

# Synthesis of $\beta$ -Phenethylamines via Ni/Photoredox Cross-Electrophile Coupling of Aliphatic Aziridines and Aryl Iodides

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Cite This: <https://dx.doi.org/10.1021/jacs.0c01724>

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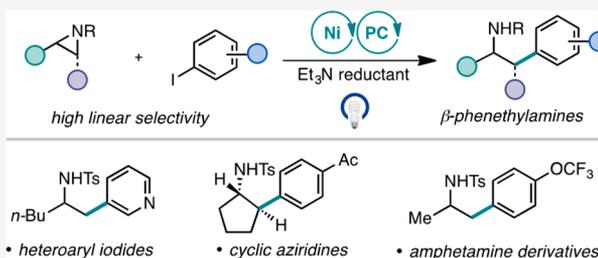
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**ABSTRACT:** A photoassisted Ni-catalyzed reductive cross-coupling between tosyl-protected alkyl aziridines and commercially available (hetero)aryl iodides is reported. This mild and modular method proceeds in the absence of stoichiometric heterogeneous reductants and uses an inexpensive organic photocatalyst to access medicinally valuable  $\beta$ -phenethylamine derivatives. Unprecedented reactivity was achieved with the activation of cyclic aziridines. Mechanistic studies suggest that the regioselectivity and reactivity observed under these conditions are a result of nucleophilic iodide ring opening of the aziridine to generate an iodoamine as the active electrophile. This strategy also enables cross-coupling with Boc-protected aziridines.



## INTRODUCTION

The  $\beta$ -phenethylamine scaffold is an important nitrogen-containing motif in medicinal chemistry, with thousands of reported derivatives possessing varied pharmacological activity (Figure 1A).<sup>1</sup> Phenethylamine itself is a monoaminergic neuromodulator. Numerous phenethylamine derivatives are naturally occurring and bioactive, such as dopamine, norepinephrine, and adrenaline.<sup>2</sup> Synthetic derivatives belong to a range of different drug classes, such as antidepressants, anti-Parkinson agents, appetite suppressants, and decongestants. For example, amphetamine and its derivatives are important for central nervous system treatments. As a result of the strong interest in accessing the  $\beta$ -phenethylamine substructure, a variety of synthetic approaches have been devised.<sup>3</sup>

The arylation of aliphatic aziridines represents a particularly attractive retrosynthetic disconnection due to its modularity, enabling the installation of diverse (hetero)aryl groups and ethyl backbone substitutions in a single C–C bond-forming step. Most examples in this context rely on the use of organocuprates, generated from aryl lithium or Grignard reagents, in combination with a strong Lewis acid, which can lead to limited functional group compatibility and poor regioselectivity (Figure 1B).<sup>4</sup> In 2013, Michael and co-workers reported a Pd-catalyzed Suzuki coupling of aliphatic aziridines with aryl boronic acids that affords  $\beta$ -phenethylamines in high regioselectivity.<sup>5a</sup> Recently, Zhao and co-workers reported a Pd-catalyzed C–H coupling of benzoic acids and aliphatic aziridines (Figure 1B).<sup>5</sup> Although these reports significantly advanced the state of the art, both methods relied on the use of a precious metal catalyst and were only applicable to terminal aliphatic aziridines.<sup>5b</sup> Additionally, the latter methodology relied on a carboxylic acid to direct C–H activation. Therefore,

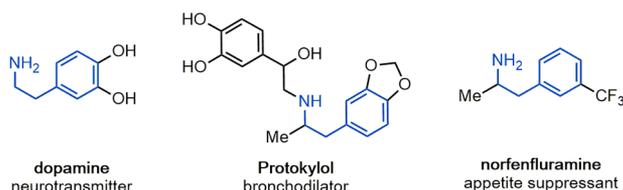
the development of complementary catalytic methods is necessary to expand the generality and practicality of this approach for the synthesis of  $\beta$ -phenethylamines.

Over the past decade, our lab and the Jamison lab have reported Ni-catalyzed Negishi cross-coupling reactions of aziridines (Figure 1B).<sup>7</sup> Moreover, Zhou and co-workers have reported a Ni/photoredox cross-coupling of styrenyl aziridines and potassium benzyltrifluoroborates.<sup>8</sup> However, identification of a general and selective protocol to access  $\beta$ -phenethylamine products, particularly  $\alpha$ -substituted phenethylamines, has been challenging.<sup>9,10</sup> Recently, we reported a reductive cross-electrophile coupling of tosyl-protected (*N*-Ts) styrenyl aziridines with aryl iodides that selectively yielded the branched isomeric product (Figure 1C).<sup>11,12</sup> The use of widely available and bench stable aryl iodide electrophiles, without the need to pregenerate organometallic reagents, provided a practical advantage over conventional Ni-catalyzed cross-coupling procedures with aziridines. Albeit, this strategy was still not applicable to the preparation of  $\alpha$ -substituted  $\beta$ -phenethylamine products, as aliphatic aziridines were unreactive.

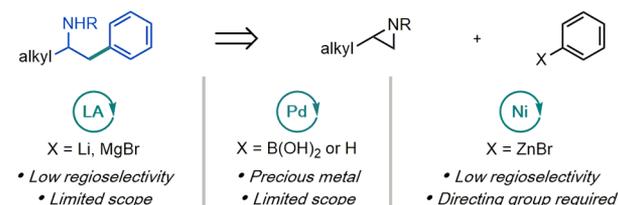
We report here the development of a photocatalytic Ni-catalyzed cross-electrophile coupling strategy with aliphatic aziridines and (hetero)aryl iodides that delivers a broad range of  $\beta$ -phenethylamine scaffolds (Figure 1D). Recent studies

Received: February 12, 2020

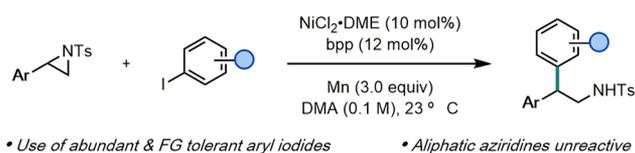
## A. Examples of bioactive and pharmaceutically relevant



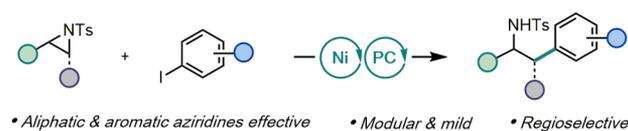
## B. Approaches to



## C. Prior work: reductive cross-coupling with styrenyl aziridines



## D. This work: photocatalytic cross-coupling with aliphatic aziridines



**Figure 1.** Bioactive and pharmaceutically relevant  $\beta$ -phenethylamines and aziridine cross-coupling methodologies. bpp = 2,6-bis(*N*-pyrazolyl)-pyridine.

have demonstrated that it is possible to use a visible-light photoredox catalyst in conjunction with an amine as the reductant in Ni-catalyzed cross-electrophile coupling reactions.<sup>13</sup> An advantage of this approach is that it addresses challenges inherent to the use of heterogeneous reductants in traditional protocols. The methodology reported here highlights that a photocatalytic cross-electrophile coupling can also impart distinct and previously inaccessible reactivity compared to cross-electrophile couplings with Mn as a reductant. Mechanistic studies were performed to probe this variation in reactivity.

## RESULTS AND DISCUSSION

**Optimization.** Our initial investigations focused on the coupling of aliphatic aziridine **1a** with 4'-iodoacetophenone jointly catalyzed by a nickel catalyst and a visible-light photoredox catalyst (Table 1). Different amine-based reductants, solvents, catalyst loadings and reaction concentrations were investigated (see SI Optimization Studies). We found that linear isomer **2a** could be obtained in 59% yield (1:b > 10:1) using NiBr<sub>2</sub>·DME/4,4'-di-*tert*-butylbipyridine (dtbbpy) as the cross-coupling catalyst, 1,2,3,5-tetrakis(carbazol-9-yl)-4,6-dicyanobenzene (4CzIPN) as the photocatalyst, and Et<sub>3</sub>N as the reductant (Table 1, entry 1).<sup>14</sup> While homocoupling is often an issue in cross-electrophile coupling reactions, therefore requiring a large excess of aryl halide, only 15% of biaryl product was observed under these conditions using 1.5

Table 1. Optimization Table

Reaction scheme: **1a** + (1.5 equiv)  $\xrightarrow[\text{Et}_3\text{N (3.0 equiv), THF (0.08 M), 24 h, 34 W blue LEDs}]{\text{NiBr}_2\cdot\text{DME (5 mol\%), dtbbpy (10 mol\%), 4CzIPN (4 mol\%)}}$  **2a**

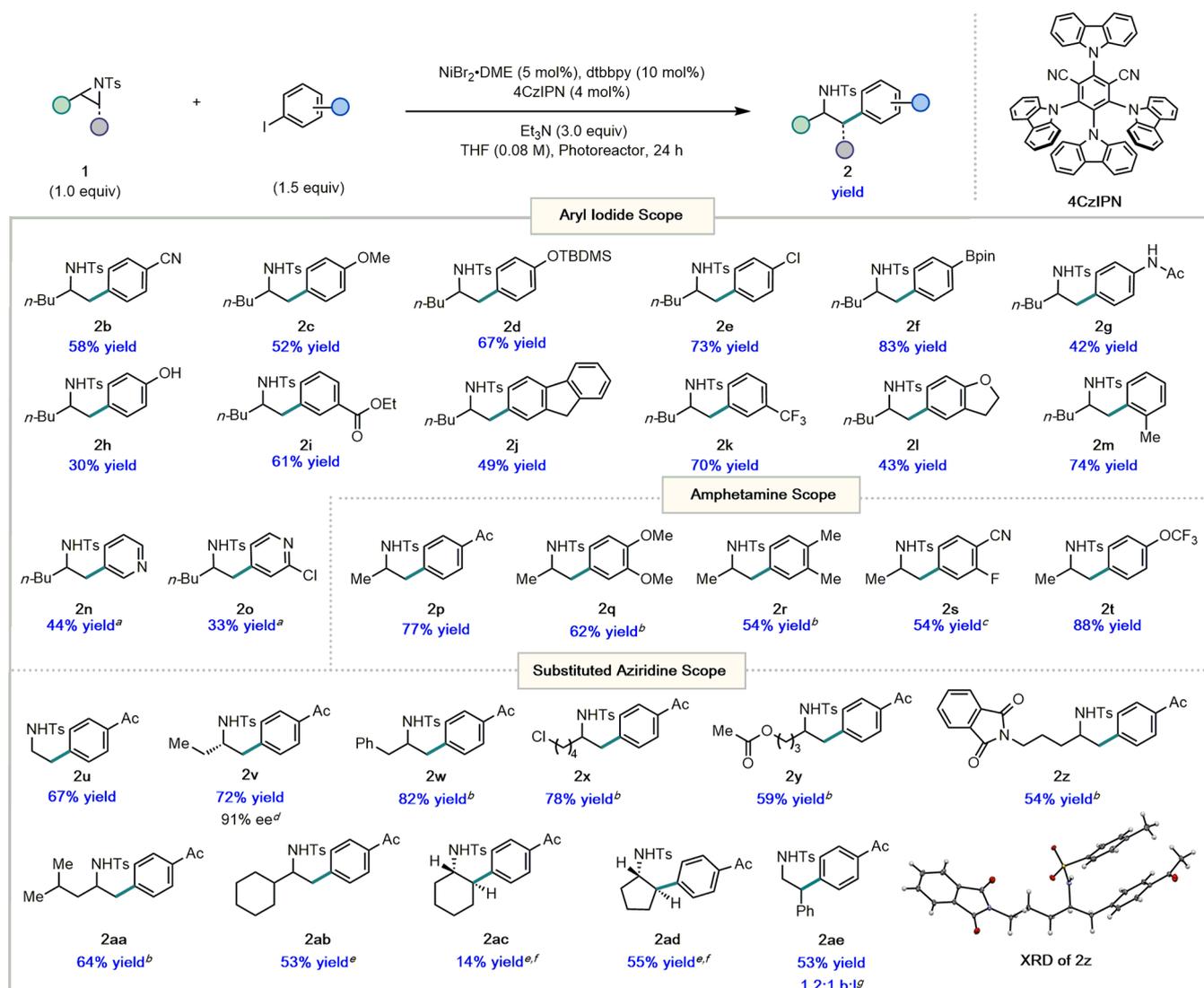
entry	deviation from standard conditions	conversion of <b>1a</b> [%]	yield [%] <sup>a</sup>
1	none	100	59
2	4'-bromoacetophenone	82	0
3	Ir(dF-CF <sub>3</sub> -ppy) <sub>2</sub> (dtbbpy)PF <sub>6</sub>	100	57
4	no Et <sub>3</sub> N	30	0
5	no dtbbpy	61	0
6	no Ni	100	0
7	no 4CzIPN	11	0
8	no light	0	0 <sup>b</sup>
9	0.5 mmol scale	70	46
10	0.5 mmol scale for 48 h	>95	76
11	photoreactor on 0.5 mmol scale	100	82 (72) <sup>c</sup>

<sup>a</sup>Reaction run on 0.1 mmol scale. Yields are the average of two runs and were determined using 1,3,5-trimethoxybenzene (1.0 equiv) as an external standard. <sup>b</sup>Reaction run at 40 °C. <sup>c</sup>Isolated yield.

equiv of aryl iodide.<sup>15</sup> Aryl bromides proved to be ineffective for the transformation (Table 1, entry 2). The use of an Ir-photocatalyst that has similar redox potentials to 4CzIPN was also successful, delivering **2a** in 57% yield (Table 1, entry 3). However, 4CzIPN was elected for further study since it is easily synthesized from inexpensive materials and avoids the use of a precious metal. Control studies showed that Ni, ligand, photocatalyst, light, and Et<sub>3</sub>N were all required in the reaction (Table 1, entry 4–8). Lastly, for larger scale reactions (0.5 mmol), 82% yield was obtained by switching from the use of 34 W blue LEDs to a 450 nm photoreactor (Table 1, entry 9–11).<sup>16</sup>

**Substrate Scope.** The generality of the transformation was evaluated under the optimized conditions (Figure 2). In all cases examined, terminal aliphatic aziridines yielded the linear coupled product in high selectivity. A wide range of *para*-substituted aryl iodides containing either electron-withdrawing or electron-donating functionality were tolerated, delivering products with nitrile (**2b**), methoxy (**2c**), and silyl ether (**2d**) groups in good yield. The reaction proceeded well with aryl iodides containing functionality that would be challenging to access with methods that use organozinc, organolithium, or Grignard reagents, including chloride (**2e**), boronate ester (**2f**), acetanilide (**2g**), protic (**2h**), and carbonyl (**2i**) groups. *Meta*- and *ortho*-substituted aryl iodides were also tolerated (**2j–m**). In contrast to previously reported aziridine cross-coupling methodologies, heteroaryl iodides, a substrate class of high value in medicinal chemistry and library drug design, were competent coupling partners, providing the desired  $\beta$ -heteroarylethylamine products **2n** and **2o**.<sup>17a</sup>

We also investigated the scope of 2-alkyl-substituted tosyl-protected aziridines. Amphetamine derivatives, which are pharmaceutically valuable motifs, were obtained in moderate to high yields (**2p–t**) from methyl-substituted aziridine with variation in aryl functionality such as trifluoromethoxy or 4-cyano-3-fluoro-phenyl groups. The unsubstituted ethylene-derived aziridine provided the corresponding phenethylamine **2u** in 67% yield. The reaction of an enantiopure aziridine afforded product **2v** with minimal erosion of enantioselectivity,



**Figure 2.** Reaction substrate scope. Reactions were run on 0.5 mmol scale and yields are the average of two runs. <sup>a</sup>10 mol % Ni, 20 mol % dtbbpy, and 1.25 equiv Ar–I. <sup>b</sup>Reaction run for 48 h. <sup>c</sup>Product contains 10% of branched isomer, reported yield is corrected to account for this. <sup>d</sup>Aziridine 95% ee. Determined by HPLC. <sup>e</sup>Reaction run for 72 h. <sup>f</sup>Selectivity determined by <sup>1</sup>H NMR. <sup>g</sup>b:l ratio determined by <sup>1</sup>H NMR.

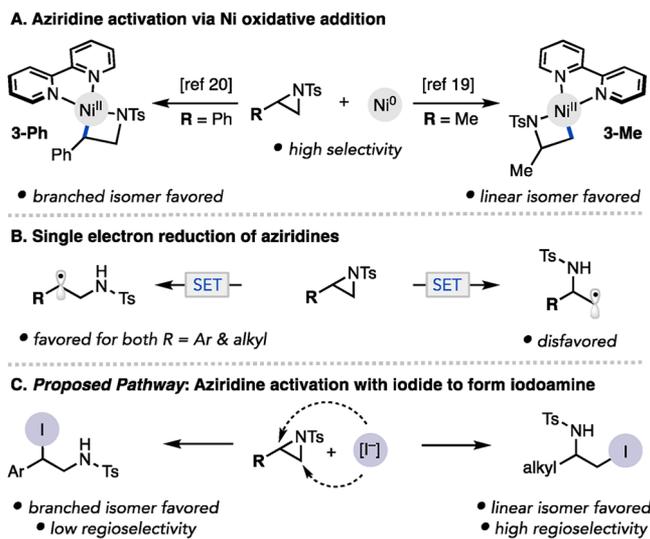
suggestive of exclusive activation at the less-substituted C–N bond. Photocatalytic cross-electrophile coupling proceeded smoothly with aziridines containing synthetically versatile functional groups such as benzylic **2w**, aliphatic chloride **2x**, ester **2y**, and phthalimide **2z**. Introduction of  $\beta$ - and even  $\alpha$ -branching to the aziridine substrate showed no deterioration in yield, with **2aa** and **2ab** generated in 64% and 53% yield, respectively. However, aliphatic 2,2-disubstituted aziridines showed limited reactivity.<sup>17b</sup>

Notably, cyclic 2,3-disubstituted aziridines were competent coupling partners. For instance, cross-coupling with cyclohexyl aziridine furnished product **2ac** in 14% yield and cyclopentyl aziridine afforded product **2ad** in 55% yield. Both products were formed exclusively as *trans* diastereomers. It is likely that the enhancement in yield of **2ad** in comparison to **2ac** arises from an increase in ring strain leading to more effective aziridine activation. To the best of our knowledge, no prior catalytic aziridine cross-coupling methods have been successful with this substrate class. Furthermore, whereas previous Ni-catalyzed methodologies have not been general for both

aromatic and aliphatic aziridines, this photocatalytic strategy is: cross-coupling with styrenyl aziridine afforded **2ae** in 53% yield as a mixture of branched and linear isomers in a 1.2:1 (b:l) ratio. The generation of the linear product under the photocatalytic coupling conditions was unexpected based on prior work. For example, under our previously reported cross-electrophile conditions with Mn, styrenyl aziridines delivered exclusively the branched isomer with bpp or dtbbpy as the ligand (Figure 1C).<sup>18</sup>

**Mechanistic Investigations.** The b:l mixture observed for styrenyl aziridine and the reactivity with cyclic aziridines are unprecedented in Ni-catalyzed cross-coupling reactions. This prompted us to examine the mechanism of the photoassisted cross-coupling.

Previous Ni-catalyzed aziridine cross-coupling methodologies were proposed to proceed via aziridine oxidative addition to Ni, an elementary step that has been studied across various ligand and aziridine classes (Figure 3A). For example, Hillhouse and Jamison have shown that oxidative addition of bpy- or phen-ligated Ni<sup>0</sup> to a *N*-Ts aliphatic aziridine occurs at



**Figure 3.** Possible pathways for aziridine activation. SET = single electron transfer.

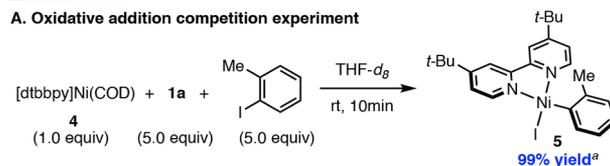
the terminal C–N bond to yield **3-Me**.<sup>19</sup> In contrast, our group has shown that for *N*-Ts styrenyl aziridines, oxidative addition occurs through cleavage of the internal C–N bond with [bpy]Ni(COD) to form **3-Ph**.<sup>20</sup> The nearly equal b:l product regioselectivity for *N*-Ts styrenyl aziridine observed under the photoassisted reaction conditions is inconsistent with this regiochemical outcome of aziridine oxidative addition. To provide additional evidence against this aziridine activation mechanism, we conducted a competition experiment between Ar–I (5.0 equiv) and aziridine **1a** (5.0 equiv) with [dtbbpy]Ni<sup>0</sup>(COD)(**4**) (1.0 equiv) (Figure 4A). Exclusive reactivity of the Ar–I was observed in less than 10 min, suggesting that aziridine activation by Ni<sup>0</sup> is unlikely under these reaction conditions.

For these reasons, we considered several alternative aziridine activation mechanisms. First, direct single-electron reduction of the aziridine by the photocatalyst could afford a radical intermediate that is intercepted by Ni in cross-coupling (Figure 3B).<sup>8b</sup> Alternatively, the aziridine could undergo in situ ring opening by iodide to generate a  $\beta$ -iodoamine, followed by photocatalytic Ni-catalyzed cross-electrophile coupling to render the product (Figure 3C).

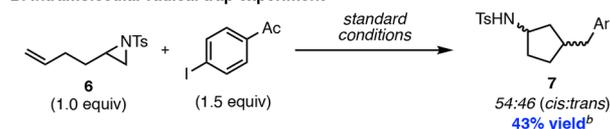
As a mechanistic probe for direct reduction of the aziridine by the photocatalyst, the reaction of aziridine **1a**, Et<sub>3</sub>N, and 4CzIPN was evaluated in the presence of light. However, no consumption of aziridine was observed. Furthermore, single-electron reduction of **1a** by either the photocatalyst or Ni would favor the generation of a 2° versus 1° radical, ultimately affording the branched cross-coupled product or racemization of enantioenriched **2v** if ring opening was reversible. Since neither of these are observed, this suggests that single-electron reduction of the aziridine is not taking place. Nevertheless, use of aziridine **6** under the reaction conditions afforded cyclized product **7** in 43% yield as a 54:46 mixture of *cis:trans* diastereoisomers (Figure 4B). This provides support for the involvement of a carbon-centered radical in cross-coupling.

In evaluating iodide ring opening as a mechanism for aziridine activation (Figure 3C), we noted that the b:l selectivity observed for the photocatalytic styrenyl and aliphatic aziridine coupling reactions is similar to that reported

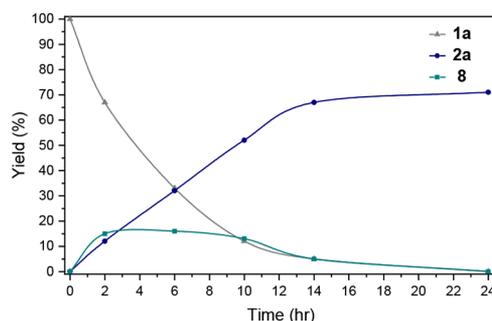
**A. Oxidative addition competition experiment**



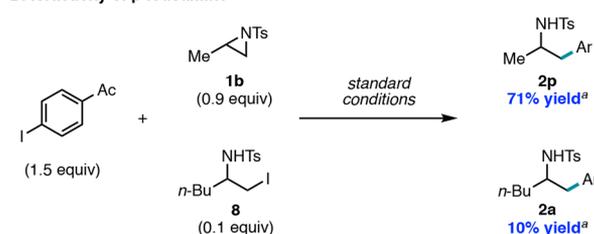
**B. Intramolecular radical trap experiment**



**C. Reaction time course**



**D. Reactivity of  $\beta$ -iodoamine**



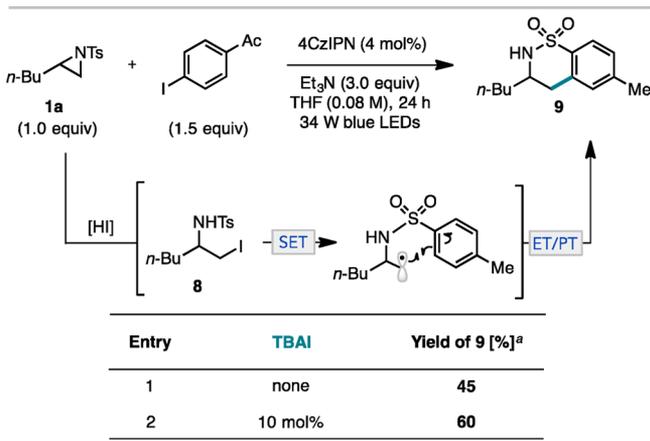
**Figure 4.** Mechanistic experiments. Standard conditions are the same as in Figure 1, entry 1. <sup>a</sup>Yields were determined by <sup>1</sup>H NMR using 1,3,5-trimethoxybenzene (1.0 equiv) as an external standard. <sup>b</sup>Isolated yield.

for halide ring opening of aziridines.<sup>21</sup> The expansion in scope to include cyclic aliphatic aziridines is also consistent with this proposal since these aziridines have not been observed to undergo oxidative addition with Ni or Pd, but secondary alkyl iodides are competent in cross-electrophile coupling reactions.<sup>22</sup> Additionally, Weix and co-workers have reported Ni-catalyzed epoxide cross-electrophile coupling reactions that are proposed to proceed through in situ formation of an iodohydrin using Et<sub>3</sub>N·HCl and NaI as exogenous additives alongside Zn as a reductant.<sup>23</sup>

To further evaluate the iodide ring-opening proposal, we sought evidence for the generation of  $\beta$ -iodoamine under the reaction conditions. Monitoring the reaction of **1a** by <sup>1</sup>H NMR, we observed formation of  $\beta$ -iodoamine **8** within the first 2 h (Figure 4C). As the reaction proceeded, **8** was present in approximately 15% yield, while a decrease of aziridine **1a** and an increase in cross-coupled product **2a** occurred. Detection of **8** in this reaction cannot be taken as direct evidence for its involvement in cross-coupling since the mass balance is such that it could be involved in unproductive chemistry. Evidence in favor of the direct involvement of the iodoamine in cross-coupling was obtained by subjecting a catalytic amount of **8** (0.1 equiv) in combination with aziridine **1b** (0.9 equiv) to the

reaction conditions (Figure 4D).<sup>24</sup> In this case, product **2a** was observed in 10% yield (quantitative yield relative to  $\beta$ -iodoamine **8**) as well as product **2p** in 71% yield.

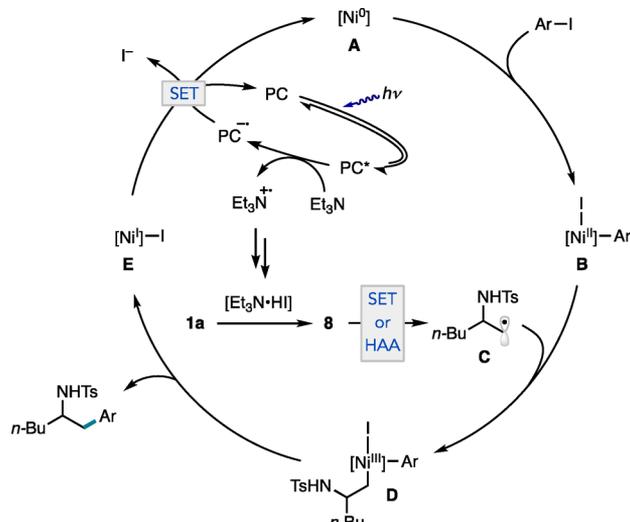
To understand whether iodoamine formation is reliant on Ni, aziridine **1a** and 4'-iodoacetophone were subjected to the photocatalytic conditions without Ni.<sup>25</sup> Complete consumption of the aziridine was observed, but the iodide-opened intermediate **8** was not detected (Figure 5). Instead, sultam **9**



**Figure 5.** Photocatalytic reactions in the absence of Ni. <sup>a</sup>Yields are the average of two runs and were determined by <sup>1</sup>H NMR using 1,3,5-trimethoxybenzene (1.0 equiv) as an external standard. ET/PT = electron transfer/proton transfer.

was obtained in 45% yield. While unexpected, the generation of sultam **9** provides indirect support for the intermediacy of iodoamine **8** and suggests that iodide ring opening can occur independent of Ni. While sultam is present in highest yields in the absence of Ni, it was also detected in trace amounts under the standard catalytic conditions (for example, see SI page S12). Sultam **9** likely arises from aziridine **1a** by iodide ring opening to form **8**, followed by photocatalytic alkyl iodide reduction and intramolecular radical cyclization.<sup>26,27</sup> Consistent with this proposal, addition of a catalytic amount of tetrabutylammonium iodide (TBAI) to the Ni-free reaction resulted in an increase in yield of **9** (Figure 5, entry 2). Moreover, subjecting iodoamine **8** directly to the photocatalytic conditions in the absence of Ni afforded **9** in 18% yield (see SI page S34). In addition to providing support for the mechanistic proposal, the photocatalytic isomerization of *N*-Ts aziridines to sultams represents an attractive synthetic approach to these medicinally valuable heterocycles.<sup>28</sup>

**Discussion.** These data suggest that iodide ring opening is a likely mechanism for aziridine activation in the photocatalytic cross-electrophile coupling. A catalytic cycle that incorporates an iodoamine and radical intermediate is proposed (Figure 6). First, facile oxidative addition of the aryl iodide with Ni<sup>0</sup> generates **B**. Concomitantly, nucleophilic iodide ring opening of **1a** is mediated by the in situ generation of HI (see SI page S37) to form **8**. SET of **8** (with either [dtbbpy]Ni<sup>I</sup>-I **E** or 4CzIPN<sup>•-</sup>) or halogen atom abstraction (HAA) from **E** generates **C**.<sup>29</sup> This radical intermediate can be trapped with **B** to generate **D**. The formation of **D** allows for reductive elimination to yield the cross-coupled product and intermediate **E**, which can be reduced by 4CzIPN<sup>•-</sup> (PC/PC<sup>•-</sup> = -1.21 vs SCE in MeCN, Ni<sup>I</sup>/Ni<sup>0</sup> = -1.17 vs SCE in THF).<sup>30</sup> While a Ni<sup>0</sup>/Ni<sup>II</sup>/Ni<sup>III</sup>/Ni<sup>I</sup> cycle is proposed, a mechanism that



**Figure 6.** Proposed catalytic cycle. HAA = halogen atom abstraction.

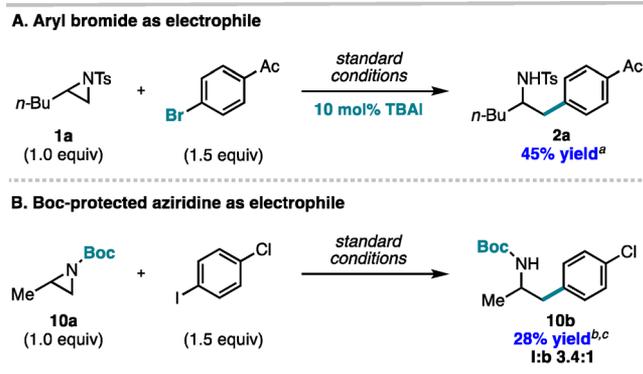
involves selective addition of Ni<sup>I</sup>-I **E** to the aryl iodide, followed by single-electron reduction and reaction of the resulting Ni<sup>I</sup>-aryl intermediate with iodoamine **8**, is also consistent with the data presented and a recent mechanistic study by Diao and co-workers (see SI page S38).<sup>31,32</sup>

As previously noted, aliphatic aziridines were not effective substrates in the Mn-mediated Ni-catalyzed reductive coupling. In light of the above mechanistic studies, we hypothesized that the difference in scope between the Mn and photocatalytic protocol was due to the generation of HI under the photocatalytic conditions, which facilitates aziridine ring opening and subsequent cross-coupling. While iodide is also a byproduct of the Mn-mediated coupling, it is likely more strongly sequestered as the MnI<sub>2</sub> salt, preventing the formation of **8**. Indeed, addition of MnI<sub>2</sub> under our previously reported Ni/Mn conditions (1.0 equiv) with aziridine **1a** did not result in any detectable cross-coupled product nor iodoamine **8**. However, the use of **8** (1.0 equiv) instead of aziridine **1a** generated **2a** in 27% yield with bpp as ligand and 60% yield using dtbbpy (see SI S35–S36).

Prior mechanistic studies on C(sp<sup>3</sup>)-C(sp<sup>2</sup>) cross-electrophile coupling reactions have implicated the importance of Ni<sup>I</sup> intermediates for selective activation of the C(sp<sup>3</sup>) electrophile. Whereas our competition experiments between aziridine and aryl iodide indicate that oxidative addition of Ni<sup>0</sup> is selective for iodoarene over aziridine, Ni<sup>I</sup>-I **E** or Ni<sup>I</sup>-Ar (as in Figure S13) is likely selective for aziridine activation.<sup>15b,29,31</sup> Under the Mn-reductive coupling conditions, Ni<sup>I</sup> or Mn could activate the aziridine via SET. Due to the stability of benzylic radicals, styrenyl aziridines are expected to be more effective reaction partners than aliphatic aziridines, thereby explaining why only styrenyl aziridines are reactive under the Mn conditions. Under the photocatalytic conditions, in situ formation of iodoamine from the aliphatic aziridine restores the ability of this substrate class to participate in cross-electrophile coupling through SET or HAA with Ni<sup>I</sup> or photocatalyst.

**Expansion of the Methodology Based on Mechanistic Findings.** The new mechanistic inference led us to hypothesize that the scope could be expanded to previously unsuccessful substrates. For example, aryl bromides did not provide the cross-coupled product presumably because

bromoamine is an ineffective electrophile under these conditions. Consistent with this hypothesis, addition of TBAI (10 mol %) to the aziridine coupling reaction with 4'-bromoacetophenone restored reactivity to give **2a** in 45% yield (Figure 7A).



**Figure 7.** Expansion in scope based on mechanistic findings. Standard conditions are the same as in Figure 1, entry 1. <sup>a</sup>Yields are the average of two runs and were determined by <sup>1</sup>H NMR using 1,3,5-trimethoxybenzene (1.0 equiv) as an external standard. <sup>b</sup>l:b ratio determined by <sup>1</sup>H NMR. <sup>c</sup>Yields are the average of two isolated runs.

For previous Ni-catalyzed aziridine cross-coupling reactions, the use of *N*-Ts protected aziridines was necessary to facilitate oxidative addition of Ni to the aziridine.<sup>9,19,20</sup> Since cross-coupling is not mediated by Ni-aziridine oxidative addition under the photocatalytic conditions, we wondered whether alternative protecting groups that are easier to deprotect but were previously unsuccessful in Ni-catalyzed aziridine cross-coupling reactions could be used.<sup>33</sup> Gratifyingly, employment of *N*-Boc aziridine **10a** yielded product **10b** in 28% yield as a 3.4:1 l:b mixture (Figure 7B). These results further highlight the opportunities available with this new strategy, which were previously not possible with Ni-catalyzed aziridine cross-coupling reactions.

## CONCLUSIONS

In summary, we have described a Ni-photoredox protocol that enables the modular assembly of a large scope of  $\beta$ -phenethylamine derivatives, allowing access to high value substrate classes for medicinal chemists. Many of the substrates have previously proven to be challenging for conventional aziridine cross-coupling methodologies. More generally, the results highlight for cross-electrophile couplings that a photocatalytic protocol can enable distinct scope compared to that using heterogeneous reductants. Mechanistic studies indicate that formation of an iodoamine through nucleophilic iodide ring opening is key for successful reactivity. This aziridine activation mode differs in comparison to those in previous TM-catalyzed methods that are reliant on oxidative C–N bond activation. On the basis of the described mechanistic details, ongoing studies are focused on utilizing this activation strategy for other strained ring systems with photocatalytic Ni cross-electrophile coupling catalysis.

## ASSOCIATED CONTENT

### Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/jacs.0c01724>.

Experimental details, optimization studies, and characterization data (PDF)

Crystallographic data (CIF)

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### Author Contributions

<sup>†</sup>J.L. and A.M. contributed equally.

### Notes

The authors declare no competing financial interest.

## ACKNOWLEDGMENTS

Financial support was provided by NIGMS R35 GM126986 and an F32 Ruth L. Kirschstein NRSA Fellowship under Award No. F32 EB027587-01 (T.J.S.). The authors gratefully acknowledge Dr. Brian P. Woods for preliminary investigations and Dr. Christoph Heinz for initial substrate scope isolations. We thank Jesus I. Martinez Alvarado for help with emission quenching studies. Dr. Phillip D. Jeffrey is acknowledged for X-ray crystallography. Lotus Separations is thanked for assistance with the purification of **7**.

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