

## Versatile Cross-Dehydrogenative Coupling of Heteroaromatics and Hydrogen Donors via Decatungstate Photocatalysis

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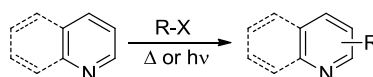
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**A facile sunlight-induced derivatization of heteroaromatics via photocatalyzed C-H activation in amides, ethers, alkanes and aldehydes is described. Tetrabutylammonium decatungstate (TBADT) was used as the photocatalyst and allowed to carry out the process under mild and acid-free conditions.**

The importance of functionalized heterocycles in medicinal chemistry is well known.<sup>1</sup> This calls for mild and efficient procedures for the introduction of substituents onto a preformed heterocycle. One dated example is the Minisci reaction, reported for the first time more than 40 years ago,<sup>2,3</sup> that is still an important tool for medicinal chemists.<sup>3</sup> The original protocol involved the thermal generation of radicals via decarboxylation of carboxylic acids mediated by an Ag<sup>I</sup> salt in the presence of persulfate anion.<sup>2</sup> Radicals then attacked the (protonated) heterocycle and gave the desired alkylated derivatives.<sup>4</sup>

Several protocols have been later developed starting from alkyl halides,<sup>5</sup> aryl<sup>6a</sup> or alkyl boronic acids,<sup>6b</sup> alkyl or alkoxyethyl trifluoroborates,<sup>6b,c</sup> zinc sulfinate salts,<sup>6d</sup> aryl diazonium salts,<sup>6e</sup> *t*Bu esters<sup>6f</sup> and aminoacids<sup>6g</sup> as radical precursors (Scheme 1, path a). A more challenging approach, however, consists in the Minisci reaction via radicals formed by activation of C-H bonds. Sparse examples were recently described, where radicals were obtained from ethers,<sup>7</sup> aldehydes,<sup>8</sup> amides,<sup>9</sup> toluenes<sup>10</sup> and even alkanes<sup>7a,11</sup> by thermal or photoinduced homolytic C-H cleavage (Scheme 1, path b). Some drawbacks are apparent in the exploitation of the latter approach. In fact, the proposed protocols are in most cases limited to the use of only a particular class of hydrogen donors (mostly ethers, due to the easy formation of  $\alpha$ -oxy radicals).<sup>7</sup> The compulsory use of high temperature<sup>7c,8,11b,c</sup> and/or hazardous organic peroxides<sup>7c,8b,c,10,11b,c</sup> and the fact that a general method for

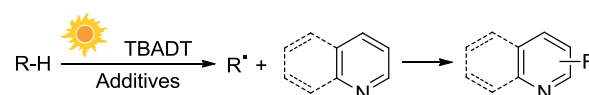
### Previous works



**Path a:** X = halogen, B(OH)<sub>2</sub>, BF<sub>3</sub>K, [SO<sub>2</sub>]<sub>2</sub>Zn, N<sub>2</sub><sup>+</sup>, COO*t*Bu, COOH

**Path b:** X = H in ethers, aldehydes, amides, toluenes, alkanes

### This work: Path c



TBADT = (nBu<sub>4</sub>N)<sub>4</sub>[W<sub>10</sub>O<sub>32</sub>]

**Scheme 1** Typical approach for the functionalization of heteroaromatics via Minisci reaction involving functionalization of a R-X bond (path a) or a R-H bond (path b). Cross-dehydrogenative coupling between hydrogen donors (R-H) and heteroaromatics via TBADT photocatalyzed activation of C-H bonds (path c).

the generation of alkyl radicals from R-H to be used in Minisci reaction is still lacking, makes the development of a milder procedure desirable. Seminal works in this field are the recent procedures based on visible light photoredox catalysis.<sup>7b,d,9b</sup>

In the last years, we (and others) had experience on the use of tetrabutylammonium decatungstate (TBADT; (nBu<sub>4</sub>N)<sub>4</sub>[W<sub>10</sub>O<sub>32</sub>]) as an efficient and robust photocatalyst able to promote photoredox reactions,<sup>12</sup> as well as hydrogen atom transfer processes, starting from different classes of organic substrates.<sup>13,14</sup> Another advantage of the use of TBADT is that it is active upon solar light irradiation, allowing to realize the so-called "window ledge chemistry".<sup>15</sup> TBADT, however, was used so far only for the functionalization of C=C (in electron-poor alkenes and fullerenes) and N=N bonds (in azodicarboxylates),<sup>16</sup> and for fluorination reactions,<sup>14g</sup> but not for the derivatization of aromatics.

We envisaged that under appropriate conditions, TBADT could be used for the (sunlight) aromatic homolytic substitution<sup>17</sup> of heterocycles via a cross-dehydrogenative coupling reaction with several hydrogen donors (R-H) as reaction partners (Scheme 1, path c).

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**Table 1** Optimization of the reaction conditions.<sup>a</sup>

entry	Bu <sub>4</sub> NBr (mol %)	conditions	GC yield (%) <sup>b</sup>	2a conversion (%) <sup>b</sup>
1	40	-	71	96
2	40	deaerated	51	77
3	40	TFA 0.1 M	trace	78
4	0	-	77	100
5	0	without TBADT	0	8
6	0	without hv	0	0
7	0	without CH <sub>2</sub> Cl <sub>2</sub>	64	85

<sup>a</sup> Reaction conditions: **1a** (40 mmol), **2a** (2.0 mmol), TBADT (4 mol%), K<sub>2</sub>S<sub>2</sub>O<sub>8</sub> (4.0 mmol), MeCN/CH<sub>2</sub>Cl<sub>2</sub> 5:1 (20 mL). Irradiation carried out by using a SolarBox equipped with a 1.5 kW Xe lamp (500 W/m<sup>2</sup>) under air equilibrated conditions.

<sup>b</sup> Determined by GC analysis using dodecane as the internal standard.

We then tested the alkylation of quinaldine (**2a**) with cyclohexane (**1a**) under different conditions. (Table 1). The reaction was performed by using a solar simulator equipped with a Xe lamp in the presence of TBADT (4 mol%) and persulfate anion in the role of oxidant<sup>6a,g,7a-b,7d-e,9b</sup> and Bu<sub>4</sub>NBr (40 mol%) as phase transfer agent.<sup>7a,18</sup> Gratifyingly, irradiation in MeCN/CH<sub>2</sub>Cl<sub>2</sub> (5:1) for 16 h under aerated conditions gave alkylated quinaldine **3a** in 71% yield with an almost total consumption of **2a** (Table 1, entry 1). The reaction was fully regioselective since no other alkylated product was formed. The absence of oxygen and the addition of a strong acid (TFA, 0.1 M) was detrimental for the process and omitting Bu<sub>4</sub>NBr did not affect the overall yield (entries 2-4). Blank experiments (entries 5-6) clearly demonstrated that the presence of light and TBADT was mandatory. The presence of CH<sub>2</sub>Cl<sub>2</sub> was important to improve the conversion of **2a**, probably thanks to a better solubility of **1a** in this solvent.

We then investigated the functionalization of **2a** with several hydrogen donors by using the conditions described in Table 1, entry 4, and the results are collected in Table 2. The reaction with cyclopentane (**1b**) and cycloheptane (**1c**) gave similar results and likewise a clean alkylation in position 4 of quinaldine occurred (entries 2-3). Next, the reaction was extended to cyclic ethers, namely THF (**1d**) and 1,4-dioxane (**1e**), and adducts **3d** and **3e** were formed in a satisfying yield (> 50%), although in the former case the presence of Bu<sub>4</sub>NBr was helpful to increase the yield (entries 4-5).

Even amides **1f** and **1g** were added photocatalytically to **2a** under the same reaction conditions to form acylated quinaldine **3f** and amidoalkylated quinaldine **3g** (entries 6-7). Acylation of the heteroaromatic was easily performed by a cross-dehydrogenative coupling with aldehydes as illustrated by the reaction of heptaldehyde **1h** with **2a** to afford **3h** in 67% yield (entry 8). Finally, the regioselective β-C-H activation in cyclopentanone **1i**<sup>14h</sup> was exploited for the synthesis of β-heteroaryl ketone **3i** in 69% yield (entry 9). To our knowledge, this is the first case where a cycloalkanone was used in the Minisci reaction.

**Table 2.** Functionalization of quinaldine **2a** via TBADT photocatalyzed C-H activation in hydrogen donors (R-H) **1a-1i**.<sup>a</sup>

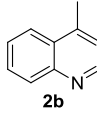
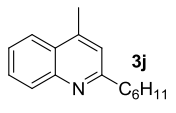
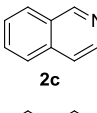
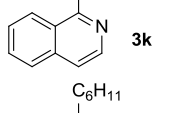
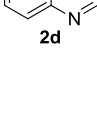
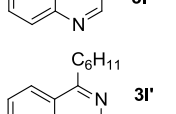
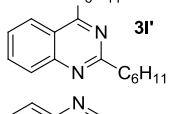
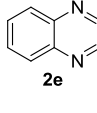
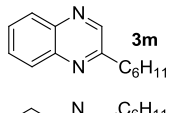
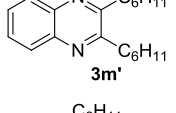
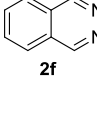
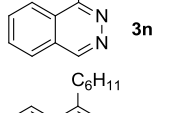
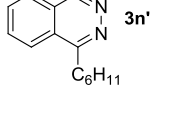

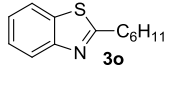
entry	1	time (h)	Product 3	Yield (%) <sup>b</sup>
1		16 h		77
2		20 h		74
3		16 h		66
4 <sup>c</sup>		16 h		53
5		20 h		73
6		16 h		47
7 <sup>c</sup>		20 h		73
8 <sup>c</sup>		16 h		67
9 <sup>c,d</sup>		24 h		69

<sup>a</sup> Reaction conditions: **1** (40 mmol), **2** (2.0 mmol), TBADT (4 mol%), K<sub>2</sub>S<sub>2</sub>O<sub>8</sub> (4.0 mmol), MeCN/CH<sub>2</sub>Cl<sub>2</sub> 5:1 (20 mL). Irradiation carried out by using a SolarBox equipped with a 1.5 kW Xe lamp (500 W/m<sup>2</sup>) under air equilibrated conditions.

<sup>b</sup> Yields of product isolated after flash chromatography on SiO<sub>2</sub>. <sup>c</sup> Bu<sub>4</sub>NBr (40 mol%). <sup>d</sup> **1i** (50 equiv.), MeCN/H<sub>2</sub>O 5:1 (20 mL).

We then focus our attention on the functionalization of other heteroaromatics (**2b-2g**, Table 3), while maintaining the same hydrogen donor (cyclohexane **1b**). The choice of **1b** was

**Table 3.** TBADT photocatalyzed addition of cyclohexane onto heteroaromatics **2b-2g**.<sup>a</sup>

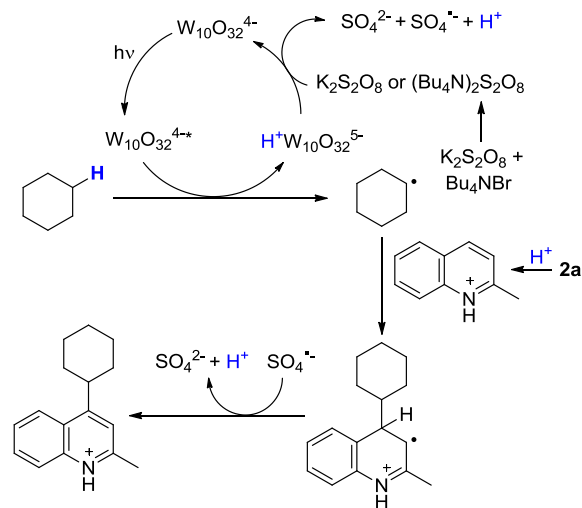
entry	<b>2</b>	time (h)	Product <b>3</b>	Yield (%) <sup>b</sup>
1		48 h		81
2		20 h		40
3 <sup>c</sup>		24 h		43
				14
4 <sup>c</sup>		48 h		60
				24
5 <sup>c</sup>		24 h		28
				20
6 <sup>c</sup>		24 h		60

<sup>a</sup> Reaction conditions: **1b** (40 mmol), **2** (2.0 mmol), TBADT (4 mol %), K<sub>2</sub>S<sub>2</sub>O<sub>8</sub> (4.0 mmol), MeCN/CH<sub>2</sub>Cl<sub>2</sub> 5:1 (20 mL). Irradiation carried out by using a SolarBox equipped with a 1.5 kW Xe lamp (500 W/m<sup>2</sup>) under air equilibrated conditions.

<sup>b</sup> Yields of product isolated after flash chromatography on SiO<sub>2</sub>. <sup>c</sup> Bu<sub>4</sub>NBr (40 mol%).

motivated by the fact that this is, among the R-H tested, the compound having the strongest C-H bond (99.5 kcal/mol).<sup>19</sup>

Alkylation of lepidine **2b** took place in a regioselective way (at position 2) and in a high yield (81%, compound **3j**, Table 3, entry 1) albeit 48 h irradiation were required to convert all the starting **2b**. Interestingly, a similar clean reaction was found in the functionalization of isoquinoline **2c**, where compound **3k** was the sole derivative formed. The situation changed when heteroaromatics containing two nitrogens were tested. The addition of cyclohexane onto quinazoline **2d** gave a mixture of mono- (**3l**) and disubstituted (**3l'**) adducts.

**Scheme 2** Proposed reaction mechanism.

Several attempts to modify the reaction conditions in order to have a clean mono- or disubstitution failed. The same holds for the experiments with quinoxaline **2e** and phthalazine **2f**, being the monoalkylated derivative (**3m** or **3n**) the main product in each case (84% overall yield in the former case). Again, a clear cut process was found in the functionalization of benzothiazole **2g** to give **3o** (60% yield). A tentative mechanism is depicted in Scheme 2 for the reaction between cyclohexane and **2a**. Excited TBADT is able to cleave homolytically the C-H bond in derivatives **1a-i**. The reduced form of the photocatalyst (H<sup>+</sup>[W<sub>10</sub>O<sub>32</sub>]<sup>5-</sup>) is oxidized by K<sub>2</sub>S<sub>2</sub>O<sub>8</sub>,<sup>20</sup> liberating an equivalent of acid along with a strong oxidant (SO<sub>4</sub><sup>-•</sup>).<sup>21</sup> The thus formed cyclohexyl radical is trapped by the protonated heterocycle and the hoped for derivative is finally formed by oxidation of the adduct radical. Minor pathways could likewise operate, however. A minor amount of SO<sub>4</sub><sup>-•</sup> could be formed directly from persulfate upon heating or by photochemical cleavage. A role of SO<sub>4</sub><sup>-•</sup> in the hydrogen abstraction of more labile C-H bonds (e.g. in ethers) could not be ruled out. Blank experiments demonstrate, however, that the presence of TBADT is mandatory for the success of the reaction. In some instances, the presence of Bu<sub>4</sub>NBr as a phase transfer agent<sup>7a,18</sup> may help to accelerate the process probably thanks to the formation of (Bu<sub>4</sub>N)<sub>2</sub>S<sub>2</sub>O<sub>8</sub> via methatesis reaction of potassium persulfate and Bu<sub>4</sub>NBr.<sup>22</sup>

The method described here compares favorably with those previously reported involving C-H activation of the alkylating agent. First of all, this is a very versatile approach since various substrates belonging to different classes of hydrogen donors (ethers, amides, aldehydes, cycloalkanones, cycloalkanes) can be activated. This is the first case of the photochemical activation of C-H bonds in aldehydes, previously obtained at a high temperature (> 100 °C)<sup>8</sup> and in cyclopentanones. As for the use of cycloalkanes and amides, these were used in a 20 equiv. amount, contrary to other cases where the hydrogen donors were used as the solvent (or, at least, co-solvent).<sup>9,11b,c</sup> However, the photocatalyzed activation of cycloalkanes for the functionalization of a heterocycle is unprecedented.

Furthermore, the reaction may be in principle carried out under natural solar light irradiation, a rare occurrence in Minisci reaction.<sup>9a</sup> Different from other procedures, the presence of a strong acid (e.g. TFA) is not required since protonation of the heterocycle took place during the reaction (Scheme 2).

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