

Sos—a sample ordering system for delivering “assay-ready” compound plates for dru...

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Abstract Many bottlenecks in drug discovery have been addressed with the advent of new assay and instrument technologies. However, storing and processing chemical compounds for screening remains a challenge for many drug discovery laboratories. Although automated storage and retrieval systems are commercially available for medium to large collections of chemical samples, these samples are usually stored at a central site and are not readily accessible to satellite research labs. Drug discovery relies on the rapid testing of new chemical compounds in relevant biological assays. Therefore, newly synthesized compounds must be readily available in various formats to biologists performing screening assays. Until recently, our compounds were distributed in screw cap vials to assayists who would then manually transfer and dilute each sample in an “ assay-ready” compound plate for screening. The vials would then be managed by the individuals in an ad hoc manner. To relieve the assayist from searching for compounds and preparing their own assay-ready compound plates, a newly customized compound storage system with an ordering software application was implemented at our research facility that eliminates these bottlenecks. The system stores and retrieves compounds in 1 mL-mini-tubes or microtiter plates, facilitates compound searching by identifier or structure, orders compounds at varying concentrations in specified wells on 96- or 384-well plates, requests the

addition of controls (vehicle or reference compounds), etc. The orders are automatically processed and delivered to the assayist the following day for screening. An overview of our system will demonstrate that we minimize compound waste and ensure compound integrity and availability. (JALA 2004; 9: 123-7) Introduction Medicinal Chemistry synthetic compounds at our Merck Frosst Research Laboratory site have traditionally been prepared in DMSO stocks in bar coded 1 dram vials and distributed to the biologists for screening. This was an ad hoc system where the vials were stored in a variety locations and conditions depending on the recipient. Since a compound may be screened in many biological assays, many aliquots of the solution were prepared in several 1 dram vials containing large dead volumes. The vials would often be misplaced requiring a new solution to be made from the stock powder. This resulted in increased waste in compound and time. For each assay, the biologist is responsible for preparing the assay compound plate for his/her screen. Until recently, this involved searching for the compound vials and preparing the drug plate containing the compounds serially diluted across columns of a 96-well plate.