



Physicochemical Analysis

Pion Analytical Services offers physicochemical characterization to help you identify the most promising small molecule drug candidates rapidly and efficiently so you can make informed decisions about candidate selection & formulation earlier in development.

Our Sirius T3 system measures physicochemical properties such as the ionization constant (pK_a), lipophilicity ($\log P/\log D$) and solubility of ionizable drugs using sub-mg amount of sample. Pion's unique, proprietary Cheqsol method enhances instrument capabilities enabling the accurate determination of kinetic and intrinsic solubilities for ionizable compounds, characterization of supersaturation behavior and the generation of pH-solubility profiles.

pK_a , LogP/D AND SOLUBILITY ASSAYS

Many drugs are weak acids or weak bases and exist in solution as an equilibrium between unionized and ionized forms. The pK_a , also known as the acid dissociation constant, is an intrinsic property of such ionizable compounds and indicates the pH at which a functional group exists in solution as a 50:50 ratio of neutral: ionized species. If the pK_a of a molecule is known, the degree of ionization of the molecule can be determined for other pH values.

LogP and logD are measures of lipophilicity. Lipophilicity is a key parameter in understanding the pharmacokinetic behavior of drugs and can influence distribution into tissues, absorption and protein binding characteristics of a drug. It is also an important factor in determining the solubility of a compound. In particular, drugs designed for oral administration require a good balance between lipophilicity and solubility in order to achieve adequate in vivo absorption.

KEY DELIVERABLES

A full study report is provided. Reports may include (per customer request): sample and customer details, table of pK_a results, presentation of logP/D results, lipophilicity profile (where appropriate,) solubility results, a logS profile and table vs. pH, distribution of species profile and statement of methodology.



The Sirius T3 physchem compound instrument

Why Use Pion

Pion scientists are proud to be the world's leading experts in the determination of physicochemical properties. We developed the Sirius T3 instrument to characterize physchem parameters such as pK_a and logP/D which they are recognised as setting the industry standard.

We know that accurate determinations are essential to select the right candidates and to discriminate others in order to define the optimal path to speed up drugs to development. Pion empowers the pharmaceutical R&D community helping to make important decisions on candidate selection based on trusted data for drug optimization, which will impact on people's lives. In other words, we help scientists to find the right answers faster to select the best strategy for a successful drug.



pK_a Analysis

Analysis	Part #	Details
Gold Standard pK _a (with a chemical structure provided)	1801010	Price per sample, 10mg
Gold Standard pK _a (without a chemical structure provided)	1811010	Price per sample, 10mg
Platinum Standard pK _a	1801210	Price per sample, 10-15mg
Upgrade from Gold Standard to Platinum	1811011	Price per sample, determined upon enquiry
MEC (molar extinction coefficient) with a Chemical structure provided	1801110	Price per sample, 10mg

LogP/D Analysis

Analysis	Part #	Details
Gold Standard pH-metric LogP (with a chemical structure)	1801012	Price per sample, 5mg
Gold Standard pH-metric LogP (without a chemical structure)	1811012	Price per sample, 10mg

Shake-Flask

Analysis	Part #	Details
Gold Standard Shake-Flask (HPLC) logP/D	1801013	Price per sample per pH, 20-50mg

Solubility Analysis

Analysis	Part #	Details
Platinum Standard pH-metric solubility CheqSol (aqueous)	1802001	Price per sample, 20-50mg
Platinum Standard pH-metric solubility CheqSol (co-solvent)	1802002	Price per sample, 20-50mg
Platinum Standard pH-metric solubility CheqSol (biorelevant)	1802410	Price per sample, 20-50mg
Platinum Standard pH-metric solubility CheqSol (in presence of excipients)	1802430	Price per sample, 20-50mg

Shake-Flask

Analysis	Part #	Details
Gold Standard shake-flask solubility (aqueous)	1802401	Price per sample per pH, 20-50mg
Gold Standard shake-flask solubility (co-solvent)	1802403	Price per sample per pH, 20-50mg
Gold Standard shake-flask solubility (biorelevant media)	1802402	Price per sample per pH, 20-50mg
Gold Standard shake-flask solubility (in presence of excipients)	1802405	Price per sample per pH, 20-50mg



With analysis that can be tailored to your specific application, Pion's Analytical Services provides the vital information missing from your research.





Screening Analysis

pK_a - High throughput pK_a measurement using the Fast UV pK_a assay (pH 2.0 to pH 12.0)

10 samples

Analysis	Part #	Details
Multi sample pK _a screening	1801201	Batch of 10 samples, 200µL /10mM stock
Additional multi sample pK _a screening	1801202	Per additional sample, 200µL /10mM stock

5 samples

Multi sample pK _a screening	1801203	Batch of 5 samples, 200µL /10mM stock
Additional multi sample pK _a screening	1801204	Per additional sample, 200µL /10mM stock

LogD - High throughput logD measurements using shake-flask HPLC methodology, based octanol/water partitioning assay at fixed pH. For ionisable & non-ionisable compounds. Performed at pH 7.4 or pH 2.5.

10 samples

Analysis	Part #	Details
Multi sample LogD screening	1801301	Batch of 10 samples, 200µL /10mM stock
Additional multi sample LogD screening	1801302	Per additional sample 200µL /10mM stock

5 samples

Multi sample LogD screening	1801303	Batch of 5 samples, 200µL /10mM stock
Additional multi sample LogD screening	1801304	Per additional sample 200µL /10mM stock

Solubility- High throughput solubility measurements using 96-well UV-plate reader methodology at fixed pH. For ionisable & non-ionisable compounds. Performed at requested pH values

10 samples

Analysis	Part #	Details
Multi sample solubility screening (DMSO stock)	1822101	Batch of 10 samples, 250µL /10mM stock
Multi sample solubility screening (DMSO free)	1822102	Batch of 10 samples, 3mg per sample