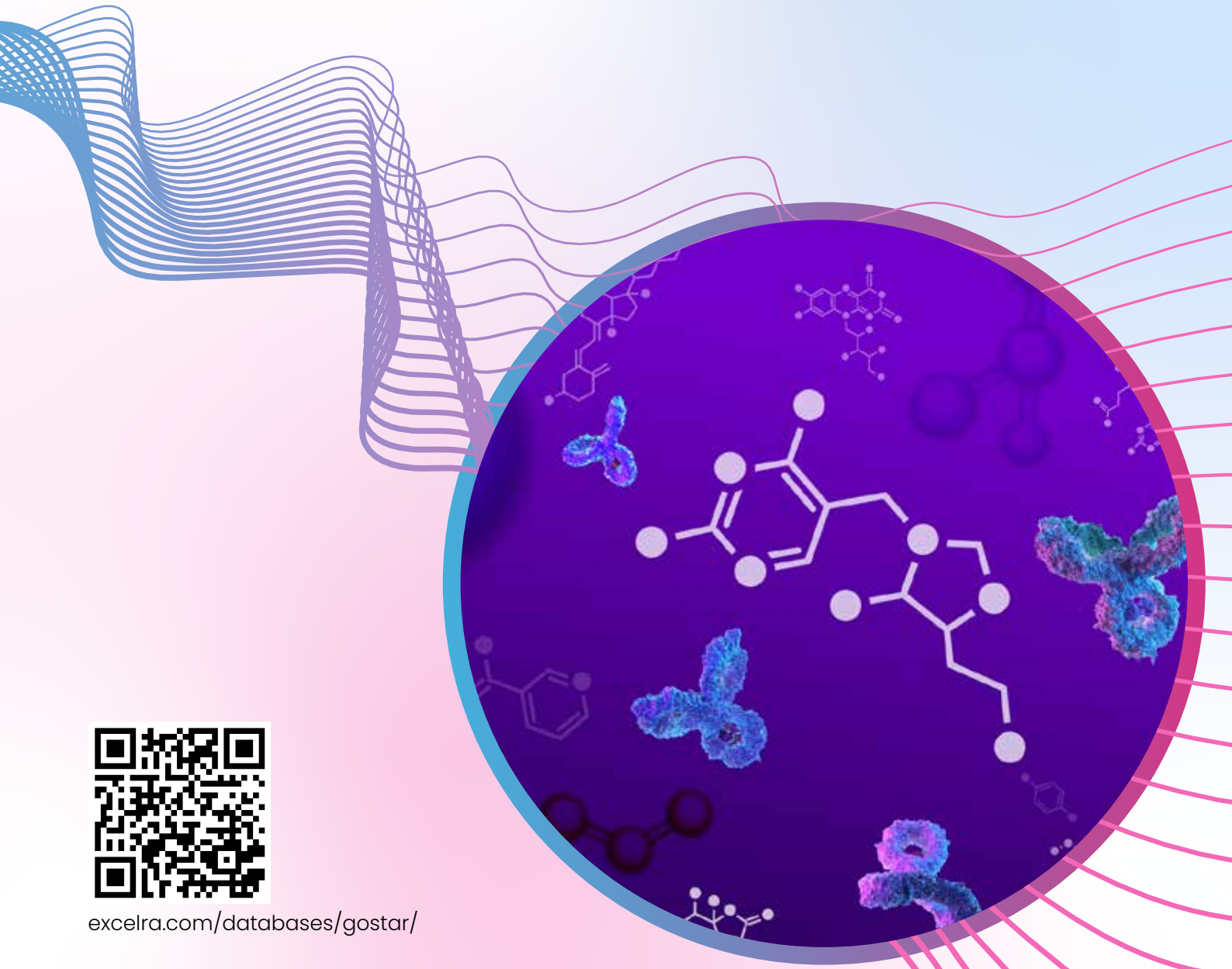
excelra

Accelerating Life-Saving Drug Discovery Breakthroughs

CURATION SERVICES

GOSTAR™



excelra.com/databases/gostar/

Empowering data-driven drug discovery

Analysis-ready SAR data curation, tailored annotations, and time-efficient solutions

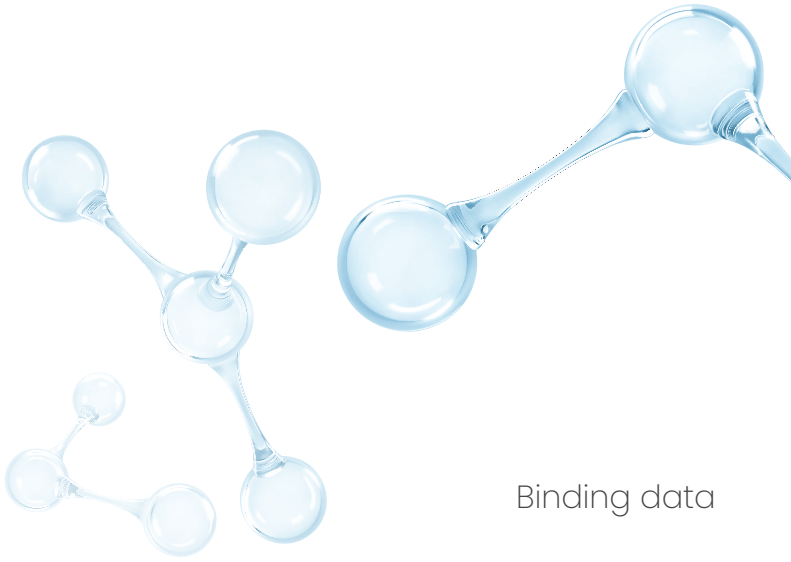
In the dynamic field of drug discovery and development, the importance of obtaining and analyzing data on molecular targets, recent patents, and journal articles cannot be overstated. These resources provide essential insights and the latest breakthroughs, keeping you at the forefront of innovation. Our comprehensive data curation services are meticulously designed to address this urgent need. They ensure the timely delivery of relevant information, relieving you from the time-consuming burden of data extraction. This streamlined approach not only optimizes your organization's efficiency but also optimizes cost-effectiveness. By embracing our curation services, you empower your scientists, whether they are medicinal or computational chemists, to focus their expertise on the core of their research, ensuring a continuous cycle of productivity.

- State of the art curation tools and platform
- Cutting-edge article screening strategies
- Highly qualified subject matter experts with masters and PhD degrees
- Three level quality check and quality assurance approach

GOSTAR™

The Excelra advantage

Scalable, modality-agnostic curation trusted by global pharma & biotech



Small Molecules

Structures
Core group details

TPD

Degrader type
Target protein and E3 ligase
Linker structures

Large Molecules

Peptides, mAbs, ADCS
Sequences (VH & VL)
Clone details and expression system
ASO structures and Modified nucleotides
Extraction of ASO in HELM format

Binding data

Pharmacokinetics

ADME & toxicity parameters

Physicochemical properties

Functional in vitro/ in vivo activity

Target & disease indication mapping

Comprehensive SAR data extraction, curation, and structuring services

The pharmaceutical and biotech industries are exploring new target classes, including the previously 'undruggable' genome and innovative disease interception mechanisms, while also finding new applications for well-known target classes like GPCRs, Kinases, Ion Channels, Hydrolases, Proteases, and more. Valuable information, however, is often scattered across unstructured data sources, making access and utilization challenging.

Emerging drug target classes, and beyond

1. **Immune checkpoints** ⟶ e.g., PD-1, PD-L1, LAG-3
2. **Epigenetic targets** ⟶ e.g., DNMT3A, HDAC2, EZH2
3. **Autophagy targets** ⟶ e.g., mTOR, Beclin-1, ULK1
4. **Protein degraders** ⟶ e.g., BRD4, AR, MDM2
5. **RNA binders** ⟶ e.g., SMN2, MAPT, FOXM1
6. **Integrins** ⟶ e.g., αvβ3, α4β1, α5β1
7. **Transcription factors** ⟶ e.g., NF-κB, PPARs, HIF-2α
8. **Synthetic lethality** ⟶ e.g., ATR-WEE1, ATM-DNA-PK, RAD52-PALB2

In addition to providing high-quality and annotated target-specific SAR data, our tailored curation services are designed to help you enhance drug development productivity and discover breakthrough therapies. Here are our allied custom chemistry solutions designed to improve the efficiency of your research.

1. **Virtual chemical library development**
   Proteome-focused or multi-target optimal libraries
2. **Chemical space analysis**
   Scaffold-based activity landscape analysis
3. **Markush enumeration**
   Markush-based overlap analysis for novelty assessment, and research prioritization
4. **Small & large molecule data curation**
   Molecular Target Activity & Affinity, ADMET Properties, Compound's Journey to Clinic, Chemical Reactions

Data delivery in flexible-file formats

Unlock the power of seamless data integration with our cutting-edge solutions for the pharmaceutical industry. Our data is expertly curated and delivered in a variety of formats, including SDF, XLS, CSV, TSV, and MRV, ensuring compatibility with the latest drug discovery software and analytical tools.

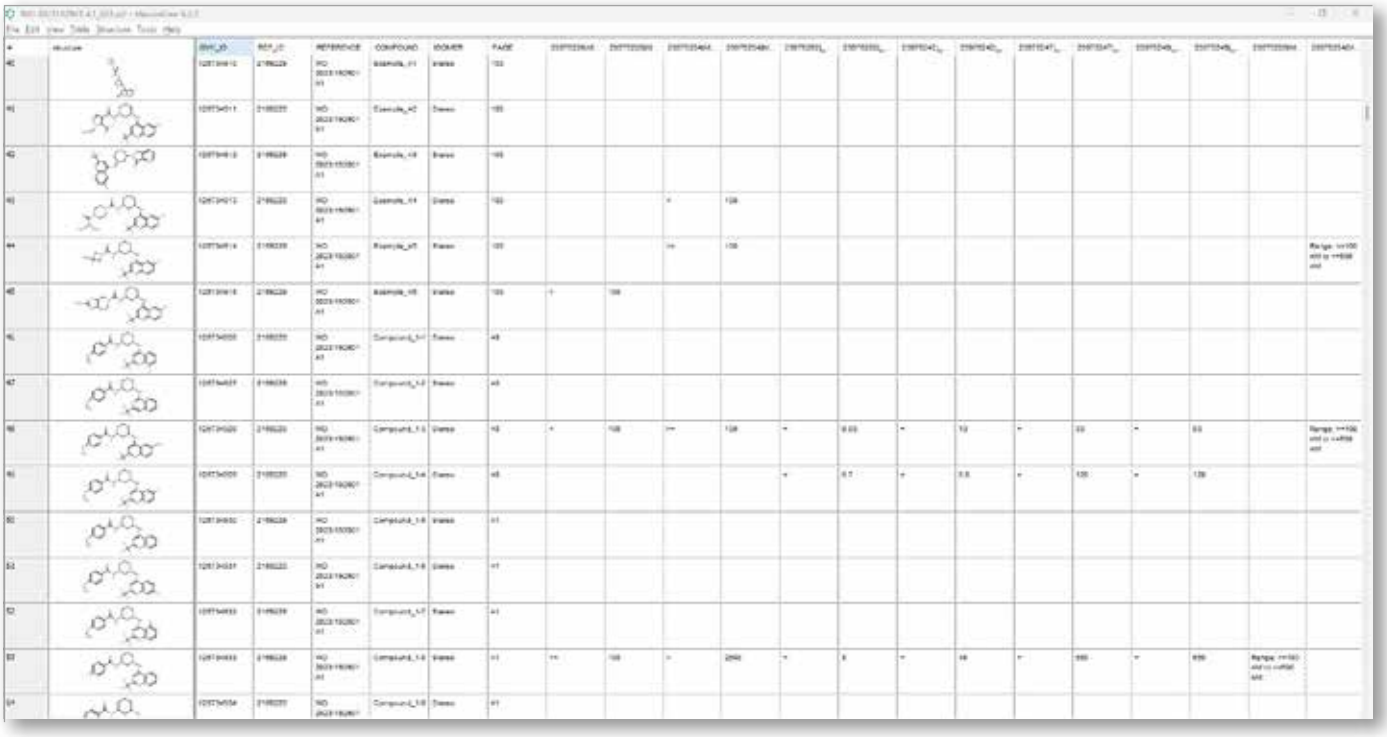


Fig 1: SDF sample data

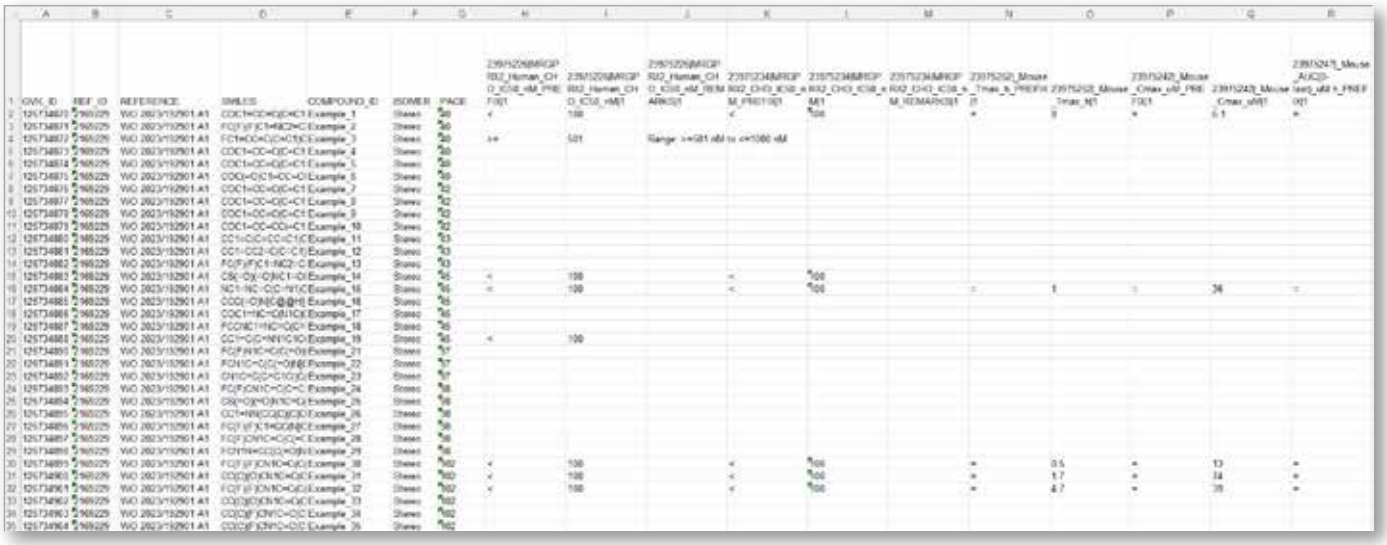


Fig 2: XLS sample data

But that's not all – for those with larger datasets and more complex needs, we offer the flexibility to choose from a range of robust relational database models, such as Oracle, PostgreSQL, or MySQL. Elevate your research, streamline your processes, and empower your team with data solutions that fit your exact requirements. Choose us for a future of limitless possibilities in pharmaceutical data management.

Case Study - 1

Patent-derived insights drive innovations in modern-day drug discovery

Background

In the dynamic field of drug discovery, researchers focused on targeted drug development for various cancers encounter the intricate landscape of kinase-targeted therapies. To navigate this complexity and foster innovation, these researchers strategically integrate scientific insights from patents and literature into their daily workflows, steering strategic decisions in their pursuit of advancements.

Challenges confronting the researchers

At the forefront of their work is the formidable task of identifying novel compounds with robust kinase inhibition profiles. The ongoing and intricate nature of efficiently extracting and interpreting nuanced information buried within patent documents, while staying abreast of the latest advancements, poses a continual challenge.

Time savings and enhanced efficiency

In a traditional setting, researchers often spend a substantial amount of time on manual extraction, curation, and structuring of information from patents. This process can consume, on average, 15-20 hours per week, diverting valuable time and resources away from the core research objectives.

Collaboration impact

By collaborating with our custom patent curation service, this arduous process is streamlined and optimized. Researchers typically experience a remarkable 60-70% reduction in time spent on data extraction and curation. This translates to an estimated time savings of 9-14 hours per week, allowing researchers to refocus on core research activities, accelerate project timelines, and drive innovation.

Immersive day-to-day workflows

1. **Patent-driven SAR exploration & innovative lead identification:**
   Leveraging the curated SAR data primarily sourced from patents, researchers employ a blend of traditional medicinal chemistry techniques and computational analyses. This fusion allows for the identification of novel chemotypes and lead-like molecules with enhanced binding affinity and selectivity, directly impacting the hit-to-lead transition. This focused, patent-specific information empowers the researcher to discern critical molecular features influencing kinase inhibition with unprecedented precision.

2. **Multiparameter optimization with patent-driven insights:**
   The curated dataset, enriched with patent-derived physicochemical insights, forms the foundation for lead optimization, ensuring potent kinase inhibition and optimal drug-like properties. Simultaneously, ADMET insights from patents, integrated through computational models and experiments, drive early-stage decision-making, minimizing late-stage attrition risks. Detailed metabolism data, extracted from patents, undergoes both traditional enzymatic studies and modern computational analyses, guiding pathway predictions and optimizing compound stability. This dual approach balances tradition and innovation in achieving precision in drug discovery.

3 Polypharmacology strategic exploration

Researchers explore polypharmacology insights derived from patents using a combination of literature review and in-house experimentation. This holistic approach aids in designing compounds that address multiple targets within, for example, oncological pathways, potentially overcoming resistance mechanisms.

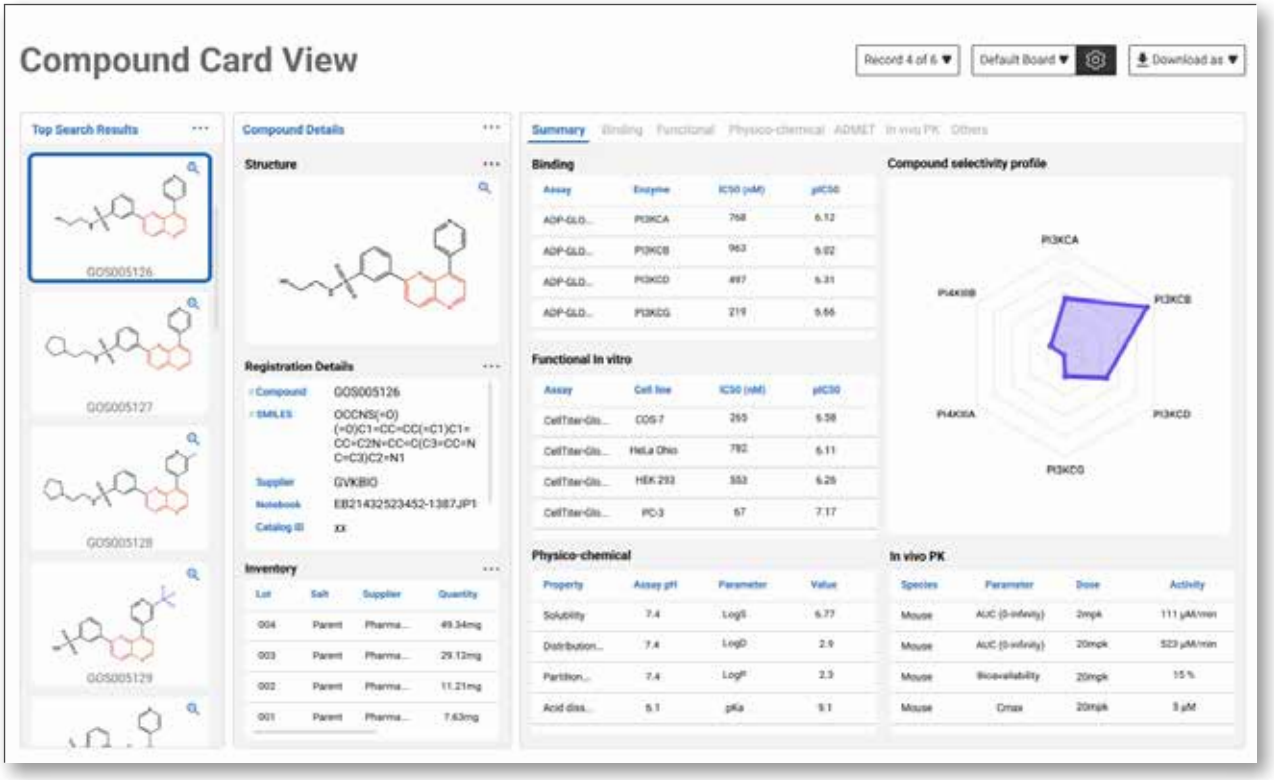


Fig 3: Conceptual representation of a 3rd-party analytical tool

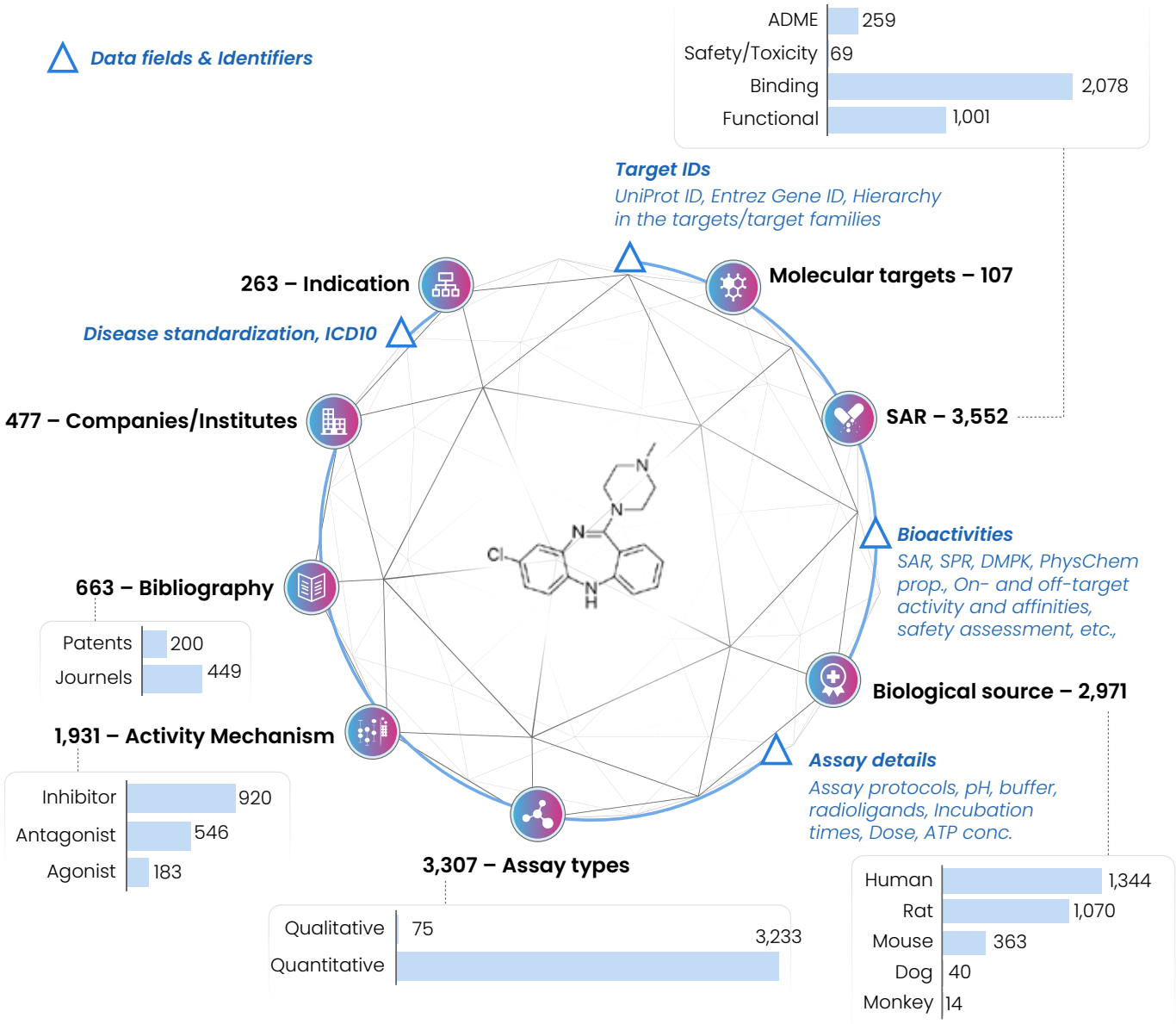
Collaboration impact

The seamless integration of patent-derived insights facilitated by our custom curation service stands as a testament to the precision and innovation required in modern-day medicinal chemistry. The fusion of traditional and computational methodologies, enriched by a wealth of patent-derived information, plays a pivotal role in elevating the researcher's effectiveness within the competitive domain of targeted drug discovery. Beyond mere timesaving, this outcome signifies a transformative pathway, guiding researchers toward groundbreaking advancements in drug discovery.

Case Study - 2

Clozapine | compound profile

Antipsychotic with a known risk of drug-induced seizures



The Excelra advantage

With a rich legacy of domain expertise, Excelra stands as the preferred partner for the top 20 pharmaceutical companies, delivering bespoke data curation services extracted from extensive journal and patent resources.

Our key advantage resides in our technologically augmented manual curation process, subject to a stringent 3-tier quality control system. Seasoned scientists with Ph.D. and MS degrees in medicinal chemistry, drug discovery, and allied life sciences oversee this meticulous procedure.

Experience the efficiency of our services with rapid project turnaround times, typically within 2-3 business days for the majority of literature sourced from journal articles and patents. We understand the value of your time and are committed to keeping your research agile and productive.

Where data means more

excelra

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Connect with our experts: marketing@excelra.com

www.excelra.com