叶俊涛课题组相关研究介绍

Topic report

汇报人：王宁　　　　时间：2025.11.28

目　录

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1. 作者简介

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教育经历：

- 2008年9月-2013年6月　中科院上海有机化学研究所，博士，导师：麻生明院士
- 2004年9月-2008年6月　华中科技大学，应用化学专业，本科

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- 2019年7月 -- 至今　上海交通大学 化学化工学院 特别研究员、博士生导师
- 2018年7月-2019年6月　美国康奈尔大学，博士后，合作导师:Tristan Lambert 教授
- 2016年1月-2018年6月　美国哥伦比亚大学,博士后,合作导师:Tomislav Rovis 教授
- 2013年11月-2015年12月 加拿大多伦多大学,博士后,合作导师:Mark Lautens 教授

研究方向：基于光催化及酶催化的新型有机合成方法学及其在高分子化学和药物化学等领域的应用。

1. 1光催化双重氢原子转移

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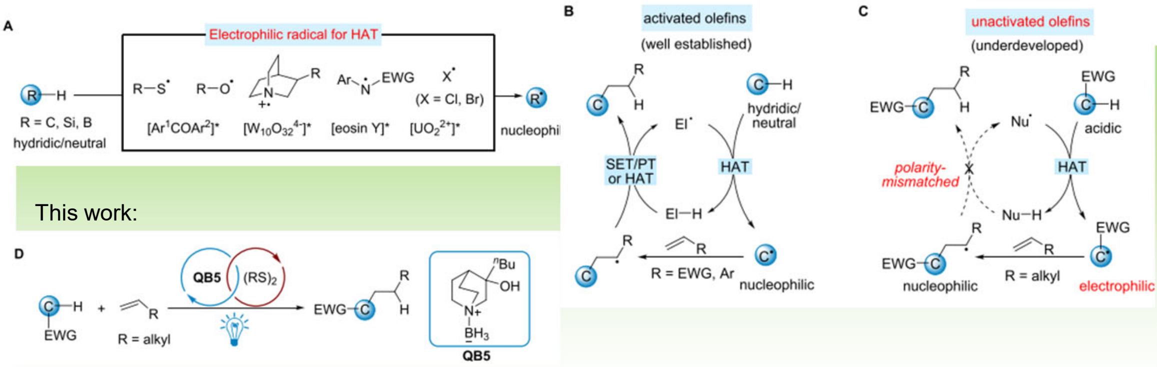
Hydroalkylation of Unactivated Olefins via Visible-Light-Driven Dual Hydrogen Atom Transfer Catalysis

Guangyue Lei,[§] Meichen Xu,[§] Rui Chang, Ignacio Funes-Ardoiz,* and Juntao Ye*

Cite This: *J. Am. Chem. Soc.* 2021, 143, 11251−11261

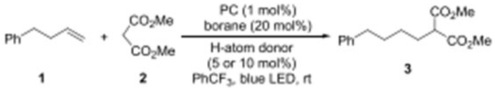
J. Am. Chem. Soc. **2021**, *143*, 11251−11261

1. 1光催化双重氢原子转移



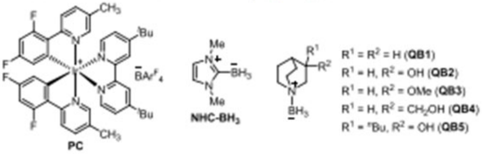
1. 1光催化双重氢原子转移

Table 1. Reaction Optimization[a]

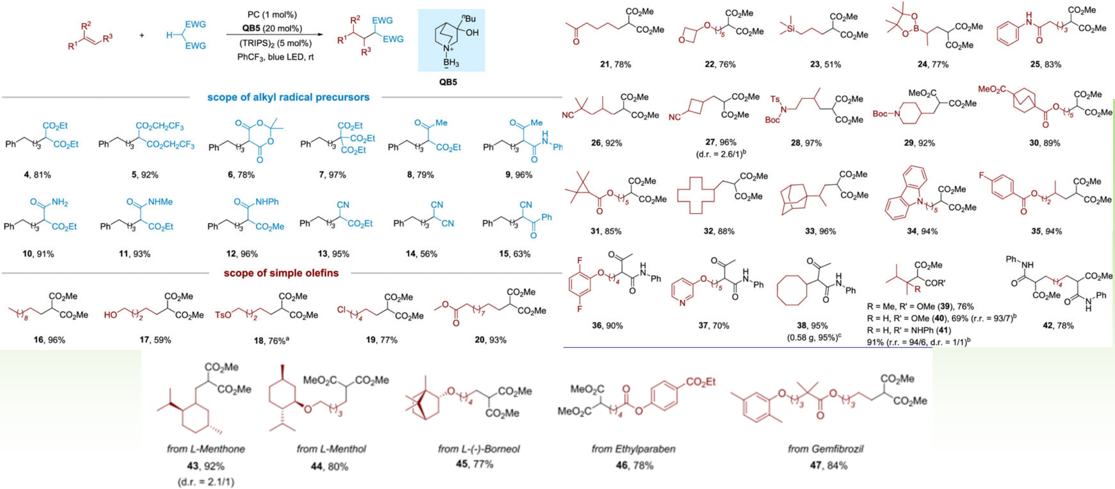


entry	borane	H atom donor	yield (%)[b]
1	NHC-BH$_3$	TRIPSH	0
2	QB1	TRIPSH	45
3	QB2	TRIPSH	75
4	QB3	TRIPSH	46
5	QB4	TRIPSH	45
6	QB5	TRIPSH	89
7	QB5	(TRIPS)$_2$	92 (91)[c]
8[d]	QB5	(TRIPS)$_2$	91
9	–	(TRIPS)$_2$	7
10	QB5	–	18
11	–	–	0
12[e]	QB5	(TRIPS)$_2$	0
13[f]	QB5	(TRIPS)$_2$	0

[a]Reaction conditions: All reactions were carried out with **1** (0.2 mmol), **2** (0.8 mmol), **PC** (1 mol %), borane (20 mol %), TRIPSH (10 mol %) or (TRIPS)$_2$ (5 mol %), and PhCF$_3$ (0.5 mL) unless otherwise noted. The reactions were irradiated with a 40-W Kessil blue LED under nitrogen atmosphere for 48 h. [b]Yields were determined by ^{1}H NMR analysis of the crude reaction mixture. [c]Isolated yield. [d]Benzene as the solvent. [e]Without PC. [f]Without light. BAr$^F_4$: tetrakis[3,5-bis(trifluoromethyl)-phenyl]borate.



1.1 光催化双重氢原子转移



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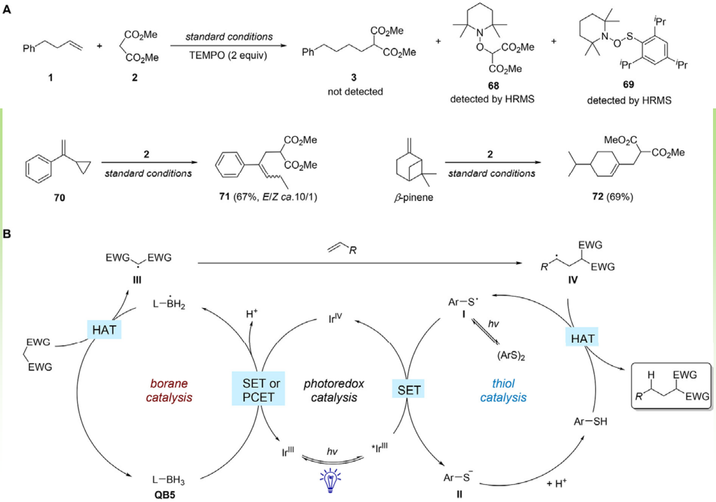

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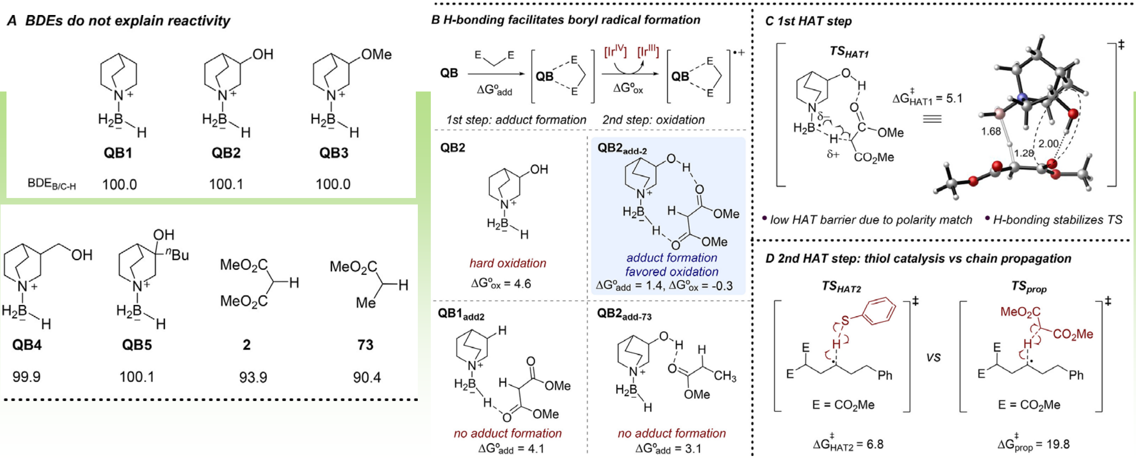


1.1 光催化双重氢原子转移

nature communications

Article https://doi.org/10.1038/s41467-022-32238-8

Visible-light mediated catalytic asymmetric radical deuteration at non-benzylic positions

Received: 30 March 2022

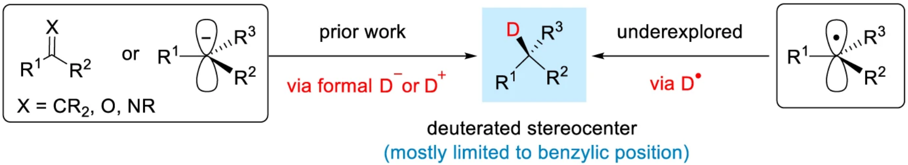
Accepted: 21 July 2022

Qinglong Shi[1,3], Meichen Xu[1,3], Rui Chang[1], Devenderan Ramanathan[1], Beatriz Peñin[2], Ignacio Funes-Ardoiz[2] & Juntao Ye[1]

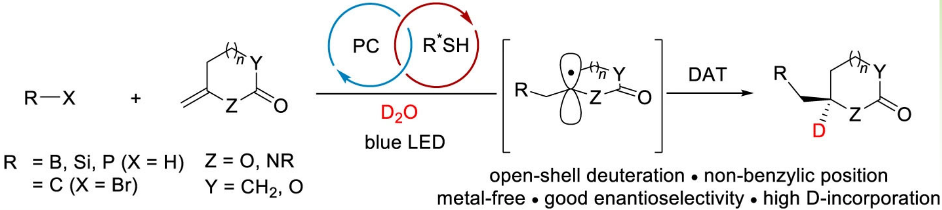
Nat. Commun. **2022**, *13*, 4453

1.1 光催化双重氢原子转移

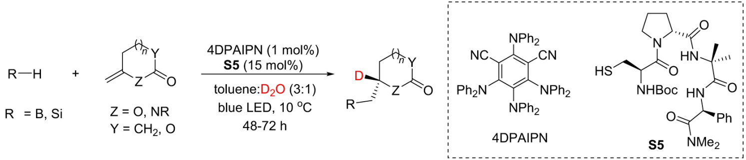
a

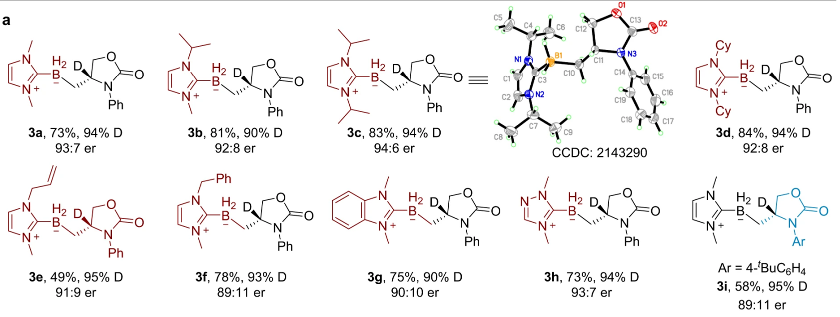


b



1.1 光催化双重氢原子转移





3a, 73%, 94% D
93:7 er

3b, 81%, 90% D
92:8 er

3c, 83%, 94% D
94:6 er

3d, 84%, 94% D
92:8 er

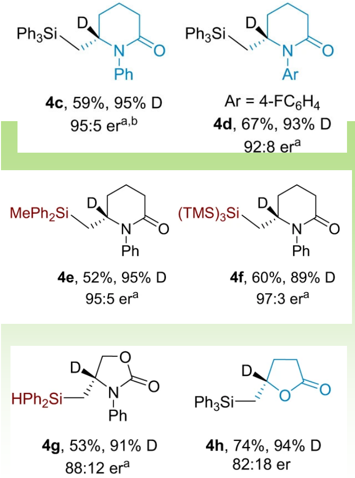
3e, 49%, 95% D
91:9 er

3f, 78%, 93% D
89:11 er

3g, 75%, 90% D
90:10 er

3h, 73%, 94% D
93:7 er

Ar = 4-^{t}BuC$_6$H$_4$
3i, 58%, 95% D
89:11 er



4c, 59%, 95% D
95:5 er[a,b]

Ar = 4-FC$_6$H$_4$
4d, 67%, 93% D
92:8 er[a]

4e, 52%, 95% D
95:5 er[a]

4f, 60%, 89% D
97:3 er[a]

4g, 53%, 91% D
88:12 er[a]

4h, 74%, 94% D
82:18 er

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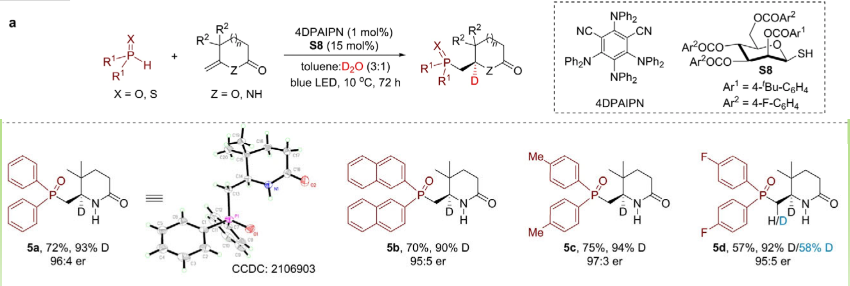

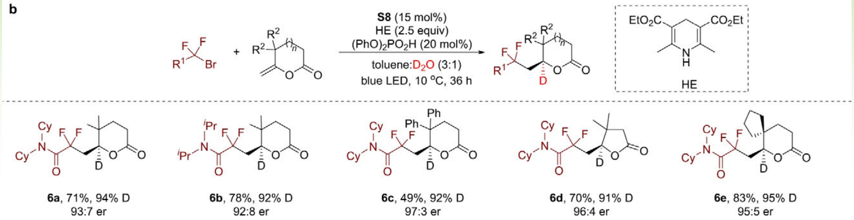

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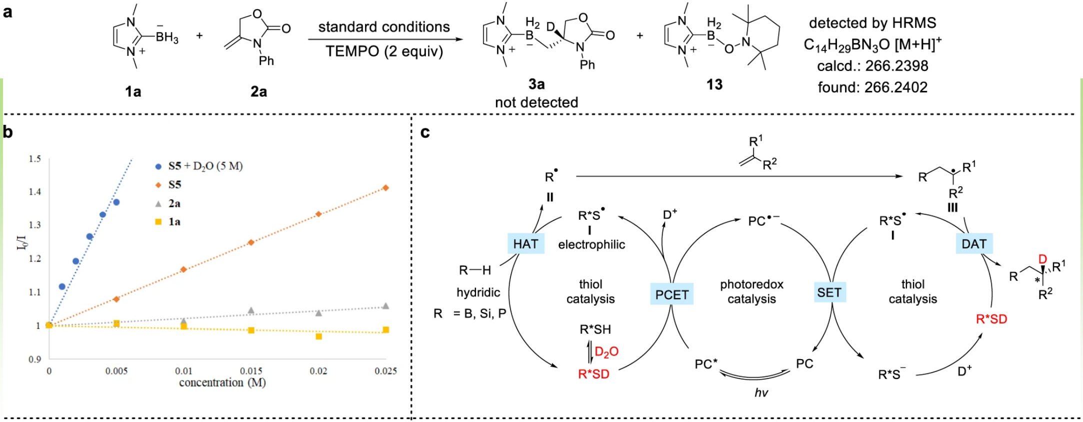

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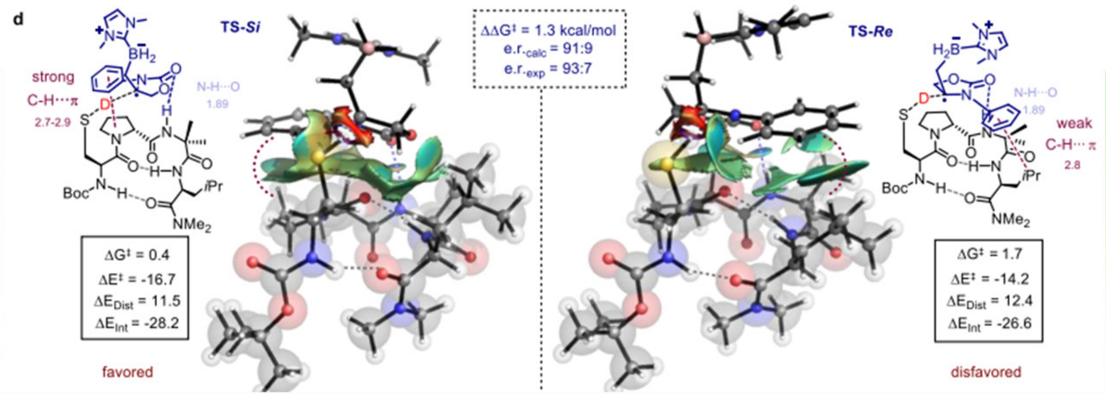

1.1 光催化双重氢原子转移

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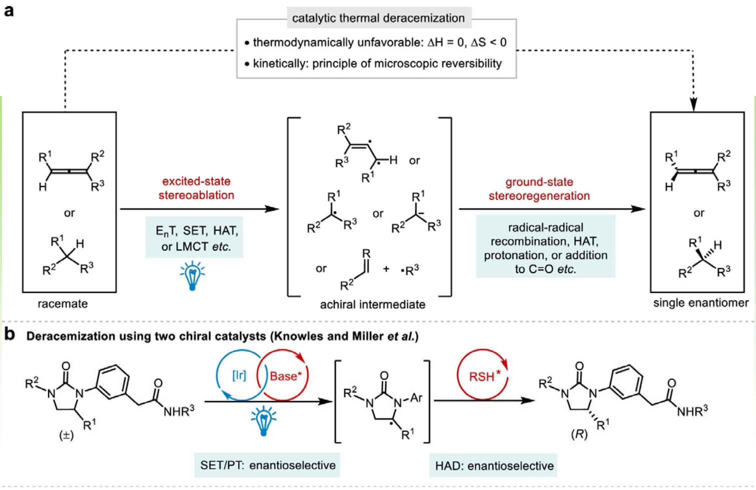
Article

Photochemical Deracemization of Lactams with Deuteration Enabled by Dual Hydrogen Atom Transfer

Xiaoyu Yan, Yubing Pang, Yutong Zhou, Rui Chang, and Juntao Ye*

Cite This: *J. Am. Chem. Soc.* 2025, 147, 1186−1196
Read Online

1.1 光催化双重氢原子转移



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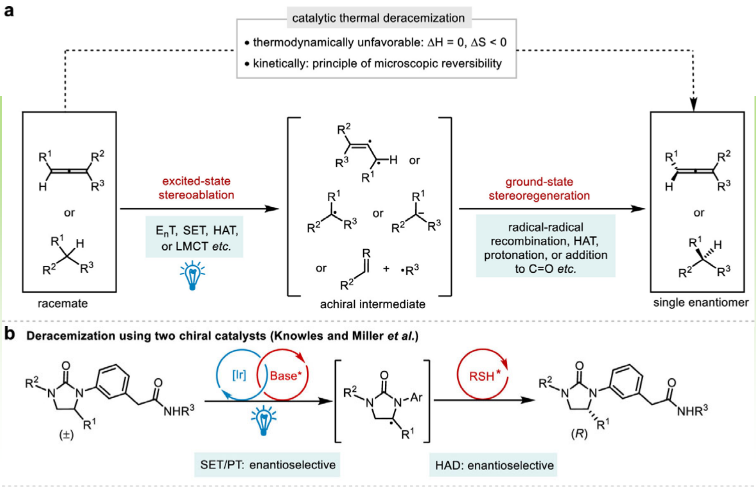
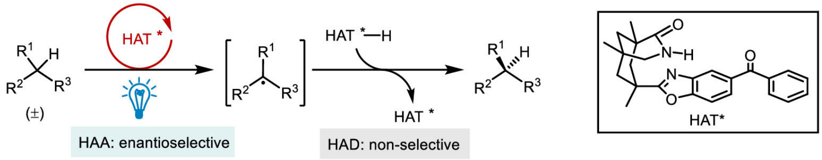
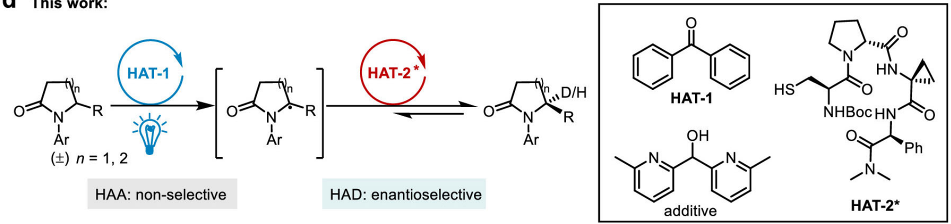


1.1 光催化双重氢原子转移

c **Deracemization using a single chiral HAT catalyst (Bach *et al.*)**



d **This work:**



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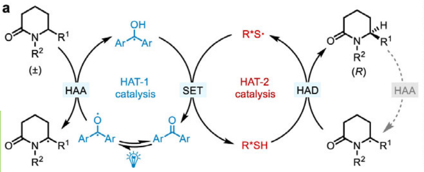
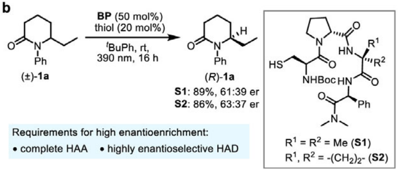
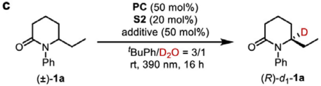
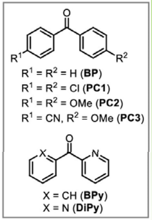
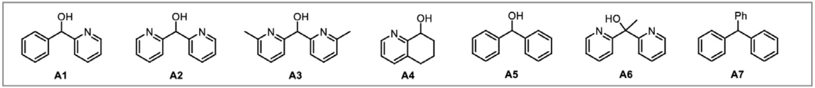






Entry	PC	additive	er	D/%	Yield/%
1	BP	-	75:25	89	85
2	BPy	-	89:11	94	89
3	DiPy	-	67:33	38	84
4	BP	A1	88:12	82	86
5	BP	A2	91:9	95	85
6	BP	A3	92:8	>95	84
7	BP	A4	92:8	91	86
8	BP	A5	71:29	82	80
9	BP	A6	81:19	90	81
10	BP	A7	75:25	63	86
11	PC1	A3	91:9	94	87
12	PC2	A3	89:11	90	91
13	PC3	A3	90:10	94	82
14[a]	BP	A3	95:5	95	87





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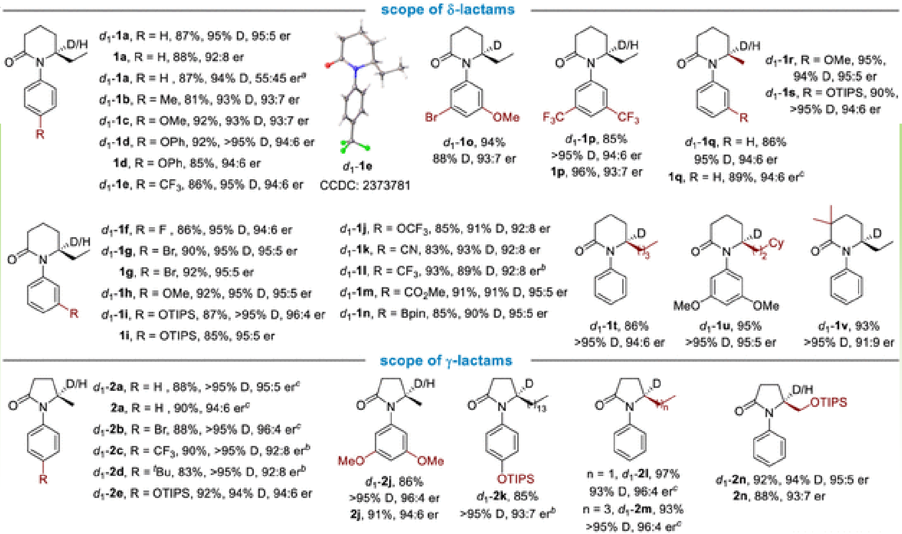
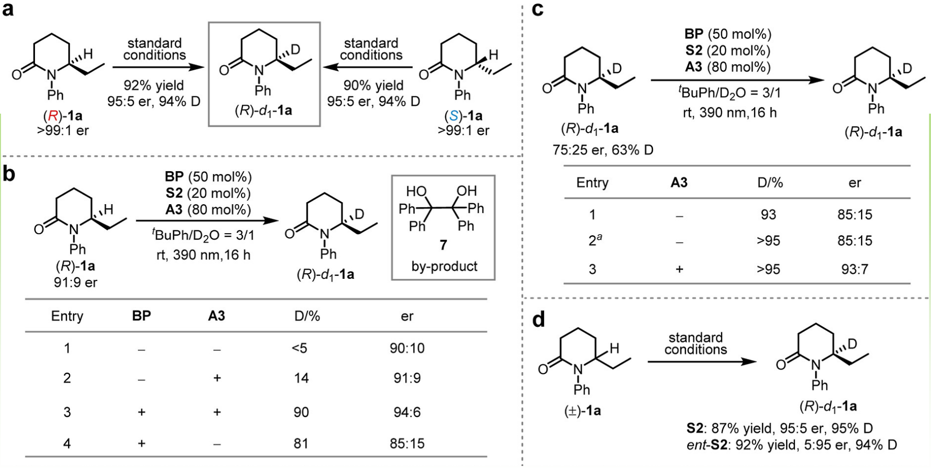


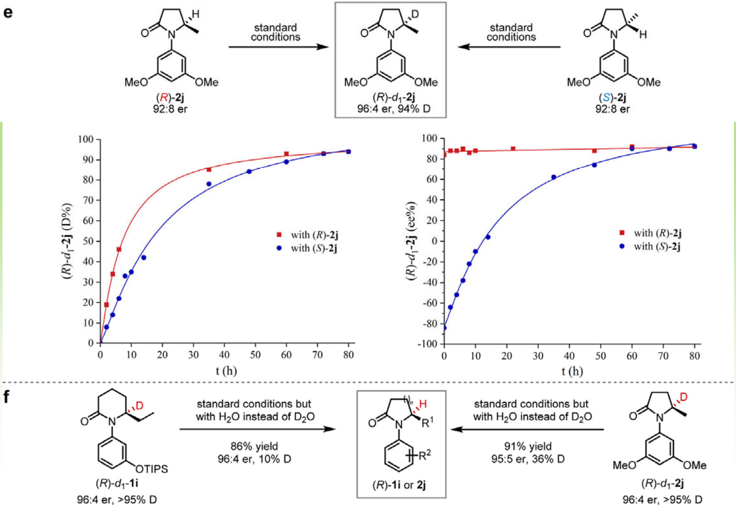
1.1 光催化双重氢原子转移



Entry	BP	A3	D/%	er
1	–	–	<5	90:10
2	–	+	14	91:9
3	+	+	90	94:6
4	+	–	81	85:15

Entry	A3	D/%	er
1	–	93	85:15
2[a]	–	>95	85:15
3	+	>95	93:7

1.1 光催化双重氢原子转移



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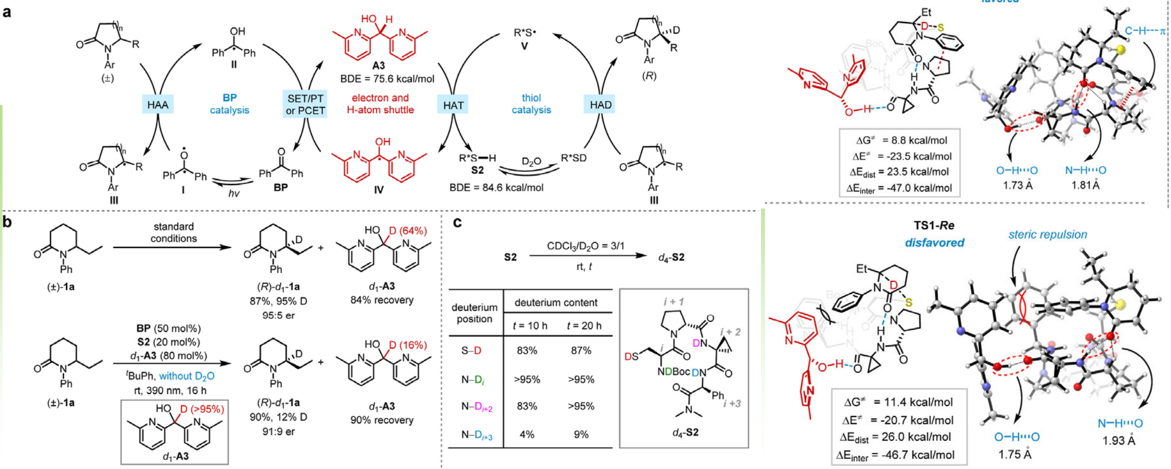

deuterium position	deuterium content	
	t = 10 h	t = 20 h
S–D	83%	87%
N–D_i	>95%	>95%
N–D_{i+2}	83%	>95%
N–D_{i+3}	4%	9%

1.2 光催化氢烷基化

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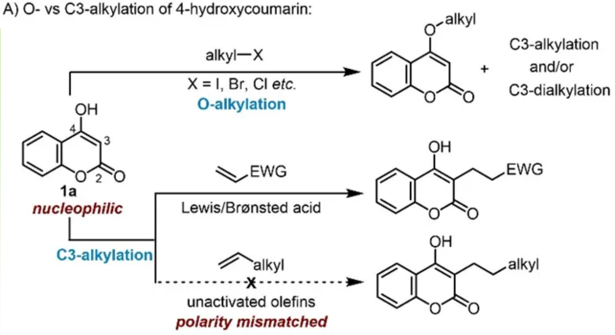
Synthetic Methods

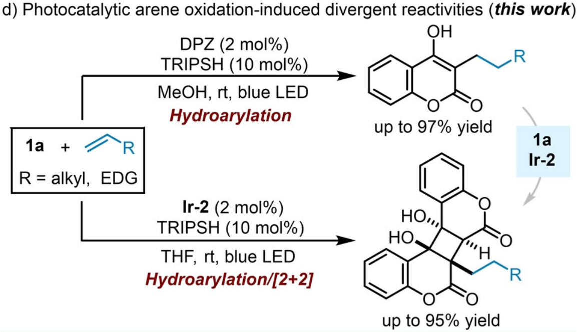
Divergent Photosensitizer Controlled Reactions of 4-Hydroxycoumarins and Unactivated Olefins: Hydroarylation and Subsequent [2+2] Cycloaddition

*Rui Chang, Yubing Pang, and Juntao Ye**

Dedicated to Professor Dennis P. Curran on the occasion of his 70th birthday

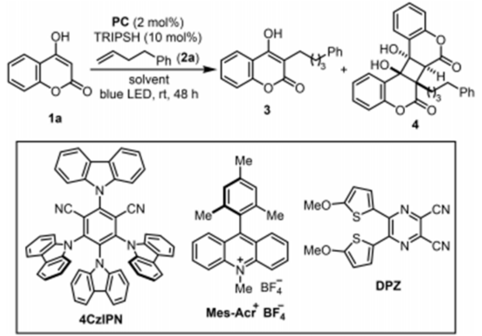
1.2 光催化氢烷基化


A) O- vs C3-alkylation of 4-hydroxycoumarin:
alkyl—X
X = I, Br, Cl etc.
O-alkylation
alkyl
C3-alkylation
and/or
C3-dialkylation
OH
1a
nucleophilic
C3-alkylation
EWG
Lewis/Brønsted acid
alkyl
unactivated olefins
polarity mismatched


d) Photocatalytic arene oxidation-induced divergent reactivities (this work)
DPZ (2 mol%)
TRIPSH (10 mol%)
MeOH, rt, blue LED
Hydroarylation
up to 97% yield
1a + R
R = alkyl, EDG
Ir-2 (2 mol%)
TRIPSH (10 mol%)
THF, rt, blue LED
Hydroarylation/[2+2]
up to 95% yield
1a
Ir-2

1.2 光催化氢烷基化

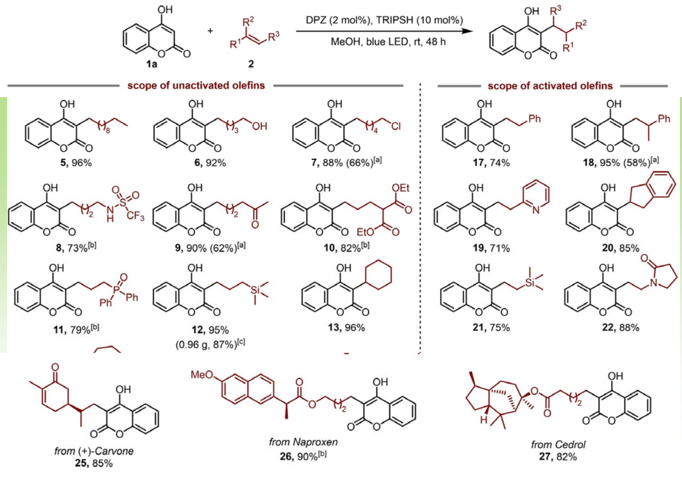
Table 1: Optimization of reaction conditions.[a]

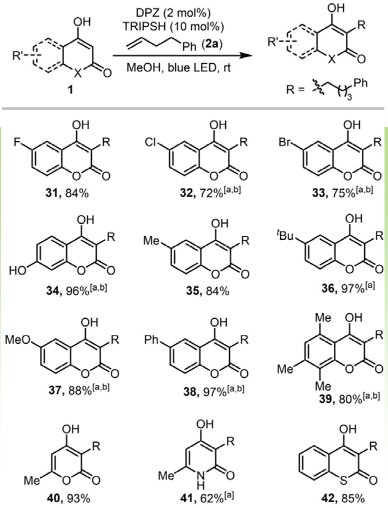


Entry	PC	Solvent	Yield of **3** [%][b]	Yield of **4** [%][b]
1[c]	4CzIPN	CH_3CN	55	10
2	4CzIPN	acetone	57	17
3	4CzIPN	MeOH	54	31
4	Mes-Acr$^+$BF$_4^-$	MeOH	20	0
5	DPZ	MeOH	97 (96)[d]	0
6	DPZ	MeOH	75[e] (61)[f]	0
7	**Ir-1**	MeOH	<5	70
8[g]	**Ir-2**	THF	0	96
9	-[h]	MeOH	0	0
10[i]	DPZ	MeOH	<5	0
11[j]	DPZ	MeOH	0	0

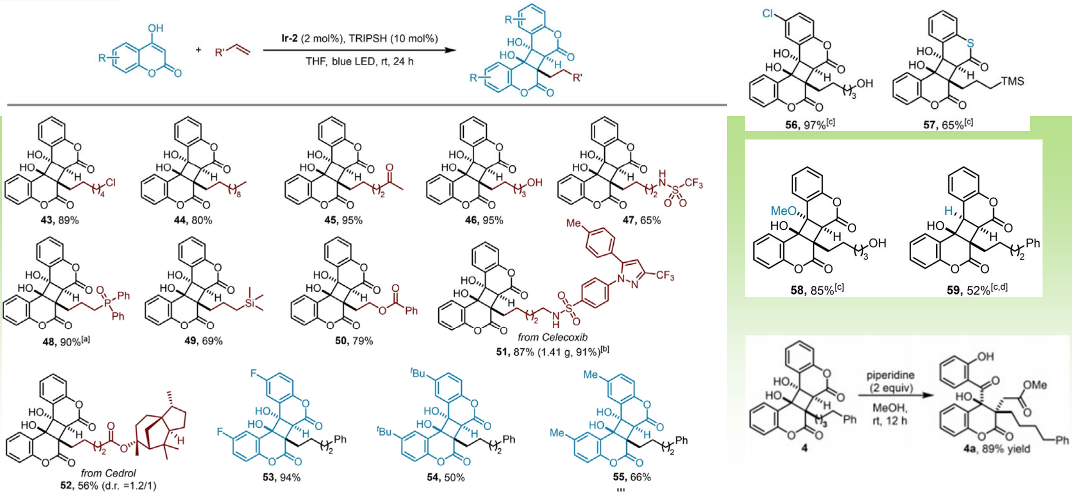
[a] All reactions were carried out with **1a** (0.4 mmol), **2a** (0.2 mmol), **PC** (2 mol%), and TRIPSH (10 mol%) in the indicated solvent (1 mL) unless otherwise noted. The reactions were irradiated with a 40-W Kessil blue LED (λ=427 nm) under nitrogen atmosphere for 48 h. [b] Yields were determined by ^{1}H NMR analysis of the crude reaction mixture. [c] 17% of **2a** remained. [d] Isolated yield. [e] **1a** (0.2 mmol) and **2a** (0.2 mmol) were used. [f] **1a** (0.2 mmol) and **2a** (0.4 mmol) were used. [g] Reaction was carried out with **1a** (0.8 mmol) for 24 h. [h] Without **PC**. [i] Without TRIPSH. [j] Without light. **Ir-1** = Ir[dF(CF$_3$)ppy]$_2$(dtbbpy)PF$_6$. **Ir-2** = Ir[dF(CF$_3$)ppy]$_2$(bpy)PF$_6$.

1.2 光催化氢烷基化

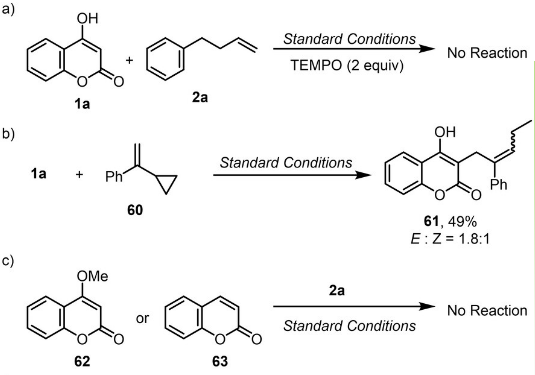

DPZ (2 mol%), TRIPSH (10 mol%)
MeOH, blue LED, rt, 48 h
1a
2
scope of unactivated olefins
scope of activated olefins
5, 96%
6, 92%
7, 88% (66%)[a]
17, 74%
18, 95% (58%)[a]
8, 73%[b]
9, 90% (62%)[a]
10, 82%[b]
19, 71%
20, 85%
11, 79%[b]
12, 95%
(0.96 g, 87%)[c]
13, 96%
21, 75%
22, 88%
from (+)-Carvone
25, 85%
from Naproxen
26, 90%[b]
from Cedrol
27, 82%

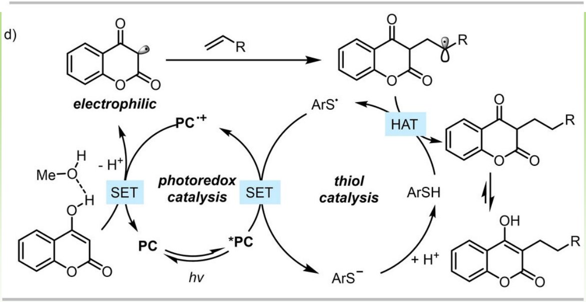

DPZ (2 mol%)
TRIPSH (10 mol%)
(2a)
MeOH, blue LED, rt
1
31, 84%
32, 72%[a,b]
33, 75%[a,b]
34, 96%[a,b]
35, 84%
36, 97%[a]
37, 88%[a,b]
38, 97%[a,b]
39, 80%[a,b]
40, 93%
41, 62%[a]
42, 85%

1.2 光催化氢烷基化


Ir-2 (2 mol%), TRIPSH (10 mol%)
THF, blue LED, rt, 24 h
43, 89%
44, 80%
45, 95%
46, 95%
47, 65%
48, 90%[a]
49, 69%
50, 79%
from Celecoxib
51, 87% (1.41 g, 91%)[b]
from Cedrol
52, 56% (d.r. =1.2/1)
53, 94%
54, 50%
55, 66%
56, 97%[c]
57, 65%[c]
58, 85%[c]
59, 52%[c,d]
piperidine
(2 equiv)
MeOH,
rt, 12 h
4
4a, 89% yield

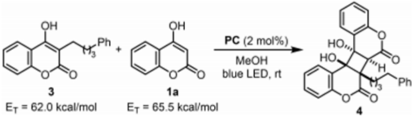
1.2 光催化氢烷基化


a)
OH
O
O
1a
+
2a
Standard Conditions
TEMPO (2 equiv)
No Reaction
b)
1a
+
Ph
60
Standard Conditions
OH
Ph
61, 49%
E : Z = 1.8:1
c)
OMe
62
or
63
2a
Standard Conditions
No Reaction


d)
electrophilic
R
ArS·
HAT
PC·+
- H+
Me–O
H
H
SET
photoredox
catalysis
SET
thiol
catalysis
ArSH
OH
PC
*PC
hν
ArS−
+ H+

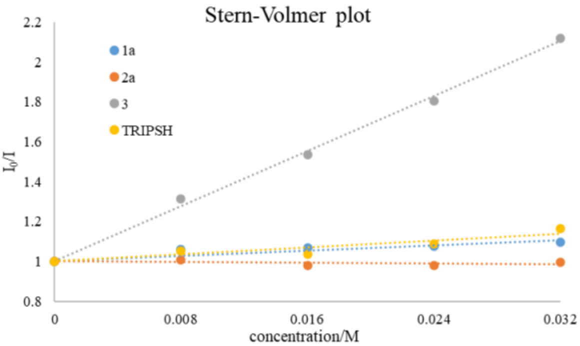
1.2 光催化氢烷基化

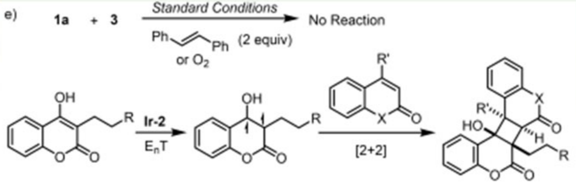
Table 2: Evaluation of photocatalyst for the [2+2] cycloaddition reaction.[a]



Entry	PC	$E_{1/2}$ (V, vs SCE) (PC*/PC•−)	(PC•+/PC*)	E_T [kcal/mol]	Yield [%][b]
1	Mes-Acr$^+$BF$_4^-$	+2.18	–	44.7	0
2	DPZ	+1.37	−1.45	46.4	0
3	*fac*-Ir(ppy)$_3$	+0.31	−1.73	58.1	0
4	**Ir-1**	+1.21	−0.89	61.8	99
5	**Ir-2**	+1.32	−1.00	62.0	99
6	**Ir-3**	+0.97	−0.92	62.9	89
7	*fac*-Ir[(dF)ppy)$_3$]	+0.34	−1.46	63.5	23

[a] All reactions were carried out with **3** (0.1 mmol), **1a** (0.2 mmol), **PC** (2 mol%), and MeOH (0.5 mL) under nitrogen atmosphere for 12 h. [b] Determined by ^{1}H NMR analysis of the crude reaction mixture. **Ir-3** = Ir[dF(Me)ppy]$_2$(dtbbpy)PF$_6$. See Supporting Information for structures of the photocatalysts.





2.1. 光酶催化烯烃氢磺酰化

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Single-Electron Oxidation-Initiated Enantioselective Hydrosulfonylation of Olefins Enabled by Photoenzymatic Catalysis

Qinglong Shi, Xiu-Wen Kang, Zhiyong Liu, Pandaram Sakthivel, Hasil Aman, Rui Chang, Xiaoyu Yan, Yubing Pang, Shaobo Dai,* Bei Ding,* and Juntao Ye*

Cite This: *J. Am. Chem. Soc.* 2024, 146, 2748−2756 Read Online

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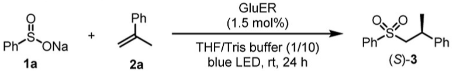
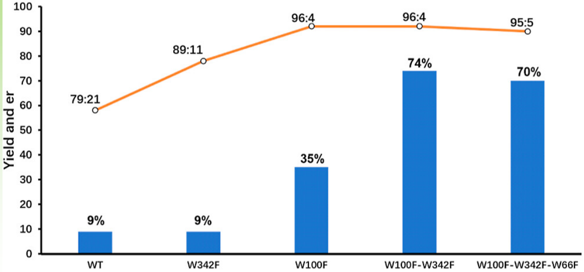
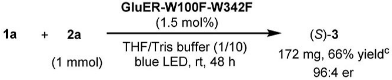
J. Am. Chem. Soc. **2024**, *146*, 2748−2756

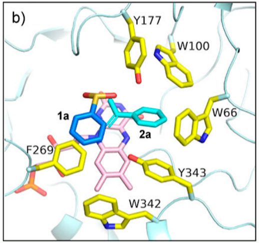
2.1. 光酶催化烯烃氢磺酰化

a) protein engineering[a,b]





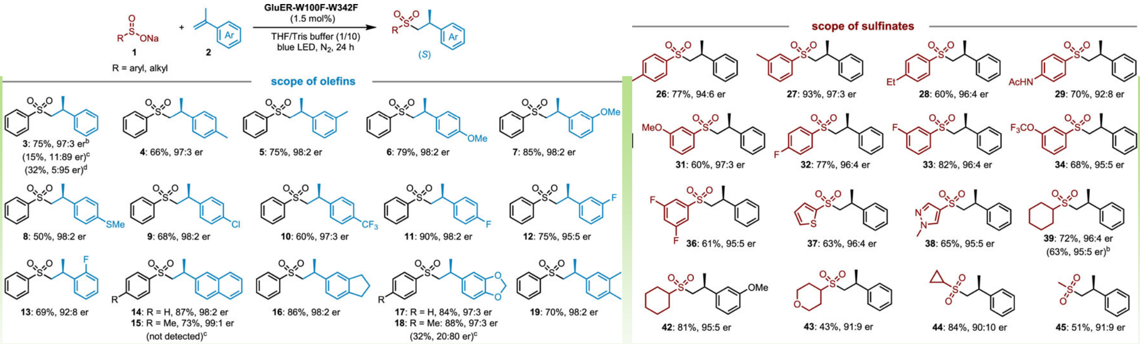




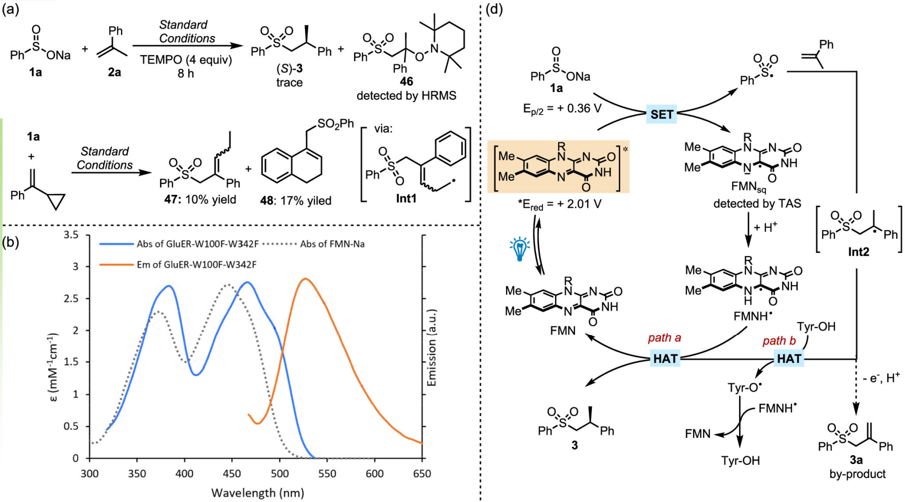
c) control experiments

entry	deverivations from optimal conditions	3
1	DMSO instead of THF	37% yield 95:5 er
2	MeCN instead of THF	55% yield 92:8 er
3	no enzyme	n.r.
4	no blue LED	n.r.

2.1. 光酶催化烯烃氢磺酰化



2.1. 光酶催化烯烃氢磺酰化



2.2. 光酶催化烯烃氢烷基化

JACS
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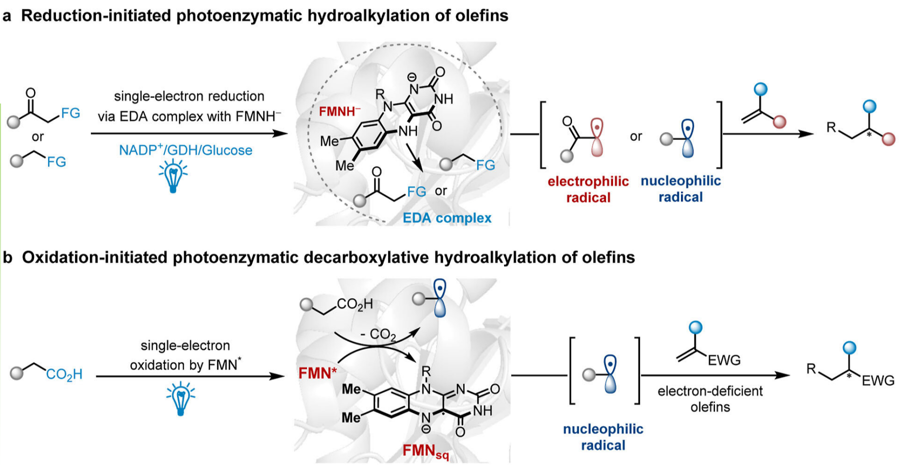
Photoenzymatic C(sp^3)−H Functionalization of 1,3-Dicarbonyls Enables Enantioselective Hydroalkylation of Styrenes

Ermeng Wang,[§] Qiaoyu Zhang,[§] Qinglong Shi,* Xiaoyu Wang, Ting Ma, Yixue Wu, Binju Wang,* and Juntao Ye*

Cite This: https://doi.org/10.1021/jacs.5c17564 Read Online

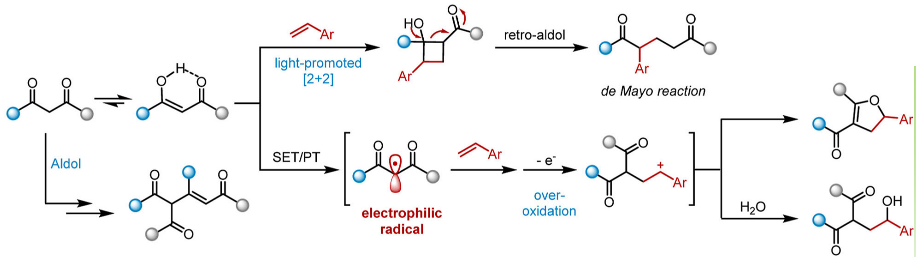
J. Am. Chem. Soc. **2025**, doi: 10.1021/jacs.5c17564.

2.2. 光酶催化烯烃氢烷基化

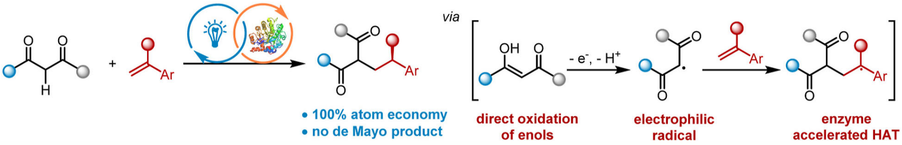


2.2. 光酶催化烯烃氢烷基化

c Challenges in photochemical hydroalkylation with 1,3-dicarbonyls

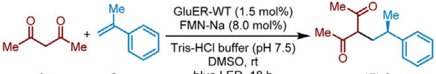


d C–H bonds as radical precursors for photoenzymatic hydroalkylation of styrenes (this work)



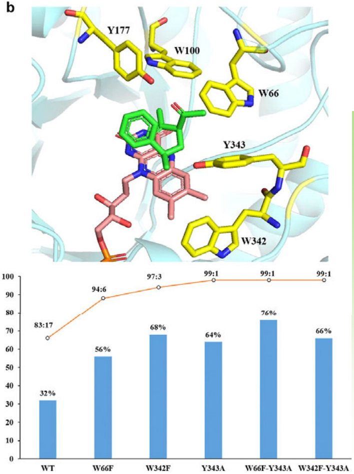
2.2. 光酶催化烯烃氢烷基化

a

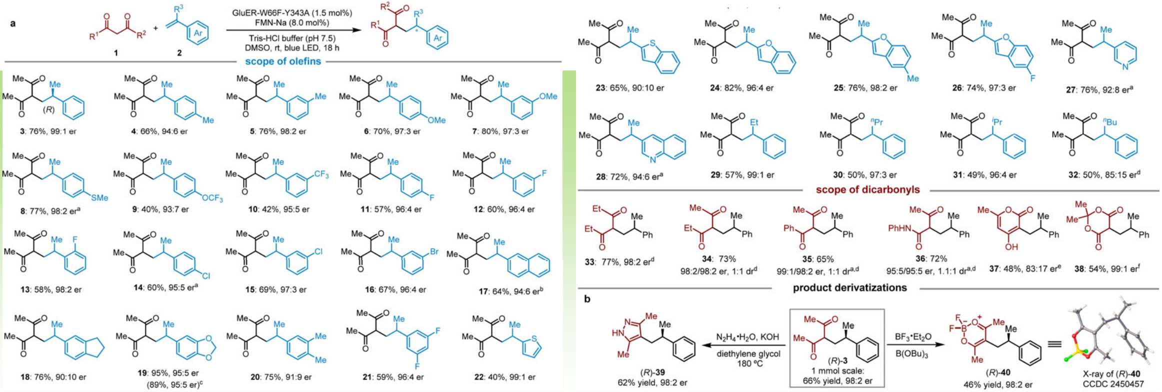


Entry	Variations from the above conditions	Yield (%)[a]	e.r.[b]
1	no FMN-Na	n.r.	-[c]
2	none	32	83:17
3	YersER -WT	28	27:73
4	GluER-W66F	56	94:6
5	GluER-Y343A	64	99:1
6	GluER-W66F-Y343A	76	99:1
7	as entry 6, THF instead of DMSO	42	98:2
8	as entry 6, Tris buffer (pH 8.0)	66	99:1
9	as entry 6, Tris buffer (pH 9.0)	56	99:1
10	as entry 6, no FMN-Na	trace	-[c]
11	as entry 6, no blue LED	n.r.	-[c]
12	no enzyme	16	50:50

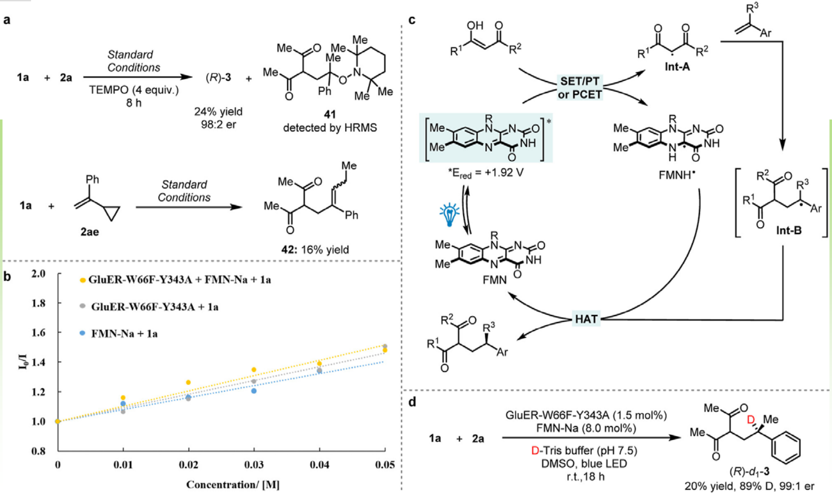
b



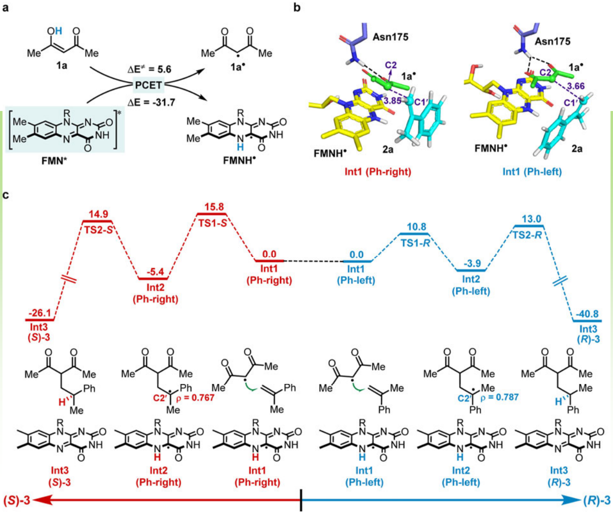
2.2. 光酶催化烯烃氢烷基化移



2.2. 光酶催化烯烃氢烷基化



2.2. 光酶催化烯烃氢烷基化



3.2 光催化硼硫键构筑

Angewandte Chemie International Edition
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Photocatalytic Boron Insertion into Thiaarenes via Boryl Radicals

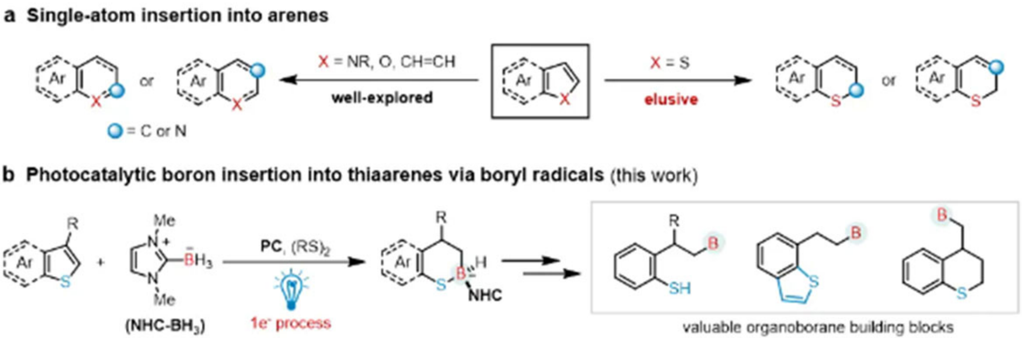
Yubing Pang, Ermeng Wang, Prof. Dr. Juntao Ye

Dedicated to Prof. Shengming Ma on the occasion of his 60th birthday

First published: 19 May 2025 | https://doi.org/10.1002/anie.202508379 | Citations: 3

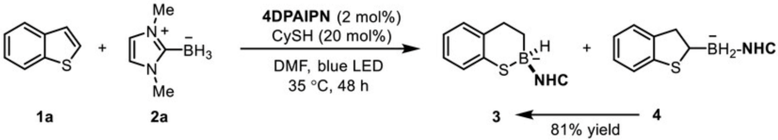
Homepage: https://www.x-mol.com/groups/Ye_Juntao

3.2 光催化硼硫键构筑

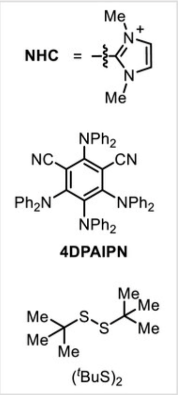

a Single-atom insertion into arenes
Ar
or
X = NR, O, CH=CH
well-explored
X = S
elusive
= C or N
b Photocatalytic boron insertion into thiaarenes via boryl radicals (this work)
R
S
Me
BH_3
(NHC-BH_3)
PC, (RS)$_2$
1e⁻ process
NHC
SH
B
valuable organoborane building blocks

3.1 光催化硼硫键构筑

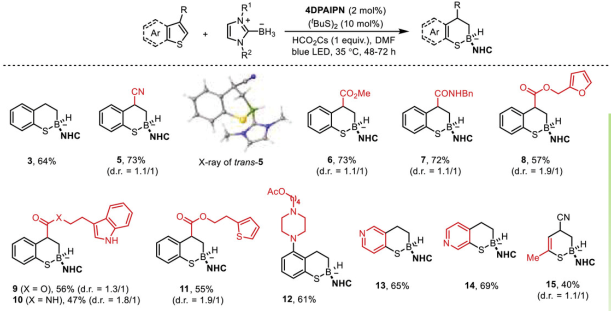
a) Reaction optimization

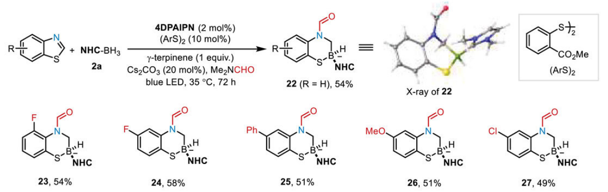


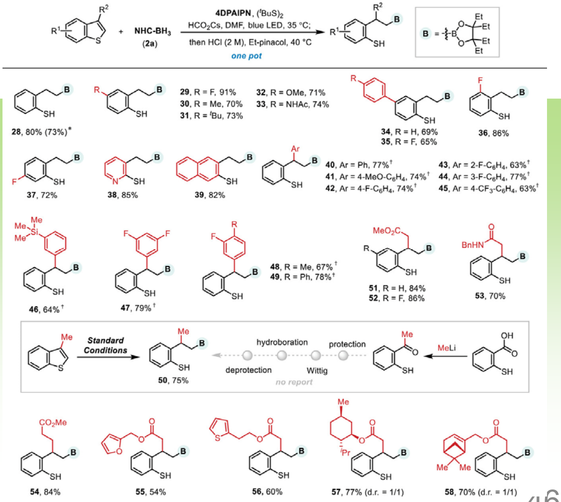
entry	variation from initial conditions	yield of 3 (%)	yield of 4 (%)
1	none	30	7
2	(^{t}BuS)$_2$ (10 mol%) instead of CySH	26	34
3	as entry 2 but with HCO_2Cs (1 equiv.)	65	4
4	as entry 3 but without light	0	0
5	as entry 3 but without **4DPAIPN**	0	0
6	as entry 3 but without (^{t}BuS)$_2$	0	6



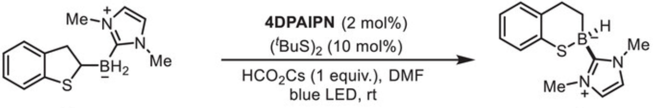
3.1 光催化硼硫键构筑


4DPAIPN (2 mol%)
(^{t}BuS)$_2$ (10 mol%)
HCO$_2$Cs (1 equiv.), DMF
blue LED, 35 °C, 48-72 h
3, 64%
5, 73% (d.r. = 1.1/1)
X-ray of trans-5
6, 73% (d.r. = 1.1/1)
7, 72% (d.r. = 1.1/1)
8, 57% (d.r. = 1.9/1)
9 (X = O), 56% (d.r. = 1.3/1)
10 (X = NH), 47% (d.r. = 1.8/1)
11, 55% (d.r. = 1.9/1)
12, 61%
13, 65%
14, 69%
15, 40% (d.r. = 1.1/1)


4DPAIPN (2 mol%)
(ArS)$_2$ (10 mol%)
γ-terpinene (1 equiv.)
Cs$_2$CO$_3$ (20 mol%), Me$_2$NCHO
blue LED, 35 °C, 72 h
22 (R = H), 54%
X-ray of 22
(ArS)$_2$
23, 54%
24, 58%
25, 51%
26, 51%
27, 49%

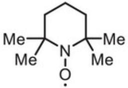

4DPAIPN, (^{t}BuS)$_2$
HCO$_2$Cs, DMF, blue LED, 35 °C;
then HCl (2 M), Et-pinacol, 40 °C
one pot
28, 80% (73%)*
29, R = F, 91%
30, R = Me, 70%
31, R = ^{t}Bu, 73%
32, R = OMe, 71%
33, R = NHAc, 74%
34, R = H, 69%
35, R = F, 65%
36, 86%
37, 72%
38, 85%
39, 82%
40, Ar = Ph, 77%†
41, Ar = 4-MeO-C$_6$H$_4$, 74%†
42, Ar = 4-F-C$_6$H$_4$, 74%†
43, Ar = 2-F-C$_6$H$_4$, 63%†
44, Ar = 3-F-C$_6$H$_4$, 77%†
45, Ar = 4-CF$_3$-C$_6$H$_4$, 63%†
46, 64%†
47, 79%†
48, R = Me, 67%†
49, R = Ph, 78%†
51, R = H, 84%
52, R = F, 86%
53, 70%
Standard Conditions
50, 75%
hydroboration
protection
deprotection
Wittig
no report
MeLi
54, 84%
55, 54%
56, 60%
57, 77% (d.r. = 1/1)
58, 70% (d.r. = 1/1)

3.1 光催化硼硫键构筑

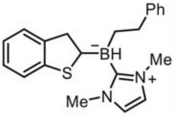


4 → 3

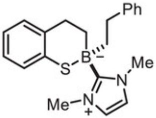
entry	variation from initial conditions	recovery of 4 (%)	yield of 3 (%)
1	none	0	81
2	no **4DPAIPN**	30	59
3	no blue LED	79	0
4	no $(^t\mathrm{BuS})_2$	61	13
5	no HCO_2Cs	0	78
6	**TEMPO** as additive	91	0
7	styrene as additive	0	0 (**68**: 72%; **69**: 9%)



TEMPO

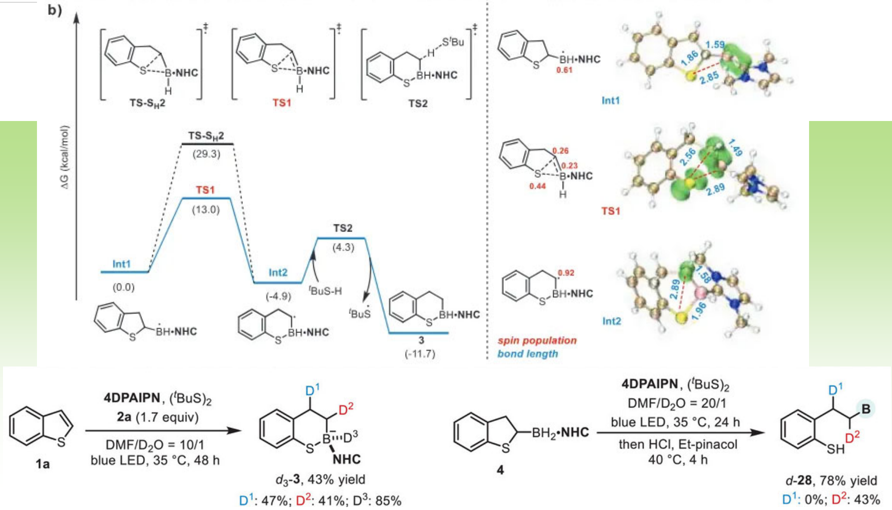


68

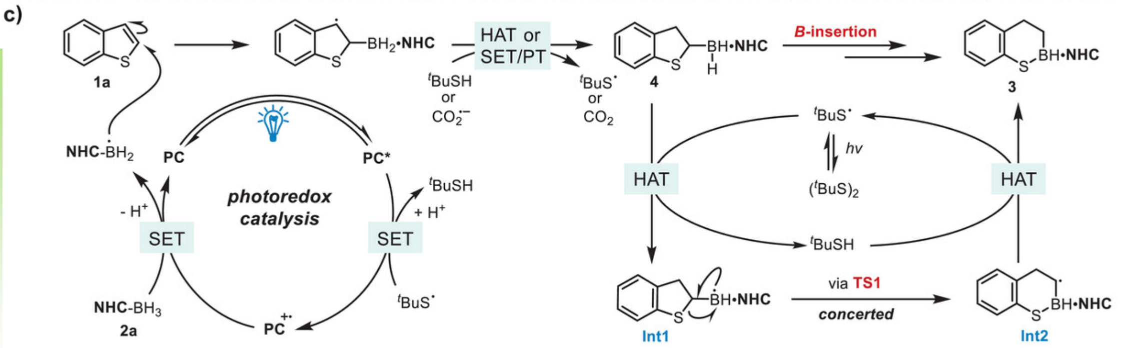


69

3.1 光催化硼硫键构筑


b)
ΔG (kcal/mol)
TS-S$_H$2
TS1
TS2
Int1
(0.0)
(29.3)
(13.0)
Int2
(-4.9)
^{t}BuS-H
TS2
(4.3)
^{t}BuS
3
(-11.7)
BH•NHC
B•NHC
S^{t}Bu
0.61
0.26
0.23
0.44
0.92
1.59
1.86
2.85
2.56
1.49
2.89
1.58
1.96
spin population
bond length
4DPAIPN, (^{t}BuS)$_2$
2a (1.7 equiv)
DMF/D$_2$O = 10/1
blue LED, 35 °C, 48 h
1a
NHC
d_3-3, 43% yield
D[1]: 47%; D[2]: 41%; D[3]: 85%
BH$_2$•NHC
4
4DPAIPN, (^{t}BuS)$_2$
DMF/D$_2$O = 20/1
blue LED, 35 °C, 24 h
then HCl, Et-pinacol
40 °C, 4 h
SH
B
d-28, 78% yield
D[1]: 0%; D[2]: 43%

3.1 光催化硼硫键构筑


c)
1a
BH2•NHC
HAT or
SET/PT
tBuSH
or
CO2•−
tBuS•
or
CO2
4
BH•NHC
H
B-insertion
3
BH•NHC
NHC-BH2
PC
PC*
photoredox
catalysis
- H+
SET
SET
tBuSH
+ H+
NHC-BH3
2a
PC•+
tBuS•
tBuS•
hv
(tBuS)2
HAT
HAT
tBuSH
BH•NHC
Int1
via TS1
concerted
BH•NHC
Int2

3.1 光催化硼硫键构筑

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Article

Spin Delocalization of Nitrile-Ligated Diarylboryl Radicals Enables Photochemical Boracycle Synthesis via *N*-Borylimidoyl Radicals

Yubing Pang, Xiaoyu Yan, Hasil Aman, Meichen Xu, and Juntao Ye*

Cite This: *J. Am. Chem. Soc.* 2025, 147, 25397−25406
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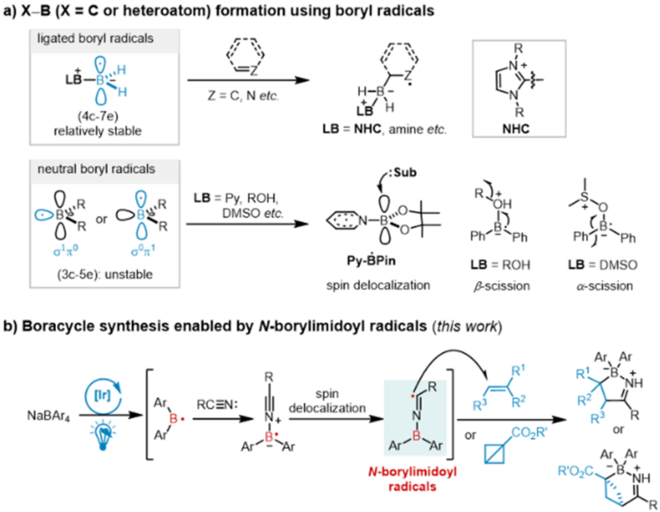
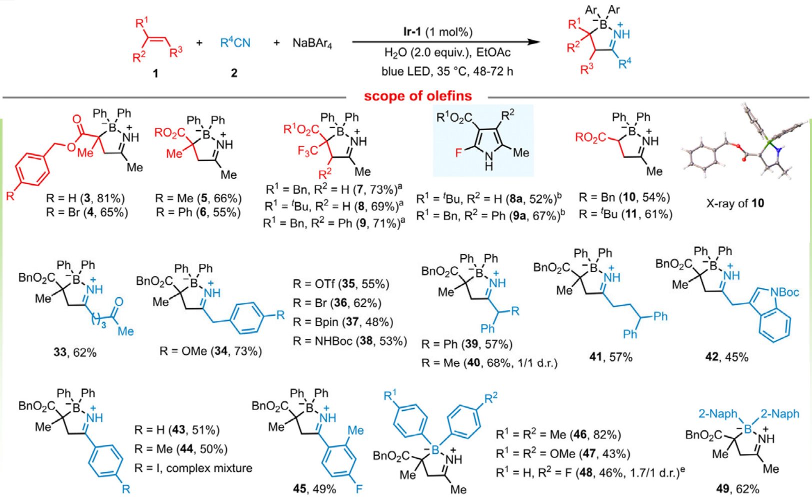
J. Am. Chem. Soc. **2025**, *147*, 25397−25406

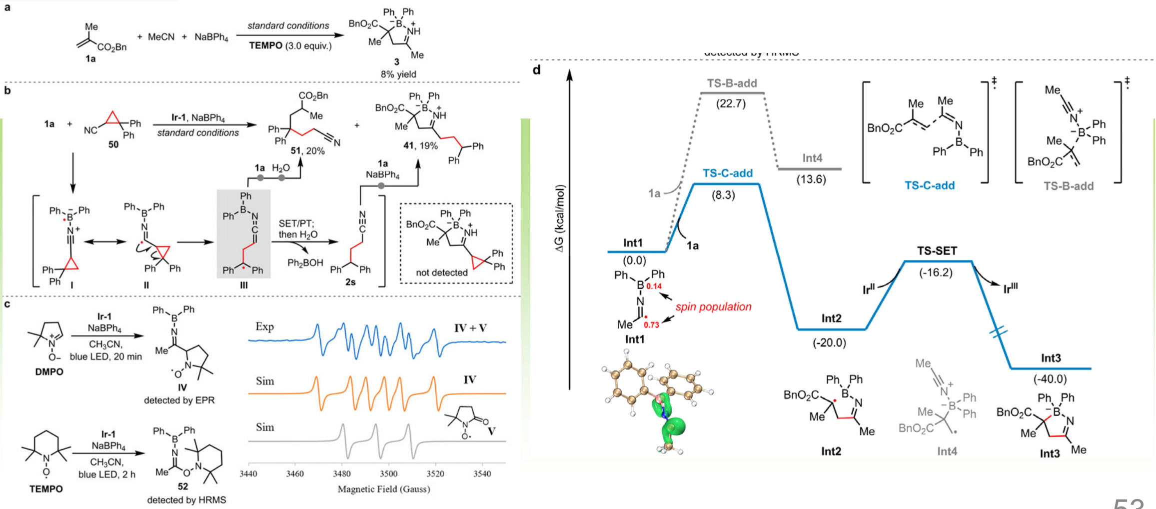
3.1 光催化硼硫键构筑


a) X–B (X = C or heteroatom) formation using boryl radicals
ligated boryl radicals
(4c-7e)
relatively stable
Z = C, N etc.
LB = NHC, amine etc.
NHC
neutral boryl radicals
(3c-5e): unstable
LB = Py, ROH, DMSO etc.
:Sub
Py-BPin
spin delocalization
LB = ROH
β-scission
LB = DMSO
α-scission
b) Boracycle synthesis enabled by N-borylimidoyl radicals (this work)
NaBAr4
[Ir]
RC≡N:
spin delocalization
N-borylimidoyl radicals
or

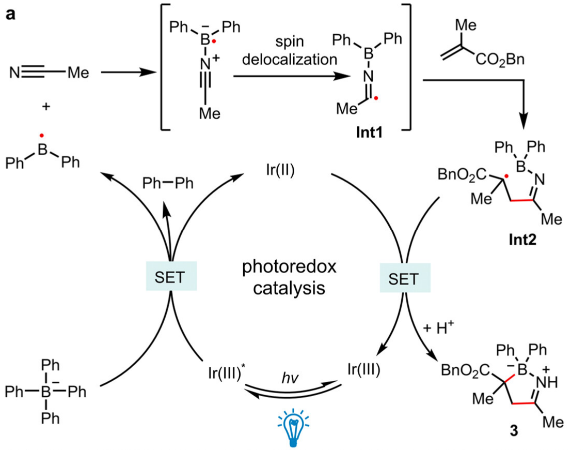
3. 3.2 光催化硼氮键构筑

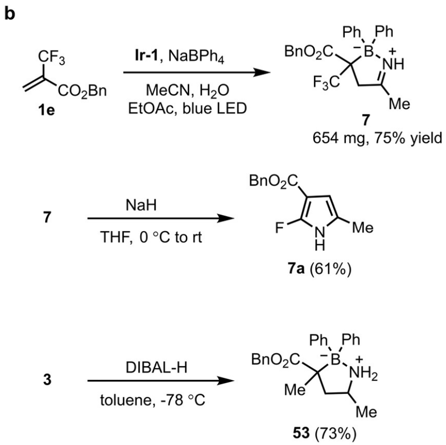


3.2 光催化硼氮键构筑

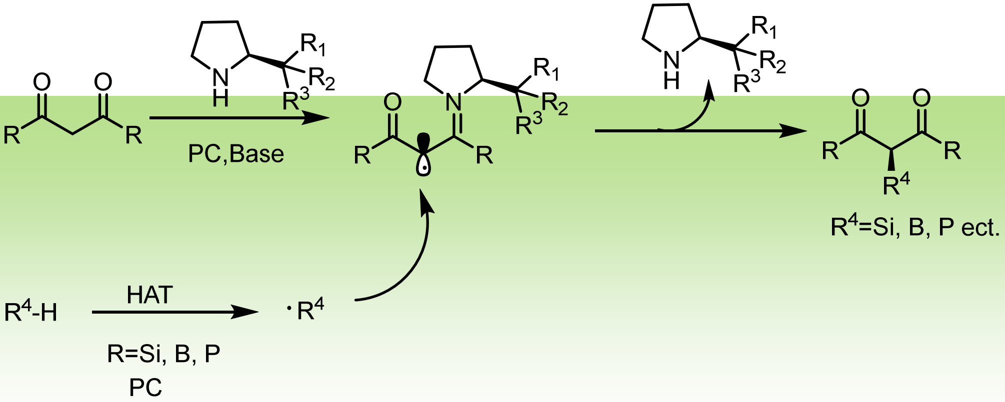

a
1a
+ MeCN + NaBPh4
standard conditions
TEMPO (3.0 equiv.)
3
8% yield
b
50
Ir-1, NaBPh4
standard conditions
51, 20%
41, 19%
SET/PT; then H2O
Ph2BOH
2s
not detected
c
DMPO
Ir-1
NaBPh4
CH3CN,
blue LED, 20 min
IV
detected by EPR
TEMPO
blue LED, 2 h
52
detected by HRMS
Exp
IV + V
Sim
IV
Sim
V
3440
3460
3480
3500
3520
3540
Magnetic Field (Gauss)
d
ΔG (kcal/mol)
TS-B-add
(22.7)
Int4
(13.6)
TS-C-add
(8.3)
Int1
(0.0)
1a
spin population
0.14
0.73
Int2
(-20.0)
TS-SET
(-16.2)
Int3
(-40.0)
TS-C-add
TS-B-add

3.2 光催化硼氮键构筑


a
N≡—Me
+
Ph–B–Ph
Ph–B–Ph
N+
Me
spin delocalization
Ph–B–Ph
N
Me
Int1
Me
CO2Bn
Ph Ph
BnO2C
B
N
Me
Me
Int2
Ph–Ph
Ir(II)
SET
photoredox catalysis
SET
+ H+
Ph
Ph–B–Ph
Ph
Ir(III)*
hv
Ir(III)
Ph Ph
BnO2C
B
+
NH
Me
Me
3


b
CF3
CO2Bn
1e
Ir-1, NaBPh4
MeCN, H2O
EtOAc, blue LED
Ph Ph
BnO2C
B
+
NH
F3C
Me
7
654 mg, 75% yield
7
NaH
THF, 0 °C to rt
BnO2C
F
N
H
Me
7a (61%)
3
DIBAL-H
toluene, -78 °C
Ph Ph
BnO2C
B
+
NH2
Me
Me
53 (73%)

4.Proposal


O
O
R
R
N
H
R1
R2
R3
PC,Base
O
N
R
R
R1
R2
R3
N
H
R1
R2
R3
O
O
R
R
R4
R4=Si, B, P ect.
R4-H
HAT
·R4
R=Si, B, P
PC

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Precise Synthesis Lab at Tongji University

谢 谢 聆 听

Topic report

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