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The geography of toxic inventions

Working Paper:
https://papers.ssrn.com/sol3/papers.cfm?abstract_id=3937284

Elisa Giuliani
(with Biggi G & Martinelli A)

RESINNREG

26 10 2021

IN SUPREMÆ DIGNITATIS 1343
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Introduction to the **talk**

- Innovation often seen as key for economic growth and catching up of poor countries
- Optimism about innovation as a fixer of grand sustainability challenges
- Evidence of unsustainable directionality of innovation (‘the dark side of innovation’; Coad et al., 2021)
  - Geography of Innovation Conference 2020: a dark side special session (with S. Iammarino)
  - More work needed to understand ‘dark innovations’

How Bill Gates aims to clean up the planet

An artists impression of what Carbon Engineering's ambitious direct air capture project would look like when completed. Photograph: Carbon Engineering

How Blockchain Could Help End Modern Day Slavery In Asia's Exploitative Seafood Industry

My own **journey**… to this talk

How companies impact development processes
Development not just econ growth (Sen,1999)

Articles

The noxious consequences of innovation: what do we know?

Gianluca Biggi & Elisa Giuliani

Pages 19-41 | Published online: 10 Feb 2020

How (small-scale) firms learn and innovate in developing countries (Giuliani & Bell, **2005**)

Cambridge Journal of Economics 2014, **38**, 479–517
doi:10.1093/cje/bet060
Advance Access publication 11 November 2013

Multinational corporations' economic and human rights impacts on developing countries: a review and research agenda

Elisa Giuliani and Chiara Macchi*

Why firms abuse human rights in the conduct of their business (Wettstein, Giuliani et al., **2019**)

Today’s **focus**

- **Pesticides** as dark innovations
- Environmental challenges: not all about climate change and circular economy!
- Environmental toxicity: a silent threat
  - Past exposure to toxic chemicals that bioaccumulate
  - Exposure to new chemicals
  - Chemical mixtures

SPECIAL SECTION CHEMISTRY FOR TOMORROW'S EARTH

REVIEW

Tracking complex mixtures of chemicals in our changing environment

Beate I. Escher[1,2]*, Heather M. Stapleton[3], Emma L. Schymanski[4]

Chemicals have improved our quality of life, but the resulting environmental pollution has the potential to cause detrimental effects on humans and the environment. People and biota are chronically exposed to thousands of chemicals from various environmental sources through multiple pathways. Environmental chemists and toxicologists have moved beyond detecting and quantifying single chemicals to characterizing complex mixtures of chemicals in indoor and outdoor environments and biological matrices. We highlight analytical and bioanalytical approaches to isolating, characterizing, and tracking groups of chemicals of concern in complex matrices. Techniques that combine chemical analysis and bioassays have the potential to facilitate the identification of mixtures of chemicals that pose a combined risk.

Motivation

- Exposure to toxic chemicals related to the emergence of numerous contemporary illnesses
  - Cancer
  - Neurodegenerative diseases
  - Endocrine regulation

  - Damages to ecosystems

- Huge liability for firms

Home ‣ News ‣ Business News

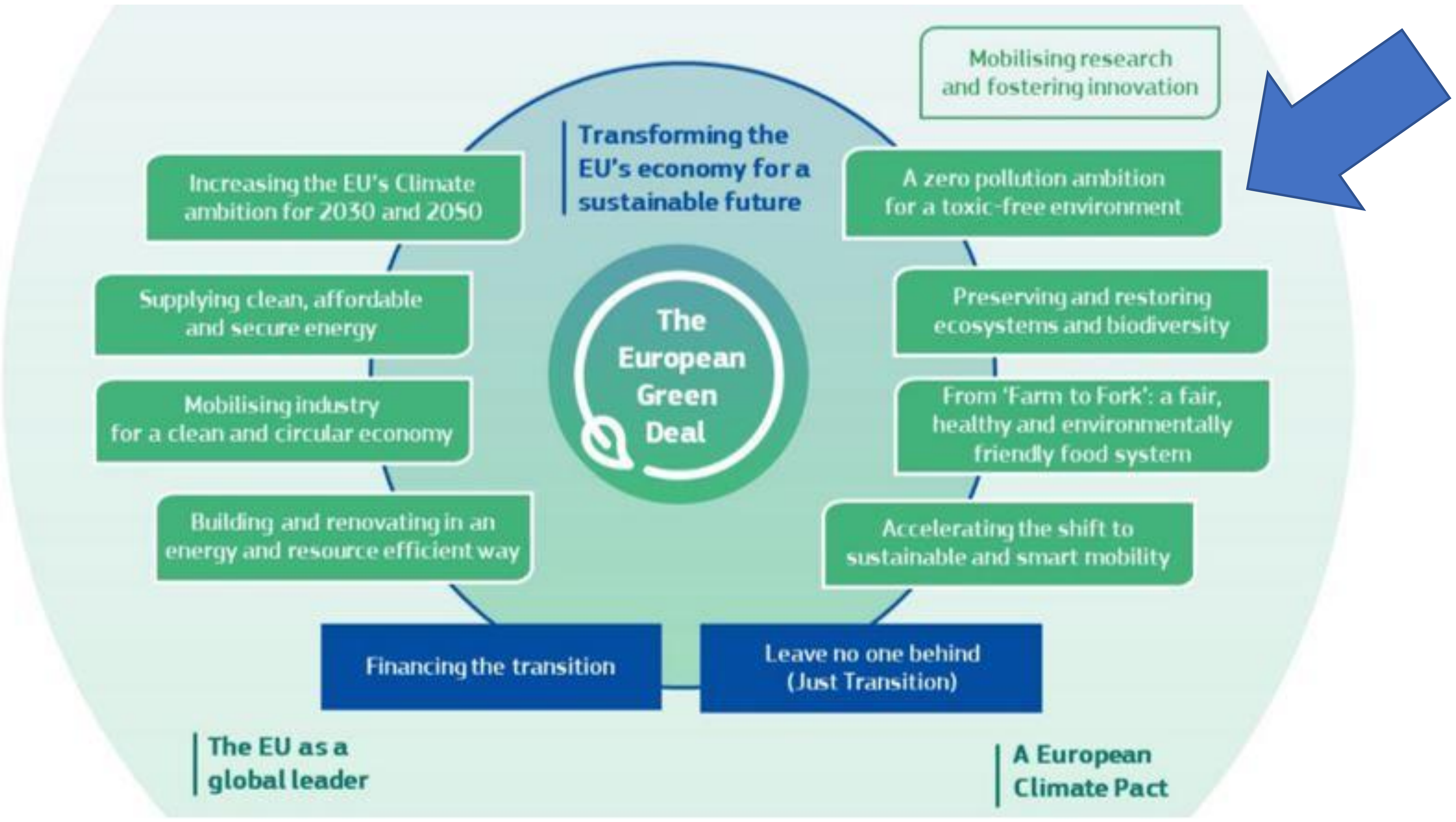
BAYER OFFERS UP TO $2 BILLION TO SETTLE FUTURE ROUNDUP LAWSUITS

By Chuck Abbott
2/4/2021

In its second proposal to settle future lawsuits that allege its Roundup weedkiller is carcinogenic, seed and ag-chemical giant Bayer said on Wednesday that it would pay up to $200 million to individual claimants and a maximum of $2 billion overall. The offer, which was submitted for approval to a U.S. district court judge in San Francisco, would cover lawsuits filed in the next four years.

"The class plan is intended to be one part of a holistic solution designed to provide further closure to the Monsanto Roundup litigation," said Bayer, based in Germany.

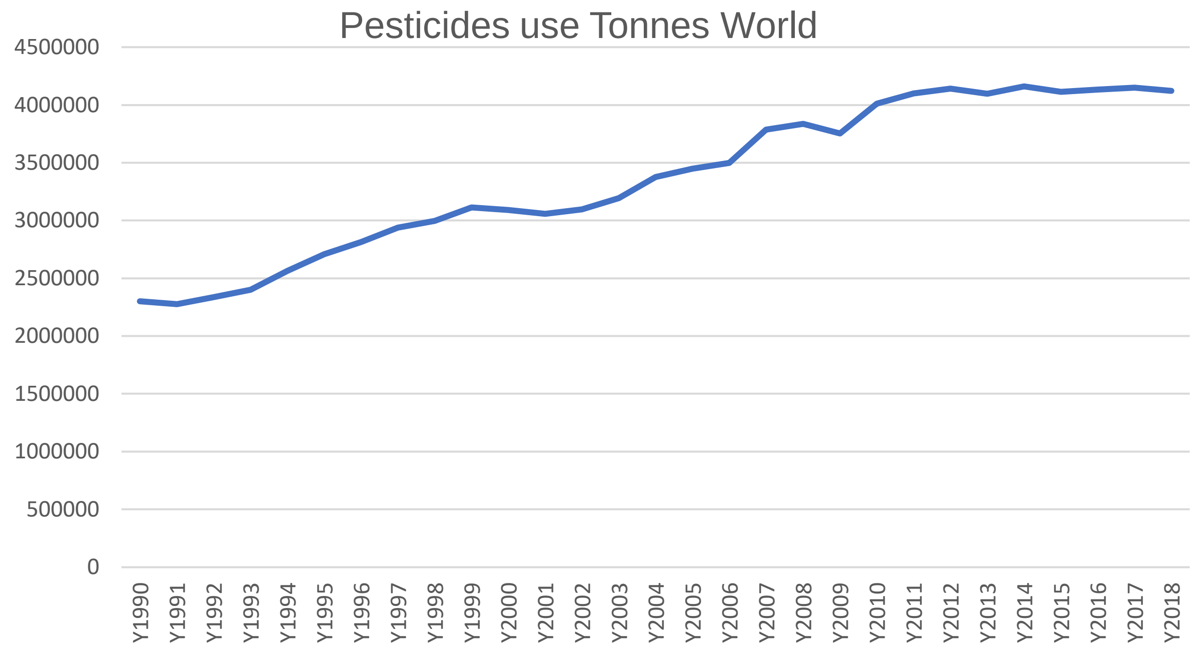
A problem of growing **policy relevance**



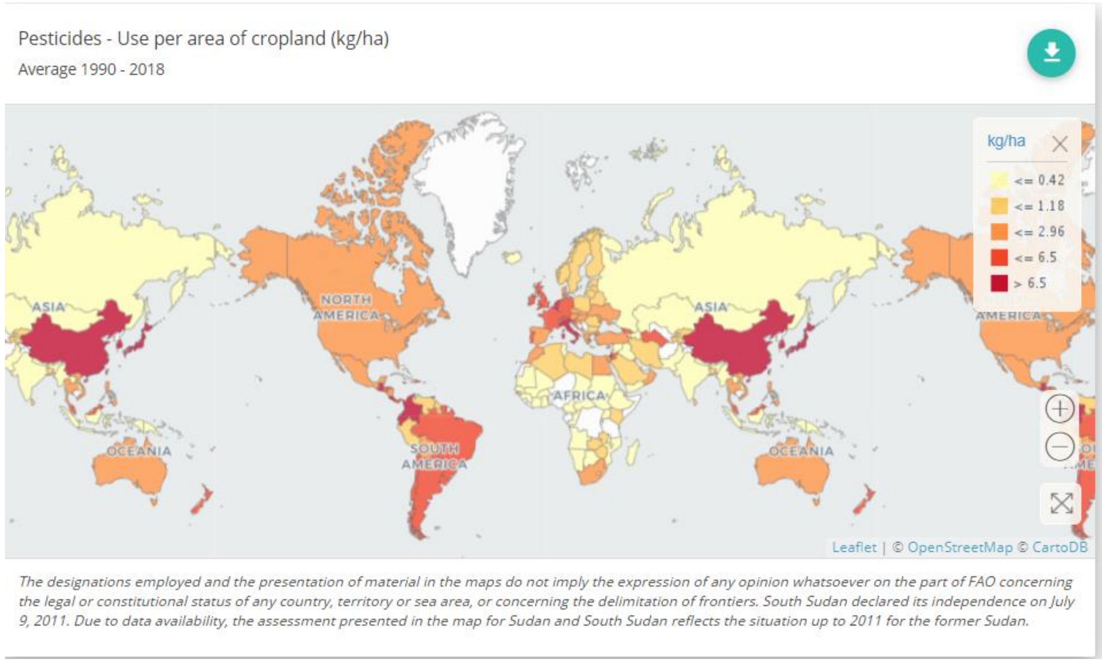
2020 EU GREEN DEAL

*"to achieve a toxic-free environment, and ensure that chemicals are produced and used in a way that maximises their contribution to society **while avoiding harm to the planet and to current and future generations**."*

Still an **open** problem



Source Own elaboration based on FAOStat 2020. The Pesticides Use database includes data on the use of major pesticide groups (Insecticides, Herbicides, Fungicides, Plant growth regulators and Rodenticides) and of relevant chemical families. Data report the quantities (in tonnes of active ingredients) of pesticides used in or sold to the agricultural sector for crops and seeds.



Source FAOStat 2020.

Pioneers of **scientific evidence**

- Early evidence of bioaccumulation properties of early pesticides (e.g. DDT) already in 1934 (Achilladelis et al 1987)
- Rachel Carlson (1962): *Silent Spring*
  - Focuses on a class of highly hazardous pesticides called **Persistent Organic Pollutants** (POPs) (persistent, travel long distance, highly toxic)
  - Prompted first regulatory steps in the US (e.g. EPA) and internationally

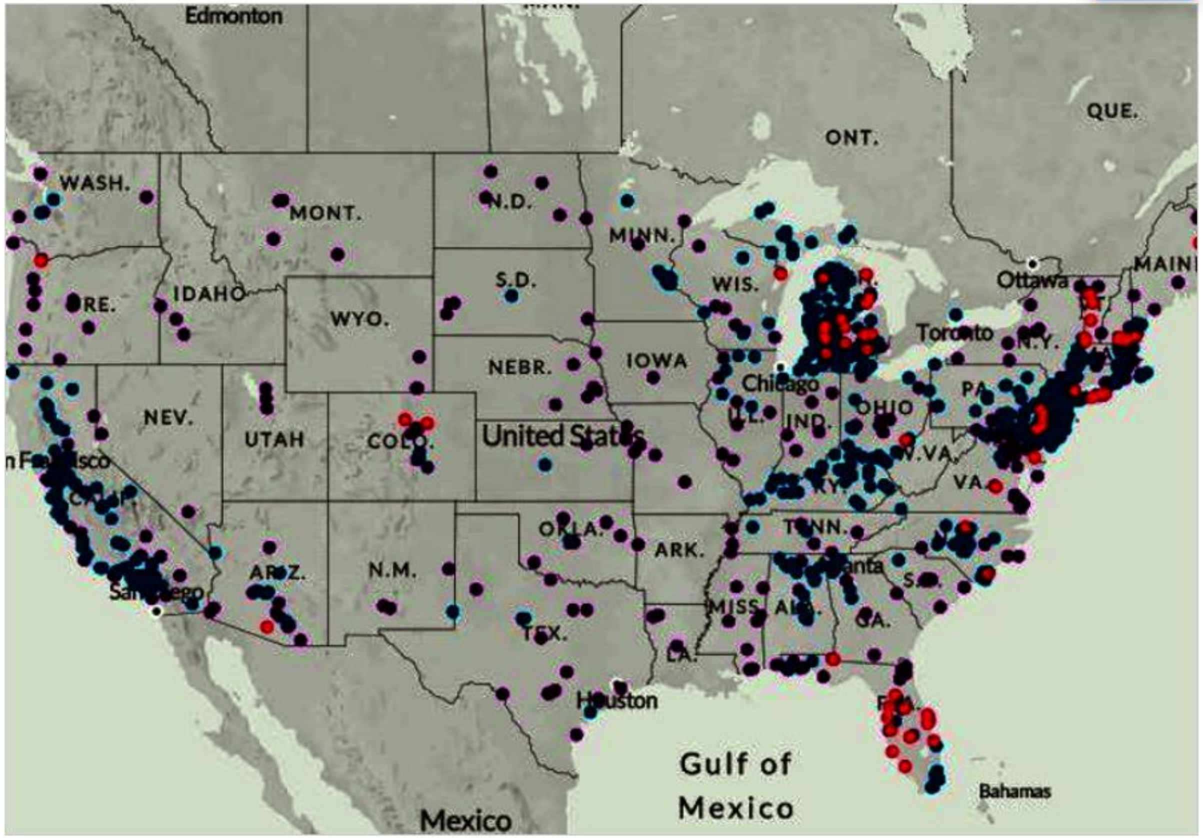
Carlson R (1962)

POPs rebranded as ‘**forever chemicals**’

US factories still discharging ‘forever chemicals’

PREMIUM

Published: 15 April 2020 Written by Simon Glover Print



The New York Times

A Move to Rein In Cancer-Causing ‘Forever Chemicals’

Michael Regan, the E.P.A. administrator, wants to limit a class of chemicals that has been linked to cancer and is found in everything from drinking water to furniture.

76

Milestones in the history of **POPs**

WW II

1962

After
Silent Spring
POPs become
a public
concern

1970s

US Environmental Protection Agency

US bans DDT in 1972

1992

1995

UNEP launched **International Working Group** to study POPs toxicity

2001-2004

Stockholm Convention
Signature and Ratification
12 POPs banned

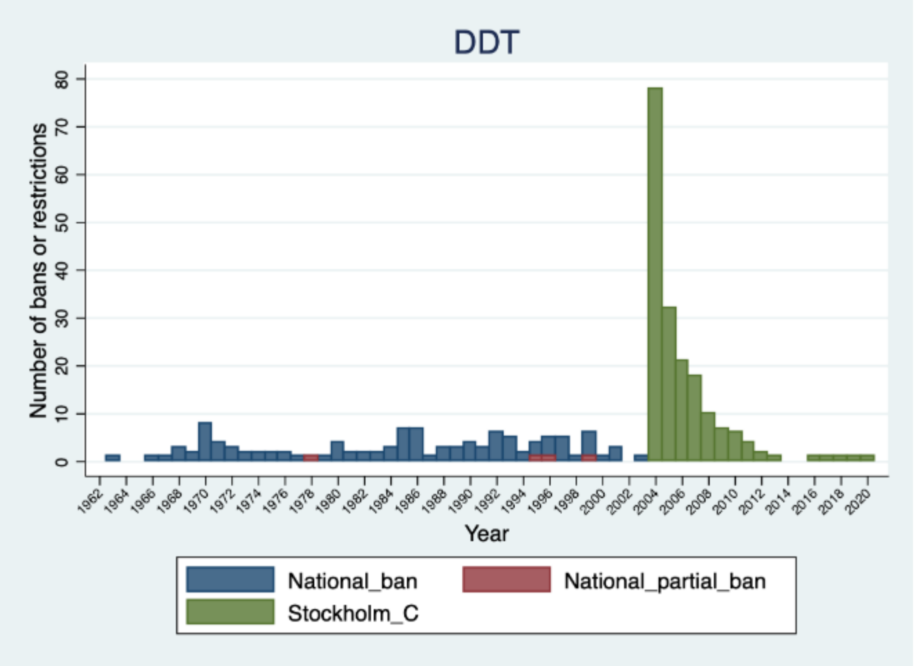
2017

Stockholm Convention bans **16 new POPs**

Regulations still imperfect

- Regulations have progressed
  - International treaties (e.g. Stockholm Convention on POPs)
  - Supra-national norms (EU REACH)
  - National norms
- But risk regulations are imperfect, slow and often subject to corporate lobby

  (Lynn, 1986; van Zwanenberg, 2020; van Zwanenberg et al., 2013; Coad et al., 2020; Millstone, 2015)
- Authorization processes based on industry evidence using GLP (good lab practices)



Note: 65,2% (120/184) of ratifying countries implemented national bans (including partial ban) before Stockholm Convention, 35% did not

This paper **goals**

- Temporal geography of pesticides
  - Which are the top patenting countries and regions?
  - How does the geography of inventions change over time?

- Focus on
  - Both the International Patent Class (IPC) of pesticides 1990-2017 and the sub-class of persistent organic pollutants (POPs)
  - top regions for pesticides inventions and compare their toxicity over time

Theory

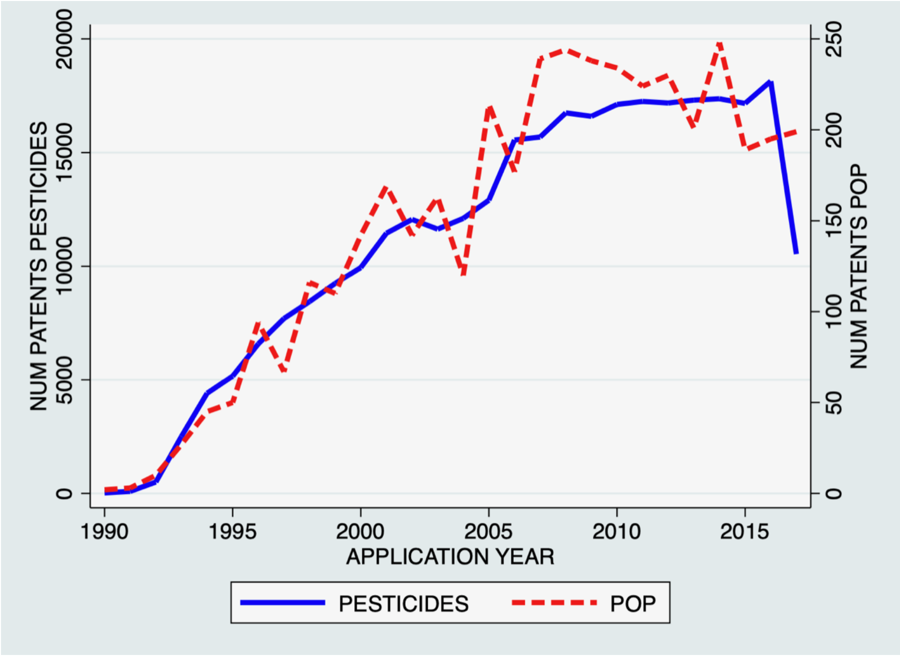
- Toxic pesticides are an increasingly socially contested category
- Vernon's (1966) product cycle theory, and the "pollution haven" hypothesis (e.g. Levinson and Taylor 2008), predict that poorer countries attract most of the polluting activities that are no longer allowed or socially accepted in richer countries
- Some developing countries have experienced technological catching up (Altenburg, Schmitz and Stamm, 2008) and have increased their R&D capacity

- We expect the **invention of (toxic) pesticides** to shift geography over time from s.c. Western countries to institutionally weaker countries (i.e. North to South)

Methodology

Methodology

- **Inventors' geo-localization:**
  - **Match** between initial set of over 93,000 pesticides patent families (IPC classes A01N and A01P - NACE class 20.2 – 'Manufacture of Pesticides and Other Agrochemical Products') from the **Derwent Chemistry Resources** (DCR) database & dataset **Rassenfosse et al. (2019)** to geo-localize inventors.
  - Geographical information for **37,503 patent families** between 1990 and 2017.
  - Sub-set of **POP inventions** based on the Stockholm Convention list of the 28 highly hazardous pesticides (**519** patent families 1990-2017)



Methodology

- Pesticides

(A01N and A01P)

- Dirty (high toxicity)
- Clean (low toxicity, green chemistry, etc.)

- Persistent Organic Pollutants (classified by the Stockholm Convention)

Methodology

- **How to identify dirty patents**
- **Toxicity analysis** on a **sample** of non-POP patent applications from top patenting regions (~ 4,000)
- Three steps (Biggi, Giuliani, Martinelli, Benfenati, *RP*, 2022):
  - Step 1. Match chemical compounds with patents
  - Step 2. Test the toxicity of chemical compounds in patent claims
  - Step 3. Measure patents toxicity

Research Policy 51 (2022) 104329

Contents lists available at ScienceDirect

Research Policy

journal homepage: www.elsevier.com/locate/respol

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Patent Toxicity

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ARTICLE INFO

Keywords:
Patents
Patent toxicity
Computational toxicology
QSAR models
Chemical inventions

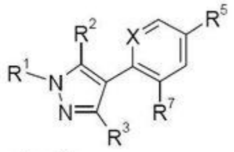
ABSTRACT

A toxic-free world is one of the goals of the European Green Deal and a key objective of the World Health Organization Inter-Organization Programme for the Sound Management of Chemicals. However, although use of some toxic chemicals is being banned, others continue to be developed. We consider this motivation for a closer examination of the toxicity of chemical inventions. We combine patent analysis with computational toxicology and develop a methodological roadmap to measure patent toxicity, that is, the extent to which a patent includes "components" (or compounds) that are toxic to humans and/or the environment. To illustrate our proposed methodology, we analyse the toxicity of ten well-known hazardous chemicals and compare it against that of other groups of chemical patents. We suggest that the measurement of patent toxicity opens up interesting avenues for future research with, potentially, strong policy implications.

Step 1 Chemical patenting

- In chemical industry, firms try to ‘patent block’ rivals from patenting or entering in their markets through Markush claim
  - A shorthand way of describing multiple different chemical constructions that achieve the same or comparable function

- The claim section account for the extent (i.e. the scope) of the protection sought in a patent document (Bekkers et al., 2016; Jayaraj and Gittelman, 2018; Kuhn and Thompson, 2019; Marco et al. 2016).



(I)

wherein

R^1 is C_1-C_4alkyl or C_1-C_4haloalkyl;

R^2 is an optionally substituted aryl or heteroaryl;

R^3 is halogen;

R^4 is hydrogen, halogen, C_1-C_4 alkyl, C_1-C_4 haloalkyl, cyano or OR^6;

R^5 is hydrogen, halogen, C_1-C_4 alkyl, C_1-C_4 haloalkyl, cyano or OR^6;

R^6 is hydrogen, C_1-C_6 alkyl, C_3-C_7 cycloalkyl, C_3-C_{10} alkylcycloalkyl, C_1-C_6 haloalkyl, C_2-C_6 alkenyl, C_2-C_6 haloalkenyl, C_3-C_7 cycloalkenyl, C_2-C_6 alkynyl, C_2-C_6 haloalkynyl, C_2-C_6 alkyloxyalkyl;

R^7 is halogen or OR^6;

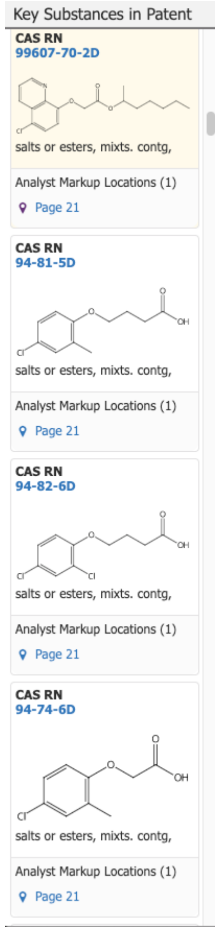
X is N or C-R^4;

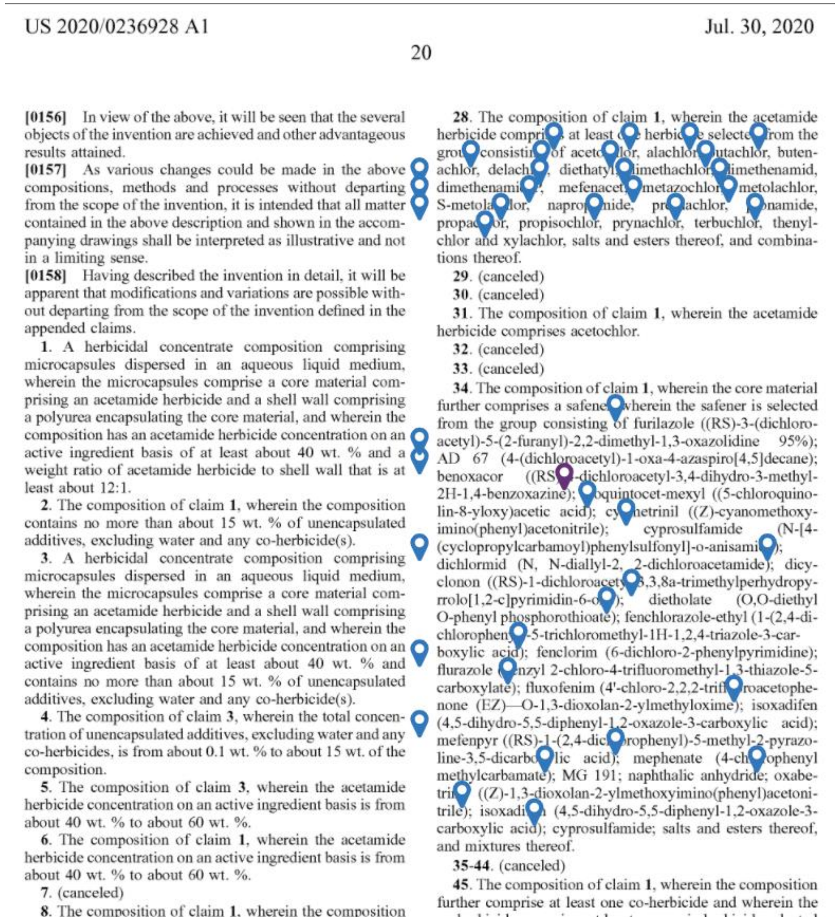
or an agrochemically usable salt form thereof.

Example of Markush claim: R1-R7 are are placeholders that can accept different chemical groups for each position. In this case R1 has 2 options while R3 have only 1 option. Instead of listing all the possible combinations, the Markush structure efficiently captures this combinatorial set of novel compounds

Step 1 Match chemicals w/ patents

- Sources
  - Derwent Chemistry Resources (Clarivate)
  - SciFinder (CAS)
  - Reaxys (Elsevier)
  - SCRIPDB (University of Toronto)
  - SureChEMBL (European Molecular Biology Laboratory)
- Patent-compounds association
- Compounds are specified through international identifiers
- Exact location the in a specific section (title, abstract, description or claims)





US 2020/0236928 A1 Jul. 30, 2020

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[0156] In view of the above, it will be seen that the several objects of the invention are achieved and other advantageous results attained.

[0157] As various changes could be made in the above compositions, methods and processes without departing from the scope of the invention, it is intended that all matter contained in the above description and shown in the accompanying drawings shall be interpreted as illustrative and not in a limiting sense.

[0158] Having described the invention in detail, it will be apparent that modifications and variations are possible without departing from the scope of the invention defined in the appended claims.

1. A herbicidal concentrate composition comprising microcapsules dispersed in an aqueous liquid medium, wherein the microcapsules comprise a core material comprising an acetamide herbicide and a shell wall comprising a polyurea encapsulating the core material, and wherein the composition has an acetamide herbicide concentration on an active ingredient basis of at least about 40 wt. % and a weight ratio of acetamide herbicide to shell wall that is at least about 12:1.

2. The composition of claim 1, wherein the composition contains no more than about 15 wt. % of unencapsulated additives, excluding water and any co-herbicide(s).

3. A herbicidal concentrate composition comprising microcapsules dispersed in an aqueous liquid medium, wherein the microcapsules comprise a core material comprising an acetamide herbicide and a shell wall comprising a polyurea encapsulating the core material, and wherein the composition has an acetamide herbicide concentration on an active ingredient basis of at least about 40 wt. % and contains no more than about 15 wt. % of unencapsulated additives, excluding water and any co-herbicide(s).

4. The composition of claim 3, wherein the total concentration of unencapsulated additives, excluding water and any co-herbicides, is from about 0.1 wt. % to about 15 wt. of the composition.

5. The composition of claim 3, wherein the acetamide herbicide concentration on an active ingredient basis is from about 40 wt. % to about 60 wt. %.

6. The composition of claim 1, wherein the acetamide herbicide concentration on an active ingredient basis is from about 40 wt. % to about 60 wt. %.

7. (canceled)

8. The composition of claim 1, wherein the composition

28. The composition of claim 1, wherein the acetamide herbicide compri[illegible] at least [illegible] herbi[illegible] selecte[illegible] from the grou[illegible] consisti[illegible] of aceto[illegible]lor, alachlor, [illegible]utachlor, butenachlor, delach[illegible], diethatyl[illegible]imethachlor[illegible]imethenamid, dimethenami[illegible], mefenacet, metazochlor, metolachlor, S-metola[illegible]lor, napro[illegible]mide, pr[illegible]achlor, [illegible]namide, propa[illegible]or, propisochlor, prynachlor, terbuchlor, thenylchlor and xylachlor, salts and esters thereof, and combinations thereof.

29. (canceled)

30. (canceled)

31. The composition of claim 1, wherein the acetamide herbicide comprises acetochlor.

32. (canceled)

33. (canceled)

34. The composition of claim 1, wherein the core material further comprises a safene[illegible] wherein the safener is selected from the group consisting of furilazole ((RS)-3-(dichloroacetyl)-5-(2-furanyl)-2,2-dimethyl-1,3-oxazolidine 95%); AD 67 (4-(dichloroacetyl)-1-oxa-4-azaspiro[4,5]decane); benoxacor ((RS[illegible]-dichloroacetyl-3,4-dihydro-3-methyl-2H-1,4-benzoxazine); [illegible]oquintocet-mexyl ((5-chloroquinolin-8-yloxy)acetic acid); cy[illegible]metrinil ((Z)-cyanomethoxyimino(phenyl)acetonitrile); cyprosulfamide (N-[4-(cyclopropylcarbamoyl)phenylsulfonyl]-o-anisami[illegible]); dichlormid (N, N-diallyl-2, 2-dichloroacetamide); dicyclonon ((RS)-1-dichloroacety[illegible]3,3,8a-trimethylperhydropyrrolo[1,2-c]pyrimidin-6-o[illegible]); dietholate (O,O-diethyl O-phenyl phosphorothioate); fenchlorazole-ethyl (1-(2,4-dichlorophen[illegible]-5-trichloromethyl-1H-1,2,4-triazole-3-carboxylic acid); fenclorim (6-dichloro-2-phenylpyrimidine); flurazole ([illegible]nzyl 2-chloro-4-trifluoromethyl-1,3-thiazole-5-carboxylate); fluxofenim (4'-chloro-2,2,2-trifl[illegible]roacetophenone (EZ)—O-1,3-dioxolan-2-ylmethyloxime); isoxadifen (4,5-dihydro-5,5-diphenyl-1,2-oxazole-3-carboxylic acid); mefenpyr ((RS)-1-(2,4-dic[illegible]rophenyl)-5-methyl-2-pyrazoline-3,5-dicarbo[illegible]lic acid); mephenate (4-ch[illegible]ophenyl methylcarbamate); MG 191; naphthalic anhydride; oxabetri[illegible] ((Z)-1,3-dioxolan-2-ylmethoxyimino(phenyl)acetonitrile); isoxadi[illegible] (4,5-dihydro-5,5-diphenyl-1,2-oxazole-3-carboxylic acid); cyprosulfamide; salts and esters thereof, and mixtures thereof.

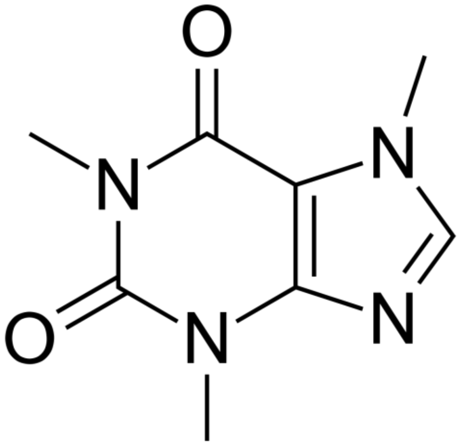
35-44. (canceled)

45. The composition of claim 1, wherein the composition further comprise at least one co-herbicide and wherein the

Step 1 Compound identifiers

Caffeine

Caffeine compound structure



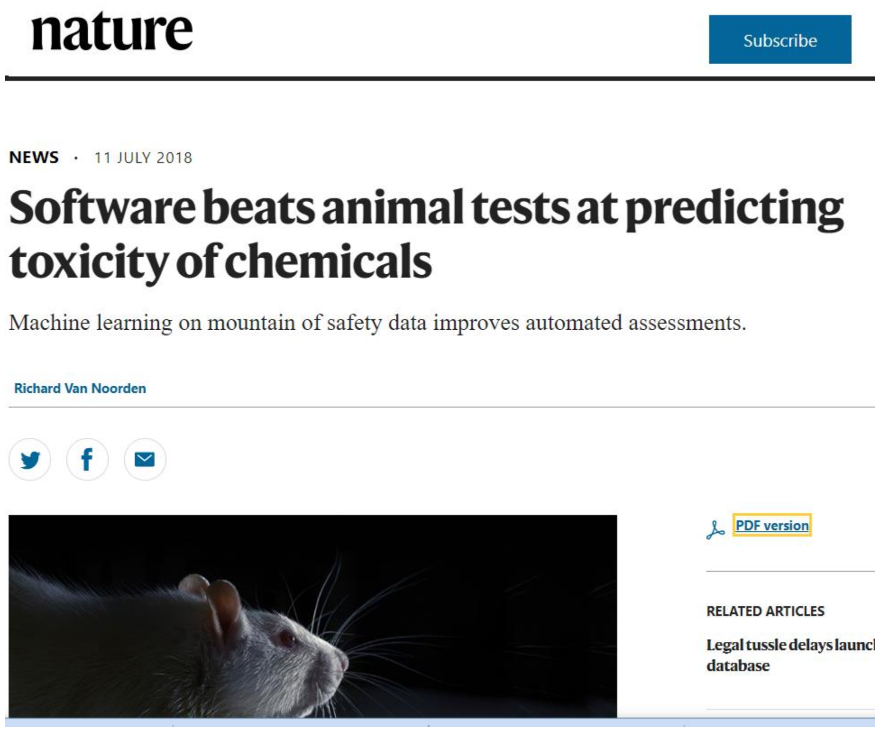
Caffeine compound identifiers

- CAS Registry Number: 58-08-2
- SMILES: CN1C=NC2=C1C(=O)N(C(=O)N2C)C
- InChIKey: RYYVLZVUVIJVGH-UHFFFAOYSA-N

Step 2 Toxicity test

- Test the toxicity of chemical compounds in patent claims (in vivo, in vitro, in silico)
- In silico toxicology: computational methods to assess potential toxicity

- **Quantitative Structure-Activity Relationship** (QSAR) models to predict potential toxicity based on the physiochemical properties and/or structural properties of the chemicals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Software beats animal tests at predicting toxicity of chemicals

Machine learning on mountain of safety data improves automated assessments.

Richard Van Noorden

PDF version

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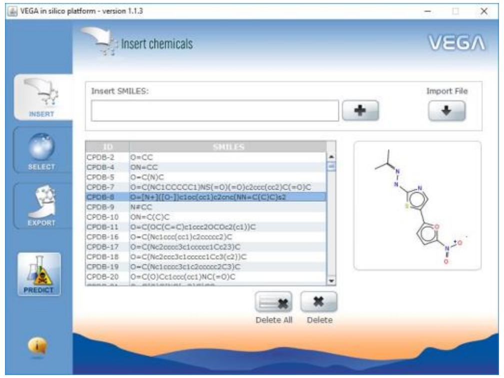
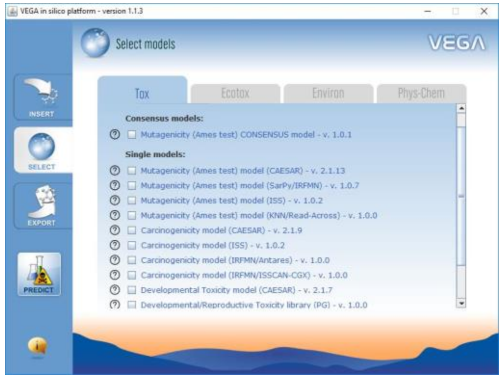
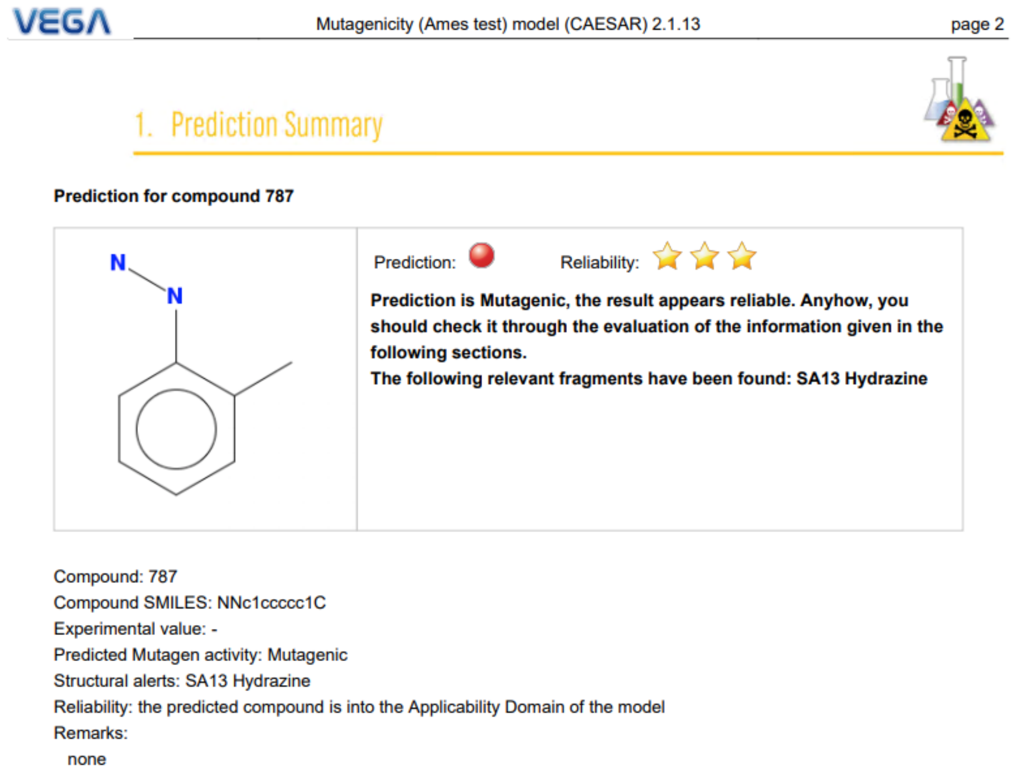
Step 2 Toxicity test

- **Toxicity endpoints**
  - On humans and natural environment

- **Here focus on human health toxicity - CMR**:
  - Carcinogenicity
  - Mutagenicity
  - Reprotoxicity
- **CMR** make the first and most toxic category of the **toxicity** classes







VEGA Mutagenicity (Ames test) model (CAESAR) 2.1.13 page 2

1. Prediction Summary

Prediction for compound 787

Prediction: Reliability:

Prediction is Mutagenic, the result appears reliable. Anyhow, you should check it through the evaluation of the information given in the following sections.
The following relevant fragments have been found: SA13 Hydrazine

Compound: 787
Compound SMILES: NNc1ccccc1C
Experimental value: -
Predicted Mutagen activity: Mutagenic
Structural alerts: SA13 Hydrazine
Reliability: the predicted compound is into the Applicability Domain of the model
Remarks:
none

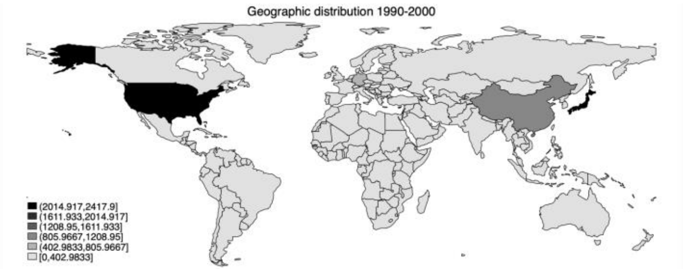
Step 3 Patent Toxicity

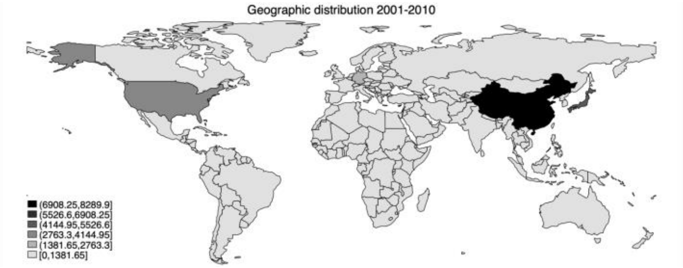
- Aggregate compounds' potential toxicity at the patent level
- A patent may include several chemical compounds in the claim
    - Active ingredient; reagent; excipient; catalyst
- Patent-level measures
    - Total Count Toxicity= Number of chemical compounds in the patent claim that are flagged as CMR toxic with high reliability

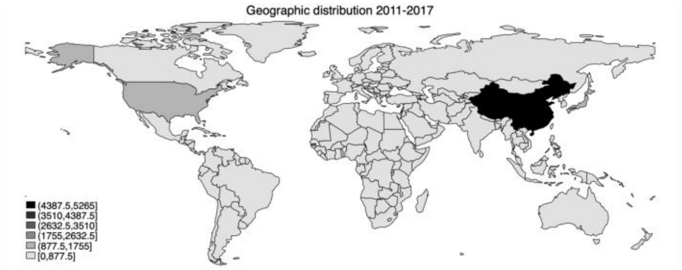
Results

All pesticides
POP pesticides
CMR pesticides (sample)

The **geography** of pesticides inventions



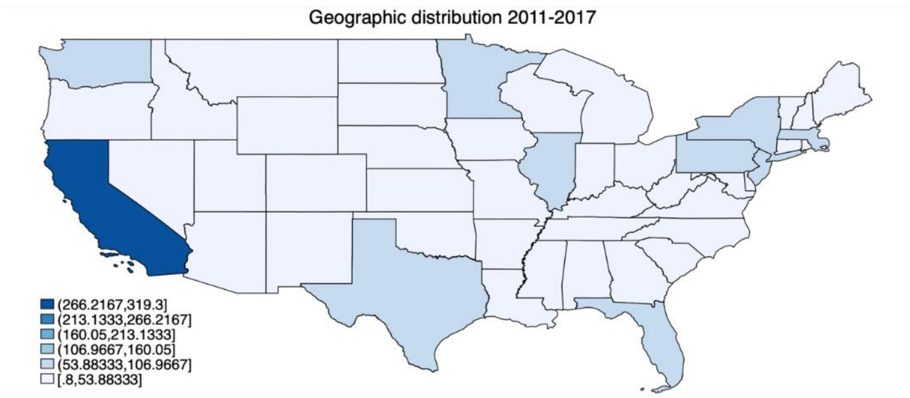


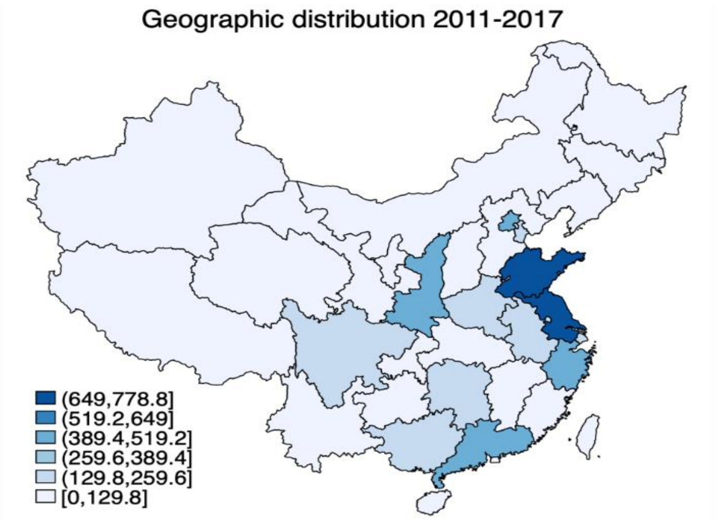


Top 4 inventing countries for pesticides-related patent families by period

Timespan	Country	Ranking	Number of patent families
1990-2000	USA	1	2570
	JPN	2	2183
	CHN	3	878
	DE	4	845
2001-2010	CHN	1	8350
	JPN	2	4595
	USA	3	4198
	DE	4	1814
2011-2017	CHN	1	5320
	USA	2	1539
	JPN	3	945
	DE	4	412

Regional focus in top inventing countries



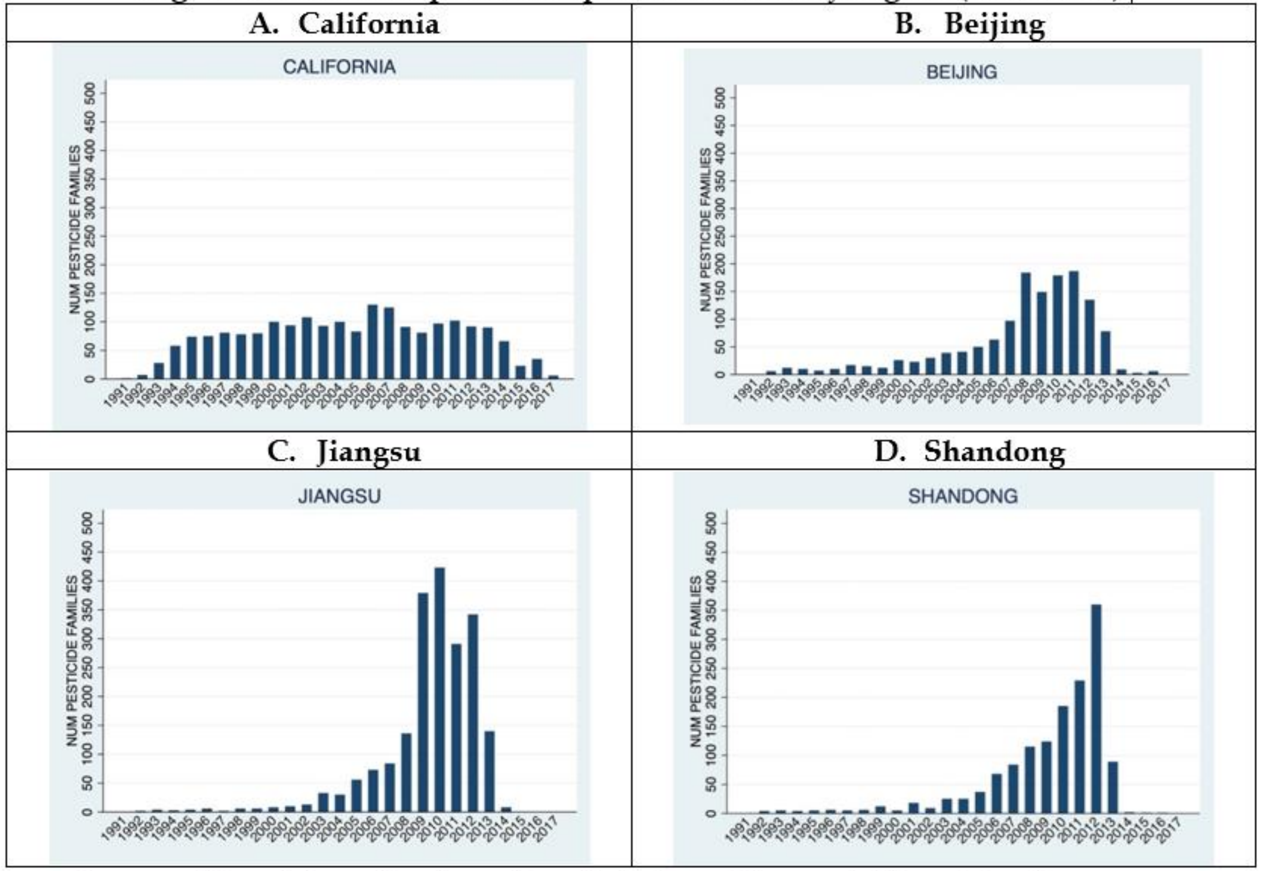


California		
Assignee Name	Number of patent families (1990-2017)	Share over the total
BAYER CROPSCIENCE AG	134	6,71%
UNIV CALIFORNIA	131	6,56%
BASF SE	82	4,11%
DOW AGROSCIENCES LLC	69	3,46%
SYNGENTA PARTICIPATIONS AG	47	2,35%
DU PONT DE NEMOURS&CO E I	38	1,90%
US SEC OF AGRIC	36	1,80%
MYCOGEN CORP	35	1,75%
ALLERGAN SALES INC	35	1,75%
DEPUY SYNTHES PROD LLC	35	1,75%

Jiangsu		
Assignee Name	Number of patent families (1990-2017)	Share over the total
JIANGSU HUIFENG Agrochemicals	503	24,45%
NANJING NO 1 Pesticides Group	165	8,02%
UNIV NANJING AGRIC	115	5,59%
NANTONG BAOYE CHEM CO LTD	77	3,74%
NANJING KABO BIOTECHNOLOGY CO LTD	75	3,65%
JIANGSU AGRIC ACAD SCI	70	3,40%
SUZHOU PACH FINE CHEM CO LTD	47	2,28%
ZHANG ZHI GAO	38	1,85%
ZHENJIANG VICTOR PHARM CO LTD	37	1,80%
CHANGSHU HENGMAO TRADE CO LTD	31	1,51%

Regional focus in top inventing countries
All pesticides

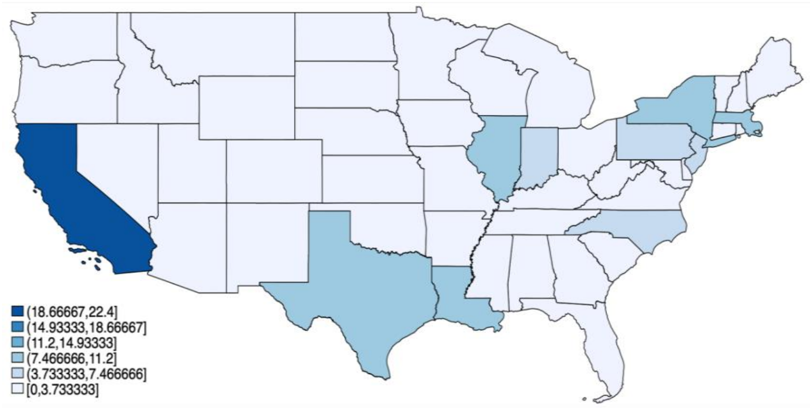
Figure 5: Trends in pesticides patent families by region (1990-2017)

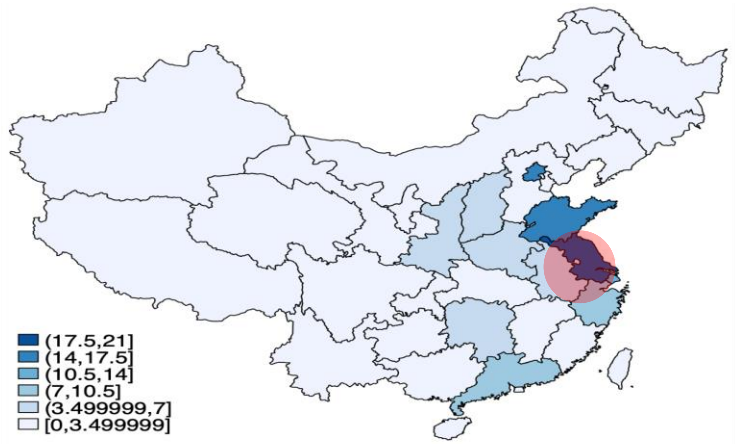


Source: Our elaboration based on data from Derwent Chemistry Resources.

Regional focus in top inventing countries

POP pesticides



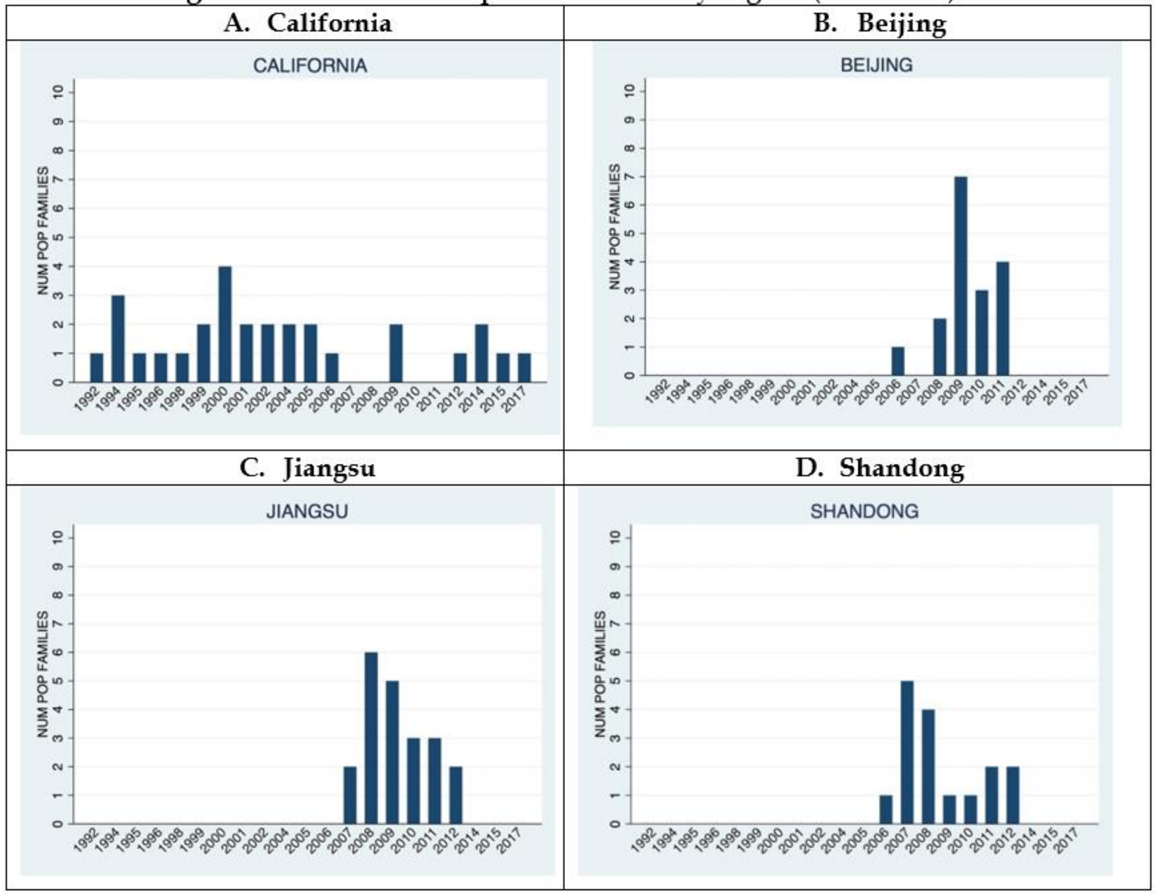


Patent Application US2017035051 (filed USPTO by Syngenta in 2017) describes "*mixtures of pesticidally active ingredients and methods of using the mixtures in the field of agriculture*" and it claims the use of an "*organochlorine compound including those selected from the group consisting of endosulfan (in particular alpha-endosulfan), benzene hexachloride, DDT, chlordane and dieldrin*"

Regional focus in top inventing countries

POP pesticides

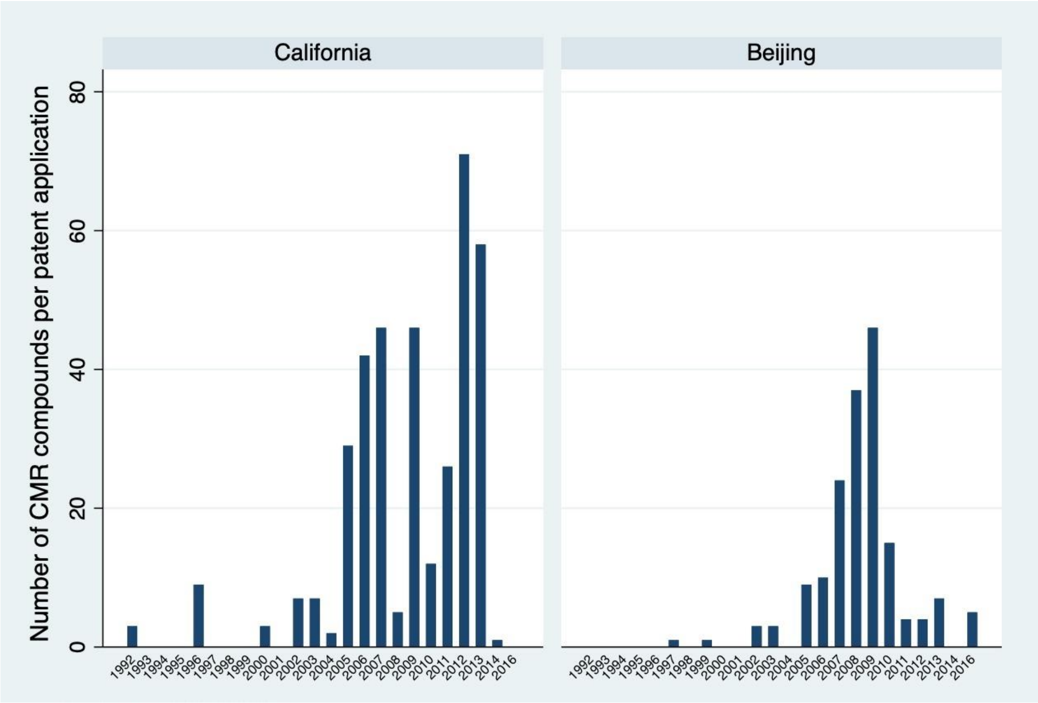
Figure 8: Trends in POP patent families by region (1990-2017)



Source: Our elaboration based on data from Derwent Chemistry Resources.

CMR toxicity of top inventing regions

CMR= carcinogenic, mutagenic, reprotoxic



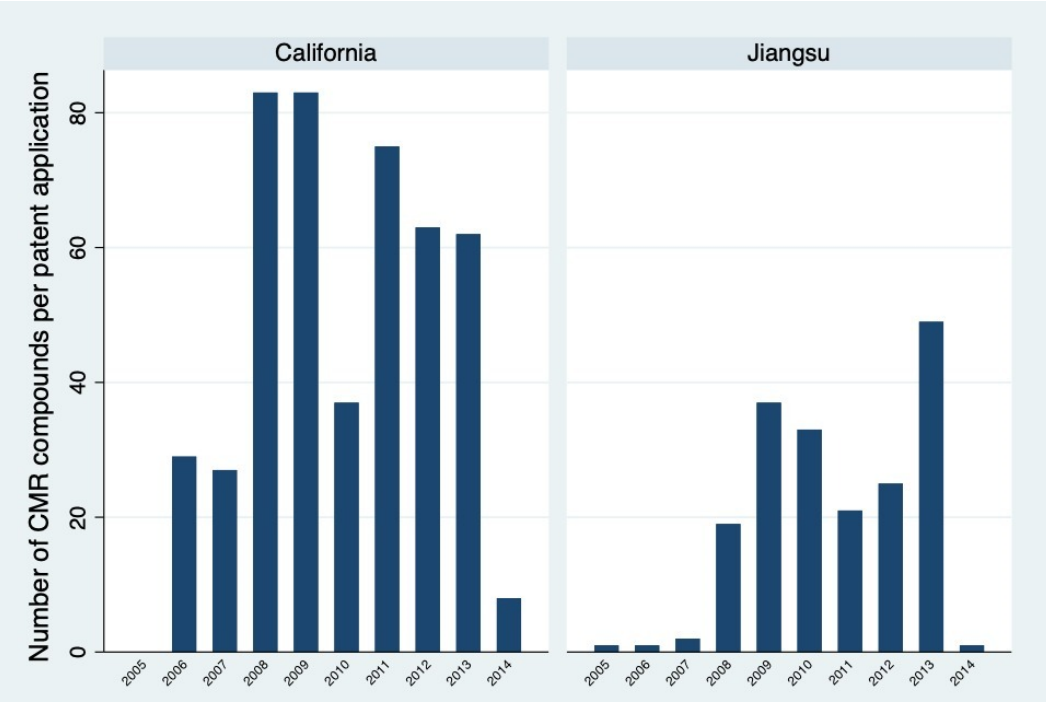


Table 3: Patents toxicity analyses: California vs. three Chinese provinces (1990-2017)

PANEL A		Carcinogenic Toxicity	Mutagenic Toxicity	Reproductive Toxicity	CMR Toxicity+
California	Cumulative number of compounds in patent claims	181	108	206	367
Beijing	Cumulative number of compounds in patent claims	50	48	104	169

California	Average number of compounds per patent family (Std. Dev.)	1.81 (3.97)	1.08 (3.42)	2.06 (4.85)	3.67 (7.57)
Beijing	Average number of compounds per patent family (Std. Dev.)	0.49 (1.01)	0.47 (1.34)	1.01. (3.14)	1.65. (3.71)
	p-value	(3.25)***	(1.67)*	(1.81)*	(2.42)**

California	Average number compounds per patent family considering all IPR legislations (Std. Dev.)	39.32 (168.01)	31.45 (146.93)	43.8 (199.78)	74.6 (288.39)
Beijing	Average number compounds per patent family considering all IPR legislations (Std. Dev.)	1.10 (2.96)	1.26 (6.15)	2.18 (6.46)	3.71(10.79)
	p-value	(2.96)**	(2.07)**	(2.10)**	(2.48)**

California/Beijing ratio	Cumulative compounds in patent claims	3.62	2.25	1.98	2.17
California/Beijing ratio	Average number compounds per patent family considering all IPR legislations	35.74	24.96	20.09	20.10

Note: p-values *** p<0.01; ** p<0.05; * p<0.1. For this analysis we compare two random samples of patents invented in California and in one of the three Chinese regions. The two random samples are matched on the filing date. (+) A compound can be classified as CMR Toxic if it results to be Carcinogenic, or Mutagenic or Reprotox or all three.

Discussion

- Stigmatized and banned categories – i.e. pesticides and POPs follow the prediction of a shifting geography of inventions from North to South (US/J/EU to China)
- The less apparent (and harder to contest) patent features in terms of CMR toxicity follow a different logic:
  - Not fully displaced to China
  - The US/California retains leadership in CMR toxic pesticides
  - IPR appropriation of California invented patents is in a bigger set of jurisdictions: Chinese inventions are for domestic use, US inventions are for global use

Conclusions

- Pesticides as dark innovations: some are ‘categorized’ and others are ‘in the making’ –two **different** geographies

- Changing geography, but persistence in toxic inventions can slow down the achievement of sustainability goals (e.g. toxic free environment)

- Contribution to the dark side of innovation, new methods to identify what is not easily visible