

SpecScreen xHTS

New technologies are revolutionizing science and the development of new pharmaceutical products. High-throughput screening, combinatorial chemistry, functional genomics and bioinformatics are accelerating the discovery of new active substances in research. Parallel to the trend towards constantly increasing the throughput of samples, there is also the demand for reducing costs in research and development.

Increasing the efficiency of system solutions offers a technological answer to these economic challenges.

RPD TOOL provides custom-made solutions within the areas of **automation, on-line analytics and screening.**

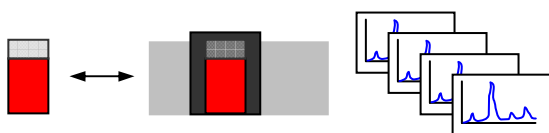
SpecScreen xHTS is designed as a dedicated platform for physical stability testing during formulation development.



SpecScreen xHTS: The system is a dedicated platform for automated physical stability testing during formulation development and is equipped with near infrared, Raman spectrometer and CCD camera, has a capacity of up to 2000 samples which can be stored under different conditions (e.g. temperature, humidity).

Concept and components of SpecScreen xHTS

SpecScreen xHTS is an automated platform for physical stability testing during pre-formulation and formulation development activities in R & D. The system consists of several temperature-controlled racks (5°C to 80°C / 40 F to 175 F) that can store up to 2000 samples in 96 or 24 well plate format glass vials under a wide range of humidity controlled atmosphere. In the standard configuration, the system is further equipped with a CCD-camera, a near infrared (NIR) and/or a Raman spectrometer. A robot transports the samples



Fully automated periodical acquisition of near infrared and/or Raman spectra of all test samples stored in SpecScreen xHTS.

between the racks and the spectrometers at intervals of hours to days. **No sample preparation is necessary and the analysis method is non-destructive to the sample.**

The acquired spectra are stored in a database for further analysis with our sophisticated software:

SpecFlash is a 1st level analysis package that automatically analyzes the vibrational spectra of the products stored in **SpecScreen xHTS**. It provides instant information about ongoing processes in the samples (i. e. morphological changes, hydrate formation or unspecific water up-take of drugs).

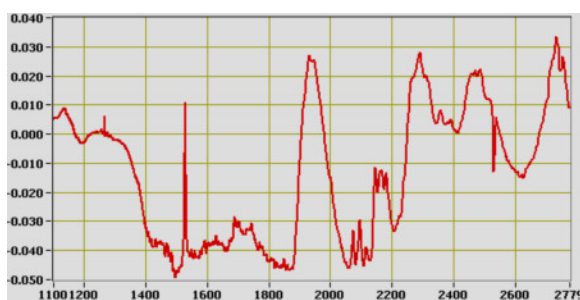
SpecAnalyzer is a 2nd level software tool and provides a level of information, previously unobtainable by conventional methods, about the physical and sometimes also chemical transformation processes in the sample.

SpecScreen xHTS Sample Manger is a software package for the management of samples stored in the system. It includes an efficient sample management system and a tool for the automated generation of data evaluation reports.

Field of application

Storage stability studies

The statistical analysis of the vibrational spectra sets provides valuable information about



Process factor calculated from a near infrared (NIR) data set of a new formulation candidate. X-axis: Wavelength [nm]. Y-axis: Absorbance.

ongoing processes in the test samples. A result of the 1st level data evaluation is the **process factor**, which is the calculated trend of systematic changes in the spectra data set. The process factor shows systematic changes in the vibrational spectra during the storage of test samples. It supports the identification of degradation or morphological changes of the active ingredient in new formulation candidates.

Additional results of the 1st level data evaluation are calculated **time profiles** showing the kinetics of significant processes in the test samples.

Time profile and process factor enable a quick qualitative overview of the behavior of a new drug substance in a set of formulation candidates. Based on this result, selected samples can be further analyzed by the interactive software package or transferred to ChromScreen xHTS for automated HPLC analysis for quantification of the degradation products of the active ingredient.



Time profiles of a test sample stored at 40°C/dry (green) and 40°C/75% relative humidity (red). Blue line: calculated linear regression of the 40°/75 % r.h. sample. X-axis: Storage time [day]. Y-axis: Calculated scores.

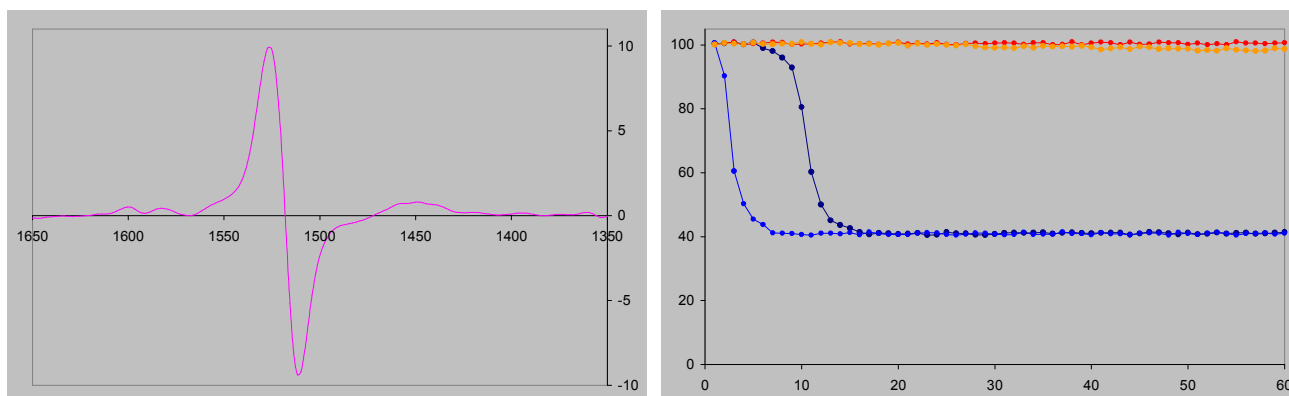
Solubility of drug candidates in semi-solid formulations

The development of a stable semi-solid formulation for poor soluble active pharmaceutical ingredients is a challenging task in pharmaceutical R & D.

RPD TOOL has developed methods to support the development of creams and ointments. Small amounts of new formulation candidates are stored under different storage conditions on **SpecScreen xHTS** and are analyzed with Raman spectroscopy.

Kinetics of dissolution and crystallization processes can be analyzed.

An example is given below. The influence of formulation preparation on drug solubility was studied using Raman spectroscopy.



Left: Difference in Raman spectra of dissolved and solid form of a new drug candidate. X-axis: Wave number [cm^{-1}], Y-axis: Raman emission

Right: Calculated kinetic profile of the solubility of four test samples. Light blue: Sample produced according to process A, sample composition 1. Dark blue: Sample produced according to process B, sample composition 1. Orange: Sample produced according to process A, sample composition 2. Red: Sample produced according to process B, sample composition 2. X-axis: Storage time [day], Y-axis: Relative solubility [%].

Our offer

If you are interested in accelerating your R & D processes in formulation development do not hesitate to contact us. We would be pleased to inform you about our products and services, which include custom analyses on our powerful in-house screening systems.

We are looking forward to your call.

Sincerely

Your RPD TOOL Team