

2-((3*R*,9*bS*)-5,5-Dioxido-2,3-dihydro-9*bH*-benzo[4,5]isothiazolo[3,2-*b*]oxazol-3-yl)-1-phenylethan-1-one

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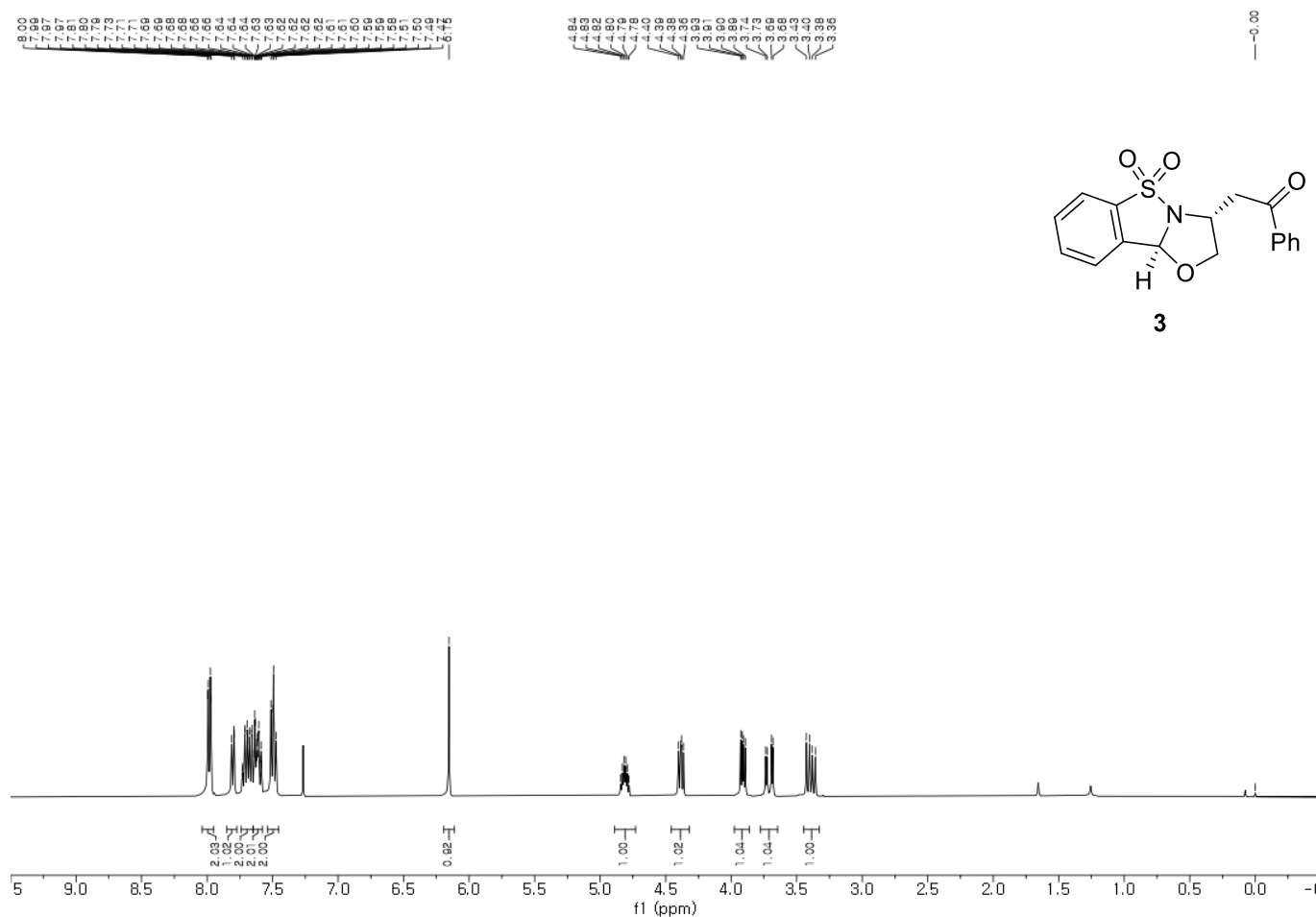


Figure S1. ¹H NMR spectrum of compound 3 (CDCl₃, 400 MHz)

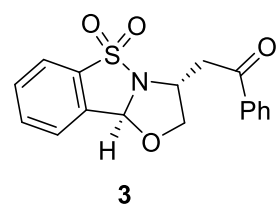
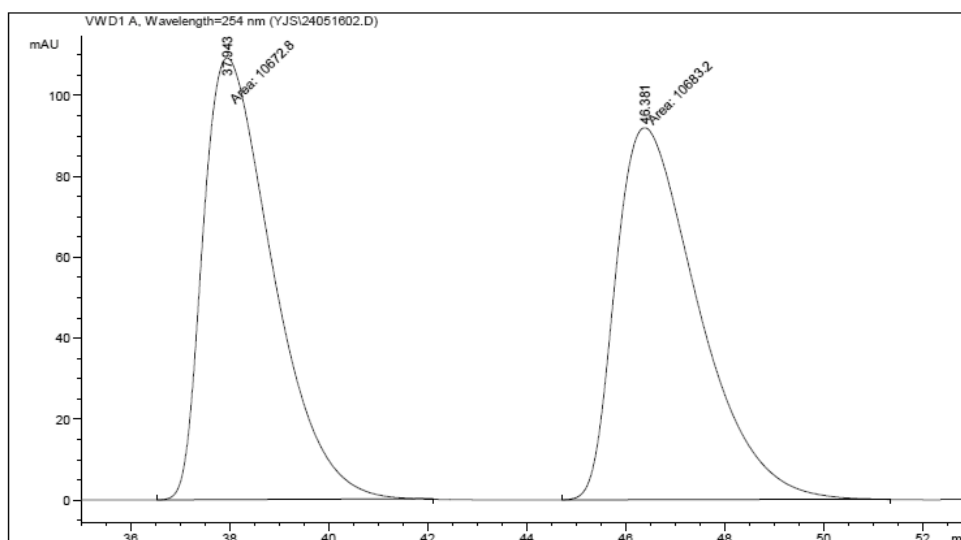
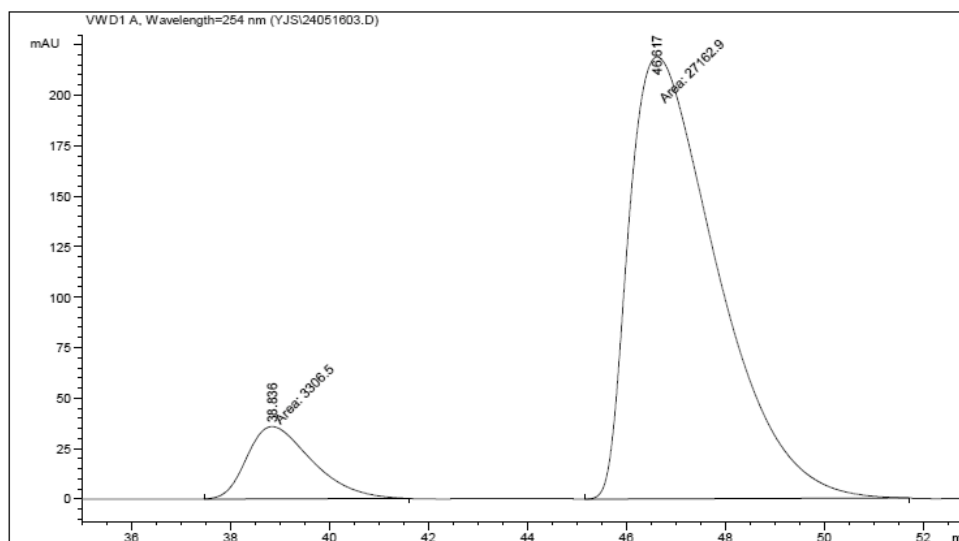


Figure S2. ^{13}C NMR spectrum of compound **3** (CDCl_3 , 100 MHz)

racemic**Area Percent Report**

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	37.943	MM	1.6310	1.06728e4		109.06538	49.9758
2	46.381	MM	1.9379	1.06832e4		91.87923	50.0242
Totals :				2.13560e4		200.94461	

enantiomerically enriched**Area Percent Report**

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	38.836	MM	1.5329	3306.50220		35.95003	10.8519
2	46.617	MM	2.0661	2.71629e4		219.11259	89.1481
Totals :				3.04694e4		255.06262	

Figure S3. HPLC chromatogram of compound 3

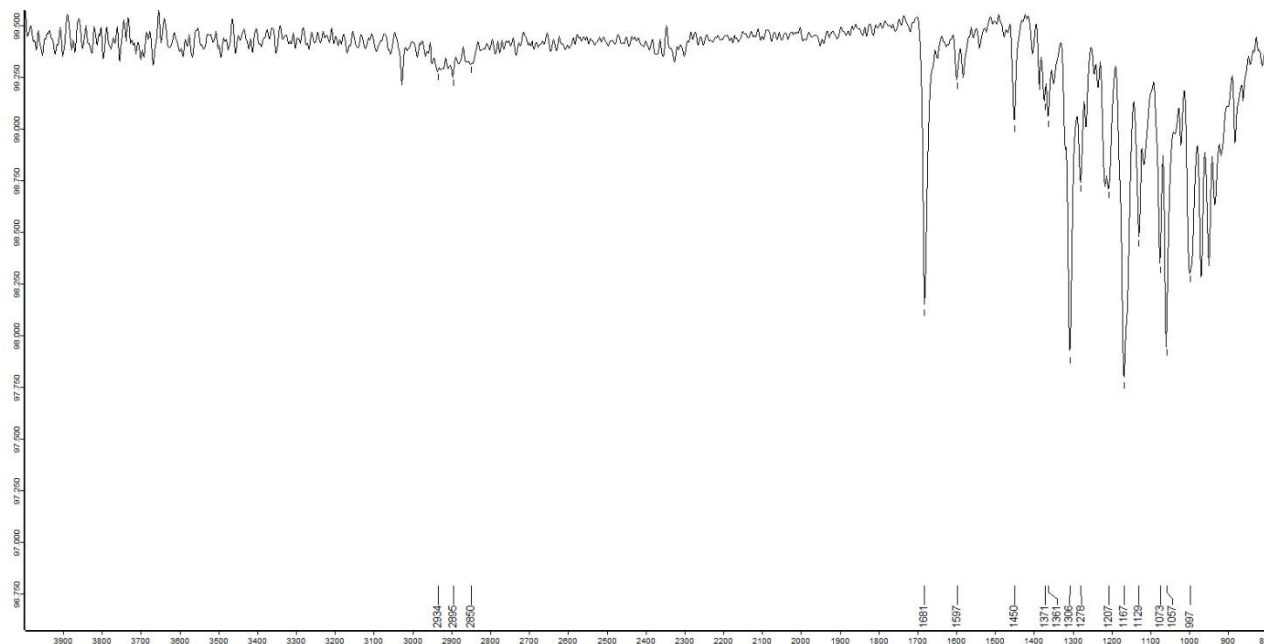


Figure S4. IR spectra of compound **3**

[Elemental Composition]

Data : YJS-24-163-001

Date : 20-May-2024 14:02

Page: 1

Sample: -

Note: -

Inlet : Direct

Ion Mode : EI+

RT : 1.24 min

Scan#: 38

Elements : C 17/0, H 15/0, N 1/0, O 4/0, S 1/0

Mass Tolerance : 1000ppm, 5mmu if m/z > 5

Unsaturation (U.S.) : 0.0 - 30.0

Observed m/z Int%

329.0721 0.1

Estimated m/z Err[ppm / mmu] U.S.

329.0722 -0.4 / -0.1 12.0

C

H

N

O

S

17

15

1

4

1

Table S1. High mass data of compound **3**