



# Synthesis and Application of Functionalized NHC-Gold-Complexes

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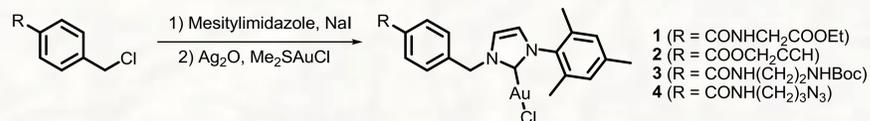
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## Introduction

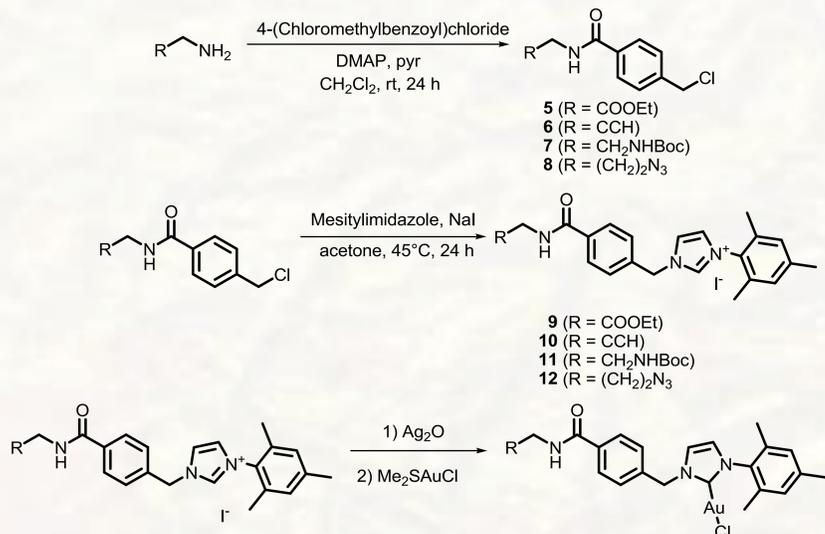
First investigated by Wanzlick and Öfele in the early 1960s,<sup>[1]</sup> **N-heterocyclic carbenes** (NHCs) are a topic of high current interest, in particular in transition metal catalysis. They are an attractive alternative to phosphine ligands, thanks to their strong  $\sigma$ -donating capability and low level of  $\pi$ -acidity. Moreover, extensive variation of the steric and electronic features of NHC's is possible.<sup>[2]</sup> Still, the number of NHCs bearing reactive functionalities, which might allow their linkage to solid supports or surfaces, is limited.

Based on precedent works by Grubbs and Nolan,<sup>[3]</sup> we developed a new route to functionalized, unsymmetrical *N*-heterocyclic carbenes which were converted into the corresponding gold complexes. All complexes catalyze the cycloisomerization of functionalized allenes.



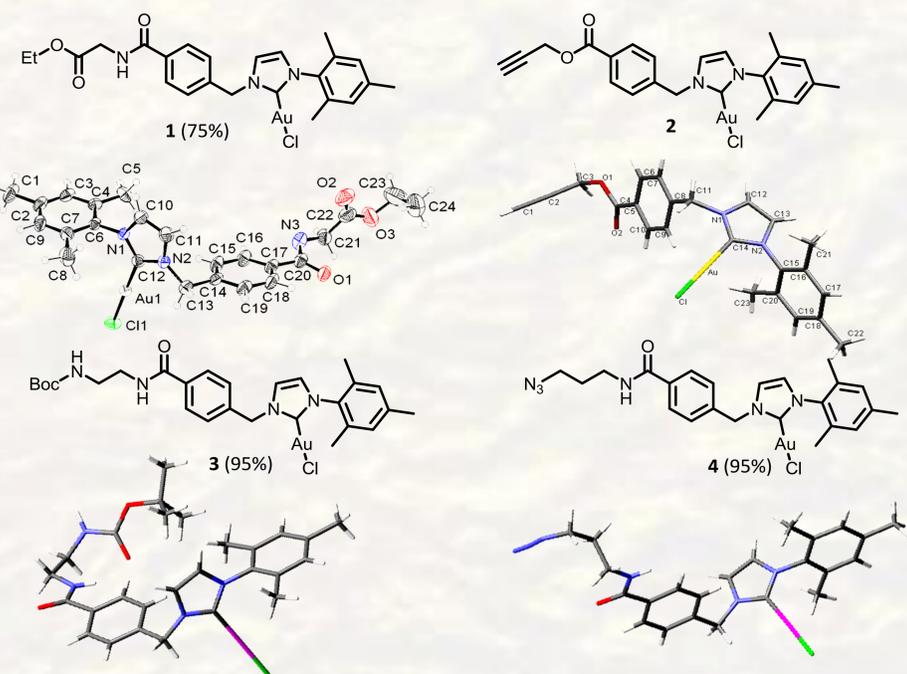
## Results

### Synthesis of the NHC-Gold-Complexes

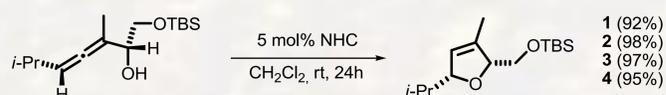


Starting from 4-(Chloromethyl)benzoylchloride, it was possible to build up four new imidazoliumsalts in a two-step-synthesis by changing the amine in the first step. In this way functional groups can be introduced easily.

The formation of the corresponding gold-complexes was carried out under conditions development by Nolan. He described the synthesis of a gold complex via a metal-exchange reaction to get higher yields.

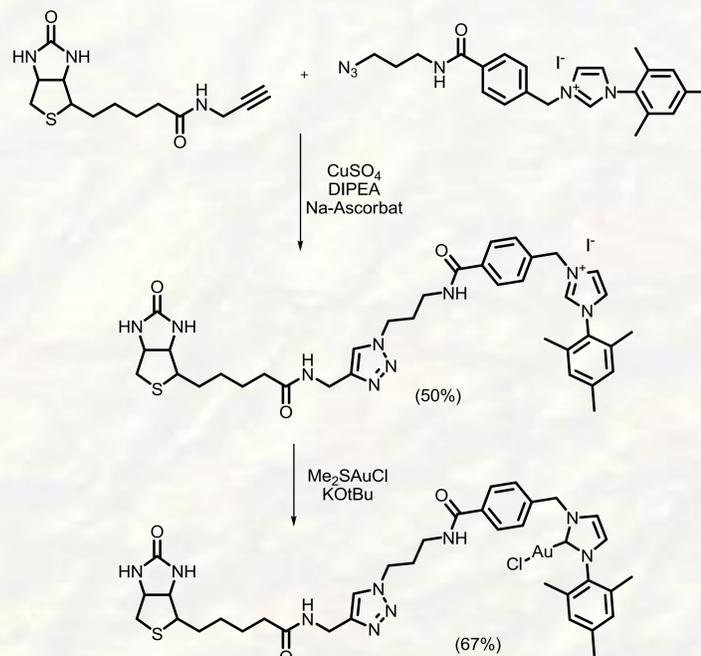


As known in literature, NHC-Metal-Complexes show a broad range of catalytic reactivity.<sup>[4]</sup> Here, we tested the cycloisomerization of a functionalized allene.<sup>[5]</sup>



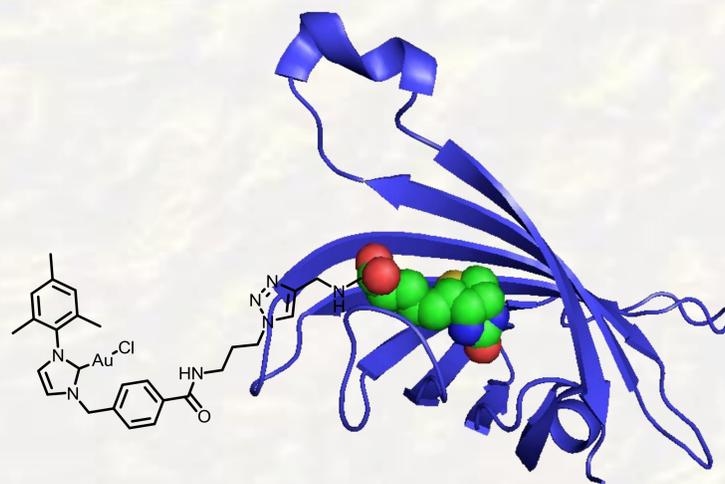
### Synthesis of a NHC-Biotin-Gold-Complex

The Huisgen 1,3-dipolar cycloaddition, also known as „Click-Chemistry“, has proven to be an efficient tool for the formation of a 1,2,3-triazole linkage between alkynes and azides.<sup>[6]</sup> The high tolerance against functional groups and the mild reaction conditions are optimal assumptions to build up a NHC-Biotin-Gold-Complex. By using CuSO<sub>4</sub>, DIPEA and Na-Ascorbate, the synthesis could be performed with moderate yields.



The complex shows catalytic reactivity in cycloisomerizations of allenes. The addition of an additive, such as AgBF<sub>4</sub>, gave high yields and faster reaction times.

Streptavidin has a high affinity to biotin and this non-covalent binding is one of the strongest known in nature. Further investigations will focus on the connection of the Biotin-NHC-Gold-Complex to a solid surface.



## References

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 (2) R. H. Grubbs, A. W. Waltman, *Organometallics*, **2004**, *23*, 3105–3107.  
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(4) S. Díez-González, N. Marion, S. P. Nolan, *Chem. Rev.* **2009**, *109*, 3612–3676.  
 (5) A. Hoffmann-Röder, N. Krause, *Org. Lett.* **2001**, *3*, 2537–2538.  
 (6) M. Meldal, W. Tornøe, *Chem. Rev.* **2008**, *108*, 2952–3015.