

TABLE 4.6

Equipment Available for Sirius for pK_a , Log P , and Solubility Measurement and Data Handling

Instrument	Features
GLpK _a : simultaneous pK_a , log P , and solubility determination	<ul style="list-style-type: none"> • pH range of 1.8–12.2 (for standard titrations) • Up to 30 samples in 24^ohour • Automated operation • Measurements below 10–4^oM • Built-in traceability and reminders • Supports D-PAS for spectrophotometric pK_a
D-PAS: spectrophotometric pK_a	<ul style="list-style-type: none"> • Concentrations as low as 10–6^oM • Sample weight down to 50^oμg • Single- or multiprotic molecules • Macro- and microconstants easily fitted to Sirius GLpK_a or PCA200
PCA200: entry-level pK_a , log P , and solubility	<ul style="list-style-type: none"> • Measures pK_a, log P, and intrinsic solubility • Ideal for smaller workloads or academic research • Uses the pH-metric technique and RefinementPro2 software • Automated addition of acid and base titrants • Supports D-PAS (UV method)
ProfilerSGA: rapid pK_a measurement	<ul style="list-style-type: none"> • Fully automated physicochemical profiling • Measures pK_a in just 2^omin • Multiwavelength spectrophotometric technique • Open access option • Automated data handling and processing • Full computer control • Microplate format • Measures below 10–5^oM concentration • 300 assays in 24 hours • MDM mixed solvent system
ProfilerLDA: log D/P octanol/water partitioning	<ul style="list-style-type: none"> • Fully automated log D determination • Multiwavelength spectrophotometric technique • Open access (administrator and user profiles) • Automated data handling and processing • Full computer control • Microplate format (96- and 384-well) • Remote network monitoring • Performance monitoring
ProfilerLDA: log D/P octanol/water partitioning	<ul style="list-style-type: none"> • Fully automated log d determination • Multiwavelength spectrophotometric technique • Open access (administrator and user profiles) • Automated data handling and processing • Full computer control • Microplate format (96- and 384-well) • Remote network monitoring • Performance monitoring

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