Supplementary Information

Cascade reactions initiated by radical addition of tetrahydrofuran to β-bromonitrostyrenes

Xin Ge, Kim Le Mai Hoang, Min Li Leow and Xue-Wei Liu*

Division of Chemistry and Biological Chemistry, School of Physical and Mathematical Sciences, Nanyang Technological University

Singapore 637371, Singapore

E-mail: xuewei@ntu.edu.sg

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4. X-ray data of compound 2h-1

Crystal data and structure refinement for compound 2h-1

Identification code: compound 2h-1
Empirical formula: C13 H15 N O5
Formula weight: 265.26
Temperature: 103(2) K
Wavelength: 0.71073 Å
Crystal system: Triclinic
Space group: P-1
Unit cell dimensions:
- a = 8.0104(6) Å
- b = 8.0179(8) Å
- c = 10.7954(7) Å
- α = 102.106(2)°
- β = 109.539(3)°
- γ = 95.818(2)°
Volume: 627.73(9) Å³
Z: 2
Density (calculated): 1.403 Mg/m³
Absorption coefficient: 0.109 mm⁻¹
F(000): 280
Crystal size: 0.40 x 0.24 x 0.20 mm³
Theta range for data collection: 2.07 to 32.02°
Index ranges:
- -11 ≤ h ≤ 11
- -11 ≤ k ≤ 11
- -16 ≤ l ≤ 16
Reflections collected: 13070
Independent reflections: 4334 [R(int) = 0.0180]
Completeness to theta = 32.02°: 99.8 %
Absorption correction: None
Max. and min. transmission: 0.9786 and 0.9578
Refinement method: Full-matrix least-squares on F²
Data / restraints / parameters: 4334 / 915 / 346
Goodness-of-fit on F²: 1.038
Final R indices [I>2sigma(I)]: R1 = 0.0462, wR2 = 0.1126
R indices (all data): R1 = 0.0675, wR2 = 0.1230
Largest diff. peak and hole: 0.223 and -0.205 eÅ⁻³
5. Isotope labeling experiments

When the reaction was conducted under an $^{18}$O$_2$ atmosphere, the ester was obtained in 52% yield. The differences in mass spectroscopy showed that an $^{18}$O atom was incorporated into the ester.

Spectrum of ESI (LRMS) of 2a
Spectrum of ESI (LRMS) of 2a-\(^{18}\)O

Spectrum of ESI (HRMS) of 2a-\(^{18}\)O

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.8, max = 50.0
Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron ions
68 formula(s) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

- C: 0.14
- H: 0.17
- N: 0.1
- O: 0.2
- 160: 0.2
- 180: 0.2

C:18H18O

222.1222

223.1222

223.1220

0.2

0.9

5.5

13.1

0.0

C13 H17 1802 180
6. $^1$H and $^{13}$C NMR spectra of compounds 2a-2s

$^1$H and $^{13}$C NMR spectra of compound 2a-1 (the anti-isomer)
$^1$H and $^{13}$C NMR spectra of compound 2a-2 (the syn-isomer)
$^1$H and $^{13}$C NMR spectra of compound 2b-1 (the anti-isomer)
$^1$H and $^{13}$C NMR spectra of compound 2b-2 (the syn-isomer)
$^1$H and $^{13}$C NMR spectra of compound 2c-1 (the *anti*-isomer)
$^1$H and $^{13}$C NMR spectra of compound 2c-2 (the syn-isomer)
$^1$H and $^{13}$C NMR spectra of compound 2d-1 (the anti-isomer)
$^1$H and $^{13}$C NMR spectra of compound 2d-2 (the syn-isomer)
$^1$H and $^{13}$C NMR spectra of compound 2e-1 (the anti-isomer)
$^1$H and $^{13}$C NMR spectra of compound 2e-2 (the syn-isomer)
$^1$H and $^{13}$C NMR spectra of compound 2f-1 (the *anti*-isomer)
$^1$H and $^{13}$C NMR spectra of compound 2f-2 (the syn-isomer)
$^1$H and $^{13}$C NMR spectra of compound 2g-1 (the anti-isomer)
$^1$H and $^{13}$C NMR spectra of compound 2g-2 (the syn-isomer)
$^1$H and $^{13}$C NMR spectra of compound 2h-1 (the anti-isomer)
$^1$H and $^{13}$C NMR spectra of compound 2h-2 (the syn-isomer)
$^1$H and $^{13}$C NMR spectra of compound 2i-1 (the anti-isomer)
$^1$H and $^{13}$C NMR spectra of compound 2i-2 (the syn-isomer)
$^1$H and $^{13}$C NMR spectra of compound 2j-1 (the anti-isomer)
$^1$H and $^{13}$C NMR spectra of compound 2j-2 (the syn-isomer)
$^1$H and $^{13}$C NMR spectra of compound 2m-1 (the anti-isomer)
$^1$H and $^{13}$C NMR spectra of compound 2m-2 (the syn-isomer)
$^1$H and $^{13}$C NMR spectra of compound 2o-1 (the *anti*-isomer)
$^1$H and $^{13}$C NMR spectra of compound 2o-2 (the syn-isomer)
$^1$H and $^{13}$C NMR spectra of compound 2p-1 (the *anti*-isomer)
$^1$H and $^{13}$C NMR spectra of compound 2p-2 (the syn-isomer)
$^1$H and $^{13}$C NMR spectra of compound 2q-1 (the *anti*-isomer)
$^1$H and $^{13}$C NMR spectra of compound 2q-2 (the syn-isomer)
$^1$H and $^{13}$C NMR spectra of compound 2r-1 (the anti-isomer)
$^1$H and $^{13}$C NMR spectra of compound 2r-2 (the syn-isomer)
\(^1\)H and \(^{13}\)C NMR spectra of compound 2s-1 (the anti-isomer)
$^1$H and $^{13}$C NMR spectra of compound 2s-2 (the *syn*-isomer)