

University of Minho
School of Engineering

Towards a Genome-Wide Transport Systems Encoding Genes Tracker

Lagoa D.¹, Liu F.², Ferreira E.C.¹, Faria J.², Henry C.² and Dias O.¹

1) CEB - Centre of Biological Engineering, Universidade do Minho, 4710-057 Braga, Portugal

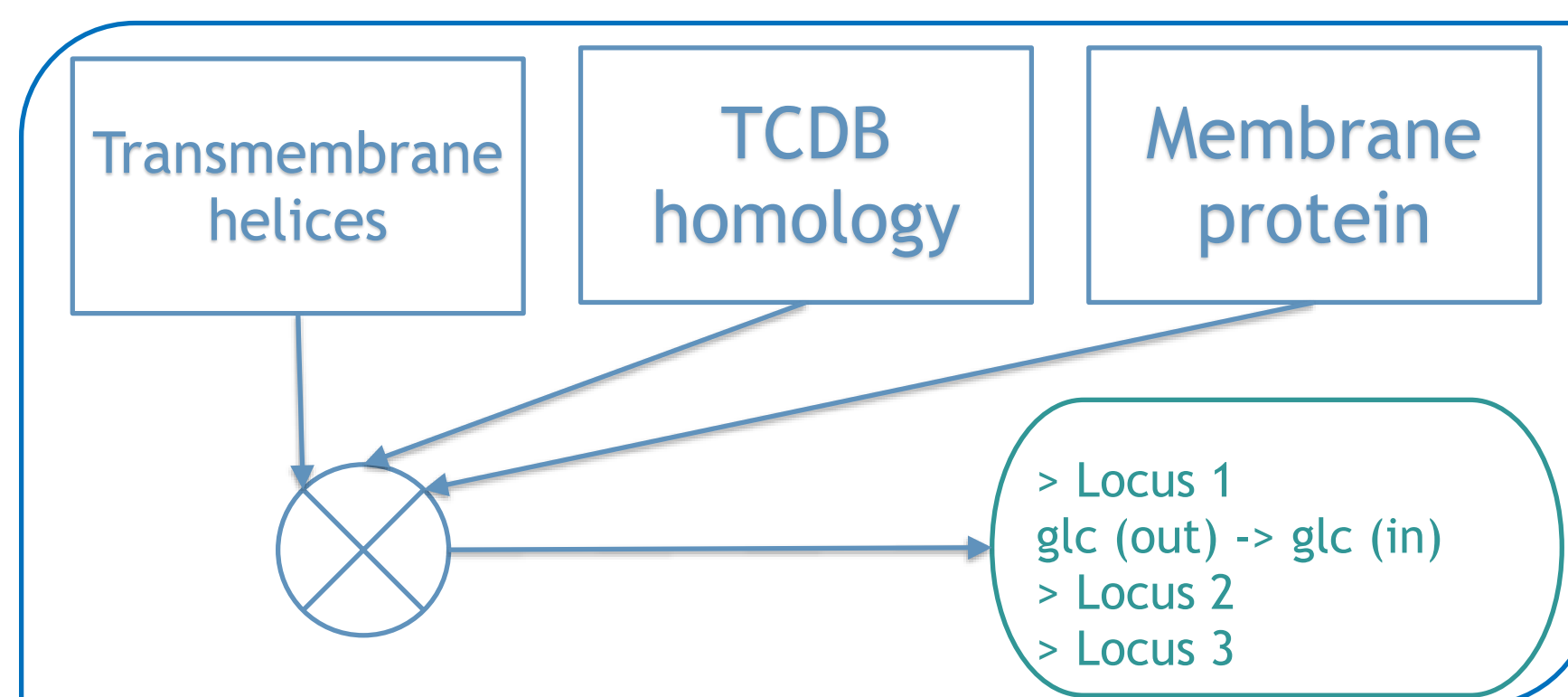
Group: BIOSYSTEMS

2) Mathematics and Computer Science Division, Argonne National Laboratory

CENTRE OF
**BIOLOGICAL
ENGINEERING**

Introduction

TRIAGE, is a tool currently embedded in *merlin*, which performs the identification of transport systems and automatically generates transport reactions for every metabolite transported by those carriers. Reactions generated by *TRIAGE* can be directly integrated in *GSM* models, as all metabolites involved have KEGG and/or ChEBI identifiers. Up to our knowledge, this is the only tool capable of identifying and generating such reactions.

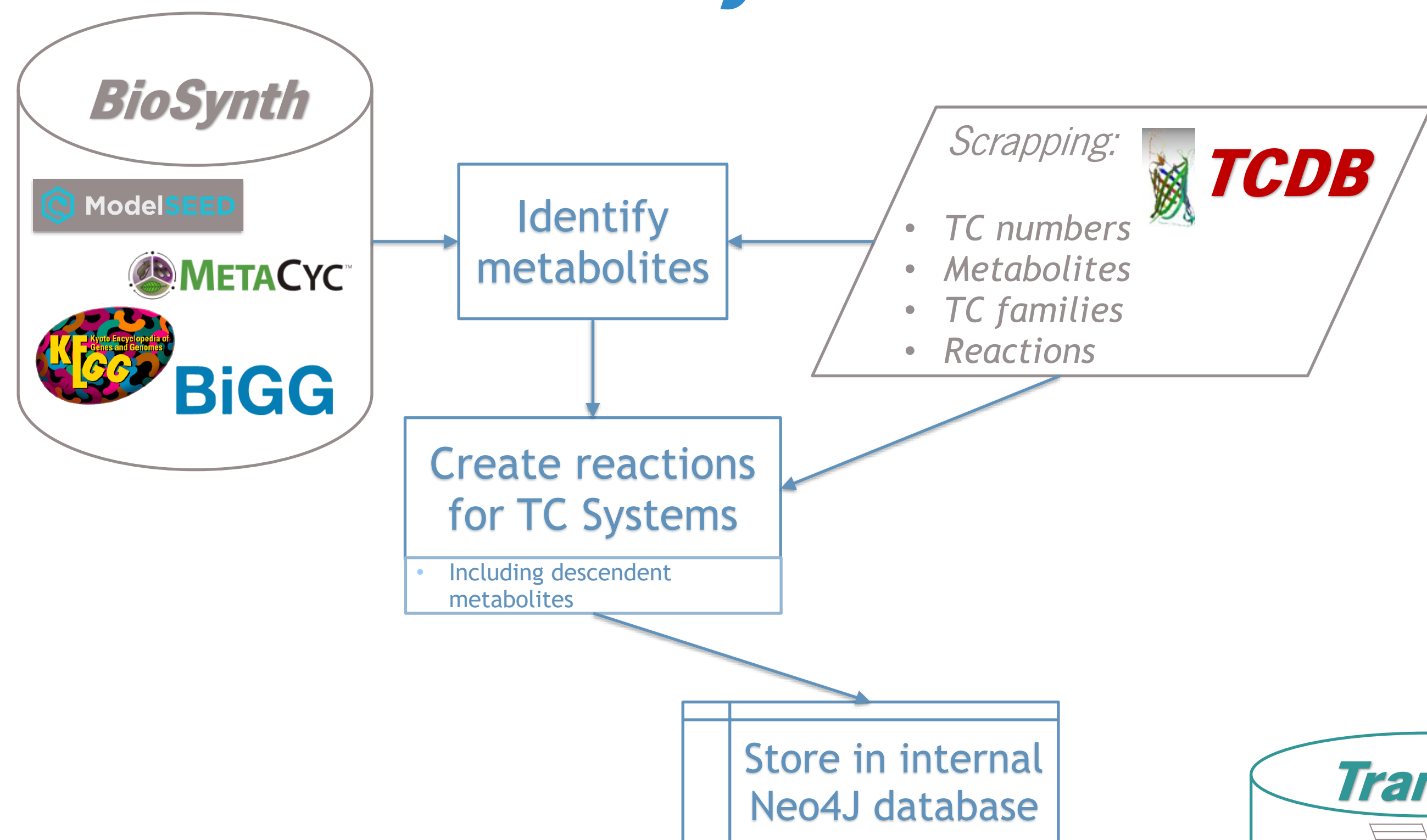


However, *TRIAGE*'s pipeline is very strict, as it combines several tools to decrease the number of false positives, which implies that a negative prediction in one of the modules will exclude the gene of the membrane transport systems encoding genes set.

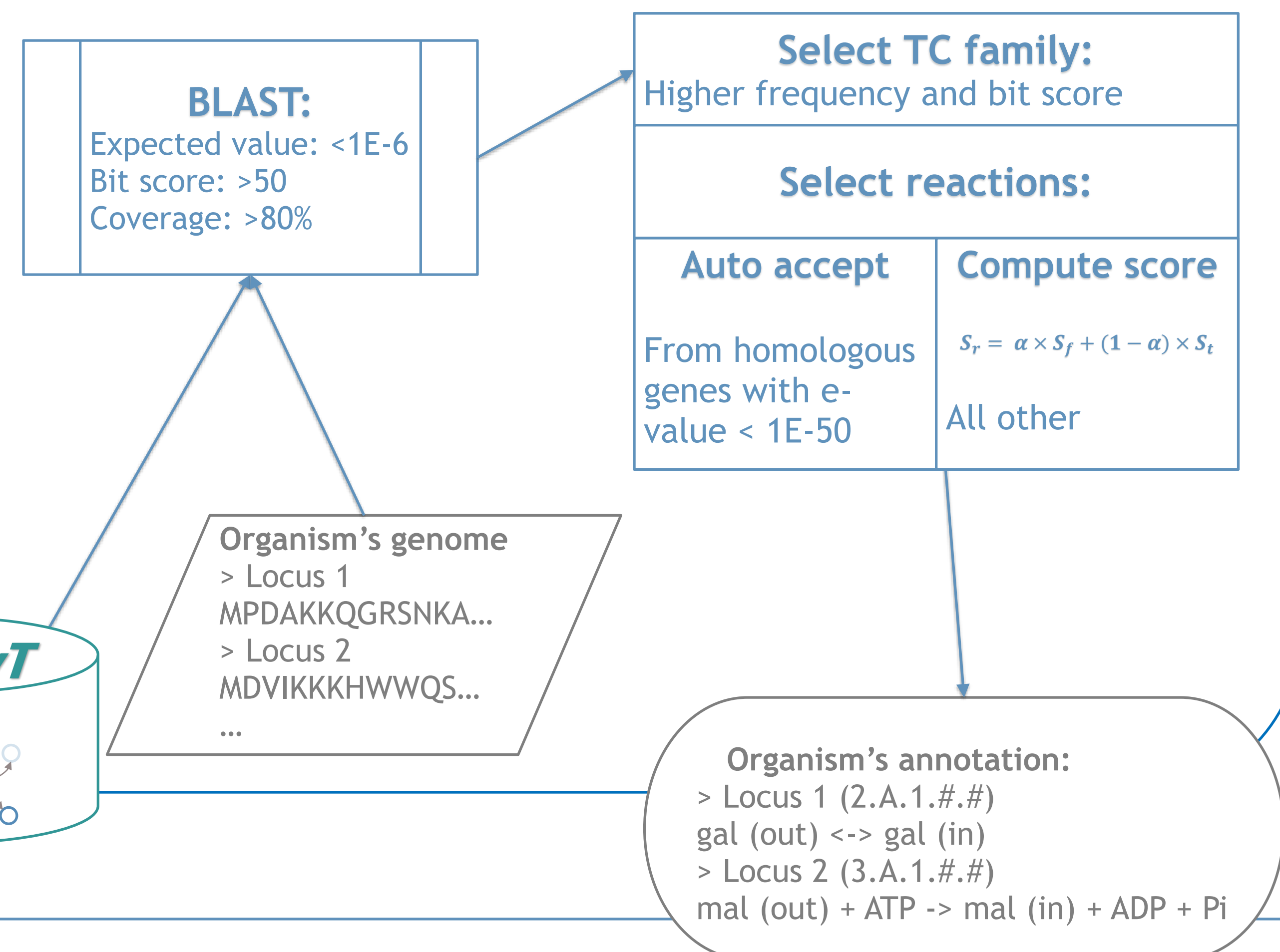
The Transport Systems Tracker (*TranSyT*) is a new approach for this problem. It was developed to perform the same tasks as *TRIAGE*, though without its major restrictions. Unlike *TRIAGE*, the information available in its database is automatically extracted from TCDB, and annotated using BioSynth. Proteins identified as transporters are annotated with Transporter Classification Database (TCDB) families numbers and reactions from its internal database.

Methods

Create *TranSyT* database



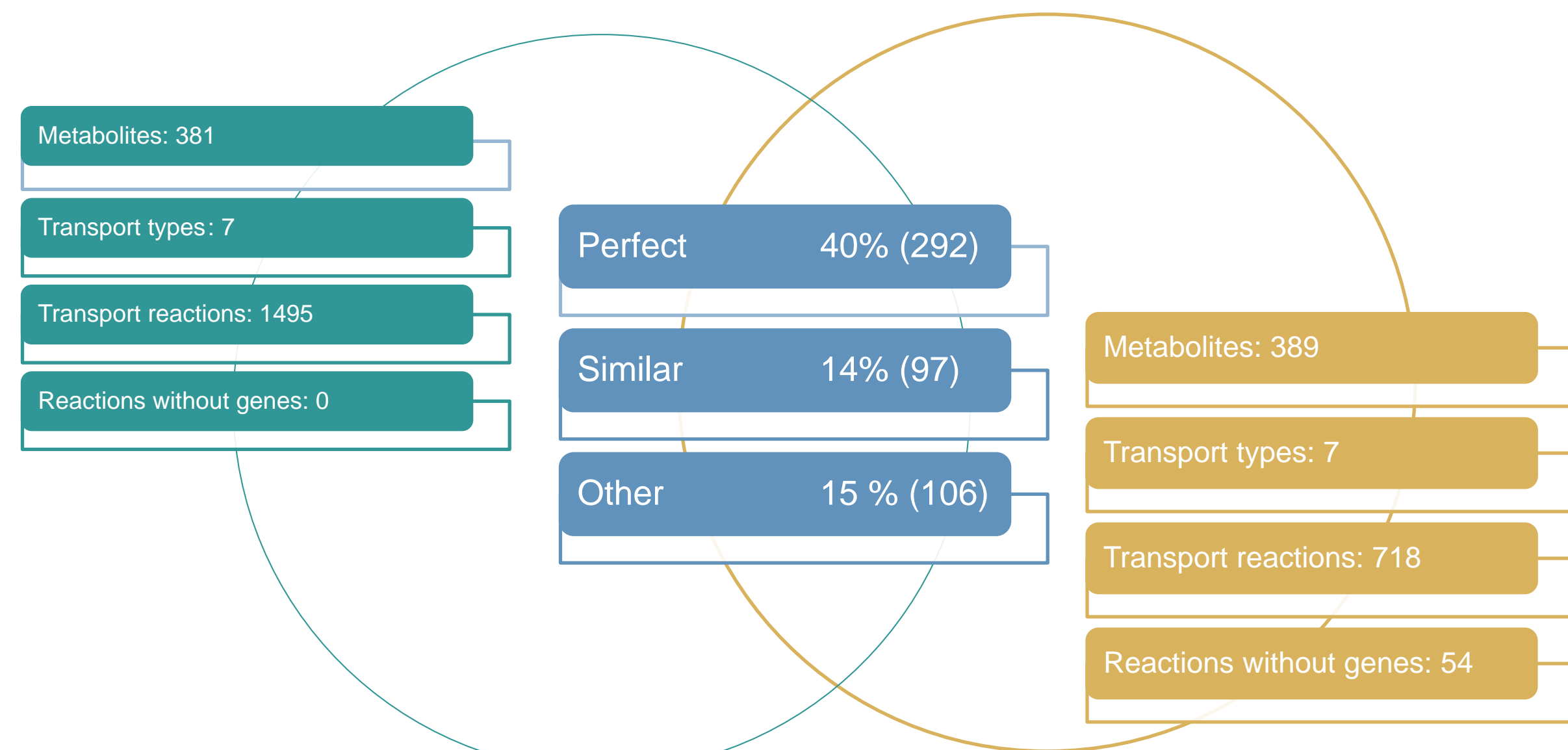
Annotate organism



TranSyT contents

TC systems (TC Number, Accession)	17321
Accessions	17221
TC Numbers	13349
TC Families	1176
Equations	428
Metabolites	6015
Descendent metabolites	5002
Reactions	58623

TranSyT versus iAF1260



Results

	mechanism			Total
	same	other	no match	
ABC	10	6	43	59
Symport	44	26	28	98
Uniport	24	55	120	199
Antiport	12	8	30	50
PEP/NAD	7	11	2	20
Total	97	106	223	

Conclusions

TranSyT's approach was able to automatically create reactions for nearly 70% the iAF1260 model transporters. Moreover, it allowed identifying transport reactions incorrectly assigned to genes unable to transport such metabolite.

TranSyT is currently being implemented in both *merlin* and KBase.

This study was supported by FCT under the scope of the strategic funding of UID/BIO/04469/2013 unit and COMPETE 2020 (POCI-01-0145-FEDER-006684) and BioTecNorte operation (NORTE-01-0145-FEDER-000004) funded by the European Regional Development Fund under the scope of Norte2020 - Programa Operacional Regional do Norte.