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Supplementary Information

Cascade reactions initiated by radical addition of

tetrahydrofuran to β-bromonitrostyrenes

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Table of Contents

1.	X-ray data of compound 2h-1	.S2
2.	Isotope labelling experiments	
3.	¹ H and ¹³ C NMR spectra of compounds 2a-2s	S5

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	C13 H15 N O5				
Formula weight	265.26	265.26				
Temperature	103(2) K	103(2) K				
Wavelength	0.71073 Å	0.71073 Å				
Crystal system	Triclinic					
Space group	P-1					
Unit cell dimensions	a = 8.0104(6) Å	a= 102.106(2)°.				
	b = 8.0179(8) Å	b= 109.539(3)°.				
	c = 10.7954(7) Å	$g = 95.818(2)^{\circ}$.				
Volume	627.73(9) Å ³					
Z	2					
Density (calculated)	1.403 Mg/m ³					
Absorption coefficient	0.109 mm ⁻¹	0.109 mm ⁻¹				
F(000)	280	280				
Crystal size	$0.40 \ge 0.24 \ge 0.20 \text{ mm}^3$	0.40 x 0.24 x 0.20 mm ³				
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 %	99.8 %				
Absorption correction	None					
Max. and min. transmission	0.9786 and 0.9578	0.9786 and 0.9578				
Refinement method	Full-matrix least-squares of	Full-matrix least-squares on F ²				
Data / restraints / parameters	4334 / 915 / 346					
Goodness-of-fit on F^2	1.038					
Final R indices [I>2sigma(I)]	R1 = 0.0462, wR2 = 0.112	R1 = 0.0462, $wR2 = 0.1126$				
R indices (all data)	R1 = 0.0675, wR2 = 0.123	30				
Largest diff. peak and hole	0.223 and -0.205 e.Å $^{-3}$	0.223 and -0.205 e $Å^{-3}$				

5. Isotope labeling experiments



When the reaction was conducted under an ¹⁸O₂ atmosphere, the ester was obtained in 52% yield. The differences in mass

spectroscopy showed that an ¹⁸O atom was incorporated into the ester.



Spectrum of ESI(HRMS) of 2a

Elementa	Composition	Report								Page
Single Ma Folerance Element pr Number of	ass Analysis = 5.0 PPM / DE ediction: Off isotope peaks us	IE: min = -' ed for i-FIT	1.8, max = 1 = 3	50.0						
Monoisotopi 6 formula(e ilements Us 2: 0-15 H:	ic Mass, Even Elect e) evaluated with 1 sed: 1-21 O: 1-4 Cl:	ron lons results withi 0-2 Br: 0-	n limits (all n 1	esults (up to	1000) for each r	mass)				
13H16O3 X-23 152 (3	.328)									1: TOF MS ES
00						221.1177				5.00010
%										
220.900	220.950	221	.000	221.050	221.10	0	221.150	221.200	221.250	221.300
inimum:		5.0	5.0	-1.8 50.0						
ax1mum:								12.1		
ass	Calc. Mass	mDa	PPM	DBE	1-FIT	1-FIT	(Norm) Form	ula		

Spectrum of ESI (LRMS) of 2a-¹⁸O



Spectrum of ESI (HRMS) of 2a-18O

Elemental Composition Report Page 1 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 66 formula(e) 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 16O: 0-2 17O: 0-2 18O: 0-2 C13H16O3 GX-17 24 (0.526) 1: TOF MS ES+ 2.84e+001 223.1222 100 % m/z 222,900 222,950 223.000 223.050 223.100 223.150 223 200 223 250 223.300 Minimum: Maximum: -1.8 50.0 5.0 5.0 PPM DBE Mass Calc. Mass mDa i-FIT i-FIT (Norm) Formula 223.1222 223.1220 C13 H17 1602 180 0.2 0.9 5.5 13.1 0.0

6. ¹H and ¹³C NMR spectra of compounds 2a-2s

¹H and ¹³C NMR spectra of compound 2a-1 (the *anti*-isomer)



¹H and ¹³C NMR spectra of compound 2a-2 (the *syn*-isomer)



¹H and ¹³C NMR spectra of compound 2b-1 (the *anti*-isomer)



¹H and ¹³C NMR spectra of compound 2b-2 (the *syn*-isomer)





¹H and ¹³C NMR spectra of compound 2c-1 (the *anti*-isomer)

¹H and ¹³C NMR spectra of compound 2c-2 (the *syn*-isomer)



¹H and ¹³C NMR spectra of compound 2d-1 (the *anti*-isomer)



¹H and ¹³C NMR spectra of compound 2d-2 (the *syn*-isomer)



¹H and ¹³C NMR spectra of compound 2e-1 (the *anti*-isomer)



¹H and ¹³C NMR spectra of compound 2e-2 (the *syn*-isomer)



¹H and ¹³C NMR spectra of compound 2f-1 (the *anti-*isomer)



¹H and ¹³C NMR spectra of compound 2f-2 (the *syn*-isomer)







¹H and ¹³C NMR spectra of compound 2g-2 (the *syn*-isomer)



¹H and ¹³C NMR spectra of compound 2h-1 (the *anti*-isomer)



¹H and ¹³C NMR spectra of compound 2h-2 (the *syn*-isomer)



¹H and ¹³C NMR spectra of compound 2i-1 (the *anti*-isomer)





¹H and ¹³C NMR spectra of compound 2i-2 (the *syn*-isomer)

¹H and ¹³C NMR spectra of compound 2j-1 (the *anti-*isomer)



¹H and ¹³C NMR spectra of compound 2j-2 (the *syn*-isomer)



¹H and ¹³C NMR spectra of compound 2m-1 (the *anti*-isomer)



¹H and ¹³C NMR spectra of compound 2m-2 (the syn-isomer)



¹H and ¹³C NMR spectra of compound 20-1 (the *anti*-isomer)







¹H and ¹³C NMR spectra of compound 2p-1 (the *anti*-isomer)







¹H and ¹³C NMR spectra of compound 2q-1 (the *anti*-isomer)







¹H and ¹³C NMR spectra of compound 2r-1 (the *anti*-isomer)





¹H and ¹³C NMR spectra of compound 2r-2 (the *syn*-isomer)

¹H and ¹³C NMR spectra of compound 2s-1 (the *anti*-isomer)



¹H and ¹³C NMR spectra of compound 2s-2 (the *syn*-isomer)

