OUR MISSION

Finest Services For You

iChemExplorer™

“Better Data Quicker”

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iChemExplorer



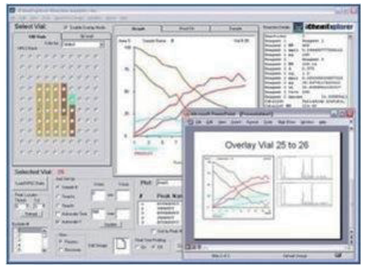
HW/SW Capabilities:

- 自动化反应与分析模块，集成HPLC取样与冷热/搅拌功能
- 反应适用在标准进样瓶 从250uL至1 mL
- 自动取样器托盘和多孔板上多达54次反应
- 直接或淬灭取样，适用于均相或多相样品
- LC数据的实时峰值分析
- 耐用结构硬件和直观的软件设计

- A module integrates cooling/heating (-20 to 150˚C) and stirring (up to 1200 rpm) into a HPLC auto-sampler
- Reaction volume 250 µL to 1 mL in standard HPLC vials
- Up to 54 reactions on the auto-sampler trays and wellplates
- Direct or quench injection of homogeneous/ heterogeneous samples
- Real-time peak profiling of LC data
- Robust hardware and intuitive software

Applications:

- 加药反应、筛选和动力学
- 强制降解以及动力学
  (Ea,k 及 $t_{1/2}$ 符合 Arrhenius 方程)
- 溶解度和温度关系 (符合 Van't Hoff 方程)
- 均匀/直接或萃取注射/适用不同种类的样品
- 更多应用价值如手性拆分，ee升级，以及杂质结晶

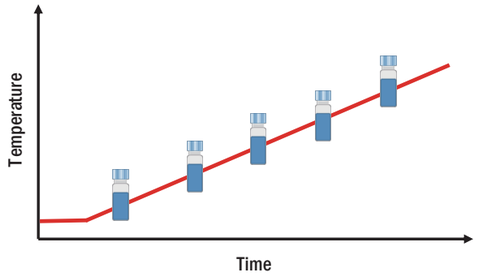


- Reaction dosing ,screening and kinetics
- Forced degradation and kinetics
  (Ea,k and $t_{1/2}$ fitting to Arrhenius Equation)
- Solubility vs.temperature (fitting to Van't Hoff Equation)
- Chiral resolution , ee upgrade ,and impurity injection by crystallization

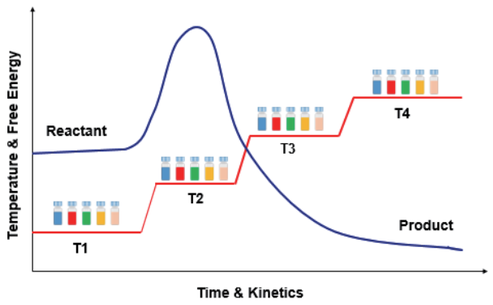
More Convenient Solutions

	Robot / Reactor	HPLC-MS	iChemExplorer
Sample Prep	✓	Bottleneck	✓
Data Acquisition	✓	✓	✓
Data Analysis	Bottleneck	✓	✓
Report	Bottleneck	Bottleneck	✓

iChemExplorer is capable of real time LC sample preparation
(quench and dilution after sampling), data acquisition, analysis and reporting



Automated Equilibration
Sampling
Quench



- User defined thermal profile
- Automated thermal profiling,stirring , sampling and recording
- Suspended stirring during sampling

- 热配置文件可自定义
- 自动热剖面分析，搅拌，取样以及记录
- 取样时能暂停搅拌

Auto-sampler Trays to Heat and Stir



24-position flow tray
(-20-80C)

24孔 FLOW槽
（-20~80℃）



24-position plate
(ambient to 80C)

24孔板
（室温~80℃）



54-position tray
(ambient to 150C)

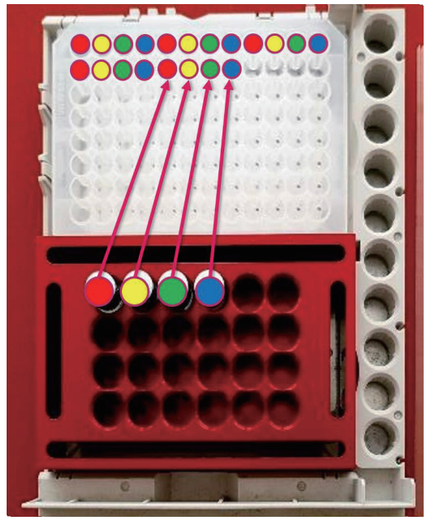
52孔托槽
（室温~150℃）





Fits to LC wellplate autosampler , i.e.
Waters Acquity
Shimadzu Nexerra

Control Quench Tool



- 淬灭溶剂以 i.e 1:100稀释预填在孔板
- 根据时间点进行样品转移,淬灭,稀释或注射
- iChemExplorer设备能降淬灭/稀释过程关联至源瓶

- Prefill back-wellplate with quench solvent at appropriate dilution, i.e 1:100
- Time-point sample transfer,quench,dilution and injection
- iChemExplorer correlates quench/diluted samples to source vials

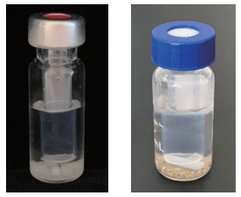
Example shown
- Four source vials
- Five time-point transfers from each source vial to back-wellplate
- Sample from back-wellplate for HPLC analysis

Experiment Samples in HPLC Vials



Reation in a vial

- Minimize reagent,solvent and waste
- Save time and resources
- Quality and reproducible results
- 最小使用样品需求量，以免造成浪费
- 节省时间和资源
- 保证质量且能够复值



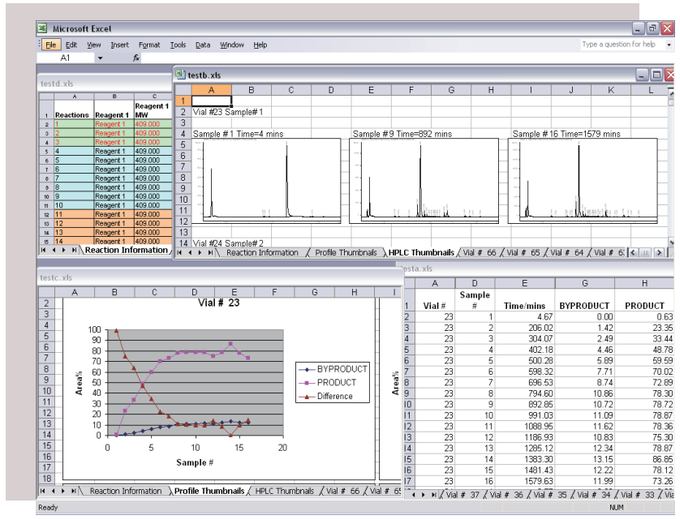
Custom filter insert

1mL glass vial with crimp seal top is also available and used for reaction screening by customers

1ml 样品瓶与顶部密封的同时，通过1um的过滤可做筛选反应

Item Number	Description
ICHEMPRO	iChemExplorer System and Quenchplate for 2ml vials with Autosampler, includes PC with 3 year iChemExplorer software license
ICHEMEX	iChemExplorer System and 54-Position Heated Tray for 2ml vials to fit Agilent Autosampler,includes PC with 3 year iChemExplorer software license
QUENCHPLATE	Heated plate for 24 two ml vials in wellplate footprint
FLOWPLATE	Well Plate to circulate heat transfer fluid for 24 two ml vials; Programmable Circulator Required; Support for Huber, Lauda and NesLab
FLOWTRAY	Well Plate to circulate heat transfer fluid for 24 two ml vials; Programmable Circulator Required; Support for Huber, Lauda and NesLab
FILTERINSERT	Filter Insert to fit two milliliter sample vial

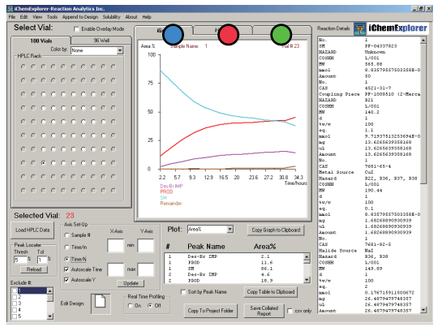
iChemExplorer Reporter/Analysis/Peak Profiling



- Easy import and REPROCESS of LC date sampled at temperatures and time points
- One-button export peak profiles,chromatographs and numerical data to Excel,eLN and SpotFile

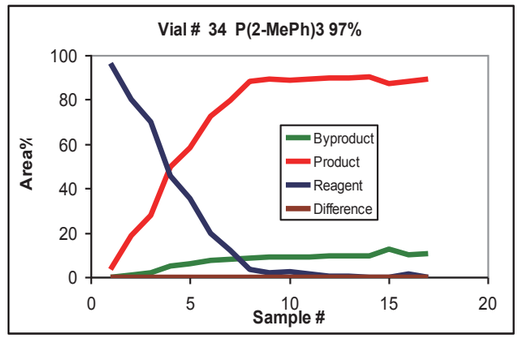
- 接入非常方便灵活
- 可记录/读取在各温度点和时间点的LC分析数据
- 一键导出峰图，色谱图和各类数据图
  支持Excel，eLN SpotFile文件类型

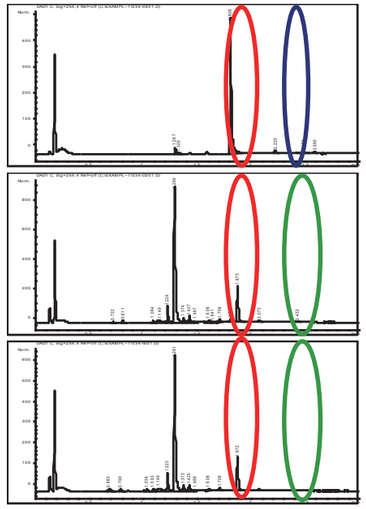
Reporter UI



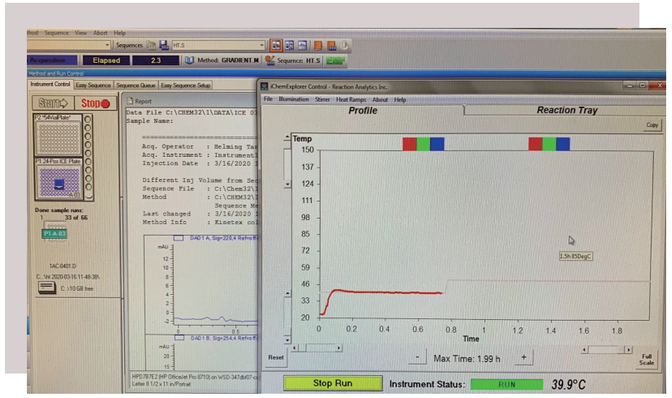
- **iGraph tab**/Create and customize Peak Profiles.Export to Excel or paste to other applications
- **iHeat tab**/Manual and automatic control of temperature
- **iSample tab**/Fill in the blanks to create sampling sequence

Follow changes in area or area % of the interested peaks from sample to sample in real time or post-analysis





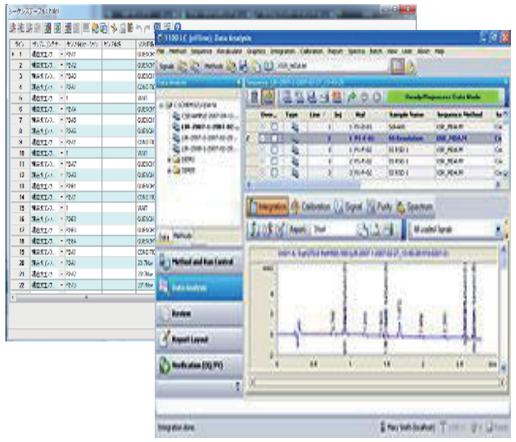
iChemExplorer Control Online Display

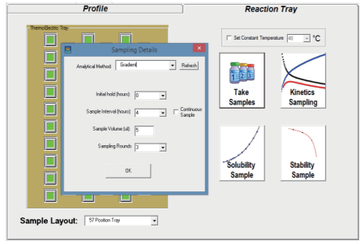


- Auto-compiled LC sequence for initial equilibration, interval wait and sample injection, coupled with temperature profile
- Customized low flow rate during equilibration or wait time
- The running sequence can be updated for uninjected samples

- 自动编译LC信息序列以达到初值平衡 自动处理间隔等待，样品注入以及温度剖面
- 可在平衡和等待中实现低流量定制
- 可以更新未注入的样本的运行顺序

HW/SW Integration
Full Compatibility with Agilent HPLC

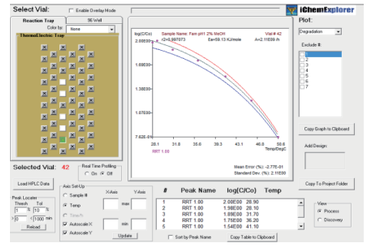




iCE Control Software

Agilent ChemStation

Perfect match use



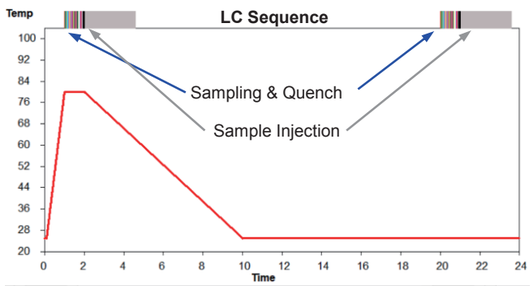
iCE Reporter Software

Agilent HPLC Model	1290	1260	1100/1200
Compatible	4226	1329	1329
Autosampler		1367	1367

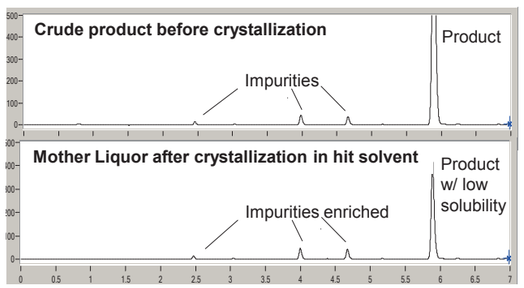
Impurity Rejection by Crystallization

Enables impurity rejection by crystallization in LC sample vials

- 24 varying solvent conditions for slurry or crysallization
- 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

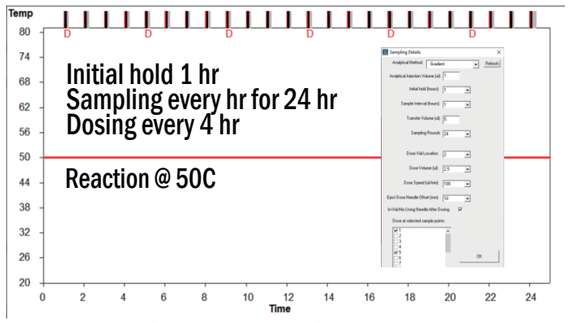


Impurity Rejection by Crystallization and LC Analysis

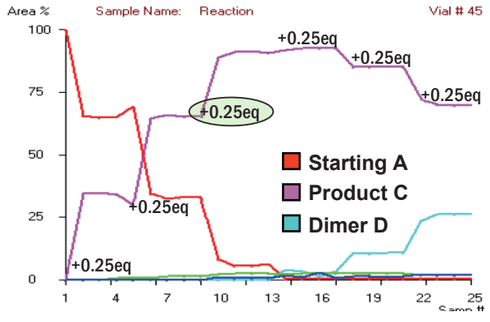
Reaction Control by Dosing

Enables reagent dosing for reaction control and kinetic study in 2ml vials

- Dedicated UI for dosing experiment
- Automated LC sequence for reagent doses and reaction sample time points,coupled with temperature program
- Sampling ,quench and LC analysis of in-vial filtered reaction mixture throughout time course
- Critical for process control to avoid unwanted by product



UI-Defined LC Sequence of Sampling and Dosing



Real Time LC Peak Profiling

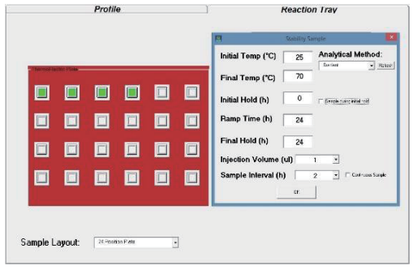
Reagent B dose : 0.25 eq=2.5 uL, 3x 0.25 eq for optimum yield of Product C in12 hr

A + B ⟶ C Desired product

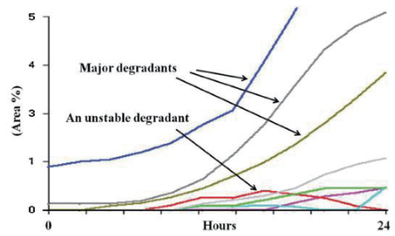
C + B ⟶ D Unwanted dimer D due to overdose of B

Forced Degradation for API Assessment

Provides "fit-for-purpose" protocols for conducting API's forced degradation in buffers



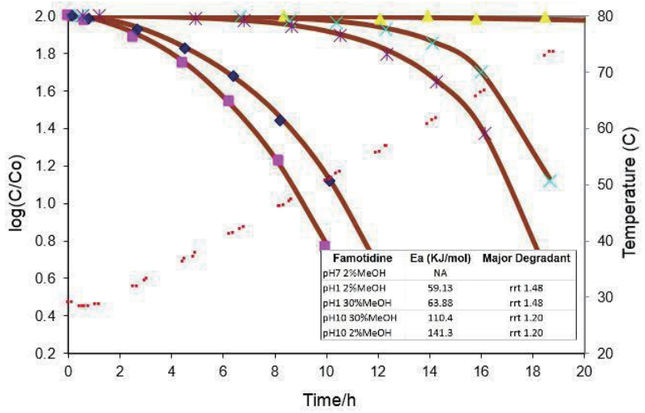
On-Plate Sampling
Quench and Analysis



Design and Control of
Temperature and Sample Profiles

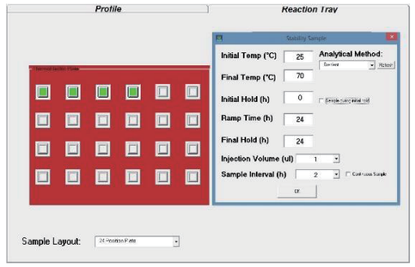
Real Time Peak Profiling
for Degradation Kinetics

- Automated LC sequence for stability time point and sample injection ,coupled with non-isothermal or staged temperature program to achieve desired degradation level
- Direct of quench injection of stability samples,appropriate for insoluble through in-vial filtration
- Real time LC peak profiling for degradation kinetics
- Estimated Ea,k and $t_{1/2}$ by plot fitting to Arrhenius Equation
- Completed stability test and report in 2 days

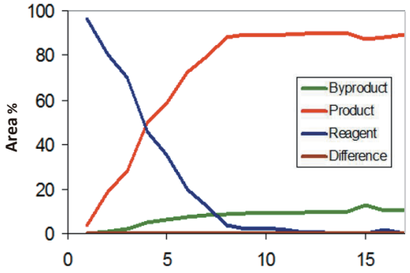


Reaction Screening and Kinetic Study

Enables reaction screening and kinetic study in LC sample vials



On-Plate Sampling
Quench / Dilution
and Analysis

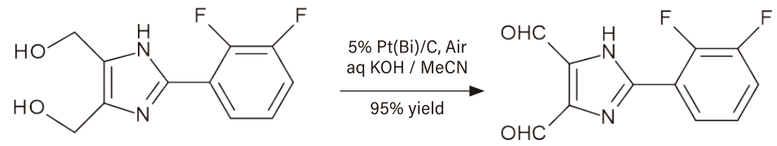


Design and Control of
Temperature and Sample Profiles

Real Time Peak Profiling
for Reaction Kinetics

- Automated LC sequence for reaction time point and sample injection ,coupled with temperature program
- Direct injection or quench/dilution of in-vial filtered reaction samples
- Realtime LC peak profiling for reaction kinetics

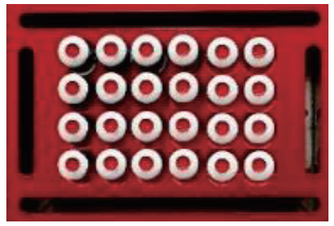
Customer example of reaction screening utilized *iChemExplorer*



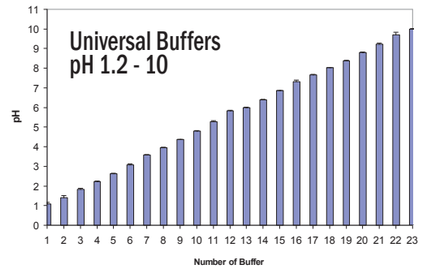
Green Oxidation: Air as Terminal Oxidant (over 106 catalysts and conditions were evaluated)
R.K. Bowman *et al., J. Org. Chem., 2013, 78, 11680*

pH Solubility and pKa Profiling

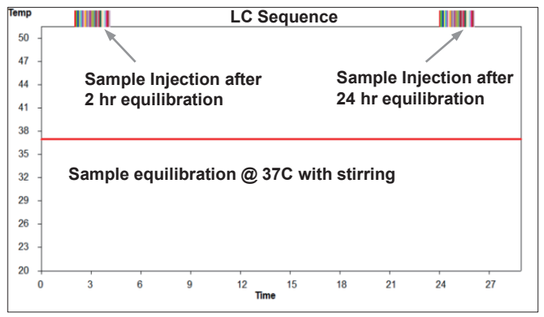
Enables pH solubility and pKa profiling in LC sample vials



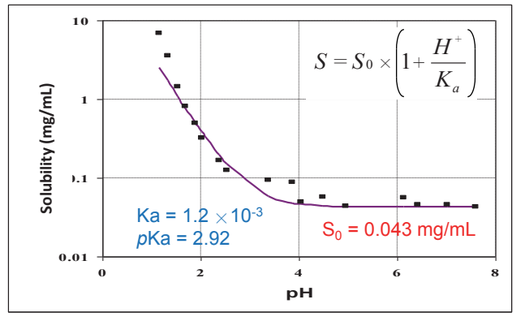
24-Vial with Filter Insert
Temperature & Stirring Control



- Up to 24 universal pH buffers to cover entire pH range
- User-defined temperature ,agitation and equilibration profiles
- Automated direct or quench/dilution injection of in-vial filtered samples
  - √ After equilibration for 2 hr to determine solubility of original or transient form
  - √ After equilibration for 24 hr to determine equilibrium solubility
- pH solubility plot to estimate S_0 and *pKa* by fitting to Henderson-Hasselbalch equation
- The equilibrium form isolated for solid state characterization as needed



Automated Equilibration and Sample Injection



pH Solubility Plot with Fitted S_0 *and pKa*

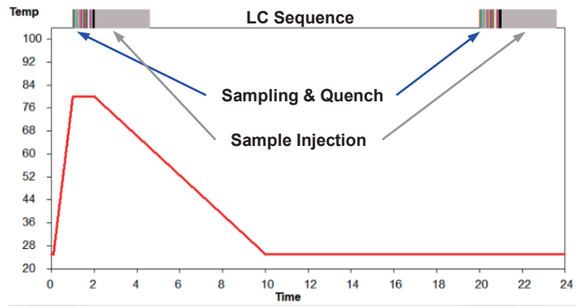
For an oral drug candidate ,the FDA requires a pH-solubility profile to be determined at 37 ± 1 C in aqueous media with a pH range of 1 - 8 and an equilibration time of 24 hours

Applications

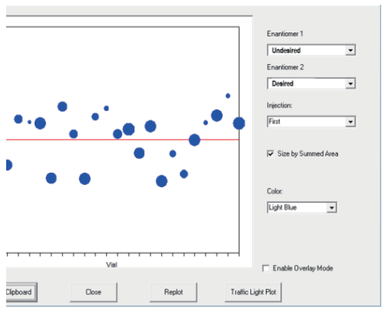
Classical Chiral Resolution

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



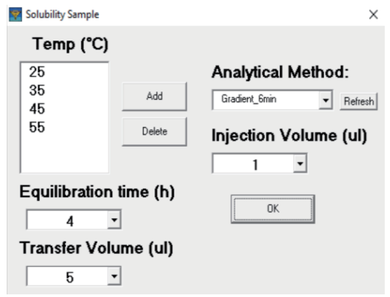
Integrated Temperature Program and LC sequence



de Plot of 24 Screening Samples

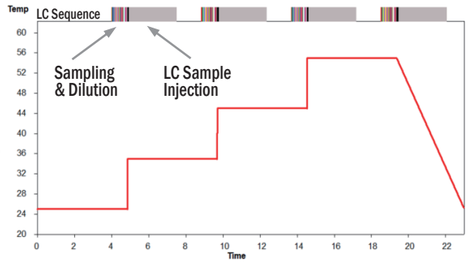
Solubility vs. Temperature

Enables solubility measurement at different temperatures in 2ml LC vials



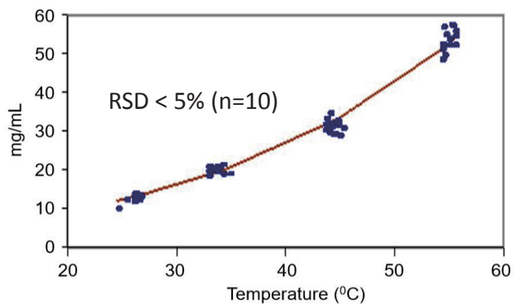
Solubility UI

On-Plate Sampling
Dilution and Analysis



Automated Equilibration
and Sample Injection

- Dedicated UI for solubility protocol
- Up to 24 solvent compositions in one experiment
- User-defined temperature,agitation and equilibration profiles
- Automated sampling ,quench/dilution and LC injection of in-vial filtered samples throughout equilibration period
- Plot of solubility vs. temperature and fitting to Van's Hoff equation



AMGEN
AstraZeneca
astellas
Boehringer Ingelheim
gsk GlaxoSmithKline
VERTEX
Pfizer
NOVARTIS
SANOFI
TEVA PHARMACEUTICALS
Takeda

Over 100 active users in US, Europe and Japan in the past 10 years

Price list

Category	RAI Item Number/Description	Unit	List Price
Hardware/ Software	**ICHEMPRO** *iChemExplorer System and Quenchplate for 2 ml vials with Autosampler; includes PC with 3 year iChemExplorer software license*	each	469,300.00
	ICHEMEX *iChemExplorer System and 54-Position Heated Tray for 2 ml vials to fit Agilent Autosampler; includes 3 year iChemExplorer software license*	each	355,100.00
Accessory	**QUENCHPLATE** *Heated plate for 24 two ml vials in wellplate footprint*	each	29,700.00
	FLOWPLATE *Well Plate to circulate heat transfer fluid for 24 two ml vials; Programmable Circulator Required; Support for Huber, Lauda and NesLab*	each	44,500.00
	FLOWTRAY *Well Plate to circulate heat transfer fluid for 24 two ml vials; Programmable Circulator Required; Support for Huber, Lauda and NesLab*	each	44,500.00
Software	**CONTROL** *One Year software license for Temperature and Stirring control with Sampling Control for Agilent Chemstation*	per year	89,500.00
	REPORTER *One Year software license to acquire, view and report data*	per year	26,400.00
	MSADD *Add capability to view data from Agilent MassHunter*	per year	48,000.00
Service	**ISERVICEDAY** *International Two Day On-Site Service and Training - REQUIRED with purchase of iCESystem*	each	65,300.00
	SILVERSERVICE *International One Year Service Plan*	each	65,300.00
Consumable	**FILTERINSERT** *Filter Insert to fit two milliliter sample vial*	each	100.00

Note