Accelerating Innovation at the Confluence of Human-Curated Content and Artificial Intelligence

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www.cas.org

Mark R. Grabau
Chief Analytics Officer, CAS

Accelerating innovation improves human outcomes

- Cure diseases
- Save resources
- Improve quality of life

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Data is both a blessing and a curse to innovation

The Data Paradox

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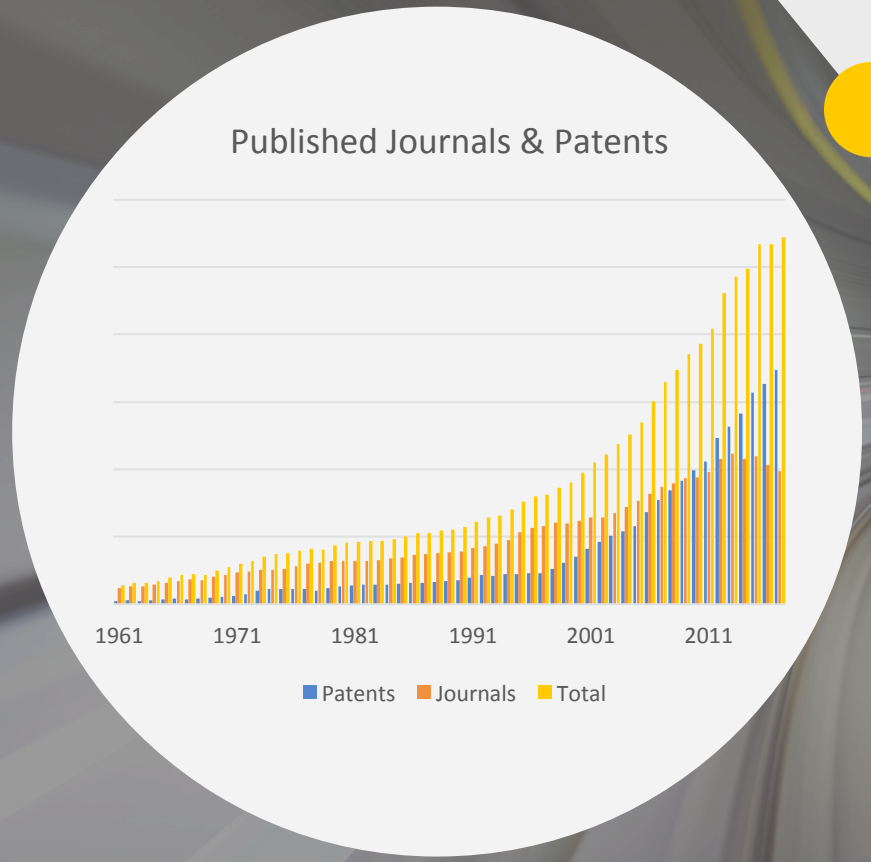
Increasing volume, complexity and connections in the information landscape require new solutions



- Volume
- Complexity
- Connectedness

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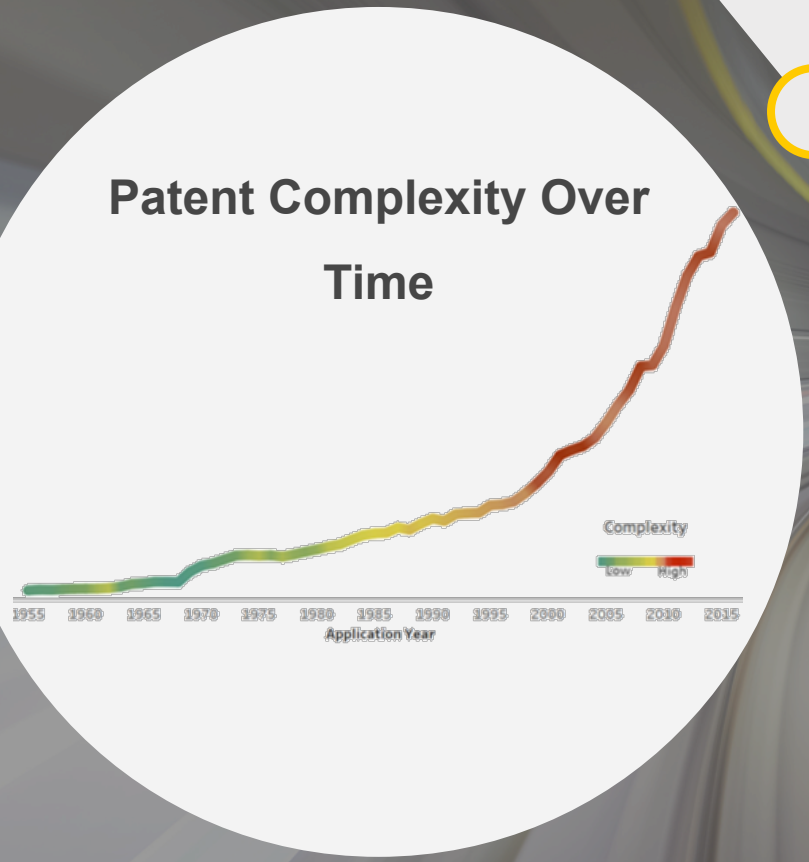
Increasing volume, complexity and connections in the information landscape require new solutions



- Volume
- Complexity
- Connectedness

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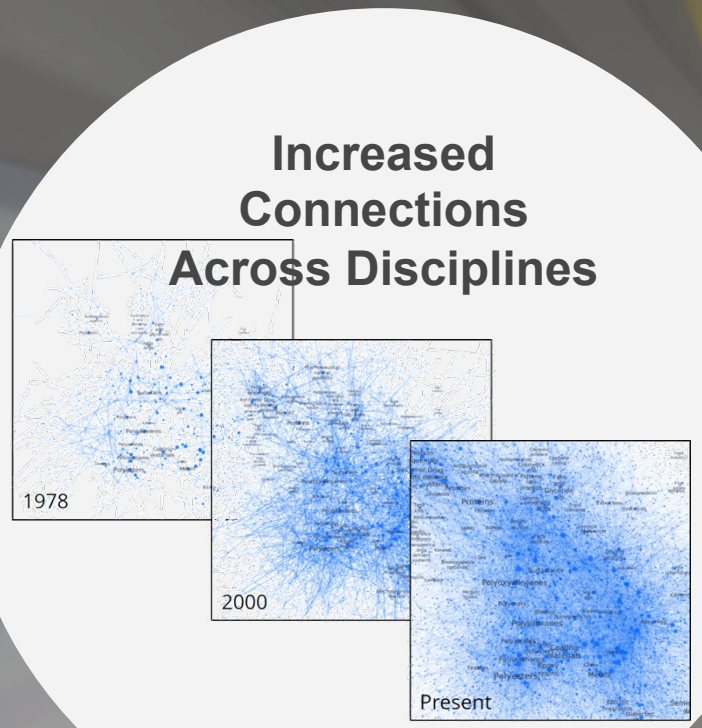

- Volume
- Complexity
- Connectedness

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Artificial Intelligence has great potential to help us leverage all of this information to accelerate innovation

- Identifying new opportunities
- Increasing efficiency
- Finding unseen connections

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It’s why everyone is investing in digitalization and AI

89% of businesses plan to invest in AI by 2020

Deloitte’s Digital Disruption Index

But 85% of AI projects are not meeting expectations

Gartner

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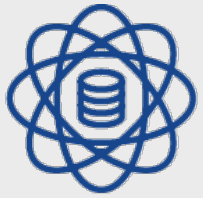
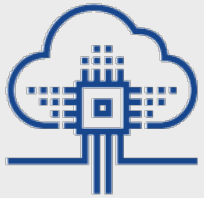
CAS is a specialist in scientific information solutions

We provide products and services that power discovery to solve our world's biggest challenges by helping organizations predict, plan and protect their innovations

With over 110 years of experience, no one knows more about scientific information and related technology than CAS



UNPARALLELED
SCIENTIFIC CONTENT



SPECIALIZED
TECHNOLOGY

UNMATCHED
HUMAN EXPERTISE

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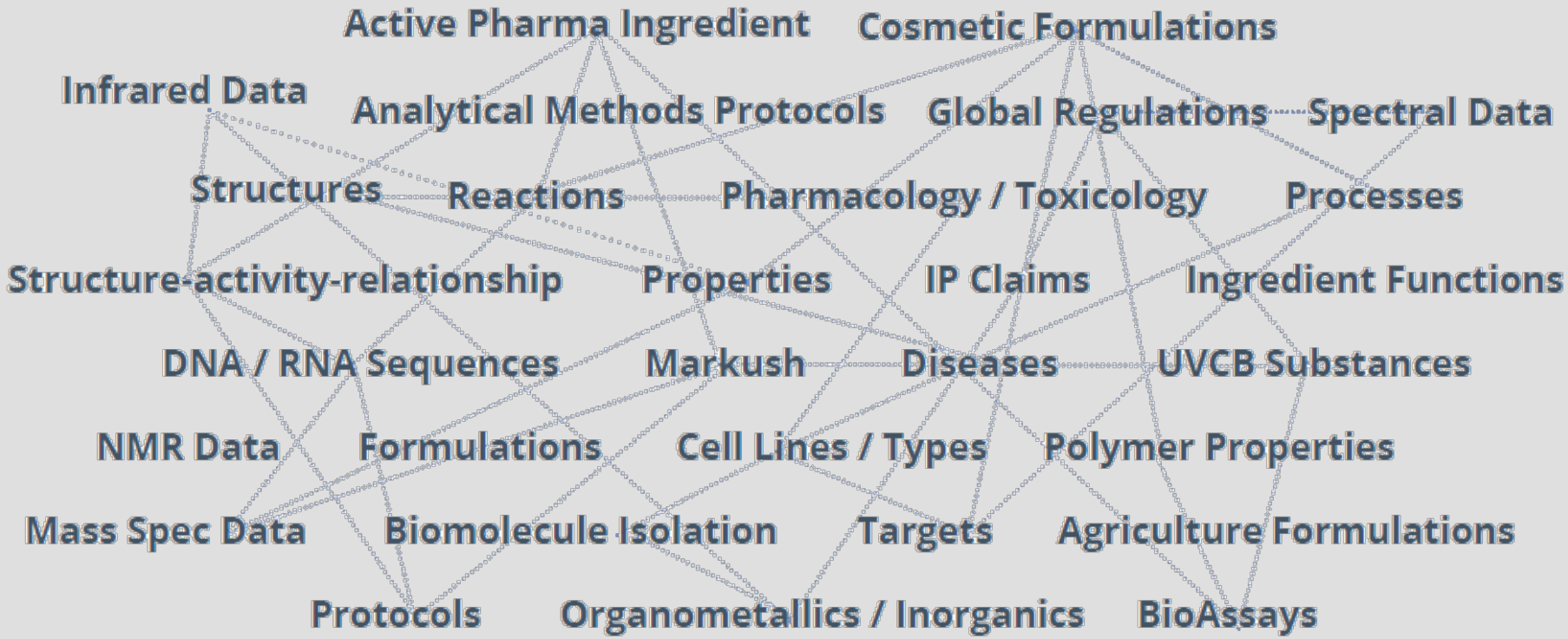
Our global scientific coverage is unmatched

50 THOUSAND scientific journals and documents

63 PATENT OFFICES worldwide

153 MILLION substances

50 LANGUAGES translated



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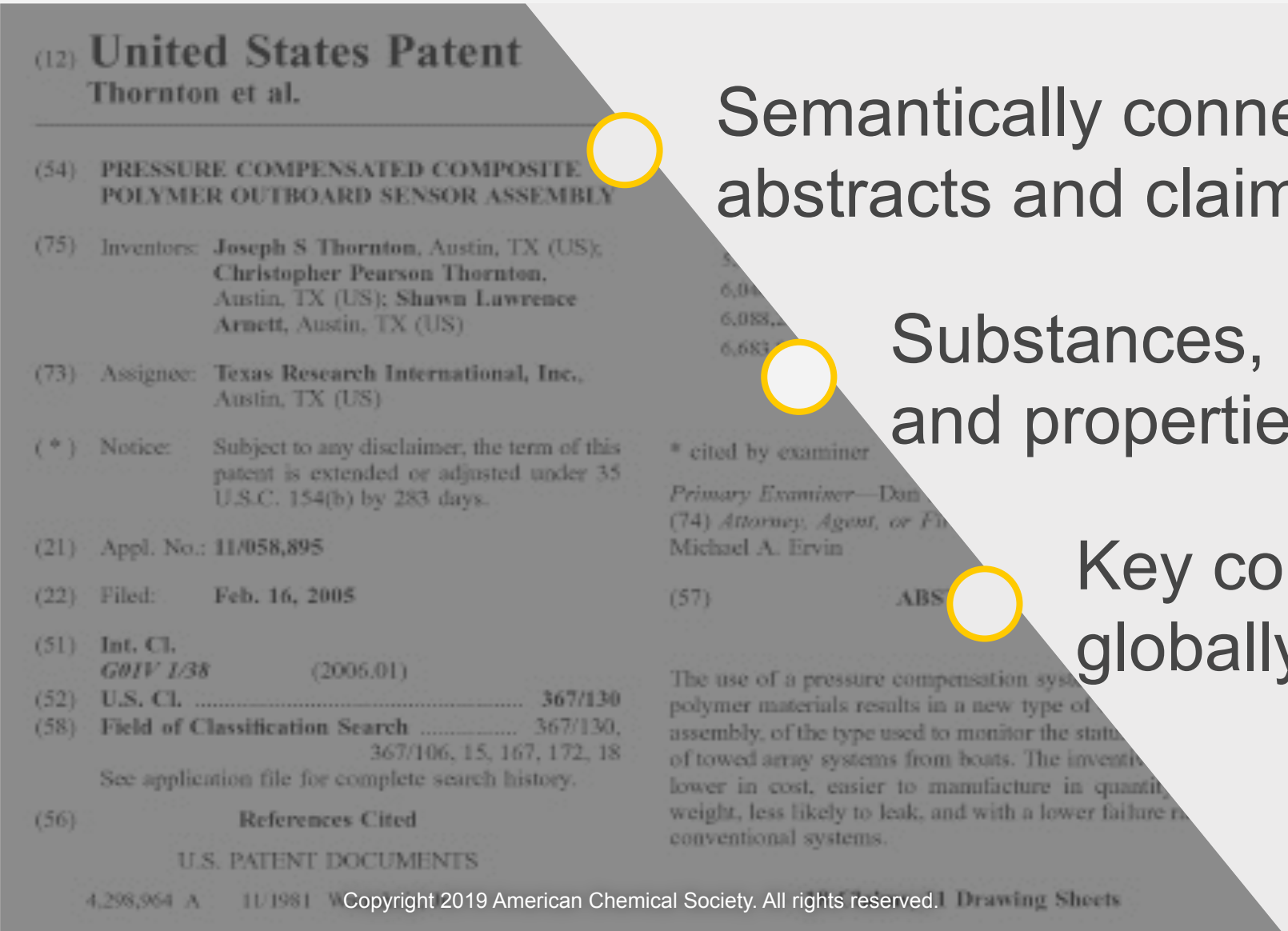
Robust, high-quality data require in-depth curation by scientists with expertise in the field and the language



(12) **United States Patent**
Thornton et al.

(54) **PRESSURE COMPENSATED COMPOSITE POLYMER OUTBOARD SENSOR ASSEMBLY**

(75) Inventors: **Joseph S Thornton**, Austin, TX (US); **Christopher Pearson Thornton**, Austin, TX (US); **Shawn Lawrence Arnett**, Austin, TX (US)

(73) Assignee: **Texas Research International, Inc.**, Austin, TX (US)

(*) Notice: Subject to any disclaimer, the term of this patent is extended or adjusted under 35 U.S.C. 154(b) by 283 days.

(21) Appl. No.: **11/058,895**

(22) Filed: **Feb. 16, 2005**

(51) **Int. Cl.**
G01V 1/38 (2006.01)

(52) **U.S. Cl.** **367/130**

(58) **Field of Classification Search** 367/130, 367/106, 15, 167, 172, 18

See application file for complete search history.

(56) **References Cited**

U.S. PATENT DOCUMENTS

4,298,964 A 11/1981 W

* cited by examiner

Primary Examiner—Dan

(74) *Attorney, Agent, or Fi*
Michael A. Ervin

(57) ABS

The use of a pressure compensation sys
polymer materials results in a new type of
assembly, of the type used to monitor the statu
of towed array systems from boats. The inventi
lower in cost, easier to manufacture in quanti
weight, less likely to leak, and with a lower failure r
conventional systems.

1 Drawing Sheets

Semantically connected titles, abstracts and claims

Substances, reactions, sequences and properties connected across pubs

Key concepts and inventions globally translated and indexed

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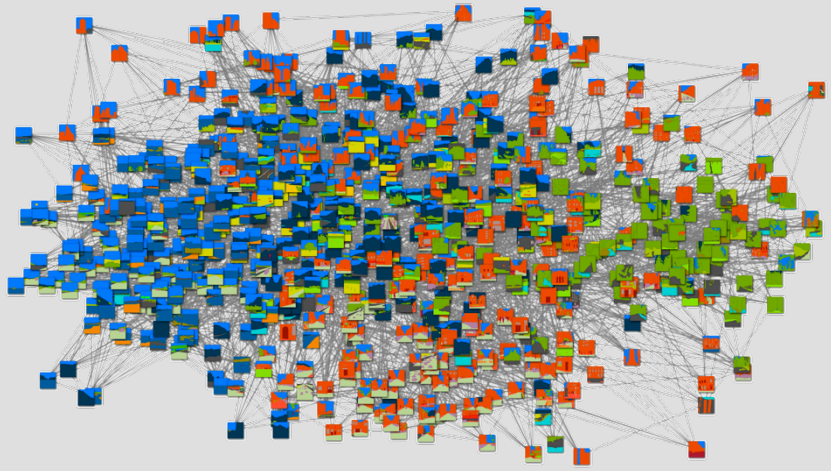
CAS conquers the chaos

- Global Translation
- Document Indexing
- Lexicon Development
- Semantic Indexing
- Reaction Indexing
- Markush Indexing



- Data Modeling
- Search Architecture
- App Development

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Algorithms miss details within scientific content that only intellectual curation delivers

	Finds all chemistry	Comprehensive retrieval	Scientific connections	50+ languages translated	Well-structured and connected	
Human Indexing	✓ (tables, text, images & Markush)	✓	✓	✓ (native speakers with scientific expertise)	✓	**HIGH CONFIDENCE**
Automated Indexing	✗ (Simple chemistry, not novel or complex)	✗ (Inconsistent)	✗ (Lacks context & connections)	✗ (limited in language and scope)	✗ (unstructured)	**LOW CONFIDENCE**

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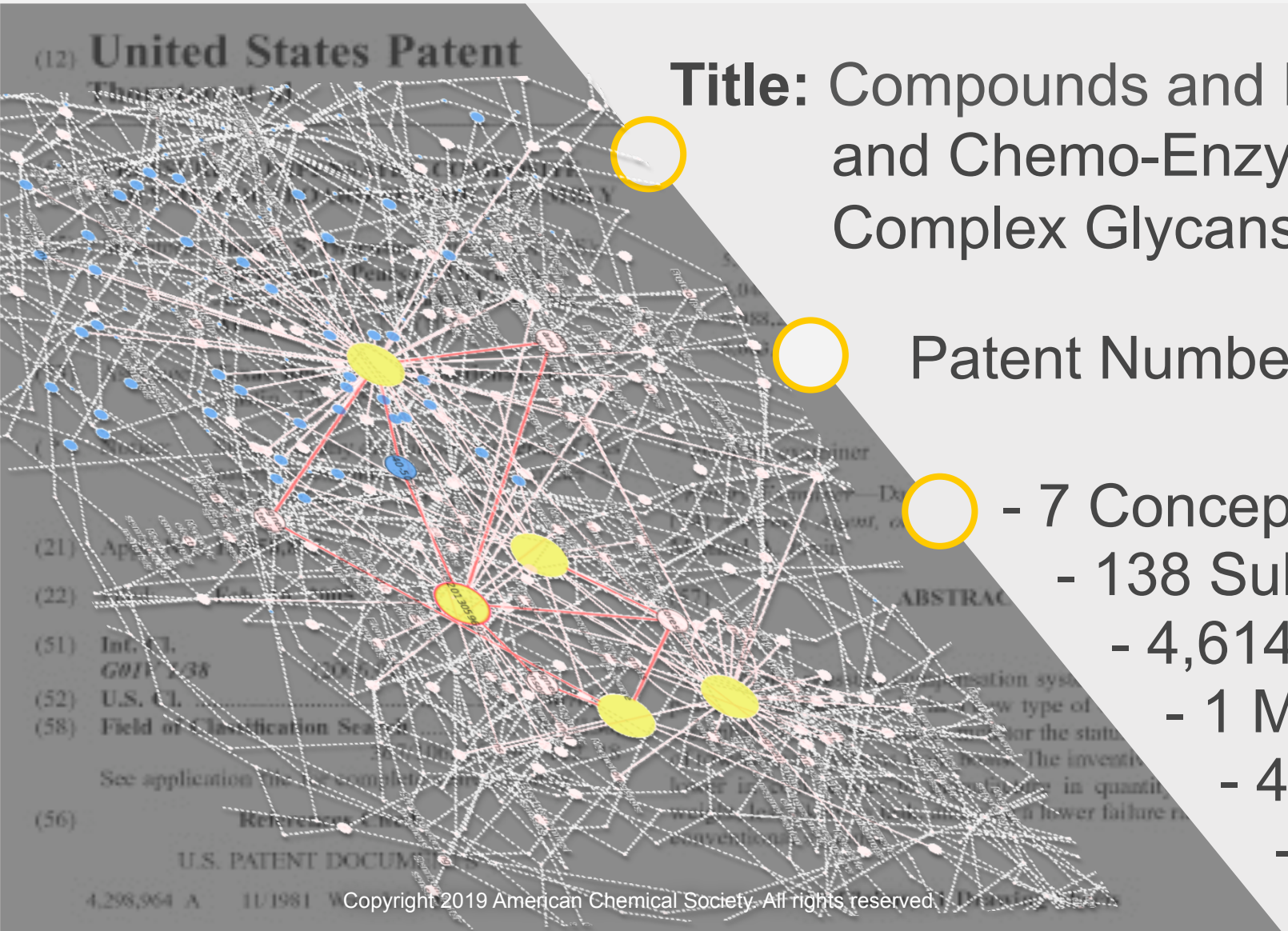
CAS captures critical details that algorithms alone miss



Title: Compounds and Methods for Chemical and Chemo-Enzymatic Synthesis of Complex Glycans

Patent Number: WO 2012135049

- 7 Concepts
  - 138 Substances
    - 4,614 Reactions
      - 1 Markush Structure
        - 4 Patent Family Members
          - 3 Cited Documents

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More data beats clever algorithms, but BETTER DATA beats more data

Peter Norvig, PhD
Director of research at Alphabet, notable author & AI expert

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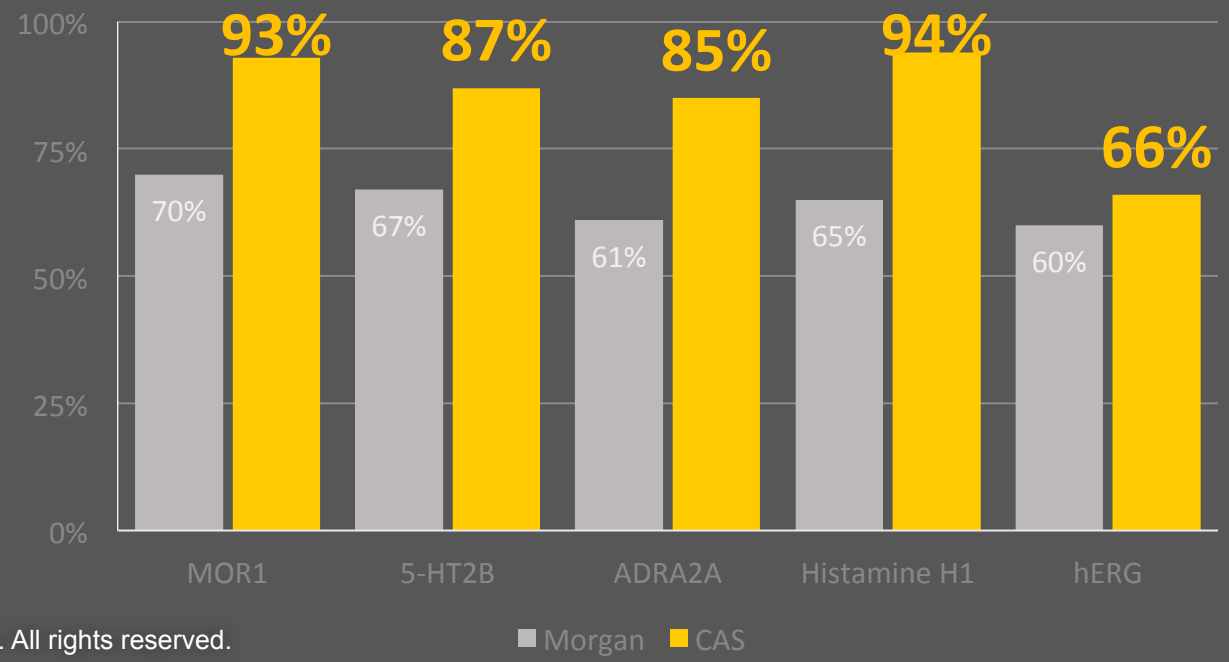
What is the measurable impact of clean, human-curated data on predictive outcomes?

CHALLENGE: A recently published paper classified almost 10,000 chemical entities on predicted biological activity to five different targets using Morgan fingerprints using a support vector machine model

OUR QUESTION: Does substituting Morgan fingerprints with CAS proprietary fingerprints have a measureable impact on prediction accuracy?

RESULTS:

The classification accuracy increased by over 30% when using higher-quality CAS data



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CAS uses knowledge graphs to leverage this data for unique insights

Outcomes:	**Literature Discovery**	**Prior Art Search**	**Decision Support**
			
Approach:	**Text-based knowledge graphs**	**AI + knowledge graphs**	**IAP + real-time analytics**

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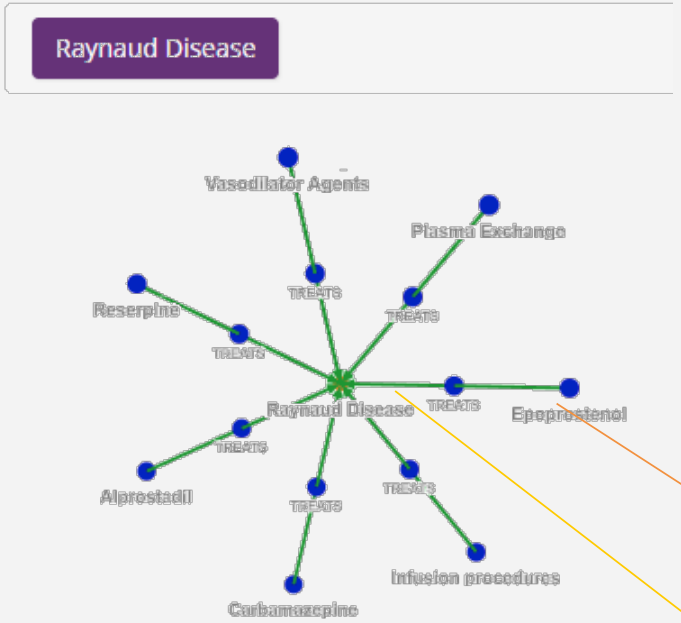
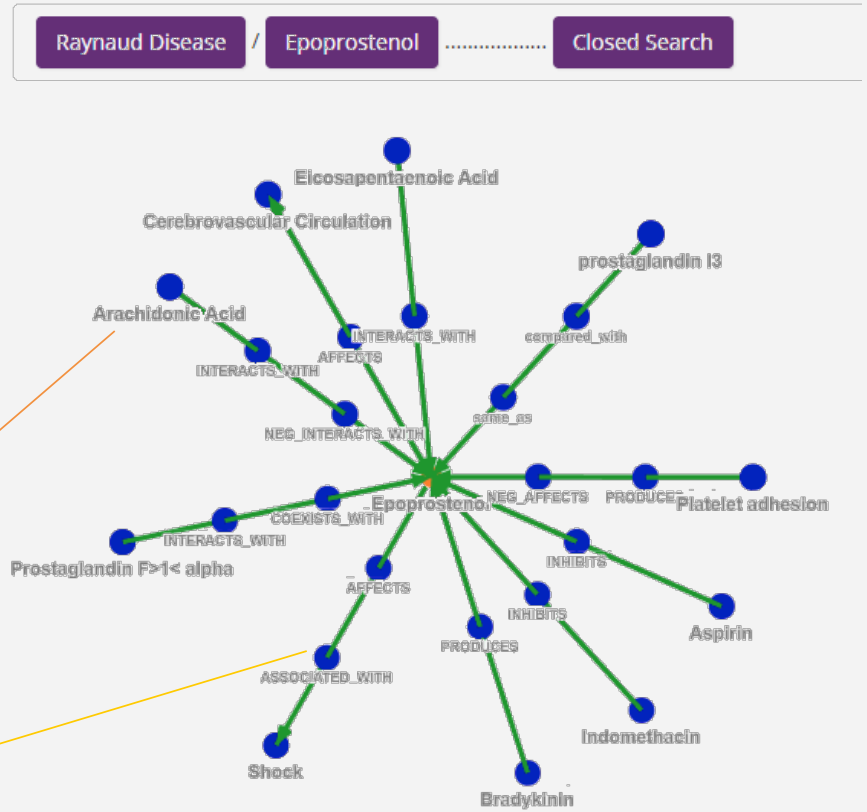
Literature based discovery via knowledge graphs allows for open exploration

Begin with a known curated concept



Explore other related concepts extracted from content



Concept and Substance Details

Source Reference Exploration

Literature Discovery

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and closed discovery

Begin by choosing several concepts

Source Concepts

Concept Name

Magnesium

Add Another Subject

AND

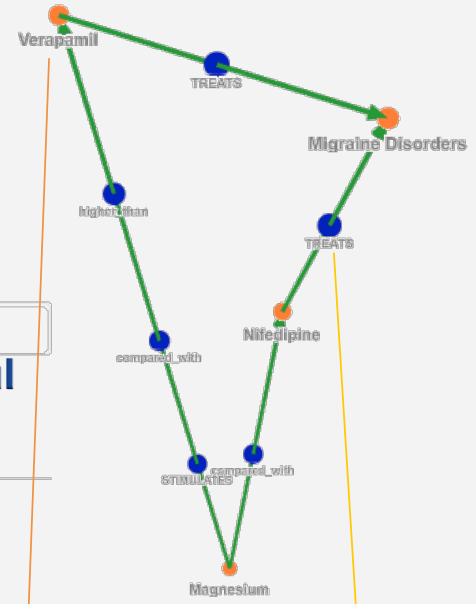
Destination Concepts

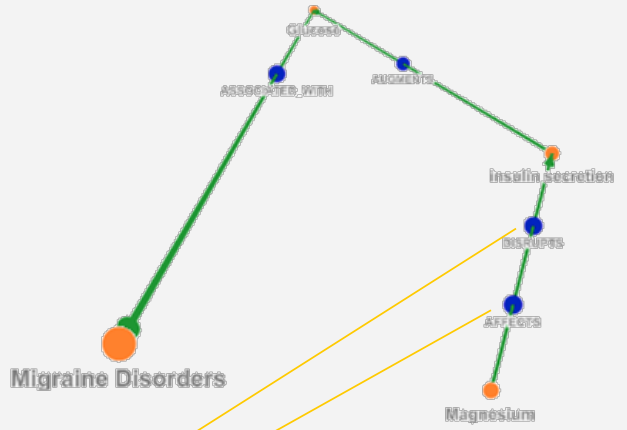
Concept Name

Migraine Disorders

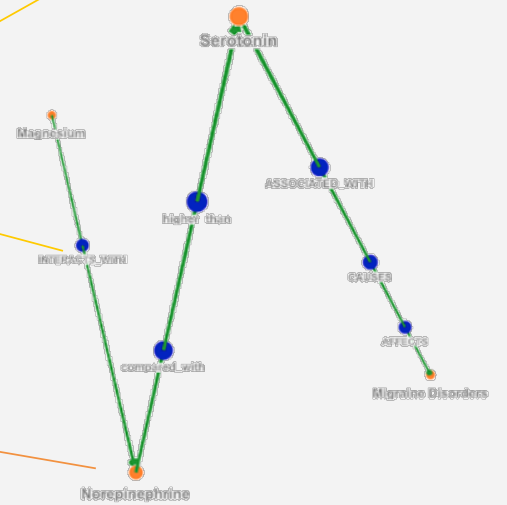
Add Another Object

Find meaningful connections





Source Reference Exploration



Concept and Substance Details

Literature Discovery

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CAS uses knowledge graphs to leverage this data for unique insights

Outcomes:	Literature Discovery	**Prior Art Search**	Decision Support
			
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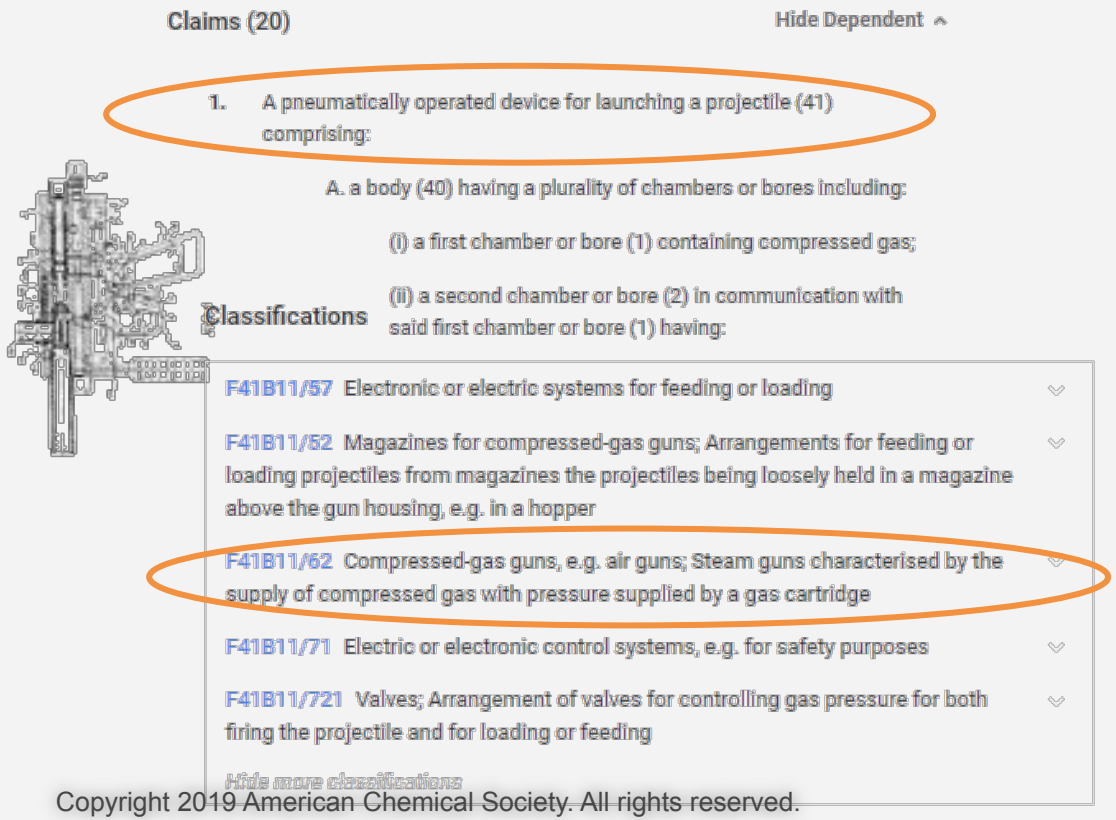
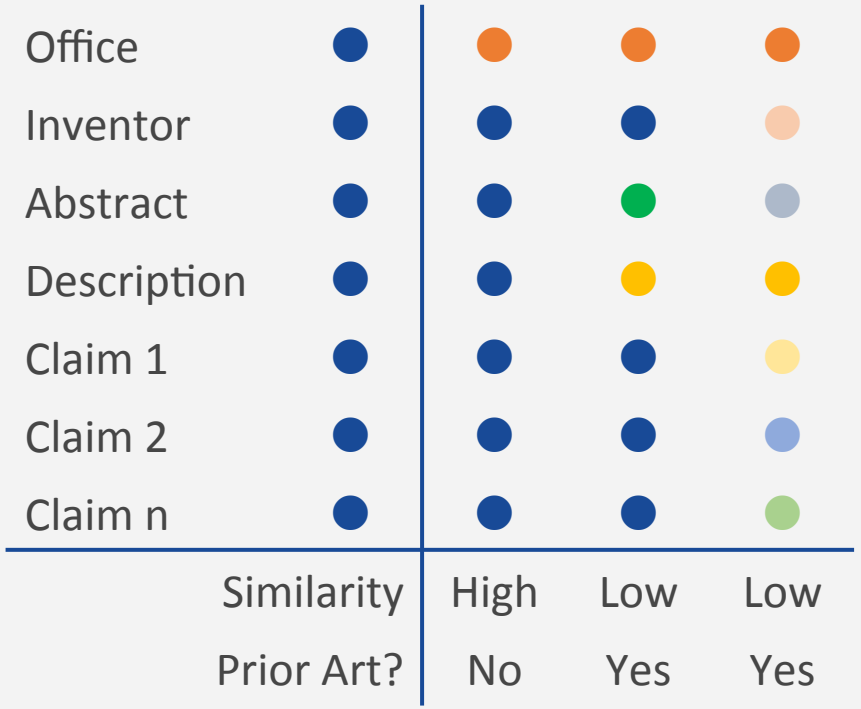
Patents have inherent challenges compared to typical text ingestion and similarity searches

Syntactic Similarity vs Semantic Similarity



Similarity vs Prior-Art



Prior Art Search

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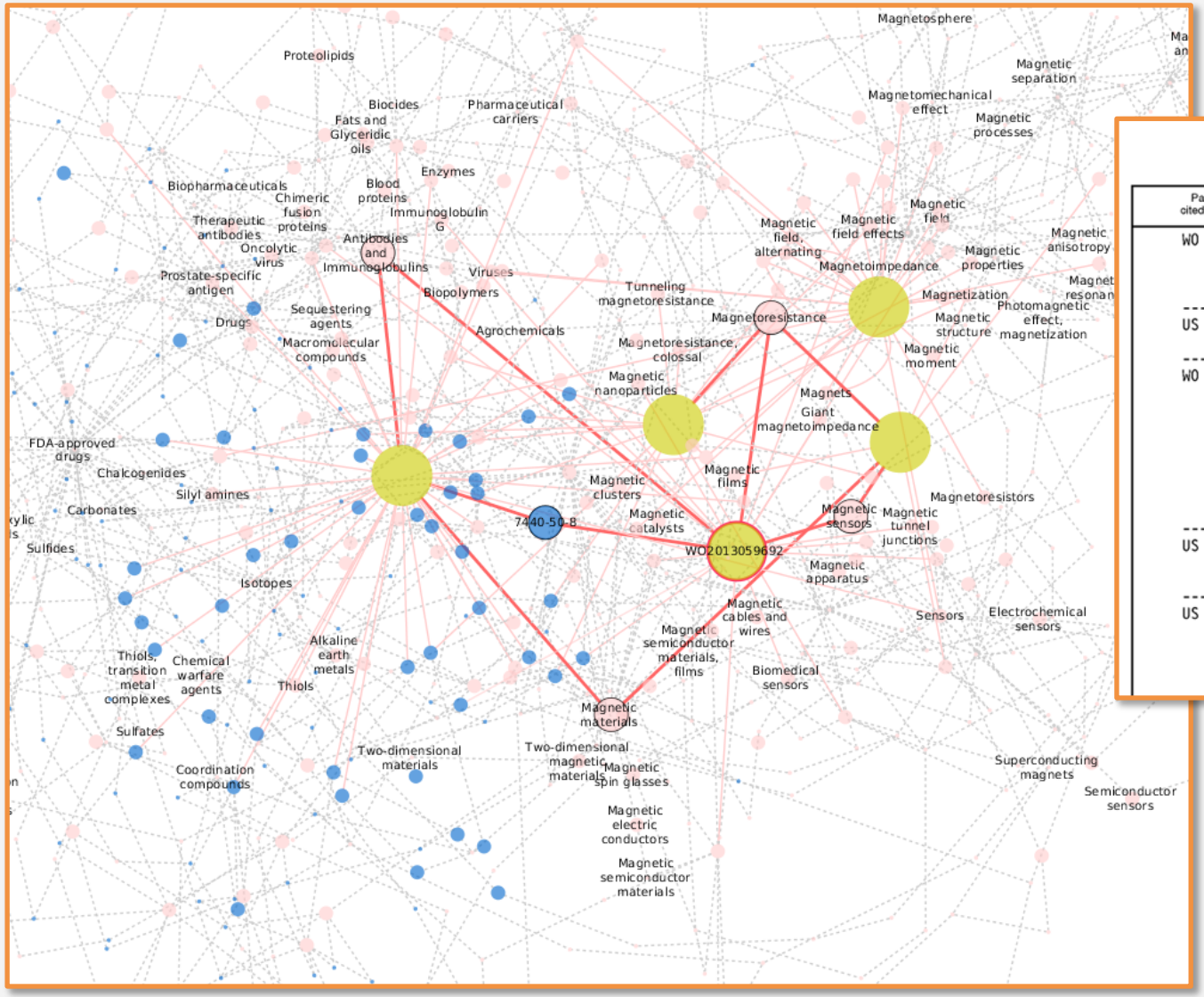
Visual representation of search reports support faster patent analysis and examination



INTERNATIONAL SEARCH REPORT

Information on patent family members

International application No PCT/US2012/061156

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Prior Art Search

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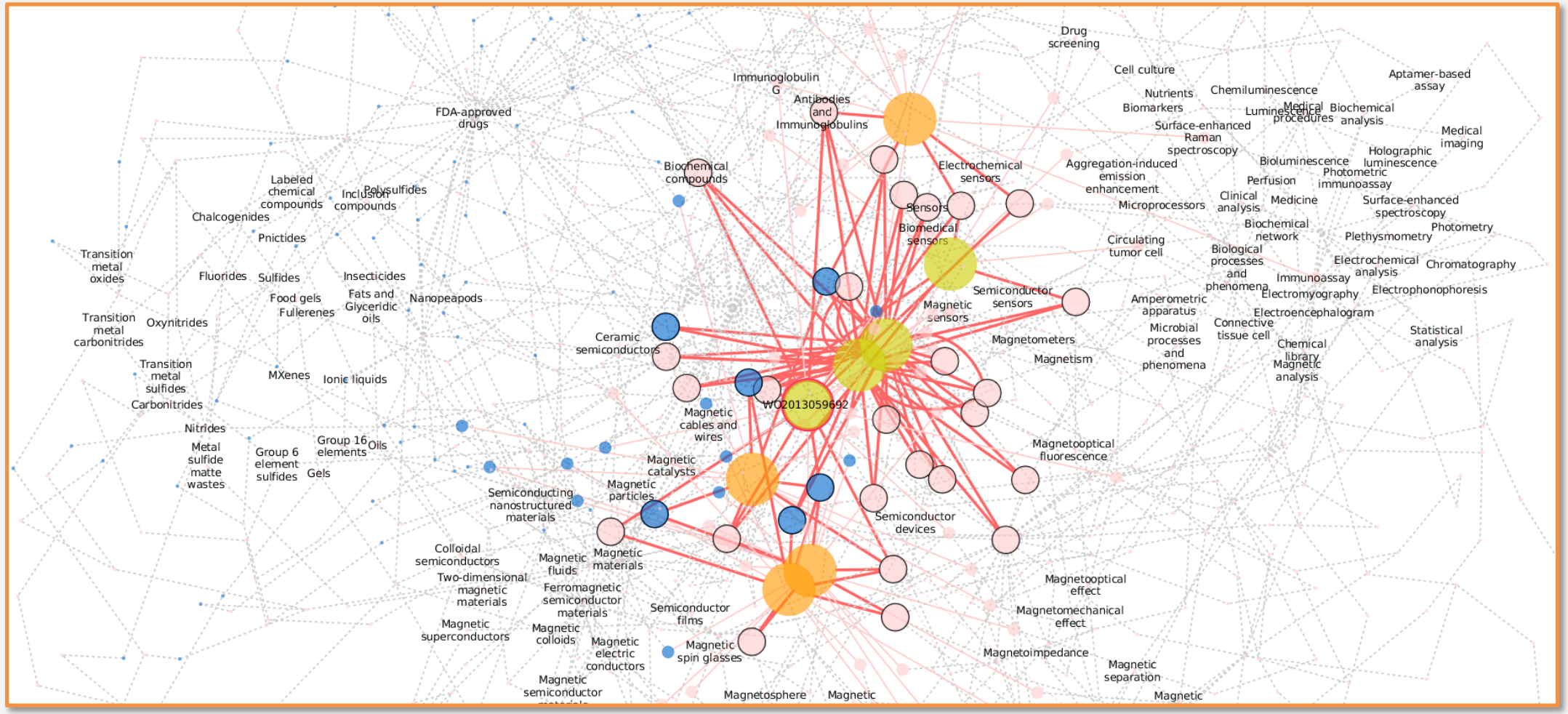
Can extend beyond search reports to include other connected patents and non-patent literature



Prior Art Search

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CAS uses knowledge graphs to leverage this data for unique insights

Outcomes:	Literature Discovery	Prior Art Search	Decision Support
			
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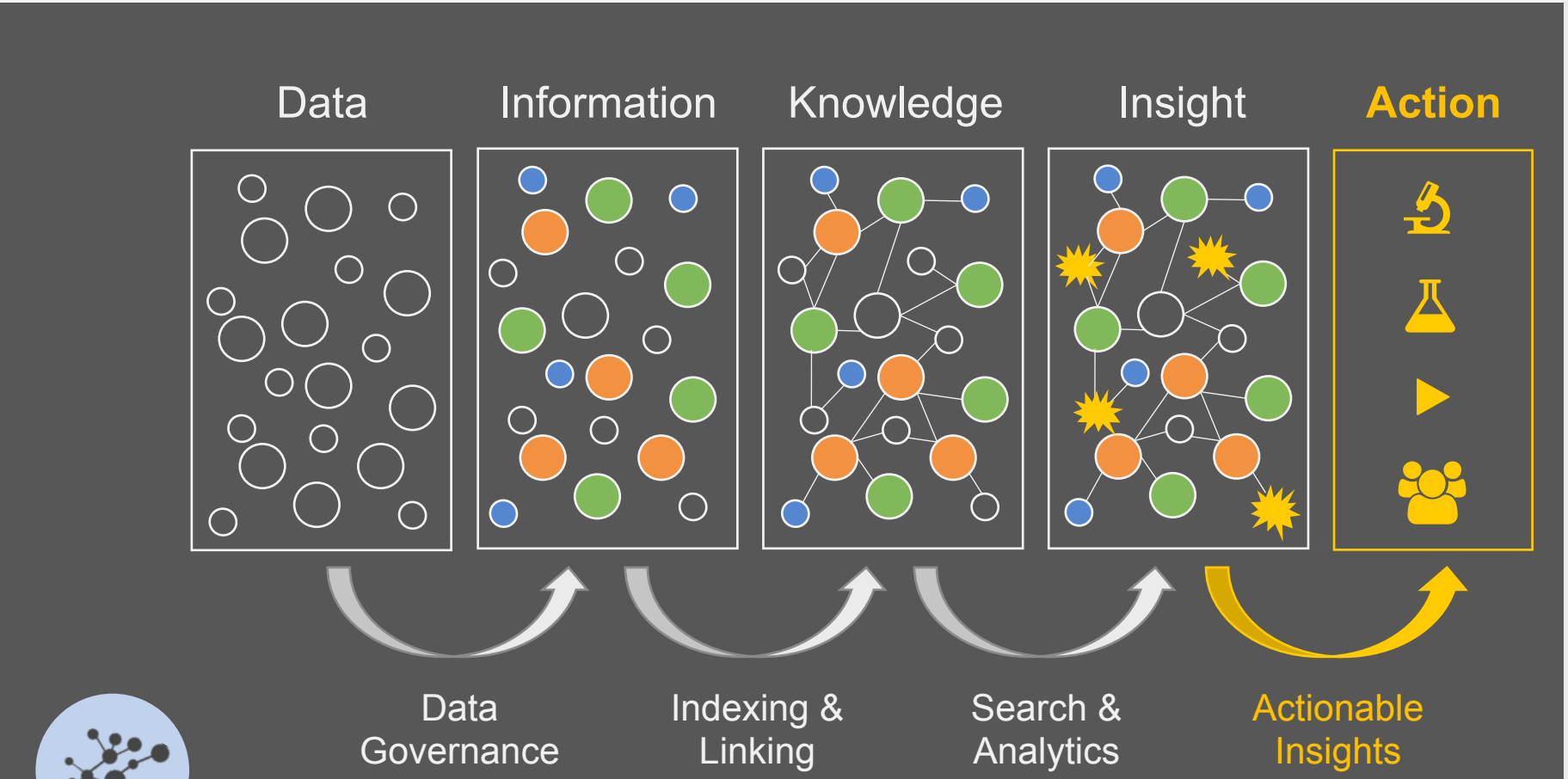
Building connections transforms data to support insights and key decisions



Actionable insights drive faster breakthroughs

Decision Support

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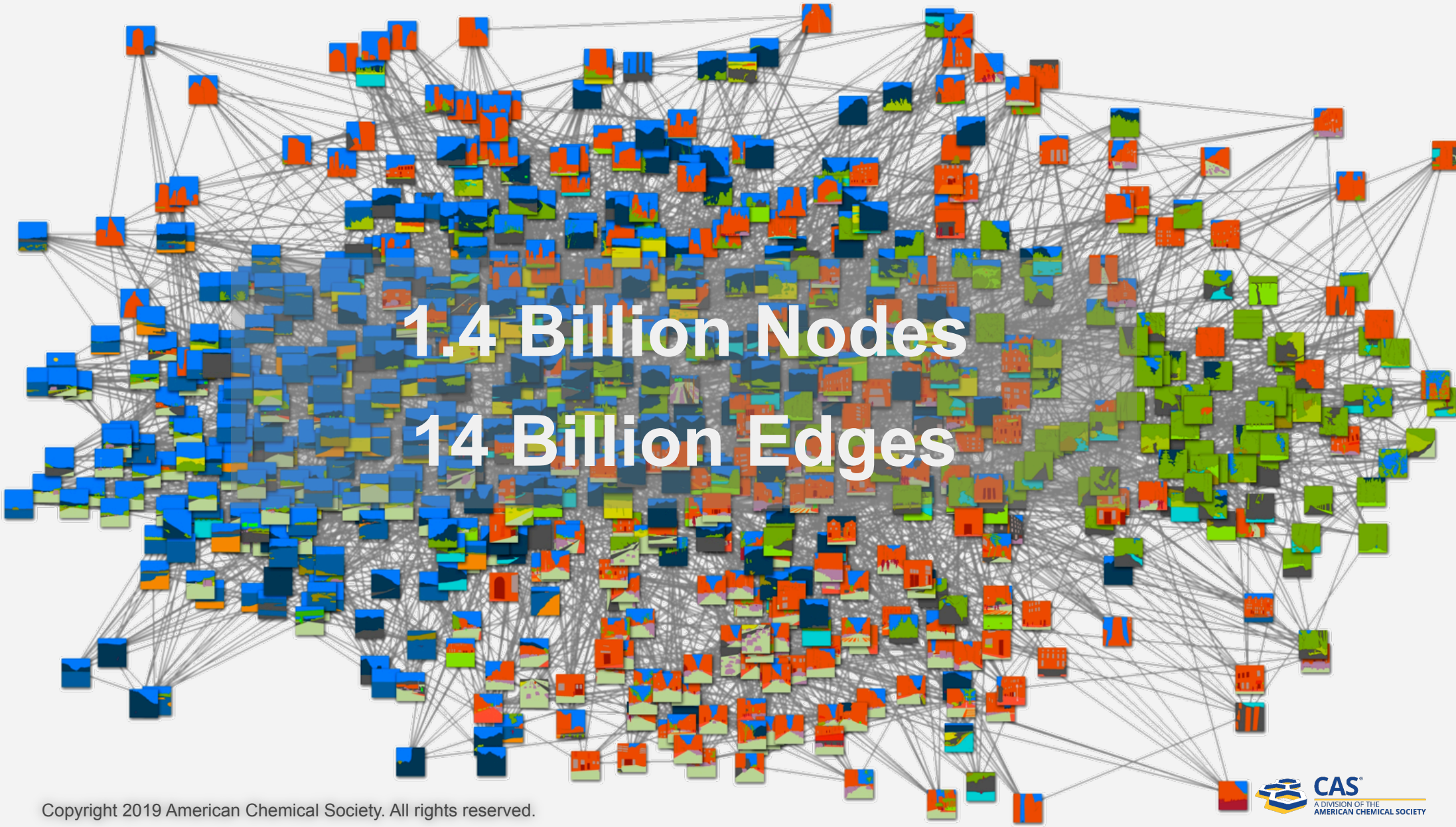
The CAS knowledge graph is enormous



Decision Support

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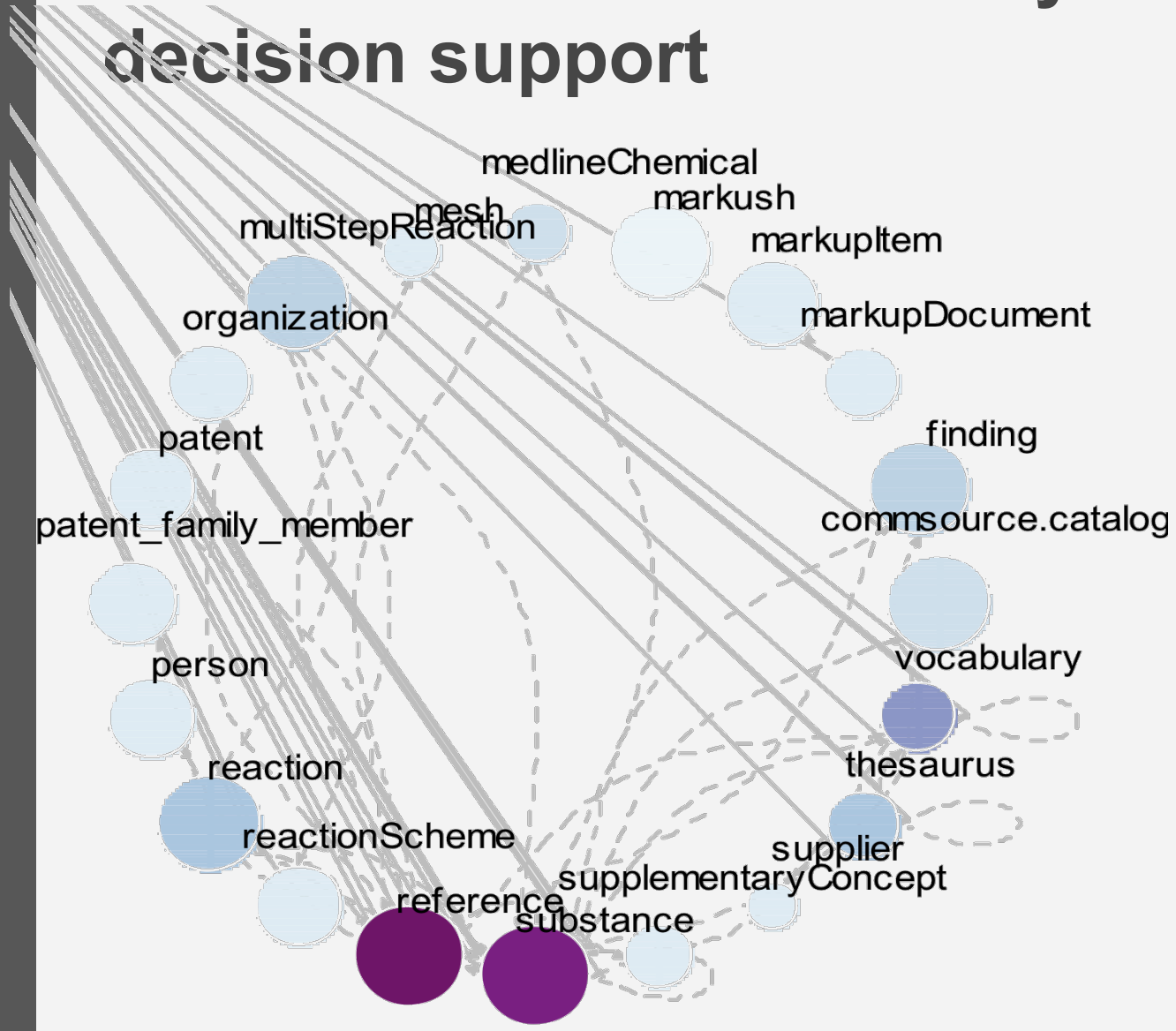
IAP enables real-time analytics for more insightful decision support



Nearly 10TB of data and >25 entities for SciFinder-n

Distributed, scalable and cloud-enabled

Integrated text search, structure search and graph traversal in near real time

Decision Support

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To Recap

The potential of emerging data technologies to accelerate scientific innovation is
HIGH

The impact of data quality on the success of these technologies is
HUGE

The ROI on human-curated data for scientific content is
MEASURABLE

The potential applications to drive insight are
UNLIMITED

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