

The many faces of reproducibility

Alexandre Hocquet^{1,2}

¹ KHK, RWTH Aachen, Germany

² Archives Henri Poincaré, Nancy, France

Recherche reproductible : état des lieux, 8 mars 2023

Autopromo

Paper in Historical and Social Studies of Science | [Published: 17 April 2021](#)

Epistemic issues in computational reproducibility: software as the elephant in the room

[Alexandre Hocquet](#) & [Frédéric Wieber](#)

[European Journal for Philosophy of Science](#) 11, Article number: 38 (2021) | [Cite this article](#)

261 Accesses | 3 Altmetric | [Metrics](#)



MIT Press Direct

Search...

Perspectives on Science

Advanced Search

Register

Perspectives on Science

Issues Online Early About Submit Subscribe

Volume 28, Issue 5
September-October 2020

October 01 2020

Models, Parameterization, and Software: Epistemic Opacity in Computational Chemistry

Frédéric Wieber, Alexandre Hocquet

[Author and Article Information](#)

Perspectives on Science (2020) 28 (5): 610–629.

https://doi.org/10.1162/posc_a_00352



Cite PDF Permissions Share

Abstract



Journals & Magazines > IEEE Annals of the History of... > Volume: 39 Issue: 4

“Only the Initiates Will Have the Secrets Revealed”: Computational Chemists and the Openness of Scientific Software

Publisher: IEEE

Cite This

PDF

Alexandre Hocquet, Frédéric Wieber [All Authors](#)

507 Full Text Views



Re: Taxol 1 Jan 93 14:11:05 ESTFrom: Francl Michelle M <mfranc1@cc.brynmawr.edu>Date: Mon, 4 Jan 93 12:36 -0800From: hcj@guil.uncc.edu (Harry C. kfz-heidelberg.de>Subject: energy contribution of hbonds?Date: 06 Jan 1993 10:55:29 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON_DOUGLAS_W@LILLY.COM>Subject: u CADD videosDate: Wed, 6 Jan 93 13:03:33 -0800From: chiremvl@andromeda!jeffh@uunet.UU.NET (Jeff Blaney)Subject: Re: Polygon-based solvent accessible surfacesDate: Thu, 7 Jan 93 !!Date: 08 Jan 1993 09:19:39 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON_DOUGLAS_W@LILLY.COM>Subject: replies to my posting about PDB searching methodsDate: F vi@tiberius.tc.cornell.edu>From: scsupham@reading.ac.ukDate: Mon, 11 Jan 93 17:54:05 GtsSubject: DMOI questionsDate: Mon, 11 Jan 1993 14:33 ESTFrom: WILLIAMS%XRAY2@ulkyvxo2.loui tcular modelingDate: wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@ e: Thu, 14 Jan 1993 11:18:26 -0500From: jle@world.std.com (Joe l.BITNET@OHSTVMA.ACS.OHIO-STATE.EDUSubject: Steric strain at T all.edu>Subject: UHF calc's on diradicals/TSDate: Mon, 18 Jan 9 wed, 20 Jan 93 10:11:36 ESTFrom: landman@hal.physics.wayne.edu l.crc.uno.edu>Subject: Re: density problemDate: wed, 20 Jan 93 >Date: 21 Jan 93 07:50:00 ESTFrom: nauss@wrair-emh1.army.milSub ant symmetry and Gaussian90Date: 22 Jan 93 13:06:32 UTFFrom: "BD : Thu, 21 Jan 93 17:31:46 -0500From: system@alchemy.chem.utoron 05:30 -0500From: chm_ramsay@emunix.emich.eduSubject: CHEMICALC: encesDate: Tue, 26 Jan 93 12:57:08 -0500From: watanabe@tammy.ha oject: Computer Assisted Chemistry Course Info RequestedDate: W .chem.utah.edu>subject: Re: Periodic Table WidgetDate: wed, 27 edavis.edu>subject: Population Analysis in GaussianFrom: mei@ve : excited statesDate: Fri, 29 Jan 1993 16:47:38 -0600From: sliu .edu>subject: Gaussian and excited statesDate: Fri, 29 Jan 93 15 te: 01 Feb 93 19:26:49-0500From: SBPM MF dielectricDate: Mon, 1 Feb 93 17:57 2D drawing?From: QINGSONG@minmet.lan. e for calculating zeta potential and e Moore <kmoore@ncsc.org>Subject: MOLSOL 2 +0100From: ivan@gandalf.ciam.unibo.i edu>Subject: Memory and CPU for Starde di Treasurywala)Subject: Coordinates o workstations and serversDate: wed, 10 rom: rickl@biosym.comSubject: DIBUG ad sa@si.fi.ameslab.gov (Theresa Windus)S K360171%EDVZ.UNI-Linz.AC.%@OHSTVMA.ACS :09 +0100 (WET)From: PREINERT@bioJan.u :01 PS S A. S /Fishe <ravi 16:49: alex@ba : Thu, ADY Thu, 2 questio 25:19 e: Tue ! Mar 9 let>Dat : Hanoc GROW ca.phy. ch (Re ul freq for UN software (pa 'om: Ge Semic her J 128@aw ja@obe1 J4:42 -

Subject: Re: Taxol modellingDate: Fri, 1 Jan 93 14:11:05 ESTFrom: Francl Michelle M <mfranc1@cc.brynmawr.edu>Date: Mon, 4 Jan 93 12:33:36 -0800From: hcj@guil.uncc.edu (Harry C. ...
!Date: 08 Jan 1993 09:19:39 -0500 (EST)From: "dwj@lilly.com" <dwj@lilly.com>Subject: Polygon-based solvent accessible surfacesDate: Thu, 7 Jan 93 ...
vi@tiberius.tc.cornell.edu>From: scsuham@readino.ac.ukDate: Mon, 11 Jan 93 17:54:05 GMTSubject: DMO1 questionsDate: Mon, 11 Jan 1993 14:33 ESTFrom: WILLIAMS%XRAY2@ulkvxv02.lou

Histoire des sciences

Terminologies for Reproducible Research

Lorena A. Barba, the George Washington University, Washington D.C.

January 2018

Introduction

Reproducible research—by its many names—has come to be regarded as a key concern across disciplines and stakeholder groups. Funding agencies and journals, professional societies and even mass media are paying attention, often focusing on the so-called “crisis” of reproducibility. One big problem keeps coming up among those seeking to tackle the issue: different groups are using terminologies in utter contradiction with each other. In July 2017, over a dozen participants

19 Feb 2018

g)Subject: Re: Hydrogen bond.Date: Wed, 24 Feb 93 17:21 EDTFrom: <PODOSNNA%NYUACF1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU>Subject: X-window terminal emulator for MacDate: Thu, ...
nl.govSubject: X-window terminal emulator for MacDate: Thu, 25 Feb 93 17:19:09 -0500From: feng@sgi.chem.temple.edu (Feng Chen)Subject: X-windows Server on MS-windowsDate: Thu, 2 ...
d.harvard.edu (jill cheney)Subject: Computer Program to Evaluate wigner 3j CoefficientsDate: Fri, 26 Feb 1993 22:08:57 +0100From: ole.swang@kjemi.uio.noSubject: language questio ...
semipirical calculations simple oxidesFrom: sender@chemdc1.tau.ac.il (Senderowitz Hanoch)Subject: MOPAC6.0Date: Sun, 28 Feb 93 13:44:41 GMT-2:00Date: Mon, 1 Mar 1993 15:25:19 ...
n.deSubject: Expert Know-How wanted !!Date: 02 Mar 1993 08:13:18 -0500 (EST)From: "DONALD B. BOYD" <BOYD_DONALD_B@LILLY.COM>Subject: new book on computational chemistryDate: Tue ...
ate.Edu (Gene Carter)Subject: Co MD parameters.Date: Tue, 2 Mar 93 17:22:53 CSTFrom: Greg Landrum <landrum@chemres.tn.cornell.edu>Subject: Re:Cache on the MacDate: Tue, 2 Mar 9 ...
lling Software: Does anyone have STELLA?Date: 04 Mar 1993 17:08:31 -0500 (EST)From: MARYJO@northeastern.eduSubject: PDB subdir organization?From: Jan Labanowski <jkl@cc1.net>Dat ...
ar 93 17:30:16 GMTDate: Sun, 7 Mar 93 12:36 ESTFrom: <SML108@PSUVM.PSU.EDU>Subject: Minimum allowable interatomic separationsFrom: sender@chemdc1.tau.ac.il (Senderowitz Hanoc ...
secc.fi.cnr.itSubject: MO Theory Made VisibleDate: Tue Mar 09 11:23:12 1993Date: Tue, 9 Mar 93 10:52:25 -0500From: gallion@auriga.rose.brandeis.edu (steve gallion)Subject: grow ...
uplingDate: Thu, 11 Mar 93 18:54 EDTFrom: <PODOSNNA%NYUACF1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU>Subject: Software for PCDate: Fri, 12 Mar 93 04:51:15 GMTFrom: jim@quanta.phy. ...
r 1993 02:33:09 -0800 (PST)From: Thomas Nhan <tom@cassandra.chem.washington.edu>Subject: PDB source file...Date: Sun, 14 Mar 93 11:06:13 +0100From: doelz@comp.bioz.unibas.ch (Re ...
MA.ACS.OHIO-STATE.EDU>Subject: partial charges for fictive atoms in G92Date: Mon, 15 Mar 1993 12:55 ESTFrom: HSUS@chemv2.mps.ohio-state.eduSubject: Problem with vibrational freq ...
, 15 Mar 1993 21:55:05 -0600 (CST)From: Chris Parkinson <mbdtsr1@hpc.ch.man.ac.uk>Subject: MM2 code for UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UN ...
ar 1993 13:58:36 -0400From: ZSHI@ac.dal.caSubject: Information about IBM RS6000Date: 17 Mar 93 16:18:00 EDTFrom: "STEPHEN R. HELLER" <srheller@asr.arsusda.gov>Subject: Software ...
st Girona Seminar on Molecular SimilarityDate: Thu, 18 Mar 93 10:40:05 CETFrom: ZSYAMP01%EBCECA1@OHSTVMA.ACS.OHIO-STATE.EDUSubject: First Congress of the ISTCP (pa ...
:11 -0500Subject: Keep the noise down, pleaseDate: 19 Mar 93 11:37:00 ESTFrom: nauss@wrair-emh1.army.milSubject: Program called GRIDDate: Fri, 19 Mar 93 14:33:18 ESTFrom: Ge ...
23 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Announcing AMPAC 4.5Date: 21 Mar 1993 17:36:57 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Semic ...
.milSubject: What about simulated annealing?Date: Wed, 24 Mar 93 14:11:32 +0100From: dufner@ws01.pc.chemie.th-darmstadt.de (Hagen Dufner)Subject: efg in g92From: "Christopher J ...
ject: SC&A Conference speakers - thanksDate: Thu, 25 Mar 93 10:18:48 -0500From: au195@cleveland.freenet.edu (Dr. Gene A. Nelson)Subject: Batching files in MOPACFrom: zrfl0128@aw ...
MO@CHEMNA.DICHI.UNINA.ITSSubject: looking for ACES programFrom: Robert Laird <mbdtsr1@hpb.ch.man.ac.uk>Subject: Fe-0 calculationDate: Mon, 29 Mar 93 15:49:03 BSTFrom: rafapa@obel ...
uk>Subject: Polyrate QueryDate: Tue, 30 Mar 1993 19:31:32 +0200From: c62@aixfile1.urz.uni-heidelberg.de (Andreas Schulz)Subject: NBO analysesDate: Tue, 30 Mar 1993 16:04:42 - ...
ulz)Subject: Stephen R. WilsonDate: Thu, 1 Apr 1993 16:33:29 +0200From: oles@gollum.uio.noSubject: BiosymDate: 01 Apr 1993 11:43:13 -0600 (CST)From: CUNDRIT@memstvx1.memst.edu

Subject: Re: Taxol modellingDate: Fri, 1 Jan 93 14:11:05 ESTFrom: Francl Michelle M <francl@cc.brynmawr.edu>Date: Mon, 4 Jan 93 12:33:36 -0800From: hcj@guil.uncc.edu (Harry C. kfz-heidelberg.de>Subject: energy contribution of hbonds?Date: 06 Jan 1993 10:55:29 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON_DOUGLAS_W@LILLY.COM>Subject: u : CADD videosDate: Wed, 6 Jan 93 13:03:33 -0800From: chiremvl and home!jeffb@uunet.UUNET (Jeff Blarey)Subject: Re: Polygon-based solvent accessible surfacesDate: Thu, 7 Jan 93 !!Date: 08 Jan 1993 09:19:39 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON_DOUGLAS_W@LILLY.COM>Subject: replies to my posting about PDB searching methodsDate: F vi@tiberius.tc.cornell.edu>From: scsupham@readino.ac.ukDate: Mon, 11 Jan 93 17:54:05 GMTSubject: DM01 questionsDate: Mon, 11 Jan 1993 14:33 ESTFrom: WILLIAMS%XRAY2@ulkvxv02.lou

Histoire des sciences

CHANGING ORDER_r Reproducible Research

*Replication and Induction
in Scientific Practice*

on University, Washington D.C.

9 Feb 2018



H. M. COLLINS

With a new Afterword

names—has come to be regarded as a key concern across Funding agencies and journals, professional societies and , often focusing on the so-called “crisis” of reproducibility. Among those seeking to tackle the issue: different groups are ion with each other. In July 2017, over a dozen participants

g)Subject: Re: Hy %NYUACF1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU>Subject: X-window terminal emulator for MacDate: Thu, -0500From: feng@sgi.chem.temple.edu (Feng Chen)Subject: X-windows Server on MS-windowsDate: Thu, 2 d.harvard.edu (jil ficientsDate: Fri, 26 Feb 1993 22:08:57 +0100From: ole.swang@kjemi.uio.noSubject: language questio semiempirical calcu itz Hanoch)Subject: MOPAC6.0Date: Sun, 28 Feb 93 13:44:41 GMT-2:00Date: Mon, 1 Mar 1993 15:25:19 n.desSubject: Exper m: "DONALD B. BOYD" <BOYD_DONALD_B@LILLY.COM>Subject: new book on computational chemistryDate: Tue ate.Edu (Gene Car TFFrom: Greg Landrum <landrum@chemres.tn.cornell.edu>Subject: Re:Cache on the MacDate: Tue, 2 Mar 9 lling Software: Dc rom: MARYJO@northeastern.eduSubject: PDB subdir organization?From: Jan Labanowski <jkl@cc1.net>Dat ar 93 17:30:16 GMT ubject: Minimum allowable interatomic separationsFrom: sender@chemdcl.tau.ac.il (Senderowitz Hanoc : Tue, 9 Mar 93 10:52:25 -0500From: gallion@auriga.rose.brandeis.edu (steve gallion)Subject: grow ACS.OHIO-STATE.EDU>Subject: Software for PCDate: Fri, 12 Mar 93 04:51:15 GMTFrom: jim@quanta.phy. >Subject: PDB source file...Date: Sun, 14 Mar 93 11:06:13 +0100From: doelz@comp.bioz.unibas.ch (Re n, 15 Mar 1993 12:55 ESTFrom: HSUS@chemv2.mps.ohio-state.eduSubject: Problem with vibrational freq uk>Subject: MM2 code for UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UN Date: 17 Mar 93 16:18:00 EDTFrom: "STEPHEN R. HELLER" <srheller@asrr.arsusda.gov>Subject: software CETFrom: ZSYAMP01%EBCESCA1@OHSTVMA.ACS.OHIO-STATE.EDUSubject: First Congress of the ISTCP (pa :11 -0500Subject: Keep the noise down, pleaseDate: 19 Mar 93 11:37:00 ESTFrom: nauss@wrair-emh1.army.milSubject: Program called GRIDDate: Fri, 19 Mar 93 14:33:18 ESTFrom: Ge 23 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Announcing AMPAC 4.5Date: 21 Mar 1993 17:36:57 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Semic .milSubject: What about simulated annealing?Date: Wed, 24 Mar 93 14:11:32 +0100From: dufner@ws01.pc.chemie.th-darmstadt.de (Hagen Dufner)Subject: efg in g92From: "Christopher J ject: SC&A Conference speakers - thanksDate: Thu, 25 Mar 93 10:18:48 -0500From: au195@cleveland.freenet.edu (Dr. Gene A. Nelson)Subject: Batching files in MOPACFrom: zrfl0128@aw MO@CHEMNA.DICHI.UNINA.ITSubject: looking for ACES programFrom: Robert Laird <mbdtsr1@hpb.ch.man.ac.uk>Subject: Fe-O calculationDate: Mon, 29 Mar 93 15:49:03 BSTFrom: rafapa@obel uk>Subject: Polyrate QueryDate: Tue, 30 Mar 1993 19:31:32 +0200From: c62@aixfile1.urz.uni-heidelberg.de (Andreas Schulz)Subject: NBO analysesDate: Tue, 30 Mar 1993 16:04:42 - ulz)Subject: Stephen R. WilsonDate: Thu, 1 Apr 1993 16:33:29 +0200From: oles@gollum.uio.noSubject: BiosymDate: 01 Apr 1993 11:43:13 -0600 (CST)From: CUNDRARIT@memstvx1.memst.edu

Subject: Re: Taxol modellingDate: Fri, 1 Jan 93 14:11:05 ESTFrom: Francl Michelle M <mfrancl@cc.brynmawr.edu>Date: Mon, 4 Jan 93 12:33:36 -0800From: hcj@guil.uncc.edu (Harry C. kfz-heidelberg.de>Subject: energy contribution of hbonds?Date: 06 Jan 1993 10:55:29 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON_DOUGLAS_W@LILLY.COM>Subject: u : CADD videosDate: Wed, 6 Jan 93 13:03:33 -0800From: chiremvl@home.com!jeffb@uunet.UUNET (Jeff Blarey)Subject: Re: Polygon-based solvent accessible surfacesDate: Thu, 7 Jan 93 !!Date: 08 Jan 1993 09:19:39 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON_DOUGLAS_W@LILLY.COM>Subject: replies to my posting about PDB searching methodsDate: F vi@tiberius.tc.cornell.edu>From: scsupham@readino.ac.ukDate: Mon, 11 Jan 93 17:54:05 GMTSubject: DM01 questionsDate: Mon, 11 Jan 1993 14:33 ESTFrom: WILLIAMS%XRAY2@ulkvxv02.lou

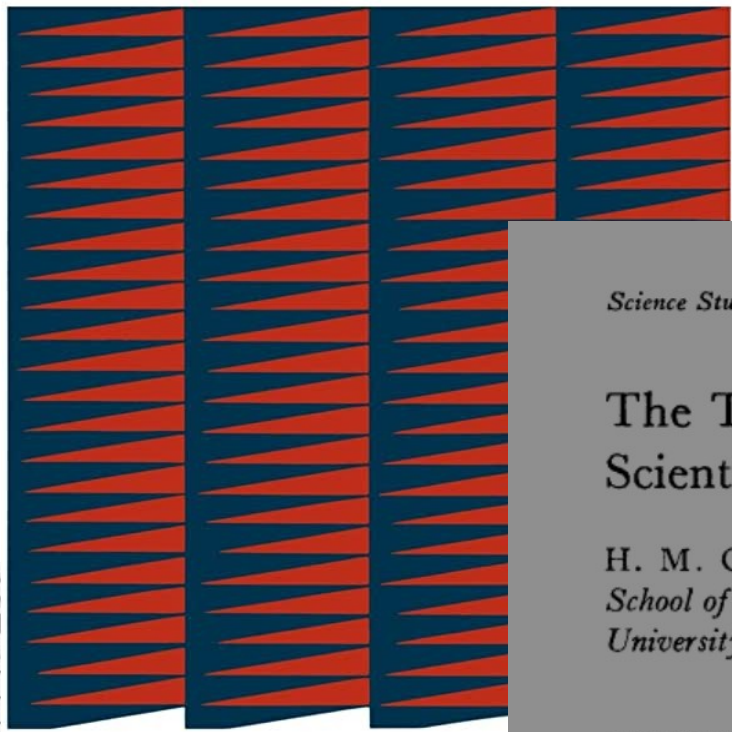
Histoire des sciences

CHANGING ORDER, Reproducible Research

*Replication and Induction
in Scientific Practice*

on University, Washington D.C.

9 Feb 2018



Science Studies, 4 (1974), 165-86.

The TEA Set: Tacit Knowledge and Scientific Networks

H. M. COLLINS
*School of Humanities and Social Sciences
University of Bath**

INTRODUCTION: METHODOLOGICAL AND THEORETICAL ARGUMENT

Thomas Kuhn's concept of 'paradigm'¹ has attracted a lot of attention from

H. M. COLLINS

With a new Afterword

g)Subject: Re: Hy
nl.govSubject: X-w
d.harvard.edu (jil
semiempirical calcu
n.desSubject: Exper
ate.Edu (Gene Car
lling Software: Dc
ar 93 17:30:16 GMT
secc.fi.cnr.itSubj
uplingDate: Tfr
r 1993 02:33:09 -C
MA.ACS.OHIO-STATE.
, 15 Mar 1993 21:5
ar 1993 13:58:36 -
st Girona Seminar
:11 -0500Subject: Keep the noise down, pleaseDate: 19 Mar 93 11:37:00 ESTFrom: nauss@wrair-emh1.army.milSubject: Program called GRIDDate: Fri, 19 Mar 93 14:33:18 ESTFrom: Ge
23 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Announcing AMPAC 4.5Date: 21 Mar 1993 17:36:57 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Semic
.milSubject: What about simulated annealing?Date: Wed, 24 Mar 93 14:11:32 +0100From: dufner@ws01.pc.chemie.th-darmstadt.de (Hagen Dufner)Subject: efg in g92From: "Christopher J
ject: SC&A Conference speakers - thanksDate: Thu, 25 Mar 93 10:18:48 -0500From: au195@cleveland.freenet.edu (Dr. Gene A. Nelson)Subject: Batching files in MOPACFrom: zrf10128@aw
MO@CHEMNA.DICHI.UNINA.ITSubject: looking for ACES programFrom: Robert Laird <mbdtsr1@hpb.ch.man.ac.uk>Subject: Fe-O calculationDate: Mon, 29 Mar 93 15:49:03 BSTFrom: rafapa@obel
uk>Subject: Polyrate QueryDate: Tue, 30 Mar 1993 19:31:32 +0200From: c62@aixfile1.urz.uni-heidelberg.de (Andreas Schulz)Subject: NBO analysesDate: Tue, 30 Mar 1993 16:04:42 -
ulz)Subject: Stephen R. WilsonDate: Thu, 1 Apr 1993 16:33:29 +0200From: oles@gollum.uio.noSubject: BiosymDate: 01 Apr 1993 11:43:13 -0600 (CST)From: CUNDARIT@memstvx1.memst.edu

oss
nd
ity.
are
nts

MacDate: Thu,
sDate: Thu, 2
anguage questio
1993 15:25:19
stryDate: Tue
Tue, 2 Mar 9
l@cc1.net>Dat
lerowitz Hanoc
Subject: grow
im@quanta.phy.
unibas.ch (Re
prational freq

uk>Subject: MM2 code for UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UN
Date: 17 Mar 93 16:18:00 EDTFrom: "STEPHEN R. HELLER" <srheller@asrr.arsusda.gov>Subject: Software
CETFrom: ZSYAMP01%EBCECA1@OHSTVMA.ACS.OHIO-STATE.EDUSubject: First Congress of the ISTCP (pa
Subject: Program called GRIDDate: Fri, 19 Mar 93 14:33:18 ESTFrom: Ge
Subject: efg in g92From: "Christopher J
Subject: Batching files in MOPACFrom: zrf10128@aw
Subject: Fe-O calculationDate: Mon, 29 Mar 93 15:49:03 BSTFrom: rafapa@obel
Subject: NBO analysesDate: Tue, 30 Mar 1993 16:04:42 -
Subject: BiosymDate: 01 Apr 1993 11:43:13 -0600 (CST)From: CUNDARIT@memstvx1.memst.edu

Subject: Re: Taxol modellingDate: Fri, 1 Jan 93 14:11:05 ESTFrom: Francis Michelle M <mfranc@cc.brynmawr.edu>Subject: u
kfz-heidelberg.de>Subject: energy contribution of hbonds?Date: 06 Jan 1993 10:55:29 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON_DOUGLAS_W@LILLY.COM>Subject: u
: CADD videosDate: Wed, 6 Jan 93 13:03:33 -0800From: chiremvl@andromeda.liaffh@unet.UU.NET (Jeff Blaney)Subject: Re: Polygon-based solvent accessible surfacesDate: Thu, 7 Jan 93
!!Date: 08 Jan 1993 09:19:39 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON_DOUGLAS_W@LILLY.COM>Subject: replies to my posting about PDB searching methodsDate: F
vi@tiberius.tc.cornell.edu>From: scsupham@reading.ac.ukDate: Mon, 11 Jan 93 17:54:05 GMTSubject: DMOI questionsDate: Mon, 11 Jan 1993 14:33 ESTFrom: WILLIAMS%XRAY2@ulkyvxo2.loui
or doubled messagesDate: Wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@watson.ibm.comSubject: data-flow programs for molecular modelingDate: wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@
GAMESS and MOPACDate: Thu, 14 Jan 1993 10:42:35 -0500 (EST)From: HERMAN@ULNA.BWH.HARVARD.EDUSubject: R

Histoire de la crise



THE TRUTH WEARS OFF? THE REPRODUCIBILITY CRISIS IN HISTORICAL PERSPECTIVE

Nicole C. Nelson
nicole.nelson@wisc.edu



Published: 28 March 2012


Drug development

Raise standards for preclinical cancer research

C. Glenn Begley & Lee M. Ellis 

Nature 483, 531–533 (2012) | [Cite this article](#)

235k Accesses | 1852 Citations | 2300 Altmetric | [Metrics](#)

 A [Clarification](#) to this article was published on 02 May 2012

Copyrighted Material
"A scorching indictment of drug companies and their research and business practices... tough, persuasive and troubling."
—JANET MASLIN, *The New York Times*

The Truth About the Drug Companies



HOW THEY DECEIVE US AND WHAT TO DO ABOUT IT

MARCIA ANGELL, M.D.

Former editor in chief of *The New England Journal of Medicine*
Winner of the Polk Award

Revised and updated
Includes tips on what you can do to protect your interests

Copyrighted Material
... (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Semic
dt.de (Hagen Dufner)Subject: efg in g92From: "Christopher J
A. Nelson)Subject: Batching files in MOPACFrom: zrfl0128@aw
alculationDate: Mon, 29 Mar 93 15:49:03 BSTFrom: rafapa@obe1
lz)Subject: NBO analysesDate: Tue, 30 Mar 1993 16:04:42 -
1993 11:43:13 -0600 (CST)From: CUNDARIT@memstvx1.memst.edu

The many faces of reproducibility: S. Leonelli

- Assumed degree of **control** over research conditions
 - choice of variables vs what can/should be stabilized
- Understanding of **variation**
 - phenomenon to be explained, confounder or signal of error?
- Dependence on **statistics** and **computation**
 - as inferential tools
- Precision of the research **goals**
 - from exploratory research to hypothesis testing
- Stability of **background knowledge** and evidence base
- Dependence on researchers' **judgment**
 - role of expertise and related training

Leonelli 2016, 2018

The many faces of reproducibility: S. Leonelli

1. Computational reproducibility
2. Direct experimental reproducibility (highly standardized experiments)
3. Scoping/Indirect/Hypothetical reproducibility (semi-standardized experiments)
4. Reproducible expertise
5. Reproducible observation

Leonelli 2018

The many faces of reproducibility: S. Leonelli

Type of Reproducibility	Assumed control	Dependence on statistics	Precision of goals	Dependence on judgement
Computational Reproducibility	total	high	high	none
Direct Experimental Reproducibility	high	high	high	low
Scoping/Indirect/Hypothetical Reprod.	limited	variable	limited	variable
Reproducible Expertise	variable	variable	variable	high
Reproducible Observation	low	low	low	high
Irreproducible Research	none	low	low	total

Overarching Gold standard

Published: 28 March 2012

Drug development

Raise standards for preclinical cancer research

C. Glenn Begley & Lee M. Ellis

Nature 483, 531–533 (2012) | [Cite this article](#)

235k Accesses | 1852 Citations | 2300 Altmetri

i A [Clarification](#) to this article was published on



OPEN ACCESS

ESSAY

Why Most Published Research Findings Are False

John P. A. Ioannidis

Published: August 30, 2005 • <https://doi.org/10.1371/journal.pmed.0020124>

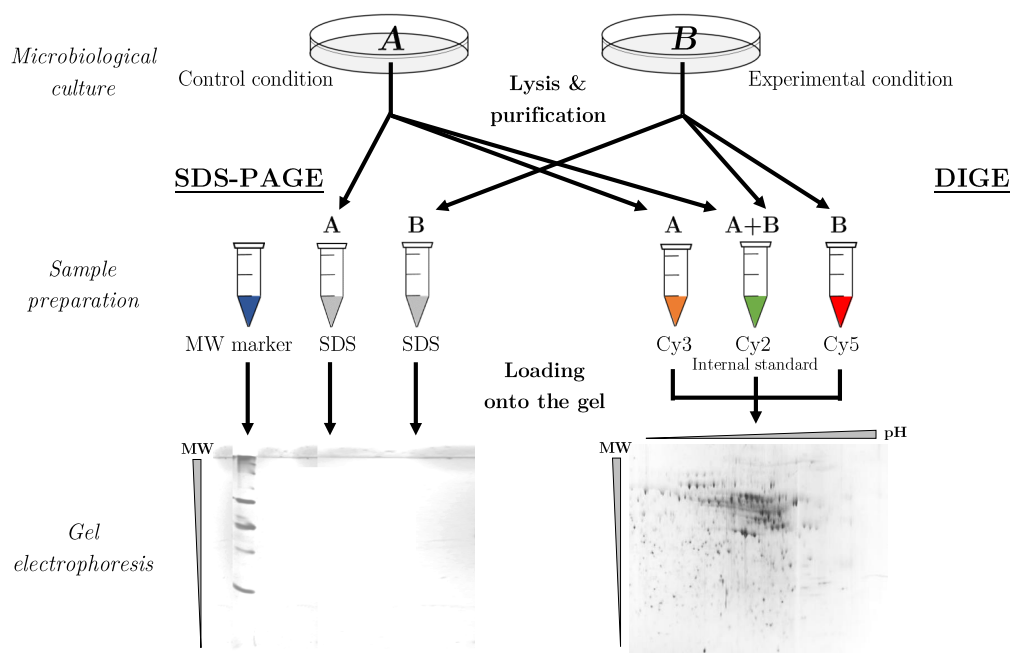
The Irreproducibility Crisis of Modern Science

Causes, Consequences, and the Road to Reform

David Randall Christopher Welsler

April 09, 2018

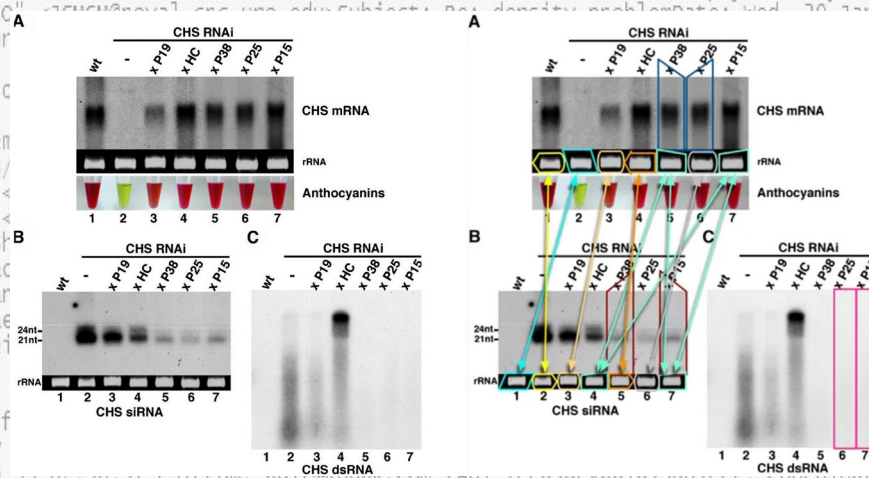
The many faces of gel electrophoresis



Visualization

Image analysis

- Visual band detection.
- Binary analysis (protein is/is not detected).
- No replicates.
- Computational spot detection.
- Calculation of abundance from normalized spot volume (Cy3/Cy2 and Cy5/Cy2) ratios.
- Statistical analysis of replicates.



12

The Voinnet Affair: Testing the Norms of Scientific Image Management

Catherine Guaspere and Emmanuel Didier

In the 1980s, it was already obvious that large companies were using metrics to track numerically the efficacy and efficiency of their employees. Management methods based on quantification gained widespread recognition during this decade (Camp, 1989; Hammer and Champy, 1993). Since the 2000s, these metrics seem to have migrated far beyond the borders of the corporate world, permeating the public bureaucracies of most liberal states, giving rise to what has come to be called the “New Public Management”.

Bibliographie

Autopromo

Hocquet, Alexandre, and Frédéric Wieber. 2021. "Epistemic Issues in Computational Reproducibility: Software as the Elephant in the Room." *Journal of Philosophy of Science* 11 (2): 38. <<https://doi.org/10.1007/s13194-021-00362-9>>

Wieber, Frédéric, and Alexandre Hocquet. 2020. "Models, Parameterization, and Software: Epistemic Opacity in Computational Chemistry." *Perspectives on Science* 28 (5): 610-29. <https://doi.org/10.1162/posc_a_00352>

Hocquet, Alexandre, and Frédéric Wieber. 2017. "'Only the Initiates Will Have the Secrets Revealed': Computational Chemists and the

Openness of Scientific Software." *IEEE Annals of the History of Computing* 39 (4): 40-58. <<https://doi.org/10.1109/MAHC.2018.1221048>>

Histoire des sciences

Barba Lorena A. 2018. "Terminologies for Reproducible Research." arXiv. <<http://arxiv.org/abs/1802.03311>>

Collins, H. M.: 1992. *Changing Order: Replication and Induction in Scientific Practice*. Chicago: University of Chicago Press.

Collins, H.M., and R.G. Harrison. 1975. "Building a TEA Laver: The Caprices of Communication." *Social Studies of Science* 5 (4): 441-50.

<<https://doi.org/10.1177/030631277500500404>>

Histoire de la crise

Begley, C. Glenn, and Lee M. Ellis. 2012. "Raise Standards for Preclinical Cancer Research." *Nature* 483 (7391): 531-33. <<https://doi.org/10.1038/483531a>>

Harvard University, dir.: 2019. *The Reproducibility Crisis in Historical Perspective* | Nicole C. Nelson | Radcliffe Institute. <<https://www.youtube.com/watch?v=DEZl0e0j9rs>>

Angell, Marcia. 2005. *The Truth about the Drug Companies: How They Deceive Us and What to Do about It: Rev. and Updated*. New York: Random House Trade Paperbacks.

The many faces of reproducibility

The Many Faces of Reproducibility - Sabina Leonelli. 2022. <<https://www.youtube.com/watch?v=dxlVk-4Llu8>>

Leonelli, Sabina. 2018. "Rethinking Reproducibility as a Criterion for Research Quality." *In Research in the History of Economic Thought and Methodology*. 36B:129-46 Emerald Publishing Limited. <<https://doi.org/10.1108/S0743-41542018000036B009>>

Overarching gold standard

Ioannidis, John P. A. 2005. "Why Most Published Research Findings Are False." *PLOS Medicine* 2 (8): e124. <<https://doi.org/10.1371/journal.pmed.0020124>>

"The Irreproducibility Crisis of Modern Science by Christopher Welsler | Report | NAS." n.d. Accessed March 8, 2023. <<https://www.nas.org/reports/the-irreproducibility-crisis-of-modern-science/full-report>>

The many faces of gel electrophoresis

Gaming the Metrics: Simulacrate and Manipulation in Academic Research. 2020. <<https://doi.org/10.7551/mitpress/11087.001.0001>>

Callaerts, Nephtali, Alexandre Hocquet, and Frédéric Wieber. n.d. "'Conducted Properly, Published Incorrectly': The Evolving Status of Gel Electrophoresis Images along Instrumental Transformations in Times of Reproducibility Crisis." *Berichte Zur Wissenschafts-Geschichte in revision* (Special Issue: The Circulation of Images in the Life Sciences 1800-present)

All images cited under fair use except when stated otherwise