SynComSim – A MATLAB Application for Simulation of Synthetic Bacterial Communities

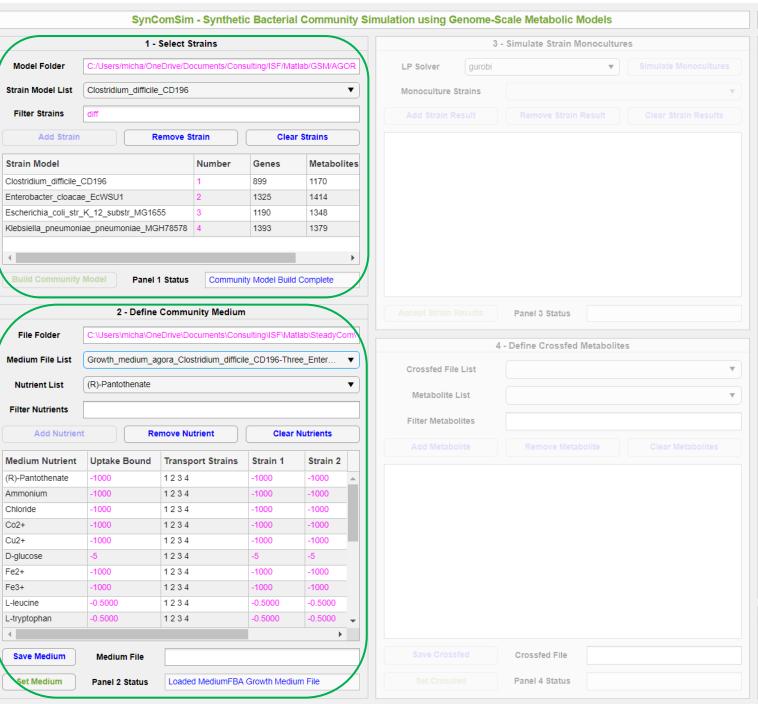
	SynCo	mSim - Synthet	ic Bacteria	I Community Si	mulation using Geno	me-Scale N	/letabolic I	lodels				li	n Silico Fe	rmentation		
1 - Select Strains					3 - Simulate Strain Monocultures					5 - Simulate Community						
Model Folder	C:/Users/micha/OneDrive/Documents/Consulting/ISF/Matlab/GSM/AGOR			LP Solver gu	LP Solver gurobi					Click Strains to Exclude Clostridium_difficile_CD196						
Strain Model List	Clostridium_difficile_0	CD196			Monoculture Strain	Strains Clostridium_difficile_CD196			FVA Percentage		Enterobacter_cloacae_EcWSU1 99 Escherichia_coll_str_K_12_substr_MG1655 Klebsiella_pneumoniae_pneumoniae_MGH78578					
Filter Strains	diff				Add Strain Result	Re	emove Strain	Result	Clear St	rain Results	Simulate Co	mmunity				
Add Strain Remove Strain Clear Strains		Nutrient or Product	Strain 1	n 1 Strain 2 S		3 S	Strain 4	Growth & Abundances		owth Rate	te Strain 1	Strain 2	Strain 3			
Strain Model		Number	Genes	Metabolites	Biomass	0.2629	0.2600	0.2505	0.	3008	FBA Solution		0.2937	0.4930	0.5070	
Clostridium difficile	CD196	1	899	1170	(R)-Pantothenate	-0.0042	-0.0016	-0.003		.0047	FVA Minimum		0.2907	0.4064	0.3183	
Enterobacter cloaca	ae EcWSU1	2	1325	1414	Ammonium	-0.8647	-1.9904	-2.010	9 -2	.9981	FVA Maximum		0.2907	0.6817	0.5872	0.13
 Escherichia_coli_str		3	1190	1348	Chloride	-0.0021	-0.0008	-0.002		.0023	4					
	iae_pneumoniae_MGH		1393	1379	Co2+	-0.0021	-0.0008	-0.002		.0023						
					Cu2+	-0.0021	-0.0008	-0.002		.0023	FBA Solution	Community	Strain 1	Strain 2	Strain 3	Strain 4
•				► -	D-glucose	-5.0000	-5.0000	-5.000		.0000	Growth rate	0.2937	0.2937	0.2937	0	0
	Model Panel 1	Status	nity Model Build	d Complete	Diphosphate	0	0	1.8314			Abundance	1.0000	0.4930	0.5070	0	0
	Paller	Status	ity would buik	a complete	Fe2+	-0.0063	0	-0.002	0 -0	.0023 🗸	(R)-Pantothenate	-0.0032	-0.0023	-0.0009	0	0
	2 Define C	ommunity Mediur			A			Ohmin Man		when the second second	(R)-lactate	0	0.5070	-0.5070	0	0
	2 - Denne C	ommunity weatur	л		Accept Strain Result	s Pan	el 3 Status	Strain Mon	oculture Res	ults Accepted	(S)-lactate	0	0.5070	-0.5070	0	0
File Folder	C:\Users\micha\OneE	Drive\Documents\Cor	isulting\ISF\M/	atlab\SteadyCom\							Ammonium	-1.6738	0.2904	-1.9642	0	0
Medium File Liet	Empty					4 - Defir	ne Crossfed	Metabolites			Chloride	-0.0016	-0.0011	-0.0005	0	0
Medium File List	Empty			▼	Crossfed File List	Cross	sfeed_amimo_	acids_agora		•	Co2+	-0.0016	-0.0011	-0.0005	0	0
Nutrient List	(R)-Pantothenate			•					Cu2+	-0.0016	-0.0011	-0.0005	0	0		
					Metabolite List	etabolite List (R)-lactate			5	-4.9998	-2.4649	-2.5349	0	0		
Filter Nutrients					Filter Metabolites						Fe2+	-0.0034	-0.0034	0	0	0
Filter Nutrients													0.0001			0
Add Nutrien	nt Rem	ove Nutrient	Clear	r Nutrients	riter metabolites						Fe3+	-0.0030	-0.0011	-0.0018	0	0
	nt Rem	ove Nutrient	Clear	Nutrients	Add Metabolite		Remove Meta	bolite	Clear I	Aetabolites	Fe3+ Formate	-0.0030 2.0187				°
Add Nutrien		ove Nutrient		r Nutrients Strain 2	Add Metabolite								-0.0011	-0.0018	0	0
Add Nutrier Medium Nutrient	Uptake Bound)							Clear I Strain 2	Aetabolites	Formate	2.0187	-0.0011	-0.0018 2.0743	0	0 0 0 0 0
Add Nutrier Medium Nutrient R)-Pantothenate	Uptake Bound	Transport Strains	Strain 1	Strain 2	Add Metabolite	Transport	Strains S	Strain 1	Strain 2 -1		Formate Glycine	2.0187 0 2.0323	-0.0011 -0.0556 -0.4930 0	-0.0018 2.0743 0.4930 2.0323	0 0 0	0 0 0 0 0 0
Add Nutrien Medium Nutrient R)-Pantothenate Ammonium	Uptake Bound -1000 -1000	Transport Strains	Strain 1 -1000	Strain 2 -1000	Add Metabolite	Transport 1234 1234	Strains S	Strain 1	Strain 2 -1 -1	Strain 3	Formate Glycine	2.0187 0 2.0323	-0.0011 -0.0556 -0.4930	-0.0018 2.0743 0.4930 2.0323	0 0 0	0 0 0 0 0 0
	Uptake Bound - -1000 - -1000 -	Transport Strains 1 2 3 4 1 2 3 4	Strain 1 -1000 -1000	Strain 2 -1000	Add Metabolite Crossfed Metabolite (R)-lactate (S)-lactate Formate	Transport 1234 1234 1234	Strains Strains - - -	Strain 1 1 1	Strain 2 -1 -1 -1	Strain 3 -1 -1 -1 -1	Formate Glycine Hvdrogen I Result Name	2.0187 0 2.0323 strains-m	-0.0011 -0.0556 -0.4930 0	-0.0018 2.0743 0.4930 2.0323 ssfeed-partial	0 0 0 0 0	0 0 0 0 0
Add Nutrien Medium Nutrient (R)-Pantothenate Ammonium Chloride	Uptake Bound -1000 -100	Transport Strains 1 2 3 4 1 2 3 4 1 2 3 4	Strain 1 -1000 -1000 -1000	Strain 2 -1000 -1000 -1000	Add Metabolite Crossfed Metabolite (R)-lactate (S)-lactate	Transport 1234 1234 1234 1234 1234	Strains S - - -	Strain 1 1 1 1 1	Strain 2 -1 -1 -1 -1	Strain 3 -1 -1 -1 -1 -1	Formate Glycine Hvdrogen	2.0187 0 2.0323 strains-m	-0.0011 -0.0556 -0.4930 0	-0.0018 2.0743 0.4930 2.0323	0 0 0 0 0	0 0 0 0 0
Add Nutrien Medium Nutrient R)-Pantothenate Ammonium Chloride Co2+ Cu2+	Uptake Bound -1000 -1000 -1000 -1000 -1000 -5	Transport Strains 1 2 3 4 1 2 3 4 1 2 3 4 1 2 3 4 1 2 3 4 1 2 3 4	Strain 1 -1000 -1000 -1000 -1000	Strain 2 -1000 * -1000 * -1000 - -1000 - -1000 - -5 -	Add Metabolite Crossfed Metabolite (R)-lactate (S)-lactate Formate Glycine L-alanine	Transport 1234 1234 1234 1234 1234 1234	Strains 5 - - - -	Strain 1 1 1 1 1 1	Strain 2 -1 -1 -1 -1 -1 -1	Strain 3 -1 -1 -1 -1 -1 -1 -1	Formate Glycine Hvdrogen I Result Name	2.0187 0 2.0323 strains-m Add	-0.0011 -0.0556 -0.4930 0	-0.0018 2.0743 0.4930 2.0323 ssfeed-partial Remove R	0 0 0 0 0	0 0 0 0 0
Add Nutrien Medium Nutrient R)-Pantothenate Ammonium Chlonde Co2+	Uptake Bound -1000 -1000 -1000 -1000 -1000 -1000 -1000 -1000 -1000 -1000 -5 -1000 -5 -1000 -5 -1000 -1000 -5 -1000 -1000 -5 -1000 -1000 -5 -1000 -1000 -5 -1000 -1000 -5 -1000 -1000 -5 -1000 -1000 -5 -1000 -5 -1000 -5 -1000 -5 -1000 -5 -1000 -5 -5 -1000 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5	Transport Strains 1234 1234 1234 1234 1234 1234 1234 1234	Strain 1 -1000 -1000 -1000 -1000 -1000 -1000 -1000 -1000 -5 -1000	Strain 2 -1000 * -1000 * -1000 * -1000 * -1000 * -1000 * -1000 * -1000 * -5 * -1000 *	Add Metabolite Crossfed Metabolite (R)-lactate (S)-lactate Formate Glycine L-alanine L-argininium(1+)	Transport 1234 1234 1234 1234 1234 1234 1234 1234	Strains 5 - - - - - - - -	Strain 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	Strain 2 -1 -1 -1 -1 -1 -1 -1	Strain 3 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1	Formate Glycine Hwdronen Result Name Discard Result Result List	2.0187 0 2.0323 strains-m Add strains-m	-0.0011 -0.0556 -0.4930 0 ninus-Kpn_cro Result ninus-Kpn_cro	-0.0018 2.0743 0.4930 2.0323 ssfeed-partial Remove R ssfeed-partial	0 0 0 0 Result	0 0 0 0 0
Add Nutrien Medium Nutrient (R)-Pantothenate Ammonium Chloride Co2+	Uptake Bound -1000 -1	Transport Strains 1234 1234 1234 1234 1234 1234 1234 1234	Strain 1 -1000 -1000 -1000 -1000 -1000 -1000 -1000 -5 -1000 -1000 -1000	Strain 2 -1000 -1000 -1000 -1000 -1000 -1000 -5 -1000 -1000	Add Metabolite Crossfed Metabolite (R)-lactate Formate Glycine L-alanine L-argininium(1+) L-aspartate(1-)	Transport 1234 1234 1234 1234 1234 1234 1234 1234	Strains 5 - - - - - - - - - - - - -	Strain 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	Strain 2 -1 -1 -1 -1 -1 -1 -1 -1 -1	Strain 3 -1 ▲ -1 ▲ -1 ▲ -1 ↓ -1 ↓ -1 ↓ -1 ↓ -1 ↓ -1 ↓ -1 ↓ -1 ↓	Formate Glycine Hvdronen Result Name Discard Result	2.0187 0 2.0323 strains-m Add strains-m	-0.0011 -0.0556 -0.4930 0 ninus-Kpn_cro Result	-0.0018 2.0743 0.4930 2.0323 ssfeed-partial Remove R	0 0 0 0 Result	0 0 0 0 0
Add Nutrien Medium Nutrient R)-Pantothenate Ammonium Chionde Co2+	Uptake Bound -1000 -1000 -1000 -1000 -1000 -1000 -5 -1000 -5 -1000 -0.500 -0.500	Transport Strains 1234 1234 1234 1234 1234 1234 1234 1234	Strain 1 -1000 -1000 -1000 -1000 -1000 -1000 -1000 -5 -1000 -1000 -0.5000	Strain 2 -1000 * -1000 * -1000 * -1000 * -1000 * -1000 * -1000 * -1000 * -5 * -1000 *	Add Metabolite Crossfed Metabolite (R)-lactate (S)-lactate Formate Glycine L-alanine L-argininium(1+) L-aspartate(1-) L-cysteine	Transport 1234 1234 1234 1234 1234 1234 1234 1234	Strains 5 - - - - - - - - - - - - - - - - - - -	Strain 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	Strain 2 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1	Strain 3 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1	Formate Glycine Hwdronen Result Name Discard Result Result List	2.0187 0 2.0323 strains-m Add strains-m	-0.0011 -0.0556 -0.4930 0 ninus-Kpn_cro 6 Status	-0.0018 2.0743 0.4930 2.0323 ssfeed-partial Remove R ssfeed-partial Simulation Re	0 0 0 0 Result	0 0 0 0 0
Add Nutrier Medium Nutrient R)-Pantothenate Ammonium Dhioride Co2+ O-glucose e2+ -e3+ -ieucine	Uptake Bound -1000 -1000 -1000 -1000 -1000 -1000 -1000 -5 -1000 -1000 -0.5000 -0.5000 -1000 -0.5000 -1000 -0.5000 -1000 -0.5000 -1000 -0.5000 -1000 -0.5000 -1000 -0.5000 -1000 -0.5000 -1000 -0.5000 -1000 -0.5000 -1000 -0.5000 -1000 -0.5000 -1000 -0.5000 -1000 -0.5000 -1000 -0.5000 -1000 -0.500 -1000 -100 -100 -1000 -1	Transport Strains 1234 1234 1234 1234 1234 1234 1234 1234	Strain 1 -1000 -1000 -1000 -1000 -1000 -1000 -1000 -5 -1000 -1000 -1000	Strain 2 -1000 -1000 -1000 -1000 -1000 -1000 -5 -1000 -1000	Add Metabolite Crossfed Metabolite (R)-lactate Formate Glycine L-alanine L-argininium(1+) L-aspartate(1-)	Transport 1234 1234 1234 1234 1234 1234 1234 1234	Strains 5 - - - - - - - - - - - - -	Strain 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	Strain 2 -1 -1 -1 -1 -1 -1 -1 -1 -1	Strain 3 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1	Formate Glycine Hwdronen Result Name Discard Result Result List	2.0187 0 2.0323 strains-m Add strains-m	-0.0011 -0.0556 -0.4930 0 ninus-Kpn_cro 6 Status	-0.0018 2.0743 0.4930 2.0323 ssfeed-partial Remove R ssfeed-partial	0 0 0 0 Result	0 0 0 0 0
Add Nutrier Medium Nutrient R)-Pantothenate Mimonium Chloride Co2+ Co2+ Co2+ Co2+ Co2+ Co2+ Co2+ Co2+	Uptake Bound -1000 -1000 -1000 -1000 -1000 -1000 -5 -1000 -5 -1000 -0.500 -0.500	Transport Strains 1234 1234 1234 1234 1234 1234 1234 1234	Strain 1 -1000 -1000 -1000 -1000 -1000 -1000 -1000 -5 -1000 -1000 -0.5000	Strain 2 -1000 -1000 -1000 -1000 -1000 -1000 -1000 -1000 -1000 -1000 -1000 -1000 -1000	Add Metabolite Crossfed Metabolite (R)-lactate (S)-lactate Formate Glycine L-alanine L-argininium(1+) L-aspartate(1-) L-cysteine	Transport 1234 1234 1234 1234 1234 1234 1234 1234	Strains 5 - - - - - - - - - - - - - - - - - - -	Strain 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	Strain 2 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1	Strain 3 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1	Formate Glycine Hwdronen Result Name Discard Result Result List	2.0187 0 2.0323 Strains-m Add strains-m s Panel	-0.0011 -0.0556 -0.4930 0 ninus-Kpn_cro Result 	-0.0018 2.0743 0.4930 2.0323 ssfeed-partial Remove R ssfeed-partial Simulation Re	0 0 0 0 Result	0 0 0 0 Clear Result
Add Nutrien Medium Nutrient R)-Pantothenate Ammonium Chionde Co2+	Uptake Bound -1000 -1000 -1000 -1000 -1000 -1000 -5 -1000 -5 -1000 -0.500 -0.500	Transport Strains 1234 1234 1234 1234 1234 1234 1234 1234	Strain 1 -1000 -1000 -1000 -1000 -1000 -1000 -1000 -5 -1000 -1000 -0.5000	Strain 2 -1000 -1000 -1000 -1000 -1000 -1000 -1000 -1000 -1000 -0.500	Add Metabolite Crossfed Metabolite (R)-lactate (S)-lactate Formate Glycine L-alanine L-argininium(1+) L-aspartate(1-) L-cysteine	Transport 1234 1234 1234 1234 1234 1234 1234 1234 1234 1234 1234 1234	Strains 5 - - - - - - - - - - - - - - - - - - -	Strain 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	Strain 2 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1	Strain 3 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1	Formate Glycine Hvidronen 4 Result Name Discard Result Result List Visualize Result	2.0187 0 2.0323 Strains-m Add strains-m s Panel	-0.0011 -0.0556 -0.4930 0 Result inus-Kpn_cro 5 Status 6 - Mana cha\OneDrive	-0.0018 2.0743 0.4930 2.0323 ssfeed-partial Remove R ssfeed-partial Simulation Re age Case	0 0 0 Result Added	Clear Result

Example – Investigate metabolite crossfeeding strategies for a 4-species community consisting of the gut pathogen *Clostridioides difficile* and three Enterobacteriaceae species

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1. Select metabolic models for the strains of interest. Strains can be removed from selected simulations later in the workflow.

2. Define nutrients contained in the culture medium. Nutrients and their uptake bounds can be added individually or loaded from a medium file created with our App MediumFBA.



3. Perform monoculture simulations to examine strain growth behavior. Fluxes of consumed nutrients and secreted products are predicted for each strain.

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4. Define metabolites allowed to be crossfed between community strains. Options include all possible metabolites, individually added metabolites, or metabolites loaded from a previously saved file.

	1 - S	elect Strains			3 - Simulate Strain Monocultures							
Model Folder	C:/Users/micha/One	Drive/Documents/Con	sulting/ISF/Ma	LP Solver gu	Simulate Monoc	mulate Monocultures						
Strain Model List	Clostridium_difficile_CD196				Monoculture Strains Clostridium_difficile_CD196							
Filter Strains	diff		Add Strain Result		Remove Strain Result Clear Strain Resul							
Add Strain	Re	move Strain	Clea	r Strains	Nutrient or Product	Strain 1	Strain 2	Strain	3 Strair	n 4		
Strain Model		Number	Genes Metabolites		Biomass	0.2629	0.2600	0.2505	0.3008			
Clostridium_difficile_(CD196	1	899	1170	(R)-Pantothenate	-0.0042	-0.0016	-0.0039				
Enterobacter_cloacae	e_EcWSU1	2	1325	1414	Ammonium	-0.8647	-1.9904	-2.0109	-2.998	31		
Escherichia_coli_str_	K_12_substr_MG165	5 3	1190	1348	Chloride	-0.0021	-0.0008	-0.0020	-0.002	23		
Klebsiella_pneumonia	ae_pneumoniae_MGH	178578 4	1393	1379	Co2+	-0.0021	-0.0008	-0.0020	-0.002	23		
					Cu2+	-0.0021	-0.0008	-0.0020				
•				► I	D-glucose	-5.0000	-5.0000	-5.0000		00		
	Model Panel 1	Statue	ity Model Build	Complete	Diphosphate	0	0	1.8314	0			
_una oonninunity	Failer	Commun	ity would build	roompiete	 [4] 	0.0000	0	0.0000	0.000	•		
Medium File List Nutrient List	(R)-Pantothenate			•	Crossfed File List		fine Crossfed Me					
Medium File List Nutrient List Filter Nutrients	(R)-Pantothenate				Metabolite List		fine Crossfed Me 4-dihydroxyphenyl)a			•		
Nutrient List		nove Nutrient	Clear		Metabolite List Filter Metabolites					•		
Nutrient List Filter Nutrients Add Nutrient	t Ren)		▼ Nutrients	Metabolite List			cetate	Clear Metabo			
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Nutrient List Filter Nutrients Add Nutrient Medium Nutrient (R)-Pantothenate Ammonium Chloride Co2+ Cu2+ D-glucose Fe2+ Fe2+ Fe3+ L-leucine	t Ren Uptake Bound -1000 -1000 -1000 -1000 -1000 -1000 -5 -1000 -1000 -00 -1000 -00 -1000 -00 -1000 -00 -	Transport Strains 1 2 3 4 1 2 3 4 1 2 3 4 1 2 3 4 1 2 3 4 1 2 3 4 1 2 3 4 1 2 3 4 1 2 3 4 1 2 3 4 1 2 3 4 1 2 3 4 1 2 3 4	Strain 1 -1000 -1000 -1000 -1000 -1000 -1000 -1000 -1000 -5 -1000 -1000 -1000	▼ Nutrients Strain 2 -1000 -100 -1000 -1	Metabolite List Filter Metabolites Add Metabolite (3,4-dihydroxyphenyl)ace (4-hydroxyphenyl)acetalo (R)-3-hydroxybutyrate (R)-Acetoin (R)-lactate (S)-lactate (S)-lactate (S)-malate(2-)	(3, (3,)))))))))))))))))))	4-dihydroxyphenyl)a Remove Metaboli ransport Strains 2 4 3 4 2 4 4 2 3 4 2 3 4 2 3 4 3 4 3 4 3 4	cetate te Strain 1 -1 NaN -1 NaN -1 NaN -1 NaN -1 NaN NaN	Strain 2 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1	Stra NaN -1 NaN NaN -1 -1 -1 -1		
Nutrient List Filter Nutrients Add Nutrient Medium Nutrient (R)-Pantothenate Ammonium Chloride Co2+ Cu2+ D-glucose Fe2+ Fe3+ L-leucine	t Ren Uptake Bound -1000 -1000 -1000 -1000 -1000 -1000 -5 -1000 -1000 -1000 -5 -1000 -1000 -0.5000	Transport Strains 1234 1234 1234 1234 1234 1234 1234 1234 1234 1234 1234 1234 1234 1234 1234	Strain 1 -1000 -1000 -1000 -1000 -1000 -1000 -1000 -5 -1000 -1000 -1000 -5 -1000 -5 -1000 -5,000	▼ Nutrients Strain 2 -1000 -1000 -1000 -1000 -1000 -1000 -5 -5 -1000 -1000 -0.5000 0 25000	Metabolite List Filter Metabolites Add Metabolite Crossfed Metabolite (3,4-dihydroxyphenyl)acetak (4-hydroxyphenyl)acetak (R)-3-hydroxybutyrate (R)-Acetoin (R)-lactate (S)-lactate (S)-lactate (S)-malate(2-) (S)-propane-1,2-diol	(3, (3,) (3,))) (3,)) (3,))) (3,))) (3,))) (3,))) (3,))) (3,))) (3,))) (3,))) (3,)))(3,))) (3,)))(3,)))(3,))(3,	4-dihydroxyphenyl)a Remove Metaboli ransport Strains 2 4 3 4 2 4 4 2 3 4 2 3 4 2 3 4 3 4 3 4 3 4	cetate te Strain 1 -1 NaN -1 NaN -1 -1 NaN -1 NaN NaN NaN	Strain 2 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1	Stra NaN -1 NaN NaN -1 -1 -1 -1 -1 -1		
Nutrient List Filter Nutrients Add Nutrient Medium Nutrient (R)-Pantothenate Ammonium Chloride Co2+ Cu2+ D-glucose Fe2+ Fe3+ L-leucine L-tryptophan 4	t Ren Uptake Bound -1000 -1000 -1000 -1000 -1000 -1000 -5 -1000 -1000 -0.5000 -0.5000 -0.5000	Transport Strains 1234 1234 1234 1234 1234 1234 1234 1234 1234 1234 1234 1234 1234 1234 1234	Strain 1 -1000 -1000 -1000 -1000 -1000 -1000 -1000 -5 -1000 -1000 -1000 -5 -1000 -5 -1000 -5,000	▼ Nutrients Strain 2 -1000 -1000 -1000 -1000 -1000 -1000 -1000 -1000 -5 -1000 -1000 -0.5000	Metabolite List Filter Metabolites Add Metabolite Crossfed Metabolite (3,4-dihydroxyphenyl)ace (4-hydroxyphenyl)ace (R)-3-hydroxybutyrate (R)-Acetoin (R)-lactate (S)-lactate (S)-malate(2-) (S)-propane-1,2-diol 1,5-Diaminopentane	(3, (3,)))))))))))))))))))	4-dihydroxyphenyl)a Remove Metaboli ransport Strains 2 4 3 4 2 4 4 2 3 4 2 3 4 2 3 4 3 4 3 4 3 4	cetate te Strain 1 -1 NaN -1 NaN -1 -1 NaN -1 NaN NaN NaN	Strain 2 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1	Stra NaN -1 NaN -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1		
Nutrient List Filter Nutrients Add Nutrient Medium Nutrient (R)-Pantothenate Ammonium Chloride Co2+ Cu2+ D-glucose Fe2+ Fe3+ L-leucine	t Ren Uptake Bound -1000 -1000 -1000 -1000 -1000 -1000 -5 -1000 -1000 -1000 -5 -1000 -1000 -0.5000	Transport Strains 1234 1234 1234 1234 1234 1234 1234 1234 1234 1234 1234 1234 1234 1234 1234	Strain 1 -1000 -1000 -1000 -1000 -1000 -1000 -1000 -5 -1000 -1000 -1000 -5 -1000 -5 -1000 -5,000	▼ Nutrients Strain 2 -1000 -1000 -1000 -1000 -1000 -1000 -1000 -1000 -5 -1000 -1000 -0.5000	Metabolite List Filter Metabolites Add Metabolite (3,4-dihydroxyphenyl)acetal (4-hydroxyphenyl)acetal (R)-3-hydroxybutyrate (R)-Acetoin (R)-lactate (S)-lactate (S)-ralate(2-) (S)-propane-1,2-diol 1,5-Diaminopentane 4	(3, (3,)))))))))))))))))))	4-dihydroxyphenyl)a Remove Metaboli ransport Strains 2 4 3 4 2 4 4 2 3 4 2 3 4 3 4 3 4 3 4 4	cetate te Strain 1 -1 NaN -1 NaN -1 -1 NaN -1 NaN NaN NaN	Strain 2 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1	Stra NaN -1 NaN -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1		

mulation using Genome-Scale Metabolic Models

	3 -	Simulate	Strain	Monocu	ltures	5		
LP Solver gu	irobi				•	Simula	te Monocultur	es
Monoculture Strain	s	Clostridiu	ım_diffici	ile_CD196	6			•
Add Strain Result		Remo	ve Strai	n Result		Clear	Strain Results	5
Nutrient or Product	Strair	n 1	Strain	2	Strair	13	Strain 4	
Biomass	0.2629	9	0.2600		0.2505	5	0.3008	
R)-Pantothenate	-0.004	2	-0.0016	; .	-0.003	9	-0.0047	
Ammonium	-0.864	7	-1.9904		-2.0109 -0.0020 -0.0020		-2.9981	10
Chloride	-0.002	1	-0.0008	; .			-0.0023	
02+	-0.002	1	-0.0008	; · ·			-0.0023	_
Cu2+	-0.002	1	-0.0008	; ·			-0.0023	
D-glucose	-5.000	0	-5.0000) .	-5.000	0	-5.0000	_
Diphosphate	0		0		1.8314	1	0	
e2+	-0.006	3	0		-0.002	0	-0.0023	- .
Accept Strain Result	4 -	Define C			olites	oculture F	Results Accepte	
	4 -	Define C	Crossfe d_amim	d Metabo	olites		Results Accepte	
Crossfed File List Metabolite List	4 -	Define C Crossfee (R)-lactat	Crossfe d_amim	d Metabo	olites		results Accepte	•
Crossfed File List Metabolite List Filter Metabolites Add Metabolite	4 -	Define C Crossfee (R)-lactat	Crossfe d_amimo re ove Met	d Metabo	olites			 • •<
Crossfed File List Metabolite List Filter Metabolites Add Metabolite	4 -	Define C Crossfee (R)-lactat Rem sport Str	Crossfe d_amimo re ove Met	d Metabo o_acids_a	igora	Clea	ır Metabolites	 • •<
Crossfed File List Metabolite List Filter Metabolites Add Metabolite Crossfed Metabolite R)-lactate	4 -	Define C Crossfee (R)-lactat Rem sport Str 4	Crossfe d_amimo re ove Met	d Metabo o_acids_a abolite Strain 1	agora	Clea Strain 2	ar Metabolites Strain 3	 • •<
Crossfed File List Metabolite List Filter Metabolites Add Metabolite Crossfed Metabolite R)-lactate S)-lactate	4 -	Define C Crossfee (R)-lactat Rem sport Str 4	Crossfe d_amimo re ove Met	d Metabo o_acids_a abolite Strain 1 -1	gora	Clea Strain 2 -1	ar Metabolites Strain 3 -1	 • •<
Crossfed File List Metabolite List Filter Metabolites Add Metabolite Crossfed Metabolite R)-lactate S)-lactate Formate	4 - 1 2 3 1 2 3	Define C Crossfee (R)-lactat Rem sport Str 4 4 4	Crossfe d_amimo re ove Met	d Metabo o_acids_a abolite Strain 1 -1 -1	gora	Clea Strain 2 -1 -1	ar Metabolites Strain 3 -1 -1	 • •<
Crossfed File List Metabolite List Filter Metabolites Add Metabolite Crossfed Metabolite R)-lactate S)-lactate S)-lactate S)-lactate	4 - Tran 123 123	Define C Crossfee (R)-lactat Rem sport Str 4 4 4 4 4	Crossfe d_amimo re ove Met	d Metabo o_acids_a abolite Strain 1 -1 -1 -1	gora	Cle: Strain 2 -1 -1 -1	ar Metabolites Strain 3 -1 -1 -1 -1	 • •<
Crossfed File List Metabolite List Filter Metabolites Add Metabolite R)-lactate S)-lactate s)-lactate -alanine	4 - Tran 123 123 123 123	Define C Crossfee (R)-lactat Rem sport Stu 4 4 4 4 4 4	Crossfe d_amimo re ove Met	d Metabo o_acids_a abolite Strain 1 -1 -1 -1 -1	gora	Clea Strain 2 -1 -1 -1 -1 -1	ar Metabolites Strain 3 -1 -1 -1 -1 -1 -1	 • •<
Crossfed File List Metabolite List Filter Metabolites Add Metabolite Crossfed Metabolite R)-lactate S)-lactate cormate S)-lactate -alanine -argininium(1+)	4 - Tran 123 123 123 123	Define C Crossfee (R)-lactat Rem sport Str 4 4 4 4 4 4 4 4 4	Crossfe d_amimo re ove Met	d Metabo o_acids_a abolite Strain 1 -1 -1 -1 -1 -1 -1 -1	gora	Cle: Strain 2 -1 -1 -1 -1 -1 -1 -1	ar Metabolites Strain 3 -1 -1 -1 -1 -1 -1 -1 -1	 • •<
Crossfed File List Metabolite List Filter Metabolites Add Metabolite Crossfed Metabolite R)-lactate S)-lactate S)-lactate cormate S)-lactate cormate S)-lactate cormate S)-lactate cormate S)-lactate cormate S)-lactate cormate S)-lactate cormate S)-lactate cormate S)-lactate cormate S)-lactate cormate S)-lactate S)-lactate Cormate S)-lactate S)-lactate Cormate S)-lactate Cormate S)-lactate Cormate S)-lactate S)-lactate Cormate S)-lactate S)-lactate S)-lactate S)-lactate S)-lactate S)-lactate Cormate S)-lactate Cormate S)-lactate S)-lactate S)-lactate S)-lactate Cormate S)-lactat	4 - Tran 123 123 123 123 123 123	Define C Crossfee (R)-lactat sport Str 4 4 4 4 4 4 4 4 4 4	Crossfe d_amimo re ove Met	d Metabo o_acids_a abolite Strain 1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1	gora	Clea Strain 2 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1	ar Metabolites Strain 3 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1	 • •<
Crossfed File List Metabolite List Filter Metabolites	4 - Tran 123 123 123 123 123 123 123	Define C Crossfee (R)-lactat sport Str 4 4 4 4 4 4 4 4 4 4 4	Crossfe d_amimo re ove Met	d Metabo o_acids_a abolite Strain 1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1	gora	Clea Strain 2 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1	ar Metabolites Strain 3 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1	 • •<
Crossfed File List Metabolite List Filter Metabolites Add Metabolite Crossfed Metabolite R)-lactate S)-lactate Formate Blycine alanine argininium(1+) aspartate(1-) cysteine	4 - Tran 123 123 123 123 123 123 123 123	Define C Crossfee (R)-lactat sport Str 4 4 4 4 4 4 4 4 4 4 4	Crossfe d_amimo re ove Met	d Metabo o_acids_a abolite Strain 1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1	gora	Clea Strain 2 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1	ar Metabolites Strain 3 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1	 • •<

						-		D	×			
In Silico Fermentation												
5 - Simulate Community												
Click Strains t	o Exclude			_	ficile_CD19							
FVA Percentage	•	99	Enterobacter_cloacae_EcWSU1 Escherichia coli str K 12 substr MG1655									
Klebsiella_pneumoniae_pneumoniae_MGH78578												
Simulate Community												
Growth & Abund	lances	Grov	wth Rate St		ain 1	Strain 2	Stra	ain 3	S			
FBA Solution	FBA Solution				0.4930	0.5070			0			
FVA Minimum			0.2907		0.4064	0.3183		0				
FVA Maximum			0.2907		0.6817	0.5872		0.1332				
4									•			
FBA Solution	BA Solution Community		Strain 1		Strain 2	Strain 3		Strain 4	4			
Growth rate	0.2937		0.2937	(0.2937	0	(D	A			
Abundance	1.0000		0.4930	(0.5070	0	(D				
(R)-Pantothenate	-0.0032		-0.0023	-	0.0009	0	(D				
(R)-lactate	0		0.5070	-	0.5070	0	(D				
(S)-lactate	0		0.5070	-	0.5070	0	(D				
Ammonium	-1.6738		0.2904	-	1.9642	0	(D				
Chloride	-0.0016		-0.0011		0.0005	0	(0				
Co2+	-0.0016		-0.0011		-0.0005 0		0					
Cu2+	-0.0016		-0.0011		0.0005	0	(0				
D-glucose	-4.9998		-2.4649	-	2.5349	0	(D				
Fe2+	-0.0034		-0.0034	()	0	(D				
Fe3+	-0.0030		-0.0011	-	0.0018	0	(D				
Formate	2.0187		-0.0556		2.0743	0	(D				
Glycine	0		-0.4930		0.4930	0	(0				
Hvdrogen	2 0323		0	5	0323	0	(0	•			
								,				
Result Name	strai	ns-min	us-Kpn_cro	ssfee	d-partial				_			
Discard Result		Add R	esult		Remove R	lesult	Clear	r Result	s			
Result List	strai	ns-min	us-Kpn_cro	ssfee	d-partial				•			
Visualize Results		anel 5	Status	Qir	nulation D	esult Added						
		aner o	Juius	3	naiadon R	coan Added						
			6 - Mana	age (Case							
Case Folder	C:\Use	rs\mich		-		onsulting\ISF\M	atlab∖	Steady	Com\			
Save Case	Ca	se File	Sta	ate_a	gora_Clost	ridium_difficile_	CD1	96-Thre	e_Er			
Load Case	Panel	6 Stat	tus Ca	se Fil	e Loaded							

5. Perform community simulation for the specified uptake bounds on medium nutrients and crossfed metabolites. Specific strains can be excluded from any simulation.
Different simulations can be stored to allow comparison through a companion visualization App.

6. Save current case tocompletely capture the currentApp state for subsequent loading.

SynComSim – Companion App for Result Visualization and Comparison

MATLAB App

