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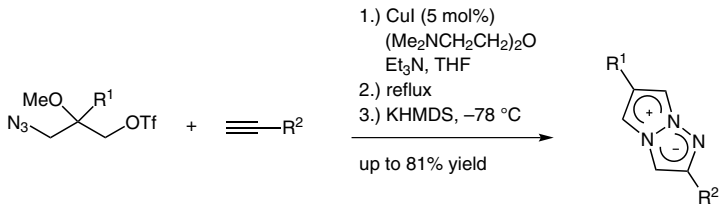
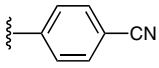
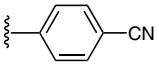
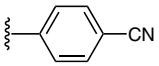
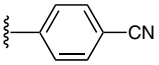
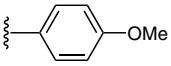
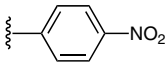
One-Pot Synthesis of Highly Fluorescent 2,5-Disubstituted-1,3a,6a-triazapentalene
Org. Lett. **2012**, *14*, 5554–5557.

Tuning The Quantum Yield of Fluorescent 2,5-Disubstituted-1,3a,6a-triazapentalene



	R^1	R^2	Product	Yield (%)
1	OMe	Ph	1a	64
2	OMe		1b	60
3	Me		1c	63
4	CN		1d	57
5[a]	Ph		1e	19
6	Me		1i	72
7	Me		1j	27

[a] The triflate was generated in situ and used without purification.

Significance: Rational design of organic molecules with improved photo-physical properties, such as high quantum yields and tunable fluorescence wavelength, is of great interest in modern science and technology. In this paper, the authors report a one-pot synthesis of 2,5-disubstituted-1,3a,6a-triazapentalenes. By a cascade sequence utilizing a copper(I)-catalyzed 1,3-dipolar cycloaddition followed by intramolecular cyclization and elimination, the authors managed to obtain the desired 1,3a,6a-triazapentalene skeleton.

Comment: The authors report the synthesis of a series of 2,5-disubstituted-1,3a,6a-triazapentalenes. These novel compounds allowed the authors to probe the effects of electron-donating and -withdrawing substituents on the photo-physical properties of 1,3a,6a-triazapentalene derivatives. Introduction of substituents in the 5-position led to a dramatically increased quantum yield. A correlation between the Hammet σ_p-value of the R^2-substituent and the quantum-yield tendency could furthermore be estimated.

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