

# iChemExplorer™

## “Better Data Quicker”



**iChemExplorer**

# Calibrated Storage Chambers



Who left the door  
OPEN???

Ovens and Aliquots Everywhere  
With Kilograms of Material



**iChemExplorer**

# Automated Batch Reactors



Complimentary Images of  
Mettler Toledo, HEL and Syrris

Limited number of  
reactions for the  
capital required

Sampling and  
Analysis must follow  
to get Results



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# Lab Workflow

	Robot/ Reactor	HPLC/ MS	iChemExplorer
• Prep	X		X
• Run	X		X
• Analyze	Bottleneck	X	X
• Data		X	X
• Report		Bottleneck	X



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# Sample Vial as Reaction Vessel



*1ml tubes, 2 ml and 6 ml vials*

- Minimize Starting Material, Solvent and Waste
- Disposable Reactor with lowest cost per reaction
- Accurate, Precise and Scalable Results
- Robust Hardware



# iChem Hardware to Heat and Stir



Flowtray



iCEplate



- Ambient to 150C with iChemExplorer iCEtray
- Stir to 1100 RPM with iChemExplorer iCEbox



iCEtray for 2 ml vials

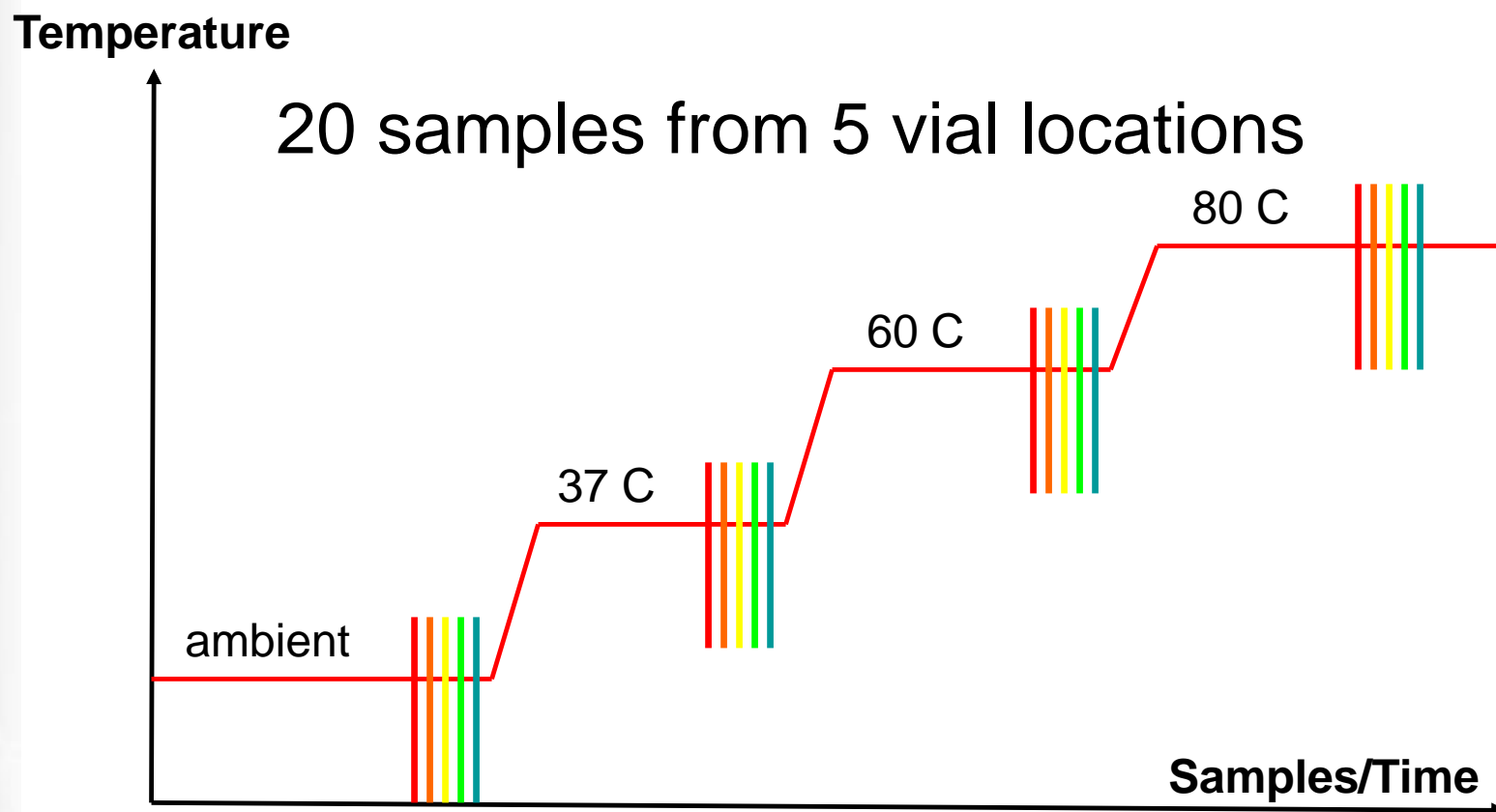


iCEtray  
6 ml vials



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# Automate Temperature & Sampling

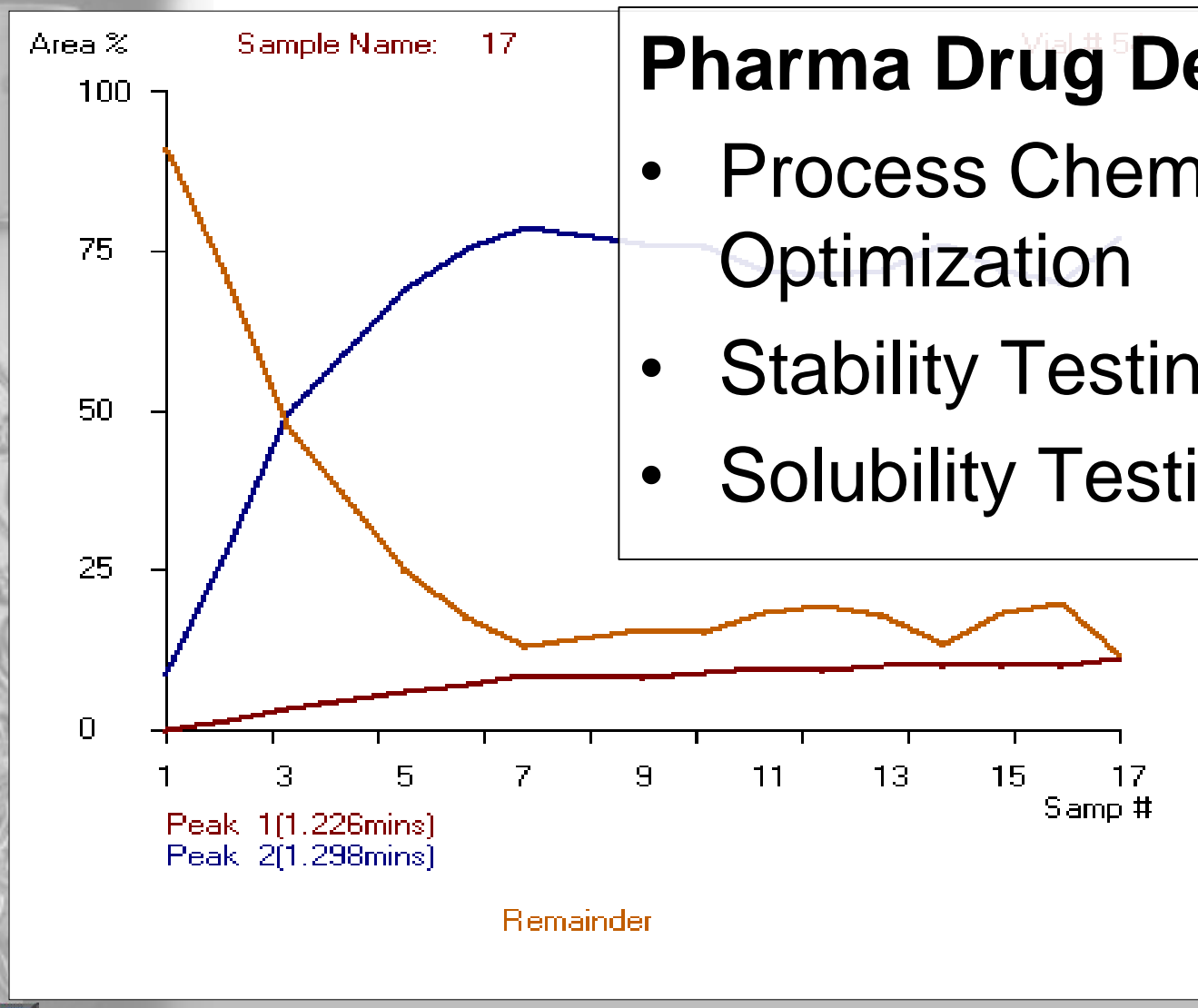


**Automate Temperature Control  
with Sampling**



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# When You Need iChemExplorer



## Pharma Drug Development

- Process Chemistry Optimization
- Stability Testing
- Solubility Testing



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# Better Chemistry w/ iChemExplorer

- Pfizer
  - Novartis
  - Merck
  - Astellas
  - Amgen
  - Teva
  - You...
- Over 100 active users
  - Users in Europe, Japan & US
  - Compatible with Agilent & Waters



**iChemExplorer**

# Faster Turnaround

**Prep > Heat/Stir > Sample > Analyze > Data > Present**

	<b>Mon</b>	<b>Tues</b>	<b>Wed</b>	<b>Thur</b>	<b>Fri</b>
<b>Traditional</b>	Prep	Run Sample	Analyze	Data	<b>Present</b>
<b>iChem</b>	Prep <b>Night –</b> Run Sample Analyze Data	<b>Present</b> Prep <b>Night –</b> Run Sample Analyze Data	<b>Present</b> Prep <b>Night –</b> Run Sample Analyze Data	<b>Present</b> Prep <b>Night –</b> Run Sample Analyze Data	<b>Present</b> Prep <b>Night –</b> Run Sample Analyze Data

**285 Experiments per Week**  
**14,250 Experiments per Year**  
**With One iChemExplorer**



**iChemExplorer**

# Better Quality of Data - QOD

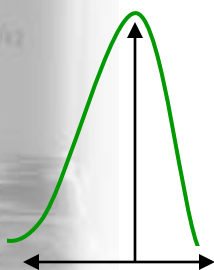
## Sources of Experimental Error

### Execution

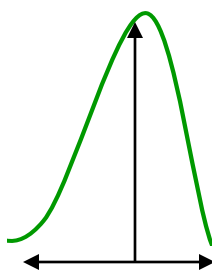
- Heating/Stirring
- Sampling
- Recording

### Analysis and Reporting

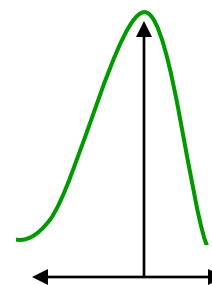
Solution  
Prep



X



X



**Minimize  
= Experiment  
Error**

**Automate with  
iChemExplorer**

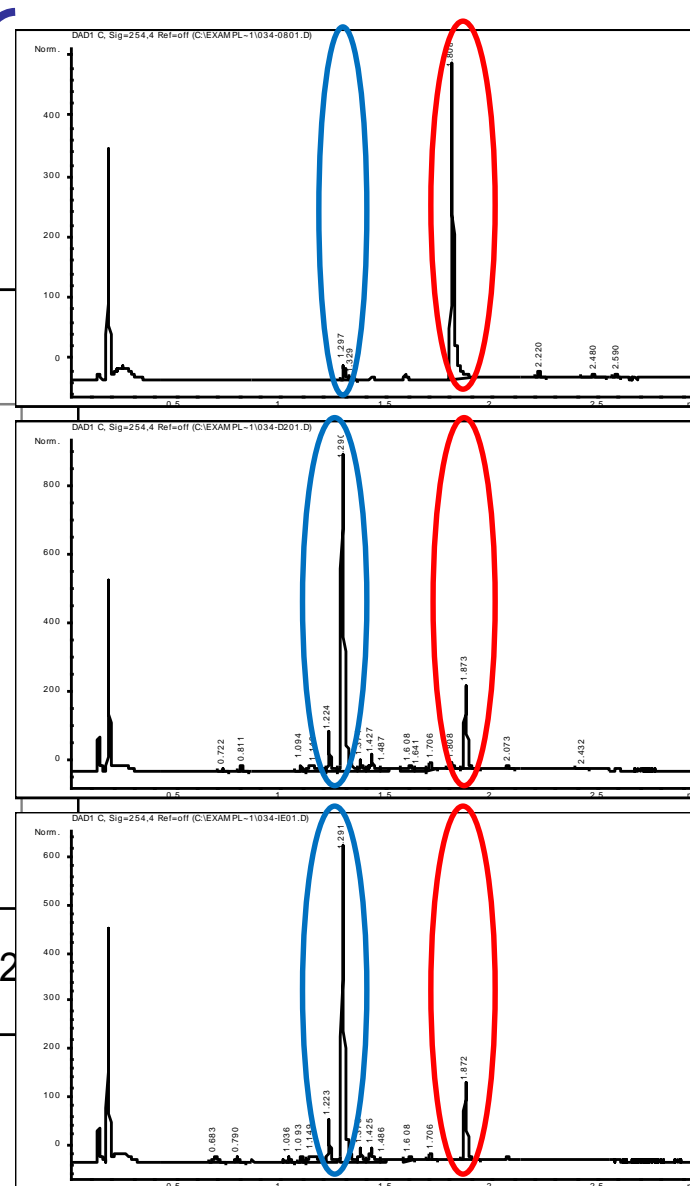
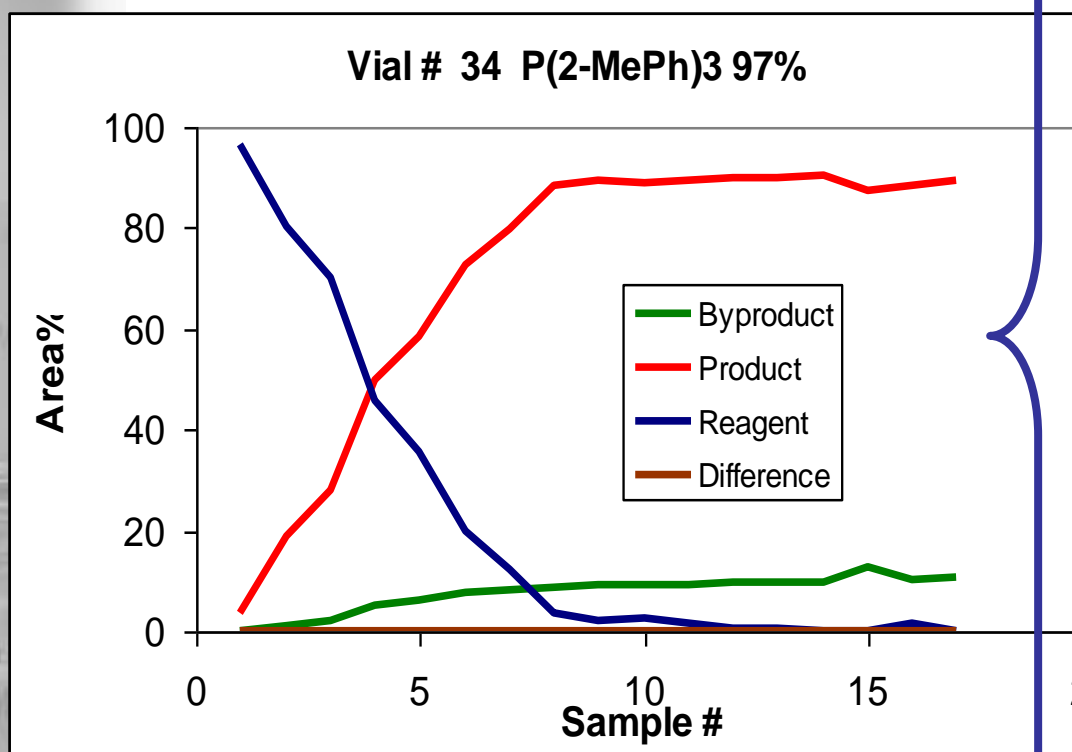


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# Immediate Presentation of Data

## PEAK PROFILES

Follow Peak Area from one sample to the next



# Export to Microsoft Excel



- One-button to Microsoft Excel
- Peak Profile and chromatographs for each sample
- Save time and reduce errors with numeric data



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# Sampling from Saturated Solution



**NEW**  
Filter Insert for  
2 ml vial



**AVAILABLE NOW**  
Filter Vial from  
Thomson Instrument



# Example: Thermodynamic Solubility

$r^2=0.98$

T(°C) mg/ml

T(0) =2.2

T(25)=10.7

T(50)=40.2

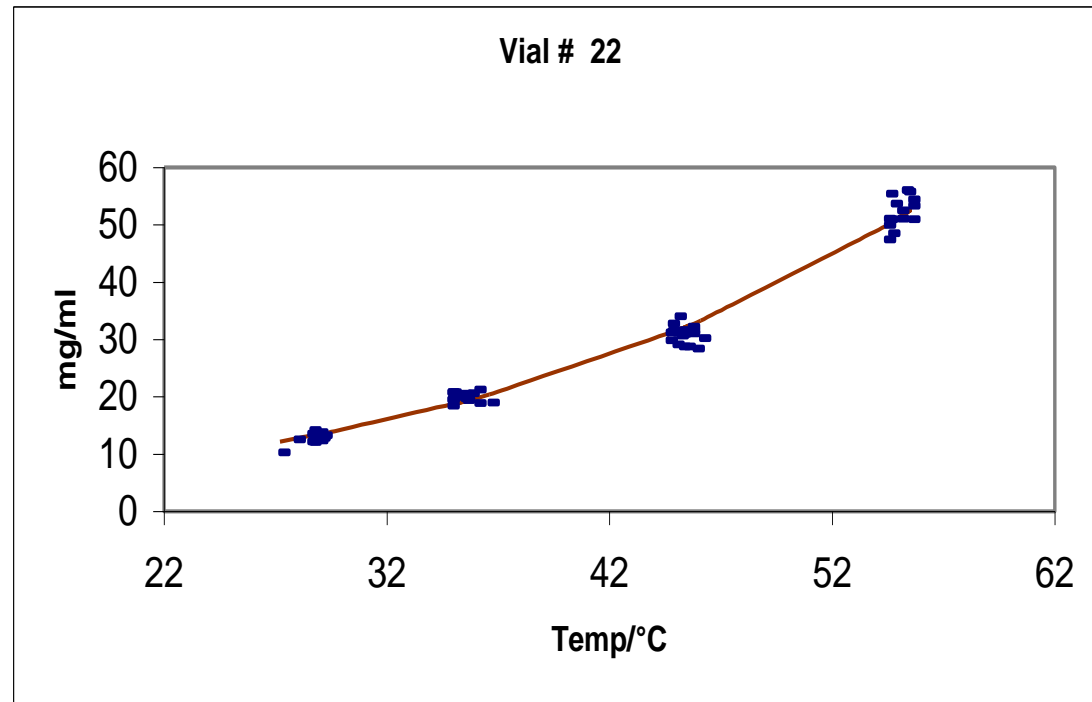
T(75)=124.9

$\ln x=A+BT^{-1}$

x/mgml<sup>-1</sup> T/K

A=19.45143

B=-5088.944



“Works well for screening solvents”

Dr. Tony Shephard  
AstraZeneca



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# iChemExplorer for Better Data Quicker



**Automate the work to  
gather more data**

**Organize the data for  
better understanding**



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