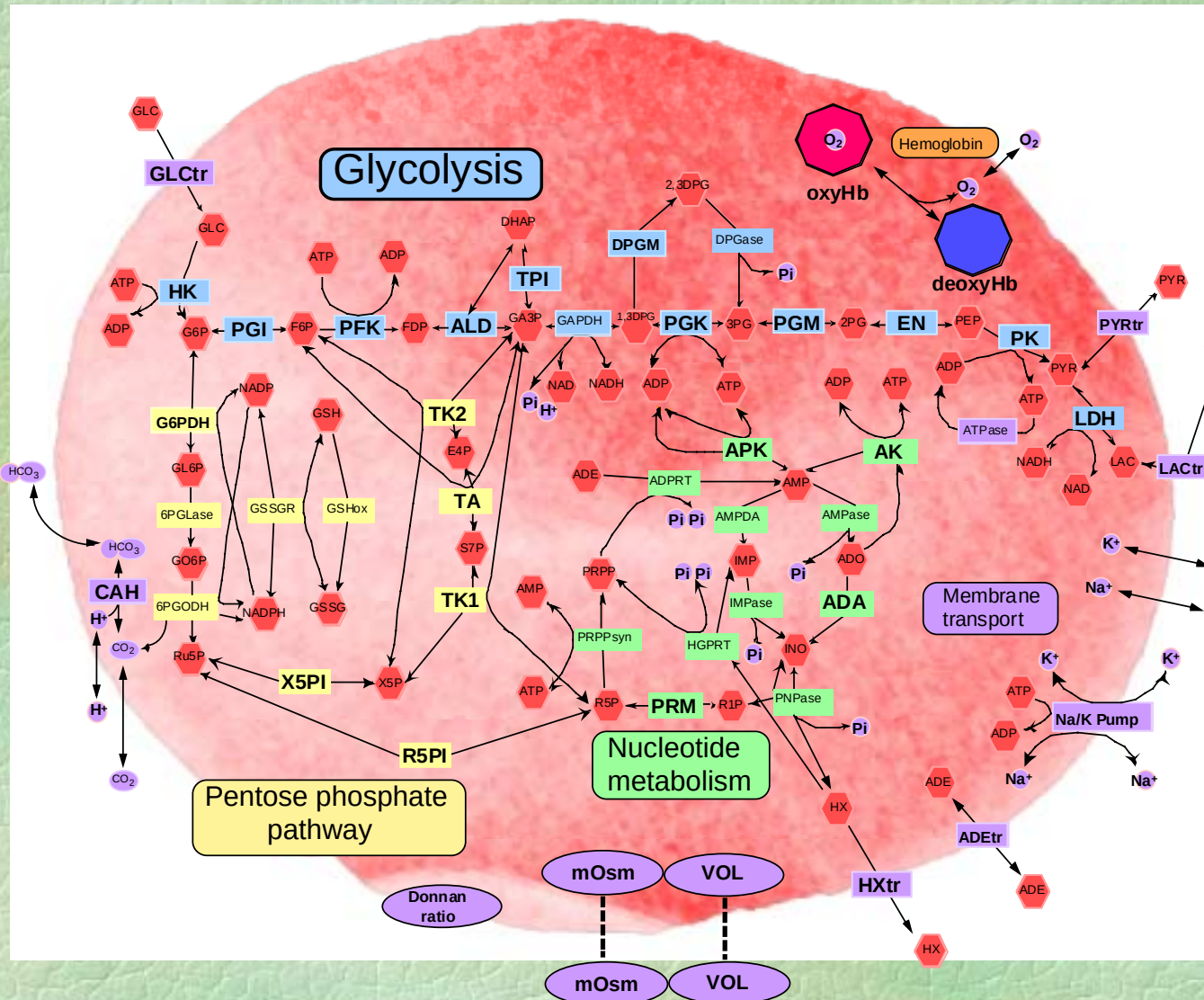


赤血球細胞コンピュータ シミュレーションによる 病理解析

慶大SFC E-CELL
プロジェクト

赤血球細胞シミュレーションの概要



酵素反応

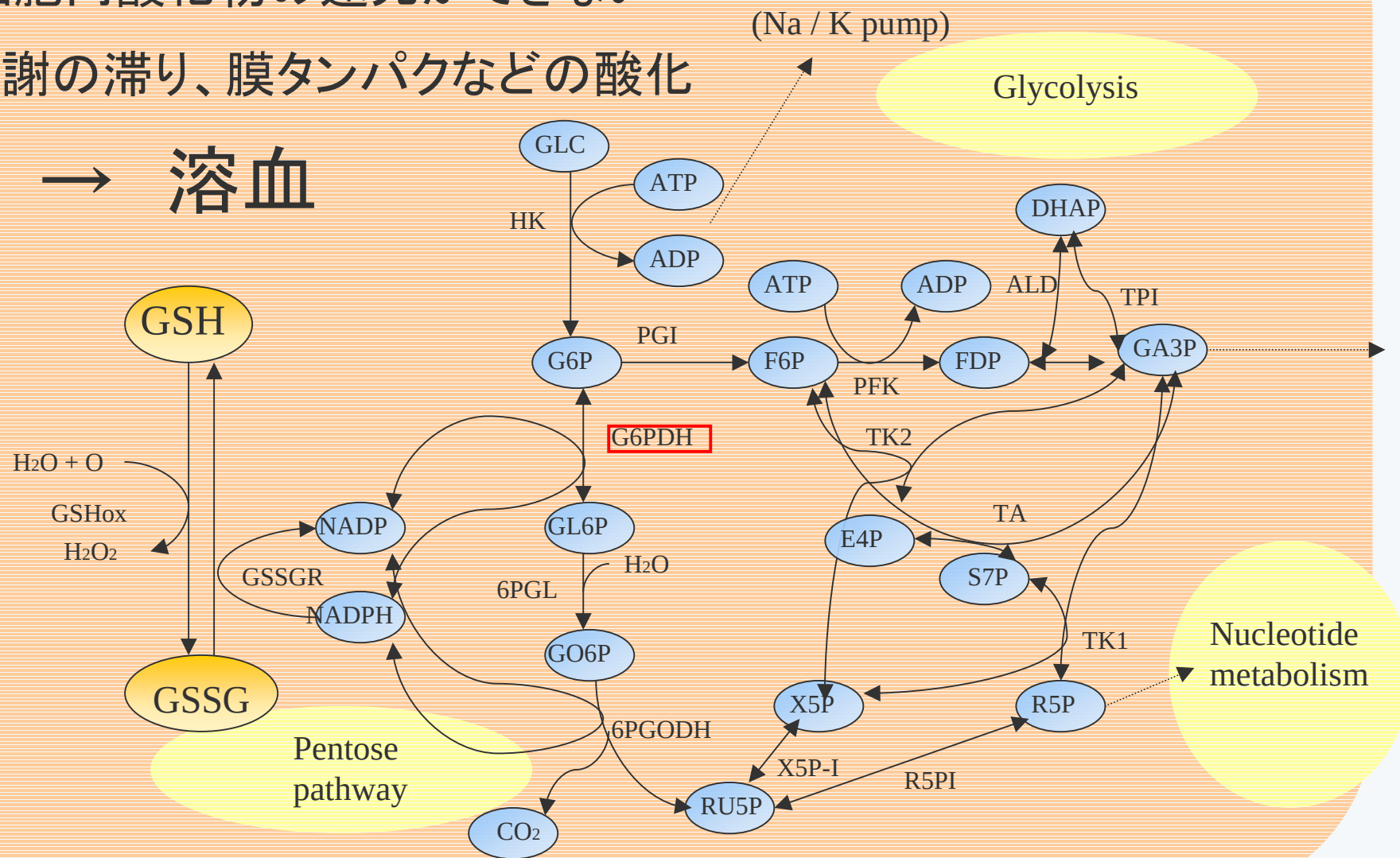
Enzyme or Reaction	ID	Group	Reactor	Reaction mechanism
Glutathione turnover	GSHox	PPP	GSHoxReactor	Mass action
Glutathione reductase (NADPH)	GSSGR	PPP	GSSGRReactor	Ordered Bi Ter mechanism
Glucose 6-phosphate dehydrogenase	G6PDH	PPP	G6PDHReactor	Ordered Bi Bi mechanism
6-Phosphogluconolactonase	6PGLase	PPP	MichaelisUniUniReactor	Michaelis Menten mechanism
6-Phosphogluconate dehydrogenase	6PGLDH	PPP	GL6PDHReactor	Ordered Bi Ter mechanism
Ribose 5-phosphate isomerase	R5PI	PPP	UniUniReactor	Uni Uni mechanism
Xylulose 5-phosphate isomerase	X5PI	PPP	UniUniReactor	Uni Uni mechanism
Transketolase I	TK1	PPP	PingPongBiBiReactor	Ping-Pong Bi Bi mechanism
Transketolase II	TK2	PPP	PingPongBiBiReactor	Ping-Pong Bi Bi mechanism
Transaldolase	TA	PPP	PingPongBiBiReactor	Ping-Pong Bi Bi mechanism
Hexokinase	HK	Glycolysis	HKReactor	
Phosphoglucoisomerase	PGI	Glycolysis	UniUniReactor	Uni Uni mechanism
Phosphofructokinase	PFK	Glycolysis	PFKReactor	
Aldolase	ALD	Glycolysis	OrderedUniBiReactor	Ordered Uni Bi mechanism
Triose phosphate isomerase	TPI	Glycolysis	UniUniReactor	Uni Uni mechanism
Glyceraldehyde phosphate dehydrogenase	GAPDH	Glycolysis	RapidEquilibriumReactor	Mass action
Phosphoglycerate kinase	PGK	Glycolysis	RapidEquilibriumReactor	Mass action
Diphosphoglycerate mutase	DPGM	Glycolysis	DPGMReactor	Michaelis Menten mechanism
Diphosphoglycerate phosphatase	DPGase	Glycolysis	MichaelisUniUniReactor	Michaelis Menten mechanism
Phosphoglyceromutase	PGM	Glycolysis	RapidEquilibriumReactor	Mass action
Enolase	EN	Glycolysis	RapidEquilibriumReactor	Mass action
Pyruvate kinase	PK	Glycolysis	PKReactor	
Pyruvate transport process	PYRtr	Transport	RapidEquilibriumReactor	Mass action
Lactate dehydrogenase	LDH	Glycolysis	RapidEquilibriumReactor	Mass action
Lactate transport process	LACtr	Transport	RapidEquilibriumReactor	Mass action
Leak of Potassium	K_Leak	Transport	LeakageReactor	
Leak of Sodium	Na_Leak	Transport	LeakageReactor	
Sodium/potassium pump	Pump	Transport	PumpReactor	
AMP phosphohydrolase	AMPase	NM	MassActionReactor	Mass action
Adenosine deaminase	ADA	NM	MichaelisUniUniReactor	Michaelis Menten mechanism
Adenosine kinase	AK	NM	MichaelisBiBiReactor	Michaelis Menten mechanism
Adenylate kinase	APK	NM	RapidEquilibriumReactor	Mass action
Adenosine triphosphate phosphohydrolase	ATPase	NM	MassActionReactor	Mass action
Adenosine monophosphate deaminase	AMPDA	NM	MichaelisUniUniReactor	Michaelis Menten mechanism
Inosine monophosphatase	IMPase	NM	MassActionReactor	Michaelis Menten mechanism
Purine nucleotide phosphorylase	PNPase	NM	RapidEquilibriumReactor	Mass action
Phosphoribosyl pyrophosphate synthetase	PRPPsyn	NM	PRPPReactor	
Adenine phosphoribosyl transferase	ADPRT	NM	MichaelisBiBiReactor	Michaelis Menten mechanism
Hypoxanthine-guanine phosphoryl transferase	HGPRT	NM	MichaelisBiBiReactor	Michaelis Menten mechanism
Hypoxanthine transport process	HXtr	NM	HXTTRReactor	
Magnesium complexation of ATP	MgATP_maker		ComplexReactor	Mass action
Magnesium complexation of AMP	MgAMP_maker		ComplexReactor	Mass action
Magnesium complexation of ADP	MgADP_maker		ComplexReactor	Mass action
Magnesium complexation of 2,3DPG	MgDPG_maker		ComplexReactor	Mass action

代謝中間物質

Metabolic intermediate	ID	Predicted	Initial	Predicted/Initial	Observed
1,3-Diphosphoglycerate	13DPG	1.83E-04	4.00E-04	4.58E-01	4.00E-04
2-Phosphoglycerate	2PG	4.16E-03	1.40E-02	2.97E-01	1.40E-02 ± 5.00E-03
3-Phosphoglycerate	3PG	4.62E-02	4.50E-02	1.03E+00	4.50E-02
Adenosine	ADO	8.93E-06	1.20E-03	7.44E-03	1.20E-03 ± 3.00E-04
Dihydroxy acetone phosphate	DHAP	1.35E-01	1.40E-01	9.62E-01	1.40E-01 ± 8.00E-02
Erythrose 4-phosphate	E4P	1.17E+00	4.70E-04	2.48E+03	-
Fructose 6-phosphate	F6P	6.39E-02	1.60E-02	3.99E+00	1.60E-02 ± 3.00E-03
Fructose 1,6-diphosphate	FDP	1.14E-02	7.60E-03	1.50E+00	7.60E-03 ± 4.00E-03
Glucose 6-phosphate	G6P	1.96E-01	3.80E-02	5.16E+00	3.80E-02 ± 1.20E-02
Glyceraldehyde 3-phosphate	GA3P	6.24E-03	6.70E-03	9.32E-01	6.70E-03 ± 1.00E-03
Gluconolactone 6-phosphate	GL6P	7.62E-06	1.17E-05	6.51E-01	-
Gluconate 6-phosphate	GO6P	2.72E+00	1.86E-01	1.46E+01	-
Glutathione	GSH	3.21E+00	3.21E+00	1.00E+00	3.21E+00 ± 1.50E+00
Glutathione	GSSG	1.03E-04	1.06E-04	9.74E-01	-
Hypoxanthine	HXi	9.32E-06	2.00E-03	4.66E-03	2.00E-03
Inosine monophosphate	IMP	5.03E-03	1.00E-02	5.03E-01	1.00E-02
Inosine	INO	3.32E-08	1.00E-03	3.32E-05	1.00E-03
Potassium	Ki	1.26E+02	1.35E+02	9.36E-01	1.35E+02 ± 1.00E+01
Lactate	LACi	1.20E+00	1.10E+00	1.09E+00	1.10E+00 ± 5.00E-01
Nicotinamide adenine dinucleotide	NAD	8.87E-02	6.20E-02	1.43E+00	-
Nicotinamide adenine dinucleotide	NADH	3.13E-04	2.70E-02	1.16E-02	-
Nicotinamide adenine phosphate	NADP	8.06E-05	9.60E-05	8.39E-01	-
Nicotinamide adenine phosphate	NADPH	6.58E-02	6.58E-02	1.00E+00	6.58E-02
Sodium	Nai	2.27E+01	1.00E+01	2.27E+00	1.00E+01 ± 6.00E+00
Phosphoenolpyruvate	PEP	1.89E-02	1.70E-02	1.11E+00	1.70E-02 ± 2.00E-03
5-Phosphoribosyl 1-phosphate	PRPP	6.91E-05	5.00E-03	1.38E-02	5.00E-03 ± 1.00E-03
Pyruvate	PYRi	6.00E-02	7.70E-02	7.79E-01	7.70E-02 ± 5.00E-02
Inorganic phosphate	Pi	1.30E-01	1.00E+00	1.30E-01	1.00E+00
Ribose 1-phosphate	R1P	2.12E-05	6.00E-02	3.53E-04	6.00E-02
Ribose 5-phosphate	R5P	2.81E-04	3.30E-02	8.52E-03	-
Ribulose 5-phosphate	RU5P	1.48E-04	1.29E-02	1.15E-02	-
Sedoheptulose 7-phosphate	S7P	7.49E-02	2.30E-01	3.26E-01	-
Xylulose 5-phosphate	X5P	4.30E-04	3.90E-02	1.10E-02	-
2,3-Diphosphoglycerate	2,3-DPG	4.21E+00	4.50E+00	9.36E-01	4.50E+00 ± 5.00E-01
Adenosine diphosphate	ADP	2.20E-01	2.70E-01	8.16E-01	2.70E-01 ± 1.20E-01
Adenosine monophosphate	AMP	2.42E-02	8.00E-02	3.02E-01	8.00E-02 ± 9.00E-03
Adenosine triphosphate	ATP	1.57E+00	1.54E+00	1.02E+00	1.54E-00 ± 2.50E-01

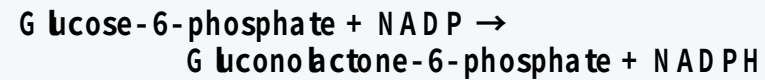
Human Erythrocyte

→ 溶血



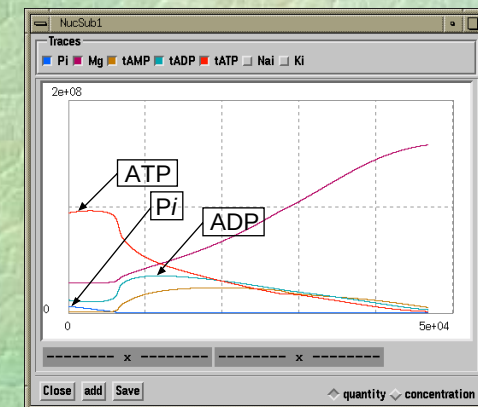
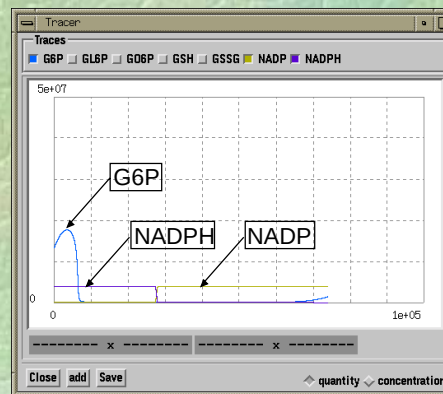
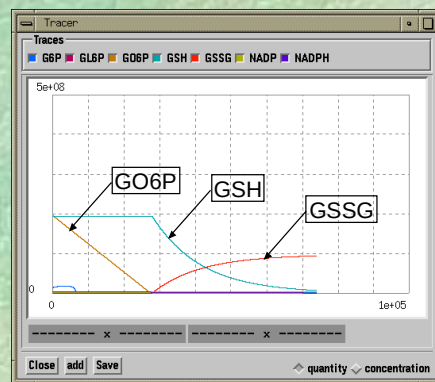
G6PDH 欠損症のシミュレーション

G lucose-6-phosphate dehydrogenase



Parameters used in the simulation experiment (G .Jacobasch *et al*, 1987)

	t/2 d	Vmax	KmG6P	KmNADP	KiNADPH	KiATP	Ki2,3-DPG
Normal	27	575	67	3.7	3.1	749	2289
We.G	2.5	10	152	3.8	0.62	180	520



E-CELL プロジェクト

- ❧ システム開発 (高橋・石川・斉藤・米田・岩田)
- ❧ 最適化手法 (斉藤・高橋・岩田)
- ❧ S-System (岩田・高橋)
- ❧ 代謝制御解析 (岡山)
- ❧ 時系列解析 (米田・高橋)
- ❧ ミトコンドリア (柚木)
- ❧ 赤血球 (中山・木下・喜田)
- ❧ 糖尿病 (内藤)
- ❧ 化学走性 (松崎)
- ❧ 遺伝子ネットワーク (橋本・三由・妹尾)
- ❧ 光合成 (汪・中山)
- ❧ 概日リズム (三由・中山)
- ❧ 細胞周期 (藤田)
- ❧ DNA複製 (藤田・松尾・山田・三由)