

Supplementary materials

Cytotoxicity, mitochondrial functionality, and redox status of human conjunctival cells after short and chronic exposure to preservative-free bimatoprost 0.03% and 0.01%: an *in vitro* comparative study.

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Table S1. List of the input molecules used for drug network prediction using the STITCH database. ^aPubChem CID for chemicals, UniProt code for proteins.

Molecule	Code ^a	Description
bimatoprost	127909	bimatoprost
PGE2	158	prostaglandin E2 (PGE2)
GOT2	P00505	glutamic-oxaloacetic transaminase 2, (mitochondrial aspartate aminotransferase 2)
MDH2	P40926	malate dehydrogenase 2, NAD (mitochondrial)
SLC1A3	P43003	solute carrier family 1 (glial high-affinity glutamate transporter), member 3
SLC25A11	Q02978	solute carrier family 25 (mitochondrial carrier; oxoglutarate carrier), member 11
UCP1	P25874	uncoupling protein 1 (mitochondrial, proton carrier)
UCP2	P55851	uncoupling protein 2 (mitochondrial, proton carrier)
UCP3	P55916	uncoupling protein 3 (mitochondrial, proton carrier)

Table S2. Predicted drug network functional partners from STITCH database (<http://stitch.embl.de/>) ranked by combined score, using the input molecules reported in Table S1. ^aPubChem CID for chemicals, UniProt code for proteins.

Node	Code ^a	Description	Neighbourhood	Gene Fusion	Co-occurrence	Co-expression	Experiments	Databases	Text-mining	Prediction	Homology	Combined score
PTGER4	P35408	<i>prostaglandin E receptor 4 (subtype EP4)</i>					•	•	•			0.999
PTGER3	P43115	<i>prostaglandin E receptor 3 (subtype EP3)</i>					•	•	•			0.999
PTGER1	P34995	<i>prostaglandin E receptor 1 (subtype EP1)</i>					•	•	•			0.998
PTGER2	P43116	<i>prostaglandin E receptor 2 (subtype EP2)</i>					•	•	•			0.998
CS	O75390	<i>citrate synthase</i>	•		•	•	•	•	•			0.996
PTGS2	P35354	<i>prostaglandin-endoperoxide synthase 2 (prostaglandin G/H synthase and cyclooxygenase)</i>						•	•			0.995
FH	P07954	<i>fumurate hydratase</i>	•		•	•	•	•	•			0.994
oxaloacetate	970	<i>oxaloacetic acid</i>					•	•	•			0.993
glutamic acid	611	<i>monopotassium glutamate (MPG)</i>					•	•	•			0.992
pyridoxal phos.	1051	<i>pyridoxal phosphate</i>					•	•	•			0.990
malate	525	<i>magnesium malate</i>					•	•	•			0.990
carboxy	283	<i>formate, (alias fatty acids)</i>					•	•	•			0.989
phosphate	1003	<i>Phosphoric acid</i>					•	•	•			0.989
IL8	P10145	<i>interleukin 8</i>						•	•			0.988
MDH1	P40925	<i>malate dehydrogenase 1</i>	•					•	•	•		0.987
rosiglitazone	77998	<i>rosiglitazone is an antidiabetic drug in the thiazolidinedione class of drugs</i>						•	•			0.987
CXCR6	O00574	<i>chemokine (C-X-C motif) receptor 6</i>					•	•	•			0.986
LDHC	P07864	<i>lactate dehydrogenase C</i>	•					•	•	•		0.984

LDHB	P07195	<i>lactate dehydrogenase B</i>	•	•	•	0.984
ADCY2	Q08462	<i>adenylate cyclase 2</i>	•	•	•	0.983

Table S3. Predicted drug network functional partners from STITCH database (<http://stitch.embl.de/>) ranked by combined score, including rosiglitazone as input molecule. ^aPubChem CID for chemicals, UniProt code for proteins.

Node	Code ^a	Description	Neighbourhood	Gene Fusion	Co-occurrence	Co-expression	Experiments	Databases	Text-mining	Prediction	Homology	Combined score
PTGER4	P35408	<i>prostaglandin E receptor 4 (subtype EP4)</i>				•	•	•	•			0.999
PPARG	P37231	<i>peroxisome proliferator-activated receptor gamma</i>			•	•	•	•				0.999
PTGER3	P43115	<i>prostaglandin E receptor 3 (subtype EP3)</i>			•	•	•	•				0.999
PPARA	Q07869	<i>peroxisome proliferator-activated receptor alpha</i>			•	•	•	•				0.999
PTGER1	P34995	<i>prostaglandin E receptor 1 (subtype EP1)</i>			•	•	•	•				0.998
PTGER2	P43116	<i>prostaglandin E receptor 2 (subtype EP2)</i>			•	•	•	•				0.998
CS	O75390	<i>citrate synthase</i>	•		•	•	•	•				0.996
RETN	Q9HD89	<i>resistin</i>					•	•				0.996
PTGS2	P35354	<i>prostaglandin-endoperoxide synthase 2 (prostaglandin G/H synthase and cyclooxygenase)</i>					•	•				0.995
FH	P07954	<i>fumarate hydratase</i>	•		•	•	•	•				0.994
oxaloacetate	970	<i>oxaloacetic acid</i>			•	•	•	•				0.993
glutamic acid	611	<i>monopotassium glutamate (MPG)</i>			•	•	•	•				0.992
ADIPOQ	Q15848	<i>adiponectin</i>					•	•				0.991
malate	525	<i>magnesium malate</i>			•	•	•	•				0.990
pyridoxal phos.	1051	<i>pyridoxal phosphate</i>			•	•	•	•				0.990
carboxy	283	<i>formate, (alias fatty acids)</i>			•	•	•	•				0.989
phosphate	1003	<i>phosphoric acid</i>			•	•	•	•				0.989
LEP	P41159	<i>leptin</i>					•	•				0.989
CD36	P16671	<i>platelet glycoprotein 4</i>					•	•				0.988
IL8	P10145	<i>interleukin 8</i>					•	•				0.988