

# iChemExplorer Application

## pH Solubility and pKa Profiling

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

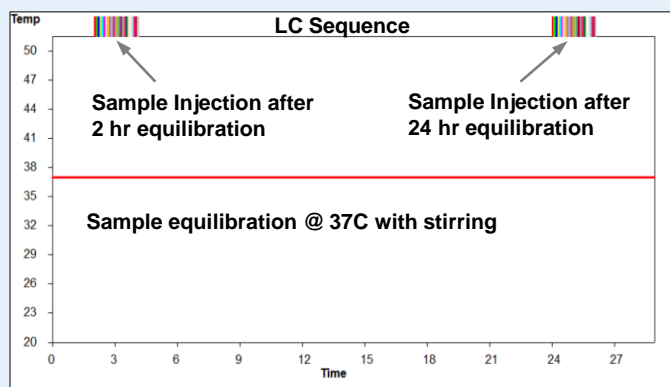
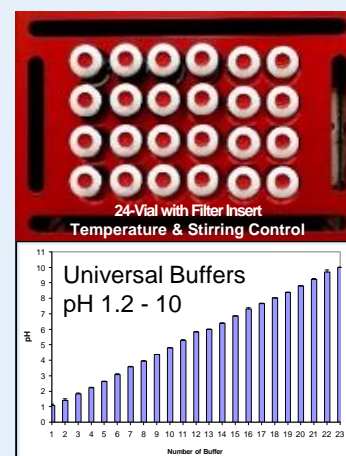


**iChemExplorer** is an innovative hardware/software module integrated into your HPLC autosampler:

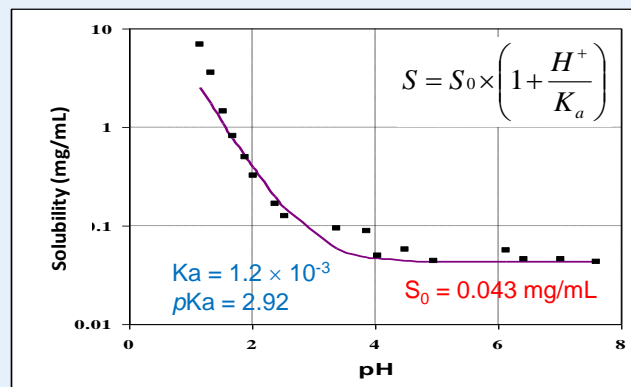
- Temperature and stirring control
- Proprietary in-vial filter insert technology
- Intuitive interface for experiment design and execution
- Application specific data analysis and reporting

**iChemExplorer** enables pH solubility and pKa profiling in LC sample vials:

- 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  $pK_a$  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  $pK_a$

For an oral drug candidate, the FDA requires a pH-solubility profile to be determined at  $37 \pm 1^\circ\text{C}$  in aqueous media with a pH range of 1 - 8 and an equilibration time of 24 hours