Molbank **2014**, M816; doi:10.3390/M816

OPEN ACCESS

molbank

ISSN 1422-8599

www.mdpi.com/journal/molbank

Short Note

2,3-Bis(4-(3-(trifluoromethyl)-3*H*-diazirin-3-yl)phenyl)oxirane

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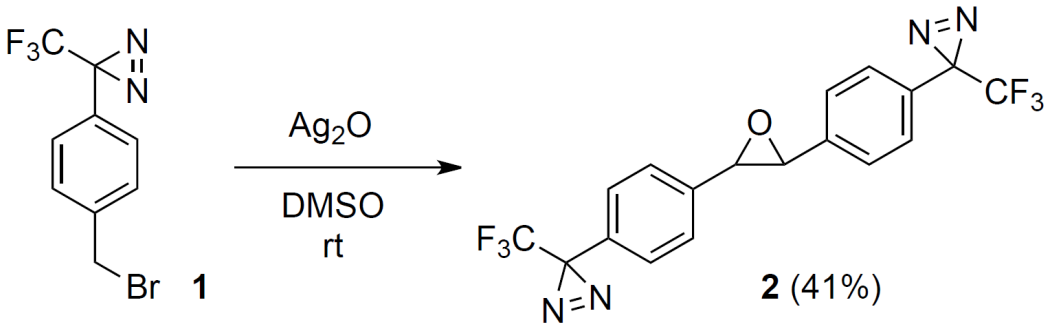
Received: 20 January 2014 / Accepted: 18 February 2014 / Published: 24 February 2014

Abstract: The title compound, which has two photoreactive groups in a molecule, was synthesized by the coupling reaction of 3-(4-(bromomethyl)phenyl)-3-(trifluoromethyl)-3*H*-diazirine in the presence of silver oxide in DMSO.

Keywords: diazirine; oxirane; photoaffinity label

Diazirine based photoaffinity labeling is a useful chemical biology method to elucidate interactions between low molecular weight bioactive compounds and biomolecules [1]. Photoreactive compound contained two photophores [2,3] is one of the attractive tools for comprehensive analysis of ligand-biomolecule interactions by photoaffinity labeling.

Scheme 1. Synthesis of 2,3-bis(4-(3-(trifluoromethyl)-3*H*-diazirin-3-yl)phenyl)oxirane (**2**).



We have synthesized a new two photophores containing compound, 2,3-bis(4-(3-(trifluoromethyl)-3*H*-diazirin-3-yl)phenyl)oxirane **2**, from 4-[3-(trifluoromethyl)-3*H*-diazirin-3-yl]benzyl bromide **1** with silver oxide in DMSO [4] without decomposition of diazirinyl ring. ^{1}H- and ^{13}C-NMR chemical shifts for

oxirane moiety (3.83 and 62.17 ppm) strongly indicated that the purified compound is *trans*- isomer [5,6]. The 2,3-*trans* two-photophores containing oxirane ring is utilized for introduction of **2** to ligand.

Experimental

Synthesis of 2,3-bis(4-(3-(trifluoromethyl)-3H-diazirin-3-yl)phenyl)oxirane (**2**)

To a solution of 4-[3-(trifluoromethyl)-3*H*-diazirin-3-yl]benzyl bromide (**1**) [7,8] (0.10 g, 0.36 mmol) in anhydrous DMSO (1 mL), silver oxide (0.09 g, 0.39 mmol) was added. The resulting mixture was stirred overnight at room temperature until TLC showed the reaction to be complete. The reaction was filtered by Celite and treated with H_2O, which was extracted with diethyl ether. The combined oil layer was dried over $MgSO_4$ and subjected to rotary evaporation to remove the solvent. The crude product was purified by silica gel column chromatography (CH_2Cl_2/hexane, 1:1) to afford **2** (0.06 g, 41%) as a yellow solid. $[\alpha]_D$ −20 (c 0.5, $CHCl_3$). UV($CDCl_3$) λ_{max} (ε) 250 (2120), 356 (1170). ^{1}H-NMR (270 MHz, $CDCl_3$): δ 7.37 (4H, d, J = 8.1 Hz,), 7.22 (4H, d, J = 8.1 Hz), 3.83 (2H, s). ^{13}C-NMR (68 MHz, $CDCl_3$): δ 138.54, 129.48, 126.91, 126.02, 122.14 (q, $^1J_{CF}$ = 274.7 Hz), 62.17, 28.24 (q, $^2J_{CF}$ = 40.6 Hz). ^{19}F-NMR (470 MHz, $CDCl_3$): δ −65.22. HRMS (FD): *m/z* calcd for $C_{18}H_{10}F_6N_4O$: 412.0759; found: 412.0744.

Acknowledgments

This research was partially supported by the Fugaku Foundation for financial support. Part of this work was performed under the Cooperative Research Program of "Network Joint Research Center for Materials and Devices".

Conflicts of Interest

The authors declare no conflict of interest.

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