

## Networked Purification System Increases Productivity for Medicinal Chemists

In the highly competitive race to develop useful new compounds, medicinal chemists are responsible for advancing synthesis projects to a decision point as quickly as possible. In some companies, quotas for compounds to be synthesized and delivered for screening have reportedly doubled in recent years. This gives chemists a strong incentive to look for innovative ways to multi-task and to reduce the time spent on repetitive and routine activities. Since purification of target compounds typically accounts for 30–40% of the chemist's time (Fig. 1) when done by traditional manual methods, it offers a great opportunity for time savings and increased productivity.

### Automated Purification

Many medicinal chemists have only recently made the transition from fully manual flash chromatography to instrument systems that automate solvent gradients and fraction collection. These systems free the chemist to work on additional syntheses in the lab while a purification is running. Flash chromatography systems with on-line UV detection can additionally reduce the amount of TLC work required

on separated compounds. However, the chemist still typically runs purifications only when he or she will be in the lab to monitor the collection of precious compounds throughout the run.

### Flexible Communication and Control Provides Additional Time Savings

The same computer and communication technologies that allow universal Internet access can also give chemists the

freedom to monitor and control an instrument from any location. The Combi-Flash Companion from Isco, Inc. (Fig. 2) is the first flash chromatography system to implement this type of next-generation networked interface.

This flexibility is due to an internal Linux-based Web server and network hardware that serves a thin-client application. The Companion thus incorporates its own powerful internal processor that automates its operation and processes the data. XML data allows the interchange of control instructions and chromatographic results between the instrument and chemist at a Windows-based computer. Windows-based computers can range from a PDA running the Pocket PC operating system, mobile notebook computers on a wireless network, to the ubiquitous desktop computer. Though the design opens itself to nearly limitless connection possibilities, operat-

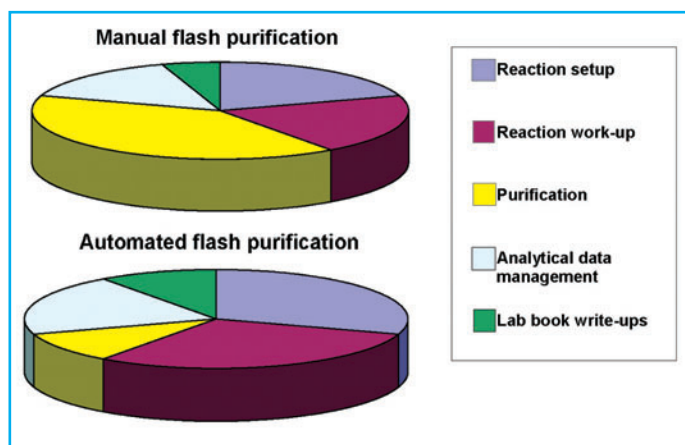


Fig. 1: Manual Flash purification is typically the most time-consuming task for the medicinal chemist performing organic syntheses. Automated flash chromatography with network control can provide an 80% time savings in purification, increasing the number of synthesis projects that can be successfully advanced to a decision point.

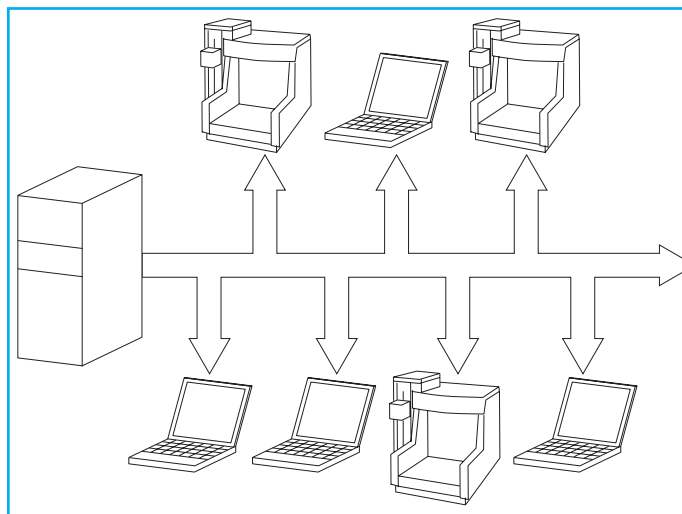


Fig. 2: Multiple automated Flash chromatography systems with network connectivity. Each system is accessible from any web browser connection.



**Fig. 3:** The Isco CombiFlash Companion fits conveniently in a hood, and includes a lockable mount that holds a standard touchscreen PDA for on-board control via the PDA's browser software.

ing the instrument in any environment from direct connection to a computer to a site-wide network is as simple as starting Windows Internet Explorer.

This technology offers a number of advantages.

### Reduced Lab Space Requirement

Traditional instrument control previously required a dedicated PC for its "front panel." Now, a low-cost, space-saving PDA connected to the Companion's USB port provides front panel control. Often the other role of the dedicated PC was to automate the instrument operation and perform complex data processing. Again, these functions are internal to the Companion. The very same PDA can display the real time operational parameters and the results of the data processing.

### Convenient Data Access

Ethernet and Universal Serial Bus (USB) communications allow for high-speed connections to the instrument. The built-in Ethernet Network Interface Card (NIC) and TCP/IP support make it easy to directly connect to the instrument, or to add the instrument to a corporate net-



**Fig. 4:** Here, a chemist uses a wireless tablet PC to check the status of a separation running in a remote lab. Because CombiFlash Companion has its own built-in Linux-based web server, it is easy to implement wireless connectivity using standard, readily-available personal computer accessories.

work for control by any PC (Fig. 3). With the addition of standard consumer wireless products, Companion can be incorporated into Wi-Fi networks. Whether the connection is wired or wireless, a Network Administrator can restrict access to certain users or groups, or allow for plant-wide or even off-site access to the instrument.

### Data Delivery and Storage to Suit Your Workflow

With Companion connected as a network node, chromatographic data are easily transferred, stored, and backed-up to meet requirements. The instrument will save the data in formats easily integrated with Microsoft Office products, as an Adobe Acrobat PDF file, or as raw text. Whatever format is chosen, the instrument can also post the file to a network folder or deliver them to an E-mail inbox.

### Conclusions

So what does the combination of Ethernet, Web Servers, PDAs, and open connectivity do for productivity? Quite sim-



**Fig. 5:** An optional expansion module allows CombiFlash Companion to run 4 samples unattended, using columns from 4–330 g for milligram to multi-gram purifications.

ply, laboratory instrument monitoring and control no longer requires the time and presence of the chemist. Compound purification takes place while the chemist is performing synthesis, maintaining a laboratory notebook, or even attending a meeting.

Chemists stay in touch with their instruments from wherever their other work takes them. Data from previous chromatographic separations are equally accessible from any internet connection, and delivered in convenient formats. However, when there is a need to return to the instrument, the space-saving PDA provides touch-screen control. Eliminating the traditional, dedicated PC once again allows the space in and around the fume hood to be used for chemistry, not computing. The overall savings in time spent on compound purification enables the medicinal chemist to advance more synthesis projects to the next stage.

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