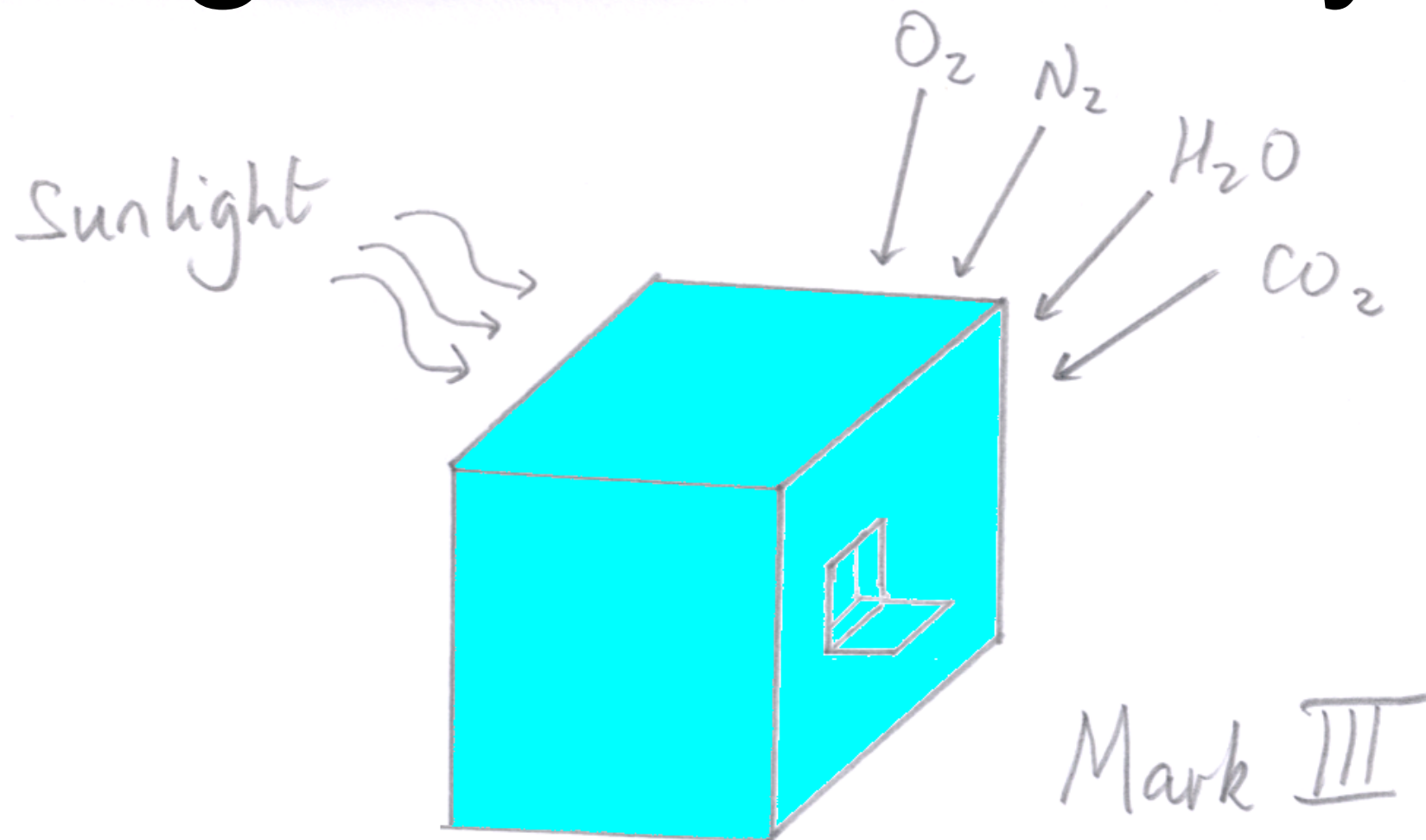


Big data chemistry

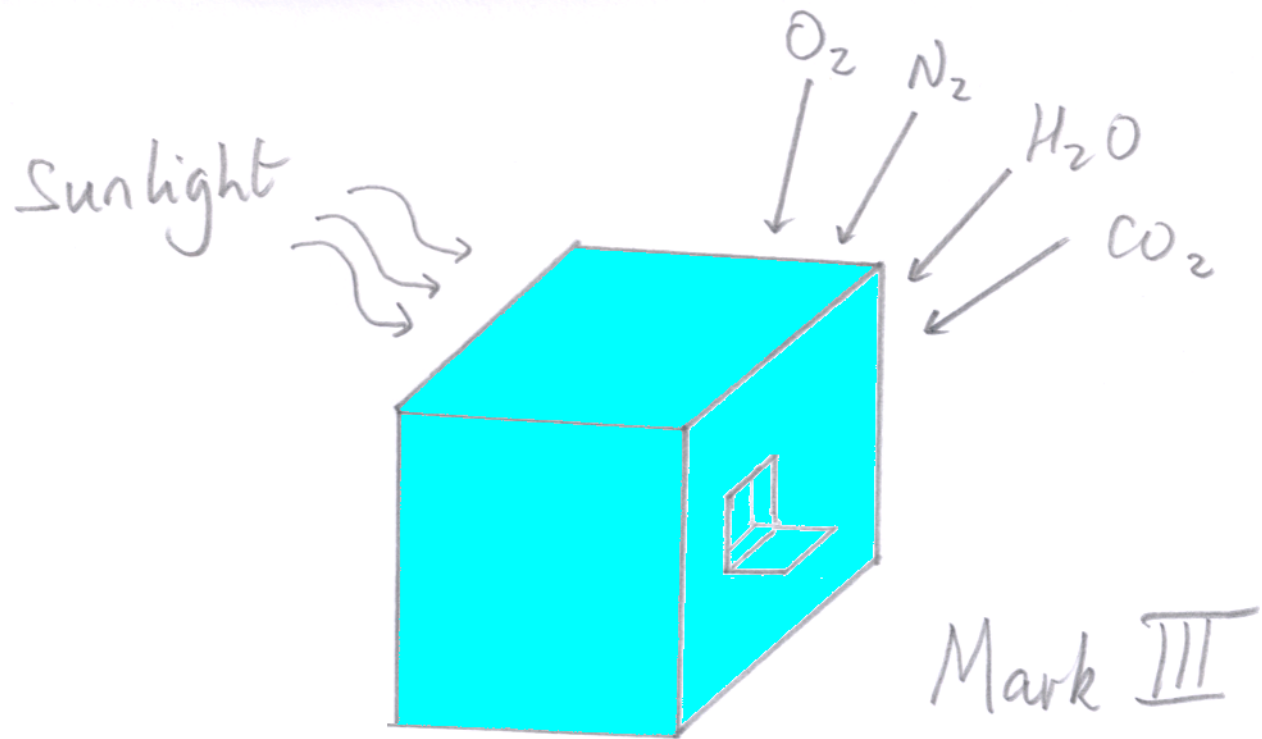


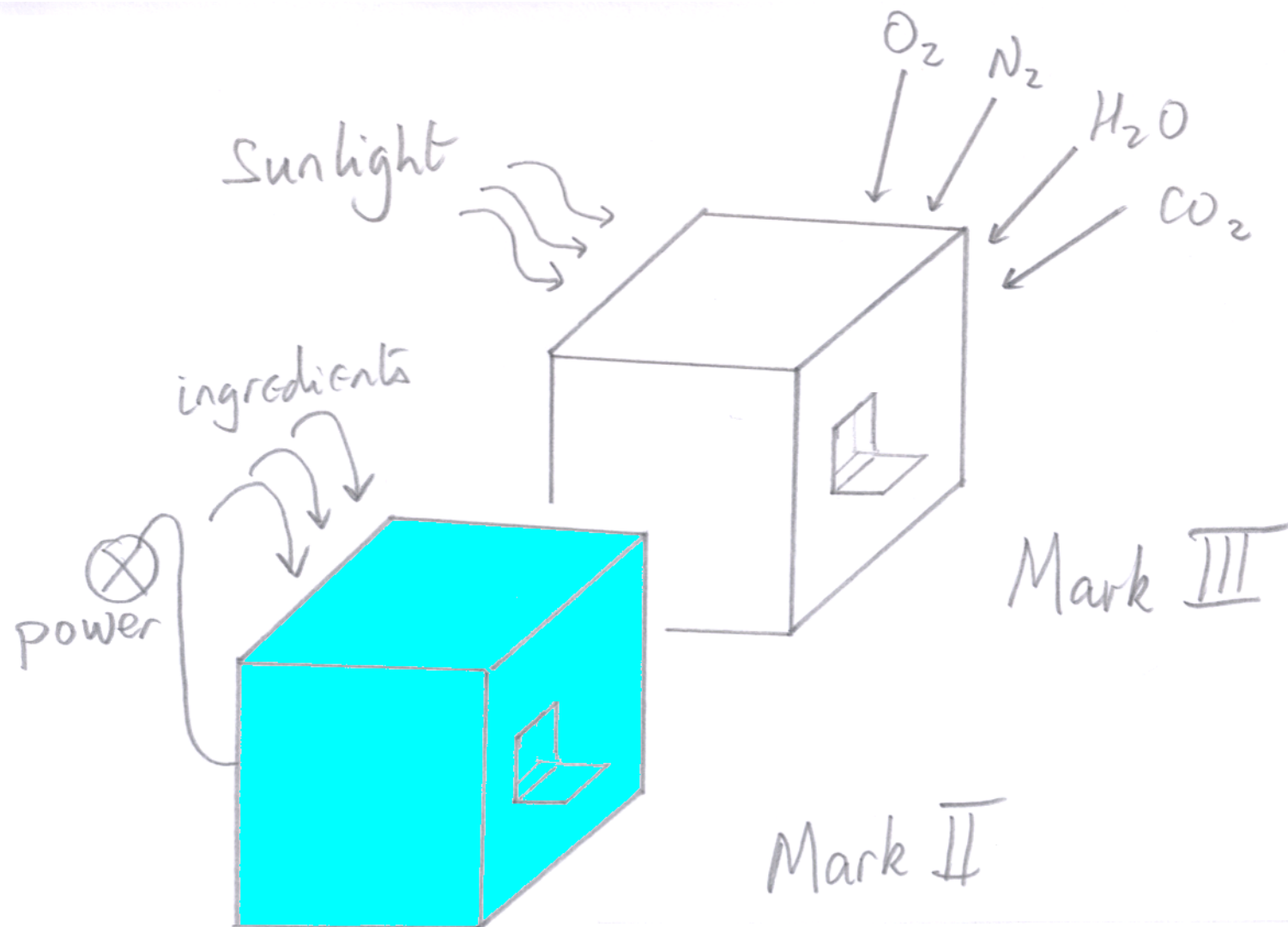
Jonathan M Goodman
Department of Chemistry
University of Cambridge

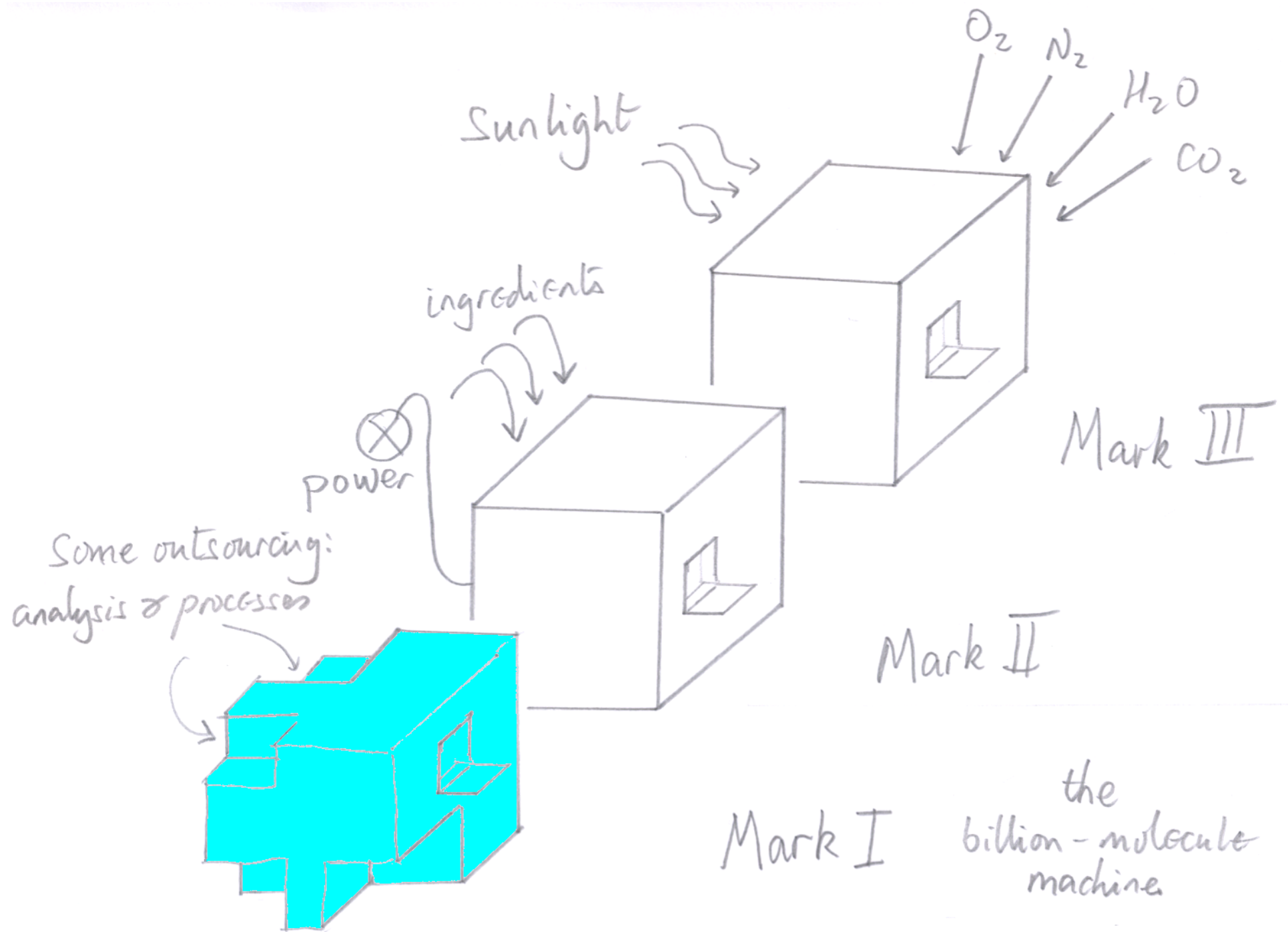
Wikipedia:

Big data

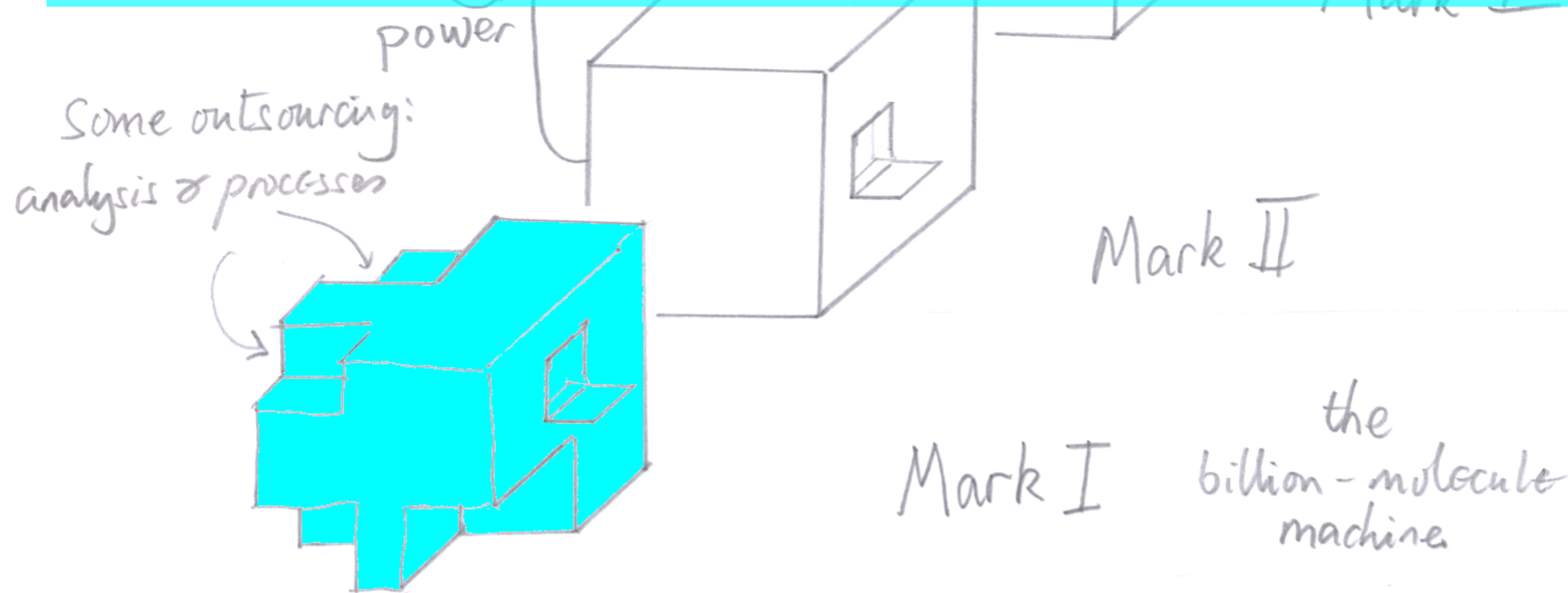
is an all-encompassing term
for any collection of data sets
so large and complex that
it becomes difficult to process them
using traditional
data processing applications







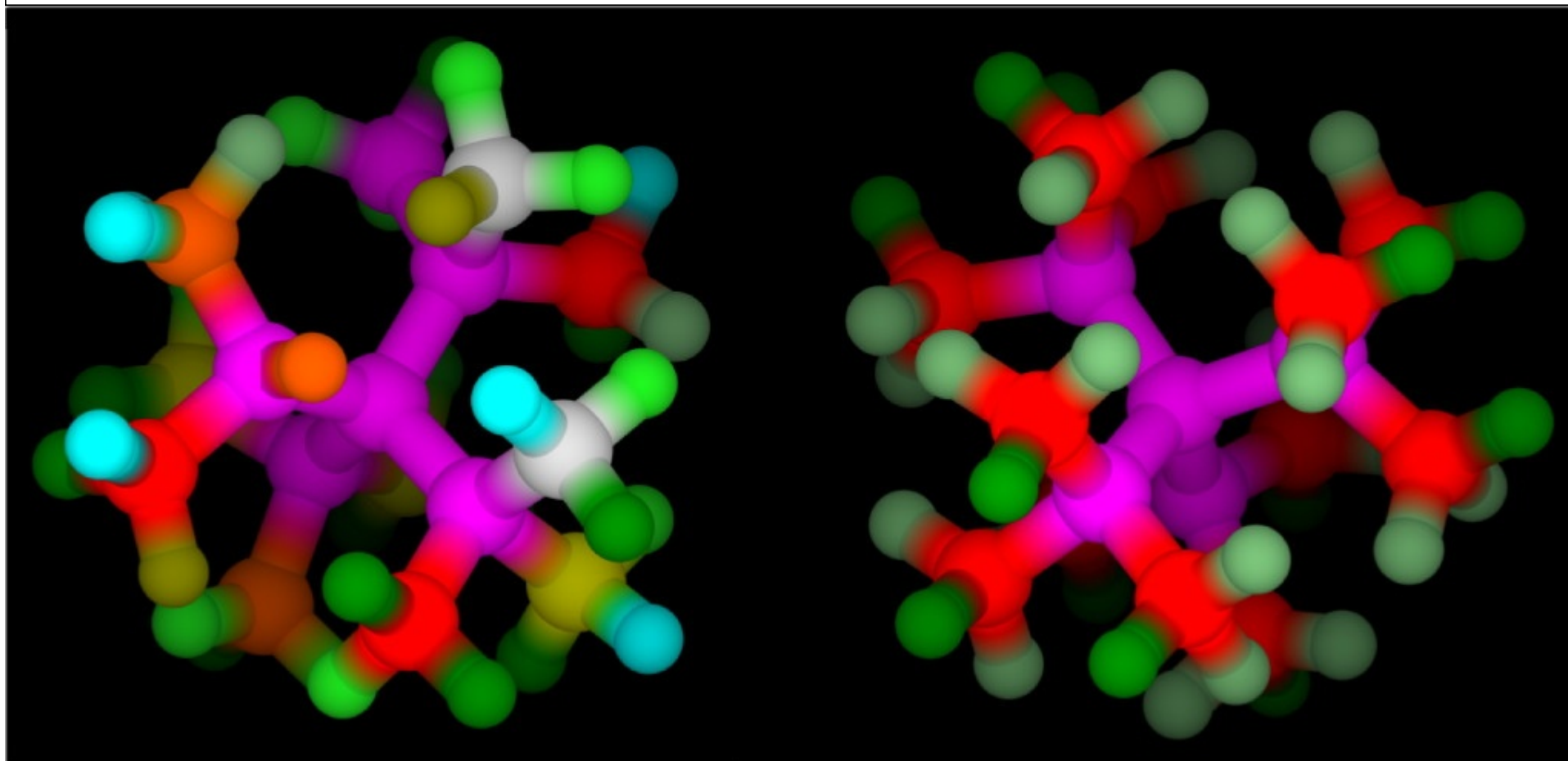
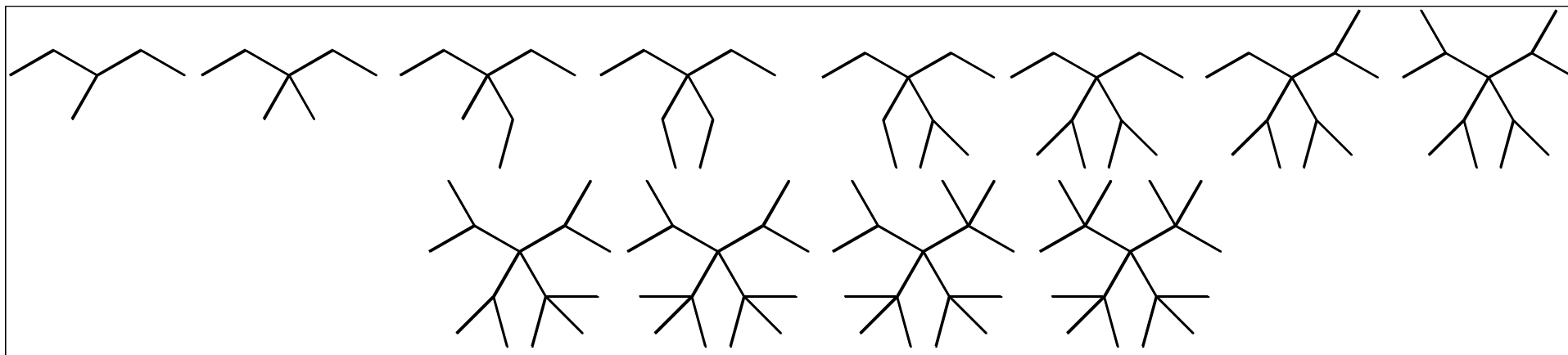
- (1) Make a molecule
- (2) Make a process for a library
- (3) Make the best molecules with specific properties





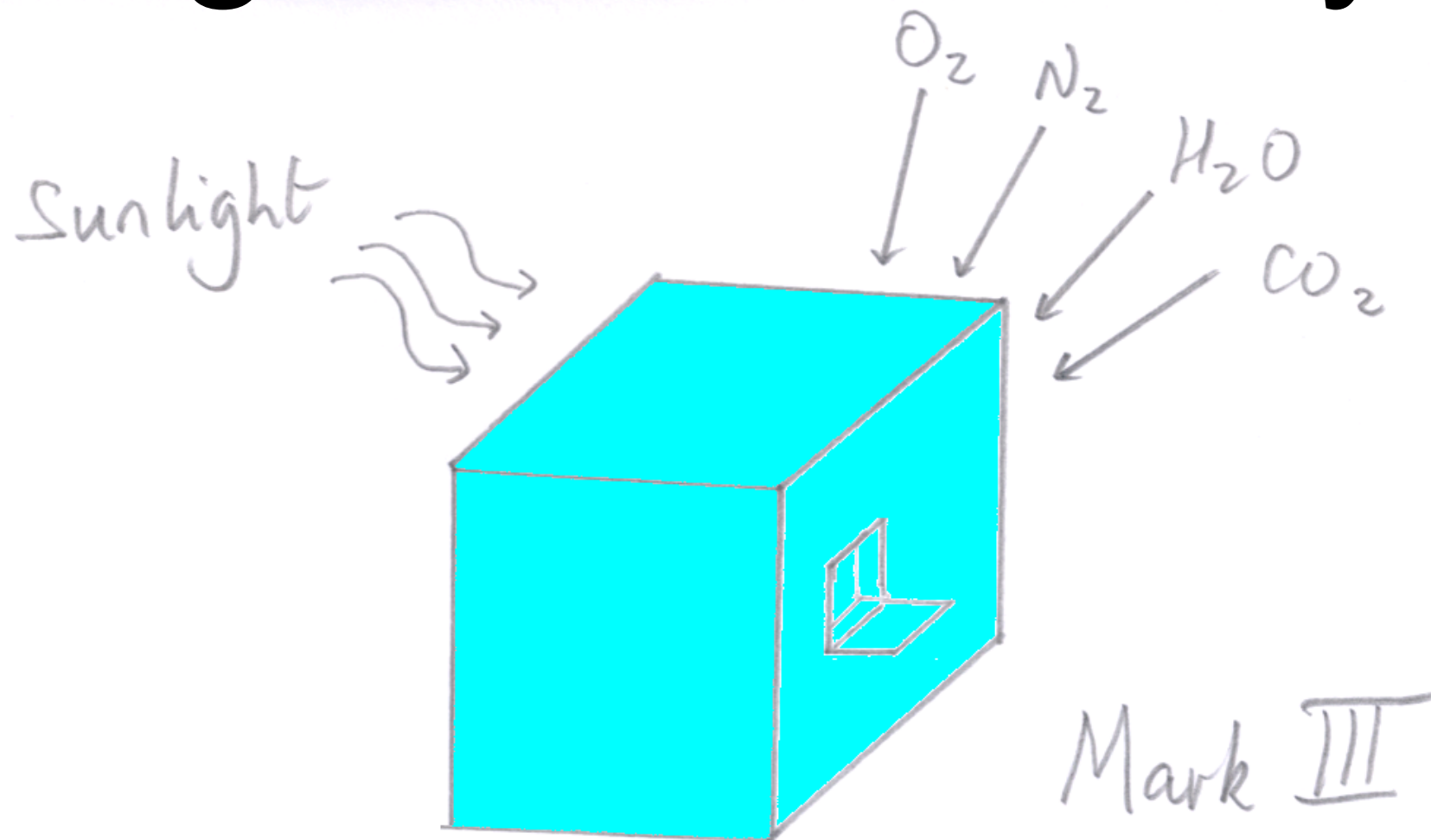
What is the simplest molecule
that cannot be made?

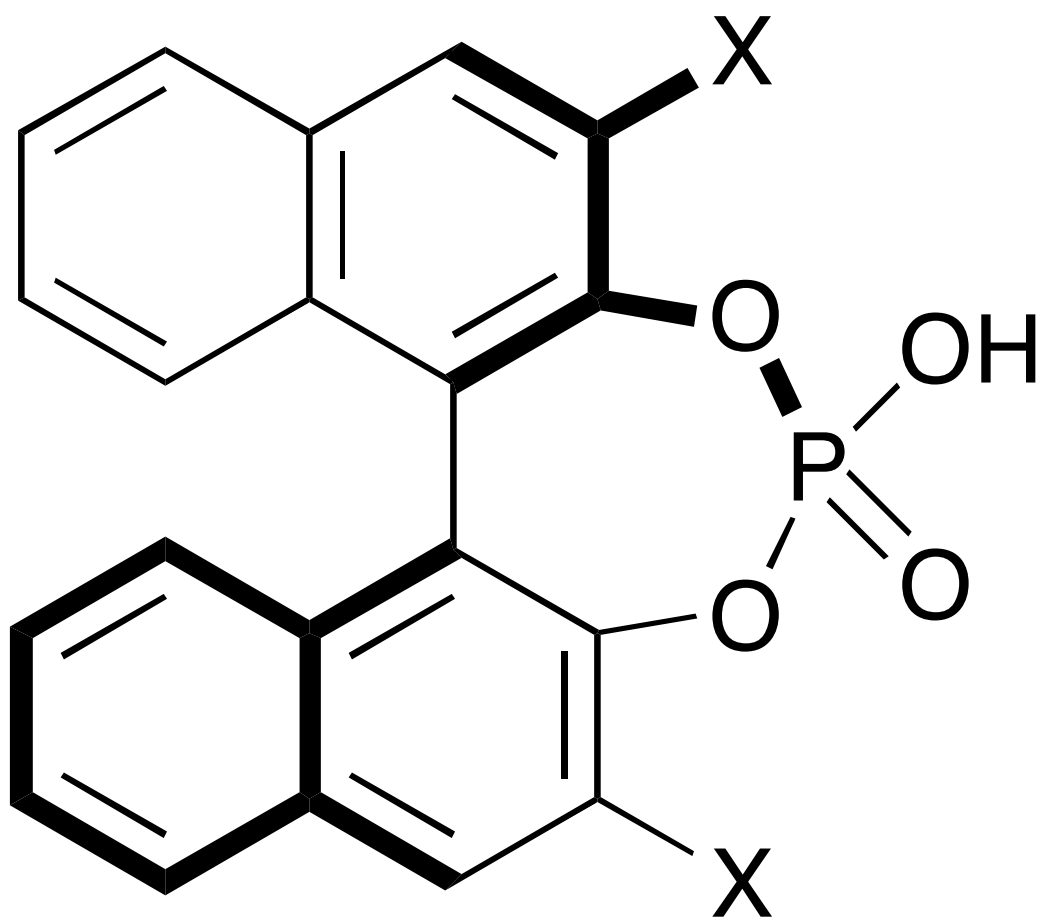
Hydrocarbons only
All valencies satisfied
No rings
Must exist under normal conditions

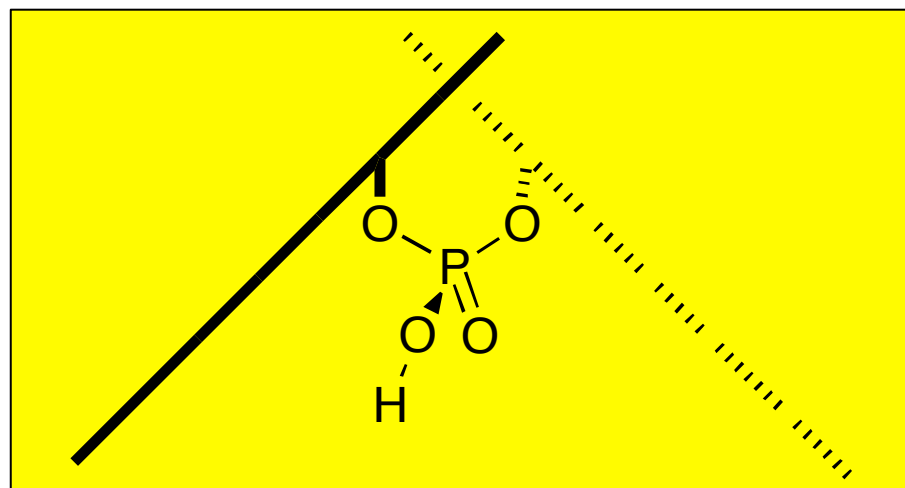
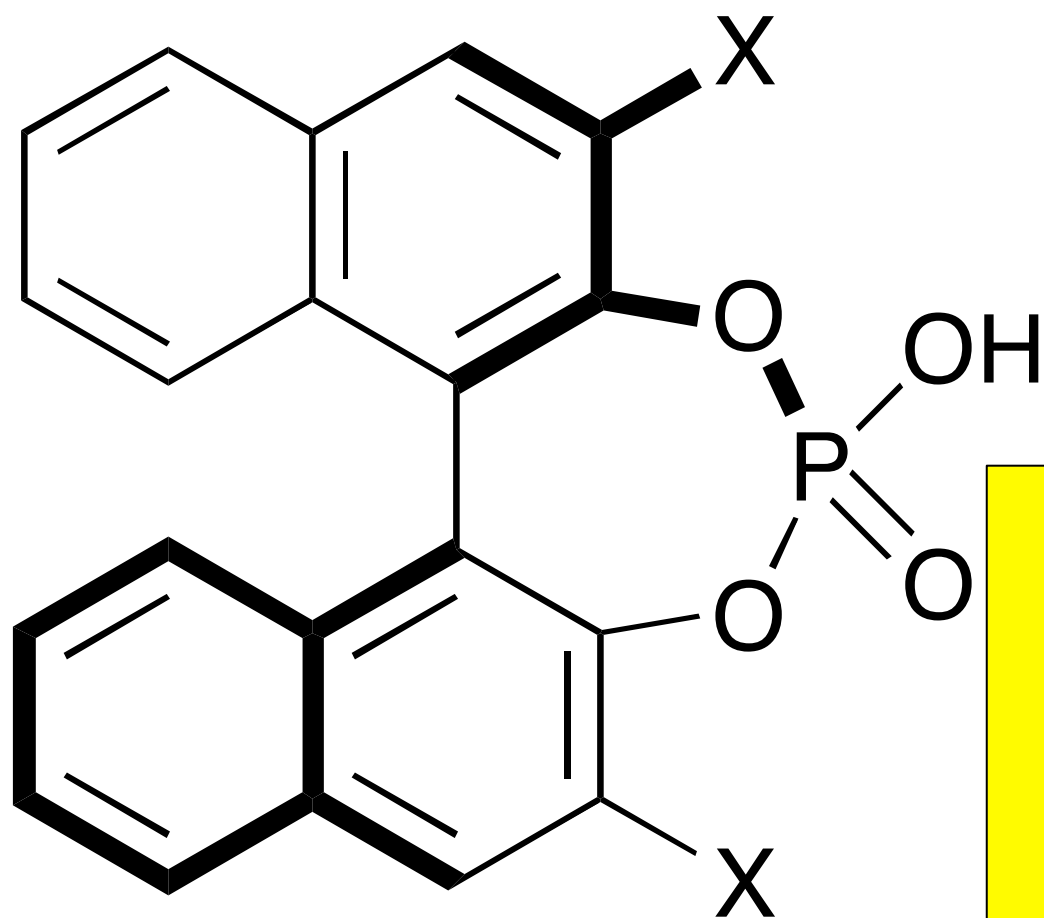


J. Chem. Inf. Model. 2005, **45**, 81-87; *J. Chem. Inf. Model.* 2007, **47**, 2124-2132.

Big data chemistry





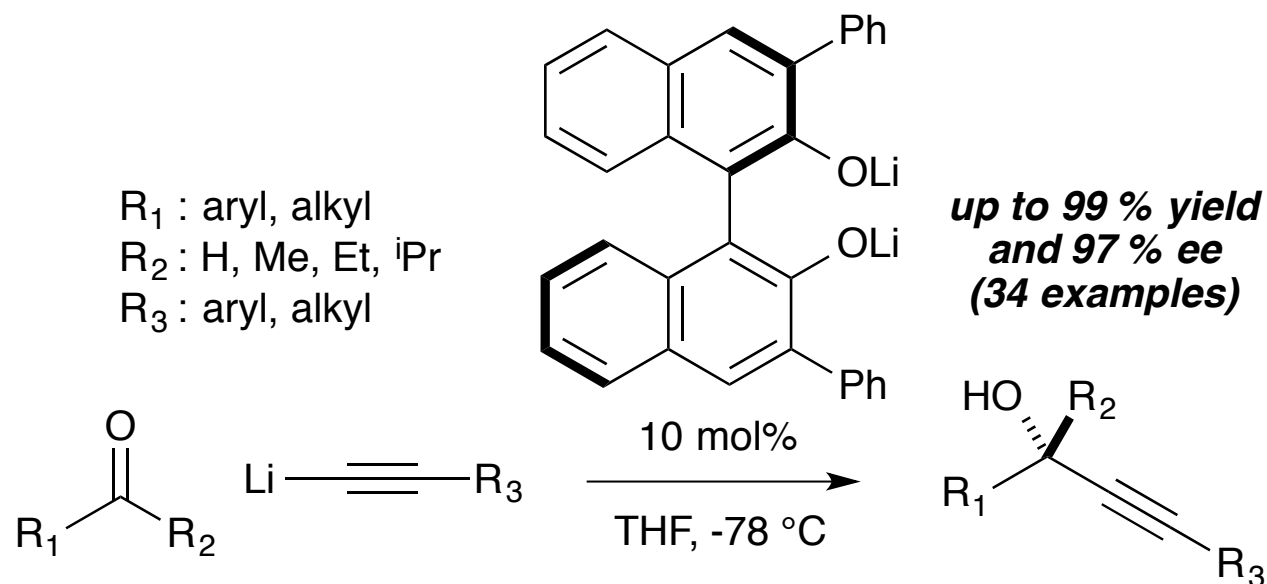


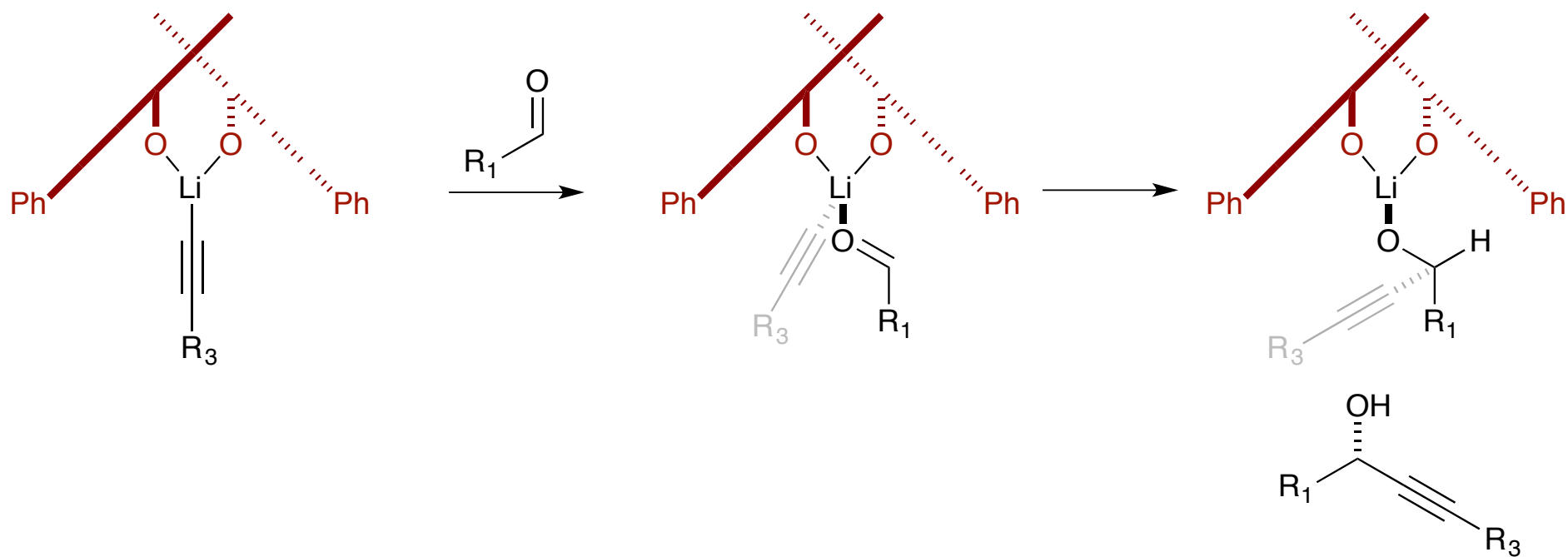
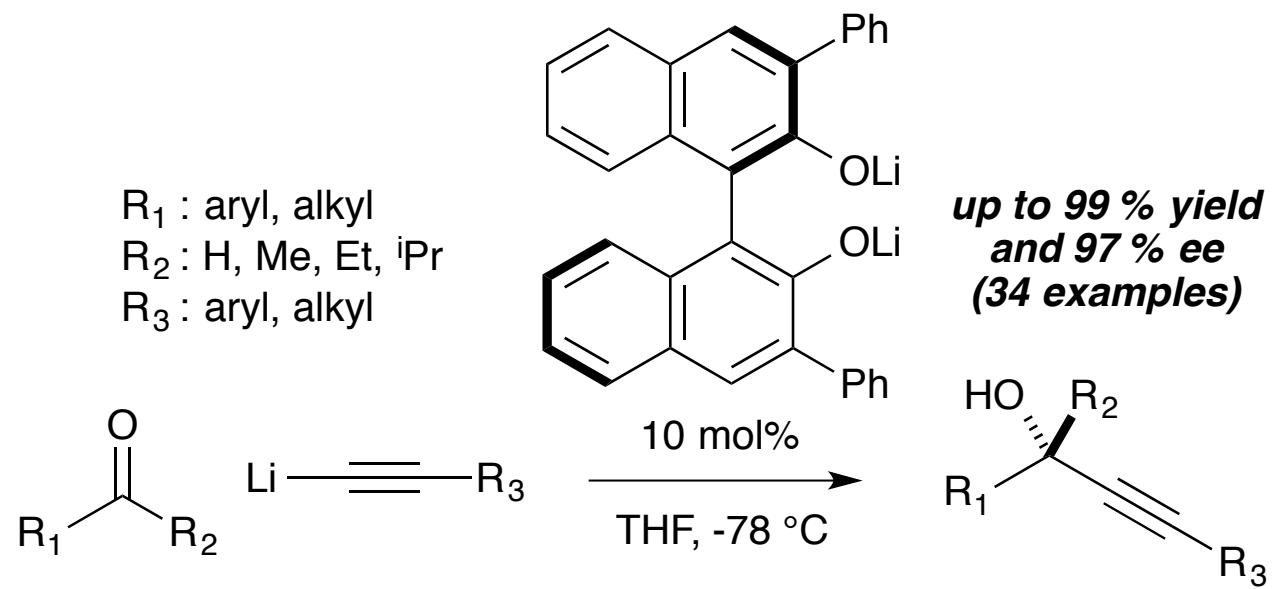
Lithium Binaphtholate-Catalyzed Asymmetric Addition of Lithium Acetylides to Carbonyl Compounds

Shunsuke Kotani, Kenji Kukita, Kana Tanaka, Tomonori Ichibakase, and Makoto Nakajima

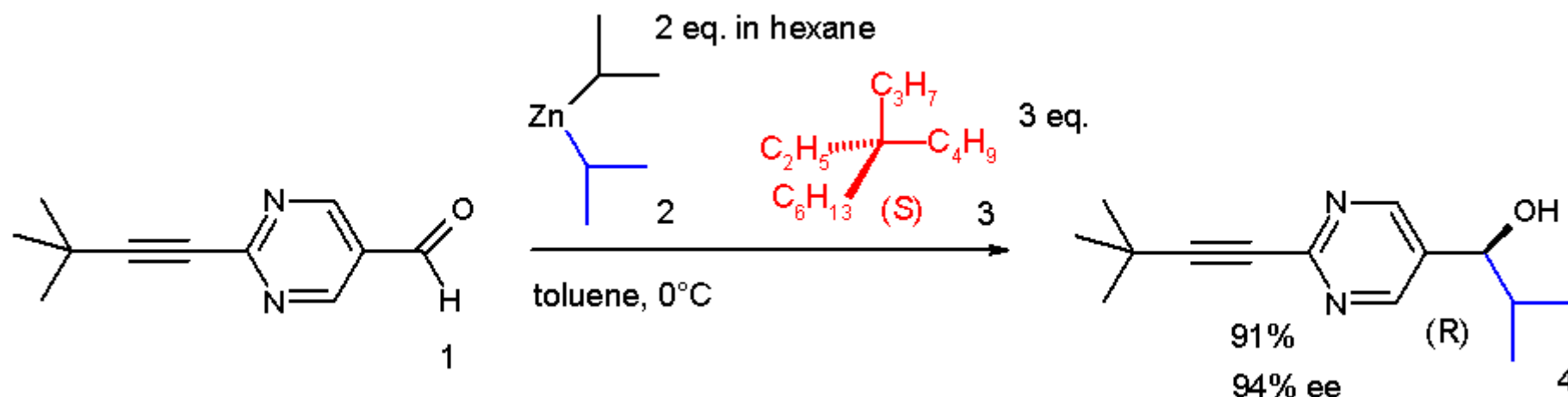
J. Org. Chem., **2014**, 79 (11), pp 4817–4825

DOI: 10.1021/jo5005394





Soai reaction

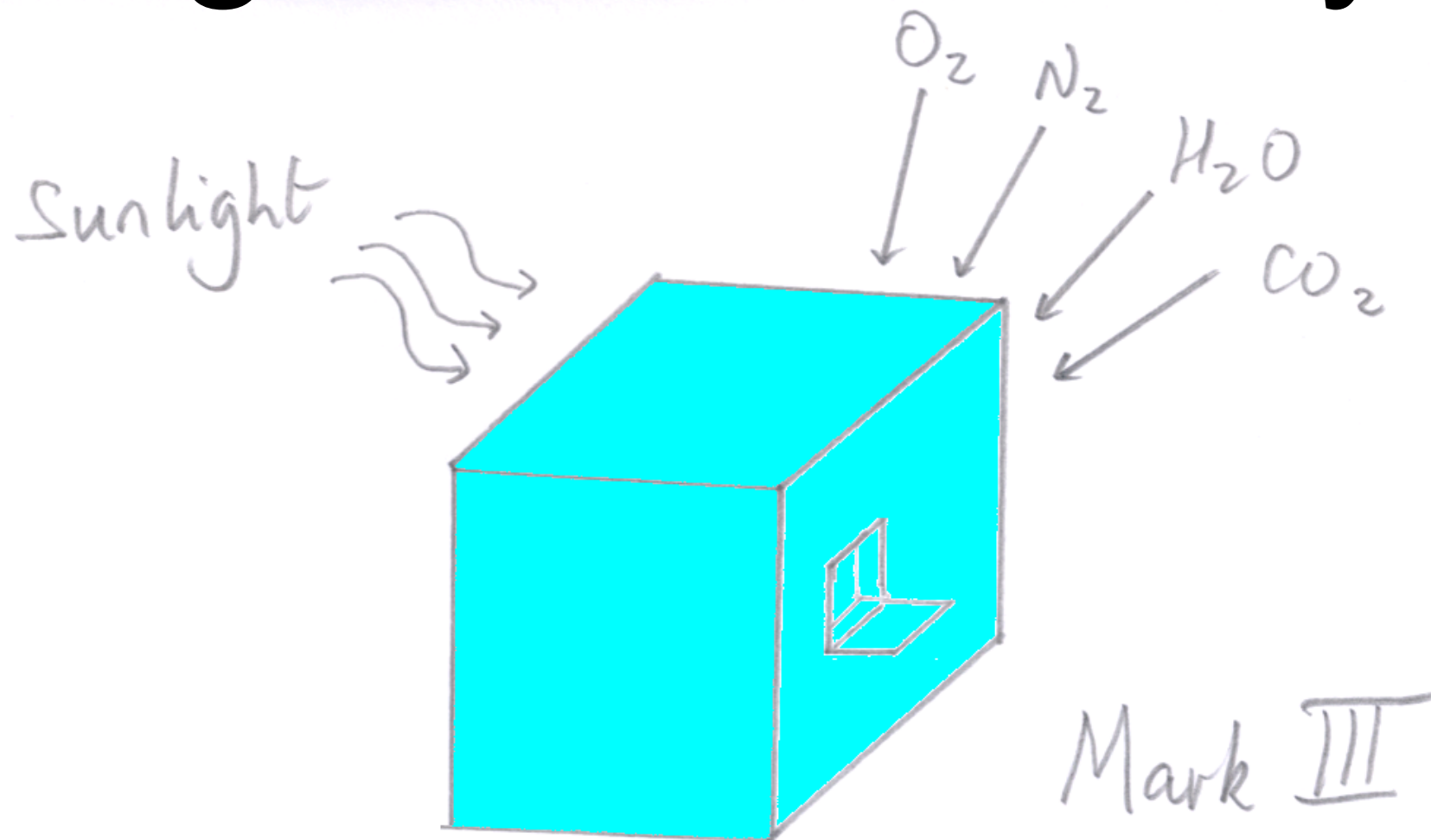


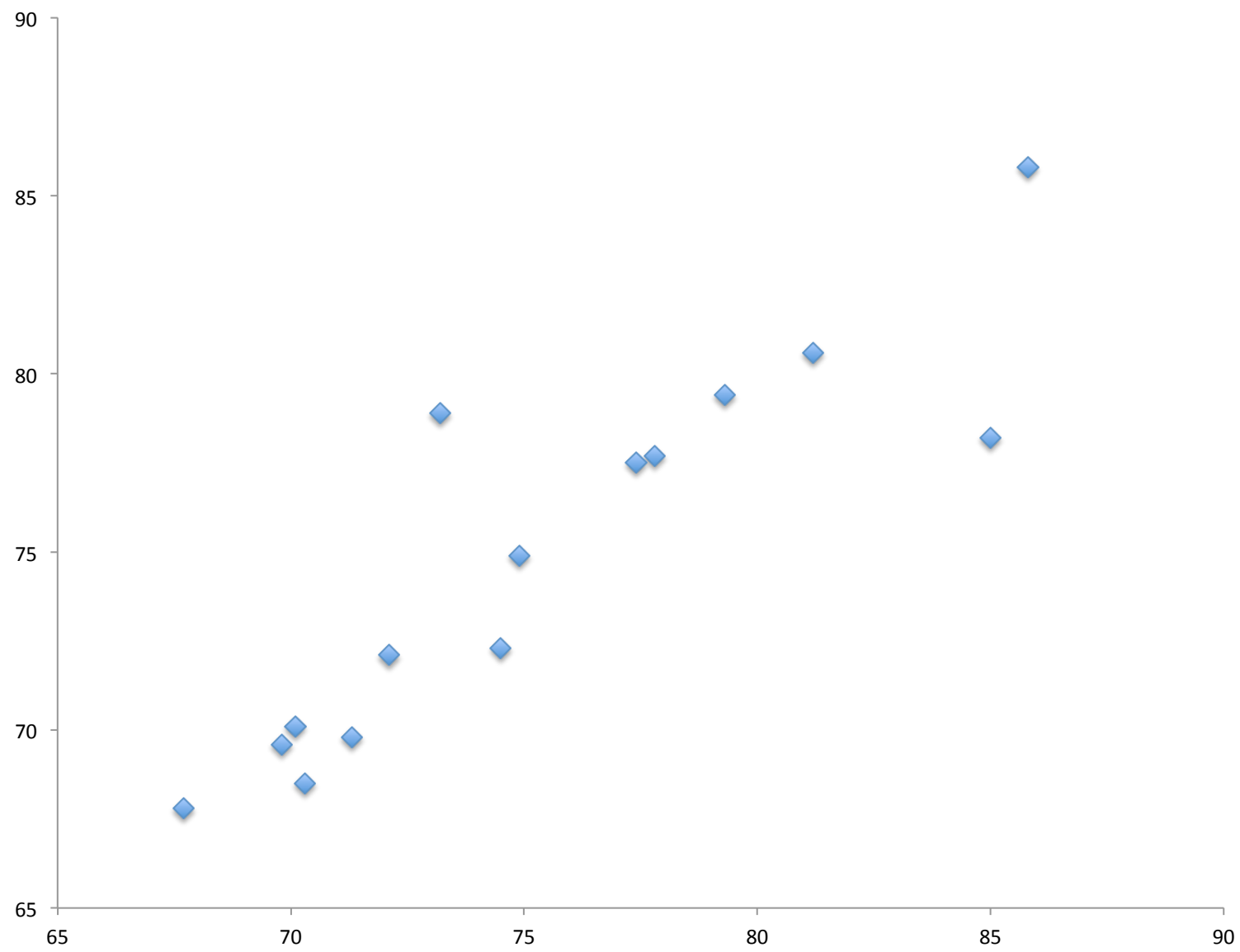
Permission details

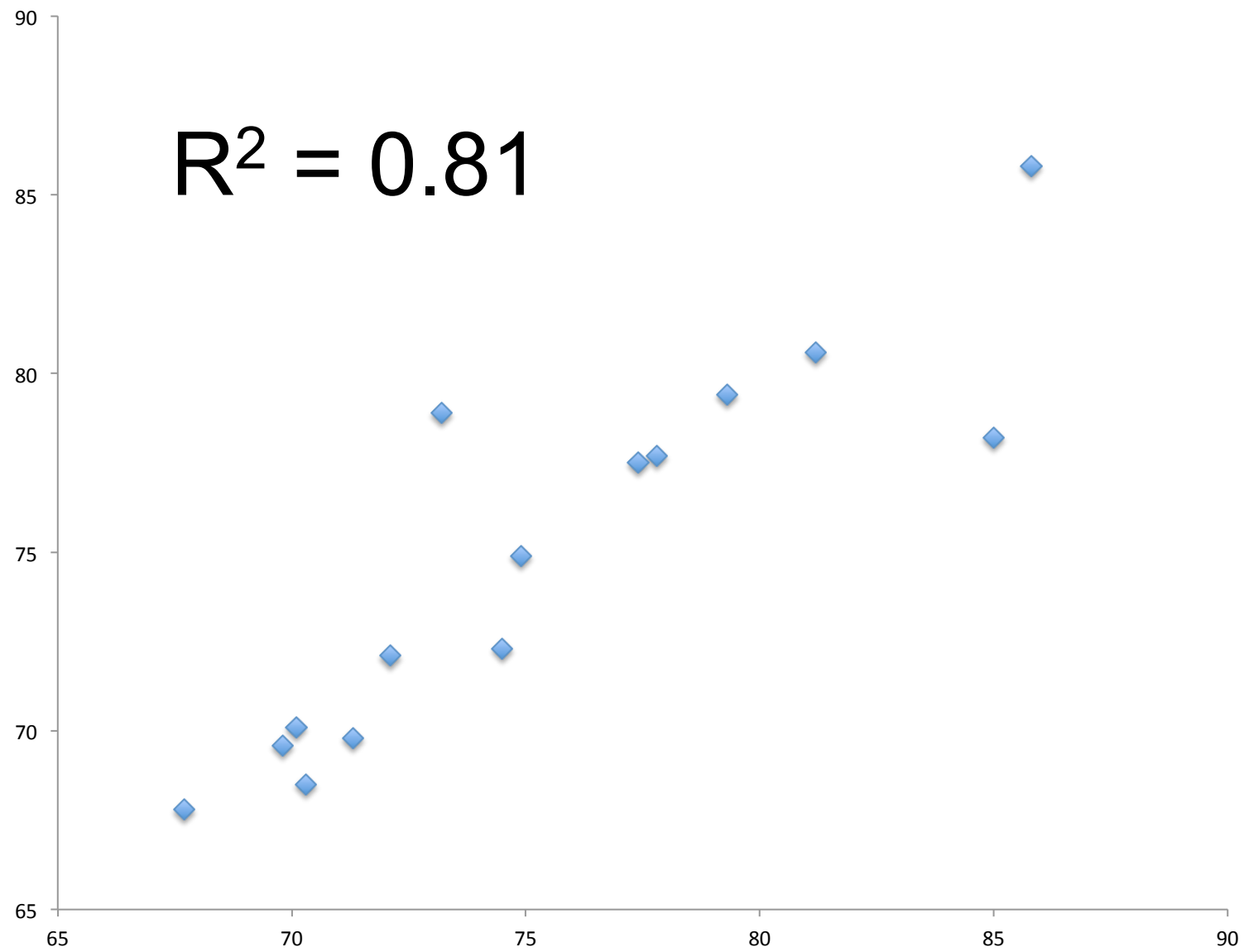
CC-BY-SA-3.0-MIGRATED; Released under the [GNU Free Documentation License](https://www.gnu.org/licenses/fdl-1.3.html).

Shibata, Takanori; Morioka, Hiroshi; Hayase, Tadakatsu; Choji, Kaori; Soai, Kenso.
Highly Enantioselective Catalytic Asymmetric Automultiplication
of Chiral Pyrimidyl Alcohol
Journal of the American Chemical Society 1996, **118**, 471.
doi:10.1021/ja953066g

Big data chemistry







On the Structure of Maitotoxin

K. C. Nicolaou and Michael O. Frederick

Angewandte Chemie International Edition Volume 46, Issue 28, pages 5278–5282, July 9, 2007

DOI: 10.1002/anie.200604656

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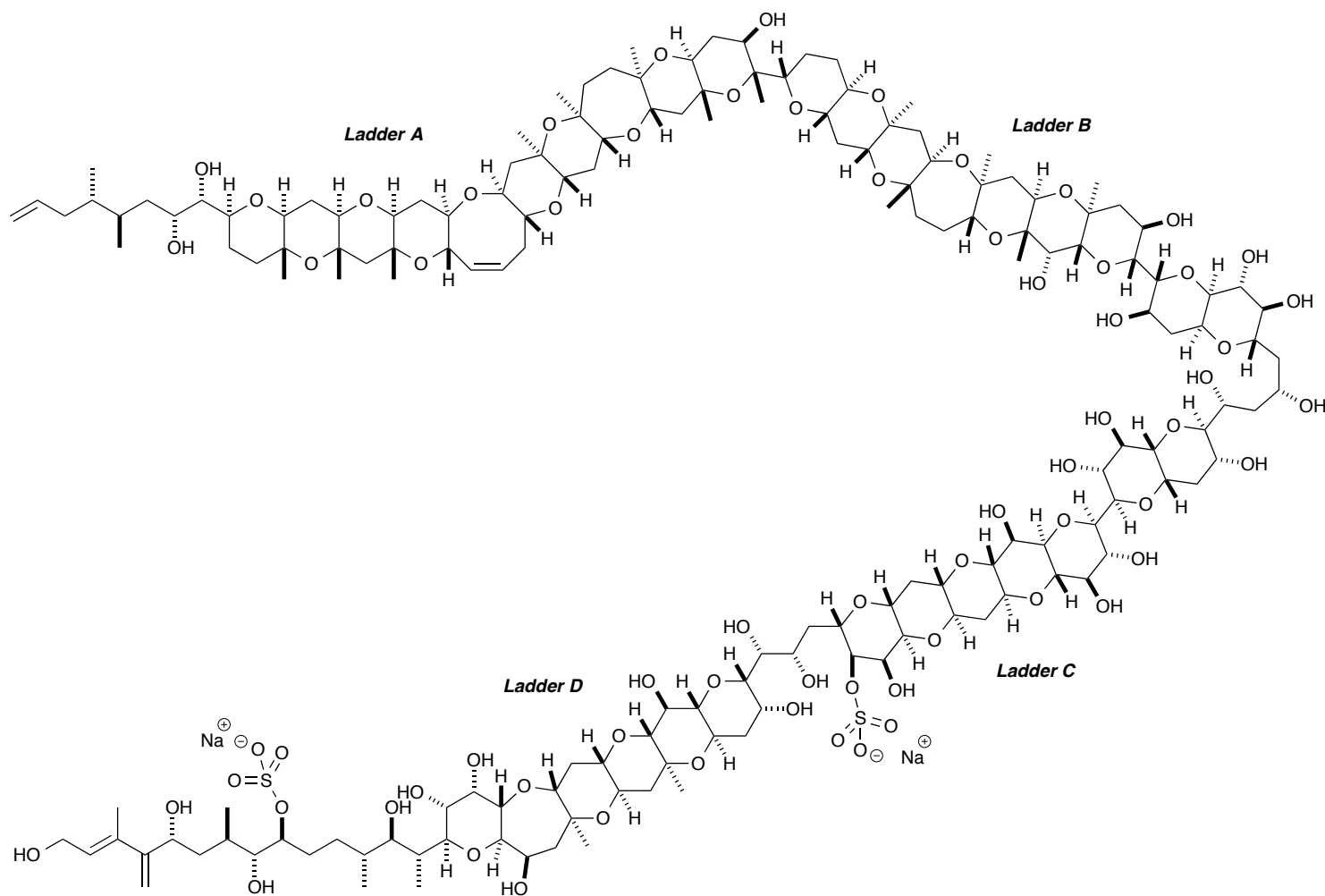
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Stereochemical Uniformity in Marine Polyether Ladders – Implications for the Biosynthesis and Structure of Maitotoxin

Andrew R Gallimore and Jonathan B Spencer

Angewandte Chemie International Edition 2006, 45, 4406–4413.

DOI: 10.1002/anie.200504284

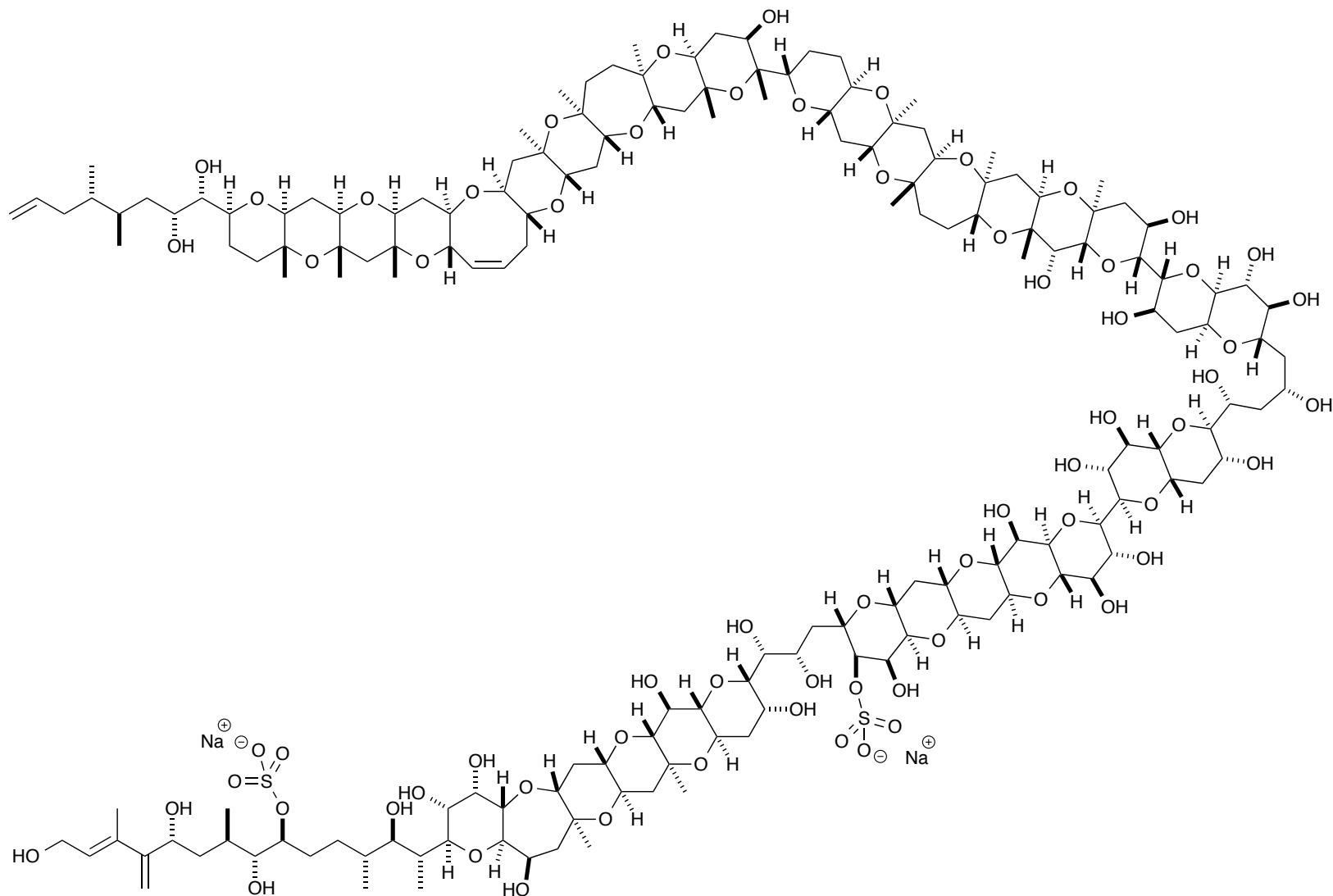


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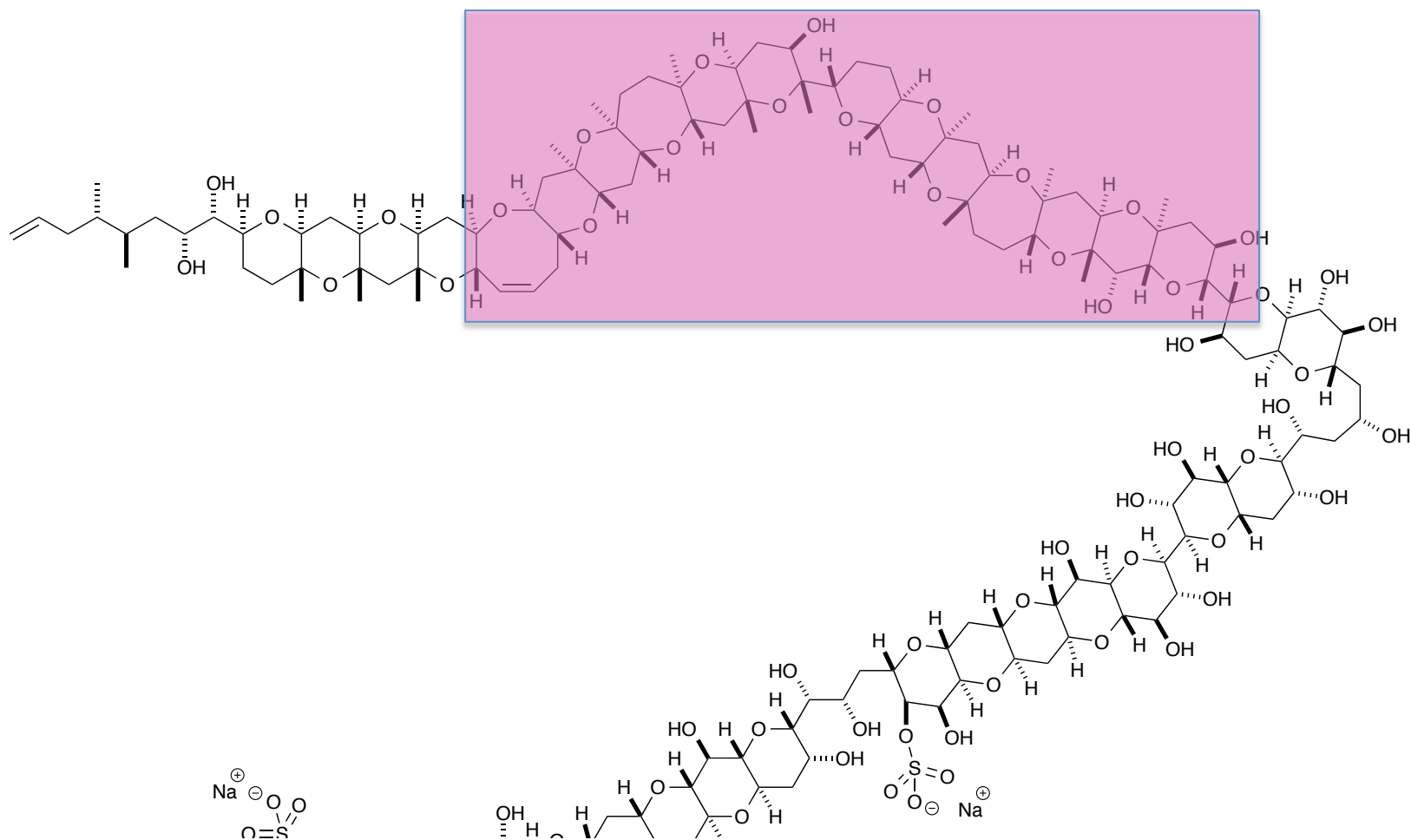


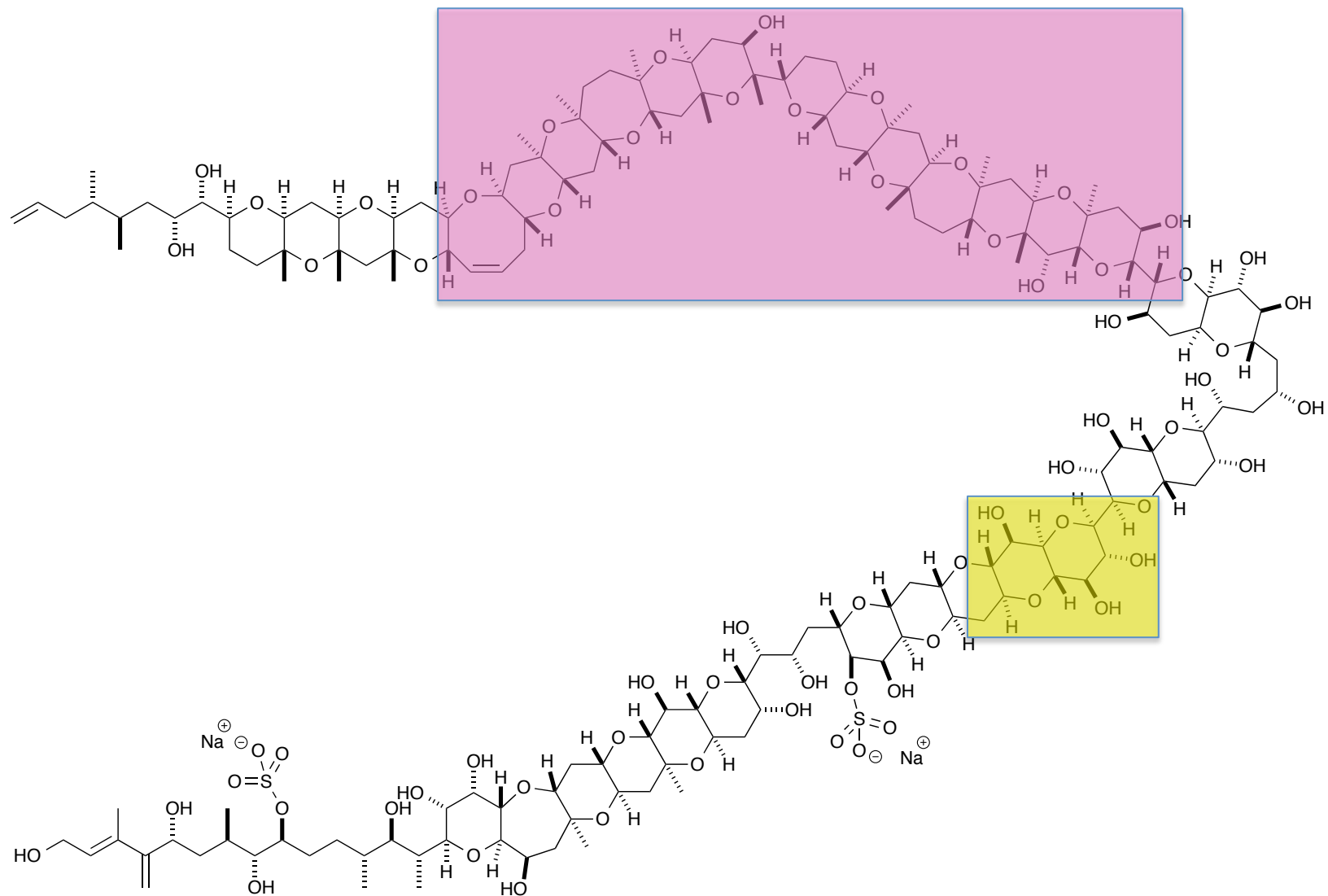
Synthesis and Biological Evaluation of QRSTUVWXYZA' Domains of Maitotoxin

K. C. Nicolaou, Philipp Heretsch, Tsuyoshi Nakamura,
Anna Rudo, Michio Murata, and Keiichi Konoki

J. Am. Chem. Soc., 2014, **136** (46), pp 16444–16451

DOI: 10.1021/ja509829e



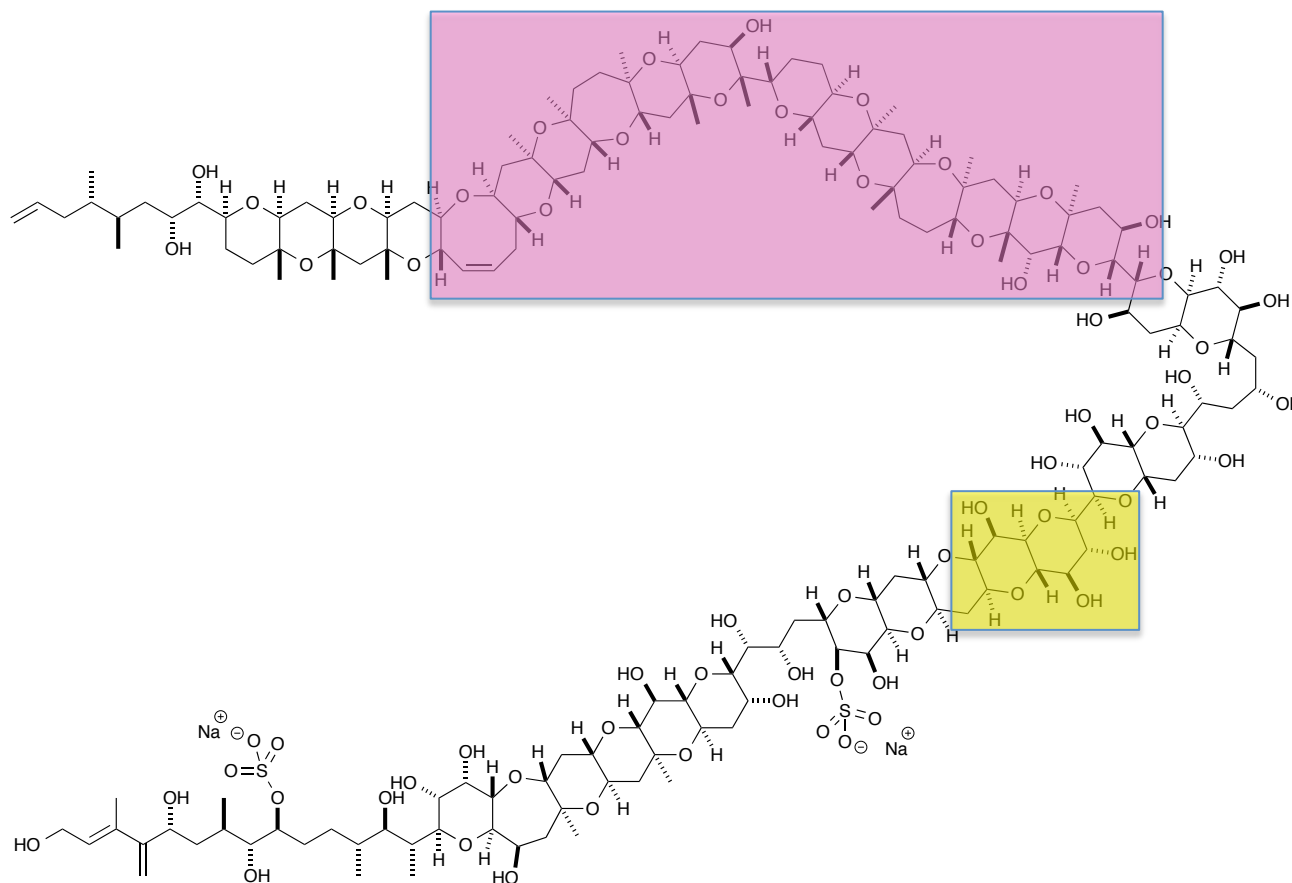


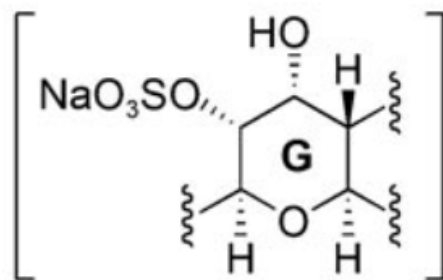
Chemical Synthesis of the GHIJK Ring System and Further Experimental Support for the Originally Assigned Structure of Maitotoxin

K. C. Nicolaou, Kevin P. Cole, Michael O. Frederick, Robert J. Aversa and Ross M. Denton

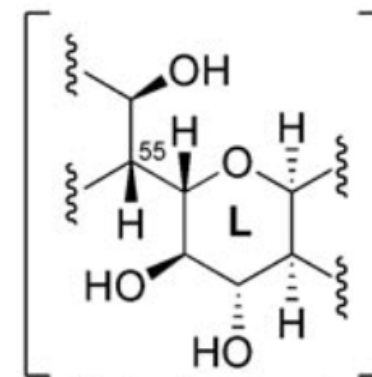
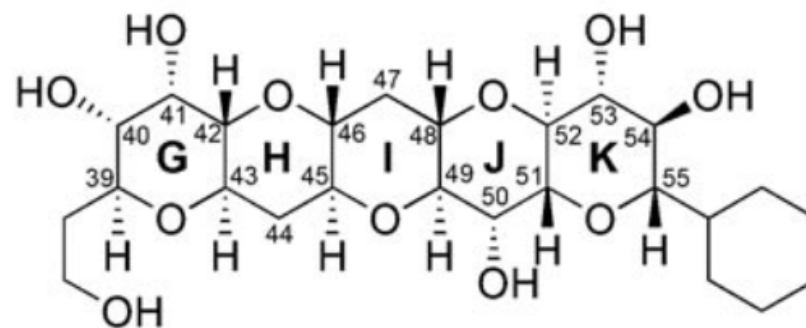
Angewandte Chemie International Edition 2007,46, 8875–8879.

DOI: 10.1002/anie.200703742

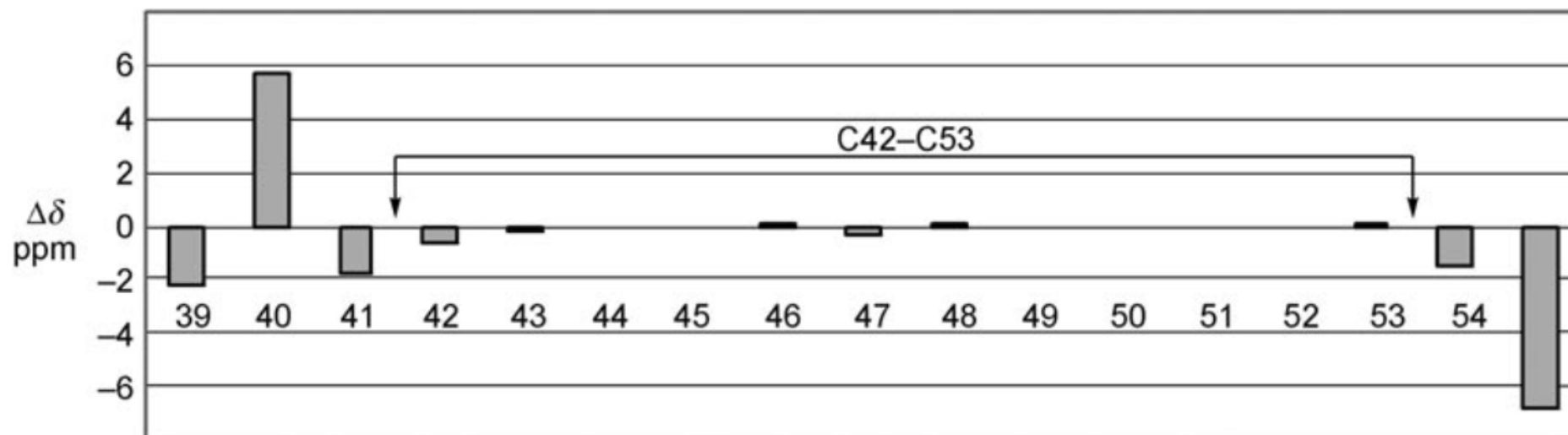


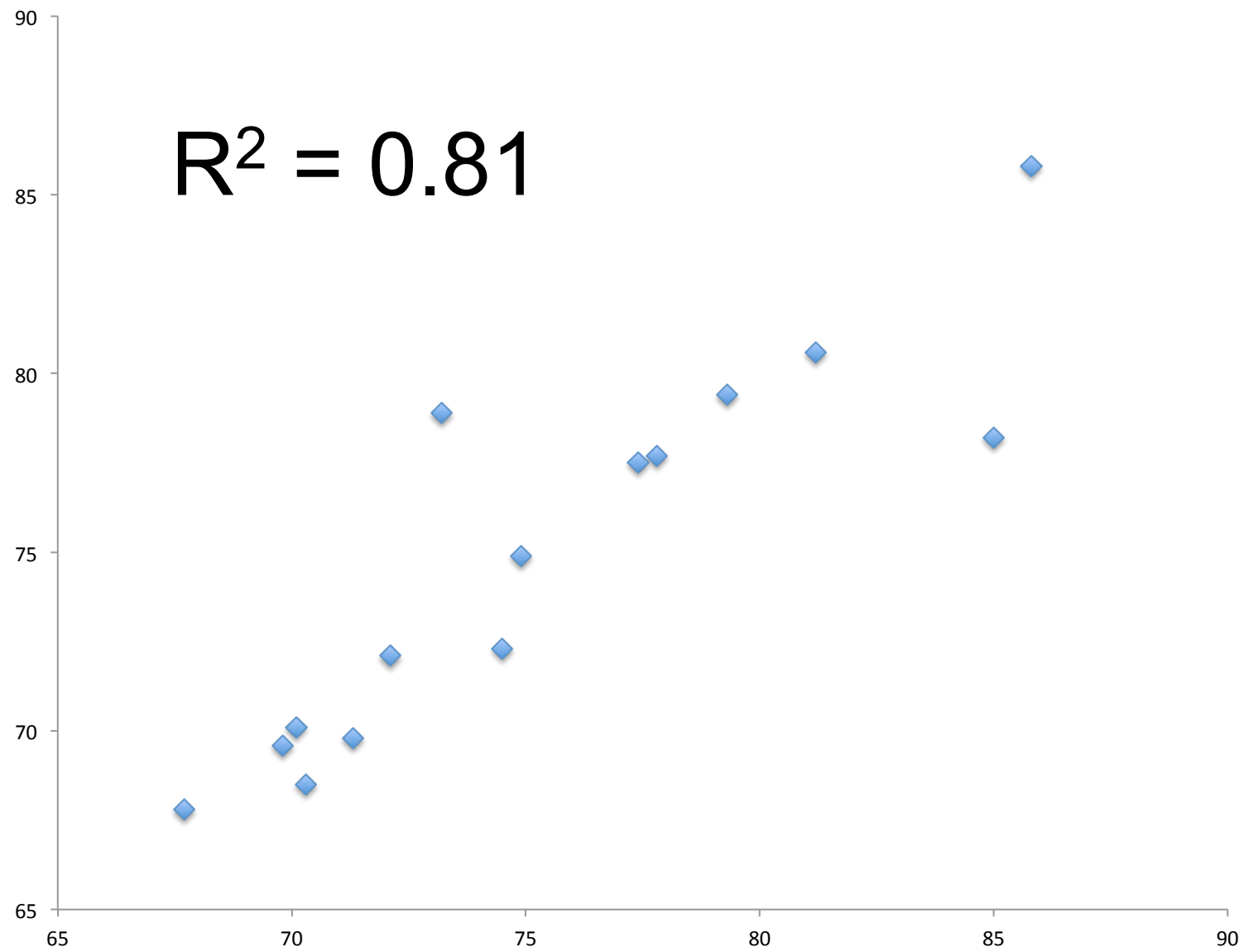


maitotoxin structure



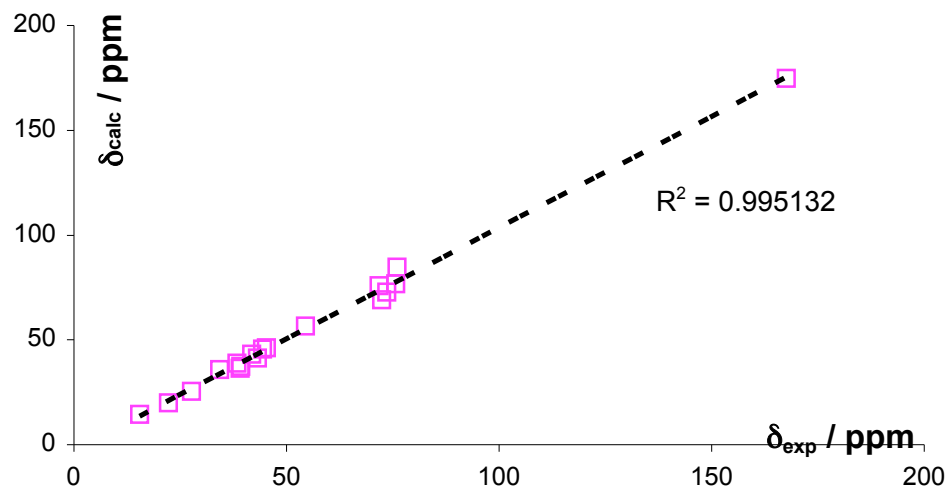
maitotoxin structure



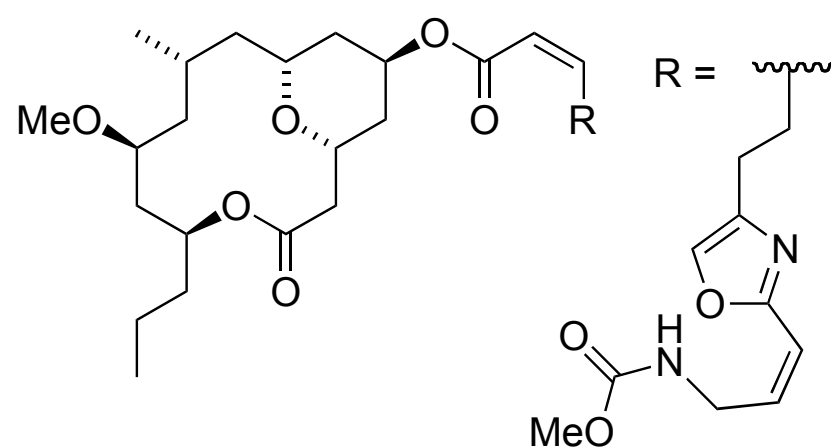
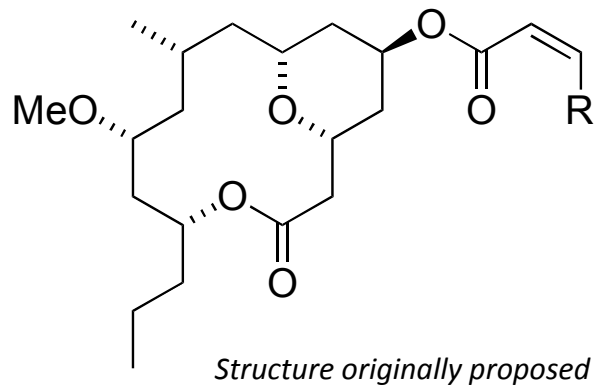
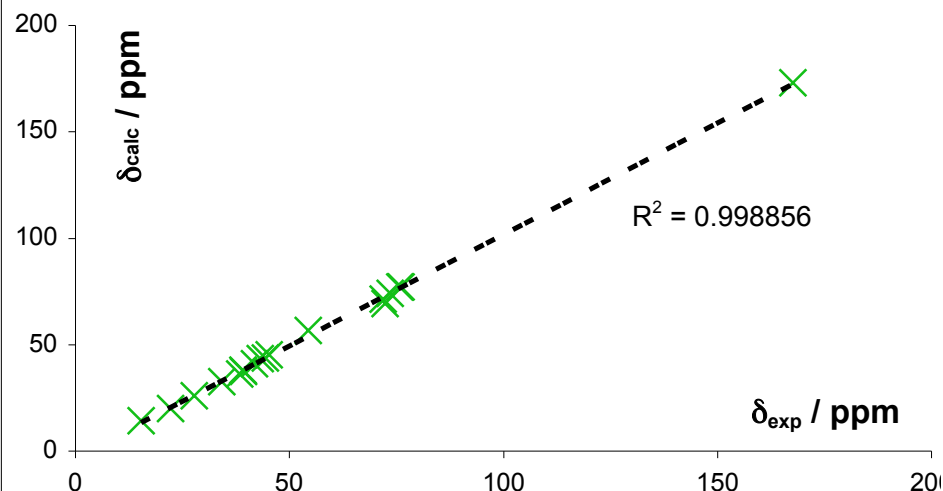


Simulating spectroscopic properties: *Neopeltolide*

Calculated vs Experimental shifts: Carbon data

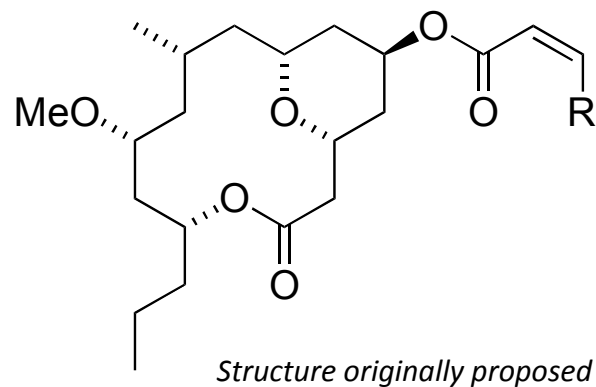
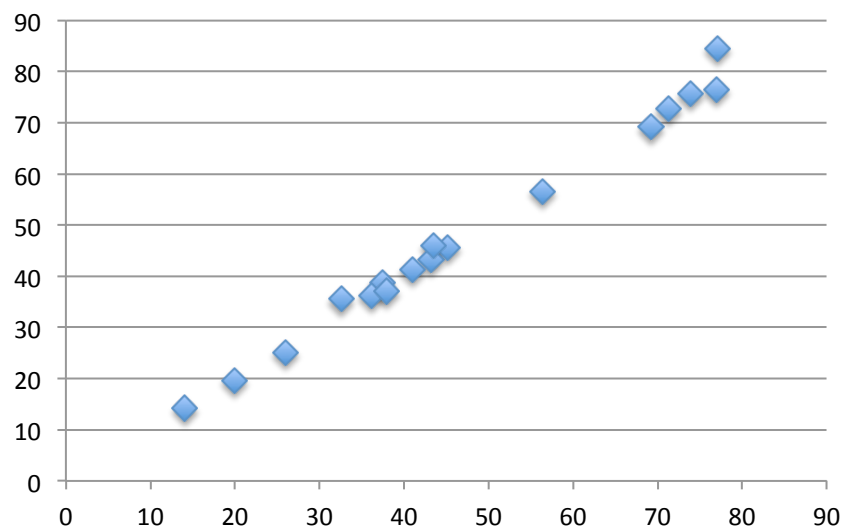


Calculated vs Experimental shifts: Carbon data

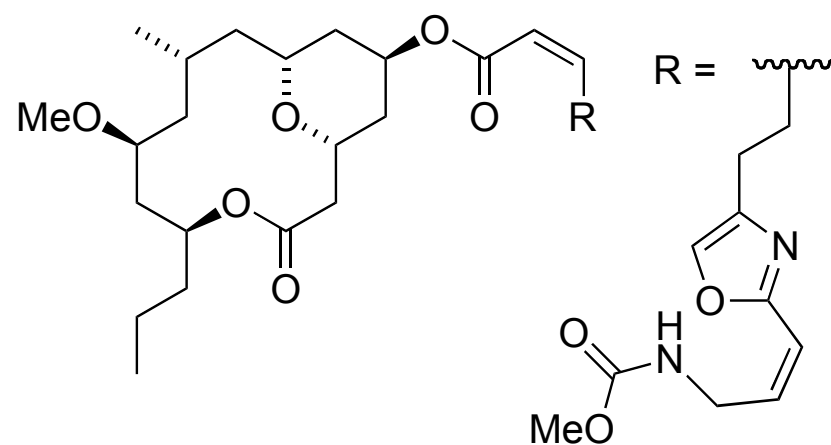
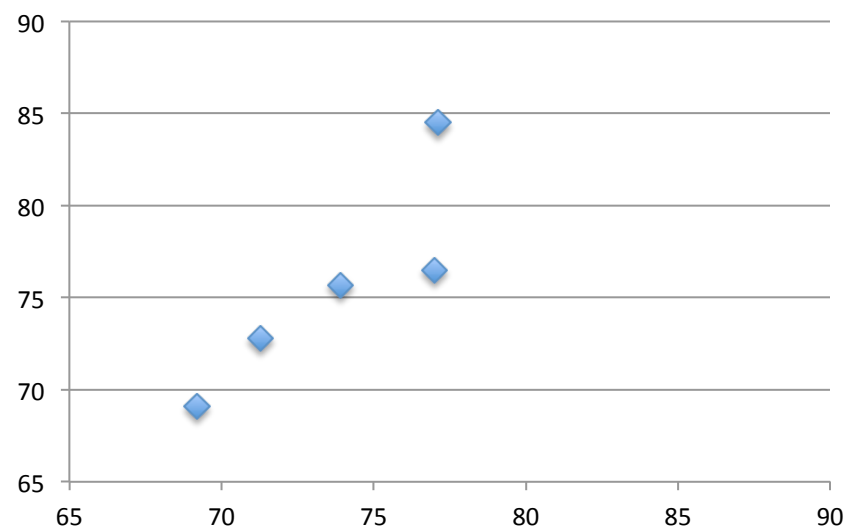


Simulating spectroscopic properties: *Neopeltolide*

$$R^2 = 0.99$$

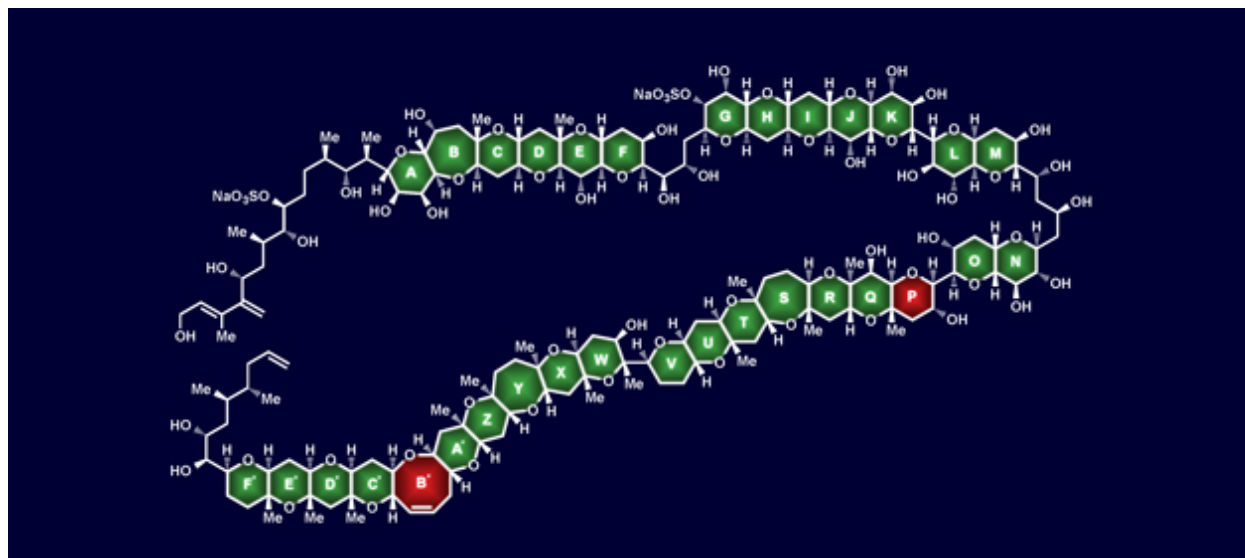


$$R^2 = 0.76$$



Chemistry's toughest total synthesis challenge put on hold by lack of funds

15 January 2015 **Katrina Kramer**

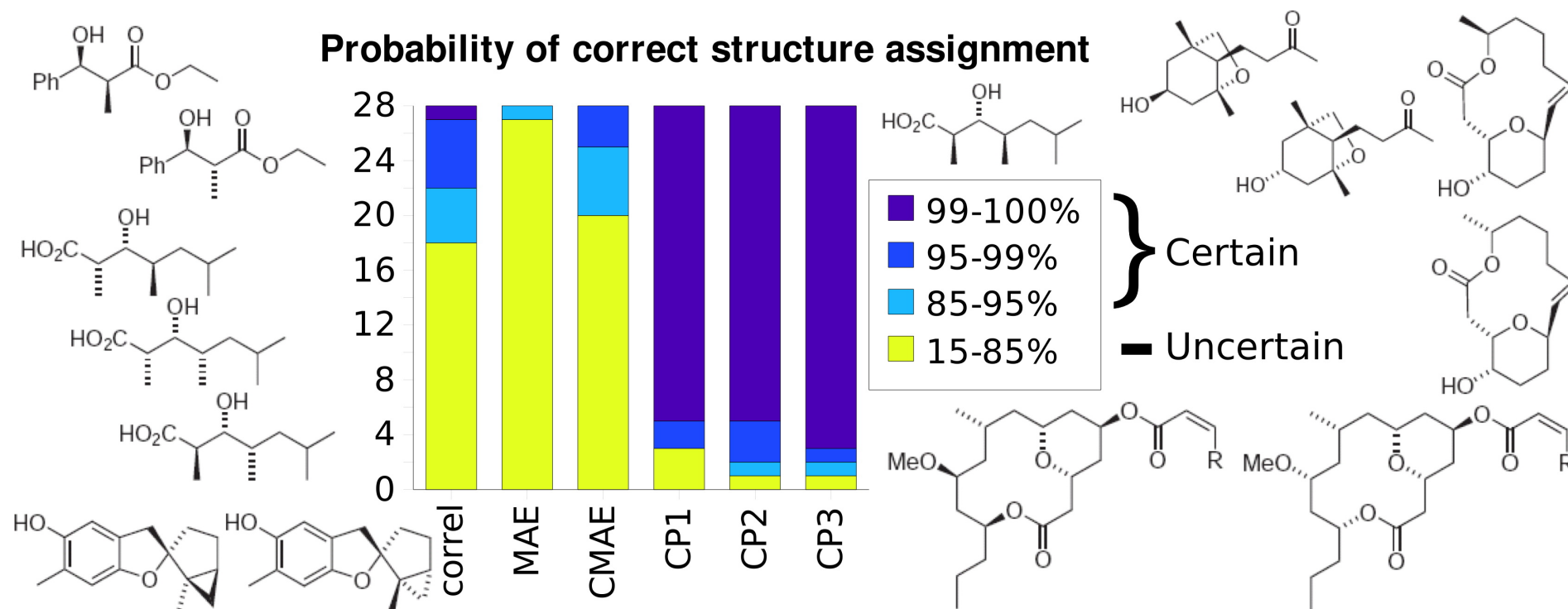


Synthesising maitotoxin is one of the hardest chemistry challenges out there © ACS

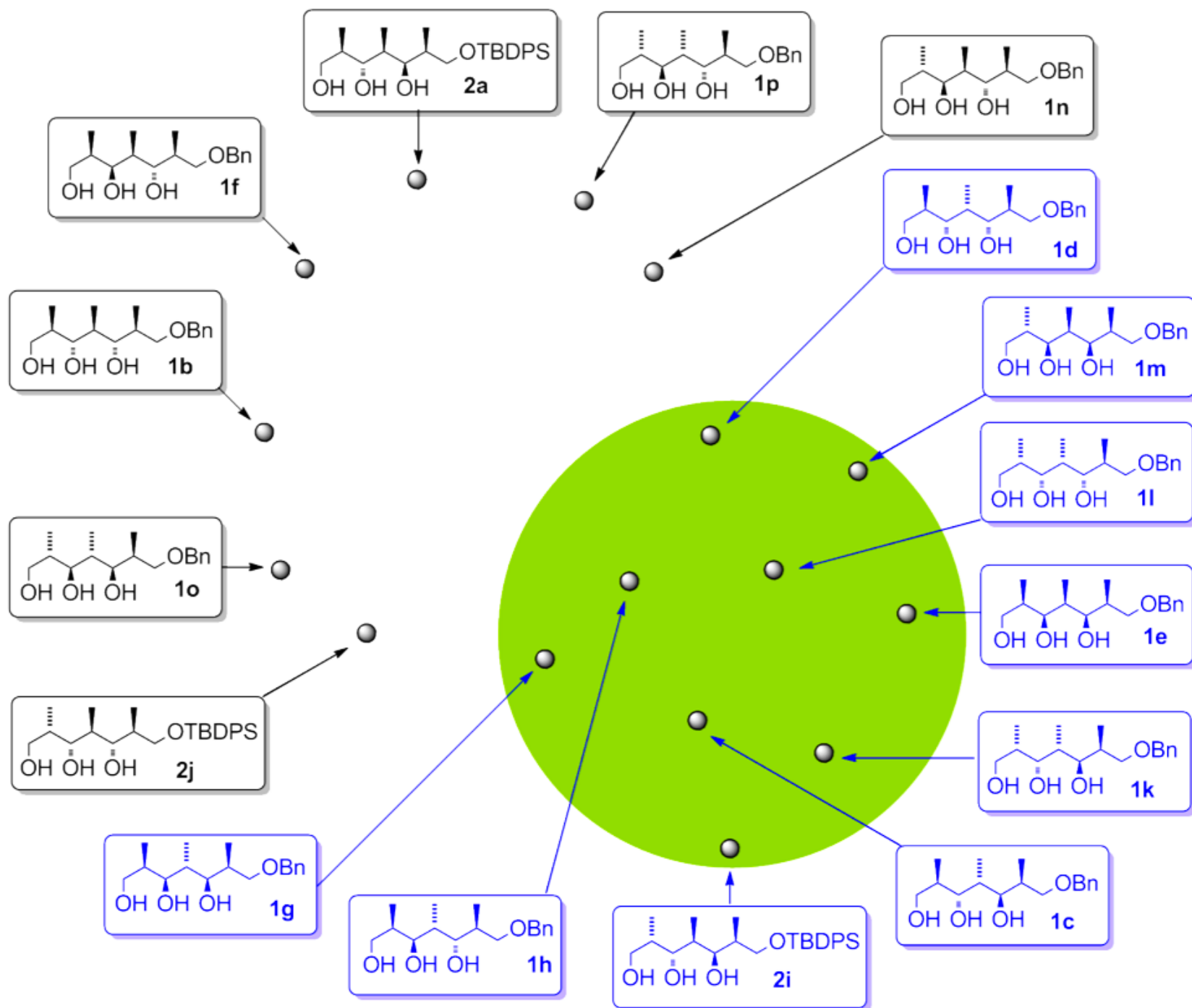
How many chemists does it take to synthesise a molecule? The answer is 20, at least when it comes to **maitotoxin**, quite possibly the toughest total synthesis challenge around. With 32 rings and 98 stereocentres, maitotoxin is the largest and most complex natural product that is neither a protein nor a polysaccharide, consisting mostly of fused cyclic ethers. Now, after eight years of research, **KC Nicolaou** and his group from Rice University, Texas, US, have almost completed its total synthesis. But the completion of possibly the greatest chemical challenge out there now faces a funding crisis that has halted the synthesis just as the finishing line is in sight.

Maitotoxin's physiological effects have been known for decades. It can cause ciguatera, a common form of seafood poisoning that can result from eating Pacific Ocean coral reef fish. Scientists isolated the compound from the gut of the striated surgeonfish – *maito* in Tahitian, hence the molecule's name – but later found that it is not the fish producing the neurotoxin but the plankton species *Gambierdiscus toxicus*, that surgeonfish feed on. However, maitotoxin's chemical structure remained elusive until, in 1993, Japanese researchers

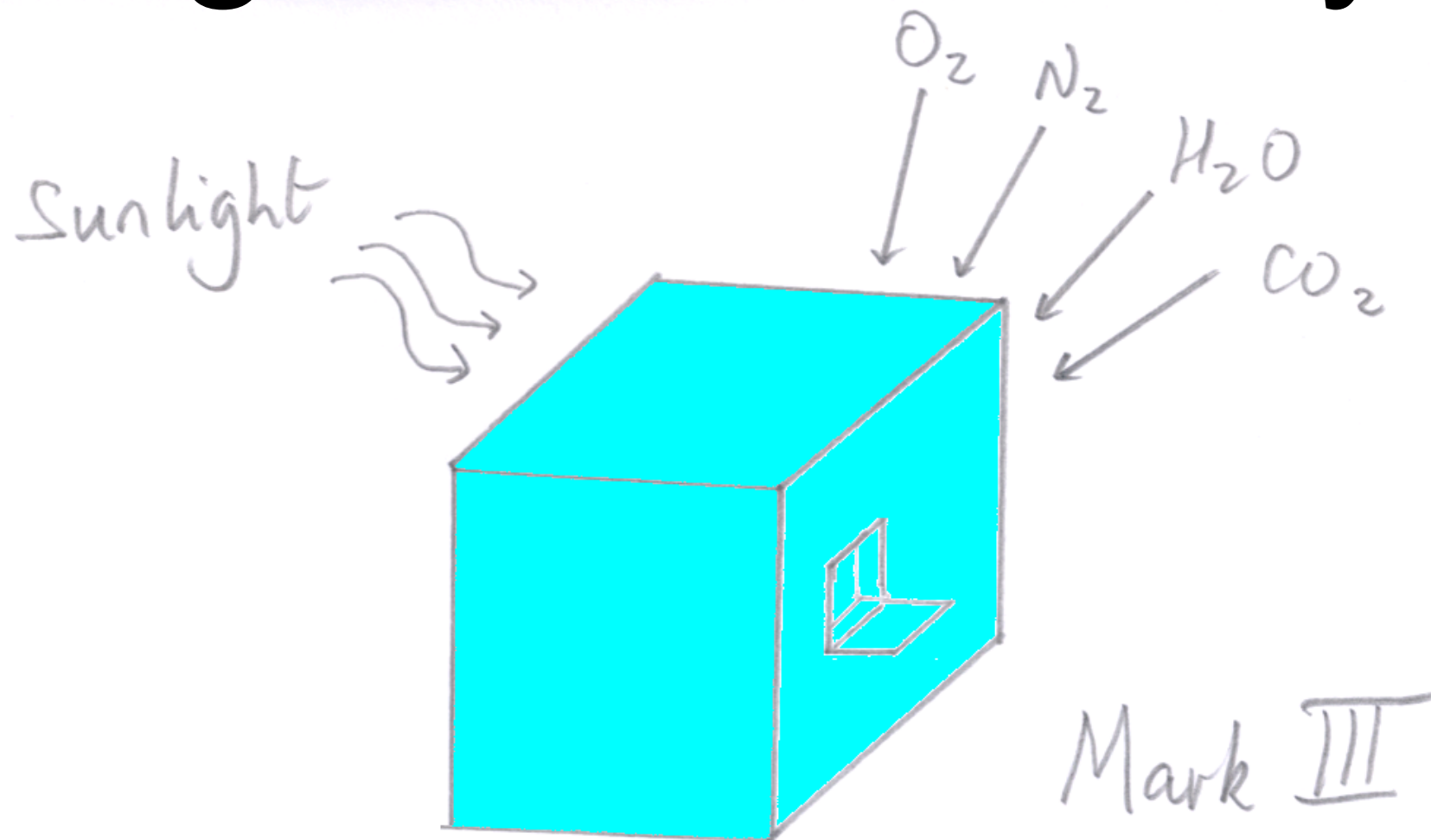
Simulating spectroscopic properties



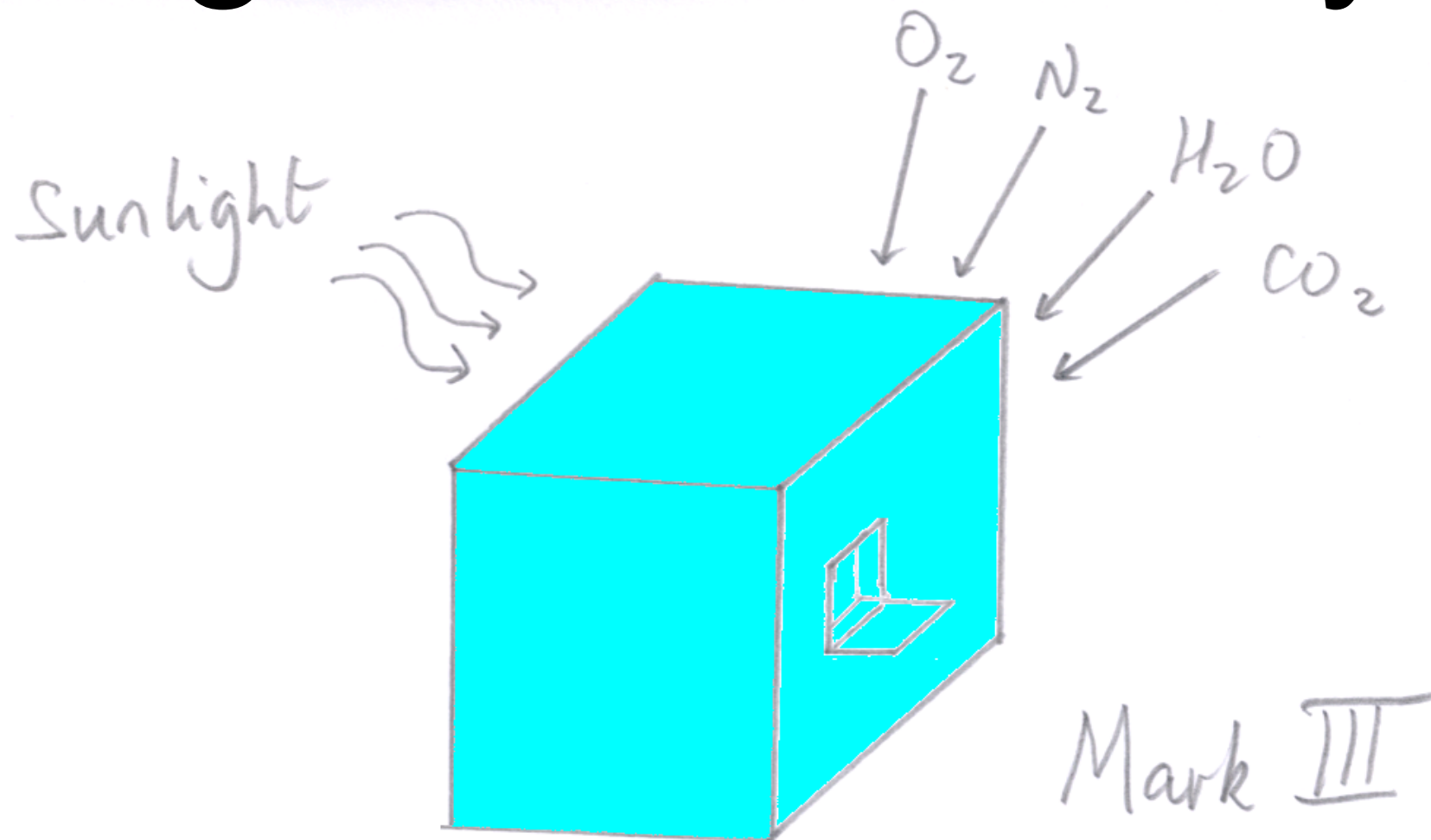
Probabilities based on a collection of calculated and experimental NMR data

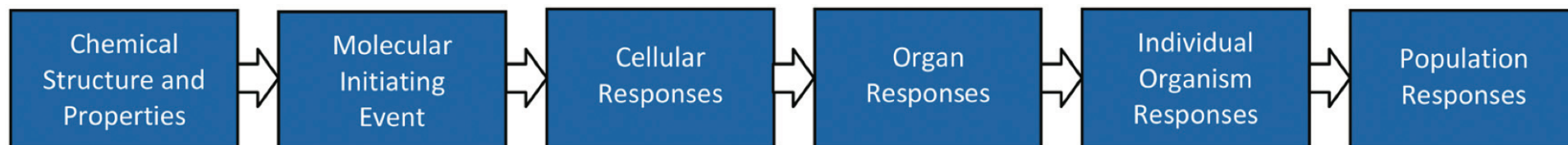
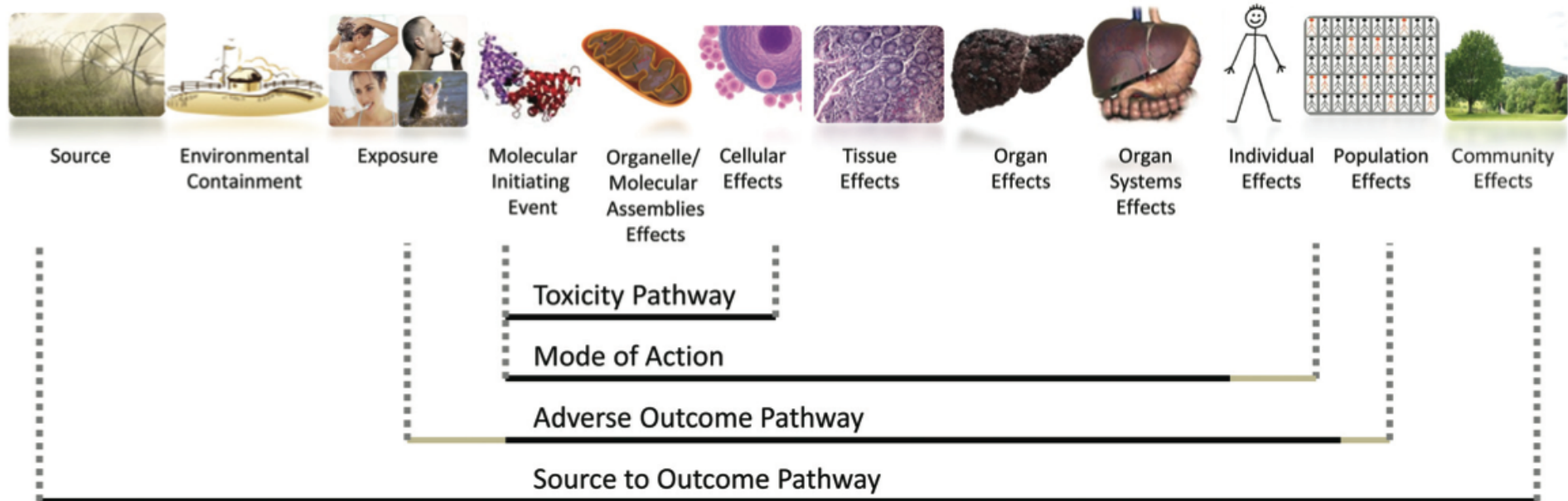


Big data chemistry



Big data chemistry





The role of chemistry in developing understanding of adverse outcome pathways and their application in risk assessment

Steve Gutsell and Paul Russell

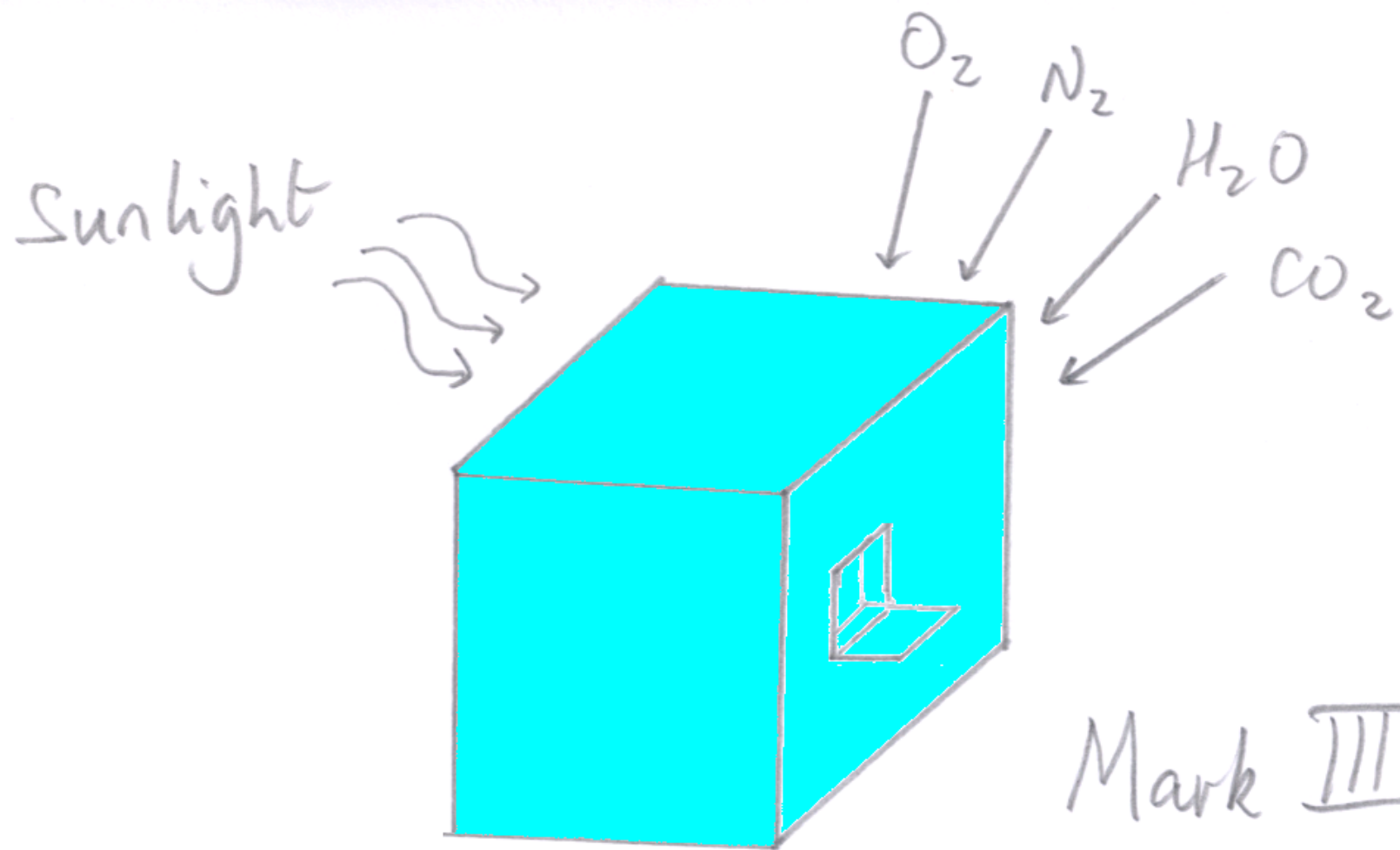
Toxicol. Res., 2013, **2**, 299

G. T. Ankley, *et al*,

Adverse outcome pathways: a conceptual framework to support ecotoxicology research and risk assessment

Environ. Toxicol. Chem., 2010, **29**, 730–741.

Compound	Acetaminophen	Amiodarone	Chlorpromazine	Kojic acid	Methotrexate
No. of MIEs	10	11	6	8	12
No. of AOs	22	47	34	26	38

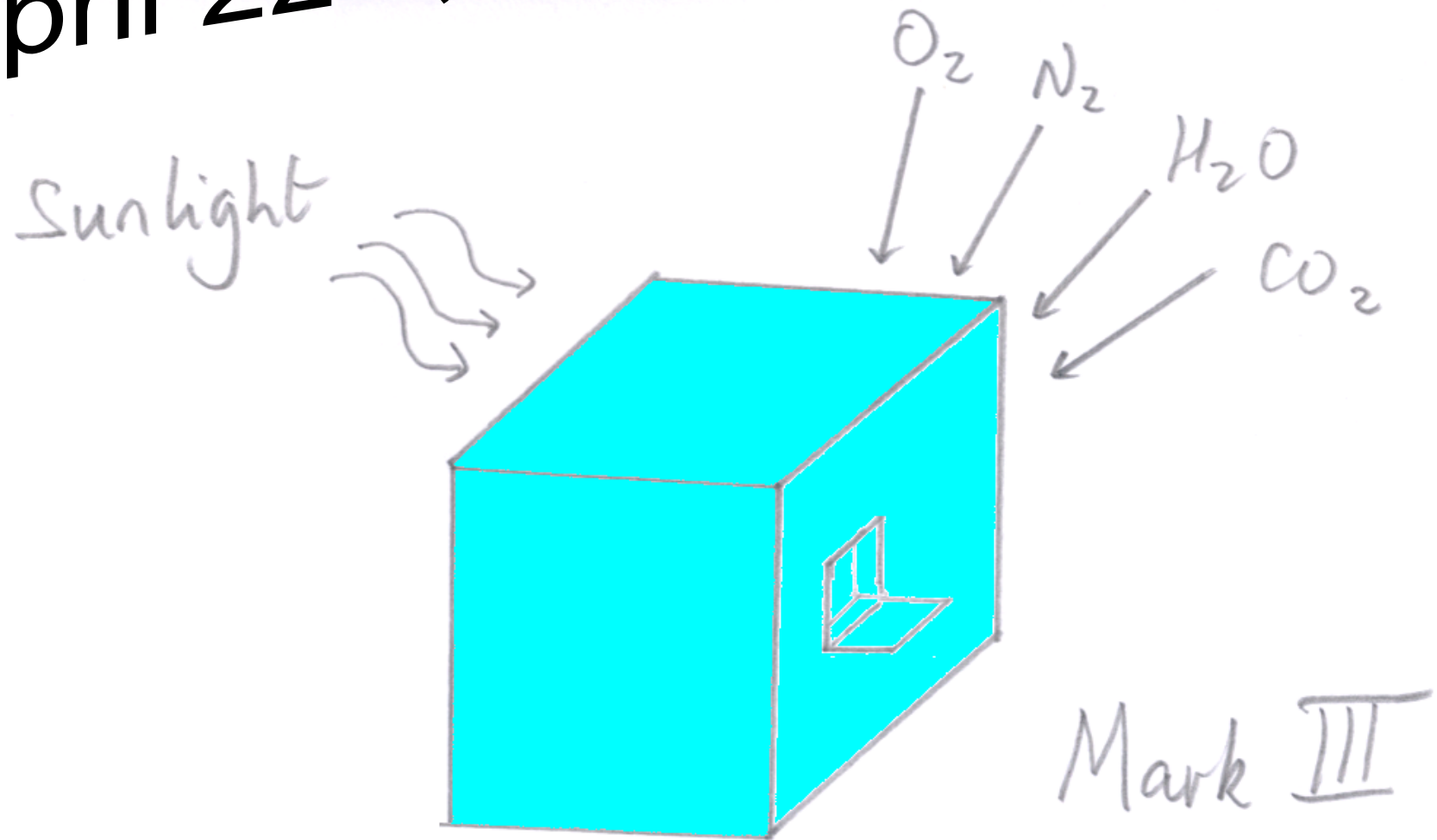


Bill Gates:

*We always
overestimate
the change that will occur
in the next two years and
underestimate
the change that will occur
in the next ten.*

*Don't let yourself be
lulled into inaction.*

April 22nd, 2025



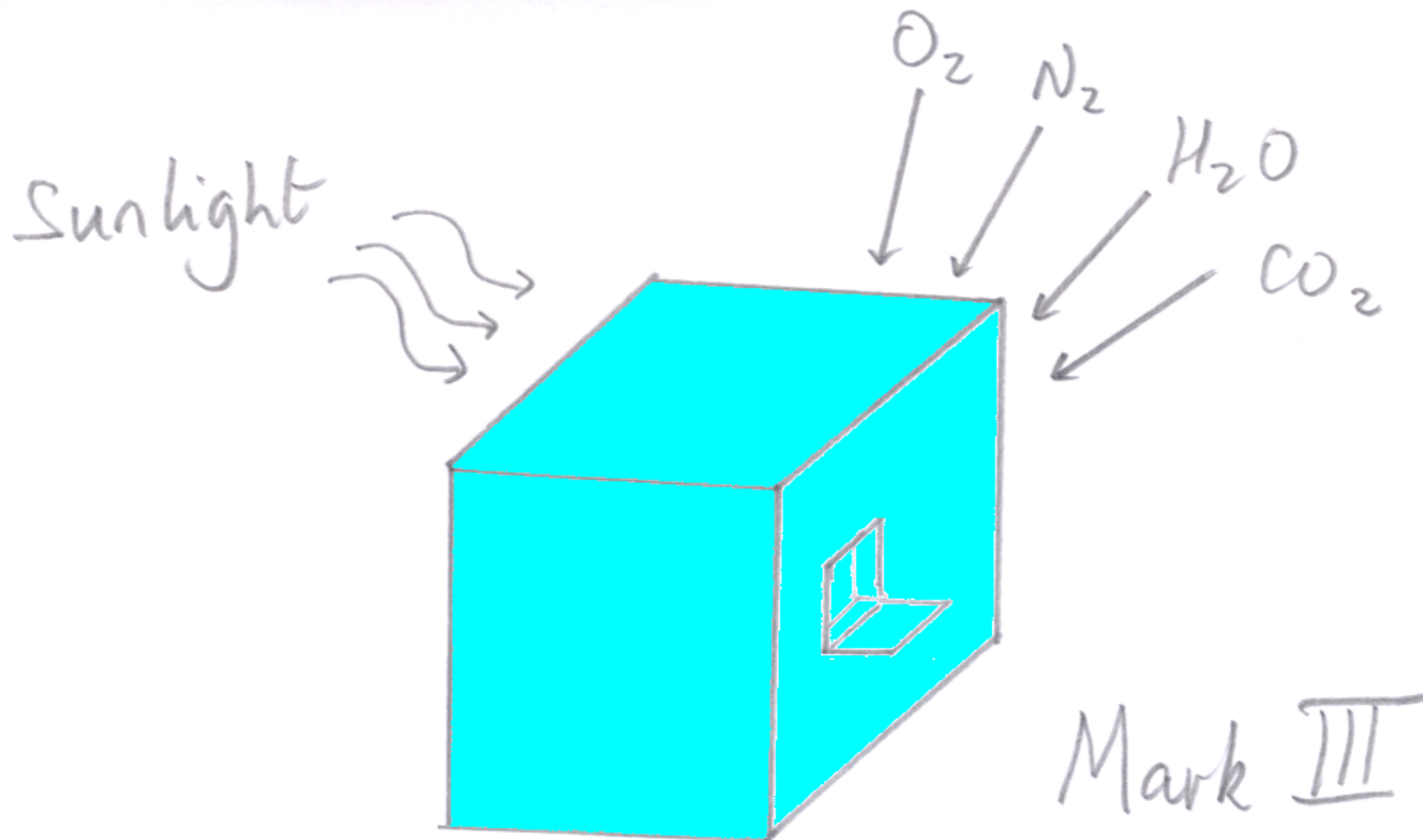
[illegible]

Invention	First made	Tesco
Teflon	1940	1960
Electronic Computers	1940	1980
Lasers	1960	1990
Light Emitting Polymers	1990	2000

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Molecule-Making Machines	2025	???

Invention	First made	Tesco
Teflon	1940	1960
Electronic Computers	1940	1980
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Light Emitting Polymers	1990	2000
Molecule-Making Machines	2025	???
Nuclear Fusion	1950	???

Ten Years of Big Data Chemistry



Jonathan M Goodman
Department of Chemistry
University of Cambridge