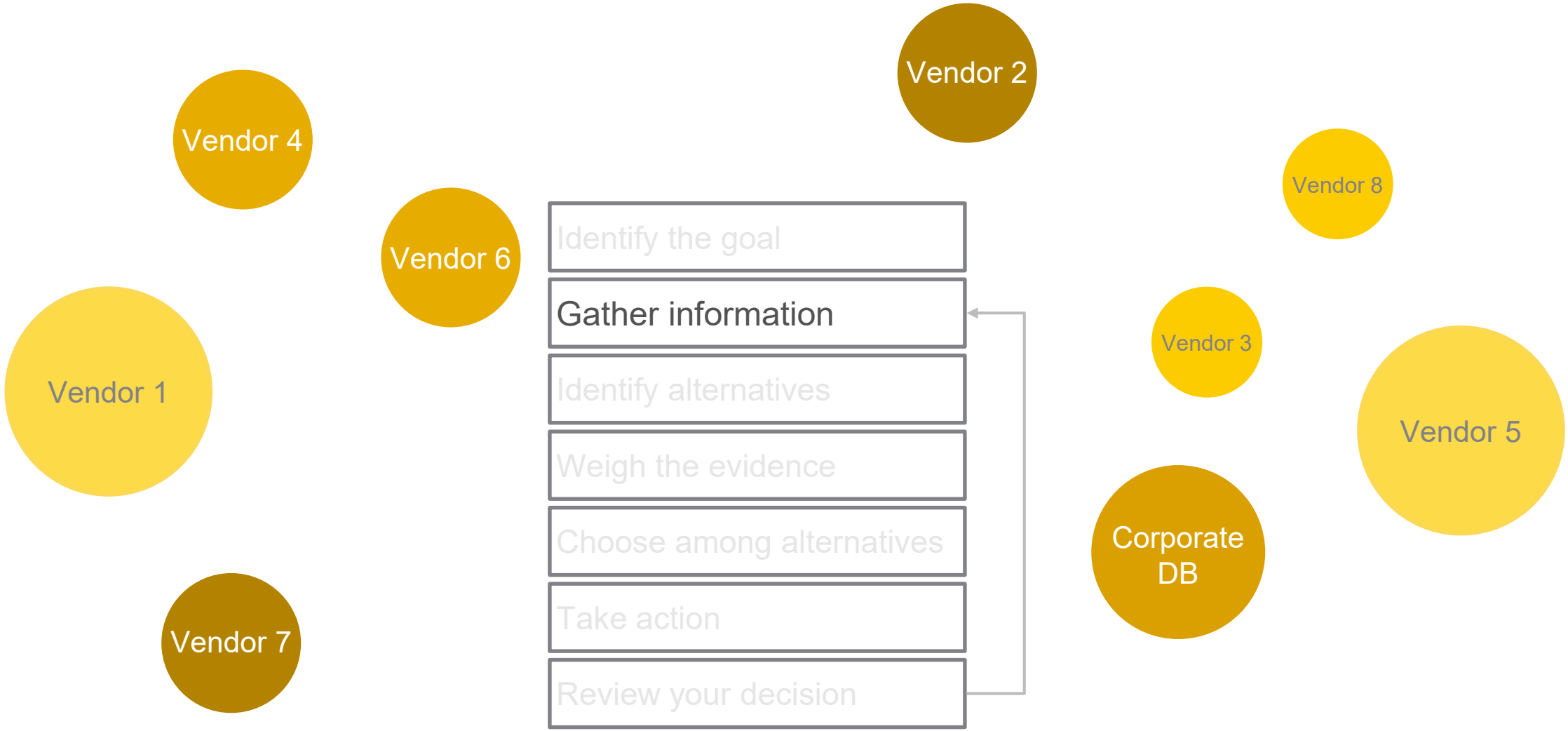
ChemAxon

Ivan Solt

SHRINKING THE HAYSTACK

Budapest, Hungary


Identify the goal
Gather information
Identify alternatives
Weigh the evidence
Choose among alternatives
Take action
Review your decision


Vendor 2
Vendor 4
Vendor 8
Vendor 6
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Vendor 3
Vendor 1
Vendor 5
Corporate DB
Vendor 7

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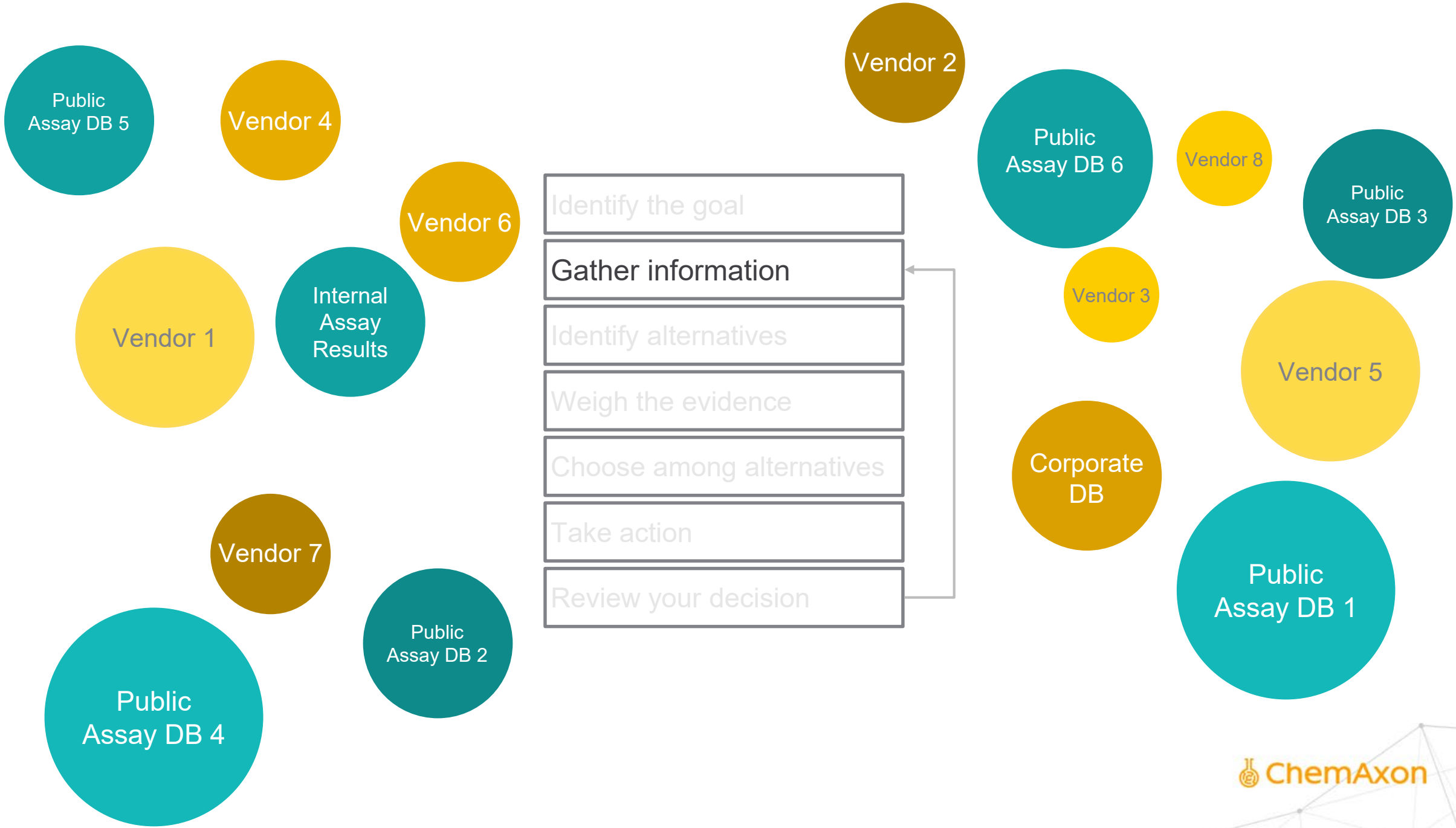
Public Assay DB 5
Vendor 4
Vendor 2
Public Assay DB 6
Vendor 8
Public Assay DB 3
Vendor 6
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Vendor 1
Internal Assay Results
Vendor 3
Vendor 5
Corporate DB
Vendor 7
Public Assay DB 1
Public Assay DB 2
Public Assay DB 4
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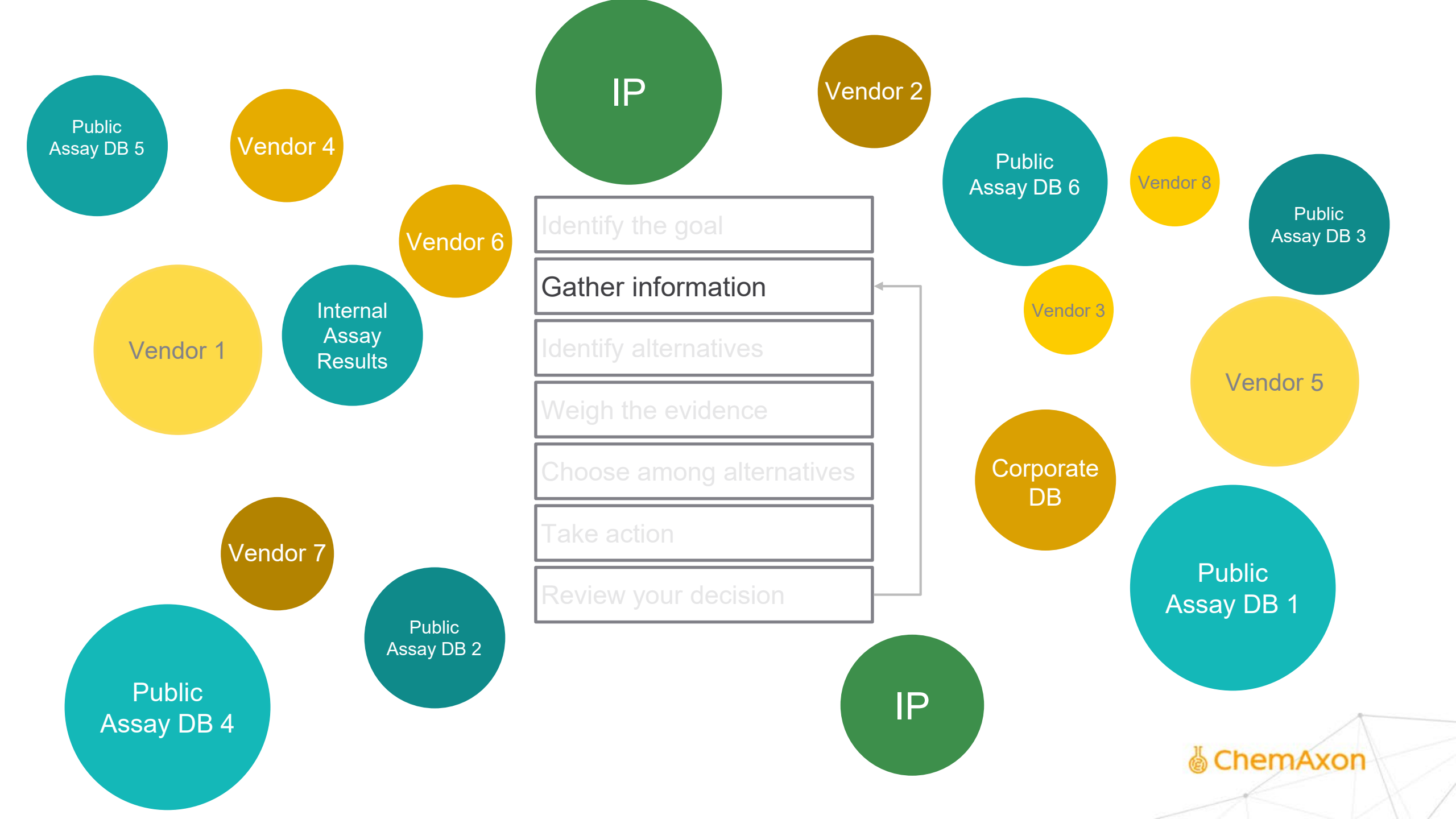
Public Assay DB 5
Vendor 4
IP
Vendor 2
Public Assay DB 6
Vendor 8
Public Assay DB 3
Vendor 6
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Public Assay DB 4
IP
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Ursus Wehrli

Ursus Wehrli

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ENAMINE REAL

171M

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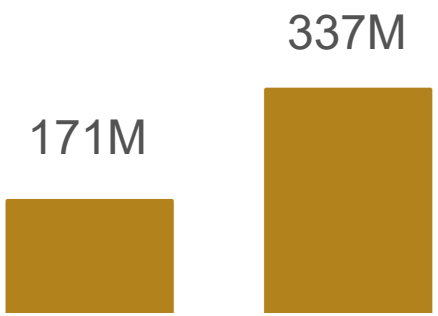
ENAMINE REAL



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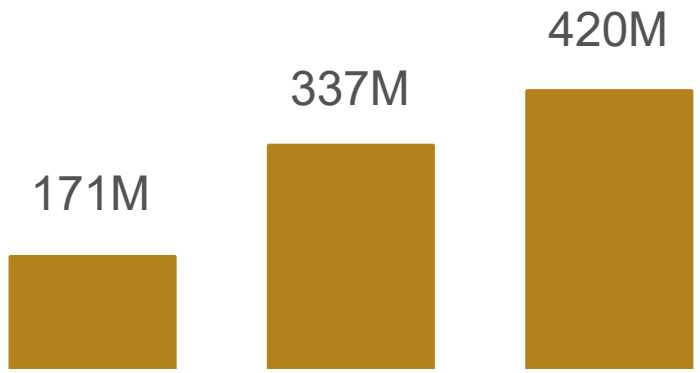

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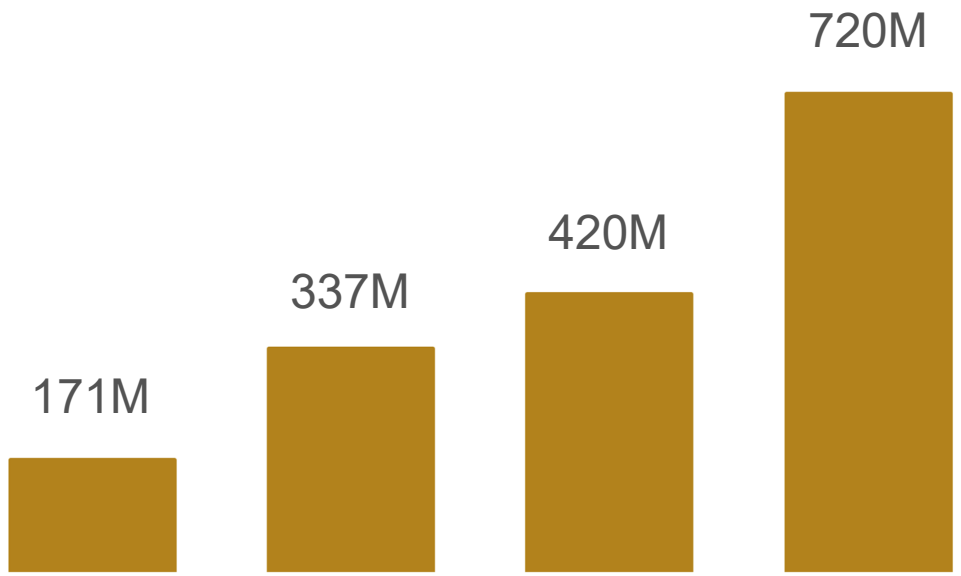

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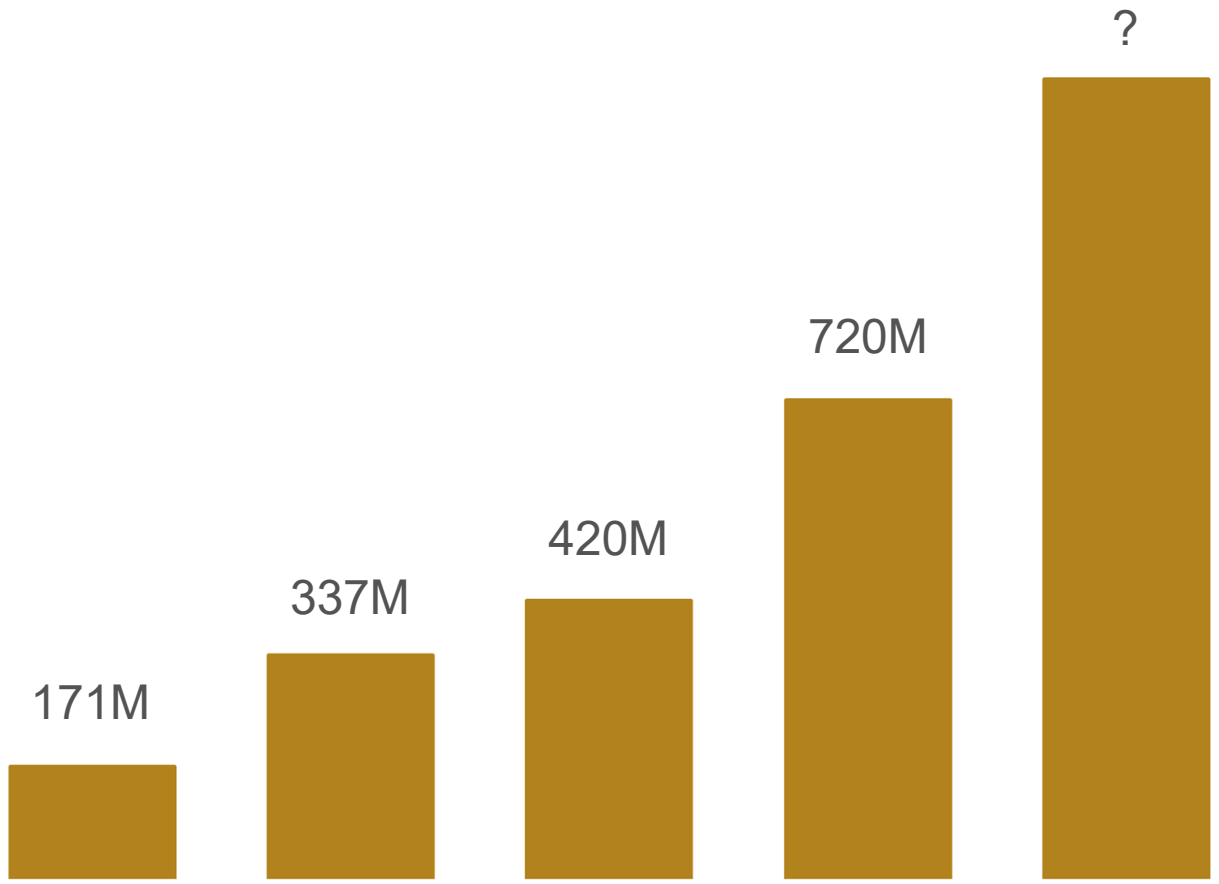

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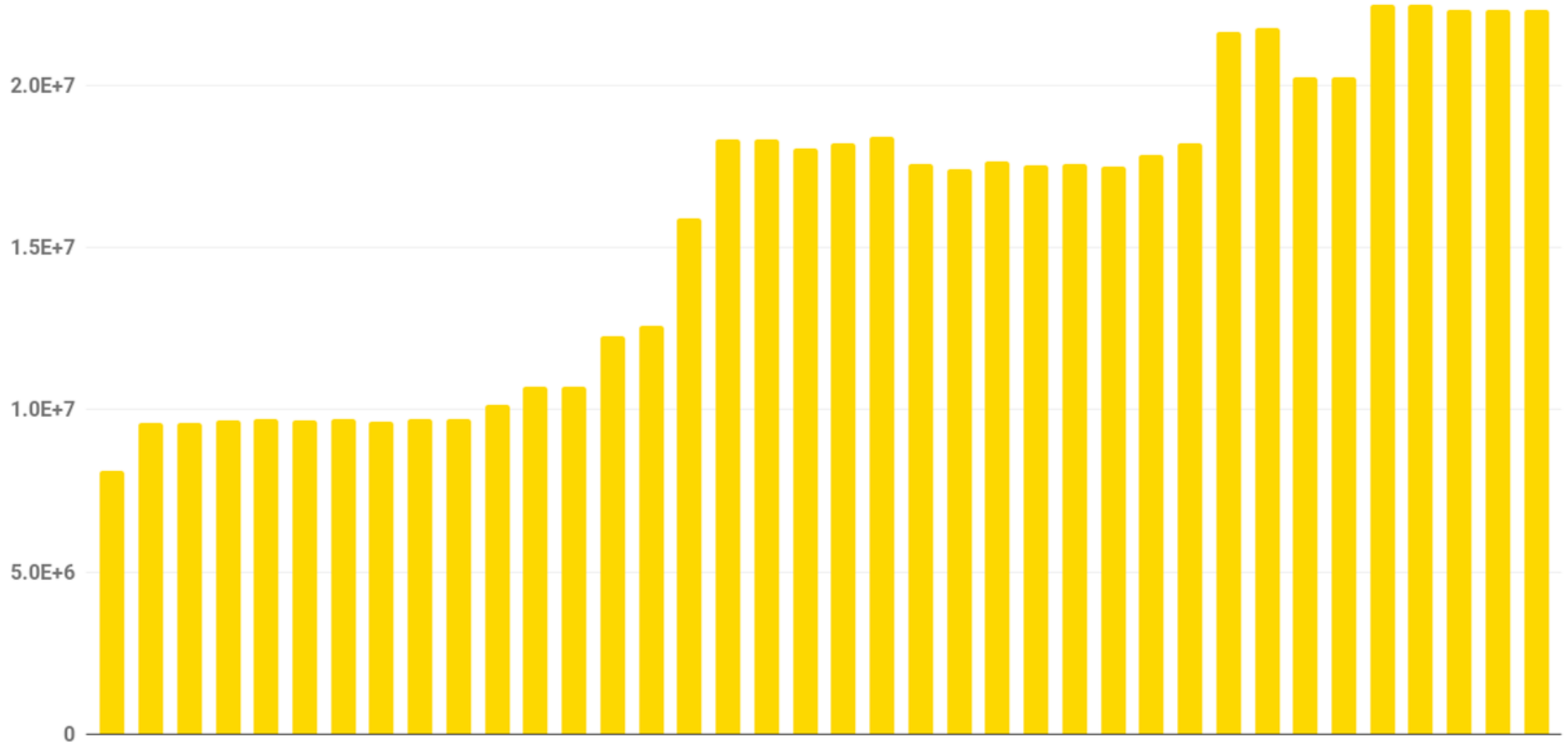
EMOLECULES



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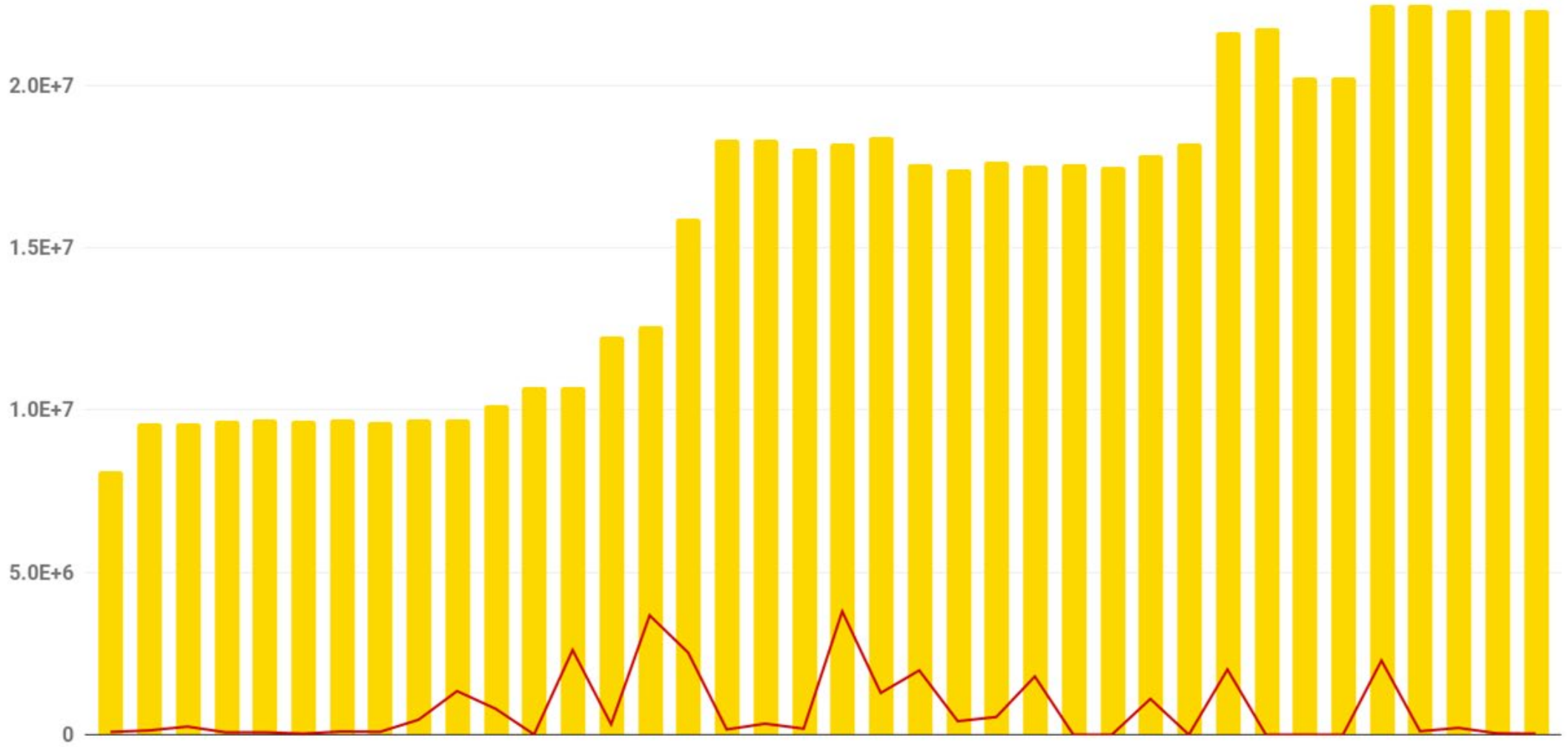
EMOLECULES



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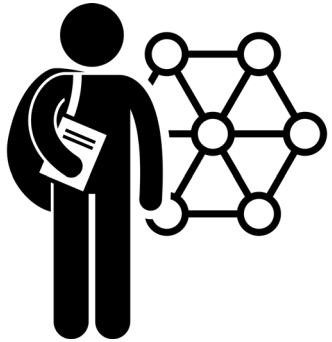
Corporate Compound Repository 1.5M – 3M

MolPort All Stock ~7M

Enamine REAL ~720M

ChEMBL 1.8M

SureChEMBL ~18M



BindingDB 651K

Namiki Shoji ~6M

Screening library 250k – 1M

PubChem Compounds ~95M

eMolecules ~22M

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Haystack Prototype

- Corporate Compound Repository
  1.5M – 3M
- MolPort All Stock
  ~7M
- eMolecules
  ~22M
- BindingDB
  651K
- ChEMBL
  1.8M
- SureChEMBL
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- PubChem Compounds
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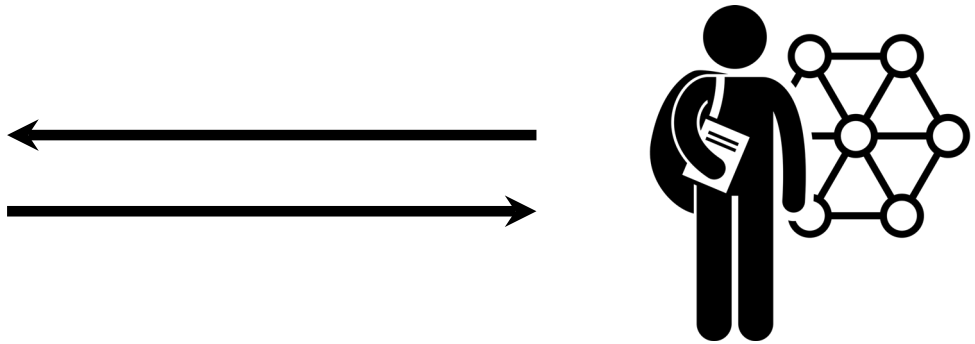
- Enamine REAL ~720M
- +



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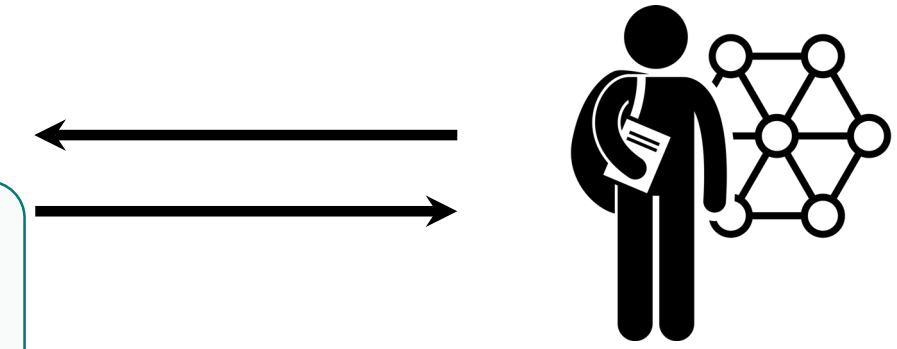
- Enamine REAL ~720M
- +

Design Application Layer



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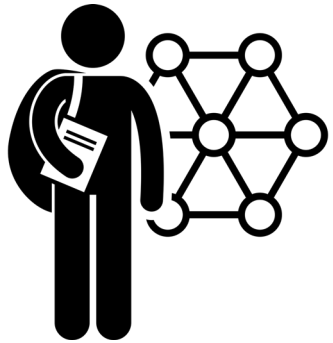
Stuff

Design Application Layer



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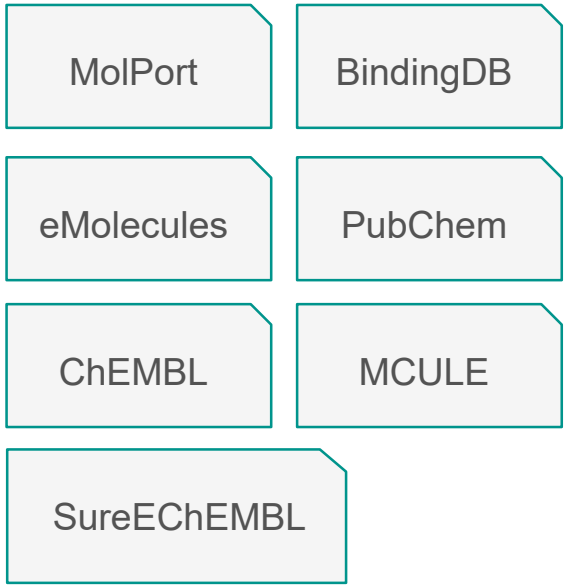
THE HAYSTACK DATABASE- PROTOTYPE



~140M in total

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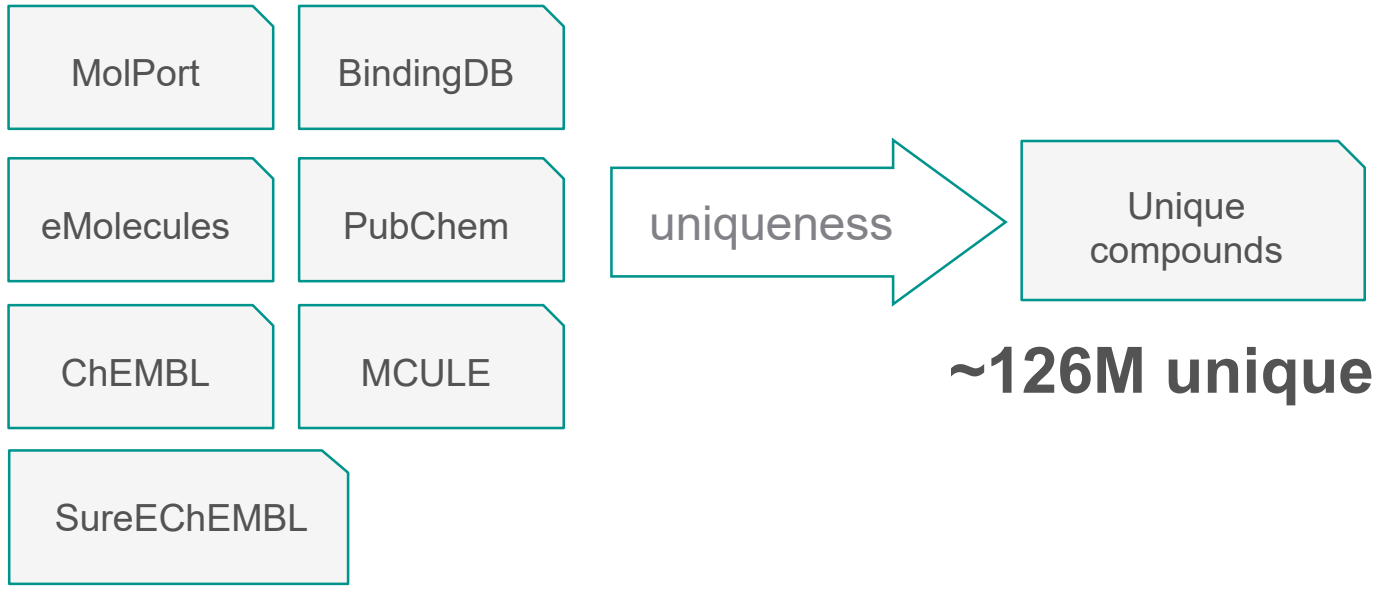

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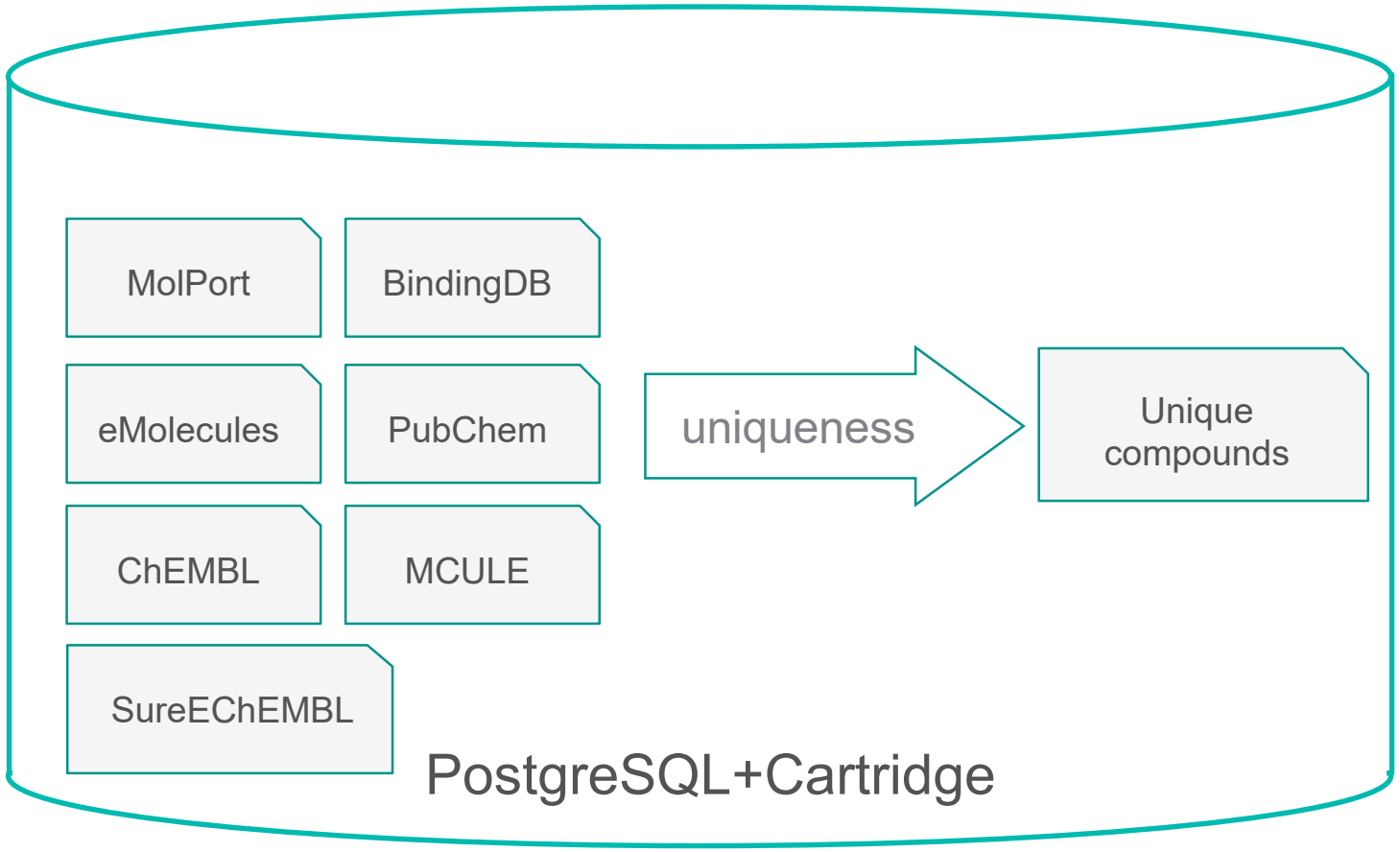

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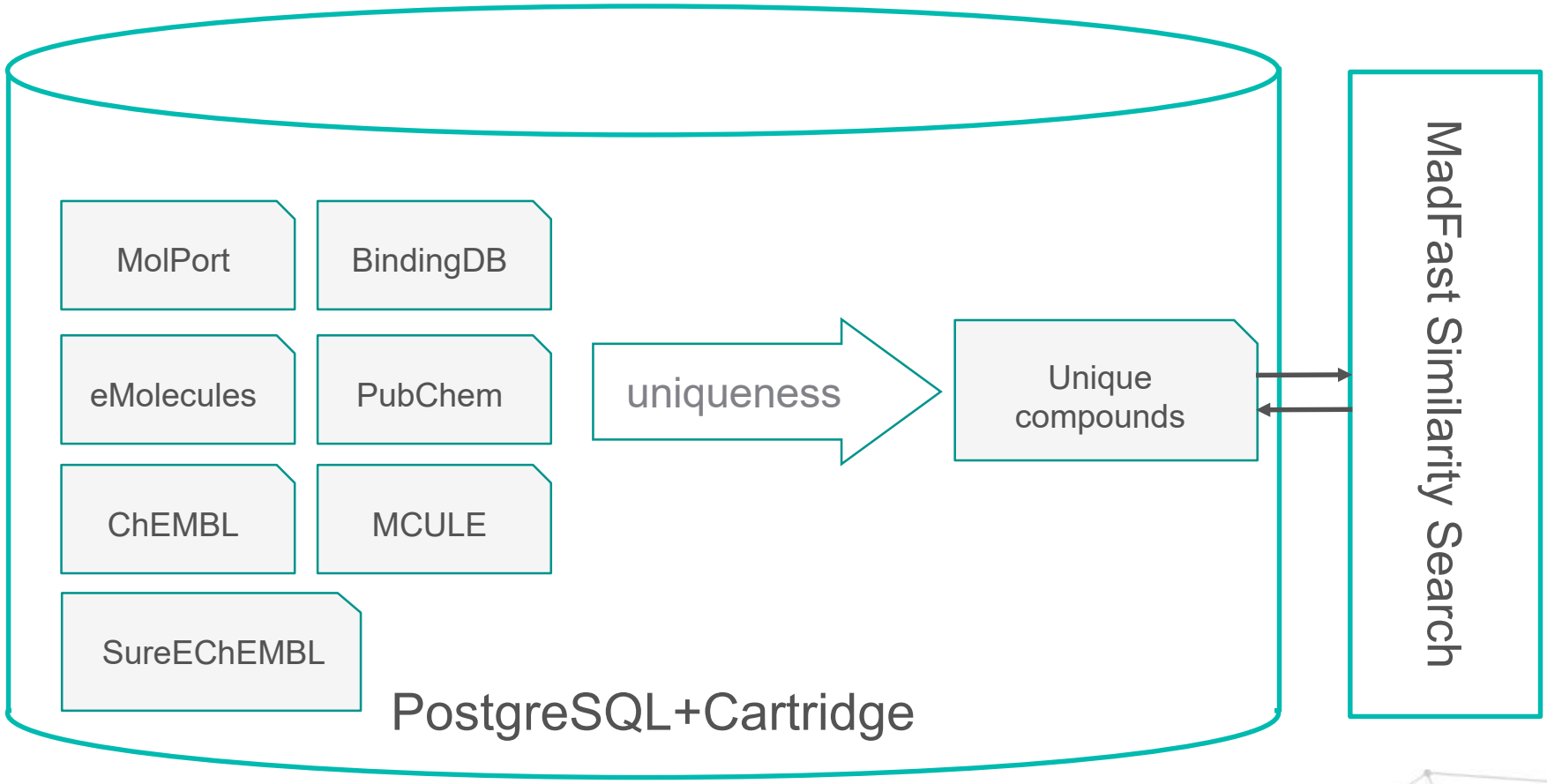

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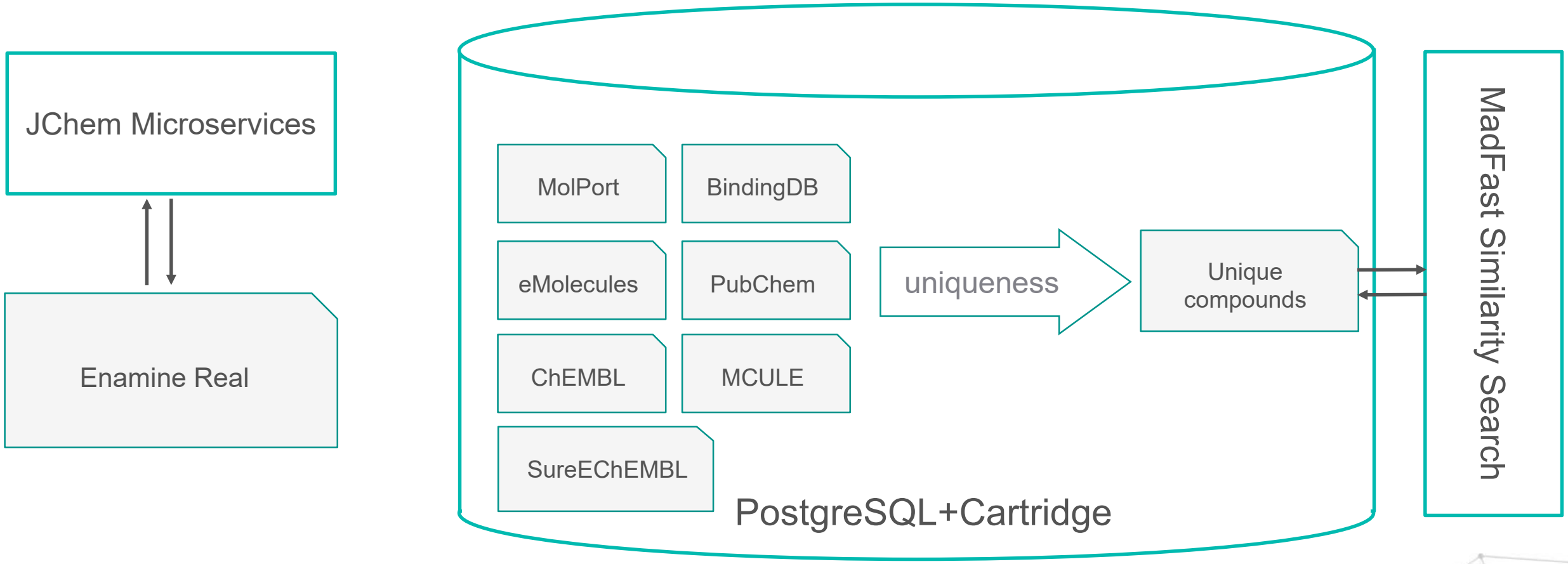

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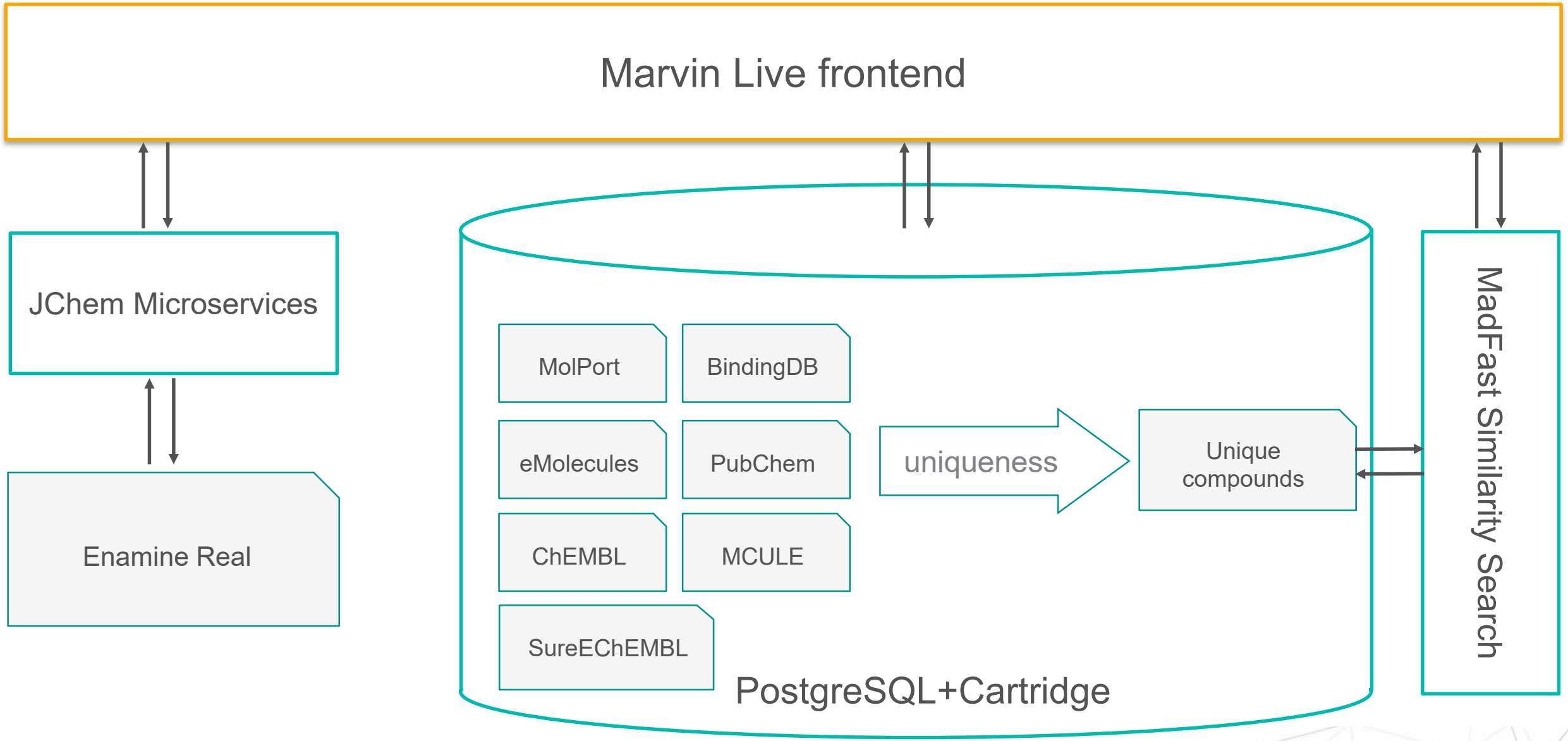
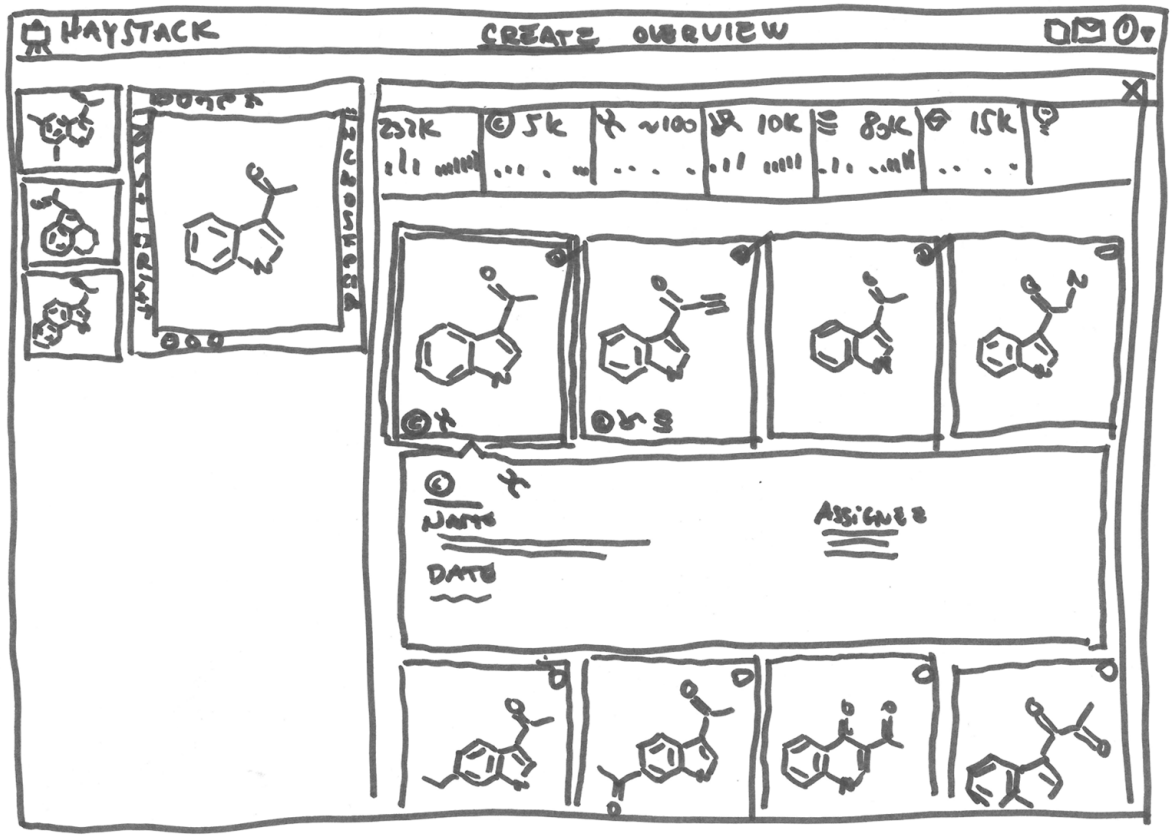


SO WHAT NEXT?



Q1

- Validation
- Work out requirements

Q2

- Consolidating backend
- API layer
- GUI design and early development starts

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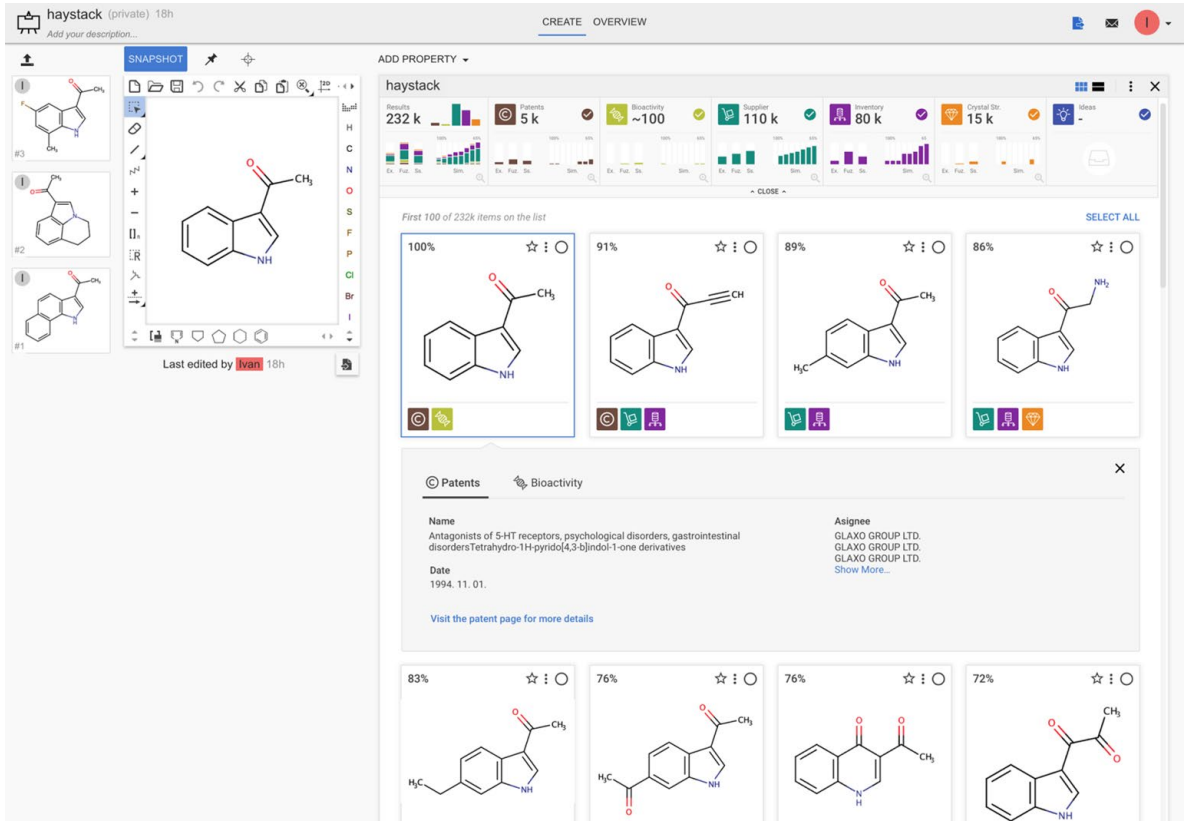

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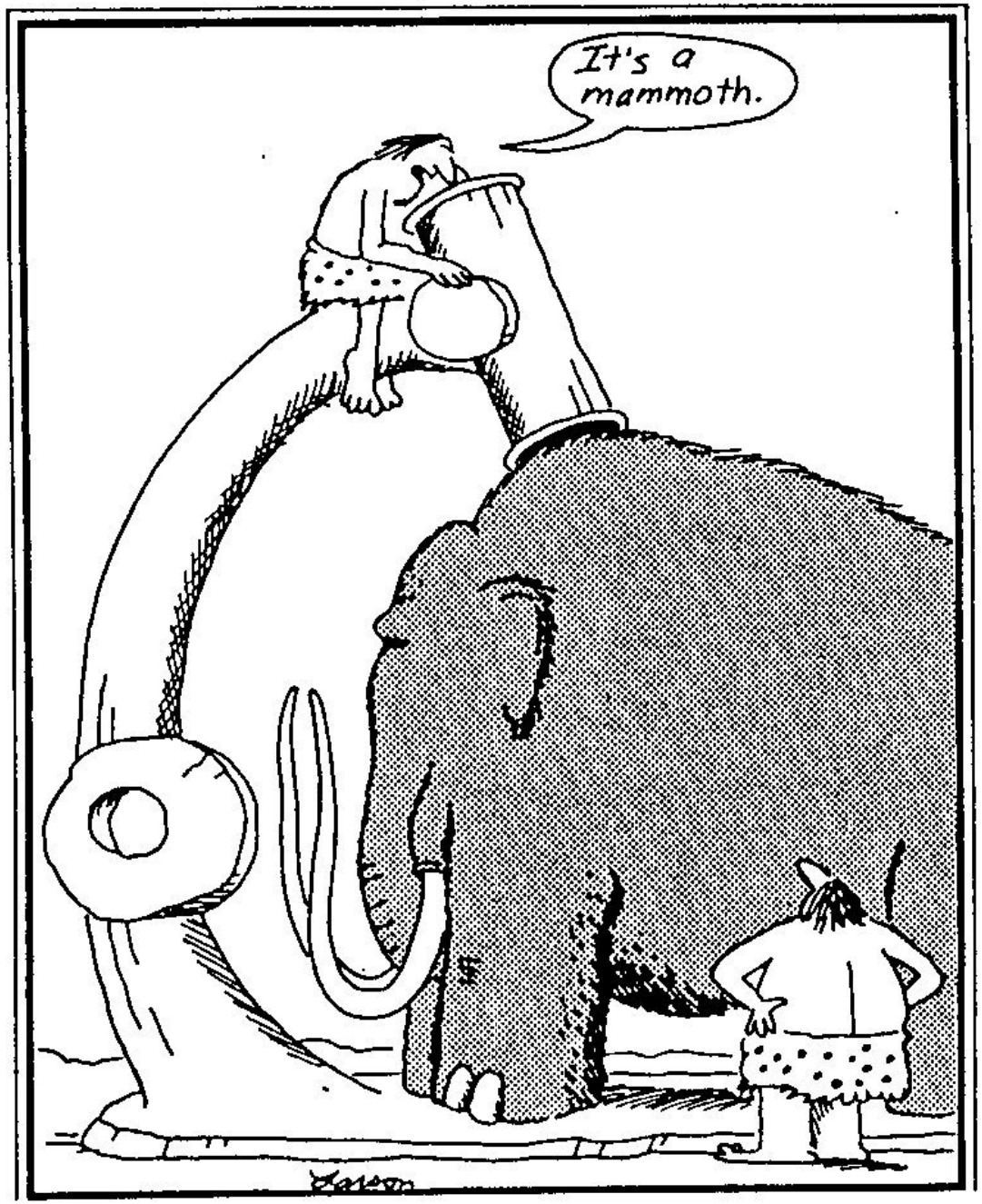

Early microscope

Talk to us

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Thank you

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