# *iChemExplorer* Application

## Impurity Rejection by Crystallization

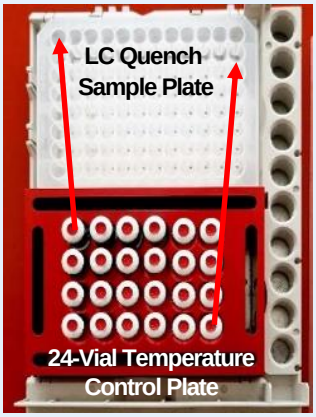
*Turn your LC and LC/MS into an Automated Screening System*
*Chemistry to Results in a LC Sample Vial*

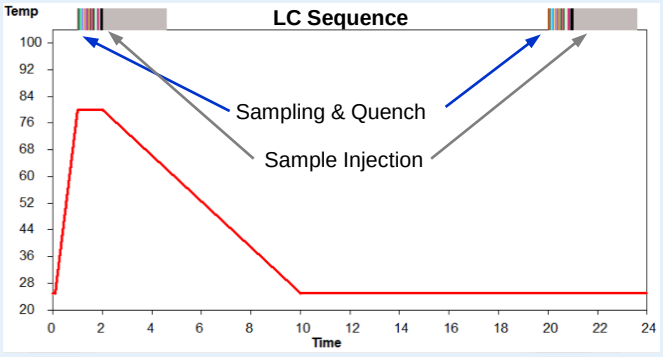
***iChemExplorer*** is an innovative hardware/software module integrated into your HPLC autosampler:

- Heating and cooling (5 to 150 $^0$C)
- Stirring up to 1200 rpm
- Proprietary in-vial filter insert technology
- Intuitive software interface for experiment design and execution
- Application specific data analysis and reporting

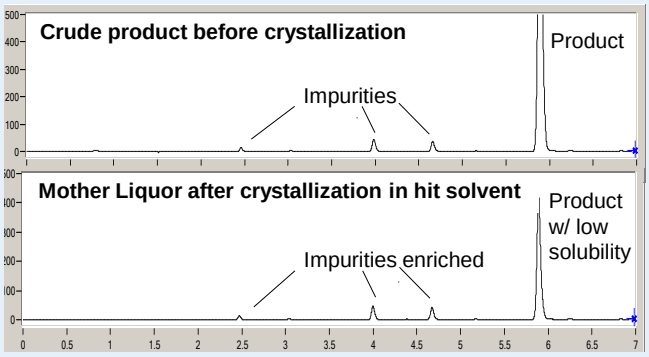
***iChemExplorer*** enables impurity rejection by crystallization in LC sample vials:

- 24 varying solvent conditions for slurry or crystallization
- User-defined heat-cool and equilibration profile
- Automated sampling, quench, dilution and LC injection of plate samples
  - ✓ After equilibration at hot temperature for solubility or dissolution
  - ✓ At the end of crystallization for solubility and impurity enrichment in mother liquor
- Calculate maximum yield and purity of crystallized solid based on mass balance
- Automated crystallization and LC analysis in real time




Integrated Temperature Program and LC Sequence




Impurity Rejection by Crystallization and LC Analysis

**A Case Study of Impurity Rejection by Crystallization**

An Integrated High-Throughput Screening Approach for Purification of Solid Organic Compounds by Trituration and Crystallization in Solvents

H. Tan *et al.*, *Org. Pro. Res. Dev.* 2008, 12, 58

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