

1 Using MR-Chordless Circuits for Efficient
2 Enumeration of Autocatalytic Cores in Large
3 Chemical Reaction Networks - Supplementary
4 Information

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1 Metabolic Networks

Metabolic networks in SBML - format were downloaded as .xml-files from the BIGG database [1] and from each network a set of small molecules with high connectivity removed, co-factors, catalysts, as well as energy providing or electron transferring molecules. The overall list of molecules fed to *autogatito* was derived from the union of species from all metabolic networks of the BIGG-database. However, since not each metabolite is present in each metabolic network, the list of removed molecules may differ from species to species. In each case, we provide here the list of BIGG-identifiers and refer to the BIGG-website for complete names of the chemical molecules. The prefix "M" always refers to metabolite and the suffixes "c", "e", "g" "h", "m", and "r" to the compartments, cytosol, extracellular, golgi apparatus, chloroplast, mitochondrial, and endoplasmic reticulum, respectively.

1.1 Helicobacter Pylori

The set of species removed from the metabolic network of *Helicobacter pylori* [2] comprised M.fmn_c, M.dctp_c, M.ppi_c, M.pro_L_e, M.fadh2_c, M.na1_e, M.pi_c, M.h2s_c, M.pa.Hp_c, M.fum_e, M.succ_e, M.ump_c, M.gmp_c, M.dtmp_c, M.ctp_c, M.dttp_c, M.aa_e, M.imp_c, M.ribflv_c, M.so3_c, M.cdp_c, M.datp_c, M.core_lps_hp_c, M.dcdp_c, M.dump_c, M.mqn6_c, M.hco3_c, M.dgmp_c, M.dutp_c, M.trnaglu_c, M.h2o_c, M.damp_c, M.h2co3_e, M.pime_e, M.dudp_c, M.mql6_c, M.gdp_c, M.h2_e, M.o2_c, M.h2co3_c, M.cmp_c, M.ala_L_e, M.co2_c, M.na1_c, M.dadp_c, M.atp_c, M.nadph_c, M.no_c, M.thmpp_c, M.ACP_c, M.nh4_c, M.so4_c, M.nad_c, M.adp_c, M.dnad_c, M.dgdp_c, M.dcamp_c, M.no3_c, M.fmnh2_c, M.nmn_c, M.no2_c, M.fe2_c, M.nadp_c, M.nadh_c, M.nmn_e, M.h_c, M.h2o2_c, M.coa_c, M.btn_c, M.o2s_c, M.udp_c, M.fad_c, M.utp_c, M.amp_c, M.dgtp_c, M.gtp_c, M.thmpp_c, and M.h_e.

1.2 Methanosarcina Barkeri

The set of species removed from the metabolic network of *Methanosarcina barkeri* [3] comprised M.trnaleu_c, M.ump_c, M.f430p1_c, M.h2o_c, M.dctp_c, M.k_c, M.cobya_c, M.ch4_e, M.imp_c, M.actn_R_e, M.k_e, M.trnalys_c, M.o2s_c, M.so3_e, M.cl_c, M.fmn_c, M.com_c, M.thm_c, M.cmp_c, M.f390a_c, M.udp_c, M.h_c, M.co2dam_c, M.meoh_e, M.mg2_c, M.f420_0_c, M.trnahis_c, M.ppi_c, M.f390g_c, M.idp_c, M.damp_c, M.trnaser_c, M.dcdp_c, M.co_c, M.trnaala_c, M.cob_c, M.nmn_c, M.nadph_c, M.dcmp_c, M.trnaglu_c, M.datp_c, M.ribflv_c, M.cbi_e, M.cdp_c, M.pppi_c, M.tma_e, M.gmp_c, M.ala_L_e, M.cobalt2_c, M.itp_c, M.ni2_c, M.adp_c, M.dnad_c, M.gtp_c, M.cd2_e, M.f420_1_c, M.dma_e, M.mma_e, M.dtmp_c, M.trnaile_c, M.trnagln_c, M.pac_e, M.na1_e, M.co2_c, M.btn_e, M.cu2_c, M.dump_c, M.trnatrp_c, M.ca2_e, M.thmpp_c, M.fe2_c, M.cu2_e, M.f420_2_c, M.pi_c, M.unknown_cbl1deg_e, M.coa_c, M.h_e, M.atp_c, M.trnamet_c, M.dgdp_c, M.f420_5_c, M.ctp_c, M.f420_6_c, M.no2_c, M.cbl1hbi_e, M.n2_e, M.nadp_c, M.h2o2_c, M.dgtp_c, M.alac_S_e, M.dudp_c, M.ca2_c, M.trnaasp_c, M.dcamp_c, M.dutp_c, M.dadp_c, M.f420_7_c, M.h2_e, M.thmpp_c, M.cl_e, M.f420_2h2_c, M.trnaphe_c, M.na1_c, M.trnapro_c, M.trnatyr_c, M.cd2_c, M.f430p2_c, M.dms_e, M.btn_c, M.trnagly_c, M.trnacys_c, M.utp_c, M.h2_c, M.s_e, M.ch4s_e, M.dtdp_c,

67 M_ind3ac_e, M_s_c, M_trnaarg_c, M_co1dam_c, M_f420_4_c, M_nh4_c, M_f420_3_c,
 68 M_camp_c, M_trnathr_c, M_hco3_c, M_nad_c, M_gdp_c, M_trnaval_c, M_o2_c,
 69 M_unknown_rbfdeg_e, M_h2s_c, M_glyald_e, M_f430p3_c, M_so3_c, M_nadh_c, M_f430_c,
 70 M_tsul_c, M_amp_c, and M_dttp_c.

71 1.3 Staphylococcus Aureus

72 The set of species removed from the metabolic network of Staphylococcus aureus
 73 [4] comprised M_h_c, M_trnagly_c, M_thmmp_c, M_cdp_c, M_fmn_c, M_dgmp_c,
 74 M_dctp_c, M_mqn8_c, M_amp_c, M_nadh_c, M_nadp_c, M_dgtp_c, M_no3_c, M_datp_c,
 75 M_itp_c, M_pi_e, M_fadh2_c, M_h2s_c, M_btn_c, M_nad_c, M_dtmp_c, M_pppi_c,
 76 M_glyc3p_e, M_apoACP_c, M_atp_c, M_mql8_c, M_gmp_c, M_pro_L_e, M_udp_c,
 77 M_dump_c, M_fad_c, M_nadph_c, M_fe2_c, M_dudp_c, M_dadp_c, M_hco3_c, M_ncam_e,
 78 M_dcamp_c, M_na1_c, M_gdp_c, M_trnaser_c, M_fmnh2_c, M_o2_c, M_dcmp_c,
 79 M_arg_L_e, M_ump_c, M_na1_e, M_dcdp_c, M_trnaala_c, M_h2o2_c, M_ribflv_c,
 80 M_dttp_c, M_idp_c, M_trnaile_c, M_s_c, M_so3_c, M_pi_c, M_dnad_c, M_damp_c,
 81 M_dgdp_c, M_ACP_c, M_trnalys_c, M_adp_c, M_trnaglu_c, M_dutp_c, M_imp_c,
 82 M_utp_c, M_trnamet_c, M_ctp_c, M_ppi_c, M_cmp_c, M_trnaasp_c, M_thmpp_c,
 83 M_ptrc_e, M_trnaasn_c, M_acnam_e, M_h_e, M_no2_c, M_orn_e, M_trnaarg_c, M_btn_e,
 84 M_gtp_c, M_dtdp_c, M_cu2_c, M_nh4_c, M_coa_c, M_q8h2_c, M_o2s_c, M_rbfivr_c,
 85 M_so4_c, M_cu2_e, M_glyald_e, M_nh4oh_c, M_q8_c, M_co2_c, M_h2o_c, M_trnathr_c,
 86 and M_trnacys_c.

87 1.4 Lactococcus Lactis

88 The set of species removed from the metabolic network of Lactococcus Lac-
 89 tis [5] comprised M_pi_c, M_cellb_e, M_o2s_c, M_trnaval_c, M_trnapro_c, M_acp_c,
 90 M_amp_c, M_dttp_c, M_trnaasn_c, M_arg_L_e, M_trnaarg_c, M_glc_D_e, M_trnaleu_c,
 91 M_thmpp_c, M_h2o2_c, M_mqn8_c, M_glu_L_e, M_hco3_c, M_trnaala_c, M_trnaasp_c,
 92 M_utp_c, M_ACP_2_c, M_PROT_LLA_c, M_actn_R_e, M_ppi_c, M_apoACP_c,
 93 M_PROT_LLA_v3_c, M_dgmp_c, M_dtmp_c, M_4abut_e, M_trnahis_c, M_dcdp_c,
 94 M_nmn_c, M_itp_c, M_CPS_LLA_c, M_gtp_c, M_dump_c, M_glyc3p_e, M_trnagln_c,
 95 M_dtdp_c, M_nadph_c, M_pa_LLA_c, M_trnathr_c, M_mql7_c, M_ribflvRD_c, M_idp_c,
 96 M_dgtp_c, M_o2_c, M_trnagly_c, M_dutp_c, M_ump_c, M_nadp_c, M_dgdp_c, M_nh4_c,
 97 M_trnaglu_c, M_ribflv_c, M_co2_c, M_atp_c, M_dadp_c, M_hqn_c, M_acgala_e,
 98 M_dudp_c, M_cdp_c, M_ctp_c, M_nmn_e, M_h2s_c, M_cmp_c, M_trnaile_c, M_thm_c,
 99 M_trnacys_c, M_dnad_c, M_pppi_c, M_adp_c, M_gdp_c, M_dcamp_c, M_h_e, M_ACP_c,
 100 M_ch4s_e, M_fadh2_c, M_trnatyr_c, M_fad_c, M_trnaser_c, M_nadh_c, M_damp_c,
 101 M_dctp_c, M_h2o_e, M_trnalys_c, M_dimp_c, M_udp_c, M_nh3_c, M_orn_L_e,
 102 M_fmn_c, M_gmp_c, M_h2o_c, M_trnamet_c, M_datp_c, M_mqn7_c, M_thmmp_c,
 103 M_diact_e, M_nad_c, M_pi_e, M_dcmp_c, M_coa_c, M_imp_c, M_trnatrp_c, M_trnaphe_c,
 104 M_RNA_LLA_c, and M_h_c.

105 1.5 Plasmodium Falciparum

106 The set of species removed from the metabolic network of Plasmodium falciparum [8] comprised M_h_e, M_mqn4_c, M_o2s_l, M_amp_m, M_ca2_c, M_imp_c,
 107

108 M_ca2_e, M_datp_c, M_hco3_c, M_camp_c, M_hco3_h, M_35cimp_c, M_ribflv_c,
 109 M_q8h2_m, M_cdp_c, M_dttp_c, M_Lcyst_e, M_lys_L_e, M_h_g, M_pa_pf_18_0_20_4_c,
 110 M_dttp_e, M_nad_c, M_atp_m, M_dudp_c, M_o2s_m, M_4hba_e, M_pa_pf_16_0_16_0_c,
 111 M_fmnn_c, M_dcmp_c, M_dsbcrd_r, M_gmp_c, M_mql4_m, M_ppi_h, M_udp_c,
 112 M_coa_h, M_dimp_c, M_no3_c, M_mqn4_m, M_nadh_h, M_Hb_l, M_h_m, M_asn_L_e,
 113 M_h2o_l, M_amp_c, M_ser_L_e, M_ppi_c, M_pa_pf_18_0_18_1_c, M_nad_h, M_nh4_c,
 114 M_dsbgox_r, M_nadh_m, M_no_c, M_h2o_h, M_dnad_c, M_no3_m, M_thm_e, M_nadp_h,
 115 M_apoACP_h, M_o2_m, M_dadp_c, M_atp_c, M_gdp_c, M_asp_L_e, M_dtmp_c,
 116 M_35cgmp_c, M_seln_c, M_thmpp_c, M_nadp_m, M_pa_pf_16_0_18_2_c, M_xolest_16_0_e,
 117 M_ncam_e, M_nadph_h, M_gtp_m, M_35ccmp_c, M_pi_c, M_h_l, M_dtdp_c, M_cys_L_e,
 118 M_na1_e, M_thm_c, M_chsterol_e, M_dutp_c, M_pa_pf_18_2_18_2_c, M_h2o2_c,
 119 M_dna5mtc_c, M_cmp_c, M_adp_h, M_dgtp_c, M_damp_c, M_o2s_c, M_4fe4s_h,
 120 M_btn_c, M_ctp_c, M_adp_c, M_dcamp_c, M_dcdp_c, M_pa_pf_18_1_18_2_c, M_nadp_c,
 121 M_didp_c, M_fe2_m, M_nh4_h, M_ctp_h, M_o2_l, M_nmn_c, M_cu2_e, M_arg_L_e,
 122 M_atp_h, M_fadh2_m, M_chol_e, M_ppi_m, M_leu_L_e, M_gtp_c, M_met_L_e,
 123 M_pa_pf_20_4_20_4_c, M_utp_c, M_2fe2s_h, M_na1_c, M_fad_m, M_no2_m, M_thmmp_c,
 124 M_nadph_c, M_co2_m, M_cmp_h, M_ACP_h, M_gln_L_e, M_dsbcox_r, M_co2_c,
 125 M_pppi_c, M_coa_c, M_nad_m, M_cu2_c, M_adp_m, M_ump_c, M_pa_pf_18_0_18_0_c,
 126 M_h2o2_l, M_pa_pf_16_0_20_4_c, M_glu_L_e, M_pa_pf_16_0_18_1_c, M_dna_c,
 127 M_h2o2_m, M_q8_m, M_h_c, M_dctp_c, M_nadh_c, M_h2o_g, M_pa_pf_16_0_18_0_c,
 128 M_pa_pf_18_1_20_4_c, M_gly_e, M_dgdp_c, M_ile_L_e, M_pi_h, M_gthrd_e, M_dgmp_c,
 129 M_dsbgrd_r, M_gdp_m, M_nh4_m, M_h_r, M_h2o_m, M_5fthf_e, M_fe2_c, M_gthox_e,
 130 M_h2o2_h, M_4pyrdx_e, M_ala_L_e, M_o2_c, M_co2_h, M_h_h, M_nadph_m,
 131 M_35cdamp_c, M_thr_L_e, M_dump_c, M_pa_pf_18_1_18_1_c, M_pi_m, M_no2_c,
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