

Supramolecular catalysis in the dearomative Michael addition involving nitro-group-activated benzofurans

Aleksandra Topolska,^a Artur Przydacz,^a Anna Skrzyńska,^{a*} and Łukasz Albrecht^{a*}

^a Institute of Organic Chemistry
Faculty of Chemistry
Lodz University of Technology
Żeromskiego 116, 90-924 Łódź, Poland
E-mail: lukasz.albrecht@p.lodz.pl

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1. Materials and methods

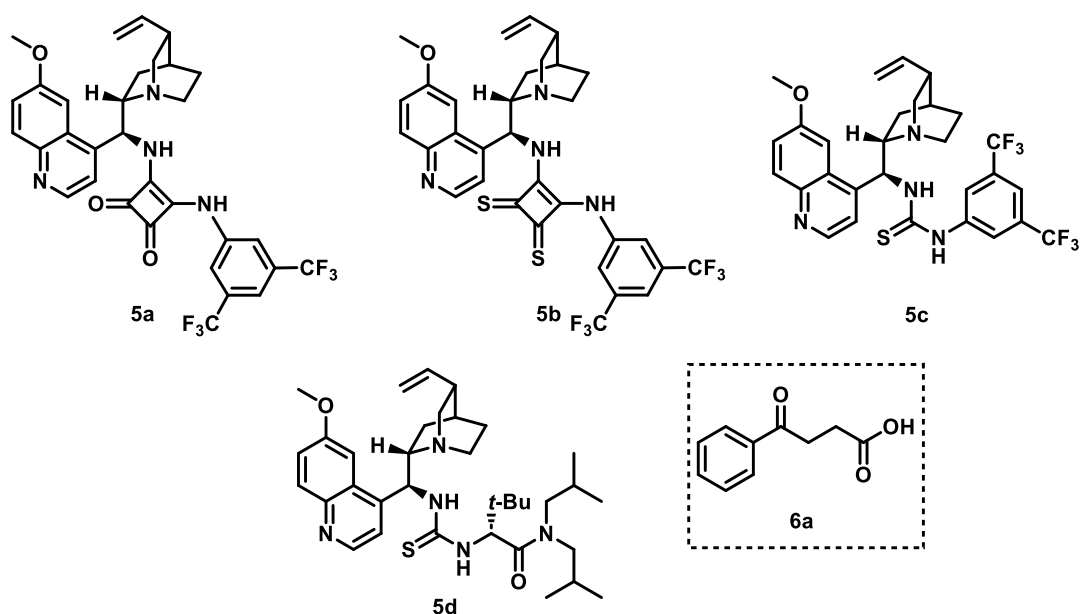
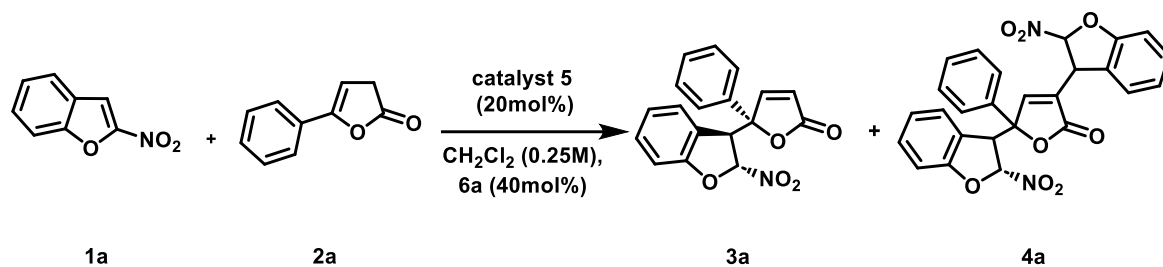
NMR spectra were acquired on a Bruker Ultra Shield 700 instrument, running at 700 MHz for ^1H and 176 MHz for ^{13}C , respectively. Chemical shifts (δ) are reported in ppm relative to residual solvent signals (CDCl_3 : 7.26 ppm for ^1H NMR, 77.16 ppm for ^{13}C NMR). Highresolution mass spectra (HRMS) were obtained on Bruker ESI-Q-TOF Impact II spectrometer using electrospray (ESI+) ionization. Optical rotations were measured on a Perkin-Elmer 241 polarimeter and $[\alpha]_D$ values are given in $\text{deg}\cdot\text{cm}\cdot\text{g}^{-1}\cdot\text{dm}^{-1}$; concentration c is listed in $\text{g}\cdot(100\text{ mL})^{-1}$. Analytical thin layer chromatography (TLC) was performed using pre-coated aluminum-backed plates (Merck Kieselgel 60 F254) and visualized by ultraviolet irradiation or Hanessian's stain. Unless otherwise noted, analytical grade solvents and commercially available reagents were used without further purification. For column chromatography silica gel (Silica gel 60, 230-400 mesh, Fluka). The enantiomeric ratio (er) of the products were determined by Ultra Performance Convergence Chromatography (UPC²) using Daicel Chiralpak IB or IC column as chiral stationary phases. 2-Nitrobenzofurans **1** were synthesized according to the literature procedure.¹ 5-Substituted-furan-2(3*H*)-ones **2** were prepared from the corresponding starting materials following the literature procedure.²

(1) L. Lei, H.-Y. Niu, D.-C. Wang, X.-H. Yang, G.-R. Qu, H.-M. Guo, *Chem. Commun.* 2019, **55**, 553-556.

(2) A. Tsolomitis, C. J. Sandris, *Heterocycl.Chem.* 1983, **20**, 1545-1548.

2. Reaction conditions optimizations

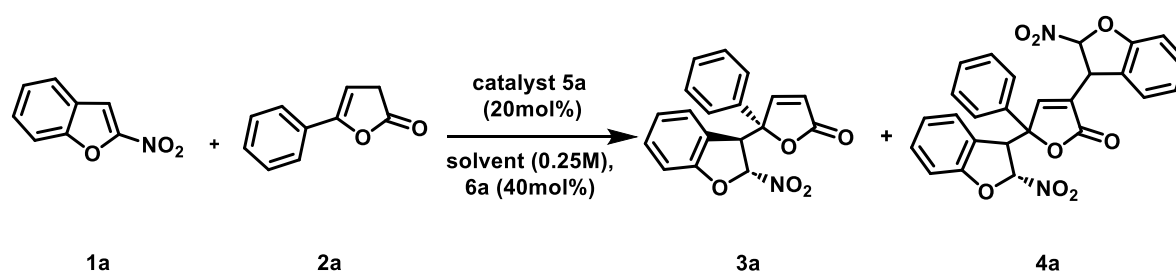
Table S1. Investigation of catalyst.



Entry	Cat.	Solvent	Add. (40mol%)	Conv.[%] ^b 3a/4a	dr ^c	er ^d
1-4	5a-5d	CH_2Cl_2	-	<5/<5	-	-
5	5a	CH_2Cl_2	6a	80/14	4:1	85:15
6	5b	CH_2Cl_2	6a	35/18	1.8:1	-
7	5c	CH_2Cl_2	6a	81/18	1.2:1	-
8	5d	CH_2Cl_2	6a	63/17	4.7:1	70:30

Reaction conditions: The reactions were performed in 0.05 mmol scale using 1.0 equiv of **1a** and 1.2 equiv. **2a**, 20mol% of **5** in 0.2 mL of the solvent in room temperature. ^b Determined by ^1H NMR spectroscopy of a crude reaction mixture after 18 h. In parentheses isolated yield is given. ^c Determined by ^1H NMR spectroscopy of a crude reaction mixture. ^d Determined by CSP UPC².

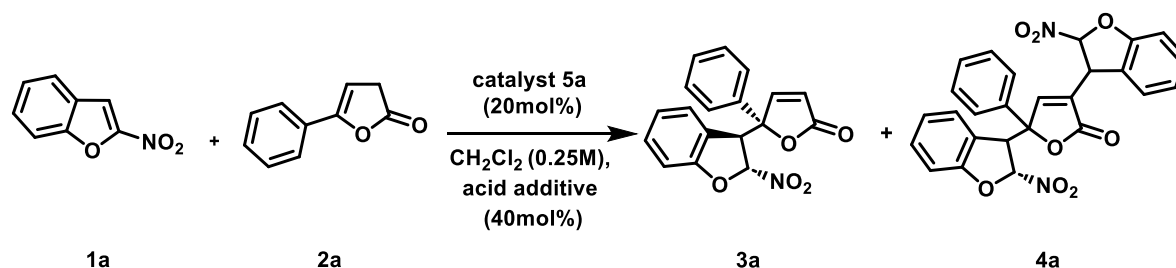
Table S2. Investigation of solvent.



Entry	Cat.	Solvent	Add. (40mol%)	Conv.[%] ^b 3a/4a	dr ^c	er ^d
1	5a	CH ₂ Cl ₂	6a	80/14	4:1	85:15
2	5a	Et ₂ O	6a	72/28	3:1	-
3	5a	THF	6a	74/36	3:1	-
4	5a	toluene	6a	65/28	-	-
5 ^e	5a	CH ₂ Cl ₂	6a	70/0	2:1	85:15
6 ^f	5a	CH ₂ Cl ₂	6a	75/10	-	-
7 ^g	5a	CH ₂ Cl ₂	6a	45/7	-	-

Reaction conditions: The reactions were performed in 0.05 mmol scale using 1.0 equiv of **1a** and 1.2 equiv. **2a**, 20mol% of **5** in 0.2 mL of the solvent in room temperature. ^b Determined by ¹H NMR spectroscopy of a crude reaction mixture after 18 h. In parentheses isolated yield is given. ^c Determined by ¹H NMR spectroscopy of a crude reaction mixture. ^d Determined by CSP UPC². ^e The reaction was conducted in -5°C. ^f Reaction carried out using **1a** (1.0 equiv.) and **2a** (2.0 equiv.). ^g Reaction performed using **1a** (2.0 equiv.) and **2a** (1.0 equiv.).

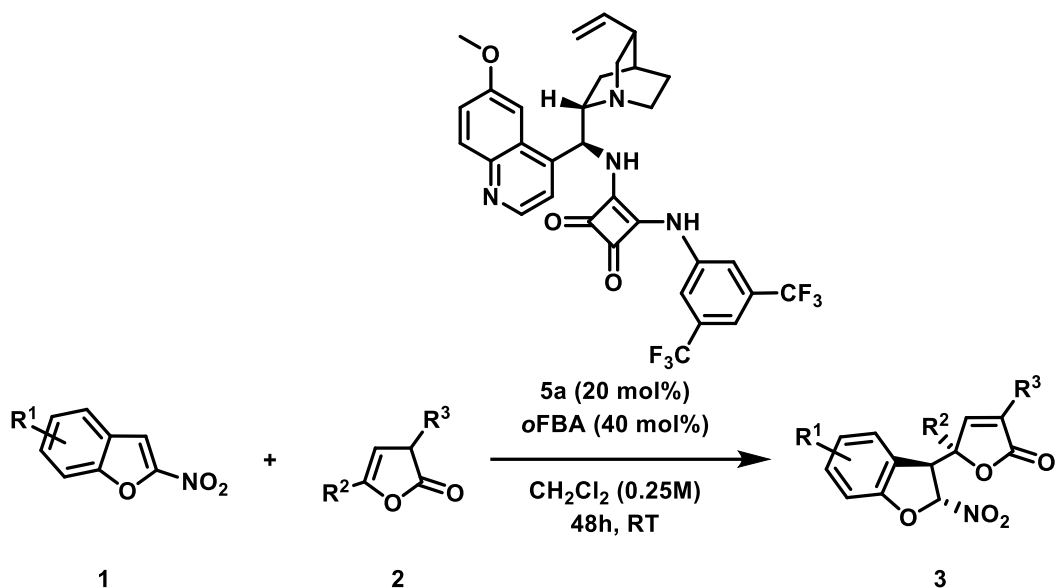
Table S3. Investigation of acid additive.



Entry	Cat.	Solvent	Add. (40mol%)	Conv.[%] ^b 3a/4a	dr ^c	er ^d
1	5a	CH_2Cl_2	AcOH	52/0 (43)	>20:1	97:3
2	5a	CH_2Cl_2	DMABA	81/0 (40)	>20:1	95:5
3	5a	CH_2Cl_2	PhCOOH	84/0 (75)	>20:1	94:6
4	5a	CH_2Cl_2	PicOH	78/0 (60)	>20:1	98.5:1.5
5	5a	CH_2Cl_2	<i>o</i> -FBA	70/0 (68)	>20:1	98:2
6 ^e	5a	CH_2Cl_2	<i>o</i> -FBA	>95/0 (85)	>20:1	98:2

Reaction conditions: The reactions were performed in 0.05 mmol scale using 1.0 equiv of **1a** and 1.2 equiv. **2a**, 20mol% of **5** in 0.2 mL of the solvent in room temperature. ^b Determined by ¹H NMR spectroscopy of a crude reaction mixture after 18 h. In parentheses isolated yield is given. ^c Determined by ¹H NMR spectroscopy of a crude reaction mixture. ^d Determined by CSP UPC². ^e Reaction time 48h. DMABA – 4-(dimethylamino)benzoic acid; PicOH – picolinic acid; *o*-FBA - *ortho*-fluorobenzoic acid.

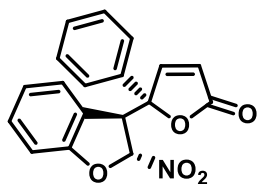
3. General procedure for dearomative Michael addition



In an ordinary 4 mL glass vial equipped with a magnetic stirring bar 2-nitrobenzofuran **1** (0.1 mmol, 1.0 equiv.) and 5-substituted-furan-2(3H)-one **2** (0.15 mmol, 1.5 equiv.) were dissolved in CH₂Cl₂ (0.4 mL). Cinchona alkaloid catalyst **5** (12.6 mg, 0.02 mmol, 0.2 equiv.) and *o*-fluorobenzoic acid (5.6 mg, 0.04 mmol, 0.4 equiv.) were added and the reaction mixture was stirred in room temperature for 48h. The progress of the reaction was controlled by ¹H NMR spectroscopy. After full conversion of the starting material **1**, the reaction mixture was directly subjected to column chromatography on silica gel (hexanes : ethyl acetate 4:1) to afford pure product **3**.

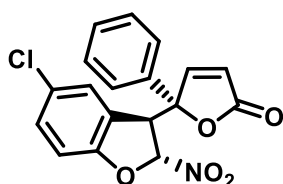
4. Characterization data of products 3

(*R*)-5-((2*R*,3*S*)-2-Nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(5*H*)-one **3a**



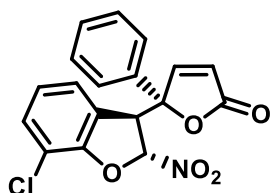
Following the general procedure product **3a** (>20:1 dr in a crude reaction mixture) was isolated in 85% yield as light-yellow oil (27.5 mg). ¹H NMR (700 MHz, CDCl₃) δ 7.63 (d, *J* = 5.7 Hz, 1H), 7.52 – 7.48 (m, 2H), 7.48 – 7.43 (m, 3H), 7.37 – 7.31 (m, 1H), 7.10 (d, *J* = 8.1 Hz, 1H), 6.95 (t, *J* = 7.5 Hz, 1H), 6.75 (d, *J* = 7.5 Hz, 1H), 6.18 (d, *J* = 5.7 Hz, 1H), 5.83 (d, *J* = 1.4 Hz, 1H), 4.51 (s, 1H). ¹³C NMR (176 MHz, CDCl₃) δ 170.3, 159.2, 155.2, 135.7, 131.2, 129.8, 129.6 (2C), 126.4, 126.1 (2C), 122.9, 122.9, 119.9, 111.4, 106.9, 90.4, 57.4. The er was determined by UPC² using a chiral Chiralpack IC column gradient from 100% CO₂ up to 40%; *i*-PrOH, 2.5 mL/min; *t*_R = 3.245 (major), *t*_R = 3.458 (minor) : 98:2 er. [α]_D²¹ = - 51.5 (c = 1.0, CHCl₃). HRMS *m/z* [M+Na]⁺ Calculated for C₁₈H₁₃NO₅Na⁺: 346.0686; found 346.0683.

(*R*)-5-((2*R*,3*S*)-5-Chloro-2-nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(5*H*)-one **3b**



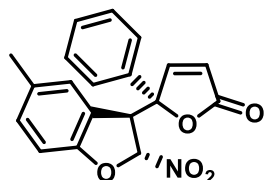
Following the general procedure product **3b** (>20:1 dr in a crude reaction mixture) was isolated in 74% yield as light-yellow oil (26.3 mg). ¹H NMR (700 MHz, CDCl₃) δ 7.64 (d, *J* = 5.7 Hz, 1H), 7.53 – 7.50 (m, 2H), 7.49 – 7.45 (3H), 7.31 (dd, *J* = 8.6, 2.2 Hz, 1H), 7.03 (d, *J* = 8.6 Hz, 1H), 6.76 (d, *J* = 2.2, 1H), 6.22 (d, *J* = 5.7 Hz, 1H), 5.85 (d, *J* = 1.5 Hz, 1H), 4.47 (s, 1H). ¹³C NMR (176 MHz, CDCl₃) δ 170.1, 157.9, 154.9, 135.2, 131.3, 129.9, 129.8 (2C), 128.0, 126.4, 125.9 (2C), 123.0, 121.8, 112.4, 107.1, 90.1, 57.2. The er was determined by UPC² using a chiral Chiralpack IC column gradient from 100% CO₂ up to 40%; *i*-PrOH, 2.5 mL/min; *t*_R = 3.078 (major), *t*_R = 3.242 (minor) : 97:3 er. [α]_D²¹ = - 71.3 (c = 1.0, CHCl₃). HRMS *m/z* [M+Na]⁺ Calculated for C₁₈H₁₂ClNO₅Na⁺ : 380.0296; found 380.0292.

(*R*)-5-((2*R*,3*S*)-7-Chloro-2-nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(5*H*)-one **3c**



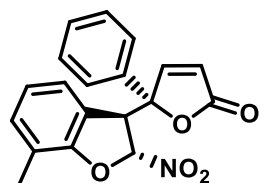
Following the general procedure product **3c** (>20:1 in a crude reaction mixture) was isolated in 80% yield as yellow oil (28.4 mg). ¹H NMR (700 MHz, CDCl₃) δ 7.65 (d, *J* = 5.7 Hz, 1H), 7.52 – 7.49 (m, 2H), 7.48 – 7.44 (m, 3H), 7.34 – 7.30 (m, 1H), 6.91 (t, *J* = 7.8 Hz, 1H), 6.65 (m, 1H), 6.20 (d, *J* = 5.7 Hz, 1H), 5.89 (d, *J* = 1.6 Hz, 1H), 4.55 (s, 1H). ¹³C NMR (176 MHz, CDCl₃) δ 170.0, 155.3, 154.9, 135.4, 131.6, 129.9, 129.7 (2C), 126.0 (2C), 124.5, 123.8, 123.2, 121.8, 117.0, 106.5, 90.1, 58.0. The er was determined by UPC² using a chiral Chiralpack IC column gradient from 100% CO₂ up to 40%; *i*-PrOH, 2.5 mL/min; *t*_R = 3.375 (major) *t*_R = 3.544 (minor) : 93:7 er. [α]_D²¹ = - 49.9 (c = 1.0, CHCl₃). HRMS *m/z* [M+Na]⁺ Calculated for C₁₈H₁₂ClNO₅Na⁺ : 380.0294; found 380.0293.

(*R*)-5-((2*R*,3*S*)-5-Methyl-2-nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(5*H*)-one
3d



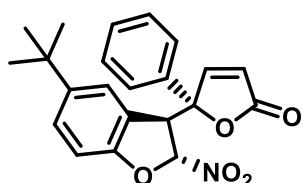
Following the general procedure product **3d** (>20:1 in a crude reaction mixture) was isolated in 50% yield as light-yellow oil (16.7 mg). ¹H NMR (700 MHz, CDCl₃) δ 7.63 (d, *J* = 5.7 Hz, 1H), 7.50 – 7.48 (m, 2H), 7.46 – 7.44 (m, 3H), 7.11 (d, *J* = 8.3 Hz, 1H), 6.97 (d, *J* = 8.3 Hz, 1H), 6.52 (s, 1H), 6.18 (d, *J* = 5.7 Hz, 1H), 5.80 (d, *J* = 1.4 Hz, 1H), 4.45 (s, 1H), 2.23 (s, 3H). ¹³C NMR (176 MHz, CDCl₃) δ 170.4, 157.2, 155.3, 135.7, 132.4, 131.7, 129.7, 129.5 (2C), 126.8, 126.1 (2C), 122.8, 119.8, 110.8, 107.2, 90.4, 57.4, 21.0. The er was determined by UPC² using a chiral Chiralpack IC column gradient from 100% CO₂ up to 40%; *i*-PrOH, 2.5 mL/min; *t*_R = 3.292 (major) *t*_R = 3.638 (minor) : 97:3 er. [α]_D²¹ = - 61.7 (c = 1.0, CHCl₃). HRMS *m/z* [M+Na]⁺ Calculated for C₁₉H₁₅NO₅Na⁺ : 360.0842 ; found 360.0846.

(*R*)-5-((2*R*,3*S*)-7-Methyl-2-nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(5*H*)-one
3e



Following the general procedure product **3e** (>20:1 in a crude reaction mixture) was isolated in 46% yield as brown oil (15.3 mg). ¹H NMR (700 MHz, CDCl₃) δ 7.63 (d, *J* = 5.7 Hz, 1H), 7.51 – 7.48 (m, 2H) 7.13 (d, *J* = 7.6 Hz, 1H), 6.84 (t, *J* = 7.5 Hz, 1H), 6.55 (d, *J* = 7.6 Hz, 1H), 6.17 (d, *J* = 5.7 Hz, 1H), 5.82 (d, *J* = 1.4 Hz, 1H), 4.54 – 4.48 (m, 1H), 2.34 (s, 3H). ¹³C NMR (176 MHz, CDCl₃) δ 170.4, 157.7, 155.4, 135.8, 132.4, 129.7 (2C), 129.5, 126.1 (2C), 123.6, 122.8, 122.7, 121.7, 119.2, 106.8, 90.4, 57.7, 15.1. The er was determined by UPC² using a chiral Chiralpack IC column gradient from 100% CO₂ up to 40%; *i*-PrOH, 2.5 mL/min; *t*_R = 3.138 (major) *t*_R = 3.274 (minor) : 93:7. [α]_D²¹ = - 85.5 (c = 1.0, CHCl₃). HRMS *m/z* [M+Na]⁺ Calculated for C₁₉H₁₅NO₅Na⁺ 360.0842; found 360.0835.

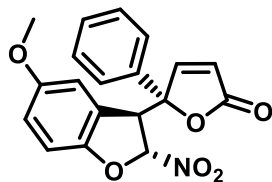
(*R*)-5-((2*R*,3*S*)-5-(*tert*-Butyl)-2-nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(5*H*)-one
3f



Following the general procedure product **3f** (>20:1 in a crude reaction mixture) was isolated in 58% yield as yellow oil (21.9 mg). ¹H NMR (700 MHz, CDCl₃) δ 7.59 (d, *J* = 5.7 Hz, 1H), 7.50 – 7.46 (m, 2H), 7.46 – 7.42 (m, 3H), 7.35 – 7.31 (m, 1H), 7.00 (d, *J* = 8.5 Hz, 1H), 6.57 (d, *J* = 2.1 Hz, 1H), 6.20 (d, *J* = 5.7 Hz, 1H), 5.76 (d, *J* = 1.3 Hz, 1H), 4.50 (d, *J* = 1.3 Hz, 1H), 1.18 (s, 9H). ¹³C NMR (176 MHz, CDCl₃) δ 170.2, 156.8, 155.1, 145.9, 135.9, 129.7 (2C), 129.5, 127.9, 126.4 (2C), 123.7, 123.1, 119.6, 110.3, 107.1, 90.5, 57.7, 34.5, 31.5 (3C). The er was determined by UPC² using a chiral Chiralpack IC column gradient from 100% CO₂ up to 40%; *i*-PrOH, 2.5 mL/min; *t*_R = 3.176 (major) *t*_R = 3.531 (minor)

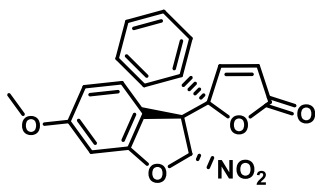
: 98:2 er. $[\alpha]_D^{21} = -26.2$ ($c = 1.0$, CHCl_3). HRMS m/z $[\text{M}+\text{Na}]^+$ Calculated for $\text{C}_{22}\text{H}_{21}\text{NO}_5\text{Na}^+$: 379.1419; found 379.1757.

(*R*)-5-((2*R*,3*S*)-5-Methoxy-2-nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(5*H*)-one
3g



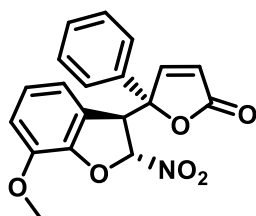
Following the general procedure product **3g** (>20:1 in a crude reaction mixture) was isolated in 63% yield as orange oil (22.2 mg). ^1H NMR (700 MHz, CDCl_3) δ 7.61 (d, $J = 5.7$ Hz, 1H), 7.52 – 7.47 (m, 3H), 7.48 – 7.43 (m, 3H), 7.00 (d, $J = 8.8$ Hz, 1H), 6.85 (dd, $J = 8.8, 2.7$ Hz, 1H), 6.23 (d, $J = 5.7$ Hz, 1H), 5.78 (d, $J = 1.3$ Hz, 1H), 4.48 (s, 1H), 3.66 (s, 3H). ^{13}C NMR (176 MHz, CDCl_3) δ 170.3, 155.4, 155.1, 153.1, 135.8, 129.8, 129.6 (2C), 126.3 (2C), 123.2, 120.9, 116.0, 112.5, 111.5, 107.4, 90.3, 57.7, 56.0. The er was determined by UPC² using a chiral Chiralpack IC column gradient from 100% CO_2 up to 40%; *i*-PrOH, 2.5 mL/min; $t_R = 3.344$ (major) $t_R = 3.650$ (minor) : 93:7 er. $[\alpha]_D^{21} = -69.6$ ($c = 1.0$, CHCl_3). HRMS m/z $[\text{M}+\text{Na}]^+$ Calculated for $\text{C}_{18}\text{H}_{12}\text{ClNO}_5\text{Na}^+$: 376.0791; found 376.0788.

(*R*)-5-((2*R*,3*S*)-6-Methoxy-2-nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(5*H*)-one
3h



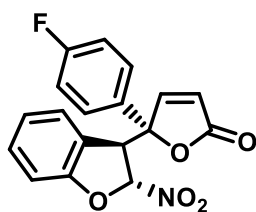
Following the general procedure product **3h** (>20:1 in a crude reaction mixture) was isolated in 43% yield as orange oil (15.3 mg). ^1H NMR (700 MHz, CDCl_3) δ 7.61 (d, $J = 5.7$ Hz, 1H), 7.50 – 7.48 (m, 2H), 7.47 – 7.45 (m, 3H), 6.66 (d, $J = 2.3$ Hz, 1H), 6.61 (d, $J = 8.4$ Hz, 1H), 6.48 (dd, $J = 8.4, 2.3$ Hz, 1H), 6.17 (d, $J = 5.7$ Hz, 1H), 5.82 (d, $J = 1.4$ Hz, 1H), 4.47 – 4.39 (m, 1H), 3.80 (s, 3H). ^{13}C NMR (176 MHz, CDCl_3) δ 170.4, 162.4, 160.7, 155.3, 135.8, 129.7, 129.6 (2C), 126.5, 126.1 (2C), 122.9, 111.4, 109.2, 107.6, 97.3, 90.5, 57.0, 55.8. The er was determined by UPC² using a chiral Chiralpack IB column gradient from 100% CO_2 up to 40%; *i*-PrOH, 2.5 mL/min; $t_R = 3.810$ (major) $t_R = 4.111$ (minor) : 93:7 er. $[\alpha]_D^{21} = -62.1$ ($c = 1.0$, CHCl_3). HRMS m/z $[\text{M}+\text{Na}]^+$ Calculated for $\text{C}_{19}\text{H}_{15}\text{NO}_6\text{Na}^+$: 376.0791; found 376.0784.

(*R*)-5-((2*R*,3*S*)-7-Methoxy-2-nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(5*H*)-one
3i



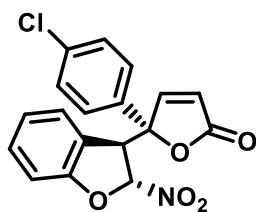
Following the general procedure product **3i** (>20:1 in a crude reaction mixture) was isolated in 40% yield as brown oil (14.3 mg). ^1H NMR (700 MHz, CDCl_3) δ 7.62 (d, $J = 5.6$ Hz, 1H), 7.49 – 7.48 (m, 2H), 7.47 – 7.45 (m, 3H), 6.95 – 6.85 (m, 2H), 6.32 – 6.29 (m, 1H), 6.18 (d, $J = 5.6$ Hz, 1H), 5.83 (d, $J = 1.4$ Hz, 1H), 4.58 – 4.51 (m, 1H), 3.93 (s, 3H). ^{13}C NMR (176 MHz, CDCl_3) δ 170.3, 155.2, 147.6, 145.0, 135.8, 129.7, 129.6 (2C), 126.2 (2C), 123.7, 123.0, 121.4, 118.0, 114.6, 107.0, 90.3, 57.9, 56.6. The er was determined by UPC² using a chiral Chiralpack IC column gradient from 100% CO_2 up to 40%; *i*-PrOH, 2.5 mL/min; $t_R = 3.778$ (major) $t_R = 4.067$ (minor) : 78:22 er. $[\alpha]_D^{21} = -44.8$ ($c = 1.0$, CHCl_3). HRMS m/z $[\text{M}+\text{Na}]^+$ Calculated for $\text{C}_{19}\text{H}_{15}\text{NO}_6\text{Na}^+$: 376.0791; found 376.0783.

(*R*)-5-(4-Fluorophenyl)-5-((2*R*,3*S*)-2-nitro-2,3-dihydrobenzofuran-3-yl)furan-2(5*H*)-one
3j



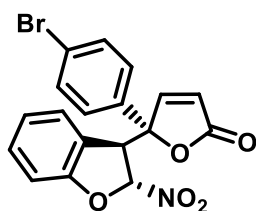
Following the general procedure product **3j** (>20:1 in a crude reaction mixture) was isolated in 43% yield as orange oil (14.6 mg). ¹H NMR (700 MHz, CDCl₃) δ 7.59 (d, *J* = 5.7 Hz, 1H), 7.46 – 7.43 (m, 2H), 7.36 – 7.33 (m, 1H), 7.21 – 7.16 (m, 2H), 7.10 (d, *J* = 8.2 Hz, 1H), 6.96 (td, *J* = 7.5, 1.0 Hz, 1H), 6.76 – 6.74 (m, 1H), 6.20 (d, *J* = 5.7 Hz, 1H), 5.80 (d, *J* = 1.4 Hz, 1H), 4.47 (s, 1H). ¹³C NMR (176 MHz, CDCl₃) δ 170.0, 163.3 (d, *J*_{C-F} = 250.2 Hz), 159.2, 154.9, 131.6 (d, *J*_{C-F} = 3.2 Hz), 131.3, 128.2, (d, *J*_{C-F} = 8.6 Hz, 2C), 126.3, 123.1, 123.0, 119.7, 116.7 (d, *J*_{C-F} = 22.1 Hz, 2C), 111.4, 106.7, 89.9, 57.4. The er was determined by UPC² using a chiral Chiralpack IC column gradient from 100% CO₂ up to 40%; *i*-PrOH, 2.5 mL/min; *t*_R = 3.043 (major) *t*_R = 3.200 (minor) : 87:13 er. [α]_D²¹ = - 70.5 (c = 1.0, CHCl₃). HRMS *m/z* [M+Na]⁺ Calculated for C₁₈H₁₂FNO₅Na⁺: 364.0591; found 364.0586.

(*R*)-5-(4-Chlorophenyl)-5-((2*R*,3*S*)-2-nitro-2,3-dihydrobenzofuran-3-yl)furan-2(5*H*)-one
3k



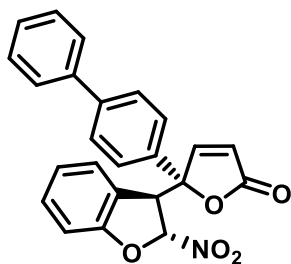
Following the general procedure product **3k** (>20:1 in a crude reaction mixture) was isolated in 65% yield as yellow oil (23.0 mg). ¹H NMR (700 MHz, CDCl₃) δ 7.59 (d, *J* = 5.6 Hz, 1H), 7.47 (d, *J* = 8.5 Hz, 2H), 7.40 (d, *J* = 8.5 Hz, 2H), 7.34 (t, *J* = 7.8 Hz, 1H), 7.10 (d, *J* = 8.1 Hz, 1H), 6.97 (t, *J* = 7.5 Hz, 1H), 6.77 (d, *J* = 7.5 Hz, 1H), 6.19 (d, *J* = 5.6 Hz, 1H), 5.90 – 5.86 (m, 1H), 4.47 (s, 1H). ¹³C NMR (176 MHz, CDCl₃) δ 169.9, 159.2, 154.8, 136.0, 134.2, 131.4, 129.8 (2C), 127.5 (2C), 126.4, 123.2, 123.0, 119.6, 111.4, 106.7, 89.8, 57.2. The er was determined by UPC² using a chiral Chiralpack IC column gradient from 100% CO₂ up to 40%; *i*-PrOH, 2.5 mL/min; *t*_R = 3.316 (major) *t*_R = 3.490 (minor) : 94:6 er. [α]_D²¹ = - 49.1 (c = 1.0, CHCl₃). HRMS *m/z* [M+Na]⁺ Calculated for C₁₈H₁₂ClNO₅Na⁺ : 380.0296; found 380.0292.

(*R*)-5-(4-Bromophenyl)-5-((2*R*,3*S*)-2-nitro-2,3-dihydrobenzofuran-3-yl)furan-2(5*H*)-one
3l



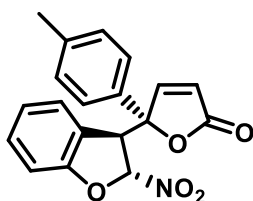
Following the general procedure product **3l** (>20:1 in a crude reaction mixture) was isolated in 65% yield as brown oil (25.9 mg). ¹H NMR (700 MHz, CDCl₃) δ 7.65 – 7.61 (m, 2H), 7.59 (d, *J* = 5.6 Hz, 1H), 7.38 – 7.30 (m, 3H), 7.10 (d, *J* = 8.2 Hz, 1H), 6.97 (t, *J* = 7.5 Hz, 1H), 6.78 (d, *J* = 7.5 Hz, 1H), 6.19 (d, *J* = 5.6 Hz, 1H), 5.81 – 5.78 (m, 1H), 4.46 (s, 1H). ¹³C NMR (176 MHz, CDCl₃) δ 169.9, 159.2, 154.7, 134.7, 132.8 (2C), 131.4, 127.8 (2C), 126.3, 124.1, 123.2, 123.0, 119.58, 111.4, 106.7, 89.9, 57.2. The er was determined by UPC² using a chiral Chiralpack IC column gradient from 100% CO₂ up to 40%; *i*-PrOH, 2.5 mL/min; *t*_R = 3.482 (major) *t*_R = 3.671 (minor) : 95:5 er. [α]_D²¹ = - 89.4 (c = 1.0, CHCl₃). HRMS *m/z* [M+Na]⁺ Calculated for C₁₈H₁₂BrNO₅Na⁺ : 423.9791; found 423.9773.

(*R*)-5-([1,1'-Biphenyl]-4-yl)-5-((2*R*,3*S*)-2-nitro-2,3-dihydrobenzofuran-3-yl)furan-2(5*H*)-one 3m



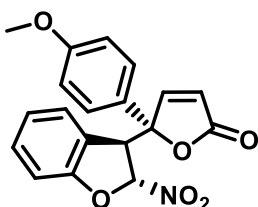
Following the general procedure product **3m** (>20:1 in a crude reaction mixture) was isolated in 91% yield as orange oil (36.3 mg). ¹H NMR (700 MHz, CDCl₃) δ 7.72 (d, *J* = 8.3 Hz, 2H), 7.66 (d, *J* = 5.6 Hz, 1H), 7.64 – 7.58 (m, 2H), 7.54 (d, *J* = 8.3 Hz, 2H), 7.48 (t, *J* = 7.7 Hz, 2H), 7.40 (t, *J* = 7.4 Hz, 1H), 7.35 (t, *J* = 7.7 Hz, 1H), 7.11 (d, *J* = 8.1 Hz, 1H), 6.97 (t, *J* = 7.5 Hz, 1H), 6.81 (d, *J* = 7.5 Hz, 1H), 6.19 (d, *J* = 5.6 Hz, 1H), 5.89 – 5.87 (m, 1H), 4.56 (s, 1H). ¹³C NMR (176 MHz, CDCl₃) δ 170.3, 159.2, 155.2 (2C), 142.6, 139.8, 134.4, 131.2, 129.1 (2C), 128.2 (2C), 127.3 (2C), 126.6 (2C), 126.4, 122.9 (2C), 119.9, 111.4, 107.0, 90.3, 57.2. The er was determined by UPC² using a chiral Chiralpack IC column gradient from 100% CO₂ up to 40%; *i*-PrOH, 2.5 mL/min; *t*_R = 4.155 (major) *t*_R = 4.316 (minor) : 96:4 er. [α]_D²¹ = - 124.2 (c = 1.0, CHCl₃). HRMS *m/z* [M+Na]⁺ Calculated for C₂₄H₁₇NO₅Na⁺ 422.0999; found 422.1000.

(*R*)-5-((2*R*,3*S*)-2-Nitro-2,3-dihydrobenzofuran-3-yl)-5-(*p*-tolyl)furan-2(5*H*)-one 3n



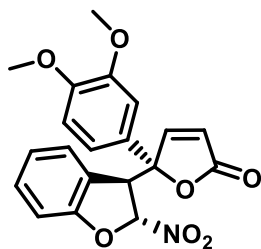
Following the general procedure product **3n** (>20:1 in a crude reaction mixture) was isolated in 66% yield as orange oil (22.1 mg). ¹H NMR (700 MHz, CDCl₃) δ 7.60 (d, *J* = 5.5 Hz, 1H), 7.36 – 7.31 (m, 3H), 7.30 – 7.27 (m, 2H), 7.09 (d, *J* = 8.1 Hz, 1H), 6.95 (t, *J* = 7.5 Hz, 1H), 6.76 (d, *J* = 7.5 Hz, 1H), 6.15 (d, *J* = 5.5 Hz, 1H), 5.83 (s, 1H), 4.50 (s, 1H), 2.40 (s, 3H). ¹³C NMR (176 MHz, CDCl₃) δ 170.4, 159.2, 155.4, 139.8, 132.6, 131.1, 130.2 (2C), 126.4, 126.0 (2C), 122.8, 122.7, 120.0, 111.3, 107.0, 90.4, 57.3, 21.3. The er was determined by UPC² using a chiral Chiralpack IC column gradient from 100% CO₂ up to 40%; *i*-PrOH, 2.5 mL/min; *t*_R = 3.613 (major) *t*_R = 3.770 (minor) : 97:3 er. [α]_D²¹ = - 79.0 (c = 1.0, CHCl₃). HRMS *m/z* [M+Na]⁺ Calculated for C₁₉H₁₅NO₅Na⁺ : 360.0842; found : 360.0837.

(*R*)-5-(4-Methoxyphenyl)-5-((2*R*,3*S*)-2-nitro-2,3-dihydrobenzofuran-3-yl)furan-2(5*H*)-one 3o



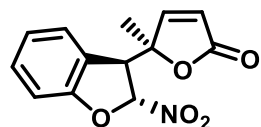
Following the general procedure product **3o** (>20:1 in a crude reaction mixture) was isolated in 83% yield as light-yellow oil (29.2 mg). ¹H NMR (700 MHz, CDCl₃) δ 7.58 (d, *J* = 5.7 Hz, 1H), 7.37 – 7.35 (m, 2H), 7.35 – 7.28 (m, 1H), 7.09 (d, *J* = 8.1 Hz, 1H), 7.02 – 6.97 (m, 2H), 6.94 (td, *J* = 7.5, 1.0 Hz, 1H), 6.81 – 6.70 (d, *J* = 7.5 Hz, 1H), 6.16 (d, *J* = 5.7 Hz, 1H), 5.82 (d, *J* = 1.4 Hz, 1H), 4.48 (s, 1H), 3.85 (s, 3H). ¹³C NMR (176 MHz, CDCl₃) δ 170.4, 160.5, 159.1, 155.4, 131.1, 127.5, 127.5 (2C), 126.4, 122.9, 122.8, 120.1, 114.9 (2C), 111.3, 107.0, 90.3, 57.4, 55.6. The er was determined by UPC² using a chiral Chiralpack IC column gradient from 100% CO₂ up to 40%; *i*-PrOH, 2.5 mL/min; *t*_R = 3.613 (major) *t*_R = 3.770 (minor) : 97:3 er. [α]_D²¹ = - 69.1 (c = 1.0, CHCl₃). HRMS *m/z* [M+Na]⁺ Calculated for C₁₉H₁₅NO₆Na⁺ : 376.0791; found 376.0788.

(R)-5-(3,4-Dimethoxyphenyl)-5-((2R,3S)-2-nitro-2,3-dihydrobenzofuran-3-yl)furan-2(5H)-one 3p



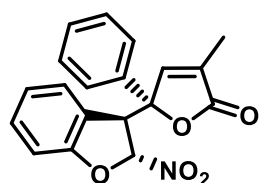
Following the general procedure product **3p** (>20:1 in a crude reaction mixture) was isolated in 56% yield as dark-pink oil (20.5 mg). ¹H NMR (700 MHz, CDCl₃) δ 7.62 (d, *J* = 5.7 Hz, 1H), 7.36 – 7.28 (m, 1H), 7.09 (d, *J* = 8.1 Hz, 1H), 6.96 (td, *J* = 7.5, 1.0 Hz, 1H), 6.93 – 6.91 (m 3H), 6.84 – 6.77 (m, 1H), 6.17 (d, *J* = 5.7 Hz, 1H), 5.84 (d, *J* = 1.4 Hz, 1H), 4.48 (s, 1H), 3.91 (s, 3H), 3.88 (s, 3H). ¹³C NMR (176 MHz, CDCl₃) δ 170.4, 159.2, 155.4, 150.1, 149.8, 131.1, 127.7, 126.5, 122.9, 122.6, 120.1, 118.8, 111.4, 111.3, 109.1, 107.0, 90.2, 57.3, 56.3, 56.1. The er was determined by UPC² using a chiral Chiralpack IC column gradient from 100% CO₂ up to 40%; *i*-PrOH, 2.5 mL/min; *t*_R = 3.883 (major) *t*_R = 4.061 (minor) : 96:4 er. [α]_D²¹ = - 94.1 (c = 1.0, CHCl₃). HRMS *m/z* [M+Na]⁺ Calculated for C₂₀H₁₇NO₇Na⁺ 406.0897; found 406.0907.

(R)-5-Methyl-5-((2R,3S)-2-nitro-2,3-dihydrobenzofuran-3-yl)furan-2(5H)-one 3r



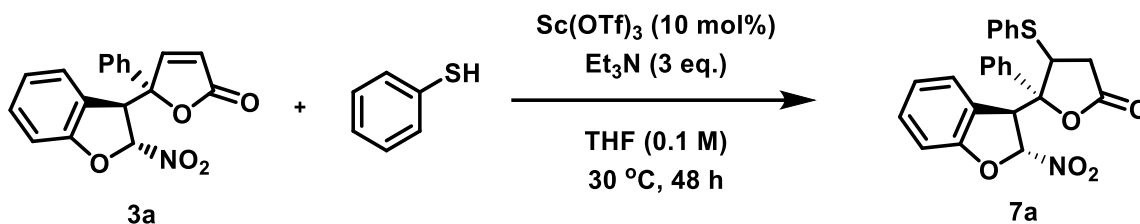
Following the general procedure product **3r** (>20:1 in a crude reaction mixture) was isolated in 65% yield as light-yellow oil (16.9 mg). ¹H NMR (700 MHz, CDCl₃) δ 7.38 – 7.34 (m, 1H), 7.30 (d, *J* = 5.7 Hz, 1H), 7.23 – 7.21 (m, 1H), 7.13 – 7.09 (m, 1H), 7.08 – 7.05 (m, 1H), 6.16 (d, *J* = 5.7 Hz, 1H), 5.92 (d, *J* = 1.7 Hz, 1H), 4.21 – 3.87 (m, 1H), 1.68 (s, 3H). ¹³C NMR (700 MHz, CDCl₃) δ 170.6, 158.7, 156.6, 131.1 (2C), 129.1, 128.3, 126.3, 111.3, 106.4, 87.4, 56.8, 22.3. The er was determined by UPC² using a chiral Chiralpack IC column gradient from 100% CO₂ up to 40%; *i*-PrOH, 2.5 mL/min; *t*_R = 3.214 (major) *t*_R = 3.493 (minor) : 95:5 er. [α]_D²¹ = - 38.9 (c = 1.0, CHCl₃). HRMS *m/z* [M+Na]⁺ Calculated for C₁₃H₁₁NO₅Na⁺ : 284.0529; found 284.0527.

(R)-3-Methyl-5-((2R,3S)-2-nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(5H)-one 3s



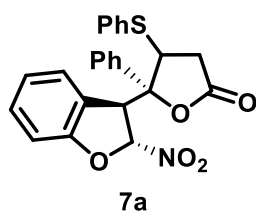
Following the general procedure product **3s** (>20:1 in a crude reaction mixture) was isolated in 58% yield as light-yellow oil (19.7 mg). ¹H NMR (700 MHz, CDCl₃) δ 7.51 – 7.47 (m, 2H), 7.46 – 7.43 (m, 3H), 7.32 (t, *J* = 7.8 Hz, 1H), 7.22 (s, 1H), 7.09 (d, *J* = 8.1 Hz, 1H), 6.94 (t, *J* = 7.5 Hz, 1H), 6.72 (d, *J* = 7.5 Hz, 1H), 5.81 (s, 1H), 4.46 (s, 1H), 1.90 (s, 3H). ¹³C NMR (176 MHz, CDCl₃) δ 171.6, 159.3, 147.6, 136.3, 132.0, 131.1, 129.5, 129.4 (2C), 126.3, 126.1 (2C), 122.7, 120.2, 111.3, 107.0, 88.0, 57.7, 10.8. The er was determined by UPC² using a chiral Chiralpack IC column gradient from 100% CO₂ up to 40%; *i*-PrOH, 2.5 mL/min; *t*_R = 3.055 (major) *t*_R = 3.389 (minor) : 95:5 er. [α]_D²¹ = - 102.1 (c = 1.0, CHCl₃). HRMS *m/z* [M+Na]⁺ Calculated for C₁₉H₁₅NO₅Na⁺ : 360.0842; found 360.0839.

5. Transformations of the product 3a

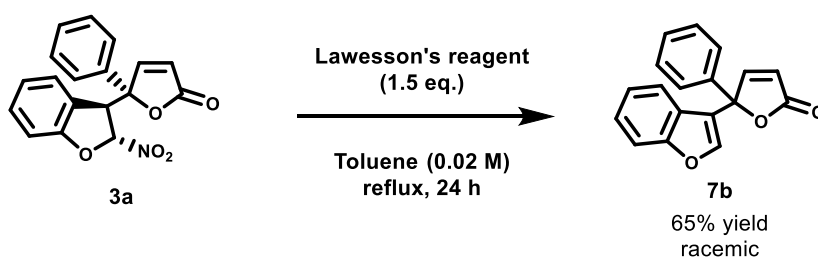


In an ordinary 4 mL glass vial equipped with a magnetic stirring bar **3a** (32.3 mg, 0.1 mmol), Sc(OTf)₃ (4.9 mg, 0.01 mmol) were stirred in THF (1 mL) at 30 °C for 30 min. Then benzenethiol (0.1 mL, 1 mmol) was added, followed by Et₃N (0.04 mL, 0.30 mmol) and the reaction mixture was stirred at 30 °C for 48 h. After full conversion of starting material **3a**, the reaction mixture was purified by column chromatography on silica gel (gradient elution: petroleum ether:ethyl acetate 8:1 to 4:1) to obtain product **4a** in 74% yield (32 mg) with 2:1 dr (in a crude reaction mixture) as pale yellow solid.

(5R)-5-((2R,3S)-2-Nitro-2,3-dihydrobenzofuran-3-yl)-5-phenyl-4-phenylthio-2,3-dihydrofuran-2-one **7a**

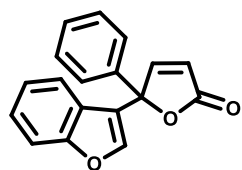


Following the general procedure product **4a** was isolated in 74% yield as pale yellow solid (32 mg) (2:1 dr in a crude reaction mixture). Major diastereoisomer: ¹H NMR (700 MHz, CDCl₃) δ 7.62 – 7.58 (m, 2H), 7.56 – 7.52 (m, 2H), 7.44 – 7.29 (m, 7H), 7.17 (d, *J* = 7.5 Hz, 1H), 7.10 (d, *J* = 8.1 Hz, 1H), 7.03–7.00 (m, 1H), 5.83 (d, *J* = 1.3 Hz, 1H), 4.70 (s, 1H), 4.41 (dd, *J* = 9.6, 7.9 Hz, 1H), 2.93 – 2.67 (m, 1H), 2.58 (dd, *J* = 17.9, 9.6 Hz, 1H). ¹³C NMR (176 MHz, CDCl₃) δ 172.5, 159.7, 134.7, 132.3, 131.2, 129.8 (2C), 129.7 (2C), 129.2, 128.8 (2C), 128.7, 126.9 (2C), 125.9, 123.3, 120.5, 111.7, 107.9, 89.7, 56.5, 49.4, 36.7. Minor diastereoisomer: ¹H NMR (700 MHz, CDCl₃) δ 7.98 (d, *J* = 7.5 Hz, 1H), 7.69 – 7.62 (m, 2H), 7.51 – 7.48 (m, 2H), 7.44 – 7.29 (m, 7H), 7.15–7.12 (m, 1H), 7.05 (d, *J* = 8.1 Hz, 1H), 5.81 (d, *J* = 1.2 Hz, 1H), 4.96 (s, 1H), 4.13–4.10 (m, 1H), 2.93 – 2.67 (m, 2H). ¹³C NMR (176 MHz, CDCl₃) 171.69, 159.85, 140.00, 135.25 (2C), 132.80 (3C), 132.74 (2C), 131.35, 129.19, 128.71, 127.69, 124.48 (2C), 123.05, 120.15, 111.51, 108.59, 90.27, 55.76, 54.26, 37.49. HRMS *m/z* [M+Na]⁺ Calculated for C₂₄H₁₉NNaO₅S⁺: 456.0877; found 456.0865.



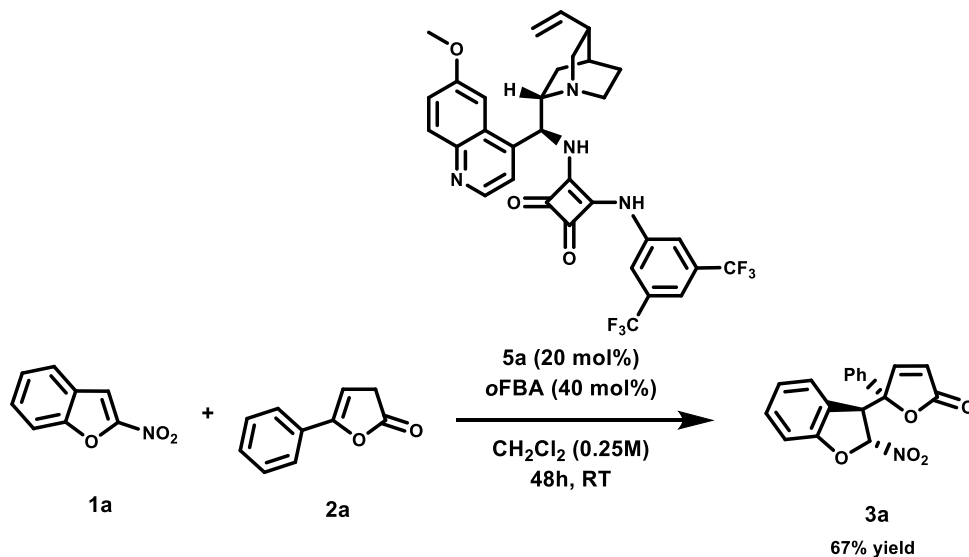
In an ordinary 25 mL round-bottomed flask equipped with a magnetic stirring bar the compound **3a** (32.2 mg, 0.1 mmol, 1 equiv.) was dissolved in toluene (5.0 mL). Then Lawesson's reagent (60.7 mg, 0.15 mmol, 1.5 equiv) was added and the reaction mixture was stirred in reflux with condenser for 24h. After full conversion of starting material **3a**, the reaction mixture was extracted with CH₂Cl₂ (3x10 mL), washed with water (2x5 mL), dried over anhydrous sodium sulfate, filtered and concentrated under reduced pressure. and column chromatography on silica gel (eluent: petroleum ether:ethyl acetate 4:1) to obtain pure product **4a** in 65% yield (17.9 mg) as light – yellow solid.

5-(Benzofuran-3-yl)-5-phenylfuran-2(5H)-one **7b**



Following the general procedure product **3s** was isolated in 65% yield as light – yellow solid (17.9 mg). ¹H NMR (700 MHz, CDCl₃) δ 7.91 (d, *J* = 5.5 Hz, 1H), 7.53 (s, 1H), 7.51 – 7.48 (m, 1H), 7.45 – 7.41 (m, 2H), 7.39 – 7.36 (m, 3H), 7.33 – 7.28 (m, 2H), 7.18 – 7.12 (m, 1H), 6.28 (d, *J* = 5.5 Hz, 1H). ¹³C NMR (176 MHz, CDCl₃) δ 171.9, 157.7, 155.9, 143.1, 137.4, 129.2, 129.1 (2C), 126.2 (2C), 125.2, 125.1, 123.4, 121.1, 120.6, 120.2, 112.0, 88.2. HRMS *m/z* [M+Na]⁺ Calculated for C₁₈H₁₂O₃Na⁺: 277.0820; found 277.0857.

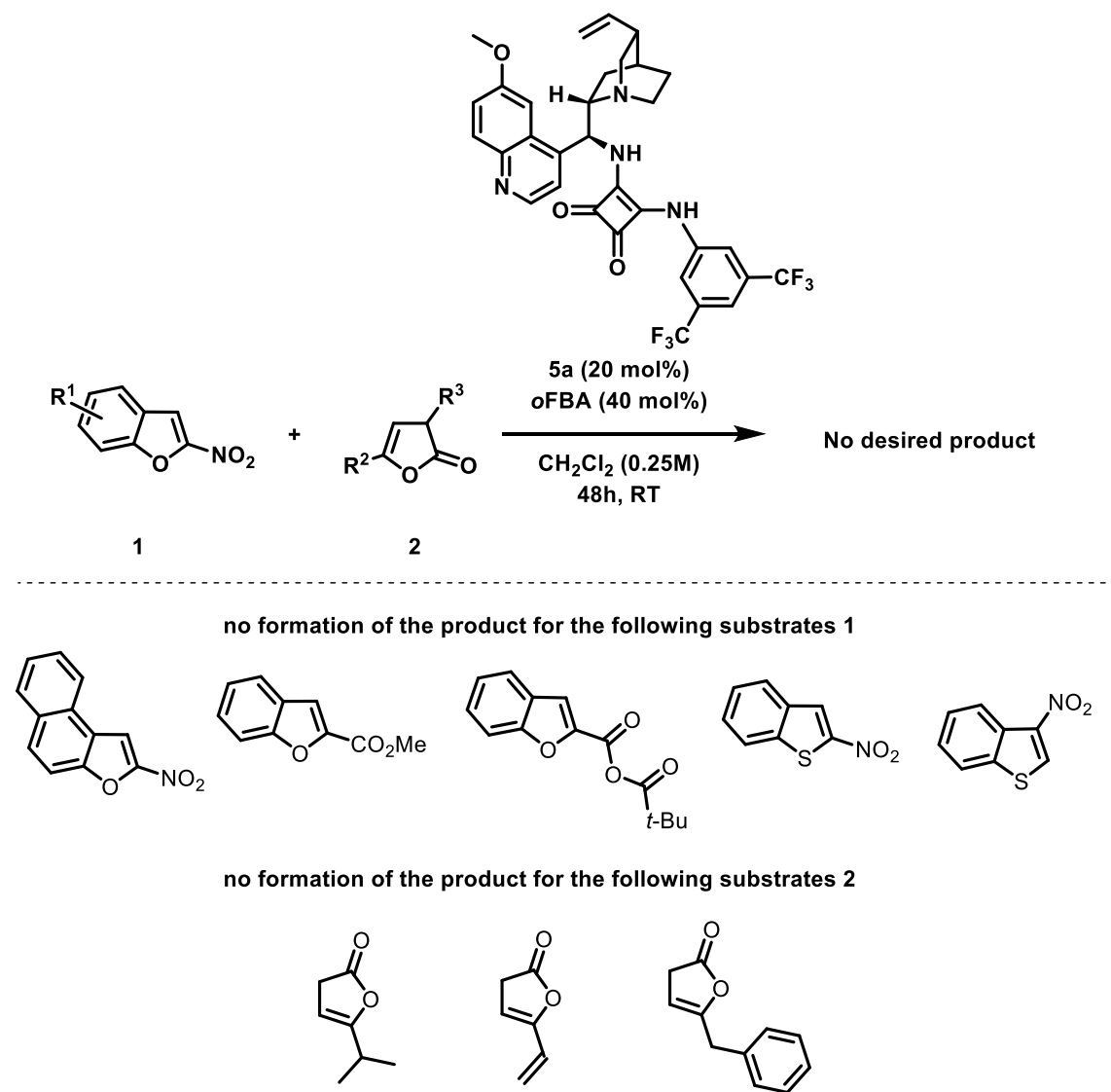
6. Enantioselective synthesis of (*R*)-5-((2*R*,3*S*)-2-nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(5*H*)-one **3a** on a 1 mmol scale



In an ordinary 8 mL glass vial equipped with a magnetic stirring bar heteroaromatic 2-nitrobenzofuran **1a** (163 mg, 1.0 mmol, 1.0 equiv.) and 5-substituted-furan-2(3*H*)-one **2a** (243 mg, 1.5 mmol, 1.5 equiv.) were dissolved in CH₂Cl₂ (4 mL). Cinchona alkaloid catalyst **5a** (126.0 mg, 0.2 mmol, 0.2 equiv.) and *o*-fluorobenzoic acid (56.0 mg, 0.4 mmol, 0.4 equiv.) were added and the reaction mixture was stirred in room temperature for 48h. The progress of the reaction was controlled by ¹H NMR spectroscopy. After full conversion of the starting material **1**, the reaction mixture was directly subjected to column chromatography on silica gel (hexanes : ethyl acetate 4:1) to afford final product **3a** with 67% yield.

7. Scope studies – unsuccessful attempts

To further expand the substrate scope, 5-substituted-2(3*H*)-furanones **2** and electron-withdrawing-group-activated heteroarenes **1** were tested. Unfortunately, no conversion was observed under standard conditions for the following substrates:



8. Crystal and X-ray data for 3a

The crystal structure of the compound (*R*)-5-((2*R*,3*S*)-2-nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(5*H*)-one **3a**, C₁₈H₁₃NO₅, was established by single-crystal X-ray diffraction at 100 K. The compound crystallizes in the non-centrosymmetric monoclinic space group *P*2₁ (*Z* = 4), with two crystallographically independent formula units per unit cell (Figure 1).

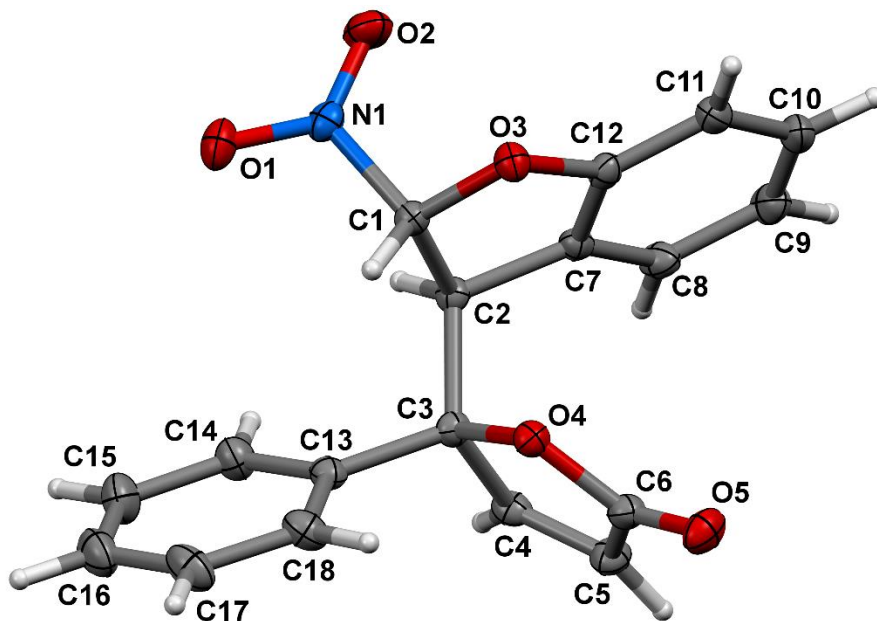


Figure 1. The molecular structure of the compound **3a** at 100 K (one of two independent molecules), showing 50% probability displacement ellipsoids. Hydrogen atoms are drawn with an arbitrary radius.

Single crystal X-ray diffraction data were collected at 100 K by the ω -scan technique using a RIGAKU XtaLAB Synergy, Dualflex, Pilatus 300K diffractometer³ with PhotonJet micro-focus X-ray Source Cu-K α (λ = 1.54184 Å). Data collection, cell refinement, data reduction and absorption correction were performed using CrysAlis PRO software.³ The crystal structure was solved using direct methods and the SHELXT 2018/2 program,⁴ with atomic scattering factors taken from the International Tables for X-ray Crystallography. Positional parameters of non-H-atoms were refined by a full-matrix least-squares method on F^2 with anisotropic thermal parameters by using the SHELXL 2019/2 program.⁵ All hydrogen atoms were positioned geometrically in calculated positions (C–H = 0.95–1.00 Å) and constrained to ride on their parent atoms with isotropic displacement parameters set to 1.2 times the U_{eq} of the parent atom.

In one of two molecules the ester group was refined as disordered over two sets of sites with an occupancy ratio of 0.829(5): 0.171(5).

(*R*)-5-((2*R*,3*S*)-2-nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(5*H*)-one **3a**: Formula C₁₈H₁₃NO₅, monoclinic, space group *P*2₁, *Z* = 4, unit cell constants *a* = 9.2613(1), *b* = 15.6804(1), *c* = 11.1987(1) Å, β = 109.808(1)°, *V* = 1530.06(3) Å³. The integration of the data yielded a total of 55453 reflections with θ angles in the range of 4.20 to 67.74°, of which 5534 were unique (*R*_{int} = 1.93%).

The final anisotropic full-matrix least-squares refinement on *F*² with 434 parameters. The final *R*₁ was 0.0212 (for *I* > 2σ(*I*)) and *wR*₂ was 0.0542 (all data). The largest peak in the final difference electron density synthesis was 0.177 eÅ⁻³ and the largest hole was -0.124 eÅ⁻³. The goodness-of-fit was 1.038. The absolute configuration was unambiguously established from anomalous scattering, by calculating the *x* Flack parameter⁶ of 0.0021(2) using 2622 quotients.

CCDC 2326286 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures.

(3) OD. Rigaku CrysAlis PRO. Rigaku Oxford Diffraction Ltd, Yarnton, Oxfordshire, England, 2019.

(4) G. M. Sheldrick, "SHELXT - integrated space-group and crystal-structure determination", *Acta Cryst.* 2015, **A71**, 3-8.

(5) G. M. Sheldrick, "Crystal structure refinement with SHELXL", *Acta Cryst.* 2015, **C71**, 3-8.

(6) S. Parsons, H. D. Flack, T. Wagner, "Use of intensity quotients and differences in absolute structure refinement" *Acta Cryst.* 2013, **B69**, 249-259.

9. Computational Data

All DFT calculations were carried out using ORCA 5.0.4 package⁷. Visualization of calculated structures was done using ChemCraft (v. b648b) graphical software. Calculations included PCM (geometry optimization, vibrational frequency analysis and IRC) or SMD (Single Point) solvation model⁸ to account for the effects exerted by CH₂Cl₂. The ground-state structures of minima and transition states were found assuming the r2scan-3c composite method.⁹ The harmonic vibrational frequencies were computed for located structures at the same level of theory to confirm the character of the located stationary points. For each located transition state intrinsic reaction coordinate (IRC) analysis was performed to confirm the connection between reactants and products. Single-point energy calculations were performed assuming the ω B97M-V range-separated hybrid meta-GGA density functional with VV10 nonlocal correlation¹⁰ and def2-qzvpp basis set¹¹ utilizing RIJCOSX approximation and def2/J auxiliary basis set¹² as implemented in ORCA software. Final energies are ZPE-corrected.

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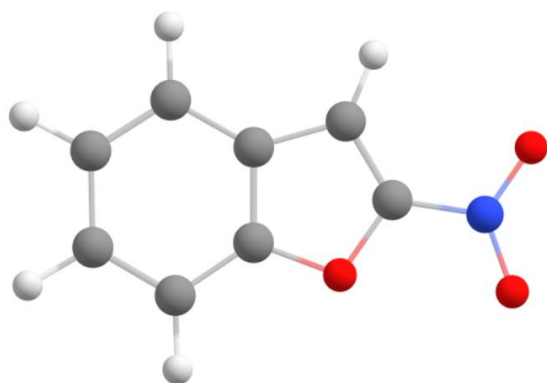
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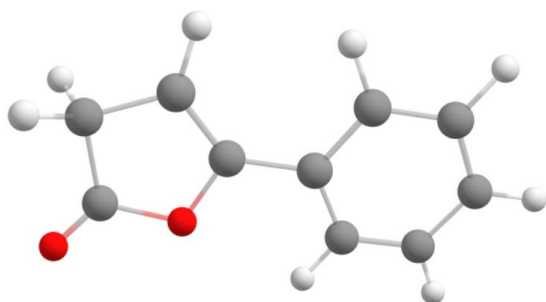
Cartesian coordinates

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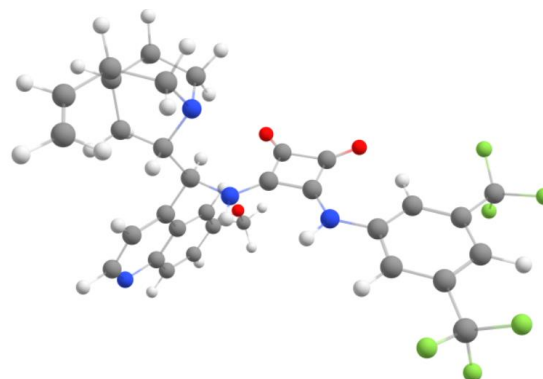
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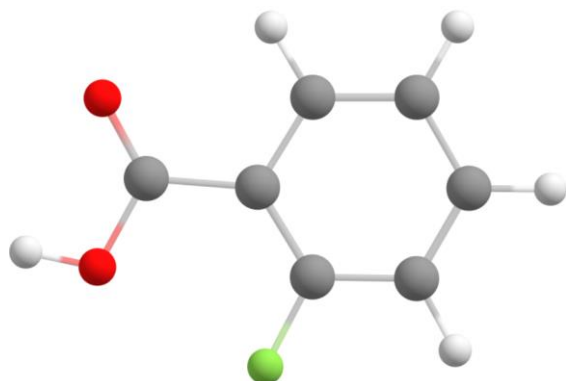
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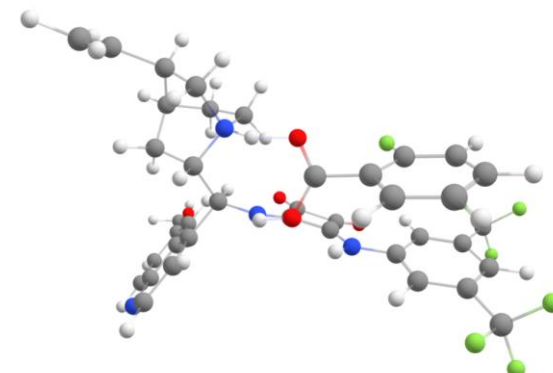
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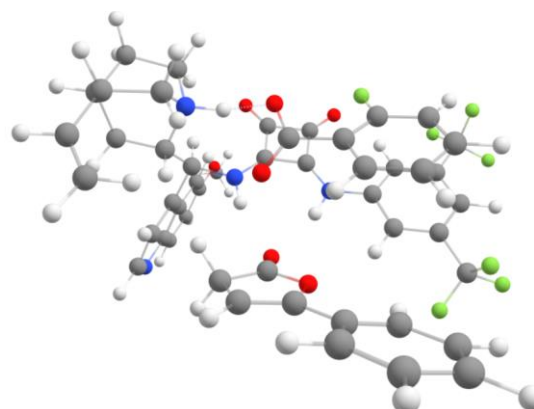
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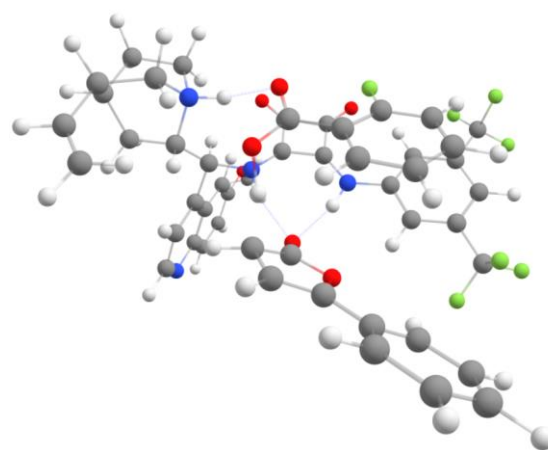
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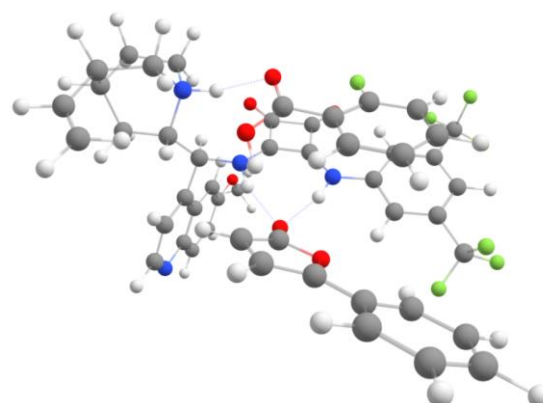


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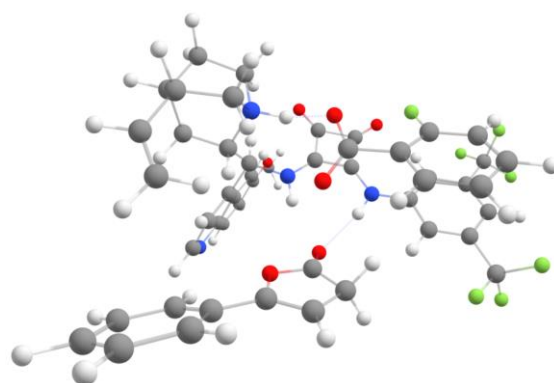


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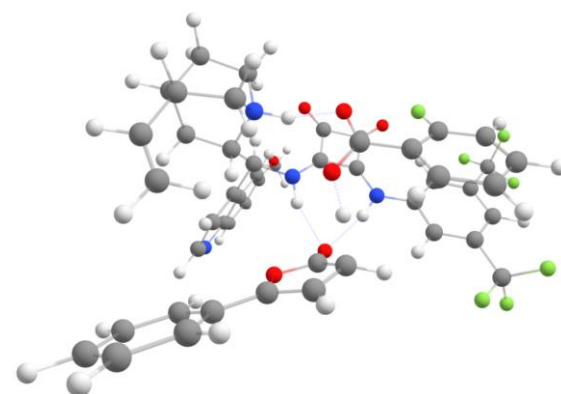


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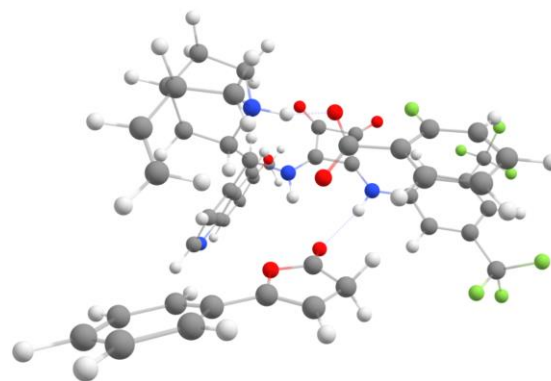


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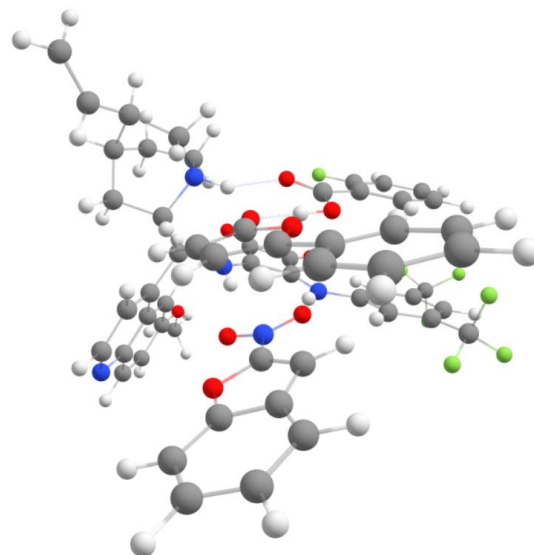


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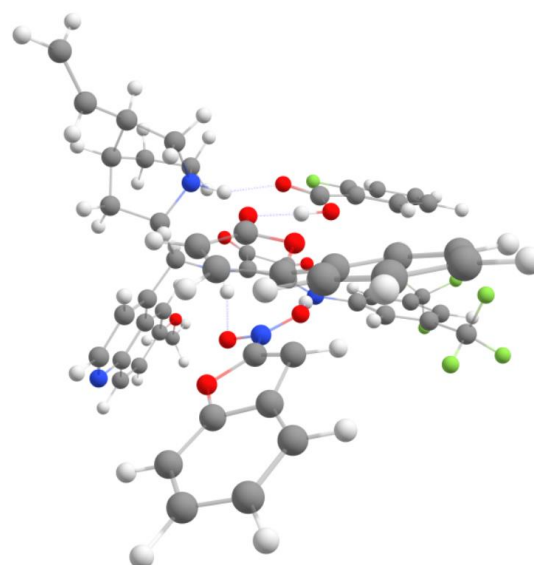


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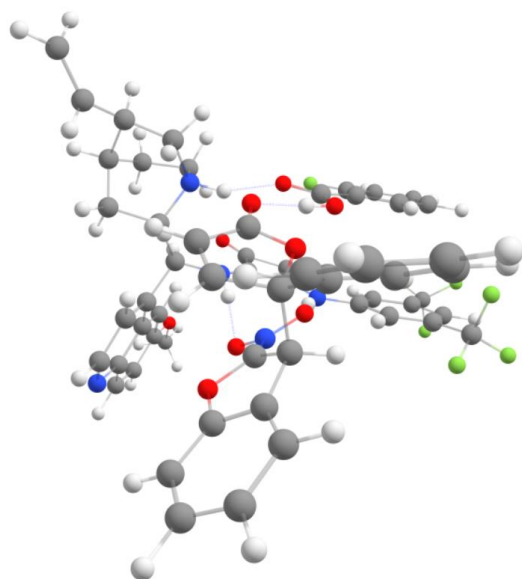
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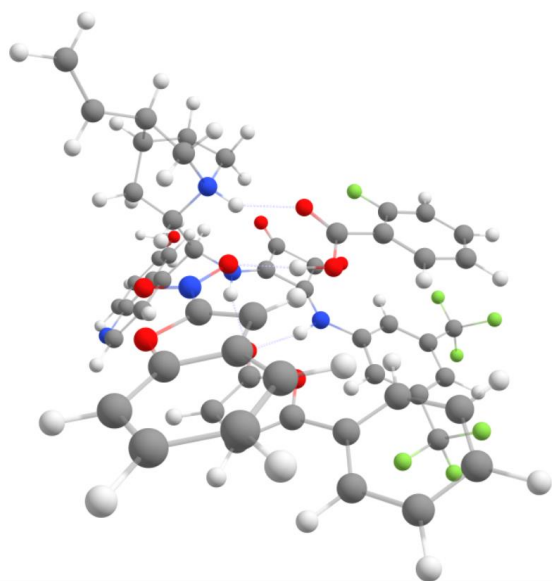


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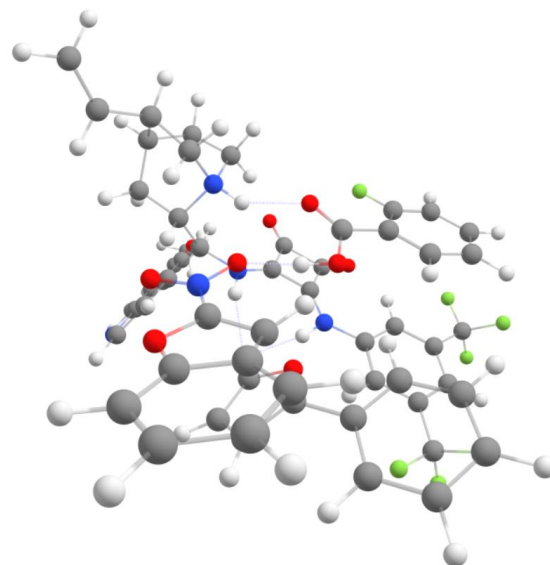


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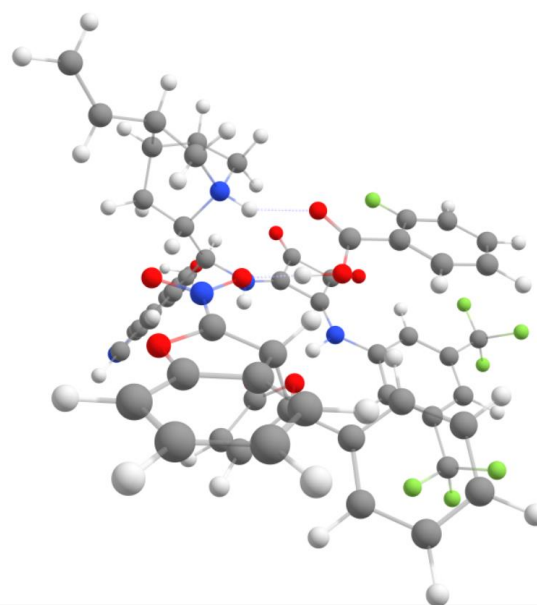


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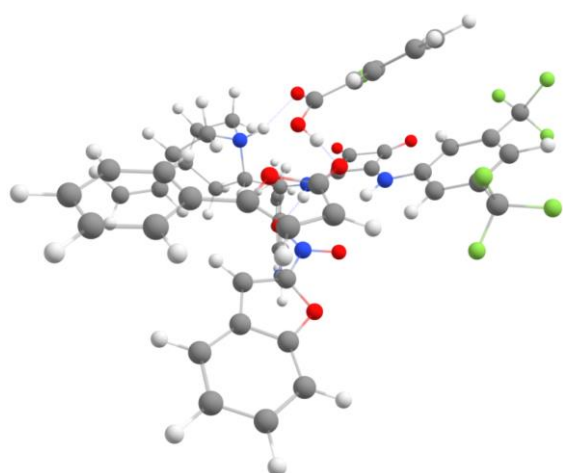
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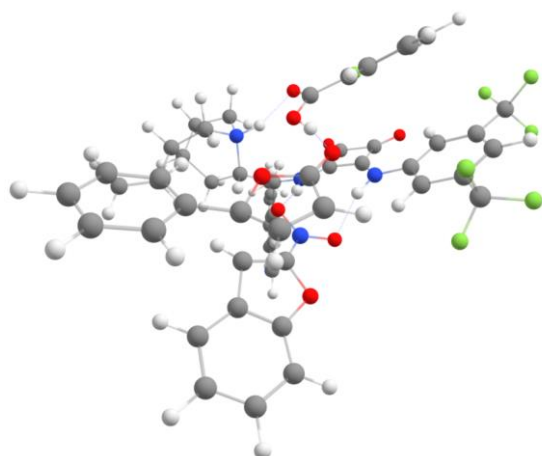


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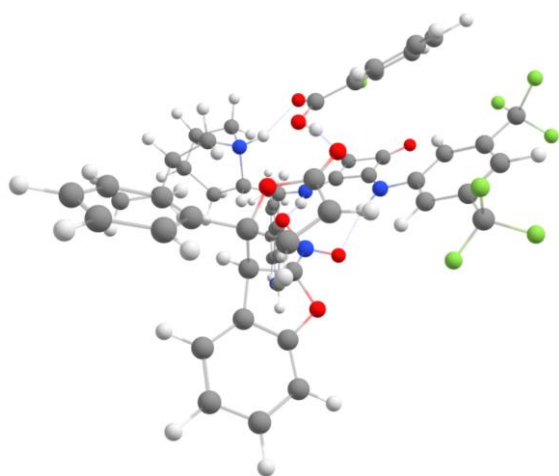


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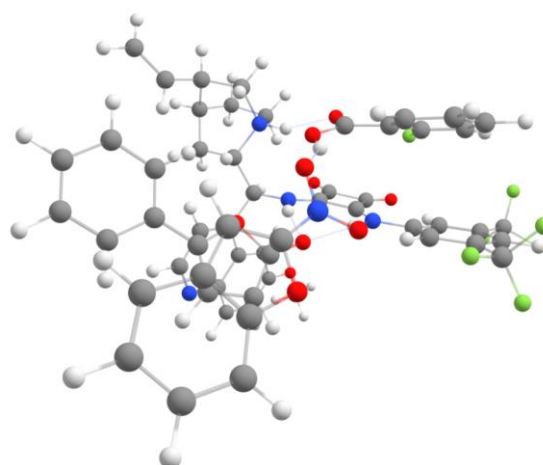


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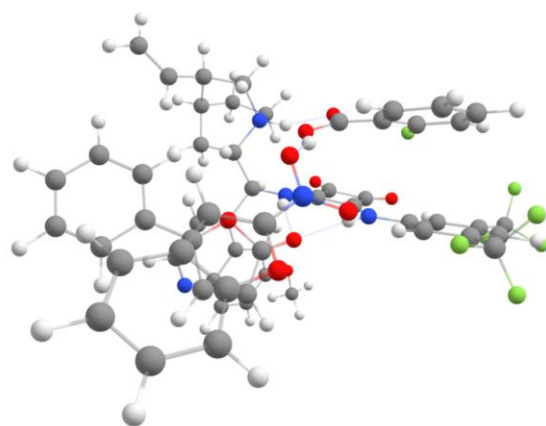


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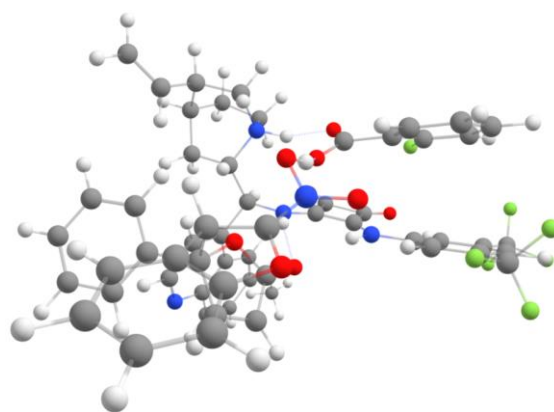


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PC-2b

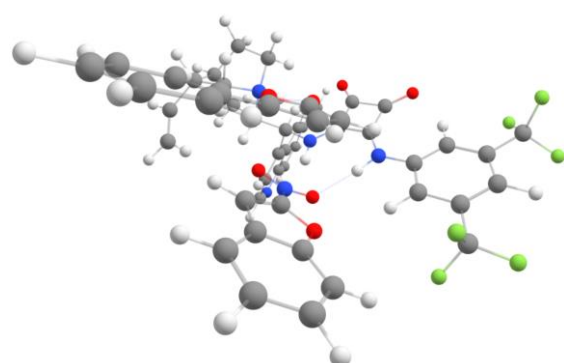


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Reaction without acid co-catalyst – major enantiomer

Reactants

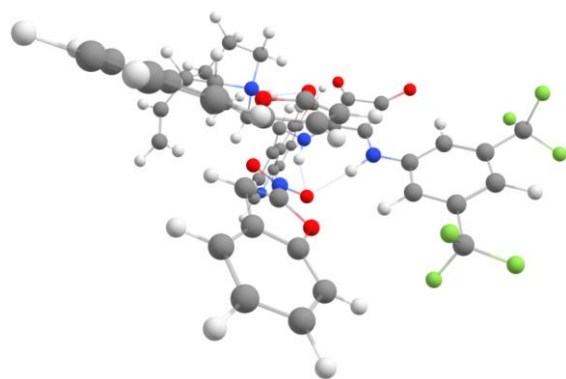


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Transition State

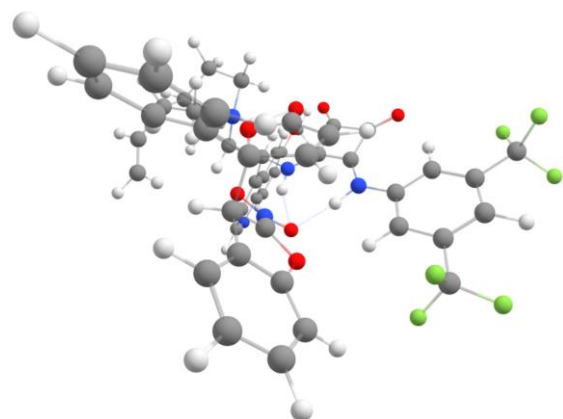


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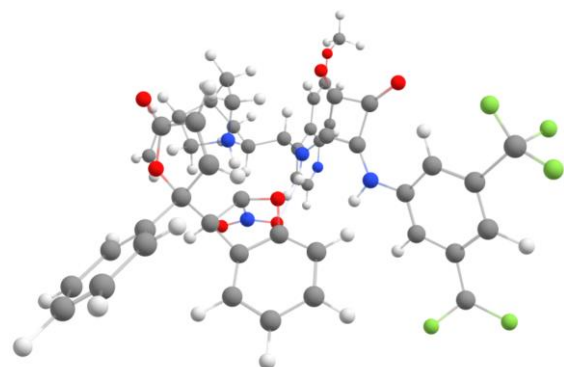


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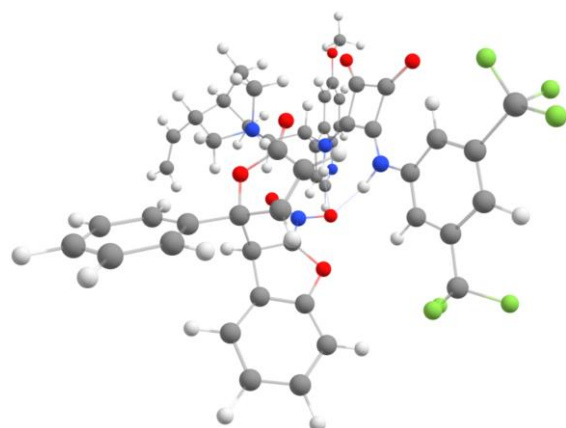


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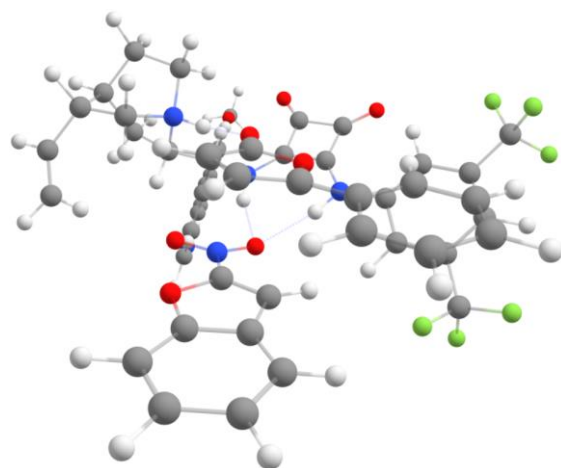
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Reaction without acid co-catalyst – minor enantiomer

Reactants

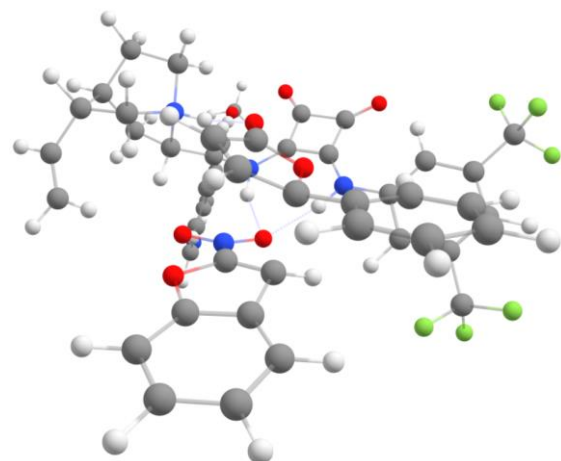


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Transition State

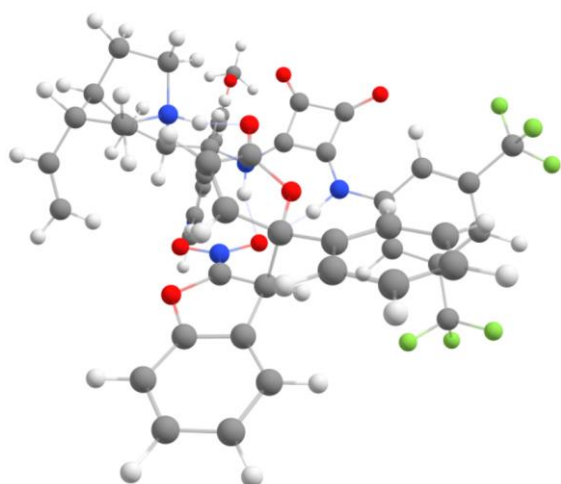


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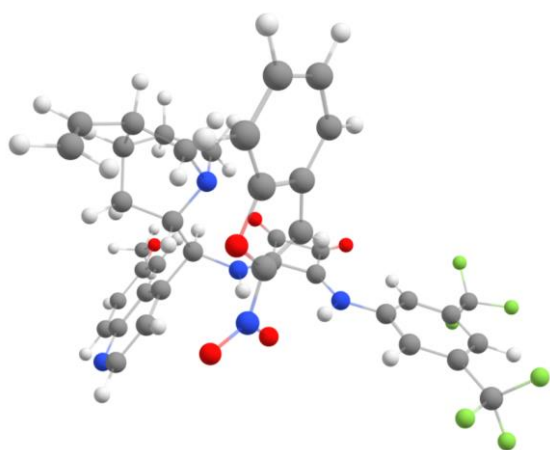
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Nucleophilic activation of 2a by quinuclidine

Reactants

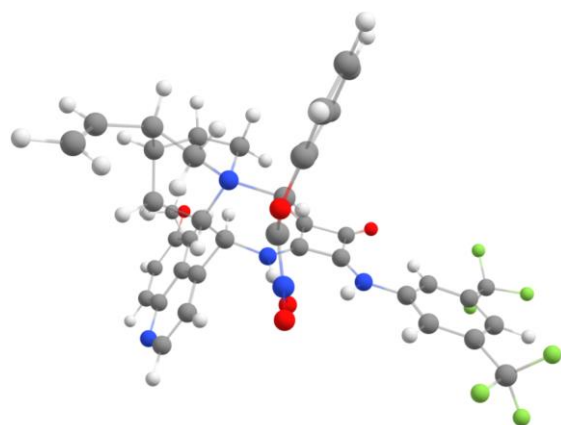


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Transition State

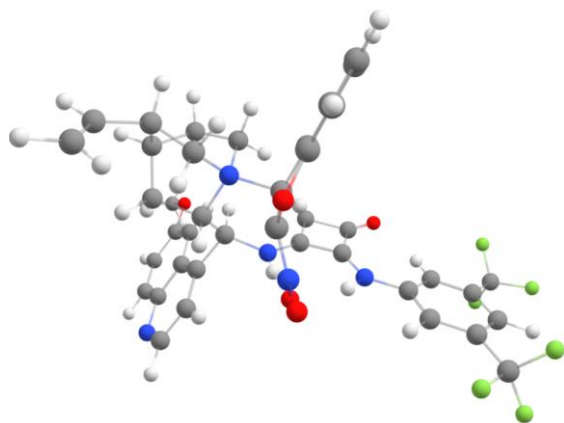


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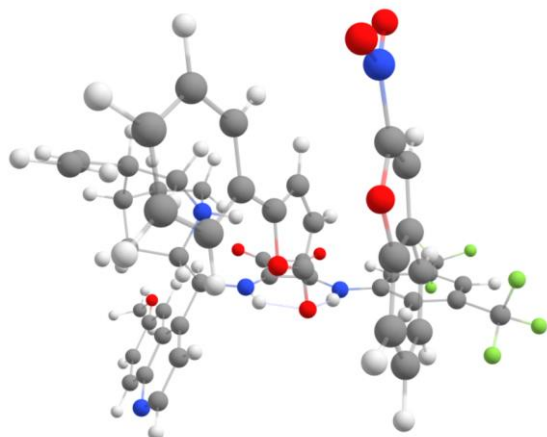


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Polymerization of 2a

Reactants 1st step

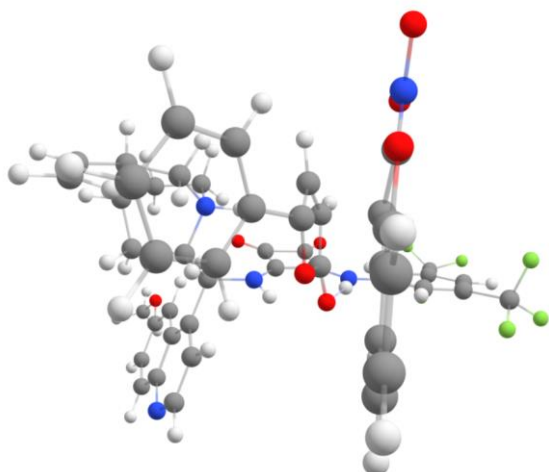


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Transition State 1st step

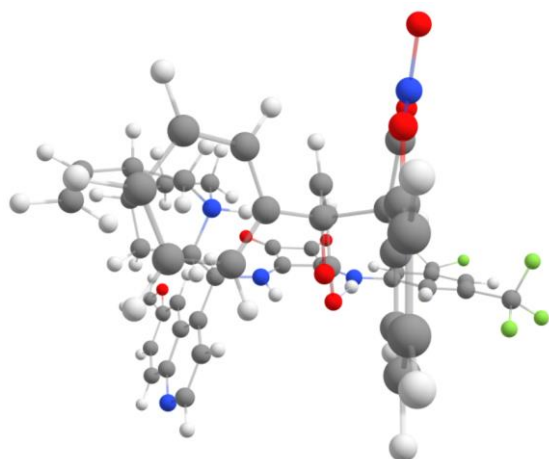


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Product 1st step

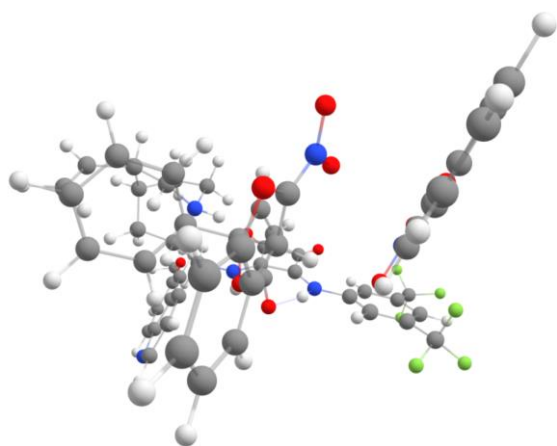


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Reactants 2nd step

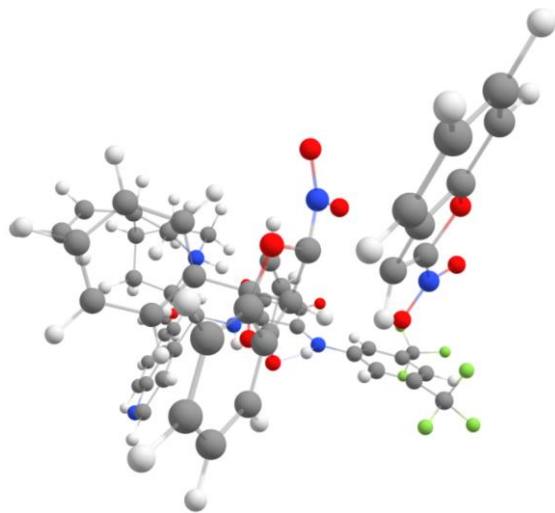


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Transition State 2nd step

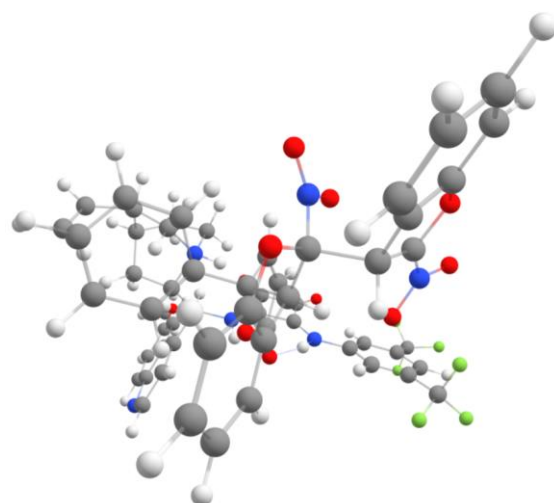


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Product 2nd step



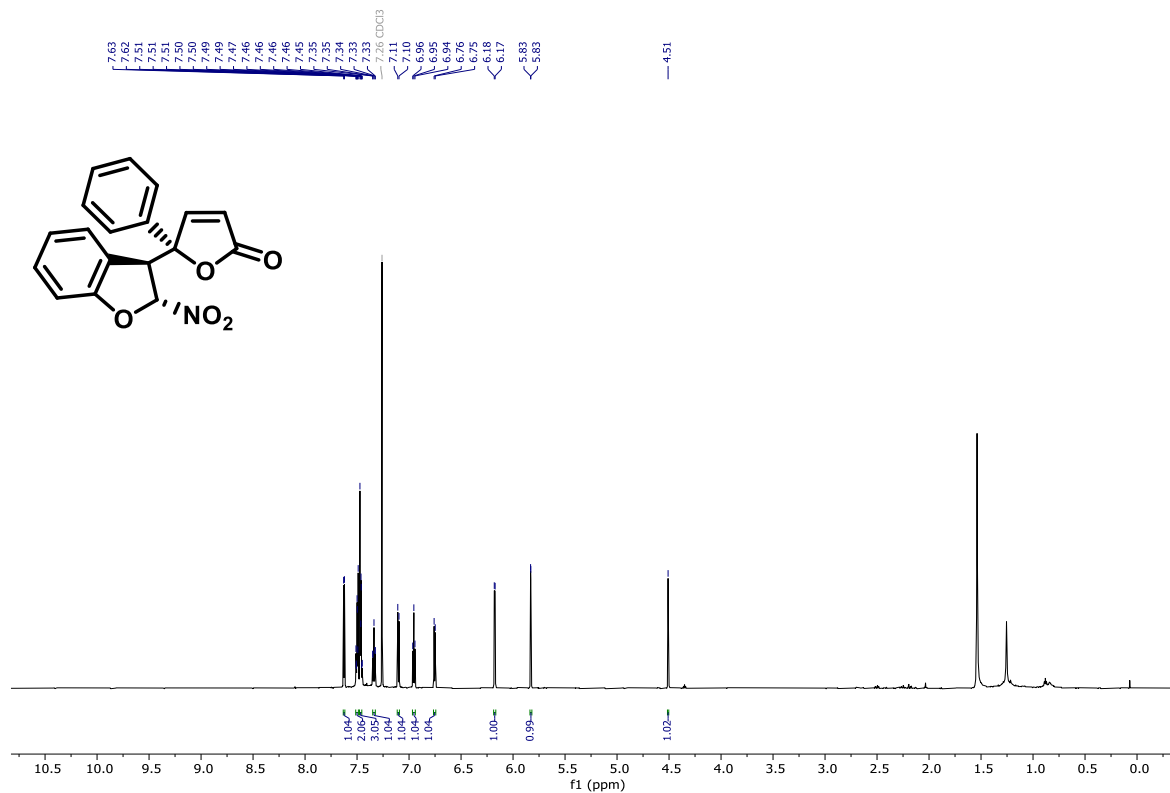
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6	-5.886150000	1.297427000	1.275969000	1	-4.820181000	-6.163502000	1.449388000
1	-4.210497000	-0.019031000	1.572262000	8	-6.277594000	-6.051628000	-1.417728000
6	-5.460313000	3.282429000	0.022910000	7	-5.776411000	-4.108826000	-0.227015000
1	-3.443622000	3.577573000	-0.669131000	8	-6.614572000	-3.487429000	-0.955025000
6	-6.360021000	2.482038000	0.718168000	8	-5.144094000	-3.500413000	
1	-7.398617000	2.772189000	0.824393000		0.718693000		
6	-5.915032000	4.594593000	-0.554249000				
6	-6.840304000	0.379015000	1.988985000				
9	-5.601407000	5.634241000	0.264320000				
9	-5.329365000	4.852314000	-1.746542000				
9	-7.250984000	4.636873000	-0.745244000				
9	-7.865231000	1.053103000	2.557952000				
9	-7.388919000	-0.524770000	1.138188000				
9	-6.230763000	-0.325242000	2.969493000				
6	-1.489048000	-2.264732000	-0.454631000				
6	-1.333177000	-2.108222000	0.989068000				
6	-1.366645000	-3.564538000	-0.747735000				
6	-1.206181000	-4.359642000	0.516637000				
8	-1.092395000	-3.321593000	1.537265000				
1	-1.372633000	-3.999589000	-1.735655000				
1	-1.668005000	-1.437237000	-1.131335000				
8	-1.348267000	-1.101411000	1.684514000				
6	0.012953000	-5.255527000	0.546639000				
6	0.786595000	-5.367178000	1.704940000				
6	0.317903000	-6.051570000	-0.560218000				
6	1.833053000	-6.282999000	1.759429000				
1	0.564415000	-4.750548000	2.568371000				
6	1.362007000	-6.968993000	-0.498533000				
1	-0.252578000	-5.970661000	-1.479618000				
6	2.116292000	-7.094247000	0.664221000				
1	2.424507000	-6.364613000	2.667039000				
1	1.584376000	-7.584707000	-1.365085000				
1	2.930092000	-7.812205000	0.711977000				
6	-2.306559000	-5.788570000	2.288565000				
6	-2.248774000	-7.155765000	2.043195000				
6	-1.954397000	-8.091658000	3.016632000				
6	-1.725748000	-7.600190000	4.303923000				
6	-1.810351000	-6.235743000	4.585489000				
6	-2.098820000	-5.314567000	3.575494000				
6	-2.540361000	-5.086816000	0.975394000				
6	-3.089335000	-6.287393000	0.167993000				
1	-1.913703000	-9.151982000	2.789635000				
1	-1.494463000	-8.299559000	5.102213000				
1	-1.648920000	-5.885675000	5.600386000				
1	-2.151859000	-4.252324000	3.791411000				

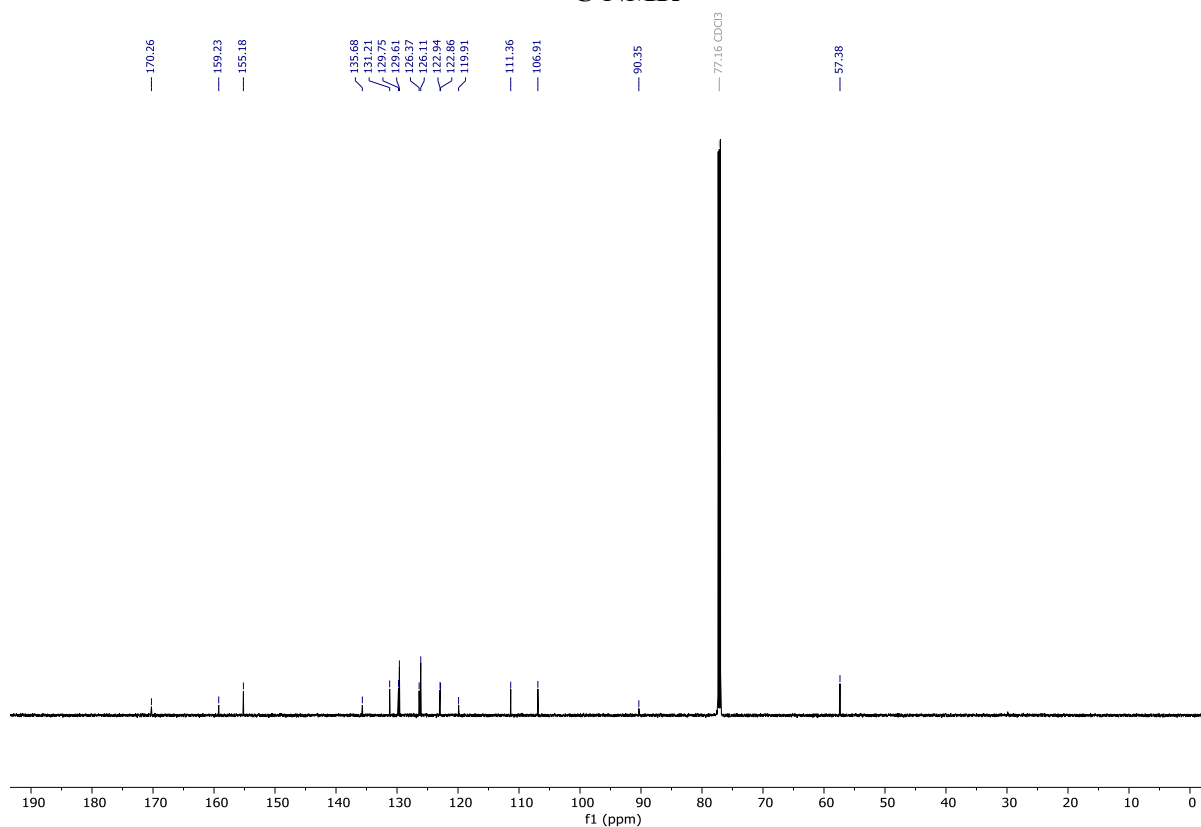
10. NMR data

(*R*)-5-((2*R*,3*S*)-2-Nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(*5H*)-one 3a

¹H NMR

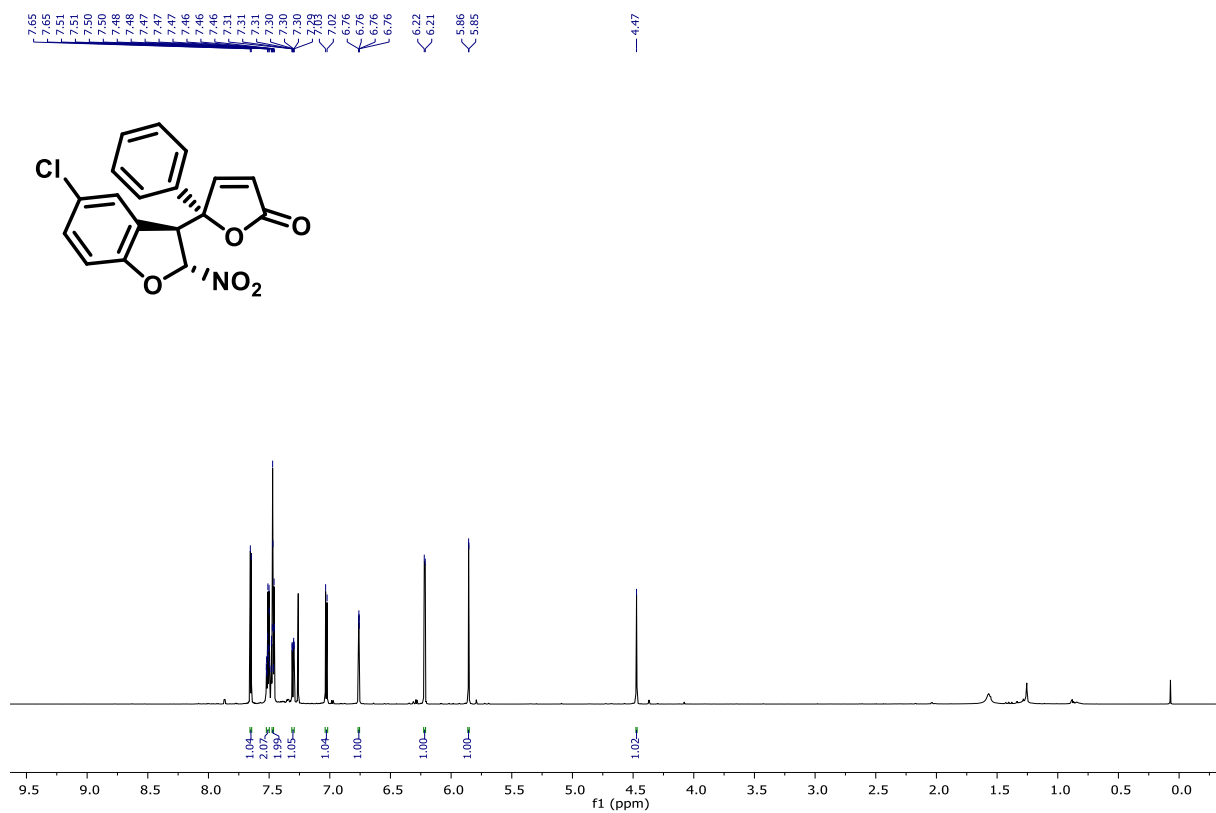


¹³C NMR

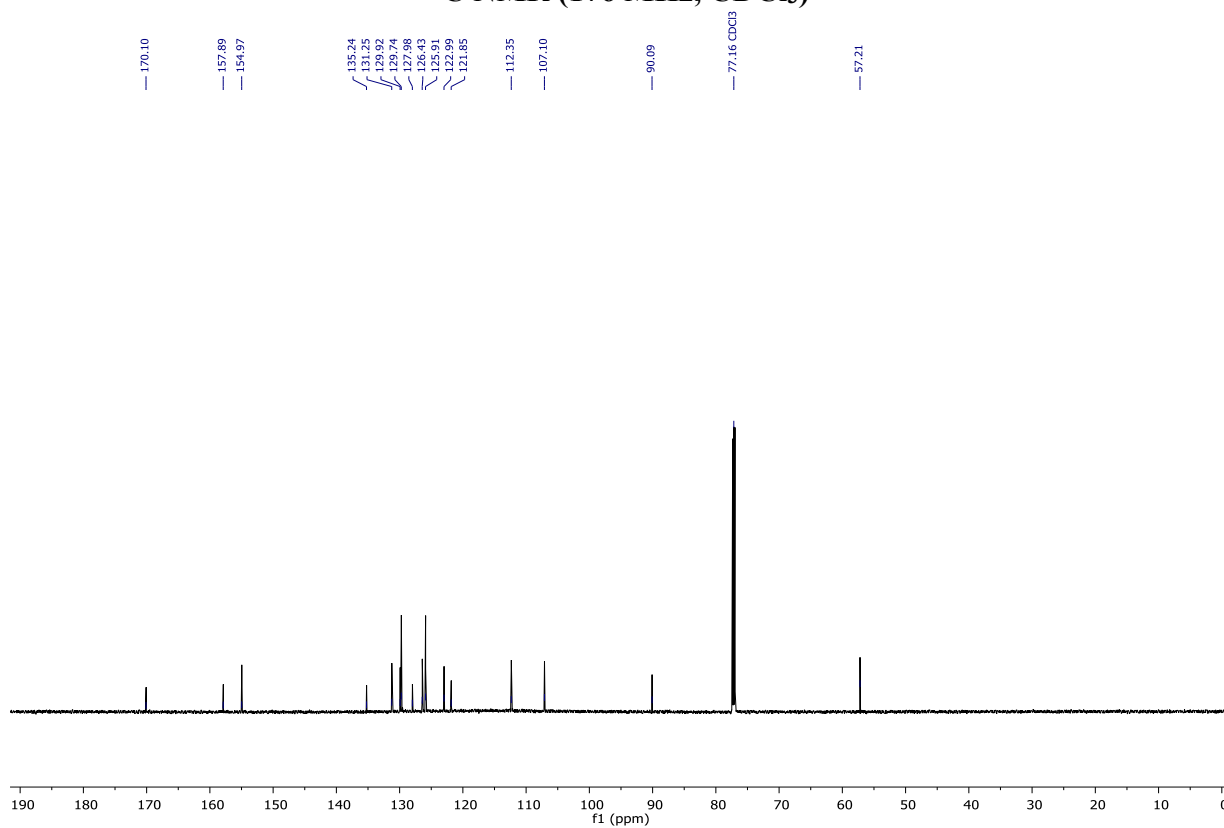


(*R*)-5-((2*R*,3*S*)-5-Chloro-2-nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(*5H*)-one
3b

¹H NMR (700 MHz, CDCl₃)

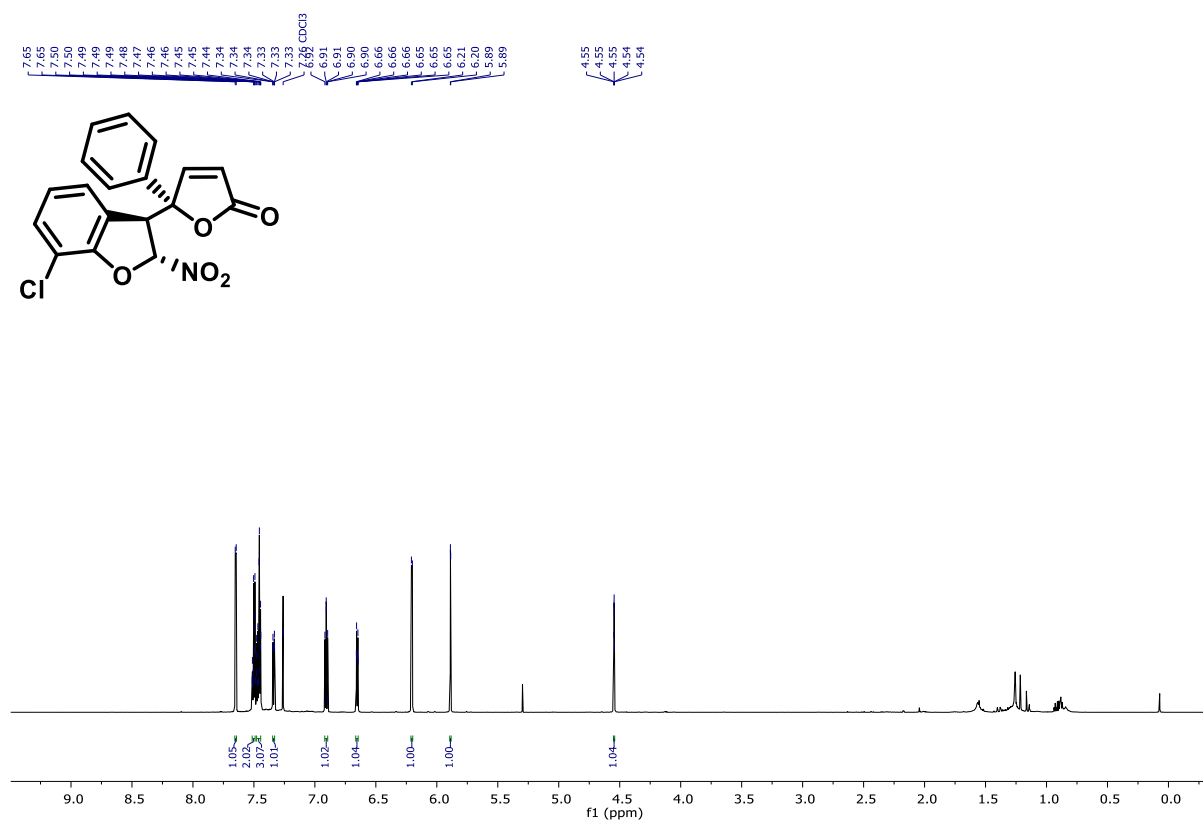


¹³C NMR (176 MHz, CDCl₃)

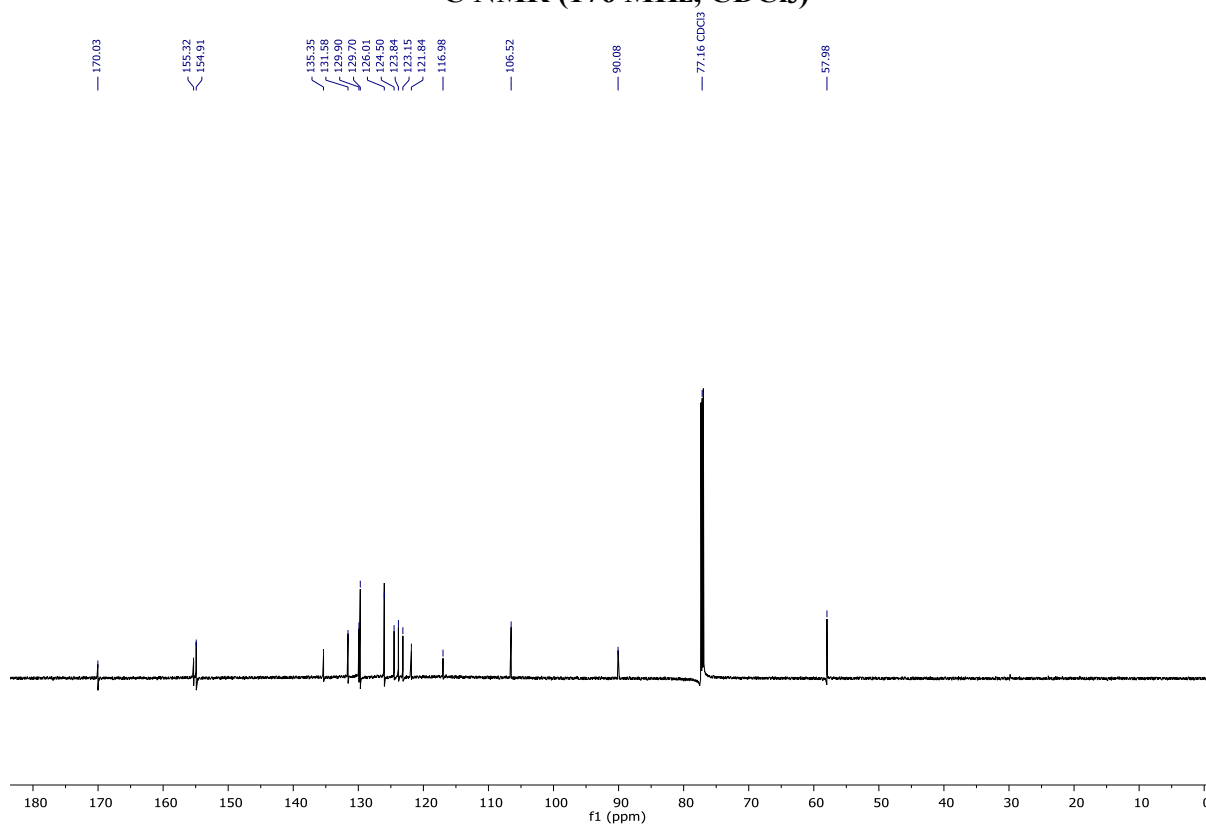


(*R*)-5-((2*R*,3*S*)-7-Chloro-2-nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(*5H*)-one
3c

¹H NMR (700 MHz, CDCl₃)

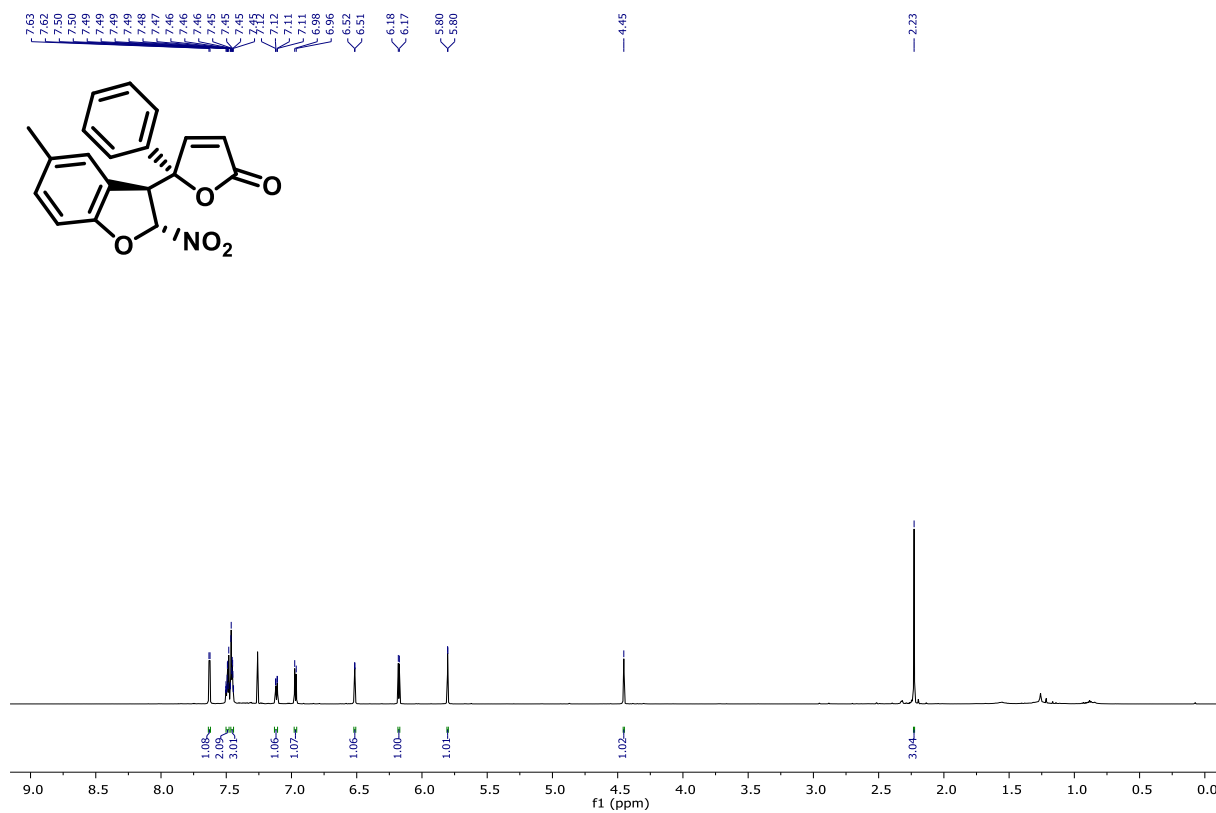


¹³C NMR (176 MHz, CDCl₃)

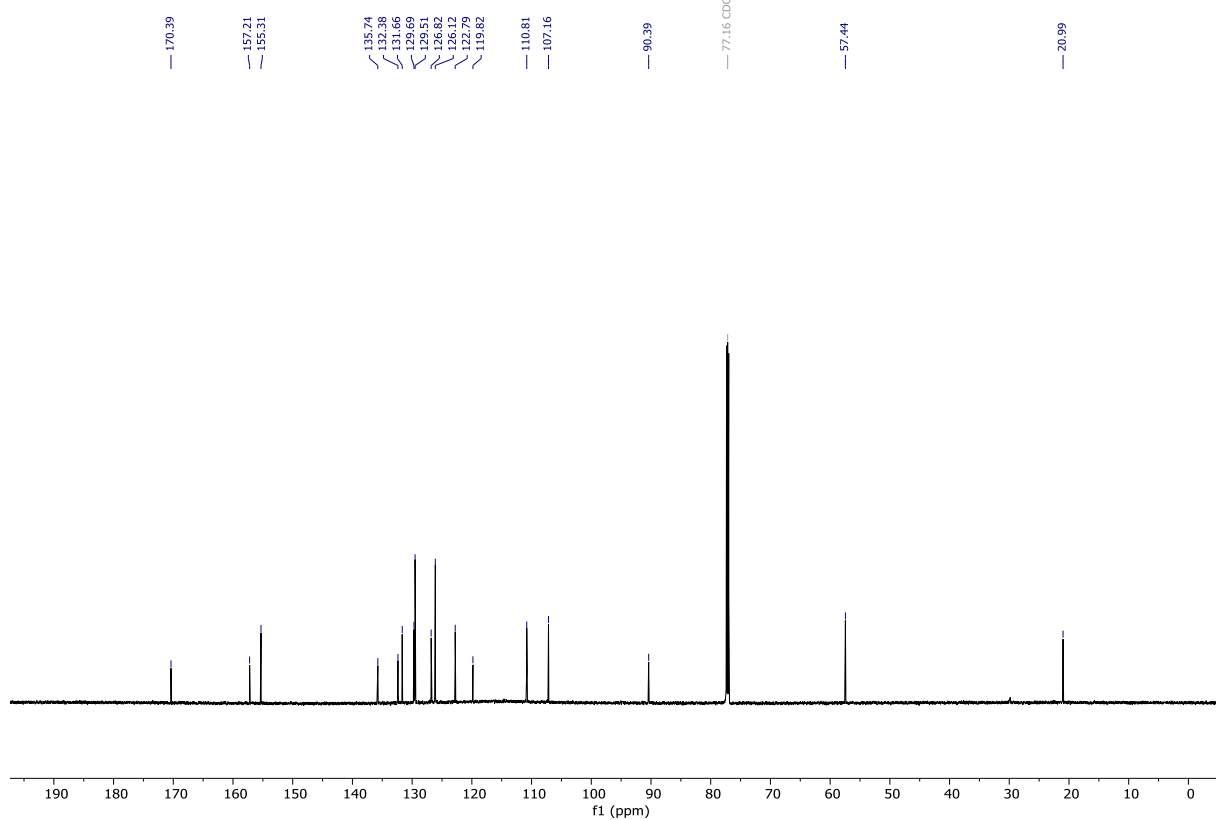


(*R*)-5-((2*R*,3*S*)-5-Methyl-2-nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(*5H*)-one
3d

¹H NMR (700 MHz, CDCl₃)

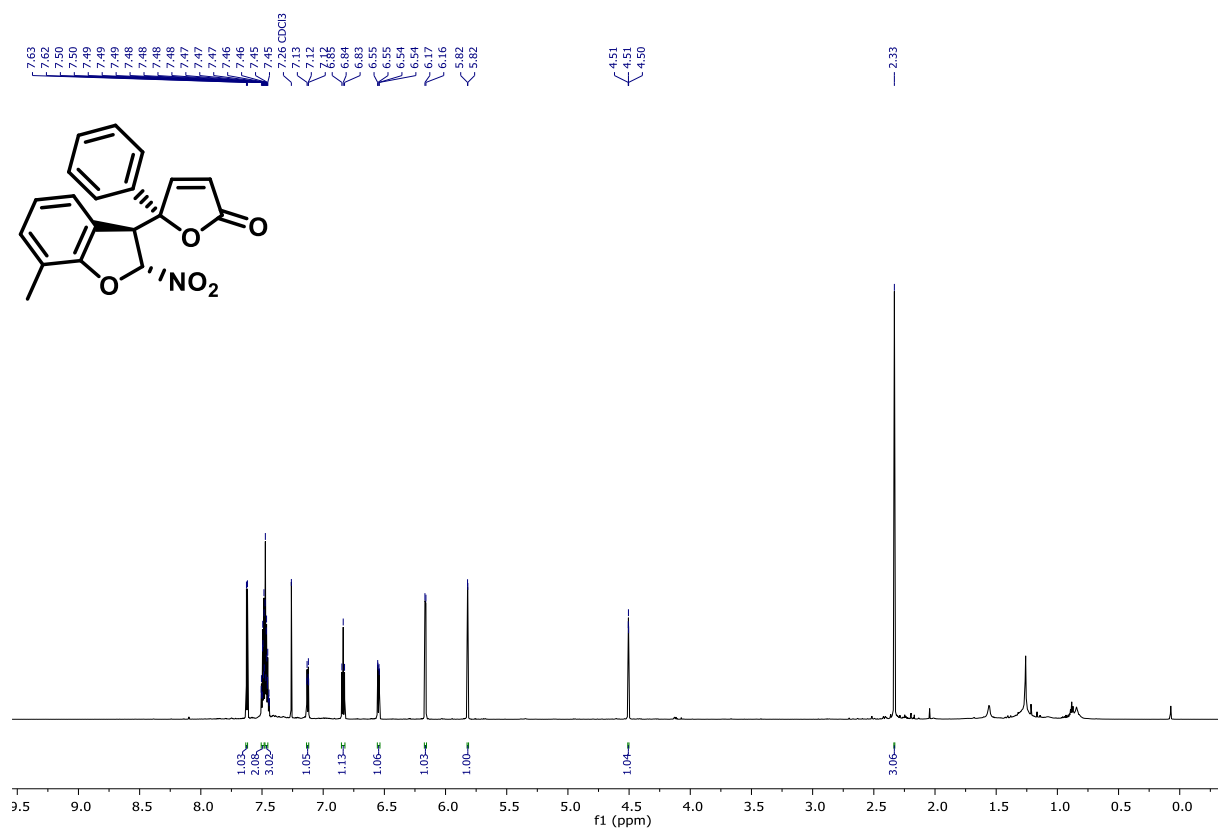


¹³C NMR (176 MHz, CDCl₃)

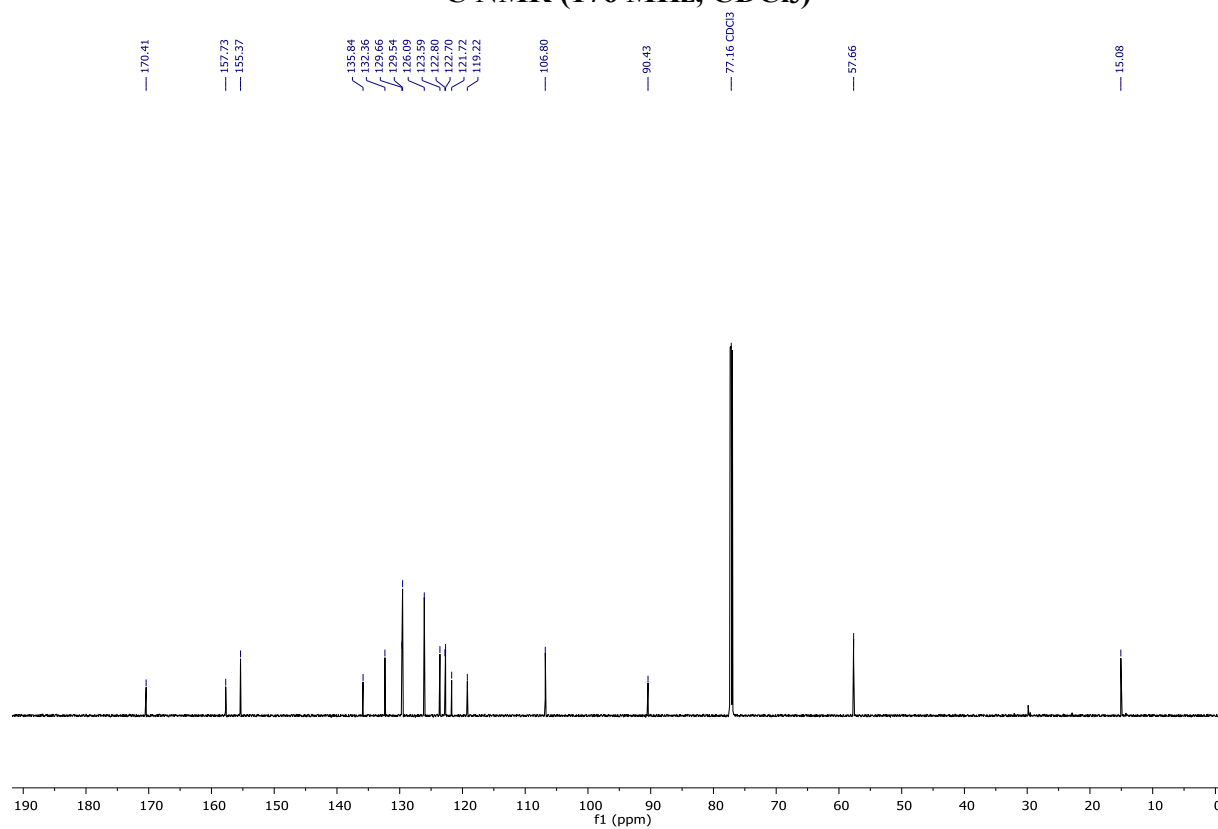


(*R*)-5-((2*R*,3*S*)-7-Methyl-2-nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(*5H*)-one
3e

¹H NMR (700 MHz, CDCl₃)

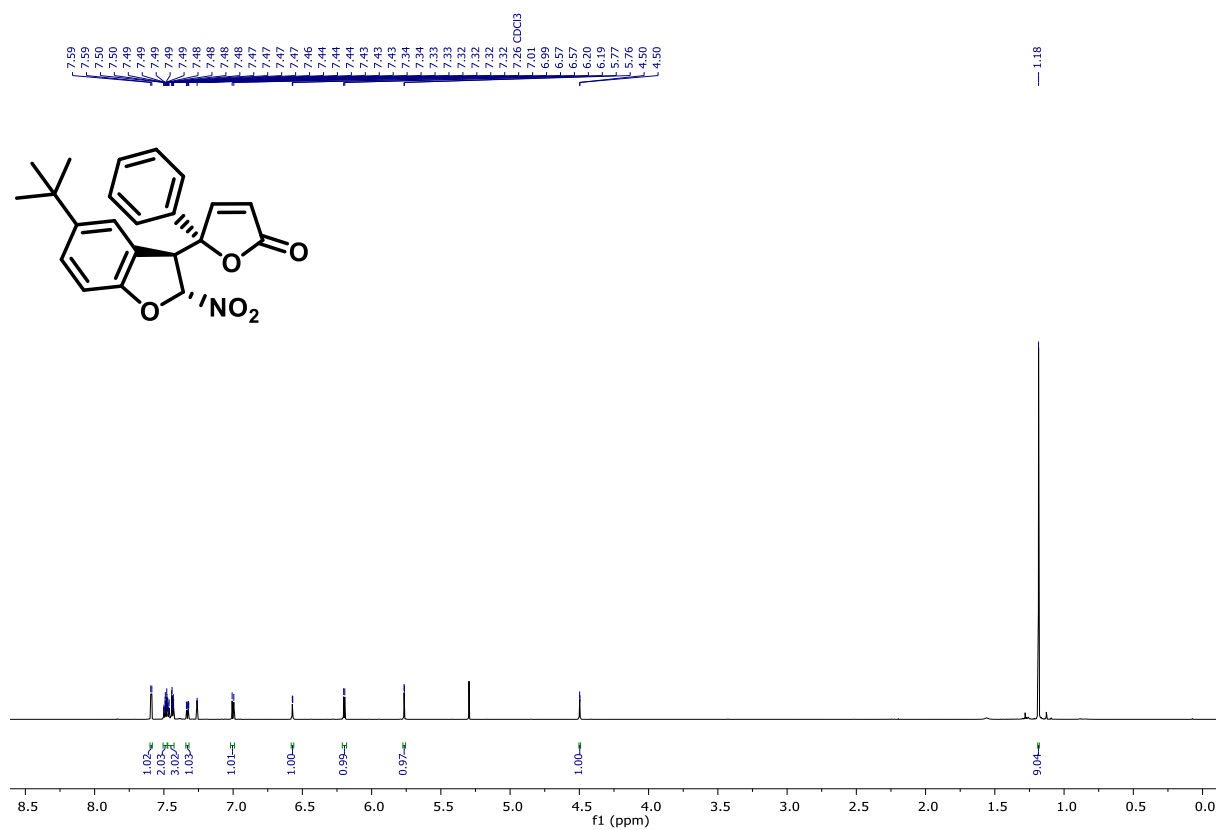


¹³C NMR (176 MHz, CDCl₃)

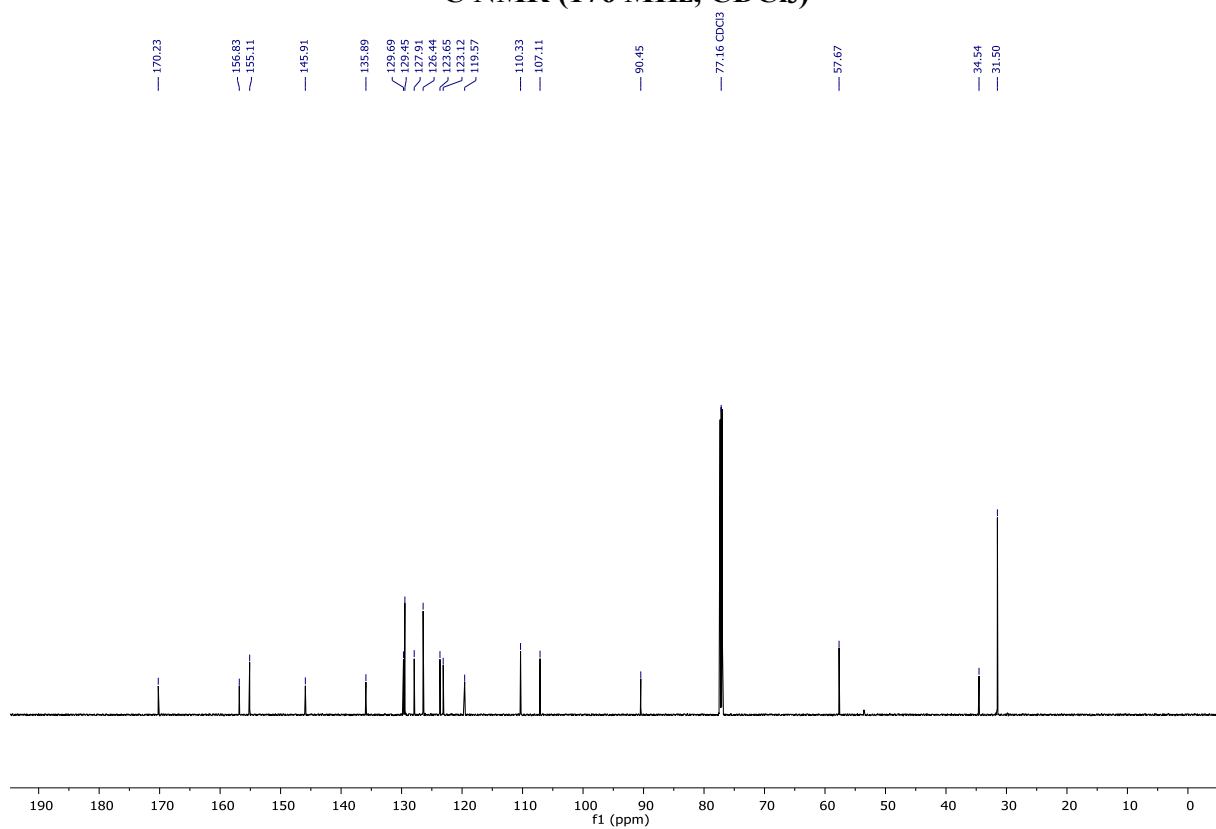


(*R*)-5-((2*R*,3*S*)-5-(*tert*-Butyl)-2-nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(*5H*)-one 3f

^1H NMR (700 MHz, CDCl_3)

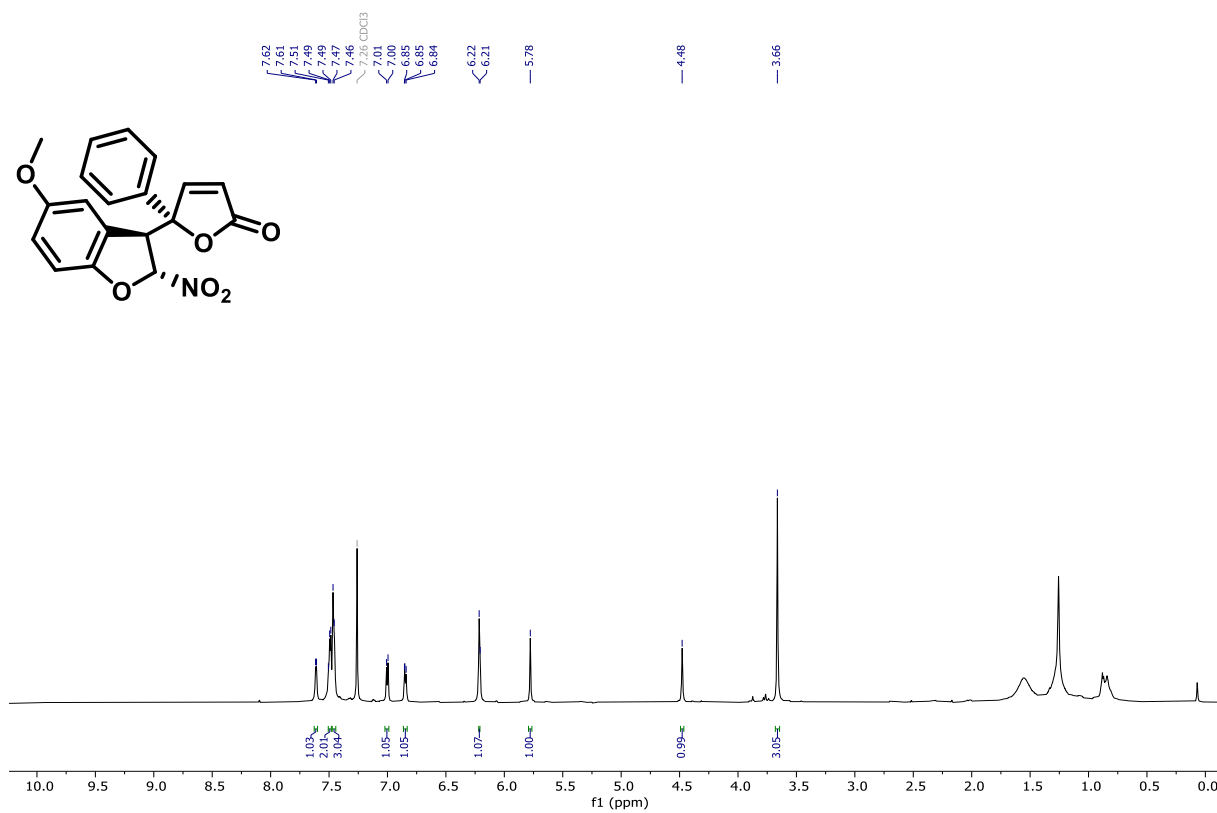


^{13}C NMR (176 MHz, CDCl_3)

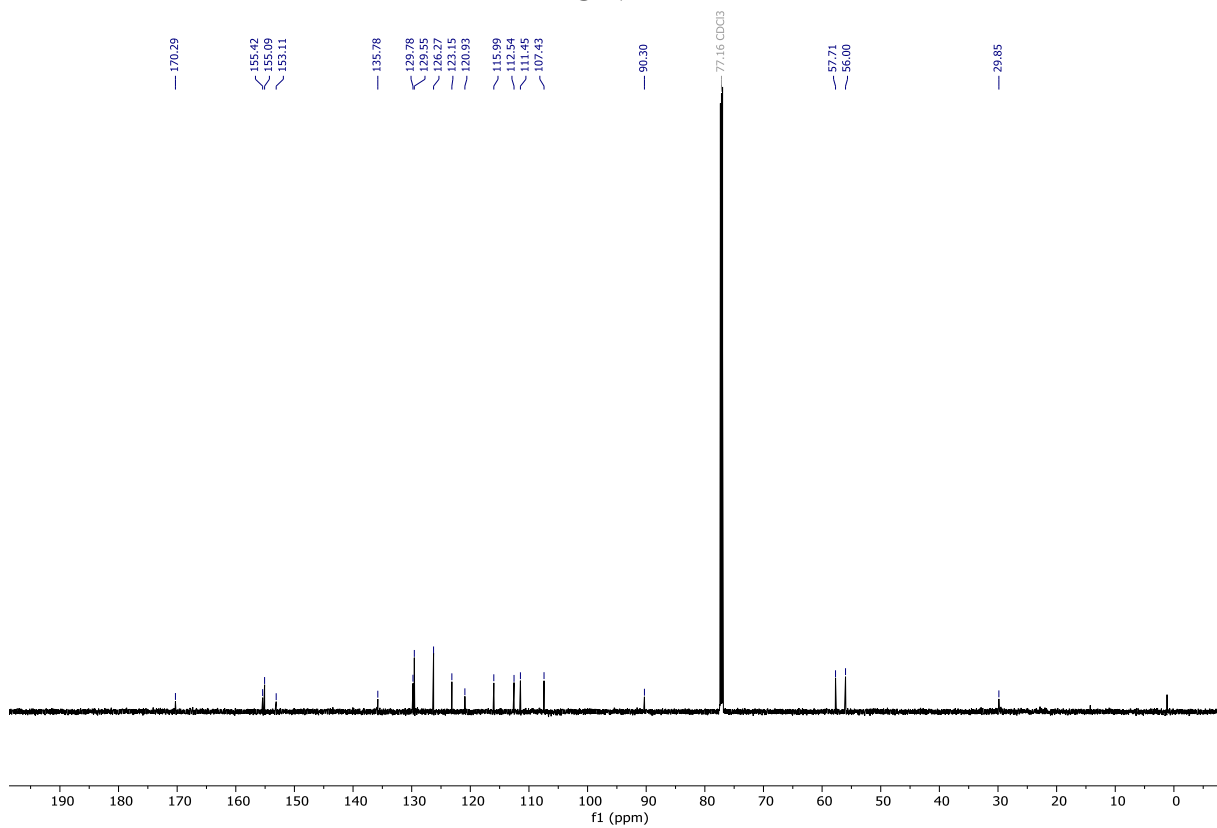


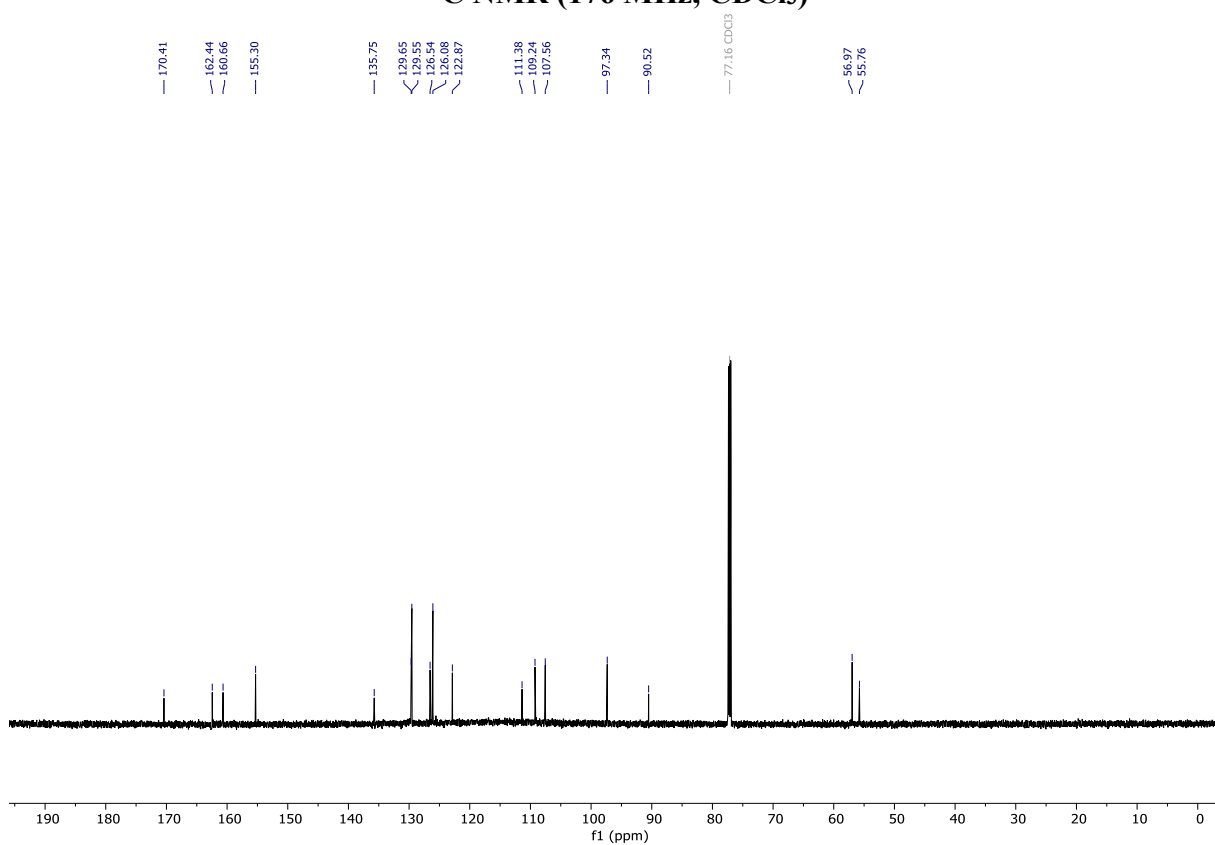
(*R*)-5-((2*R*,3*S*)-5-Methoxy-2-nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(*5H*)-one
3g

^1H NMR (700 MHz, CDCl_3)



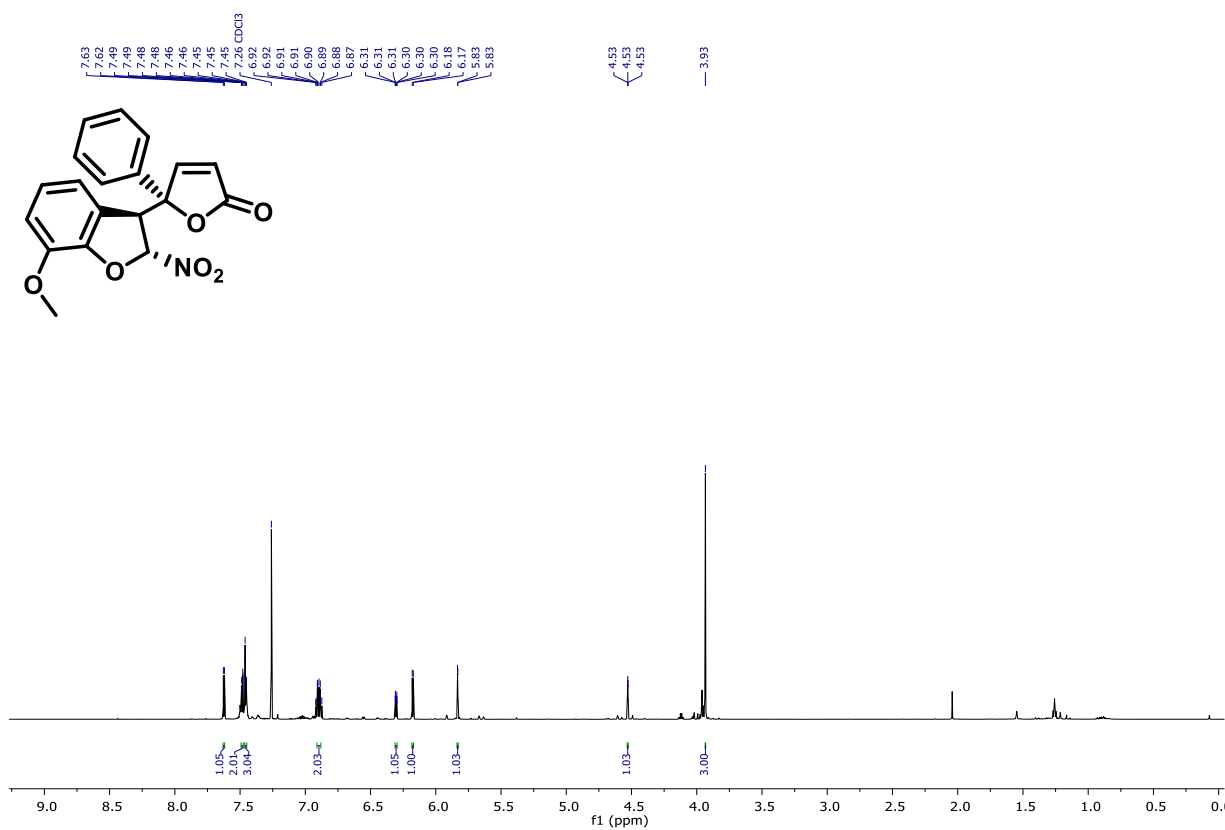
^{13}C NMR



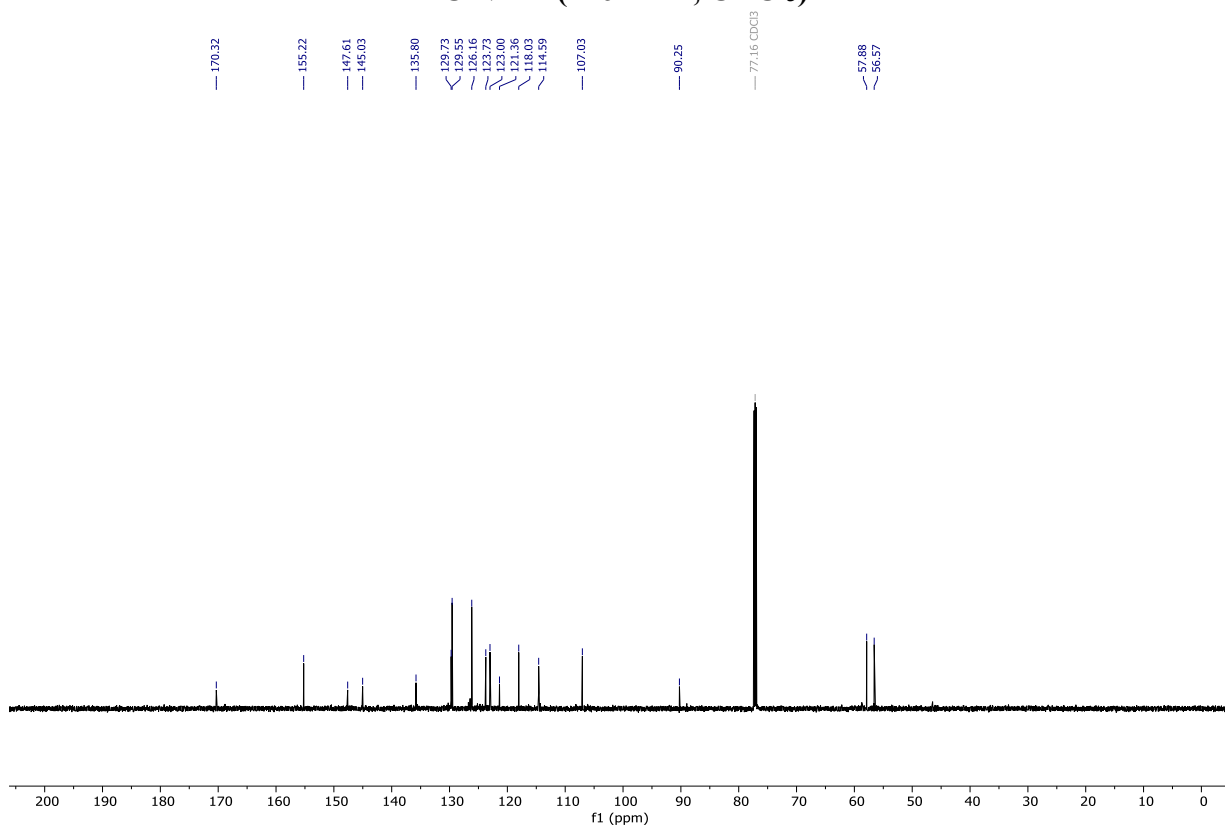
¹H NMR (700 MHz, CDCl₃)

(*R*)-5-((2*R*,3*S*)-7-Methoxy-2-nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(*5H*)-one
3i

¹H NMR (700 MHz, CDCl₃)

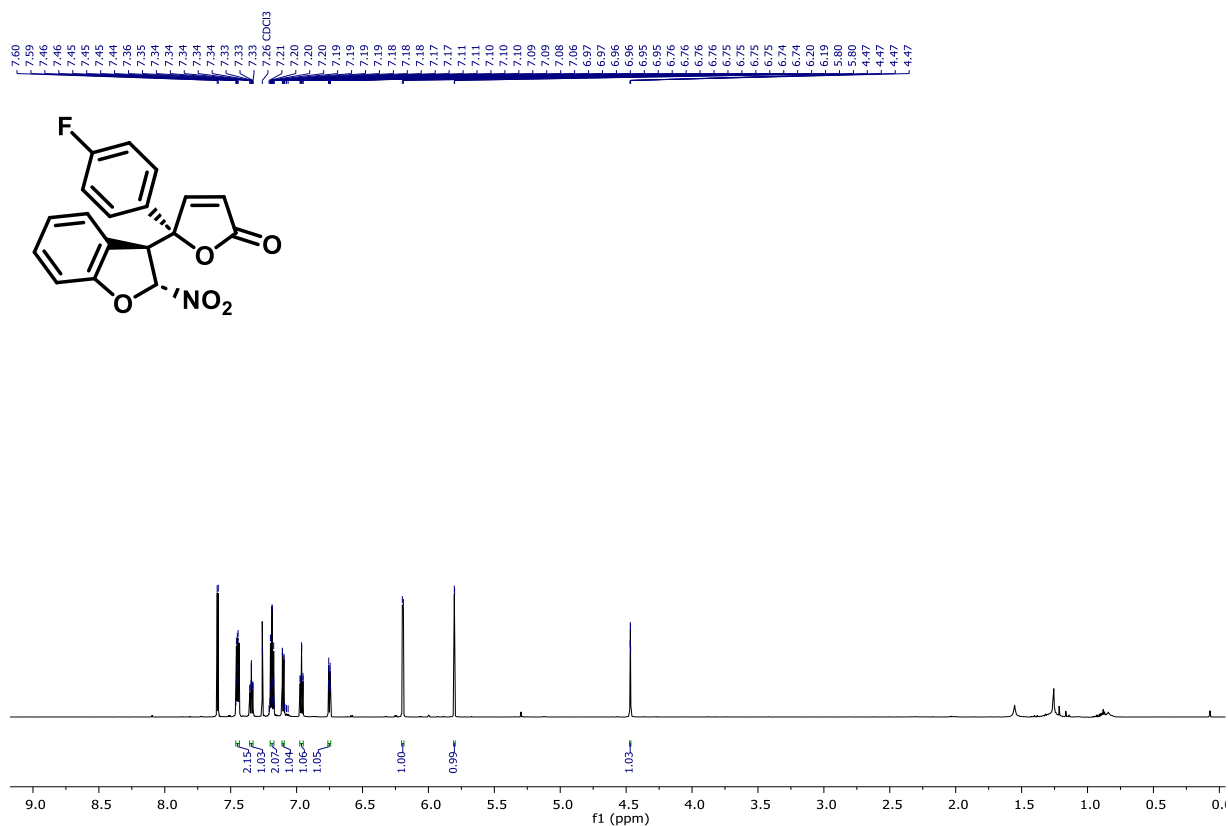


¹³C NMR (176 MHz, CDCl₃)

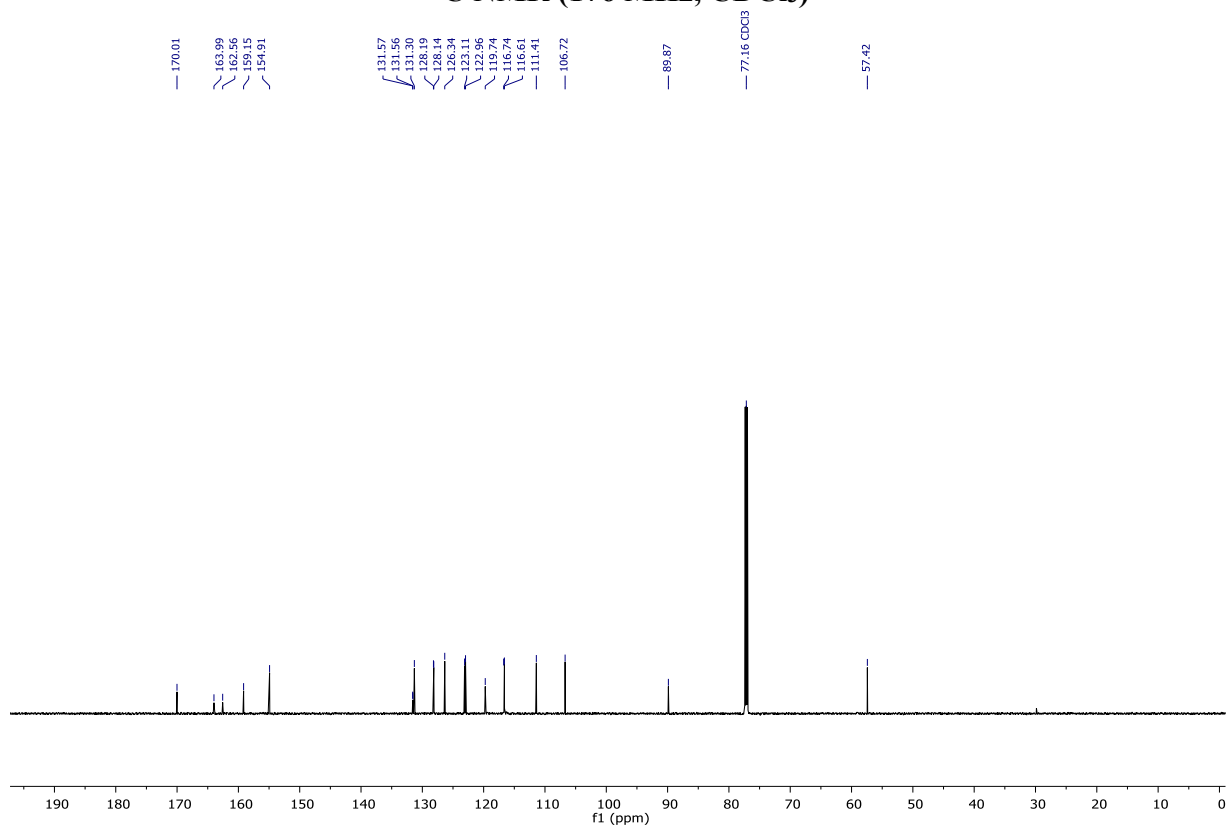


(*R*)-5-(4-Fluorophenyl)-5-((2*R*,3*S*)-2-nitro-2,3-dihydrobenzofuran-3-yl)furan-2(*5H*)-one
3j

^1H NMR (700 MHz, CDCl_3)

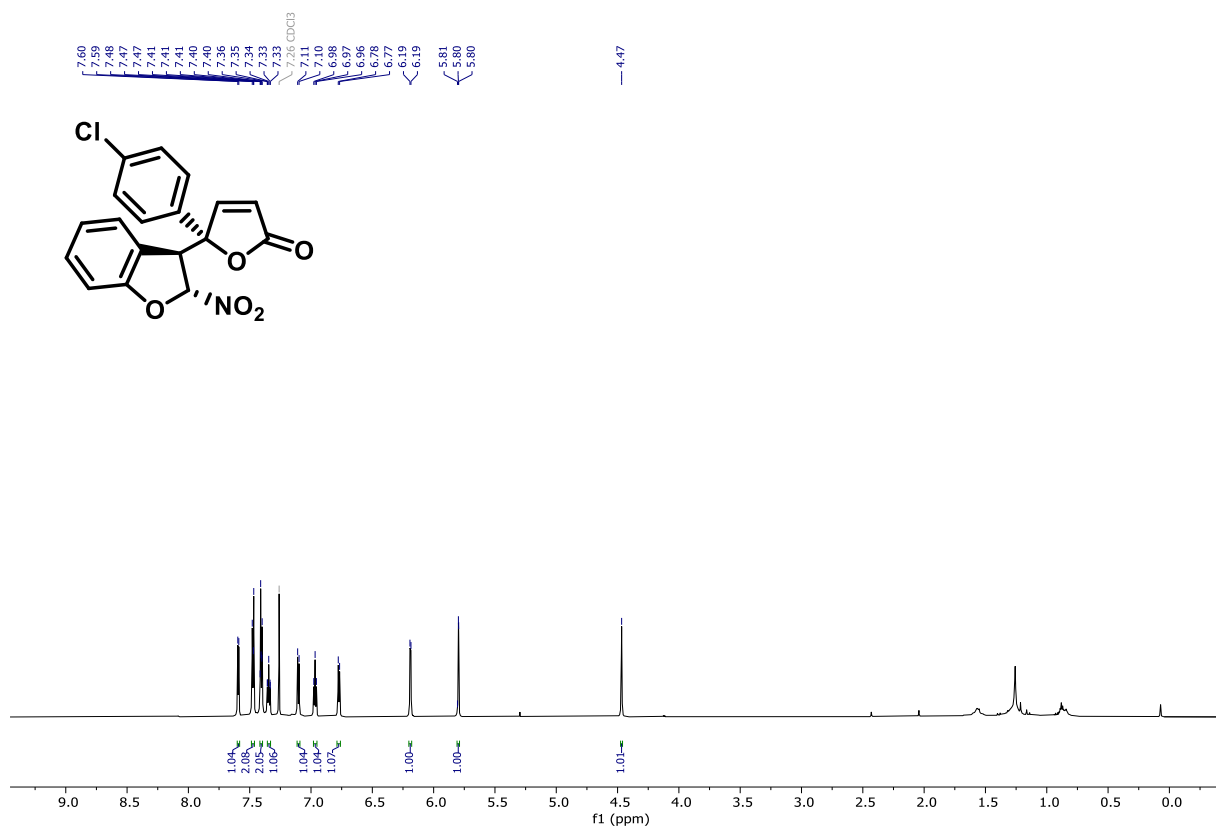


^{13}C NMR (176 MHz, CDCl_3)

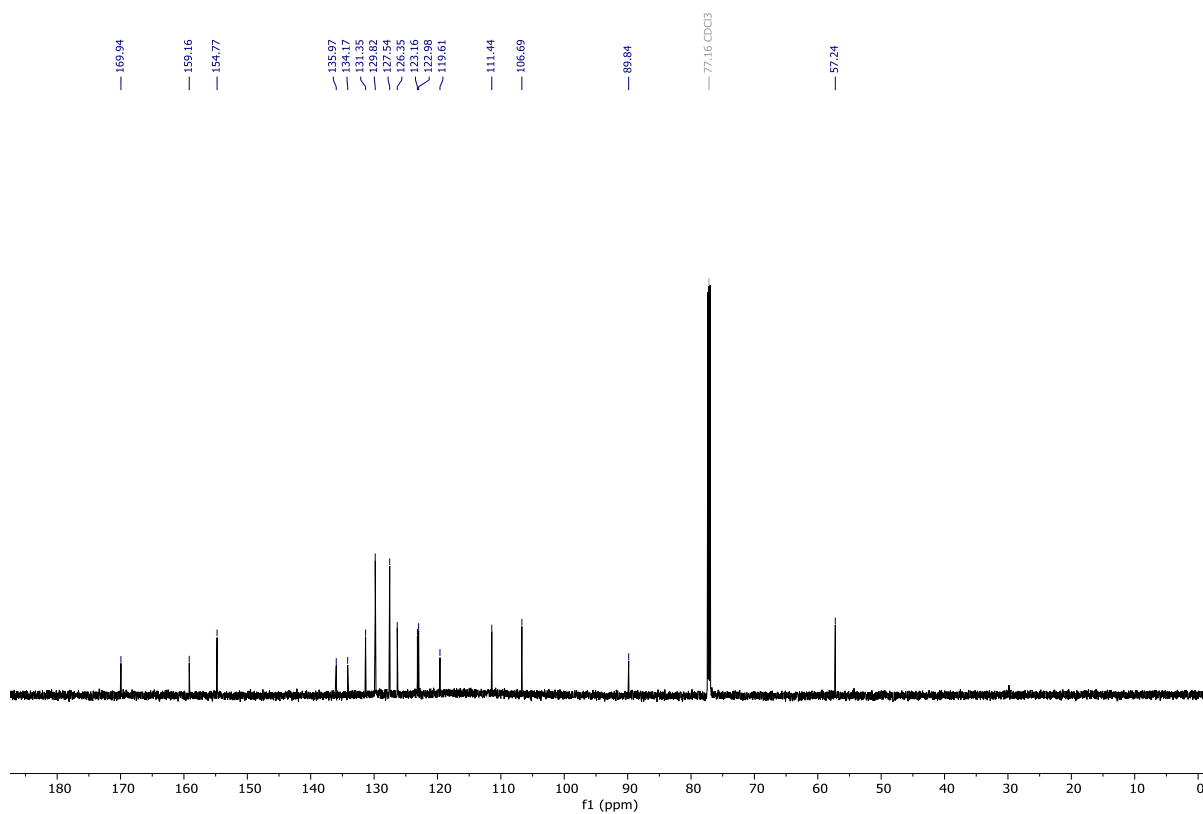


(*R*)-5-(4-Chlorophenyl)-5-((2*R*,3*S*)-2-nitro-2,3-dihydrobenzofuran-3-yl)furan-2(*5H*)-one
3k

^1H NMR (700 MHz, CDCl_3)

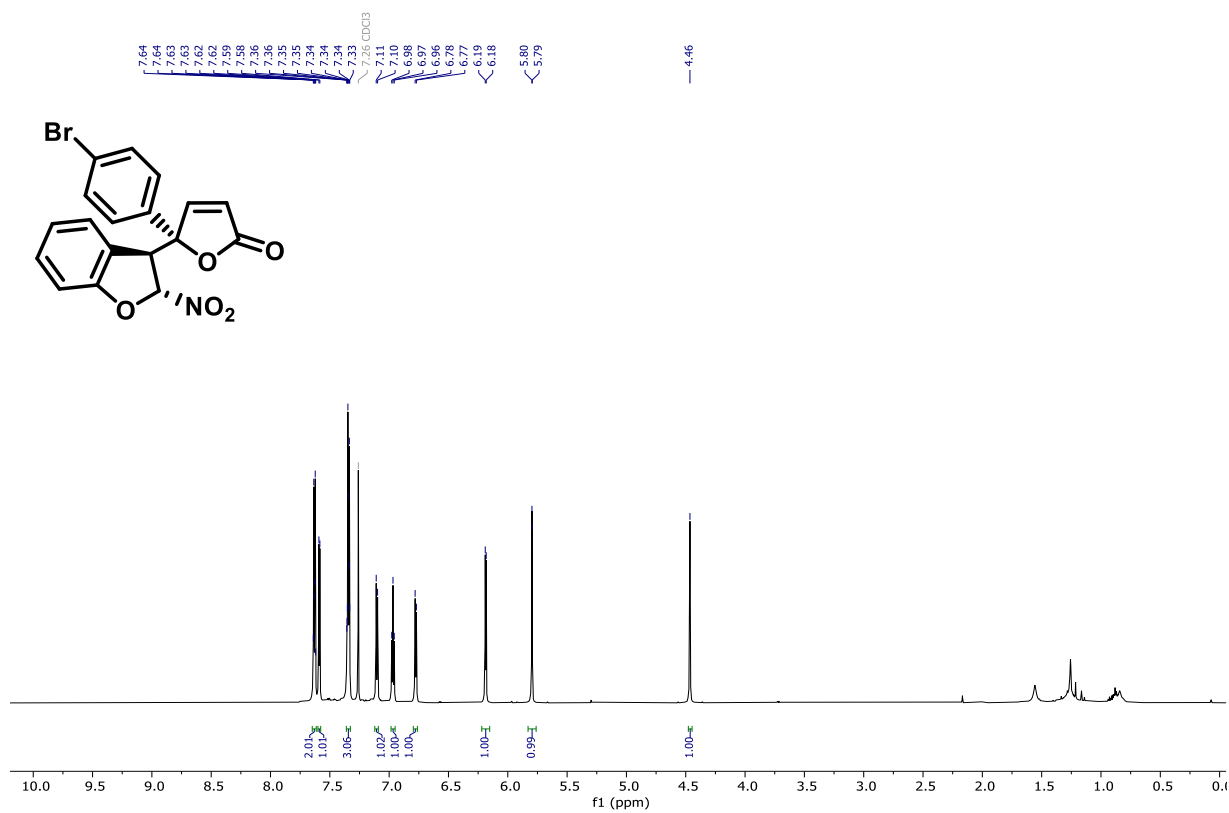


^{13}C NMR (176 MHz, CDCl_3)

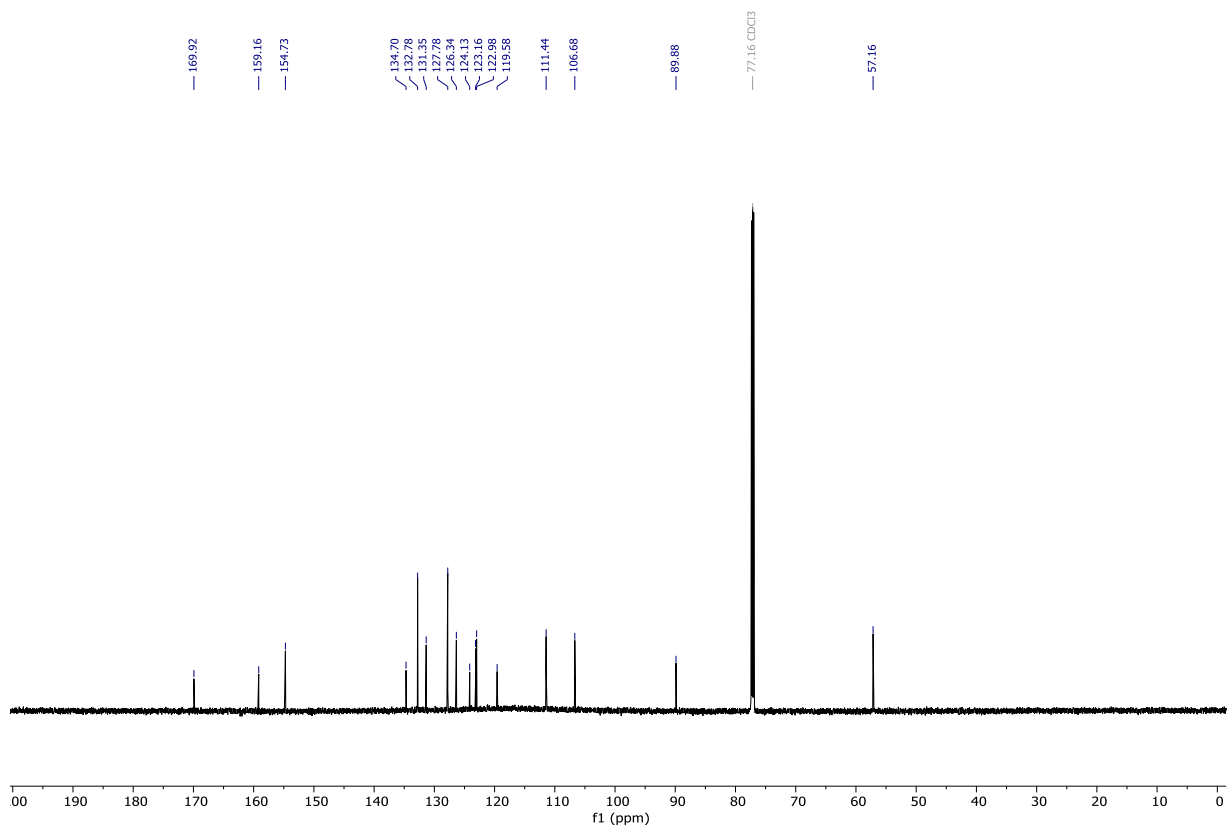


(*R*)-5-(4-Bromophenyl)-5-((2*R*,3*S*)-2-nitro-2,3-dihydrobenzofuran-3-yl)furan-2(*5H*)-one
3l

¹H NMR (700 MHz, CDCl₃)

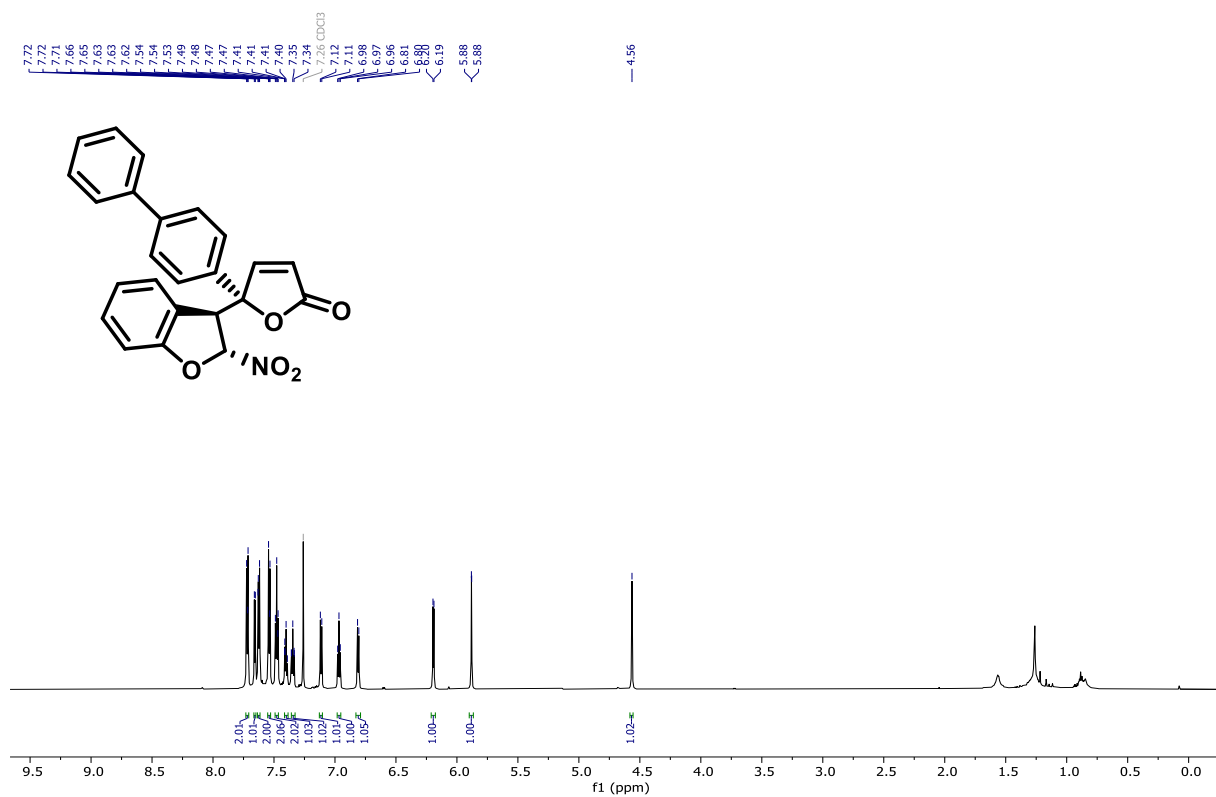


¹³C NMR (176 MHz, CDCl₃)

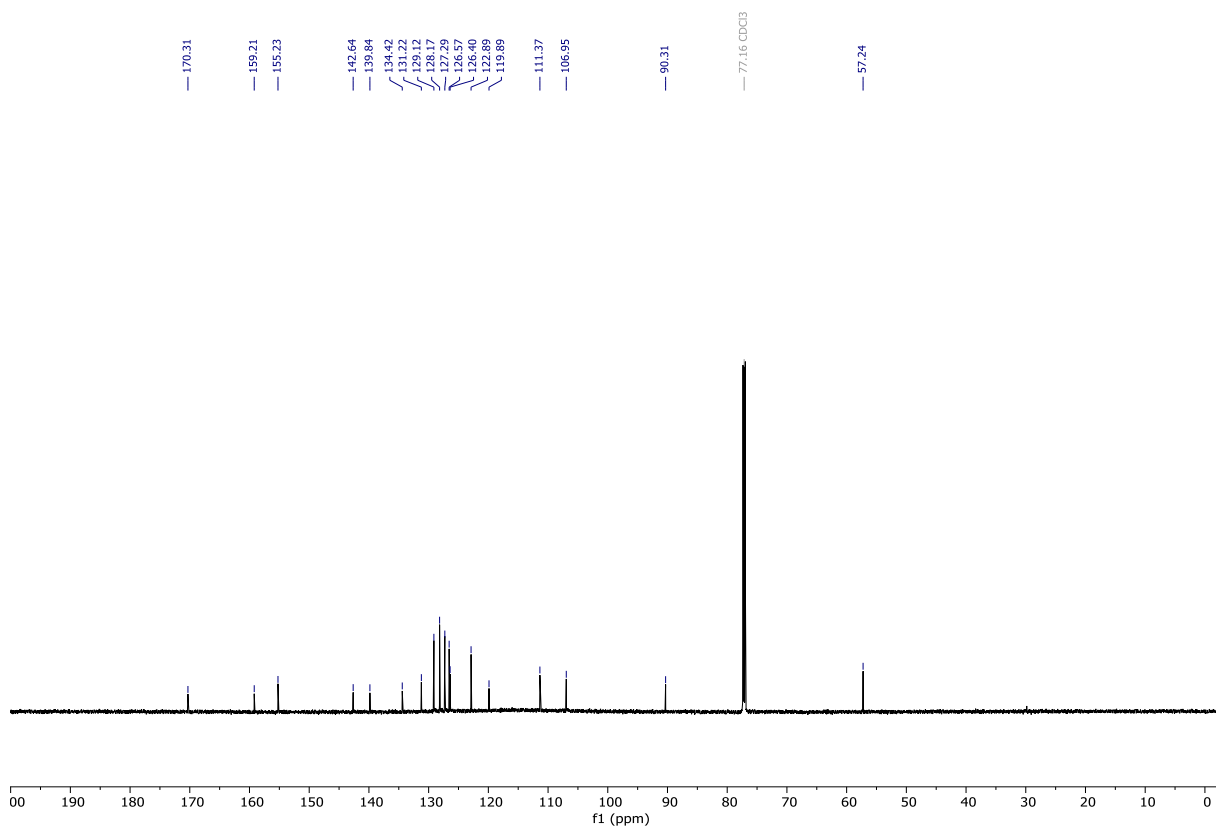


(*R*)-5-([1,1'-Biphenyl]-4-yl)-5-((2*R*,3*S*)-2-nitro-2,3-dihydrobenzofuran-3-yl)furan-2(*5H*)-one 3m

¹H NMR (700 MHz, CDCl₃)

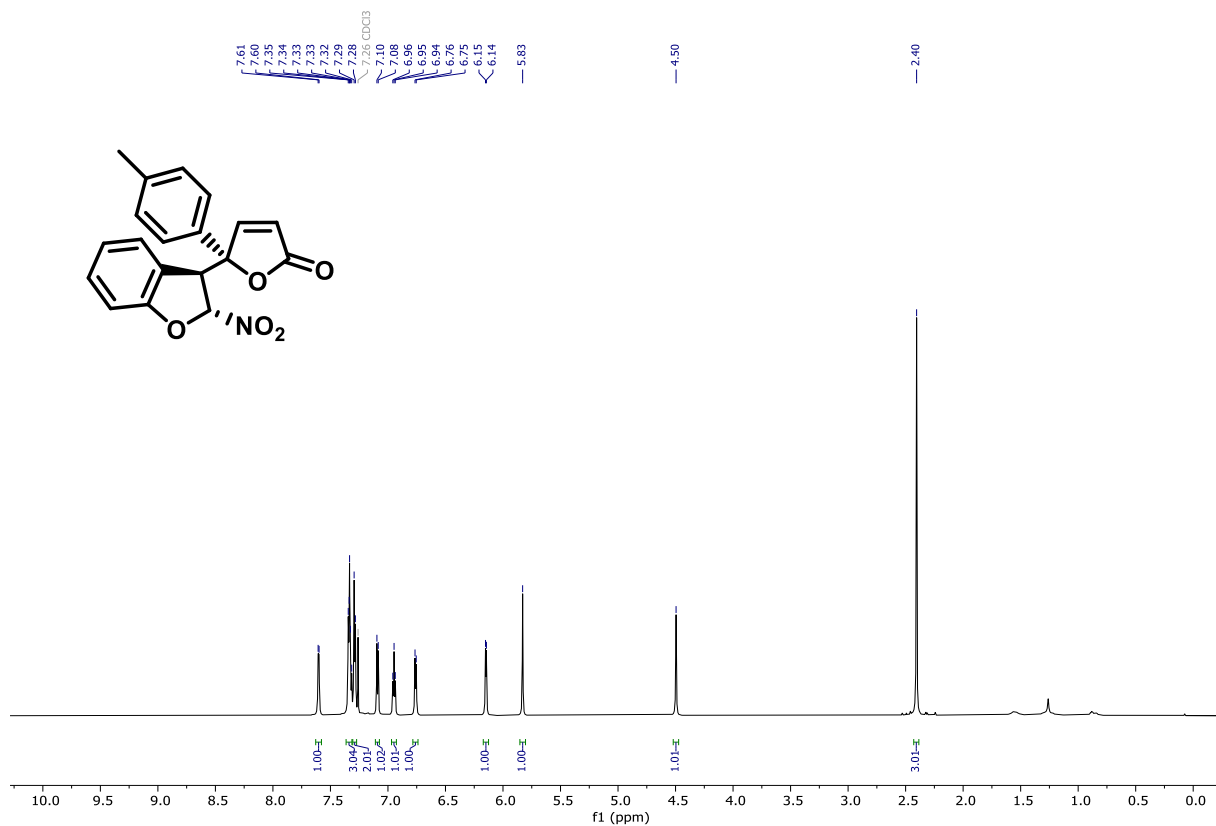


¹³C NMR (176 MHz, CDCl₃)

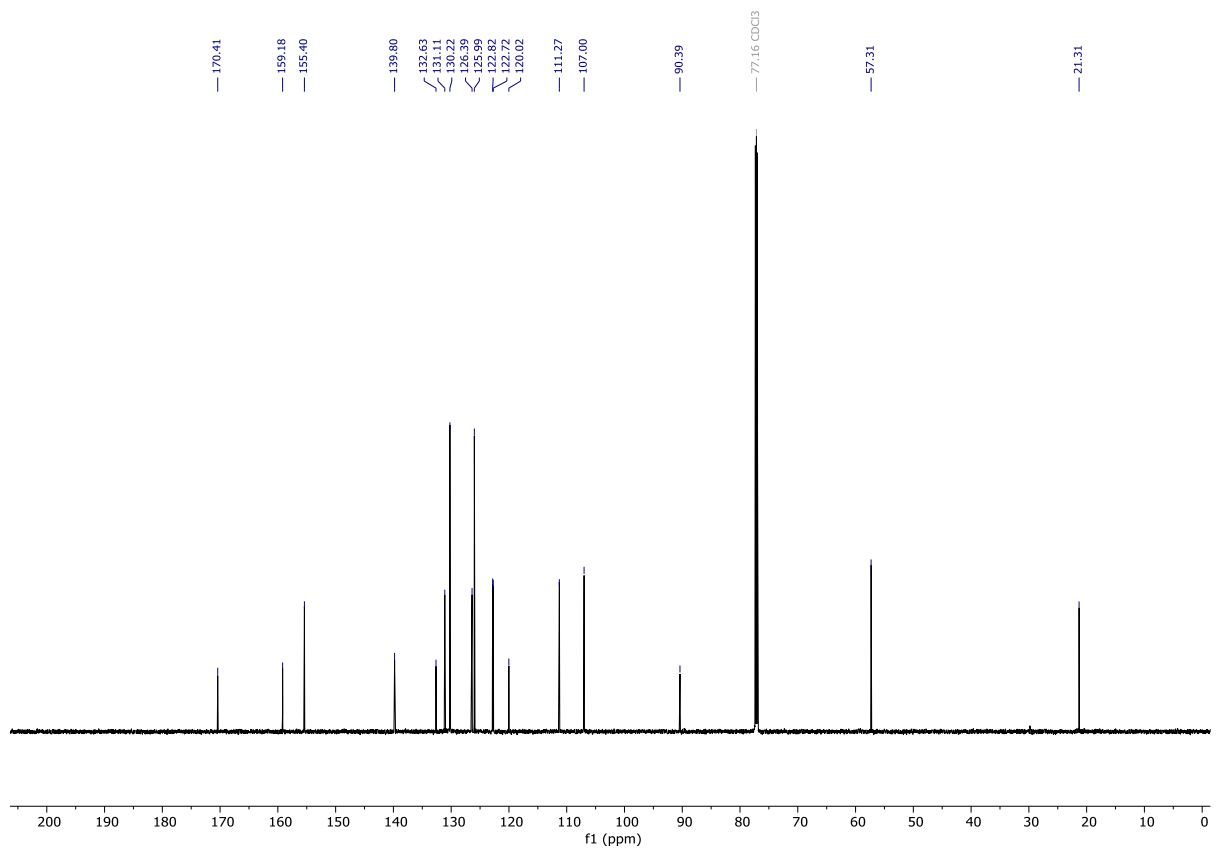


(R)-5-((2R,3S)-2-Nitro-2,3-dihydrobenzofuran-3-yl)-5-(p-tolyl)furan-2(5H)-one 3n

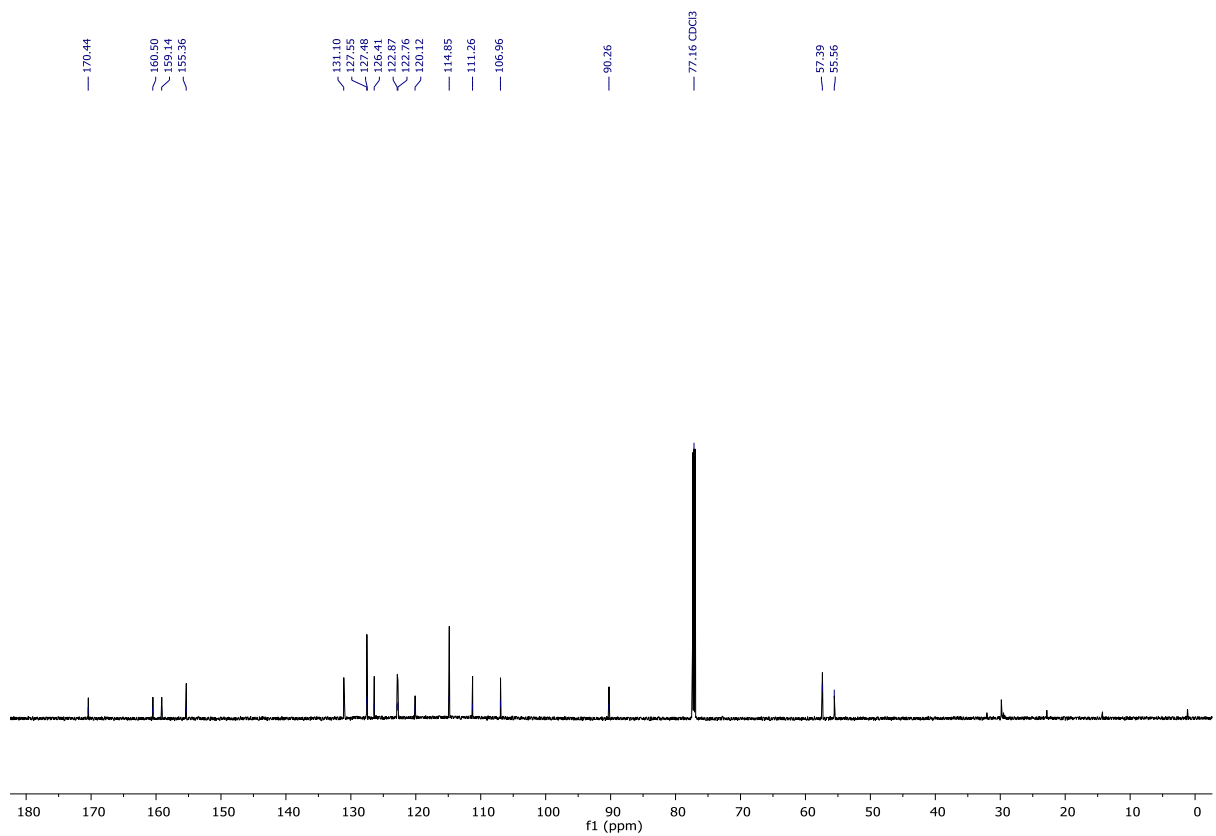
¹H NMR (700 MHz, CDCl₃)



¹³C NMR (176 MHz, CDCl₃)

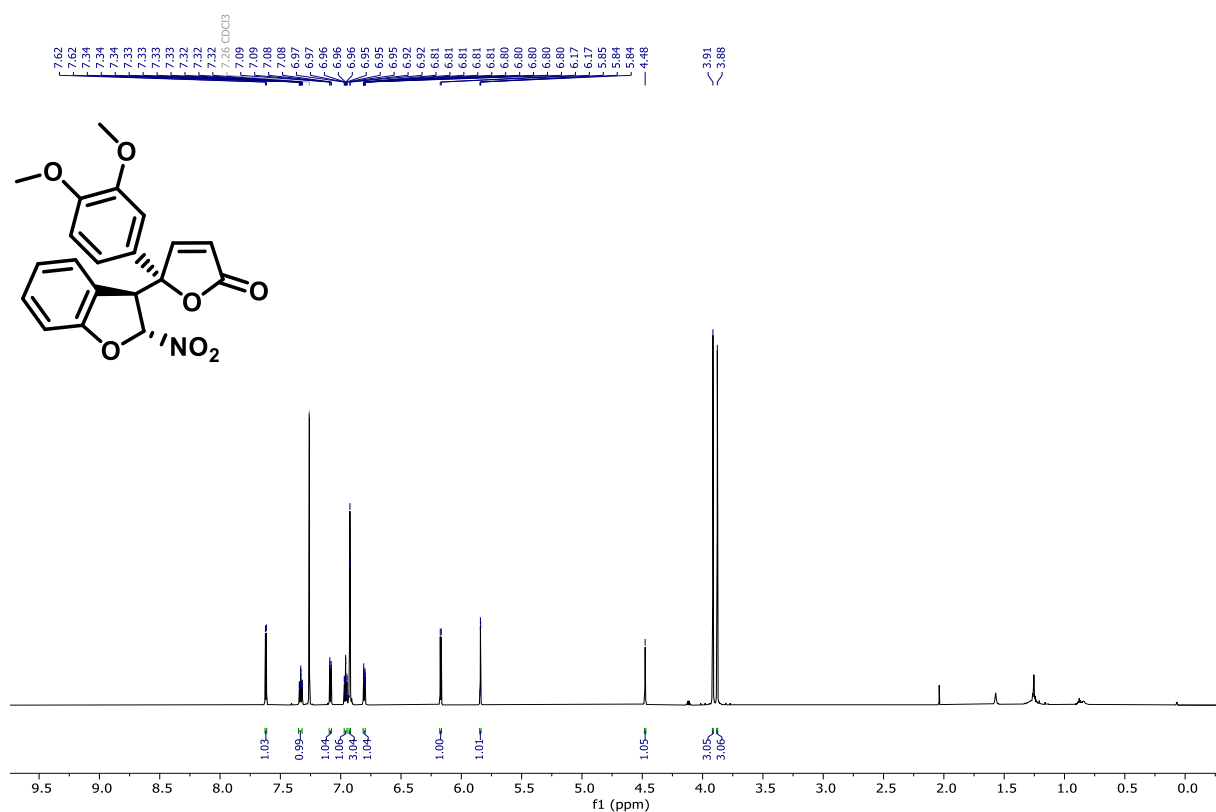


¹H NMR (700 MHz, CDCl₃)

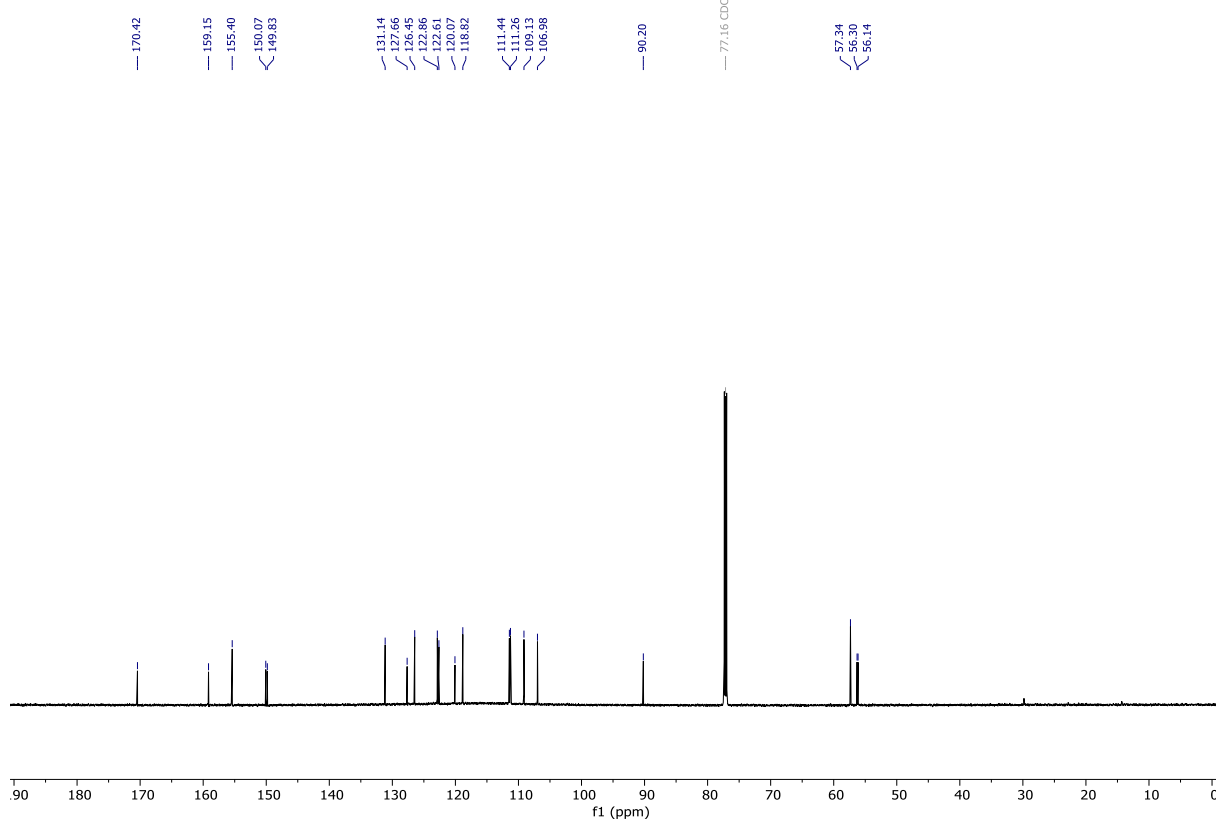


(*R*)-5-(3,4-Dimethoxyphenyl)-5-((2*R*,3*S*)-2-nitro-2,3-dihydrobenzofuran-3-yl)furan-2(*5H*)-one 3p

¹H NMR (700 MHz, CDCl₃)

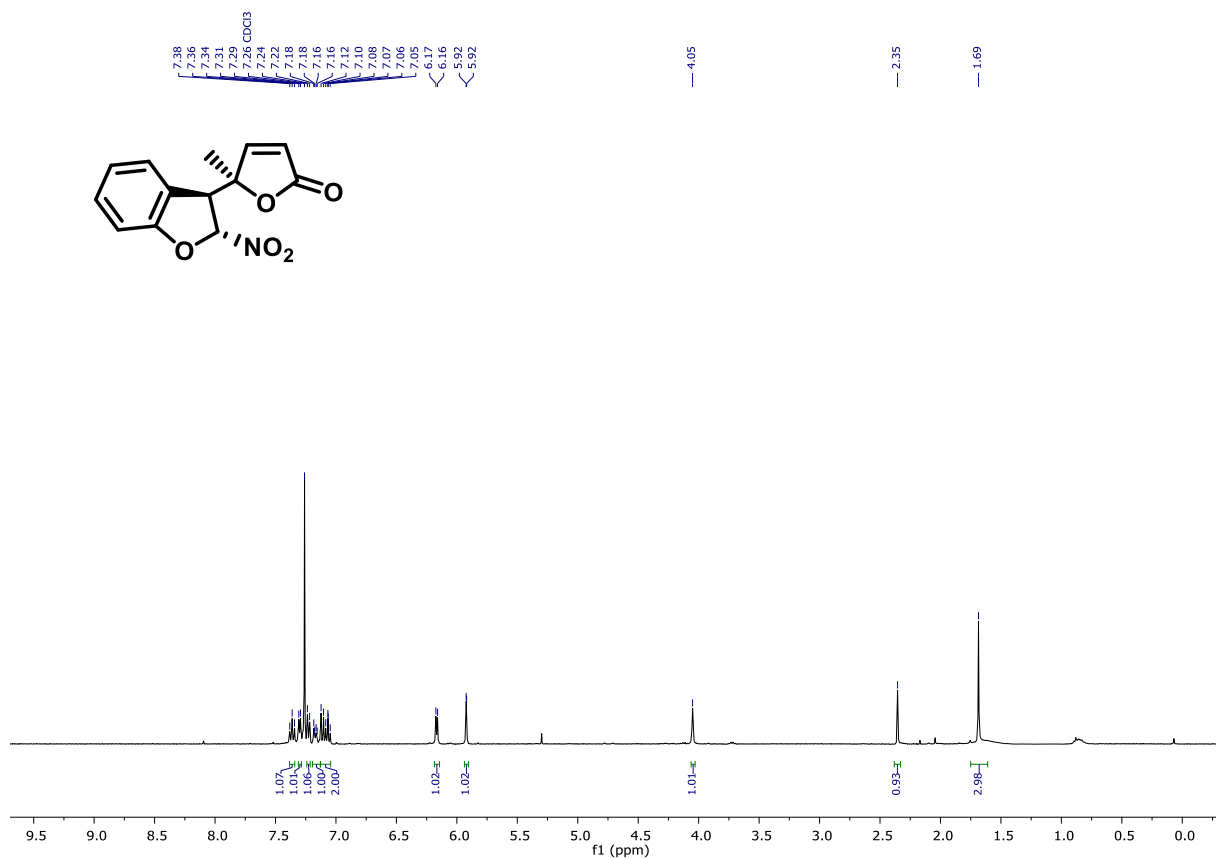


¹³C NMR (176 MHz, CDCl₃)

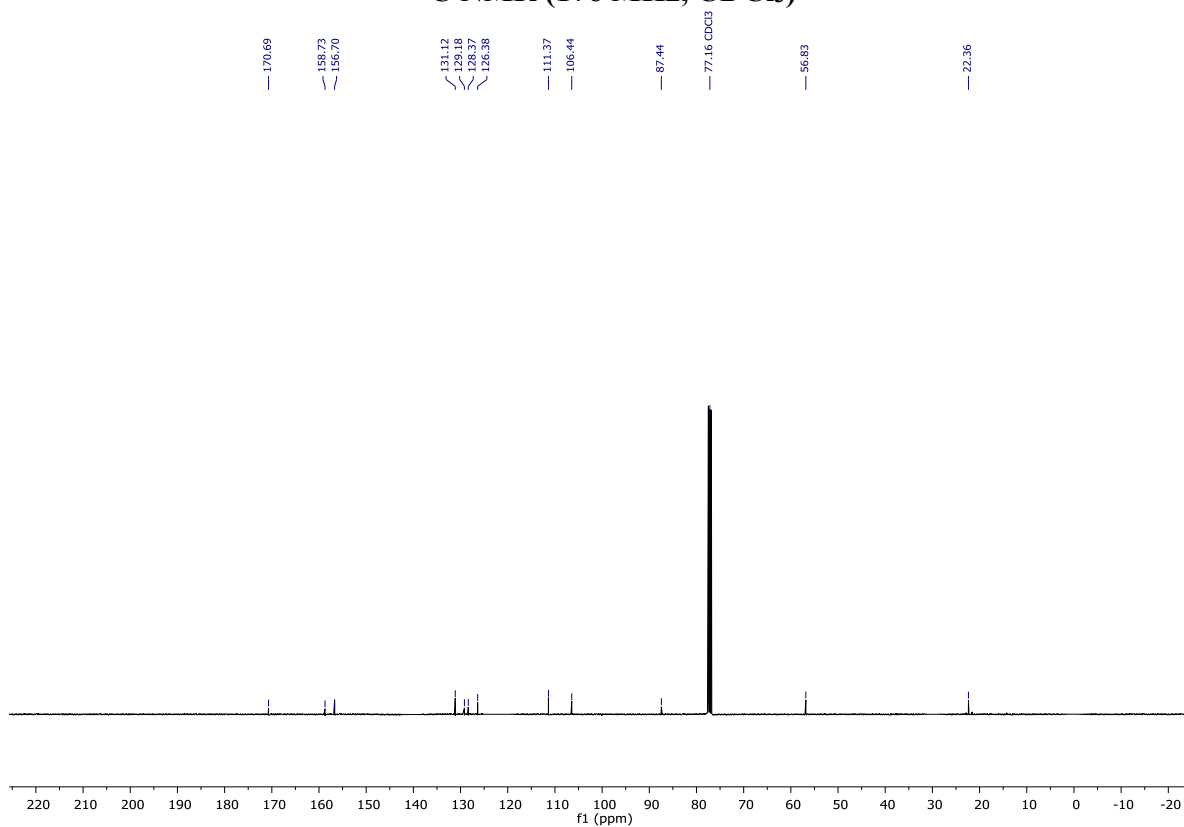


(R)-5-Methyl-5-((2R,3S)-2-nitro-2,3-dihydrobenzofuran-3-yl)furan-2(5H)-one 3r

¹H NMR (700 MHz, CDCl₃)

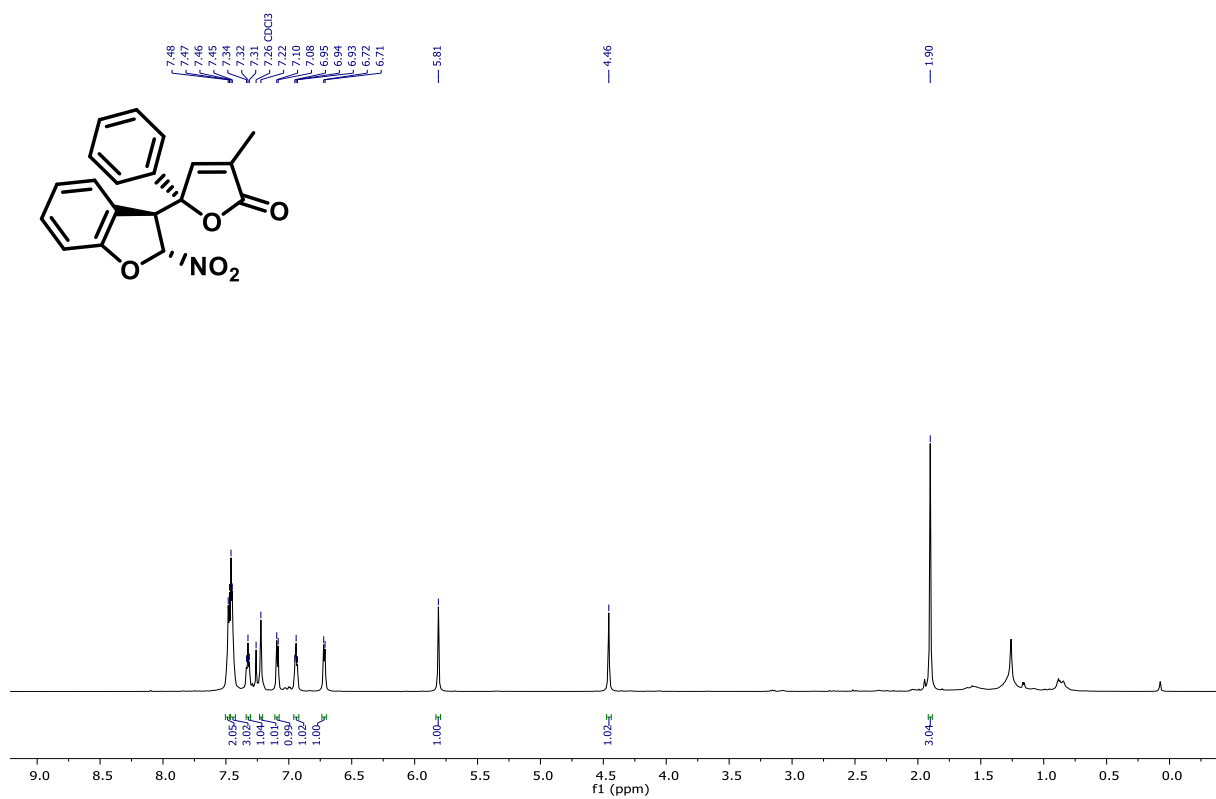


¹³C NMR (176 MHz, CDCl₃)

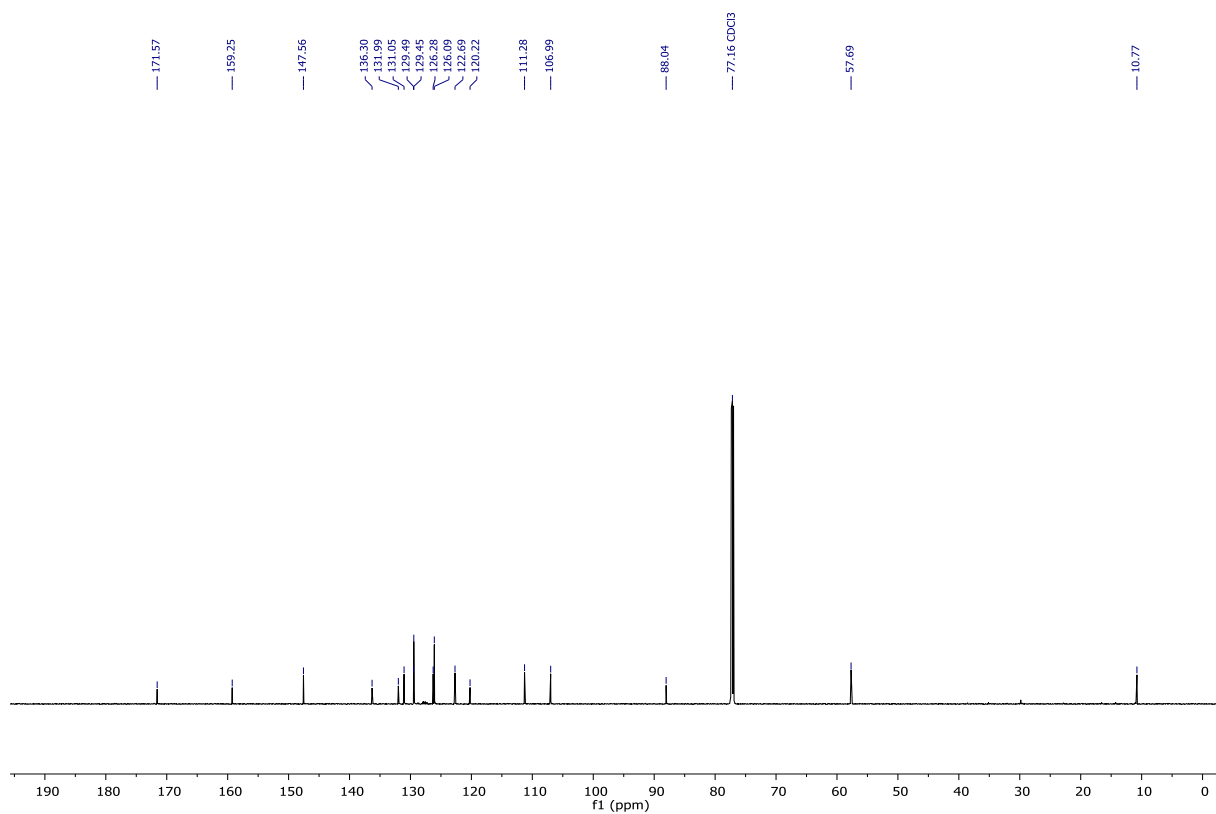


(*R*)-3-Methyl-5-((2*R*,3*S*)-2-nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(*5H*)-one
3s

^1H NMR (700 MHz, CDCl_3)

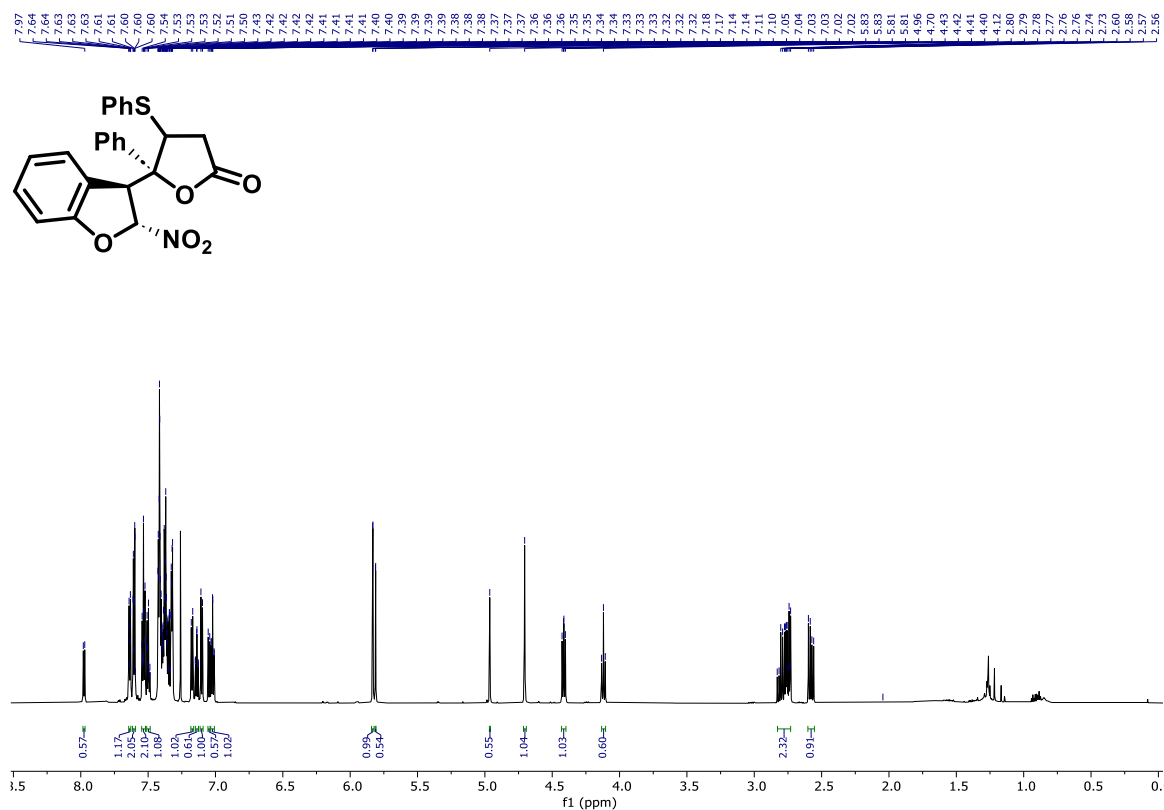


^{13}C NMR (176 MHz, CDCl_3)

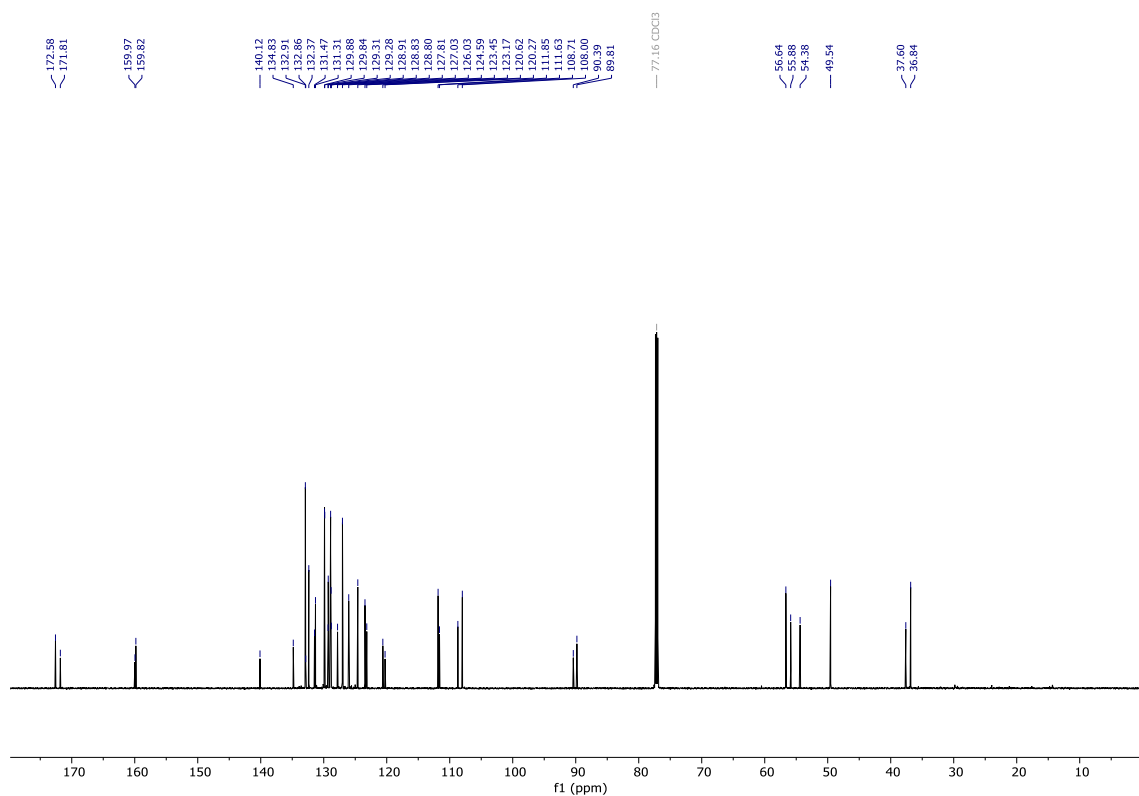


(5*R*)-5-((2*R*,3*S*)-2-Nitro-2,3-dihydrobenzofuran-3-yl)-5-phenyl-4-(phenylthio)dihydrofuran-2(3*H*)-one 7a (mixture of diastereoisomers)

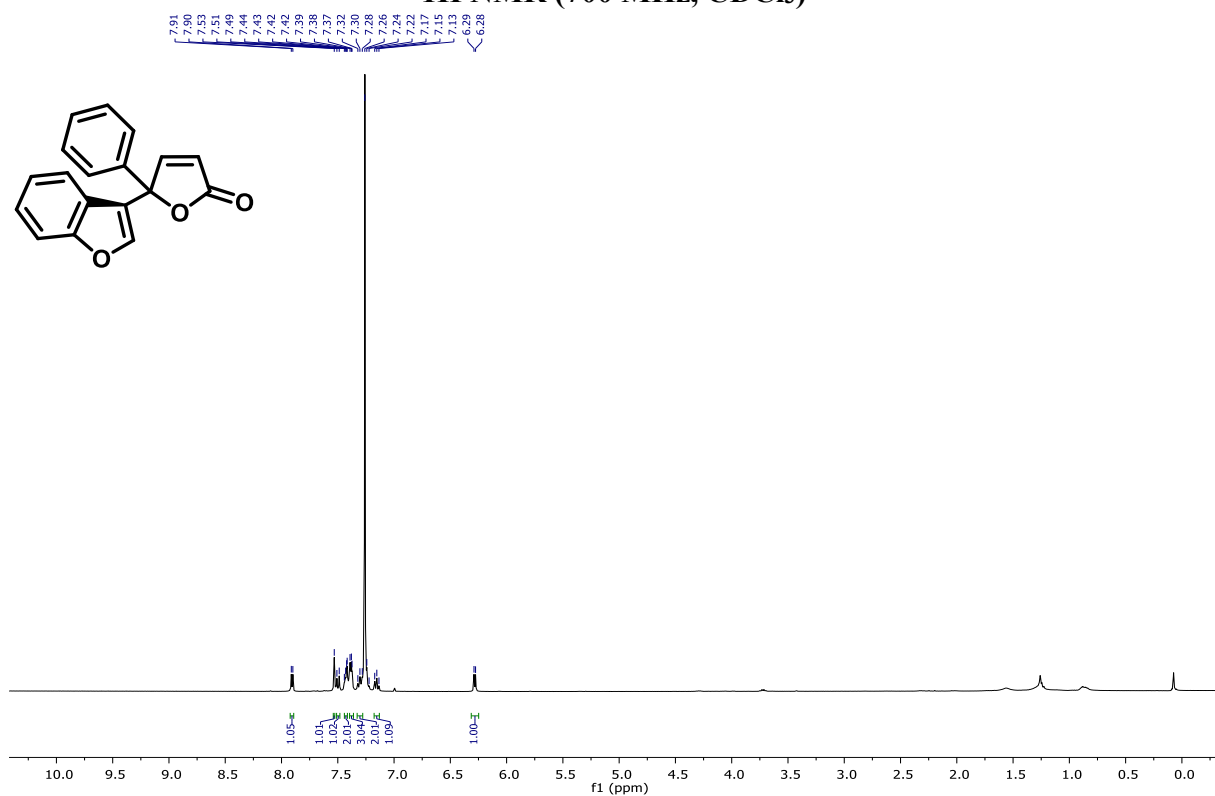
¹H NMR (700 MHz, CDCl₃)



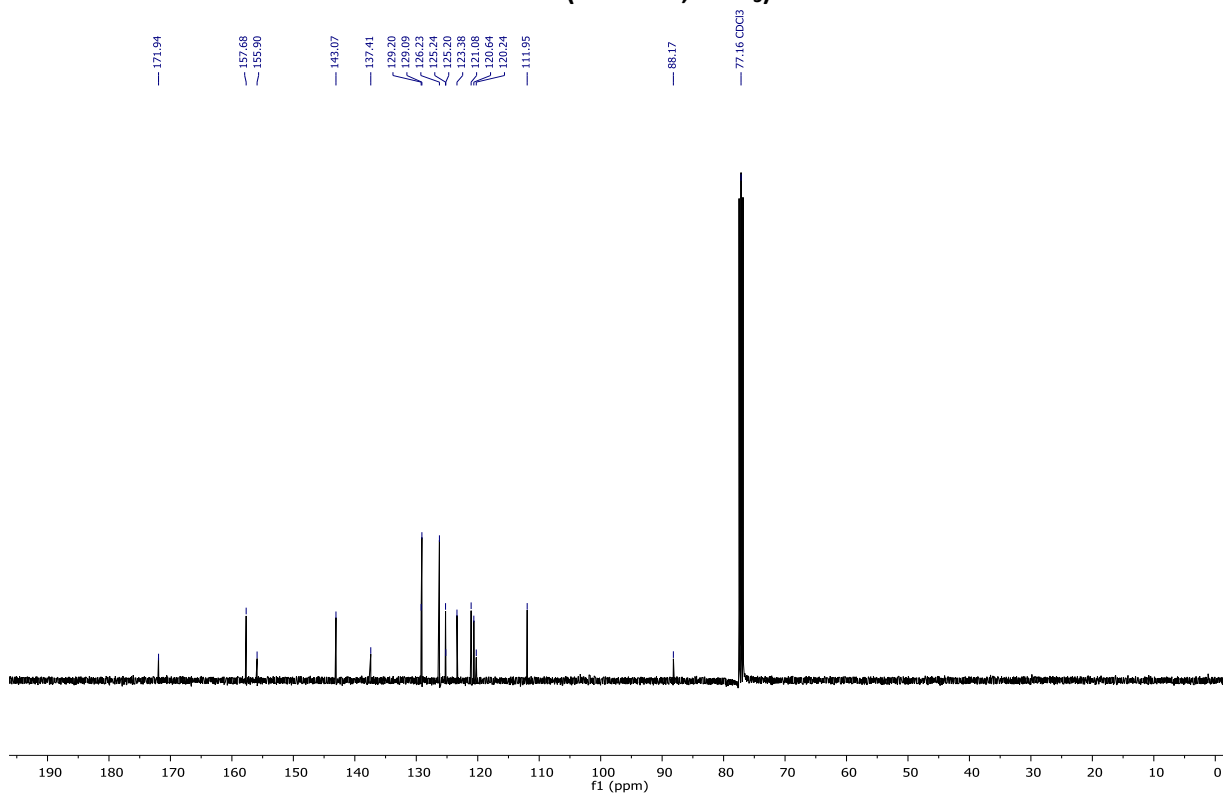
¹³C NMR (176 MHz, CDCl₃)



5-(Benzofuran-3-yl)-5-phenylfuran-2(5H)-one 7b
¹H NMR (700 MHz, CDCl₃)



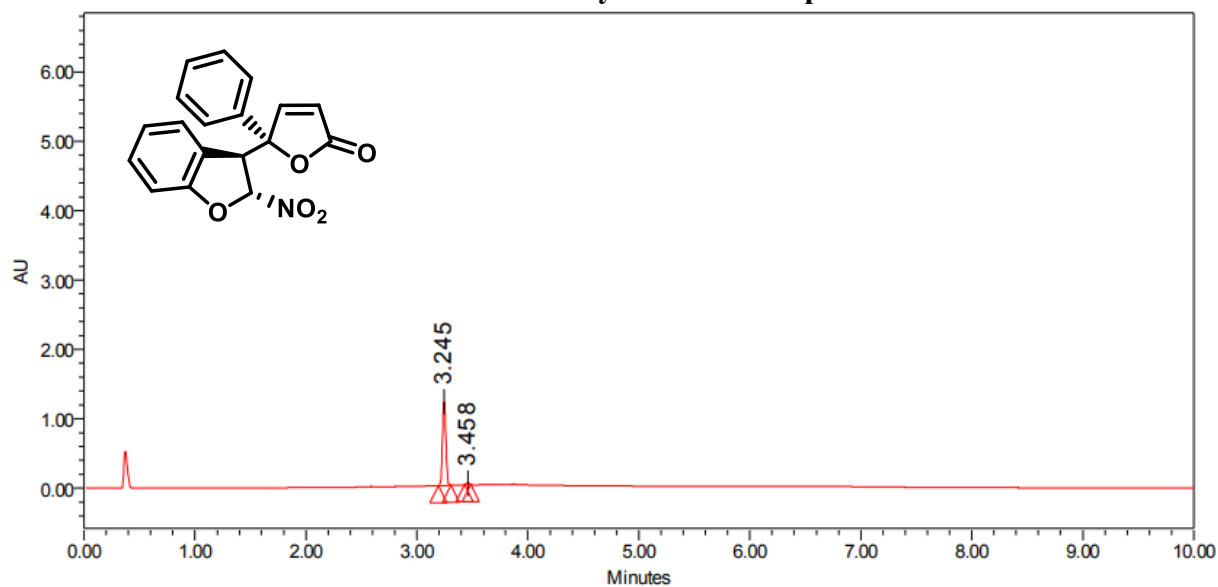
¹³C NMR (176 MHz, CDCl₃)



11. UPC² data

(*R*)-5-((2*R*,3*S*)-2-Nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(*H*)-one 3a

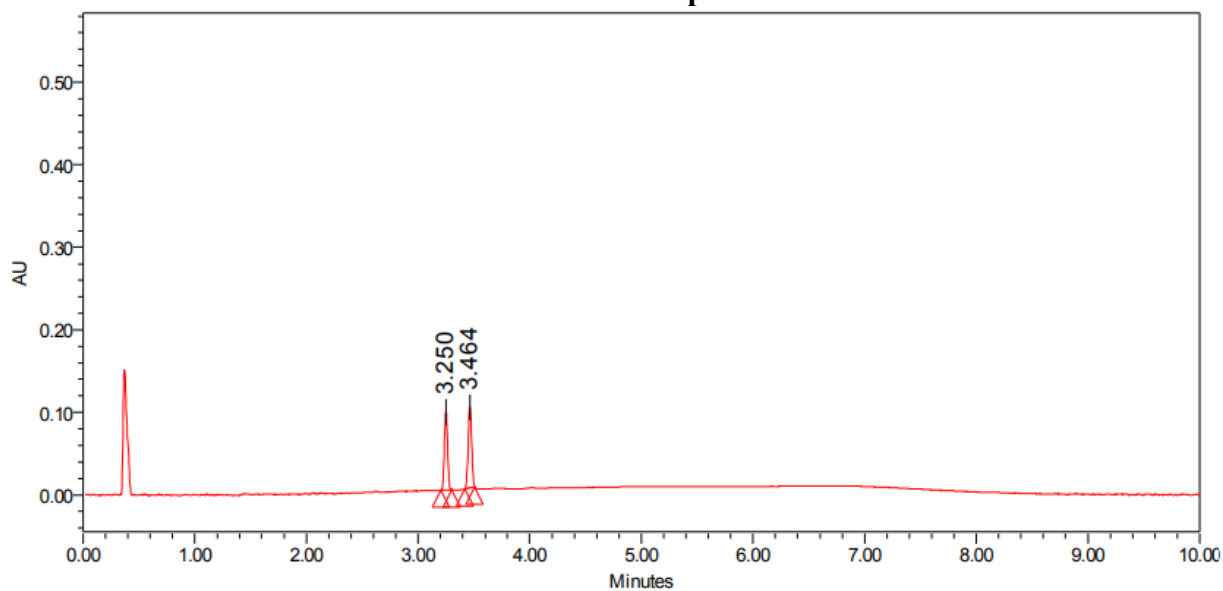
Enantiomerically enriched sample



Peak Results

	RT	% Area
1	3.245	98.24
2	3.458	1.76

Racemic sample

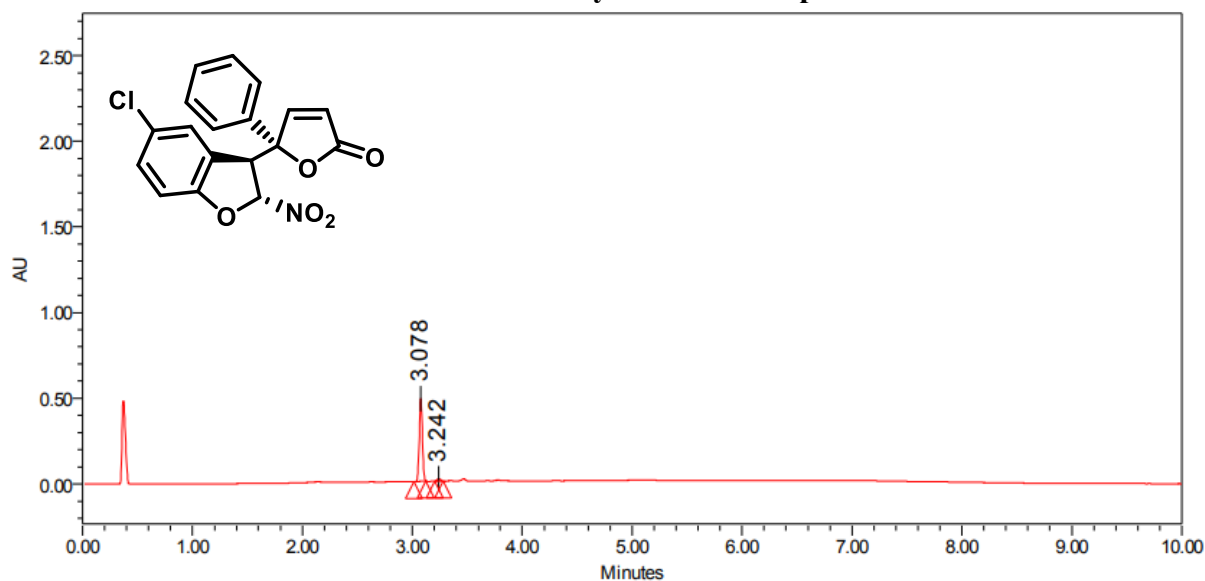


Peak Results

	RT	% Area
1	3.250	47.10
2	3.464	52.90

(*R*)-5-((2*R*,3*S*)-5-Chloro-2-nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(*5H*)-one
3b

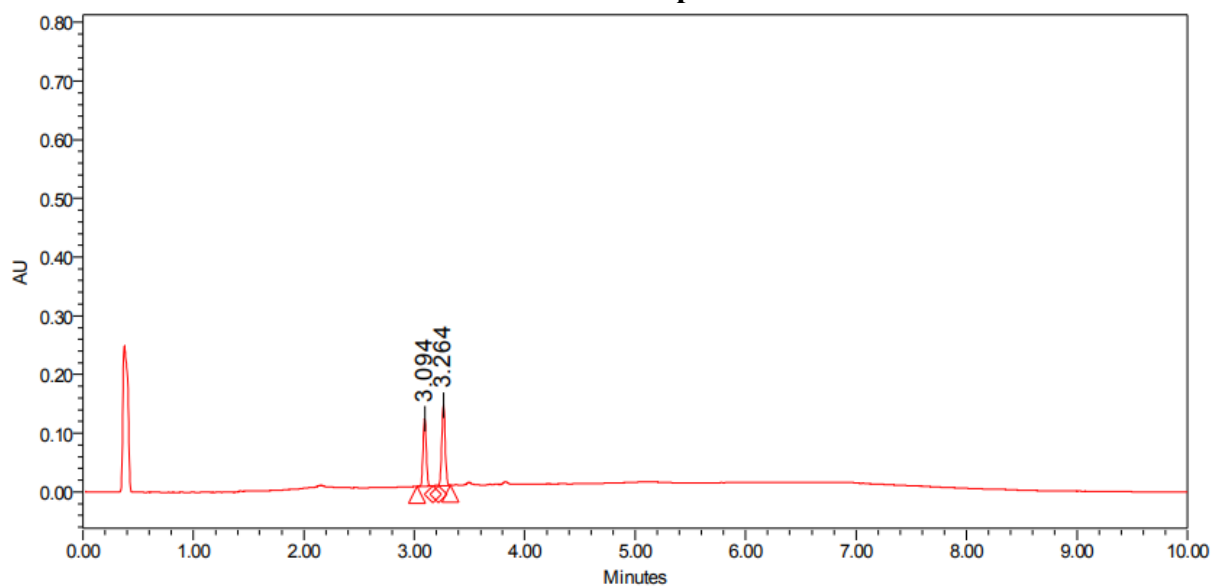
Enantiomerically enriched sample



Peak Results

	RT	% Area
1	3.078	96.97
2	3.242	3.03

Racemic sample

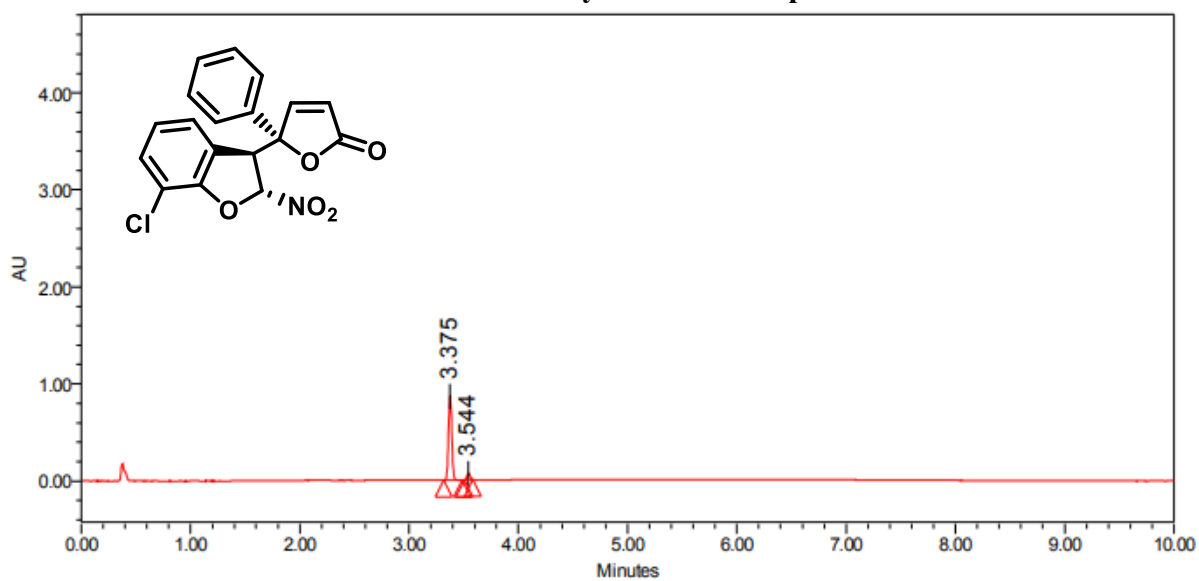


Peak Results

	RT	% Area
1	3.094	43.99
2	3.264	56.01

(*R*)-5-((2*R*,3*S*)-7-Chloro-2-nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(*5H*)-one
3c

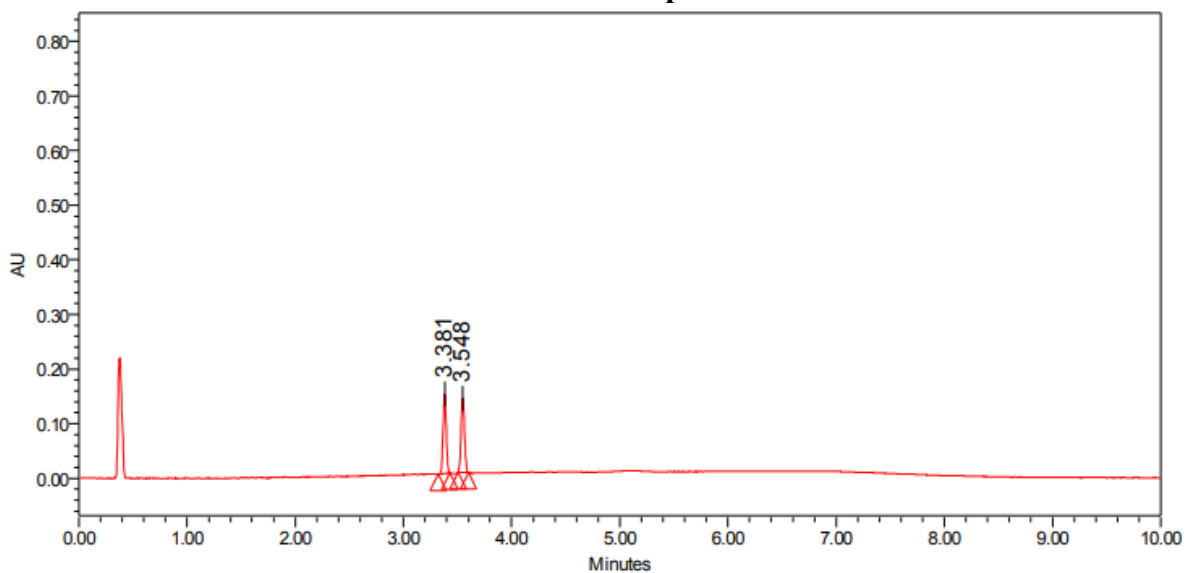
Enantiomerically enriched sample



Peak Results

	RT	% Area
1	3.375	93.08
2	3.544	6.92

Racemic sample

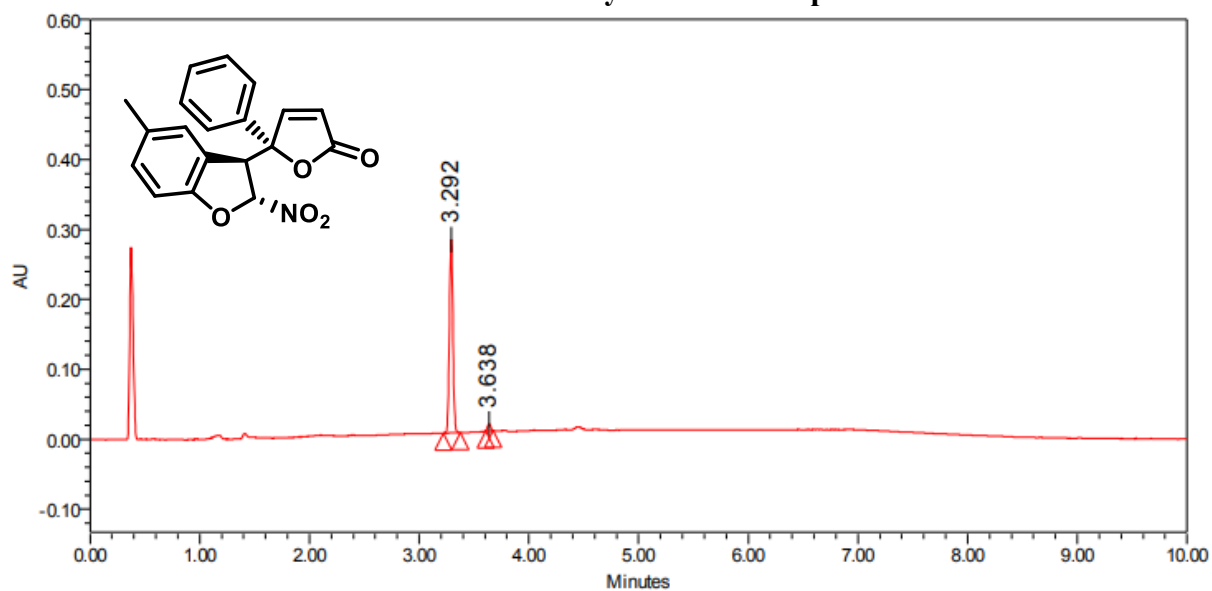


Peak Results

	RT	% Area
1	3.381	50.09
2	3.548	49.91

(*R*)-5-((2*R*,3*S*)-5-Methyl-2-nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(*5H*)-one
3d

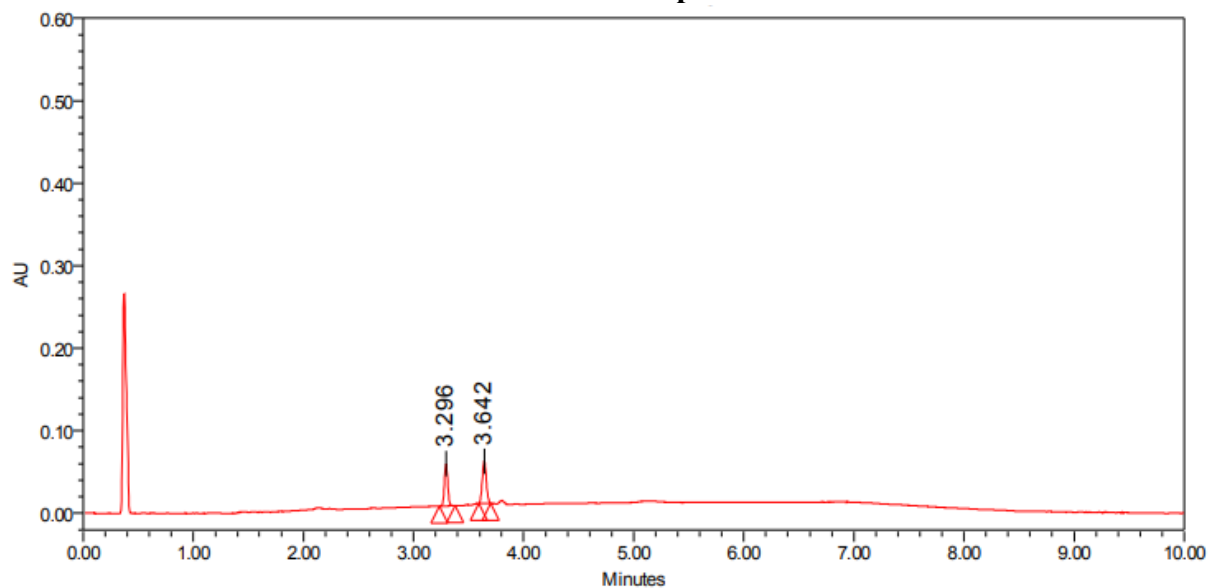
Enantiomerically enriched sample



Peak Results

	RT	% Area
1	3.292	96.75
2	3.638	3.25

Racemic sample

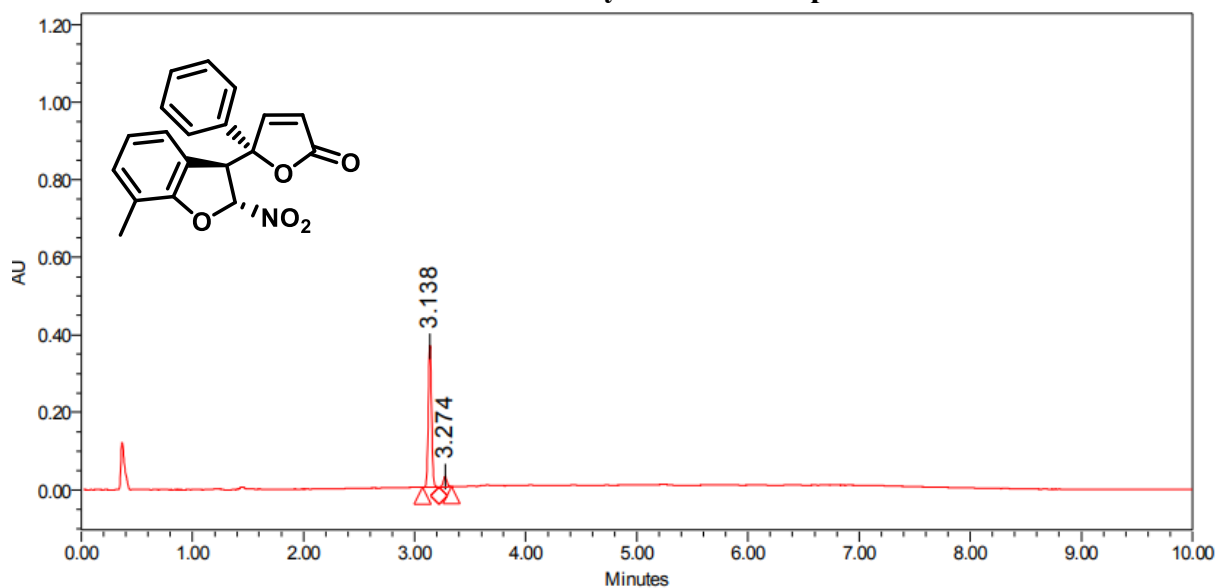


Peak Results

	RT	% Area
1	3.296	45.43
2	3.642	54.57

(*R*)-5-((2*R*,3*S*)-7-Methyl-2-nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(*5H*)-one
3e

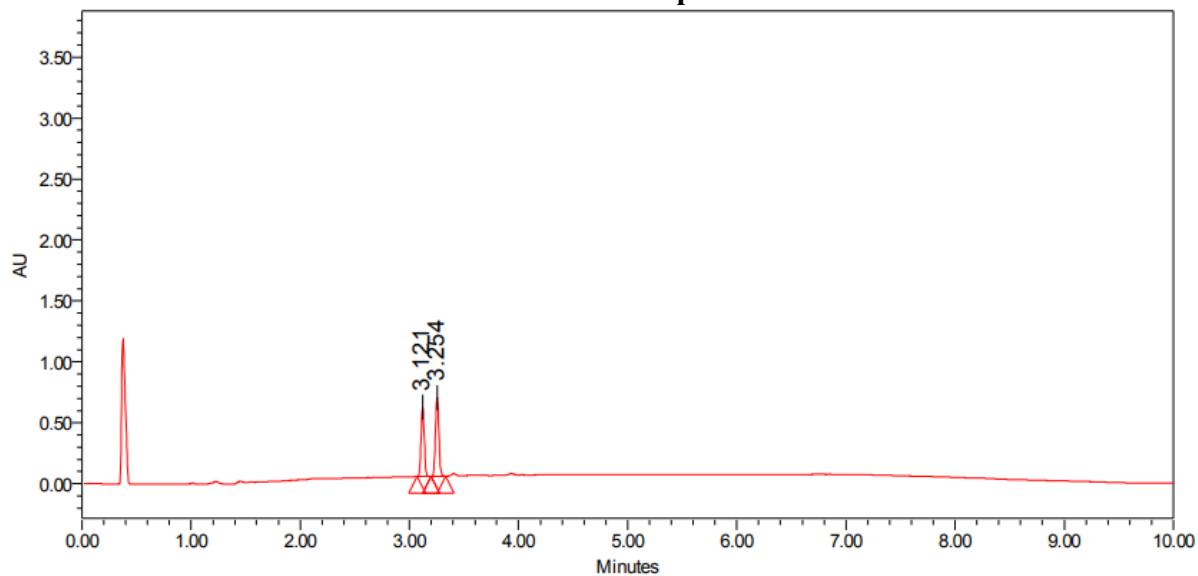
Enantiomerically enriched sample



Peak Results

	RT	% Area
1	3.138	92.73
2	3.274	7.27

Racemic sample

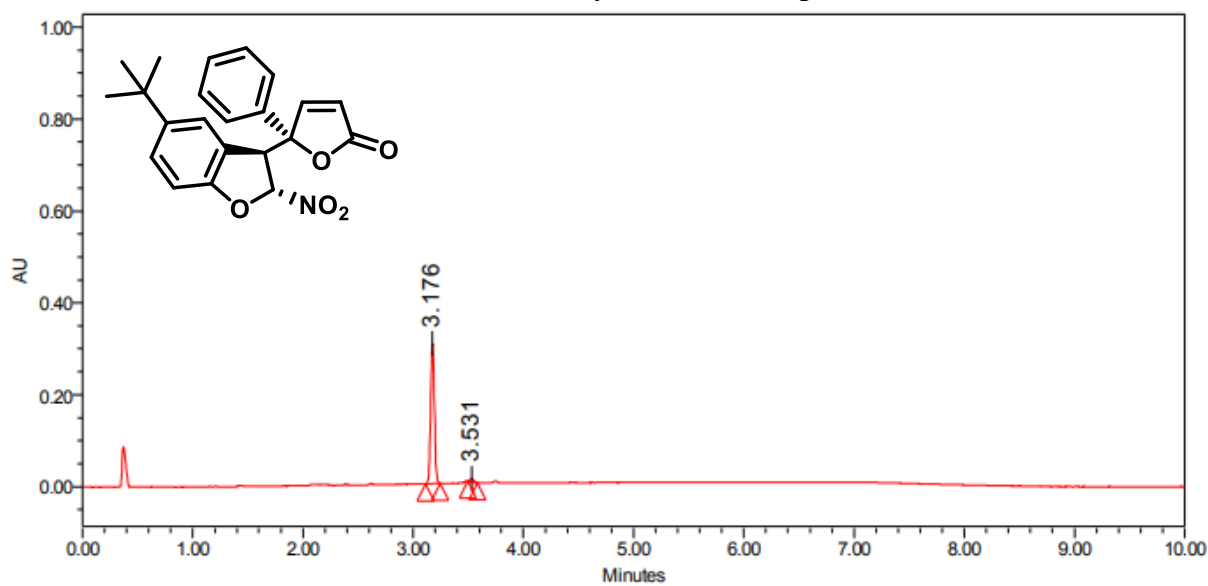


Peak Results

	RT	% Area
1	3.121	45.43
2	3.254	54.57

(*R*)-5-((2*R*,3*S*)-5-(*tert*-Butyl)-2-nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(*5H*)-one 3f

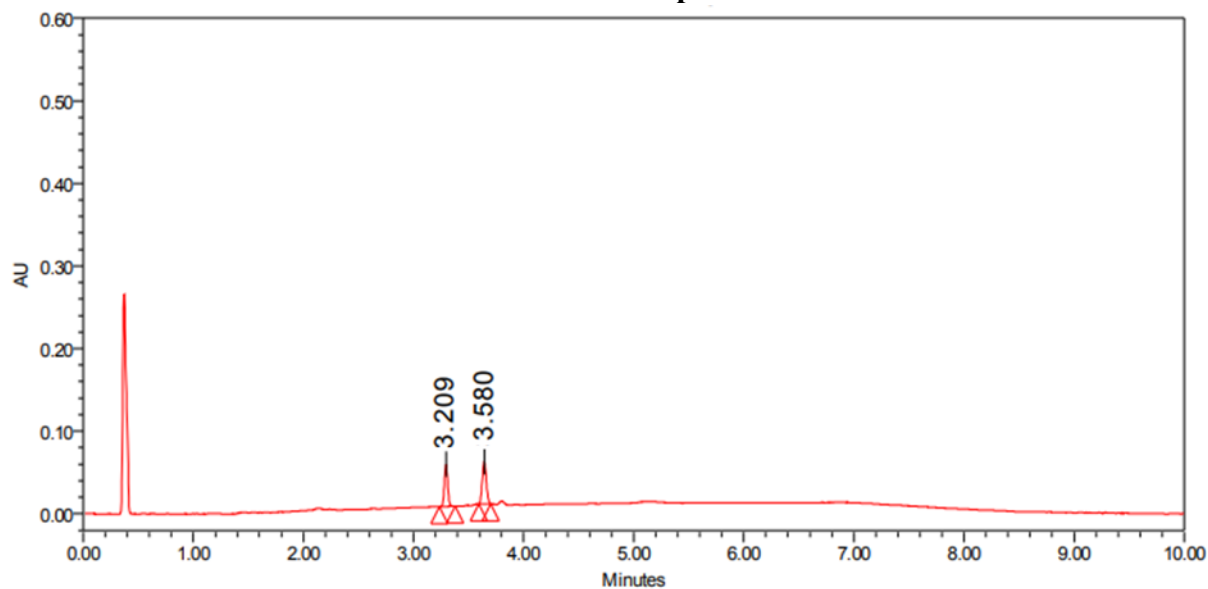
Enantiomerically enriched sample



Peak Results

	RT	% Area
1	3.176	97.76
2	3.531	2.24

Racemic sample

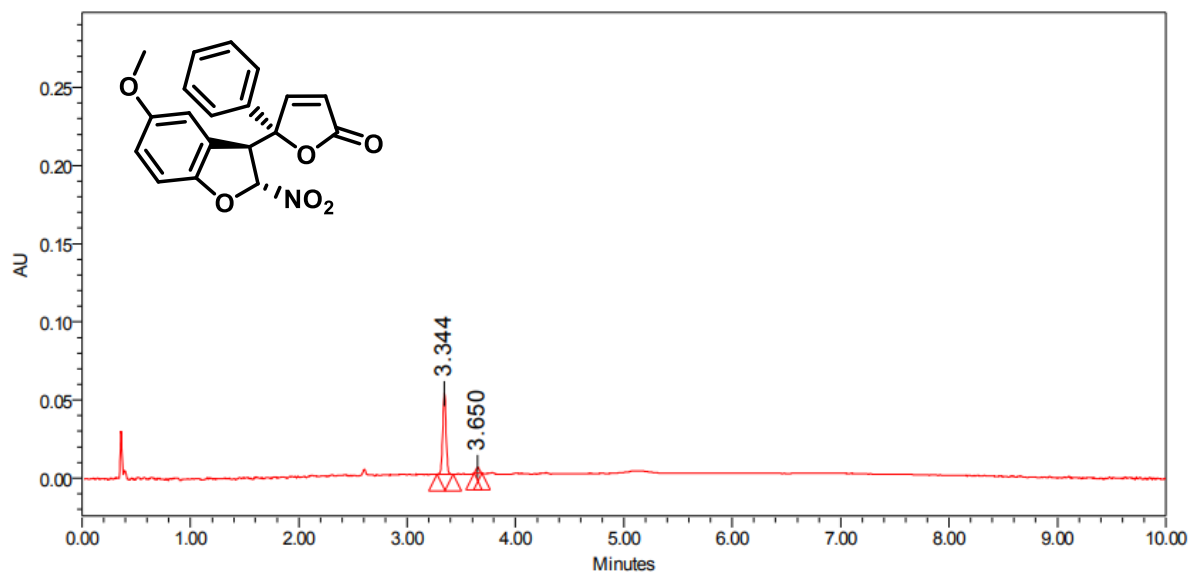


Peak Results

	RT	% Area
1	3.209	45.64
2	3.580	54.36

(*R*)-5-((2*R*,3*S*)-5-Methoxy-2-nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(*5H*)-one
3g

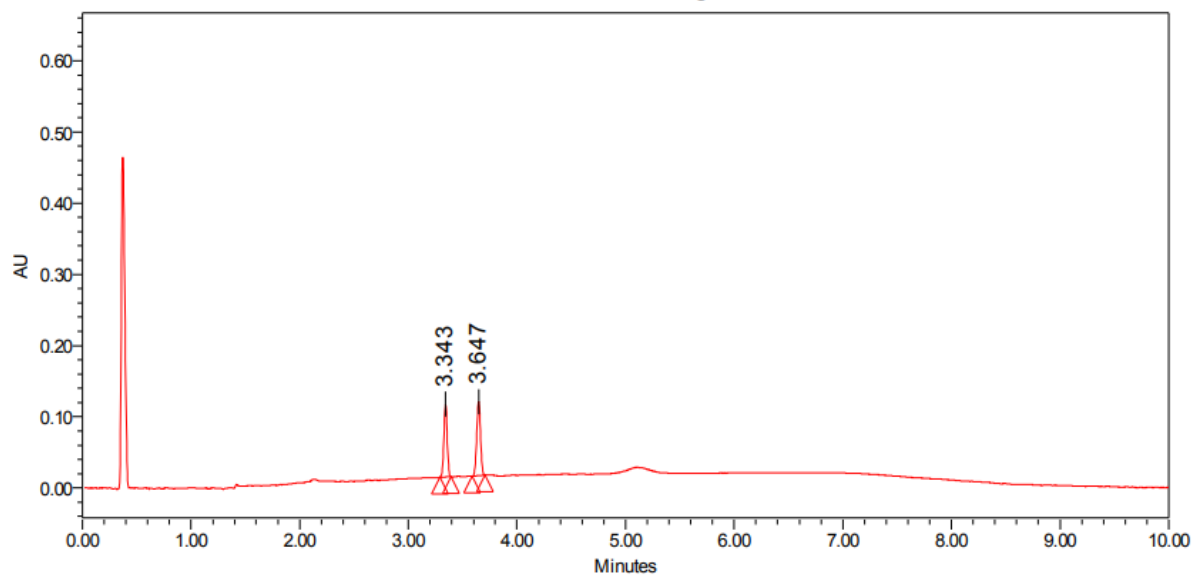
Enantiomerically enriched sample



Peak Results

	RT	% Area
1	3.344	93.06
2	3.650	6.94

Racemic sample

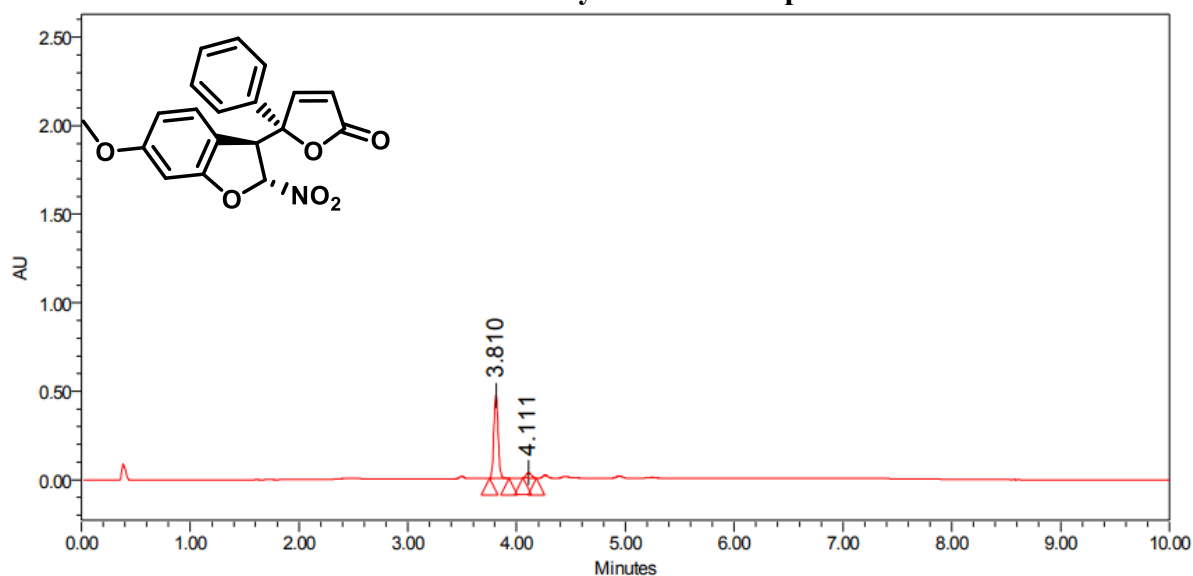


Peak Results

	RT	% Area
1	3.343	46.01
2	3.647	53.99

(*R*)-5-((2*R*,3*S*)-6-Methoxy-2-nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(*5H*)-one
3h

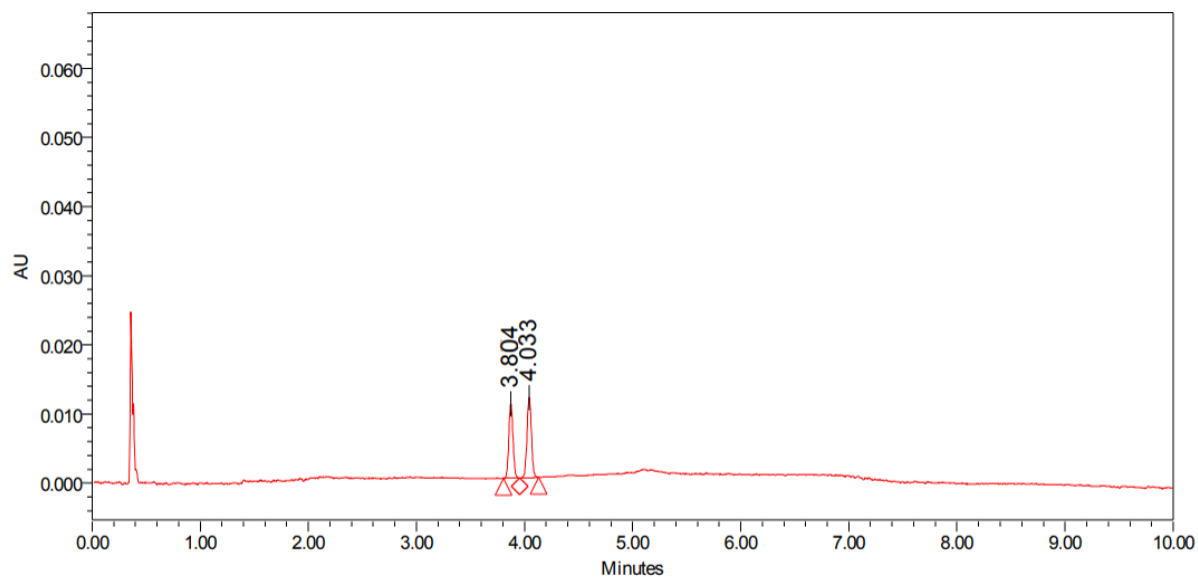
Enantiomerically enriched sample



Peak Results

	RT	% Area
1	3.810	92.77
2	4.111	7.23

Racemic sample

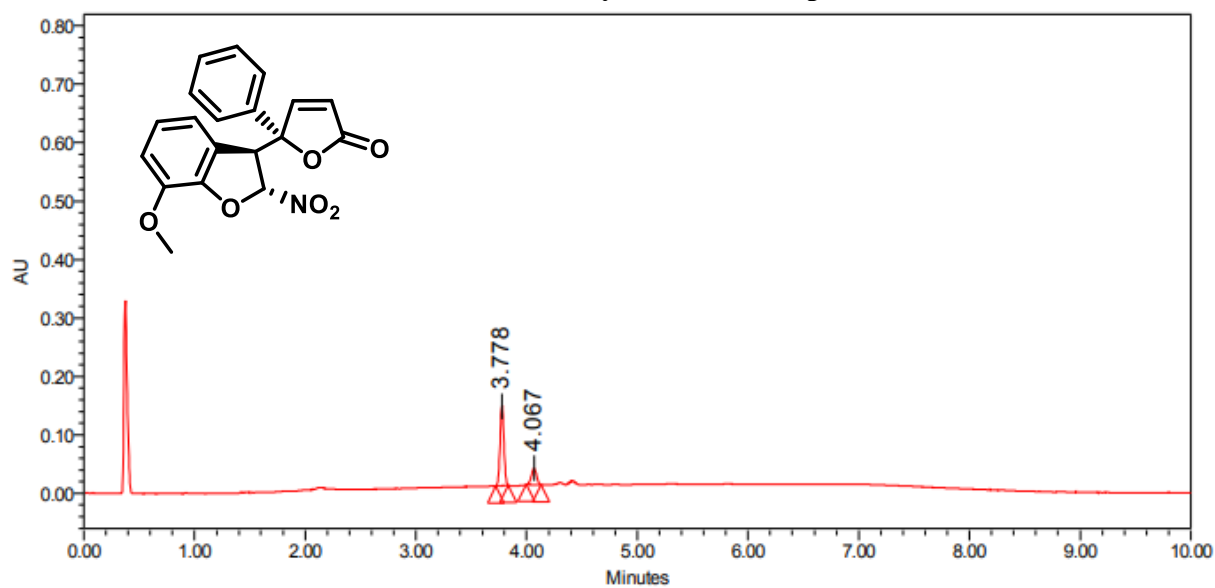


Peak Results

	RT	% Area
1	3.804	54.17
2	4.033	45.83

(*R*)-5-((2*R*,3*S*)-7-Methoxy-2-nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(*5H*)-one
3i

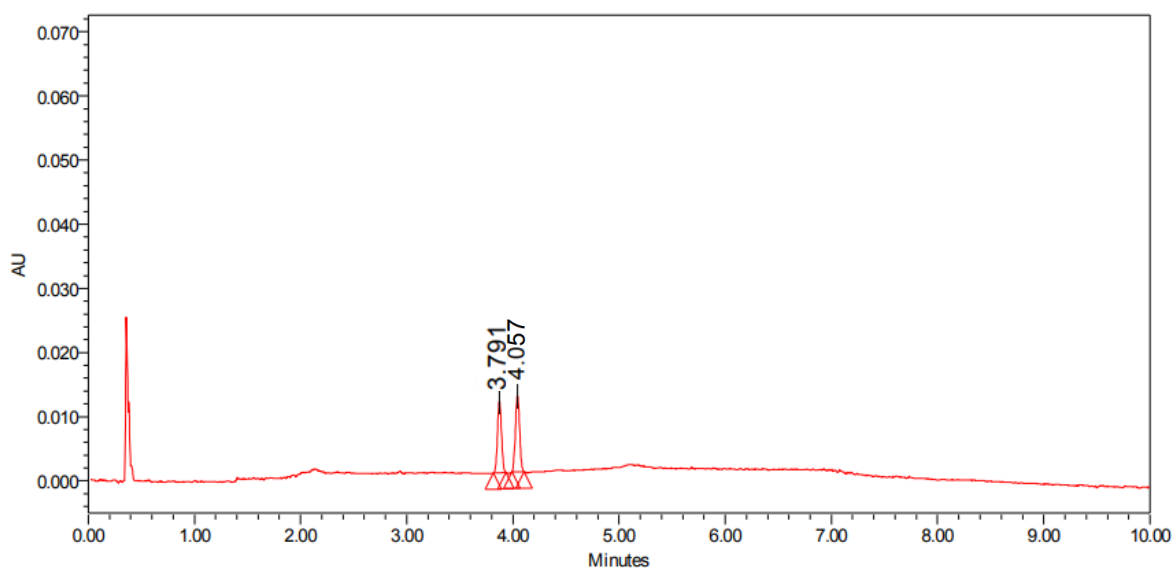
Enantiomerically enriched sample



Peak Results

	RT	% Area
1	3.778	78.48
2	4.067	21.52

Racemic sample

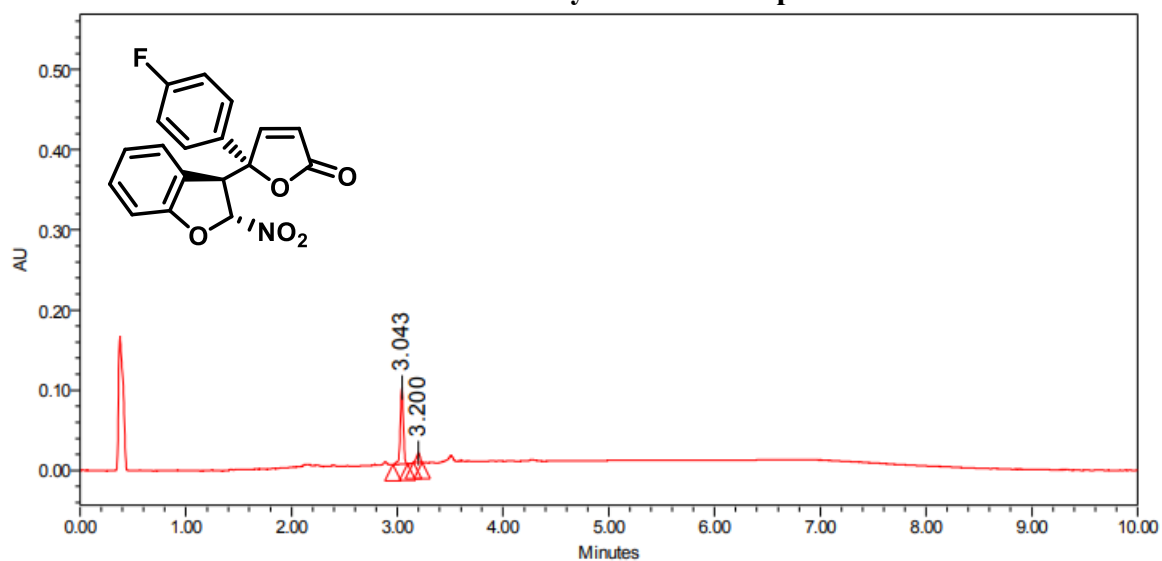


Peak Results

	RT	% Area
1	3.791	47.30
2	4.057	52.70

(*R*)-5-(4-Fluorophenyl)-5-((2*R*,3*S*)-2-nitro-2,3-dihydrobenzofuran-3-yl)furan-2(*5H*)-one
3j

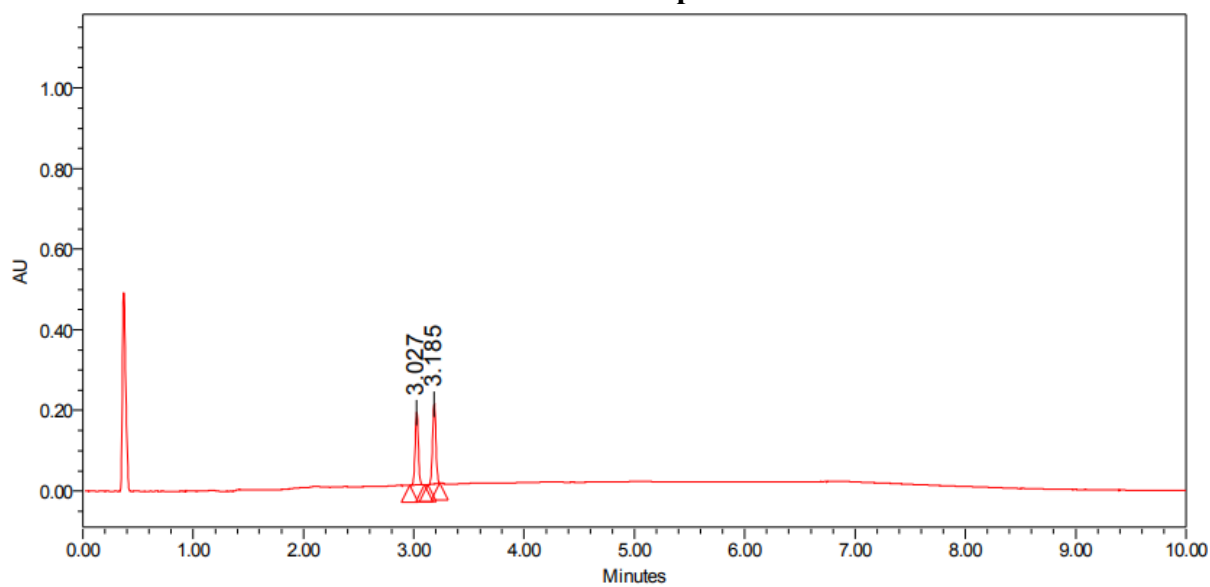
Enantiomerically enriched sample



Peak Results

	RT	% Area
1	3.043	87.03
2	3.200	12.97

Racemic sample

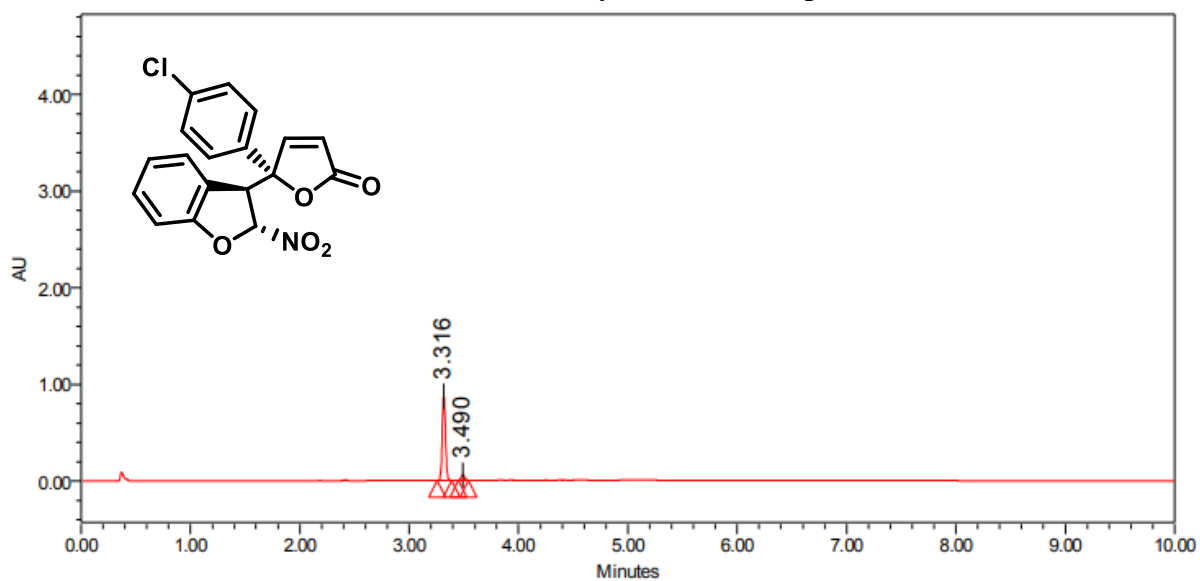


Peak Results

	RT	% Area
1	3.027	46.33
2	3.185	53.67

(*R*)-5-(4-Chlorophenyl)-5-((2*R*,3*S*)-2-nitro-2,3-dihydrobenzofuran-3-yl)furan-2(*5H*)-one
3k

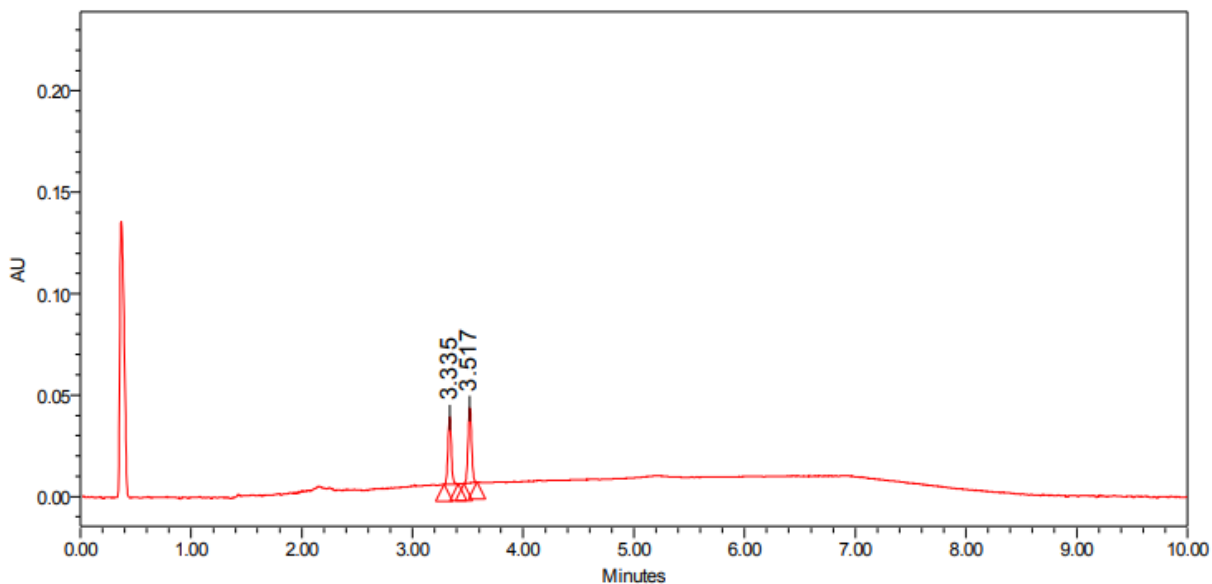
Enantiomerically enriched sample



Peak Results

	RT	% Area
1	3.316	93.93
2	3.490	6.07

Racemic sample

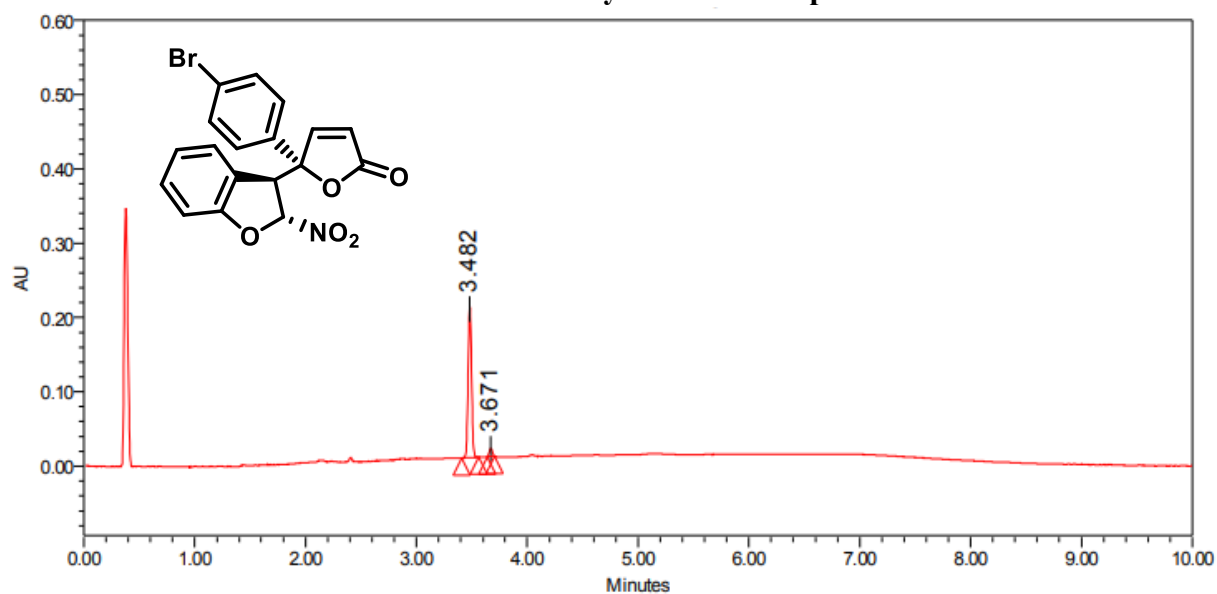


Peak Results

	RT	% Area
1	3.335	45.16
2	3.517	54.84

(*R*)-5-(4-Bromophenyl)-5-((2*R*,3*S*)-2-nitro-2,3-dihydrobenzofuran-3-yl)furan-2(*5H*)-one
3l

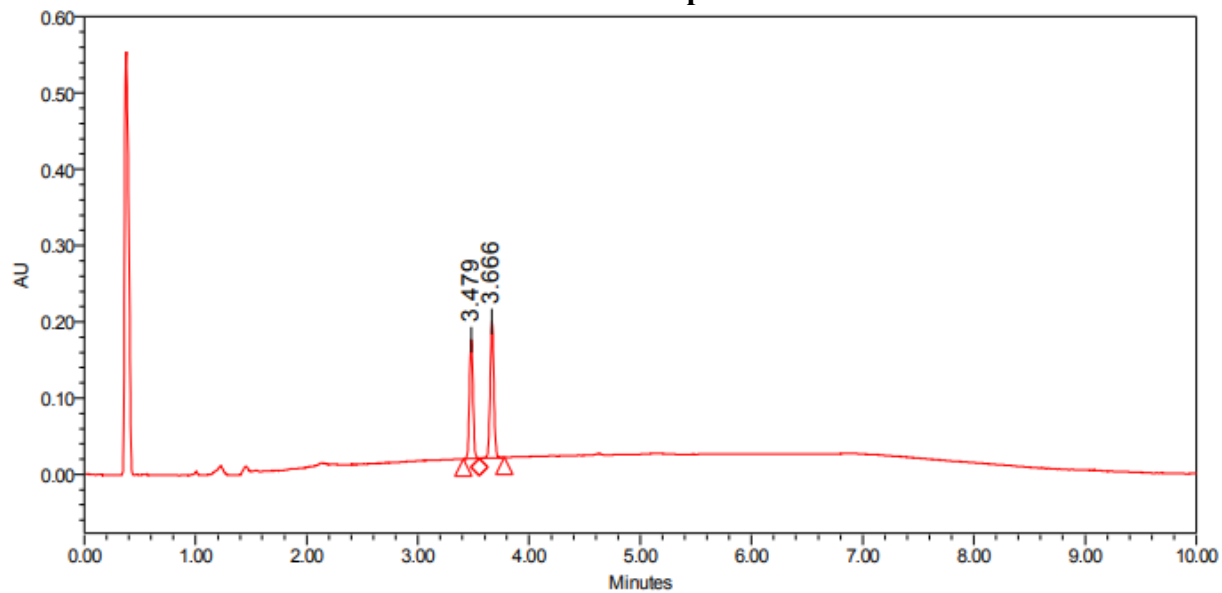
Enantiomerically enriched sample



Peak Results

	RT	% Area
1	3.482	95.04
2	3.671	4.96

Racemic sample

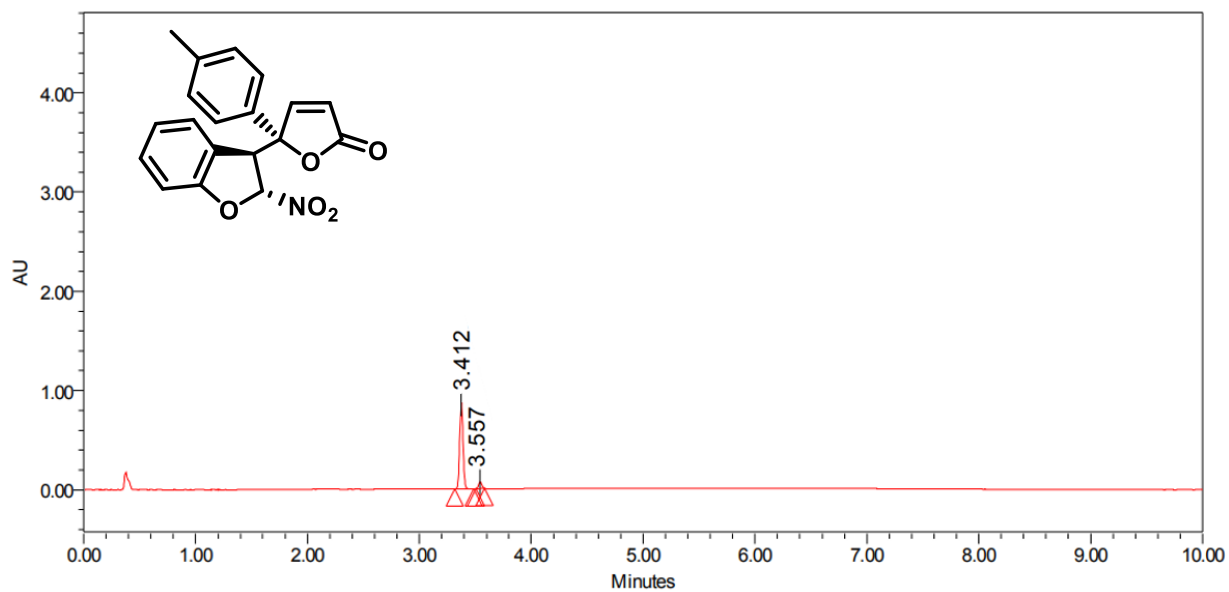


Peak Results

	RT	% Area
1	3.479	44.31
2	3.666	55.69

(*R*)-5-((2*R*,3*S*)-2-Nitro-2,3-dihydrobenzofuran-3-yl)-5-(*p*-tolyl)furan-2(*5H*)-one 3m

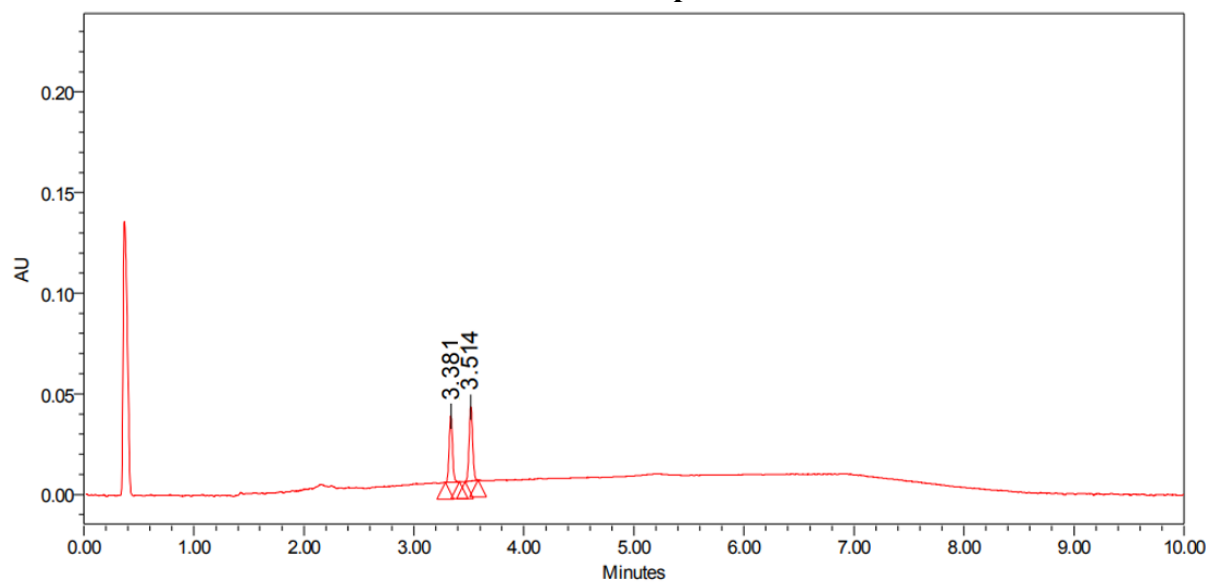
Enantiomerically enriched sample



Peak Results

	RT	% Area
1	3.412	97.24
2	3.557	2.76

Racemic sample

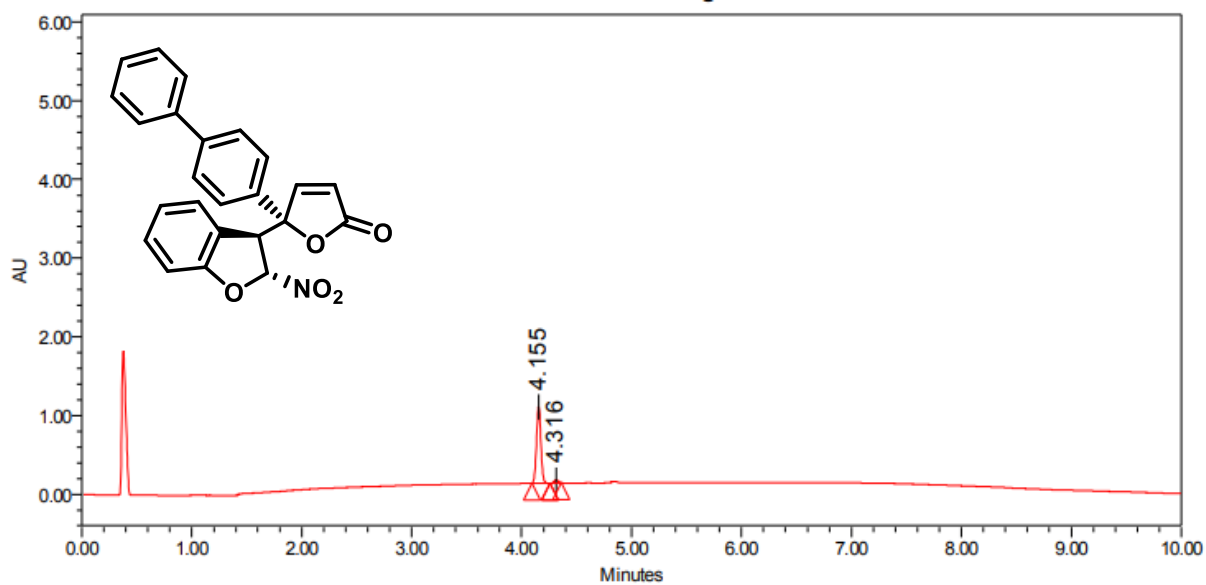


Peak Results

	RT	% Area
1	3.381	56.06
2	3.514	43.94

(*R*)-5-([1,1'-Biphenyl]-4-yl)-5-((2*R*,3*S*)-2-nitro-2,3-dihydrobenzofuran-3-yl)furan-2(*5H*)-one 3n

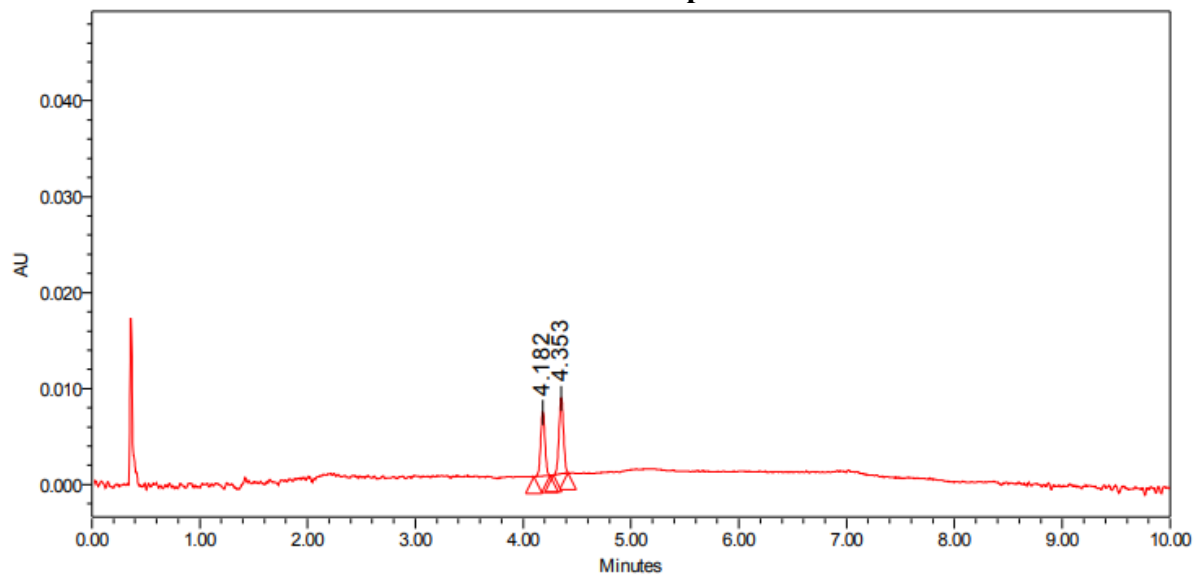
Enantiomerically enriched sample



Peak Results

	RT	% Area
1	4.155	96.40
2	4.316	3.60

Racemic sample

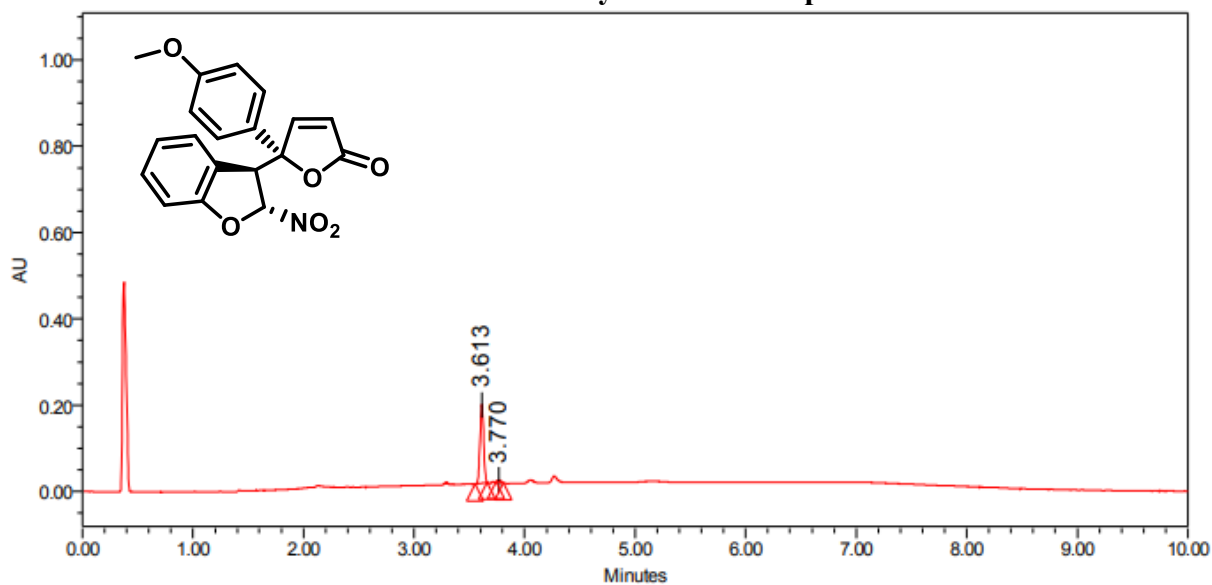


Peak Results

	RT	% Area
1	4.182	44.83
2	4.353	55.17

(*R*)-5-(4-Methoxyphenyl)-5-((2*R*,3*S*)-2-nitro-2,3-dihydrobenzofuran-3-yl)furan-2(5*H*)-one 3o

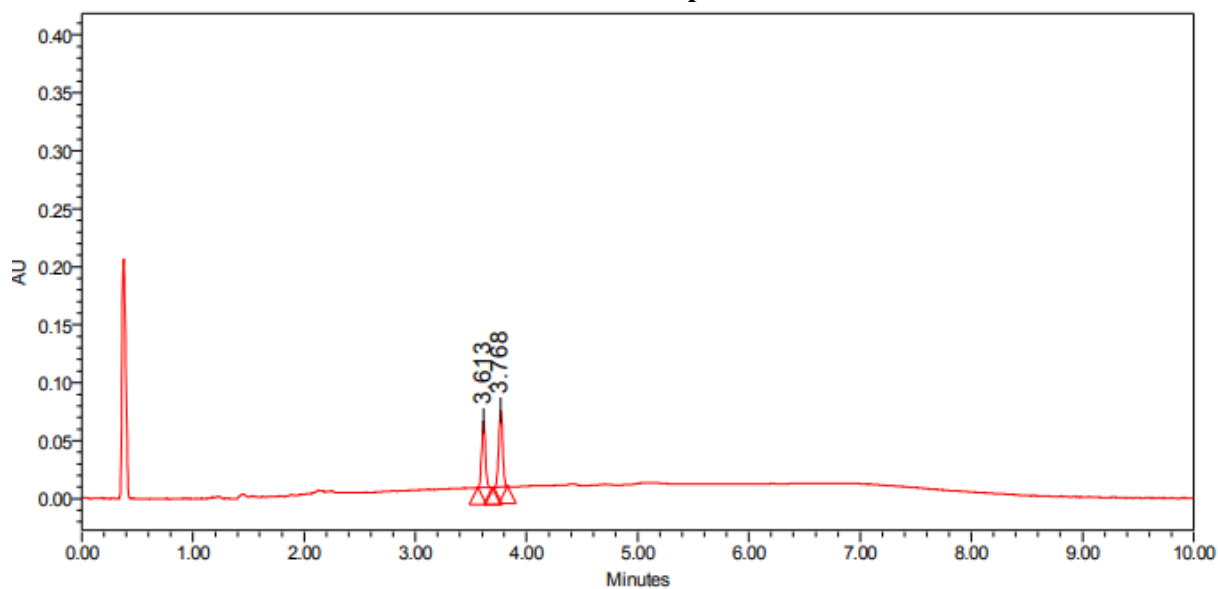
Enantiomerically enriched sample



Peak Results

	RT	% Area
1	3.613	96.94
2	3.770	3.06

Racemic sample

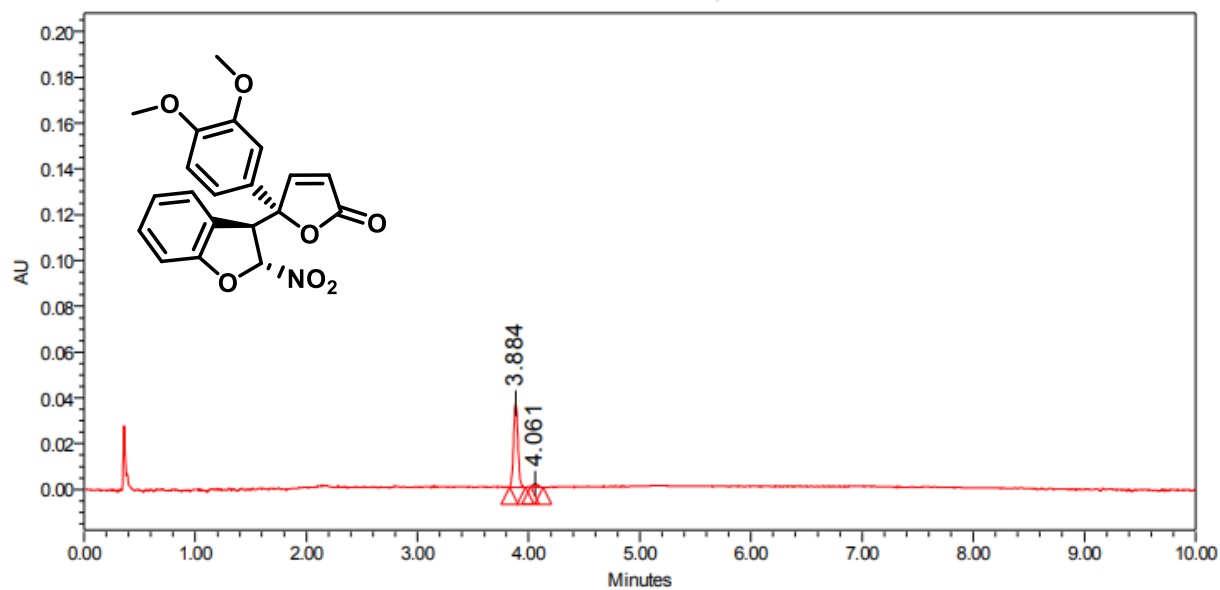


Peak Results

	RT	% Area
1	3.613	44.58
2	3.768	55.42

(*R*)-5-(3,4-Dimethoxyphenyl)-5-((2*R*,3*S*)-2-nitro-2,3-dihydrobenzofuran-3-yl)furan-2(*5H*)-one 3p

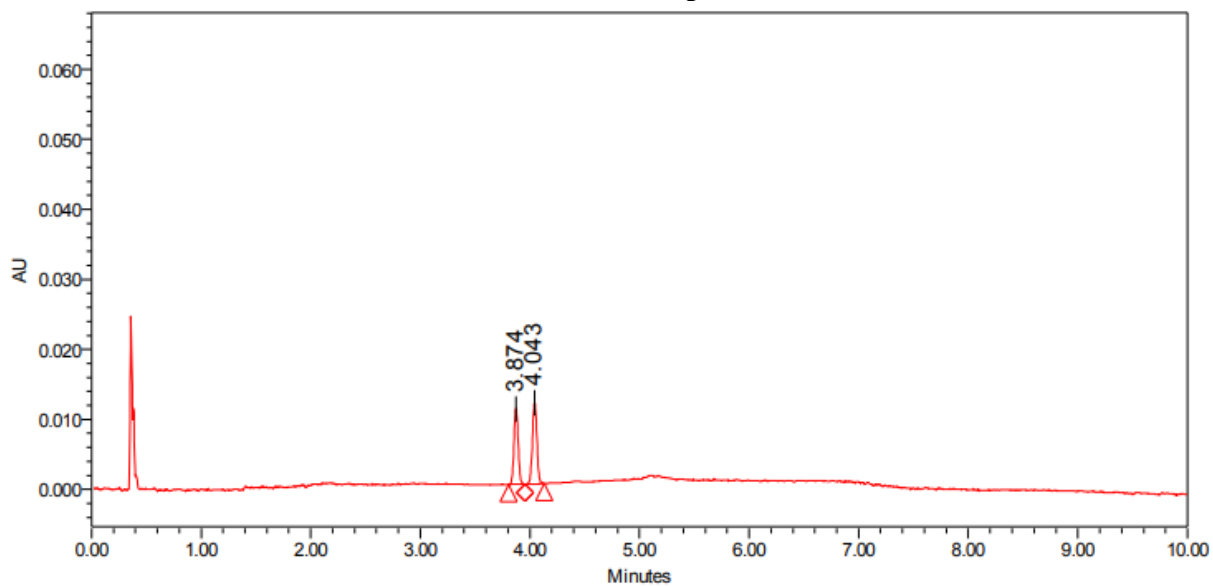
Enantiomerically enriched sample



Peak Results

	RT	% Area
1	3.884	96.07
2	4.061	3.93

Racemic sample

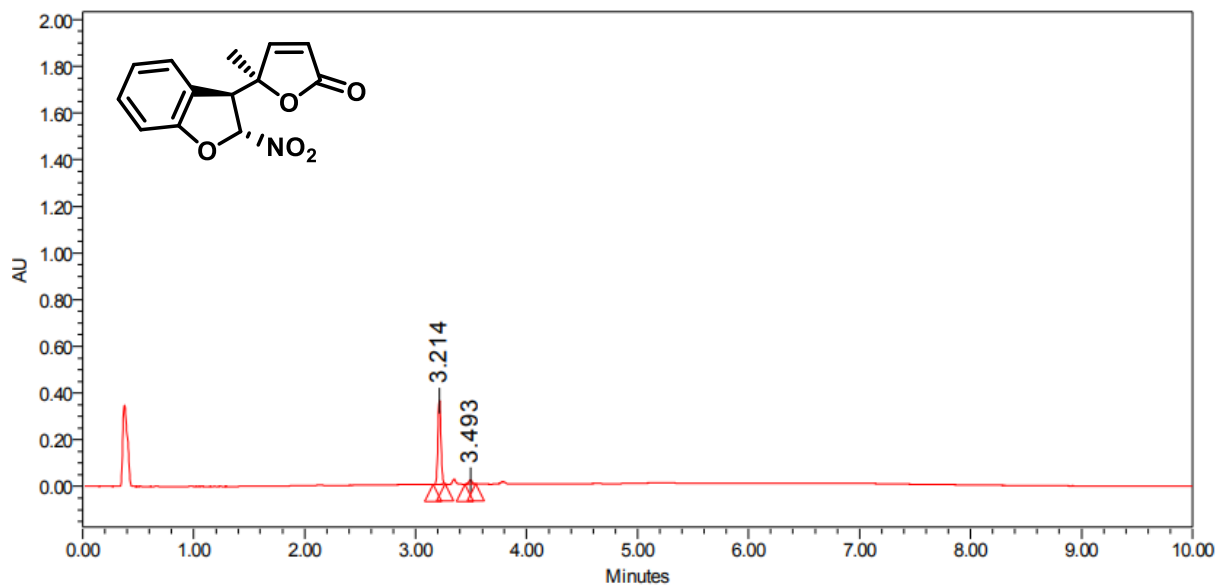


Peak Results

	RT	% Area
1	3.874	46.53
2	4.043	53.47

(*R*)-5-Methyl-5-((2*R*,3*S*)-2-nitro-2,3-dihydrobenzofuran-3-yl)furan-2(5*H*)-one 3r

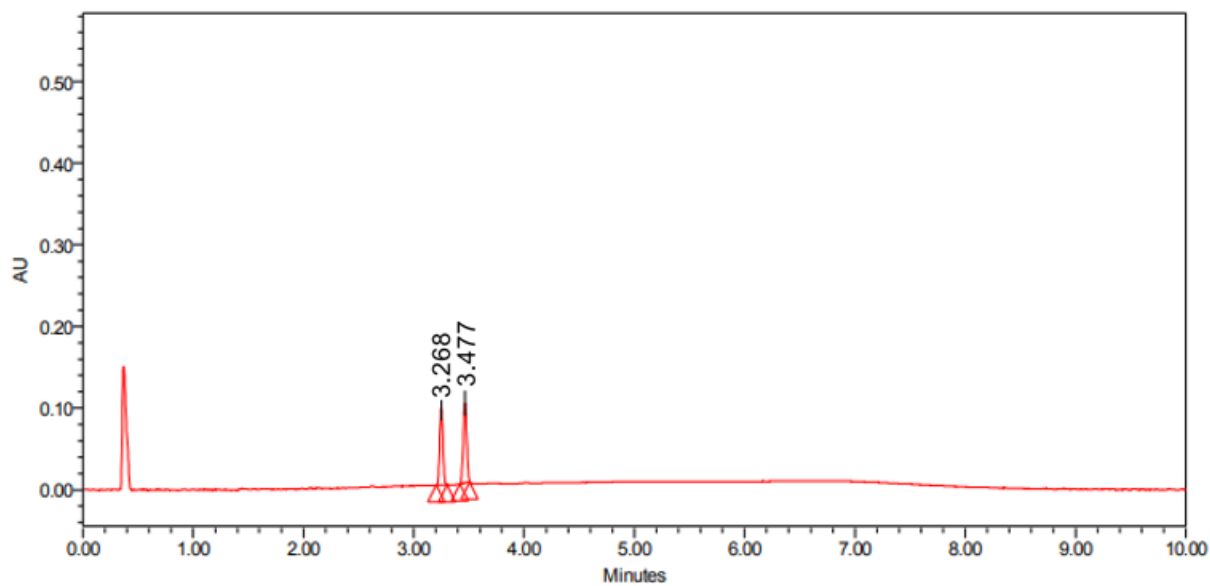
Enantiomerically enriched sample



Peak Results

	RT	% Area
1	3.214	95.08
2	3.493	4.92

Racemic sample

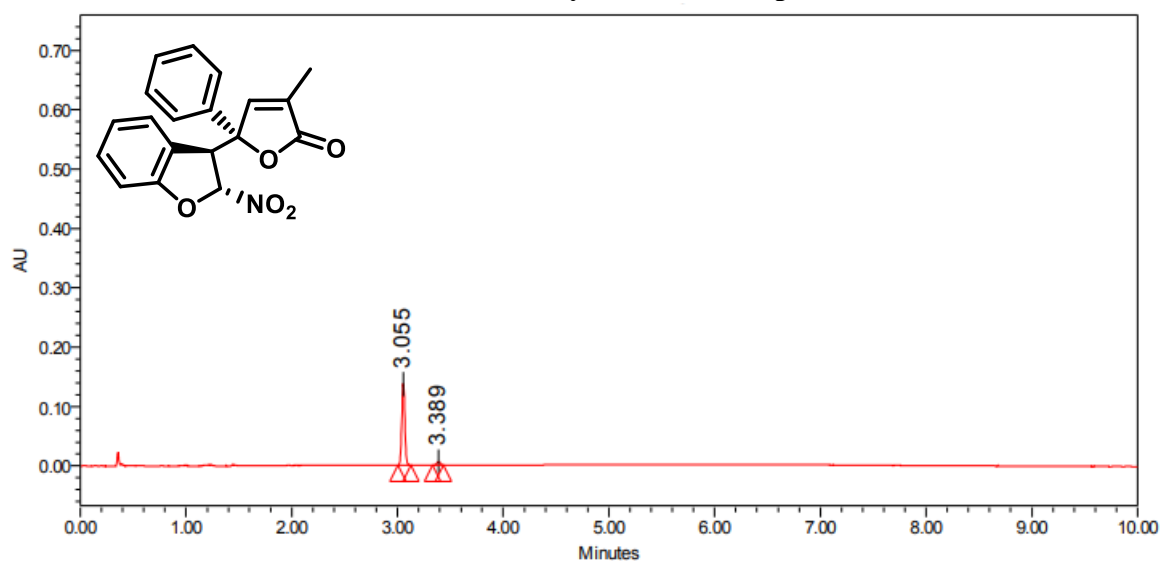


Peak Results

	RT	% Area
1	3.268	44.17
2	3.477	55.83

(*R*)-3-Methyl-5-((2*R*,3*S*)-2-nitro-2,3-dihydrobenzofuran-3-yl)-5-phenylfuran-2(*5H*)-one
3s

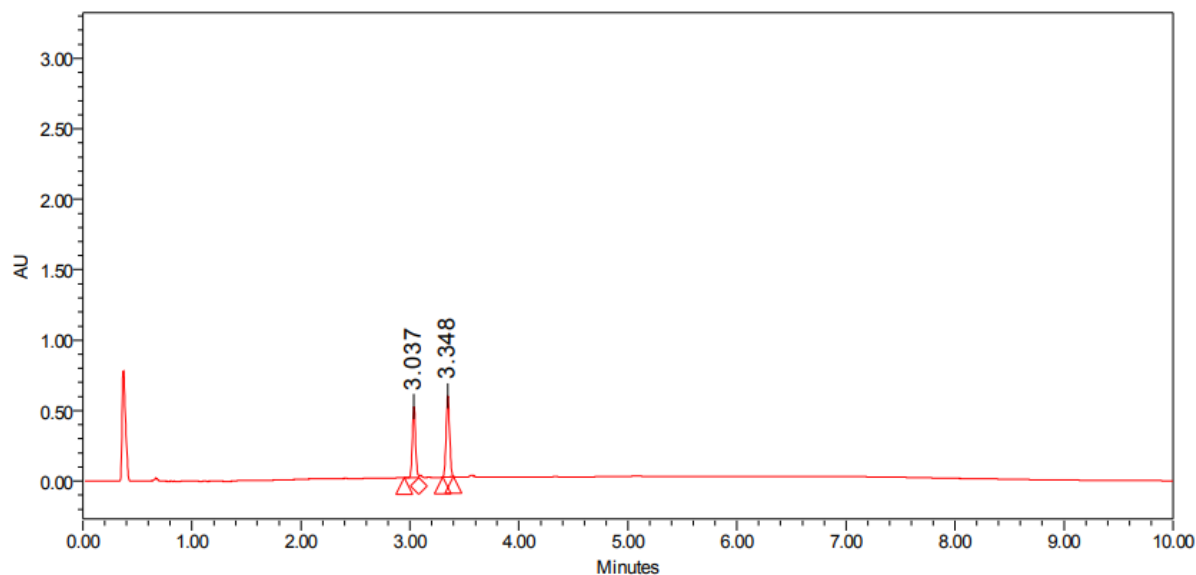
Enantiomerically enriched sample



Peak Results

	RT	% Area
1	3.055	95.49
2	3.389	4.51

Racemic sample



Peak Results

	RT	% Area
1	3.037	44.38
2	3.348	55.62