Supporting Information

Synthesis of Furanone-Fused 1,2-Benzothiazine by Rh(III)-Catalyzed C-H Activation: Regioselective Oxidative Annulation Leading to in Situ Lactonization in One Pot

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Contents:

1.	Mechanistic experiments	SI - 3
2.	Unsuccessful substrate	SI - 5
3.	Crystal structure data for compound 3ba	SI - 6
4.	Characterization data	SI - 8

Mechanistic experiments

Deuterium incorporation studies:

In a 8-mL screw cap reaction vial, sulfoximine **1b** (0.2 mmol), D_2O (10 equiv), rhodium catalyst (5 mol %), $Cu(OAc)_2 \cdot H_2O$ (1.0 equiv), Ag_2CO_3 (1.0 equiv) and $AgBF_4$ (20 mol %) were added followed by the addition of toluene (2 mL). This vial was sealed with a screw cap, placed in a pre-heated metal block at $100^\circ C$ for 4 h. After completion of the reaction, the reaction mixture was cooled to room temperature. The crude reaction mixture was purified on a flash column using EtOAc/ petroleum (1:1) ether to give the desired product **deuterio-1b** in 45% yield. The deuterium incorporation was calculated from 1H NMR spectroscopy (see the following 1H NMR spectra).

Kinetic isotopic studies:

In a 8-mL screw cap reaction vial, 1:1 ratio of **deuterio-1b** (100% D) [ie. by weighing 0.123 mmol of **deuterio-1b** 77% D, which contains 0.1 mmol of **1b-d₂** (100% D) and 0.027 mmol of **1b**] and **1b** (0.073 mmol) were taken. (Now the reaction vial contains 0.1 mmol of each of **1a** and **deuterio-1b** (100% D)). Then were added **2a** (0.1 mmol), rhodium catalyst (5 mol %), Cu(OAc)₂.H₂O (0.2 equiv), Ag₂CO₃ (1.0 equiv) and AgBF₄ (20 mol %) and toluene (2 mL) and the vial was flushed with argon and sealed with a screw cap immediately. Then the reaction mixture was stirred at 100 °C for 12 h and concentrated under vacuum. The crude reaction mixture was purified on a column chromatography using EtOAc/petroleum ether mixture (1:1). The obtained product was subjected to ¹H NMR measurement (See the following ¹H NMR spectrum).

Unsuccessful substrate

nd

nd

nd

nd

nd

nd

Crystal structure for compound 3ba (50% ellipsoid probability): **Crystal data for compound 3ba:**

Bond precision: C-C = 0.0040 Å Wavelength: 0.71073

Cell: a= 9.9108(6) b= 23.4525(13) c= 7.8620(5)

alpha= 90 beta= 90.494(6) gamma= 90

Temperature: 296K

	Calculated	Reported
Volume	1827.32(19)	1827.32(19)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C ₂₀ H ₁₉ NO ₃ S	
Sum formula	C ₂₀ H ₁₉ NO ₃ S	C ₂₀ H ₁₉ NO ₃ S
Mr	353.42	353.42
Dx, g cm ⁻³	1.285	1.285
Z	4	4
Mu (mm ⁻¹)	0.195	0.195
F000	744.0	744.0

F000'	744.82	
h, k, lmax	12,30,10	12,30,10
Nref	4186	4181

Data completeness= 0.999 Theta (max)= 27.480

R (reflections) = 0.0631(2773) wR2 (reflections) = 0.1676(4181)

S = 1.044 Npar= 226

The ORTEP diagram and Crystal Parameters of **3ba** in thermal ellipsoids are drawn at 50% probability level. The crystal of suitable quality was obtained from slow evaporation of solution of **3ba** in ethyl acetate, and was analyzed by single crystal diffractometer. Atomic coordinates, bond lengths, bond angles, and thermal parameters for this compound have been deposited at the Cambridge Crystallographic Data Centre. **CCDC 1920397** contains supplementary crystallographic data.

v

— 174.24
— 169.12

138.45
133.14
132.76
131.15
130.65
130.03
129.70
127.20
125.92
117.13

— 92.58

83.59
77.48
77.16
76.84

25.14
24.78

— 174.25
— 170.09
— 164.29
— 163.71

— 133.91
— 131.47
— 130.40
— 127.66

— 117.30
— 114.81
— 111.65
— 103.88

— 92.57

— 83.29
— 77.48
— 77.16
— 76.84

— 56.04
— 56.00

— 25.21
— 24.92

— 173.64
— 169.71

— 134.74
— 131.44
— 127.75
— 124.50
— 123.50
— 117.81

— 93.08

— 83.12
— 77.48
— 77.16
— 76.84

— 46.72

— 25.12
— 24.84

-63.33
-63.55

95.75

88.58

77.48
77.16
76.84

30.04
29.28

22.11
21.78

7.59
7.29

173.44
173.11
170.79

145.78
145.72
145.24
145.14
136.77
136.62
131.31
131.12
128.78
128.47
128.43
125.76
125.63
122.80
116.75
116.38

94.08
93.95
87.61
87.54
77.48
77.16
76.84

34.70
34.10
22.56
22.12
22.06
21.81
16.95
16.83
16.77
16.70

175.13
170.50

145.67
145.15
137.20
131.41
130.18
128.66
128.22
125.73
122.81
116.74

92.05
87.99
77.48
77.36
77.16
76.84

37.62
37.59
29.21
29.18
22.84
22.08
21.78

NOE studies, **4bj**

H_a irradiated at 2.07 δ ppm

H_c did not observed

H_a

NOE Studies, **4bk**

ppm