

innovations in digital research

kaitlin thaney

stm innovations - 30 april 2013

@kaythaneey ; @digitalsci

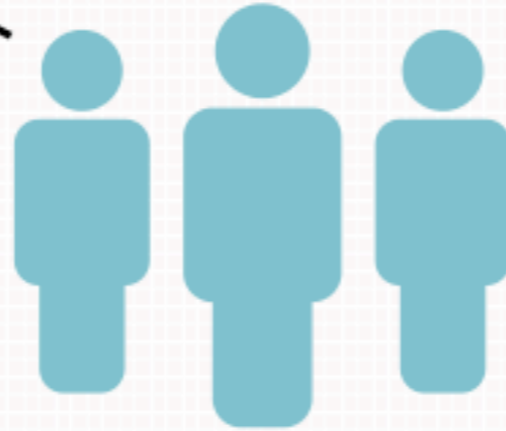


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“ traditions last not because they are excellent, but because influential people are **averse** to change and because of the sheer burdens of **transition to a better state** ... ”

- Cass Sunstein

(3)

machines

researchers

decision makers

machines

researchers

decision makers

discovery is still
sub-optimal.
(an example in chemistry)

still the starting point

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



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The E111 has been replaced by the European Health Insurance Card.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

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Results of Search in US Patent Collection db for:

diazepin: 1102 patents.

Hits 1 through 50 out of 1102

[Next 50 Hits](#)











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diazepin

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](#)

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

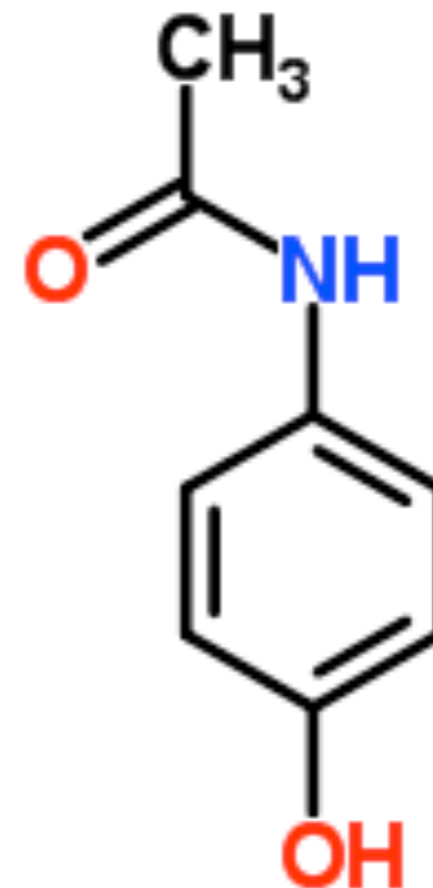
N-(4-Hydroxyphényl)acétamide

N-(4-Hydroxyphenyl)acetanilide

N-(p-hydroxyphenyl)acetamide

N-Acetyl-4-aminophenol

N-Acetyl-p-aminophenol ...



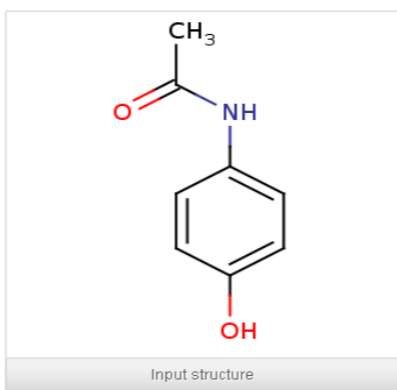
and the list goes on ...



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streamline search

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Input structure

SUBSTRUCTURE SEARCH TYPE

- Substructure
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- Exact
- Similarity

SEARCH FOR STRUCTURE IN PATENT FIELD(S)

- All
- Title
- Abstract
- Claims
- Description

Structure searches in document sections are coming soon

SEARCH AUTHORITIES

- All (inc. DocDB)
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- US Granted
- EP Applications
- EP Granted
- WO

DATE

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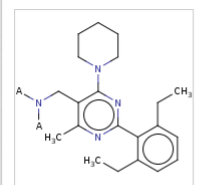
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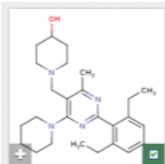
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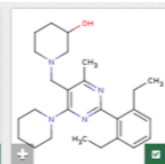


Dataset
 Patents
 Structure search type
 Substructure

Go back to structure results

Publication Number	Publication Date and Title	IPCR	Assignee(s)/Applicant(s)	Inventor(s)
US-8128395-B2	2012-03-06 4,5-disubstituted-2-aryl pyrimidines	C07D 403/00	NOVARTIS INTERNATIONAL PHARMACEUTICAL LTD [EP] NOVARTIS INT PHARM LTD [EM]	CURRIE KEVIN S [US] GHOSH MANUKA [US] GUO QIN [US] MAYNARD GEORGE D [US] MITCHELL SCOTT [US] YUAN JUN [US] ZHAO HE [US] Currie, Kevin S. Ghosh, Manuka Guo, Qin Maynard, George D. Mitchell, Scott Yuan, Jun Zhao, He

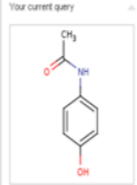




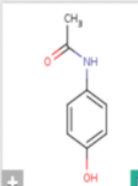
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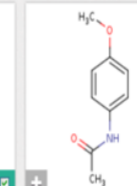
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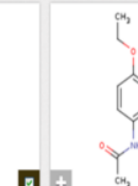
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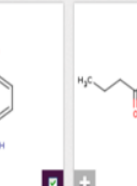


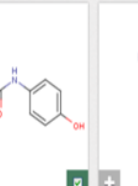
Dataset
 Patents
 Structure search type
 Query
 Paracetamol

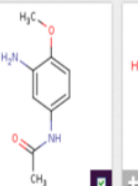












Publication Number	Publication Date and Title	IPCR	Assignee(s)/Applicant(s)	Inventor(s)
EP-1526980-A1	2012-01-10 DISPOSITIFS MEDICAUX IMPLANTABLES OU INGERABLES CONUS POUR ADMINSTRER DES MEDICAMENTS DE MANIERE REGULEE IMPLANTABLE OR INGESTIBLE MEDICAL DEVICES FOR CONTROLLED DRUG DELIVERY IMPLANTIERE ODER ENFUHRBARE MEDIZINISCHE VORRICHTUNGEN ZUR KONTROLLIERTEN ARZNEITELFREISETZUNG	A61L 29/16	BOSTON SCIENTIFIC LTD [EP] Boston Scientific Limited [EP]	BUCHY-COUTO WENNA [US] CONLEY DANIELLE [US] DAO CANG OUY [US] DAVOUDI HAMD [US] LAREAU RAYMOND [US] LI JIANMIN [US] MILLER KATHLEEN M [US] BUCHY-COUTO, WENNA [US] CONLEY, DANIELLE [US] DAO, CANG, OUY [US] DAVOUDI, HAMD [US] LAREAU, RAYMOND [US] LI, JIANMIN [US] MILLER, KATHLEEN, M [US]
US-2012005240-A1	2012-01-12 File for Delivery of a Therapeutic Agent	A61K 9/00	BROOM DANIEL EBBSOLE GARRETT ELACHOABI AMIN STOPEK JOSHUA	BROOM DANIEL [US] EBBSOLE GARRETT [US] ELACHOABI AMIN [US] STOPEK JOSHUA [US] Broom, Daniel Eberstele, Garrett Elachochabi, Amin Stopek, Joshua
WO-2011018105-A2	2011-12-29 COMPOSITIONS HERBICOIDES HERBICIDAL COMPOSITIONS	A01P 13/00	BASF SE [DE] BOWE STEVEN [US] EHRHARDT THOMAS [DE] GROSSMANN ALAUS [DE] HARMENIA SYLVE [DE] HARENZA SYLVE [DE] HUTZLER JOHANNES [DE] ISHAGLE MICHAEL [DE] KELLER KYLIE [US] MANGEN PHIL [US] NEWTON TREVOR WILLIAM [DE] REINHARD ROBERT [DE] SIMON ANJIA [DE]	BOWE STEVEN [US] EHRHARDT THOMAS [DE] GROSSMANN ALAUS [DE] HARMENIA SYLVE [DE] HUTZLER JOHANNES [DE] ISHAGLE MICHAEL [DE] KELLER KYLIE [US] MANGEN PHIL [US] NEWTON TREVOR WILLIAM [DE] REINHARD ROBERT [DE] SIMON ANJIA [DE]
US-8128382	2012-03-06 High affinity antibodies against HMD2B and methods of use thereof		MEZIMUNE, LLC (US, Gaithersburg, MD) INSTITUTE FOR MEDICAL RESEARCH (US, Marhasset, NY)	Cao, Anthony Guo, Changshou Kleier, Peter Mao, Su-Yao O'Reilly, Theresa Qi, Shishu Tian, Jane

ethyl 1-[2-(2,6-diethylphenyl)-6-methyl-5-((methyl[(1S)-1,2,3,4-tetrahydronaphthalen-1-yl]amino)methyl)pyrimidin-4-yl]piperidin-4-carboxylate

ethyl 1-[2-(2,6-diethylphenyl)-6-methyl-5-((methyl[(1S)-1,2,3,4-tetrahydronaphthalen-1-yl]amino)methyl)pyrimidin-4-yl]piperidin-4-carboxylate

ethyl 1-[2-(2,6-diethylphenyl)-6-methyl-5-((methyl[(1S)-1,2,3,4-tetrahydronaphthalen-1-yl]amino)methyl)pyrimidin-4-yl]piperidin-4-carboxylate

ethyl 1-[2-(2,6-diethylphenyl)-6-methyl-5-((methyl[(1S)-1,2,3,4-tetrahydronaphthalen-1-yl]amino)methyl)pyrimidin-4-yl]piperidine-4-carboxylate

ethyl 1-[2-(2,6-diethylphenyl)-6-methyl-5-((methyl[(1S)-1,2,3,4-tetrahydronaphthalen-1-yl]amino)methyl)pyrimidin-4-yl]-D-proline;

ethyl 1-[2-(2,6-diethylphenyl)-6-methyl-5-((methyl[(1S)-1,2,3,4-tetrahydronaphthalen-1-yl]amino)methyl)pyrimidin-4-yl]piperidin-4-carboxylate

ethyl 1-[2-(2,6-diethylphenyl)-6-methyl-5-((methyl[(1S)-1,2,3,4-tetrahydronaphthalen-1-yl]amino)methyl)pyrimidin-5-yl]methyl]-N-methyl-1,2,3,4-tetrahydronaphthalen-1-amine

ethyl 1-[2-(2,6-diethylphenyl)-4-methyl-6-piperidin-1-ylpyrimidin-5-yl]methyl]-N-methyl-1,2,3,4-tetrahydronaphthalen-1-amine

ethyl 1-[2-(2,6-diethylphenyl)-4-methyl-6-piperidin-1-ylpyrimidin-5-yl]methyl]-N-methyl-1,2,3,4-tetrahydronaphthalen-1-amine

ethyl 1-[2-(2,6-diethylphenyl)-4-methyl-6-piperidin-1-ylpyrimidin-5-yl]methyl]-N-methyl-1,2,3,4-tetrahydronaphthalen-1-amine

ethyl 1-[2-(2,6-diethylphenyl)-4-methyl-6-piperidin-1-ylpyrimidin-5-yl]methyl]-N-methyl-1,2,3,4-tetrahydroisoquinoline;

ethyl 1-[2-(2,6-diethylphenyl)-6-methyl-5-((methyl[(1S)-1,2,3,4-tetrahydronaphthalen-1-yl]amino)methyl)pyrimidin-4-yl]piperidin-3-ol;

ethyl 1-[2-(2,6-diethylphenyl)-6-methyl-5-((methyl[(1S)-1,2,3,4-tetrahydronaphthalen-1-yl]amino)methyl)pyrimidin-4-yl]pyrrolidin-3-ol

ethyl 1-[2-(2,6-diethylphenyl)-5-((3,3-dimethylpiperidin-1-yl)methyl)-4-methyl-6-piperidin-1-yl]pyrimidine;

ethyl 1-[2-(2,6-diethylphenyl)-4-methyl-6-piperidin-1-yl]pyrimidin-5-yl]methyl]-N-methyl-1,2,3,4-tetrahydronaphthalen-1-amine

Back to search results

Front-page Claims Description

All structure search results

⏪ ⏩ 3/4 ⏪ ⏩

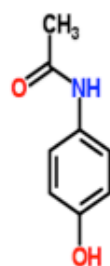
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eg. Pyridine Search



paracetamol

ChemSpider ID: 1906

Molecular Formula: C₉H₉NO₂

Monoisotopic mass: 151.063324 Da

Systematic name

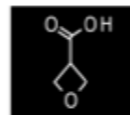
N-(4-Hydroxyphenyl)acetamide

SMILES and InChIs

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Names and Identifiers

Names and Synonyms Database ID(s)

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103-90-2 [RN]

254-465-1 [EINECS]

4-(Acetylamino)phenol

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

Patents

Google Patents USPTO Granted (26994) USPTO Applications European Granted European Applications WO/PCT Japanese Abstracts

26994 patents found in USPTO Granted

Patent No.	Title
6737256	Overcoming DAPA aminotransferase bottlenecks in biotin vitamers biosynthesis
7943170	Sustained release paracetamol containing compositions
7253108	Process for forming a thin film of TISN, in particular for phase change memory devices

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Chem. Commun., 2009, 3181-3183
DOI: 10.1039/B822882E, Communication

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Can crystal structure prediction guide experimentalists to a new polymorph of paracetamol?
Marcus Aurelius Neumann and Marc-Antoine Perrin
CrystEngComm, 2009, 11, 2475-2479
DOI: 10.1039/B909819D, Paper

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Adsorption from aqueous solutions on opened carbon nanotubes—organic compounds speed up delivery of water from inside
Artur P. Terzyk, Piotr A. Gauden, Sylwester Furmaniak, Radosław P. Wesolowski, Peter J. F. Harris and Piotr Kowalczyk
Phys. Chem. Chem. Phys., 2009, 11, 9341-9345
DOI: 10.1039/B916067A, Communication

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Direct analysis of dried blood spots utilizing desorption electrospray ionization (DESI) mass spectrometry
Justin M. Wiseman, Christopher A. Evans, Chester L. Bowen and Joseph H. Kennedy
Analyst, 2010, 135, 720-725
DOI: 10.1039/B922329K, Paper
From themed issue Ambient mass spectrometry

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The biological potential of flavones
Alok Kumar Verma and Ram Pratap
Nat. Prod. Rep., 2010, 27, 1571-1593
DOI: 10.1039/C004698C, Review

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machines

researchers

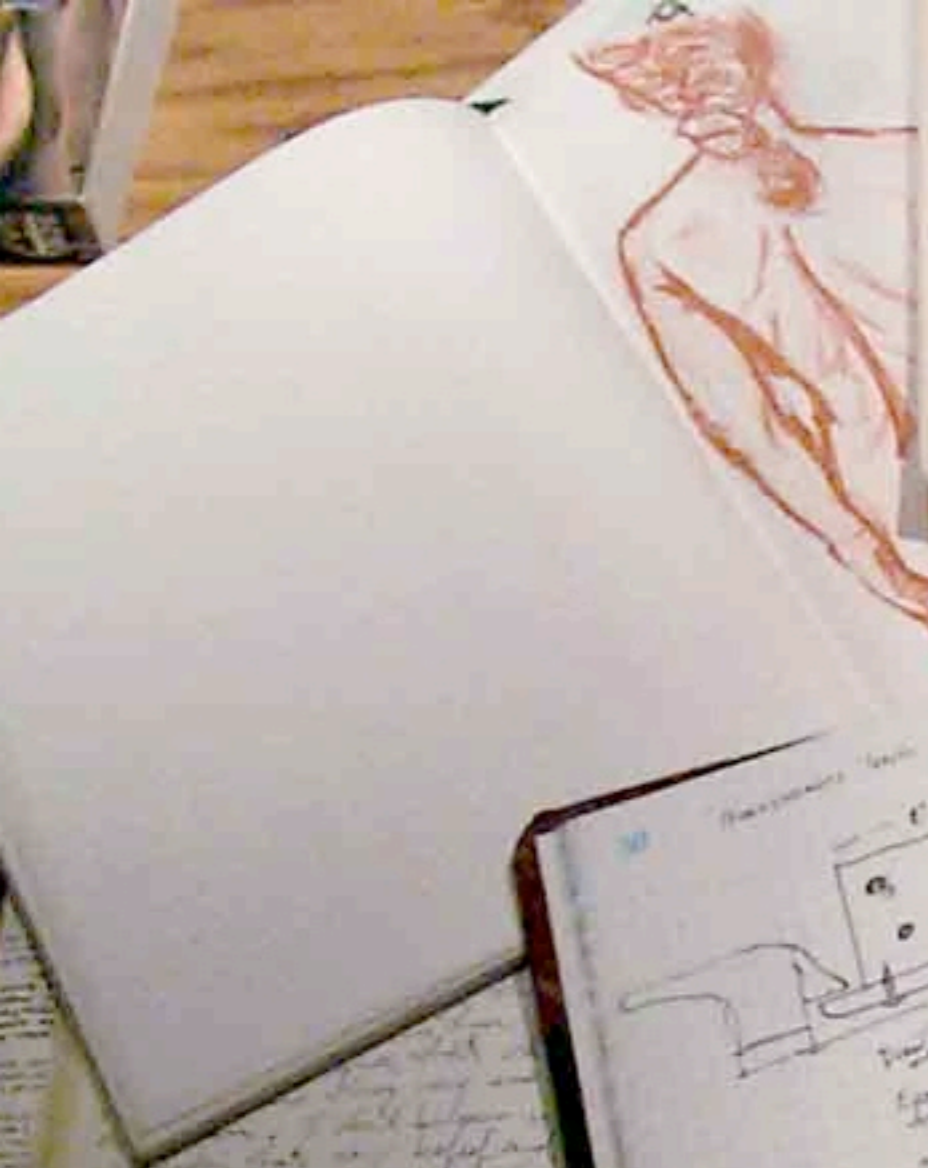
decision makers

our definition of
“information” is evolving.

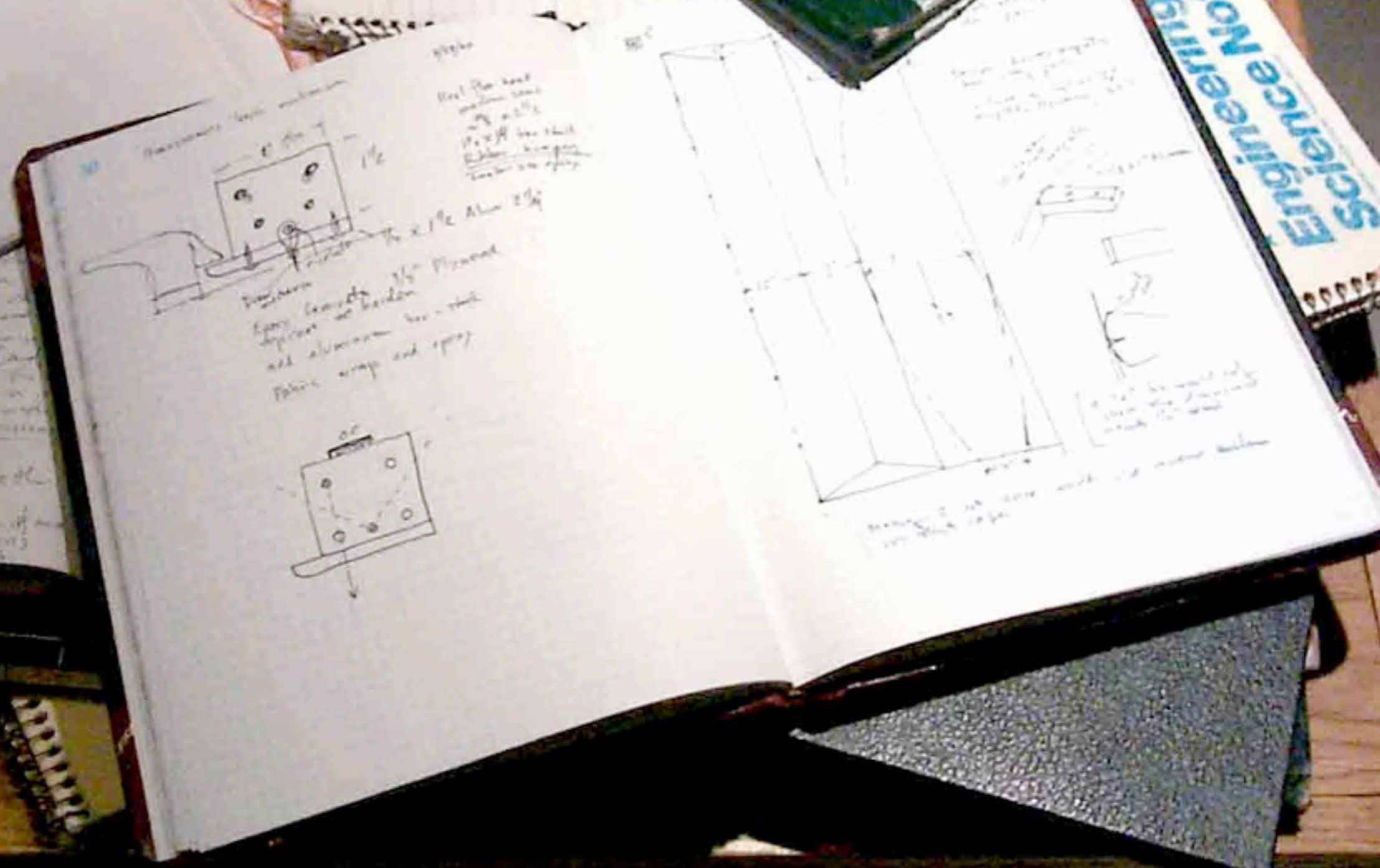
(our systems are still playing catch up.)



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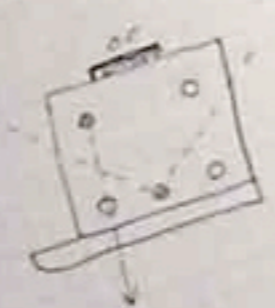
March 2
F493
April 194



Maximum load
1/2
1/4

Keep the load
uniform
1/2 x 1/4
1/4 x 1/4
1/4 x 1/4
1/4 x 1/4

Maximum
Every 1/4 inch
1/4 inch
add aluminum bar - 1/4
Fabric wrap and epoxy



Science
Engineering
and
Technology

Handwritten notes on the left edge of the notebook, including the word 'Experiment' and other illegible text.



B177-08 E

B177-08 E

[Illegible black ink scribble]

[Illegible black ink scribble]

JELLYFISH IN ARMOUR



CHRIS HENDRICKS © 2009

HOW MILK CONTAINERS SHOULD BE

186. Pork Spread Rillettes

12 first course servings

The word *rillettes* implies different preparations of cooked meats, particularly different pork preparations. In France, ham, etc. By extension the word *rillettes* is also used for dishes of fish, shellfish, etc. In addition some *rillettes* are made of cheese, black pudding, chattering sausage, etc. The following techniques are available from *rillettes*.

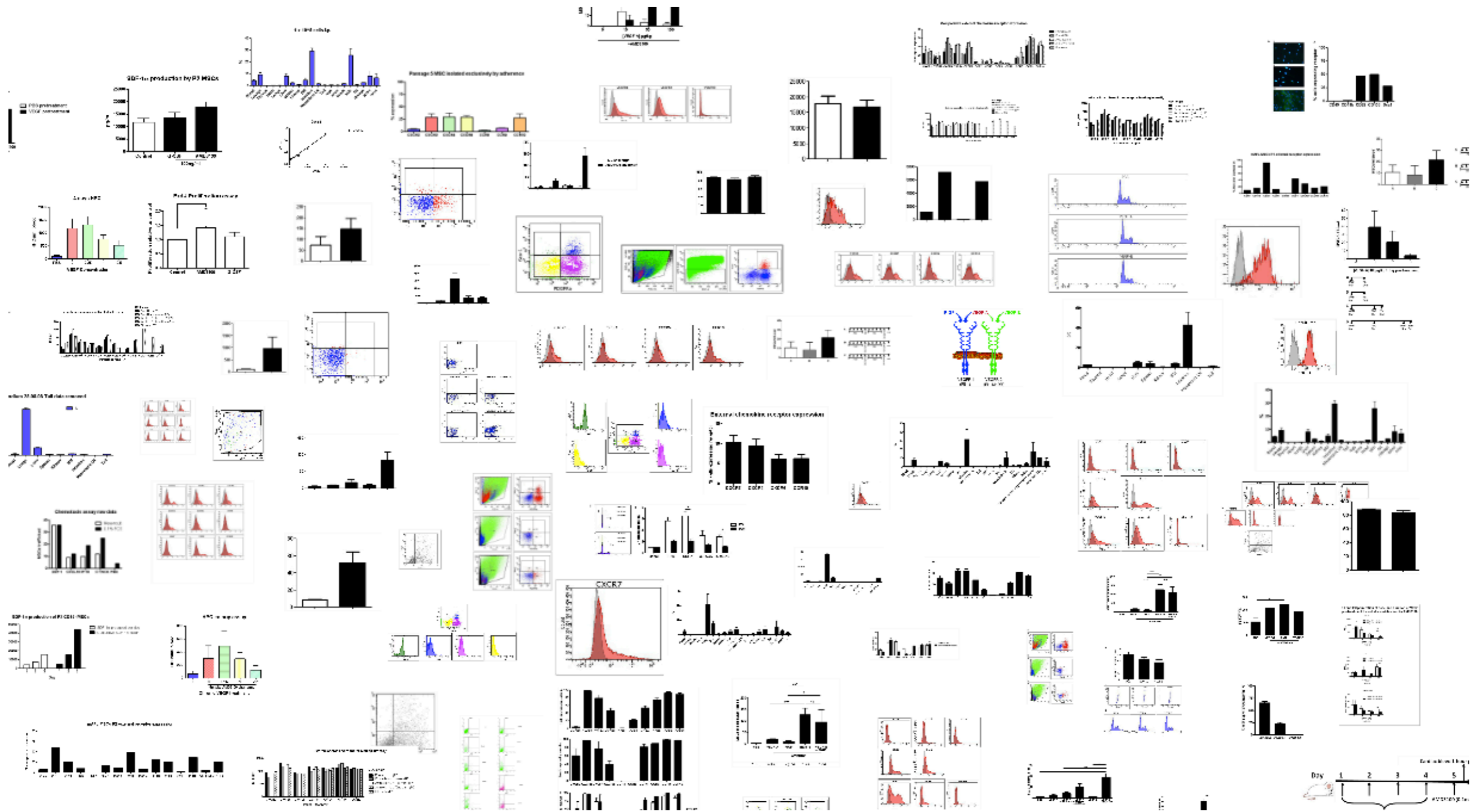
Rillettes consist of seasoned pork cooked in tiny pieces, bound together by fat and seasoned lightly with salt and pepper. They are eaten cold with Dijon mustard and country bread cut to a course or as a snack. The *rillettes* can also be made with duck, and make it the right consistency. The *rillettes* are cooked in crocks and served as such with bread, or with a stock, thyme, bay leaf, etc., but the simple recipe gives the true taste of that country dish. The crocks should be kept refrigerated up to 10 days. To keep water retains the plastic wrap and kept refrigerated up to 10 days. To keep longer the crocks have to be sealed. When frozen the taste changes and the taste tends to grow.

2 1/4 pounds fresh pork from the chuck, butt or neck (the meat should have about one-third lean meat to two-thirds fat)
1/2 teaspoon salt
1/2 teaspoon freshly ground black pepper

protocols
parameters
calibration
misc. lit

A photograph of a warehouse or factory floor. In the foreground, a large, plain brown cardboard box sits on a metal conveyor belt. The background is filled with industrial machinery, including yellow overhead cranes and various metal structures, all slightly out of focus. A semi-transparent yellow rectangular box is overlaid on the right side of the image, containing the text 'ordering + processing' in a bold, black, sans-serif font.

**ordering
+
processing**



use data to better
optimise, enable
(behaviour, productivity, reproducibility...)



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



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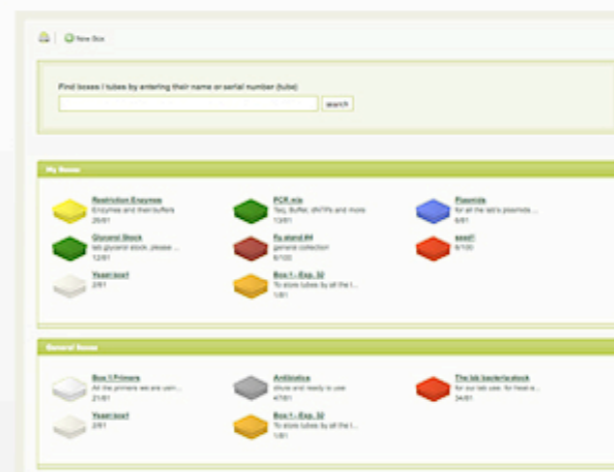
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Open Experiment

Project One

Cloning DNA fragment into expressio...

Cloning ErbB4 into expression vector

Analysis of protein fragments by LC...

Colony PCR - identify lacZ expressin...

Cloning DNA fragment over-expressi...

GFP gene

chemical compound

Kinase activity assay with wt ErbB4

Protein Purificatio - Take 1.

Protein purification

Extraction of the RBP-mRNA comple...

Cloning TAP-tag constructs for 5 Puf...

All

Ongoing

Today

▶ Start

HOURS

MIN.

SEC.

Reset

3

Add 500 ul 70% Ethanol. Spin 2 min, (RT or 4 C) and remove supernatant

analysis-4

Completed

chemical compound-12

Step 5 / 5

Kinase activity assay with wt ErbB4-14

Step 2 / 5

Add Experiment

Result

Done

analysis-4

Completed

chemical compound-12

Step 5 / 5

Kinase activity assay with wt ErbB4-14

Step 2 / 5

Add Experiment

analysis-4

Completed

chemical compound-12

Step 5 / 5

Kinase activity assay with wt ErbB4-14

Step 2 / 5

Add Experiment

ACIDIC-NATIVE GEL Protocol

For Basic Proteins (pI>7.0)
 USE ONLY FRESH GELS

Stock Solutions

- 1) 1.5M Acetate-KOH pH 4.3 (48ml 1MKOH + 17.2ml AcH + H2O up to 200ml) - Keep RT.
- 2) 30% Acrylamide 0.8% Methylene bis Acrylamide. Keep 4°C.
- 3) 0.25M Acetate-KOH pH 6.8 (48ml 1MKOH + 2.9ml AcH + H2O up to 200ml) - Keep RT.
- 4) 10% Ammonium Persulfate (APS). Keep 4°C less than 1 month.

Running Buffer x1

β-Alanine	0.35M	18.7gr
AcH	0.14M	4.8ml
H2O up to		600ml
Adjust pH to		4.3

Keep at RT

Sample Buffer x5

Glycerol 50%	1.45ml
0.25M Acetate-KOH pH 6.8	0.5ml
Methyl Green	traces

Keep in aliquots of 1ml at -20C

Separating Gel

% Acrylamide	10%	15%	7%	Gradient 7.5%	Gradient 20%
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Protocol Steps

Notes

Result

1 Add 200 ul Solution 2. Vortex and wait 1-2 min.

2 Invert to mix and spin for 3 min at room temperature or 4C. You should see a white pellet now.

Done

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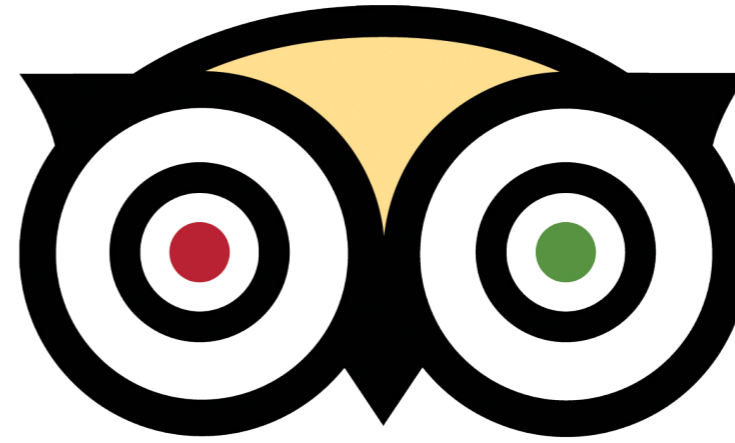
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Anti-HTT

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Sz.: 100 ul

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Monoclonal Mouse anti-HTT antibody

Anti-Huntingtin Protein, a.a. 181-810, clone 1HU-4C8

EMD Millipore

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Anti-Huntingtin Protein, clone mEM48

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doi:10.1038/nature10414

Multiple reference genomes and transcriptomes for *Arabidopsis thaliana*

Xiangchao Gan^{1*}, Oliver Stegle^{2*}, Jonas Behr^{3*}, Joshua G. Steffen^{4*}, Philipp Drewe^{3*}, Katie L. Hildebrand⁵, Rune Lyngsoe⁶, Sebastian J. Schultheiss³, Edward J. Osborne⁴, Vipin T. Sreedharan³, André Kahles³, Regina Bohnert³, Géraldine Jean³, Paul Derwent⁷, Paul Kersey⁷, Eric J. Belfield⁸, Nicholas P. Harberd⁸, Eric Kemen⁹, Christopher Toomajian⁵, Paula X. Kover¹⁰, Richard M. Clark¹, Gunnar Rättsch³ & Richard Mott¹

Genetic differences between *Arabidopsis thaliana* accessions underlie the plant's extensive phenotypic variation, and until now these have been interpreted largely in the context of the annotated reference accession Col-0. Here we report the sequencing, assembly and annotation of the genomes of 18 natural *A. thaliana* accessions, and their transcriptomes. When assessed on the basis of the reference annotation, one-third of protein-coding genes are predicted to be disrupted in at least one accession. However, re-annotation of each genome revealed that alternative gene models often restore coding potential. Gene expression in seedlings differed for nearly half of expressed genes and was frequently associated with *cis* variants within 5 kilobases, as were intron retention alternative splicing events. Sequence and expression variation is most pronounced in genes that respond to the biotic environment. Our data further promote evolutionary and functional studies in *A. thaliana*, especially the MAGIC genetic reference population descended from these accessions.

Interpreting the consequences of genetic variation has typically relied on a reference sequence, relative to which genes and variants are annotated. However, this may cause bias, because genes may be inactive in the reference but expressed in the population¹, suggesting that sequencing and re-annotating individual genomes is necessary. Advances in

suitable for annotation. Accessions were sequenced with Illumina paired-end reads² (Supplementary Table 1), generally with two libraries with 200-bp and 400-bp inserts and reads of 36 and 51 bp, respectively, to between 27-fold and 60-fold coverage. Each genome was assembled by using five cycles of iterative read mapping¹⁴ com-

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Pdx1⁺ progenitor cells, coupled with an inability of the remaining cells to compensate for this reduced cell number, causes the pancreas to be small at birth. The distal stomach and proximal intestine, which normally express *Pdx1* during development and which therefore might be expected to show some loss, were not noticeably affected in tTA/DTA embryos under any ablation conditions; this may be a result of silencing of the *tetO^{DTA}* locus in these tissues (data not shown).

One potential explanation for a small pancreas after transient progenitor ablation is the possibility that a subset of progenitor cells was selectively eliminated. Because exocrine cells constitute over 80% of tissue mass, loss of exocrine progenitor cells might account for the reduced size¹². To address this possibility, we determined the relative

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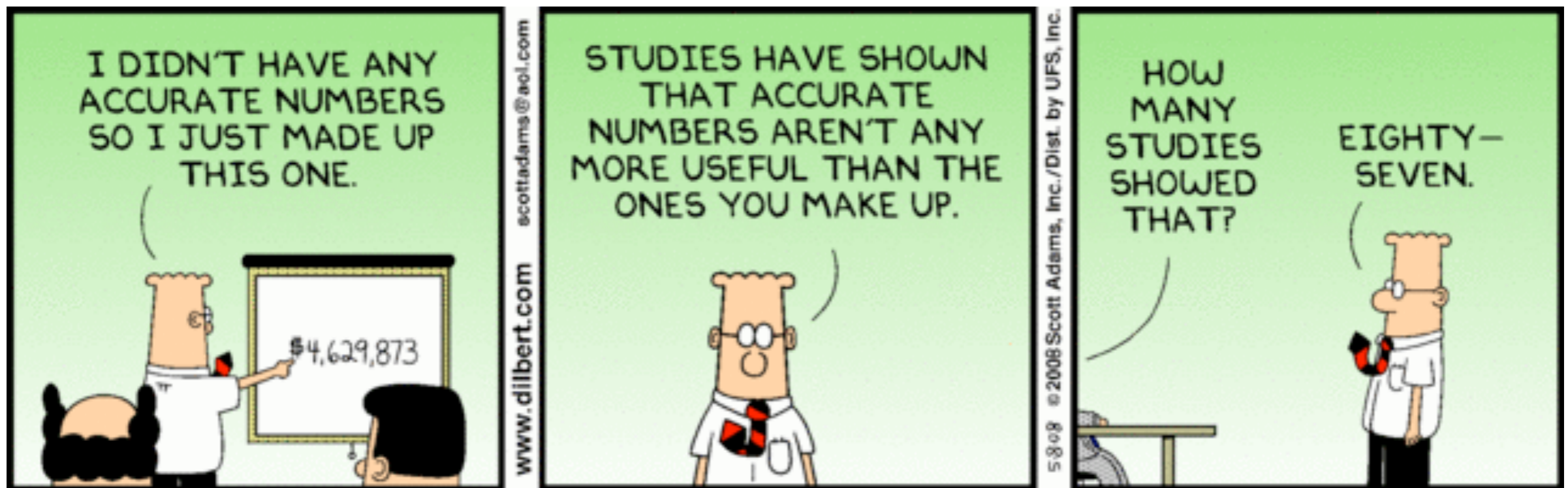
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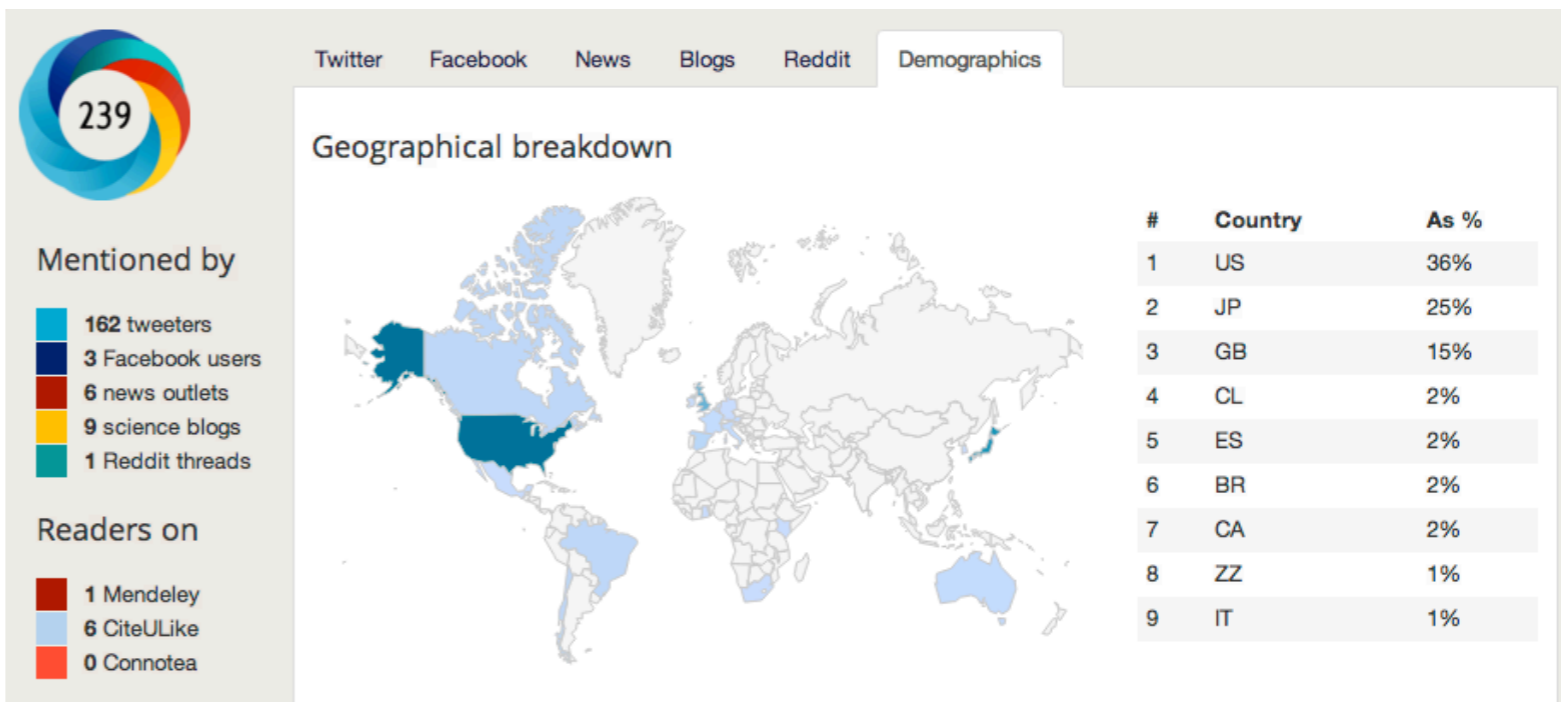
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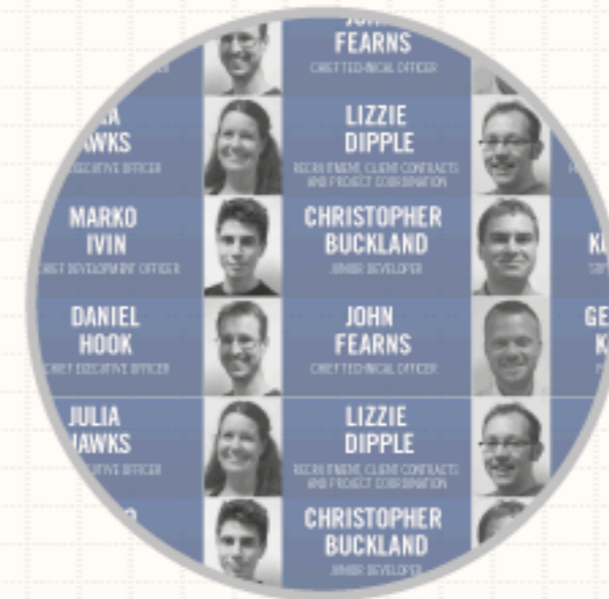
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Symplectic was founded in 2003 by four theoretical physicists studying for their PhD's at Imperial College. During their studies, they quickly realised that university staff and researchers were in need of simple, effective software to harmonise their internal processes.

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We have posted the current administrator and user guides for Symplectic Elements version 3.7.17. For up-to-date information please subscribe to our **SUPPORT** site.



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