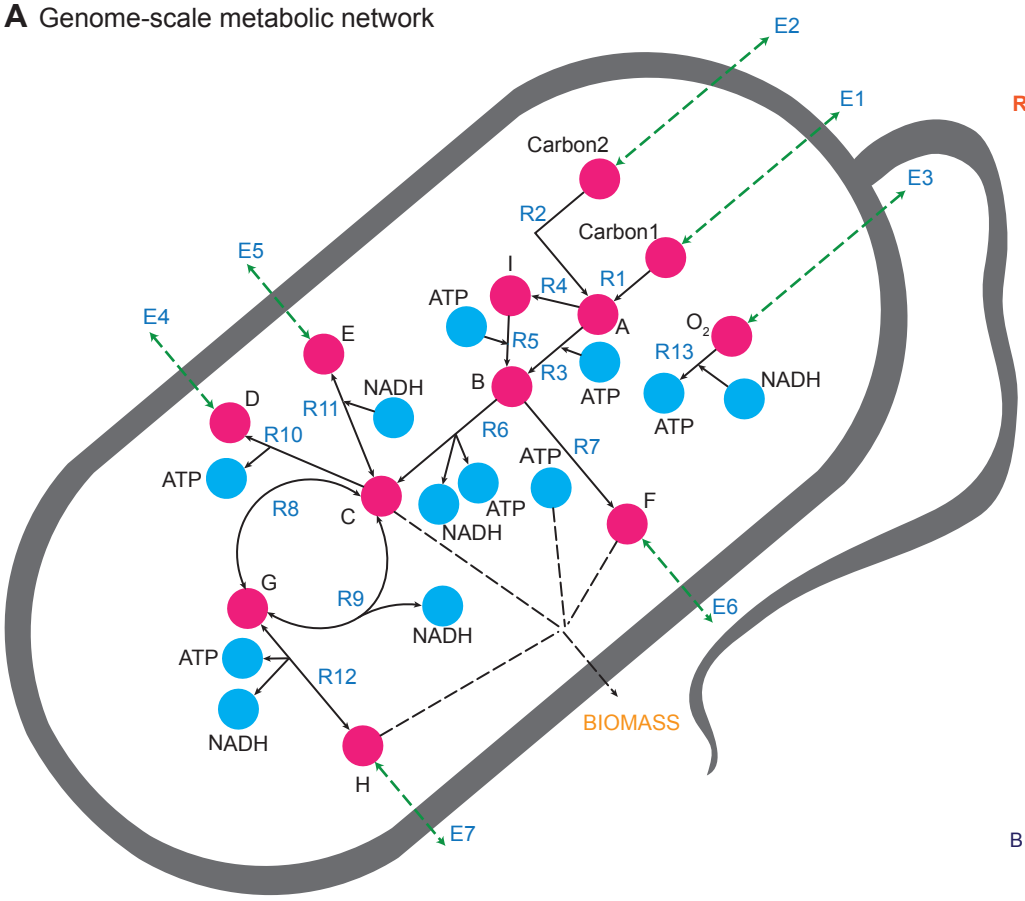
A Genome-scale metabolic network



Reaction	Equation	GPR Association
R1	Carbon1 → A	G_a
R2	Carbon2 → A	G_b
R3	A + ATP → B	G_c
R4	A → I	G_a
R5	I + ATP → B	G_d
R6	B → C + (2) ATP + (2) NADH	G_e AND G_h
R7	B → F	G_h
R8	C ↔ G	G_i
R9	G ↔ (0.8) C + (2) NADH	G_j
R10	C → (3) D + (2) ATP	G_k
R11	C + (4) NADH ↔ (3) E	G_l OR G_m
R12	G + ATP + (2) NADH ↔ H	G_n
R13	O2 + NADH → ATP	G_o
E1	Carbon1 ↔	
E2	Carbon2 ↔	
E3	O2 ↔	
E4	D ↔	
E5	E ↔	
E6	F ↔	
E7	H ↔	
BIOMASS	C + F + H + (10) ATP → Biomass	

B Mathematical representation and constraints

Balances
Stoichiometric constraints

m x n

	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	E1	E2	E3	E4	E5	E6	E7	Biomass
Carbon1	-1	0	0	0	0	0	0	0	0	0	0	0	0	-1	0	0	0	0	0	0	0
Carbon2	0	-1	0	0	0	0	0	0	0	0	0	0	0	0	-1	0	0	0	0	0	0
A	1	1	-1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
B	0	0	1	0	1	-1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C	0	0	0	0	0	1	0	-1	0.8	-1	-1	0	0	0	0	0	0	0	0	0	-1
D	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	-1	0	0	0	0
E	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	-1	0	0	0
F	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	-1	0	-1
G	0	0	0	0	0	0	0	1	-1	0	0	-1	0	0	0	0	0	0	0	0	0
H	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	-1	-1
I	0	0	0	1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
O_2	0	0	0	0	0	0	0	0	0	0	0	0	-1	0	0	-1	0	0	0	0	0
ATP	0	0	-1	0	-1	2	0	0	0	2	0	-1	1	0	0	0	0	0	0	0	-10
NADH	0	0	0	0	0	2	0	0	2	0	-4	-2	-1	0	0	0	0	0	0	0	0

S

Number of metabolites m: 14 Number of reactions n : 21

n x 1

Flux vector

V_{R1} V_{R2} V_{R3} V_{R4} V_{R5} V_{R6} V_{R7} V_{R8} V_{R9} V_{R10} V_{R11} V_{R12} V_{R13} V_{E1} V_{E2} V_{E3} V_{E4} V_{E5} V_{E6} V_{E7} $V_{BIOMASS}$

$\bullet$ V $= 0$

Bounds
Thermodynamic and other constraints

Flux	LB	UB	Constraint
V_{R1}	0	∞	Irreversible
V_{R2}	0	∞	Irreversible
V_{R3}	0	∞	Irreversible
V_{R4}	0	∞	Irreversible
V_{R5}	0	∞	Irreversible
V_{R6}	0	∞	Irreversible
V_{R7}	0	∞	Irreversible
V_{R8}	-∞	∞	Reversible
V_{R9}	0	10	Enzyme capacity
V_{R10}	0	∞	Irreversible
V_{R11}	0	∞	Reversible
V_{R12}	-∞	∞	Reversible
V_{R13}	0	∞	Irreversible
V_{E1}	-10	0	Uptake
V_{E2}	0	1000	Excretion
V_{E3}	-1000	1000	Uptake/Excretion
V_{E4}	0	∞	Reversible
V_{E5}	0	∞	Reversible
V_{E6}	0	∞	Reversible
V_{E7}	0	∞	Reversible
$V_{BIOMASS}$	0	∞	Irreversible

C Feasible solution space and linear optimization