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Short Note

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

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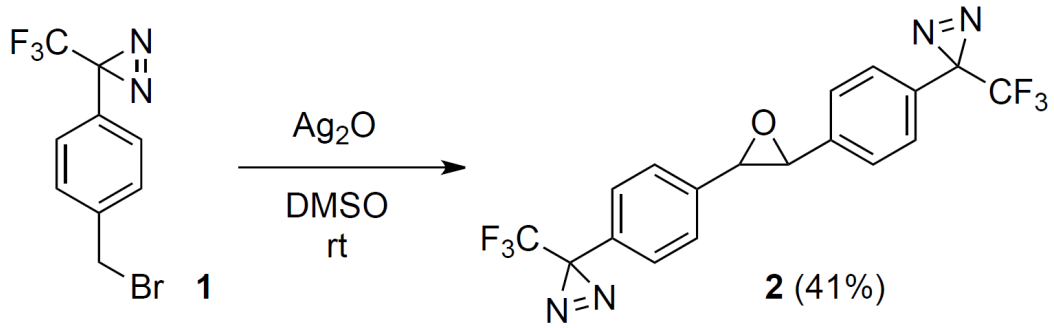
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Abstract: The title compound, which has two photoreactive groups in a molecule, was synthesized by the coupling reaction of 3-(4-(bromomethyl)phenyl)-3-(trifluoromethyl)-3*H*-diazirine in the presence of silver oxide in DMSO.

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

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Conflicts of Interest

The authors declare no conflict of interest.

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