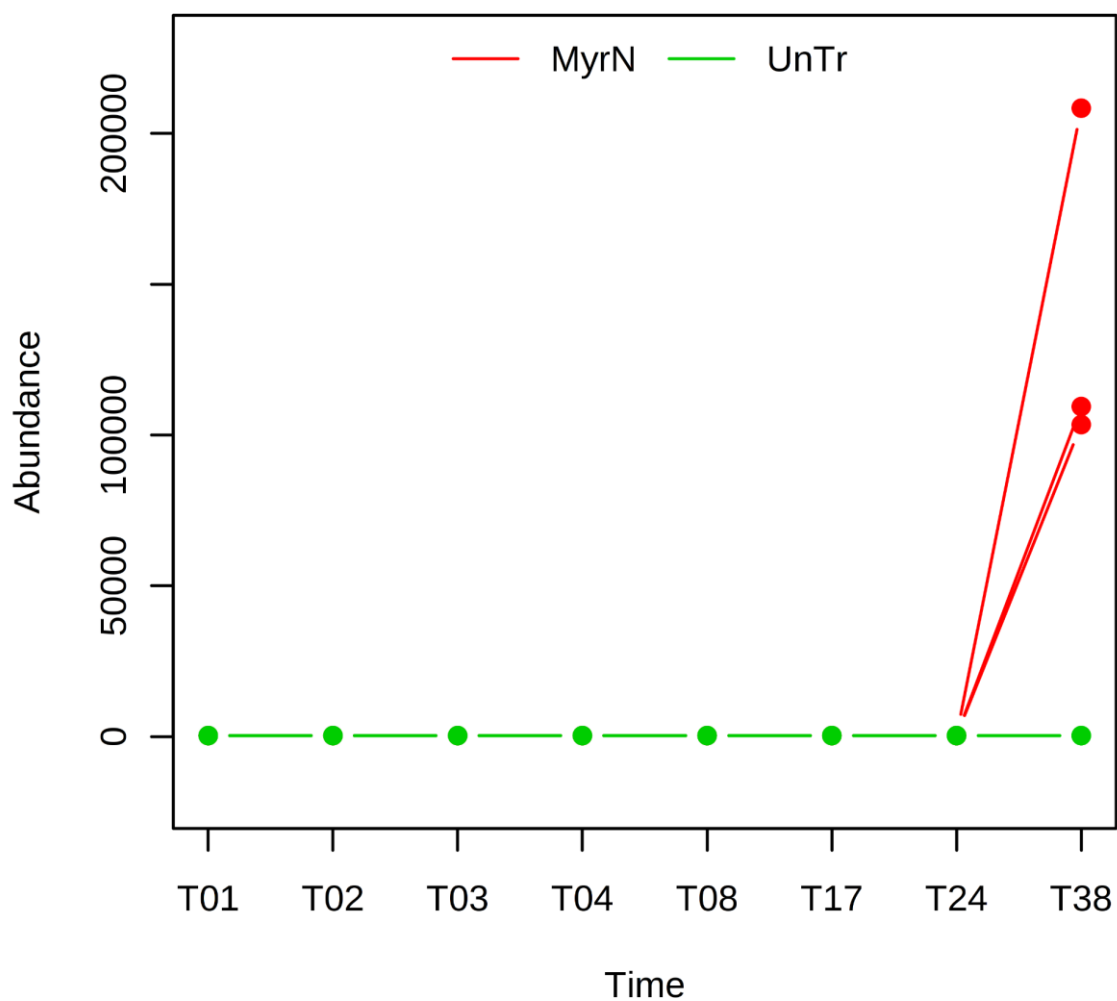


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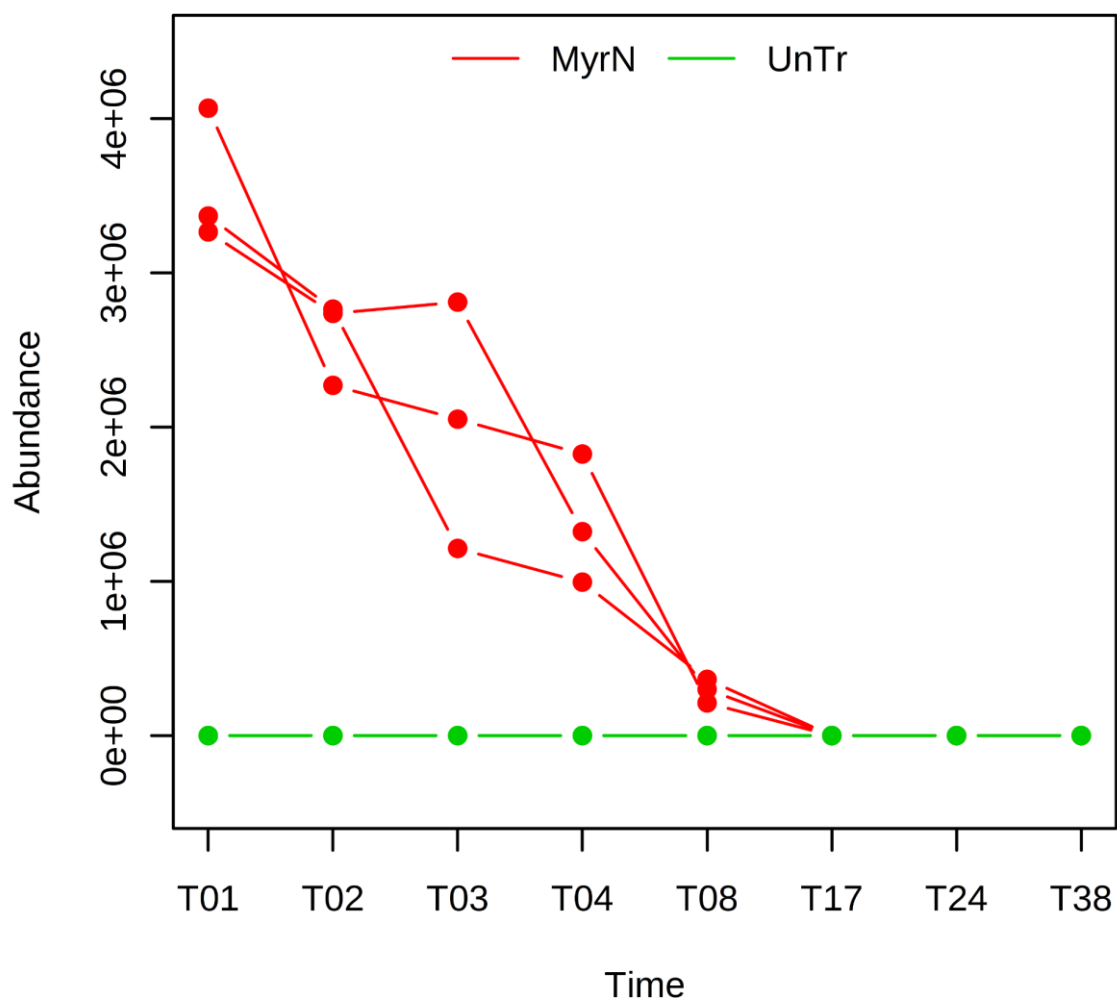




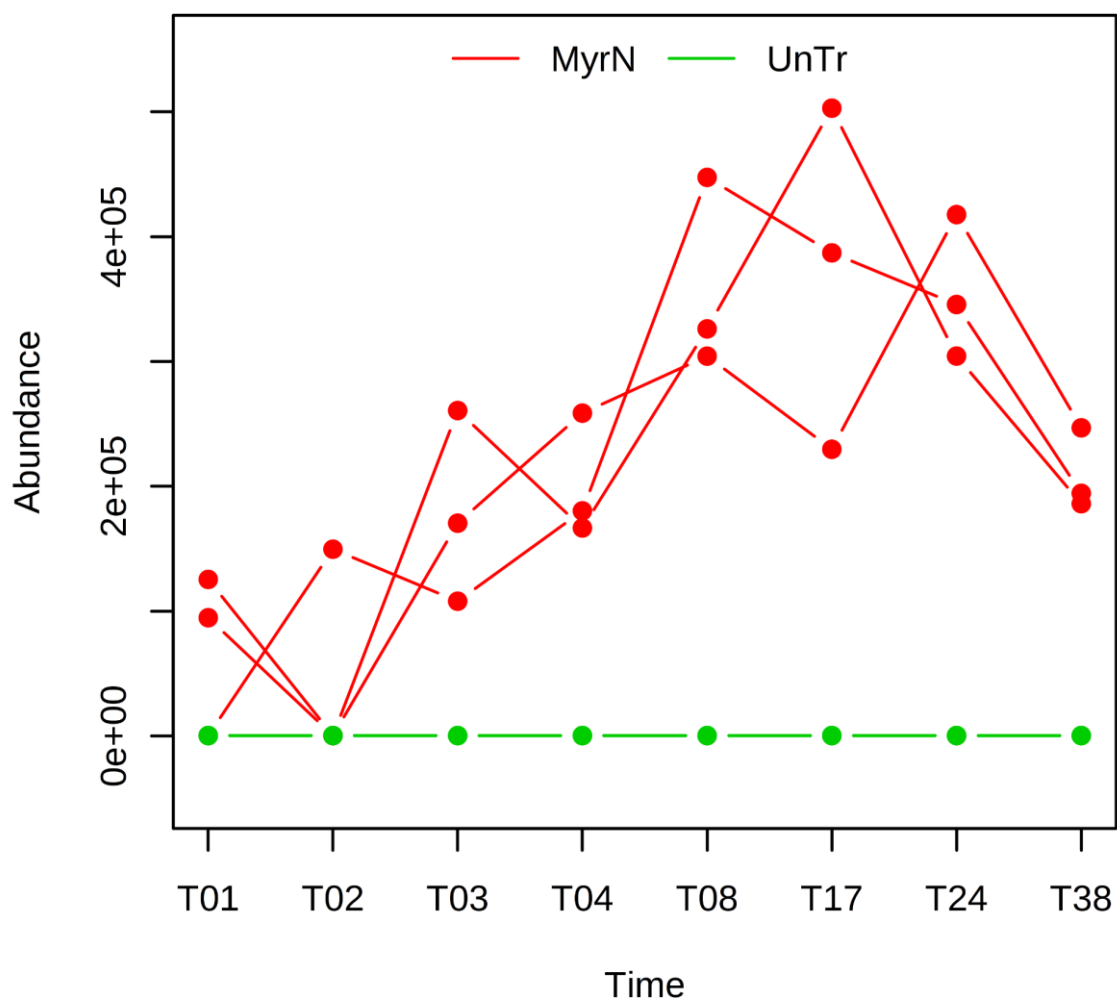
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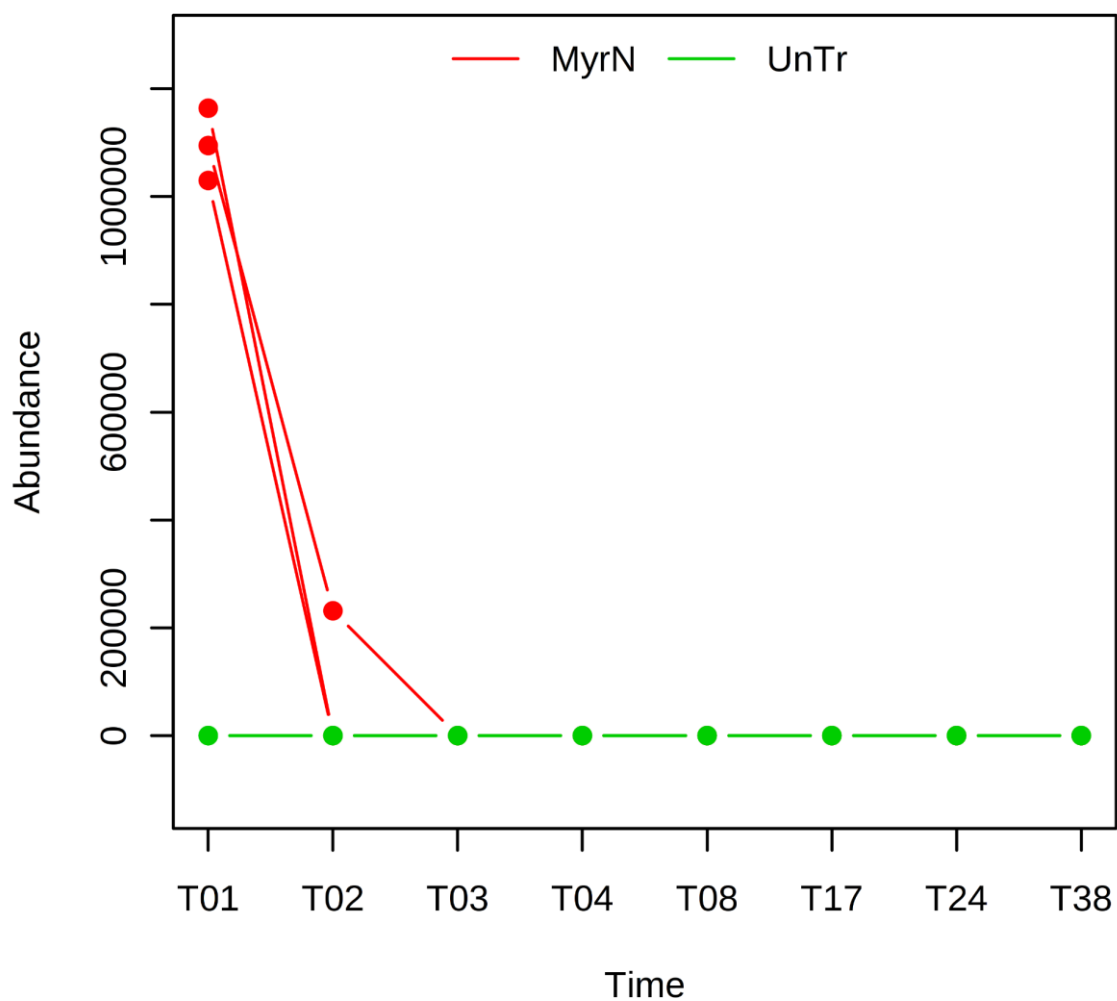
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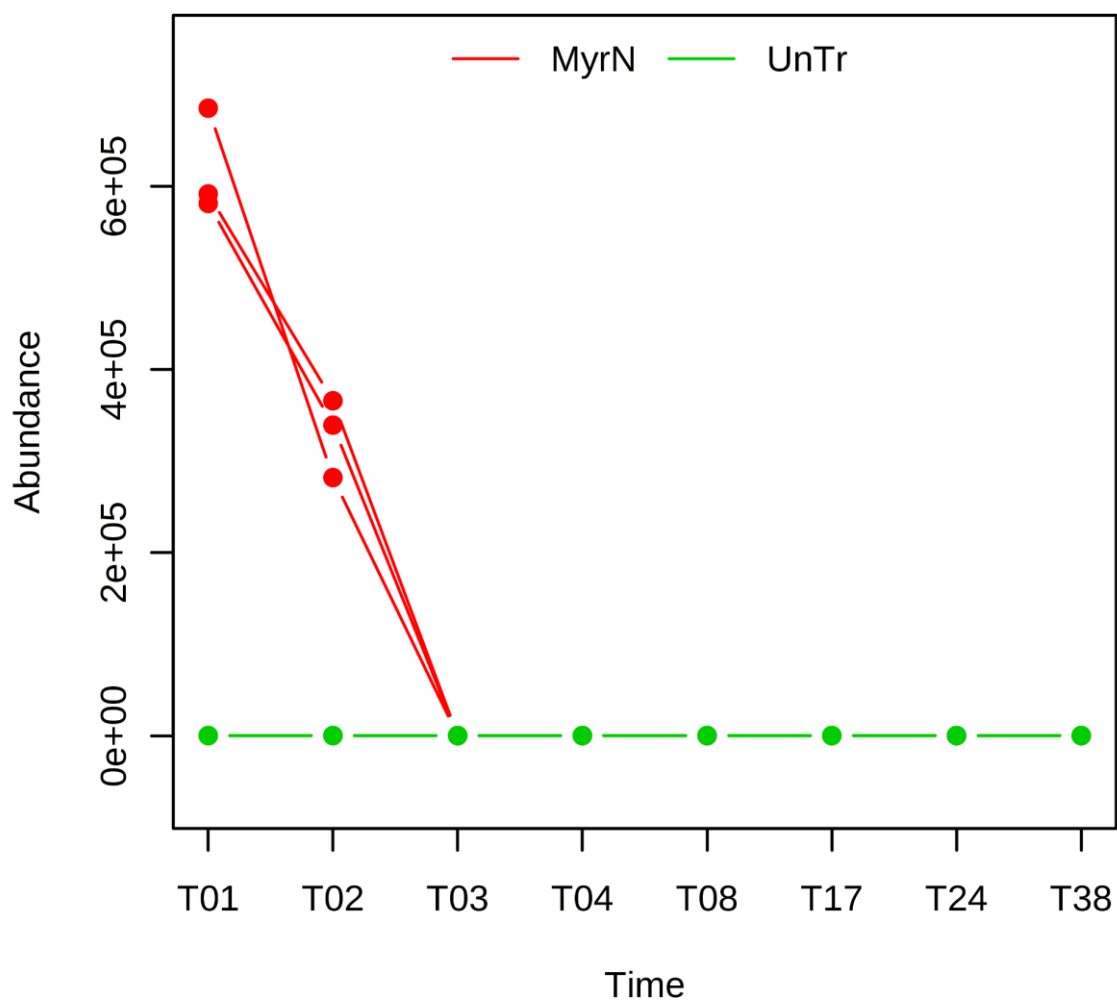
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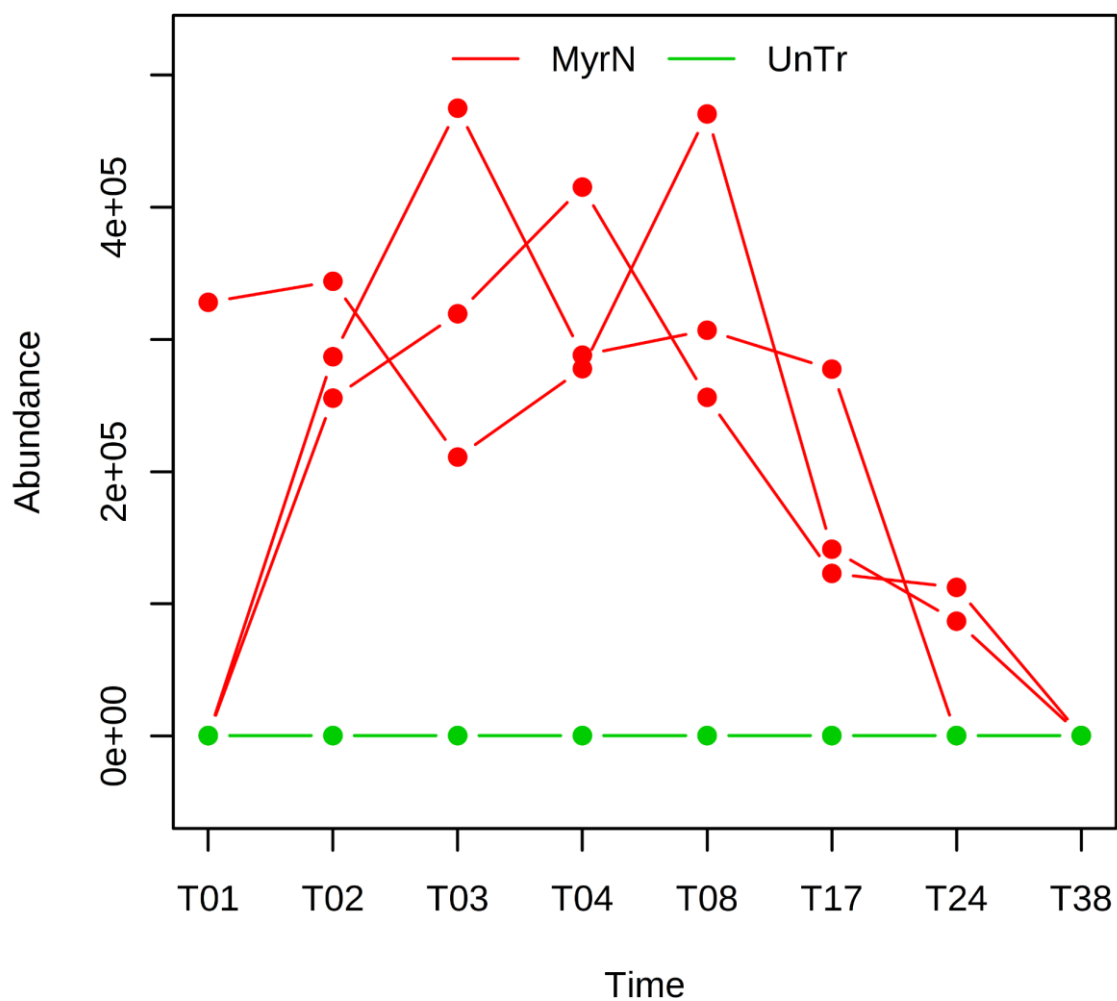
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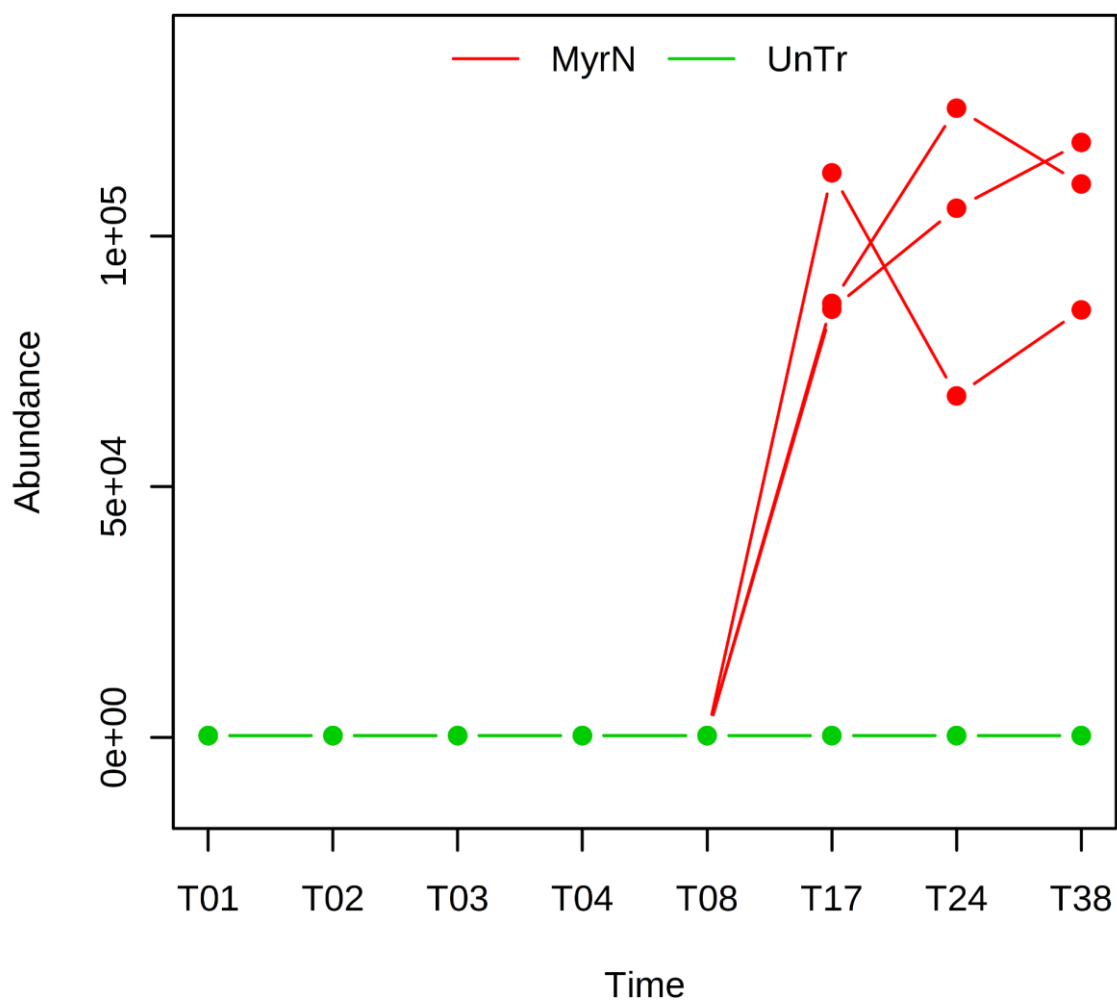
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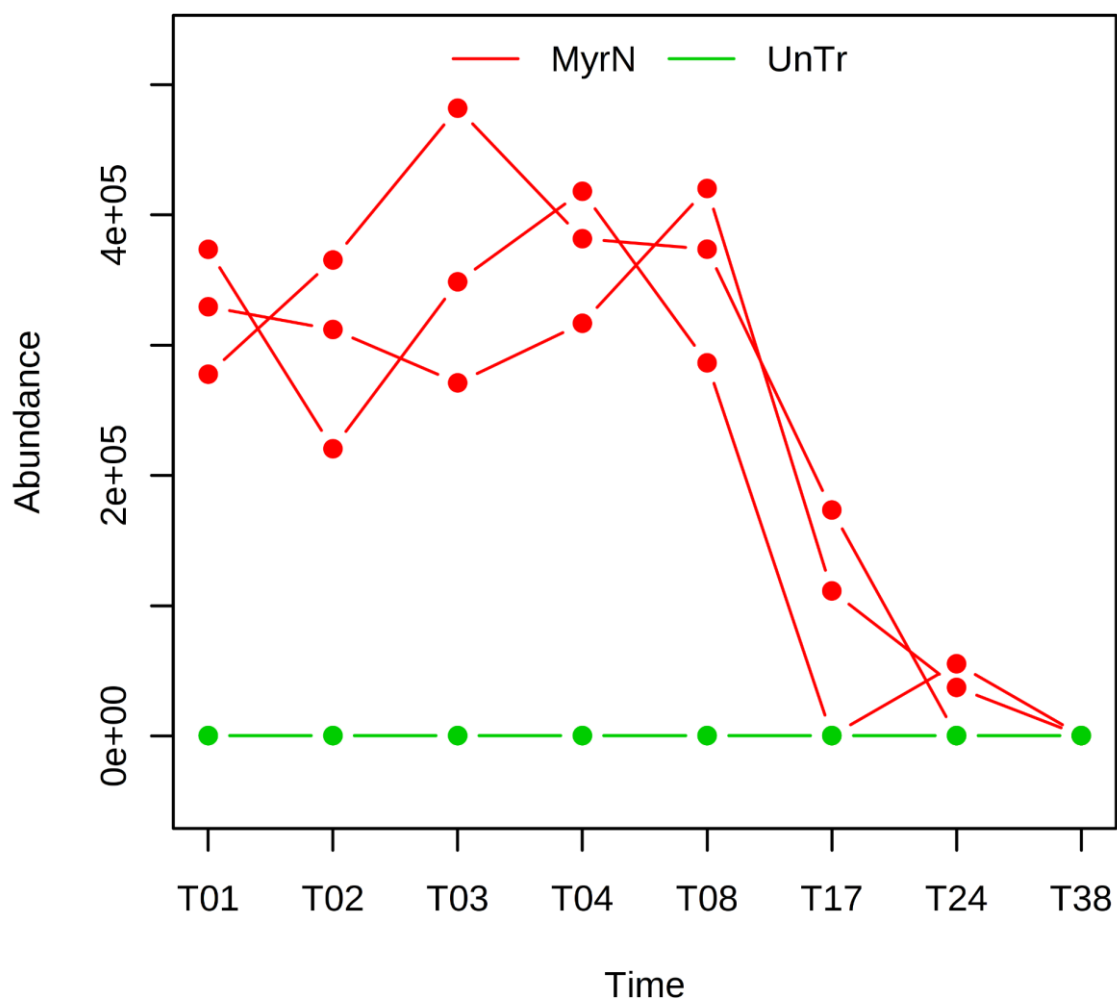
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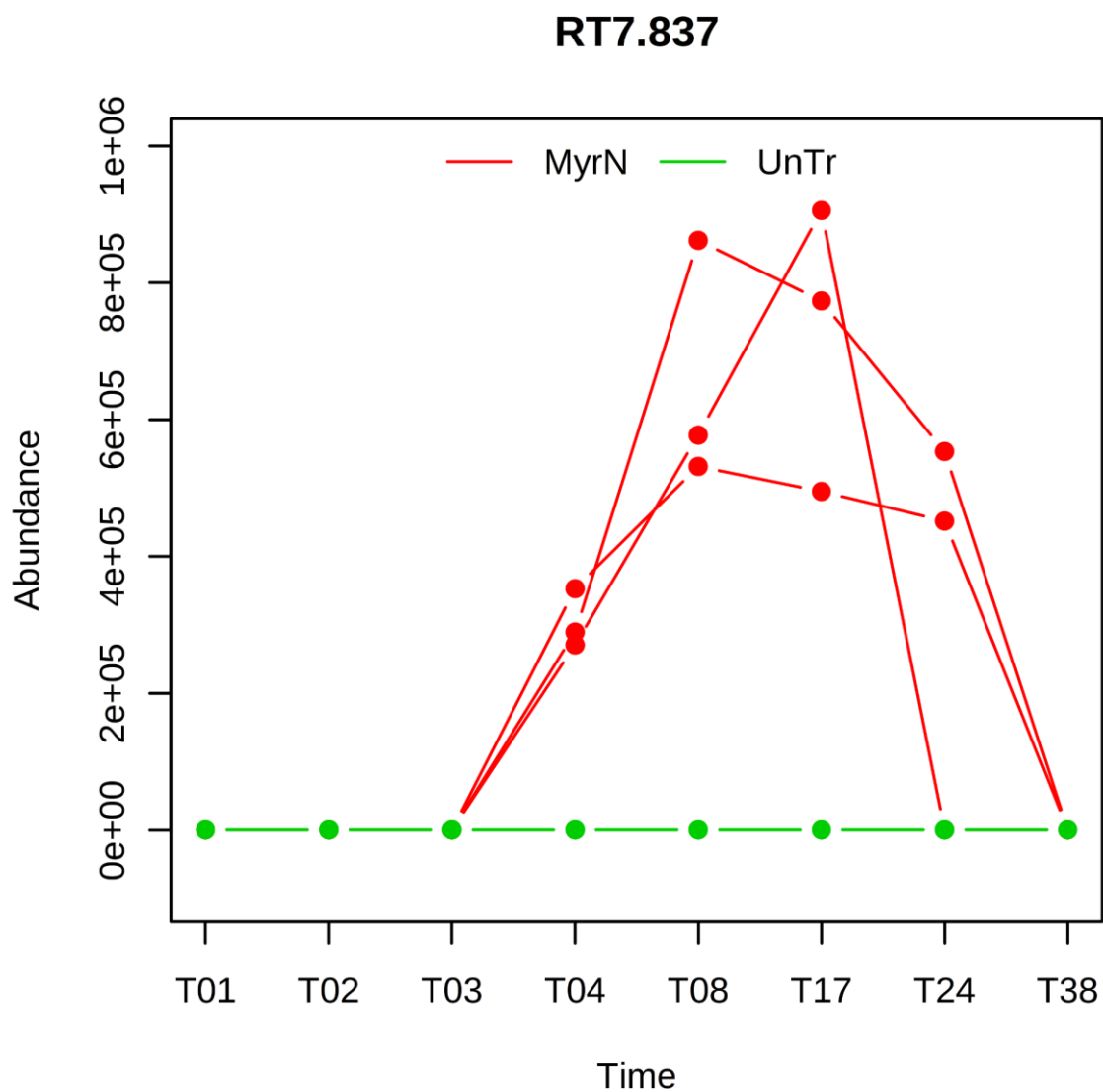


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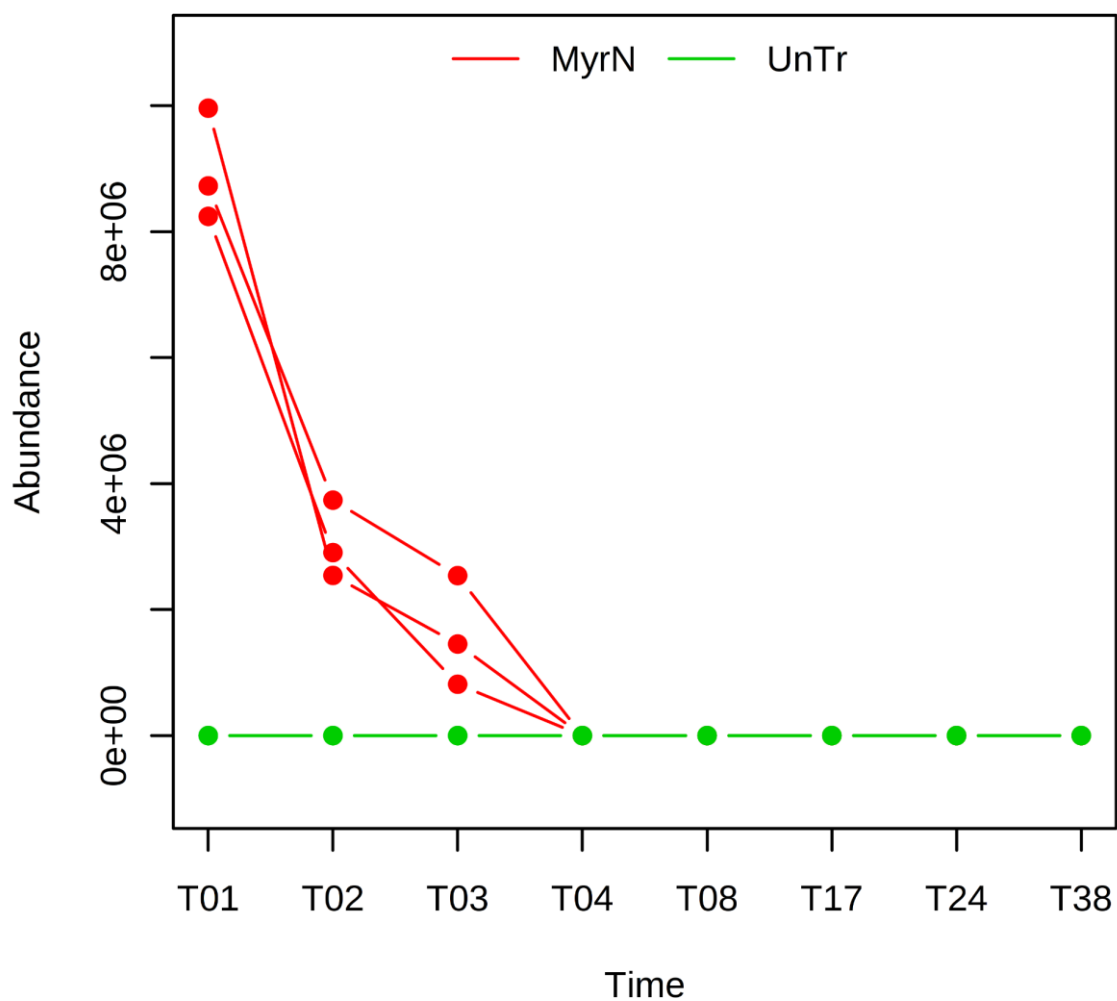


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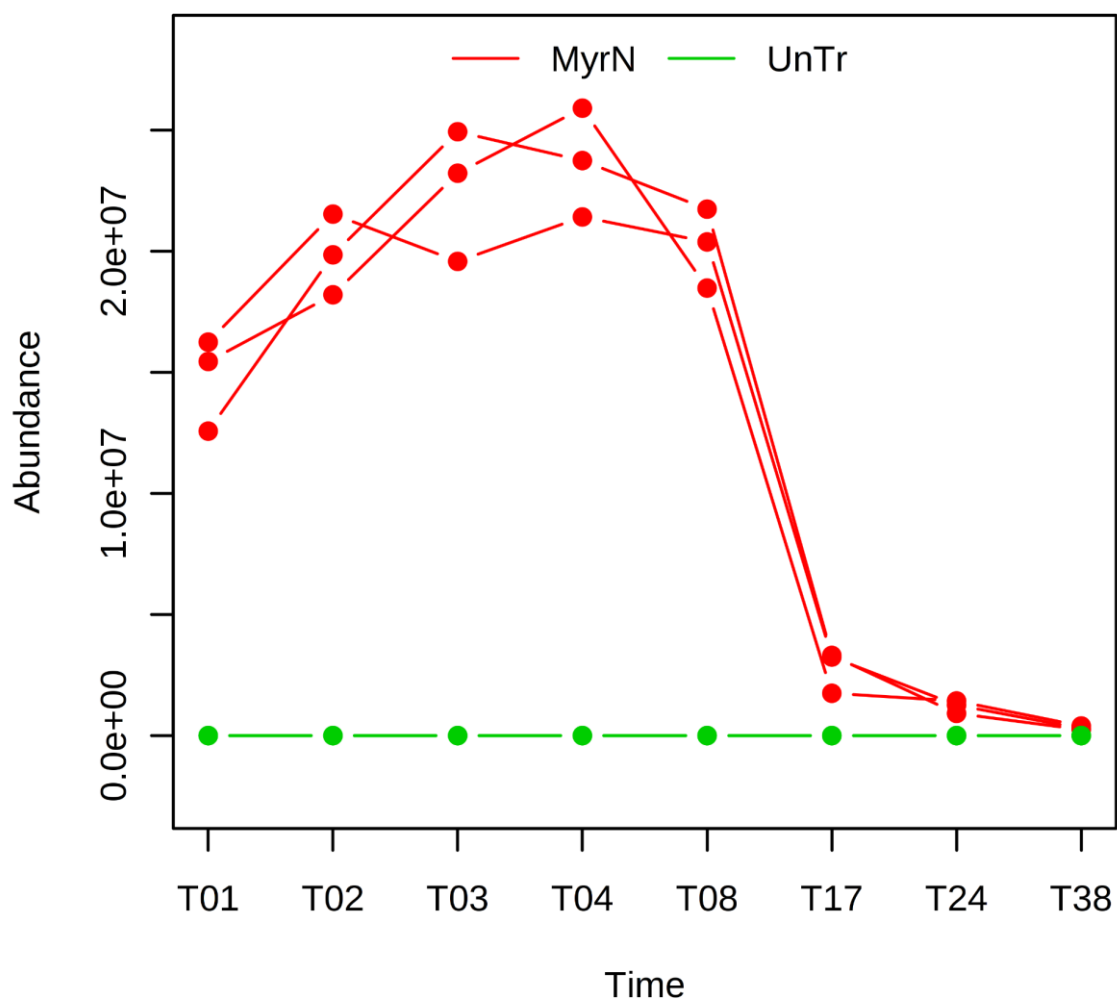




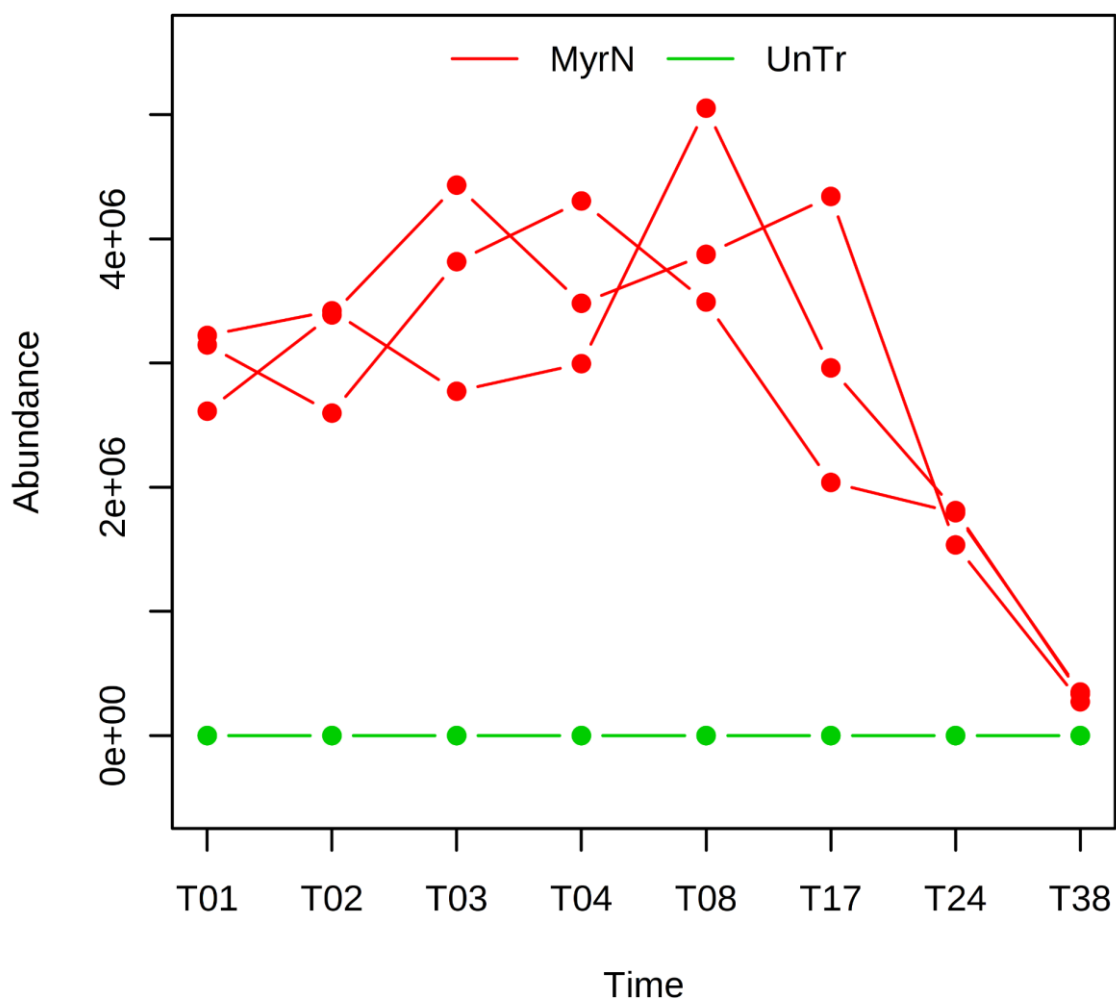
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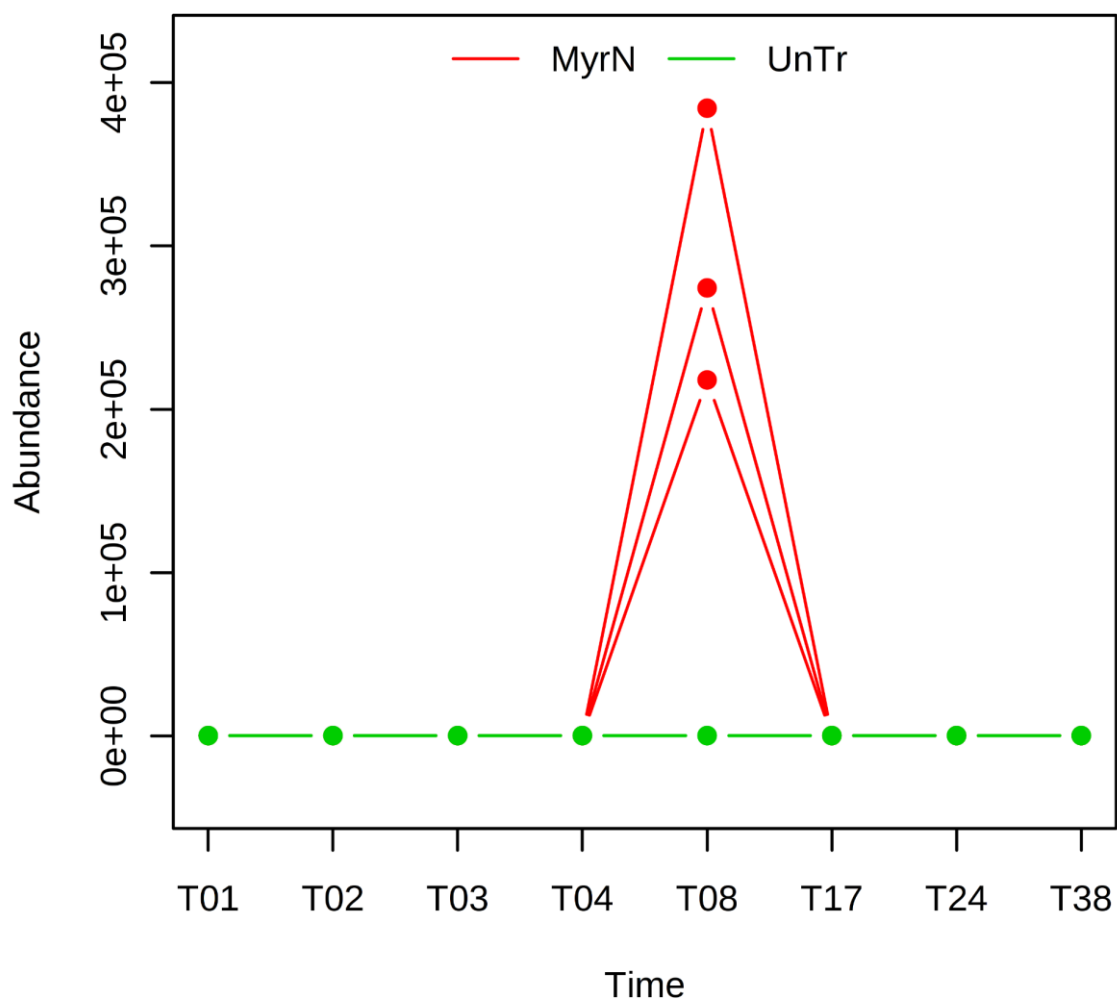
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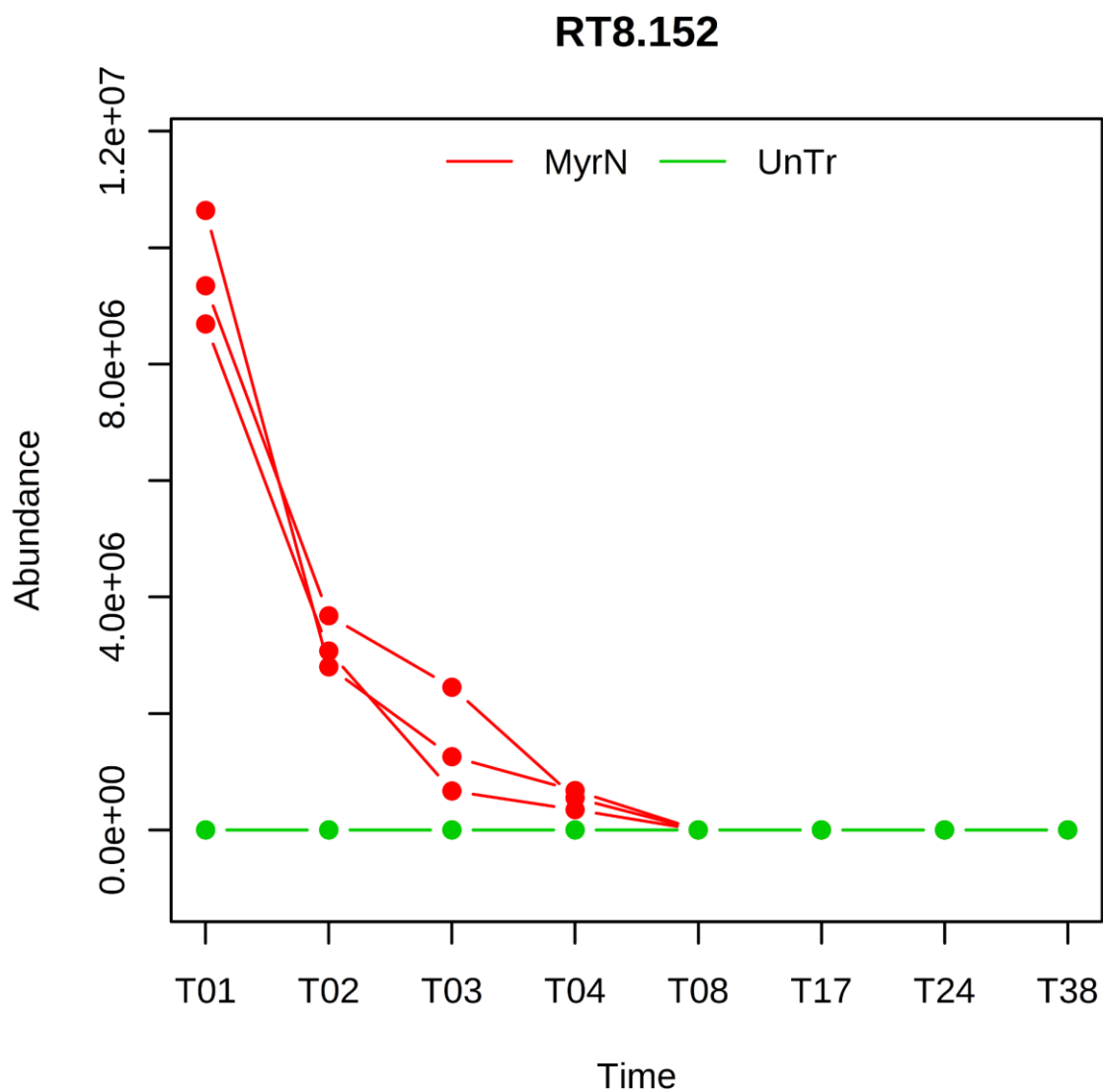


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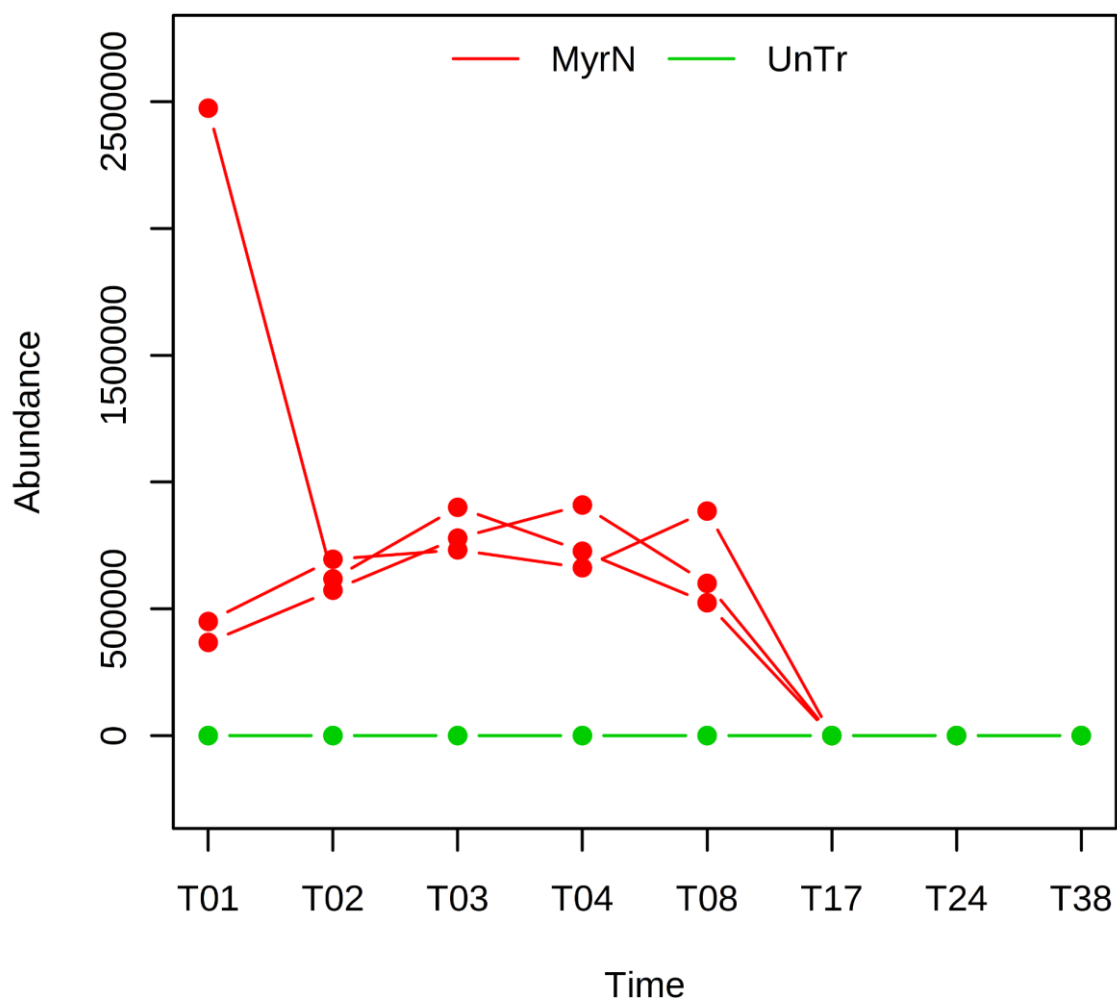


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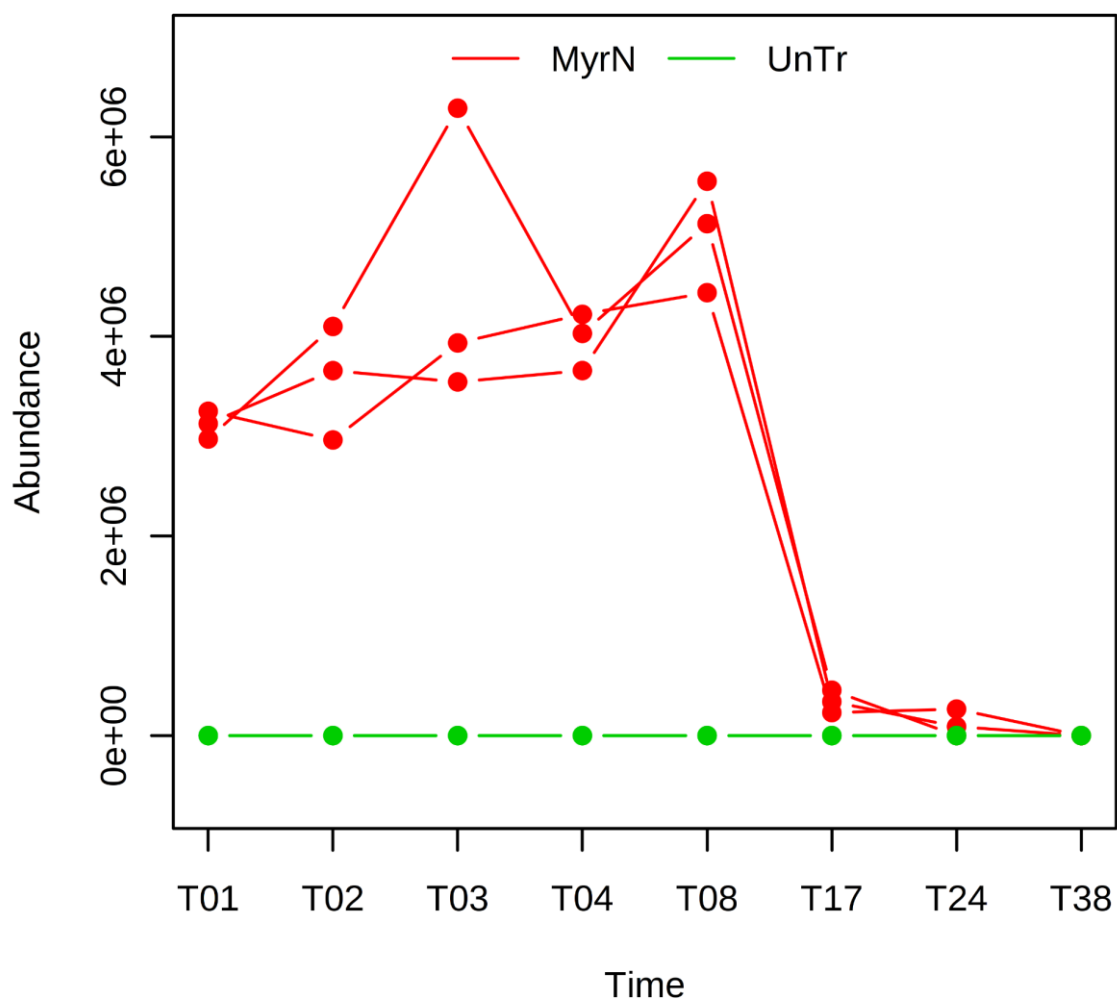




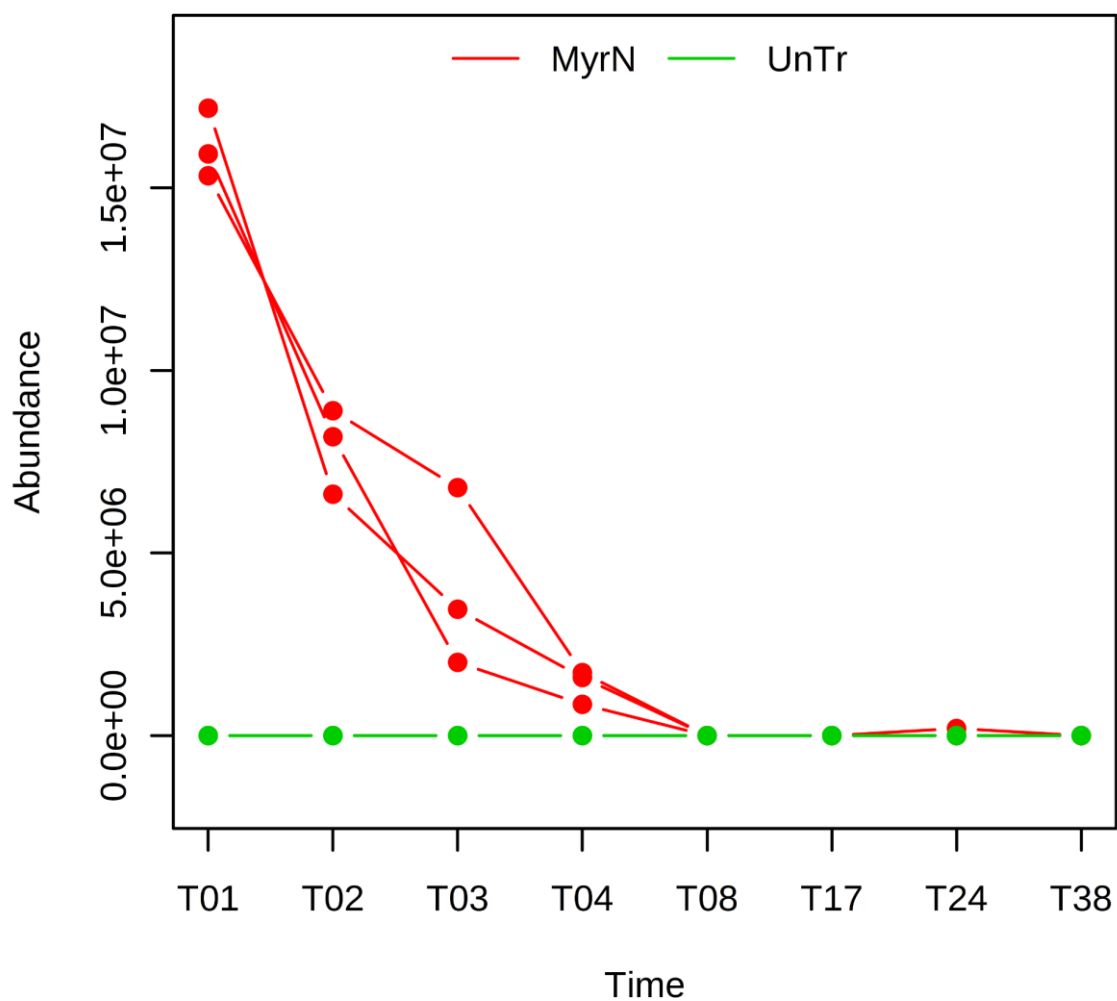
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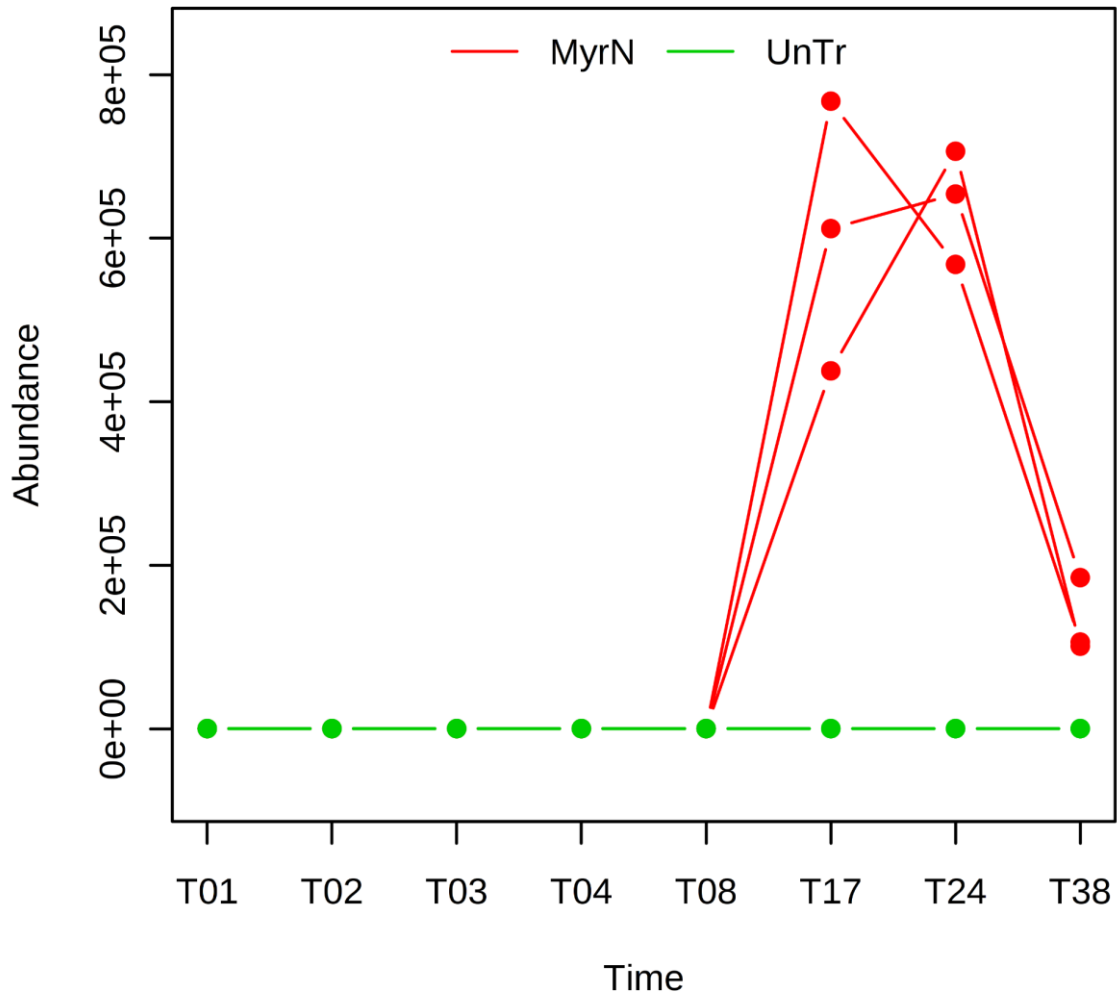
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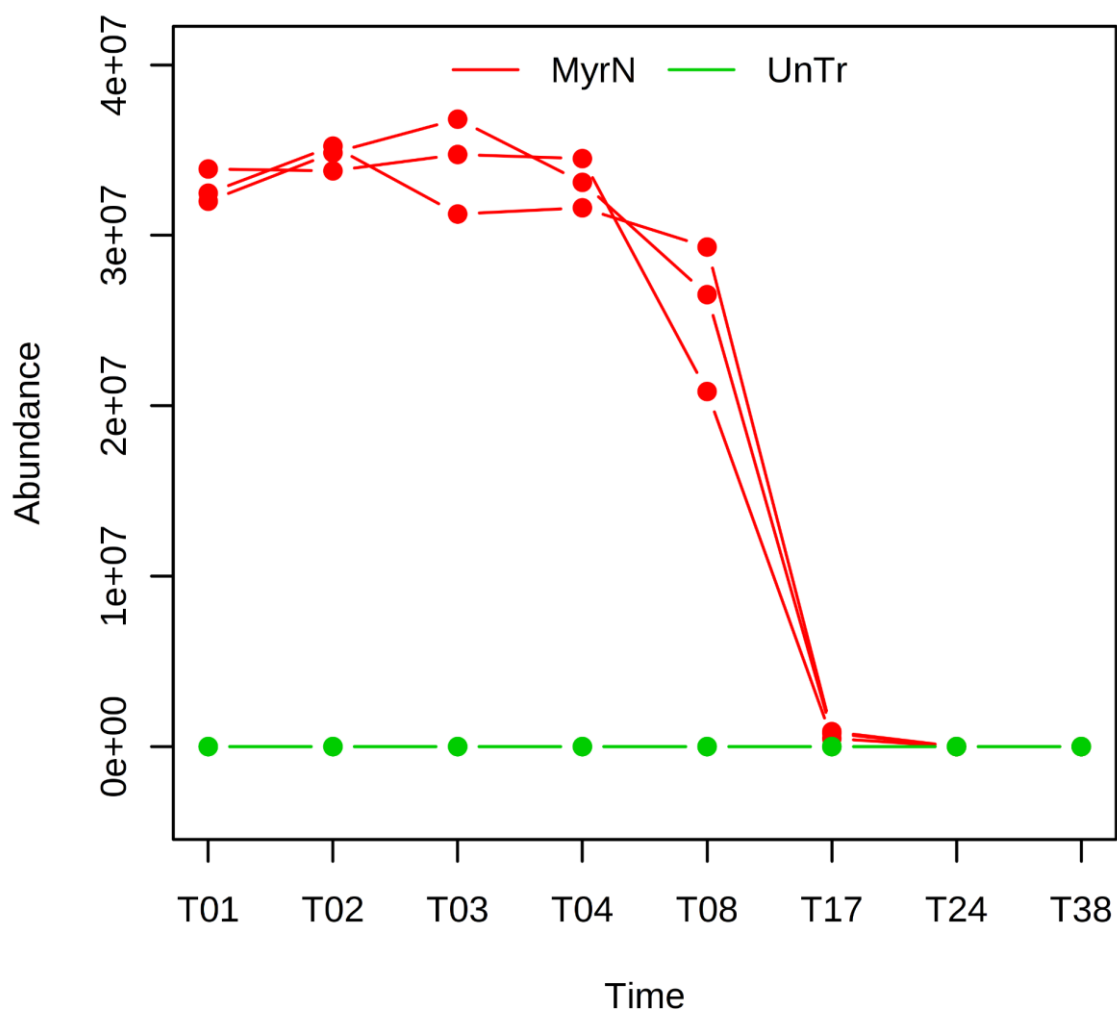
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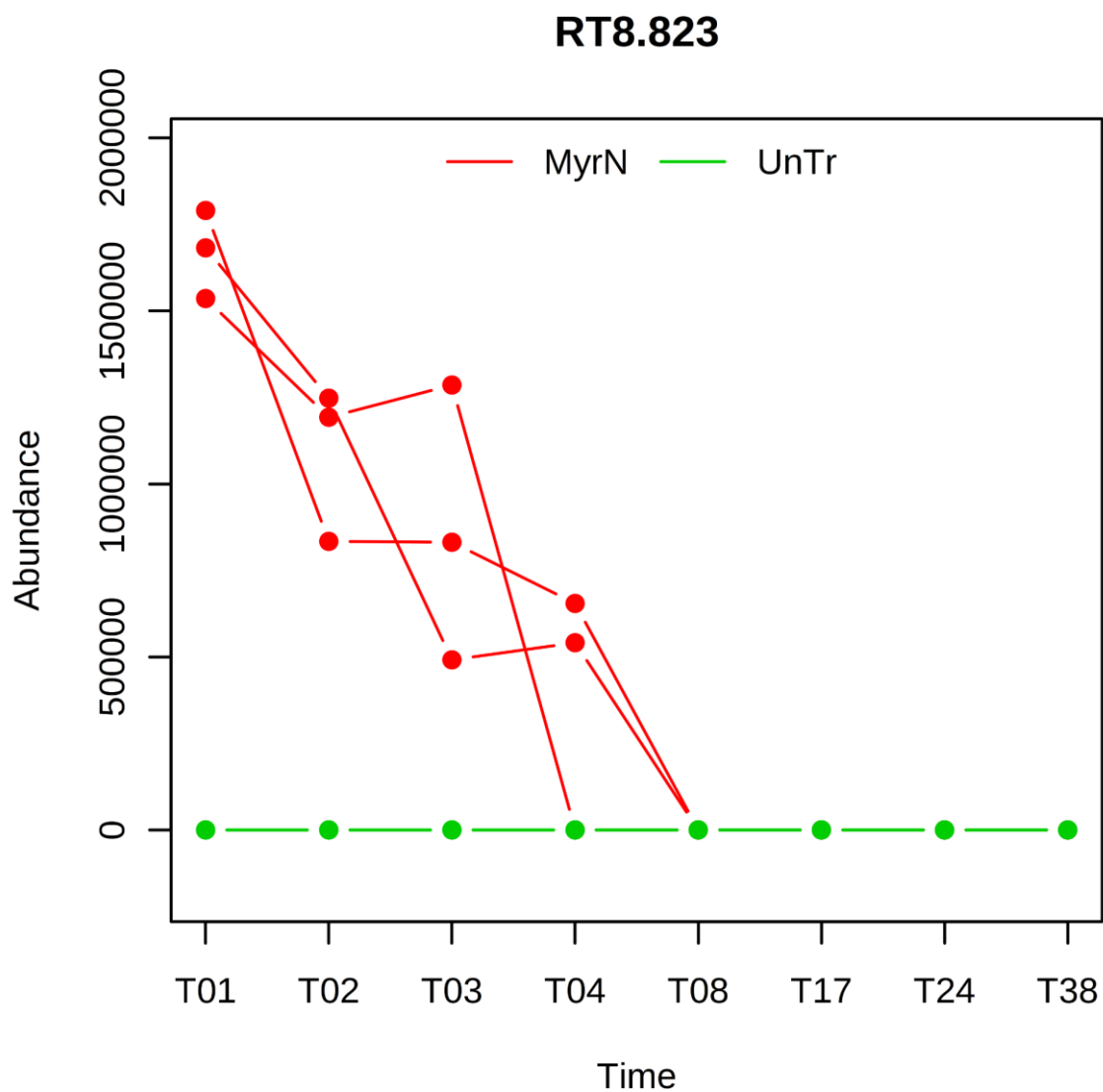


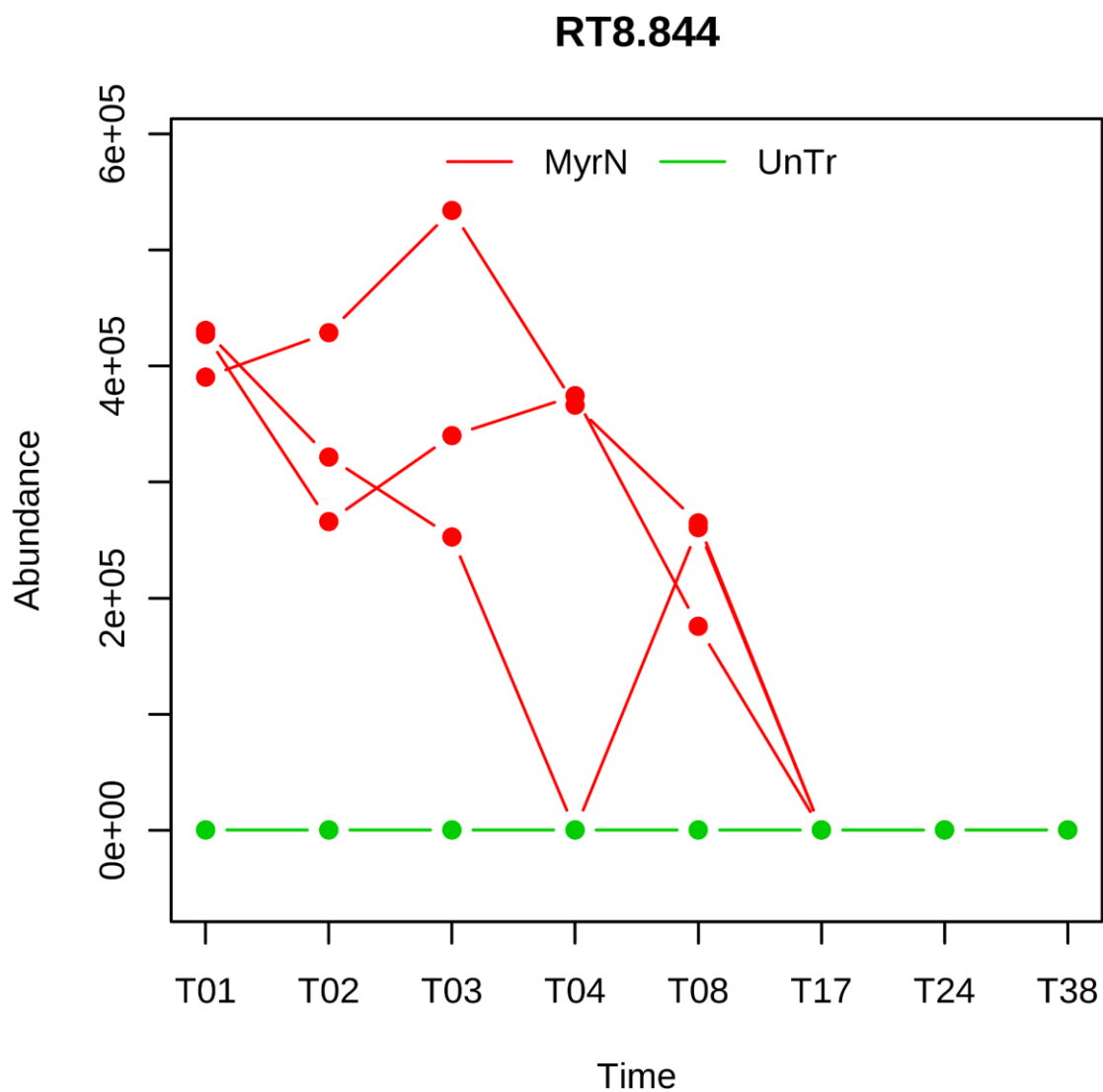
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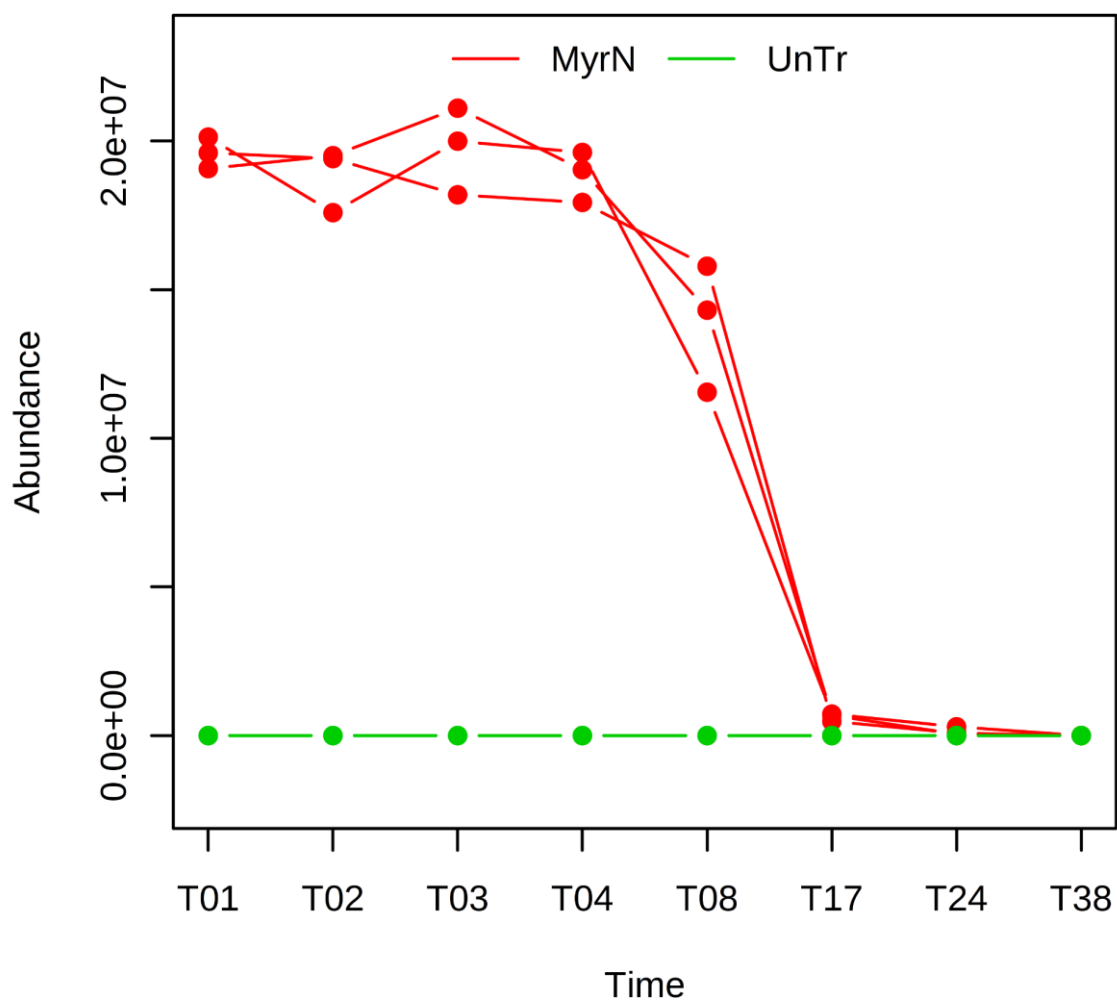
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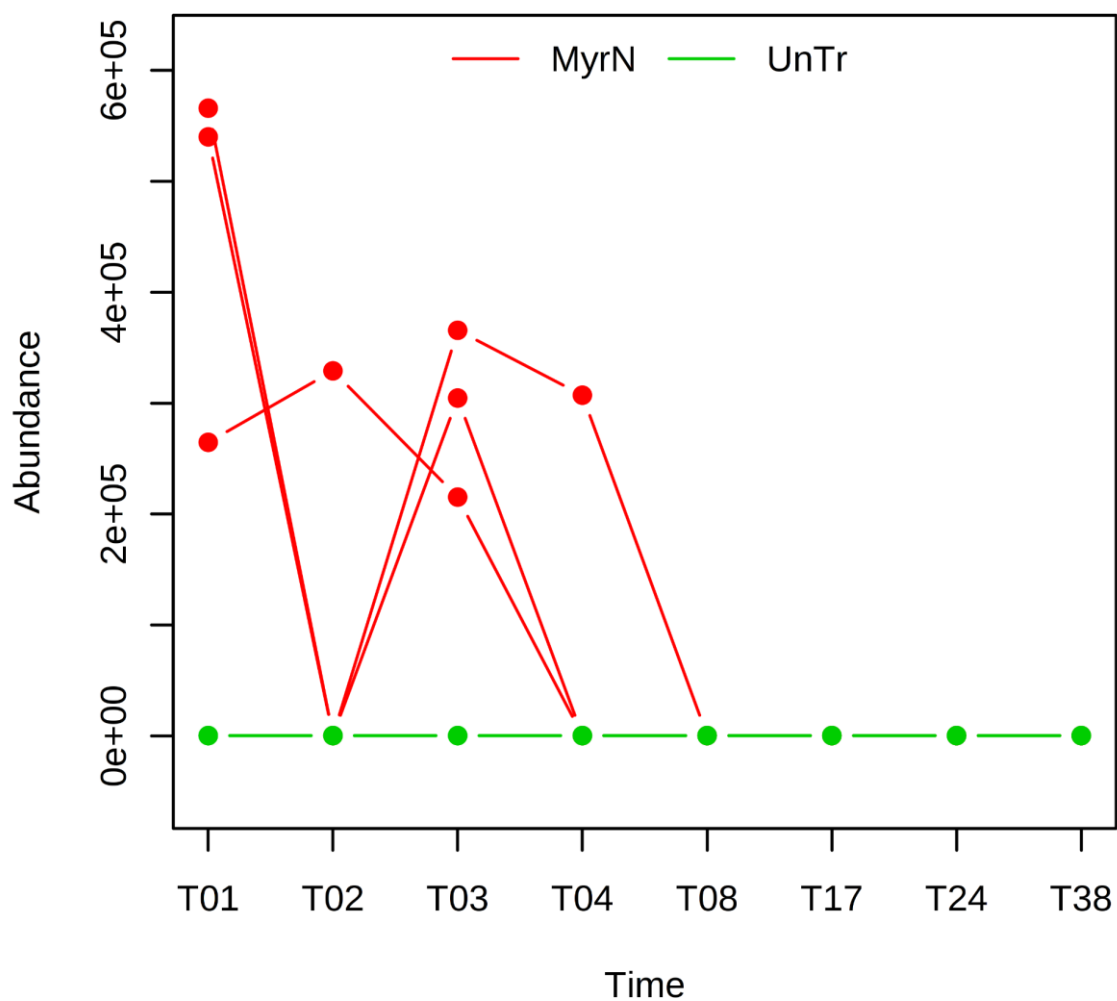


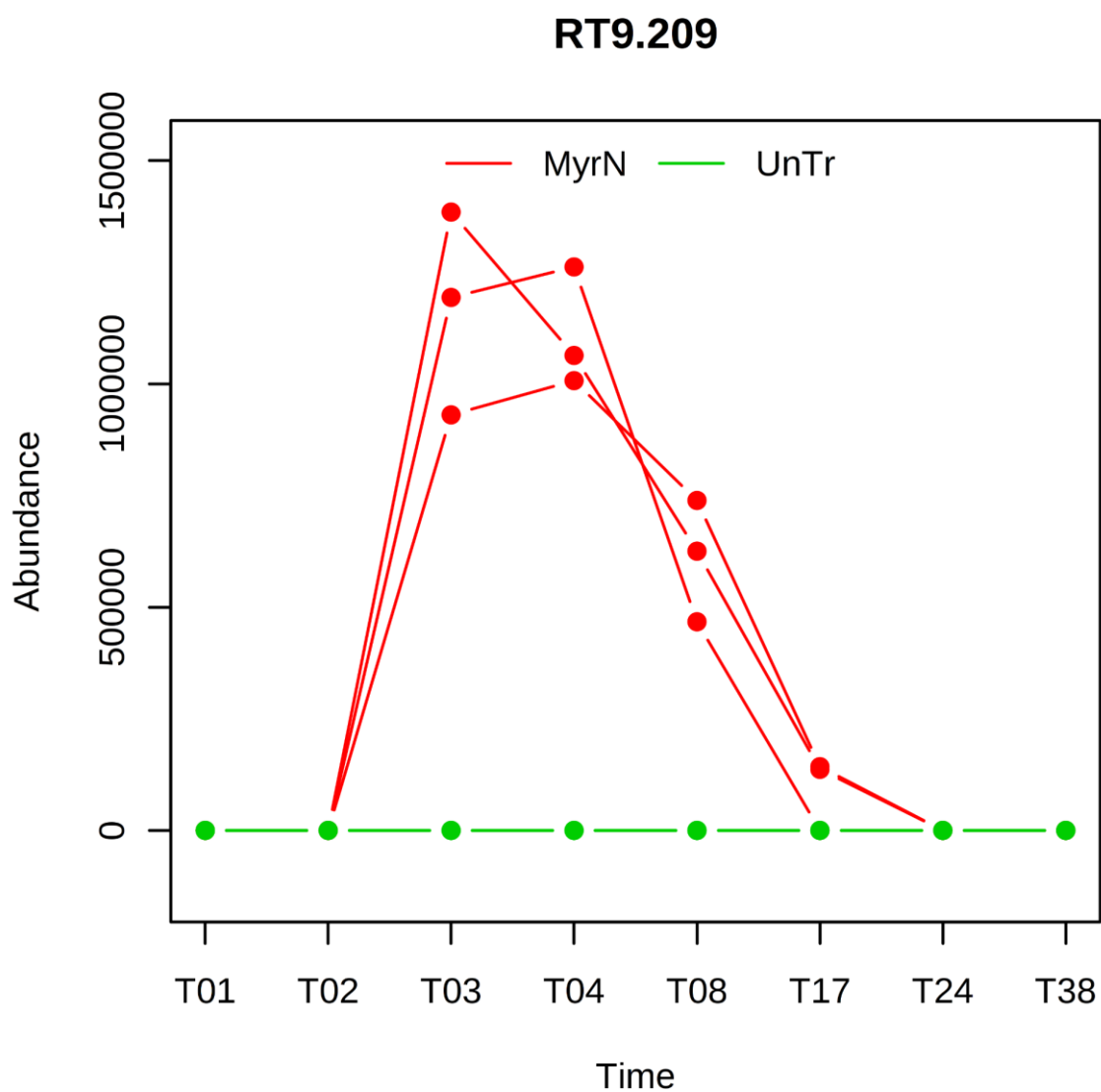


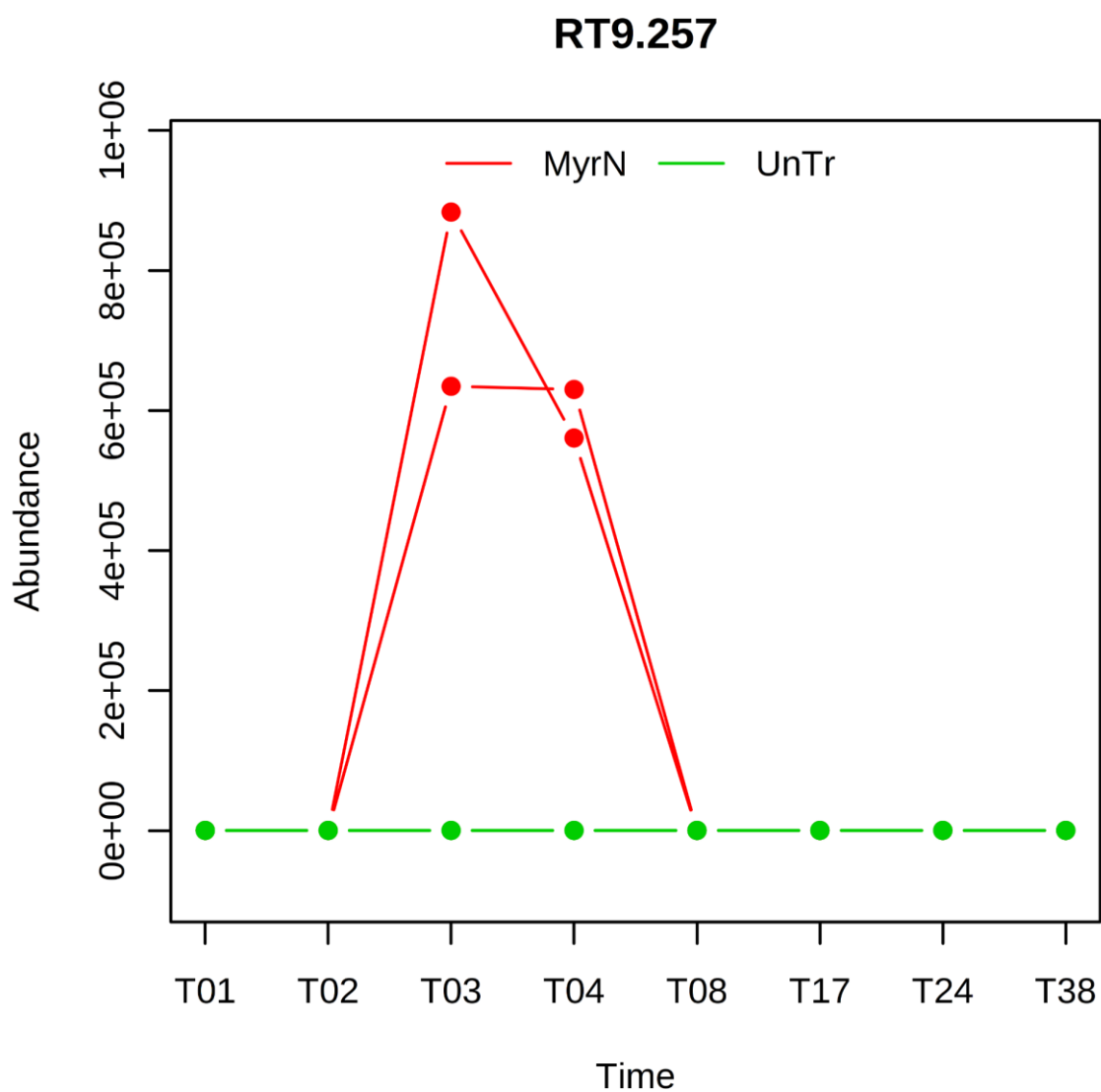
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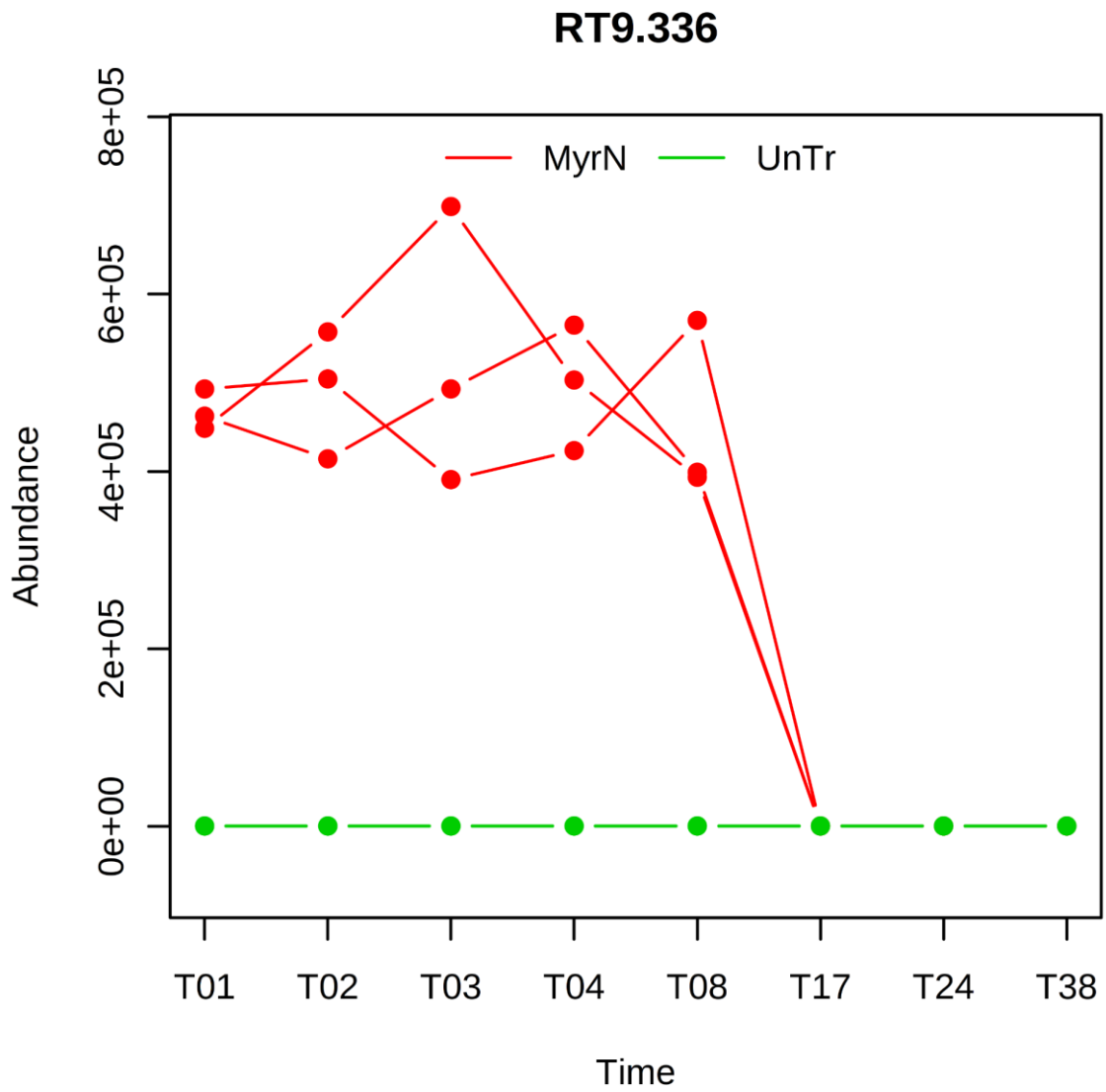


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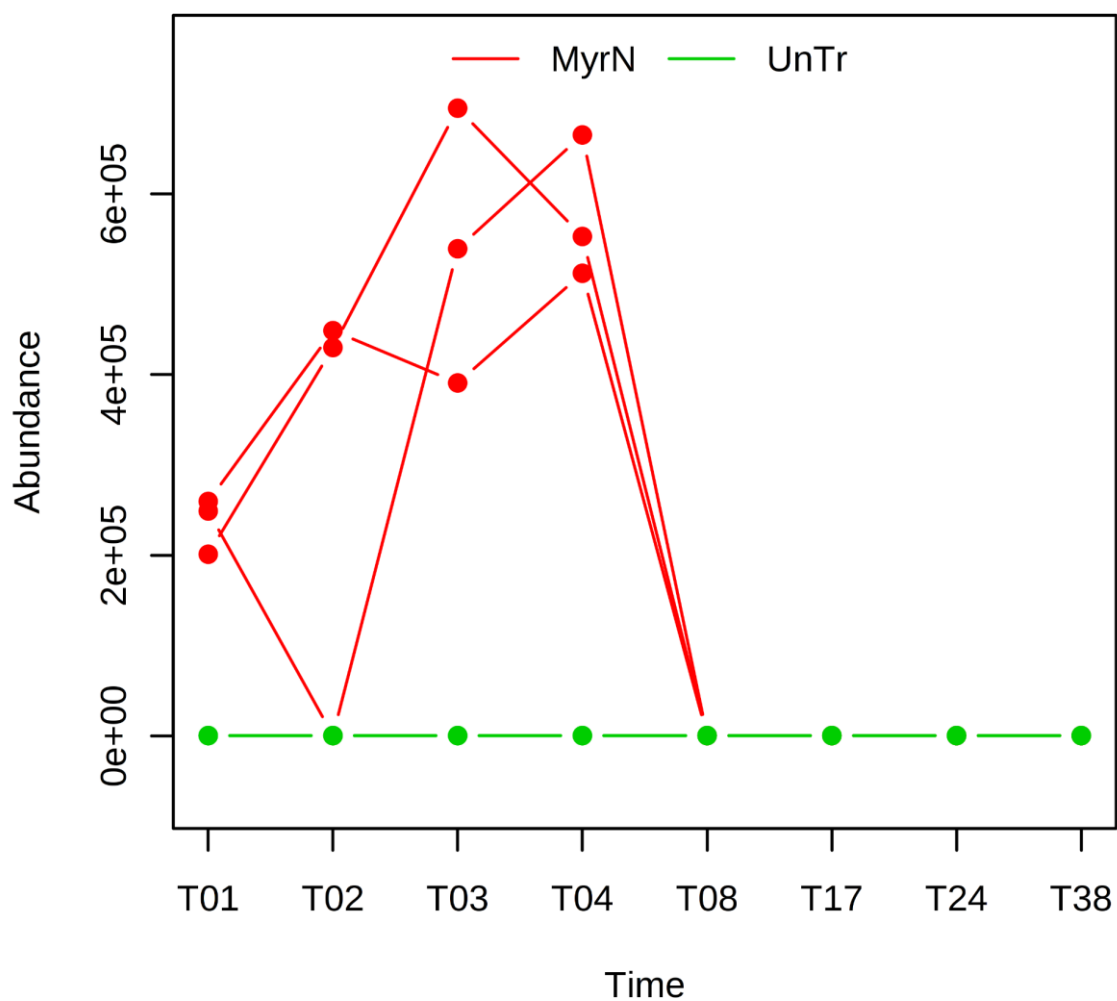




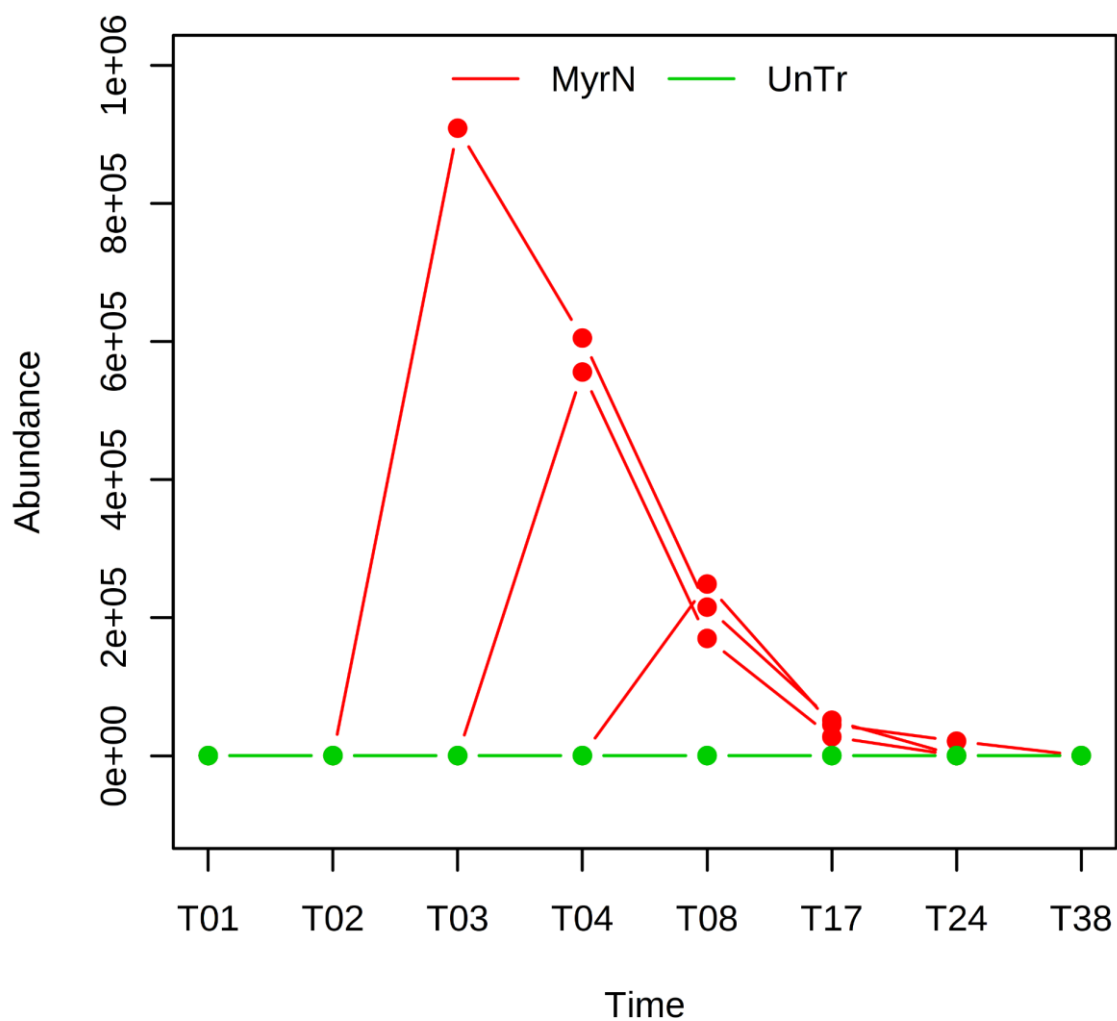




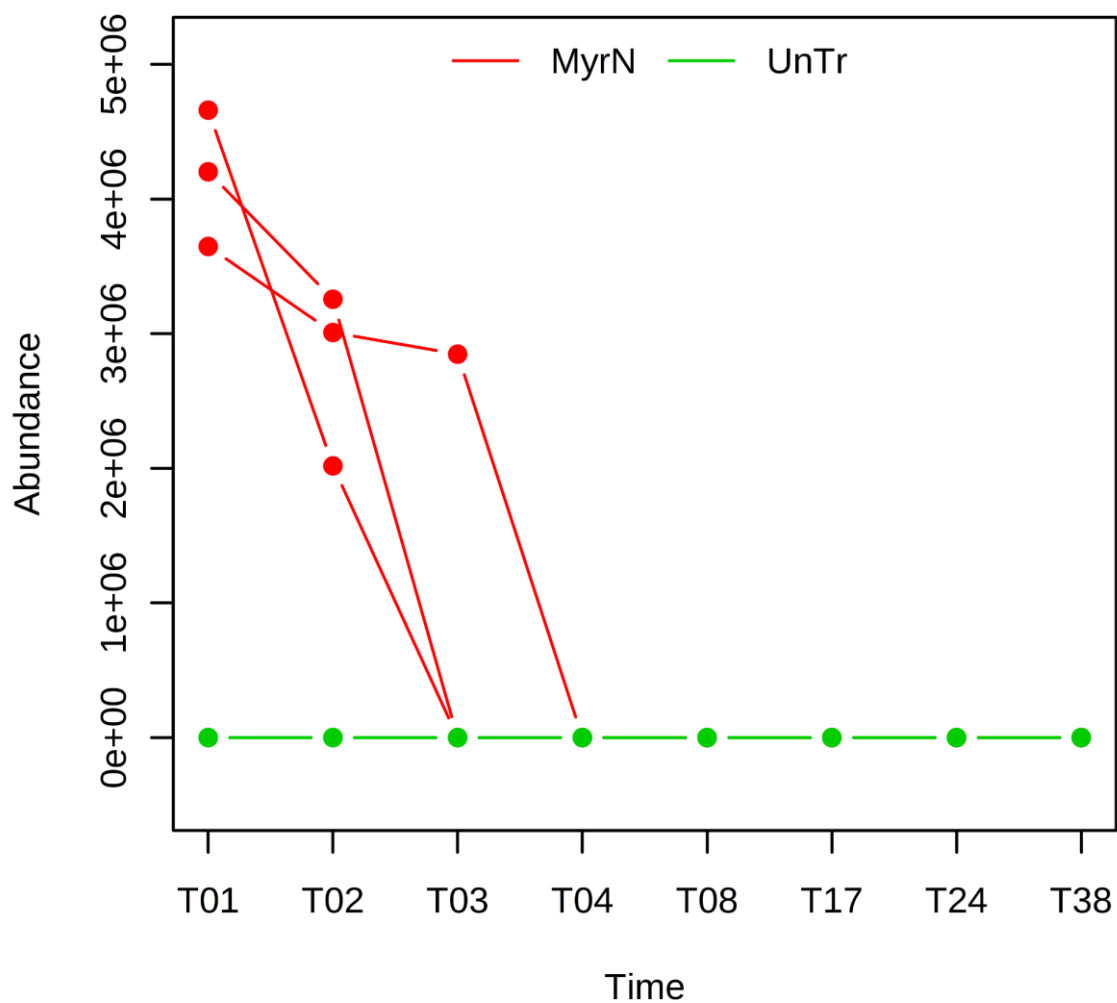
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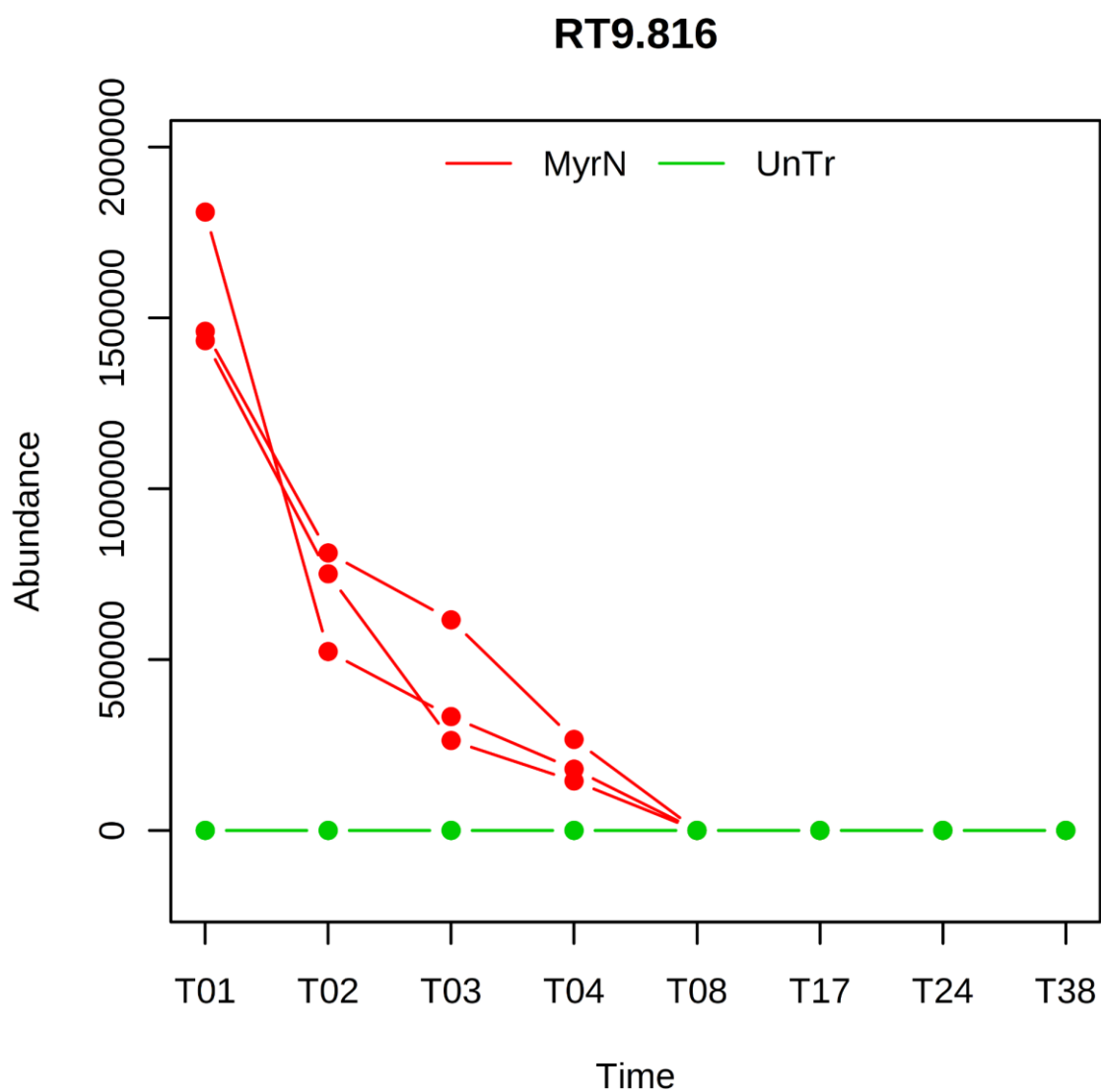


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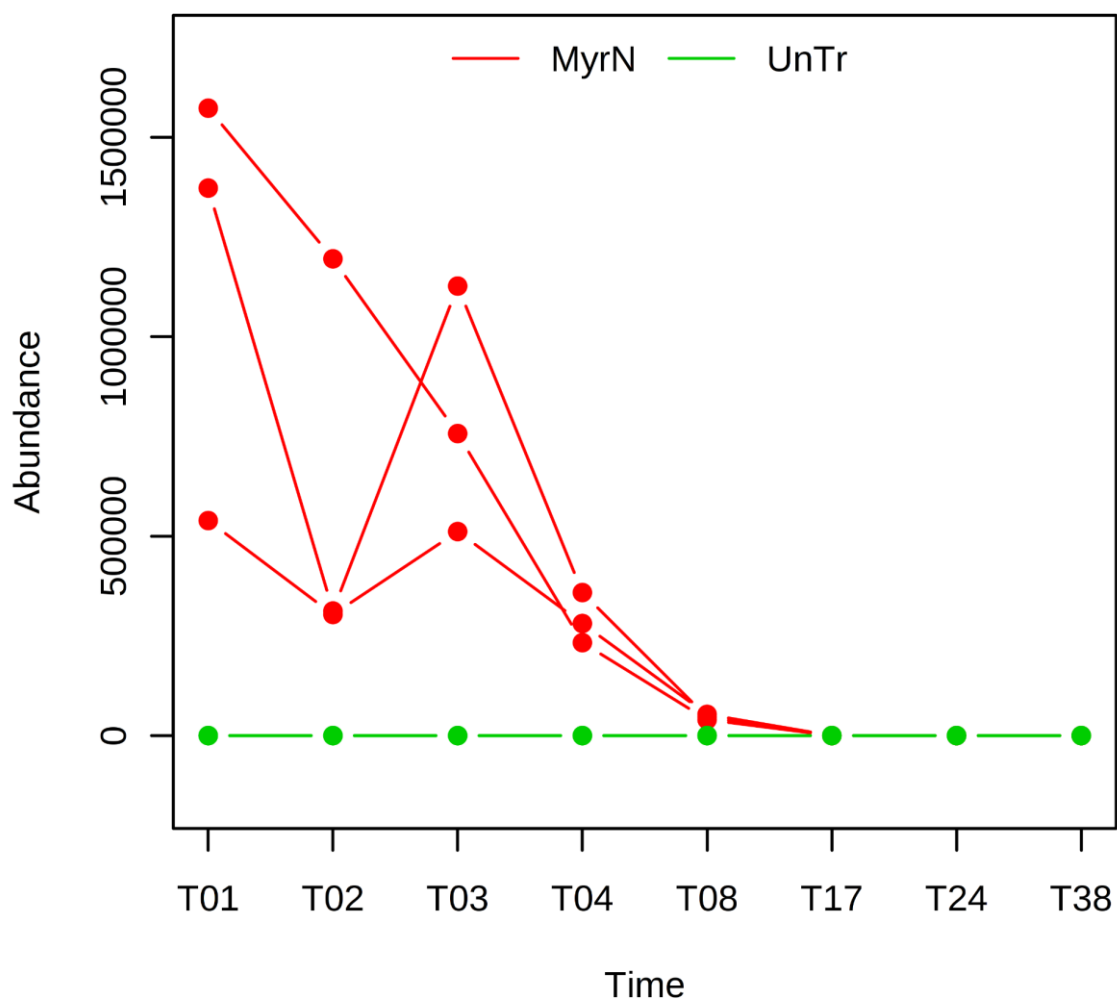


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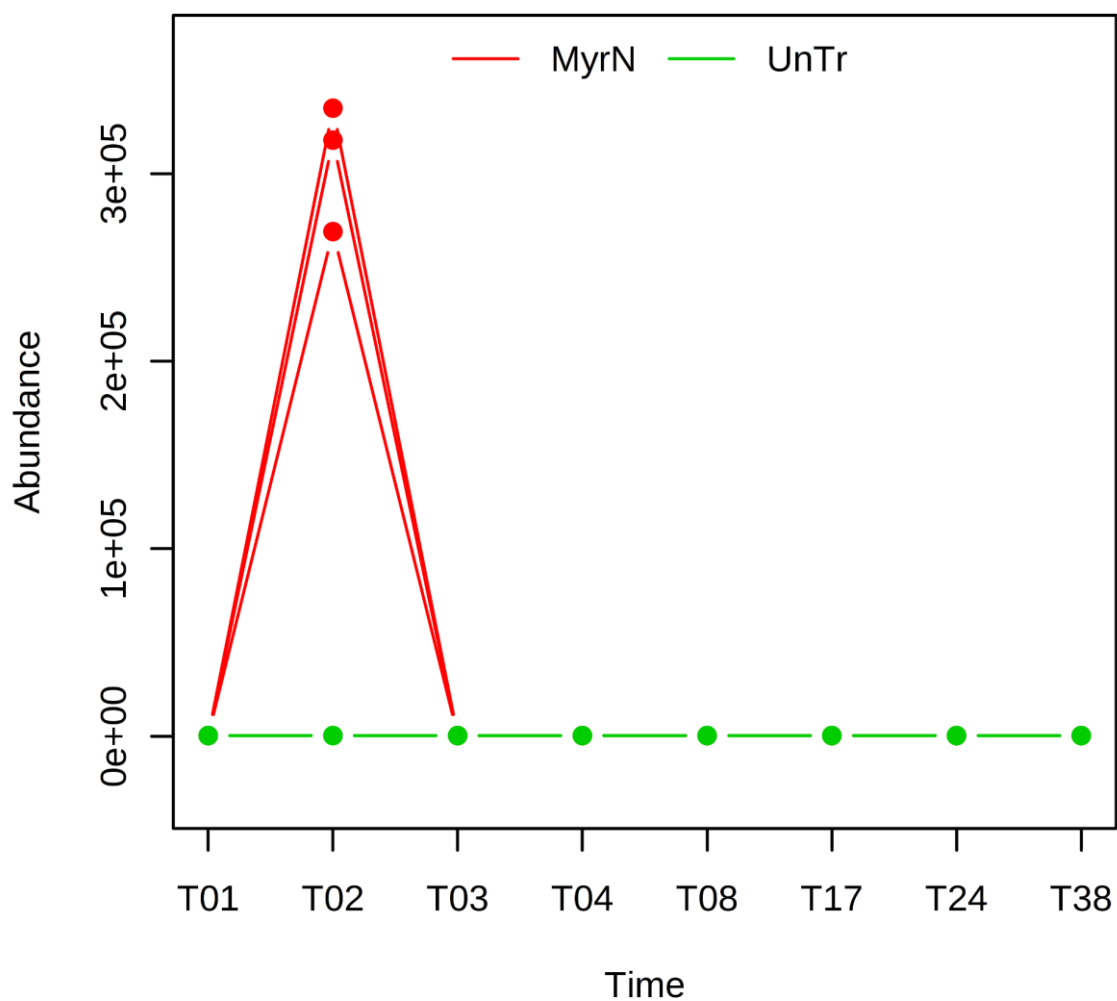




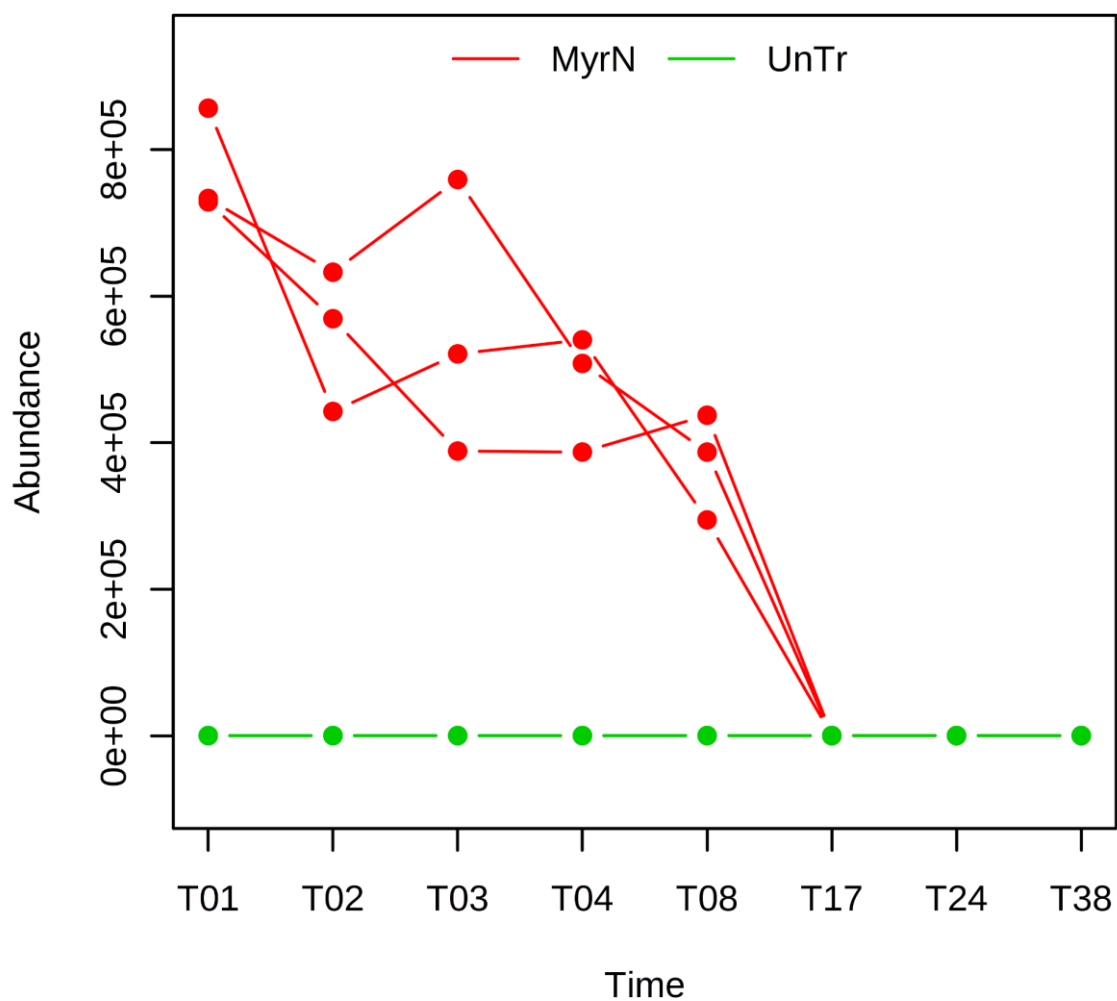
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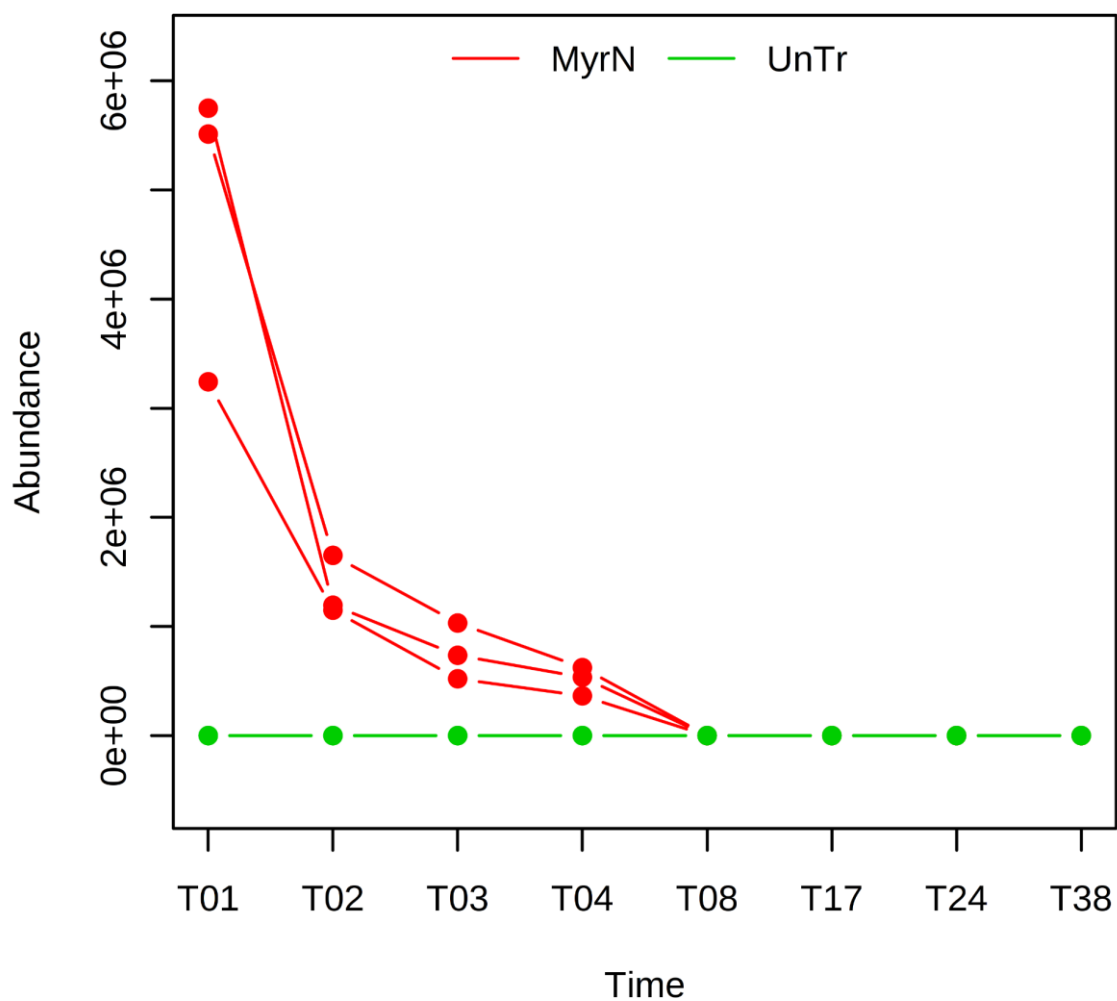
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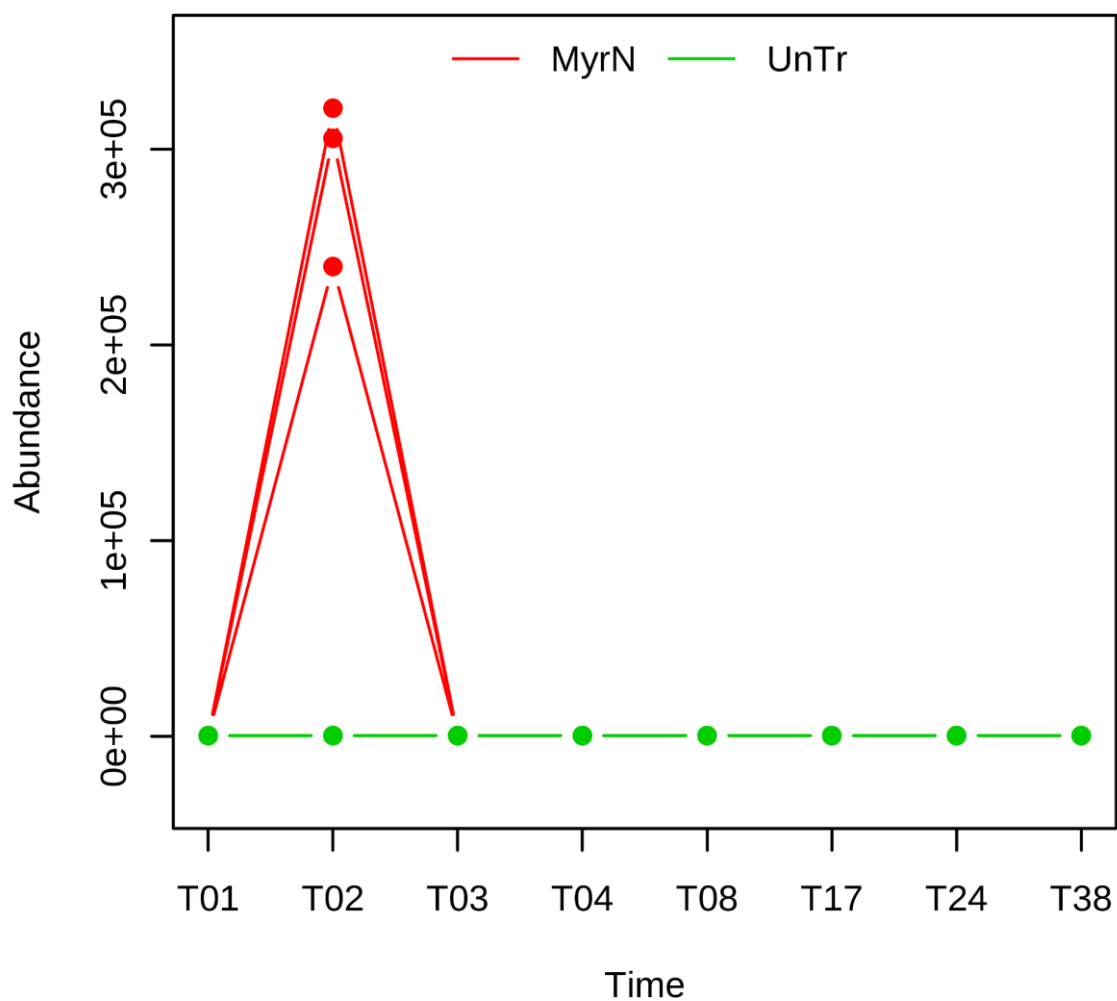
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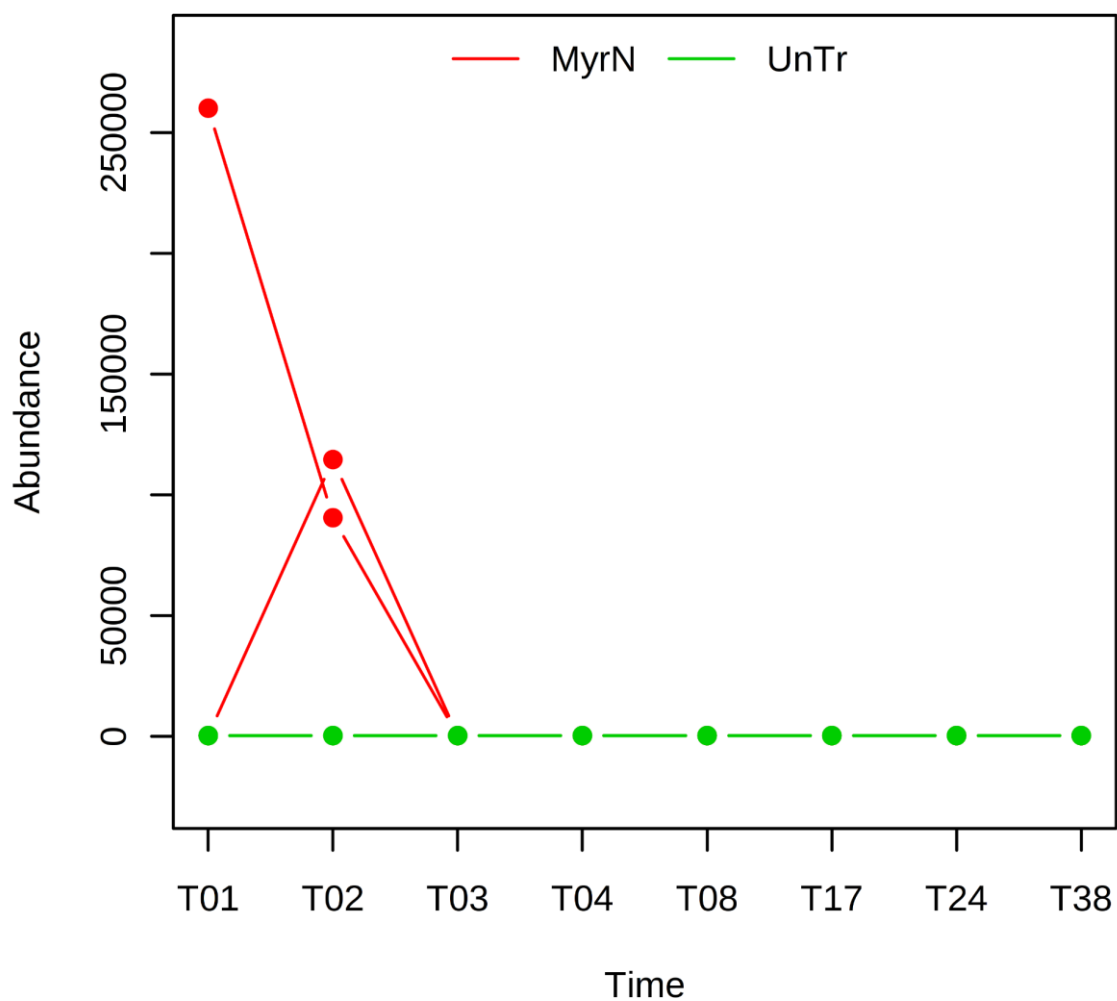
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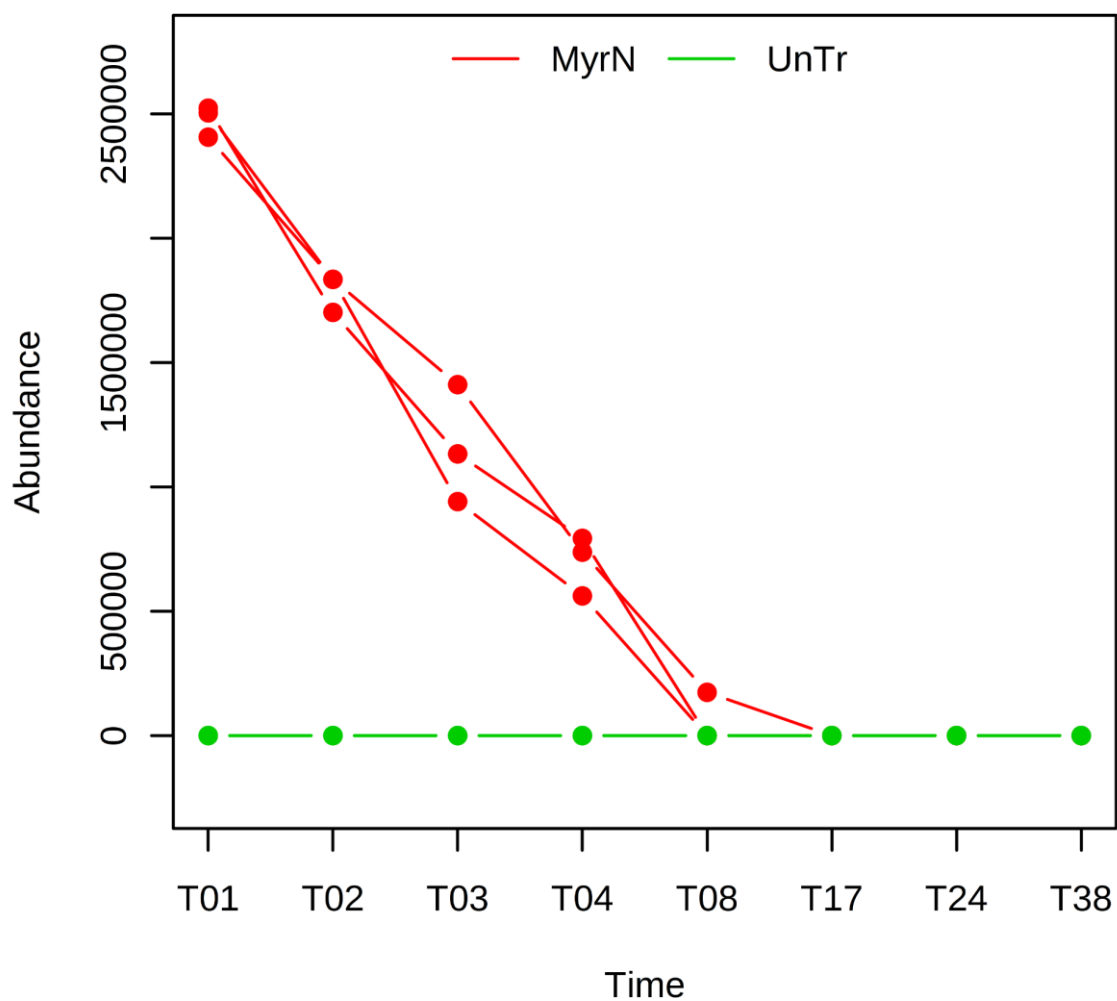
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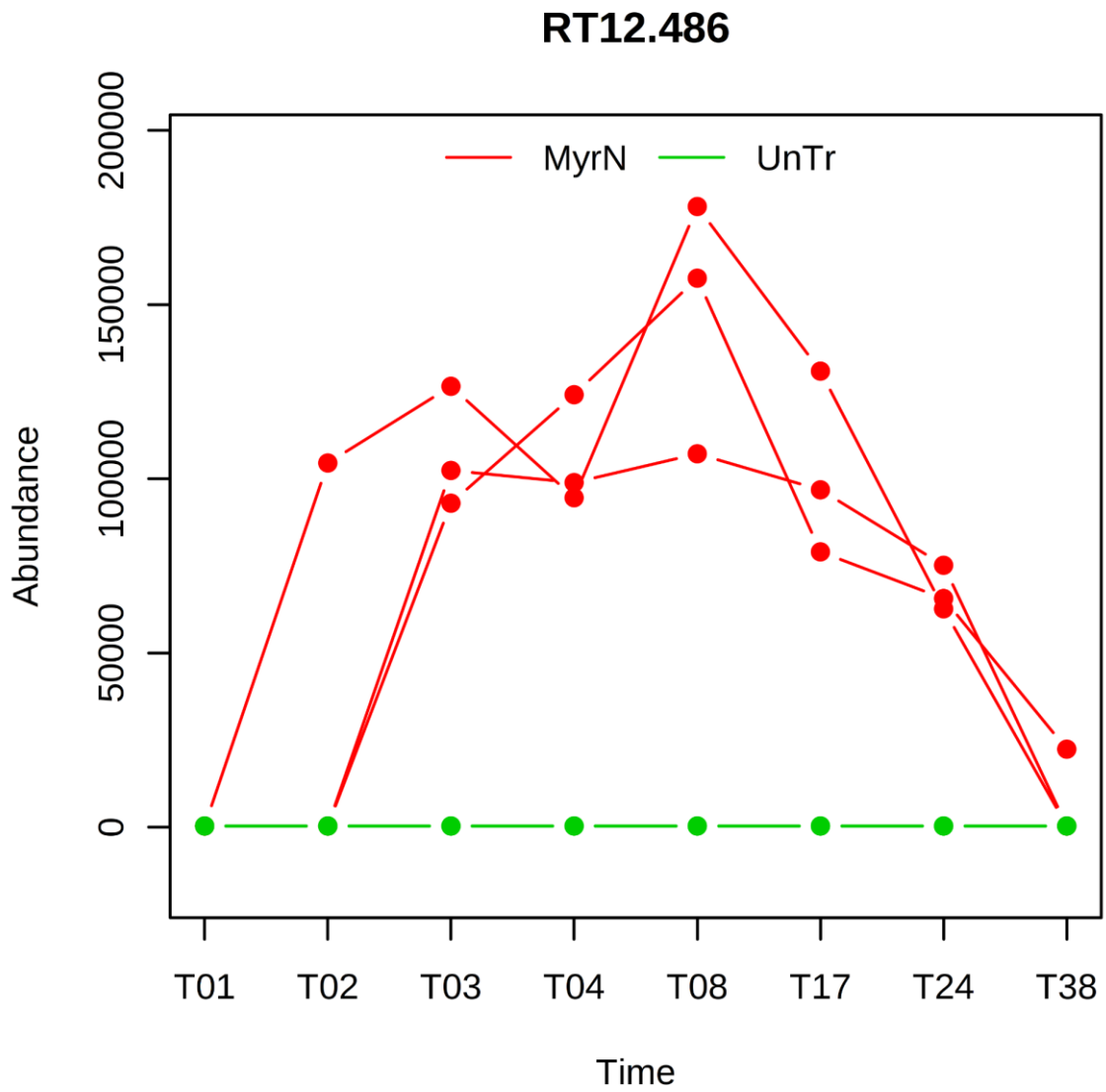


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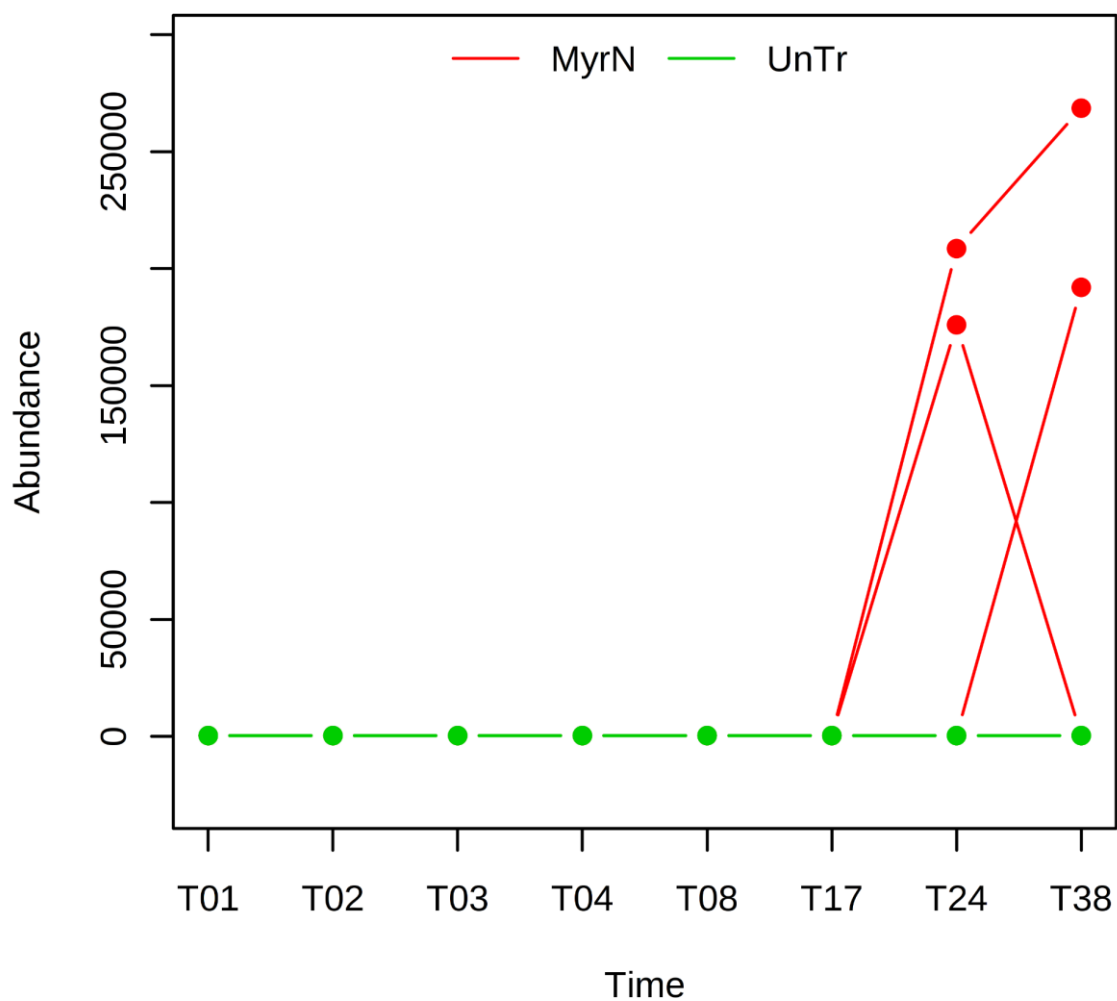


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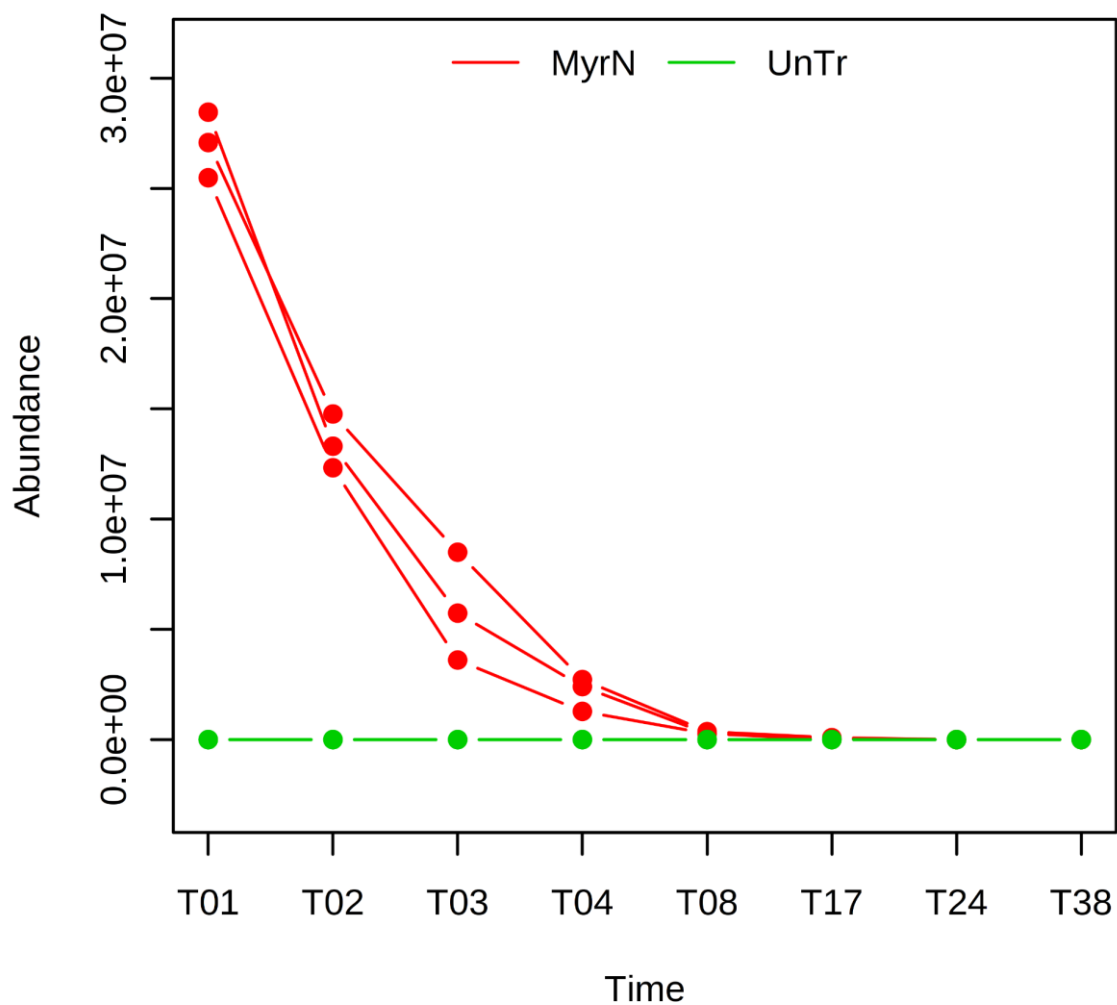




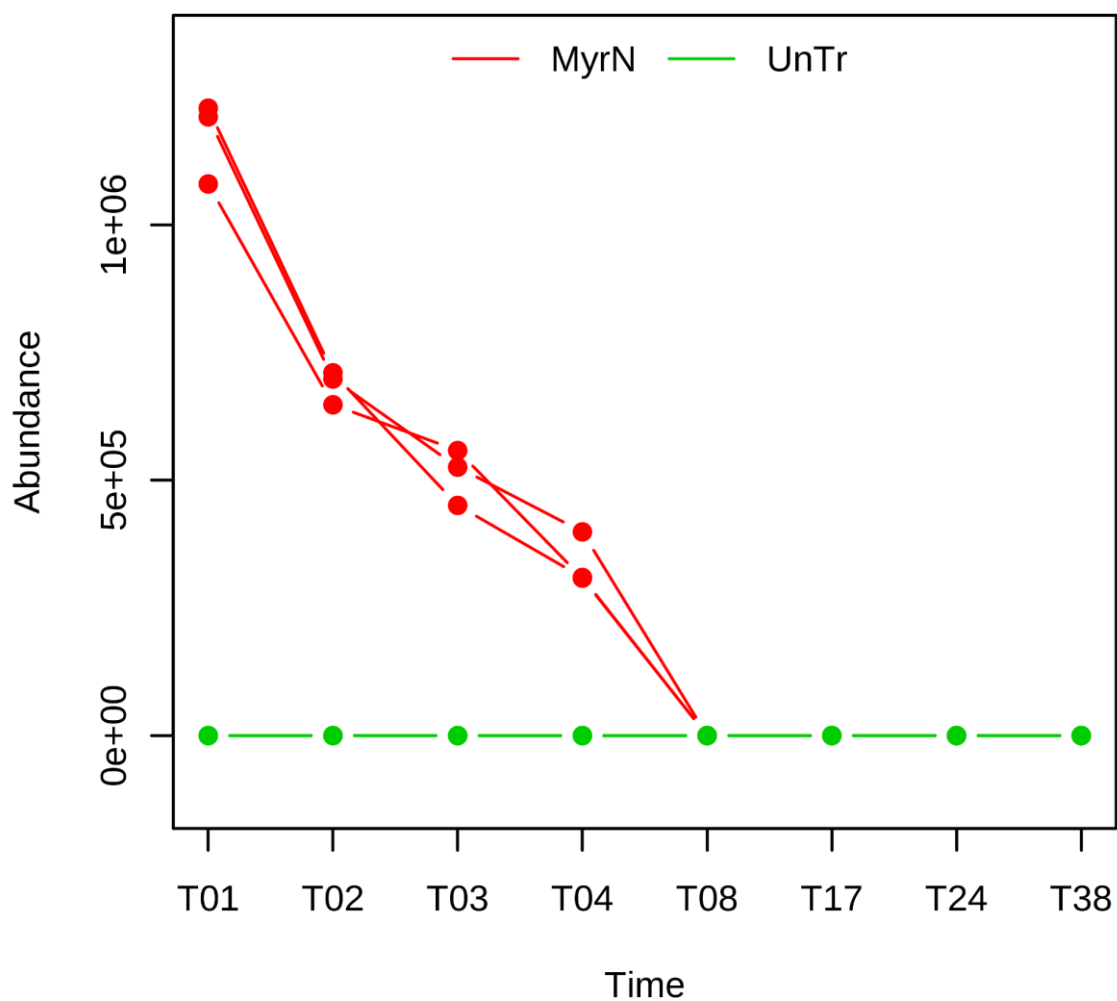
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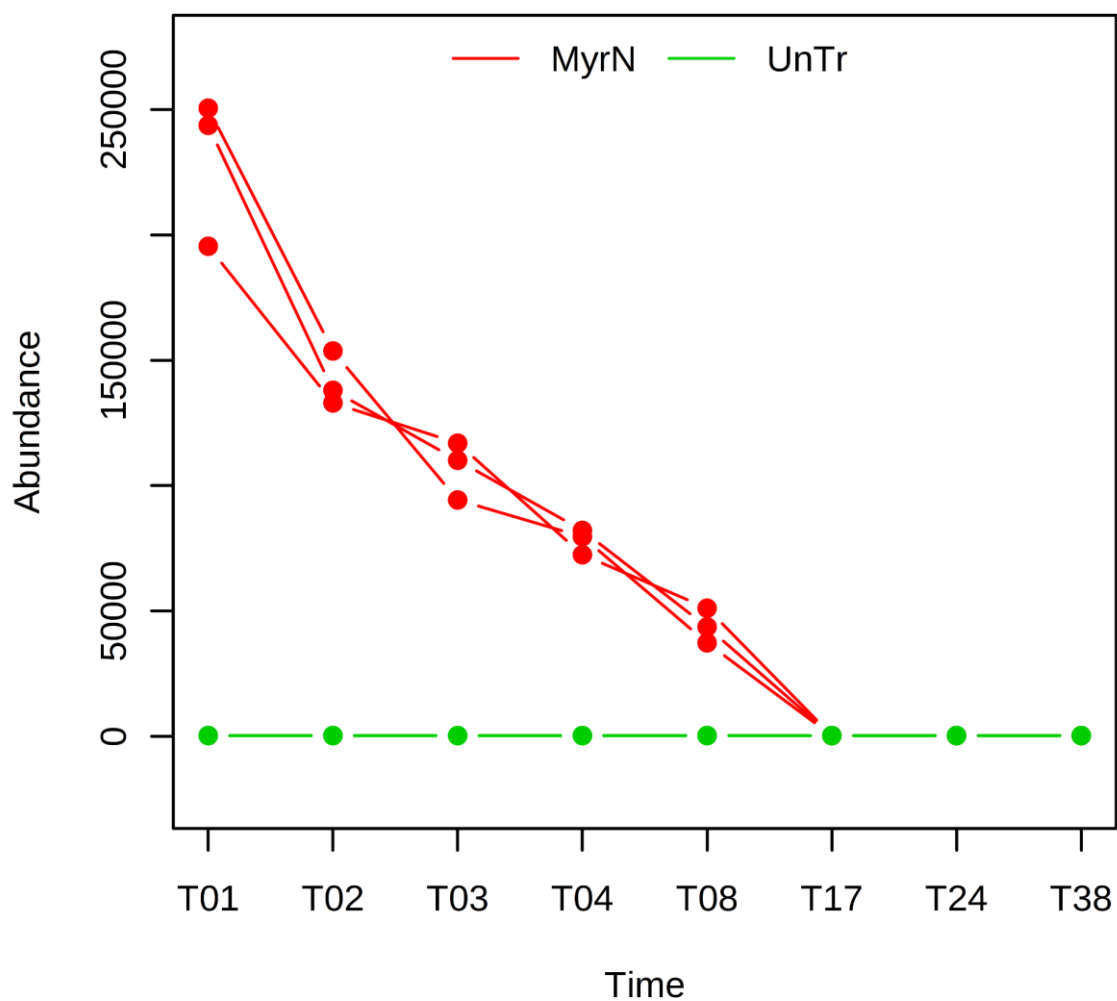
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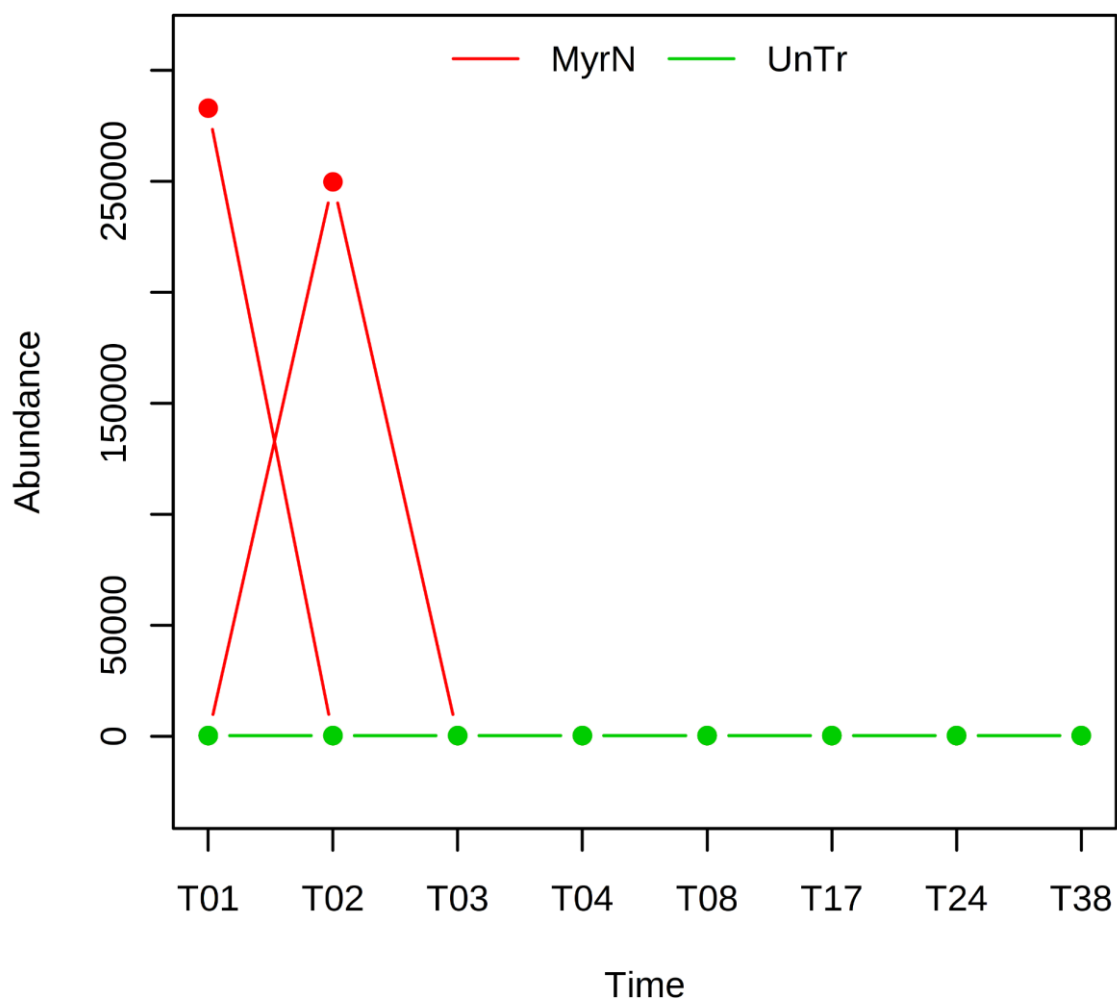
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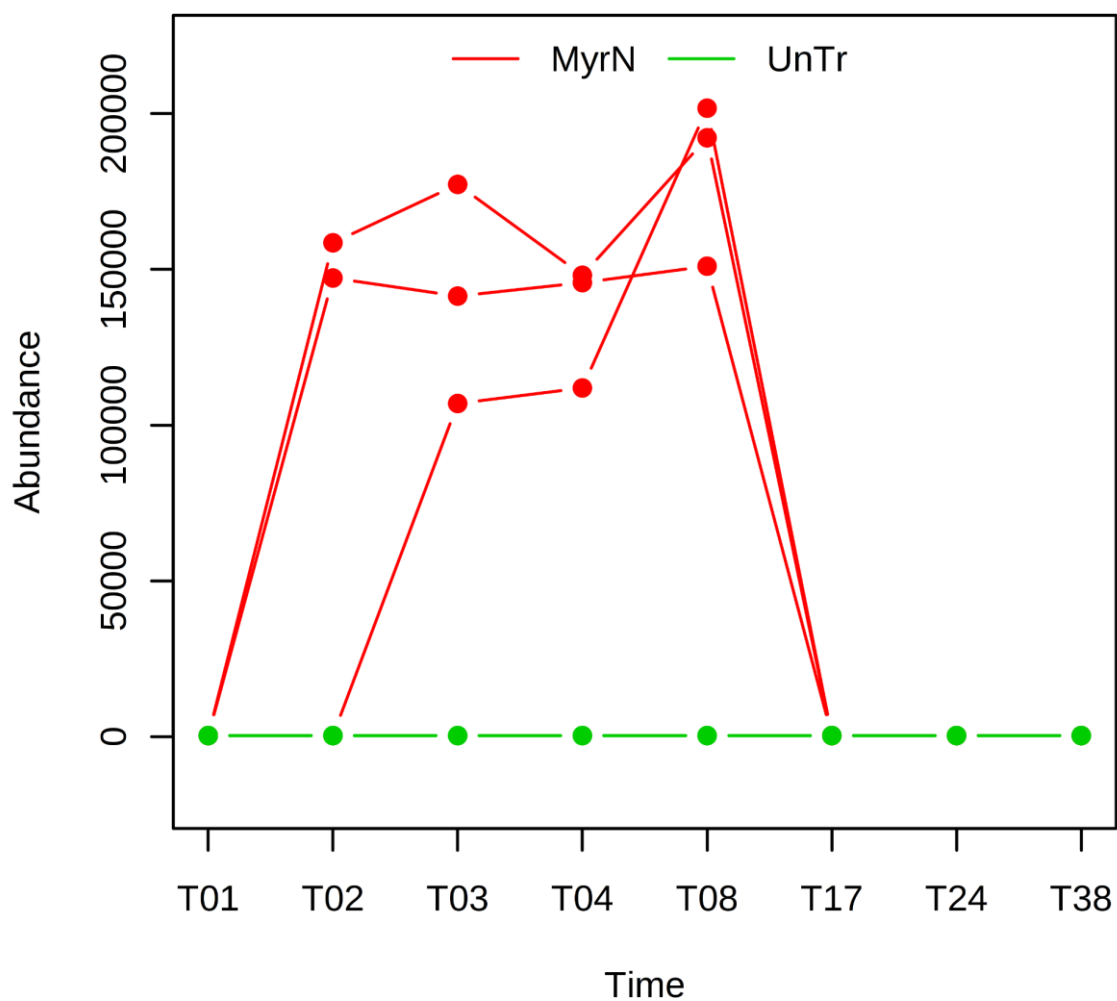
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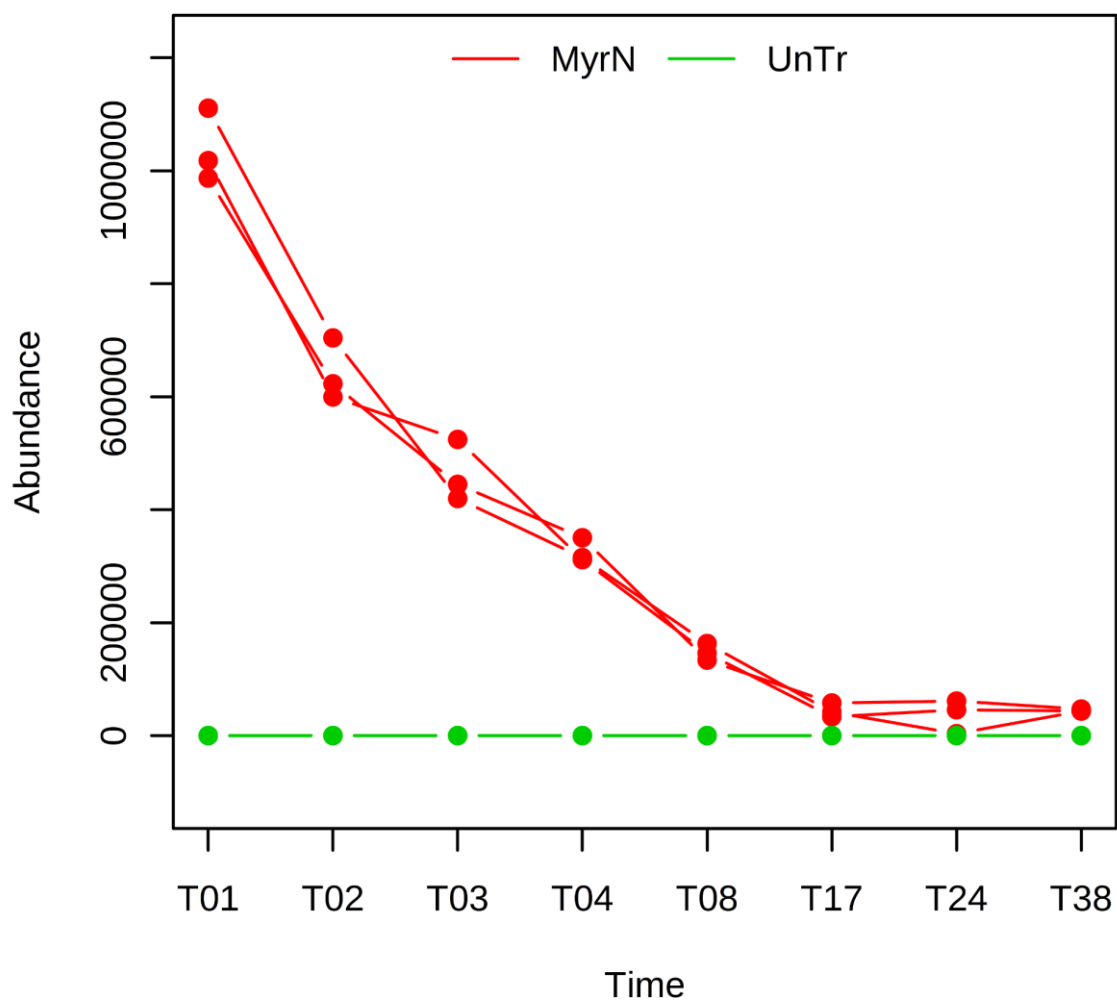
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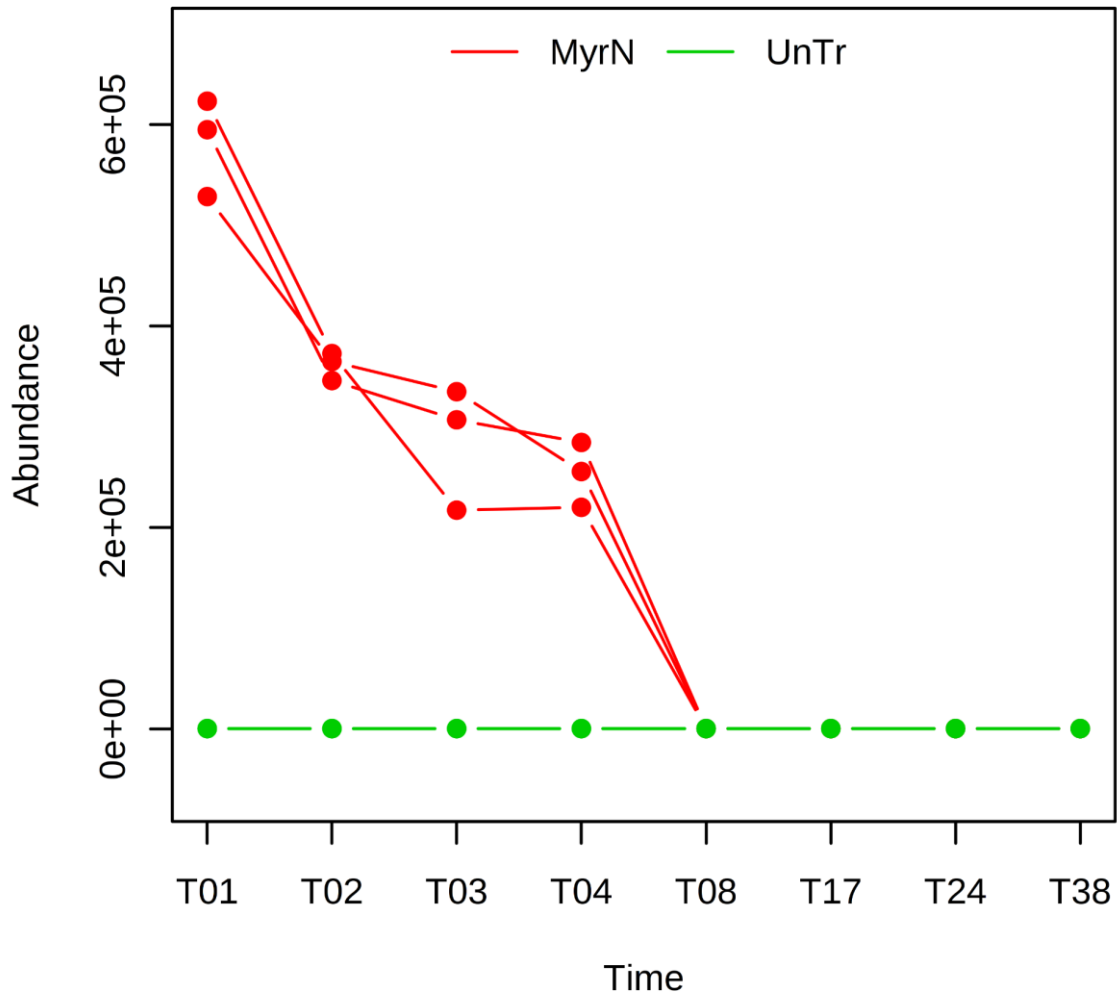
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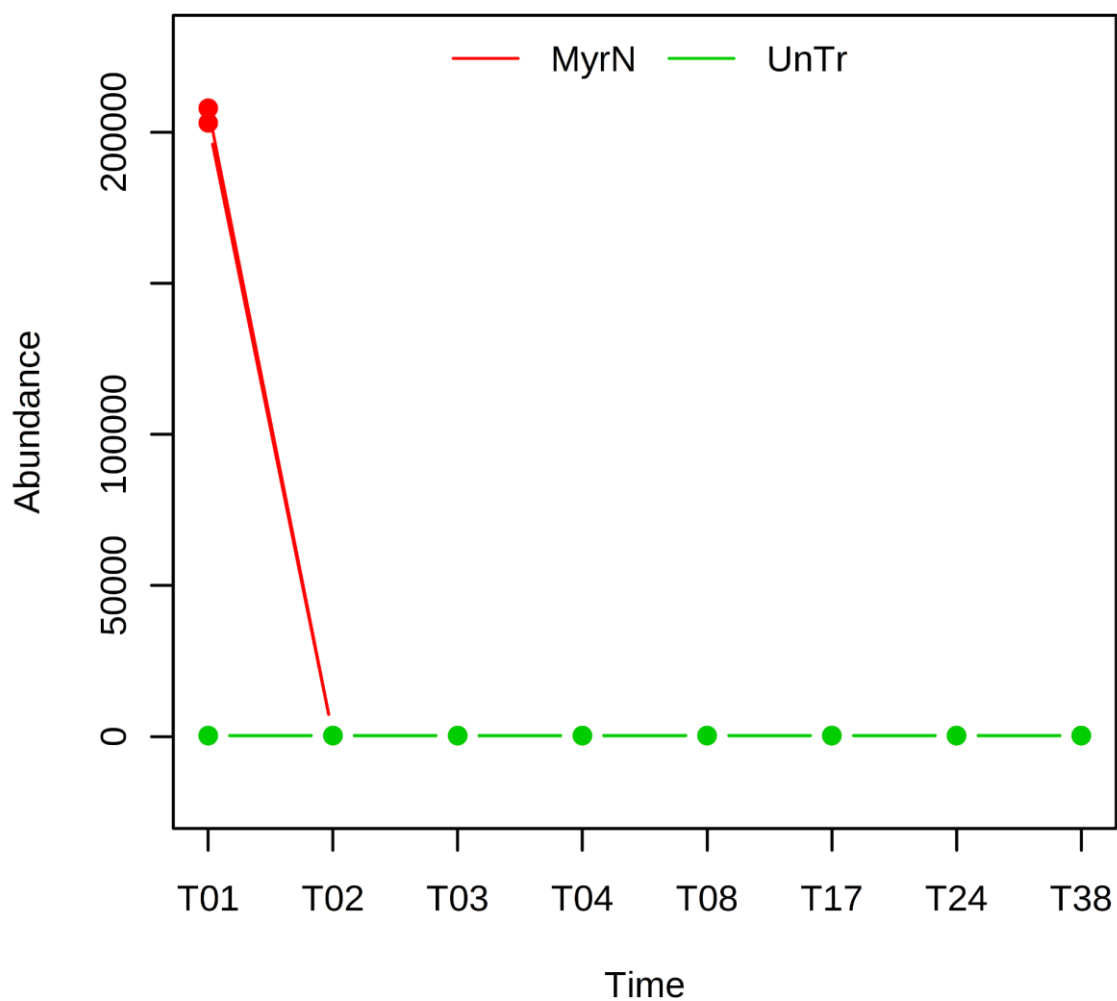
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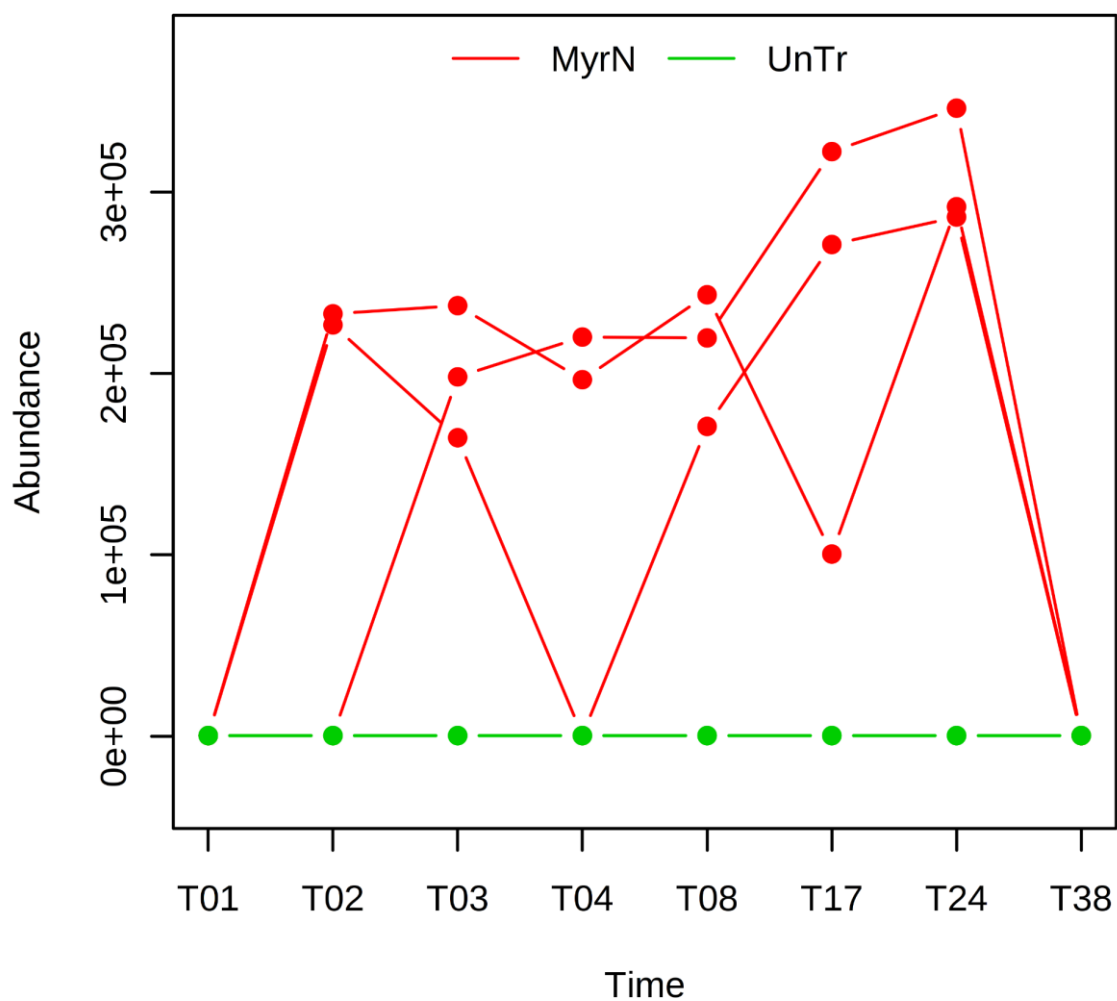
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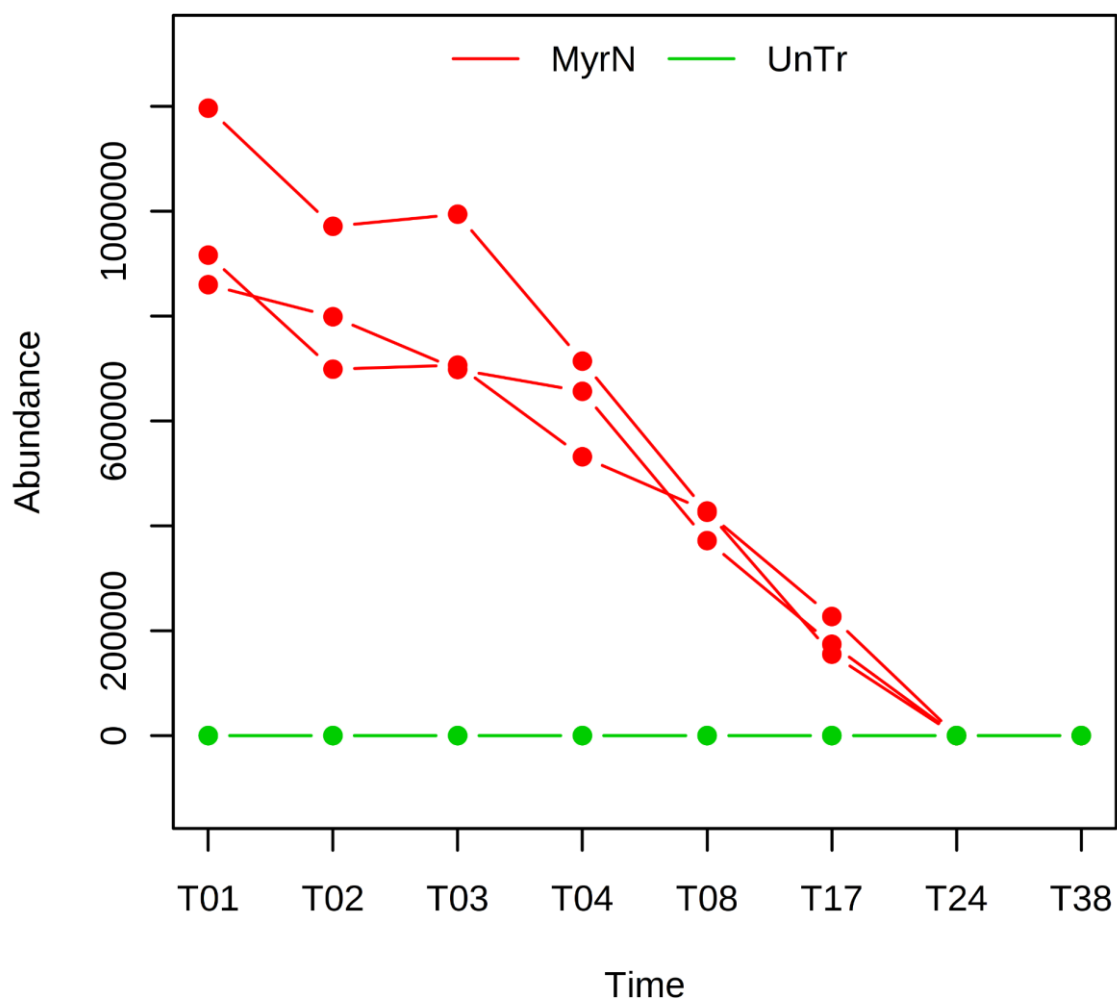
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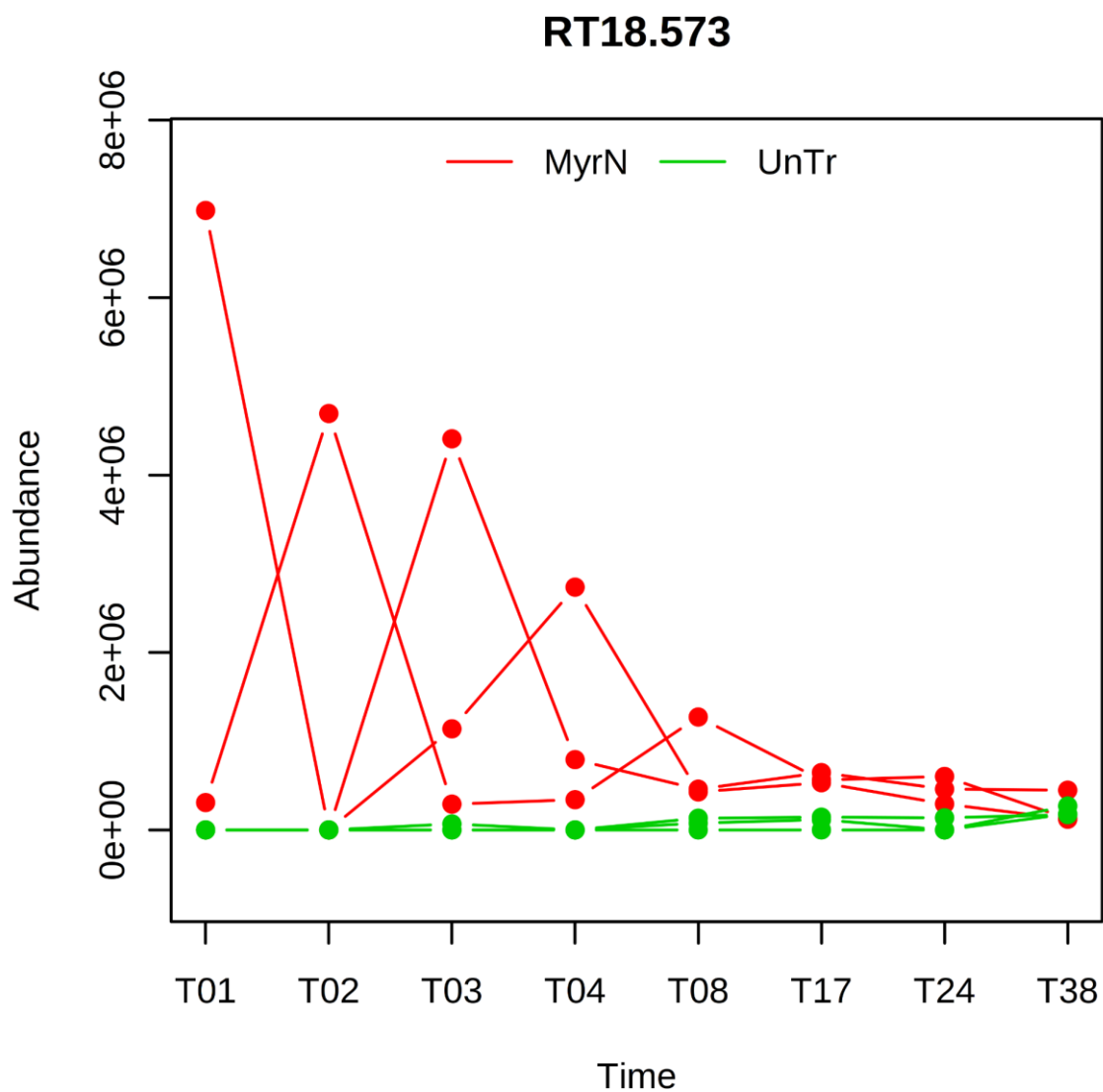


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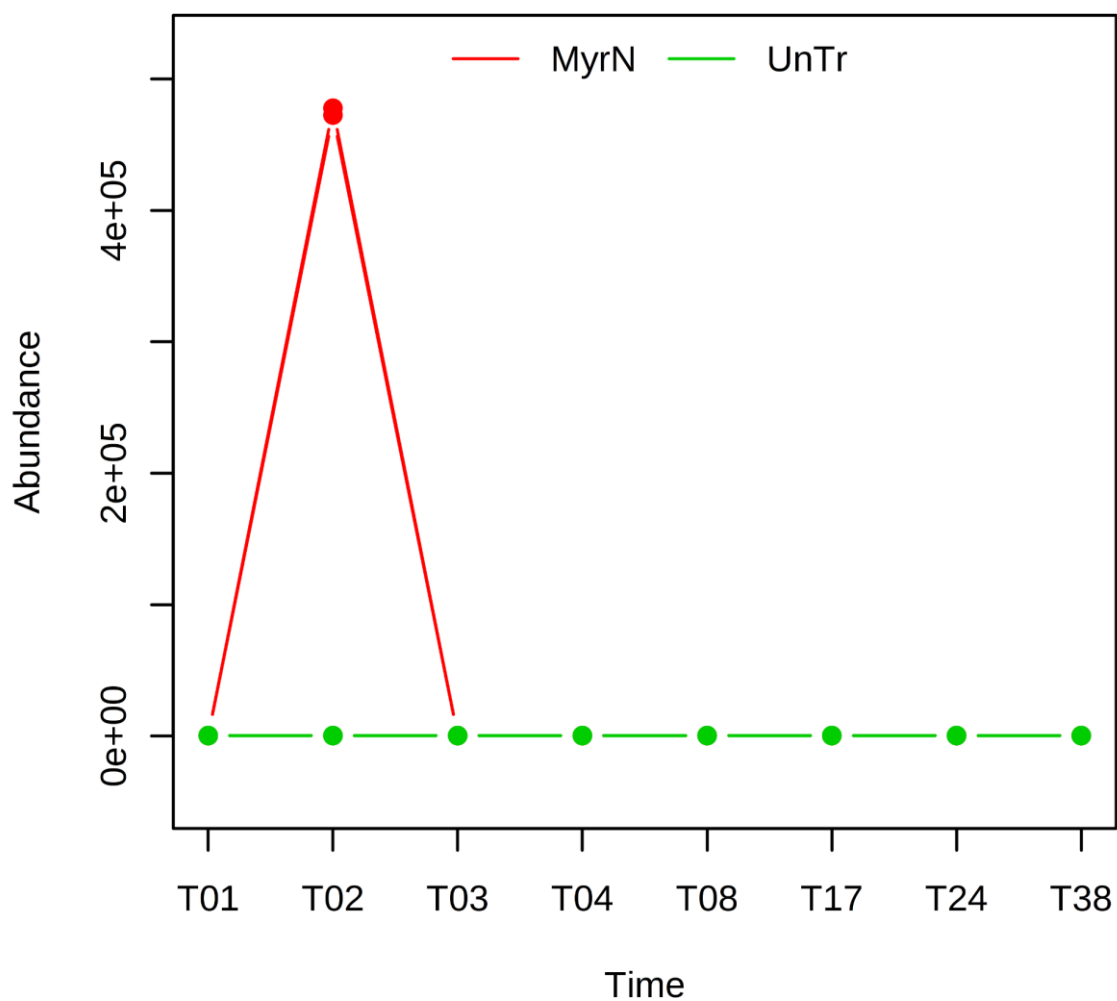


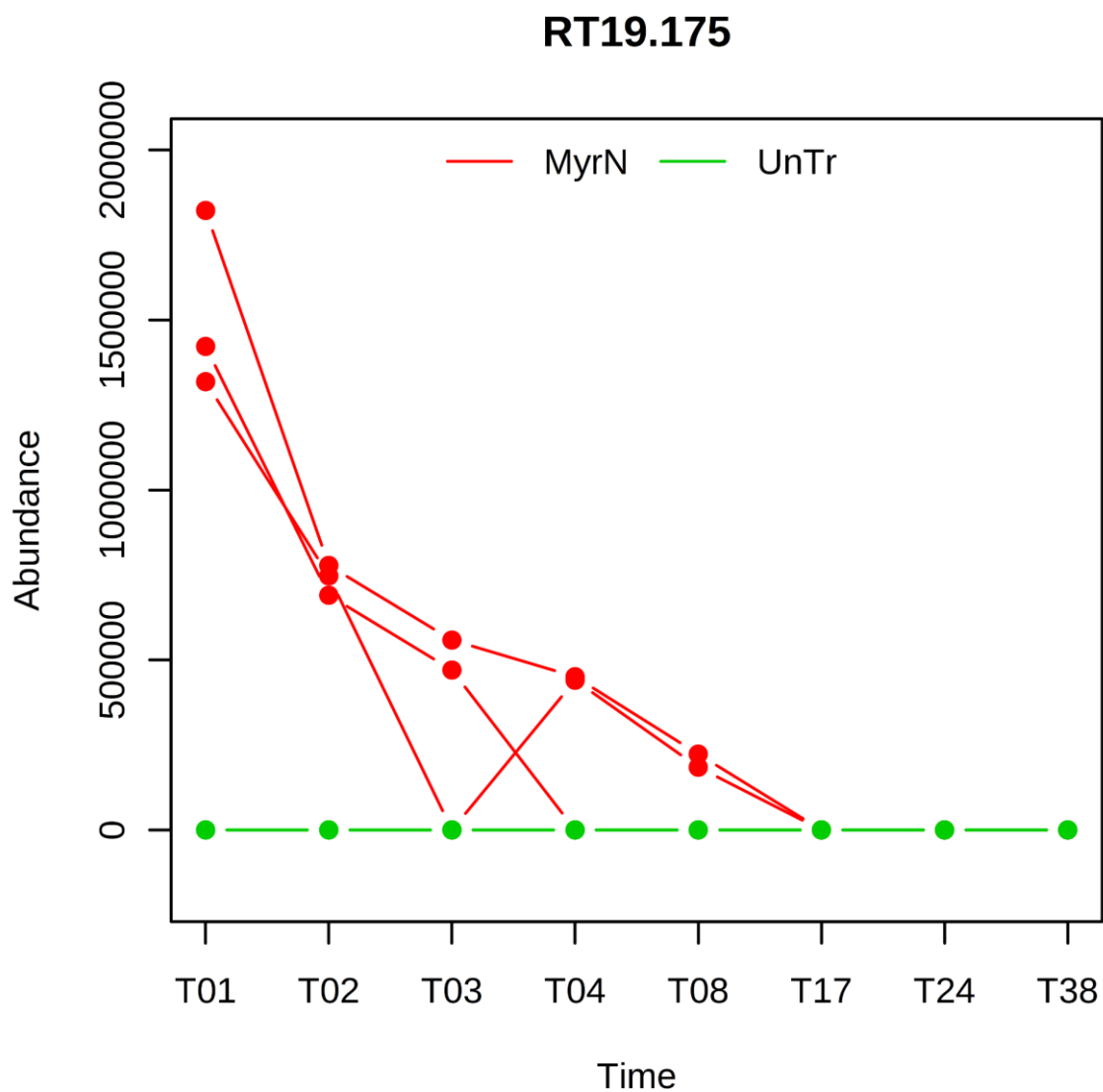
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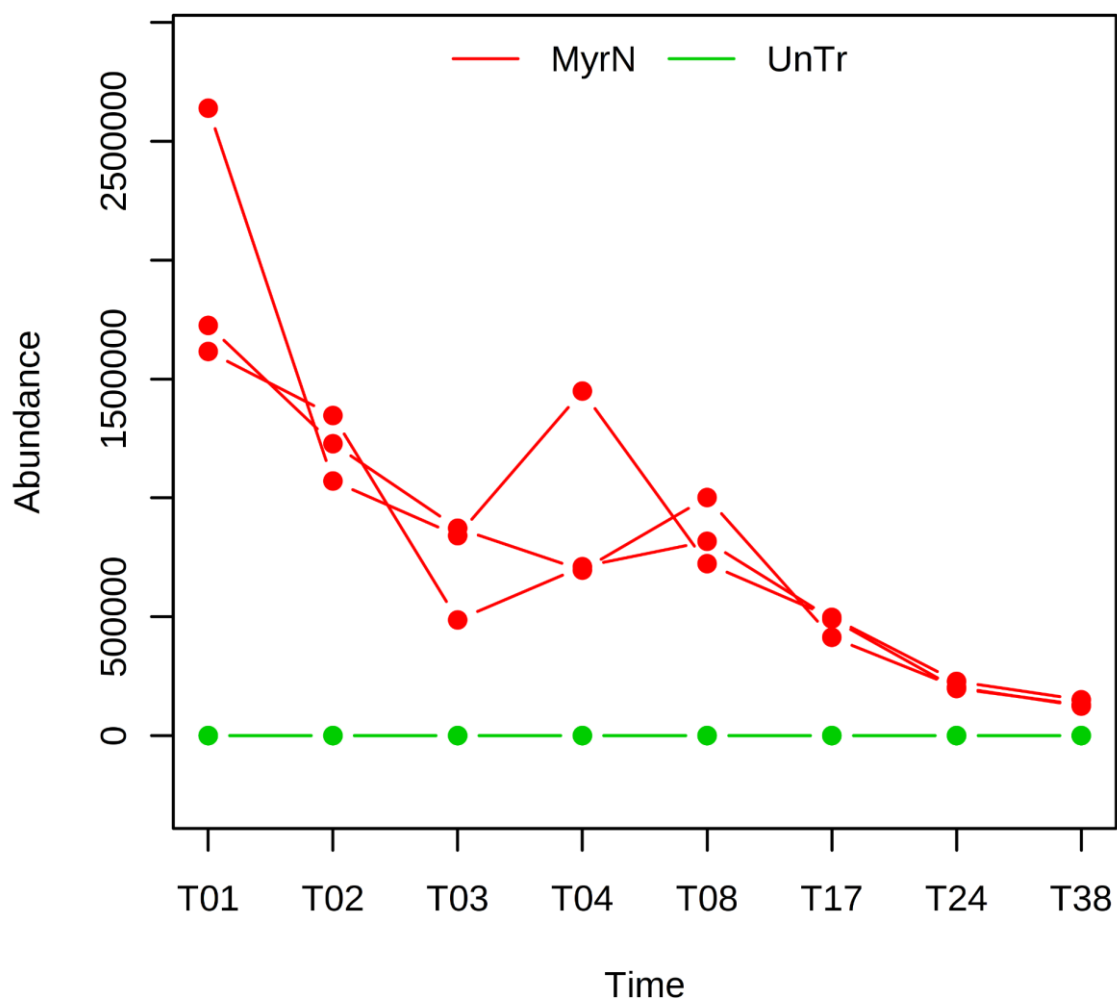


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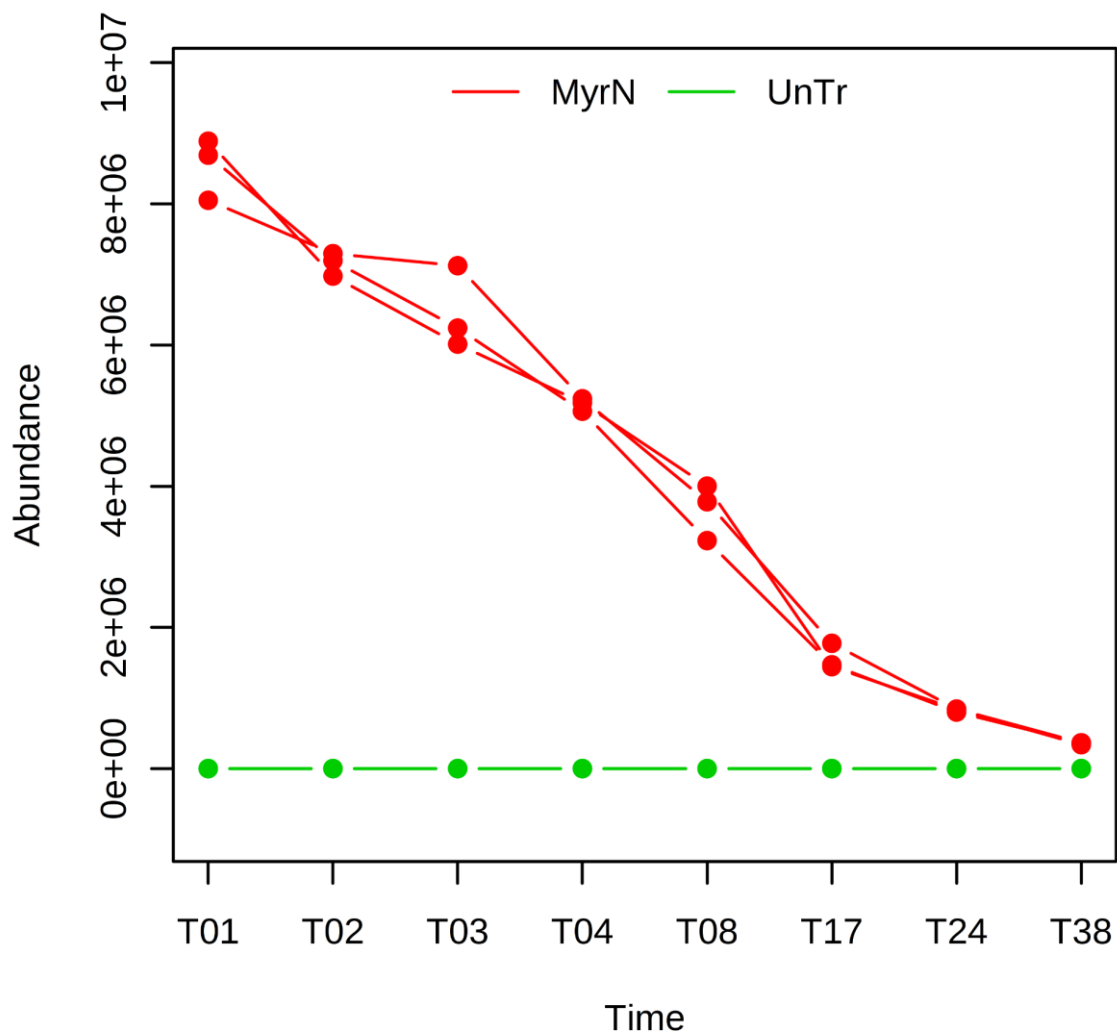




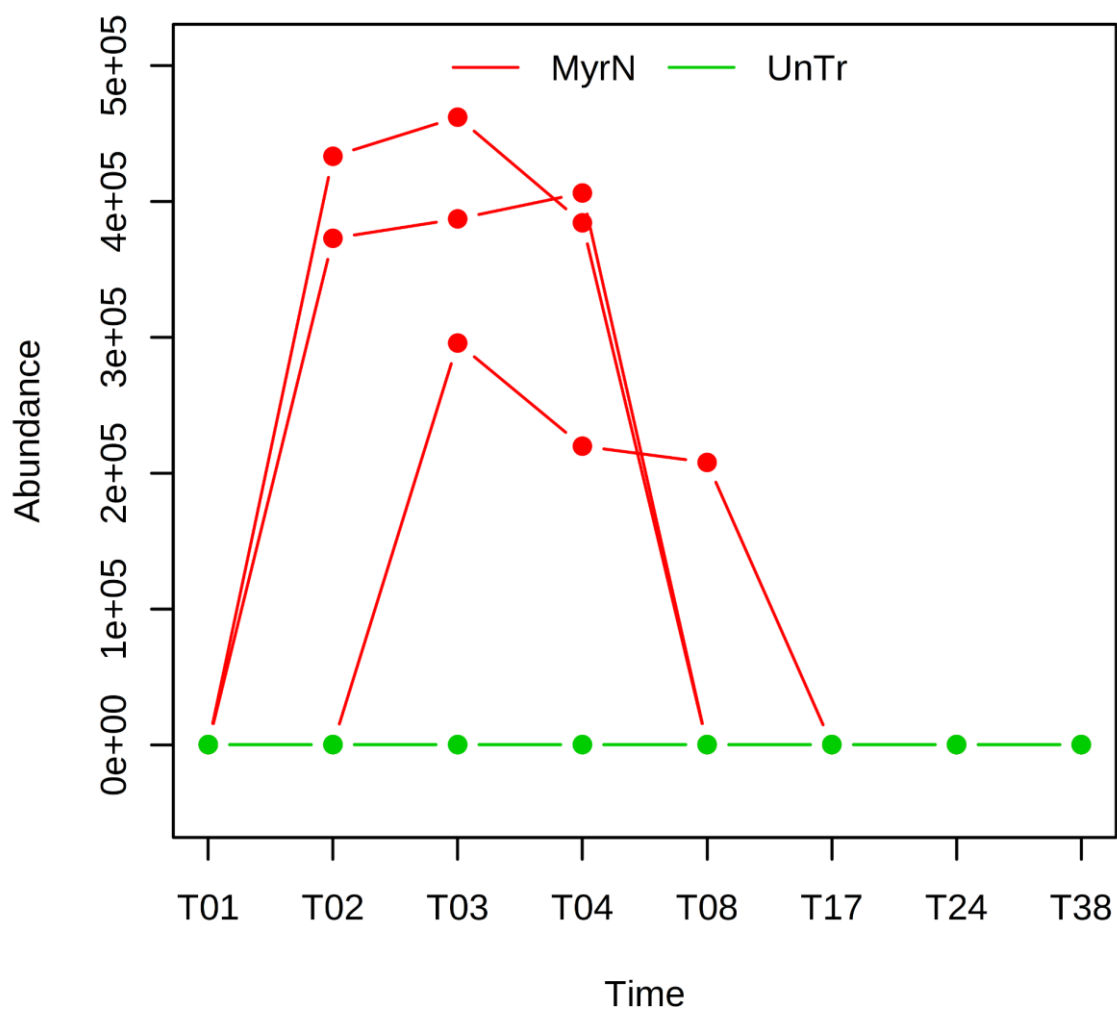
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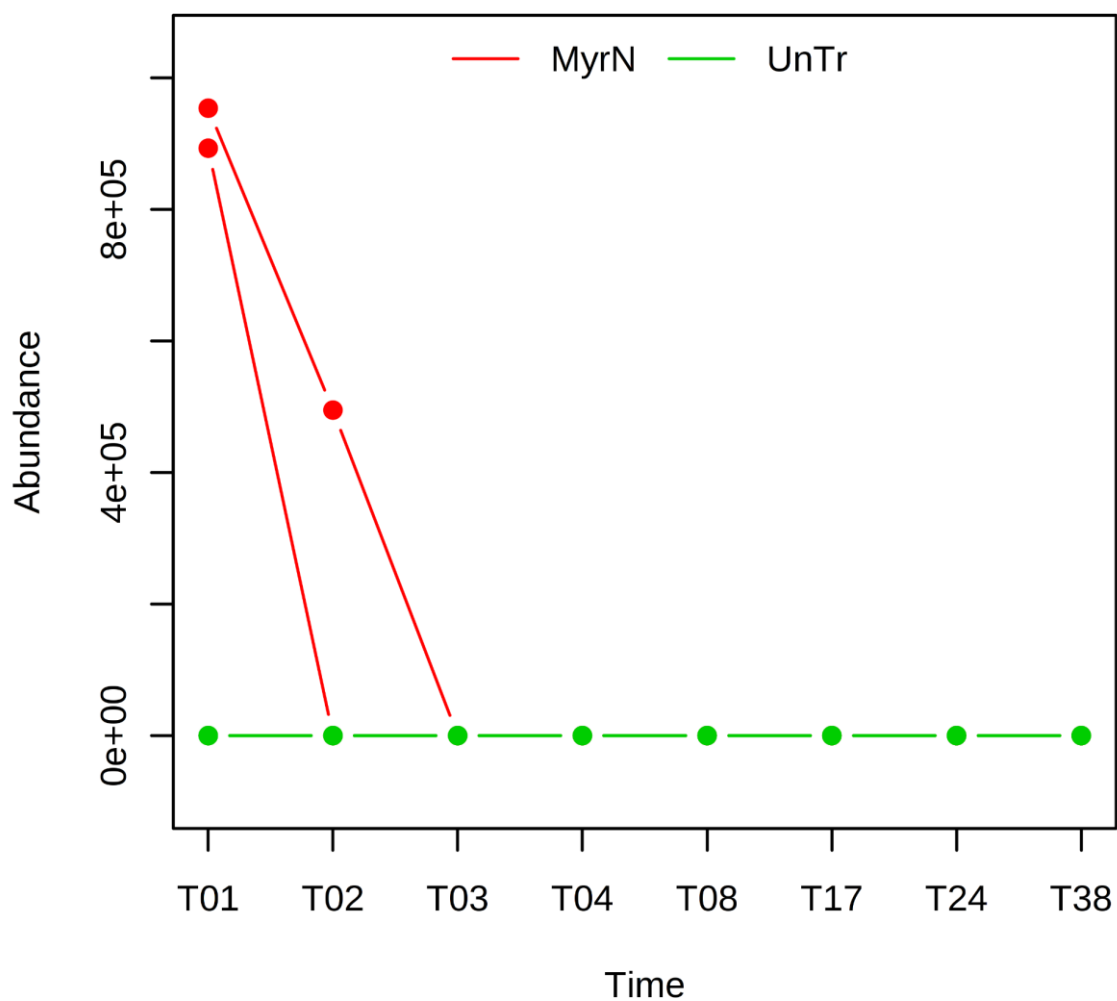
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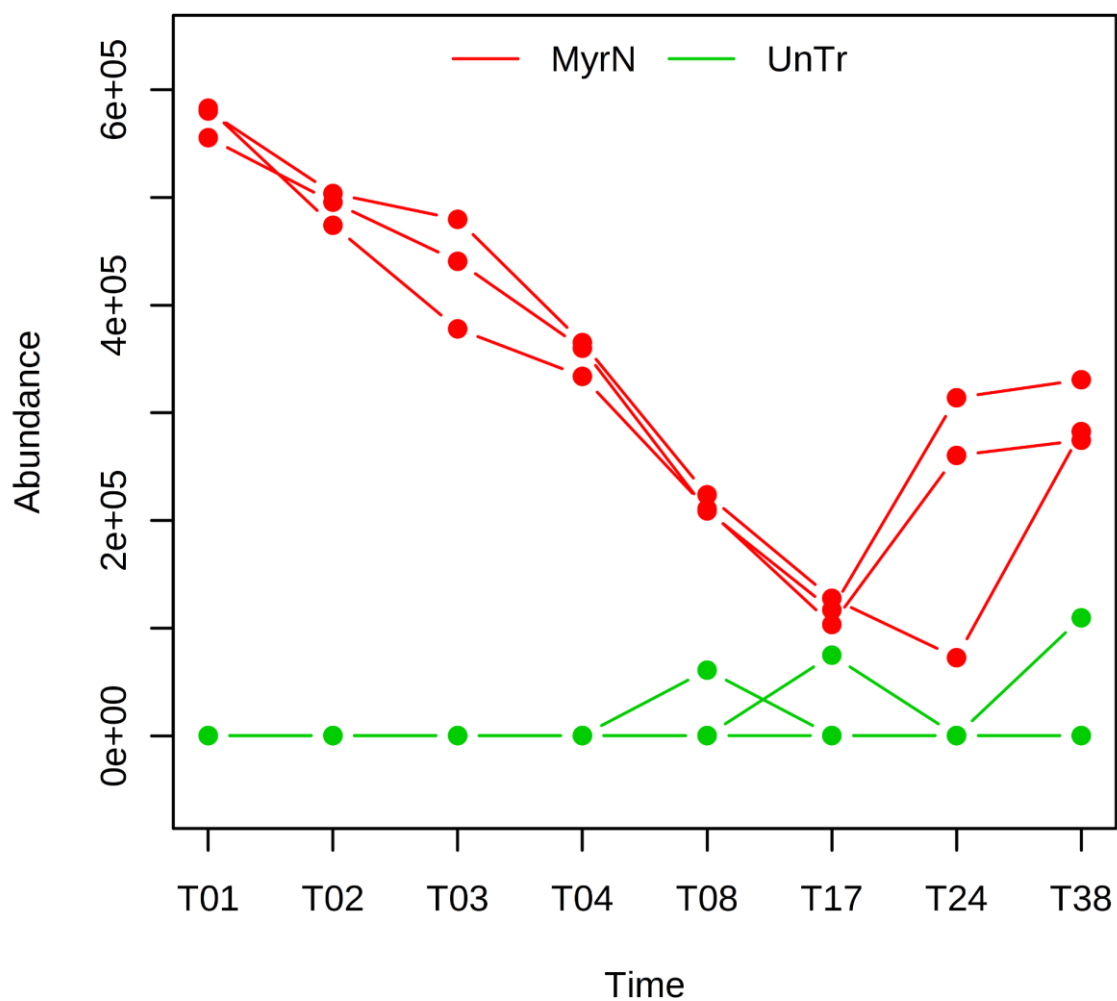
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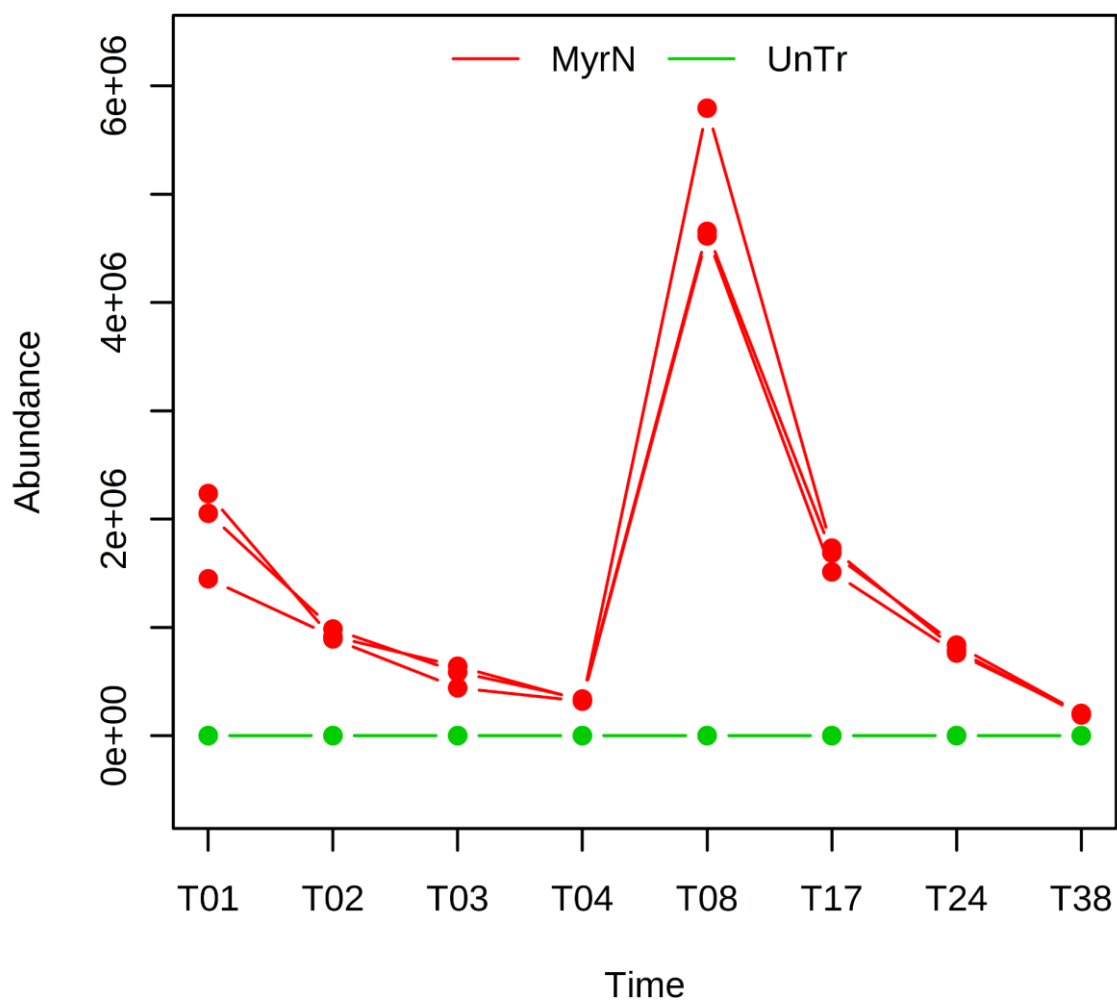
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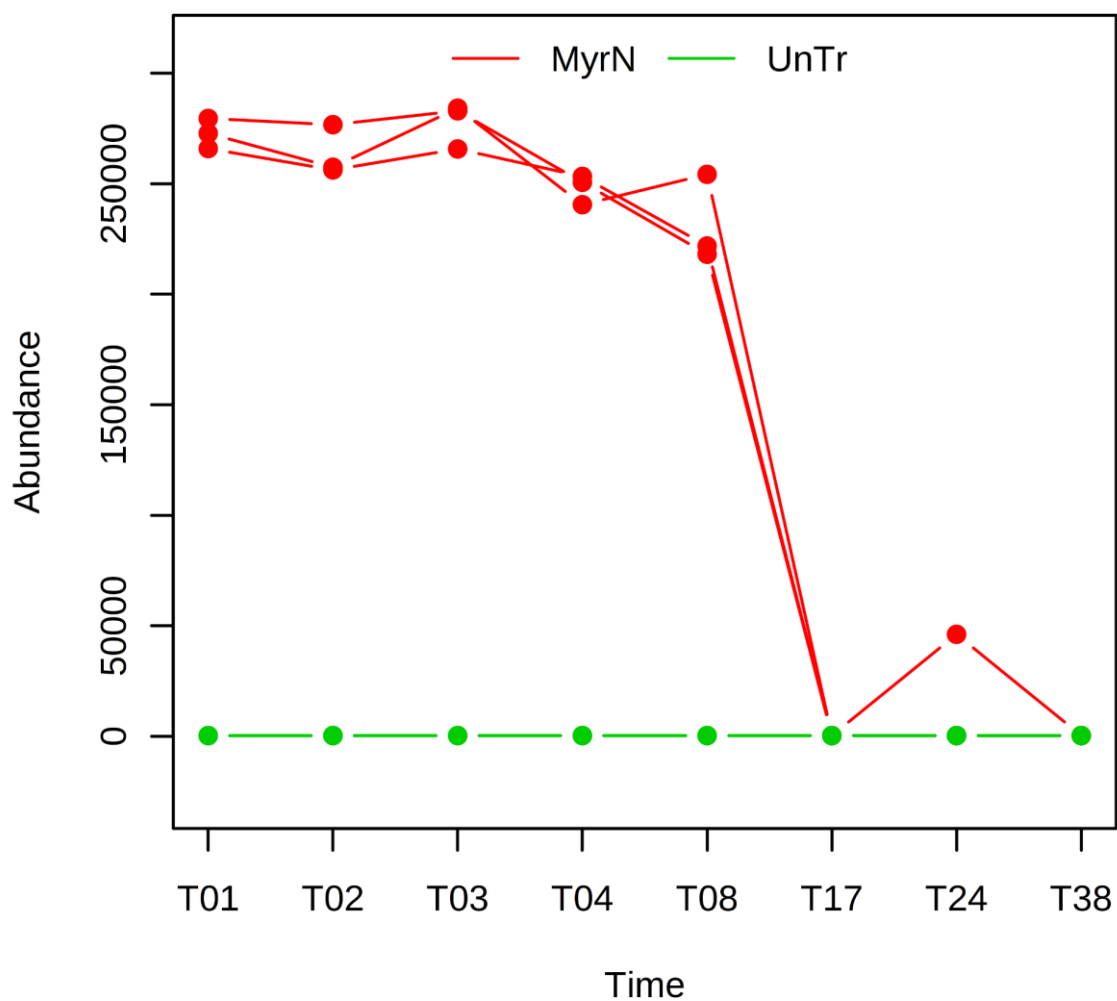
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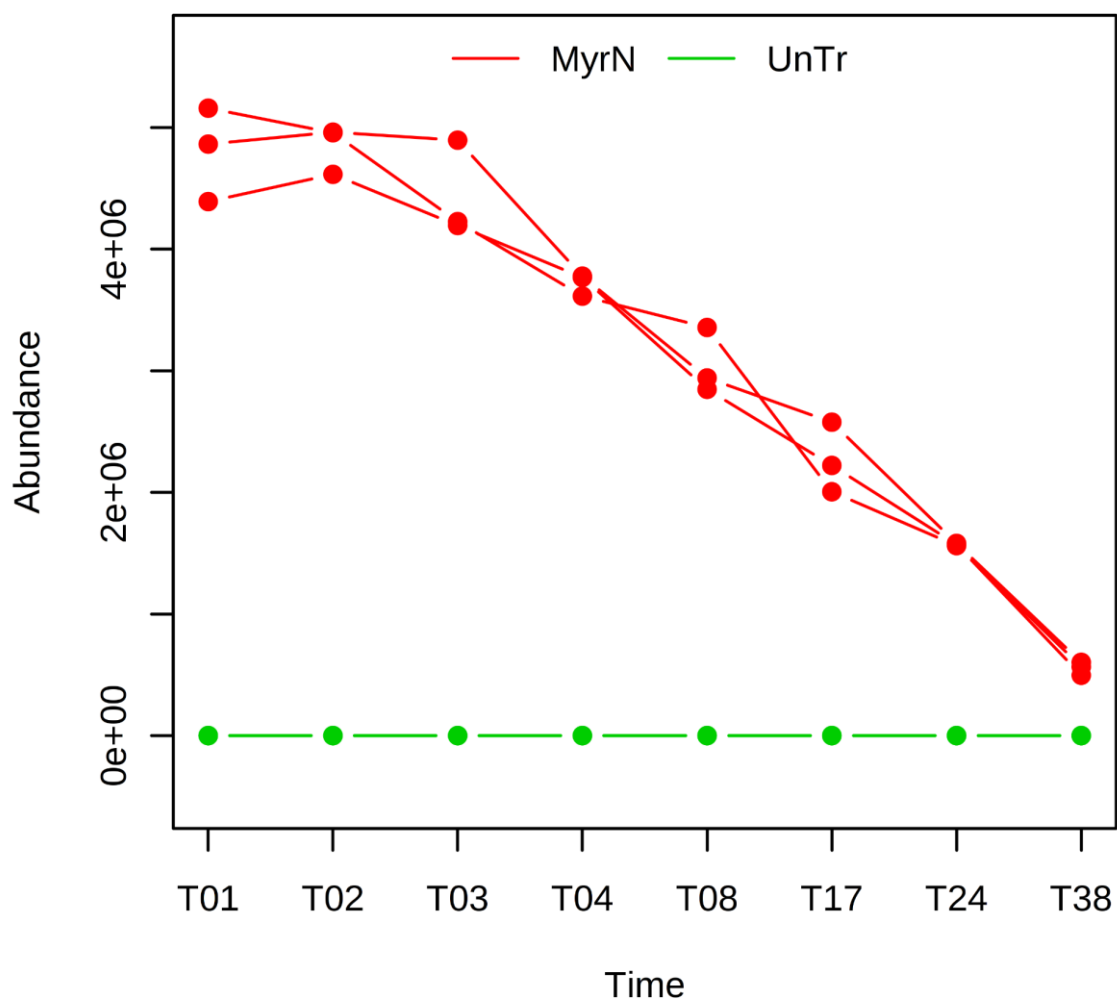
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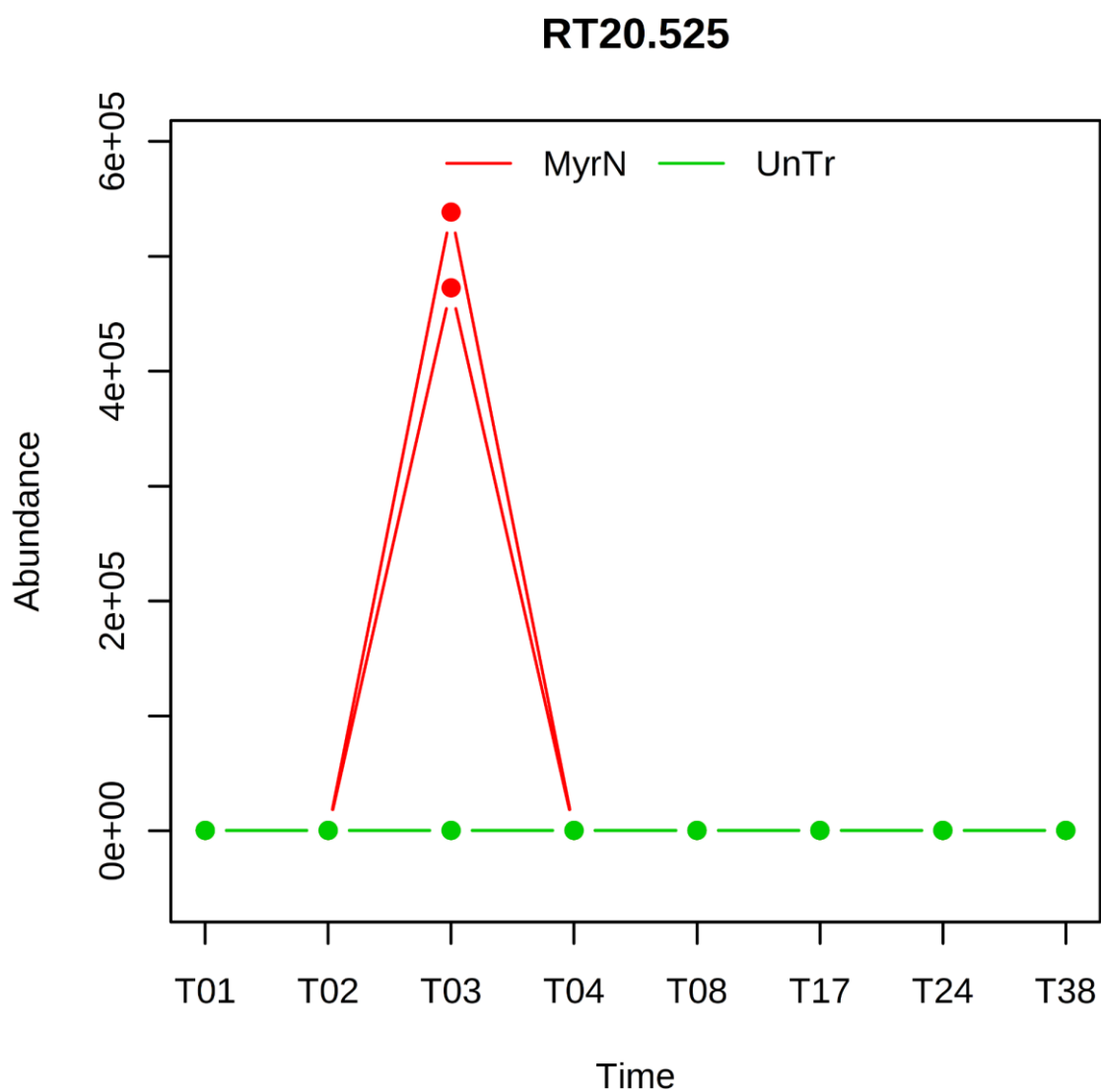


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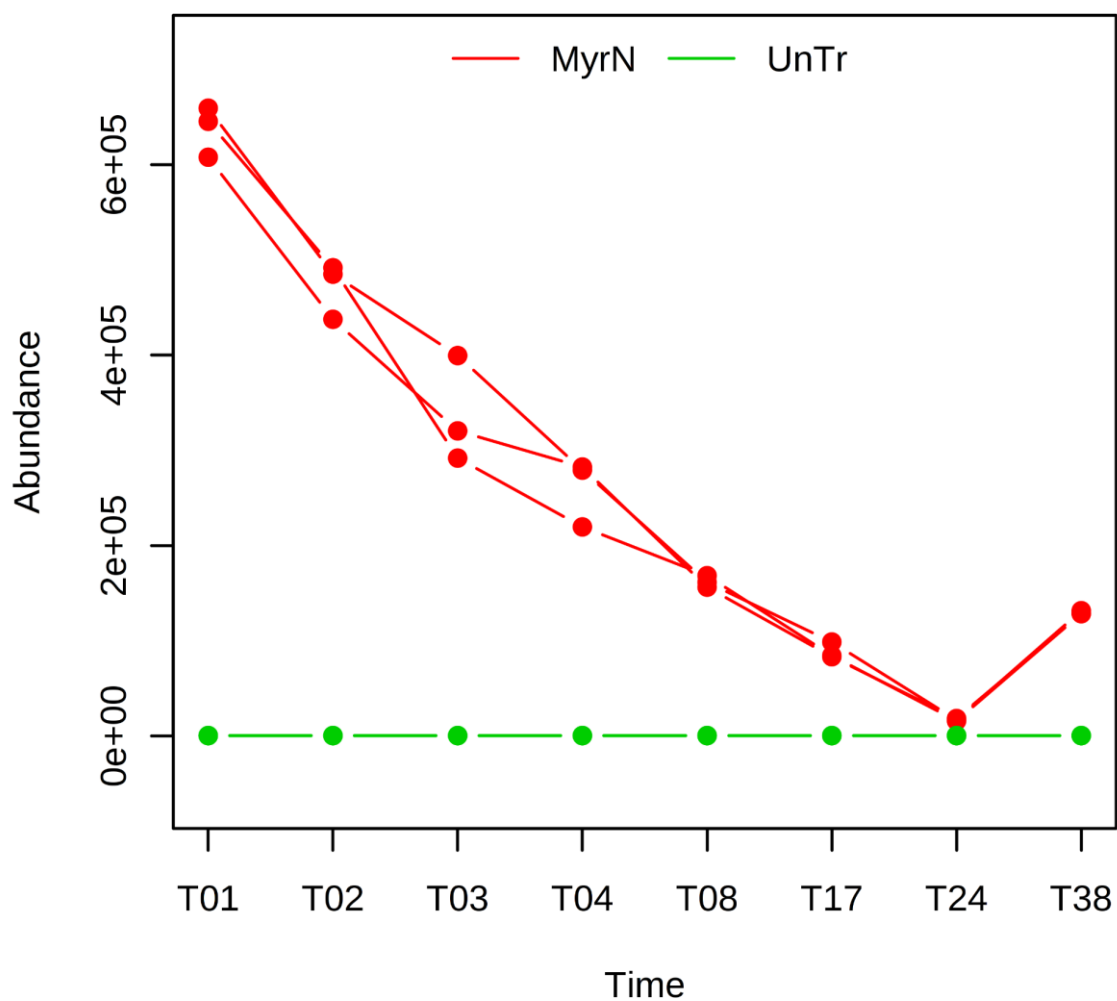


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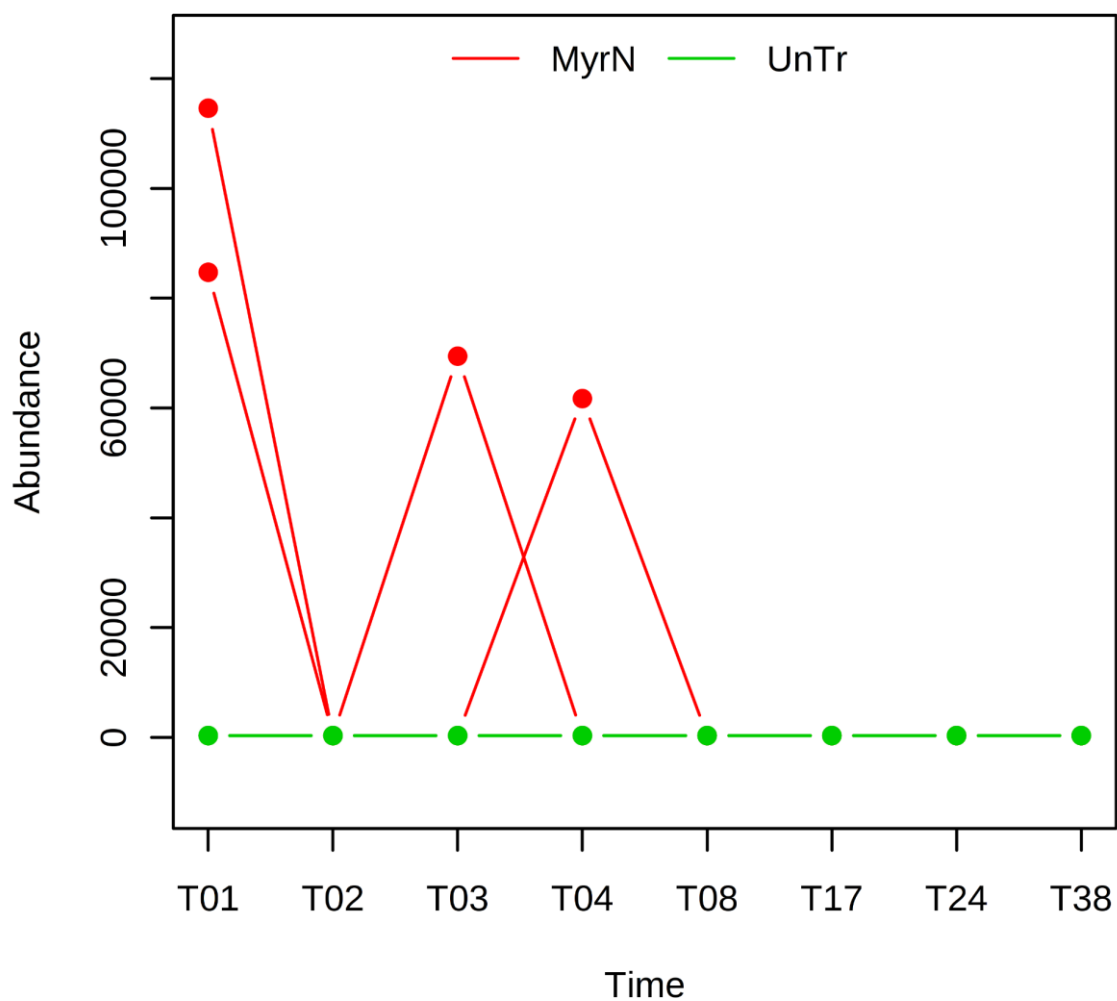




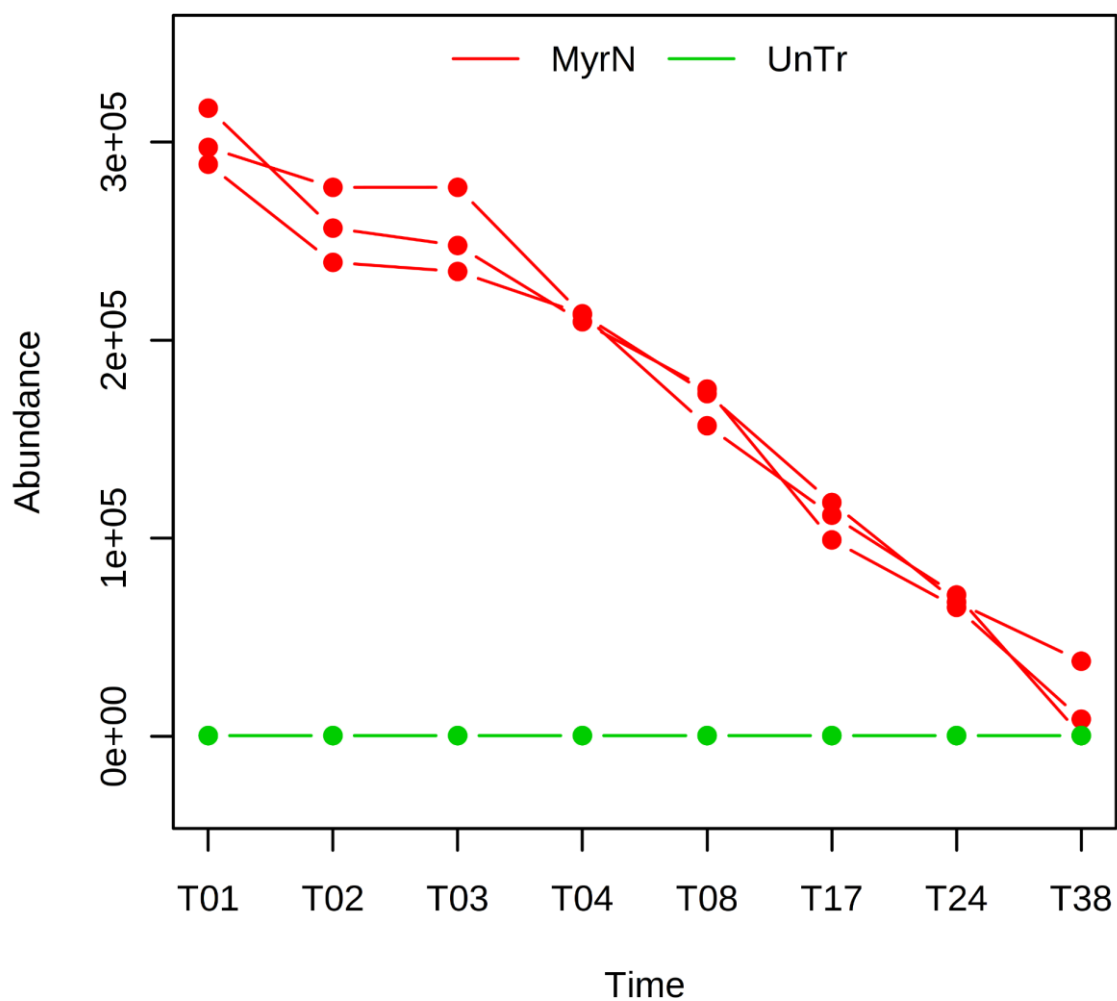
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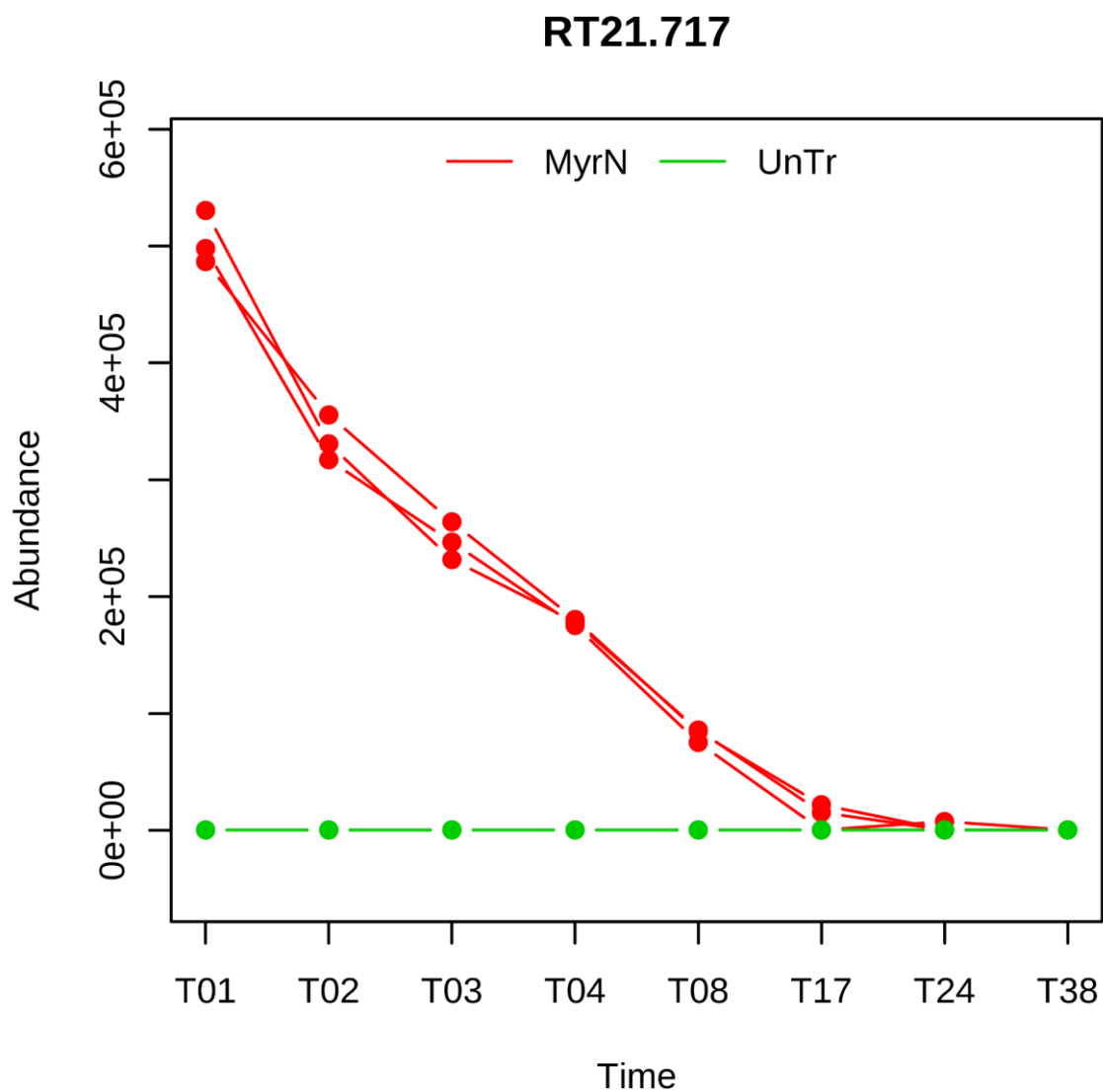


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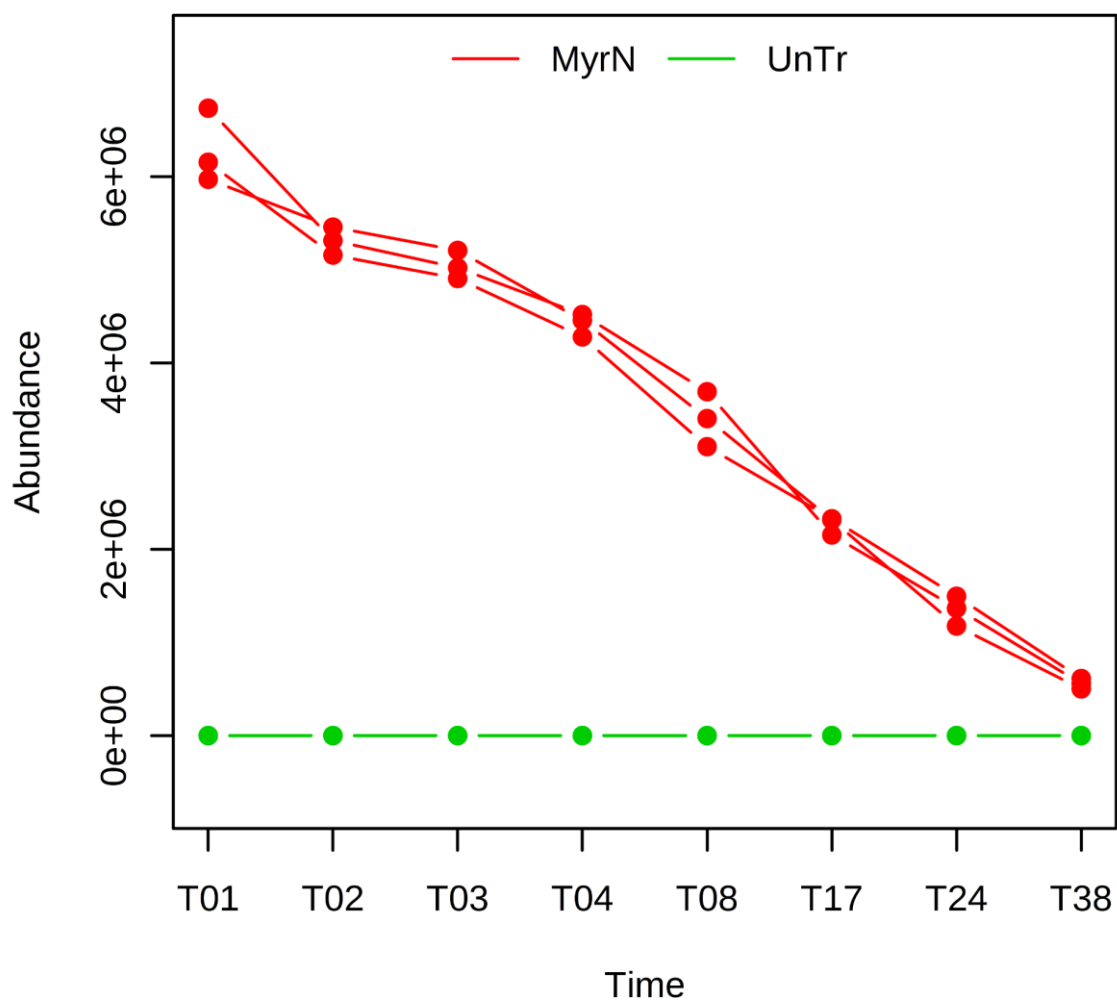


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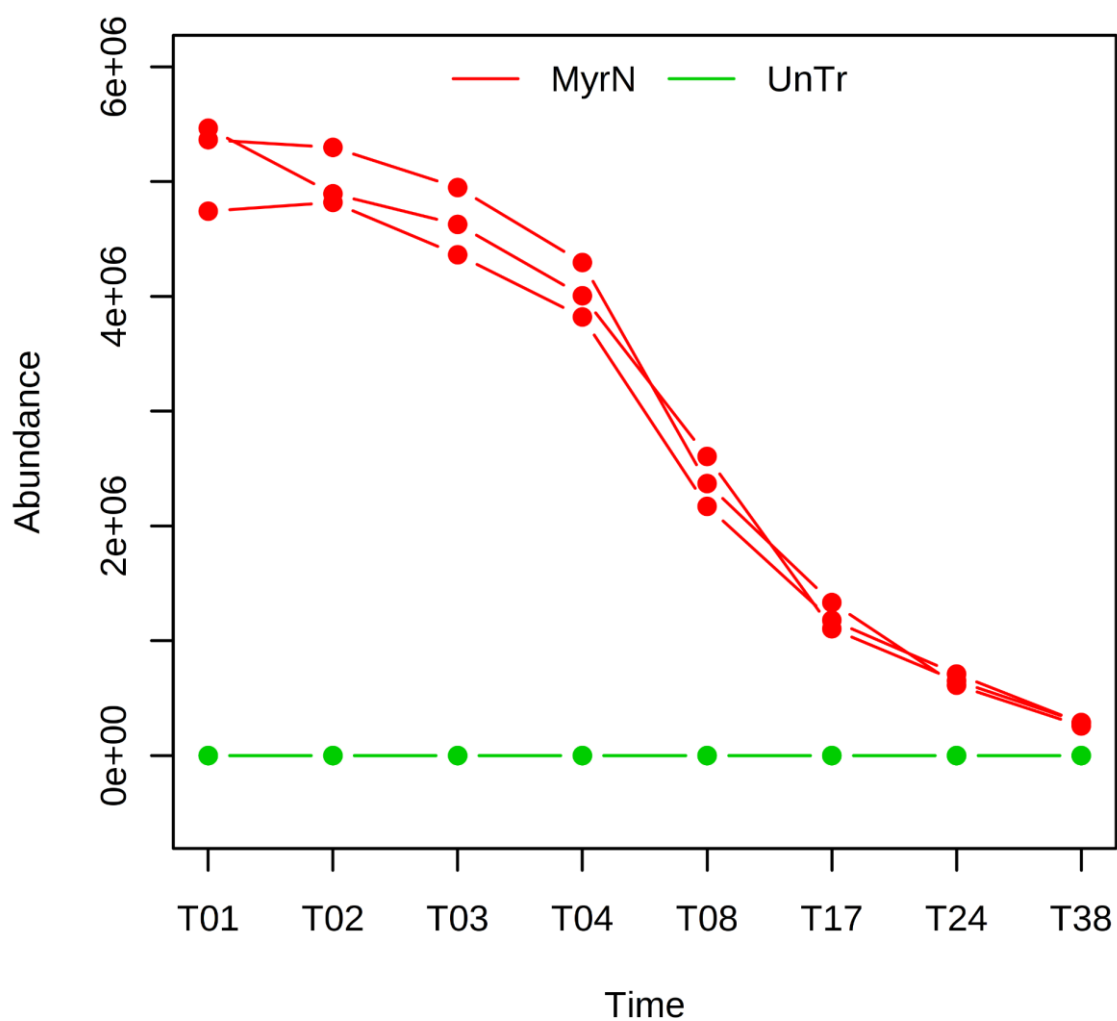




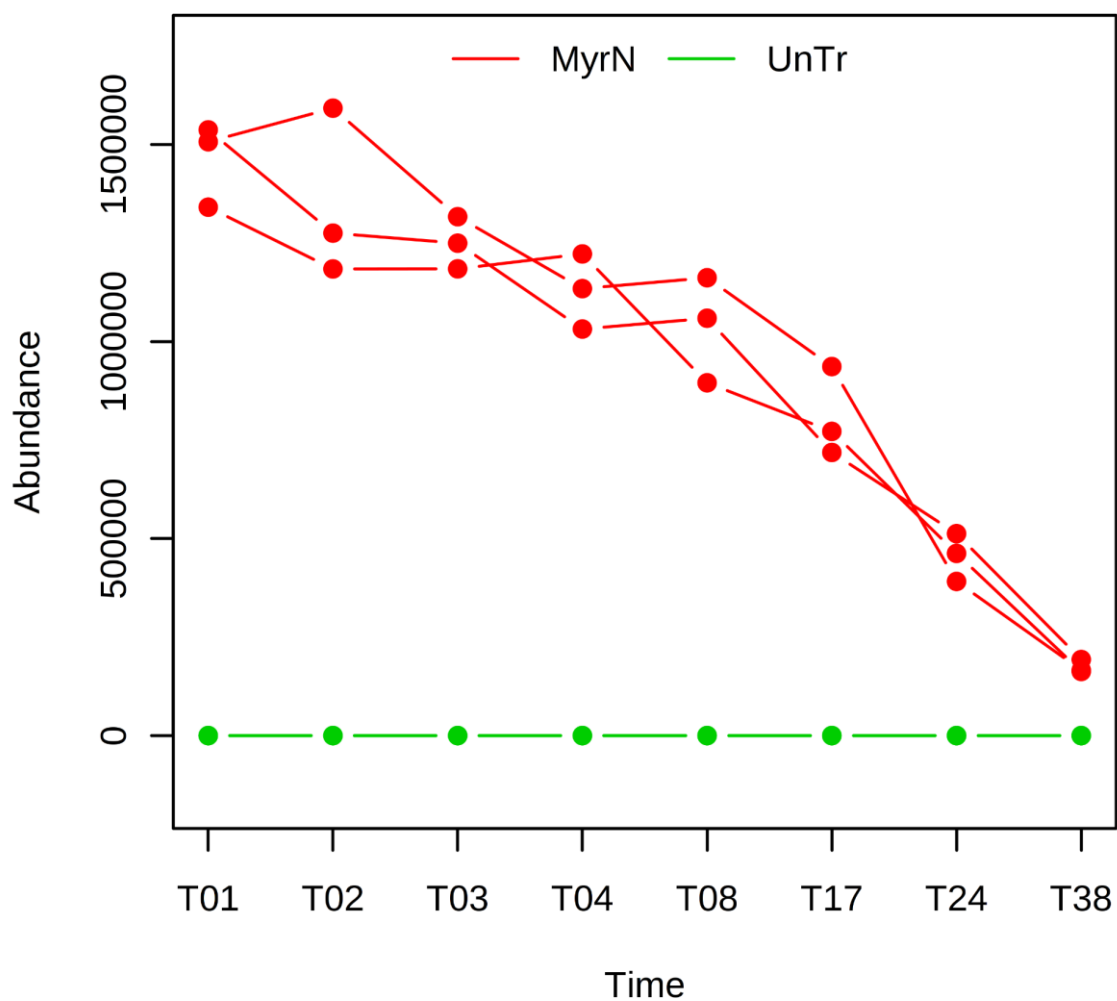
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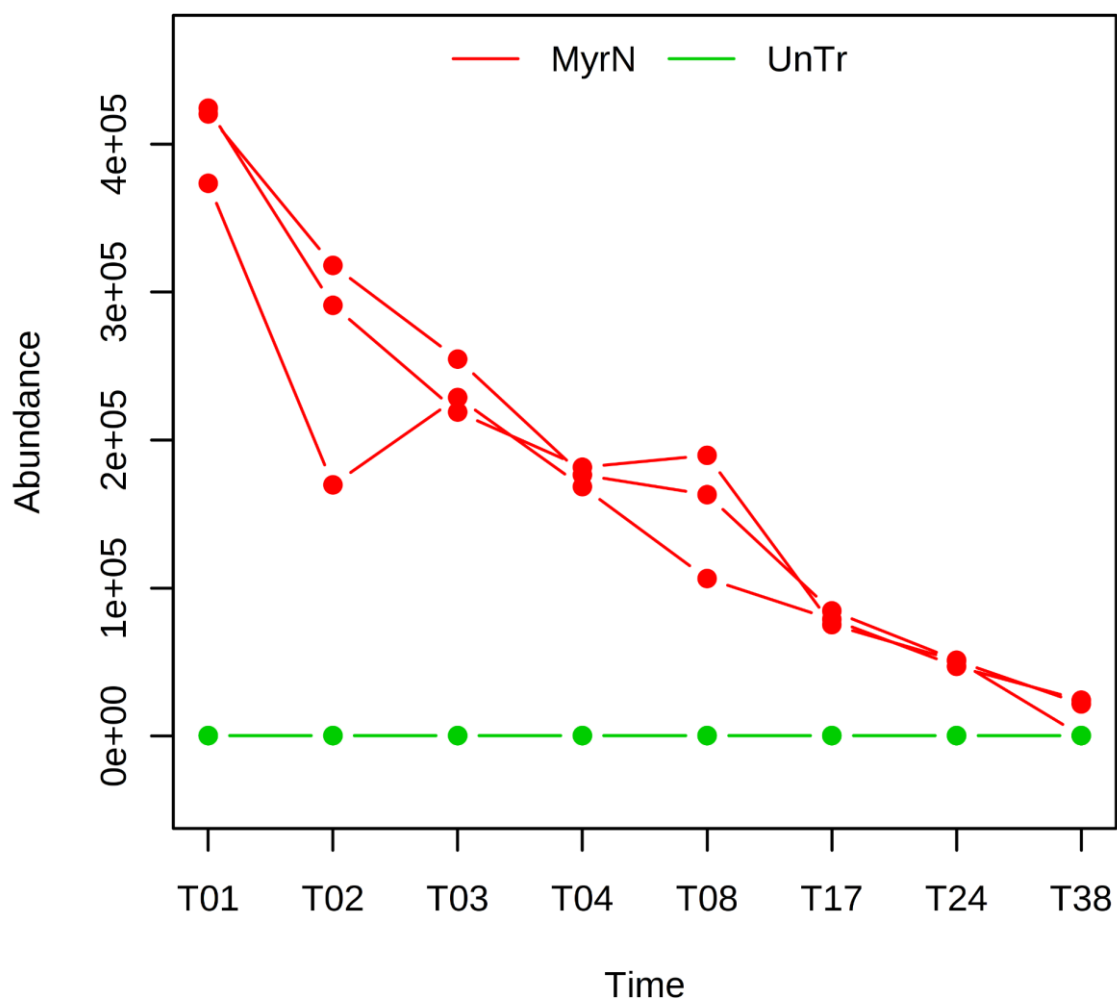
RT22.148



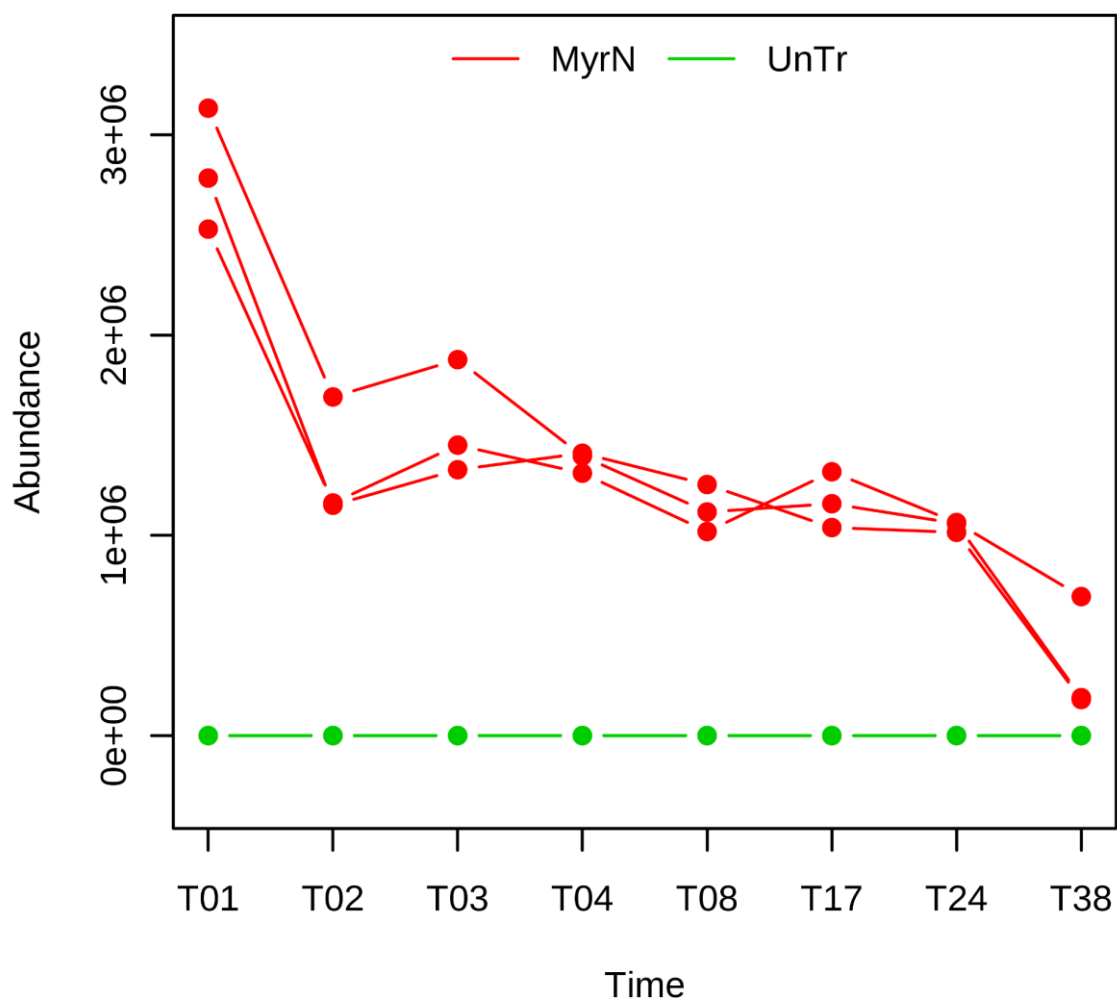
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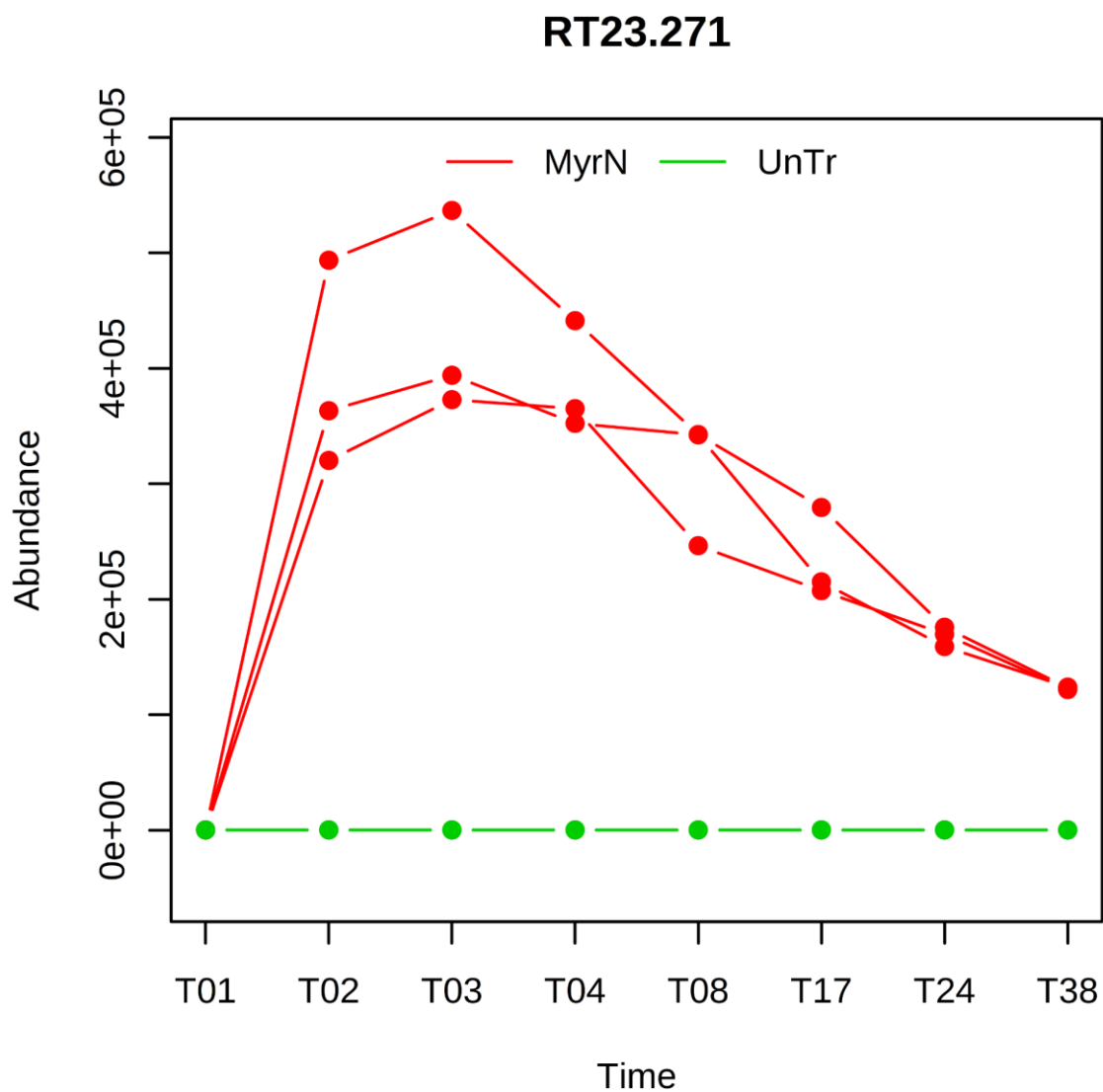


RT22.687

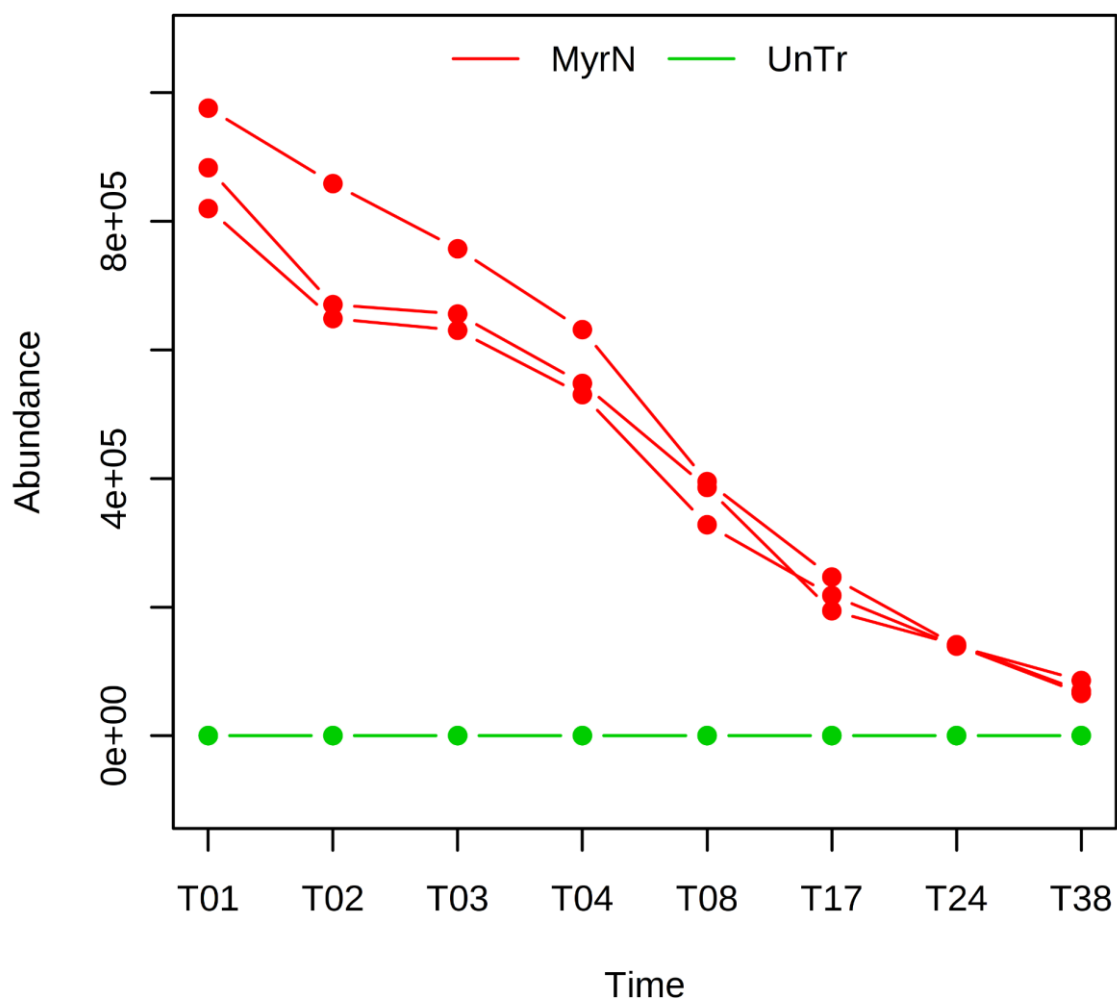


RT23.095

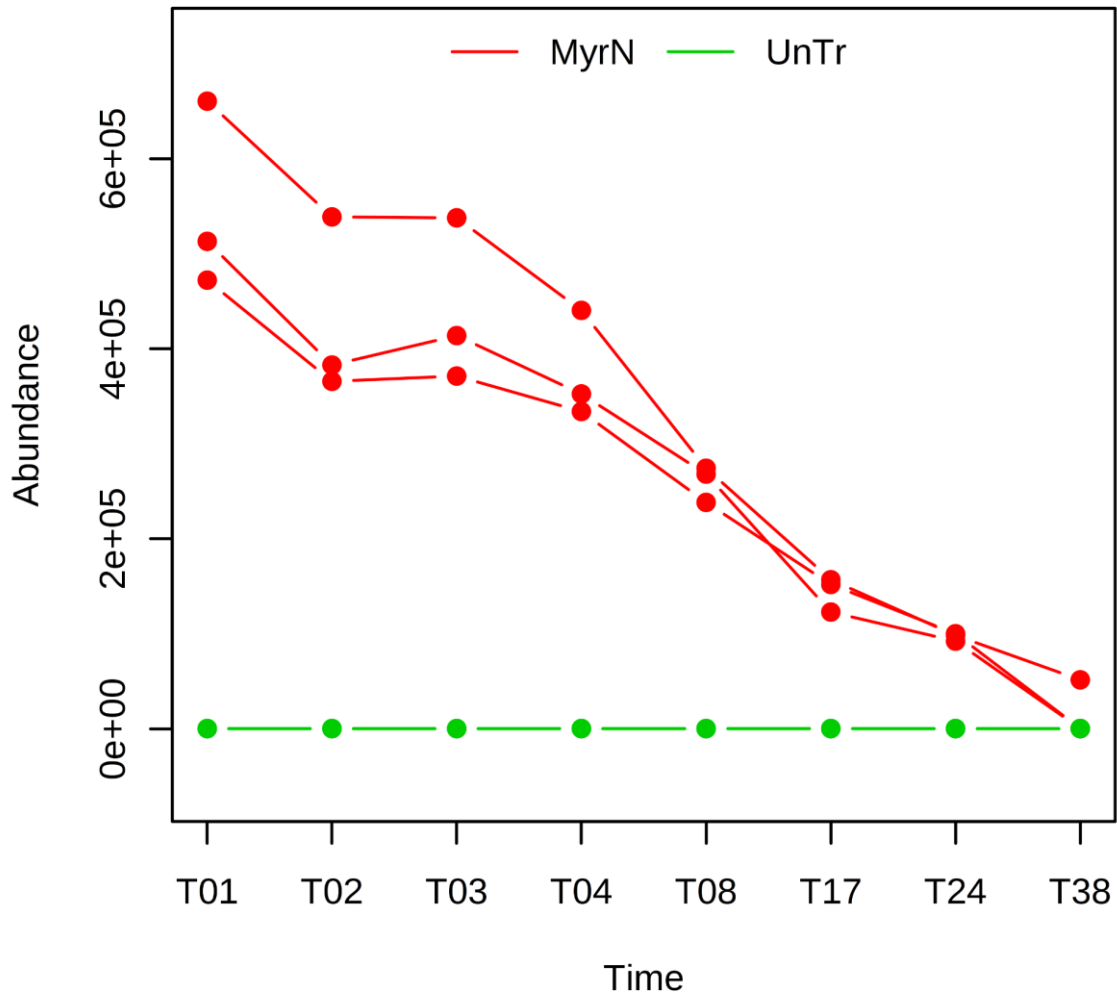




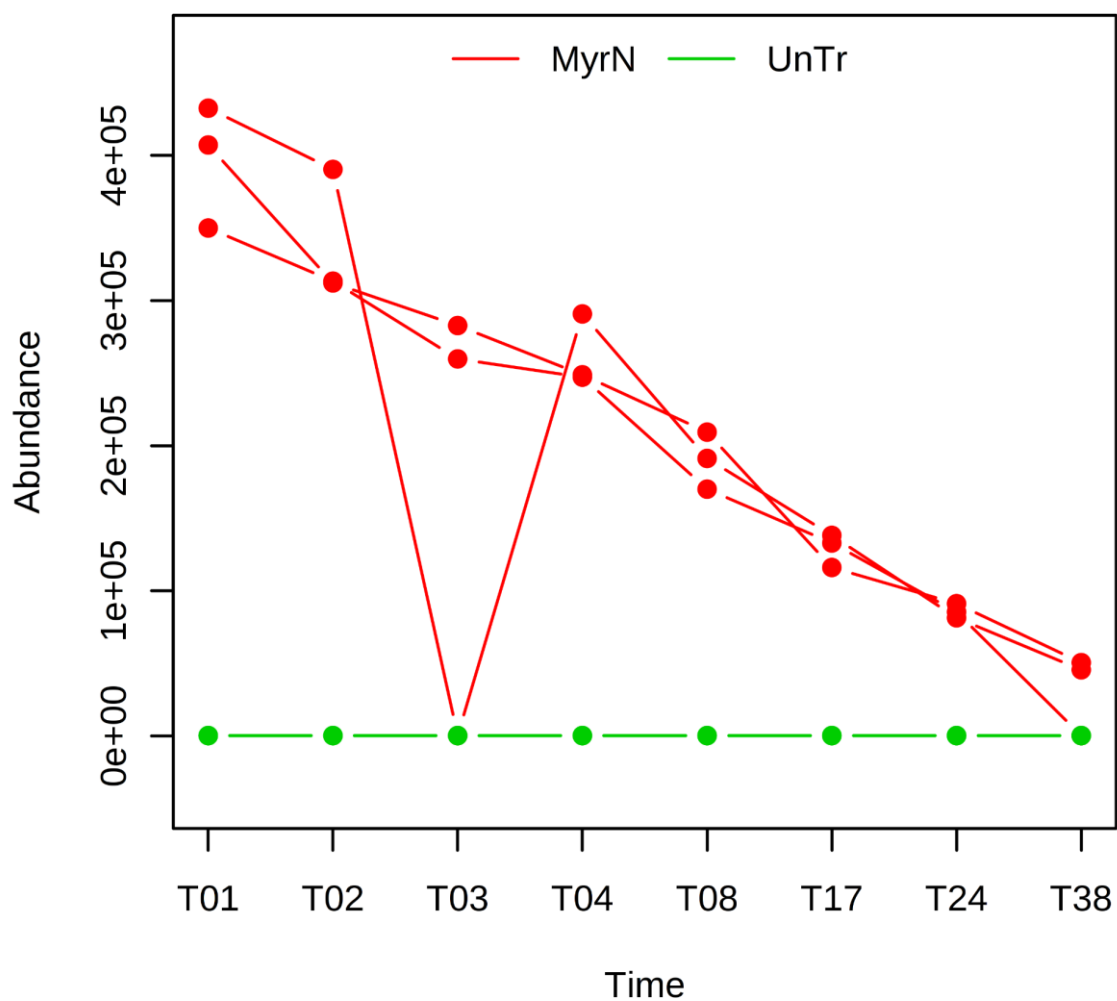
RT24.1



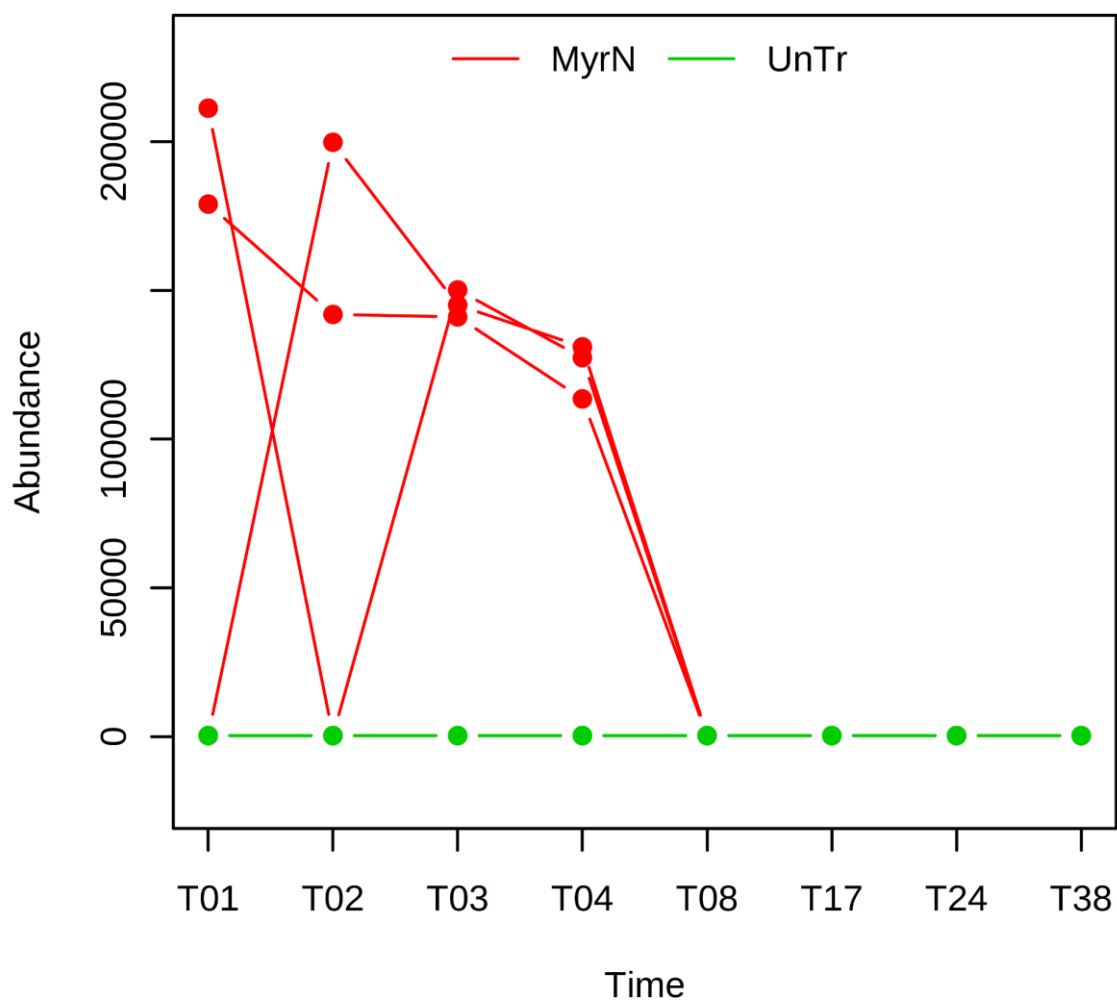
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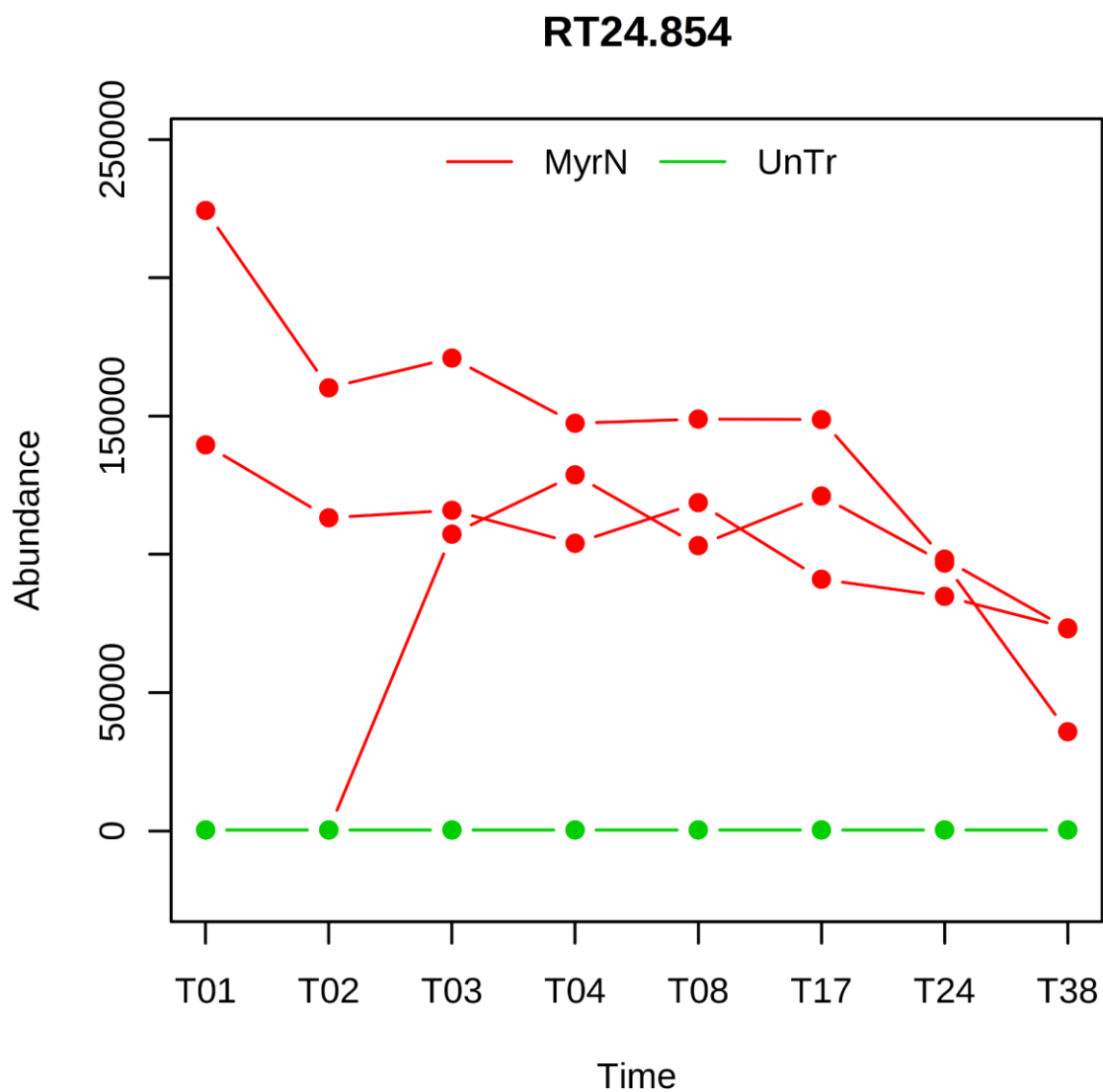


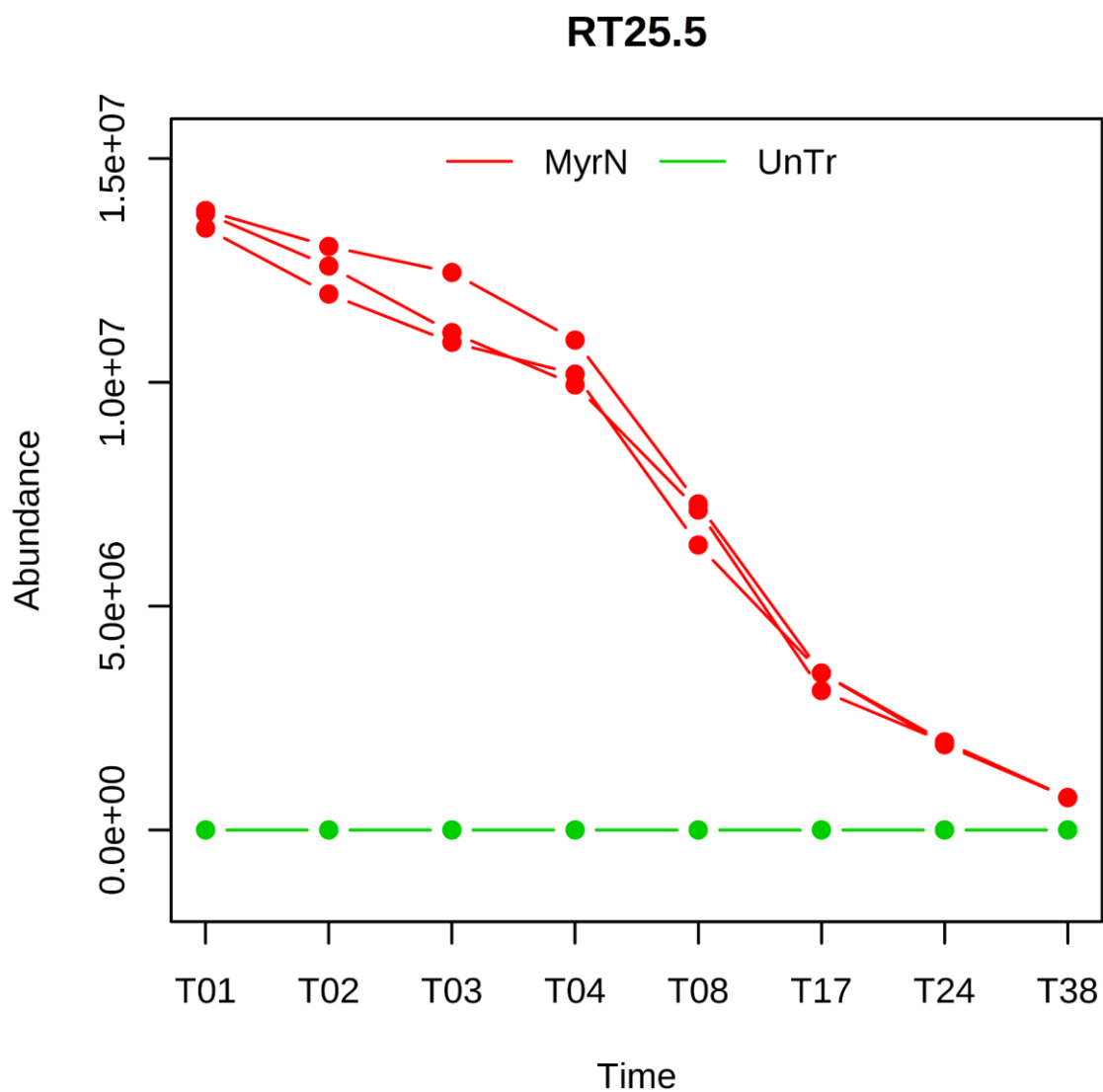
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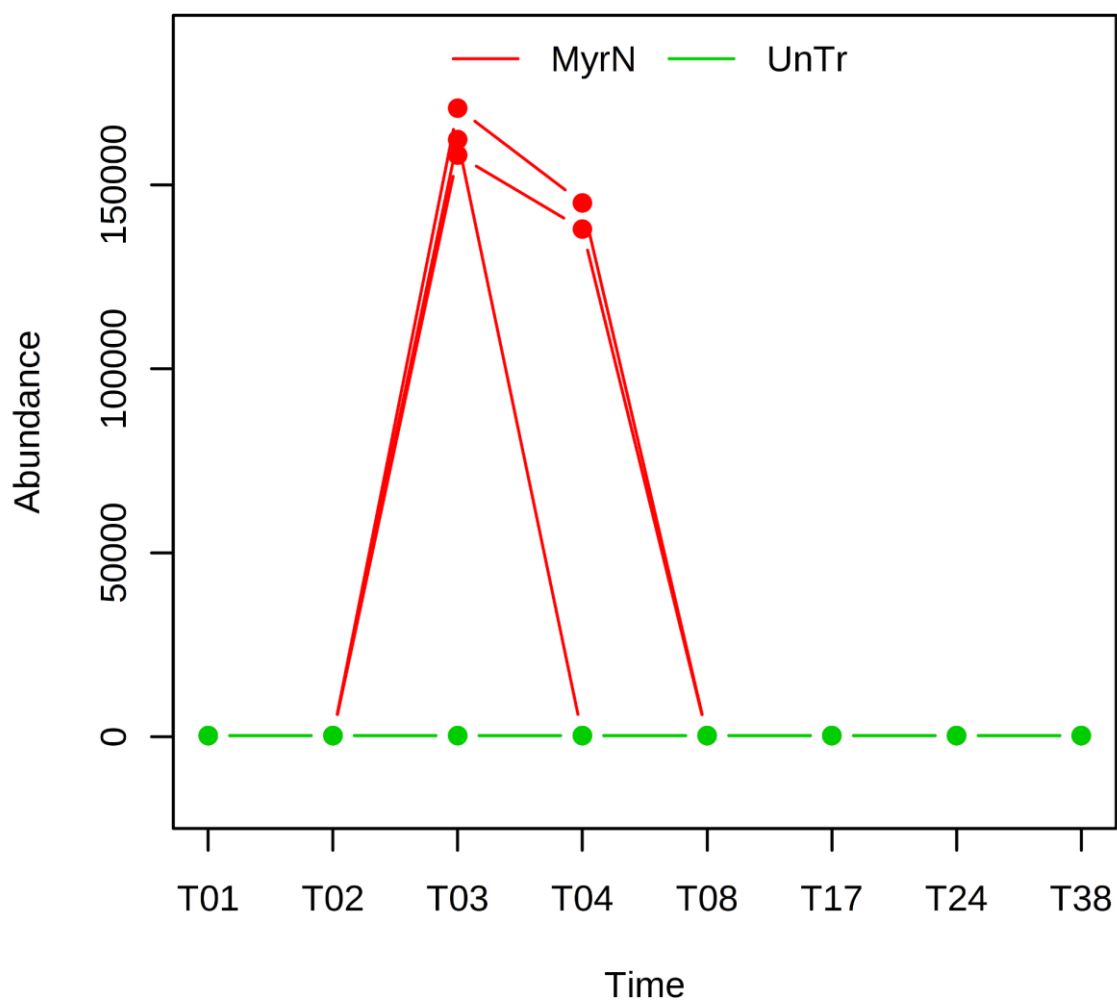
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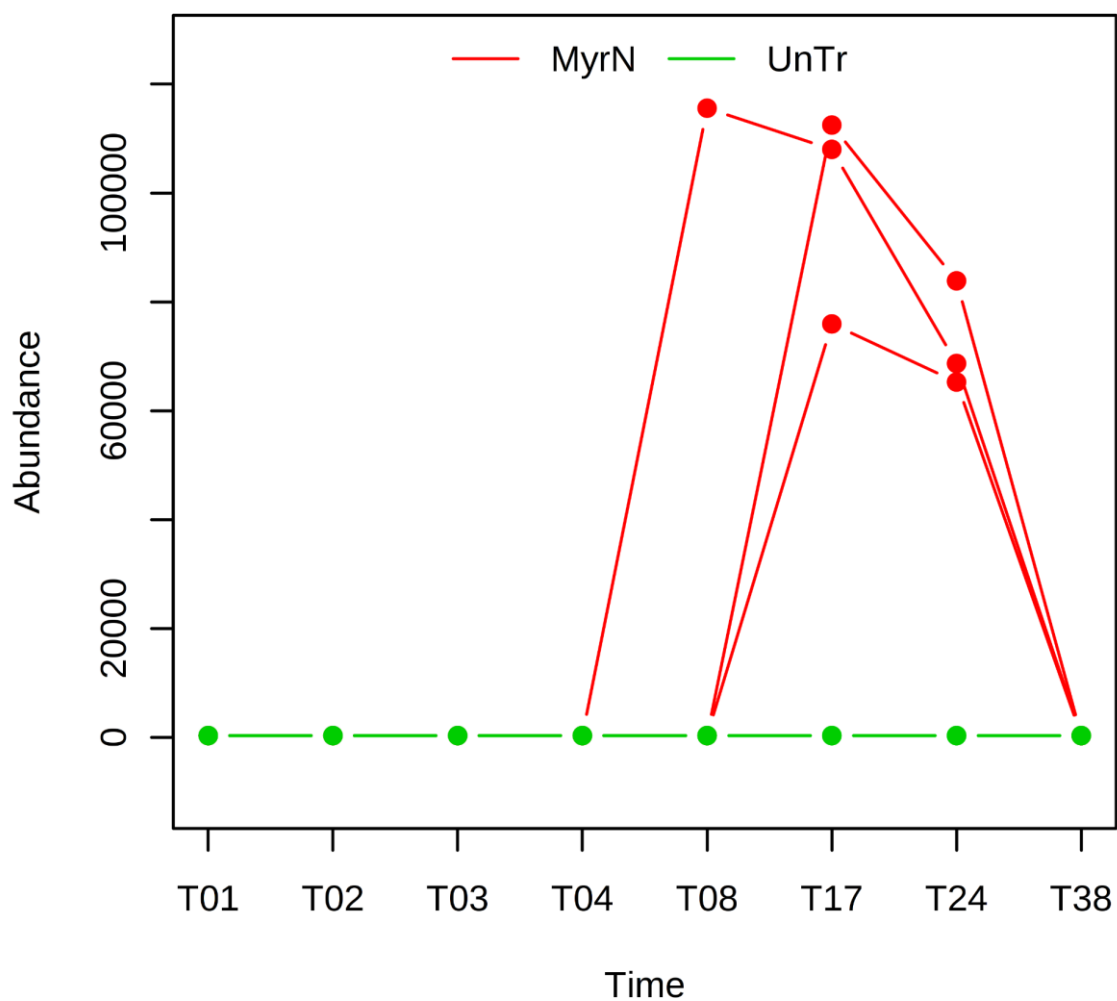


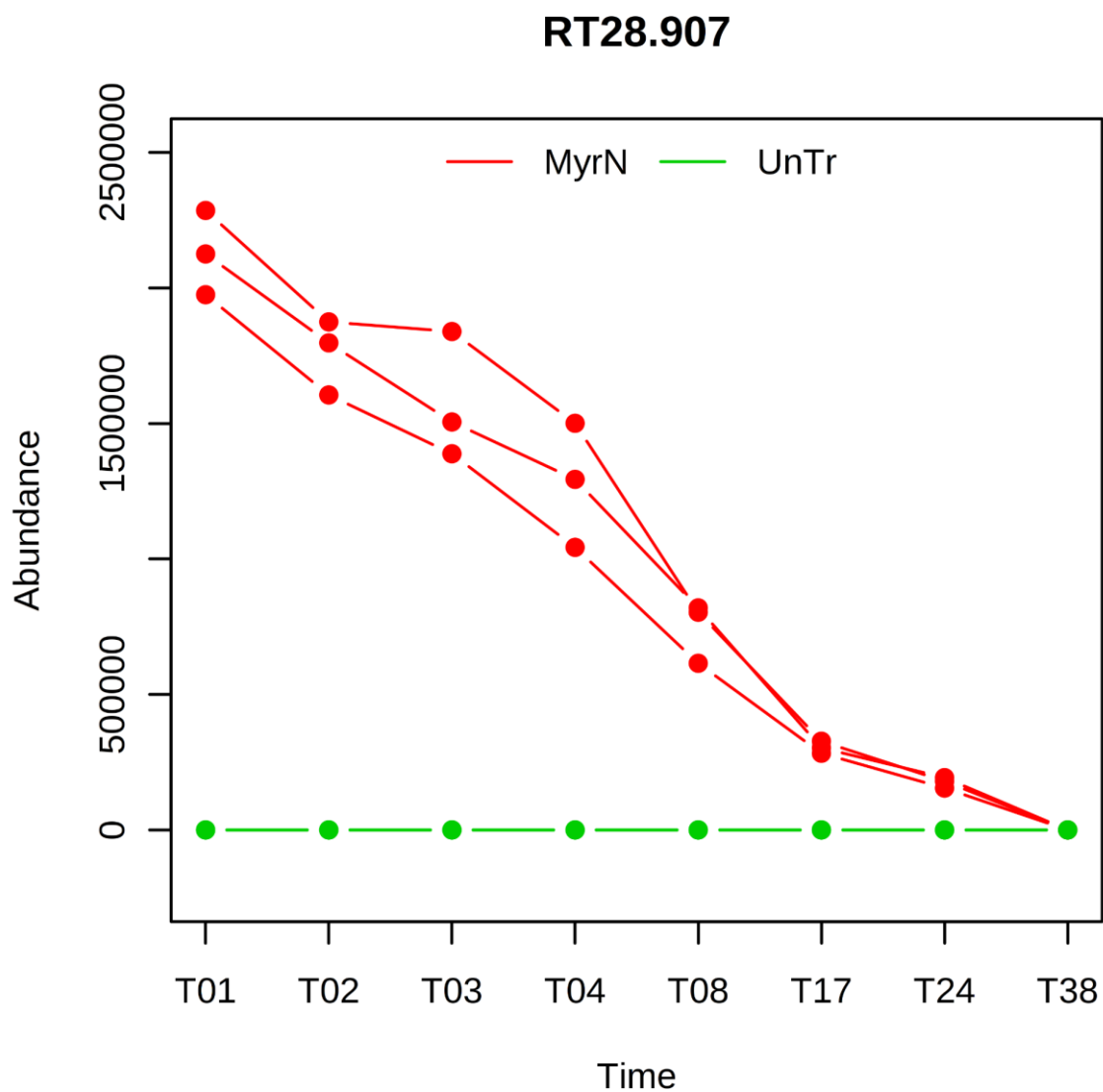


RT25.513

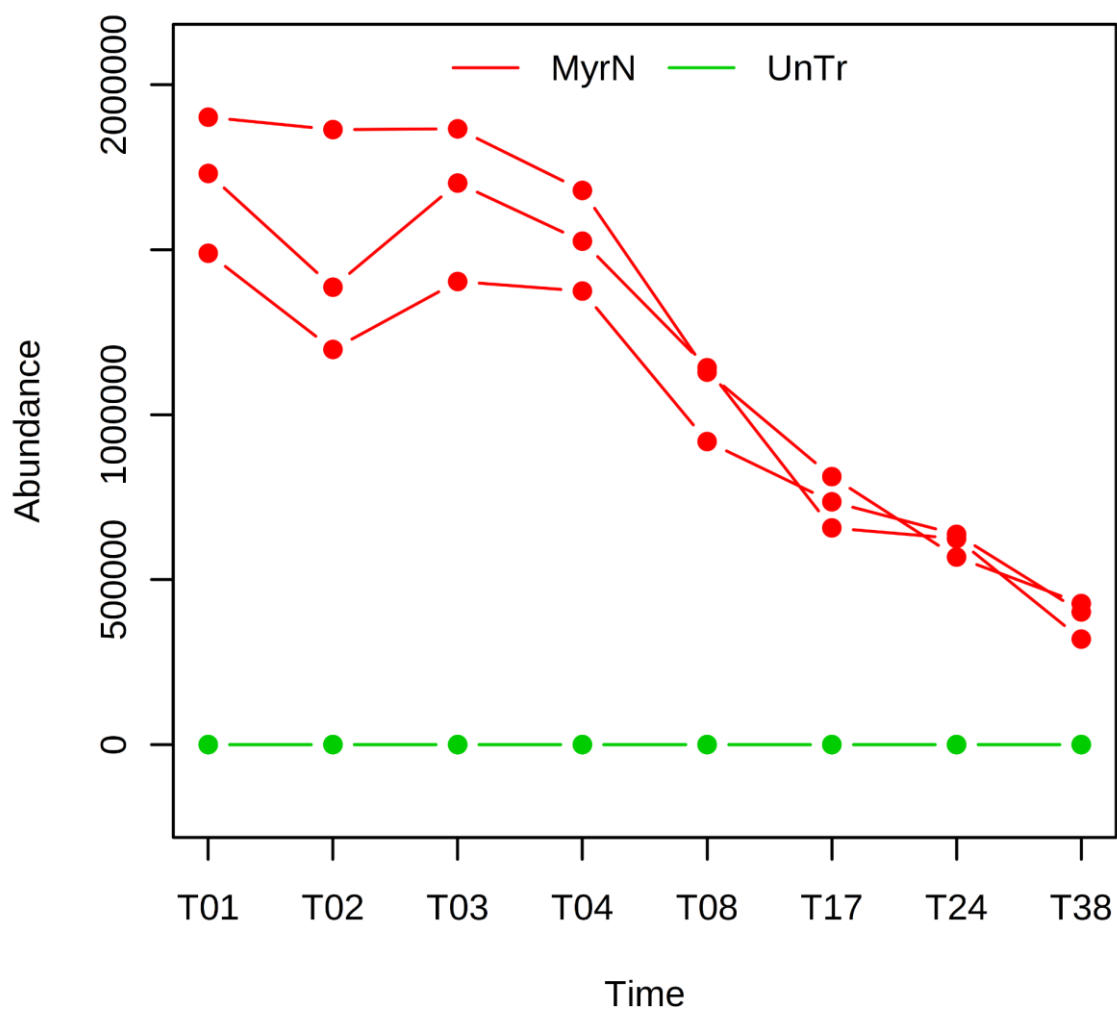


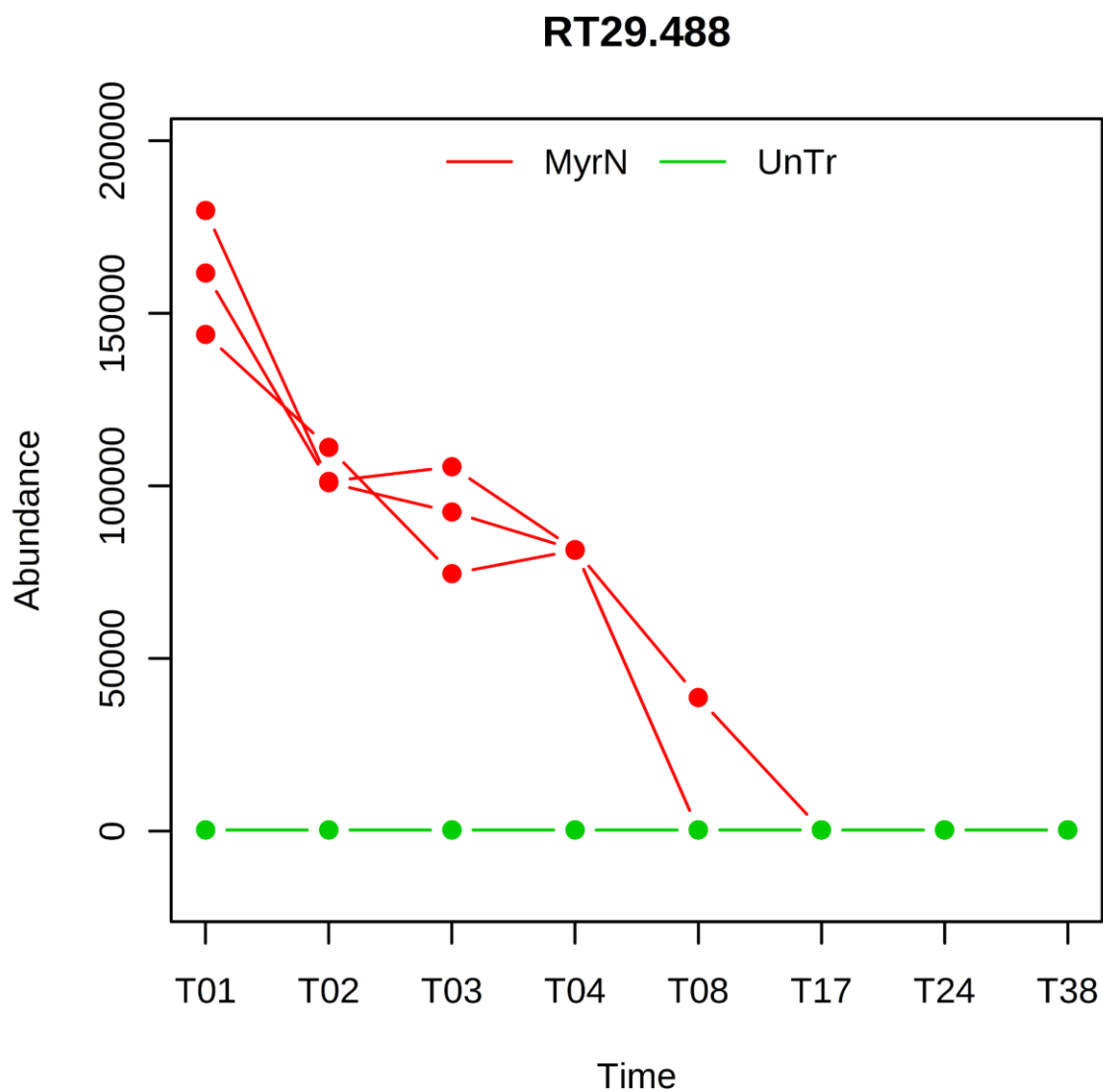
RT28.197





RT29.14





RT29.523

