

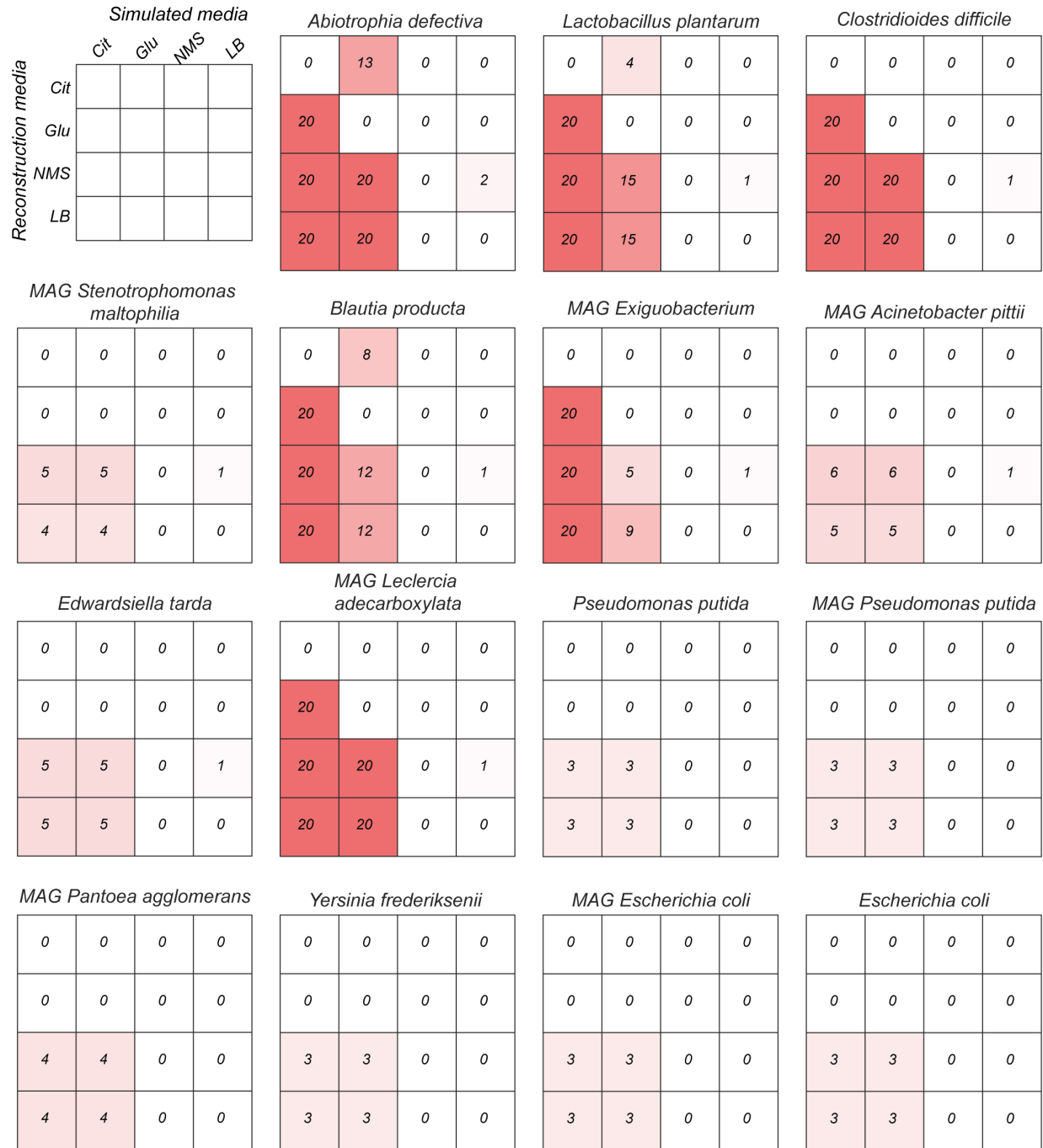
Supplementary material to: "The media composition as a crucial element in high-throughput metabolic network reconstruction"

Benedict Borer¹, Stefania Magnúsdóttir²

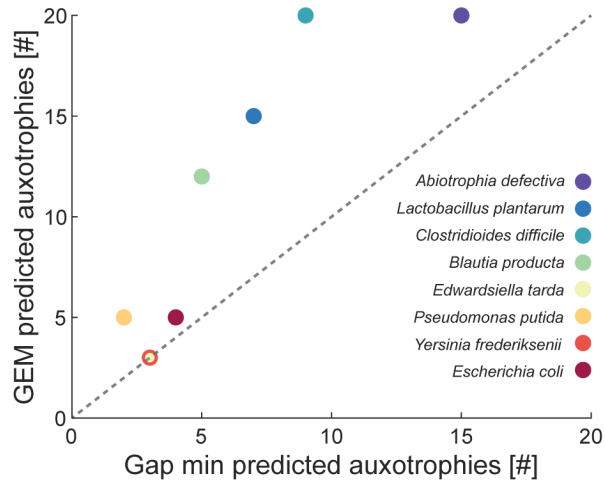
1: Earth, Atmospheric and Planetary Sciences Department, Massachusetts Institute of Technology
Cambridge, Massachusetts, USA

2: Department of Environmental Microbiology, Helmholtz Centre for Environmental Research-UFZ,
Leipzig, Germany

Corresponding authors: Stefania Magnúsdóttir, stefania.magnusdottir@ufz.de



Supplementary figure S1: Predicted number of auxotrophies for each species. Predicted auxotrophies are resolved by the media composition used for gap filling during network reconstruction (y-axis) and the media composition used for simulating growth (x-axis). For most species, reconstruction in complex media and simulation in defined media (lower left quadrant) resulted in the majority of predicted auxotrophies whereas reconstruction in minimal media and simulation in complex media (top right quadrant) resulted in no predicted auxotrophies.



Supplementary figure S2: Comparison of GapMind and GEM predicted auxotrophies. GEM predicted auxotrophies are taken from reconstructions on complex rich media (LB) simulated in glucose minimal media. NCBI genomes are used directly for the prediction of auxotrophies using GapMind for the same species using the web-interface. Overall, the GEM approach predicts a higher number of auxotrophies for the same species when compared with GapMind albeit at a similar trend.



Supplementary figure S3: Pathway resolved gap filled reactions for low quality MAGs. Low quality MAGs that required negligible gap filling (CTOTU49143, CTOTU49788 and CTOTU50314) show no unique pattern when compared to medium quality MAGs where substantial gap filling was required for growth (CTOTU46971 and CTOTU47750). Gap filled reactions are shown as the sum for all reconstructions across all different media compositions used for gap filling.

Supplementary table S1: Average number of auxotrophies for all GEMs derived from MAGs depending on the reconstruction media and simulation media differentiated by the MAG quality. Each row corresponds to a reconstruction media, the corresponding simulated media are shown as columns. Data is shown as mean with standard deviation in brackets. HQ = high quality MAGs ($\geq 90\%$ complete), MQ = medium quality MAGs ($< 90\%$ complete).

		Simulation media							
		Citrate		Glucose		NMS		LB	
		HQ	MQ	HQ	MQ	HQ	MQ	HQ	MQ
Reconstruction media	Citrate	0 (0)	0 (0)	0.18 (0.86)	0.80 (1.69)	0 (0)	0 (0)	0 (0)	0 (0)
	Glucose	0.63 (3.50)	0.40 (1.26)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)
	NMS	4.32 (3.83)	4.30 (2.79)	4.01 (2.76)	4.70 (3.20)	0 (0)	0 (0)	0.05 (0.22)	0.10 (0.32)
	LB	4.36 (3.83)	4.30 (2.79)	4.08 (2.77)	4.90 (3.78)	0 (0)	0 (0)	0 (0)	0 (0)

Supplementary table S2: Fraction of GEMs derived from MAGs that are able to produce biomass depending on the reconstruction media and simulation media. Each row corresponds to a reconstruction media, the corresponding simulated media are shown as columns.

		Simulation media			
		Citrate	Glucose	NMS	LB
Reconstruction media	Citrate	1	0.94	1	1
	Glucose	0.96	1	1	1
	NMS	0	0	1	0.94
	LB	0	0	1	1