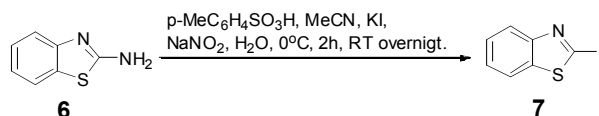


Supporting Information
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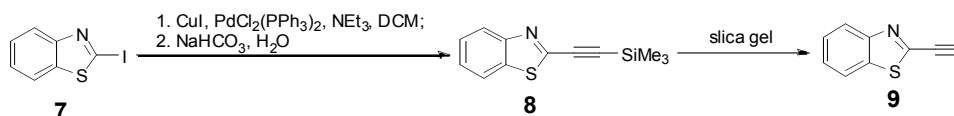
Organic synthetic experiment

2-iodobenzo[d]thiazole (**7**)¹



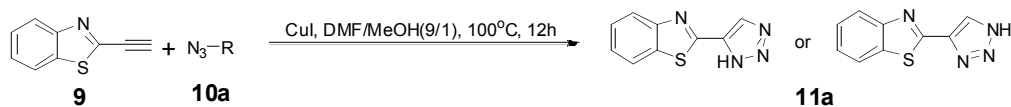
To a solution of 2-aminobenzo[d]thiazole (**6**) (3.75g, 25mol) and p-TsOH (15g, 75mmol) in acetonitrile (100ml) was added a mixture solution of KI (10.5g, 65mmol) and NaNO₂ (3.5g, 50mol) in water (15ml) at 0°C. The reaction solution was stirred at 0°C for 2h, and then at RT overnight. To the reaction solution was added around 350ml of water, adjust the solution pH to 8-9 with NaHCO₃ and added Na₂S₂O₃, filtered and the solid was washed to give brown solid 5.52g (yield 84.7%). TLC: Rf: 0.6 (hexane/ethyl acetate=6/1). MS (ESI) m/z 262 (M⁺+H); ¹HNMR (CDCl₃, 300MHz) δ 8.06 (1H, dd, J₁=7.5Hz, J₂=1.8Hz), 7.87 (1H, dd, J₁=6.9Hz, J₂=1.5Hz), 7.50~7.38 (2H, m).

2-ethynylbenzo[d]thiazole (**9**)²



To a mixture solution of **7** (0.87g, 3.33mmol), and trimethylsilylazide **10a** (0.65g, 6.66mmol) in triethylamine (3.3ml) and DCM (7ml) was added Pd(PPh)₂Cl₂ (47mg) and CuI (14mg), and stirred at 65°C for 4h. The reaction solution was diluted with EtOAc, and filtered. The filtrate was concentrated and purified by silica gel column to give 120 mg of solid **9** (yield 22.6%). Rf: 0.45 (hexane/ethyl acetate=6/1). MS (ESI) m/z 160(M⁺+H), ¹HNMR (CDCl₃, 300MHz) δ 8.11 (1H, d, J=7.8Hz), 7.89 (1H, dd, J₁=7.8Hz, J₂=1.5Hz), 7.59~7.40 (2H, m), 3.61(1H, s).

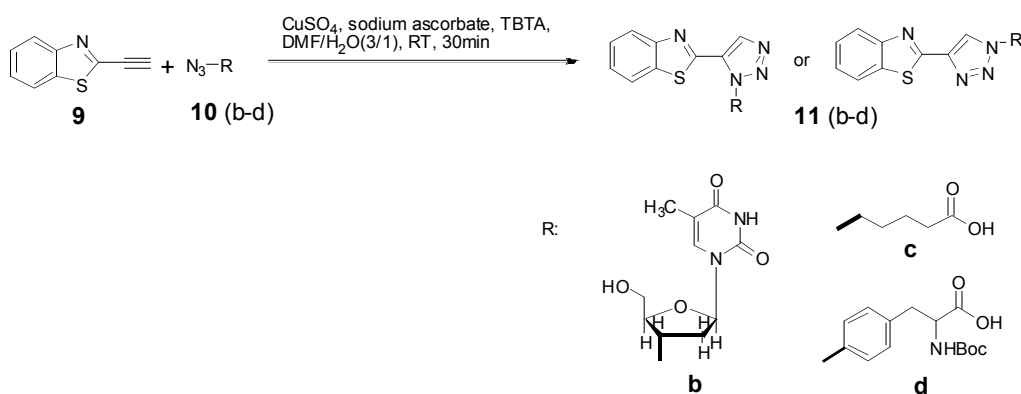
Method A: Click reaction (11a)³



To a solution of Benzothiazole alkyne (**9**) (80mg, 0.5mmol) and trimethylsilyl azide (0.1ml, 0.75mmol) in DMF/MeOH (9/1, 1ml) was added CuI (4.8mg, 0.025mmol). The reaction solution was stirred at 100°C for 12h. Around 20% starting material **9** was converted to product, checked by TLC. Part of the reaction solution was purified by preparative TLC to give 6 mg of white solid **11a**.

The MS and ¹HNMR data were summary in table S1.

Method B: Click reaction (11b-d)⁴

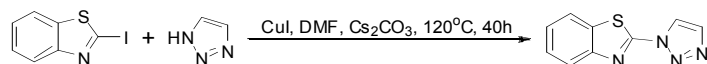


To a solution of AZT (**10b**) (28mg, 0.105mmol) in DMF (6ml) and H₂O (2ml) was added Benzothiazole alkyne (**9**) (16.7mg, 0.105mmol), CuSO₄ (3.3mgmg), sodium ascorbate (5mg), and TBTA (8mg), stirred 30min at RT, followed by TLC and HPLC. Starting material **9** was disappeared completely (100% conversion). Only the desired product peaks were found in HPLC. The reaction solution was extracted with EtOAc and washed with brine, dried over Na₂SO₄.

After removing solvent under reduced pressure, the residue was purified by silica gel column, eluted with 5% MeOH in EtOAc to give 40mg white solid **11b**, yield 89.4%.

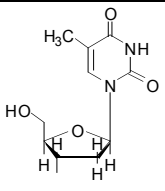
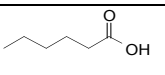
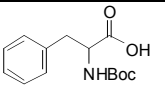
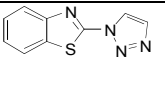
Same procedure was used to prepare **11c** and **11d**.

Method C: 2-(1H-1,2,3-triazol-1-yl)benzo[d]thiazole⁵



To a solution of 2-iodobenzo[d]thiazole (130mg, 0.5mmol) and 1,2,3-triazole (35mg, 0.75mmol) in DMF (2ml) was added Cs₂CO₃ (0.33g, 1mmol) and CuI (19mg, 0.1mmol) at RT and then stirred at 120°C for 40h. The reaction solution was extracted with ethyl acetate, washed with brine, dried over Na₂SO₄ and concentrated. The residue was purified by silica gel column to give white solid (43mg, yield 42.6%). TLC Rf: 0.32 (Hexane/EtOAc=3/1). MS and ¹HNMR data see in table S1.

Table S1. The reaction condition, conversion and Mass ¹HNMR data

	R	method ^a	conversion ^b	MS	¹ HNMR
11a	H	A	~20%	203(M ⁺ +H)	CDCl ₃ : 12.11 (1H, br), 8.43 (1H, s), 8.12 (1H, d, J=7.8Hz), 7.97 (1H, d, J=8.1Hz), 7.60-7.52 (1H, m), 7.50-7.40 (1H, m)
11b		B	100%	427 (M ⁺ +H)	MeOD: 8.79 (1H,s), 8.10-8.00 (2H, m), 7.95 (1H, d, J=1.2Hz), 7.60-7.40 (2H, m), 6.57 (1H, t, J=6.6Hz), 5.61-5.57 (1H, m), 4.52-4.48 (1H, m), 3.97 (1H, dd, J1=12.3Hz, J2=3.0Hz), 3.85 (1H, dd, J1=12.3Hz, J2=3.0Hz), 3.10-2.78 (3H, m), 1.94 (3H, d, J=1.2Hz)
11c		B	100%	303 (M ⁺ +H)	MeOD: 8.67 (1H,s), 8.07-8.00 (2H, m), 7.6-7.40 (2H, m), 4.57 (2H, t, J=7.2Hz), 2.25 (2H, t, J=7.5Hz), 2.10-1.99 (2H, m), 1.74-1.60 (2H, m)
11d		B	100%	446 (M ⁺ +H)	MeOD: 9.13(1H, s), 8.09-8.03 (2H, m), 7.84 (2H, d, J=8.4Hz), 7.60-7.40 (4H, m), 4.30-4.20 (1H, m), 3.30-3.25 (1H, d, J=4.8Hz), 3.09-3.01 (1H, m), 1.41 (9H, s).
16		C	~50%	203(M ⁺ +H)	CDCl ₃ : 8.12-8.08 (1H, m), 7.99 (2H, s), 7.90 (1H, m), 7.60-7.52 (1H, m), 7.48-7.42 (1H, m)

^aReaction conditions: A: CuSO₄, sodium ascorbate, DMF/H₂O (3/1), RT, overnight. B: CuSO₄, sodium ascorbate, TBTA, DMF/H₂O (3/1), RT, 30min. ^bConversion was estimated by TLC.

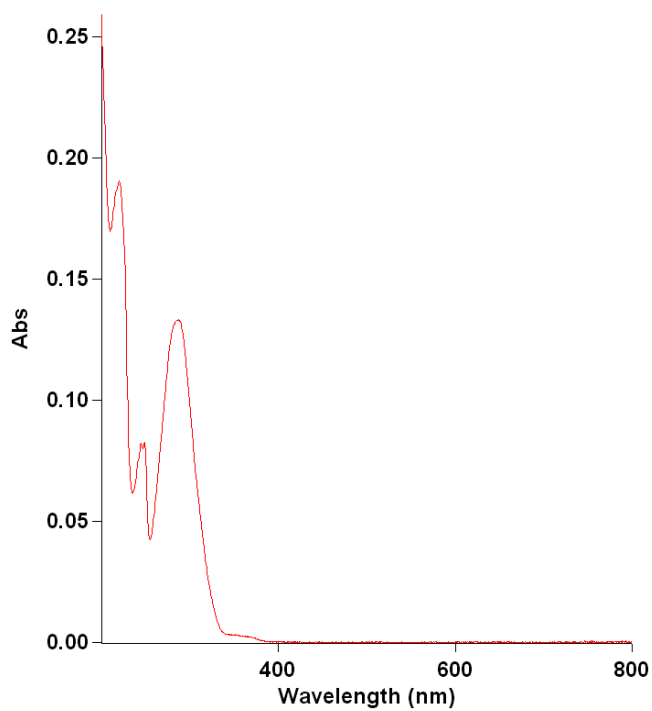


Figure S1. The UV absorption spectra of compound **9** in H₂O (10 μM), $\lambda_{\max(\text{abs})}$: 286nm.

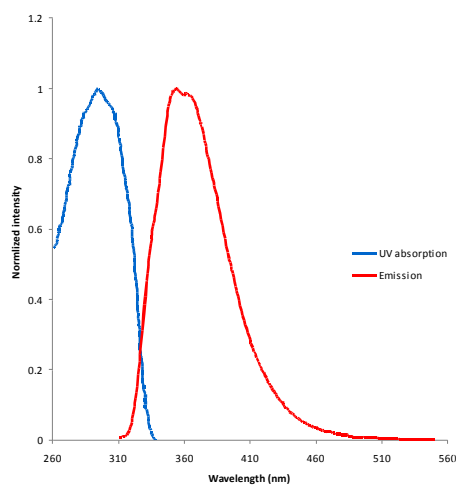


Figure S2. Absorption (blue line, $\lambda_{\max(\text{abs})}$ =294nm) and fluorescence (red line $\lambda_{\max(\text{em})}$ =354nm) of compound **11d** in MeOH

Reference

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