

EXALT controlled crystallisation toolkit

- Saves time when scaling-up crystallisation conditions compared to taking an iterative first principles synthetic route
- Produces crystals from amorphous form during late stage medicinal chemistry to enable better early pre-clinical testing
- Screens to identify the optimum solvent for process scale crystallisation using just 100mg of sample for 20 solvents, producing high quality single crystals
- Modular design enables a wide range of solvents to be evaporated at the same time, all at the same slow rate, under the same conditions
- Confirms stable forms of crystalline structure through slow evaporation
- Non-destructive – 100% recovery of active

Introduction

EXALT is a unique toolkit developed by Genevac and researchers in the field to assist with evaporative crystallisation studies in a number of ways. Such studies, either solvent screening or searching for metastable and stable forms, can be time consuming and difficult to conduct. By enabling a wide range of solvents to be evaporated at the same time and at the same slow rate, the **EXALT** system can deliver crystalline forms of a chemical in a controlled and reproducible manner.

When combined with a chemist's experience, **EXALT** can give answers when screening multiple samples very quickly, saving time when carrying out scale-up reactions, compared with taking a synthesis route.



Ibuprofen crystallised from acetone (L) and ethyl acetate (R).



EXALT also enables more solvents and conditions to be screened, helping to confirm the predictions. It also enables chemists in the late stages of projects to complete them with some crystal forms, instead of going forward with just an amorphous form. Stable forms of crystalline structure can also be confirmed by using the **EXALT** slow evaporation method.

Configuration

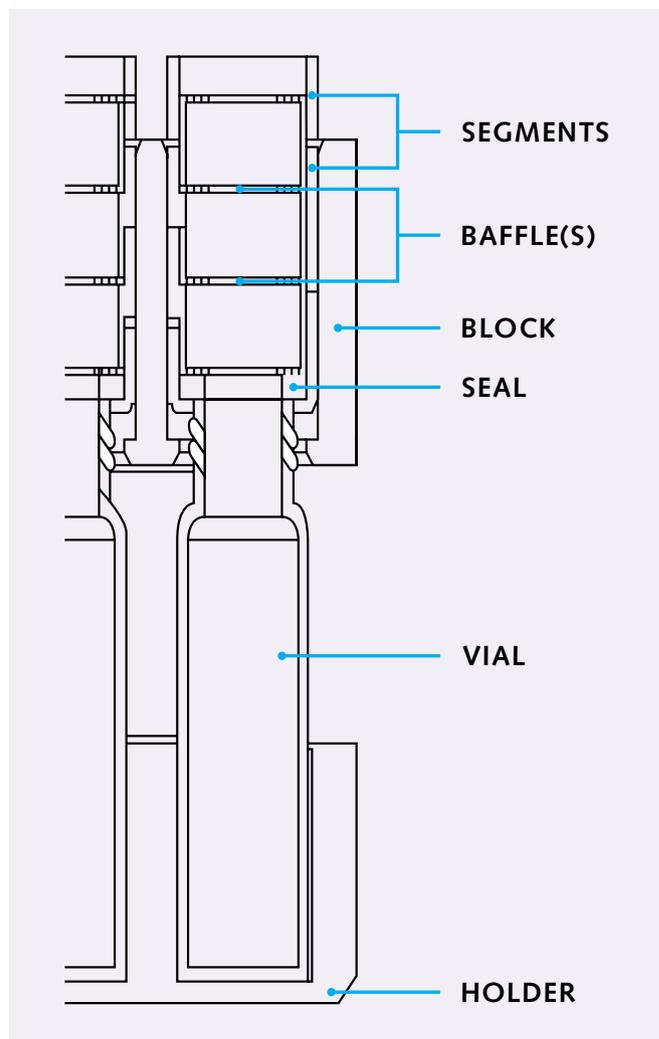
The system uses a special holder for vials, which allows selected baffles to be placed on top of the vials in order to restrict the evaporation rate of various solvents – the size and number of baffles varying according to the degree of solvent volatility. Then the holder is placed in a Genevac HT series evaporator, which cycles the samples at atmosphere and at a slightly reduced pressure for the duration of the process.



In this way, a wide range of solvents can be evaporated all at the same time and at the same slow rate. For example, DCM and Toluene can be placed in the vial holder and evaporated to sample dryness at the same time. **EXALT** may be used for solvents with a boiling point of 40°C to 165°C – DCM to DMAc. Evaporation time can be controlled in a normal range from six to 72 hours, or more, as required for most solvents in this boiling point range, delivering crystals from a range of solvents in a controlled and reproducible way.

The **EXALT** toolkit is entirely modular, allowing researchers to create their own baffle configurations to achieve the desired evaporation time profile for a set of solvents. This provides the ultimate in flexibility for experimental design.

Increasing the evaporation temperature can speed up the evaporation rate, although care must be taken not to exceed the boiling point of the most volatile solvent present. The HT series software allows the pressure drop from atmosphere, the time at atmospheric pressure and the time at reduced pressure to be specified.



Requirements

EXALT supports 15mm diameter x 45mm vials (also known as 1 dram vials) and accepts up to 24 vials per holder.

Evaporation system: a recent Genevac HT series evaporator with auto defrost and drain and the latest version of Genevac software.

