cyprotex AN EVOTEC COMPANY

Physicochemical Profiling

Physicochemical properties provide an insight into the relationship between a molecule's structure and its physical behavior within a system influencing its dissolution, absorption, distribution, metabolism, elimination, protein affinity and toxicity. The early determination of physicochemical properties is a well-established strategy to support rational compound design within drug discovery.

Cyprotex offer a comprehensive range of physicochemical profiling services. Our expert team of physical scientists can assist in designing screening strategies and can adapt assays to meet your needs.

Cyprotex offers a wide range of capabilities at hit-to-lead and lead optimization stages for small molecules and diverse modalities.

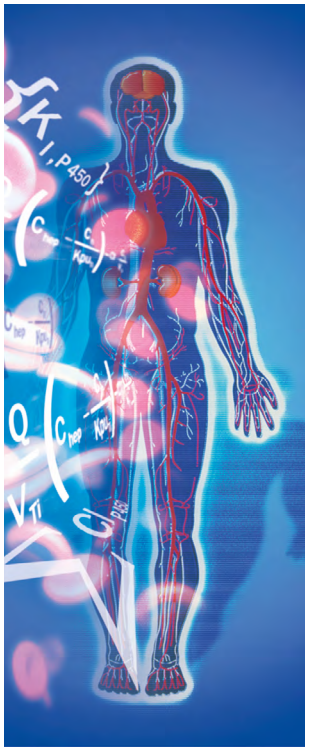
- **Solubility:** Dissolution and precipitation approaches
- **Ionization:** pK_a via potentiometric and UV approaches (+/- co-solvent)
- **Lipophilicity:** $logD_{shake\text{-}flask}$, CHI (chromatographic hydrophobicity index), potentiometric logP
- **Chemical Stability:** Range of buffers, redox additives and time frames

	Hit-to-lead	Lead optimization
Solubility	Turbidimetric	High throughput solubility (mass spectrometry or UV)
Ionization	Rapid UV	UV method Potentiometric method
Lipophilicity	Chromatographic hydrophobicity index (CHI)	$logD_{shake\ flask}$ logP
Chemical Stability	Profiling approach	Focused approach

Your Partner in Physicochemical Profiling

- **Extensive experience.** Our team of experts have decades of combined industry experience in physical chemistry to plan optimal screening strategies and assist with data interpretation and future project planning.
- **Project support.** Dedicated study managers are assigned to your project and are on hand to support you with logistics, data delivery and any technical questions.
- **Comprehensive range of services.** We offer a wide range of flexible services which can be specifically designed for your needs.
- **Secure high quality data delivery.** Our laboratories based in the USA and Europe follow strict quality procedure to ensure your data are robust and are stored and delivered securely.

In Silico Modeling Expertise – Using Physicochemical Data to Underpin AI



Machine Learning Pattern Recognition	PD and PK/PD Modeling	Simulation Modeling
Off-the-shelf and bespoke statistical modeling using structural descriptors (QSAR/QSPR) and/or measured properties	**Link PD effects to PK** drivers of efficacy **for optimal dosing regime** selection	Physiologically-based pharmacokinetic (**PBPK**) modeling Systems biology and quantitative systems pharmacology (**QSP**) modeling
Prioritize chemistry early by developing virtual screening capabilities: maximize value of existing datasets	**Simulate PD** effects by applying mechanistic, semi-mechanistic and/or empirical modeling	**Drive compound selection** by predicting properties in human or preclinical species

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