

# Leveraging Accessible Synthetic Methodologies for *In-Silico* Exploration of Novel Medicinally Relevant Small Molecules

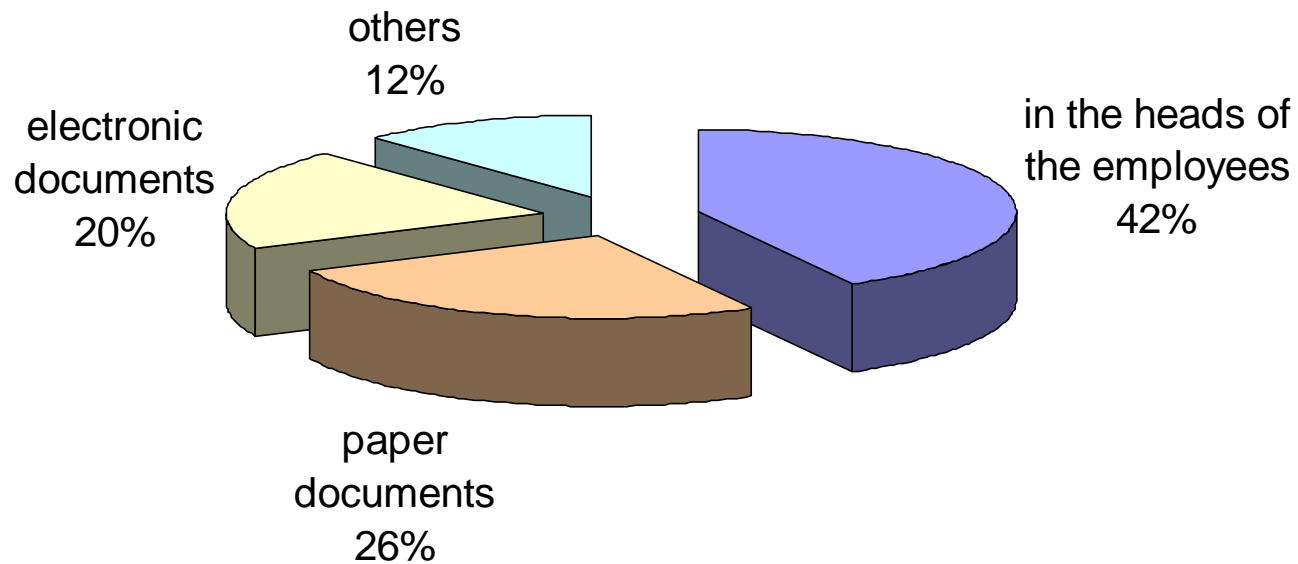
**Dr. Stephan Schürer**

Director, Content Development

**Sertanty, Inc.**

Sertanty

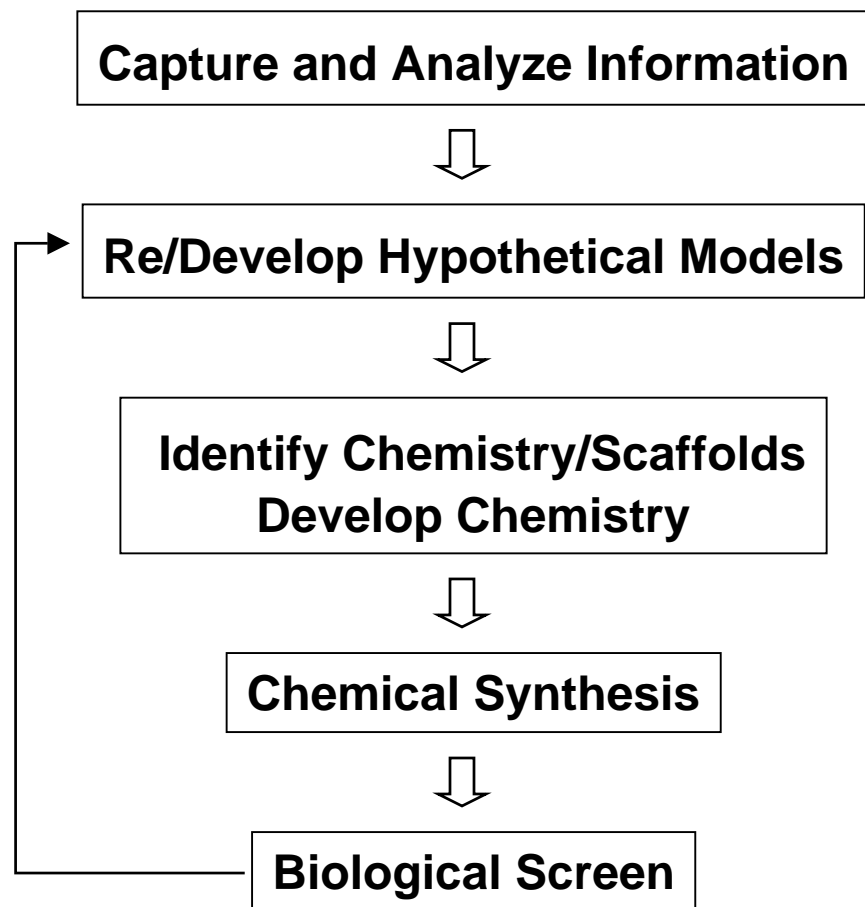
# Distribution of Knowledge



*Nachr. Chem.* **2002**, 12, 1416

In many companies only 20 to 40 % of existing knowledge is utilized

# Development Workflow



**Chemistry & SAR Knowledge Base**



**Predictive Models (QSAR,  
eScreen, docking, etc.)**



**Generate *in-silico* libraries and prioritize  
via models – multiple cycles**

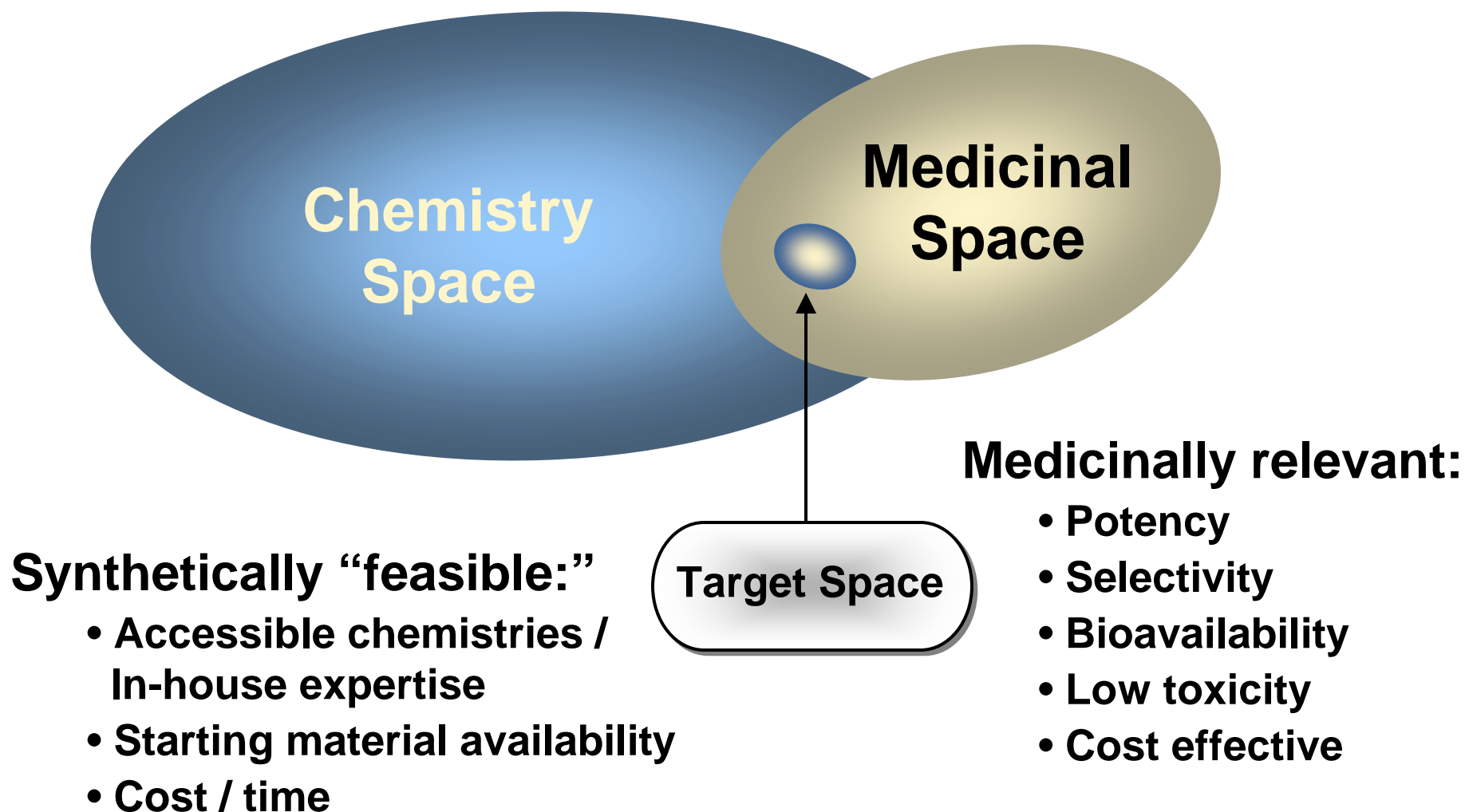


**Accessible chemistry, e.g.  
microwave synthesis**

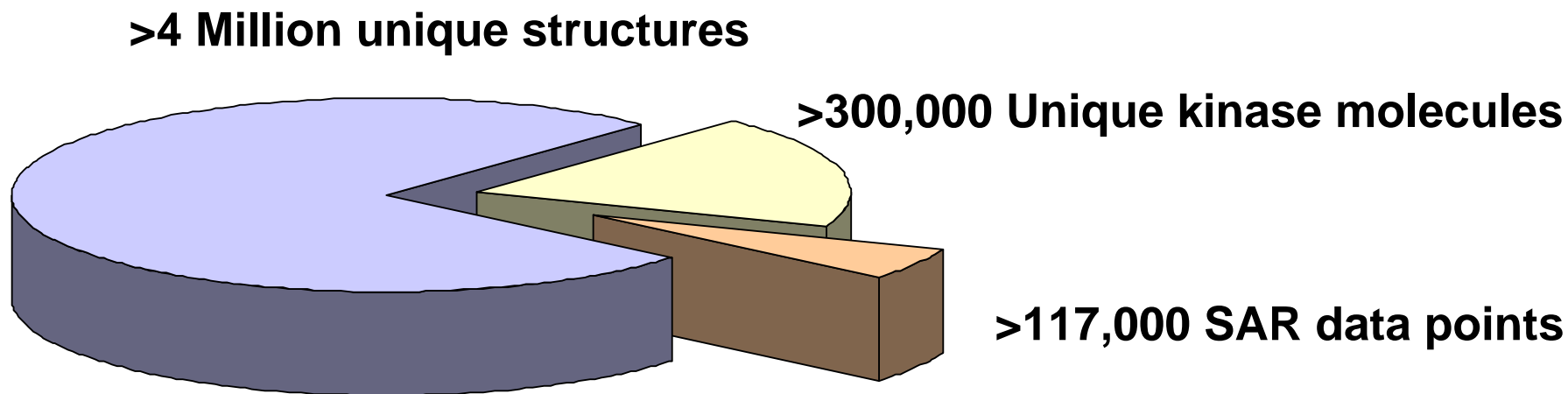


**Novel Structures**

# What can be made – What is relevant?



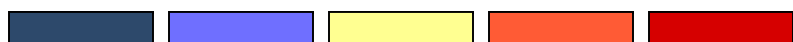
# SAR and reaction chemistry archive



- >10,000 HTS reactions with experimental procedures  
(>1,500 associated with heterocyclic Kinase inhibitors)
- >8,500 Assay protocols with detailed information
- >45 Kinase target SAR training sets
- >45 Predictive eScreen™ models

# Theoretically accessible chemical space

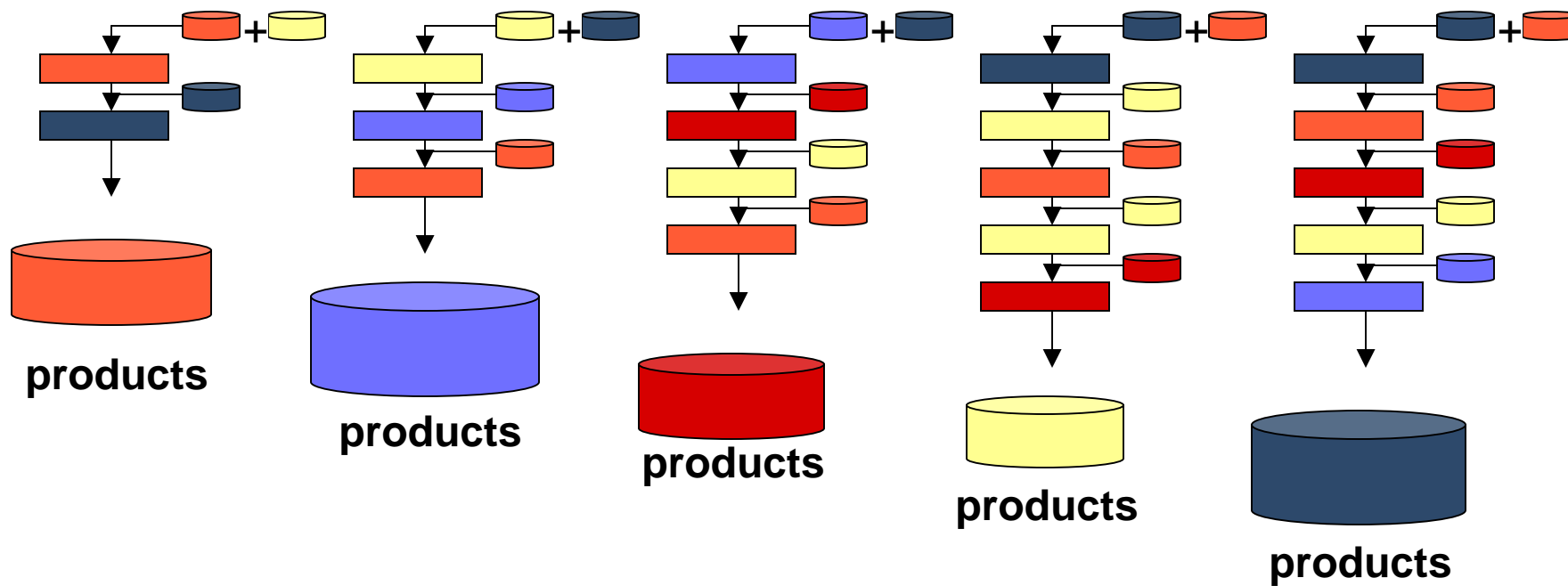
Chemical transformation types:



Available building blocks:



Potential synthetic strategies:

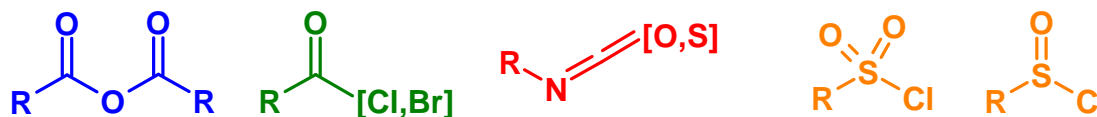


# Basic chemistry 101

## Chemical (in)-compatibility:

- Cross reactivity of functional groups
- Incompatible functional groups at given reaction type and conditions
- Avoid side reactions, catalyst poisoning, etc.

E.g. Acylators:



$\text{C};\$(\text{C}(=\text{O})\text{OC}(=\text{O})) ; !\$(\text{C}(=\text{O})\text{OC}(=\text{O}) [!#6]) ; !\$(\text{C}(=\text{O})(\text{OC}(=\text{O})) [!#6]) ]$

OR

$\text{C};\$(\text{C}(=\text{[O,N,S]}) [\text{F,Cl,Br}]) ]$

OR

$[\text{C};\$(\text{C}(=\text{[O,S]})=\text{N}) ]$

OR

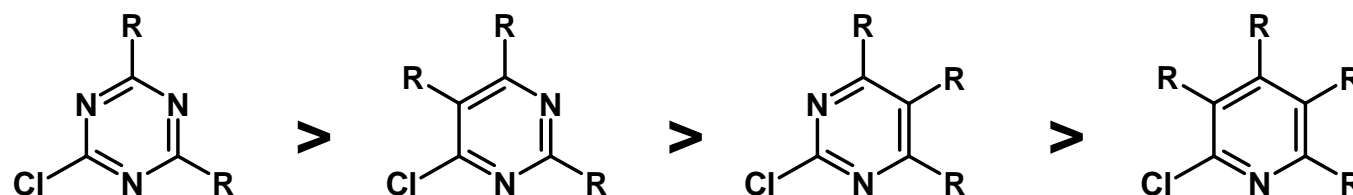
$\text{S};\$(\text{S}(=\text{O}) [\text{Cl,Br,F,I}]) ]$

**Incompatibility filters – applied to starting materials**

## Chemical reactivity:

- Reaction-type specific differences in reactivity
- Usually influenced by reaction center environment
- Definition of the reaction center details

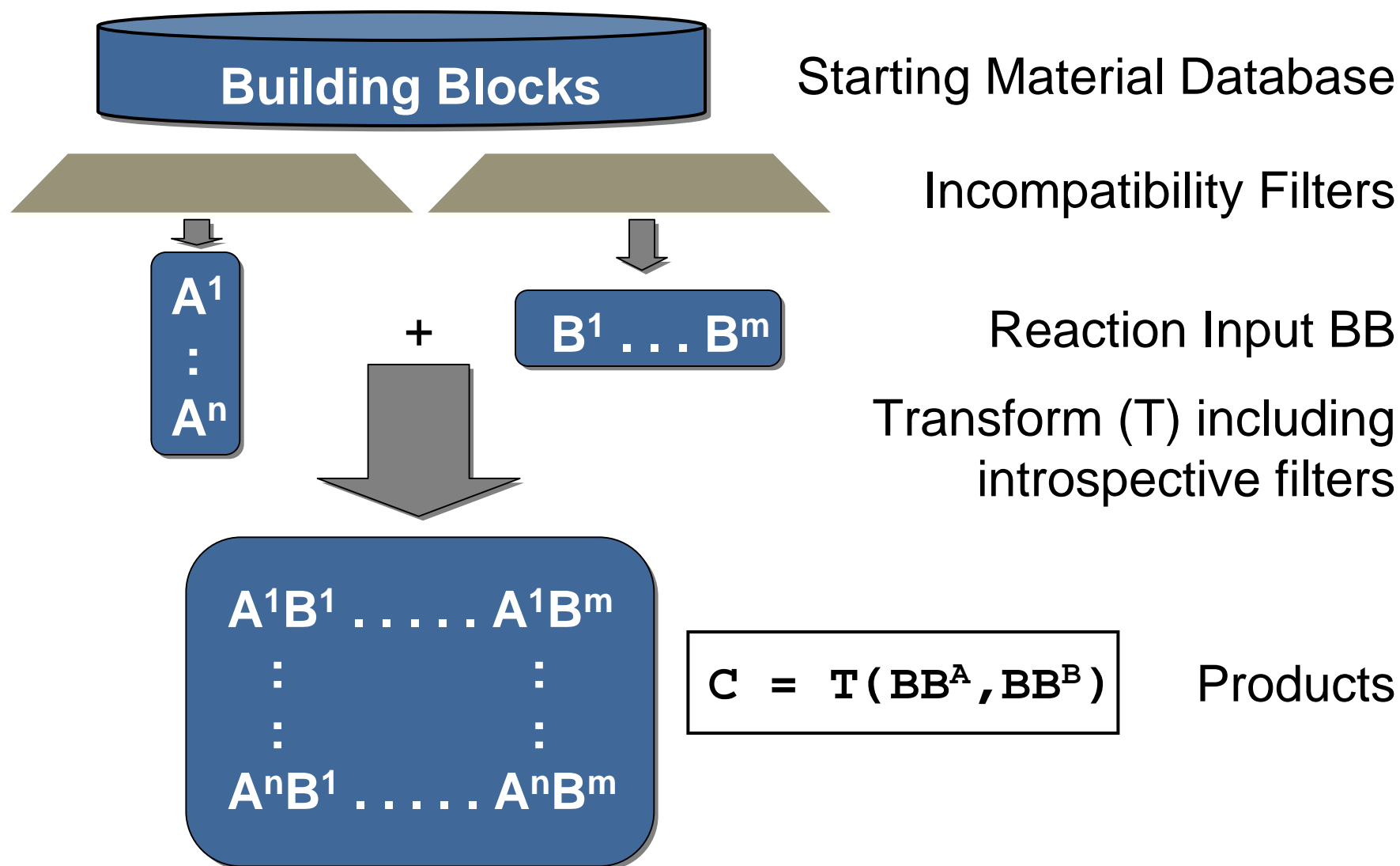
E.g. Nucleophilic aromatic substitution:



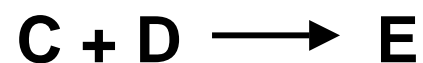
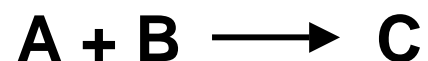
Nucleophilicity of aliphatic primary vs. secondary vs. aromatic amines

**Introspective filters (transform embedded)**

# Chemical transforms and filters



## Transforms and filters - cont'd



$$C = T_1(BB^A, BB^B)$$

$$E = T_2(C, BB^D)$$

$$= T_2[T_1(BB^A, BB^B), BB^D]$$

Filtration of final products: Lipinski -  $F^{Lip}$ , structural filters (undesired functional groups or fragments) -  $F^{BadFrag}$ , QSAR -  $F^{QSAR}$

$$E^{final} = F^{QSAR} \{ F^{BadFrag} \{ F^{Lip} ( E ) \} \}$$

$$= F^{QSAR} \{ F^{BadFrag} \{ F^{Lip} ( T_2 [ T_1 ( BB^A, BB^B ) , BB^D ] ) \} \}$$

## ChIP – Chemical intelligence platform

- Forward, prospective exploration of existing and newly coupled synthetic strategies
- Dynamic recombination of synthetic pathways to generate novel synthetically accessible molecules
- Pre- and post-synthesis filtering and prioritization
- Synthesis strategies guided towards novel and medicinally relevant molecules using ePotency, eSelectivity, and eADMEtox models
- Diversity-oriented or directed evolution of molecules

# Chemical transformations explored

- Subset 1: Nucleophilic aromatic substitution reactions
- Subset 2: Pd-catalyzed aromatic substitutions
- Subset 3: Functional group transformations
- Subset 4: Amine acylation reactions (amides / carbamates)
- Subset 5: Amine acylation reactions (ureas / thioureas)
- Subset 6: Formation of diverse (annelated) heterocyclic systems (quinazolinones, -diones, benzoimidazoles, -oxazoles, thiazoles)
- Subset 7: Formation of thioimidazoles
- Subset 8: Standard deprotection steps (Fmoc, Boc, *t*-Butyl, Trityl, )

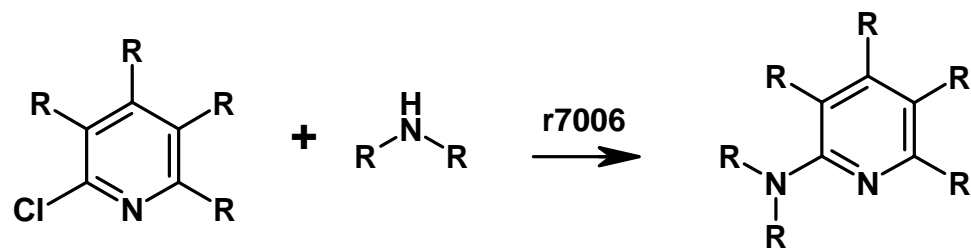
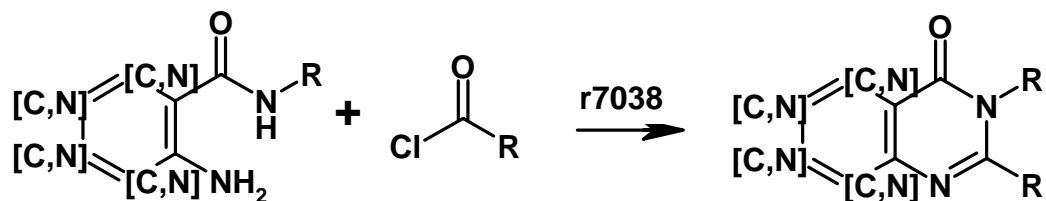
## Systematic vs. directed exploration - GA

- Systematic Exploration is not feasible: too many reaction combinations and building blocks – many of them not productive or not relevant
- Directed exploration leveraging a genetic algorithm (GA):
  - Uses text-based representation of reaction step transform
  - Starts with random sequence (starting gene) and generate products for this sequence starting from pre-filtered commercial building blocks
  - Apply Lipinski (MWT, HBA/HBD, ClogP, TPSA, rotBond) and structural filters like reactive functionalities (alkylators / acylators, electrophiles, nucleophiles, etc.) and undesired motifs (non-standard elements, >2 halo or >1 nitro per aryl, thioesters / ureas, un-branched chains, etc.)
  - Evaluate remaining structures by predicted activity (or other scoring function), e.g.:  $100 - 15 * \text{Max}(\text{eActivity})$
  - Optimization of reaction sequences by crossover mutation of highest scoring sequences
- Throughout the simulation best sequences and their products are captured

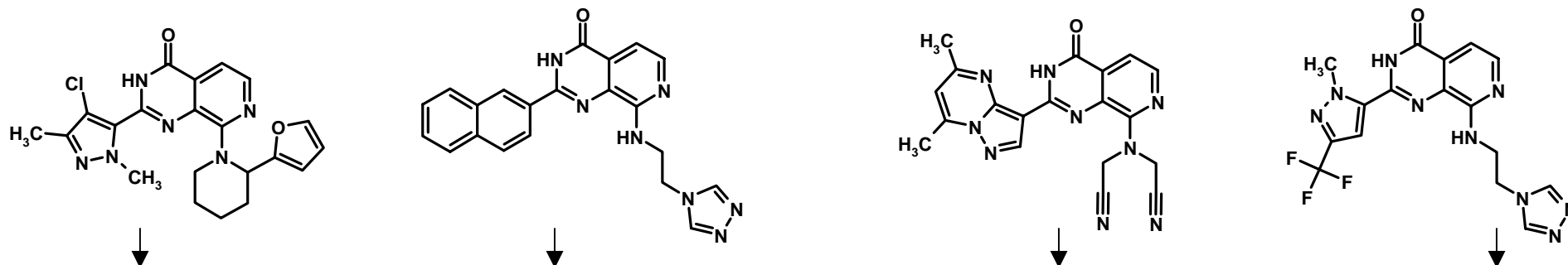


# ATP-binding site-directed simulations

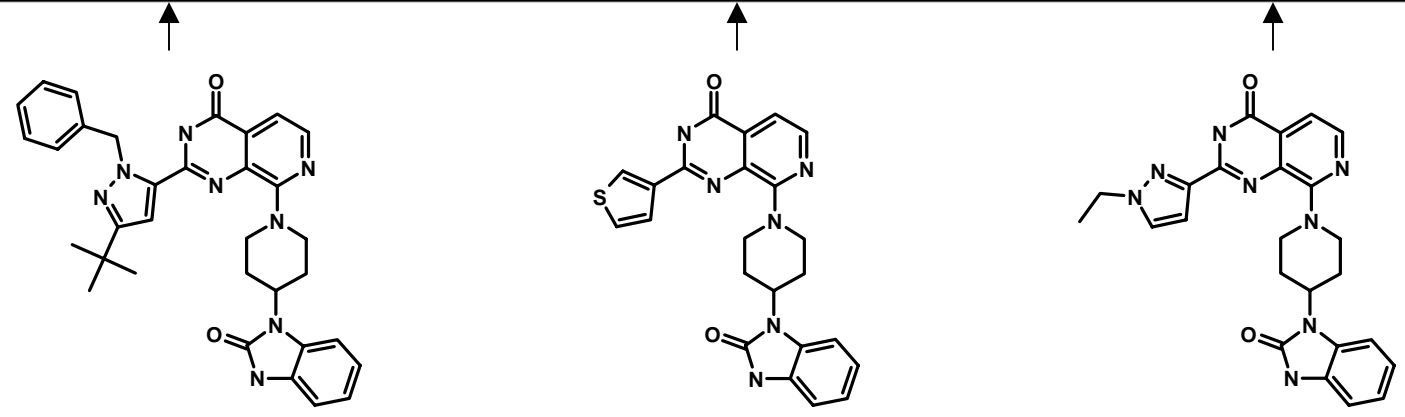
vProtocol for the Synthesis of 4-aminopyridopyrimidinones:



# Results

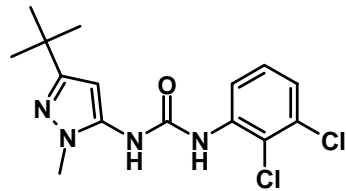


PKC	5.2	5.0	4.7	5.3	4.8	4.7	4.5	4.6	6.4	5.8	5.4	4.1	4.9	4.7	4.3	5.2	5.8	5.2	5.2	4.2	5.0	5.3	5.1	5.0	5.6	5.7	5.1	5.6	5.3	5.6	5.4	5.0	5.8	5.7	5.4	5.1	6.3	5.1	5.8	6.1	5.5	5.4	5.7	6.0	6.4	5.4	6.4	5.8	5.7	6.2
CDK1 B	6.6	5.7	6.3	6.3	6.2	6.1	6.0	6.0	5.6	6.0	5.3	5.3	5.3	5.3	5.8	5.5	5.8	5.8	5.8	5.7	5.6	5.6	5.6	5.5	5.5	5.5	5.5	5.6	5.5	5.0	5.4	5.3	4.7	5.3	5.3	5.3	5.2	5.2	5.4	5.2	5.1	5.0	5.0	4.3	4.8	4.7	4.7	4.7	4.2	
CDK4 D1	4.3	5.3	4.8	5.7	5.5	4.3	4.7	4.3	5.5	4.8	6.2	5.3	6.4	5.8	5.5	5.5	5.3	5.3	5.3	5.6	5.8	6.1	5.7	5.3	5.8	4.5	5.3	5.7	6.2	5.7	6.1	6.0	5.3	5.6	5.0	6.0	5.3	5.8	5.1	5.1	5.4	5.1	6.1	5.2	5.2	5.3	5.7	5.0	5.3	5.1
CDK5	6.6	6.5	5.7	7.3	6.3	6.0	5.3	5.4	5.7	6.6	6.3	6.1	6.2	6.4	6.4	5.4	6.0	6.4	5.5	6.0	6.6	6.1	5.6	5.3	6.3	5.3	5.8	5.8	5.5	6.1	5.3	6.6	6.2	5.3	6.0	5.7	6.2	6.5	6.0	6.4	6.2	6.1	5.3	6.4	5.3	5.7	6.2	6.2	6.2	6.2
GSK3B	6.4	5.5	6.6	6.4	5.5	6.3	5.3	5.8	6.3	6.7	5.2	5.2	5.6	6.2	5.5	6.0	6.4	5.3	6.0	5.6	5.3	5.6	5.5	5.2	5.8	6.0	5.0	5.4	5.1	5.1	5.2	5.3	5.3	5.4	5.4	6.0	5.7	5.0	6.3	5.8	5.4	5.3	5.4	6.0	6.7	5.1	6.5	6.0	5.3	6.2
MAPK14	7.5	5.1	6.8	7.1	7.4	7.1	6.3	6.5	7.3	6.7	6.1	7.1	6.7	6.1	7.6	6.2	6.6	7.0	5.1	7.4	6.6	6.2	7.6	7.4	8.3	7.1	5.3	5.7	5.8	5.3	5.7	7.6	5.1	5.1	5.8	6.1	6.4	6.1	7.3	6.8	7.3	6.0	5.5	5.4	6.6	6.1	6.6	5.1	5.1	7.1
ABL	5.8	5.0	5.4	5.4	5.3	5.2	5.7	5.5	6.1	5.3	5.3	5.5	5.8	5.1	5.3	5.6	5.8	5.3	4.8	5.4	5.2	5.8	5.2	5.7	6.5	5.9	6.0	5.5	5.5	4.8	5.6	6.3	5.1	4.3	5.8	5.5	6.8	5.8	5.4	6.4	6.4	5.7	4.3	5.5	5.5	6.5	5.2	5.5	5.1	5.1
CSK	5.3	5.8	6.3	5.9	6.8	6.6	6.3	6.3	5.8	5.7	5.4	7.0	5.2	6.0	5.8	5.5	5.7	5.4	6.0	6.1	5.5	5.7	6.2	6.4	6.8	5.6	5.2	5.2	5.7	5.6	5.6	5.4	6.3	5.8	5.6	6.2	6.4	5.6	5.8	6.0	5.6	5.4	5.8	6.4	5.3	4.3	4.3	6.6	6.2	5.6
EGFR	4.3	4.3	5.0	4.1	5.0	5.3	5.3	5.3	4.3	5.5	5.1	6.4	6.4	5.1	5.8	6.2	5.2	5.5	5.8	6.7	6.6	5.2	6.3	5.3	6.6	6.0	5.4	5.0	4.8	5.5	4.8	5.8	4.6	4.8	5.8	6.6	4.4	6.0	5.3	4.0	5.8	6.1	5.0	5.2	5.8	5.7	5.3	5.4	5.0	5.3
PDGFRB	4.8	4.3	5.2	5.1	5.3	5.2	5.1	5.0	5.3	4.3	5.2	5.5	4.8	5.6	5.4	5.4	4.8	5.3	5.0	5.2	5.1	5.1	5.0	5.1	5.7	5.1	4.7	4.3	5.1	5.3	5.3	5.6	5.3	5.2	5.2	5.4	5.5	5.0	5.2	5.5	5.1	5.3	5.4	5.2	5.0	4.6	5.0	5.2	5.3	5.2

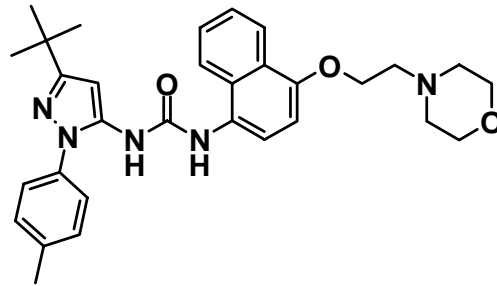


pIC50	
3.0 to 4.0	3
4.0 to 5.0	4
5.0 to 6.0	5
6.0 to 7.0	6
7.0 to 8.0	7
8.0 to 9.0	8

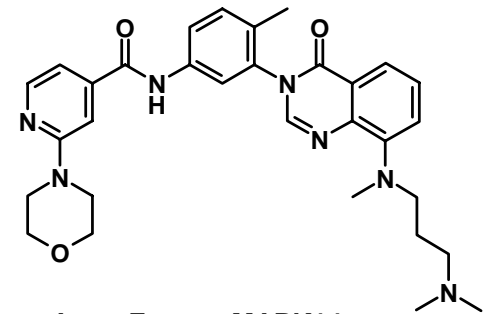
# Tanimoto similarities



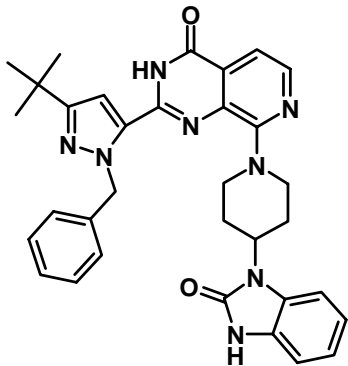
Bayer MAPK14 inhibitor  
IC50 = 53 nM



Boehringer Ingelheim MAPK14  
IC50 = 18 nM



Astra Zeneca MAPK14  
IC50 = 100 nM



Simulation result MAPK14

0.40

0.49

0.62

structural

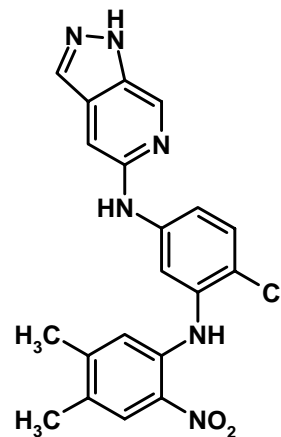
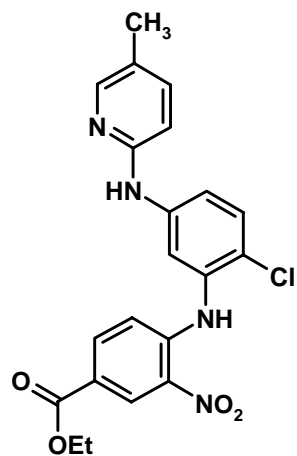
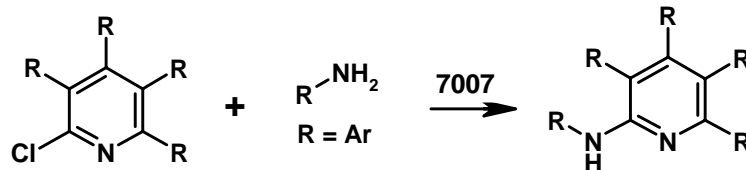
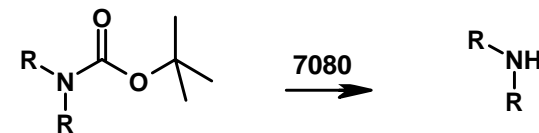
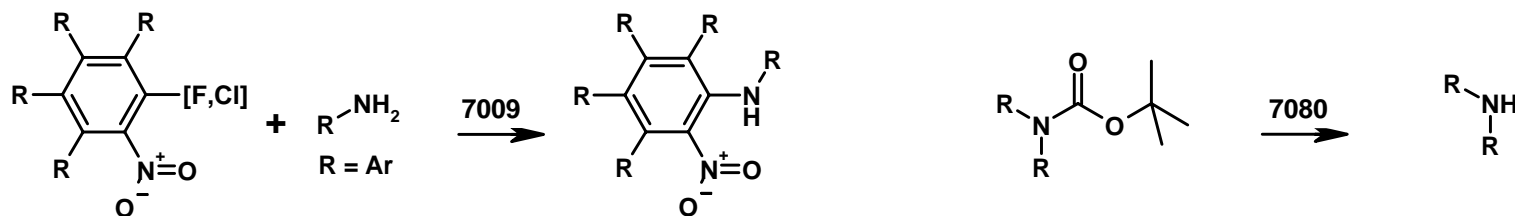
0.28

0.64

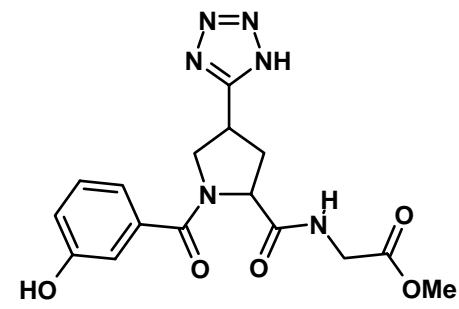
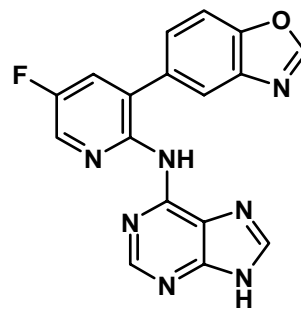
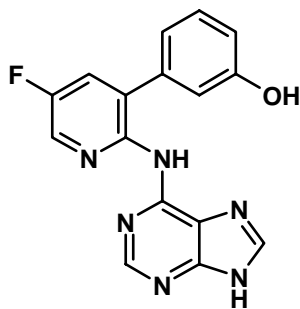
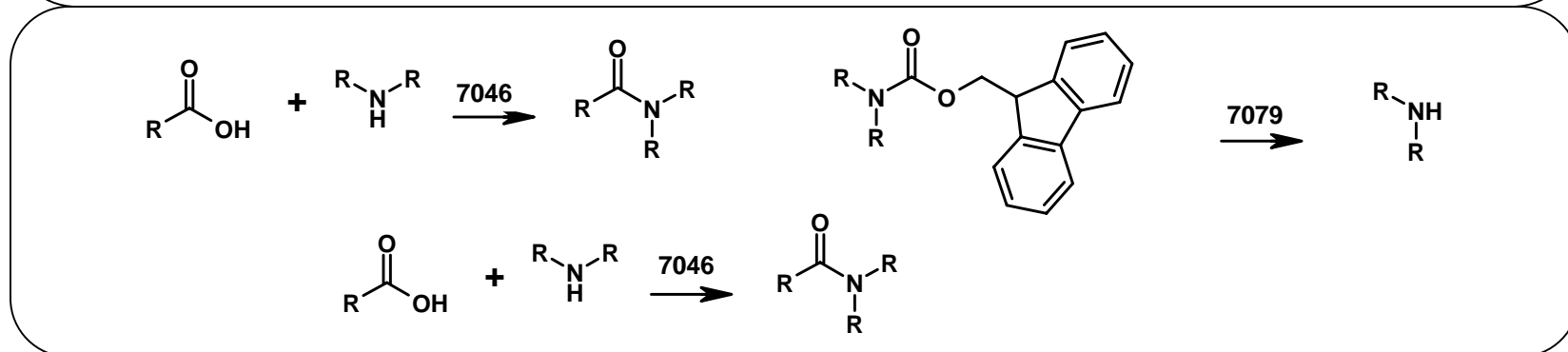
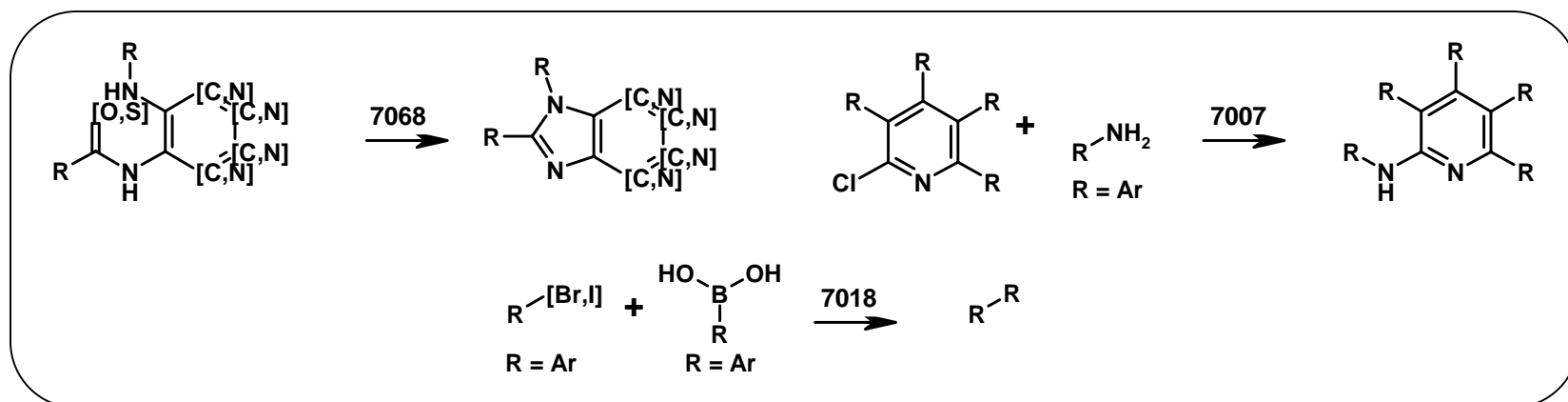
0.44

pharmacophoric

# Similarity-directed simulations I



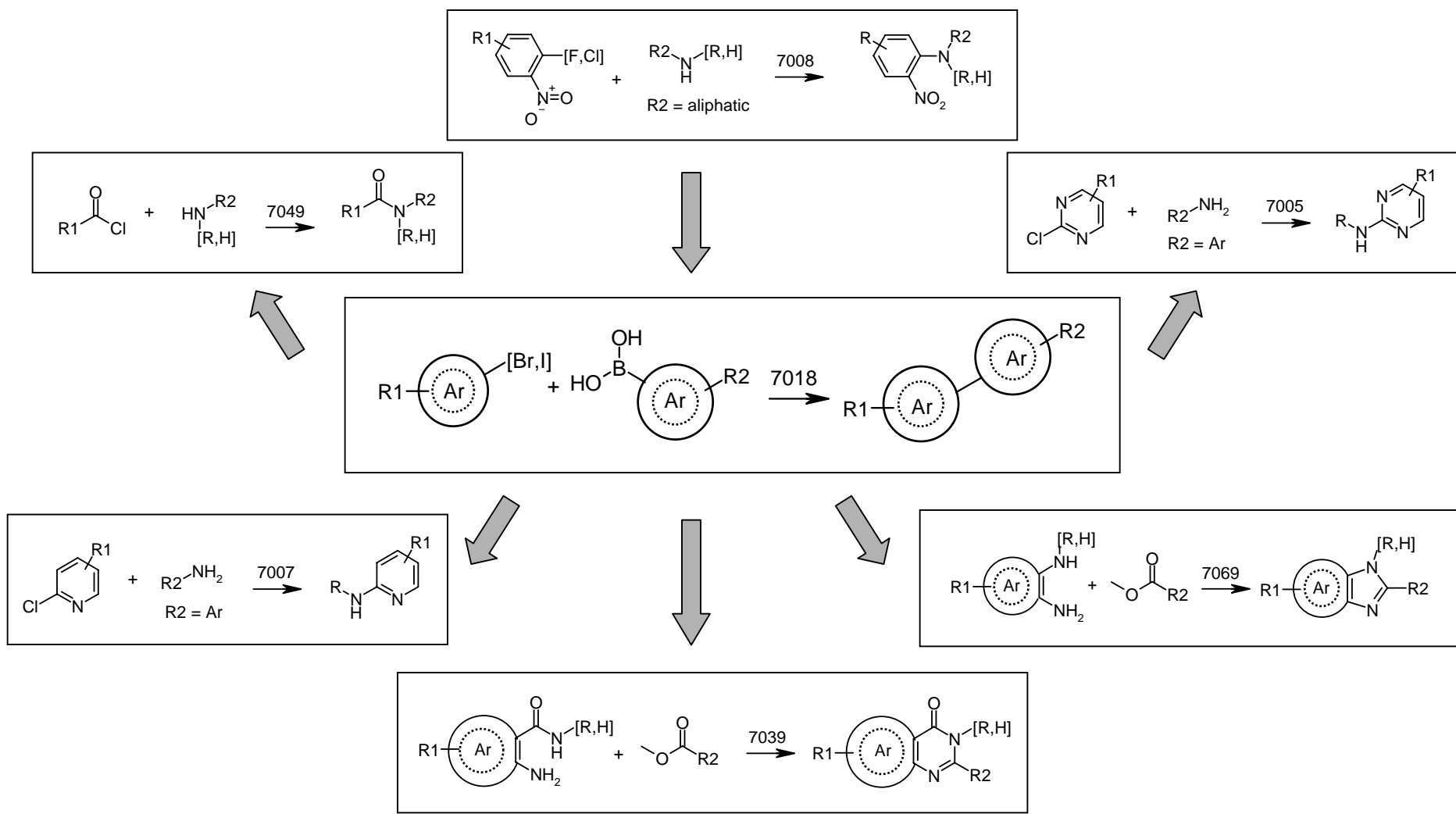
# Similarity-directed simulations I - cont'd



# Results – predicted activity matrix

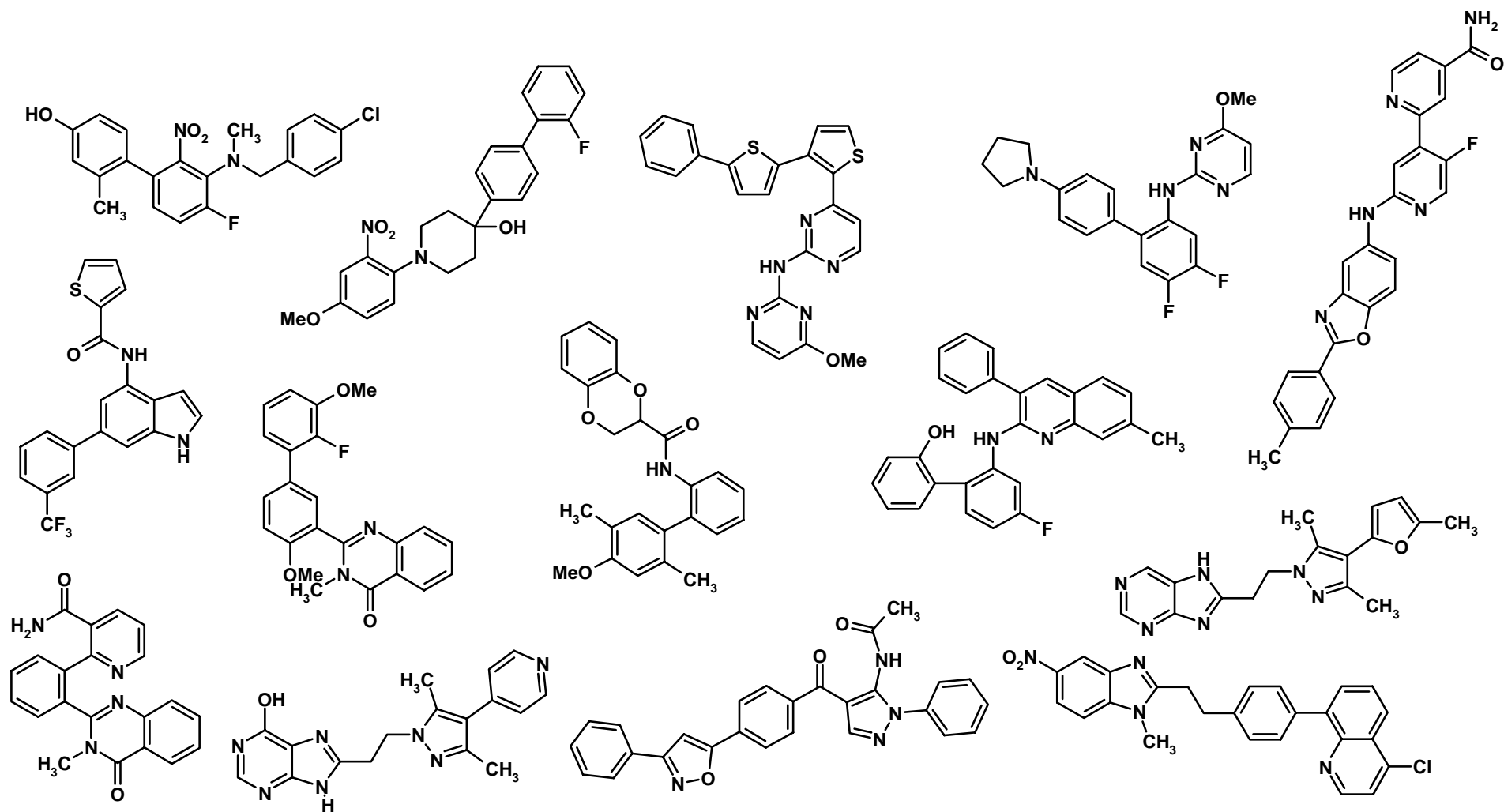
		PKA	PKC	PRKCA	PRKCB1	PRKCD	PRKCA_DAG	PRKCB1_DAG	PRKCE_DAG	PRKCG_DAG	PRKCH_DAG	PDK	CDC2	CDK1_B	CDK2	CDK2_A	CDK2_E	CDK4_D1	CDK4_D2	CDK5	CDK5_p25	CDK5_p35	MAPK14	ADK	GSK3A	GSK3B	CSK	SRC	FYN	LCK	ABL	SYK	ZAP_70_SH2	Grb2_SH2	EGFR	ERBB2	FGFR	EGFR_Substrate	PDGFR	PDGFRB	FLT1	KDR	TEK	RAF1	MAP2K	PPK	PIK4CA	
r7009	10557855	4.9	4.7	5.6	6.6	5.0	4.4	4.4	4.0	4.6	5.4	5.7	7.0	6.4	6.2	6.3	6.2	6.1	5.8	7.0	7.2	6.3	7.5	7.8	7.7	6.1	5.2	6.4	5.2	6.0	5.4	6.8	4.2	4.4	6.1	5.8	5.1	5.5	5.2	5.0	6.7	6.5	5.8	5.8	6.8	7.0	3.8	
	10557857	4.8	4.6	5.2	6.8	5.2	4.5	4.5	4.0	4.6	5.4	6.4	6.1	5.7	5.6	6.5	6.4	5.7	5.0	6.5	7.3	6.5	7.6	7.4	7.5	5.7	6.4	5.3	5.0	6.0	5.7	5.9	4.2	4.4	6.4	5.4	5.6	5.6	5.3	5.2	6.5	6.0	5.7	5.9	6.6	7.3	3.8	
	10557860	4.8	4.6	5.8	6.1	5.1	4.5	4.4	4.0	4.6	5.5	7.0	6.3	5.7	5.9	6.1	6.1	6.1	6.8	5.5	6.6	6.6	7.3	7.2	7.4	5.5	5.7	6.2	4.7	6.3	5.6	6.2	4.2	4.4	5.9	5.9	6.0	5.6	5.4	5.0	7.0	6.1	6.1	6.3	7.0	6.8	3.4	
	r7007	10557864	5.1	4.9	6.0	6.1	5.3	4.5	4.4	3.9	4.7	5.5	6.9	6.8	6.2	6.7	6.2	6.7	6.7	6.5	6.7	7.4	6.5	7.1	8.2	8.0	6.0	6.0	5.9	4.6	6.6	5.5	6.3	4.1	4.4	7.1	6.1	6.2	5.6	5.3	5.3	7.3	6.1	6.5	6.3	7.0	7.2	4.0
		10557865	5.0	5.2	5.3	5.9	5.5	4.6	4.6	4.1	4.6	5.4	6.5	6.9	7.0	6.8	6.9	6.9	5.9	6.3	7.2	7.4	6.5	6.1	6.5	7.7	6.3	6.8	6.2	5.2	6.1	5.5	6.2	4.1	4.4	6.6	6.0	5.6	5.6	5.0	5.3	7.3	6.2	6.4	6.3	6.9	7.3	4.4
		10557866	4.9	5.3	5.9	5.5	5.4	4.6	4.4	4.1	4.7	5.6	7.1	6.7	6.6	6.7	6.3	7.2	6.4	6.8	6.6	7.2	6.5	7.2	8.5	7.8	6.1	5.4	6.3	5.1	6.8	5.4	6.6	4.1	4.4	6.1	6.6	6.0	5.5	4.7	5.1	7.5	5.9	6.6	6.1	7.1	7.0	3.9
		10557858	5.0	5.0	6.3	6.1	5.1	4.5	4.5	4.0	4.7	5.7	6.1	6.0	5.3	5.9	5.9	5.9	5.8	7.0	5.4	6.4	6.5	7.9	7.8	7.4	5.4	5.6	6.2	4.5	6.7	5.7	6.5	4.2	4.4	5.9	6.4	5.8	5.5	5.6	5.0	7.2	6.1	6.3	6.3	7.1	6.7	3.5
		10557859	4.9	5.2	6.1	6.3	5.1	4.6	4.4	4.0	4.8	5.5	7.1	6.9	5.2	5.6	6.2	5.8	6.1	7.3	5.7	6.4	6.5	7.1	7.8	7.6	5.7	5.6	6.2	4.3	6.4	5.1	6.3	4.3	4.4	5.8	6.3	5.4	5.6	5.1	4.7	7.4	6.4	6.4	6.2	7.2	6.6	3.6
		10557861	4.8	4.7	5.5	6.5	5.0	4.4	4.4	4.0	4.6	5.4	5.7	6.8	5.8	6.1	6.2	5.8	5.8	5.9	6.3	6.8	6.3	7.6	7.5	7.7	5.9	5.1	6.5	5.3	6.0	5.6	6.8	4.2	4.4	5.6	5.7	5.3	5.5	5.2	4.9	6.7	6.7	5.8	5.8	6.7	7.0	3.8
		10557866	5.2	5.5	5.6	6.8	5.0	4.3	4.4	3.8	4.5	5.3	5.7	6.2	5.6	5.5	6.2	5.6	5.8	4.8	5.3	6.8	5.9	7.4	7.9	7.5	5.8	5.7	6.1	5.2	5.9	5.6	6.5	4.2	4.3	6.4	5.9	5.1	5.4	5.5	5.1	6.5	5.7	5.6	5.9	6.7	7.0	3.8
10557862		4.7	5.4	6.8	5.9	5.0	4.5	4.5	4.0	4.7	5.6	6.2	7.4	6.3	7.3	5.5	6.1	5.7	6.8	6.4	6.4	6.5	7.0	8.9	8.0	6.4	5.6	6.6	4.9	7.0	5.5	7.3	4.1	4.3	4.8	6.2	5.3	5.5	4.8	4.6	7.4	6.5	6.4	6.3	7.2	6.8	3.9	
10557853		5.1	4.8	5.3	6.2	5.0	4.6	4.6	4.0	4.8	5.6	6.1	6.5	5.9	5.7	5.6	5.2	5.6	6.7	4.7	6.2	5.6	7.6	7.8	7.4	6.5	4.7	6.5	4.7	5.0	6.1	6.0	4.4	4.2	5.9	6.5	4.5	5.6	6.4	4.8	6.9	6.7	6.3	5.5	6.6	6.5	3.4	
10557863		4.9	4.9	4.9	5.8	5.2	4.5	4.5	4.1	4.5	5.3	6.8	7.2	6.5	6.0	6.3	6.2	5.8	5.7	6.8	7.1	6.2	6.9	7.1	7.2	6.3	5.8	6.1	5.8	5.9	5.4	6.7	4.1	4.3	5.8	5.3	5.4	5.3	5.3	5.0	6.6	5.7	5.8	6.2	7.0	7.2	4.5	
10557854	4.7	4.3	5.0	6.1	5.0	4.5	4.5	4.1	4.6	5.3	6.2	5.9	5.3	5.1	5.7	5.7	5.5	6.0	5.1	6.5	5.8	7.6	6.9	7.4	5.7	5.5	6.0	5.1	5.8	6.4	6.0	4.3	4.3	6.9	6.1	5.3	5.5	6.2	5.1	6.4	6.6	5.9	6.3	6.6	6.7	3.8		
r7068	10557881	4.4	4.5	4.6	5.8	5.1	4.5	4.5	4.1	4.5	5.4	5.1	5.7	5.0	5.2	6.7	5.4	5.1	3.9	5.5	6.1	5.4	6.7	7.5	7.2	5.6	6.5	6.5	6.4	5.6	6.4	7.0	4.2	4.3	6.1	5.5	5.1	5.1	5.4	5.2	6.2	5.4	5.3	5.5	6.4	7.0	4.0	
	10557879	4.4	4.7	5.0	5.9	5.2	4.6	4.6	4.1	4.6	5.5	6.1	6.2	5.4	5.4	6.7	5.4	5.1	3.8	5.4	6.5	5.6	7.1	7.9	7.2	5.9	6.5	6.0	6.6	5.7	6.1	6.9	4.1	4.3	5.9	5.8	5.4	5.2	5.3	5.3	6.7	5.8	5.6	5.7	6.5	7.4	4.2	
	10557886	4.6	4.9	5.2	5.9	5.3	4.6	4.6	4.1	4.6	5.5	6.6	6.4	5.9	5.4	7.1	6.0	5.9	4.3	6.0	7.1	6.0	7.2	7.5	7.2	5.6	6.7	6.3	6.6	6.2	5.8	6.7	4.1	4.3	6.2	5.8	5.8	5.3	5.4	5.4	7.0	5.5	5.7	6.2	6.5	7.5	4.1	
	r7018	10557885	4.8	5.5	5.2	5.7	5.4	4.6	4.5	4.1	4.5	5.4	6.5	6.5	5.7	5.8	6.4	6.2	5.6	4.7	6.2	6.8	5.9	5.8	6.9	7.2	6.0	5.8	6.6	6.9	6.1	5.4	6.9	4.1	4.3	6.0	5.9	5.7	5.3	5.3	5.5	6.7	5.4	5.8	5.8	6.9	7.3	4.4
		10557874	4.7	5.2	5.1	5.5	5.1	4.5	4.5	4.0	4.5	5.4	6.5	6.0	5.7	5.6	6.7	6.5	5.7	4.8	5.8	6.8	5.9	7.4	7.7	7.1	5.3	6.0	6.8	6.5	6.9	6.1	7.1	4.1	4.3	6.4	6.0	5.6	5.3	5.2	5.1	6.6	6.1	5.6	6.0	6.8	7.3	4.2
		10557888	4.5	4.6	5.0	6.3	5.1	4.4	4.4	3.9	4.5	5.4	5.8	5.6	5.2	5.6	6.7	5.8	5.6	4.4	5.6	6.4	5.7	6.2	7.6	7.0	4.8	6.5	5.9	5.5	6.6	6.4	6.8	4.2	4.3	6.5	5.5	4.8	5.3	5.6	5.2	6.3	5.6	5.5	5.9	6.6	7.2	3.8
		10557877	4.5	4.4	4.8	6.1	5.1	4.5	4.5	4.1	4.6	5.5	5.4	5.7	5.0	5.3	6.7	5.6	5.2	4.0	5.3	6.1	5.5	6.4	7.6	7.1	5.3	6.2	6.7	5.9	6.1	6.4	7.0	4.2	4.3	6.3	5.5	4.8	5.2	5.3	5.2	6.2	5.6	5.4	5.5	6.4	7.0	3.7
		10557880	4.3	4.3	4.6	5.6	5.2	4.6	4.6	4.1	4.6	5.5	6.0	6.3	5.7	5.6	6.7	5.8	4.9	4.0	5.4	6.4	5.7	6.9	7.5	7.3	6.0	6.8	5.9	6.6	5.8	6.4	6.8	4.1	4.3	5.9	5.5	5.4	5.1	5.3	5.3	6.5	5.9	5.5	5.5	6.6	7.3	4.2
		10557863	4.8	4.9	4.8	5.8	5.2	4.5	4.5	4.1	4.5	5.4	6.2	5.7	5.7	5.5	6.9	6.3	5.7	4.3	5.8	6.7	5.6	6.9	7.4	7.0	5.5	6.0	6.1	6.4	6.3	6.2	7.0	4.1	4.3	6.5	5.8	5.5	5.2	5.2	5.1	6.5	5.4	5.6	5.9	6.6	7.3	4.4
		10557878	4.9	4.8	5.1	6.1	5.2	4.6	4.5	4.1	4.6	5.5	6.3	5.6	5.6	5.4	7.0	6.2	5.6	4.2	5.6	6.8	5.7	6.4	7.4	7.1	5.3	6.0	6.5	5.9	6.4	6.1	6.8	4.2	4.3	6.6	5.8	5.3	5.3	5.2	5.5	6.4	5.4	5.5	5.9	6.4	7.3	4.0
10557884		4.4	4.7	4.9	5.7	5.1	4.5	4.5	4.1	4.5	5.4	5.5	5.6	5.1	5.6	6.5	5.9	5.2	4.2	5.3	6.1	5.6	7.2	7.8	6.9	5.3	5.9	6.1	6.5	6.5	6.3	7.2	4.1	4.3	6.3	5.6	5.2	5.2	5.2	5.0	6.3	5.5	5.6	5.4	6.7	7.1	4.3	
10557876		4.6	5.7	5.0	5.8	5.4	4.6	4.5	4.1	4.5	5.4	6.4	6.6	6.0	5.6	6.6	5.7	5.8	5.0	6.1	6.7	5.6	5.6	6.7	7.6	6.2	6.2	6.9	6.9	5.7	5.0	6.6	4.2	4.3	5.9	5.8	5.8	5.2	5.1	5.7	6.8	5.0	5.6	6.0	6.7	7.2	4.1	
10557887		4.6	4.9	5.2	6.3	5.1	4.4	4.4	3.8	4.6	5.5	6.1	5.5	5.5	5.4	6.2	6.6	5.8	5.3	5.8	6.8	5.9	7.0	7.9	7.0	4.6	5.6	6.1	4.6	7.4	6.5	6.5	4.2	4.3	6.8	6.0	4.8	5.6	5.9	4.8	6.5	5.4	6.0	6.2	6.6	7.1	3.6	
10557875	5.0	5.5	5.4	6.3	5.1	4.4	4.5	3.8	4.7	5.5	7.8	5.4	5.9	5.6	5.9	6.2	5.9	5.8	5.9	6.9	5.7	7.6	8.4	7.3	5.2	5.9	5.5	4.6	7.2	6.3	6.4	4.2	4.3	6.9	6.7	5.0	5.6	6.1	4.9	6.8	5.9	6.2	6.5	6.4	7.1	3.5		
10557882	4.9	4.8	5.3	6.7	5.1	4.4	4.4	3.9	4.5	5.4	5.5	5.5	5.7	5.0	6.0	5.8	6.1	4.9	5.7	6.6	5.3	5.9	7.2	7.6	5.7	5.2	5.6	5.5	5.9	5.6	6.5	4.2	4.3	6.4	5.7	5.1	5.3	5.6	5.3	6.2	6.0	5.4	5.8	6.2	6.7	4.1		
r7046	10557871	4.9	4.3	4.8	6.4	6.1	5.0	4.4	4.0	5.1	5.4	8.0	7.3	6.8	6.1	5.7	5.3	5.3	6.2	6.5	7.1	7.0	5.8	7.0	7.3	5.4	6.9	5.4	4.4	6.6	4.8	5.2	4.4	5.2	5.3	5.2	6.0	5.8	5.3	6.0	7.7	6.8	6.4	6.5	6.6	7.6	4.1	
	10557869	4.4	4.6	4.4	5.0	6.0	4.9	4.4	4.1	4.7	5.5	7.1	6.6	5.9	6.0	5.3	5.1	4.5	6.6	6.1	6.5	6.5	5.4	7.3	7																							

# Simulations II - selected reaction sequences



orthogonal building blocks and cross compatibility

# Simulations II - selected compounds





# ChIP partnerships

## Chip Strategic Partnership Program

- Microwave ChIP Module
- Early collaborative applications of the technology
- Experimental proof of concept studies
- Early access to ChIP technology
- Access to current LUCIA system (ChIP precursor)

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