# Analytical Services for Small Molecules

Apart from being your premium partner for protein X-ray structures, CRELUX offers a large number of hit finding, hit validation and biophysical screening technologies. We now offer easy access to analytical services for your small molecule ligands. The service is available directly from CRELUX. Determination of identity, mass, purity, solubility, stability or ADME parameters of your compound for instance, can accompany any of our products or can be amended to any of our service agreements. The lab work will be performed by the computational and medicinal chemistry expert **4SC Discovery GmbH** who is also our partner within the i2c drug discovery platform (www.i2c-discovery.com).

## Analytical Services

Individual analytical services are available to support all steps in the drug discovery process of new chemical entities for medicinal chemistry. With our well established analytical technology platform we provide a wide range of methods. State-of-the-art equipment in combination with our highly professional data management enables high throughput in sample analysis. The range of analytical techniques and methods we offer includes a fully automated NMR, LC-DAD, LC-UV-MS, LC-MS/MS and melting point equipment. Our experienced team supports you right through the drug discovery process, additionally offering bioanalytical services for the quantitation of small molecules in biological matrices and the estimation of solubility, permeability, absorption and bioavailability.

**Figure 1: fully automated NMR**

## Analytical Chemistry

Analytical **LC-UV-MS** measurements allow for fast and accurate reaction control during synthesis of small molecules or for fast identity check of large substance libraries. We operate within a mass range of 80-2000 Da in $ESI^+$ or $ESI^-$ mode with simultaneous UV detection at 200-400 nm. LC-UV-MS instruments with fully automated sample analysis and short generic RP-HPLC gradient guarantee short turnaround times.

## ADME

Absorption, distribution, metabolism and excretion (**ADME**) of a drug substance influence the levels and kinetics of drug exposure. *In vitro* assays like parallel artificial membrane permeability assay (PAMPA), plasma protein binding and microsomal stability during lead optimisation can help to avoid compound failure in preclinical studies or early clinical trials. We offer all mentioned assays, which are performed with our LC-MS/MS equipment and by experienced scientists. Furthermore we offer quantitative analysis of small molecules in biological matrices like plasma as well as the determination of small molecules, metabolites or endogenous substances out of cell cultures or other biological matrices, e.g. as read out for IC50 experiments.

**Figure 2: LC-MS**

## NEW WEBSITE

Please have a look at our new website which is also optimized for mobile devices.

You will find there our products: PRIME PROTEIN, INTRACT (assays and biophysics), XPRESS, XPEDITE or XPERT X-ray structures, and i2c as well as our services like Hit finding or Hit validation.

http://www.crelux.com

## MEET US AT

**RICT,** July 1-3, Avignon, France http://www.ldorganisation.com

**BIO EUROPE,** November 2-4, Munich, Germany http://www.ebdgroup.com/bioeurope/index.php

## CONTACT

CRELUX GmbH, Am Klopferspitz 19a, D-82152 Martinsried, Germany

Dr. Michael Schaeffer, schaeffer@crelux.com, +49 (0) 89 700760170, www.crelux.com