Developing Data Science and ML Tools for Synthetic Chemists



Ischia Advanced School of Organic Chemistry

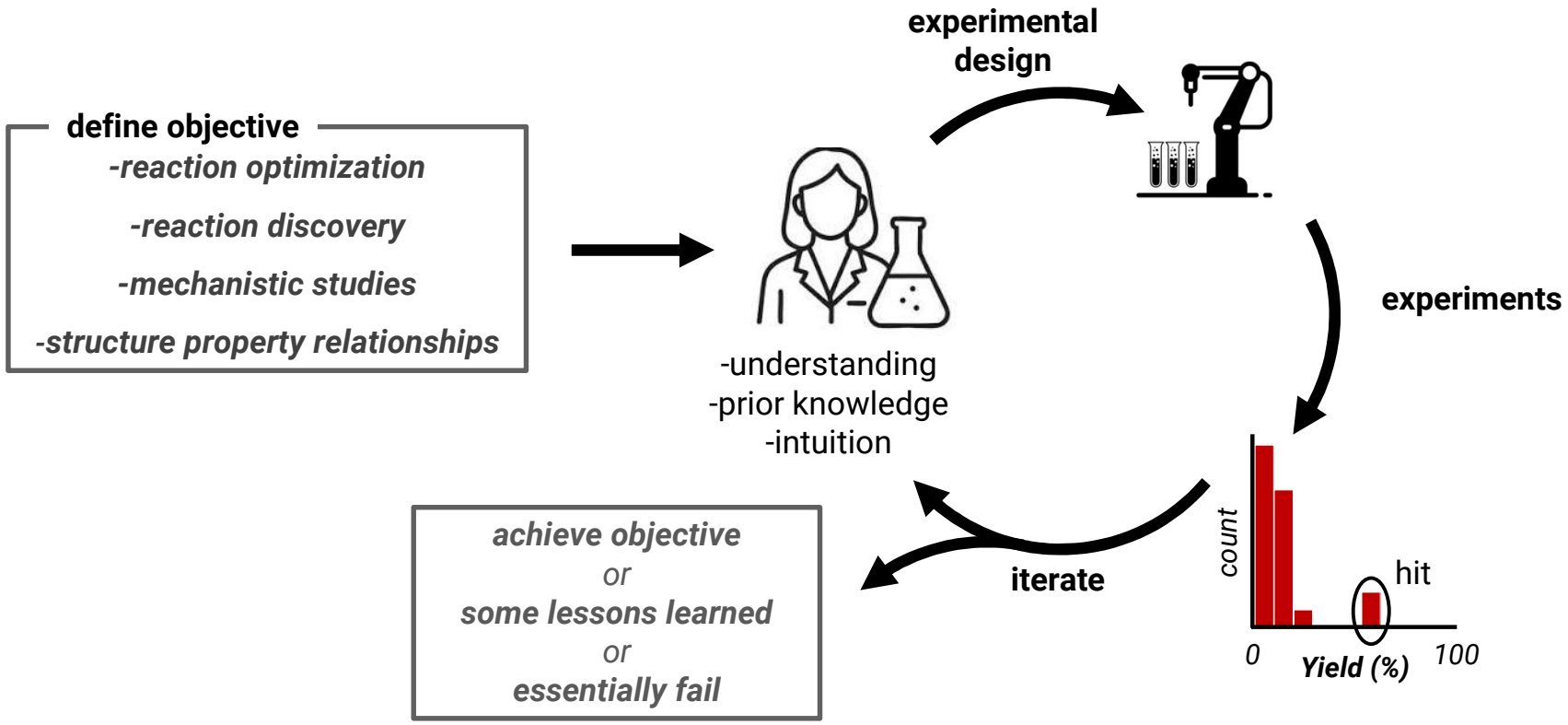
Ischia, Italy

September 20th, 2026

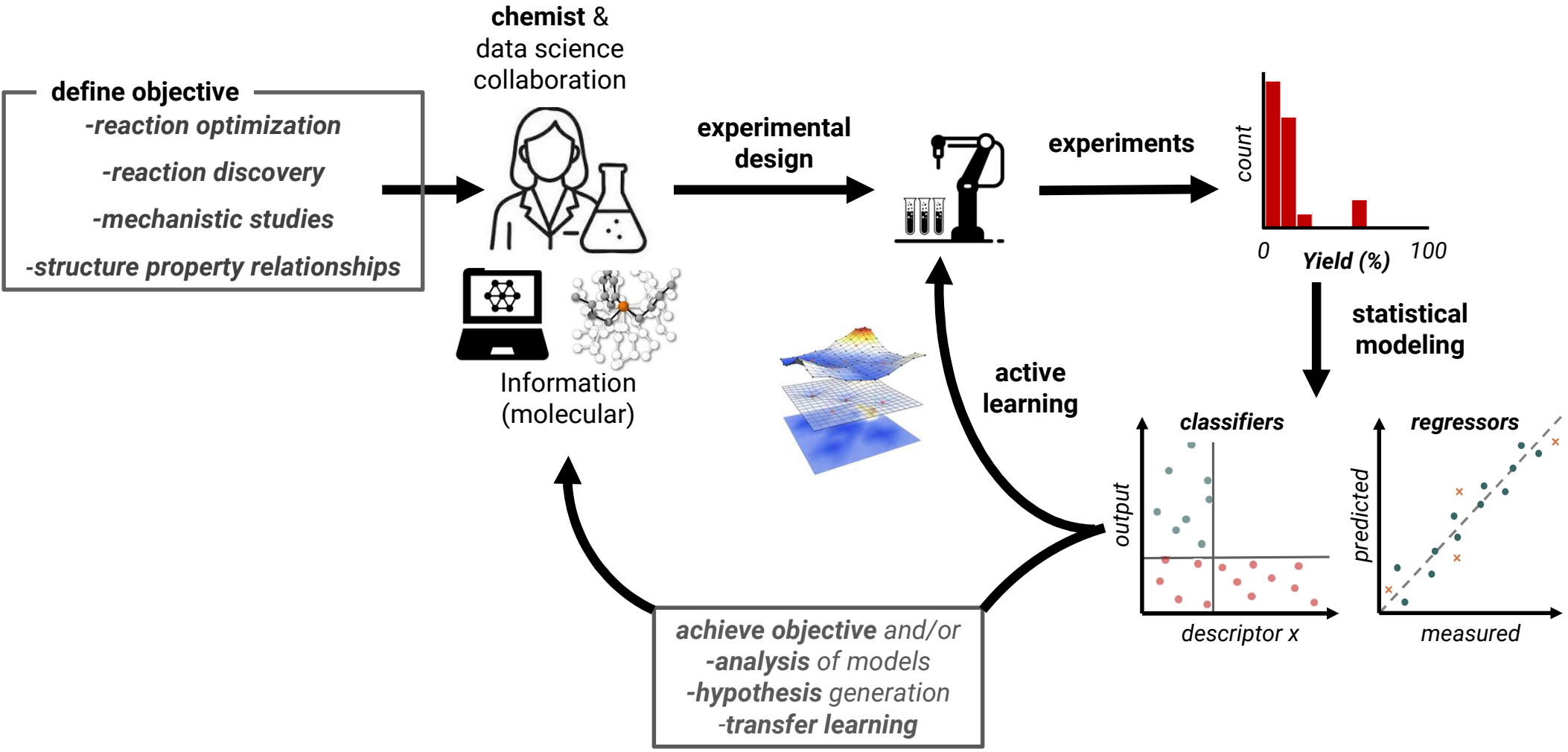
Matt Sigman



Chemist in the loop – traditional workflow



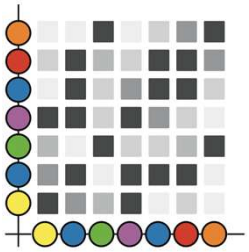
Our machine learning and data science frameworks in organic chemistry

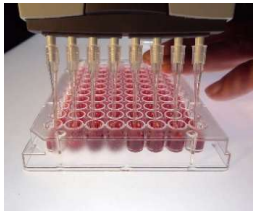


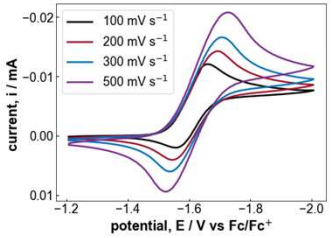
Recent contributors: Aspuru-Guzik, Burke, Cernak, Coley, Denmark, Doyle, Duarte, Gomes, Gensch, Glorius, Grzybowski, Milo, Paton, Reid, Schwaller, + many others!

General requirements to use ML/Data science in organic chemistry

data collection



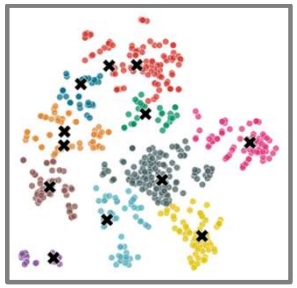




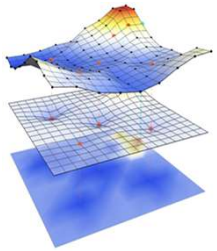
high quality, structured, diverse

machine learning algorithms

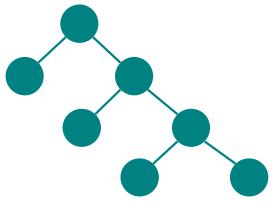
unsupervised



active



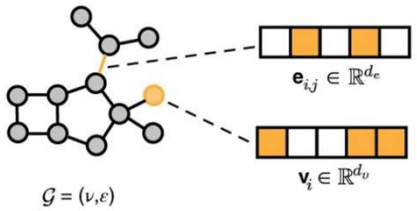
supervised



data and objective dependent

feature representation



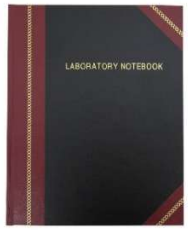


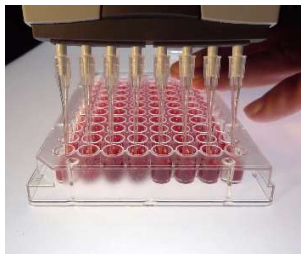
machine readable, chemical features

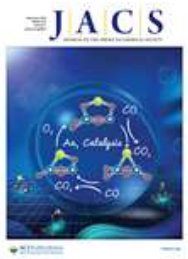
History: Williams, W. L.; Zeng, L.; Gensch, T.; Sigman, M. S.; Doyle, A. G.; Anslyn, E. V. *ACS Central Science*, **2021**, *7*, 1622.

Key challenges: data and domain of applicability

***data challenge**: Sparsity, bias of data, data outputs*

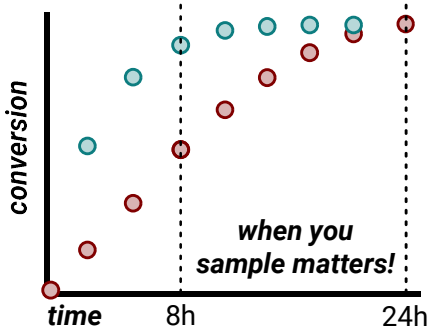






***Scalar**: enantioselectivity, rate*
**easier to correlate and relate to mechanism*

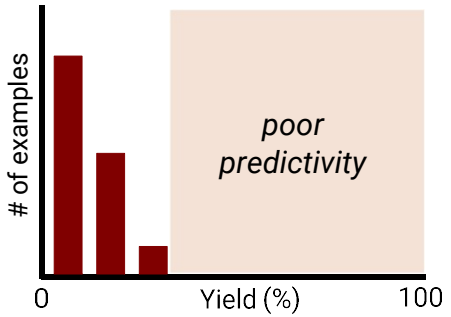
***Bounded**: yield, conversion*
**time dependent, many reasons influenced*

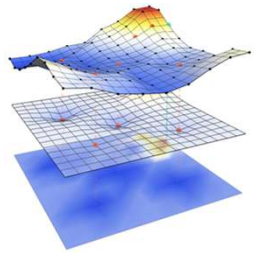


** reproducibility, purification, heterogeneous*

*with **Coley, Doyle, Reisman**, ACS Cent. Sci.* **2023**, *9*, 2196.

skewed data distribution — ***active learning***

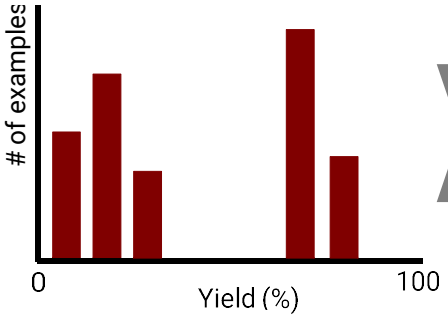


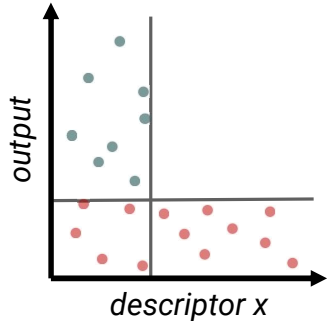


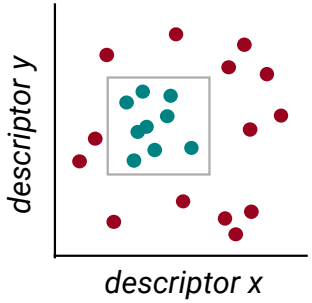
Bayesian optimization (BO)
Reaction condition optimization for yield and selectivity

Doyle group:
Nature ***2021***, 590, 89.
JACS **2022**, *144*, 19999.

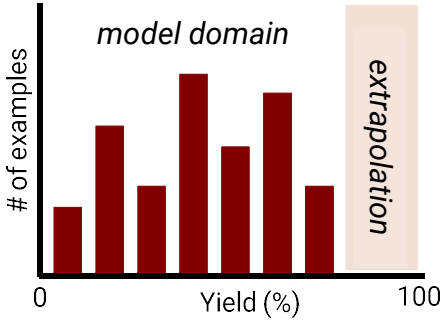
binned data distribution — ***classifiers***

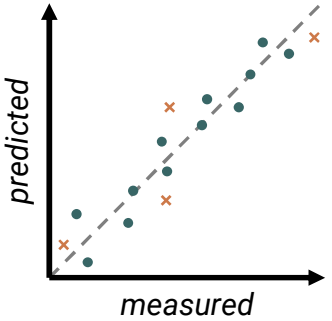






distributed data — ***regressors***

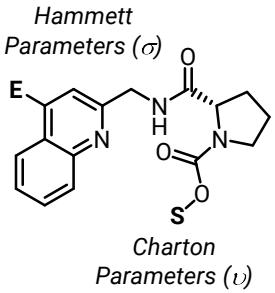




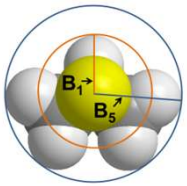
Reviews:
Chem. Sci. **2018**, *9*, 2398-2412
Sci. Adv. **2025**, *11*, eadt3013

Evolution of physical organic feature development in our group

2009-2011
Charton/ Hammett



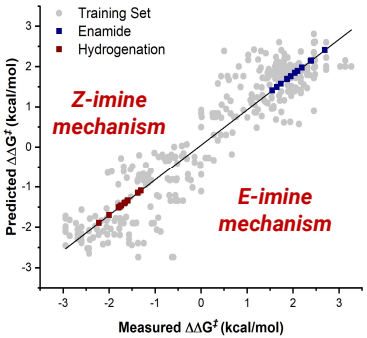
2012
Sterimol



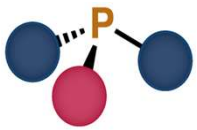
2014
DFT descriptors



2019
mechanistic connections

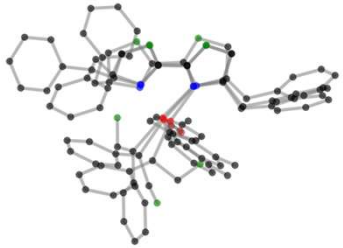


2022
kraken database



1 558 P(III)-compounds (kraken library)

2026
transition state featurization



Miller, J. J.
ACIE **2008**
47, 771-774
Harper
Science **2011**,
333, 1875-*1878*

Harper, Bess
Nature Chem.
2012, 366-374

Milo, Bess
Nature **2014**,
507, 210-214

Reid
Nature **2019**,
571, 343-348

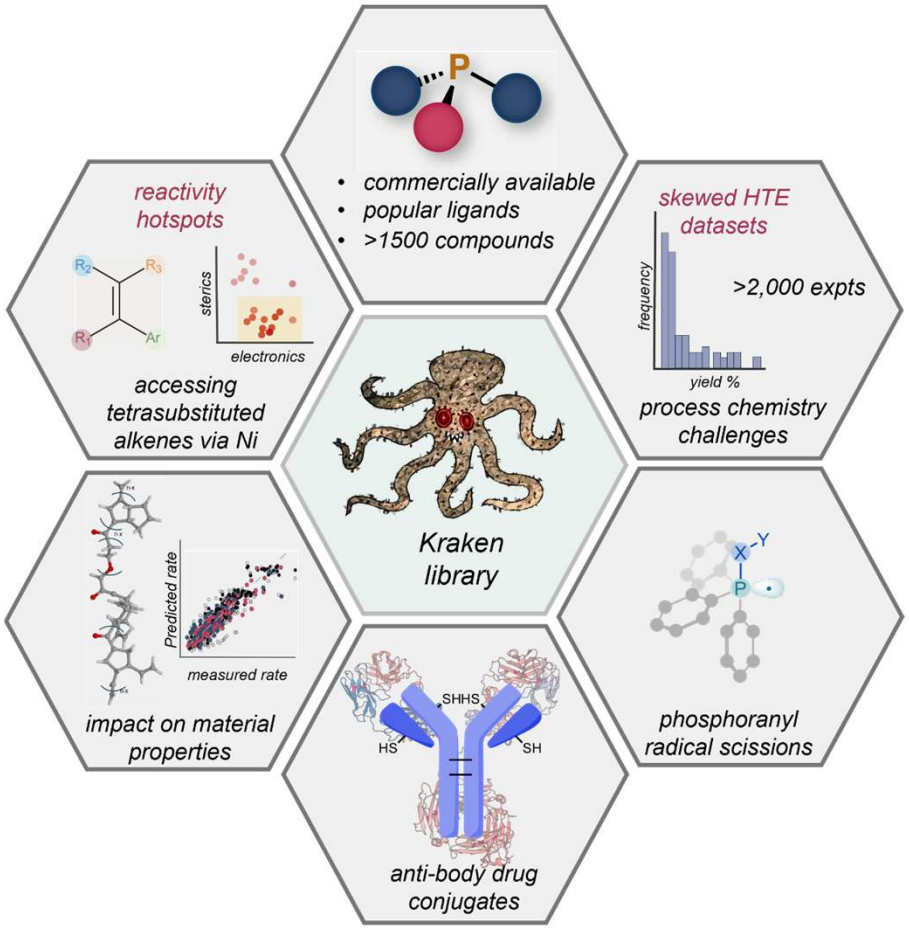
Gensch
JACS **2022**,
144, 1205-1217

Gallarati, Bucci & Doyle
Nature **2026,**
651, 637-646

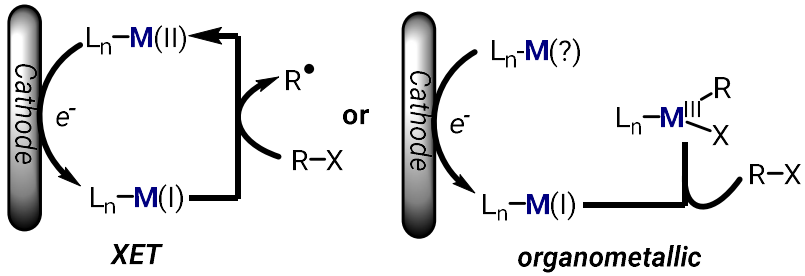
Reviews: Sigman, M. S. ; Harper, K. C.; Bess, E. N.; Milo, A. *Acc. Chem. Res.* **2016**, *49*, 1292
Santiago, C. B.; Guo, J.-Y.; Sigman, M. S. *Chem. Sci.* **2018**, *9*, 2398
Reid, J. L.; Sigman, M. S. *Nature Rev. Chem.* **2018**, *2*, 290
Crawford, J. M.; Kingston, C.; Toste, F. D.; Sigman, M. S. *Acc. Chem. Res.* **2021**, *54*, 3136
Paton and coworkers, *Acc. Chem. Res.* **2021**, *54*, 827
Fey *and coworkers:* Organometallics **2008**, *27*, 1372–1383; *Acc. Chem. Res.* **2021**, *54*, 837

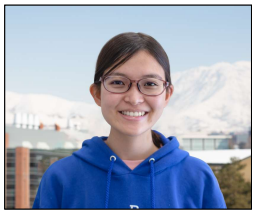
Todays lecture

Part 1: the tools and pipeline development



Part II: applications to catalysis: electrochemistry





Haruka Takenaka

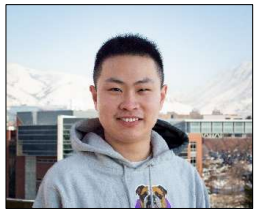


Avijit Hazra

Previous coworkers:
Dr. Chris Sandford (UT San Antonio)
Dr. David Hickey (Michigan State)



Alex Ring

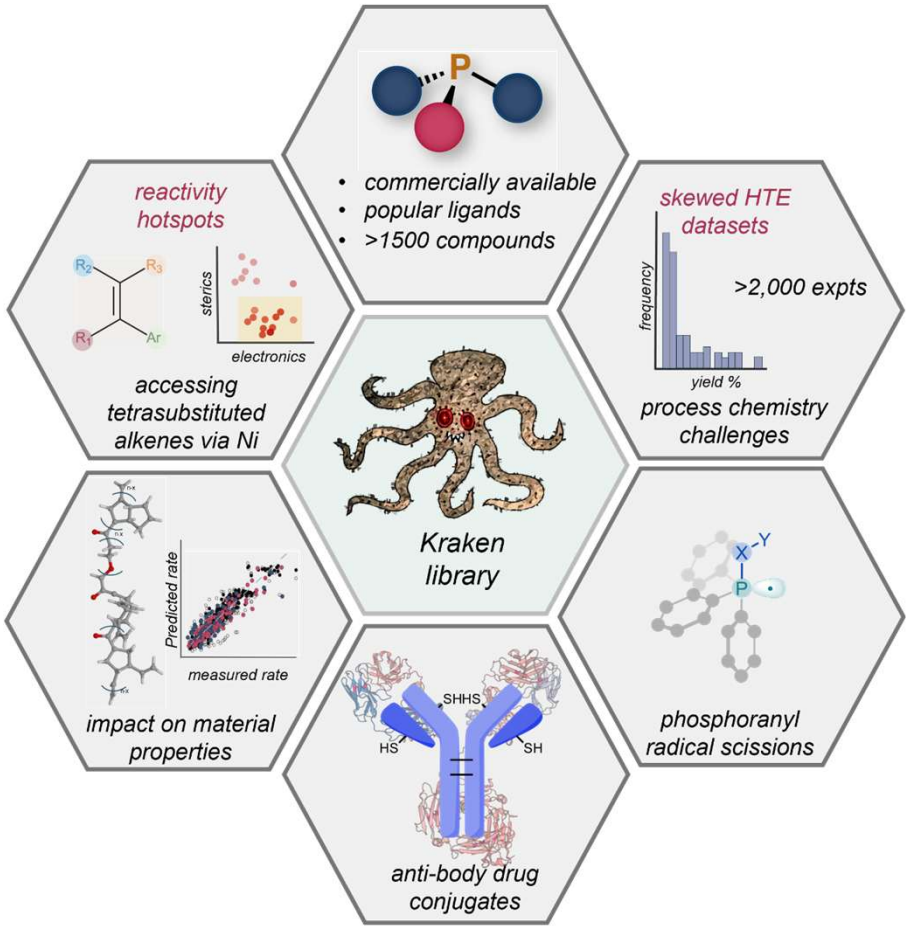


Josh Tang

w/Doyle, Reisman & Minteer labs

Kraken

***K**olossal vi**R**tual d**A**tabase for mole**K**ular d**E**scriptors of orga**N**ophosphorus ligands*



***Aspuru-Guzik Group (Toronto)**: Gabe Gomes, Pascal Friederich, Théophile Gaudin, Robert Pollice, Kjell Jorner, AkshatKumar Nigam*
***AbbVie Team**: Jeremy Henle, Andrew Ickes, Brian Kotecki, Matthew Ravn, Shashank Shekhar, Rafal Swiatowiec, Dennie Welch*
***Biscoe Group (CCNY)**: Shibin Zhao, Benjamin Murray*
***Buchwald Group (MIT)**: Kaibo Feng, Elaine Raguram*
***Doyle Group (UCLA)**: Julia Borowski, Sam Newman-Stonebraker, Daniel Min, Nari Tao, Jason Wang, Emily Wearing, Sam Hugie*
***Genentech Team**: Janis Jermaks, Lauren Sirois, Francis Gosselin, Chong Han, Jana Wassmer, Daniel Zell, Haiming Zhang*
***GSK Team:** Jennifer Crawford, Jennifer Elward, Janelle Steves*
***Hein Team (UBC):** Tara Zepel, Lars P. E. Yunker*
***Merck Team:** Melodie Christensen, Heather Johnson*
***Millipore Sigma Team:** Tom Colacot, Yam Timsina, Guolin Xu, Ben Glasspoole*
***REMAT Team**: Leah Appelhans, Ren Bean, Jacob Lessard, Jeff Moore*
***Pfizer Team**: Neal Sachs*
***Reisman Group (Cal-tech)**: Cedric Lozano*
***Sanford Group (Michigan)**: Jonathan Hall, Taylor Spiller*

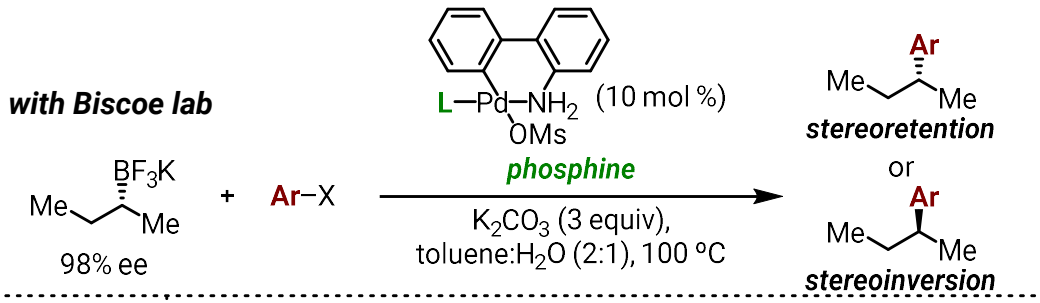
***Sigman Group**: Jamie Cadge, Aleria Garcia-Roca, **Tobias Gensch**, James Howard, Niharika Kaushik, Cian Kingston, Austin LeSuer, Jordan Liles, Tim McFadden, Zach Niemeyer, Ellyn Peters, Natalie Romer, Samantha Sloane, Sleight Smith*

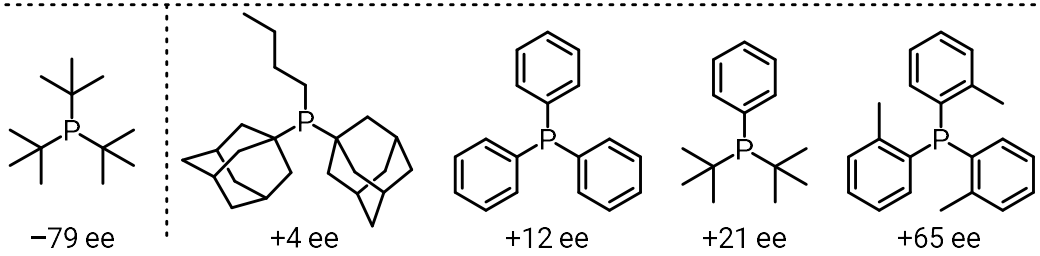
Genentech A Member of the Roche Group · abbvie · C-CAS Center for Computer Assisted Synthesis · MERCK · gsk GlaxoSmithKline · MilliporeSigma · REMAT · U.S. Department of Energy Office of Science

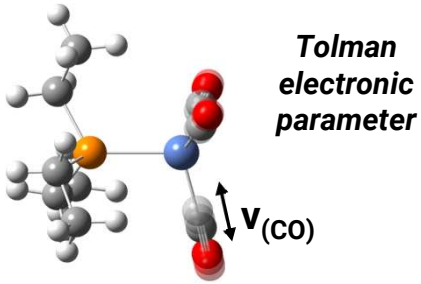
Backstory (2016): building predictive models for enantiospecific cross-coupling reactions

preliminary results from Biscoe lab

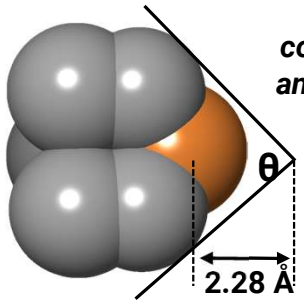
with Biscoe lab







Tolman electronic parameter

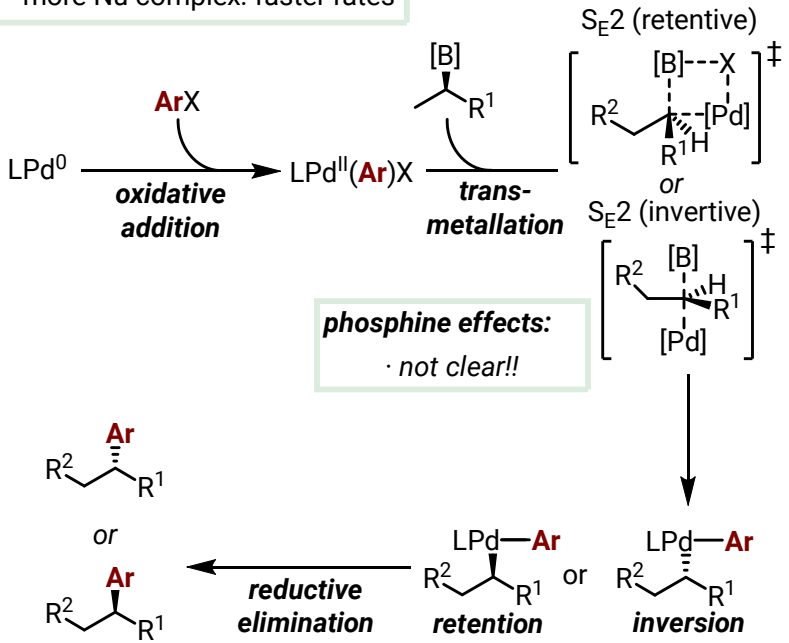


cone angle

Tolman *Chem. Rev.* **1977**, *77*, 313-348.
Fey *Organometallics* **2010**, *29*, 6245-6258.
Doyle *Nat. Chem.* **2017**, *9*, 779-784.

How does phosphine structure impact mechanism?

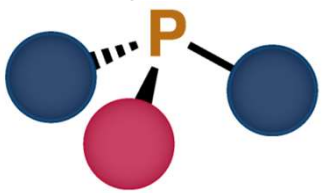
phosphine effects:
· speciation (LPd vs L_2Pd)
· more Nu complex: faster rates



phosphine effects:
· sterics: larger faster
· electronics: easier to reduce

Mechanism inspires inclusion of conformational info into descriptor database

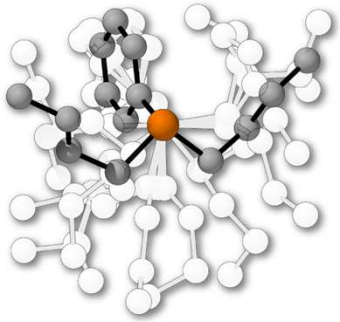
define ligands



1 558 P(III)-compounds

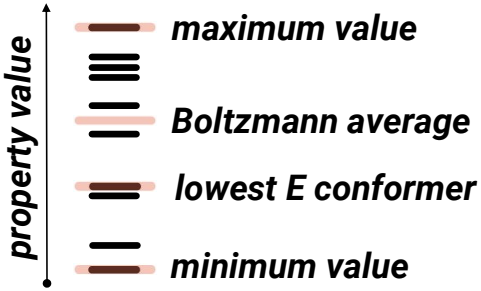
Descriptor libraries:
https://descriptor-libraries.molssi.org/

conformer ensembles



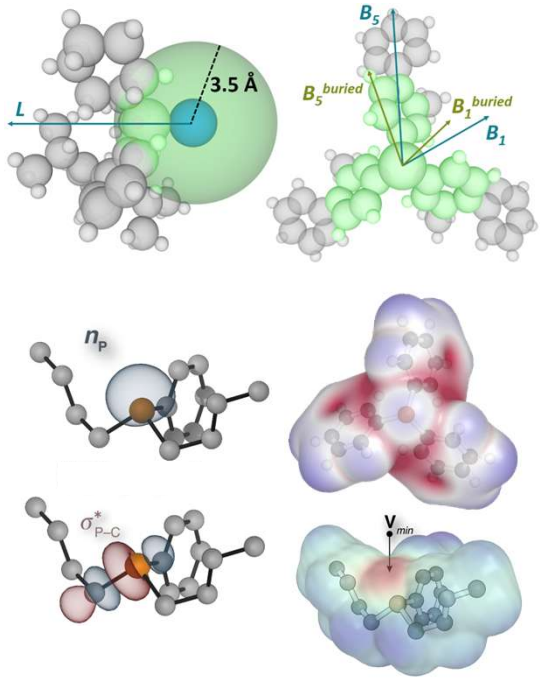
21,417 unique conformers
conformer search: *CREST, GFN2-xTB*

condensed properties capture distribution across ensemble



190 descriptors / ligand

ligand properties

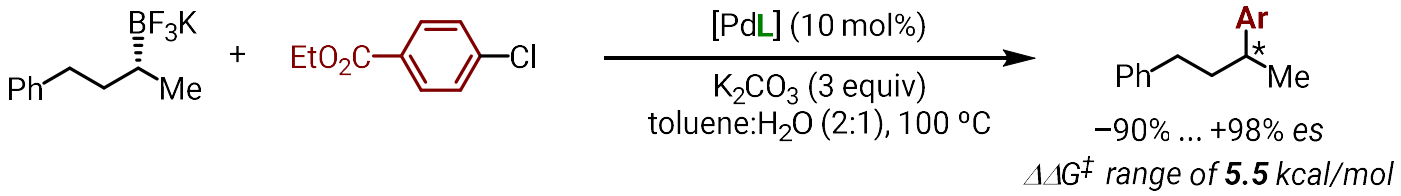


78 properties / conformer

geometry optimization
PBE-D3/6-31+G(d)
property calculation
PBE0-D3/def2-TZVP

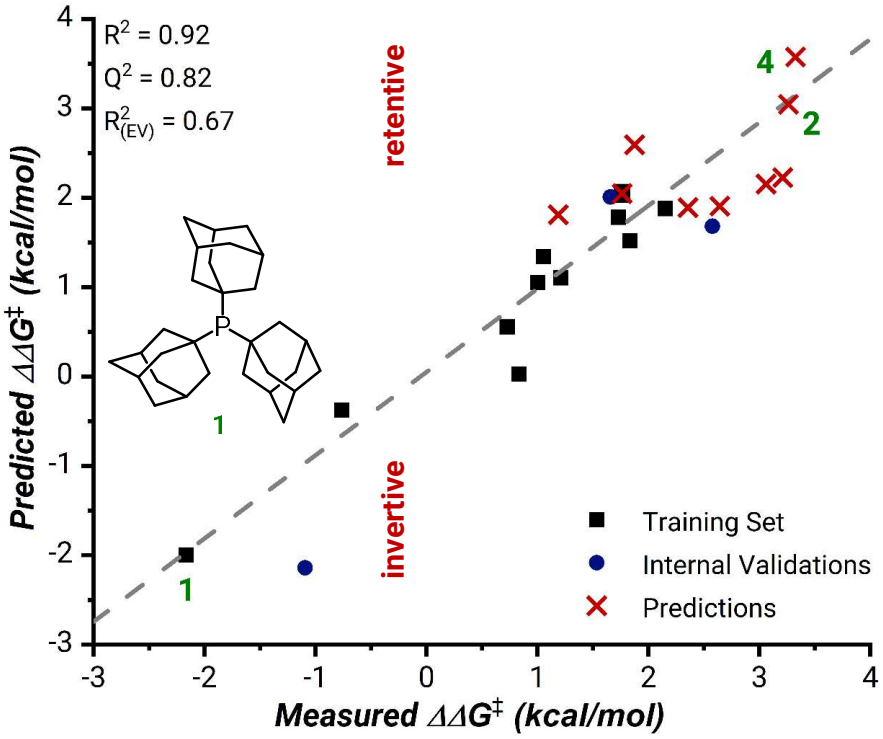
V1 (no conformers): Niemeyer, Z. L.; Milo, A.; Sigman, M. S. *Nature Chem.* **2016**, *8*, 610.
V2: Zhou, S.; **Gensch, T.**; Sigman, M.S.; Biscoe, M. *Science*, ***2018***, *362*, 670.
Kraken: Gensch, T.; dos Passos Gomes, G.; Friederich, P.; Peters, E.; Gaudin, T.; Pollice, R.; Jorner, K.; Nigam, A.; Lindner-D'Addario, M.; Sigman, M. S.; Aspuru-Guzik, A. *J. Am. Chem. Soc.* **2022**, *144*, 1205.

Proof of concept for database



Predictive model using an electronic feature

$$\Delta\Delta G^{\ddagger} = 1.5 + 0.62\, E_{\sigma^*(P-C)avg}{}^{Boltz} - 1.2\, E_{LP(P)}{}^{Boltz}$$

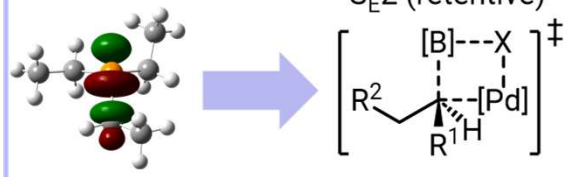


Mechanistic analysis

Electronics: Transmetallation

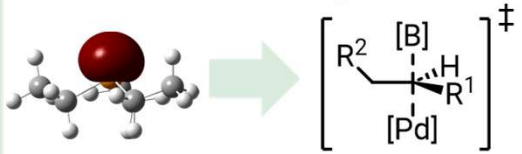
$E_{\sigma^*(P-C)avg}{}^{Boltz}$: *average energies of P–C antibonding orbitals*

related to π-back bonding



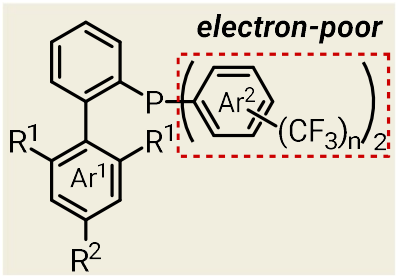
$E_{LP(P)}{}^{Boltz}$: *energy of the phosphorus lone pair orbital*

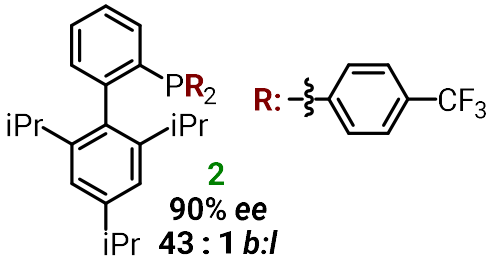
related to σ-donation



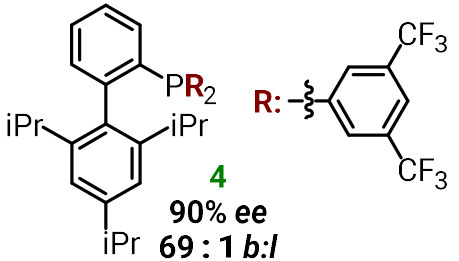
Zhou, S.; **Gensch, T.**; Sigman, M.S.; Biscoe, M. *Science*, ***2018***, *362*, 670.

extrapolations





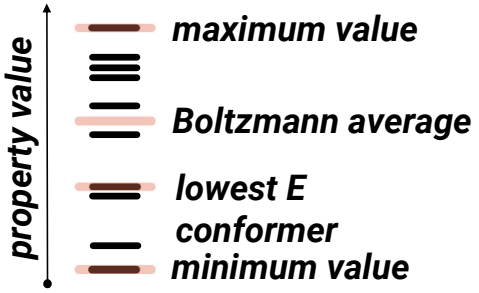
2
90% *ee*
43 : 1 *b:l*



4
90% *ee*
69 : 1 *b:l*

Uses of a large data base: training set design principles

condensed properties capture distribution across ensemble



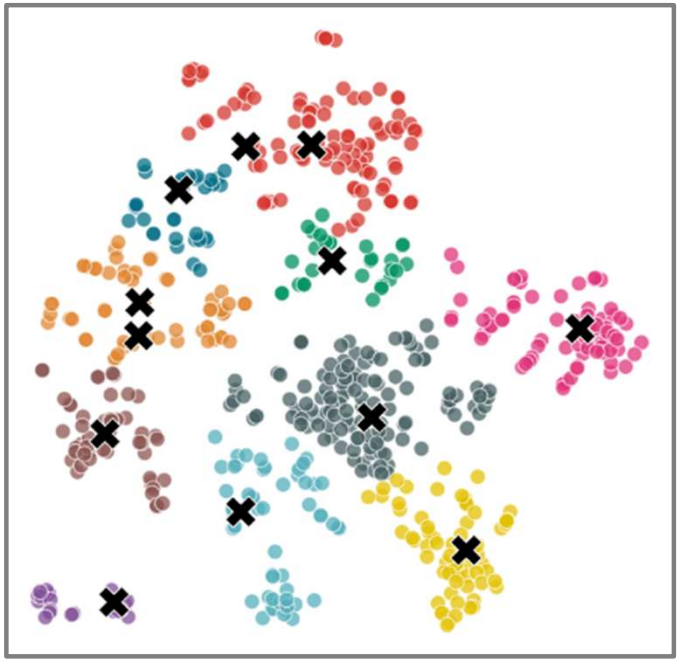
>1800 ligands
78 properties / conformer
190 descriptors / ligand
(300,000 in virtual ML library)

Step 1. *Dimensionality reduction (PCA, TSNE, UMAP)*



Step 2. *Clustering (hierarchical, k-means)*

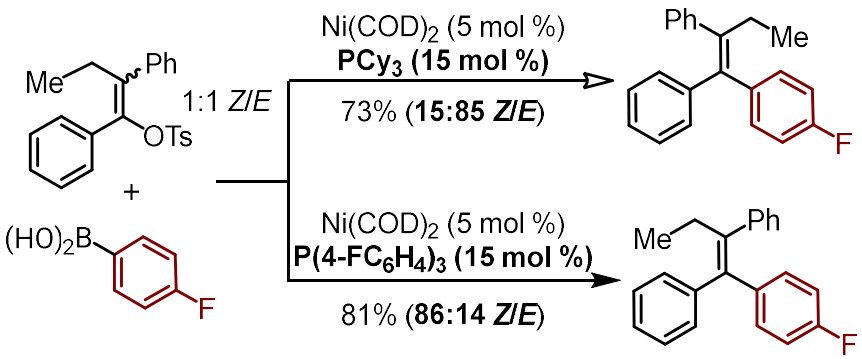
Step 3. *filter by commercial availability*



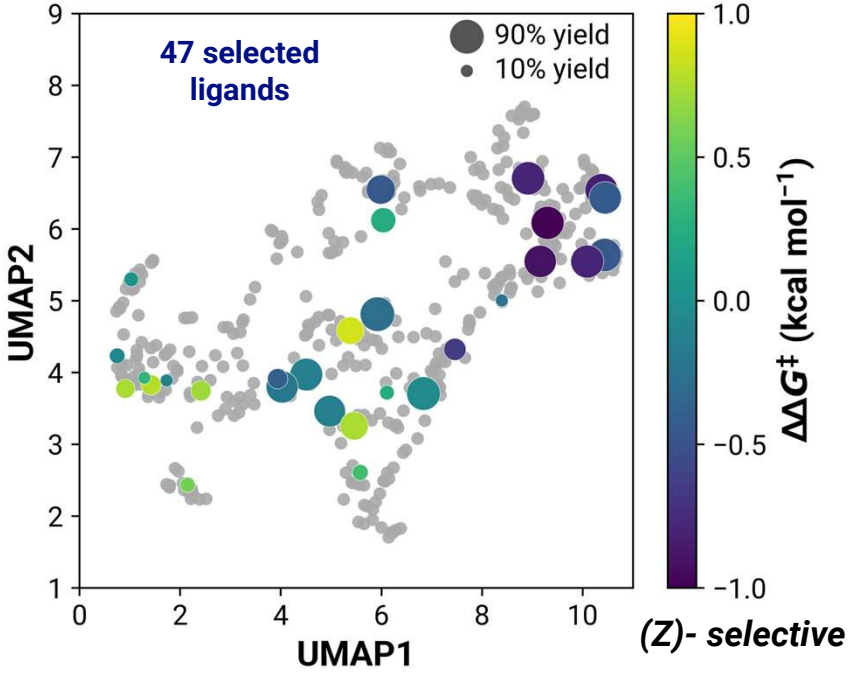
Select diverse examples for intentional data science applications (regression, classification)

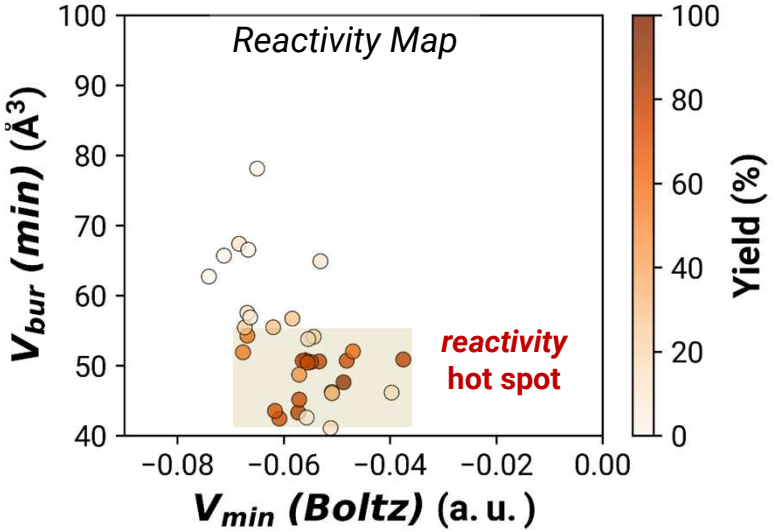
With Genentech: Zell, D.; Kingston, C.; Jermaks, J.; Smith, S. R.; Seeger, N.; Wassmer, J.; Sirois, L. E.; Han, C.; Zhang, H.; Gosselin, F. *JACS,* **2021**, *143*, 19078.
with Millipore - SigmaAldrich: Gensch, T.; Smith, S. R.; Colacot, T. J.; Timsina, Y.; Xu, G.; Glasspoole, B. W.; *ACS Catalysis*, **2022**, 12, 7773.
with GSK: Crawford, J. M.; Gensch, T.; Elward, J. M.; Steves, J. E. *Org. Process Res. Dev.* **2022**, *26,* 1115.
Review: Raghavan, P.; Haas, B. C.; Ruos, M. E.; Schleinitz, J.; Doyle, A. G.; Reisman, S. E.; Sigman, M. S.; Coley, C. W. *ACS Central Science* **2023**, *9*, 2196.
Recent approach with Bayesian optimization (ScopeBO): Roediger, S.; Sigman, M. S.; Doyle, A. G.; *J. Am. Chem. Soc.* **2026**, *128*, accepted.

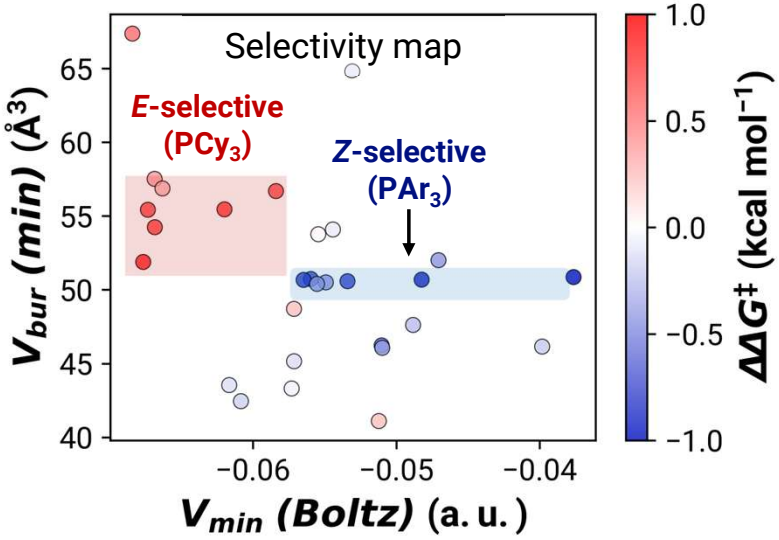
Using training set design to initiate and analyze experimental campaigns



Genentech
A Member of the Roche Group

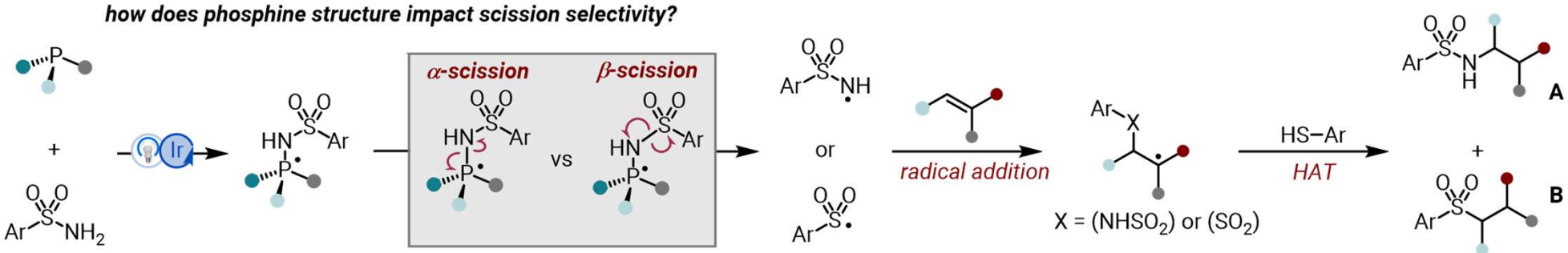


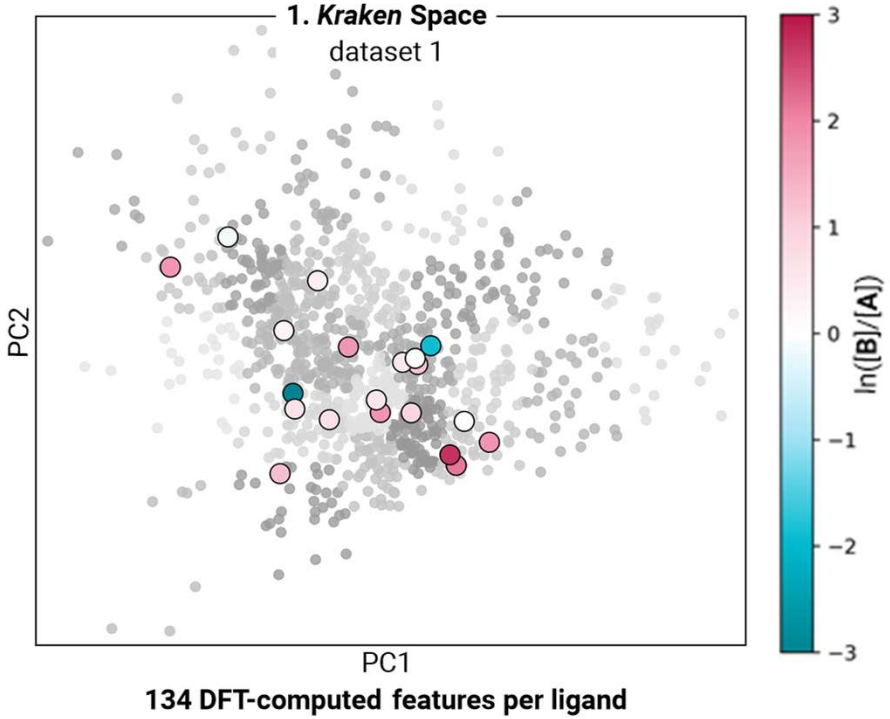




Zell, D.; Kingston, C.; Jermaks, J.; Smith, S. R.; Seeger, N.; Wassmer, J.; Sirois, L. E.; Han, C.; Zhang, H.; Gosselin, F.; Sigman, M. S. *JACS*, **2021**, *143*, 19078.

Using training set design to initiate analysis and active learning



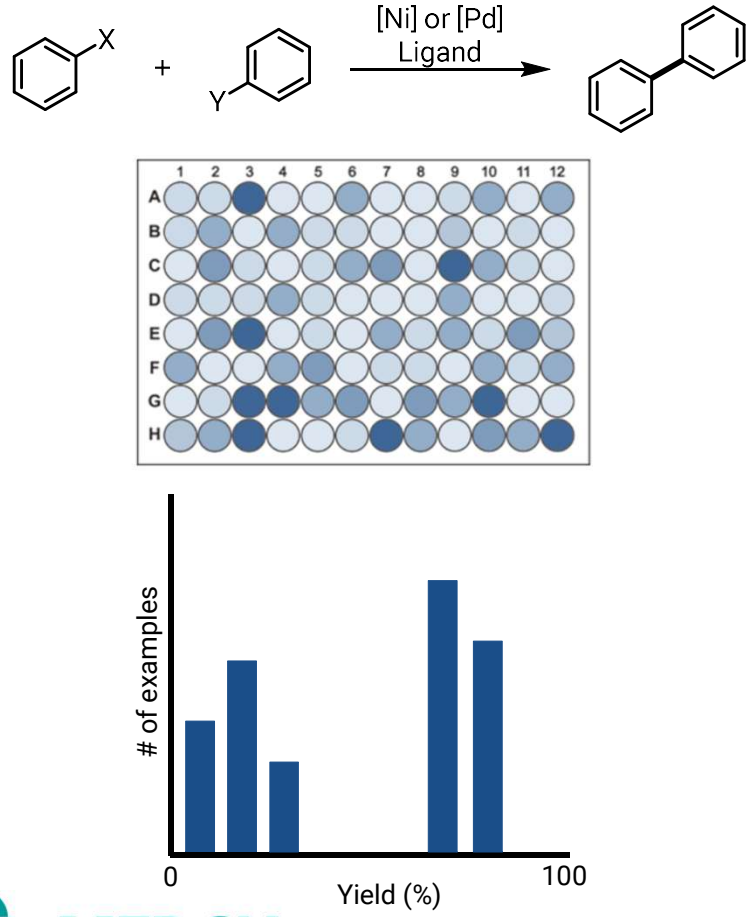


134 DFT-computed features per ligand

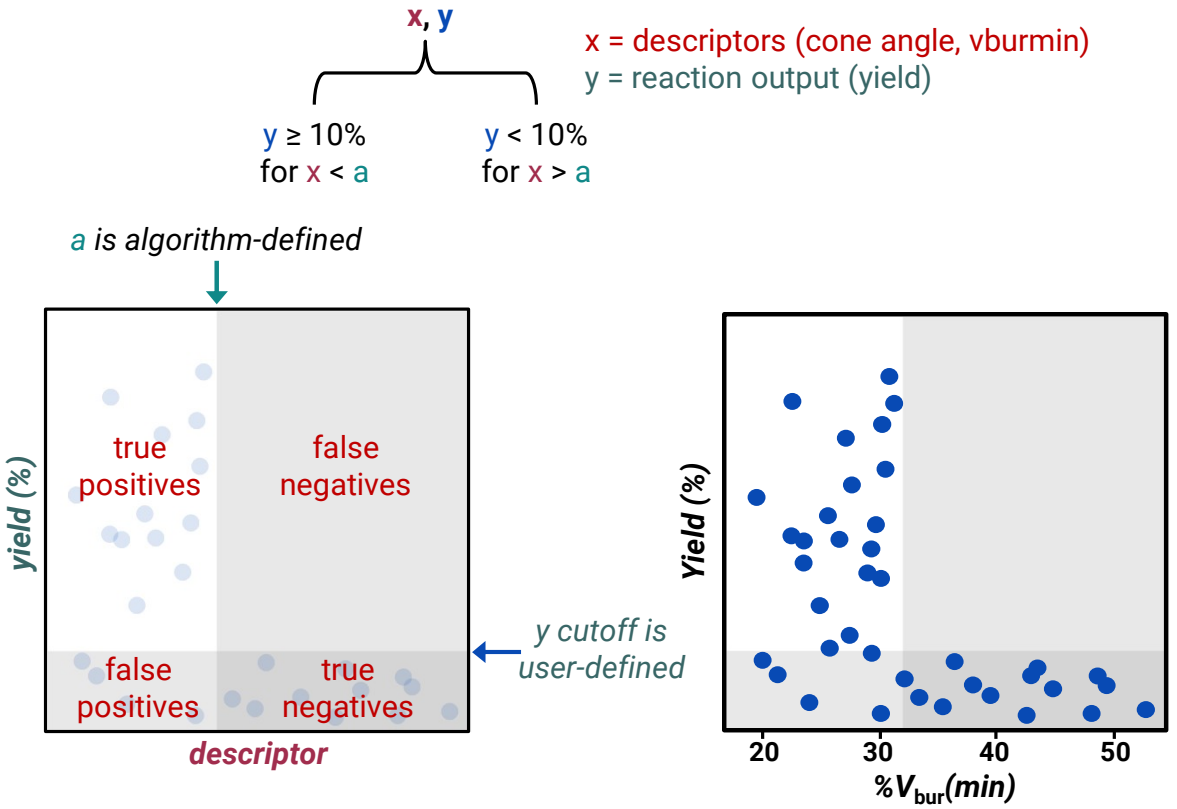
Wearing, E. R.; Kaushik, N. P.; Hugie, S. T.; Sigman, M. S.; Doyle, A. G. *J. Am. Chem. Soc.* **2026**, *148*, 37121–37133

Using kraken to analyze reactivity: classification and mechanistic tools

binned data from HTE



classification of poor performers: reactivity cliff/threshold

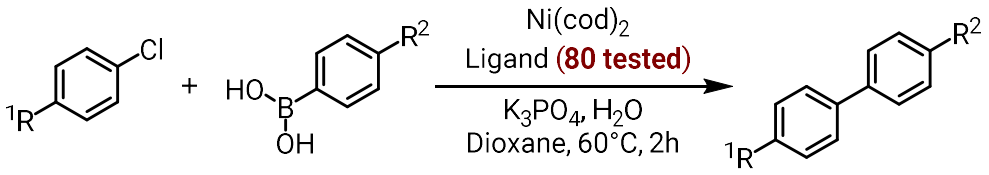


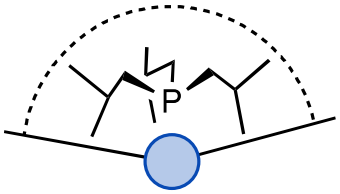
MERCK

Newman-Stonebraker, S.H.; Smith, S.R.; Borowski, J.E.; Peters, E.; Gensch, T.; Johnson, H.C.; Sigman, M.S.; Doyle, A.G. *Science*, **2021**, *374*, 301.

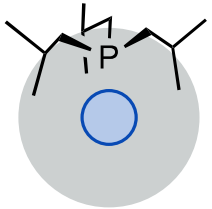
"**Double threshold**": LeSueur, A.; Tao, N.; Doyle, A.; Sigman, M. S. *Eur. J. Org. Chem* **2024**, *27*, e202400428.

Features matter - kraken descriptors are key

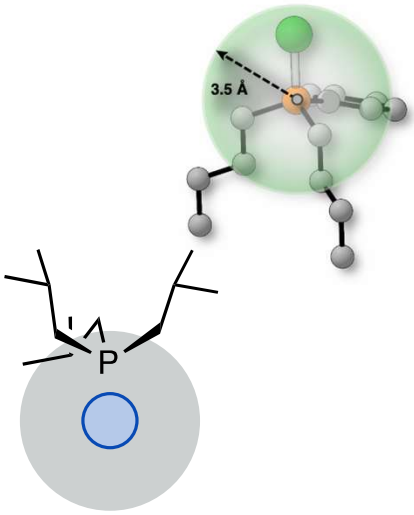




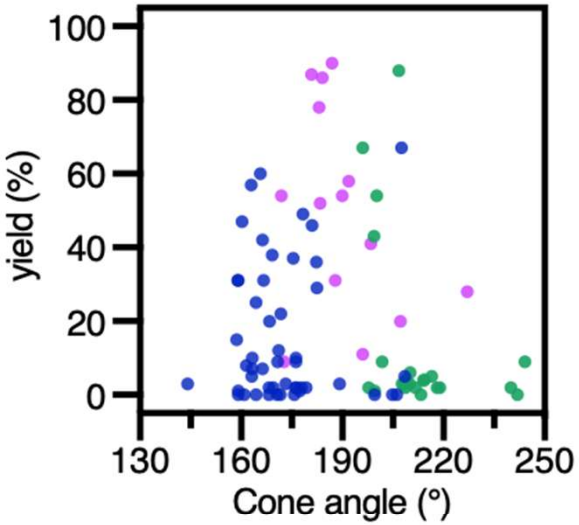
Cone angle

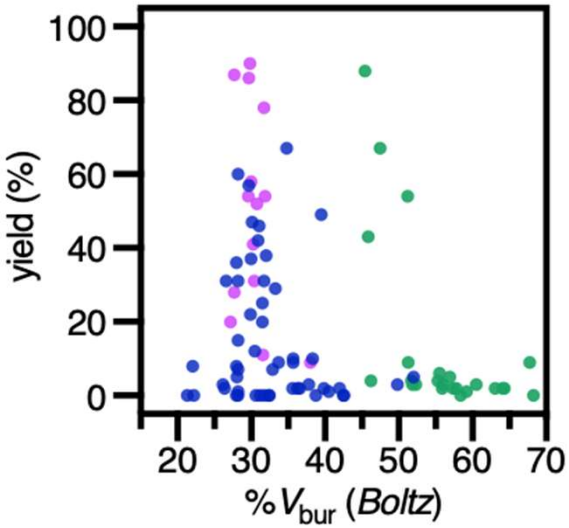


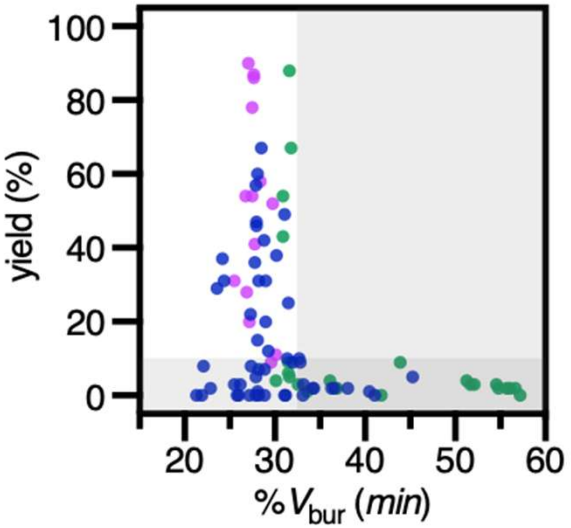
%V$_{bur}$ (Boltz)



%V$_{bur}$ (min)

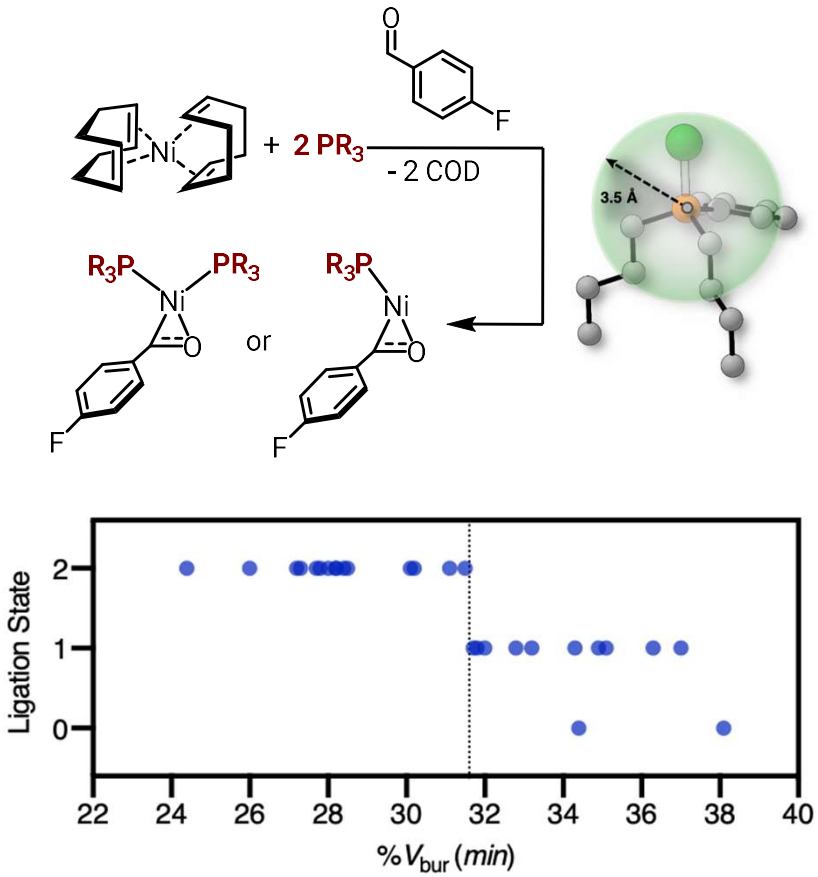


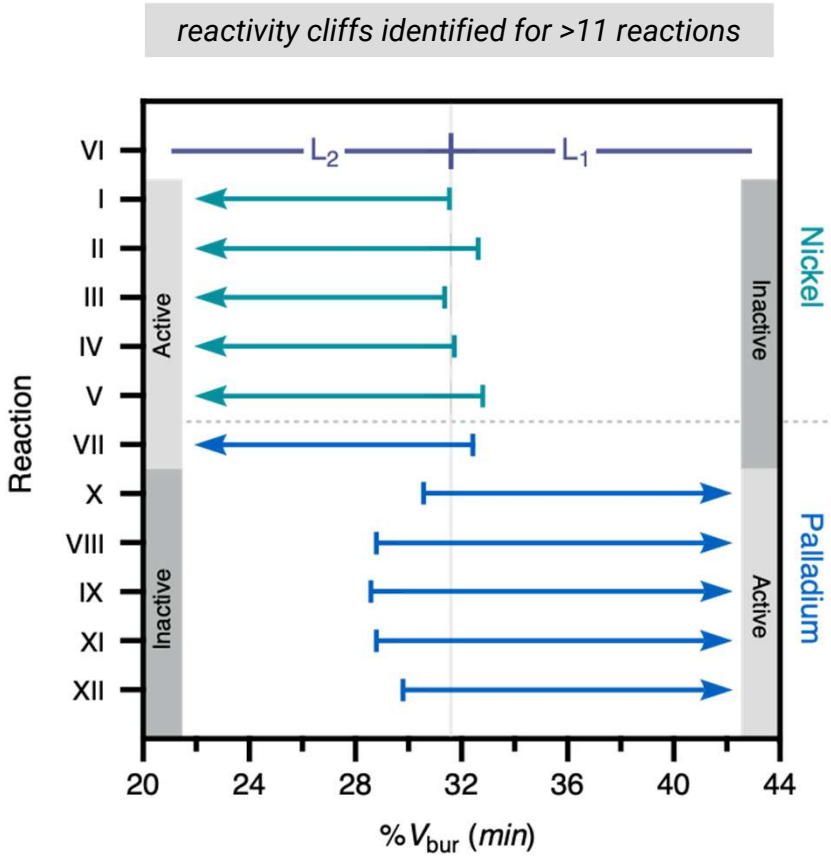




DinoPhos-type Buchwald-type All others

Mechanistic analysis & broad assessment

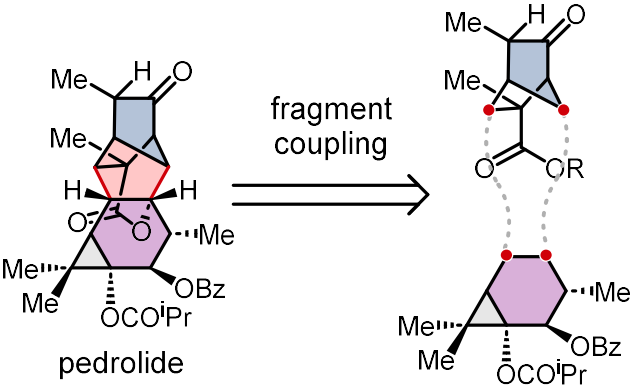




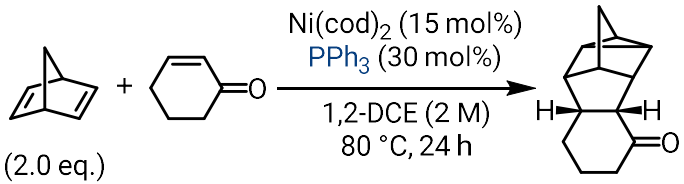
Newman-Stonebraker, S.H.; Smith, S.R.; Borowski, J.E.; Peters, E.; Gensch, T.; Johnson, H.C.; Sigman, M.S.; Doyle, A.G. *Science*, **2021**, *374*, 301.

Using kraken to warm starting an old reaction

Reisman disconnection strategy



homo-Diels-Alder strategy to core

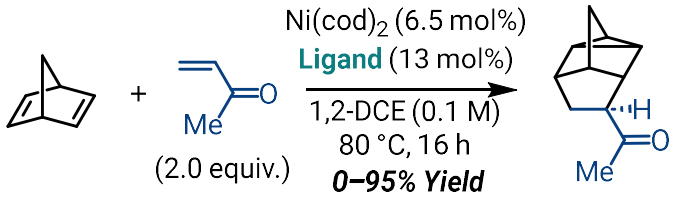


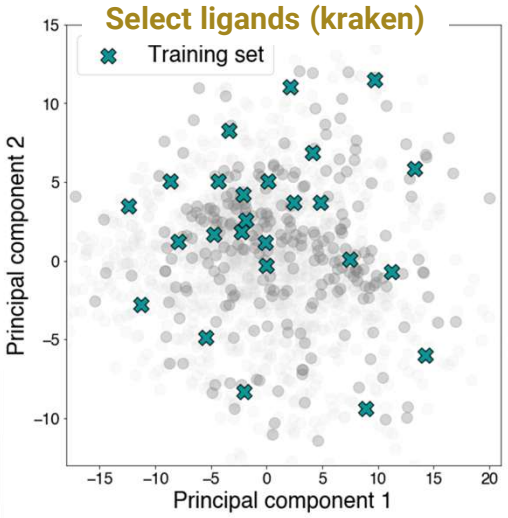
Lautens *et al. J. Am. Chem. Soc.* **1995**, *117*, 10276

Objectives:

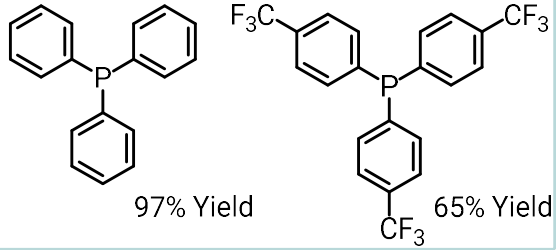
- *improve yield*
- *identify enantioselective rxns*

data science guided approach to ligand discovery

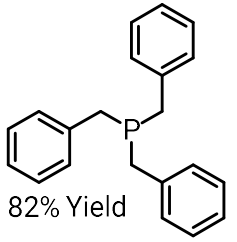




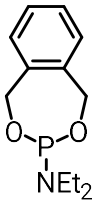
triaryl phosphines



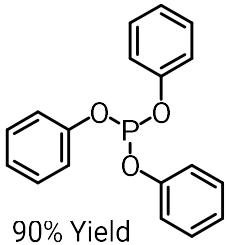
trialkyl phosphines



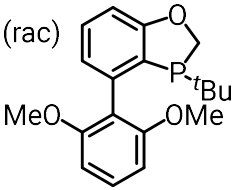
phosphoramidite



phosphites



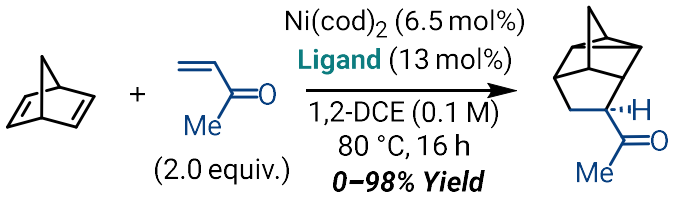
BiDIME ligands



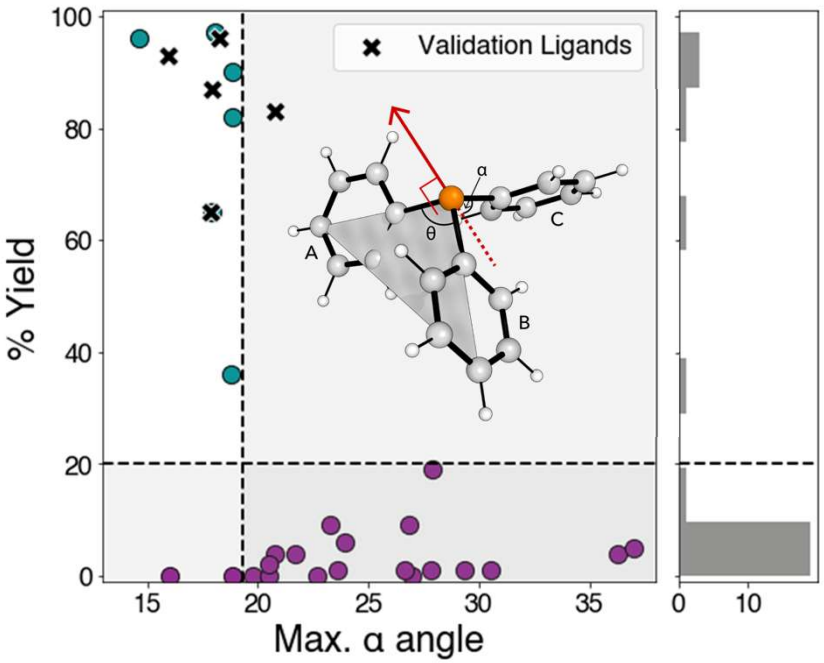
>15 phosphines gave less than 20% yield

Jamie Cadge, Cedric Lozano, Sarah Reisman

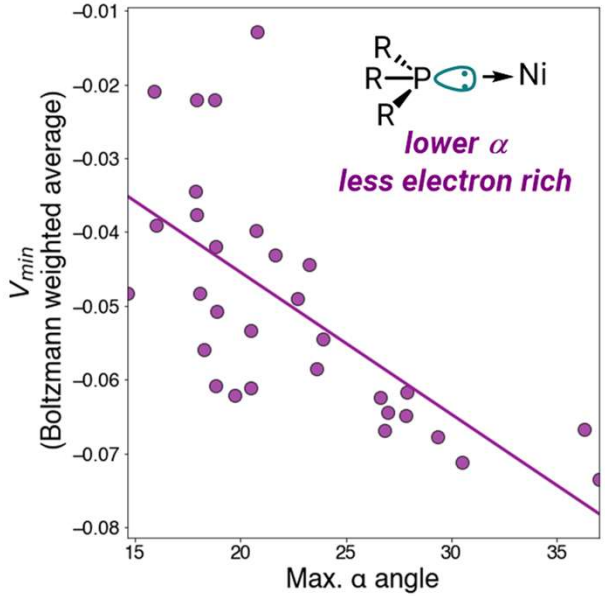
Using classifiers to design and understand diverse phosphine performance

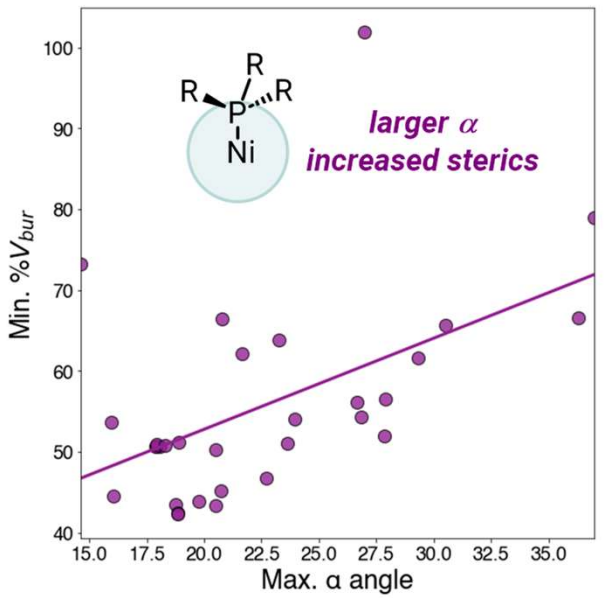


yield classification (20%)



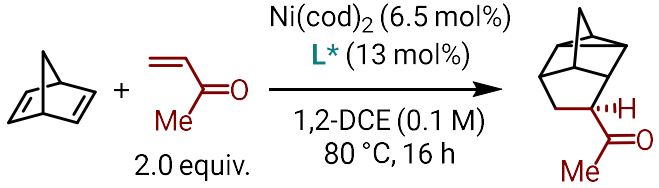
understanding ligand pyramidalization descriptor

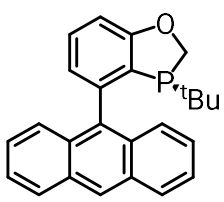




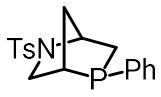
Data set design and classifier facilitates enantioselective catalyst discovery

ligand screen informed from classifier

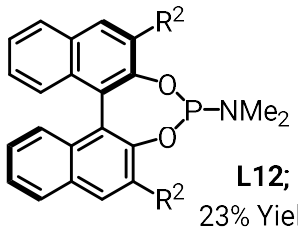




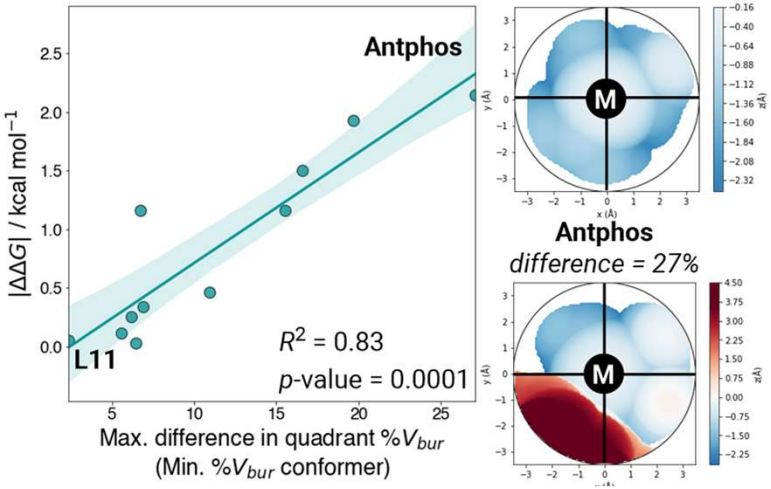
Antphos
95% Yield,
91% *ee*



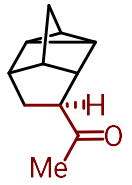
L11
69% Yield
4% *ee*



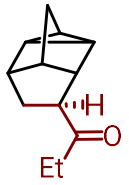
L12; R^2 = H;
23% Yield, 68% *ee*
L13; R^2 = Me;
99% Yield, 8% *ee*



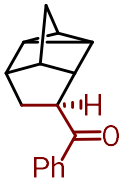
selected scope



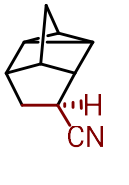
99% Yield
>20:1 *exo*:*endo*
94% *ee*



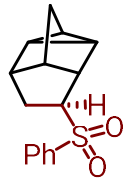
75% Yield
10:1 *exo*:*endo*
exo: 90% *ee*;
endo: 70% *ee*



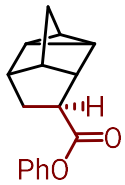
65% Yield
20:1 *exo*:*endo*
88% *ee*



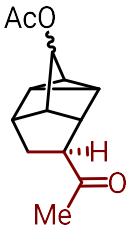
91% Yield
20:1 *exo*:*endo*
93% *ee*



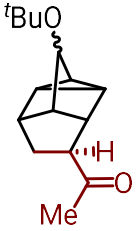
81% Yield
10:1 *exo*:*endo*
exo: 90% *ee*;
endo: 33% *ee*



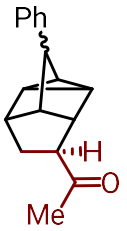
71% Yield
20:1 *exo*:*endo*
74% *ee*



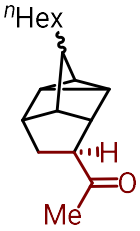
62% Yield
4.5:1 *dr*
20:1 *exo*:*endo*
91% *ee*



71% Yield
20:1 *dr*
20:1 *exo*:*endo*
70% *ee*



73% yield
1.2:1 *dr*
20:1 *exo*:*endo*
82% *ee*

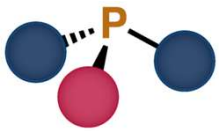


75% yield
1:1 *dr*
10:1
exo:*endo*
40% *ee*

Cadge, J. A.; Lozano, C.; Merriman, M. T.; Oblad, P.; Sigman, M. S.; Reisman, S. E. *J. Am. Chem. Soc.* **2025**, *147*, 31175–31186.

Feature libraries and training sets (evolving)

monophosphines



>1700 compounds
190 descriptors
>300,000 ML virtual library

JACS **2022**, *144*, 1205-1217
TS: *ACS Catalysis*, **2022**, 12, 7773
OPRD **2022**, *26*, 1115
kraken

bisphosphines



>700 compounds
>300 descriptors

w/Genentech
JACS **2023**, *145*, 110
TS: *JACS* **2023,** *145*, *20959*
V2: *Chem. Sci.* **2025,** *16*, 20473
V3: *update coming soon*

P,N-ligands



>400 compounds
>300 descriptors

manuscript in prep
(Sierra Hart, Bayer)

N,N-ligands



>1200 compounds
bipy, box, biox, pyrox, etc.
>300 descriptors

(w/ Doyle & Reisman)
ACS Catal., **2026**, *16*, *11532*
BUNNY

open access libraries

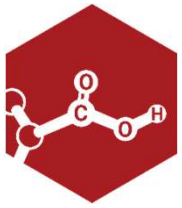
https://descriptor-libraries.molssi.org/

amines



4272/3849
primary/secondary amines
170/145 descriptors

carboxylic acids



8528 compounds
275 descriptors

PNAS **2022**, 119, e2118451119
ML descriptor prediction tool:
Digit. Discov. **2025**, *4*, 222
w/ Coley & Paton

aryl halides



>11000 compounds
>100 descriptors

w/Doyle
JACS ***2023***,*145*, *20959*
V2: *update coming soon*

sulfonyl fluorides



3600 compounds
>250 descriptors

w/Doyle & Genentech
JACS ***2025***,*147*, 25815

quinones



592 compounds
88 descriptors

w/Kwabi
ACS Energy Lett.
2026, *11*, 5227

sulfonates

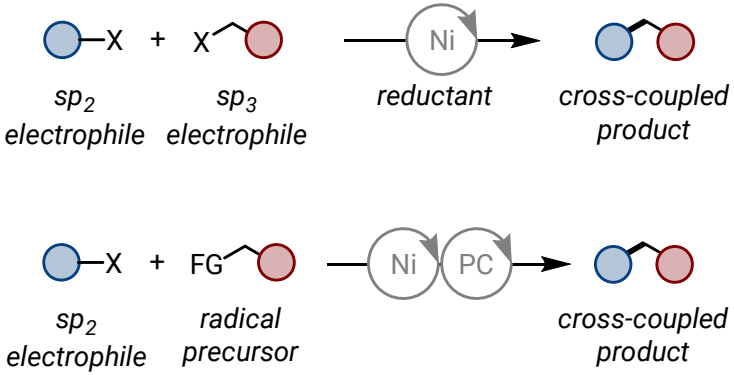


722 compounds
288 descriptors

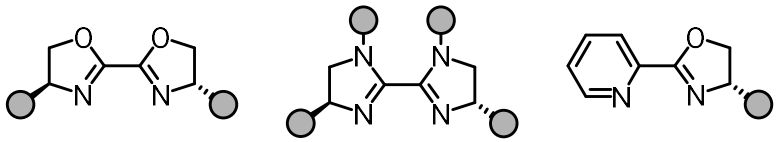
w/Bischak group
JACS **2026**, *148*, *20611*

Developing Ni-catalyzed cross-coupling reactions – challenges and questions

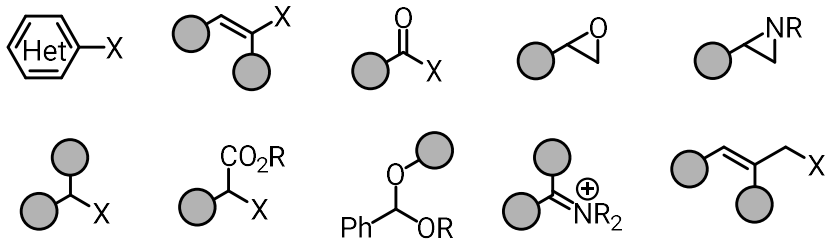
so many reactions, so many optimizations, so little data



many ligands



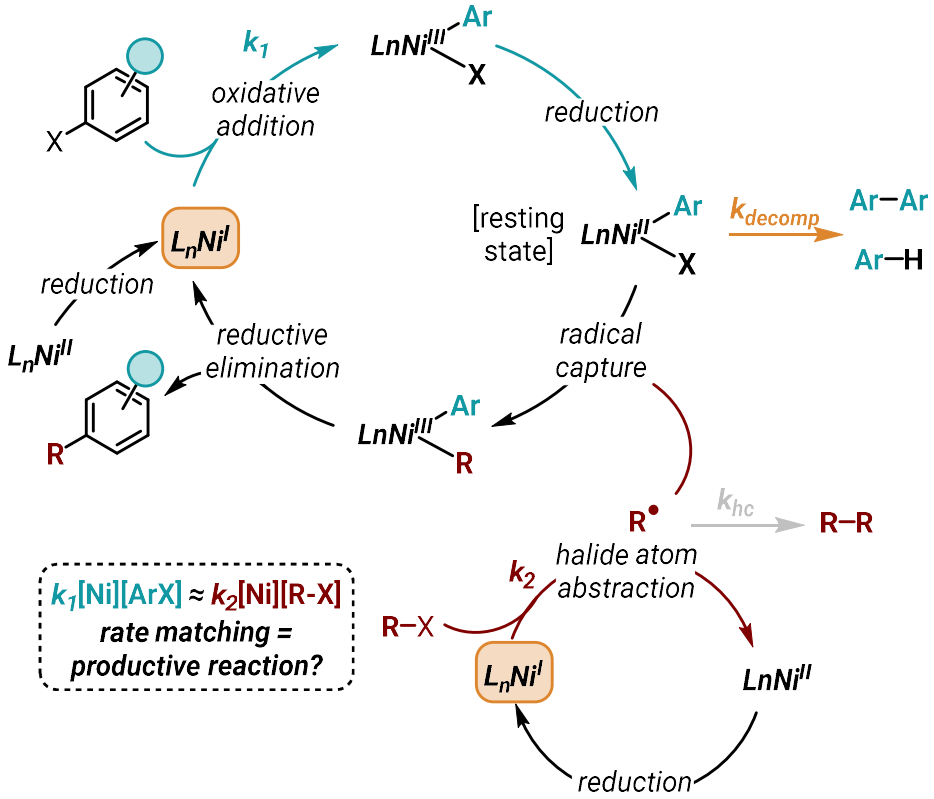
many coupling partners



Cross-electrophile coupling

Baran, Doyle, Minteer, Reisman, Weix and many others

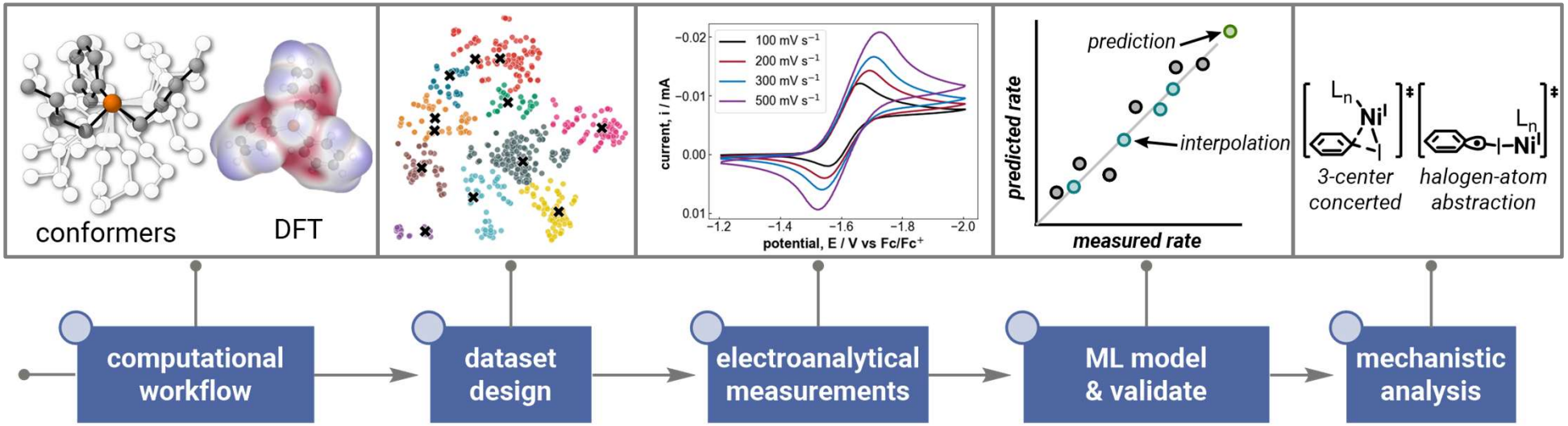
mechanistic complexities



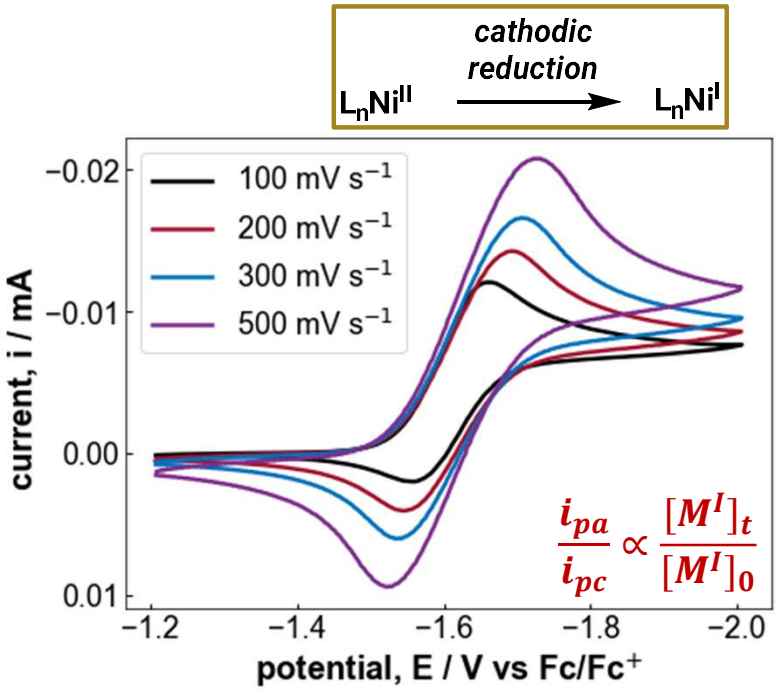
Questions:

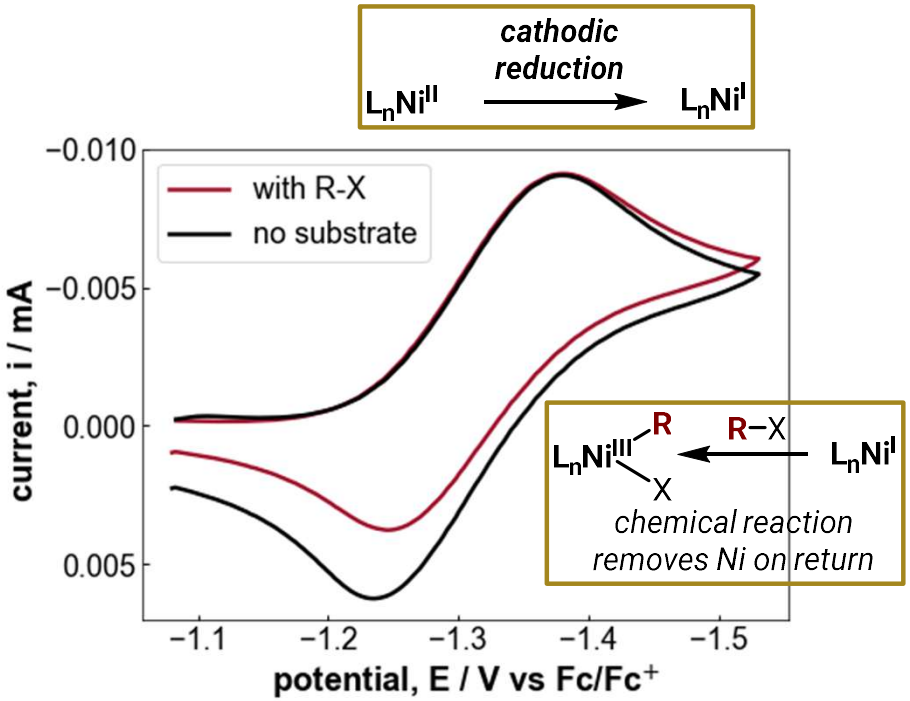
- *What is the mechanism of Ni(I) oxidative addition of aryl electrophiles?*
- *Can we build a catalyst/substrate rate predictors?*
- *Can we understand "rate matching" through predictive modeling?*

Proposed workflow



Key electroanalytical tool: peak ratio analysis to determine relative rates





Advantages:

- fast measurement of *relative rates (up to 10-20 per day)*
- *In-situ generation of low valent metal species*

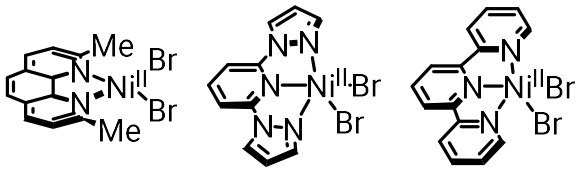
Limitations

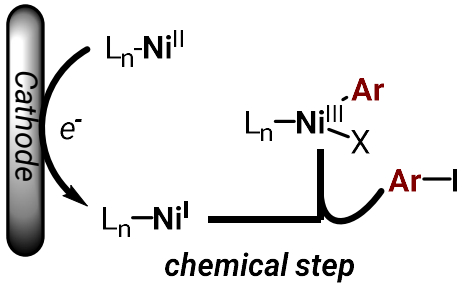
- *generally well-behaved CV required*
- *relies on many assumptions (relative k best result)*

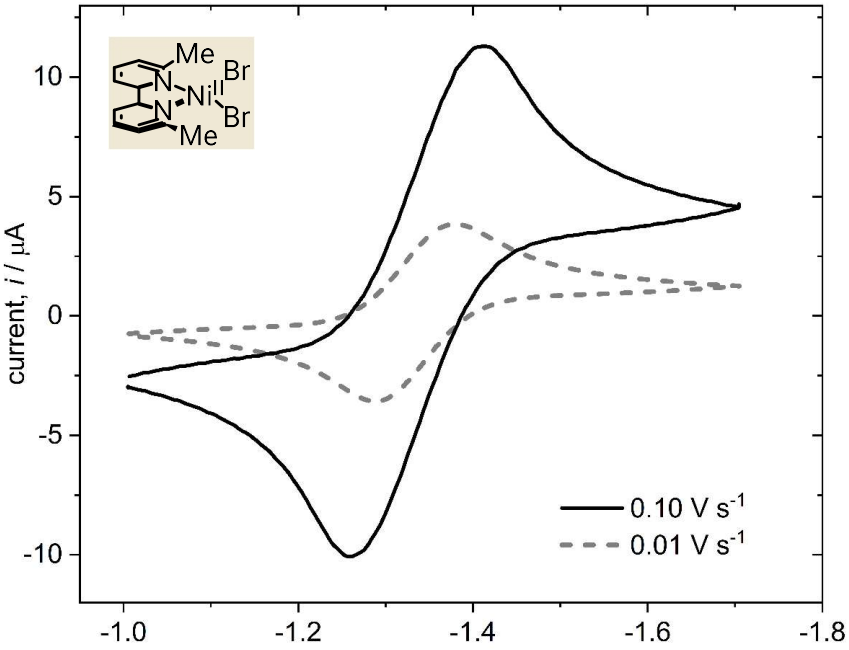
Hickey, D. P.; Sandford, C; Rhodes, Z; Gensch, T; Fries, L. R.; Sigman, M. S.; Minteer, S. D. *J. Am. Chem. Soc.* **2019**, *141*, 3, 1382-1392

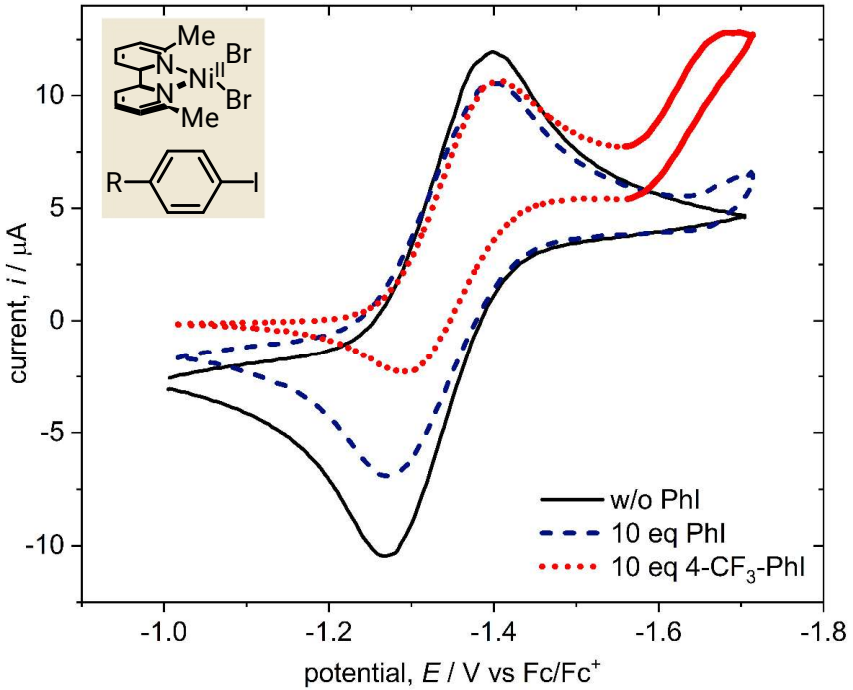
Examples of use: J. Am. Chem. Soc. **2019**, 141¸ 18877-18889; *Chem. Sci.* **2021**, 4771; *Eur. J. Org. Chem.* **2022**. doi.org/10.1002/ejoc.202200064; *J. Am. Chem. Soc.* **2022**, *143*, 20056; with Sheng,*,[1] Sun,[1] …, Liu* *Nat. Commun.* **2024**, *15*, 2781 (**autonomously**).

Identification of reported, CV reliable Ni-complexes



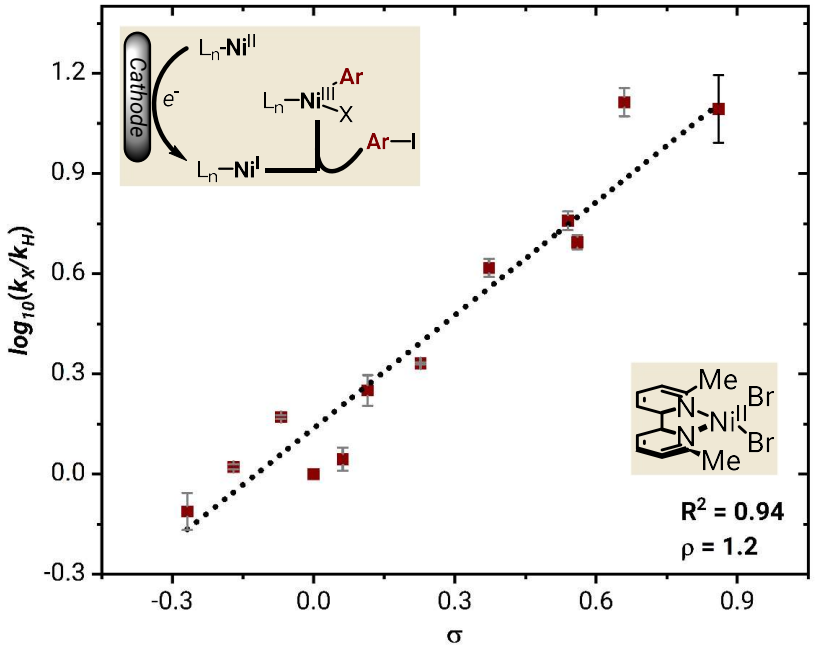


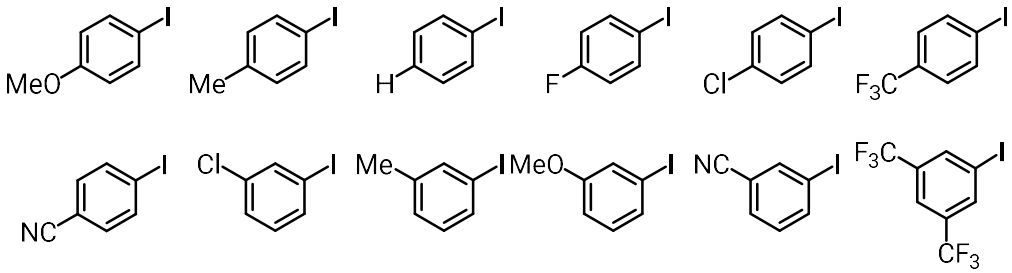




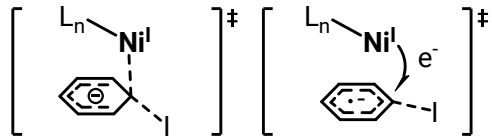
Initiate with Hammett study

Hammett plot and mechanistic proposal



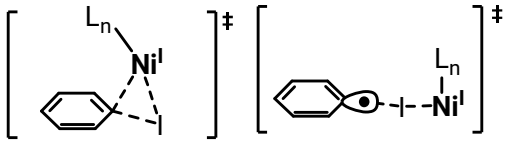


previous Hammett studies



S_NAr *Sinlge-electron transfer*

ρ ~ **4**



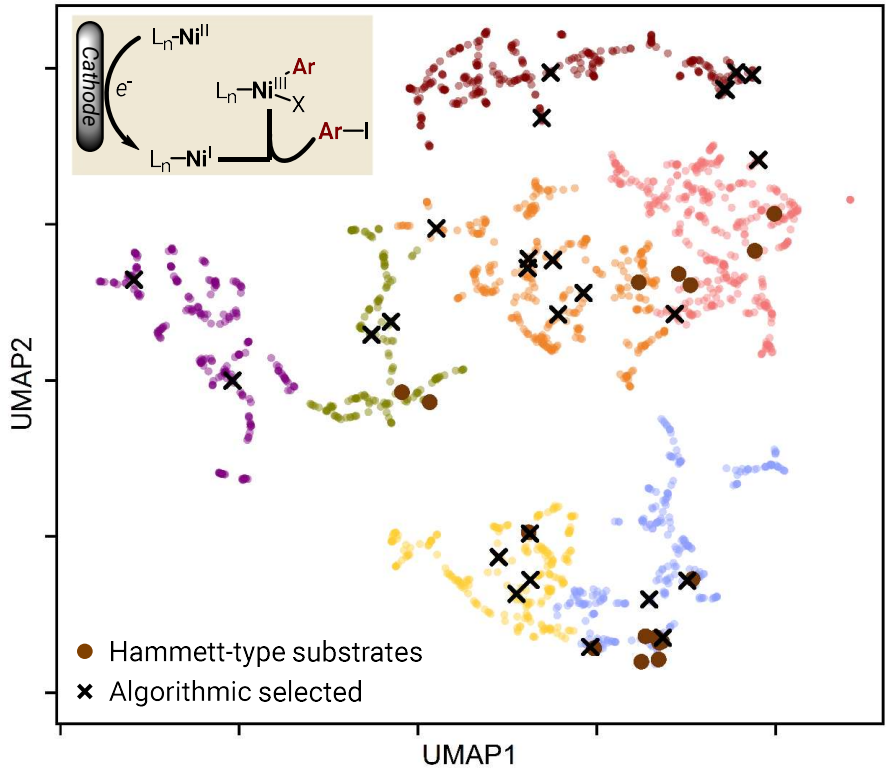
3-center concerted *Halogen-atom abstraction*

ρ ~ **1**

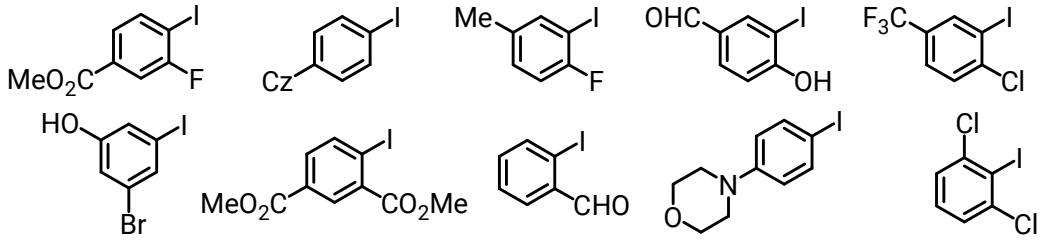
MacMillan, D. W. C. and coworkers *J. Am. Chem. Soc.* **2021**, *143*, 9332–9337.
Ting, S. I.; Williams, W. L.; Doyle, A. G. *J. Am. Chem. Soc*. **2022**, 5575.

Algorithmic selection of scope (beyond Hammett) and statistical model

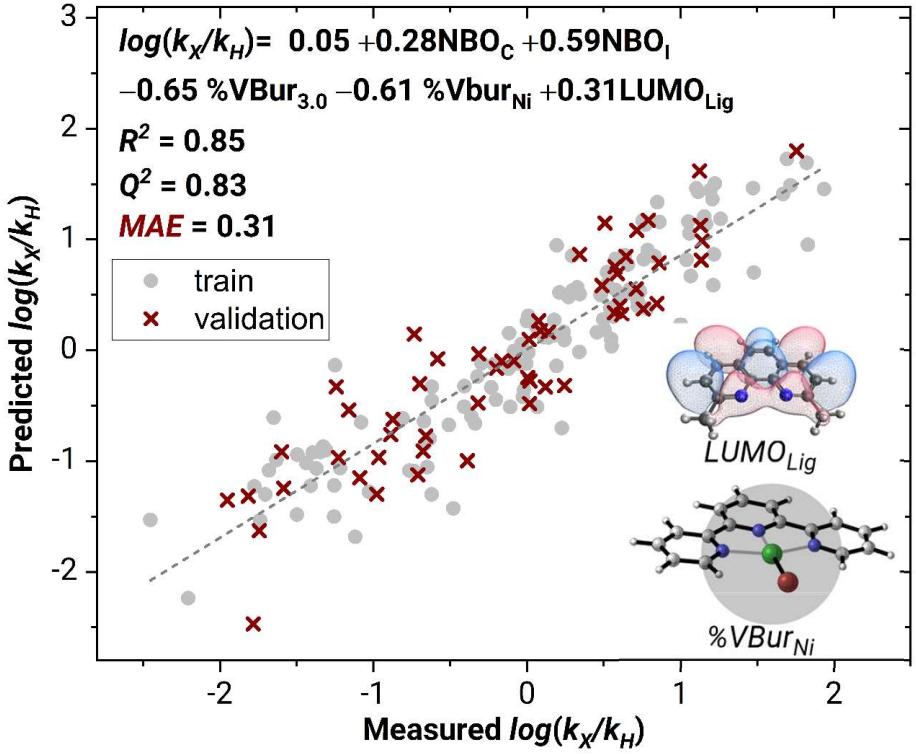
chemical space informed substrate expansion

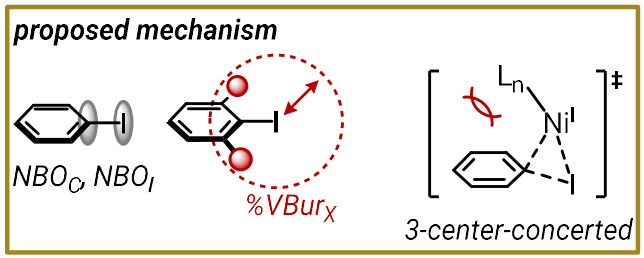


examples



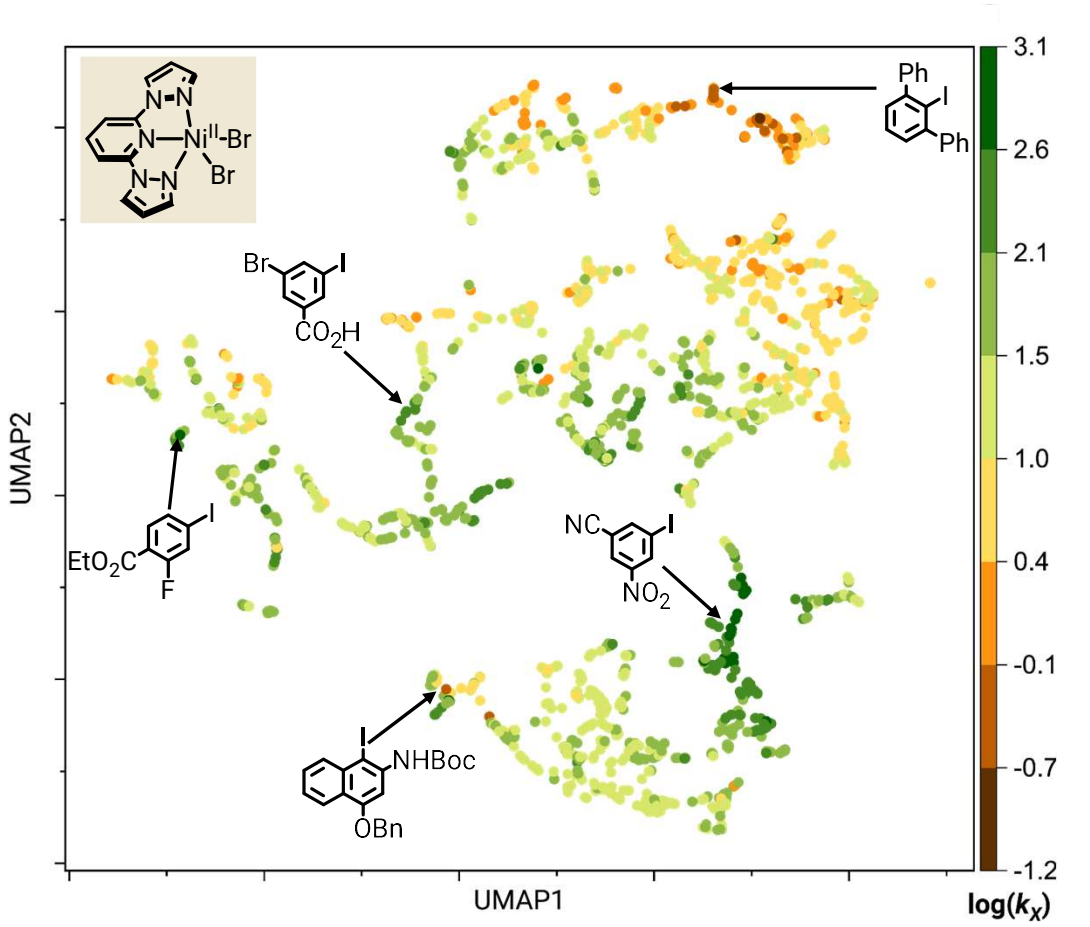
MLR model (12 catalysts and 59 substrates)



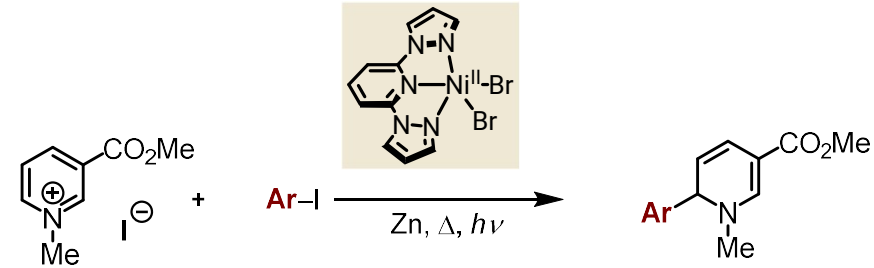


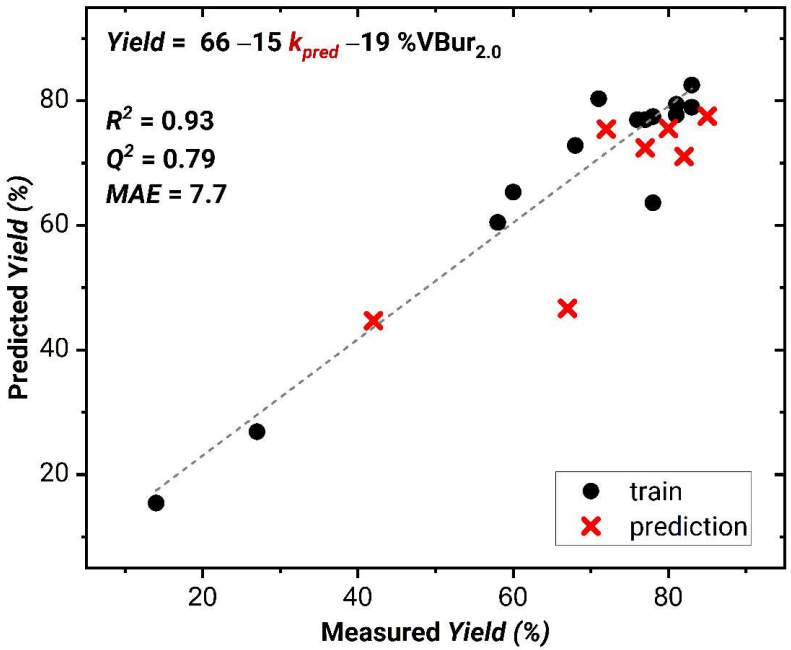
Using these correlations to predict rates of unseen substrates

heat map of predicted rates for aryl iodide oxidative addition



use for yield prediction of a new reaction

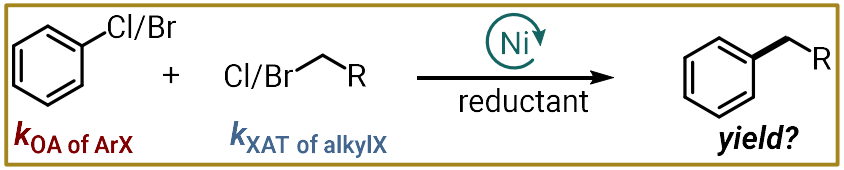




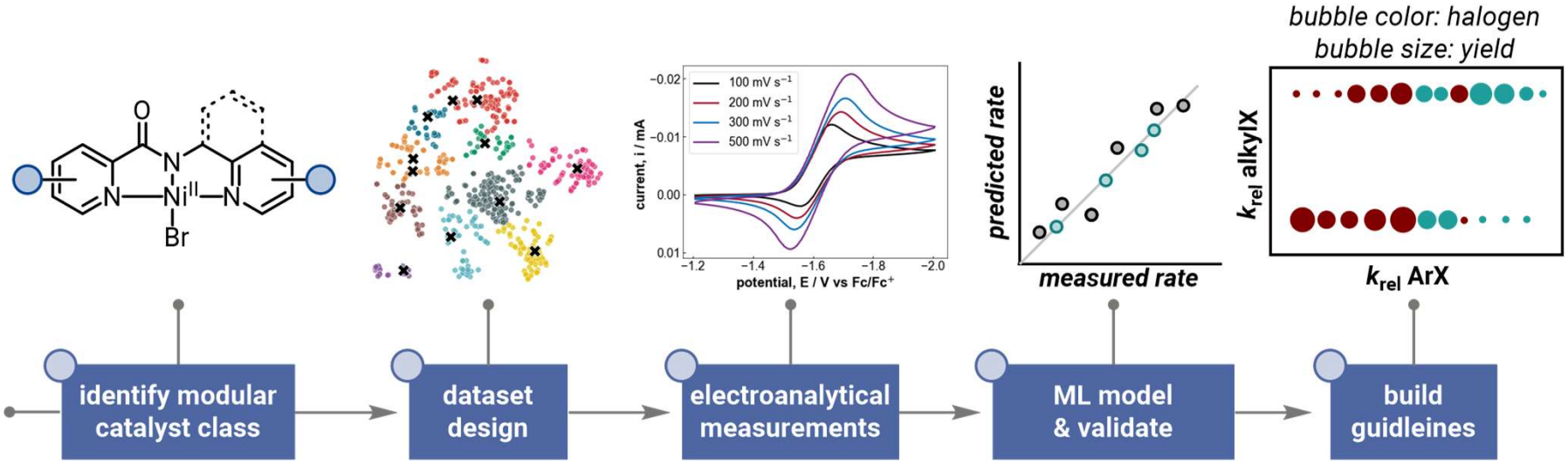
Nallagonda, R.; Musaev, D. G.; Karimov, R. R *ACS Catal*. **2022**, *12*, 1818–1829.

Tang, T.; Hazra, A. ; Min, D.; Williams, W.; Jones, E.; Doyle, A. G.; Sigman, M. S. *J. Am. Chem. Soc.* **2023**, 145, 8689–8699.

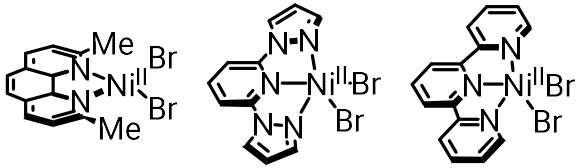
Building guidelines for "rate matching" and reaction discovery in reductive coupling

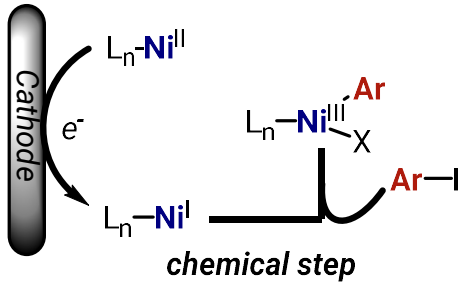


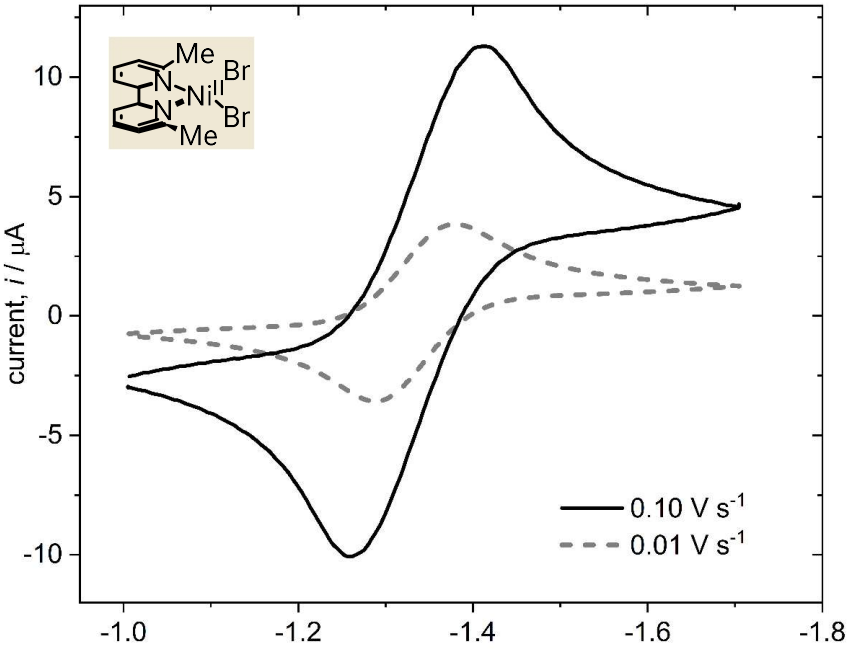
Can catalysts or halide identity be predictively used to enhance cross-electrophile coupling efficiency?
Can we use microscopic rates to inform this decision?
***Interesting synthetic question**: can we achieve alkylCl/arylCl coupling?*

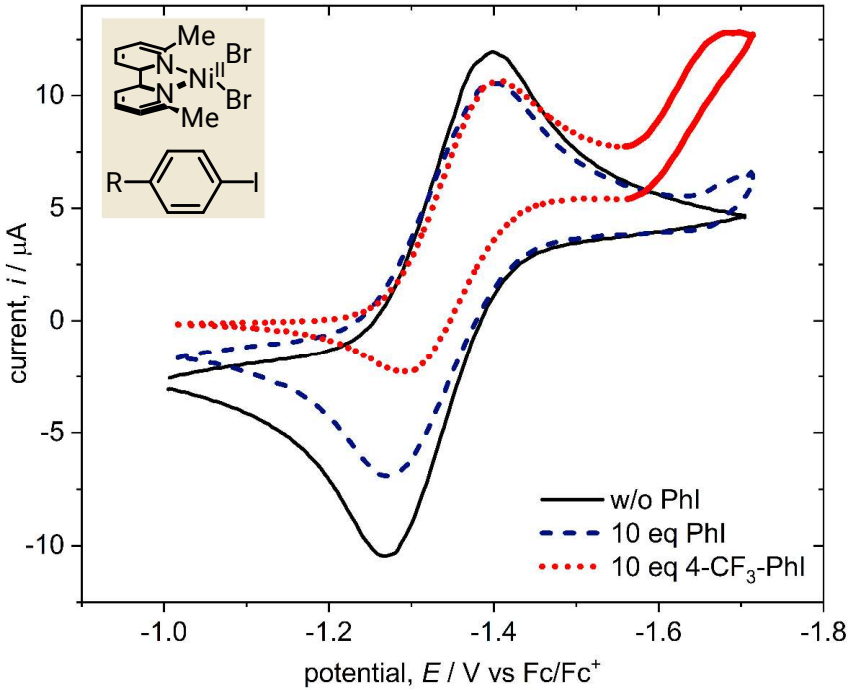


Identification of reported, CV reliable Ni-complexes



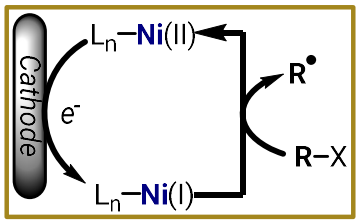


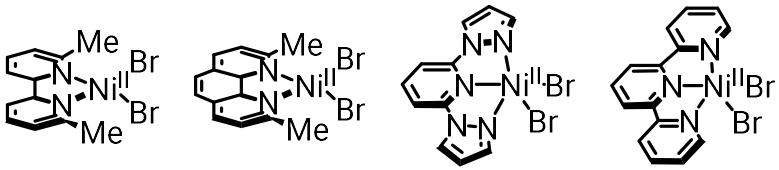


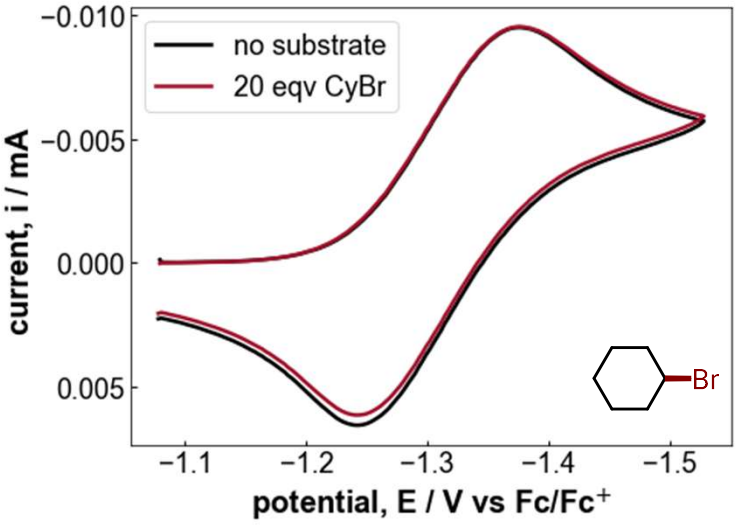


Inspiration for new catalyst design – multidentate anionic ligands

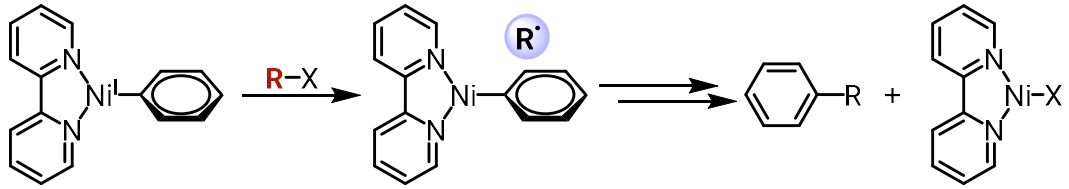
some unreactive complexes with alkyl bromides







design of modular ligand sets for electroanalytical workflow

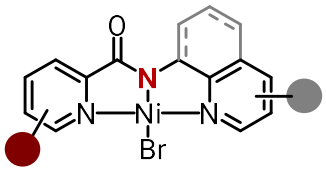


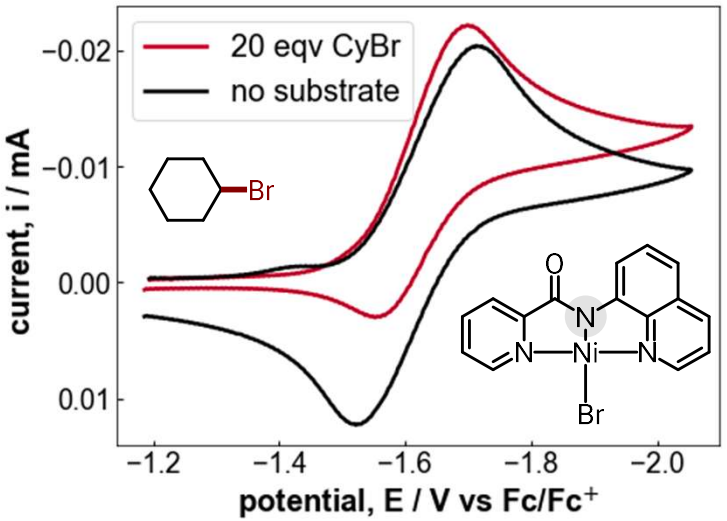
Can anionic complexes act as XAT mediators?

possible intermediate

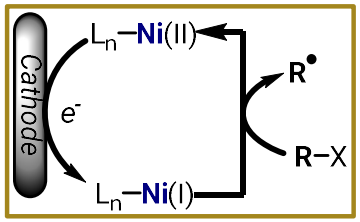
Peters, Diao, Sevov, Weix, others

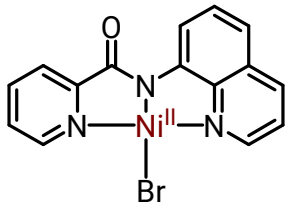
Modular tridentate monoanionic ligand

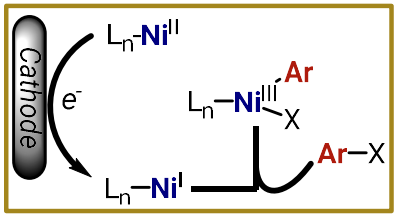


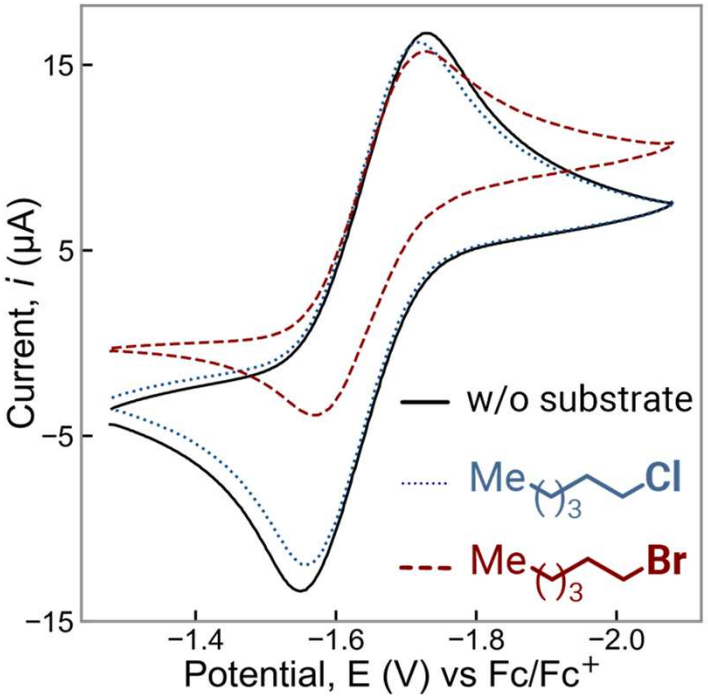


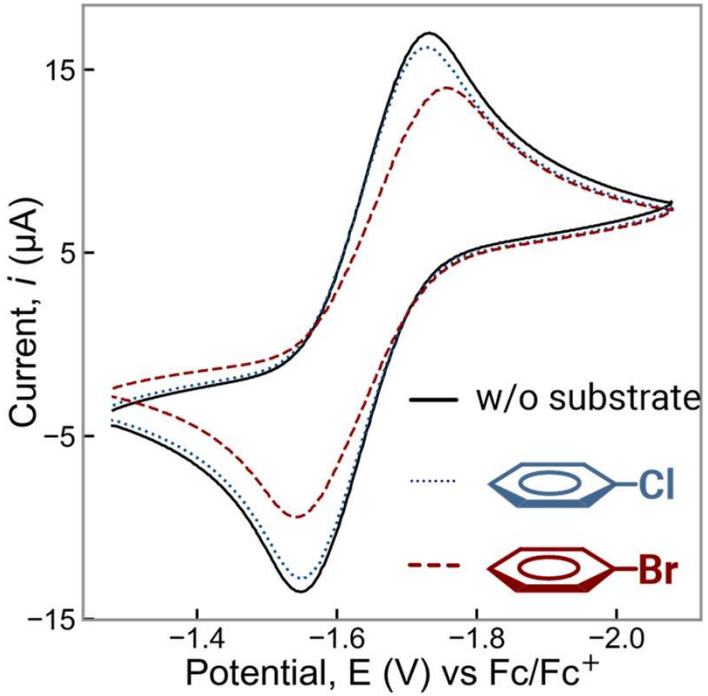
Reductive coupling of alkyl and aryl chlorides: proof of concept





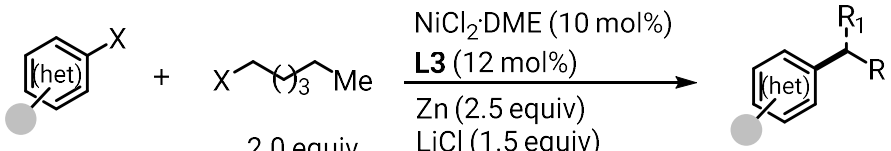


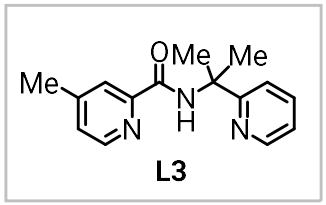




Alex Ring, Haruka Takenaka, Avijit Hazra, Sarah Reisman

Further evidence of rate matching



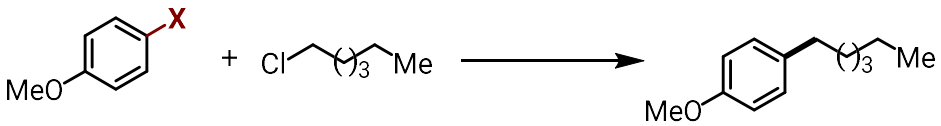


lnk_{rel} = ln(k_x/k_{ref}) where k_{ref} = 1 $M^{-1}s^{-1}$

Cl–(CH$_2$)$_3$–Me with **L3·Ni(I)**

k_x = 1.1 $M^{-1}s^{-1}$

slow aryl halide



too slow → X = Cl: lnk_{rel} = 0.9

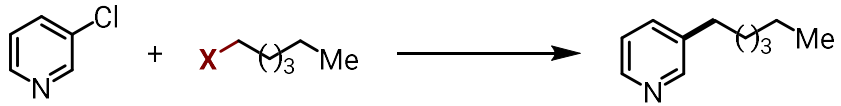
X = Br: lnk_{rel} = 3.4

lnk_{rel} = 0.1

X = Cl: 33% yield

X = Br: 80% yield

moderate aryl halide



lnk_{rel} = 1.9

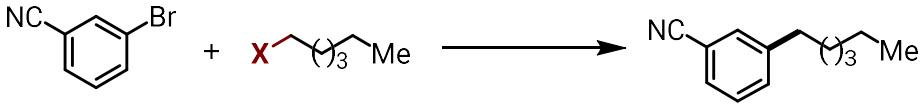
X = Cl: lnk_{rel} = 0.1

X = Br: lnk_{rel} = 7.8

X = Cl: 84% yield

X = Br: 36% yield

fast aryl halide



lnk_{rel} = 6.2

X = Cl: lnk_{rel} = 0.1

X = Br: lnk_{rel} = 7.8

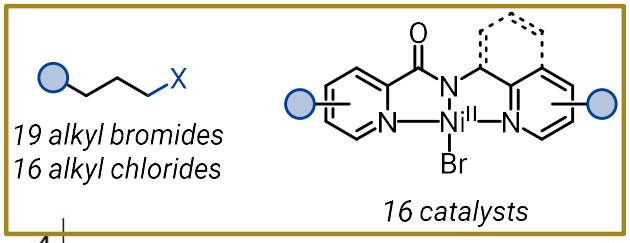
X = Cl: 27% yield

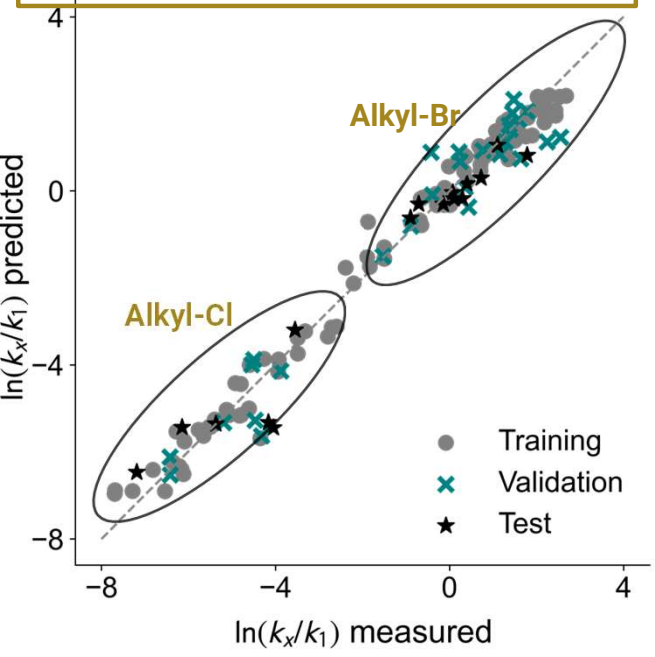
X = Br: 60% yield

Alex Ring, Haruka Takenaka, Avijit Hazra, Sarah Reisman

Building relative rate predictors: alkyl substrates

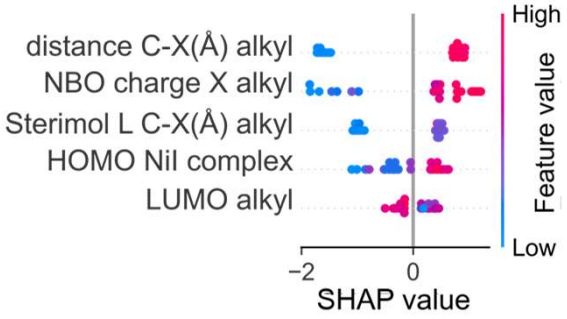
Random forest regressor



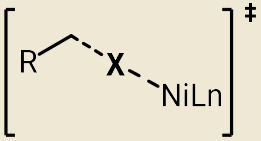


Training R^2: 0.98
Training MAE: 0.29
Validation R^2: 0.97
Validation MAE: 0.42
Test R^2: 0.96
Test MAE: 0.45

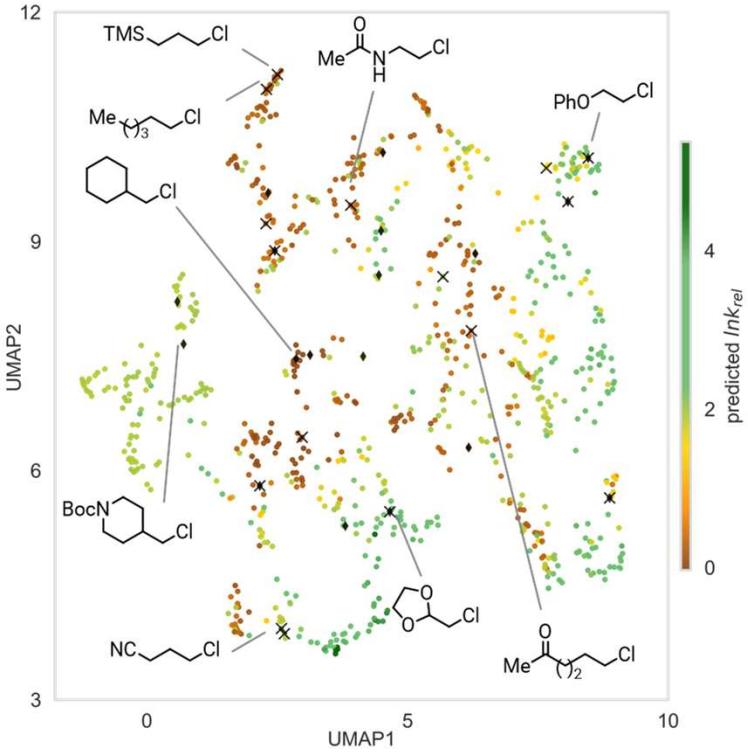
Mechanistic analysis



Halogen Atom Abstraction

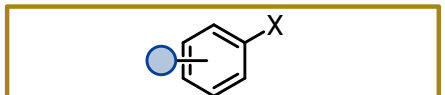


Predicted rate chemical space (AlkylCl)

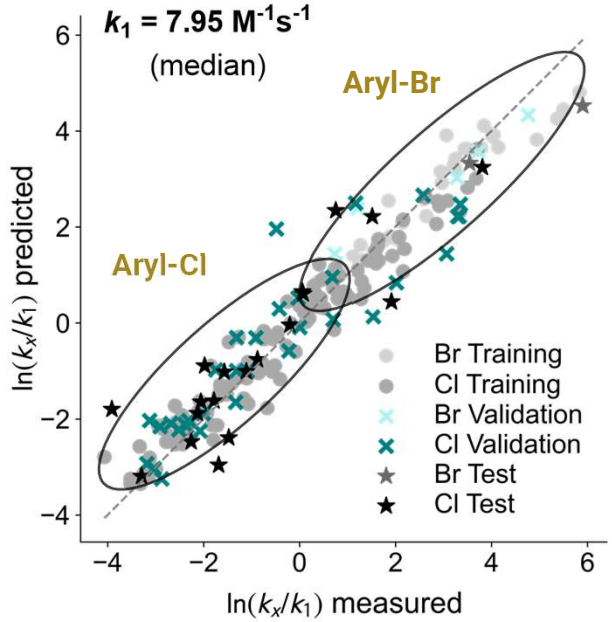


Building relative rate predictors: aryl substrates

Random forest regressor

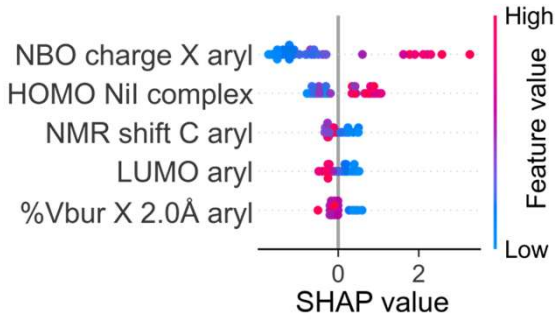


29 aryl chlorides, 15 aryl bromides
6 catalysts

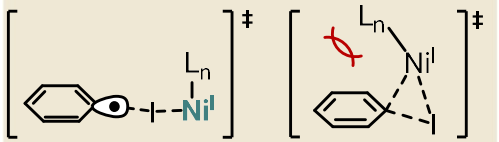


Training R^2: 0.96
Training MAE: 0.35
Validation R^2: 0.88
Validation MAE: 0.63
Test R^2: 0.86
Test MAE: 0.69

Mechanistic analysis



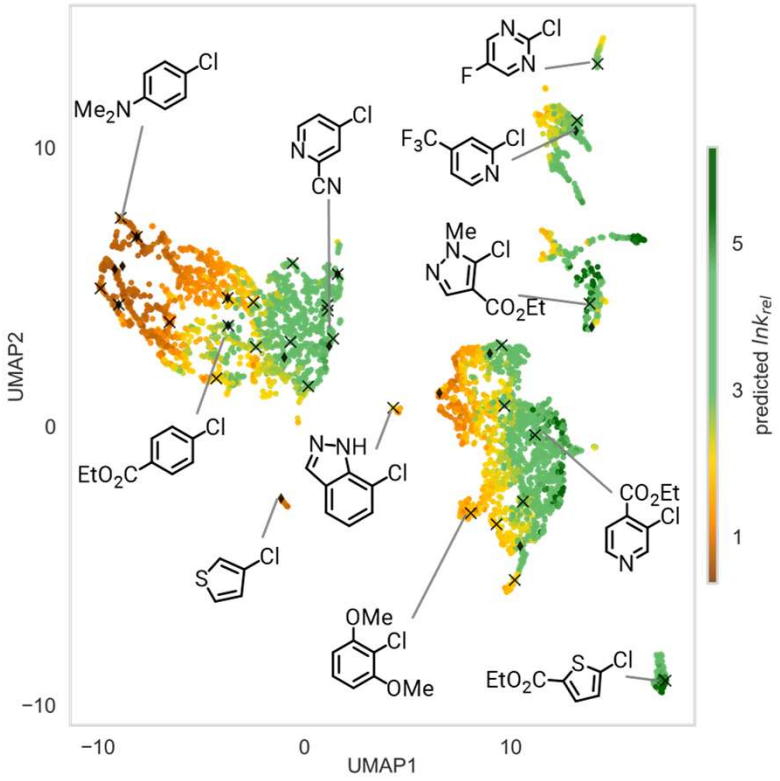
consistent with both mechanisms



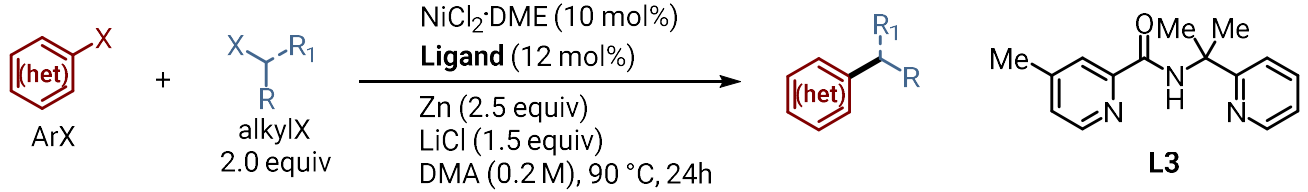
Halogen-atom abstraction

3-center-concerted

Predicted rate chemical space (ArCl)

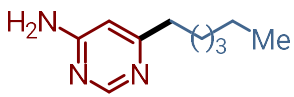


Representative scope

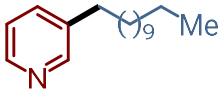


L3

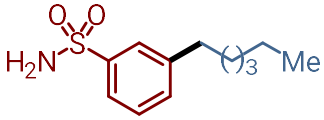
aryl chloride/alkyl chloride matched



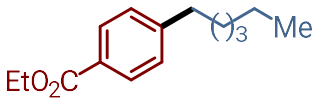
P1, 65%



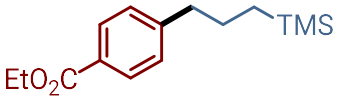
P2, 53%



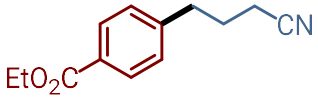
P3, 73%



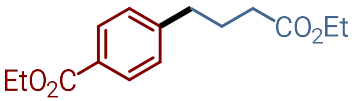
P4, 84%



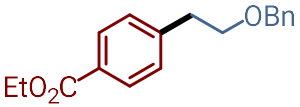
P5, 60%



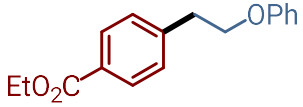
P6, 55%



P7, 82%

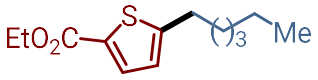


P8, 65%

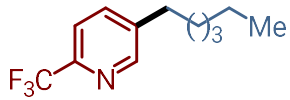


P9, 68% (L2)

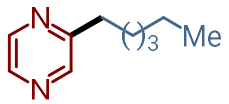
aryl chloride/alkyl bromide matched



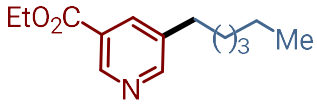
P10, 76%
with alkylCl 11%



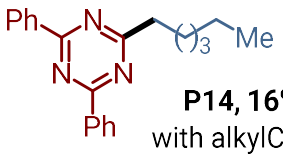
P11, 78%
with alkylCl 28%



P12, 26%
with alkylCl 15%

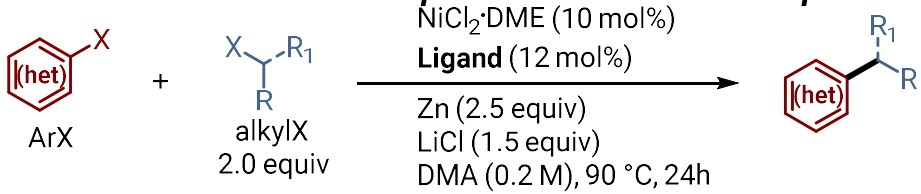


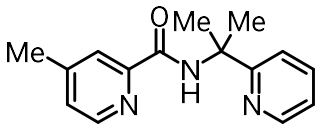
P13, 62%
with alkylCl 18%



P14, 16% (L15)
with alkylCl 8% (L3)

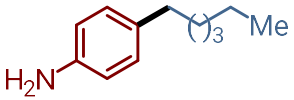
Representative scope



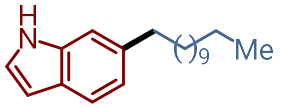


L3

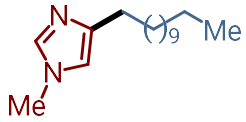
aryl bromide/ alkyl chloride matched



P15, 91%
ArCl and alkylCl 82%
ArCl and alkylBr 26%
ArBr and alkylBr 87%

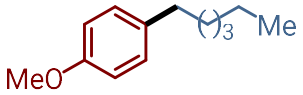


P16, 72%
ArCl and alkylCl 26%
ArCl and alkylBr 56%
ArBr and alkylBr 87%

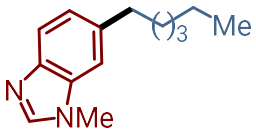


P17, 72% (L14)
with alkylBr 15% (L3)

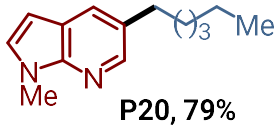
aryl bromide/ alkyl bromide matched



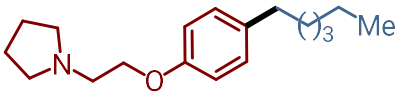
P18, 85%
ArCl and alkylCl 33%
ArCl and alkylBr 35%
ArBr and alkylCl 80%



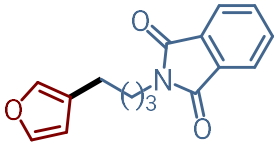
P19, 48%
with alkylCl: 38%



P20, 79%
with alkylCl:99%

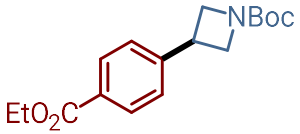


P21, 64%
with alkylCl: 48%

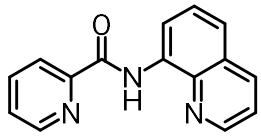


P22, 71% (L2)
with alkylCl 29% (L3)

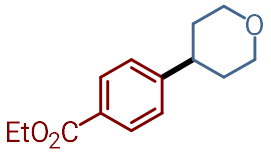
secondary



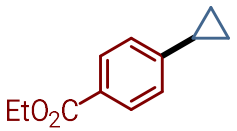
P23, 61% (L1)



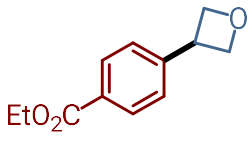
L1



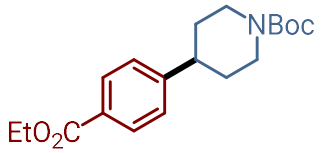
P24, 72% (L1)



P25, 81% (L1)

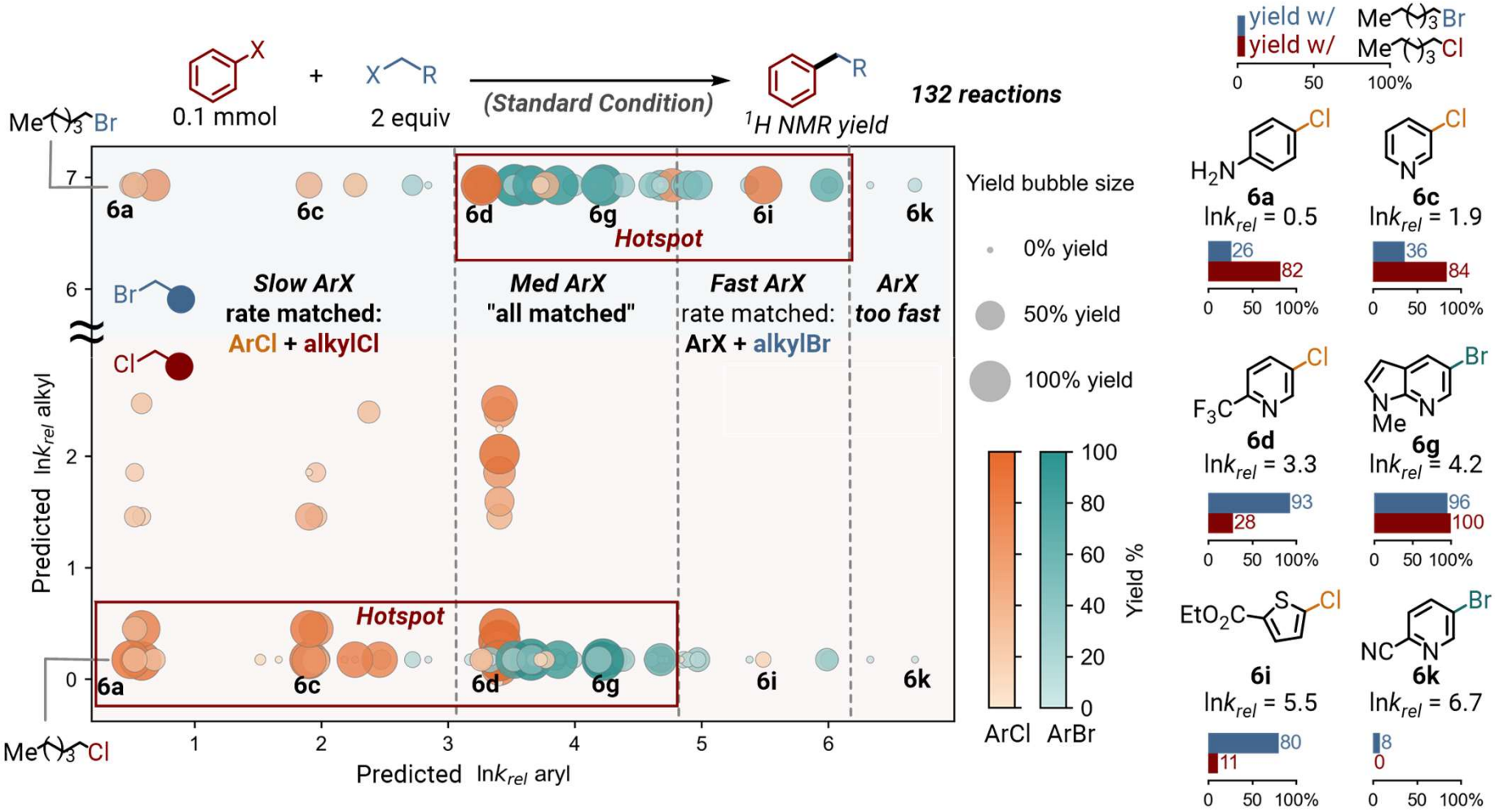


P26, 58% (L1)



P27, 74% (L1)

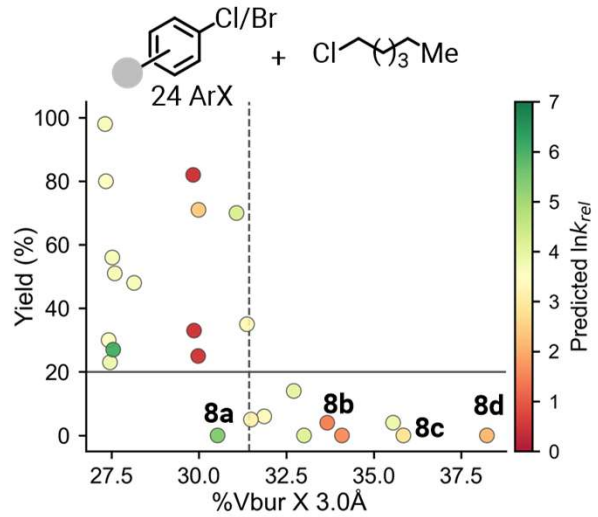
Analysis of rate matching



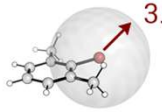
Takenaka, H.; Ring, A. J.; Hazra, H.; Wild, T. H.; Powell, S. M. R.; Tang, T.; Reisman, S. E.; Sigman, M. S. *J. Am. Chem. Soc.* **2026**, *148*, accepted.

Classification to identify more nuance

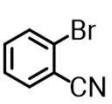
aryl couplings



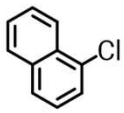
% Vbur X 3.0 Å



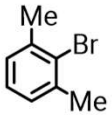
high sterics = low yields



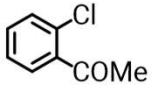
8a 0%



8b 4%

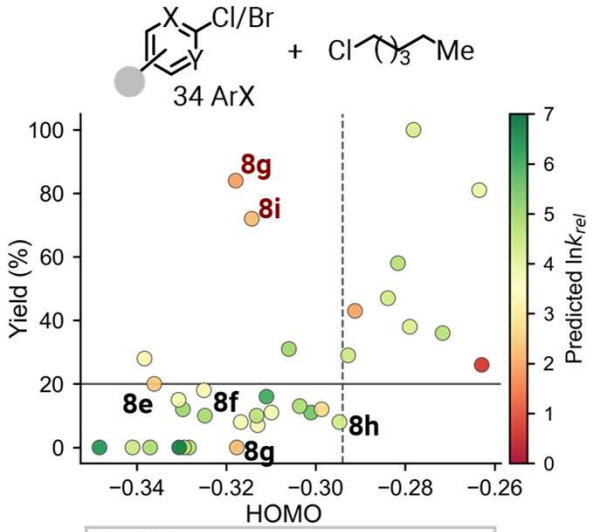


8c 0%

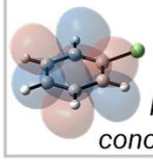


8d 0%

heteroaryl halides

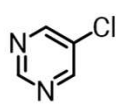


HOMO

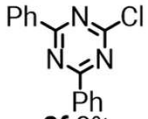


lower HOMO = low yields

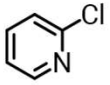
Hypothesis: slow concerted radical capture



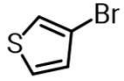
8e 20%



8f 8%



8g 0%

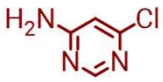


8h 8%

misclassified substrates:



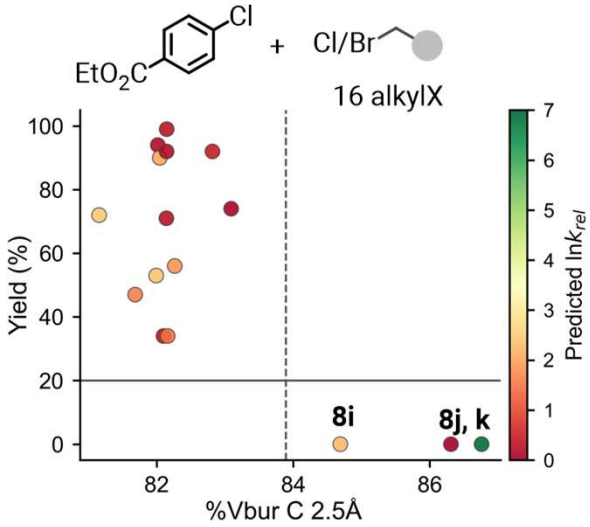
8g 84%



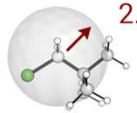
8h 72%

slow rate of OA matches slow radical capture

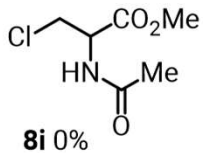
alkyl halides



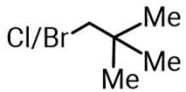
%Vbur C 2.5Å



high sterics = low yields

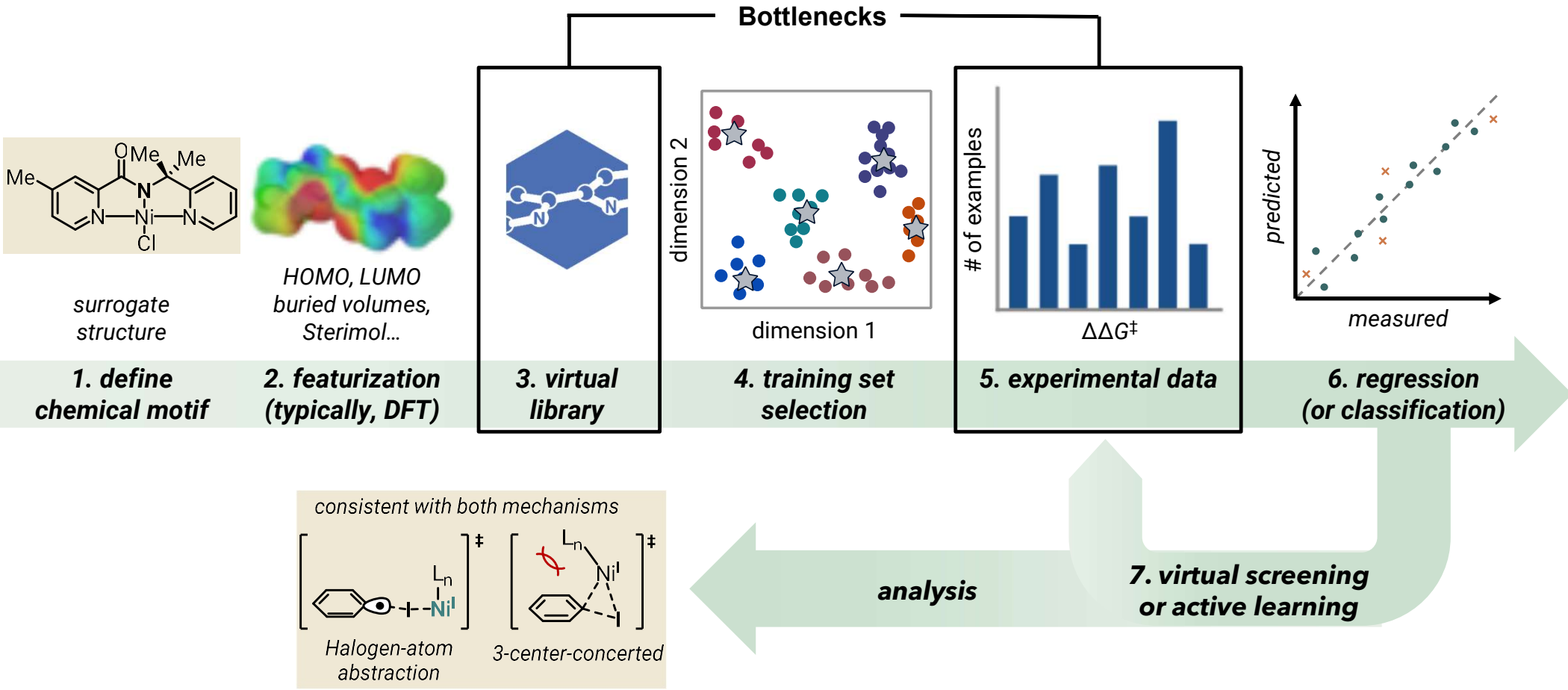


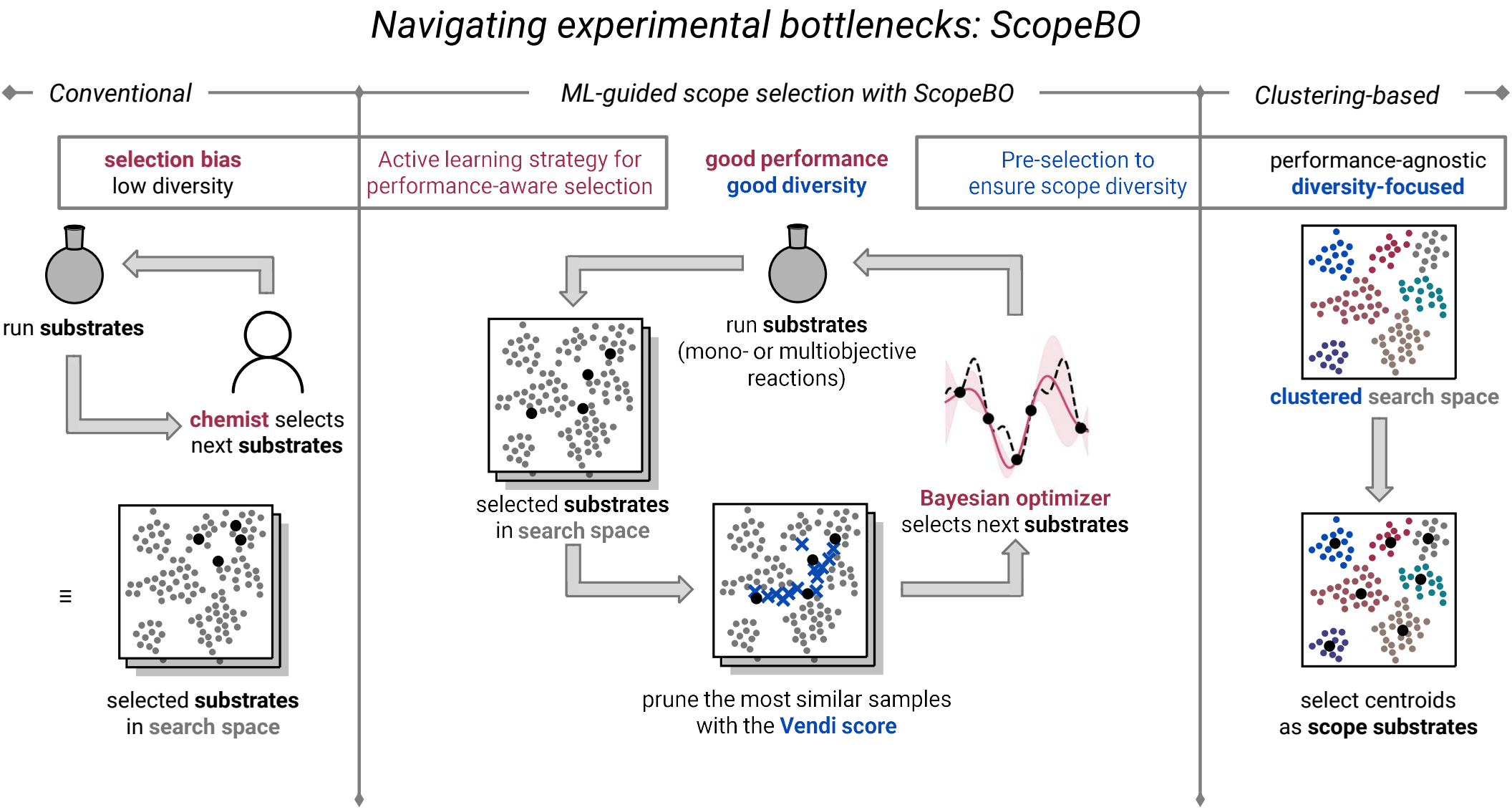
8i 0%



8j,k 0%

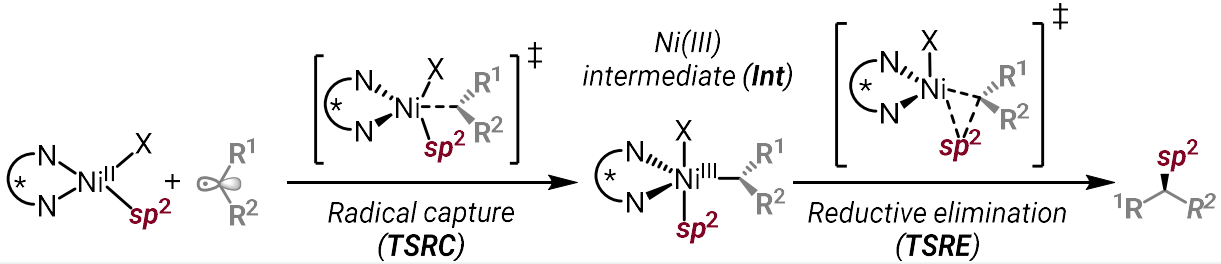
Our data science general workflow for catalysis





Roediger, S.; Sigman, M. S.; Doyle, A. G. *J. Am. Chem. Soc.* **2026**, *148*, DOI 10.1021/jacs.6c10981.

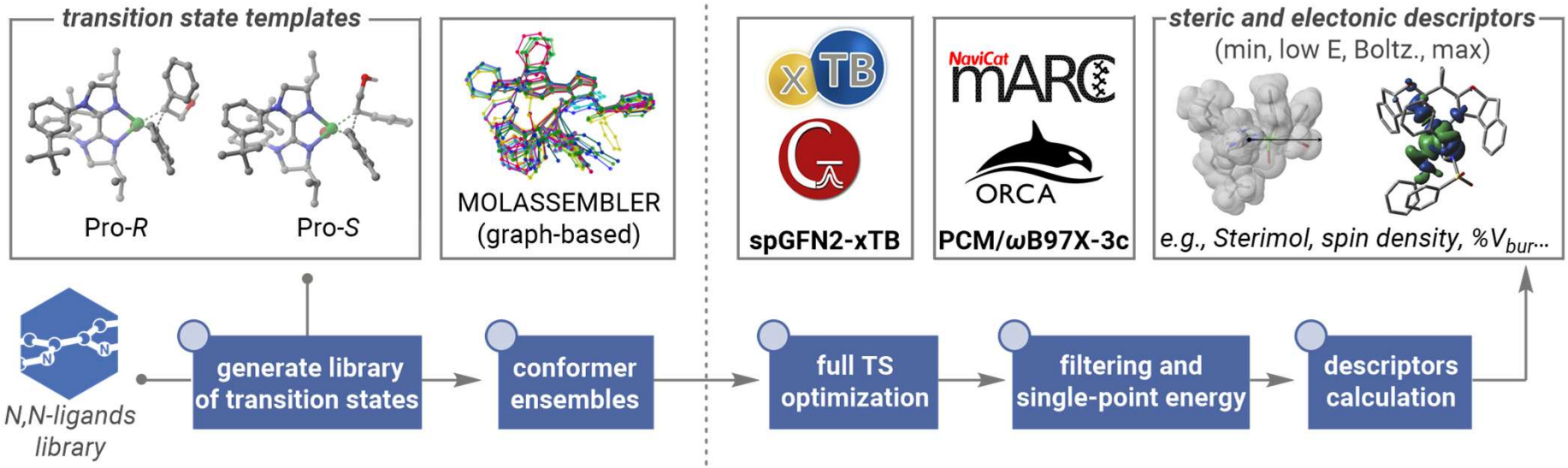
Navigating limitations in workflows: using sparse data for transfer learning (warm start)



***hypothesis**: Training models with features from TSRC, Int, TSRE should increase their domain of applicability*

***training:** on catalyst optimization and substrate scope data (already reported)*

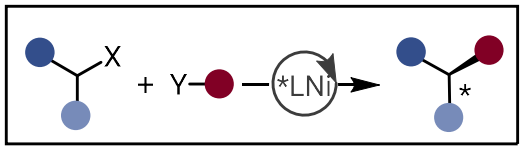
***requirement:** high throughput computational workflow*

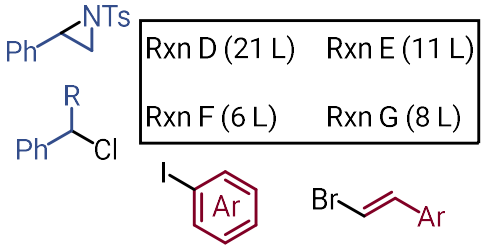


Gallarati, S. Bucci, E. M.; Doyle, A G.; Sigman, M. S. *Nature* **2026,** *651*, 637-646

Emerging workflows: towards transfer learning

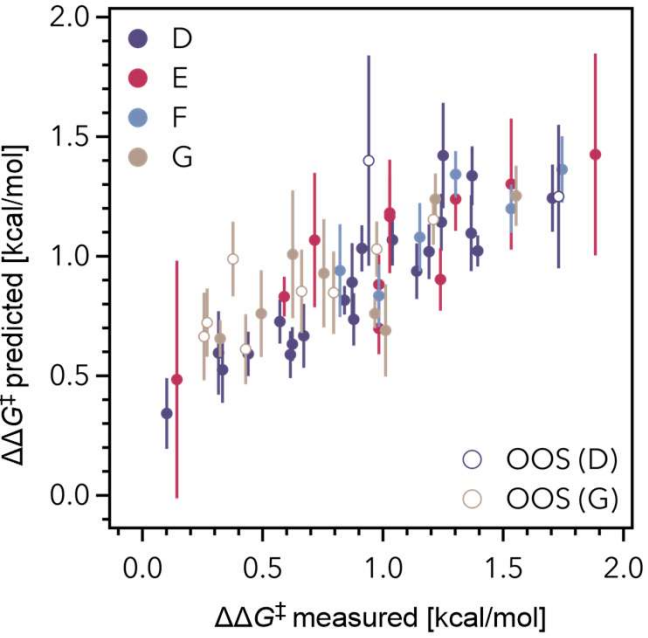
train model: diverse ligands/substrates



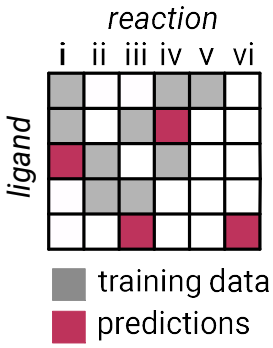


enantiodetermining TS likely ligand- and substrate-dependent

Nat. Commun. **2023**, *14*, 2322
JACS **2023**, *145*, 6270
JACS **2017**, *139*, 5684
JACS **2014**, *136*, 14365



MAE: (train) = 0.20; (OOS) = 0.29

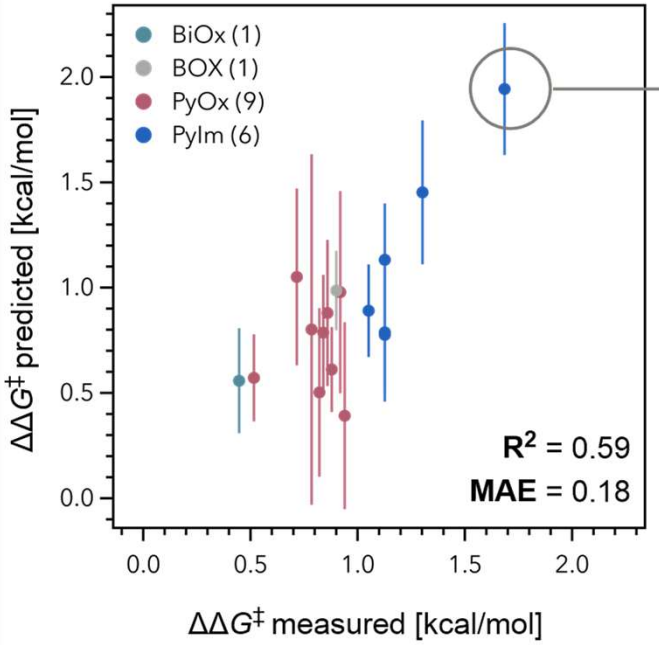


Trained on13 BiOx,
12 Bilm, 11 BOX, 1 PyOx

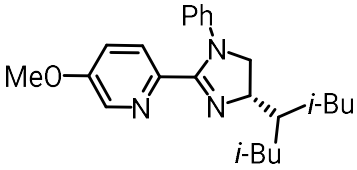
transfer learning to unseen reaction



Lan, Y et. al.*JACS* **2024**, *146*, 25426



*optimal L** **(PyIm)**



$\Delta\Delta G^{\ddagger}$ predicted = 1.94 ± 0.31
$\Delta\Delta G^{\ddagger}$ measured = 1.68
(89% ee)

trained on 1 PyOx ligand & 0 PyIm ligands

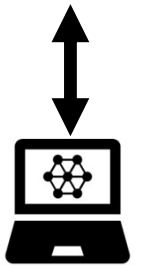
predictions on 15 PyOx/PyIm ligands

Gallarati, S. Bucci, E. M.; Doyle, A G.; Sigman, M. S. *Nature* **2026,** *651*, 637-646

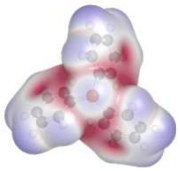
Final thoughts

chemist & data science collaboration



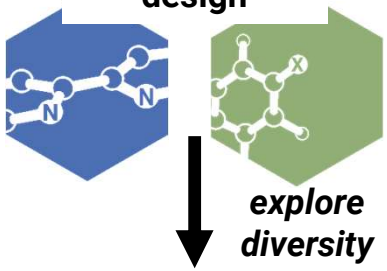




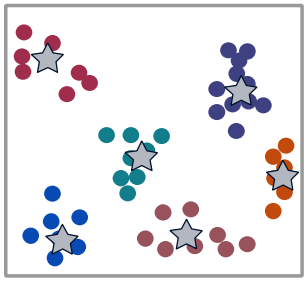


molecular features

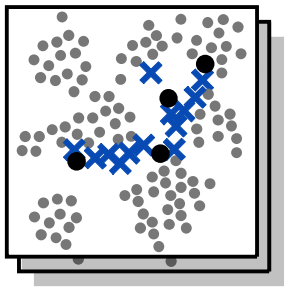
experimental design



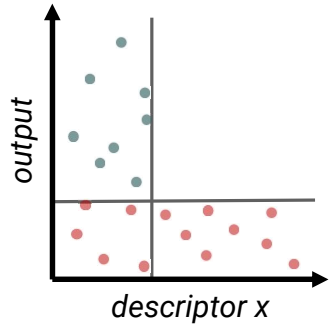
explore diversity

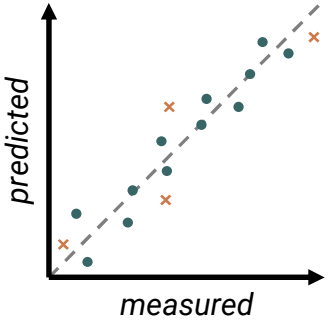


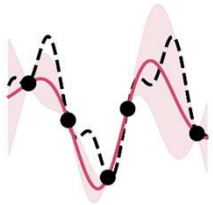
ScopeBO



optimization/ modeling

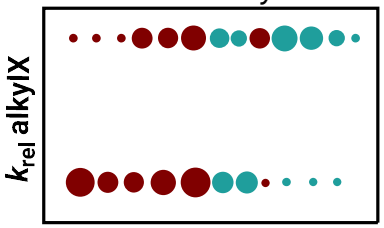


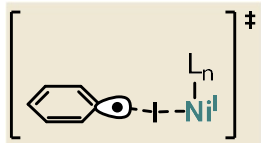




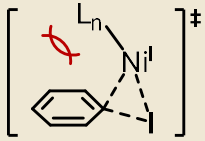
interpretation/ validation

bubble color: halogen
bubble size: yield



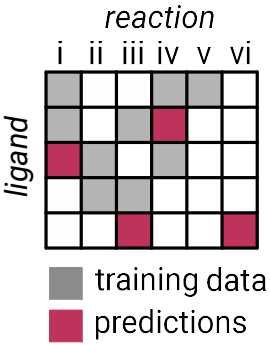


Halogen-atom abstraction



3-center-concerted

transfer learning





chemist & data science collaboration



The Group: December 2025

https://www.sigmanlab.com/

Descriptor libraries:
https://descriptor-libraries.molssi.org/

Github
https://github.com/SigmanGroup

92 U 238.03 | 73 Ta 180.95 | 1 H 1.01
CHEMISTRY

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Kaylaa Gutman (Genentech)
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