



***InChI:
A Cambridge View***

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Present InChI and RInChI

Present InChI and RInChI

1) Present InChI

2) Present InChI

3) InChI Present

Present InChI and RInChI

1) Present InChI

What is the state of the art?

2) Present InChI

How can we communicate science?

3) InChI Present

What can InChI give the world?

Present InChI and RInChI

IUPAC:

Effectively contributes to the worldwide understanding and application of the chemical sciences, to the betterment of humankind

ACS:

To advance the broader chemistry enterprise and its practitioners for the benefit of Earth and its people

RSC:

We're working to shape the future of the chemical sciences – for the benefit of science and humanity

Present InChI and RInChI

InChI are successful
because people use them

Present InChI and RInChI

InChI are successful
because people use them

*Reaction-InChI (RInChI) will be
successful if it is used*

Present RInChI

What is RInChI?

Present RInChI

What is RInChI?

International chemical identifier for reactions (RInChI)

G. Grethe, J. M. Goodman and C. H. G. Allen

Journal of Cheminformatics 2013, 5, 45.

DOI: 10.1186/1758-2946-5-45

Present RInChI

**International chemical identifier for reactions
(RInChI)
Version 1.00**

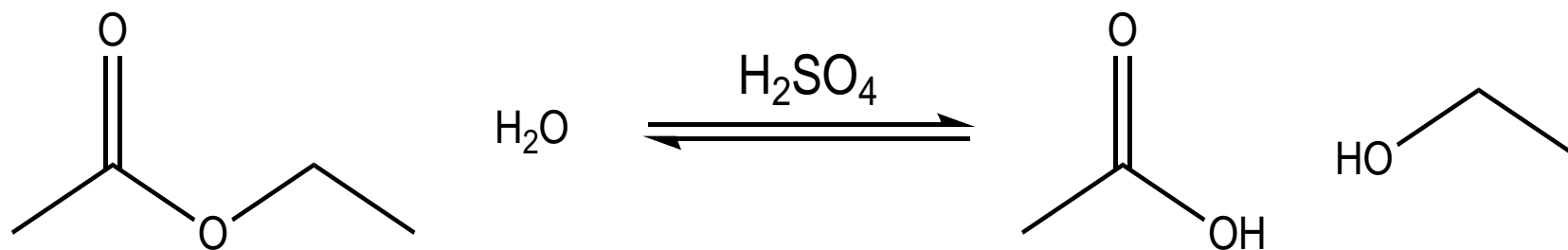
International chemical identifier for reactions (RInChI)

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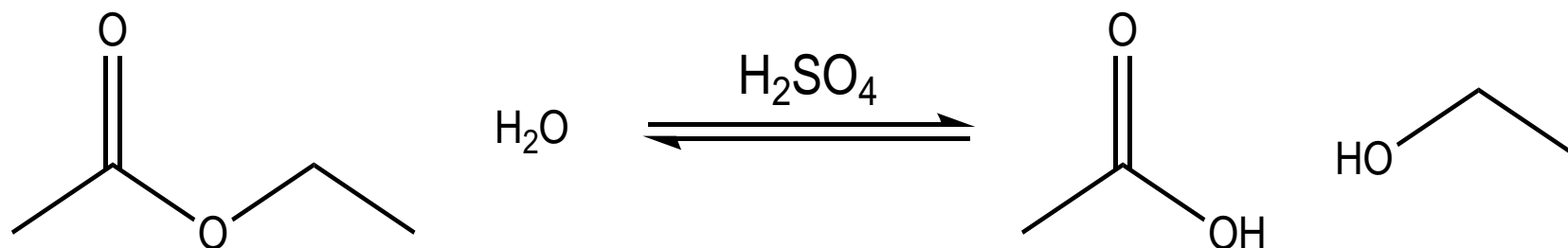
Journal of Cheminformatics 2013, 5, 45.

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Present RInChI



Present RInChI



RInChI=1.00.1S/

C2H4O2/c1-2(3)4/h1H3,(H,3,4)

!C2H6O/c1-2-3/h3H,2H2,1H3

<>

C4H8O2/c1-3-6-4(2)5/h3H2,1-2H3

!H2O/h1H2

<>

H2O4S/c1-5(2,3)4/h(H2,1,2,3,4)

/d=

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Open Access Publishing



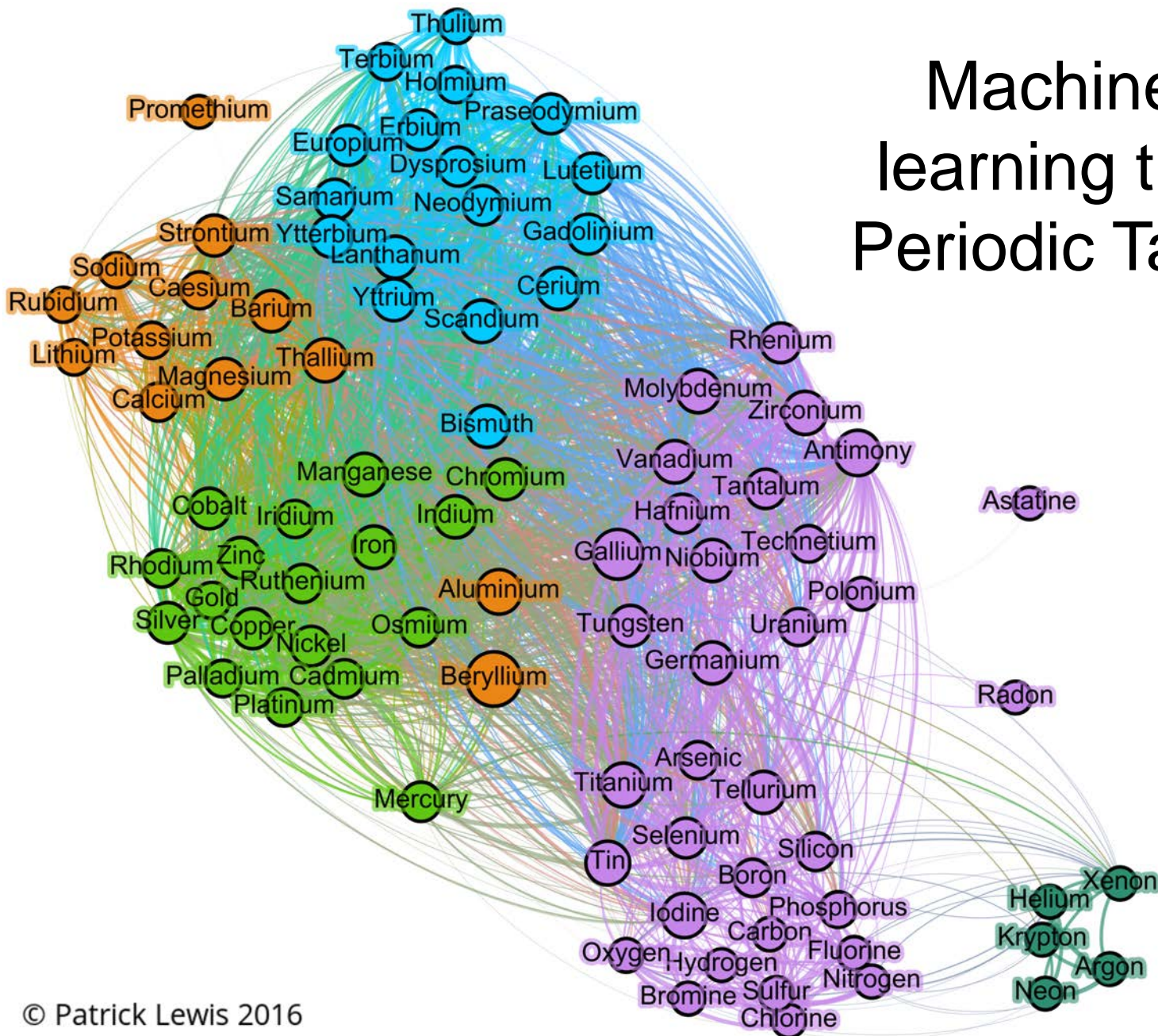
Open Access Publishing

Open Data

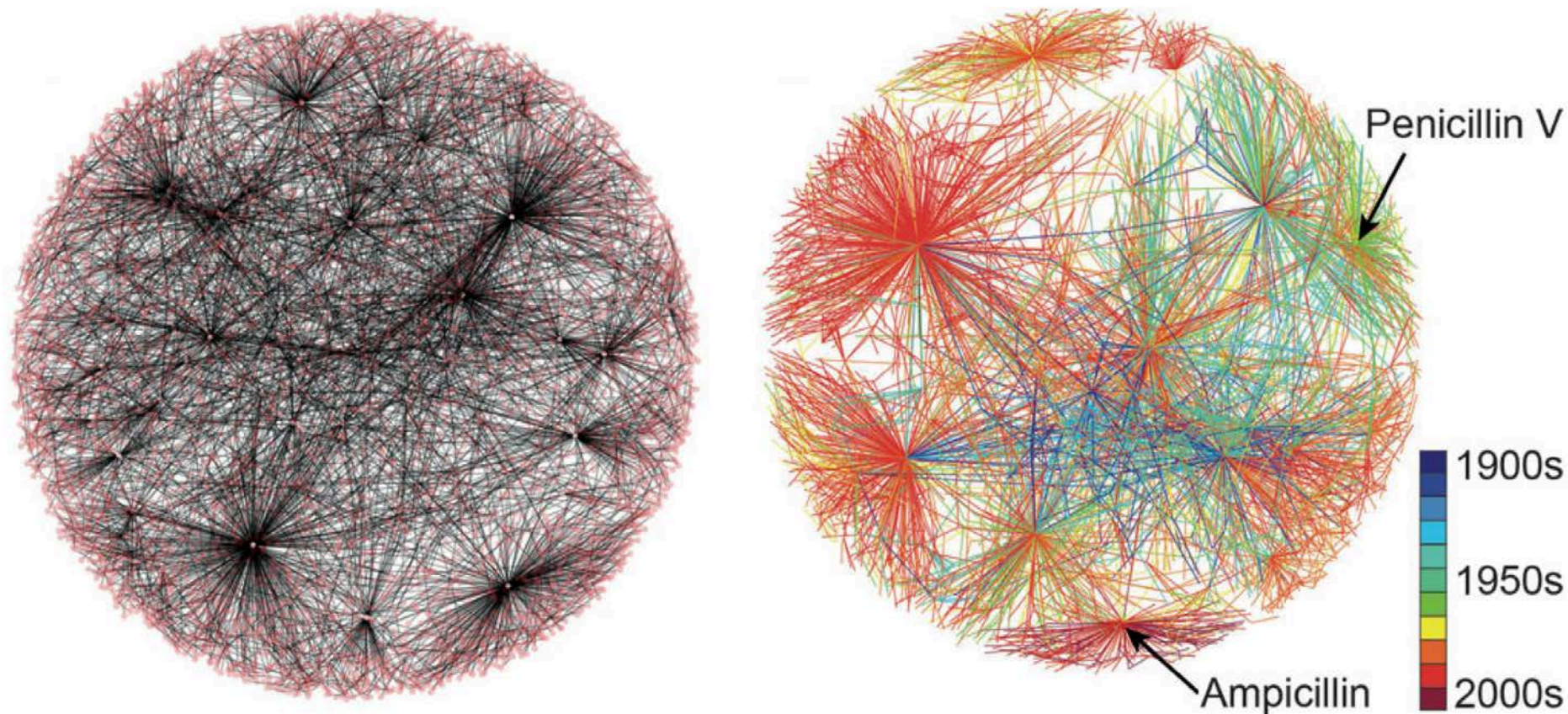


University
Data
Repositories

Machine learning the Periodic Table



© Patrick Lewis 2016



0.1 % of the Beilstein Database
Bartosz A. Grzybowski *et al.*
Angew. Chem. Int. Ed. 2012, **51**, 7922–7927

“The Trouble with quotes on the internet is that it’s difficult to determine whether or not they are genuine.”

-Abraham Lincoln

Molecule of Interest

You are being watched.

The government has a secret system:
a machine that spies on you every hour of every day.

I know, because I built it. I designed the machine
to study specific reactions, but it sees everything.

Molecules affecting ordinary people; people like you.

Molecules the authorities considered 'irrelevant'.

They wouldn't act, so I decided I would.

But I needed partners, people with the skills to intervene.

We work in secret. You'll never find us.

But reactant or reagent, if your number's up... we'll find you.

Present InChI and RInChI

1) Present InChI

What is the state of the art?

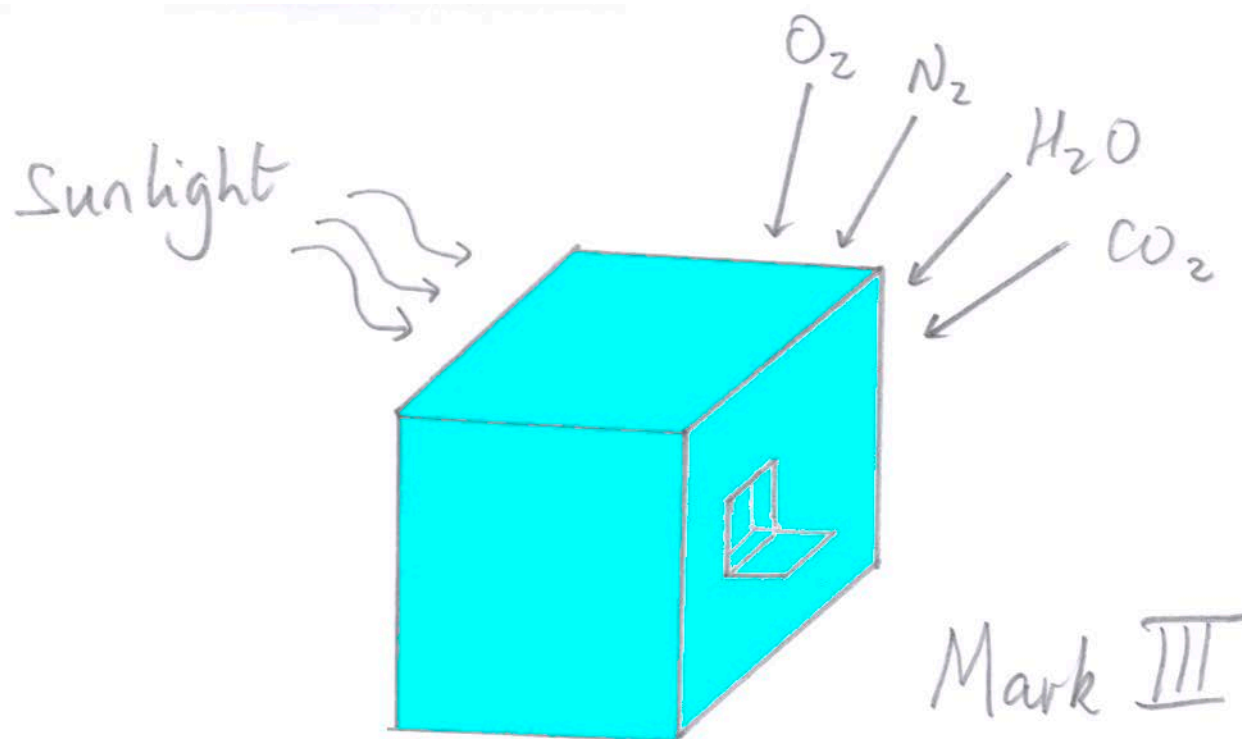
2) Present InChI

How can we communicate science?

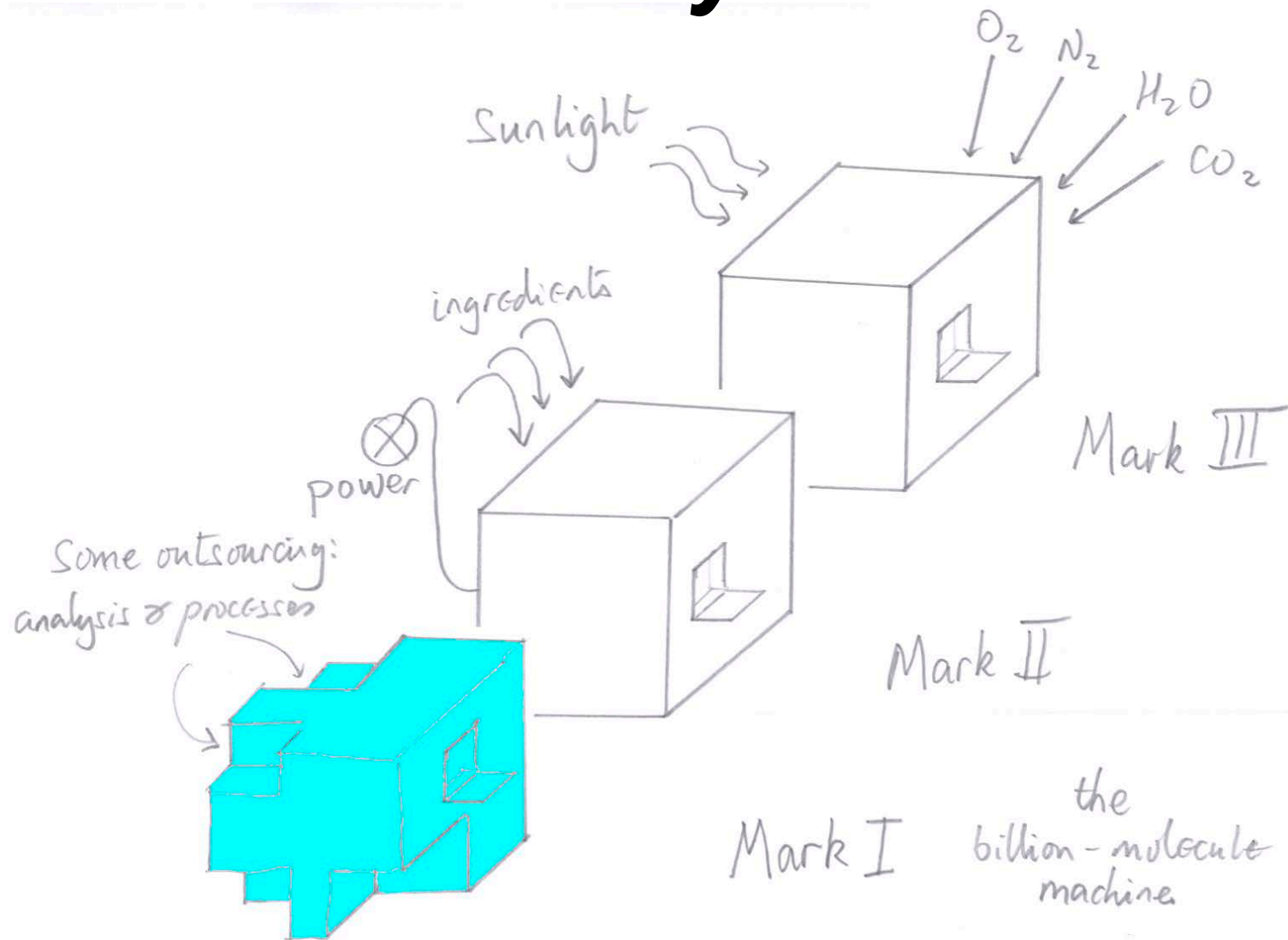
3) InChI Present

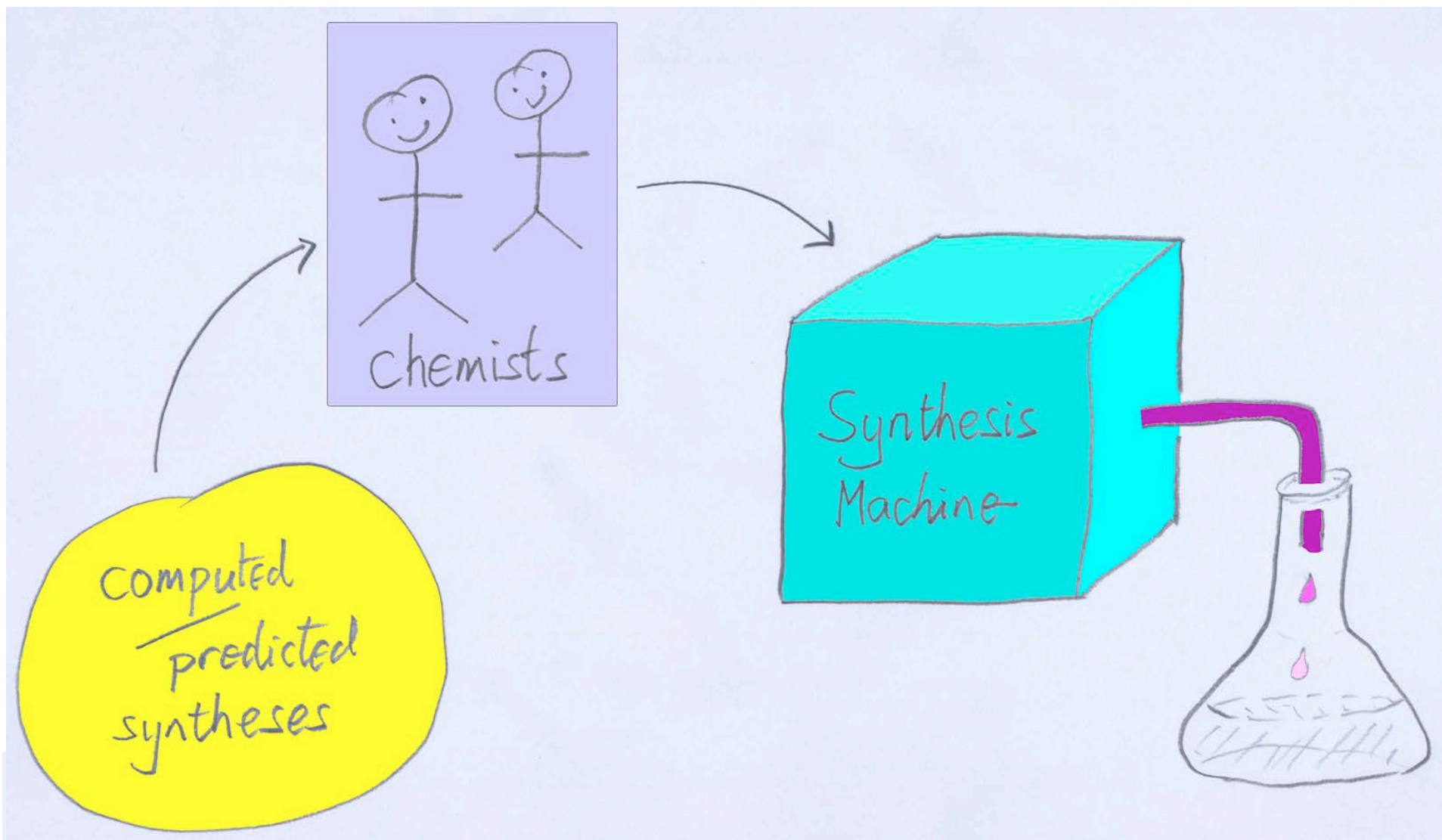
What can InChI give the world?

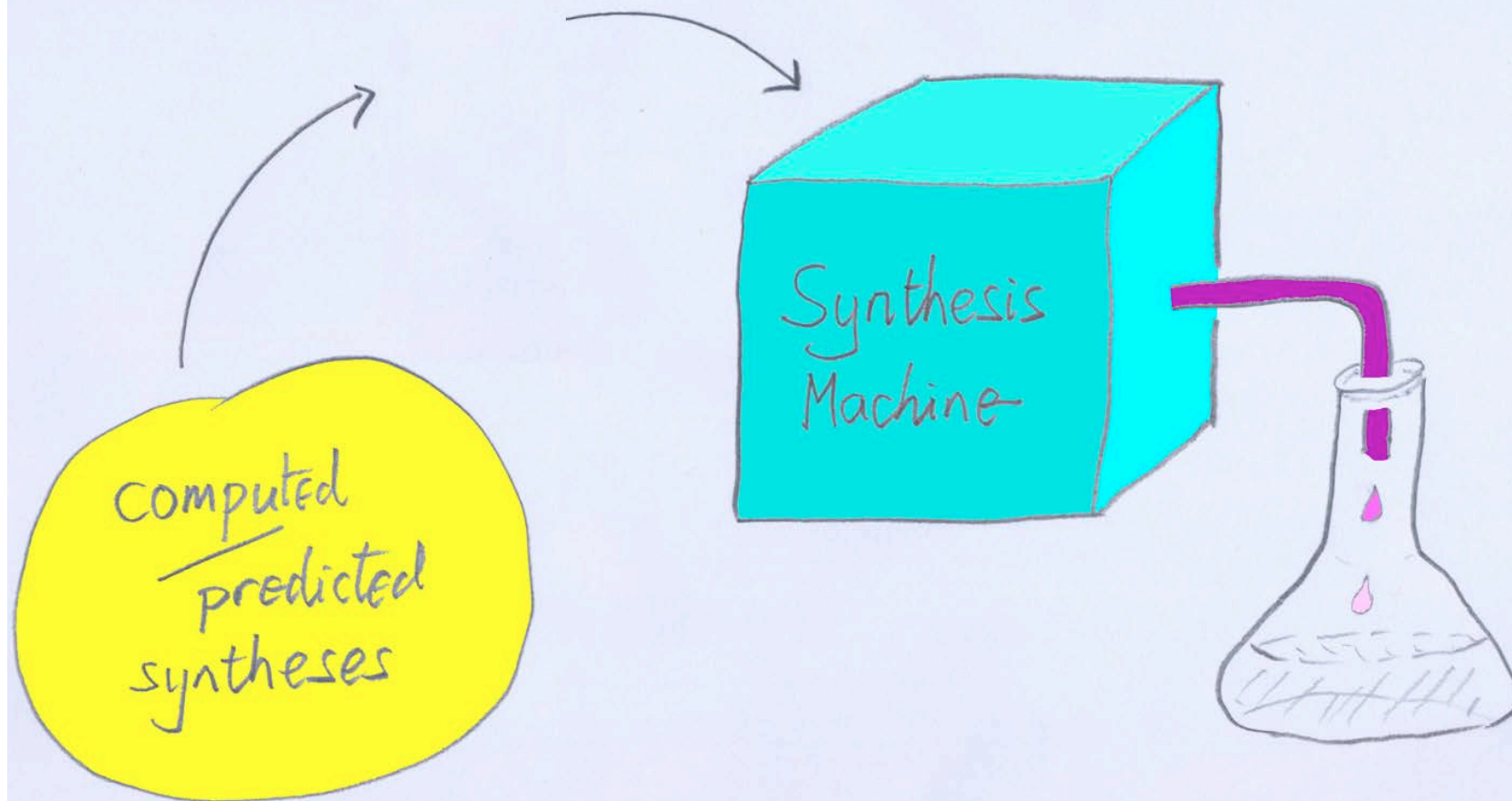
We make any molecule

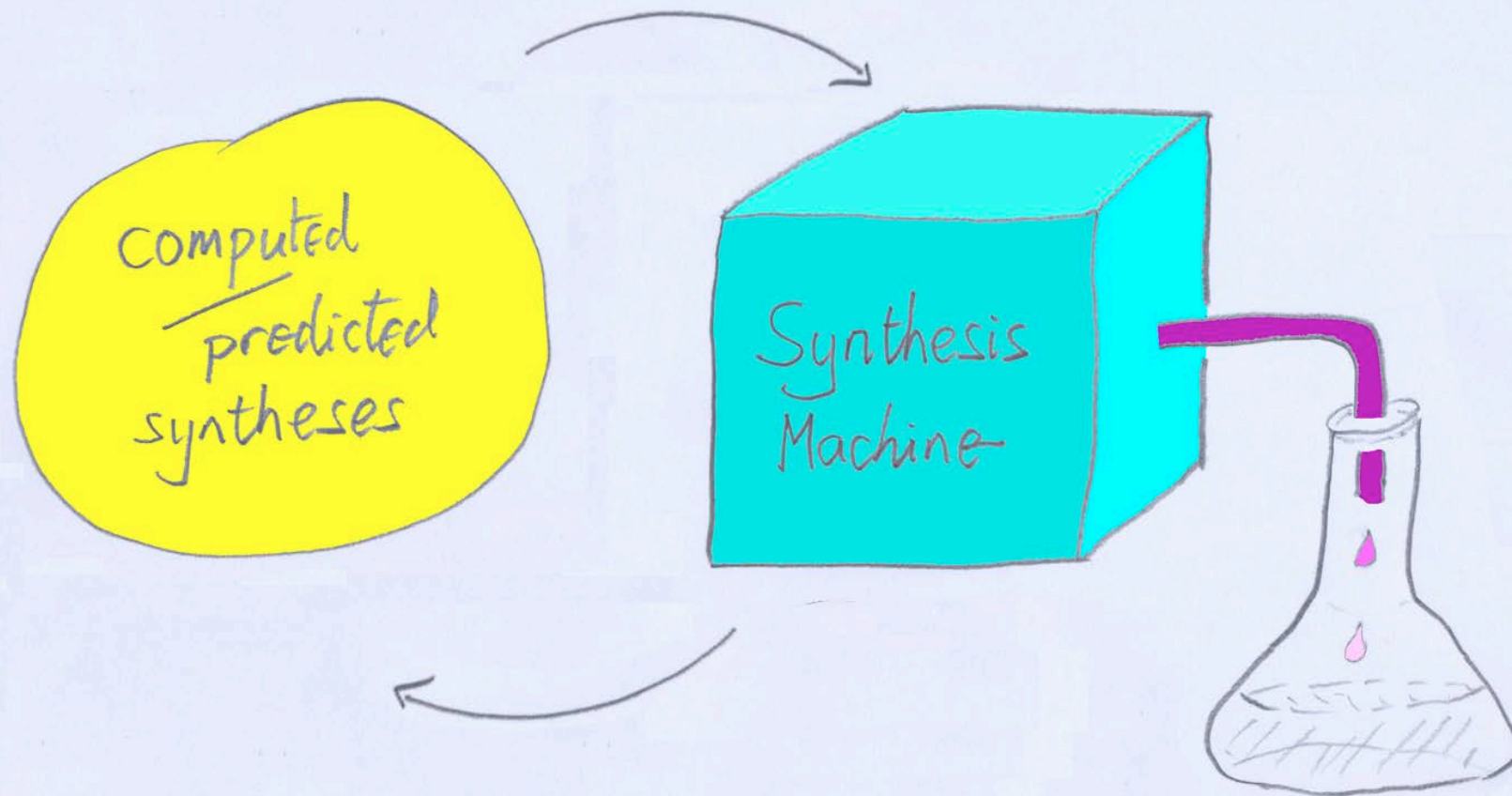


We make any molecule

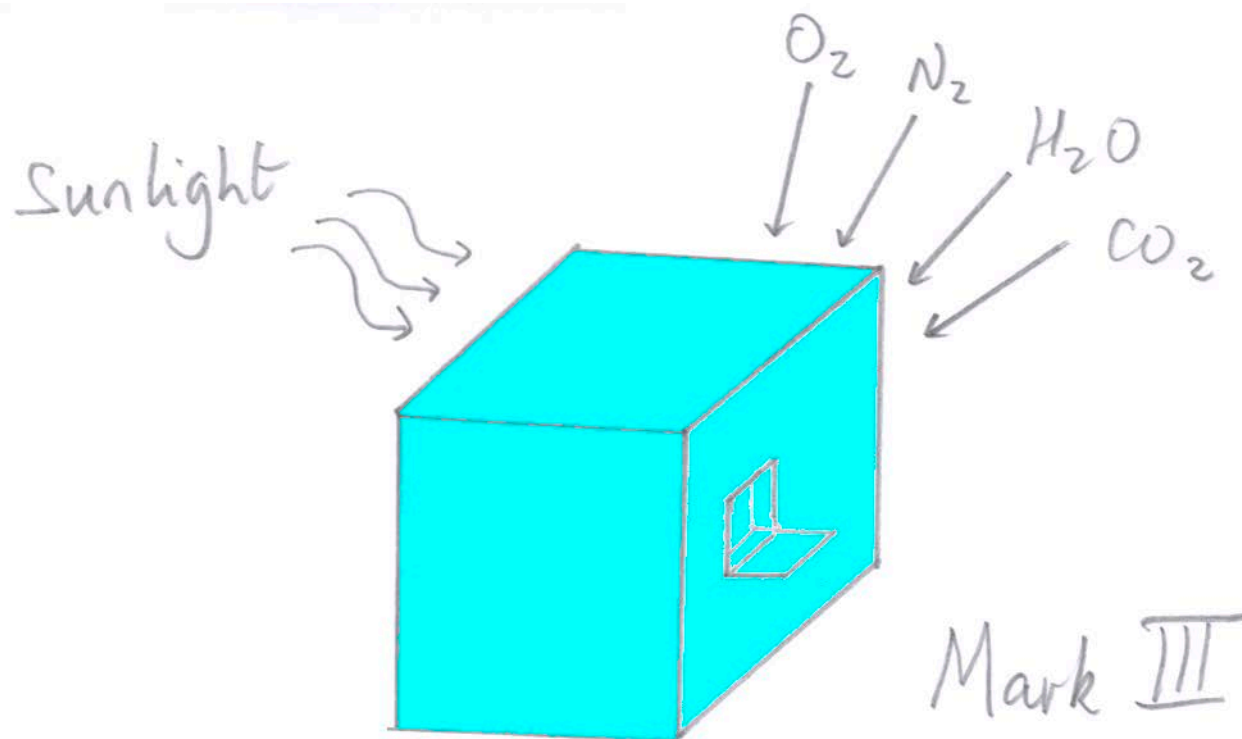








We make any molecule



*To achieve this, we need
InChI and RInChI*

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