



## Synthesis of Tetrazolo[1,5-*c*]quinazolines via Ph<sub>3</sub>PAuOTf-Catalyzed Double Hydroamination of Terminal Alkynes

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An efficient tandem process is developed by using Ph<sub>3</sub>PAuOTf-catalyzed double hydroamination of alkynes for the synthesis of new fused tetrazolo[1,5-*c*]quinazolines, with 2-(1*H*-tetrazol-5-yl)anilines and alkynes in DCE at 100 °C.

**Keywords:** Ph<sub>3</sub>PAuOTf, 2-(1*H*-Tetrazol-5-yl)anilines, Alkynes, Tetrazolo[1,5-*c*]quinazolines, Double hydroamination.

### INTRODUCTION

Metal catalyzed tandem reactions for the addition of nucleophiles to unactivated alkynes is one of the simplest and atom economical<sup>1</sup> synthetic transformation for the synthesis of various poly heterocyclic compounds<sup>2</sup>. Among all transition metals<sup>3</sup> shown significant activity for the addition of N-H bonds across unactivated C-C triple bonds<sup>4</sup>.

Metal-catalyzed double addition of nucleophiles to alkynes is playing a prominent role in the synthesis of privileged complex compounds<sup>5</sup>. In this regard we developed double hydroamination of terminal alkynes<sup>6</sup> by using tetrazole substituted anilines as nucleophiles for the formation of new fused tetrazole quinazolines.

### EXPERIMENTAL

**General method for the synthesis of fused tetrazoloquinazolines:** To a screw cap vial containing a stir bar, were added 2-(1*H*-tetrazol-5-yl)aniline (**1**) (0.621 mmol), alkyne **2** (0.745 mmol) and 2 mol % Ph<sub>3</sub>PAuOTf (Ph<sub>3</sub>PAuCl/AgOTf) in DCE (2 mL). The reaction vial was evacuated and filled with nitrogen and heated at 100 °C for 24 h. The reaction mixture was cooled to room temperature, diluted with ethyl acetate and filtered through a plug of silica gel. The filtrate was concentrated and the residue was purified by silica gel column chromatography using hexane/ethyl acetate (90/10) as an eluent to afford analytically pure compound **3**.

**5-Methyl-5-phenyl-5,6-dihydro-tetrazolo[1,5-*c*]quinazoline (**3a**):** 85 % yield; light yellow solid; m.p. = 170-172 °C; R<sub>f</sub> = 0.31 (hexane/EtOAc = 70/30); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz): δ 7.93 (d, *J* = 6.9 Hz, 1H), 7.40-7.27 (m, 6H), 7.04-

6.95 (m, 2H), 5.40 (bs, 1H), 2.38 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz): δ 149, 141.4, 133.3, 128.7, 125.8, 124.9, 120.8, 116.1, 109.1, 76.9, 28.7; IR (KBr, ν<sub>max</sub>, cm<sup>-1</sup>): 3369, 3205, 3080, 2861, 1693, 1645, 1612, 1500, 1468, 1453, 992, 910; HRMS Calcd. for C<sub>15</sub>H<sub>14</sub>N<sub>5</sub> (M<sup>+</sup> + H) 264.1249, found 264.1245.

### RESULTS AND DISCUSSION

Firstly 2-(1*H*-tetrazol-5-yl)aniline<sup>7</sup> (**1a**) when treated with ethynylbenzene (**2a**) in the presence of different metal catalysts and with various solvents, finally found that the best condition for the formation of expected product 5-methyl-5-phenyl-5,6-dihydro-tetrazolo[1,5-*c*]quinazoline (**3a**) in 85 % yield was in the presence of 2 mol % Ph<sub>3</sub>PAuOTf catalyst in DCE at 100 °C for 24 h was optimal. Likewise, treated **1a** with other alkynes oct-1-yne (**2b**) and but-3-ynylbenzene (**2c**) gave the expected products **3b** and **3c** in 78 and 79 % yield, respectively. Next to check the generality methyl substituted **1a** i.e., **1b**<sup>8</sup> reacted well with the alkynes **2a**, **2b** and **2c** afforded **3d**, **3e** and **3f** in 81, 83 and 72 % yield, respectively. Finally, 4-methoxy-2-(1*H*-tetrazol-5-yl)aniline<sup>8</sup> (**1c**) was used as the substrate to react with the alkynes **2a**, **2b** and **2c** gave the corresponding products **3g**, **3h** and **3i** in increasing yield, 89, 80 and 82 % respectively (Table-1).

### Conclusion

We have developed Ph<sub>3</sub>PAuOTf-catalyzed direct double hydroamination of alkynes for the synthesis of new fused tetrazolo[1,5-*c*]quinazolines from 2-(1*H*-tetrazol-5-yl)anilines and alkynes in the presence of 2 mol % Ph<sub>3</sub>PAuOTf catalyst in DCE at 100 °C for 24 h.

TABLE-1  
SYNTHESIS OF FUSED TETRAZOLO[1,5-c]QUINAZOLINES

Entry	1	2	3	Yield (%)
1				85
2				78
3				79
4				81
5				83
6				72
7				89
8				80
9				82

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