iChemExplorer Application

Classical Chiral Resolution

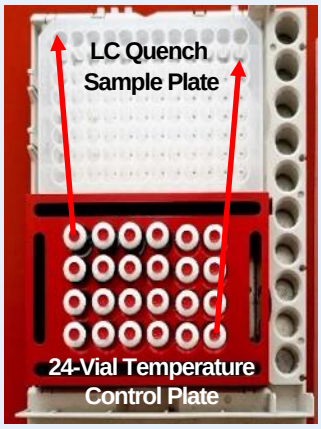
Turn your LC and LC/MS into an Automated Screening System
Chemistry to Results in a LC Sample Vial

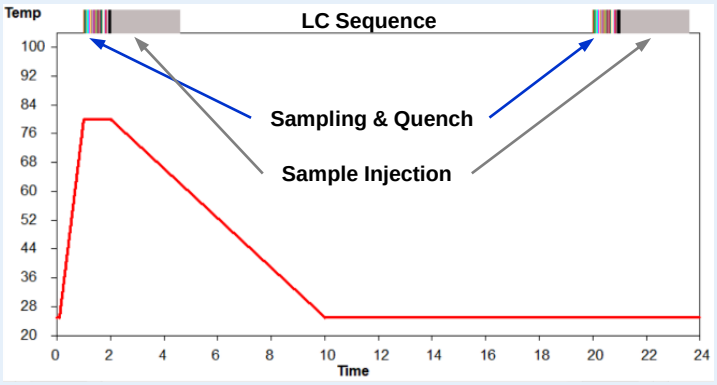
iChemExplorer is an innovative hardware/software module integrated into your HPLC autosampler:

- 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

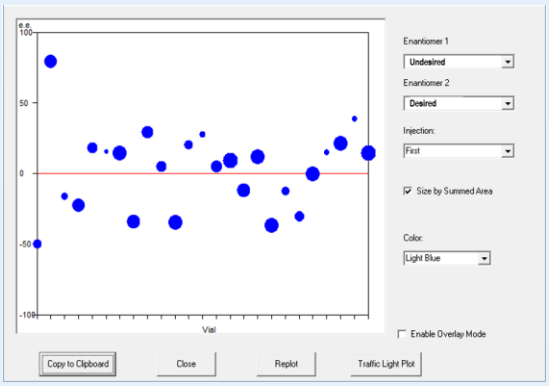
iChemExplorer enables classical chiral resolution screening by diastereomeric salt crystallization in LC sample vials:

- 24 varying resolution conditions (resolving agents, molar ratio, solvent, etc)
- 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 mother liquor *de*
- Calculate maximum yield and *de* of crystallized salts based on mass balance
- Automated crystallization and LC analysis in real time





Integrated Temperature Program and LC Sequence



de Plot of 24 Screening Samples

A Case Study of Chiral Resolution Screening

Rational Screening Approach for Classical Chiral Resolution under Thermodynamic Equilibrium
H. Tan *et al*., *Org. Pro. Res. Dev.* 2011, 15, 53

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