### Leveraging Compound Management Capabilities in Support of Drug Discovery: From Sample Archive to Sample Distribution - Driving Efficiency and Improving Productivity

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### Overview

- Vision and Responsibilities
- Support for Drug Discovery
  - Sample Archive
  - High Throughput Screening
  - Compound Ordering
  - Lead Optimization sample handling
- QC, Performance Measurement and Impact



### **Compounds as Key Strategic Assets**

"Access to chemically diverse...compound collections has been a very important competitive advantage to pharmaceutical drug companies and thus...have been considered to be one of the pharmaceutical companies carefully guarded assets" Strategic Mgmt J. 2002

For the future success of the business, it is critical that these compound assets be effectively managed and leveraged to support all drug discovery needs from lead generation through lead optimization.



### BMS Technology Investments 1998 - 2002



**Compound Management** 

High Throughput Screening





### Global Vision for Compound Management at BMS

- Improve hit identification by enhancing the quality of the content and integrity of compound collection
- Accelerate Global Drug Discovery
  - Improve cycle time for all services
  - Improve overall organizational efficiency
  - Improve quality of processes
  - Build synergies across the entire drug discovery continuum

"The impact of screening and the integrity of screening data are only as good as the compound inputs"



# BMS

### **Compound Management Responsibilities**

- Sample registration
- Archive for all discovery substances
- Sample handling needs at all stages of drug discovery
  - HTS
  - TA in vitro and in vivo
  - Liability Profiling
- Build and manage the screening deck and other compound sets to enable hit identification efforts



### **Enabling Drug Discovery**



#### **Therapeutic Area Biology**

Single Cmpds, 96 & 384 Well Custom Sets, Focused decks, Special HTS Decks

#### Lead Optimization Screening Core

Primary Screening
Secondary Screening
In vitro Selectivity Screening



# **Compound Management Environment**



### **BMS Haystack Archive**

#### **Vial Store and Tube Store Units**



#### **System Metrics**

- > 5000 scientist orders processed
- > 500,000 samples requested
- > 900,000 samples processed
- Averaged >12,000 picks & places per day (tube store)



### **Archive - Haystack Vial Store**



- Capacity: 762K Vials>75% Full
- •Barcoded Glass Vials •4°C
- Controlled humidity
- •Dry powders, oils and dry films

Bristol-Myers Squibb Company

### **Archive - Haystack Tube Store**



- Capacity: 5.2MM Tubes>85% Full
- •Non Barcoded PP tube
- •Dry tube
- •Dry HTS Deck tube
- •Wet Tubes (3 mM DMSO) •4°C
- Controlled humidity



### Volatile Solvent Transfer Process

Total Process Integration across Liquid Handlers, weigh stations Haystack and Concentrators





•Common Solvents – DCE/MeOH, AcCN, DMF, DMSO

Genesis of all Deck Sets

•60% of all orders managed through VST

Reduce manual processing
Distribute smaller amounts of material (150 nmoles)

Conservation of compound











# **Screening Support**

#### Plate Replication

- Master plate creation
  - -Dry plates
  - -VST processing
- Assay ready plates
- Cherry Picking for Retests
  - From primary archive sample
- Concentration Response Plates
  - From primary archive sample
- Data Transfer
  - Fully integrated



### **HTS - Compound Processing**



### **HTS - BioCel in Action**



		Throughput per day				
Process Type	# Tube Racks or Plates	# Compounds	# Copies	Wells Replicated	# of runs	Wells Replicated
Tube to Plate						
Master Plate Creation	80	7,040	9	63,360	2	126,720
Custom Plate Creation	220	19,360	1	19,360	2	38,720
Plate to Plate						
HTS Screening Plates	50	17,600	8	140,800	3	422,400
Assay ready Plates	400	140,800	1	140,800	2	281,600



### **Integrating CM and Screening**



### **Ordering Compounds**



Bristol-Myers Squibb Company

#### All the Compound Information You Need

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### **Seamless Data Flow**



### Leveraging CM to Improve Processes in Lead Optimization



### Goal

#### Build on our successes and experience in the lead discovery arena to reinvent how we do lead optimization

- Improve in vitro evaluation process
- Improve data and information management
- Improve sample handling



#### Lead Optimization and Profiling Sample Processing



# Quality Control and Performance Measurement



### What Do We Measure and Why?

#### Instrument performance

- Ensure quality of downstream discovery efforts
  - Quality of data
- Organizational performance and efficiency
  - Guarantee high quality service
  - Improve overall discovery productivity and efficiency
  - Drive down operating costs



# **QC - Haystack Vial Weighing**



Bristol-Myers Squibb Company

# **QC - TECAN Liquid Handling**



Weekly Accuracy and Precision Validation

Ensure accuracy of sample resupply processing



### **QC - VPrep Dispensing**







Well Accuracy: 100 nL +/- 10 nL 1 μ L +/- 0.01 μL

**Carry-over**: < 1 part in a 10,000,000

**Plate Precision**: 100 nL CV range: 4.5 - 9.7% 1 μL CV range: 2.8 - 5%





### **Service Level Agreements**

Service Level Agreements										
	# of cmpds									
Order Type	<100	<200	<500	<1000	<2000	<5000	<10000			
Custom Plate/wet	2	2	2	2	3	4	5			
Custom Plate/dry	2	2	3	4	4	5	6			
Manual re-supply	2	3	4	NA	NA	NA	NA			
Inbound TAD	1	1	1	3	4	5	10			
Inbound Inventory	2	2	2	3	4	5	5-10			
Med Chem dispensations	1	1	1	1	1	NA	NA			
Med Chem Inventory	1	1	1	1	1	NA	NA			

SLA's - expected delivery date for receipt of compound
 Based on SLA matrix - size & type

♦Goal

■*If Ordered by 11 am* - 48 hr TT irrespective of site and size



### **Productivity Gains in 5 Years**





### **Productivity Gains in 5 Years**





### Technology and Process Driven Productivity and Efficiency Gains



1999 – 143 k compounds/FTE 2004 – 990 k compounds/FTE 1998 – 1,630 compounds/FTE 2004 – 24,000 compounds/FTE



## Impact Through Automation



Automated Distribution Manual Distribution





# **Compound Management Impact**

- 20 Fold increase in the number of compounds that have become accessible for testing since 1997
- Time improvements of 30-70% for compound re-supply for all order types and sizes
- Since 1998 increased productivity by 12X and efficiency by 12X
- Efficiency gains
  - 50% less staff needed to support 12X more output
- Leveraged technology infrastructure and process analysis to improve retest rates, reduce timelines and increase hit quality
- Data and lead quality enhancements
  - 25% improvement in lead generation impact
  - 70-80% of all screens generate validated progressable leads
  - Early liability assessment on leads enable progression of best compounds into lead optimization – improved FIH success rates



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- Velocity11 Team

