SureChem

Patent chemistry when
and how **you** need it

Brought to you by the industry's most
advanced chemistry mining pipeline

DIGITAL science

ICIC 2012
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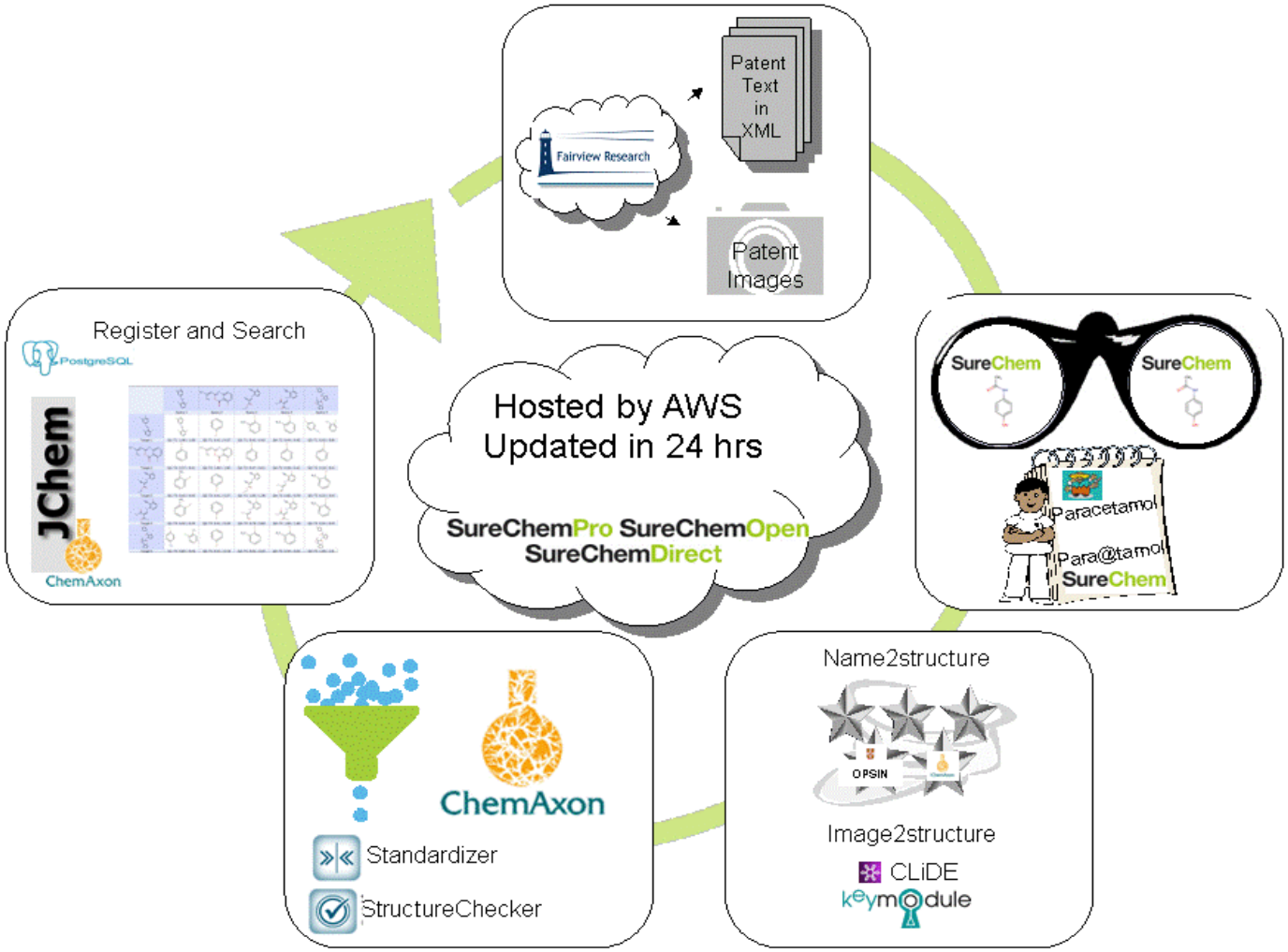
Dr. Eli Lewis explains how he has benefitted from using LabGuru at Ben-Gurion University

LabGuru in practice

SureChem Chemistry Mining Workflow



SureChem Data Collection

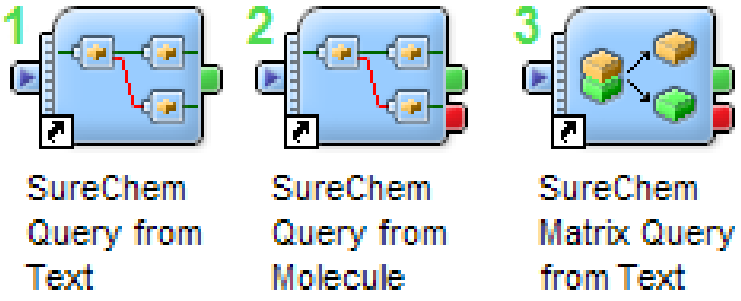
Database of automatically mined structures from text and images

- ✧ 20M annotated **US, EP, WO** full text records and Japan patent abstracts
- ✧ **12M** unique chemical structures
- ✧ MEDLINE – 19M abstracts (coming Q4)

- ✧ Structures from **text** are available 24 hours from publication
- ✧ Structures from **images** are available 2 to 3 days from publication

SureChemDirect

- API or Data Feed access to chemistry and full text
- Integrate with internal databases & workflows
- Off-the-shelf deployment including Pipeline Pilot support

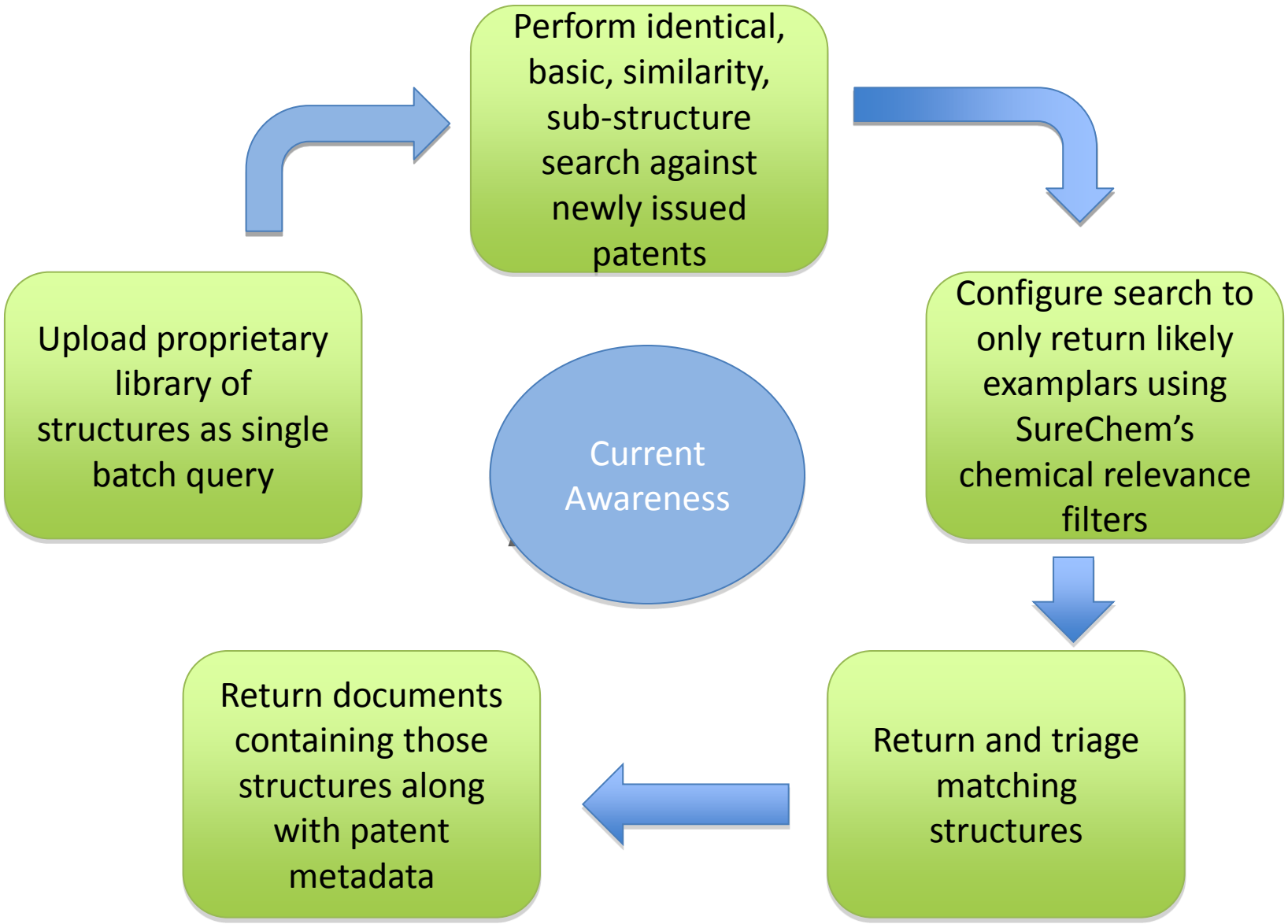


Innovative workflows:
Drug Discovery Fragment substitution

Can I perform bioisosteric replacement to improve binding and maintain freedom to operate?

1. Gather likely bioactive structures (similarity or substructure search) in combination with patent bibliographic/full text search.
2. Identify a substructure (fragment) candidate for bioisosteric replacement
3. Crop lead structure removing bioisosteric fragment
4. Perform a sub-structure search and look for hits that match compounds in your set of bioactive molecules
5. Identify matched molecular pairs of bioisosteric functional groups that maintain or improve bioactivity and are free of claims.
6. Export collected data and distribute to medicinal chemists

Batch Searching

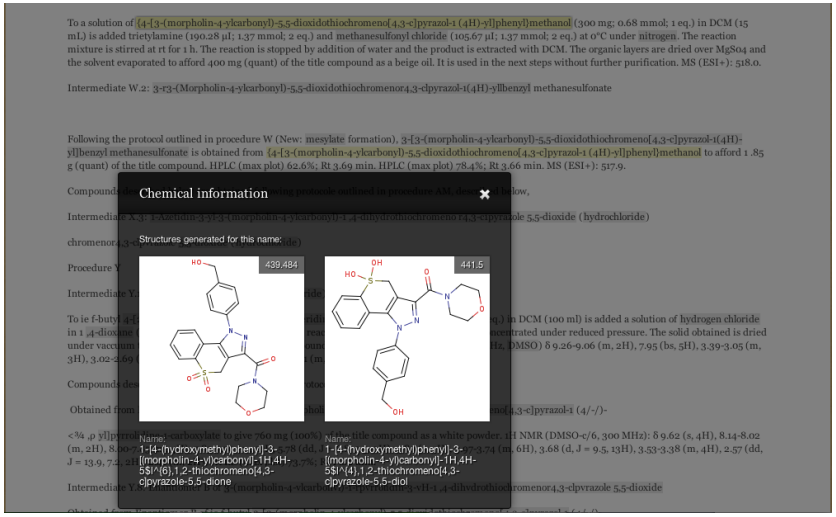


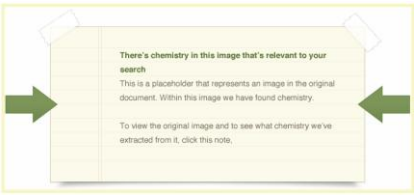
Alerts and workflow integration

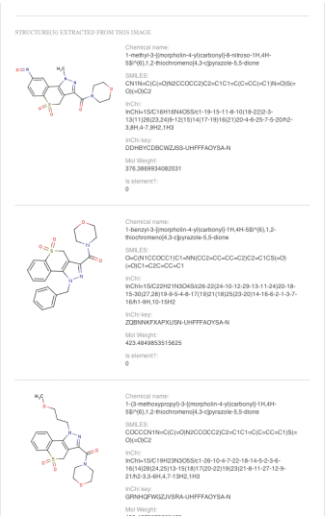
Set up daily, weekly, monthly structure and text alerts

Export structures, patent IDs and metadata to workflow tools and databases (Sharepoint, SpotFire, Seurat etc)

Distribute results to project scientists.
View structures in context using SureChemOpen/Pro



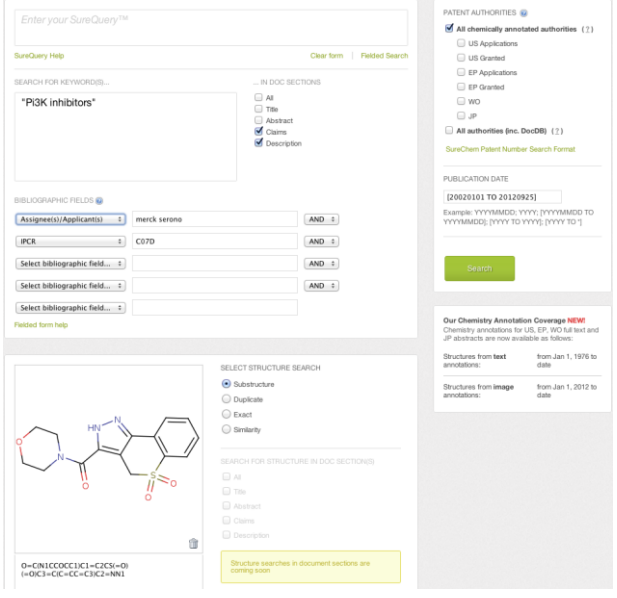


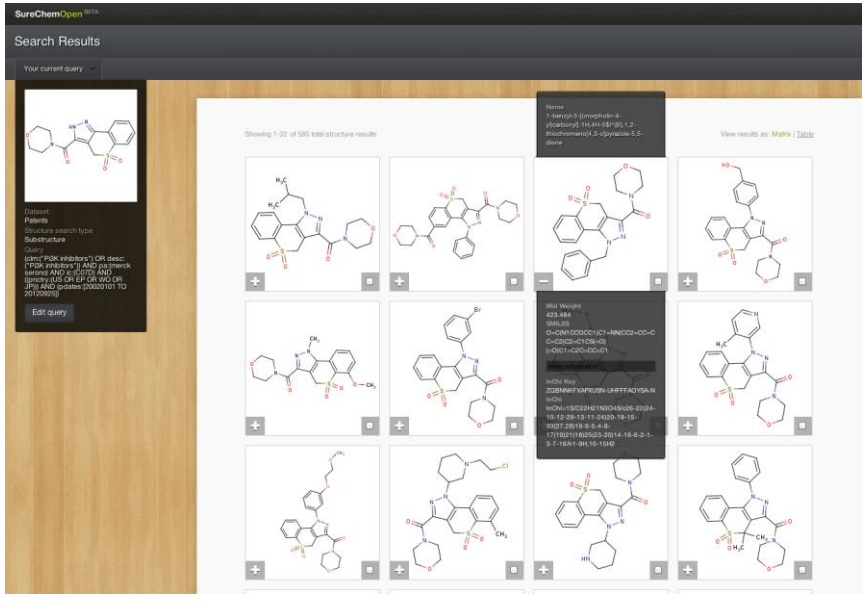


SureChem Products

SureChemOpen

- **Free resource** for researchers to search, view and navigate through the relevant chemistry in the full text of patent documents
- Enables linking to public and proprietary content



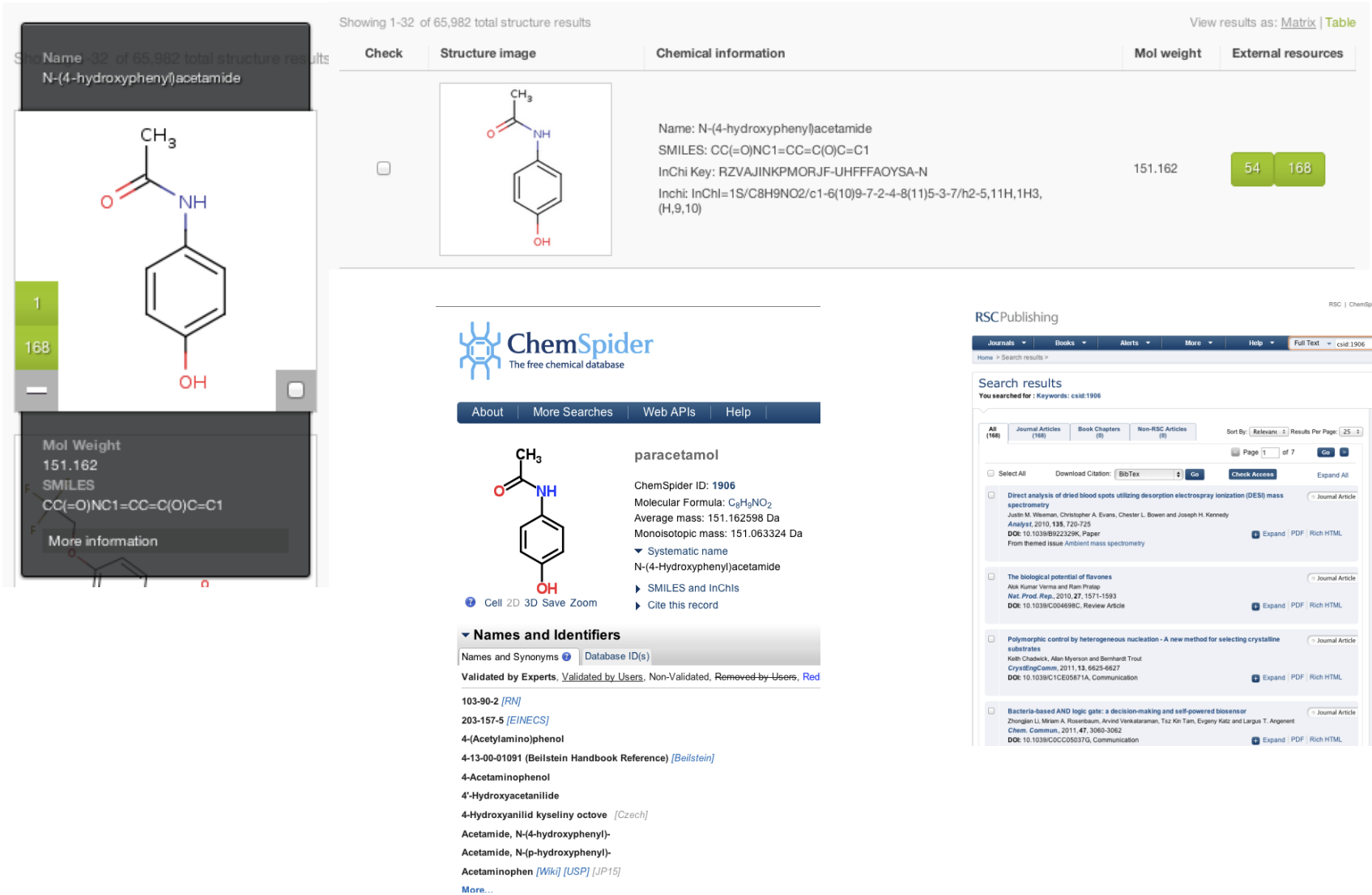


SureChemPro

Coming in Q4:

- Professional search needs
- Structure and patent metadata export, alerts, patent family search, chemical relevance filters…

SureChem Partnering



SureChem – What's next?

- Complete backfile processing of structures from images

- Implement **chemical relevance filters** to improve chemistry relevance (SCD, SCPro)
  - Frequency counts of chemicals within patent corpus
  - Advanced chemical structure filters
  - Structure location and source
  - Identification of likely exemplar and medchem relevant compounds

- **SureChem** to deposit all structures into PubChem

Please contact us to discuss your requirements or set up a free SureChemDirect evaluation

www.surechem.com

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