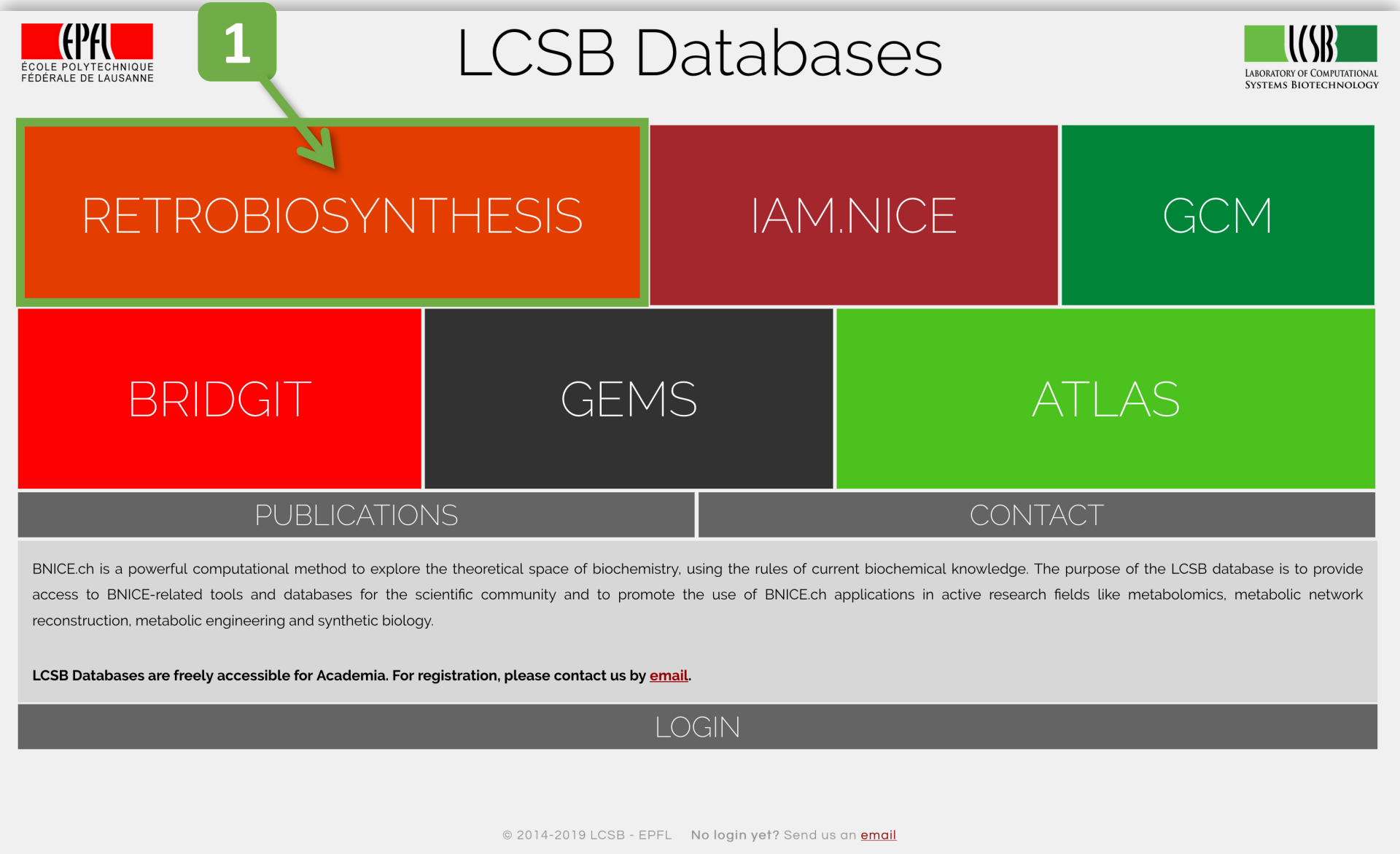
Retrobiosynthesis on **lcsb-databases.epfl.ch**

Go to retrobiosynthesis



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ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

Retrobiosynthesis

LABORATORY OF COMPUTATIONAL SYSTEMS BIOTECHNOLOGY

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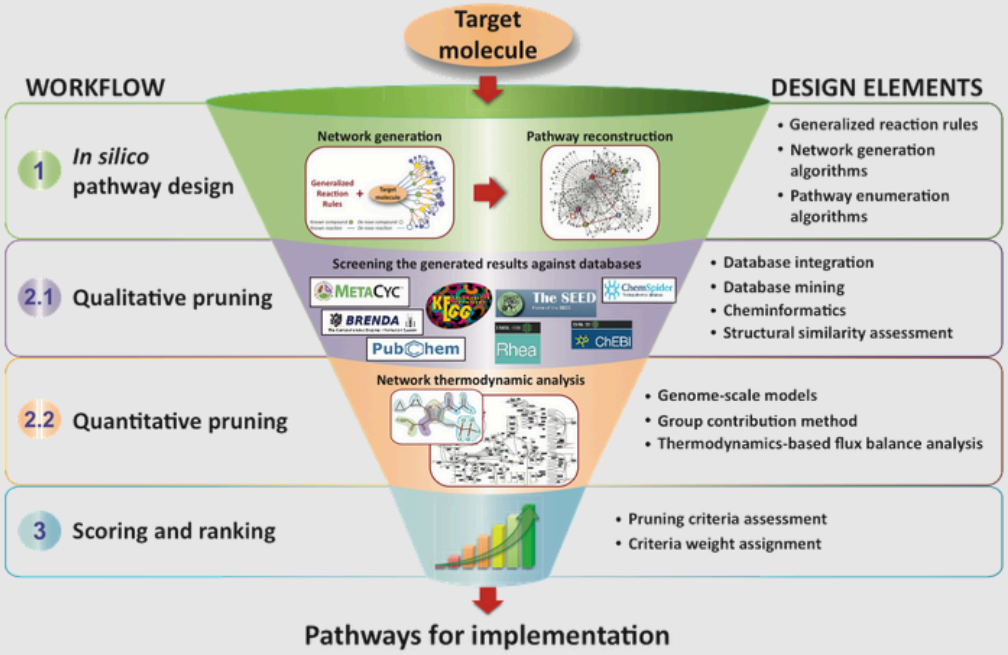
Retrobiosynthesis

The bio-production of chemicals and fuels using "modified" microorganisms is becoming a practicable substitution to the unsustainable petrochemical-based processes. However, most of natural organisms cannot directly serve as chassis organism to produce desired compounds. Therefore, the platform microorganisms need to be adapted and genetically modified through retrofitting and optimization processes introduced in synthetic biology and metabolic engineering disciplines. ***In silico* pathway design using retrobiosynthetis** is an established approach for discovering promising biosynthetic pathways.



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Retrobiosynthesis

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Available projects for your account

Search:

Entry	Name	Target	Target Name	Number of Pathways	Pathways Hash	System File Hash	Date	Pathway Map
PROJ-21	MEK_E.coli	C12201	MEK	9101	e7185c488d	d075e9f295	2016-01-15 18:12:19	Load
PROJ-22	MEK_Putida	C12201	MEK	8232	f8d37f552a	d075e9f295	2016-01-18 16:51:04	Load
PROJ-27	Propane12diol	C12035	1,2-Propanediol	1056	2f0d93408f	5f9d489a41	2016-01-19 16:07:22	Load
PROJ-28	MEK_onlyKEGG_comp_E.coli	C12201	MEK	242	d08cd9b67f	d075e9f295	2016-01-20 14:30:37	Load
PROJ-29	MEK_onlyKEGG_rxns_Ecoli	C12201	MEK	36	41c307052a	d075e9f295	2016-01-20 15:36:53	Load
PROJ-30	propane1ol_E.coli	C12143	Optal	648	d27551b0c6	5f9d489a41	2016-01-21 14:40:50	Load
PROJ-31	propane2ol_E.coli	C12024	2-Propanol	1794	e451f9a55d	5f9d489a41	2016-01-21 14:48:51	Load
PROJ-32	But3en2One	C13479	But-3-en-2-one	488	f2f320ac3c	5f9d489a41	2016-02-05 12:14:40	Load
PROJ-41	MEK2017	C12280	3-Oxopentanoate	18822	802e7720ee	fe9c442cc7	2017-03-08 11:27:46	Load

Select a project / a target molecule

4

Project PROJ-41 - List of starting compounds

Search:

Starting Compound	CPD ID	Number of feasible pathways	Shortest pathway	Length distribution	Maximal Yield	Browse all pathways
1,2-Propanediol	C12035	348	3 rxns	3:7 | 4:341	0.47	Browse
2,3-Dihydroxy-isovalerate	C12187	89	3 rxns	3:5 | 4:84	0.26	Browse
2-Dehydro-3-deoxy-D-galactonate 6-phosphate	C12340	60	4 rxns	4:60	0.47	Browse
2-keto-3-deoxygluconate	C12267	572	3 rxns	3:30 | 4:542	0.39	Browse
2-Methylcitrate	C12498	259	2 rxns	2:2 | 3:16 | 4:241	0.34	Browse
2-Oxobutyrate	C12155	568	3 rxns	3:21 | 4:547	0.55	Browse
2-Oxoglutarate	C12012	98	4 rxns	4:98	0.59	Browse
2-Oxopropanal	C12077	529	3 rxns	3:10 | 4:519	0.59	Browse

5

Select a precursor and load pathways

6

Select a pathway

Project PROJ-41 - Starting compound C 12035

Rank pathways by yield, length, BridgIT score, or overall score.

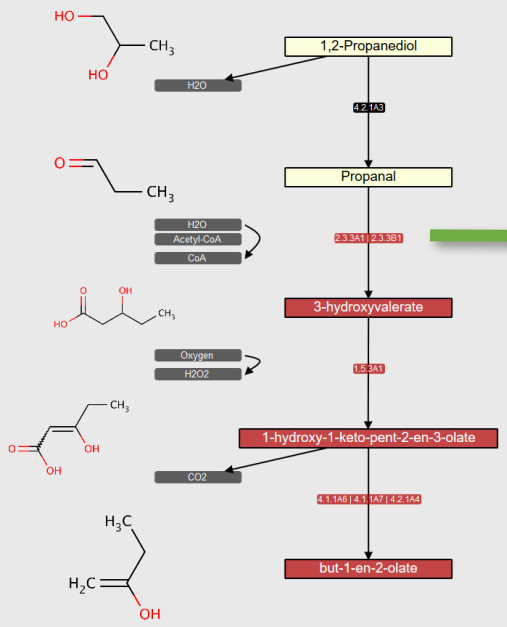
Column visibility | CSV | Excel | Show 50 entries | Search:

Pathway ID	BridgIt	Yield	Length	Known reactions	Length score	Feasibility	Kegg rxn score	Overall	Pathway	Graph
109339	0.72	0.47	4	1	0.25	1	0.25	2.69	1,2-Propanediol ↔ Propanal ↔ 3-hydroxyvalerate ↔ 1-hydroxy-1-keto-pent-2-en-3-olate ↔ but-1-en-2-olate	109339
109340	0.65	0.47	4	1	0.25	1	0.25	2.62	1,2-Propanediol ↔ Propanal ↔ 3-hydroxyvalerate ↔ 1-hydroxy-1-keto-pent-2-en-3-olate ↔ but-1-en-2-olate	109340
109351	0.57	0.47	4	1	0.25	1	0.25	2.55	1,2-Propanediol ↔ Propanal ↔ 3-hydroxy-2-methyl-butyraldehyde ↔ 2-ethylacrolein ↔ but-1-en-2-olate	109351
109388	0.72	0.47	4	1	0.25	1	0.25	2.69	1,2-Propanediol ↔ Propanal ↔ 2,3-dihydroxyvaleric acid ↔ butane-1,2-diol ↔ but-1-en-2-olate	109388
109415	0.77	0.47	4	1	0.25	1	0.25	2.75	1,2-Propanediol ↔ Propanal ↔ 2-hydroxybutyraldehyde ↔ butane-1,2-diol ↔ but-1-en-2-olate	109415
109416	0.77	0.47	4	1	0.25	1	0.25	2.75	1,2-Propanediol ↔ Propanal ↔ 2-hydroxybutyraldehyde ↔ butane-1,2-diol ↔ but-1-en-2-olate	109416
109477	0.6	0.59	4	1	0.25	1	0.25	2.69	1,2-Propanediol ↔ Propanal ↔ 3,4-dihydroxyhexan-2-one ↔ 4-hydroxyhex-3-en-2-one ↔ but-1-en-2-olate	109477

Reaction list (# IDs from Excel File)

#2531 → #177 → #152 → #957

Normal Mode | Carbon Flow



$\Delta G_r°$ in kcal/mol

ΔG = -9.17 kcal/mol

ΔG = -15.72 kcal/mol

ΔG = -13.54 kcal/mo

EC legend : novel reaction KEGG reaction

Compound legend : novel/PubChem compound KEGG compound

Click on compound or reaction to get additional information

7

Details for reaction : R212482

LCSB Reaction ID	R212482
Raw File RID	R14714
Reaction	H2O2 + 1,2-Propanediol → (2) H2O + L-Lactaldehyde
Database	Nearest KEGG entry : R00602, BridgIt score : 0.478261
Database	Nearest KEGG entry : R00602, BridgIt score : 0.307692
Energy (kcal/mol)	-71.84
Error (kcal/mol)	-0.45

Export pathway as PDF or PNG

To PDF | To PNG