cyprotex
AN EVOTEC COMPANY

AI Drug Discovery

Artificial intelligence (AI) is transforming how we identify, develop, and validate new therapies. While AI holds immense potential to revolutionize the drug discovery and development process, the availability of reliable data and the experimental validation of predictions are critical for success. We specialize in generating high-quality experimental data through flexible, cost-effective, and high-throughput workflows that improve predictive accuracy and expand the applicability of machine learning (ML) drug screening models. As a leading provider of *in vitro* ADME-Tox data, Cyprotex brings deep expertise in managing experimental variability across diverse modalities. In addition to a wide range of standard assays, we offer bespoke solutions to minimize random error and systematic bias, which are essential for ensuring reliable and accurate predictions.

Rapid Onboarding. Quick Turnaround.

Drug Metabolism
- CYP & non-CYP
- Microsomal, hepatocyte, S9, cytosolic, plasma & recombinant enzyme stability
- Reversible & time-dependent inhibition
- Nuclear receptor activation
- Metabolite identification & profiling

Drug Permeability & Transporters
- PAMPA
- Caco-2 & MDCK-MDR1 permeability
- ABC & SLC transporter evaluation

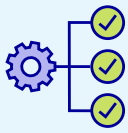
Physicochemical Profiling
- Ionization (pKa)
- Lipophilicity (log P, CHI, log D shake flask)
- Solubility & chemical stability
- Plasma, blood, microsomal & tissue binding

Bioanalysis
- Small molecules and diverse modalities

In vitro toxicology
- Mechanistic Toxicity & Cytotox Screening Panel
- Organ-Specific Toxicity
  - Cardiotoxicity
  - Neurotoxicity
  - Hepatotoxicity
  - Nephrotoxicity
- Immunotoxicology

Specialist Expertise
- High content screening (HCS)
- Electrophysiology (MEA)
- Flow cytometry
- 2D and 3D cell models
- Transcriptomics

Our Proven Approach to Partnering with AI Drug Discovery Companies



Comprehensive Project Scoping

Rapid Onboarding

Optimized Workflows

Dedicated Support

- **Comprehensive Project Scoping for Tailored Solutions.** Cyprotex provides strategic consultation on customizing every aspect from assay selection to sample management to fit your project's unique needs. Seamless LIMS integration ensures efficient data handling from the outset, aligning our capabilities with the precision and speed you need.
- **Rapid Onboarding and Flexible Pricing.** We facilitate rapid onboarding with early, clear communication of timeline estimates, indicative pricing, and all other aspects of the project lifecycle— enabling you to assess feasibility and budget alignment upfront for faster project initiation.
- **Workflow Optimization for Speed and Efficiency.** Our workflows are meticulously optimized for compound management, logistics, and assay execution. By aligning data formats and compound metadata with your ML models, we support efficient downstream analysis and predictive modeling.
- **Dedicated Support for Continuous Engagement.** Dedicated study managers and regular meetings with scientific and project leads ensure responsive, transparent communication. As projects evolve, we adapt quickly, maintaining momentum and ensuring consistency in data delivery.

Cyprotex: Enabling Smarter Drug Discovery ML Models

- **High Precision and Accuracy**
  Single-laboratory controlled assays to minimize variability. A deep understanding of systematic assay errors, combined with the capacity to handle large sample sizes, ensures data reliability.
- **Training Set Selection**
  PCA and clustering inform compound selection to broaden model applicability. Tailored strategies support both global and target-specific ML models, maximizing return on investment.
- **Data-Rich *in Vitro* Descriptors**
  Rapid, high-throughput biomimetic chromatography (~1,000/day; <3-day turnaround) provides high-quality *in vitro* descriptors, enhancing biological relevance and ML model performance.
- **Cost-Effective Data Generation**
  Strategic compound selection using replicate-based error assessment enables focused testing, delivering substantial cost savings without compromising data quality.

Explore our latest publications and expert insights on AI/ML drug discovery:

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