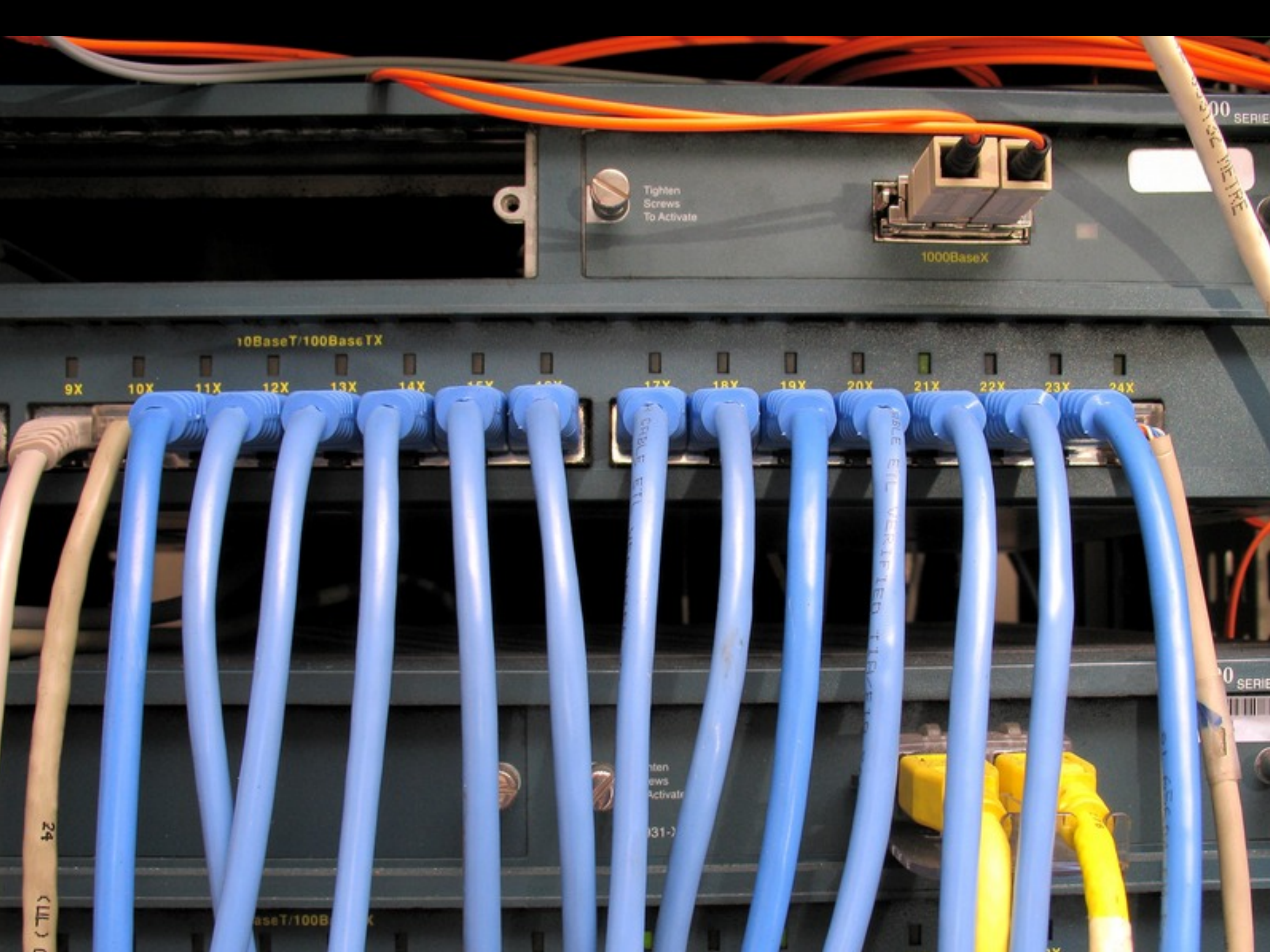


rethinking digital research

kaitlin thaney
@kaythaney ; @digitalsci
wolfram data summit



00 SERIES

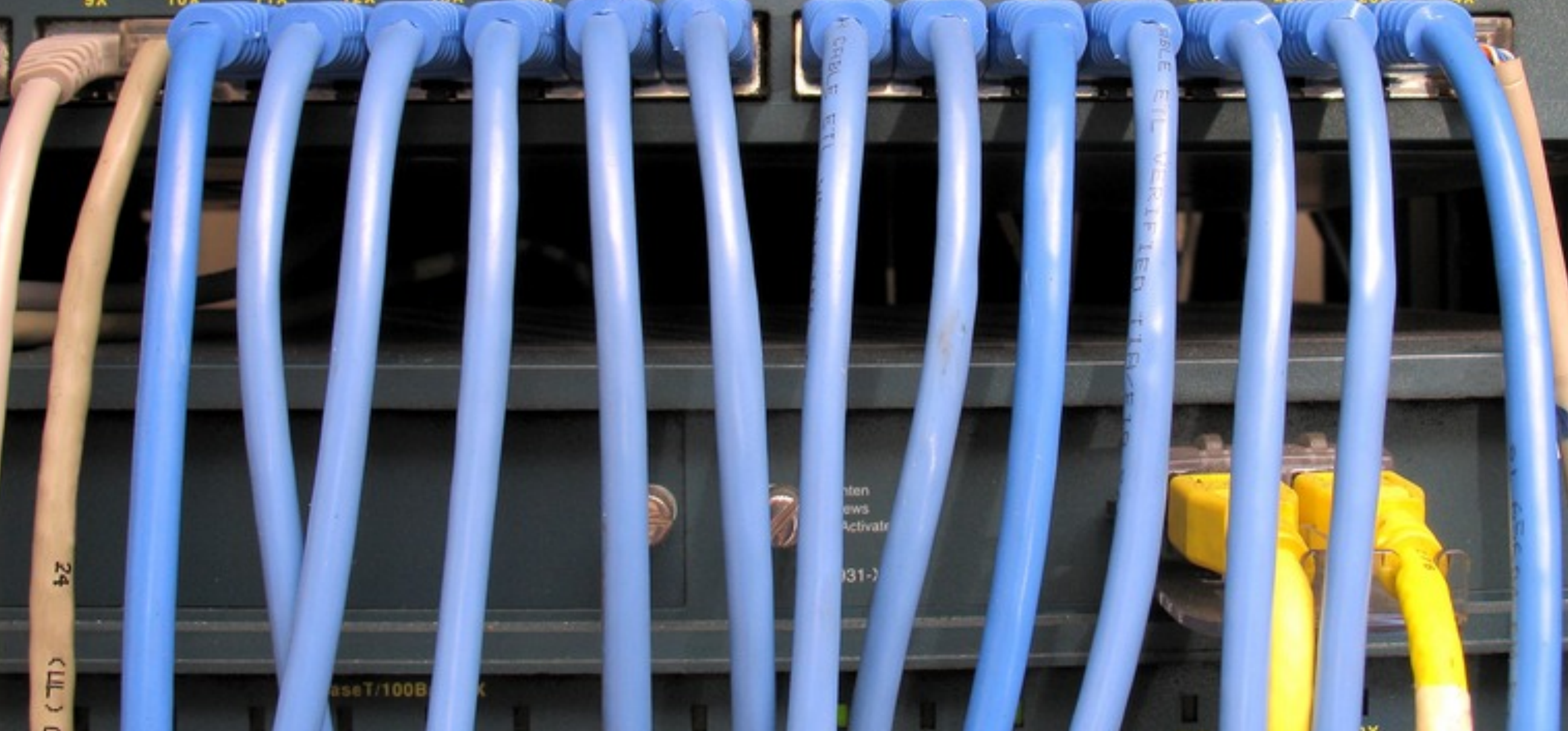
Tighten
Screws
To Activate



1000BaseX

10BaseT/100BaseTX

9X 10X 11X 12X 13X 14X 15X 16X 17X 18X 19X 20X 21X 22X 23X 24X



00 SERIES

Tighten
Screws
To Activate

31-3

10BaseT/100BaseTX

discovery



management

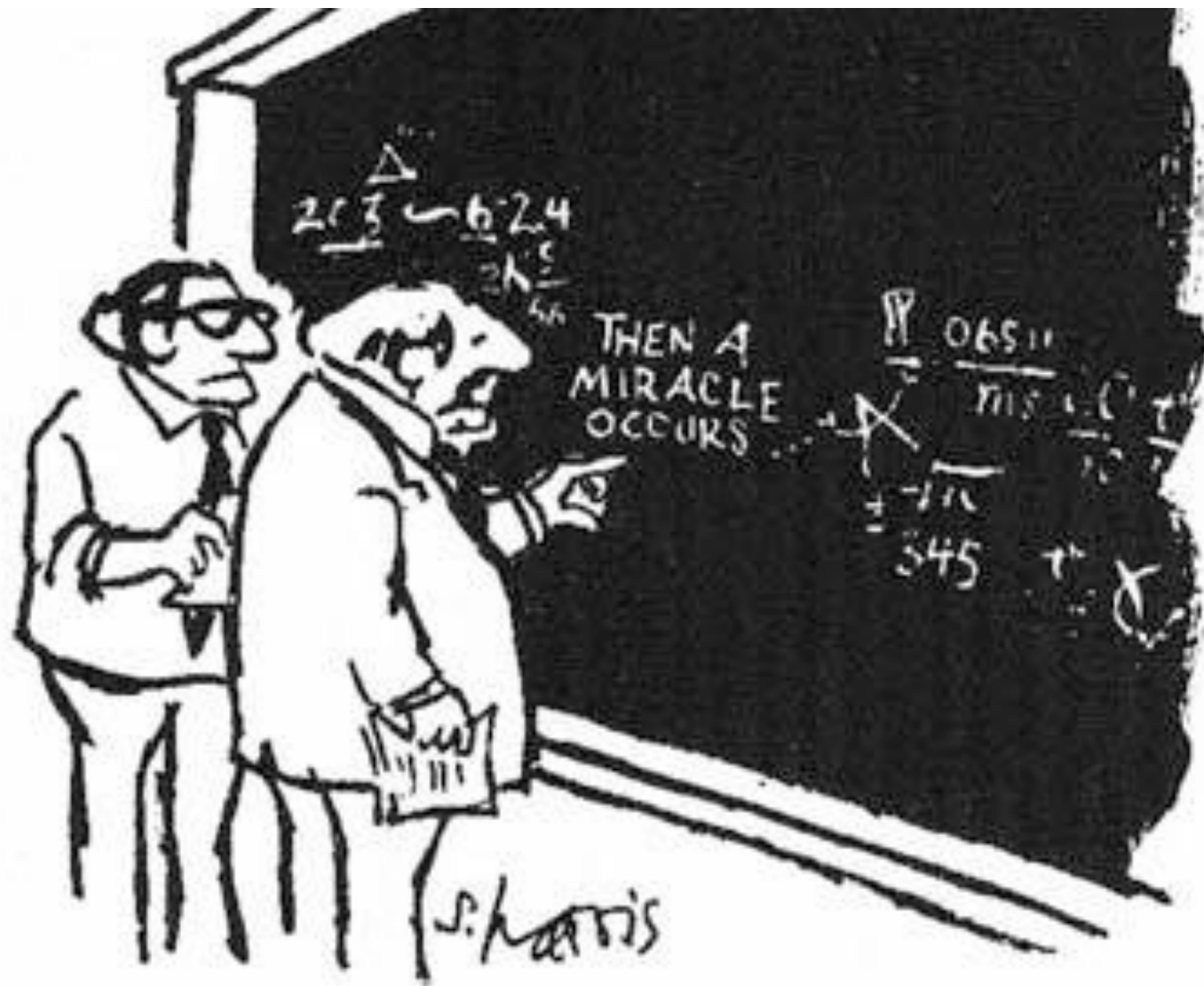
the “social”

discovery &
delivery

changes at the
workbench

annotation &
curation

social &
administrative



"I think you should be more explicit here in step two."

significant
(and somewhat silly)
gaps still exist



DIGITAL
science

what we know, is
research.

research is changing

↪ (as is the research workflow)



discovery is still
sub-optimal.

still the starting point

+Kaitlin Web Images Videos Maps News Gmail more ▾



10,11-dihydro-5-methyl-5H-dibenzo[b,e][1,4]diazepin-11-one



About 1,530,000 results (0.29 seconds)

[Go to Google.com](#) [Advanced search](#)

Everything

Images

Videos

News

Shopping

More

Search near...

Enter location

Set

The web

Pages from the UK

More search tools

▶ [E111 - Renew Online | E111-NHS.org](#)

[www.e111-nhs.org](#)

The E111 has been replaced by the European Health Insurance Card.

Ad

[Dibenzepin | 4498-32-2](#)

[www.chemicalbook.com/ChemicalProductProperty_EN_CB211059...](#) - Cached

...)ethyl]-5,10-dihydro-5-methyl-11H-dibenzo[b,e][1,4]diazepin-11-one; 10 ... -11-one; 10,11-Dihydro-10-[2-(dimethylamino)ethyl]-5-methyl-5H-dibenzo[b,e][1 ...

[11H-Dibenzo\[b,e\]\[1,4\]diazepin-11-one, 5,10-dihydro-5-\[3 ...](#)

[www.guidechem.com/products/63915-70-8.html](#) - Cached

10-Methyl-10,11-dihydro-5H-dibenzo[b,e][1,4]diazepin-11-one. 10-[2-(Diethylamino)ethyl]-5,10-dihydro-11H-dibenzo[b,e][1,4]diazepin-11-one ...

[11H-Dibenzo\[b,e\]\[1,4\]diazepin-11-one, 5,10-dihydro- suppliers ...](#)

[www.guidechem.com/products/5814-41-5.html](#) - Cached

10-Methyl-10,11-dihydro-5H-dibenzo[b,e][1,4]diazepin-11-one. 10-[3 ...

[Show more results from guidechem.com](#)

[8-Chloro-5,10-dihydrodibenzo\[b,e\]\[1,4\]diazepin-11-one, 8-Chloro-5 ...](#)

[www.chemblink.com > Chemical Listing](#) - Cached

Synonyms, 8-Chloro-5,10-dihydro-11H-dibenzo[b,e][1,4]diazepin-11-one; 8-Chloro-11-oxo-10,11-dihydro-5H-dibenzo-1,4-diazepine ... 6-Chloro-N4-[3,5-difluoro-4-[(3-methyl-1H-pyrrolo[2,3-b]pyridin-4-yl)oxy]phenyl]-2,4-pyrimidinediamine ...

[5H-Dibenzo\(b,e\)\(1,4\)diazepin-11\(10H\)-one, 10-\(2-\(dimethylamino ...](#)

[www.chemindustry.com/chemicals/0287900.html](#) - Cached

5H-Dibenzo(b,e)(1,4)diazepin-11(10H)-one, ... 10-[2-(Dimethylamino)ethyl]-5-methyl-5,10-dihydro-11H-dibenzo[b,e][1,4]diazepin-11-one, ...

USPTO PATENT FULL-TEXT AND IMAGE DATABASE

[Home](#)[Quick](#)[Advanced](#)[Pat Num](#)[Help](#)[Next List](#)[Bottom](#)[View Cart](#)

Searching US Patent Collection...

Results of Search in US Patent Collection db for:











diazepin: 1102 patents.

Hits 1 through 50 out of 1102

[Next 50 Hits](#)[Jump To](#) [Refine Search](#)

specific DBs no better
(in this case, likely worse)

PAT. NO.	Title
----------	-------

- | | |
|----|--|
| 1 | 7,973,119  Adhesive systems using imines and salts thereof and precursors to electron deficient olefins |
| 2 | 7,968,566  Pyrrolo(2,3-b) pyridine derivatives, the preparation and the pharmaceutical use thereof in the form of kinase inhibitors |
| 3 | 7,964,618  Chemical compounds |
| 4 | 7,960,556  Thiadiazole derivatives for the treatment of neuro-degenerative diseases |
| 5 | 7,960,428  Enantiomerically pure phosphoindoles as HIV inhibitors |
| 6 | 7,955,852  Expansion of renewable stem cell populations |
| 7 | 7,951,816  Compound containing basic group and use thereof |
| 8 | 7,947,718  Isoxazole compounds as histamine H.sub.3 modulators |
| 9 | 7,939,533  Dual NK1/NK3 receptor antagonists |
| 10 | 7,935,815  Imidazolyl pyridine compounds and salts thereof |

11 7,935,800  [Dual NK1/NK3 receptor antagonists](#)

name disambiguation

103-90-2

254-465-1

4-(Acetylamino)phenol

4-13-00-01091 (Beilstein Handbook Reference)

4-Acetaminophenol

4'-Hydroxyacetanilide

4-Hydroxyanilid kyseliny octove

Acetamide, N-(4-hydroxyphenyl)-

Acetamide, N-(p-hydroxyphenyl)-

Acetanilide, 4'-hydroxy-

APAP

N-(4-Hydroxyphenyl)acetamid

N-(4-Hydroxyphenyl)acetamide

N-(4-Hydroxy-phenyl)-acetamide

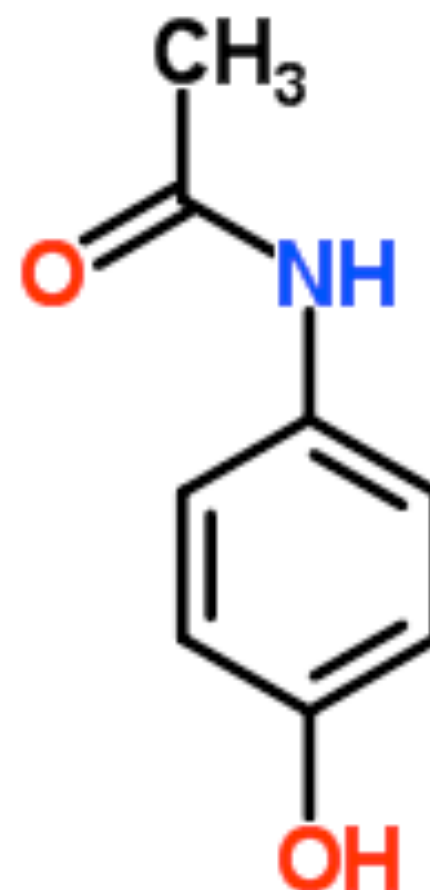
N-(4-Hydroxyphényl)acétamide

N-(4-Hydroxyphenyl)acetanilide

N-(p-hydroxyphenyl)acetamide

N-Acetyl-4-aminophenol

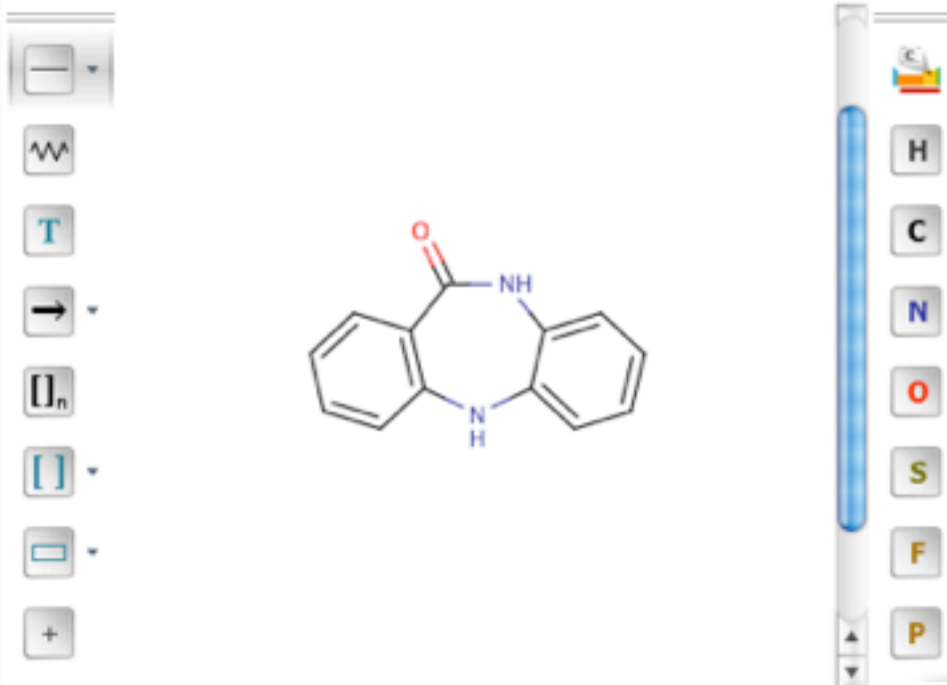
N-Acetyl-p-aminophenol ...



and the list goes on ...

STRUCTURE SEARCH

File Edit View Insert Atom Bond Structure Tools Help



Search using:

Substructure

Limit search to:

All fields

Display:

Structures

SEARCH

H

C

N

O

S

F

P



Structure search and drawing powered by ChemAxon

streamline search

EXAMPLE 21

[3-\(4-hydroxy-3-methoxyphenyl\)-8-\[\(3-hydroxy-1-pyrrolidinyl\)carbonyl\]-5,10-dihydro-11H-dibenzo\[b,e\]\[1,4\]diazepin-11-one](#)

The

DM

J=8

EXA

[3-\(4](#)

The

NM

3H),

7.01

6.87

3.34-3.44

3.86

1.84-1.92

(m, 4H).

EXAMPLE 23

[3-\(4-hydroxy-3-methoxyphenyl\)-8-\[\(2-\(hydroxymethyl\)-1-piperidinyl\)carbonyl\]-5,10-dihydro-11H-dibenzo\[b,e\]\[1,4\]diazepin-11-one](#)

The

desired

product

was

prepared

by

substituting

[2-piperidinylmethanol](#)

for

[3-pyrrolidin-1-ylpropylamine](#)

in

Example

14.

MS

(DCI)

m/e

474

(M+H)⁺; ¹H

NMR

(500

MHz,

DMSO-*d*₆)

δ

9.84

(s,

1H),

9.29

(br

s,

1H),

8.08

(s,

1H),

7.72

(d,

J=8.3

Hz,

1H),

7.25

(d,

J=1.5

Hz,

1H),

7.16-7.21

(m,

2H),

7.09

(m,

1H),

6.98-7.03

(m,

2H),

6.88

(d,

J=8.0

Hz,

1H),

4.35

(m,

1H),

3.86

(s,

3H),

3.28-3.34

(m,

4H),

1.48-1.80

(m,

6H).

EXAMPLE 24

[ethyl 1-\[\(3-\(4-hydroxy-3-methoxyphenyl\)-11-oxo-10,11-dihydro-5H-dibenzo\[b,e\]\[1,4\]diazepin-8-yl\)carbonyl\]-2-piperidinecarboxylate](#)

The

desired

product

was

prepared

by

substituting

[ethyl 2-piperidinecarboxylate](#)

for

[3-pyrrolidin-1-ylpropylamine](#)

in

Example

14.

MS

(DCI)

m/e

516

(M+H)⁺; ¹H

NMR

(500

MHz,

DMSO-*d*₆)

δ

9.89

(s,

1H),

9.28

(s,

1H),

8.14

(s,

1H),

7.73-7.74

(d,

J=8.2

Hz,

1H),

7.24

(d,

J=1.2

Hz,

1H),

7.17-7.19

(m,

2H),

7.07-7.09

(dd,

J=8.2,

2.1

Hz,

1H),

6.95-7.05

(m,

3H),

6.88

(d,

J=8.2

Hz,

1H),

4.16

(br

s,

2H),

3.86

(s,

3H),

3.61

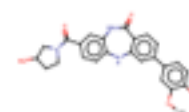
(m,

1H),

1.29-1.79

(m,

11H).



m/e 446 (M+H)⁺; ¹H NMR (500 MHz, DMSO-*d*₆) δ 9.84 (s, 1H), 9.29 (br s, 1H), 8.08 (s, 1H), 7.72 (d, J=8.3 Hz, 1H), 7.25 (d, J=1.5 Hz, 1H), 7.16-7.21 (m, 2H), 7.09 (m, 1H), 6.98-7.03 (m, 2H), 6.88 (d, J=8.0 Hz, 1H), 4.35 (m, 1H), 3.86 (s, 3H), 3.28-3.34 (m, 4H), 1.48-1.80 (m, 6H).

4. MS (DCI) m/e 460 (M+H)⁺; ¹H NMR (500 MHz, DMSO-*d*₆) δ 9.89 (s, 1H), 9.28 (s, 1H), 8.14 (s, 1H), 7.73-7.74 (d, J=8.2 Hz, 1H), 7.24 (d, J=1.2 Hz, 1H), 7.17-7.19 (m, 2H), 7.07-7.09 (dd, J=8.2, 2.1 Hz, 1H), 6.95-7.05 (m, 3H), 6.88 (d, J=8.2 Hz, 1H), 4.16 (br s, 2H), 3.86 (s, 3H), 3.61 (m, 1H), 1.29-1.79 (m, 11H).

our definition of
“data” is changing.

(or, at least, is long overdue to.)


The background image is a collage of various analog and digital media. It includes a sketch of a human figure in red ink, a green notebook, a spiral-bound notebook with a drawing of a box and handwritten notes, a book titled 'Empire Science', and a page with a grid and handwritten notes. The text 'mix of digital and analog mediums' is overlaid on the collage.

***mix of digital and
analog mediums***

CC-BY-2.0 - Plaxco Lab - <http://www.flickr.com/photos/34857812@N04/>

the non-digital





the non-digital

A photograph of a warehouse interior. In the foreground, a large, plain brown cardboard box sits on a metal conveyor belt. The belt extends into the background, where other boxes and industrial equipment are visible but out of focus. The lighting is bright and even. A semi-transparent yellow rectangular box is overlaid on the upper right portion of the image, containing the text 'ordering + processing' in a bold, black, italicized serif font.

ordering + processing

JELLYFISH IN ARMOUR



HOW MILK CONTAINERS SHOULD BE

tracking
expiration
calibration

wasted ...

\$\$\$

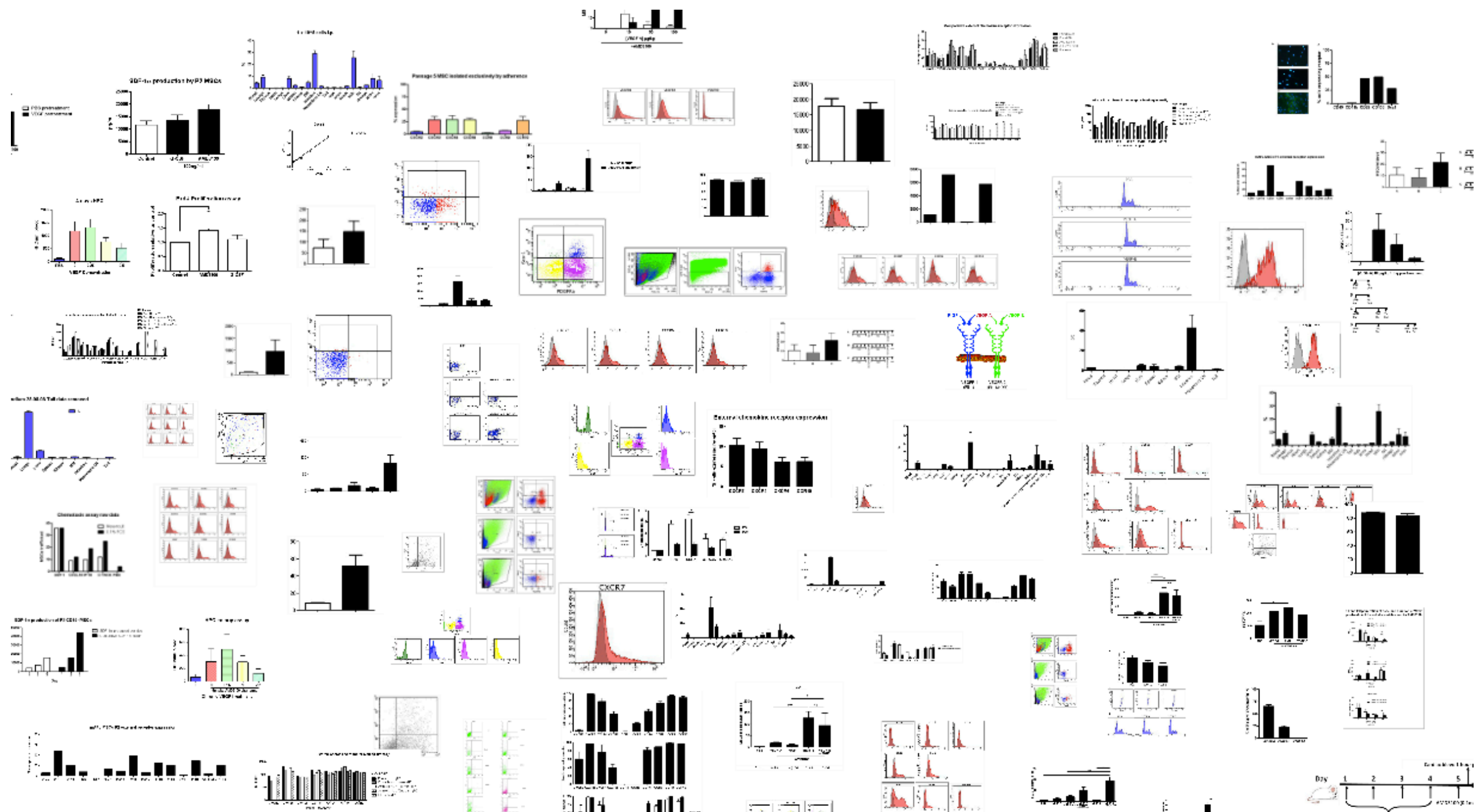
time

resource



our practices are
limiting us.

(and in some cases, harming.)



3 Gb/year

9 Gb / PhD

3 Gb / year

30,000,000 Gb / all*

9 Gb / PhD

3 Gb / year

** roughly*

how much made available?

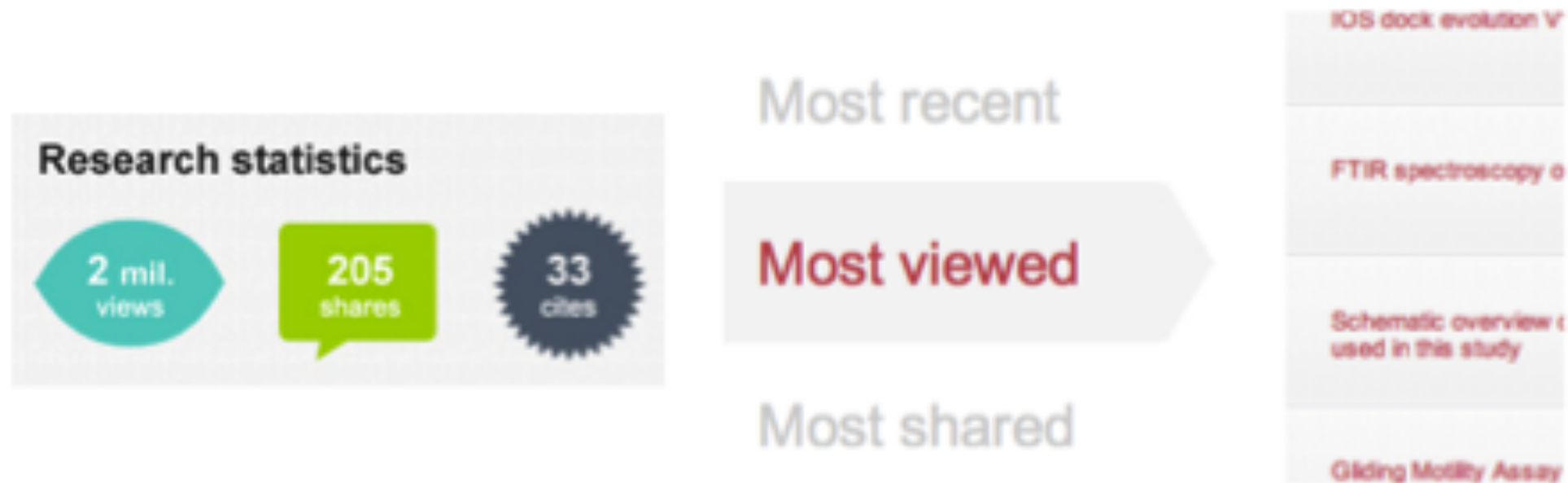
30,000,000 Gb/all*

9 Gb/PhD

3 Gb/year

** roughly*

make stupidly simple



... and part of the process.

“Non-reproducible single occurrences are of no significance to science.”

- Karl Popper



“That’s Dr. Arnold Moore. He’s conducting an experiment to test the theory that most great scientific discoveries were hit on by accident”

CRU Data Availability - Mozilla Firefox

File Edit View History Bookmarks Tools Help

http://74.125.95.13: Google ABP

Gmail ABH login Patterico Facebook NCT Blogs Log In AP Watch

Hot tim... Full text ... Patteric... CRU hac... CRU ... x

We are not in a position to supply data for a particular country not covered by the example agreements referred to earlier, as we have never had sufficient resources to keep track of the exact source of each individual monthly value. Since the 1980s, we have merged the data we have received into existing series or begun new ones, so it is impossible to say if all stations within a particular country or if all of an individual record should be freely available. Data storage availability in the 1980s meant that we were not able to keep the multiple sources for some sites, only the station series after adjustment for homogeneity issues. We, therefore, do not hold the original raw data but only the value-added (i.e. quality controlled and homogenized) data. The priorities we use when merging data from the same station from different sources are discussed in some of the literature cited below. Parts of series may have come from restricted sources, whilst the rest came from other sources. Furthermore, as stated in <http://www.cru.uea.ac.uk/cru/data/landstations/> we have never kept track of changes to country names as it is only the location and the station's

rethink the way we
rank researchers.

(the big, hairy “social” issue.)

“ What Des-Cartes did was a good step. You have added much several ways, & especially in taking ye colours of thin plates into philosophical consideration.

If I have seen further it is by standing on **ye shoulders of Giants.**”

- Isaac Newton, 1676



locked in old mechanisms.

WONKA'S
GOLDEN TICKET

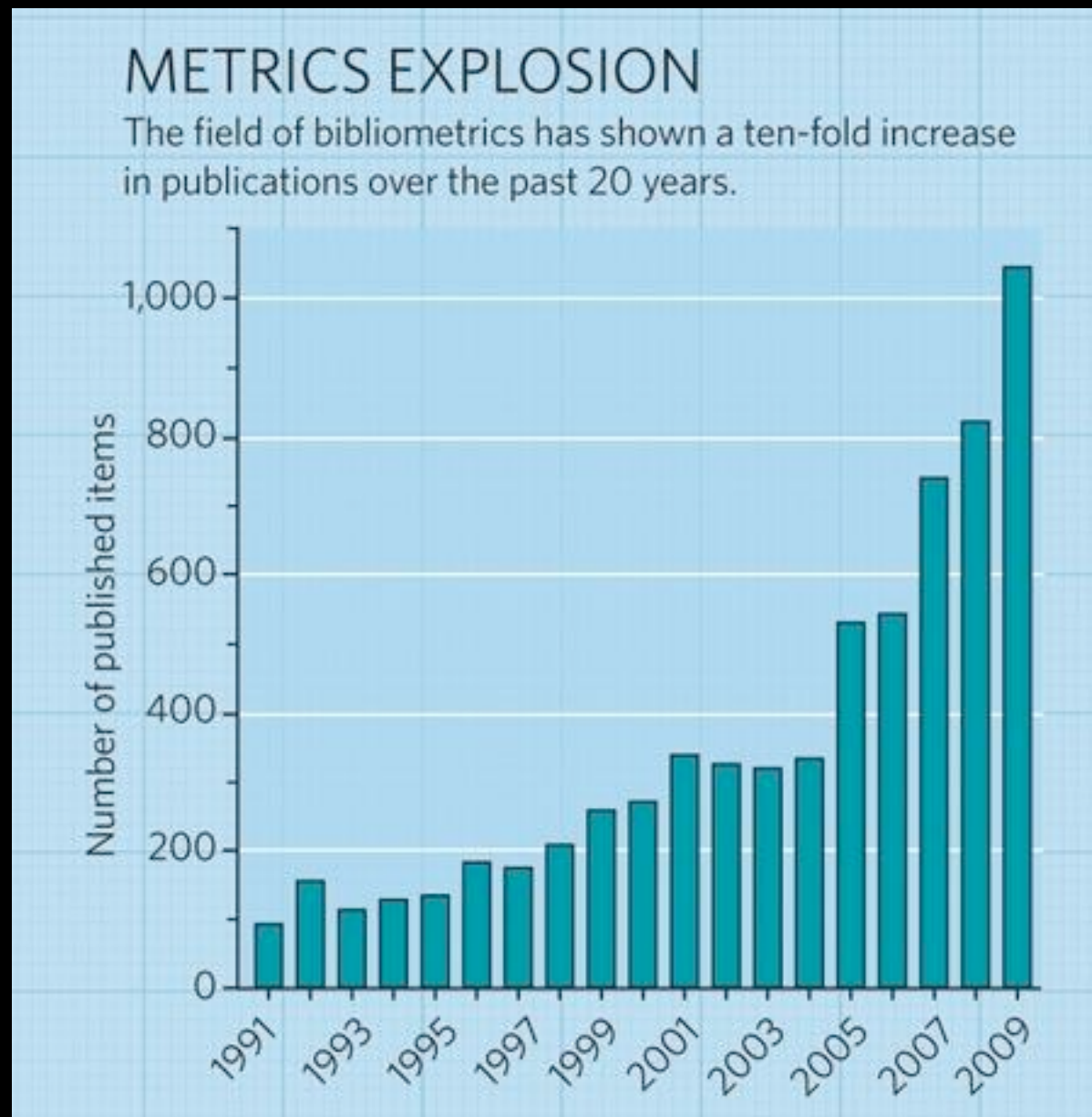
GREETINGS TO YOU, THE LUCKY FINDER OF THIS
GOLDEN TICKET FROM MR. WILLY WONKA.

PRESENT THIS TICKET AT THE FACTORY GATES AT TEN O'CLOCK
IN THE MORNING OF THE FIRST DAY OF OCTOBER AND DO NOT
BE LATE. YOU MAY BRING WITH YOU ONE MEMBER OF YOUR
OWN FAMILY... AND ONLY ONE... BUT NO ONE ELSE...

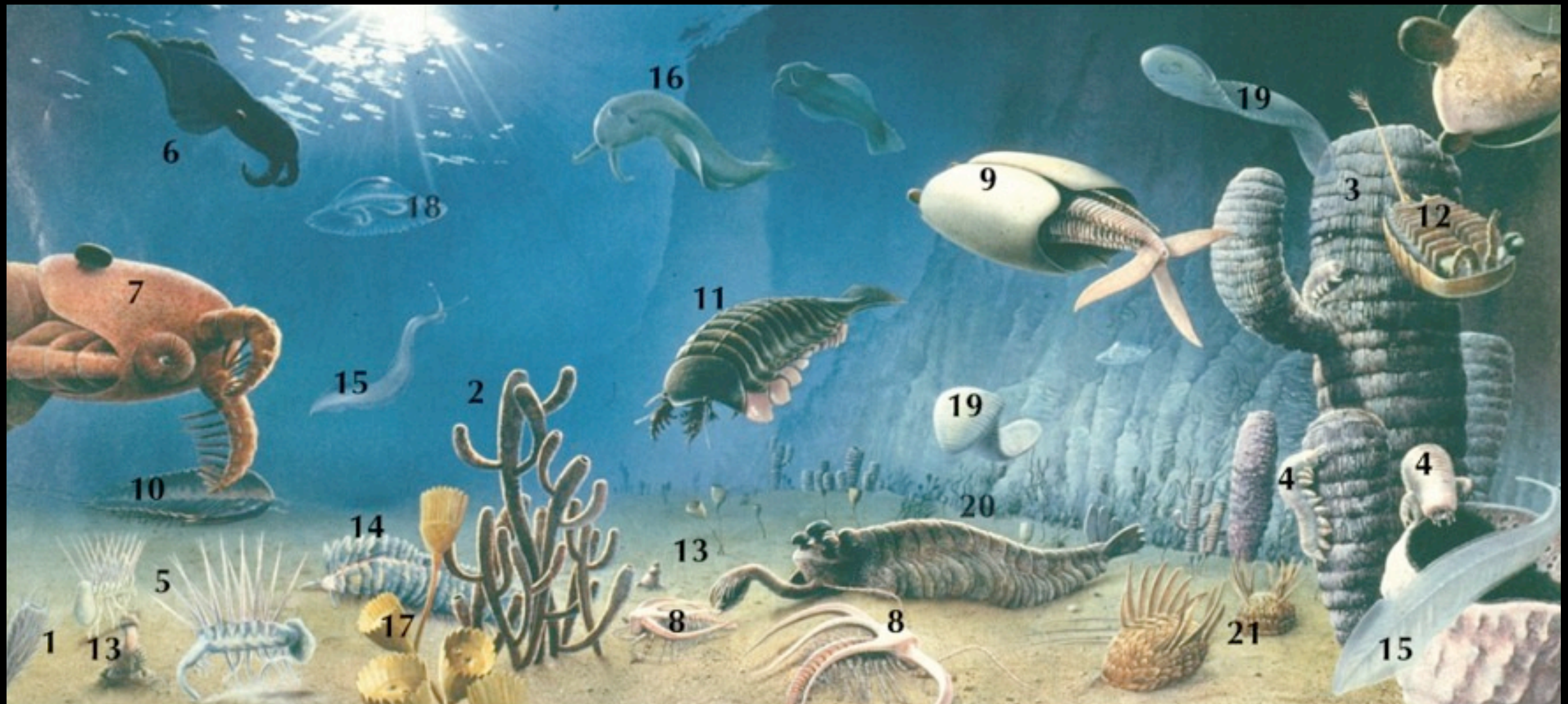
*In your wildest dreams you could not imagine the marvelous surprises
that await YOU.*

“Right now we're going through a Cambrian explosion of metrics.”

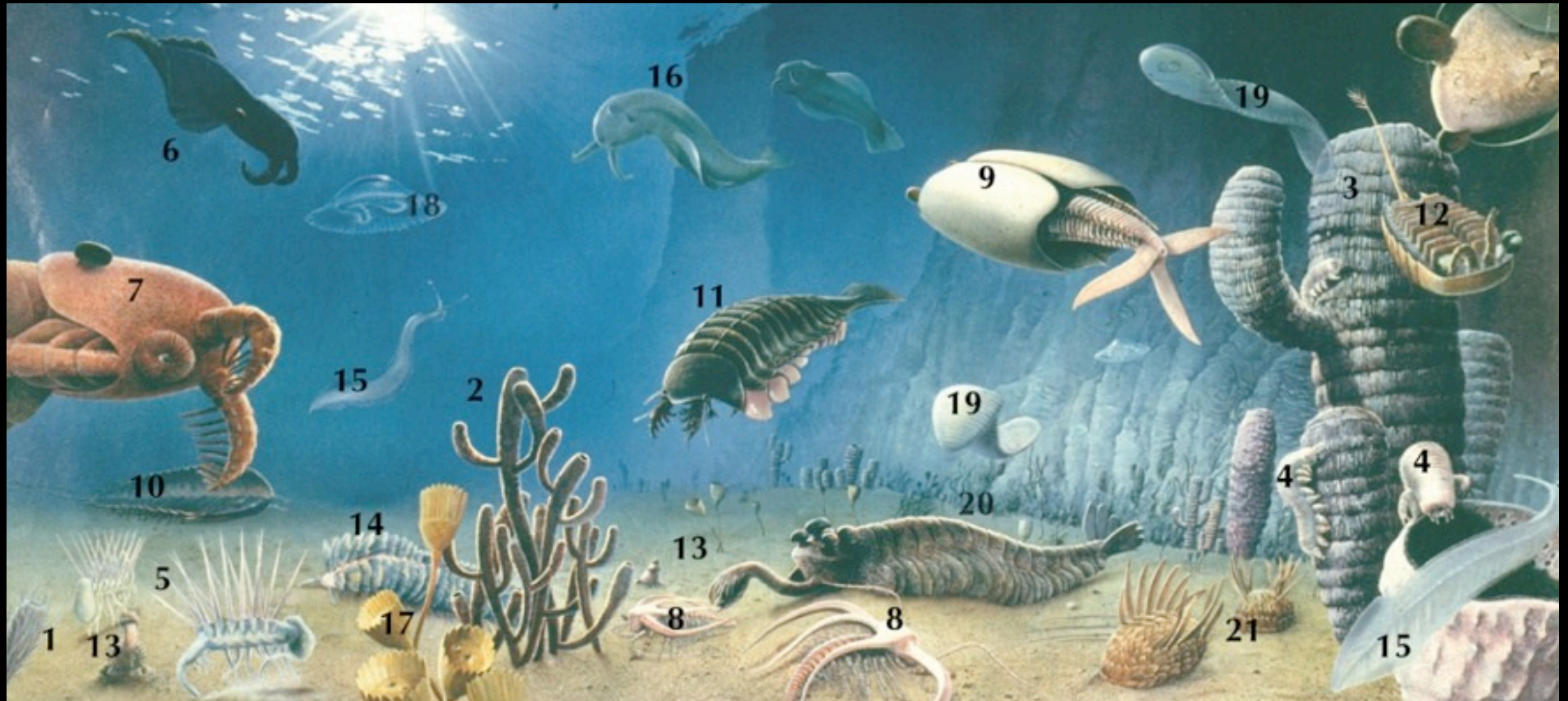
- *Johan Bollen*



Nature **465**, 864-866 (2010) | doi:10.1038/465864a



there's been a drastic spike in terms of
sheer ***volume*** and ***type***



citation / impact factor
 h - index

weighted citations (eigenfactor, sjr)
“betweenness centrality”
alt-metrics, etc.

difficult to ...
harmonise
track / maintain / map
understand
(even still measure)



ASAHI
PENTAX

K1000

SMC PENTAX-M 1:2 50mm
3987726 ASAHI OPTICAL CO.

administrators /
funders
as ***influencers***



drivers of
behavioral change

we're battling
tradition, not just
technology.

www.digital-science.com

kaitlin@digital-science.com
[@kaythaney](mailto:kaythaney@kaythaney.com)