

A vinylogous Michael reaction of 2-Furanones Dimers to α , β -unsaturated nitroolefins for constructing chiral γ,γ -disubstituted butenolides†

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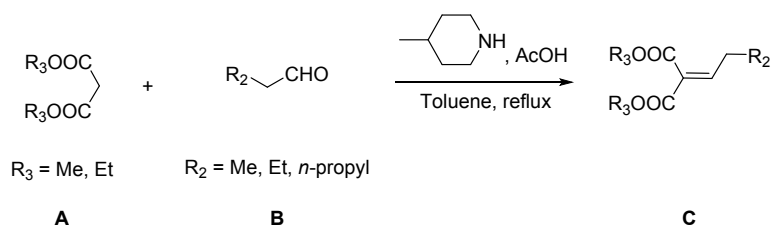
1. General methods

¹H NMR spectra and ¹³C NMR spectra were recorded on a Bruker AVANCE III 400 (400MHz) or Bruker AVANCE III 600 (600MHz) spectrometer in needful D-reagents with tetramethylsilane (TMS) as an internal reference. Data for ¹H NMR were reported as follows: chemical shift (ppm), and multiplicity (s= singlet, d= doublet, t= triplet, dd= double of doublet, br= broad, m= multiplet), coupling constants (Hz) and integration; Data for ¹³C NMR were reported as ppm. HPLC analyses were performed using a Lux 5u Cellulose-2 purchased, . HRMS of vinylogous Michael products were carried out Bruker Apex IV FTMS.

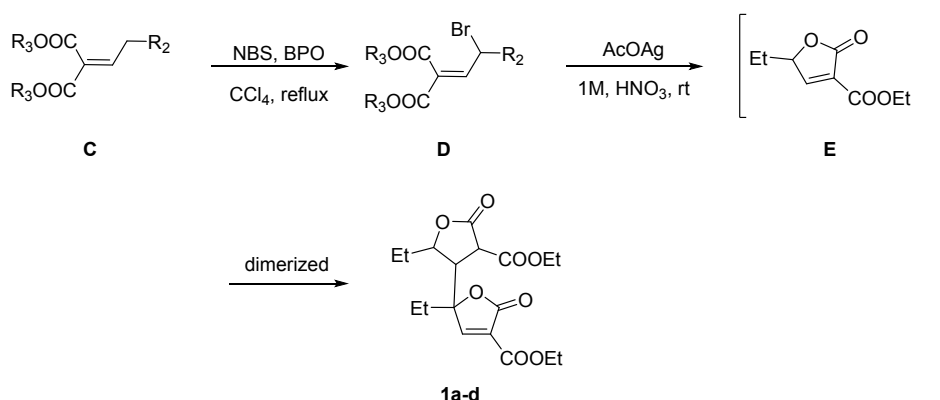
1.1 Materials

Unless otherwise stated, all reagents were purchased from commercial suppliers and were used, including catalysts **IV**, **V** and **VI**. Catalysts **I** [1], **II** [1], **III** [2] and **VII**[3] were prepared to literature procedures and all the spectral data matches with the desire compounds. α , β -Unsaturated nitroalkenes **2a-x**, were prepared accordingly to standard literature procedures[4]. Reactions were monitored by thin layer chromatography (TLC) on GF254 silica gel plates.

Dimeric 2-Furanones **1a-d** were prepared according to following procedures .



To the solution of diethylmalonate **A** (1.0 mol) in toluene (500mL) was added 4-methylpiperidine (0.156 mol) and acetic acid (20mL). While the mixture was heated to reflux with a water segregator, Aldehyde **B** (1.2 mol) was added in 12 batches within 2 hours. After extra 6 hours of reflux, the mixture was cooled down and then diluted with ethyl acetate (500mL) . The solution was washed with H₂O(500mL), 10% (w/w) NaHCO₃ solution (500mL) and saturated NaCl solution (500mL) successively, dried over anhydrous Na₂SO₄ and concentrated in vacuo. The residue was purified by silica gel chromatography (EA:PE=1:20) to afford **C** (yield 81.2%-92.5%) as colorless oil.

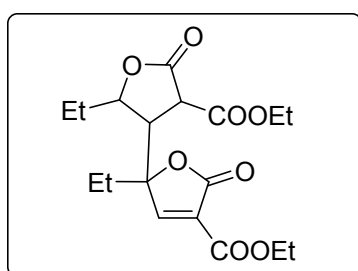


To the solution of **C** (100 mmol) obtained from previous steps in CCl₄ (100 mL) was added NBS (250 mmol) and benzoyl peroxide (2 mg). After 4 hours' reflux, the reaction mixture was cooled down and concentrated on a rotary evaporator. The residue was diluted with mL mixed solvent (petroleum ether:

ethyl acetate = 10:1, 200 mL) and the suspension was filtered. The filtrate was concentrated in vacuo to give crude product **D** which was used in the next step directly. Crude product **D** and AcOAg (100 mmol) were stirred in 1M dilute HNO₃ (200 mL) away from light under room temperature for 36 hours. The reaction mixture was diluted with ethyl acetate (250 mL) and the suspension was filtered. The solution was washed with H₂O(250mL), 10% (w/w) NaHCO₃ solution (250mL) and saturated NaCl solution (250mL) successively, dried over anhydrous Na₂SO₄ and concentrated in vacuo. The residue was purified by silica gel chromatography (EA:PE=1:4)to afford **1a-d** (39.1%-47.1% for 2 steps) as white solid or colorless oil.

ethyl 5-(4-(ethoxycarbonyl)-2-ethyl-5-oxotetrahydrofuran-3-yl)-5-ethyl-2-oxo-2,5-dihydrofuran-3-carboxylate(1a):

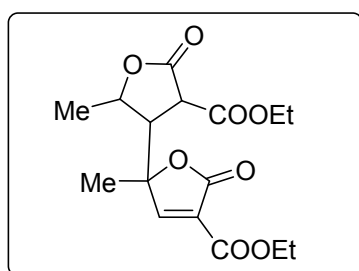
Obtained in 38% yield; Light yellow oil; purified by silica gel column chromatography(EA/Petroleum =



1:4); ¹H NMR (400 MHz, CDCl₃) δ (ppm):δ 7.97 (s, 1H), 7.92 (s, 2H), 4.42 – 4.39 (m, 1H), 4.35 (ddd, *J* = 9.5, 7.3, 3.8 Hz, 7H), 4.26 (dd, *J* = 13.9, 6.8 Hz, 6H), 4.00 (td, *J* = 7.4, 4.3 Hz, 1H), 3.28 (d, *J* = 9.2 Hz, 2H), 3.20 (ddd, *J* = 13.3, 8.8, 7.2 Hz, 3H), 2.04 – 1.81 (m, 4H), 1.82 – 1.60 (m, 4H), 1.37 (ddd, *J* = 9.6, 7.1, 4.7 Hz, 6H), 1.29 (dd, *J* = 15.3, 8.2 Hz, 6H), 1.05 (dt, *J* = 24.7, 7.3 Hz, 6H),

0.87 (dd, *J* = 14.2, 7.1 Hz, 6H). ¹³C NMR (100 MHz, CDCl₃) δ 169.32, 168.91, 167.45, 166.95, 165.84, 165.60, 162.30, 162.14, 159.29, 159.24, 127.66, 127.57, 86.97, 86.79, 80.74, 79.62, 62.98, 62.30, 62.20, 49.21, 49.17, 48.46, 48.28, 29.54, 28.92, 28.82, 28.51, 14.09, 14.03, 14.00, 9.73, 9.62, 7.70, 7.53. HRMS (ESI): *m/z* calcd for C₁₈H₂₄O₈ (M+H)⁺: 369.1471. found: 369.1523.

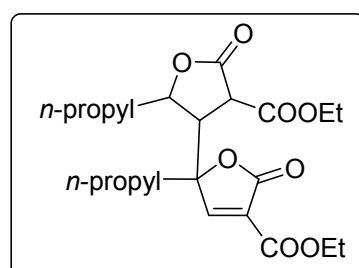
ethyl 5-(4-(ethoxycarbonyl)-2-methyl-5-oxotetrahydrofuran-3-yl)-5-methyl-2-oxo-2,5-dihydrofuran-3-carboxylate(1b):



Obtained in 29% yield; Light yellow oil; purified by silica gel column chromatography(EA/Petroleum = 1:5); ¹H NMR (400 MHz, DMSO) δ (ppm):δ 8.59 (s, 1H), 8.57 (s, 1H), 4.63 – 4.39 (m, 2H), 4.28 – 4.22 (m, 4H), 4.16 (dd, *J* = 7.1, 1.0 Hz, 4H), 3.93 (d, *J* = 9.5 Hz, 1H), 3.86 (d, *J* = 9.5 Hz, 1H), 3.12 – 3.08 (m, 1H), 3.05 (d, *J* = 7.7 Hz, 1H), 1.49 (s, 2H), 1.48 (s, 2H), 1.41 (d, *J* = 6.2 Hz,

3H), 1.39 – 1.39 (m, 3H), 1.37 (d, *J* = 6.2 Hz, 3H), 1.30 – 1.24 (m, 6H), 1.21 (dd, *J* = 7.1, 3.3 Hz, 6H). ¹³C NMR (100 MHz, DMSO) δ 170.5, 170.4, 168.2, 168.0, 166.1, 165.8, 165.7, 160.0, 159.9, 125.1, 125.0, 85.1, 85.0, 76.5, 75.8, 62.4, 61.6, 52.9, 52.2, 49.8, 49.4, 22.4, 22.0, 22.0, 21.5, 14.5, 14.4, 14.3, 14.2. HRMS (ESI): *m/z* calcd for C₁₆H₂₀O₈ (M+H)⁺:341.1158.found: 341.1202.

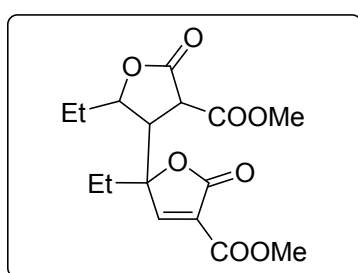
ethyl 5-(4-(ethoxycarbonyl)-5-oxo-2-propyltetrahydrofuran-3-yl)-2-oxo-5-propyl-2,5-dihydrofuran-3-carboxylate(1c):



Obtained in 15% yield; Light yellow oil; purified by silica gel

column chromatography(EA/Petroleum = 1:5); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ (ppm): δ 7.99 (s, 1H), 7.92 (s, 1H), 4.49 – 4.41 (m, 1H), 4.40 – 4.32 (m, 4H), 4.26 (ddd, $J = 13.1, 5.3, 3.8$ Hz, 4H), 4.09 – 3.92 (m, 1H), 3.77 (d, $J = 8.8$ Hz, 1H), 3.27 (d, $J = 9.2$ Hz, 1H), 3.22 – 3.17 (m, 1H), 3.16 – 3.08 (m, 1H), 1.91 – 1.69 (m, 6H), 1.67 – 1.44 (m, 6H), 1.42 – 1.33 (m, 8H), 1.32 – 1.13 (m, 8H), 0.98 (t, $J = 7.5$ Hz, 6H), 0.94 – 0.87 (m, 6H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 169.3, 168.9, 167.5, 167.0, 165.8, 165.6, 162.6, 162.4, 159.3, 159.3, 127.2, 127.2, 86.7, 86.4, 79.3, 78.1, 63.0, 62.9, 62.3, 62.2, 50.0, 49.2, 49.0, 48.3, 38.8, 38.1, 37.7, 37.4, 18.8, 18.7, 16.9, 16.7, 14.1, 14.1, 14.0, 13.9, 13.9, 13.7, 13.5. HRMS (ESI): m/z calcd for $\text{C}_{20}\text{H}_{28}\text{O}_8$ ($\text{M}+\text{H}$) $^+$: 397.1784. found: 397.1826.

methyl 5-ethyl-5-(2-ethyl-4-(methoxycarbonyl)-5-oxotetrahydrofuran-3-yl)-2-oxo-2,5-dihydrofuran-3-carboxylate(1d):



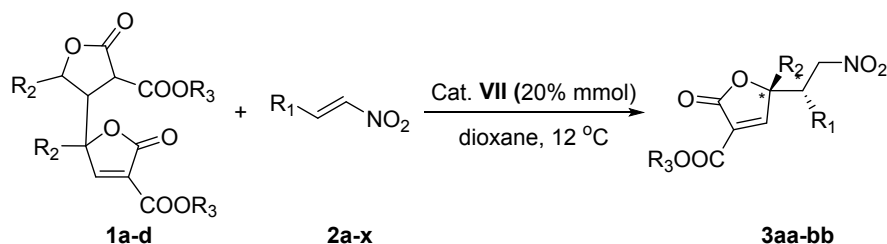
Obtained in 11% yield; Light yellow oil; purified by silica gel column chromatography(EA/Petroleum = 1:5); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ (ppm): δ 7.99 (s, 1H), 7.94 (s, 1H), 4.39 (td, $J = 7.7, 3.4$ Hz, 1H), 3.92 (s, 1H), 3.91 (s, 3H), 3.87 (s, 3H), 3.80 (d, $J = 7.1$ Hz, 3H), 3.78 (d, $J = 8.5$ Hz, 3H), 3.30 (d, $J = 8.9$ Hz, 1H), 3.20 (dd, $J = 15.8, 7.6$ Hz, 1H), 2.07 – 1.94 (m, 1H), 1.88 (dt, $J = 14.3, 6.4$ Hz, 2H), 1.81 – 1.69 (m, 1H), 1.66 (dd, $J = 16.6, 9.4$ Hz, 2H), 1.08 (t, $J = 7.3$ Hz, 4H), 1.02 (t, $J = 7.3$ Hz, 4H), 0.87 (t, $J = 7.4$ Hz, 6H), 0.86 – 0.81 (m, 6H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 168.7, 167.4, 162.6, 162.6, 159.7, 127.4, 87.1, 86.9, 80.8, 79.6, 53.8, 53.7, 53.0, 52.9, 49.1, 49.0, 48.4, 48.3, 29.6, 29.0, 28.9, 28.4, 9.7, 7.7, 7.5. HRMS (ESI): m/z calcd for $\text{C}_{16}\text{H}_{20}\text{O}_8$ ($\text{M}+\text{H}$) $^+$: 341.1158. found: 341.1195.

1.2 Reference:

- [1] C. B. Tripathi, S. Kayal and S. Mukherjee, *Org. Lett.*, 2012, **14**, 3296.
- [2] F. Yu, Z. Jin, H. Huang, T. Ye, X. Liang and J. Ye, *Org. Biomol. Chem.*, 2010, **8**, 4767.
- [3] M. S. Manna, V. Kumar and S. Mukherjee, *Chem. Commun.*, 2012, **48**, 5193.
- [4] (a) D. M. Mampreian and A. H. Hoveyda, *Org. Lett.*, 2004, **6**, 2829.; (b) X. Xia, K. Shu, Y. Ji, A. Yang, X. Shaukat, Y. Liang, *J. Org. Chem.*, 2010, **75**, 2893.

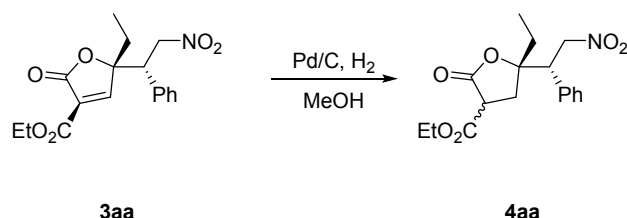
2. Synthesis and characterization of 3 and 4

2.1 General procedure for the vinylogous Michael reaction



To a solution of nitroalkenes **2a-x** (0.5 mmol) and catalyst **VII** (10% mol) in dioxane (2 mL) was added γ -butenolide **1a-d** (0.25 mmol) at 12 °C. The resulting solution was stirred at 12 °C for 24h. After removal of solvent under reduced pressure, the crude material was purified by silica gel column chromatography(Ethyl acetate/Petroleum = 1:5).

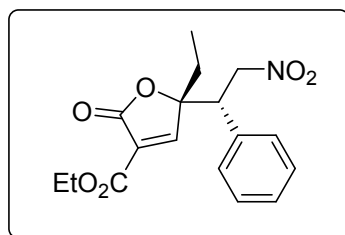
2.2 General procedure for synthetic transformation



The vinylogous Michael addition product **3aa**, 167 mg (0.5 mmol), was dissolved in 5 ml of methanol, 20% of Pd/C by wt. was added, and the mixture was stirred for 5 h under hydrogen with bubbling. When the initial compound disappeared (TLC), the mixture was filtered, and the filtrate was evaporated. the crude material was purified by silica gel column chromatography(Ethyl acetate/Petroleum = 1:5).

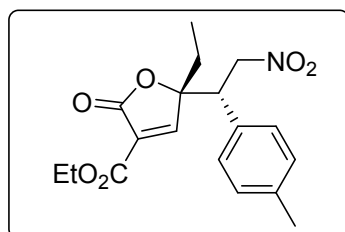
2.3 Scope of the vinylogous Michael reaction

(S)-ethyl 5-ethyl-5-((S)-2-nitro-1-phenylethyl)-2-oxo-2,5-dihydrofuran-3-carboxylate (**3aa**):



Obtained in 95% yield; Light yellow oil; purified by silica gel column chromatography(EA/Petroleum = 1:5); ¹H NMR (400 MHz, CDCl₃) δ 7.88 (1 H, s), δ 7.39 – 7.28 (3 H, m), δ 7.20 – 7.15 (2 H, m), δ 4.85 (1 H, dd, J = 13.4, 5.0Hz), δ 4.76 (1 H, dd, J = 13.3, 10.0Hz), δ 4.27 (2 H, q, J = 7.1Hz), δ 4.11 (1 H, dd, J = 9.9, 5.0Hz), δ 2.02 (1 H, dq, J = 14.8, 7.4Hz), δ 1.85 (1 H, dq, J = 14.7, 7.4Hz), δ 1.31 (3 H, t, J = 7.1Hz), δ 0.88 (3 H, t, J = 7.4 Hz). ¹³C NMR (100 MHz, CDCl₃) δ 166.0, 162.9, 159.3, 133.7, 129.4, 129.0, 128.3, 127.0, 88.4, 75.2, 61.9, 49.6, 28.9, 14.0, 7.6. HPLC(Lux 5u Cellulose-2, hexane: i-PrOH = 80:20, 1.0mL/min, t_{R1} (major)=24.09 min, t_{R1} (minor)=44.04 min, t_{R2} (major)=49.90 min, t_{R2} (minor)=54.62min). dr=9.7:1. 92% ee. ES-HRMS: Calcd for C₁₇H₂₀NO₆ [M+H], 334.1285, Found 334.1292.

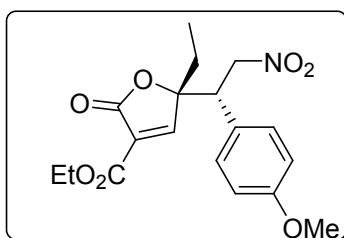
(S)-ethyl 5-ethyl-5-((S)-2-nitro-1-(p-tolyl)ethyl)-2-oxo-2,5-dihydrofuran-3-carboxylate (**3ab**):



Obtained in 94% yield ; Light yellow oil; purified by silica gel column chromatography (EA/Petroleum = 1:5); ¹H NMR (400

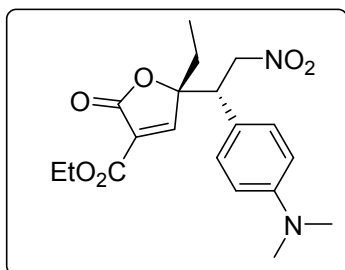
MHz, CDCl₃) δ 7.91 (1 H, s), δ 7.16 (2 H, d, J =7.9 Hz), δ 7.07 (2 H, d, J =8.0 Hz), δ 4.84 (1 H, dd, J =13.2, 5.0 Hz), δ 4.74 (1 H, dd, J =13.2, 10.1 Hz), δ 4.30 (2 H, q, J =7.1 Hz), δ 4.09 (1 H, dd, J =10.1, 5.0 Hz), δ 2.33 (3 H, s), δ 2.02 (1 H, td, J =14.5, 7.1 Hz), δ 1.85 (1 H, dq, J =14.8, 7.4 Hz), δ 1.33 (4 H, t, J =7.1 Hz), δ 0.89 (4 H, t, J =7.4 Hz). ¹³C NMR (100 MHz, CDCl₃) δ 166.0, 163.0, 159.4, 138.9, 130.5, 130.1, 128.2, 126.9, 88.6, 75.2, 61.9, 49.2, 28.9, 21.0, 14.0, 7.6. HPLC(Lux 5u Cellulose-2, hexane: i-PrOH =80:20, 1.0mL/min, t_{R1} (major)=27.961 min, t_{R1} (minor)=50.287 min, t_{R2} (major)=52.843 min, t_{R2} (minor)=65.880min). dr=7.2:1. 92% ee. ES-HRMS: Calcd for C₁₈H₂₂NO₆ [M+H], 348.1442, Found 348.1448.

(S)-ethyl-5-ethyl-5-((S)-1-(4-methoxyphenyl)-2-nitroethyl)-2-oxo-2,5-dihydrofuran-3-carboxylate (3ac):



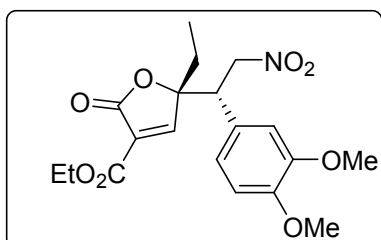
Obtained in 92% yield; Light yellow oil; purified by silica gel column chromatography (EA/Petroleum = 1:5); ¹H NMR (400 MHz, CDCl₃) δ 7.92 (1 H, s), δ 7.11 (2 H, d, J =8.6 Hz), δ 6.88 (2 H, d, J =8.6 Hz), δ 4.84 (1 H, dd, J =13.1, 4.9 Hz), δ 4.73 (1 H, dd, J =13.1, 10.3 Hz), δ 4.30 (2 H, dd, J =13.7, 6.7 Hz), δ 4.08 (1 H, dd, J =10.5, 5.1 Hz), δ 2.02 (1H, td, J =14.6, 7.2 Hz), δ 1.87 (1 H, td, J =14.8, 7.4 Hz), δ 1.34 (3H, t, J =7.1 Hz), δ 0.90 (3 H, t, J =7.4 Hz). ¹³C NMR (100 MHz, CDCl₃) δ 166.1, 163.23, 159.9, 132.3, 129.4, 125.4, 114.8, 113.8, 88.7, 75.4, 62.0, 55.3, 48.8, 28.8, 14.0, 7.7. HPLC(Lux 5u Cellulose-2, hexane: i-PrOH =80:20, 1.0mL/min, t_R (major)=78.736 min, t_{R2} (minor)=94.351 min). dr=12.5:1. 91% ee. ES-HRMS: Calcd for C₁₈H₂₂NO₇ [M+H], 364.1391, Found 364.1397.

ethyl (S)-5-((S)-1-(4-(dimethylamino)phenyl)-2-nitroethyl)-5-ethyl-2-oxo-2,5-dihydrofuran-3-carboxylate (3ad):



Obtained in 89% yield; Light yellow oil; purified by silica gel column chromatography (EA/Petroleum = 1:5); ¹H NMR (400 MHz, CDCl₃) δ 7.94 (s, 1H), 7.01 (d, J =8.8 Hz, 2H), 6.64 (d, J =8.8 Hz, 2H), 4.77 (dd, J =13.0, 5.0 Hz, 1H), 4.66 (dd, J =12.8, 10.5 Hz, 1H), 4.30 (q, J =7.1 Hz, 2H), 4.02 (dd, J =10.3, 5.0 Hz, 1H), 2.93 (s, 6H), 2.02 – 1.93 (m, 1H), 1.87 – 1.77 (m, 1H), 1.33 (t, J =7.1 Hz, 3H), 0.86 (t, J =7.4 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 165.2, 163.5, 162.6, 158.5, 149.5, 149.5, 128.9, 128.0, 125.7, 119.3, 119.1, 111.6, 111.4, 88.3, 88.2, 74.8, 74.4, 61.0, 60.9, 48.1, 47.9, 39.3, 39.2, 28.7, 27.9, 13.1, 13.1, 6.6, 6.4. HPLC(CHIRAL-OD-H, 259nm, hexane: i-PrOH =85:15, 2.0mL/min, t_{R1} (major) = 13.598 min, t_{R1} (minor) = 16.113 min, t_{R2} (minor) = 19.163 min, t_{R2} (major) = 25.232 min). dr=9.1:1. 91 % ee. ES-HRMS: Calcd for C₁₉H₂₄N₂NaO₆ [M+Na], 399.1532, Found 399.1508.

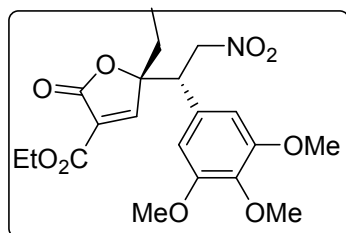
ethyl (S)-5-((S)-1-(3,4-dimethoxyphenyl)-2-nitroethyl)-5-ethyl-2-oxo-2,5-dihydrofuran-3-carboxylate(3ae):



Obtained in 95% yield; Light yellow oil; purified by silica gel column chromatography (EA/Petroleum = 1:5); major diastereoisomer: ¹H NMR (400 MHz, CDCl₃) δ 7.89 (s, 1H), 6.88 – 6.76 (m, 2H), 6.64 (d, J =2.1 Hz, 1H), 4.87 (dd, J =13.2,

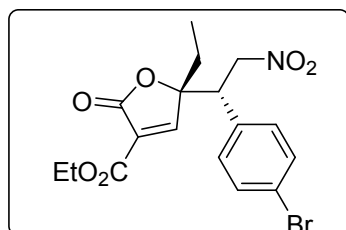
4.9 Hz, 1H), 4.77 (dd, $J = 13.2, 10.2$ Hz, 1H), 4.27 (q, $J = 7.1$ Hz, 2H), 4.02 (dd, $J = 10.3, 5.1$ Hz, 1H), 3.86 (s, 3H), 3.85 (s, 3H), 2.02 (dt, $J = 14.9, 7.4$ Hz, 1H), 1.93 (dt, $J = 14.4, 7.4$ Hz, 1H), 1.31 (t, $J = 7.1$ Hz, 3H), 0.90 (t, $J = 7.5$ Hz, 3H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 166.3, 163.5, 159.3, 149.5, 149.4, 126.6, 125.9, 120.7, 111.5, 111.0, 88.7, 75.5, 61.9, 56.1, 55.9, 49.0, 28.8, 14.0, 7.8. HPLC(CHIRAL-OJ-H, 210nm, hexane: i-PrOH =70:30, 2.0mL/min, t_{R1} (minor)=21.645 min, t_{R1} (major)=34.698 min). dr=8.3:1. 99% ee. ES-HRMS: Calcd for $\text{C}_{19}\text{H}_{24}\text{NO}_8$ [M+H], 394.1502, Found 394.1484.

ethyl (S)-5-ethyl-5-((S)-2-nitro-1-(3,4,5-trimethoxyphenyl)ethyl)-2-oxo-2,5-dihydrofuran-3-carboxylate(3af):



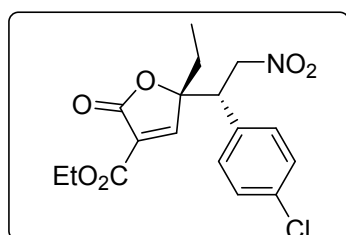
Obtained in 94% yield; Light yellow oil; purified by silica gel column chromatography (EA/Petroleum = 1:5); major diastereoisomer: $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.86 (s, 1H), 6.33 (s, 2H), 4.91 (dd, $J = 13.4, 4.9$ Hz, 1H), 4.81 (dd, $J = 13.4, 9.9$ Hz, 1H), 4.25 (q, $J = 7.1$ Hz, 2H), 3.99 (dd, $J = 9.9, 4.9$ Hz, 1H), 3.83 (s, 6H), 3.79 (s, 3H), 2.04 (dt, $J = 14.5, 7.2$ Hz, 1H), 1.97 (dt, $J = 14.4, 7.3$ Hz, 1H), 1.29 (t, $J = 7.1$ Hz, 3H), 0.92 (t, $J = 7.4$ Hz, 3H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 166.4, 163.2, 159.3, 153.8, 138.4, 129.3, 126.4, 105.2, 88.4, 75.4, 62.0, 60.9, 56.3, 49.4, 28.7, 14.0, 7.9. HPLC(CHIRAL-AD-H, 210nm, hexane: i-PrOH =90:10, 2.0mL/min, t_{R1} (minor)=12.764 min, t_{R1} (major)=315.663 min, t_{R2} (minor)=17.695 min, t_{R2} (minor)=18.697 min). dr=14.3:1. 97% ee. ES-HRMS: Calcd for $\text{C}_{20}\text{H}_{26}\text{NO}_9$ [M+H], 424.1608, Found 424.1583.

(S)-ethyl 5-((S)-1-(4-bromophenyl)-2-nitroethyl)-5-ethyl-2-oxo-2,5-dihydrofuran-3-carboxylate (3ag).



Obtained in 87% yield; Light yellow oil; purified by silica gel column chromatography (EA/Petroleum = 1:5); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.87 (1 H, s), δ 7.50 (2 H, d, $J = 7.8$ Hz), δ 7.08 (2 H, d, $J = 7.6$ Hz), δ 4.92 – 4.84 (1 H, m), δ 4.76 (1 H, t, $J = 11.9$ Hz), δ 4.30 (2 H, dd, $J = 13.6, 6.6$ Hz), δ 4.13 – 4.05 (1 H, m), δ 1.33 (3 H, t, $J = 7.1$ Hz), δ 0.91 (3 H, t, $J = 7.1$ Hz). $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 165.8, 162.6, 159.2, 132.6, 129.9, 127.2, 123.3, 110.0, 88.0, 75.0, 62.1, 48.9, 28.8, 14.0, 7.7. HPLC(CHIRAL-OD-H, hexane: i-PrOH =65:35, 254nm, 1.0mL/min, t_{R1} (major)=13.769 min, t_{R1} (minor)=15.381 min, t_{R2} (major)=22.234 min, t_{R2} (minor)=33.377min). dr=8.7:1. 92% ee. ES-HRMS: Calcd for $\text{C}_{17}\text{H}_{19}\text{BrNO}_6$ [M+H], 412.0390, Found 412.0400.

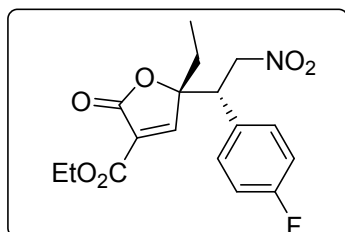
(S)-ethyl-5-((S)-1-(4-chlorophenyl)-2-nitroethyl)-5-ethyl-2-oxo-2,5-dihydrofuran-3-carboxylate (3ah)



Obtained in 90% yield; Light yellow oil; purified by silica gel column chromatography(EA/Petroleum = 1:5) ; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.88 (1 H, s), 7.37 – 7.32 (2 H, d, $J = 8.5$), 7.15 (2 H, d, $J = 8.5$ Hz), 4.89 (1 H, dd, $J = 13.5\text{Hz}, 4.9\text{Hz}$), 4.77 (1 H, dd, $J = 13.4$ Hz, 10.3 Hz), 4.30 (2 H, q, $J = 7.1$ Hz), 4.10 (1H, dd, $J = 10.3$ Hz, 4.8 Hz), 2.08 – 1.98 (1 H, m), 1.89 (1 H, m), 1.33 (3 H, t, $J = 7.1$ Hz), 0.91 (3 H, t, $J = 7.4$ Hz). $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 165.8,

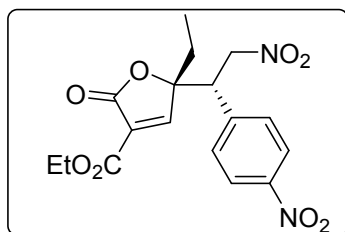
162.7, 159.2, 135.1, 132.2, 129.7, 129.6, 127.2, 88.1, 75.1, 62.1, 48.8, 28.8, 14.0, 7.7. HPLC(CHIRAL-OD-H, hexane: i-PrOH =80:20, 1.0mL/min, t_{R1} (major) = 19.70 min, t_{R1} (minor) = 21.73 min, t_{R2} (major) = 45.15 min, t_{R2} (minor) = 33.50 min). dr= 10.1:1. 88% ee. ES-HRMS: Calcd for $C_{17}H_{19}ClNO_6$ [M+H], 368.0895, Found 368.0903.

ethyl (S)-5-ethyl-5-((S)-1-(4-fluorophenyl)-2-nitroethyl)-2-oxo-2,5-dihydrofuran-3-carboxylate (3ai)



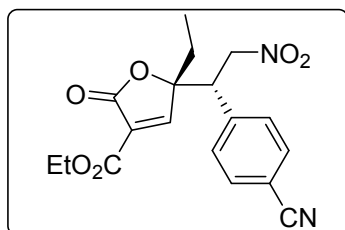
Obtained in 91% yield; Light yellow oil; purified by silica gel column chromatography(EA/Petroleum = 1:5) ; 1H NMR (400 MHz, $CDCl_3$) δ 7.86 (s, 1H), 7.20 – 7.13 (m, 2H), 7.05 (t, J = 8.5 Hz, 2H), 4.88 (dd, J = 13.4 Hz, 4.8 Hz, 1H), 4.76 (dd, J = 13.3 Hz, 10.3 Hz, 1H), 4.27 (q, J = 7.1 Hz, 2H), 4.09 (dd, J = 10.3Hz, 4.9 Hz, 1H), 2.02 (dq, J = 14.8 Hz, 7.4 Hz, 1H), 1.89 (dq, J = 14.7 Hz, 7.4 Hz, 1H), 1.31 (t, J = 7.1 Hz, 3H), 0.90 (t, J = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.9, 163.4(d, J = 122 Hz), 159.21, 130.1(d, J = 9 Hz), 127.1, 116.5(d, J = 21 Hz) , 88.3, 75.2, 62.1, 48.7, 28.8, 14.0, 7.7. HPLC(Lux 5u Cellulose-2, hexane: i-PrOH =80:20, 1.0mL/min, t_{R1} (major)=24.87 min, t_{R1} (minor)=41.67 min, t_{R2} (major)=43.68 min, t_{R2} (minor)=51.10 min). dr=19.2:1. 90%ee. ES-HRMS: Calcd for $C_{17}H_{19}FNO_6$ [M+H], 352.1191, Found 352.1197.

ethyl (S)-5-ethyl-5-((S)-2-nitro-1-(4-nitrophenyl)ethyl)-2-oxo-2,5-dihydrofuran-3-carboxylate (3aj):



Obtained in 89% yield; Light yellow oil; purified by silica gel column chromatography (EA/Petroleum = 1:5); 1H NMR (600 MHz, $CDCl_3$) δ 8.20 (d, J = 8.6 Hz, 1H), 7.86 (s, 1H), 7.39 (d, J = 8.7 Hz, 2H), 4.96 (dd, J = 13.8, 4.6 Hz, 1H), 4.85 (dd, J = 13.8, 10.4 Hz, 1H), 4.23 (q, J = 7.3 Hz, 1H), 4.20 (dd, J = 10.6, 4.8 Hz, 1H), 2.04 (td, J = 14.9, 7.5 Hz, 1H), 1.96 – 1.89 (m, 1H), 1.27 (t, J = 6.7 Hz, 3H), 0.91 (t, J = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.4, 162.6, 162.0, 140.9, 130.5, 129.4, 124.6, 124.4, 87.6, 74.8, 62.2, 49.0, 28.9, 14.0, 7.8. HPLC(CHIRAL-OD-H, hexane: i-PrOH =90:10, 1.0mL/min, t_{R1} (minor)=21.38 min, t_{R1} (major)=44.08 min). dr=5.0:1. 94% ee. ES-HRMS: Calcd for $C_{17}H_{19}N_2O_8$ [M+H], 379.1141, Found 379.1128.

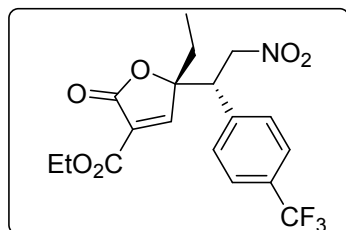
ethyl (S)-5-((S)-1-(4-cyanophenyl)-2-nitroethyl)-5-ethyl-2-oxo-2,5-dihydrofuran-3-carboxylate (3ak):



Obtained in 81% yield; Light yellow oil; purified by silica gel column chromatography (EA/Petroleum = 1:5); 1H NMR (600 MHz, $CDCl_3$) δ 7.83 (s, 1H), 7.66 (d, J = 8.4 Hz, 2H), 7.34 (d, J = 8.3 Hz, 2H), 4.94 (dd, J = 13.8, 4.6 Hz, 1H), 4.84 (dd, J = 13.7, 10.4 Hz, 1H), 4.27 (q, J = 7.1 Hz, 2H), 4.15 (dd, J = 10.4, 4.7 Hz, 1H), 2.04 (m, 1H), 1.93 (dq, J = 14.8, 7.4 Hz, 1H), 1.31 (t, J = 7.2 Hz, 3H), 0.92 (t, J = 7.4 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 165.5, 162.1, 158.8, 139.1, 133.2, 133.0, 129.2, 127.5, 87.7, 75.3, 62.3, 49.3, 28.8, 14.1, 7.8. HPLC(CHIRAL-OD-H, hexane: i-PrOH =70:30,

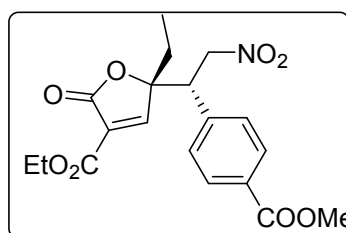
2.0mL/min, $t_{R1}(\text{major}) = 9.61$ min, $t_{R1}(\text{minor}) = 10.76$ min, $t_{R2}(\text{major}) = 13.02$ min, $t_{R2}(\text{minor}) = 18.25$ min). dr= 5.0:1. 84% ee. ES-HRMS: Calcd for $C_{18}H_{18}N_2NaO_6$ [M+Na], 381.1063, Found 381.1043.

ethyl (S)-5-ethyl-5-((S)-2-nitro-1-(4-(trifluoromethyl)phenyl)ethyl)-2-oxo-2,5-dihydrofuran-3-carboxylate (3al):



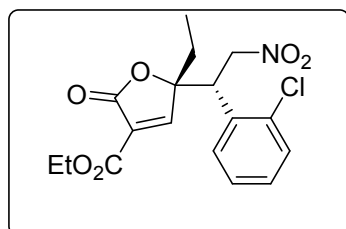
Obtained in 80% yield; Light yellow oil; purified by silica gel column chromatography (EA/Petroleum = 1:5); 1H NMR (600 MHz, $CDCl_3$) δ 7.83 (s, 1H), δ 7.61 (d, $J = 8.1$ Hz, 2H), 7.32 (d, $J = 8.1$ Hz, 2H), 4.91 (dd, $J = 13.6, 4.7$ Hz, 1H), 4.81 (dd, $J = 13.6, 10.3$ Hz, 1H), 4.27 – 4.22 (m, 2H), 4.16 (dd, $J = 10.3, 4.7$ Hz, 1H), 2.03 (dq, $J = 14.9, 7.5$ Hz, 1H), 1.88 (dq, $J = 14.8, 7.4$ Hz, 1H), 1.28 (t, $J = 7.2$ Hz, 3H), 0.90 (t, $J = 7.5$ Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 165.7, 163.1, 162.4, 159.2, 138.1, 137.9, 127.4, 126.5, 124.5, 88.0, 74.9, 62.2, 49.3, 28.9, 14.0, 7.8. HPLC(CHIRAL-OD-H, hexane: i-PrOH =65:35, 1.0mL/min, $t_{R1}(\text{major}) = 9.424$ min, $t_{R1}(\text{minor}) = 11.056$ min, $t_{R2}(\text{minor}) = 14.619$ min, $t_{R2}(\text{major}) = 22.735$ min). dr= 11.1:1. 89.0% ee. ES-HRMS: Calcd for $C_{18}H_{19}F_3NO_6$ [M+H], 402.1164, Found 402.1140.

ethyl (S)-5-ethyl-5-((S)-1-(4-(methoxycarbonyl)phenyl)-2-nitroethyl)-2-oxo-2,5-dihydrofuran-3-carboxylate (3am):

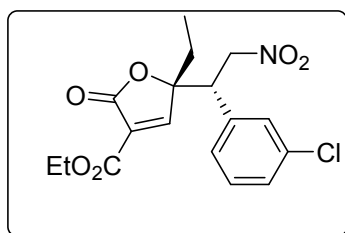


Obtained in 87% yield; Light yellow oil; purified by silica gel column chromatography (EA/Petroleum = 1:5); 1H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, $J = 8.3$ Hz, 2H), 7.87 (s, 1H), 7.28 (d, $J = 9.4$ Hz, 2H), 4.94 – 4.87 (m, 1H), 4.81 (dd, $J = 13.5, 10.1$ Hz, 1H), 4.26 (q, $J = 7.2$ Hz, 2H), 4.17 (dd, $J = 10.0, 4.9$ Hz, 1H), 3.92 (s, 3H), 2.08 – 1.98 (m, 1H), 1.94 – 1.83 (m, 1H), 1.30 (t, $J = 7.1$ Hz, 3H), 0.90 (t, $J = 7.5$ Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.2, 165.7, 162.5, 159.1, 138.7, 130.9, 130.6, 128.4, 127.2, 88.0, 74.9, 62.1, 52.4, 49.3, 29.0, 14.0, 7.7. HPLC(CHIRAL-OD-H, hexane: i-PrOH =65:35, 1.0mL/min, $t_{R1}(\text{minor}) = 16.302$ min, $t_{R1}(\text{major}) = 18.529$ min, $t_{R2}(\text{minor}) = 24.237$ min, $t_{R2}(\text{major}) = 32.231$ min). dr= 7.0:1. 89% ee. ES-HRMS: Calcd for $C_{19}H_{22}NO_8$ [M+H], 392.1345, Found 392.1320.

(S)-ethyl-5-((S)-1-(2-chlorophenyl)-2-nitroethyl)-5-ethyl-2-oxo-2,5-dihydrofuran-3-carboxylate (3an).



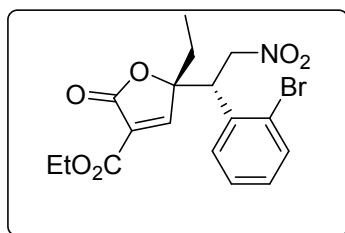
Obtained in 85% yield; Light yellow oil; purified by silica gel column chromatography (EA/Petroleum = 1:5); 1H NMR (400 MHz, $CDCl_3$) δ 8.03 (s, 1H), 7.44 – 7.33 (m, 2H), 7.27 – 7.23 (m, 2H), 5.05 – 4.88 (m, 2H), 4.47 – 4.31 (m, 1H), 4.28 – 4.18 (m, 2H), 2.12 – 2.05 (m, 2H), 1.28 (t, $J = 7.1$ Hz, 3H), 0.98 (t, $J = 7.4$ Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.1, 162.4, 159.1, 134.3, 131.7, 130.3, 130.1, 128.0, 127.8, 126.86, 88.55, 74.81, 61.82, 43.65, 28.49, 13.98, 8.01; HPLC(Lux 5u Cellulose-2, hexane: i-PrOH =80:20, 1.0mL/min, $t_{R1}(\text{major})=23.73$ min, $t_{R1}(\text{minor})=36.22$ min, $t_{R2}(\text{major})=45.00$ min, $t_{R2}(\text{minor})=66.87$ min). dr=9.5:1. 90% ee. ES-HRMS: Calcd for $C_{17}H_{19}ClNO_6$ [M+H], 368.0895, Found 368.0901.



(S)-ethyl-5-((S)-1-(3-chlorophenyl)-2-nitroethyl)-5-ethyl-2-oxo-2,5-dihydrofuran-3-carboxylate (3ao).

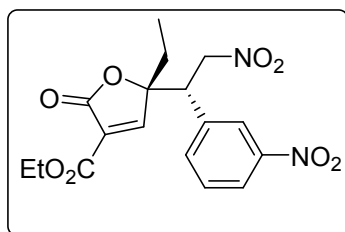
Obtained in 85% yield; Light yellow oil; purified by silica gel column chromatography (EA/Petroleum = 1:5); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.90 (1 H, s), δ 7.33 – 7.29 (2 H, m), δ 7.20 (1 H, s), δ 7.11 (1 H, dd, $J=6.0$ Hz, 2.4 Hz), δ 4.88 (1 H, dd, $J=13.6$ Hz, 4.8 Hz), δ 4.77 (1 H, dd, $J=13.5$ Hz, 10.2 Hz), δ 4.29 (2 H, dd, $J=14.3$ Hz, 7.1 Hz), δ 4.10 (1 H, dd, $J=10.1$ Hz, 4.8 Hz), δ 2.03 (1 H, dq, $J=14.8$ Hz, 7.4 Hz), δ 1.88 (1 H, dq, $J=14.7$ Hz, 7.4 Hz), δ 1.33 (3 H, t, $J=7.1$ Hz), δ 0.90 (3 H, t, $J=7.4$ Hz). $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 165.8, 162.5, 159.2, 135.8, 135.3, 130.7, 129.3, 128.8, 127.1, 126.1, 88.1, 74.9, 62.0, 49.1, 28.8, 14.0, 7.6. HPLC(Lux 5u Cellulose-2, hexane: i-PrOH =80:20, 1.0mL/min, t_{R1} (major)=20.82 min, t_{R1} (minor)=44.57 min, t_{R2} (major)=47.94 min, t_{R2} (minor)=50.54min). dr=12.3:1. 90% ee. ES-HRMS: Calcd for $\text{C}_{17}\text{H}_{19}\text{ClNO}_6$ [M+H], 368.0895, Found 368.0903.

(S)-ethyl-5-((S)-1-(2-bromophenyl)-2-nitroethyl)-5-ethyl-2-oxo-2,5-dihydrofuran-3-carboxylate (3ap).



Obtained in 82% yield; Light yellow oil; purified by silica gel column chromatography (EA/Petroleum = 1:5); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.10 (s, 1H), 7.61 – 7.53 (m, 1H), 7.32 (t, $J=7.1$ Hz, 1H), 7.26 – 7.23 (m, 1H), 7.20 – 7.13 (m, 1H), 5.03 (dd, $J=12.2$ Hz, 3.5 Hz, 1H), 4.97 – 4.87 (m, 1H), 4.33 (dd, $J=8.7$ Hz, 4.7 Hz, 1H), 4.28 – 4.18 (m, 2H), 2.10 (q, $J=7.4$ Hz, 2H), 1.38 – 1.17 (m, 3H), 1.03 – 0.95 (m, 3H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 165.0, 162.5, 159.1, 133.7, 133.4, 130.9, 130.4, 128.9, 128.6, 127.9, 88.5, 75.0, 61.8, 46.5, 28.6, 14.0, 8.1. HPLC(Lux 5u Cellulose-2, hexane: i-PrOH =80:20, 1.0mL/min, t_{R1} (major)=25.83 min, t_{R1} (minor)=39.60 min, t_{R2} (major)=50.48 min, t_{R2} (minor)=74.98 min). dr=11.0:1. 91% ee. ES-HRMS: Calcd for $\text{C}_{17}\text{H}_{19}\text{BrNO}_6$ [M+H], 412.0390, Found 412.0399.

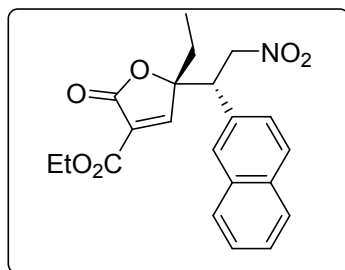
(S)-ethyl-5-ethyl-5-((S)-2-nitro-1-(3-nitrophenyl)ethyl)-2-oxo-2,5-dihydrofuran-3-carboxylate (3aq).



Obtained in 84% yield; Light yellow oil; purified by silica gel column chromatography (EA/Petroleum = 1:5); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.22 (1 H, d, $J=3.5$ Hz), δ 8.10 (1 H, s), δ 7.92 (1 H, s), δ 7.60 (2 H, d, $J=5.1$ Hz), δ 5.00 (1 H, dd, $J=13.7$, 4.7 Hz), δ 4.90 (1 H, dd, $J=13.5$, 10.4 Hz), δ 4.26 (3 H, m), δ 2.08 (1 H, td, $J=14.7$, 7.4 Hz), δ 1.96 (1 H, td, $J=14.6$, 7.3 Hz), δ 1.30 (3 H, t, $J=7.1$), δ 0.95 (3 H, t, $J=7.4$ Hz). $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 165.5, 162.0, 158.9, 148.5, 136.0, 133.8, 130.6, 127.5, 124.1, 123.8, 87.7, 74.8, 62.2, 49.0, 28.7, 14.0, 7.7. HPLC(CHIRAL-OD-H, hexane: i-PrOH =80:20, 1.0mL/min, t_{R1} (minor)=49.457 min, t_{R1} (major)=55.166 min, t_{R2} (major)=61.024 min, t_{R2} (minor)=82.746). dr=5.0:1. 85% ee. ES-HRMS: Calcd for $\text{C}_{17}\text{H}_{19}\text{N}_2\text{O}_8$

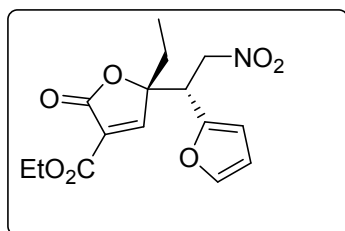
[M+H], 379.1136, Found 379.1144.

(S)-ethyl-5-ethyl-5-((S)-1-(naphthalen-2-yl)-2-nitroethyl)-2-oxo-2,5-dihydrofuran-3-carboxylate (3ar).



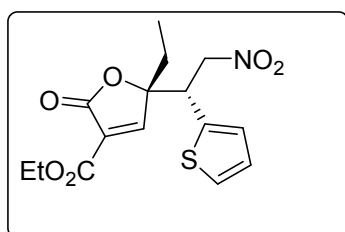
Obtained in 89% yield; Light yellow oil; purified by silica gel column chromatography (EA/Petroleum = 1:5); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.98 (1 H, s), δ 7.89 – 7.82 (3 H, m), δ 7.77 – 7.72 (1 H, m), δ 7.68 (1H, s), δ 7.58 – 7.53 (2 H, m), δ 4.95 (1 H, dd, J =13.4, 5.4 Hz), δ 4.89 (1 H, dd, J =13.4, 9.8 Hz), δ 4.35 – 4.29 (1 H, m), δ 4.24 (2 H, q, J =7.2 Hz), δ 1.97 – δ 1.84 (1 H, m), δ 1.73 (1 H, dd, J =14.8, 6.9 Hz), δ 1.29 – 1.23 (3 H, m), δ 0.92 (3 H, t, J =7.4 Hz). $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 166.0, 162.8, 159.3, 133.2, 133.2, 131.0, 130.9, 129.5, 128.9, 128.1, 128.0, 127.7, 127.0, 126.9, 88.6, 75.3, 61.9, 49.8, 29.1, 13.9, 7.6. HPLC(CHIRAL-OD-H, hexane: i-PrOH =70:30, 2.0mL/min, t_{R1} (minor)=53.03 min, t_{R1} (major)=94.60 min, t_{R2} (major)=103.56 min, t_{R2} (minor)=134.02 min). dr=11.8:1. 94% ee. ES-HRMS: Calcd for $\text{C}_{21}\text{H}_{22}\text{NO}_6$ [M+H], 384.1442, Found 384.1448.

ethyl (S)-5-ethyl-5-((S)-1-(furan-2-yl)-2-nitroethyl)-2-oxo-2,5-dihydrofuran-3-carboxylate (3as).



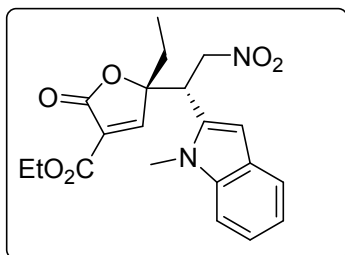
Obtained in 82% yield; Light yellow oil; purified by silica gel column chromatography (EA/Petroleum = 1:5); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.14 (s, 1H), 7.44 (s, 1H), 6.37 (s, 2H), 4.60 (d, J = 7.5 Hz, 2H), 4.37 (q, J = 7.3 Hz, 2H), 4.30 (t, J = 7.5 Hz, 1H), 1.95 (dt, J = 22.4, 7.6 Hz, 1H), 1.74 (td, J = 14.6, 7.3 Hz, 1H), 1.39 (t, J = 7.1 Hz, 3H), 0.91 (t, J = 7.4 Hz, 3H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 165.8, 162.9, 159.4, 147.1, 143.5, 126.9, 111.0, 110.9, 87.6, 73.5, 62.1, 43.3, 29.1, 14.1, 7.4. HPLC(CHIRAL-OJ-H, 210 nm, hexane: i-PrOH =70:30, 1.0mL/min, t_{R1} (major) = 34.875 min, t_{R1} (minor) = 44.793 min, t_{R2} (major) = 60.858 min, t_{R2} (minor) = 73.100 min). dr=16.5:1 . 91% ee. ES-HRMS: Calcd for $\text{C}_{15}\text{H}_{18}\text{NO}_7$ [M+H], 324.1083, Found 324.1066.

(S)-ethyl-5-ethyl-5-((S)-2-nitro-1-(thiophen-2-yl)ethyl)-2-oxo-2,5-dihydrofuran-3-carboxylate (3at).



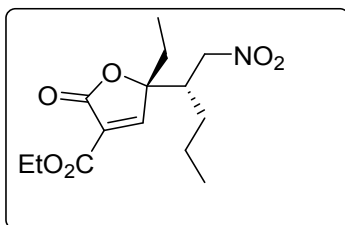
Obtained in 90% yield; Light yellow oil; purified by silica gel column chromatography (EA/Petroleum = 1:5); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.01 (1 H, s), δ 7.28 (1 H, s), δ 6.98 (2 H, s), δ 4.84 (1 H, dd, J =13.2, 4.4 Hz), δ 4.67 (1 H, dd, J =15.0, 8.6 Hz), δ 4.46 (1 H, dd, J =10.1, 4.3 Hz), δ 4.32 (2 H, q, J =7.0), δ 2.04 (1 H, td, J =14.7, 7.4 Hz), δ 1.91 (1 H, td, J =14.9, 7.6 Hz), δ 1.35 (3 H, t, J =7.1 Hz), δ 0.94 (3 H, t, J =7.4 Hz). $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 165.9, 162.4, 159.3, 135.4, 127.8, 127.6, 127.1, 126.4, 88.1, 76.3, 62.0, 44.7, 28.8, 14.0, 7.7. HPLC(Lux 5u Cellulose-2, hexane: i-PrOH =80:20, 1.0mL/min, t_{R1} (major)=26.86 min, t_{R1} (minor)=49.29 min, t_{R2} (major)=52.97 min, t_{R2} (minor)=68.43min). dr=8.9:1. 90% ee. ES-HRMS: Calcd for $\text{C}_{15}\text{H}_{18}\text{NO}_6\text{S}$ [M+H], 340.0849, Found 340.0855.

ethyl (S)-5-ethyl-5-((S)-1-(1-methyl-1H-indol-2-yl)-2-nitroethyl)-2-oxo-2,5-dihydrofuran-3-carboxylate (3au).



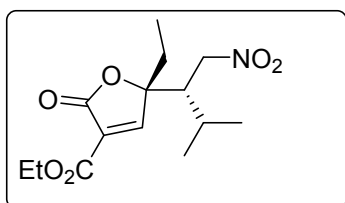
Obtained in 79% yield; Light yellow oil; purified by silica gel column chromatography (EA/Petroleum = 1:5); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.97 (s, 1H), 7.52 (d, $J = 7.9$ Hz, 1H), 7.32 – 7.27 (m, 1H), 7.24 – 7.15 (m, 2H), 6.98 (s, 1H), 4.89 (dd, $J = 12.9, 5.2$ Hz, 1H), 4.73 (dd, $J = 12.9, 10.0$ Hz, 1H), 4.49 (dd, $J = 10.0, 5.2$ Hz, 1H), 4.22 (q, $J = 7.5$ Hz, 2H), 3.76 (s, 3H), 2.14 – 2.03 (m, 1H), 2.01 – 1.90 (m, 1H), 1.25 (t, $J = 7.1$ Hz, 3H), 0.88 (t, $J = 7.4$ Hz, 3H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 166.5, 163.6, 159.4, 136.9, 127.6, 126.8, 126.7, 122.6, 120.2, 118.4, 109.8, 106.9, 89.4, 75.6, 61.8, 41.3, 33.1, 28.9, 14.0, 7.8. HPLC(CHIRAL-OD-H, 210 nm, hexane: i-PrOH =80:20, 2.0mL/min, t_{R1} (major) = 14.370 min, t_{R1} (minor) = 18.319). dr= 4.8:1. 94% ee. ES-HRMS: Calcd for $\text{C}_{20}\text{H}_{22}\text{N}_2\text{NaO}_6$ [M+Na], 409.1376, Found 409.1366.

ethyl (S)-5-ethyl-5-((S)-1-nitropentan-2-yl)-2-oxo-2,5-dihydrofuran-3-carboxylate (3av):



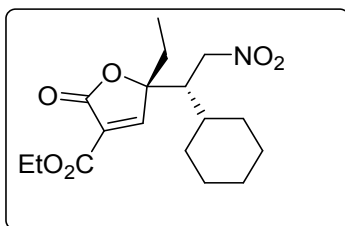
Obtained in 93% yield; Light yellow oil; purified by silica gel column chromatography (EA/Petroleum = 1:5); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.00 (s, 1H), 4.48 (dd, $J = 13.9, 5.6$ Hz, 1H), 4.37 (q, $J = 7.1$ Hz, 2H), 4.28 (dd, $J = 13.9, 5.8$ Hz, 1H), 2.87 (ddd, $J = 9.2, 7.3, 4.6$ Hz, 1H), 2.05-1.85 (m, 2H), 1.44 – 1.35 (m, 7H), 1.26 (t, $J = 7.1$ Hz, 3H), 0.88 (t, $J = 7.3$ Hz, 3H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 166.1, 163.3, 159.6, 127.1, 89.3, 75.1, 62.1, 42.8, 30.8, 28.4, 20.6, 14.1, 13.9, 7.6. HPLC(CHIRAL-OJ-H, 210 nm, hexane: i-PrOH =92:8, 1.0mL/min, t_{R1} (minor) = 63.660 min, t_{R1} (major) = 69.698 min). dr>20:1. 88% ee. ES-HRMS: Calcd for $\text{C}_{14}\text{H}_{22}\text{NO}_6$ [M+H], 300.1447, Found 300.1415.

ethyl (S)-5-ethyl-5-((S)-3-methyl-1-nitrobutan-2-yl)-2-oxo-2,5-dihydrofuran-3-carboxylate (3aw):



Obtained in 83% yield; Light yellow oil; purified by silica gel column chromatography (EA/Petroleum = 1:5); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.07 (s, 1H), 4.48 (dd, $J = 14.6, 6.1$ Hz, 1H), 4.40 – 4.31 (m, 3H), 2.95 (ddd, $J = 6.4, 4.4, 2.3$ Hz, 1H), 2.03 – 1.84 (m, 2H), 1.38 (t, $J = 7.1$ Hz, 3H), 1.03 (d, $J = 7.0$ Hz, 3H), 0.84 (t, $J = 7.4$ Hz, 3H), 0.82 (d, $J = 6.8$ Hz, 3H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 166.1, 163.8, 159.7, 126.9, 90.2, 71.9, 62.1, 47.8, 29.4, 28.2, 22.4, 17.7, 14.1, 7.6. HPLC(CHIRAL-OD-H, 210 nm, hexane: i-PrOH =95:5, 1.0mL/min, t_{R1} (minor) = 13.179 min, t_{R1} (major) = 18.070 min, t_{R2} (minor) = 49.909 min, t_{R2} (major) = 51.397 min). dr>20:1. 96 % ee. ES-HRMS: Calcd for $\text{C}_{14}\text{H}_{22}\text{NO}_6$ [M+H], 300.1447, Found 300.1436.

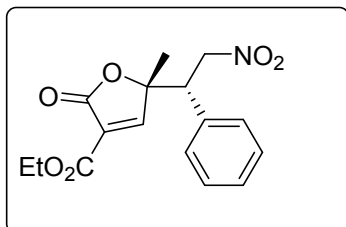
ethyl (S)-5-((S)-1-cyclohexyl-2-nitroethyl)-5-ethyl-2-oxo-2,5-dihydrofuran-3-carboxylate (3ax):



Obtained in 92% yield; Light yellow oil; purified by silica gel column chromatography (EA/Petroleum = 1:5); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.06 (s, 1H), 4.41 (d, $J = 5.5$ Hz, 2H), 4.38 (q, $J = 7.5$ Hz, 2H), 2.91 (td, $J = 5.5, 2.0$ Hz, 1H), 2.06 – 1.83 (m, 2H), 1.81 – 1.45 (m, 8H), 1.39 (t, $J = 7.1$ Hz, 3H), 1.19 – 1.05 (m, 3H),

0.85 (t, $J = 7.4$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 166.0, 163.7, 159.7, 126.9, 90.1, 72.6, 62.1, 48.2, 38.8, 32.6, 29.5, 28.56, 26.6, 26.3, 25.8, 14.1, 7.6. HPLC(CHIRAL-OJ-H, 210 nm, hexane: i-PrOH = 92:8, 1.0mL/min, t_{R1} (major) = 50.012 min, t_{R1} (minor) = 66.758 min). dr > 20:1. 90% ee. ES-HRMS: Calcd for $\text{C}_{17}\text{H}_{25}\text{NNaO}_6$ [$\text{M}+\text{Na}$], 362.1580, Found 362.1548.

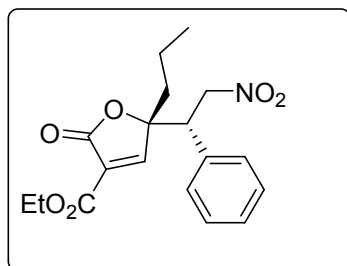
ethyl (S)-5-methyl-5-((S)-2-nitro-1-phenylethyl)-2-oxo-2,5-dihydrofuran-3-carboxylate(3ay):



White solid. Obtained in 93% yield; Light yellow oil; purified by silica gel column chromatography (EA/Petroleum = 1:5); ^1H NMR (400 MHz, CDCl_3) δ 7.89 (s, 1H), 7.35 – 7.21 (m, 3H), 7.11 (d, $J = 6.5$ Hz, 2H), 4.83 (dd, $J = 13.4, 5.1$ Hz, 1H), 4.72 (dd, $J = 13.4, 9.9$ Hz, 1H), 4.19 (q, $J = 7.1$ Hz, 2H), 3.99 (dd, $J = 9.9, 5.1$ Hz, 1H), 1.51 (s, 3H), 1.23 (t, $J = 7.1$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 164.7, 162.9, 158.4, 132.6, 128.4, 128.1, 127.2,

124.8, 84.5, 74.0, 60.9, 49.5, 22.3, 13.0. HPLC(CHIRAL-OJ-H, 254 nm, hexane: i-PrOH = 97:3, 1.0mL/min, t_{R1} (major) = 19.984 min, t_{R1} (minor) = 40.539 min, t_{R2} (minor) = 25.931 min, t_{R2} (major) = 29.097 min). dr = 14.1:1. 90% ee. ES-HRMS: Calcd for $\text{C}_{16}\text{H}_{18}\text{NO}_6$ [$\text{M}+\text{H}$], 320.1134, Found 320.1113.

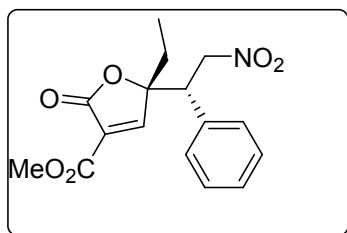
ethyl (S)-5-((S)-2-nitro-1-phenylethyl)-2-oxo-5-propyl-2,5-dihydrofuran-3-carboxylate(3az):



Obtained in 91% yield; Light yellow oil; purified by silica gel column chromatography (EA/Petroleum = 1:5); ^1H NMR (400 MHz, CDCl_3) δ 7.90 (s, 1H), 7.44 – 7.29 (m, 3H), 7.22 – 7.13 (m, 2H), 4.86 (dd, $J = 13.4, 5.0$ Hz, 1H), 4.77 (dd, $J = 13.4, 10.0$ Hz, 1H), 4.26 (q, $J = 7.1$ Hz, 2H), 4.10 (dd, $J = 10.0, 5.0$ Hz, 1H), 1.99 – 1.74 (m, 2H), 1.41 – 1.18 (m, 5H), 0.91 (t, $J = 7.3$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 166.0, 163.3, 159.3, 133.6, 129.4, 129.0, 128.3, 126.5, 88.2, 75.2, 62.0, 49.8, 37.7, 16.8, 14.1, 13.9.

HPLC(CHIRAL-OJ-H, 254 nm, hexane: i-PrOH = 97:3, 2.0mL/min, t_{R1} (minor) = 36.733 min, t_{R1} (major) = 40.539 min, t_{R2} (minor) = 45.309 min, t_{R2} (major) = 52.316 min). dr = 16.3:1. 92% ee. ES-HRMS: Calcd for $\text{C}_{18}\text{H}_{22}\text{NNaO}_6$ [$\text{M}+\text{Na}$], 370.1267, Found 370.1248.

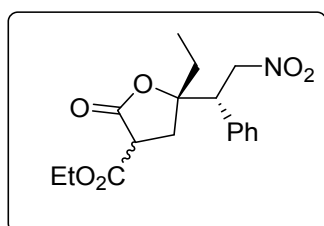
methyl (S)-5-ethyl-5-((S)-2-nitro-1-phenylethyl)-2-oxo-2,5-dihydrofuran-3-carboxylate (3ba):



Obtained in 85% yield; Light yellow oil; purified by silica gel column chromatography (EA/Petroleum = 1:5); ^1H NMR (400 MHz, CDCl_3) δ 7.87 (s, 1H), 7.32 – 7.24 (m, 3H), 7.11 (dd, $J = 7.8, 1.6$ Hz, 2H), 4.79 (dd, $J = 13.4, 5.1$ Hz, 1H), 4.70 (dd, $J = 13.4, 9.9$ Hz, 1H), 4.05 (dd, $J = 9.9, 5.1$ Hz, 1H), 3.75 (s, 3H), 1.96 (dq, $J = 14.8, 7.4$ Hz, 1H), 1.80 (dq, $J = 14.7, 7.4$ Hz, 1H), 0.81 (t, $J = 7.4$

Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 165.0, 162.6, 158.7, 132.6, 128.4, 128.1, 127.2, 125.6, 87.6, 74.1, 51.7, 48.5, 27.8, 6.6. HPLC(CHIRAL-OD-H, 210 nm, hexane: i-PrOH = 70:30, 1.0mL/min, t_{R1} (major) = 30.03 min, t_{R1} (minor) = 55.70 min). dr = 12.9:1. 80% ee. ES-HRMS: Calcd for $\text{C}_{16}\text{H}_{18}\text{NO}_6$ [$\text{M}+\text{H}$], 320.1134, Found 320.1120.

ethyl (SS)-5-ethyl-5-((S)-2-nitro-1-phenylethyl)-2-oxotetrahydrofuran-3-carboxylate(4aa):



mixture of diastereoisomers(major isomer: minor isomer = 1.7:1); Obtained in 66% yield; Light yellow oil; purified by silica gel column chromatography (EA/Petroleum = 1:5); ^1H NMR (400 MHz, CDCl_3)

δ 7.42 – 7.31 (m, 3H, major isomer + minor isomer), 7.32 – 7.25 (m, 2H, major isomer + minor isomer), 4.97 – 4.86 (m, 2H, major isomer + minor isomer), 4.21-4.08 (m, 2H, major isomer + minor isomer), 3.70(dd, J = 9.8, 5.4 Hz, 1H, major isomer), 3.61 (t, J = 10.3 Hz, 1H, minor isomer), 2.66 (dd, J = 13.6, 10.2 Hz, 1H, minor isomer), 2.53 (dd, J = 13.0, 8.7 Hz, 1H, major isomer), 2.36 – 2.14 (m, 2H, major isomer + minor isomer), 1.96 (q, J = 7.5 Hz, 2H, major isomer), 1.86 – 1.63 (m, 2H, minor isomer), 1.23 (td, J = 7.2, 3.1 Hz, 3H, major isomer + minor isomer), 1.12 (t, J = 7.5 Hz, 3H, major isomer), 1.04 (t, J = 7.4 Hz, 3H, minor isomer). ^{13}C NMR (101 MHz, CDCl_3) δ 171.2(major isomer), 170.5(minor isomer), 167.4(major isomer), 167.1(minor isomer), 134.42(minor isomer), 134.1(major isomer), 129.5(major isomer), 129.4(minor isomer), 129.2(major isomer+minor isomer), 129.0(major isomer), 128.7(minor isomer), 87.6(major isomer+minor isomer), 76.2(minor isomer), 75.7(major isomer), 62.5(minor isomer), 62.4(major isomer), 50.0(major isomer), 49.6(minor isomer), 46.8(minor isomer), 46.7(major isomer), 33.4(major isomer+minor isomer), 31.6(major isomer+minor isomer), 14.0(major isomer+minor isomer), 7.7(major isomer+minor isomer). ES-HRMS: Calcd for $\text{C}_{17}\text{H}_{21}\text{NNaO}_6$ [M+Na], 358.1267, Found 358.1274.

3. Single Crystal X-Ray Diffraction of 3ay.

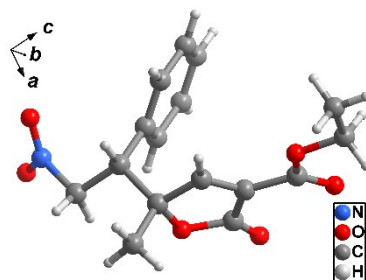


Table 1 Crystal data and structure refinement for 3ay.	
Identification code	3ay
CCDC	1958966
Empirical formula	C ₁₆ H ₁₇ NO ₆
Formula weight	319.30
Temperature/K	298.15
Crystal system	orthorhombic
Space group	<i>P</i> 2 ₁ 2 ₁ 2 ₁
<i>a</i> /Å	8.1801(8)
<i>b</i> /Å	11.5319(9)
<i>c</i> /Å	16.4021(14)
α /°	90
β /°	90
γ /°	90
Volume/Å ³	1547.2(2)
<i>Z</i>	4
ρ_{calc} /cm ³	1.371
μ /mm ⁻¹	0.891
<i>F</i> (000)	672.0
Crystal size/mm ³	0.4 × 0.15 × 0.13
Radiation	CuK α (λ = 1.54178)
2 θ range for data collection/°	9.374 to 129.972
Index ranges	-9 ≤ <i>h</i> ≤ 5, -13 ≤ <i>k</i> ≤ 8, -14 ≤ <i>l</i> ≤ 19
Reflections collected	3340
Independent reflections	2339 [<i>R</i> _{int} = 0.0379, <i>R</i> _{sigma} = 0.0757]
Data/restraints/parameters	2339/0/211
Goodness-of-fit on <i>F</i> ²	1.031

Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0501$, $wR_2 = 0.1033$
Final R indexes [all data]	$R_1 = 0.0679$, $wR_2 = 0.1163$
Largest diff. peak/hole / $e \text{ \AA}^{-3}$	0.21/-0.21
Flack parameter	0.2(4)

4. DFT calculations

4.1 Computational Information

DFT¹ studies have been performed with the Gaussian09 program² using the B3LYP³ method. The 6-31G* basis set was used for the system. The structures were optimized with SMD⁴ method in 1,4-dioxane ($\epsilon=2.2099$). Harmonic vibrational frequency calculations show that all structures were shown to be stationary points (with no imaginary frequency) or transition states (with one imaginary frequency). The 3D molecular figures were prepared using CYLView.⁵

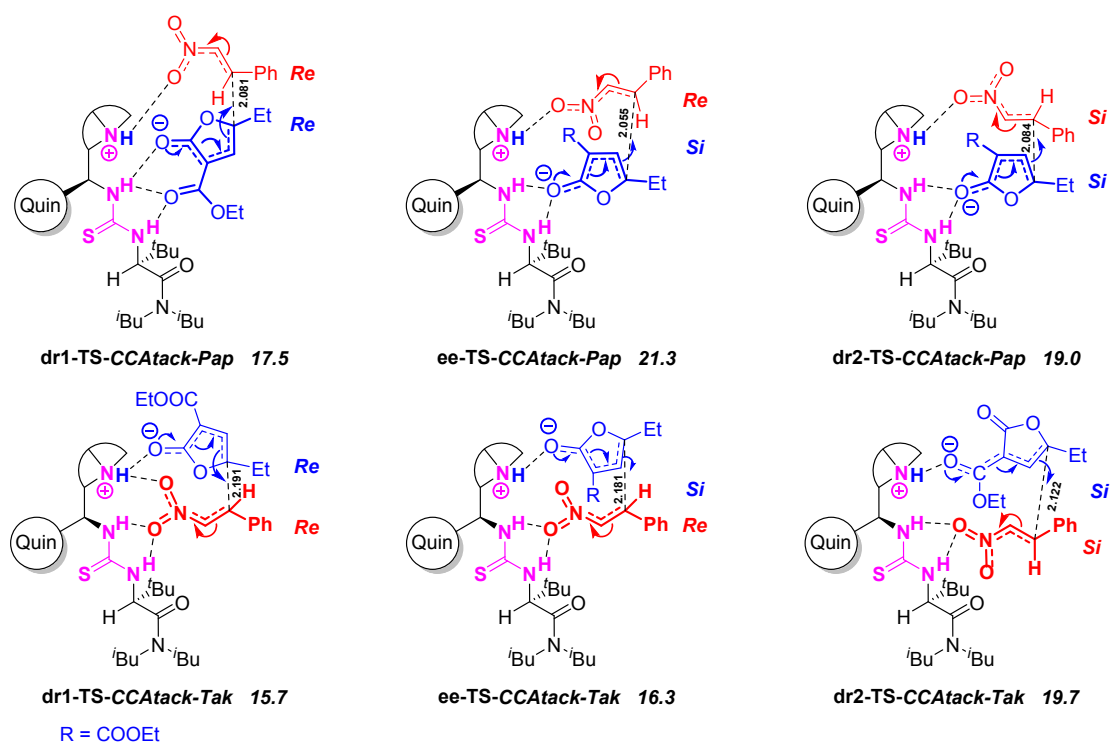


Figure 1 Transition states of the C-C bond formation leading to other chiral isomers. The relative free energies (ΔG_{sol} , 285.15 K, 1.0 atm) in 1,4-dioxane are in kcal/mol. The selected bond lengths are in Å. Calculated at the B3LYP/6-31G* level.

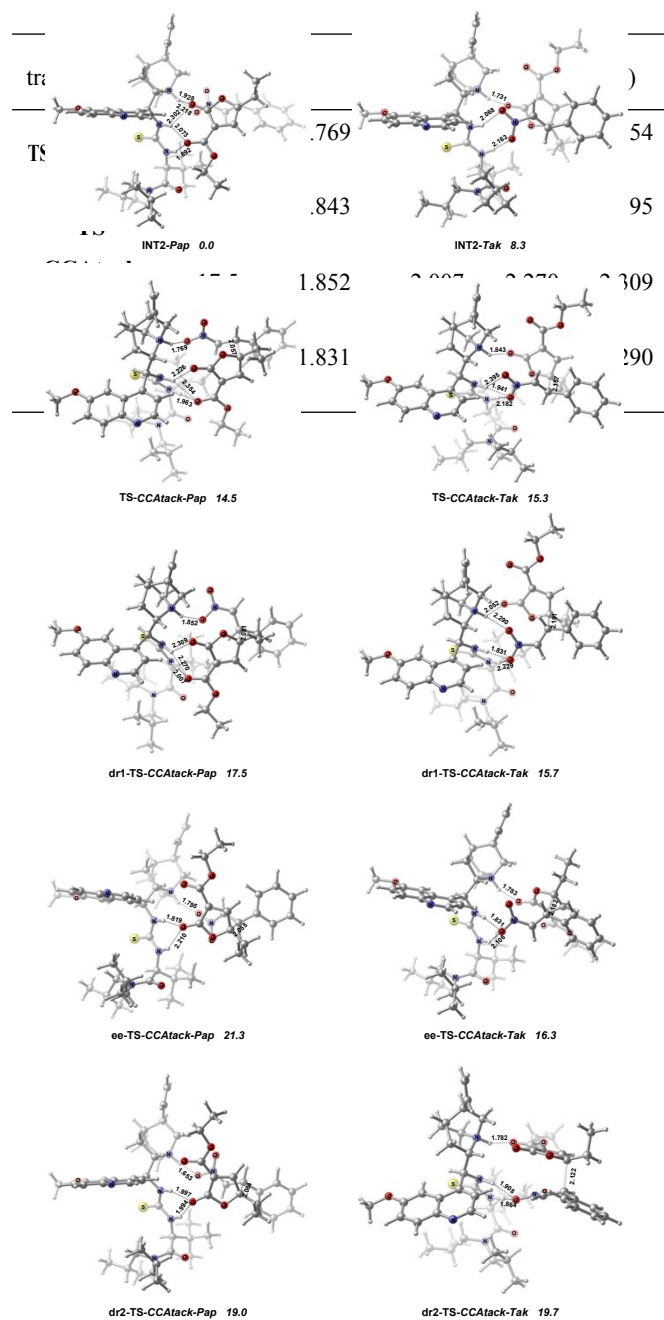


Figure 2. Optimized structures of intermediates and transition states of the C-C bond formation (*INT2-Pap*, *INT2-Tak*, *TS-CCAtack-Pap*, *TS-CCAtack-Tak*, *dr1-TS-CCAtack-Pap*, *dr1-TS-CCAtack-Tak*, *ee-TS-CCAtack-Pap*, *ee-TS-CCAtack-Tak*, *dr2-TS-CCAtack-Pap* and *dr2-TS-CCAtack-Tak*). The selected bond lengths are in Å. The relative free energies (ΔG_{sol} , 285.15 K, 1.0 atm) in 1,4-dioxane are in kcal/mol. Calculated at the B3LYP/6-31G* level.

Table 1. The distance of O.....HN in each transition state.

4.2 Calculated total energies and cartesian coordinates

INT2-Pap

E(RB3LYP)= -3353.35786666 Hartree

Sum of electronic and thermal Free Energies= -3352.273641 Hartree

C,0,-0.768544987,3.0806805862,0.0938454468
C,0,-0.7904799403,5.1211266881,-1.4050410688
C,0,-1.4660263402,4.4356807905,-0.2004960389
H,0,-0.2823566952,3.0849837276,1.0685831405
H,0,-2.5253184772,4.2776856682,-0.4254632746
H,0,-1.4286430749,5.0765983013,0.6850254243
C,0,-0.0364700182,2.8944630822,-2.3141498969
H,0,0.8830320411,2.82218409,-2.8964682565
H,0,-0.6089882828,1.9780876126,-2.4668516653
C,0,-0.8565992226,4.1697100814,-2.6165427433
H,0,-0.4633262579,4.6639128117,-3.5110193853
H,0,-1.8988368565,3.9063862479,-2.8271252412
H,0,-1.308170577,6.0575141729,-1.633426479
C,0,0.7061043673,5.4164598977,-1.1036272309
H,0,1.1696737728,5.7408898087,-2.0429091417
C,0,1.3595678485,4.0802133643,-0.6581642558
H,0,2.2551490166,3.8407447421,-1.2339683367
H,0,1.6224250165,4.0589473257,0.4000735997
N,0,0.3941543262,2.9394022535,-0.8720594463
C,0,0.9211008276,6.5049795242,-0.0844088513
H,0,0.5811085071,6.2948517467,0.9305867618
C,0,1.4914490622,7.6815460986,-0.3455424432
H,0,1.6153049546,8.4380672234,0.4253185565
H,0,1.8585468059,7.9356106388,-1.3385984968
C,0,-1.7299460198,1.8627464145,0.0262971164
H,0,-2.3341277532,1.9373587676,-0.8761448427
C,0,-2.6349960317,1.8920580671,1.2658654138
C,0,-4.0345770044,2.1993093684,1.2015219214
C,0,-2.0890240391,1.6188283083,2.5035768873

C,0,-4.7432911685,2.4781451537,0.00795395
C,0,-4.7557671888,2.2212759089,2.446160559
C,0,-2.8982191378,1.6556452107,3.662526287
H,0,-1.0385395154,1.3607591639,2.6048051209
C,0,-6.0942491661,2.7834373795,0.0298970145
H,0,-4.259252815,2.4289426274,-0.9603392855
C,0,-6.1373864721,2.5356328191,2.4320331953
H,0,-2.4530828034,1.4342653493,4.6317226135
C,0,-6.8012391636,2.8157354901,1.2597118392
H,0,-6.6571610073,2.5470778766,3.3852994522
H,0,-7.8590077862,3.0519628626,1.2841531215
N,0,-1.0150808528,0.5961582674,-0.0910072942
O,0,-6.6685925281,3.0418216671,-1.1787125126
C,0,-8.0642399055,3.3096380809,-1.230518513
H,0,-8.2974711963,3.4639085151,-2.2862601099
H,0,-8.6553480841,2.4645328172,-0.8551472231
H,0,-8.3283236367,4.2171579061,-0.6722295627
N,0,-4.1810616079,1.9523902184,3.6540406742
H,0,-0.3604611112,0.351219469,0.6607202589
C,0,-1.3840202541,-0.408950619,-0.9432320799
N,0,-0.8367827471,-1.6063941814,-0.6388488393
H,0,-0.3267198712,-1.6596375818,0.2491249454
S,0,-2.4044073349,-0.1447625365,-2.2943358051
O,0,3.731006796,1.5565893307,1.6943797165
O,0,1.5201335789,1.5811427657,1.1588382941
O,0,1.908733472,-2.4224720984,2.9665757921
O,0,0.3755320392,-1.120028116,1.9215797228
C,0,1.5476899306,-1.2846400328,2.316350747
C,0,2.4820664398,0.9390655787,1.6284934926
C,0,2.6225207523,-0.3593525989,2.177296117
C,0,4.0030933891,-0.4882575203,2.5924584175
C,0,4.630384241,0.6707696398,2.2856852785
C,0,6.0163651433,1.1785035389,2.5012741855
C,0,0.8654493092,-3.388070293,3.2201677498
C,0,1.4774143876,-4.5051170372,4.0437532569
H,0,4.4510492749,-1.3481935041,3.0720327668
H,0,6.4502916645,1.5122633461,1.5472614186
H,0,0.0483220816,-2.8957139019,3.7590976397
H,0,0.4678721733,-3.7577096933,2.2706331491
H,0,2.2928550933,-4.9954650746,3.500550458
H,0,0.7153469156,-5.2606111233,4.2674719573
H,0,1.8742285821,-4.1265987464,4.992551373
H,0,6.631352749,0.3386470007,2.8466799615

C,0,5.8345758386,0.6279439177,-2.0065697138
H,0,5.9643422723,1.4895719687,-2.6569040814
C,0,4.5824652191,0.3559533447,-1.597521474
H,0,4.2587212879,-0.4699798707,-0.9810996081
C,0,7.0330899455,-0.1303766691,-1.6785143784
C,0,8.2217795829,0.168248336,-2.3720627936
C,0,7.054486616,-1.1466023398,-0.7005861024
C,0,9.393221254,-0.5381457761,-2.1135022247
H,0,8.215280118,0.9551984632,-3.1221271871
C,0,8.2276271847,-1.8452857651,-0.4416245685
H,0,6.1595701919,-1.3698148593,-0.1274230008
C,0,9.397929895,-1.5474854776,-1.1490154325
H,0,10.300916317,-0.3003797173,-2.6608183633
H,0,8.2342784225,-2.6223851543,0.3173764633
H,0,10.311805517,-2.0974770627,-0.94179689
N,0,3.4884631797,1.1940332132,-1.9971513805
O,0,3.6987799204,2.2465924992,-2.6176666996
O,0,2.3540076987,0.8009726964,-1.6835259573
H,0,0.901504958,2.078457196,-0.5982090734
C,0,-0.9296675786,-2.8482951174,-1.4106577597
H,0,-1.6385279056,-2.6611897964,-2.2146105882
C,0,0.4335565297,-3.237655537,-2.0921159516
C,0,1.6267227302,-3.198678994,-1.117238566
H,0,1.7775593104,-2.1916393129,-0.7118976106
H,0,1.4919384648,-3.892271527,-0.2857644685
H,0,2.5449472337,-3.4732986229,-1.6527356548
C,0,0.7049018357,-2.2303887936,-3.2281173178
H,0,-0.08992915,-2.2417783055,-3.9829478814
H,0,0.7993625661,-1.2069947008,-2.8523944198
H,0,1.6466850582,-2.484460826,-3.7313143788
C,0,0.3120623775,-4.6434281411,-2.71083504
H,0,-0.5138670671,-4.696280479,-3.4310462255
H,0,1.2316685661,-4.8927984011,-3.2544800899
H,0,0.1583236936,-5.4123580043,-1.9483556006
C,0,-1.4773608836,-3.9278835297,-0.4377788679
O,0,-0.6978086009,-4.5480416328,0.296436128
N,0,-2.8239099184,-4.1565663265,-0.3631959654
C,0,-3.266329802,-5.1440779156,0.6381086042
H,0,-4.2822472425,-5.4485796319,0.365757253
H,0,-2.6224044294,-6.0242838461,0.5546541321
C,0,-3.8801874236,-3.4885079489,-1.1382343241
H,0,-4.6377936644,-3.1406904697,-0.4267535856
H,0,-3.4813667356,-2.5894520673,-1.6100393496

C,0,-3.253222949,-4.6535405642,2.101166805
H,0,-2.220402995,-4.374383892,2.3371711319
C,0,-3.6589190505,-5.8144993005,3.0195994151
H,0,-3.0003163187,-6.682080121,2.8894835408
H,0,-3.6113774365,-5.516777519,4.073823813
H,0,-4.6875267028,-6.1439353267,2.81784381
C,0,-4.1448875591,-3.4283523883,2.3346249067
H,0,-3.8326938555,-2.5744428612,1.7237911719
H,0,-5.1983952307,-3.6444649168,2.1092087781
H,0,-4.0951670381,-3.1102140652,3.3832300942
C,0,-4.5712644855,-4.3706670856,-2.2012803619
H,0,-4.9832521361,-5.2581615894,-1.6988608411
C,0,-5.745424359,-3.5881738456,-2.8061389458
H,0,-5.3954876087,-2.6831398125,-3.3189160619
H,0,-6.2886939411,-4.1963722658,-3.5391616827
H,0,-6.4619757503,-3.2764530857,-2.036099782
C,0,-3.606780032,-4.8540075632,-3.2891477325
H,0,-2.7725873201,-5.4222882799,-2.8638965141
H,0,-4.1218730064,-5.509823095,-4.0017747883
H,0,-3.1937129307,-4.010879084,-3.8578617054
C,0,6.0997508253,2.3345737193,3.5131217616
H,0,7.1353570634,2.6759308665,3.6318236311
H,0,5.4980644416,3.1880849229,3.1824285495
H,0,5.7280643647,2.0222994029,4.4957435272

INT2-Tak

E(RB3LYP)= -3353.34539888 Hartree

Sum of electronic and thermal Free Energies= -3352.260459 Hartree

C,0,-0.8450053867,2.8219329614,0.3197742666
C,0,-0.8543065065,5.2020514812,-0.5682312639
C,0,-1.4583730587,4.2432006544,0.4771894249
H,0,-0.296662577,2.5393248658,1.2189737315
H,0,-2.5429900517,4.2038568924,0.3431937054
H,0,-1.2857105492,4.6136599437,1.4916856151
C,0,-0.3271984074,3.2821937541,-2.099922575
H,0,0.5372161727,3.3462183454,-2.762092903
H,0,-0.9491413577,2.4551128475,-2.4435423297
C,0,-1.0968925071,4.6154995323,-1.9721259123
H,0,-0.7578401167,5.3157902628,-2.7422128212
H,0,-2.1687372622,4.4568028192,-2.1324386403
H,0,-1.3302640397,6.1836549458,-0.4838724214
C,0,0.679890786,5.3427273479,-0.3642155475
H,0,1.0831694491,5.8631914396,-1.2411476394

C,0,1.2700288114,3.9098457675,-0.3168334137
H,0,2.139882345,3.7632674801,-0.9583724364
H,0,1.5642920564,3.6196882519,0.6951883983
N,0,0.2254102244,2.9059485862,-0.7495941414
C,0,1.0596826044,6.138534044,0.8570520255
H,0,0.7572490358,5.7245349277,1.8204292072
C,0,1.7310722727,7.2900329657,0.8291724709
H,0,1.9754124537,7.8305989196,1.7402365298
H,0,2.0670065398,7.7366742272,-0.1050605565
C,0,-1.9002293511,1.7253572813,0.0298165168
H,0,-2.5252052943,2.0297175925,-0.8083168924
C,0,-2.7743725156,1.5467987418,1.282287236
C,0,-4.1301137066,2.0074716028,1.3665288815
C,0,-2.2311752563,0.937808018,2.395304662
C,0,-4.8334037988,2.6334365367,0.3095041262
C,0,-4.8092129601,1.8140278186,2.6199755074
C,0,-2.9970146118,0.7878413963,3.5744133518
H,0,-1.2105273479,0.5652566983,2.3833086926
C,0,-6.1394133659,3.0650563697,0.4721187091
H,0,-4.3869641635,2.7580795179,-0.6691555403
C,0,-6.1453608264,2.2679804845,2.7522851305
H,0,-2.5526084276,0.3032305767,4.4429893913
C,0,-6.8033637254,2.8839950043,1.7132349629
H,0,-6.6353247145,2.1106830485,3.7083164134
H,0,-7.8256939407,3.218355246,1.8474017395
N,0,-1.2425341557,0.488545722,-0.3774502587
O,0,-6.7153526016,3.6531307635,-0.6130097179
C,0,-8.0761819049,4.0607185422,-0.5288735663
H,0,-8.3247690947,4.4676224284,-1.5112256892
H,0,-8.7415993447,3.2149596688,-0.3143333012
H,0,-8.2213540677,4.8427790016,0.2276631252
N,0,-4.2370358194,1.2110013485,3.7018712999
H,0,-0.4162740638,0.2246737733,0.1595490956
C,0,-1.8461826031,-0.4733370107,-1.1431473966
N,0,-1.1332603896,-1.6203803151,-1.2490651918
H,0,-0.2362965417,-1.6541484171,-0.7661967456
S,0,-3.3483880503,-0.2097291176,-1.9008345649
O,0,3.0509371466,-0.8954997698,-1.7449004254
O,0,1.9557261292,1.0875390242,-1.6991678759
O,0,6.2096440764,2.2686928163,-0.9067354277
O,0,4.2070039486,3.2742230118,-1.2223680721
C,0,4.8620577252,2.235784404,-1.1559573943
C,0,3.0419846253,0.495229763,-1.5830926064

C,0,4.3905548633,0.8835293952,-1.3226024727
C,0,5.1794351121,-0.3122985207,-1.340725646
C,0,4.3447126883,-1.3601420295,-1.5872058928
C,0,4.5854679259,-2.8058926697,-1.8707139234
C,0,6.7913711972,3.575579778,-0.7667498187
C,0,8.2737937449,3.3934817902,-0.5003043531
H,0,6.2476505261,-0.3751618506,-1.1870560506
H,0,3.7920963913,-3.4093164667,-1.4109971868
H,0,6.6168453047,4.1528256771,-1.6818884727
H,0,6.2987586087,4.1095488193,0.0539824533
H,0,8.4424454926,2.8199633171,0.4178276144
H,0,8.7550216311,4.3718408982,-0.3858579268
H,0,8.761657347,2.8669579347,-1.3277654233
H,0,5.5289918715,-3.0956403621,-1.3923888554
C,0,3.8923802905,-1.6876082493,1.4672479185
H,0,3.3514773479,-2.5525127804,1.0953481923
C,0,3.1935183935,-0.5304058462,1.5740052357
H,0,3.5648177215,0.4177244519,1.9325522084
C,0,5.2623143865,-1.9084229098,1.9051324896
C,0,5.7542440421,-3.2291896167,1.9195807586
C,0,6.1170260124,-0.8691152594,2.329297319
C,0,7.0490659223,-3.5052390891,2.3510456665
H,0,5.1062655433,-4.0389971756,1.5942108872
C,0,7.4095949574,-1.1481629332,2.7561108353
H,0,5.7745728696,0.1605962219,2.3013432457
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H,0,7.4086541158,-4.5304154081,2.358147366
H,0,8.0576478884,-0.3358994327,3.0736177533
H,0,8.8926200123,-2.6780870483,3.106402025
N,0,1.8357559544,-0.4688738977,1.1941468241
O,0,1.2246671422,-1.4879982973,0.8200450275
O,0,1.2692593309,0.6494782173,1.2790173889
H,0,0.7434363104,2.0054321896,-0.8719789297
C,0,-1.5718846335,-2.8746307259,-1.87622032
H,0,-2.6219185013,-2.732322178,-2.1270833077
C,0,-0.8347892223,-3.193498759,-3.2232914225
C,0,0.6998097005,-3.177168243,-3.0965004472
H,0,1.069102037,-2.2041054609,-2.7566842622
H,0,1.0513326254,-3.9418896746,-2.4024425374
H,0,1.1447184377,-3.3666560543,-4.0819351462
C,0,-1.2439069104,-2.1304868915,-4.2626483352
H,0,-2.3263213228,-2.1171448571,-4.4327705873
H,0,-0.9421063576,-1.1242220878,-3.9558897021

H,0,-0.7541380691,-2.3446486458,-5.2210115499
C,0,-1.3045079968,-4.5717989317,-3.7296452419
H,0,-2.3955120994,-4.6097851557,-3.8448081488
H,0,-0.8679047978,-4.7755335186,-4.7150833105
H,0,-0.9974737588,-5.3771022107,-3.0562979128
C,0,-1.4150156652,-3.9742952616,-0.7869087453
O,0,-0.3721691037,-4.6302642366,-0.7061678385
N,0,-2.4196232645,-4.1606911513,0.1257497183
C,0,-2.1553845108,-5.1409363596,1.1941514523
H,0,-3.1190931199,-5.3937388528,1.6487382174
H,0,-1.7568542083,-6.05023648,0.7340328892
C,0,-3.7272896245,-3.4915133898,0.150047679
H,0,-3.8966013762,-3.1350459665,1.1729053858
H,0,-3.7010089186,-2.6000507874,-0.4778150007
C,0,-1.1792428128,-4.6641202183,2.2896155262
H,0,-0.2313285803,-4.4281539142,1.7939696118
C,0,-0.9324914409,-5.8121529242,3.2780511912
H,0,-0.5426300273,-6.7036610154,2.7713980755
H,0,-0.2031258506,-5.5216239141,4.0436936428
H,0,-1.8568064416,-6.1013527112,3.7971552655
C,0,-1.6684074143,-3.404314309,3.0140218963
H,0,-1.7996621075,-2.5652146744,2.3219520835
H,0,-2.6246183063,-3.575857918,3.5273597175
H,0,-0.9421102496,-3.0888201939,3.7736295399
C,0,-4.9177103611,-4.3811263111,-0.271756486
H,0,-4.928991173,-5.2689221854,0.3775680573
C,0,-6.225728694,-3.6125374959,-0.0389039545
H,0,-6.2675813788,-2.7058936603,-0.6558540323
H,0,-7.0947096876,-4.2301913209,-0.2952905761
H,0,-6.333780396,-3.3056195048,1.0088596588
C,0,-4.8064807214,-4.8622658053,-1.7225248981
H,0,-3.8802692045,-5.4223391065,-1.8920852208
H,0,-5.6424441469,-5.5252535796,-1.97688958
H,0,-4.8311404135,-4.0184213046,-2.4239371659
C,0,4.6533599321,-3.1324570628,-3.3740688664
H,0,4.8105702436,-4.2066226829,-3.5304365425
H,0,3.7248835399,-2.8502321663,-3.880813498
H,0,5.4776666139,-2.5928943729,-3.8542149319

TS-CCAttack-Pap

E(RB3LYP)= -3353.33970951 Hartree

Sum of electronic and thermal Free Energies= -3352.250535 Hartree

C,0,-1.8007476404,2.8000984042,0.4674842339

C,0,-3.2587940229,4.6312426568,-0.521605875
C,0,-3.0185005597,3.7371343946,0.7106037961
H,0,-0.9948544431,3.0081866594,1.1689527924
H,0,-3.9190114082,3.1454063298,0.9019138867
H,0,-2.8500623003,4.3425034353,1.605914176
C,0,-2.1547089733,2.9473474622,-2.0249641971
H,0,-1.6274579029,3.2932125306,-2.9161066617
H,0,-2.3111161904,1.8713274784,-2.1242783733
C,0,-3.4599068949,3.726608125,-1.7529121283
H,0,-3.7268250044,4.3262423506,-2.6293010145
H,0,-4.2884776625,3.0319926037,-1.5759847851
H,0,-4.1453846529,5.2514798442,-0.3592702333
C,0,-2.0260637535,5.5388821146,-0.7900992671
H,0,-2.163826546,5.996314962,-1.7774237635
C,0,-0.7776626928,4.6194319728,-0.8332143505
H,0,-0.1403860398,4.7814237813,-1.7015064555
H,0,-0.1464813863,4.7218306466,0.0518212226
N,0,-1.2034289242,3.1693633404,-0.8775795062
C,0,-1.8574880633,6.651270209,0.2117765211
H,0,-1.6688038533,6.3508117847,1.2435305115
C,0,-1.9195699809,7.9500382321,-0.0832703936
H,0,-1.7964885366,8.7148083365,0.6795318315
H,0,-2.091396425,8.3017005724,-1.0992489539
C,0,-2.1710098875,1.299083419,0.5736510419
H,0,-3.0253855733,1.0969614566,-0.0694578528
C,0,-2.5329383669,0.9842018291,2.032994134
C,0,-3.8629486663,0.6366559279,2.4449884076
C,0,-1.550294056,1.0383781139,3.0007881371
C,0,-4.9702880484,0.5159014227,1.5709188209
C,0,-4.0719122619,0.4037276189,3.8492757393
C,0,-1.867466923,0.7707189129,4.352739566
H,0,-0.5237287526,1.280896868,2.7400030962
C,0,-6.2315103093,0.1998914334,2.0493716654
H,0,-4.8596170444,0.6339679344,0.4993752606
C,0,-5.3744837213,0.0810464802,4.3042540823
H,0,-1.0802383114,0.8152884322,5.1044632153
C,0,-6.4375330977,-0.0171549918,3.4362330694
H,0,-5.5049856389,-0.088467863,5.3686732147
H,0,-7.4212411275,-0.2665171553,3.8172179816
N,0,-1.1049086307,0.4284927434,0.0876178287
O,0,-7.2217029369,0.1169356314,1.1171170946
C,0,-8.5318088756,-0.2406672284,1.5402919178
H,0,-9.1416500103,-0.2567108649,0.6344790331

H,0,-8.5532280608,-1.2363861042,2.0014963452
H,0,-8.9508386115,0.4957476877,2.2382891727
N,0,-3.0768278469,0.4741796483,4.7802072445
H,0,-0.200252123,0.51315525,0.5550009367
C,0,-1.3131503044,-0.6592790711,-0.7131834112
N,0,-0.2836891354,-1.5371177309,-0.725866424
H,0,0.4627229509,-1.3822521923,-0.0470545734
S,0,-2.7392086473,-0.859793387,-1.6381787699
O,0,3.1393631913,3.1861646448,0.785685912
O,0,1.1230181374,2.2110073363,1.1201735731
O,0,3.7659994274,-1.2676427023,1.6568081842
O,0,1.5737187319,-0.7530286244,1.4433517146
C,0,2.7563580041,-0.4137266535,1.4238487879
C,0,2.3414215154,2.0920413303,1.0199886043
C,0,3.2258217875,0.9423590548,1.159907279
C,0,4.5170666547,1.3926869498,0.9843534823
C,0,4.4626022368,2.7544134237,0.5739759365
C,0,5.4970588377,3.802795122,0.8959927878
C,0,3.4061145647,-2.644866177,1.9568268589
C,0,4.6922961974,-3.4425047389,2.02122843
H,0,5.4191202314,0.7967200382,1.0173316502
H,0,5.2772175074,4.7089644044,0.3181540143
H,0,2.8737680201,-2.6565980706,2.9142666641
H,0,2.7308699012,-3.0172707578,1.1832545824
H,0,5.2174396789,-3.420322578,1.0602668432
H,0,4.4597483411,-4.4871253672,2.2565531915
H,0,5.3658837907,-3.0575319583,2.7947323858
H,0,6.4706835044,3.4345086843,0.5536164217
C,0,4.4415336531,2.5783771585,-1.4754996214
H,0,4.400037416,3.6580370833,-1.597178829
C,0,3.227424823,1.9368732224,-1.8155274598
H,0,3.1099151444,0.8742091587,-1.9559424764
C,0,5.7395117273,1.9734712805,-1.8815550085
C,0,6.8014605742,2.8129997851,-2.2580113999
C,0,5.9506654508,0.5832625231,-1.9199627155
C,0,8.0303889143,2.2868285964,-2.6587437493
H,0,6.6553233304,3.8903871565,-2.2492360569
C,0,7.1769421347,0.0572598361,-2.3204335795
H,0,5.153177417,-0.0949653392,-1.6300522757
C,0,8.2239303405,0.9058557299,-2.69109448
H,0,8.8341477668,2.9584601021,-2.9493869522
H,0,7.315788113,-1.0206076751,-2.3439372551
H,0,9.1792737125,0.492365328,-3.0031082608

N,0,2.0619628395,2.6420493314,-1.936792307
O,0,2.0419055583,3.8988698248,-1.9052858658
O,0,0.9737124957,1.9772450929,-2.0914279502
H,0,-0.3376824752,2.6128068931,-1.0888329706
C,0,-0.1370063133,-2.7173445945,-1.5831970921
H,0,-1.0810963818,-2.8272513962,-2.1124615123
C,0,0.9717286258,-2.5328353919,-2.6824064495
C,0,2.3395062833,-2.1122172284,-2.1096989033
H,0,2.2537142746,-1.1859912066,-1.5303340168
H,0,2.7669783765,-2.8853626983,-1.470123093
H,0,3.0343134243,-1.9168162687,-2.9365183533
C,0,0.5043050582,-1.429587357,-3.6546950745
H,0,-0.4793563052,-1.6502343152,-4.0845493419
H,0,0.4526902678,-0.4512334706,-3.1665236674
H,0,1.2188877375,-1.3430447414,-4.4829107097
C,0,1.1246550238,-3.8506006766,-3.4652722695
H,0,0.1806617956,-4.1538911183,-3.9339455881
H,0,1.8604566328,-3.7244755582,-4.2687646766
H,0,1.4723797137,-4.6669212307,-2.8242414275
C,0,0.1060676624,-3.919388214,-0.6310206434
O,0,1.252182238,-4.1613040996,-0.2291038907
N,0,-0.9482292142,-4.6725810488,-0.1949741474
C,0,-0.6325367742,-5.7341566004,0.7791128149
H,0,-1.4792326578,-6.4280190111,0.7896468612
H,0,0.2405708519,-6.2818490747,0.4135586448
C,0,-2.3657939455,-4.5075688453,-0.5528877943
H,0,-2.9372425101,-4.4832078018,0.3819703071
H,0,-2.5180797022,-3.5336098567,-1.0199798009
C,0,-0.3516433641,-5.2457974915,2.2158910911
H,0,0.4955780846,-4.55320794,2.1599478742
C,0,0.0652798572,-6.4448163765,3.0788085966
H,0,0.9468728802,-6.9524604053,2.6680497004
H,0,0.3099820546,-6.1268712888,4.0993295224
H,0,-0.7421549411,-7.1864927884,3.1508182083
C,0,-1.5377345366,-4.5024392101,2.8421393785
H,0,-1.8139344588,-3.6139391621,2.2641349306
H,0,-2.423330581,-5.1479192994,2.9226001047
H,0,-1.2887025507,-4.1633640423,3.855163514
C,0,-2.9452537438,-5.6183729671,-1.4567344119
H,0,-2.7993668479,-6.5839780159,-0.9512193915
C,0,-4.4564842722,-5.3977917076,-1.611048332
H,0,-4.6702629558,-4.4438888945,-2.1098586874
H,0,-4.9093230485,-6.1956191344,-2.2116660126

H,0,-4.9648128136,-5.3851832554,-0.6388418667
C,0,-2.253433649,-5.6950715398,-2.8214485792
H,0,-1.1762958523,-5.8644721257,-2.7192150088
H,0,-2.6613047708,-6.5209904284,-3.4168701082
H,0,-2.4036718351,-4.7716432906,-3.3956252965
C,0,5.5678498286,4.1565398825,2.3892114537
H,0,6.3189238607,4.935946843,2.5639362896
H,0,4.6044204774,4.5298705618,2.7520837678
H,0,5.8406196945,3.2832909839,2.992834009

TS-CCAttack-Tak

E(RB3LYP)= -3353.33753666 Hartree

Sum of electronic and thermal Free Energies= -3352.249333 Hartree

C,0,1.2597377203,2.7561665333,-0.2637440623
C,0,1.5258697775,5.1048365434,0.6510156151
C,0,2.0619271405,4.0814567187,-0.3693633516
H,0,0.6603882422,2.5901930419,-1.1567794872
H,0,3.1233265873,3.9025409355,-0.1711472238
H,0,1.9976872893,4.4731802645,-1.3883469461
C,0,0.8321051717,3.2280742302,2.1754975335
H,0,-0.0062093702,3.3265000075,2.8666981814
H,0,1.4113171013,2.3534413463,2.473339854
C,0,1.6835492416,4.5134401374,2.0649282438
H,0,1.3641873351,5.2399552392,2.8190785695
H,0,2.7374513419,4.2887537948,2.2599331361
H,0,2.0932678675,6.0368823814,0.5709298741
C,0,0.0170394182,5.3955474478,0.412244321
H,0,-0.3346719458,6.0032101618,1.2545839348
C,0,-0.7315111139,4.0349272882,0.4320678376
H,0,-1.5648162333,4.0028200142,1.1347203108
H,0,-1.1205603366,3.7512633322,-0.5480885148
N,0,0.2226529024,2.9321517679,0.830142813
C,0,-0.2557567755,6.1618718051,-0.8560223005
H,0,-0.017039598,5.6526375915,-1.7909476629
C,0,-0.7604540166,7.3950352241,-0.9007056062
H,0,-0.9294111098,7.9077852861,-1.8443752691
H,0,-1.0273651963,7.9405346199,0.0029550766
C,0,2.1414357518,1.5009119621,-0.0375861424
H,0,2.8429804627,1.6839744782,0.7749245325
C,0,2.919292559,1.2166872169,-1.3315462986
C,0,4.3306309022,1.4377425758,-1.4614771031
C,0,2.2341135198,0.7478275759,-2.4345211765
C,0,5.1719553915,1.9020490655,-0.4217304215

C,0,4.9183772753,1.1633724567,-2.7455314833
C,0,2.9187046512,0.50328172,-3.6473578391
H,0,1.1635574481,0.5663482198,-2.3891595373
C,0,6.5267680659,2.1012264943,-0.6290018164
H,0,4.7893187837,2.0785170945,0.5760130853
C,0,6.3084357156,1.3751829233,-2.9221761294
H,0,2.363553129,0.1325464367,-4.5082583354
C,0,7.102990525,1.836062975,-1.8981953814
H,0,6.7271475016,1.1591708063,-3.9003553719
H,0,8.1629126188,1.9868825642,-2.0670261429
N,0,1.3157484652,0.3767409192,0.3900897884
O,0,7.2374102584,2.5546215995,0.4421476429
C,0,8.6469089923,2.7001802146,0.3143093849
H,0,9.0010583938,3.0323133497,1.2926105116
H,0,9.1326578146,1.7488325164,0.0625790113
H,0,8.9125149304,3.4566407903,-0.4356190657
N,0,4.2089607922,0.7036908346,-3.8166622166
H,0,0.507092624,0.1373899113,-0.1958957907
C,0,1.7646539136,-0.6207740572,1.2146799589
N,0,0.8525116416,-1.6060224513,1.4108269285
H,0,-0.0488554832,-1.489627935,0.9485690941
S,0,3.3060289086,-0.5960536021,1.9385954587
O,0,-2.9466073354,-0.55783771,1.4381252473
O,0,-1.8286779258,1.3766371935,1.784813265
O,0,-5.9295340119,2.8668907894,0.9086876307
O,0,-3.8891087521,3.6732408074,1.4629293731
C,0,-4.6172024938,2.7213880232,1.2259279902
C,0,-2.8881358835,0.8196386264,1.5079816065
C,0,-4.2309686442,1.311012544,1.2423333639
C,0,-5.0330281257,0.2062697207,1.0140930702
C,0,-4.2180574877,-0.9485672005,1.0030240458
C,0,-4.6209896962,-2.3398717144,1.4068481599
C,0,-6.4261305761,4.2225190239,0.8616525285
C,0,-7.9087699359,4.1569812844,0.5543750974
H,0,-6.089815863,0.2132544587,0.7843113436
H,0,-3.816088498,-3.0347895042,1.1409339594
H,0,-6.2322409703,4.7091742274,1.823045797
H,0,-5.8764913177,4.7762376594,0.0926351356
H,0,-8.0924471101,3.664031272,-0.4063814507
H,0,-8.3200032483,5.1714323525,0.5015266936
H,0,-8.4493929089,3.6087657575,1.3333255459
H,0,-5.4996855754,-2.6242485514,0.8170306474
C,0,-3.7907026802,-1.1007652705,-1.1056658558

H,0,-3.1661798363,-1.9657880536,-0.9017163677
C,0,-3.0730394955,0.0638628644,-1.4349453041
H,0,-3.5156981066,0.9663318758,-1.8284431051
C,0,-5.0796029968,-1.4059138871,-1.7682589291
C,0,-5.4190360239,-2.7468521557,-2.01999681
C,0,-5.9805451882,-0.4057656943,-2.1795574443
C,0,-6.6117959043,-3.0791465492,-2.6631234879
H,0,-4.731583621,-3.5335545051,-1.7197888295
C,0,-7.1708758132,-0.737885245,-2.8210384943
H,0,-5.7552327401,0.6391053936,-1.9855721007
C,0,-7.4930425838,-2.0761037852,-3.0669168297
H,0,-6.8484823213,-4.1230987729,-2.8512606187
H,0,-7.8517547768,0.0507316262,-3.1308750534
H,0,-8.4222762365,-2.3315984339,-3.5689882053
N,0,-1.7246081263,0.1630985884,-1.2548412498
O,0,-1.0214347734,-0.8349498259,-0.8915546747
O,0,-1.1591446177,1.2789236927,-1.4830543787
H,0,-0.3553734586,2.0766365485,0.9265409393
C,0,1.0914792684,-2.9148206842,2.0336865155
H,0,2.167000549,-2.9862477542,2.1871554821
C,0,0.4351561073,-3.0791746892,3.4496679668
C,0,-1.0638376248,-2.7299630672,3.4696964043
H,0,-1.2391991574,-1.6979311951,3.1493406684
H,0,-1.6355422573,-3.3949584333,2.8214233767
H,0,-1.4455016815,-2.8246238428,4.4946810384
C,0,1.1607356786,-2.1423049854,4.4358117766
H,0,2.2285686338,-2.3745392076,4.5122649656
H,0,1.0721567016,-1.0927196208,4.1395864268
H,0,0.7199370139,-2.2461423266,5.4355800768
C,0,0.6380356712,-4.5315489256,3.9254024273
H,0,1.7004575138,-4.8056345917,3.9443270922
H,0,0.255856783,-4.6468904398,4.947241811
H,0,0.1068515804,-5.2449953458,3.2886661522
C,0,0.6171042575,-3.9597054463,0.986117553
O,0,-0.5505320932,-4.3636975115,0.9927923154
N,0,1.4865811866,-4.3706783699,0.0116955862
C,0,0.9339962081,-5.2704334911,-1.0164509601
H,0,1.7802938134,-5.7449059775,-1.5243213709
H,0,0.3670352006,-6.0573705558,-0.5104370807
C,0,2.8975442547,-3.9855952659,-0.1346578015
H,0,3.0508545652,-3.6967907103,-1.1806190738
H,0,3.1033044646,-3.0925412557,0.4574396193
C,0,0.0229085759,-4.588007086,-2.0589722456

H,0,-0.7966601789,-4.1141331231,-1.5080909082
C,0,-0.5731291815,-5.6593183126,-2.9822184384
H,0,-1.1354261331,-6.4129910881,-2.4169649623
H,0,-1.2590677491,-5.2109610889,-3.7109377839
H,0,0.2102371605,-6.1826524863,-3.5477643853
C,0,0.7436789087,-3.5019908377,-2.8667034518
H,0,1.1247452503,-2.7019777909,-2.2236372077
H,0,1.5856122353,-3.9163993066,-3.4386761434
H,0,0.0561878639,-3.0377968561,-3.58427849
C,0,3.9128636114,-5.0914798293,0.2300421119
H,0,3.675999784,-5.9831645175,-0.3686824276
C,0,5.323568202,-4.6269857713,-0.1580337561
H,0,5.6086441832,-3.7208865609,0.3916319144
H,0,6.0667373478,-5.4007367367,0.0685340042
H,0,5.3941486511,-4.4011966236,-1.2292585075
C,0,3.8456014684,-5.4886836526,1.7083402869
H,0,2.841450153,-5.8239557951,1.9900618843
H,0,4.5384676176,-6.3119704701,1.9212632498
H,0,4.1228825102,-4.6488624003,2.3585302146
C,0,-4.9400883877,-2.4736693183,2.9045850654
H,0,-5.1890728346,-3.5129240678,3.149512828
H,0,-4.0850203866,-2.1789280579,3.5211387448
H,0,-5.7936799127,-1.8460032987,3.185996803

dr1-TS-CCAtack-Pap

E(RB3LYP)= -3353.33698798 Hartree

Sum of electronic and thermal Free Energies= -3352.245816 Hartree

C,0,-0.3698233758,2.6429519519,1.1144217893
C,0,0.009171668,4.989109585,0.2250969897
C,0,-0.9013520265,4.1031877166,1.0972017087
H,0,0.0548428149,2.3935436757,2.0847121966
H,0,-1.9181698947,4.1334228635,0.6920619323
H,0,-0.962616717,4.4875676661,2.1191889238
C,0,0.4925324201,2.9945450498,-1.2336614738
H,0,1.4208320071,2.8576467862,-1.7904509858
H,0,-0.2427029337,2.2849129849,-1.6184636138
C,0,-0.0196861645,4.452274825,-1.2196508951
H,0,0.6027862636,5.0778464665,-1.8681633891
H,0,-1.0414324632,4.4978859526,-1.6119211921
H,0,-0.3508782611,6.0223073226,0.2486496779
C,0,1.4764884535,4.9416764372,0.7336796372
H,0,2.0901231677,5.4880606584,0.0076447958
C,0,1.9208217249,3.4532732094,0.7375541179

H,0,2.7957006357,3.2698759108,0.1123637222
H,0,2.1250505373,3.0712093856,1.7393178412
N,0,0.8203060097,2.578003588,0.1782644116
C,0,1.672180378,5.5873043509,2.0812432048
H,0,1.1867363005,5.1009856108,2.9287566965
C,0,2.3919679907,6.6894206739,2.2939479527
H,0,2.4970995526,7.1188205891,3.2872233777
H,0,2.9067393782,7.2051522179,1.4850183421
C,0,-1.4692833836,1.6071663655,0.7752836794
H,0,-1.9664972243,1.9072071527,-0.1447698674
C,0,-2.4789589527,1.5756099855,1.9307362447
C,0,-3.8326267385,2.0301429332,1.7913772319
C,0,-2.0804927669,1.100121518,3.1639908469
C,0,-4.395145154,2.5210916775,0.5887318686
C,0,-4.6613027035,1.982802209,2.9664574118
C,0,-2.9888624144,1.0825692438,4.2478763058
H,0,-1.071182136,0.7287692761,3.3205283095
C,0,-5.707395933,2.962512925,0.5384948586
H,0,-3.8288349579,2.5335468077,-0.3349761749
C,0,-5.9989060596,2.4424870805,2.8793625945
H,0,-2.6594818161,0.7022464746,5.2141072424
C,0,-6.5197292483,2.9265310939,1.7014488582
H,0,-6.6033350836,2.3973836685,3.7801794794
H,0,-7.5476629148,3.2693838054,1.6698432161
N,0,-0.9246407215,0.2807599274,0.5017622121
O,0,-6.1406158251,3.4146840122,-0.6712309881
C,0,-7.4871745918,3.8563943818,-0.7945496326
H,0,-7.6067597099,4.154349883,-1.838304987
H,0,-8.2010363045,3.0542156004,-0.5681418362
H,0,-7.6916770569,4.7217964427,-0.1508919705
N,0,-4.2309011959,1.5131077465,4.1733237695
H,0,-0.4207905747,-0.1732557803,1.2655351539
C,0,-1.3423908693,-0.5099318094,-0.5343667787
N,0,-1.0151784736,-1.8149996933,-0.3874233495
H,0,-0.6200397752,-2.0898113284,0.512354579
S,0,-2.1665783287,0.1135503951,-1.8951103107
O,0,3.6337275288,0.1622150828,2.2214205435
O,0,1.425121143,0.5851761589,2.4268283884
O,0,1.3841847833,-3.7497560224,3.0630767141
O,0,-0.0020145328,-2.0810581051,2.4218764145
C,0,1.1336902278,-2.4887411917,2.6756889369
C,0,2.3336363472,-0.2361066154,2.4088059702
C,0,2.3414070924,-1.6815578913,2.5802611855

C,0,3.6583434105,-2.0902018537,2.4967431697
C,0,4.4677728063,-0.9751459475,2.1403563625
C,0,5.8611622091,-0.7142417627,2.6515801556
C,0,0.2414509478,-4.646951651,3.1365978282
C,0,0.7461431239,-5.9827080939,3.6414915043
H,0,4.0246897392,-3.1055657178,2.5806999561
H,0,6.3170795925,0.0765421142,2.0420049832
H,0,-0.4972979628,-4.2089629684,3.8150515749
H,0,-0.20759596,-4.7275513932,2.1430261201
H,0,1.4894897589,-6.4091617468,2.9593578844
H,0,-0.092788055,-6.6844218796,3.7100413596
H,0,1.1981439825,-5.8893921469,4.6349443323
H,0,6.4570143848,-1.6192522531,2.4965002991
C,0,4.6162373874,-1.2346377828,0.0810661078
H,0,3.6253390324,-1.6670533962,-0.0094671927
C,0,4.7085432099,0.0520433532,-0.5013980075
H,0,5.6303115523,0.5454983008,-0.7699450755
C,0,5.7205221468,-2.2112180082,-0.1120810094
C,0,5.4260667519,-3.5862238079,-0.1045856293
C,0,7.0568291117,-1.8229754807,-0.3157576806
C,0,6.4250633918,-4.53870828,-0.2975859258
H,0,4.3976721079,-3.9076021014,0.0429974278
C,0,8.0574120996,-2.7752282227,-0.5049171948
H,0,7.3213209624,-0.7700172413,-0.3301196148
C,0,7.7475276295,-4.1367376038,-0.496627857
H,0,6.1693377145,-5.5951052774,-0.2969414664
H,0,9.0828322562,-2.4510212449,-0.6626729932
H,0,8.5288293248,-4.8767778633,-0.6477190263
N,0,3.6005753442,0.7944284188,-0.7787683739
O,0,2.4301279486,0.356296515,-0.4950370422
O,0,3.7441060177,1.9207365328,-1.3451790398
H,0,1.2202509207,1.6151468473,0.1230889476
C,0,-1.1850943004,-2.888206451,-1.3713434028
H,0,-1.7979280938,-2.4751488996,-2.1701054414
C,0,0.1694334775,-3.3284844754,-2.0355242378
C,0,1.260584349,-3.6974553181,-1.0119692402
H,0,1.4778106761,-2.8510294772,-0.3503008243
H,0,0.9750309739,-4.5565132382,-0.4033194614
H,0,2.1892664388,-3.9363786301,-1.5456082515
C,0,0.6937806874,-2.1519145849,-2.884791347
H,0,-0.0365945522,-1.8336619191,-3.6369036579
H,0,0.9503991227,-1.283484197,-2.269312899
H,0,1.6063095432,-2.4568871836,-3.412504429

C,0,-0.0977244265,-4.5272701025,-2.9659463646
 H,0,-0.8395231858,-4.2816610792,-3.7359535874
 H,0,0.8258614426,-4.8108364647,-3.4850797314
 H,0,-0.4492972553,-5.4030859787,-2.4119765556
 C,0,-1.9382231368,-4.0328255347,-0.6399535173
 O,0,-1.3033137195,-4.8838218499,-0.0025578273
 N,0,-3.3039857179,-4.0672900066,-0.6646852628
 C,0,-3.9504240586,-5.1486949896,0.1013534266
 H,0,-4.9791671563,-5.2314879574,-0.2642675754
 H,0,-3.4389701974,-6.0861369746,-0.1358096382
 C,0,-4.1993645481,-3.1080058428,-1.3292866907
 H,0,-4.9466846204,-2.7954109483,-0.5911300714
 H,0,-3.6449114654,-2.2067347441,-1.5940077666
 C,0,-3.9665188273,-4.963546655,1.6337185216
 H,0,-2.9229514758,-4.9519469574,1.9678297612
 C,0,-4.6609168293,-6.1745233305,2.2720992918
 H,0,-4.17346971,-7.1161932155,1.9902922299
 H,0,-4.6428018109,-6.106327315,3.366329123
 H,0,-5.713758493,-6.2390850364,1.9649743285
 C,0,-4.6249755373,-3.6517700227,2.077651463
 H,0,-4.1068591612,-2.7776084796,1.6687622131
 H,0,-5.67823255,-3.6022379638,1.7694025856
 H,0,-4.6017115469,-3.5599355621,3.1704909877
 C,0,-4.9326507369,-3.6521909526,-2.5752637023
 H,0,-5.5026471587,-4.5444553362,-2.2775105566
 C,0,-5.9355103827,-2.5966464677,-3.0613072939
 H,0,-5.4229304323,-1.6758291276,-3.3668369935
 H,0,-6.5046521992,-2.9634743068,-3.9236687529
 H,0,-6.6546667476,-2.3306024798,-2.2766918858
 C,0,-3.9719012419,-4.062934972,-3.695808047
 H,0,-3.2617190995,-4.8255921753,-3.3583948746
 H,0,-4.5238816274,-4.4809066546,-4.5465008198
 H,0,-3.401227617,-3.2014419875,-4.06599552
 C,0,5.9080386359,-0.3071093477,4.1320379523
 H,0,6.9421472264,-0.1138545438,4.4408616307
 H,0,5.3277563388,0.6038303472,4.3115375596
 H,0,5.5059322178,-1.0968256563,4.7772800802

dr1-TS-CCAttack-Tak

E(RB3LYP)= -3353.33595263 Hartree

Sum of electronic and thermal Free Energies= -3352.248685 Hartree

C,0,-0.2462255647,2.7542638469,0.347185632

C,0,0.2627323517,4.9662910738,-0.785594695

C,0,-0.5260786683,4.2821677268,0.3480591851
H,0,0.2697056214,2.4426982039,1.2566978632
H,0,-1.5934608176,4.471072959,0.202542606
H,0,-0.2651615131,4.7088859907,1.3206023445
C,0,0.2585601937,2.8324806445,-2.1234902552
H,0,1.0795001354,2.6055890599,-2.8040930855
H,0,-0.5698947517,2.1617828053,-2.3574151517
C,0,-0.1453575938,4.3242934733,-2.1267836274
H,0,0.3431875003,4.8400367042,-2.9597301301
H,0,-1.2257544803,4.425776878,-2.2754893489
H,0,0.0350063598,6.0365391067,-0.797118441
C,0,1.7900075515,4.760517969,-0.5942077366
H,0,2.2877059944,5.1152382474,-1.5043973365
C,0,2.0401360719,3.2344244711,-0.457628399
H,0,2.7908559163,2.8698615334,-1.1595837106
H,0,2.3404834535,2.9472353884,0.5522247119
N,0,0.7659219462,2.4737233429,-0.7486048276
C,0,2.3639870477,5.5232773542,0.5713434407
H,0,2.0019973774,5.2423369507,1.5617754529
C,0,3.2691175583,6.4966855292,0.4660036488
H,0,3.6452099314,7.0219981565,1.3404296401
H,0,3.6707434487,6.8065974278,-0.4972444439
C,0,-1.5236478492,1.8875671696,0.1948746459
H,0,-2.0992270442,2.2262982552,-0.6649771758
C,0,-2.3657159364,2.0273189637,1.4723024195
C,0,-3.5887126819,2.7764983563,1.5201048798
C,0,-1.9302232285,1.4284866308,2.6374751258
C,0,-4.1796300258,3.4248163269,0.4086428448
C,0,-4.2471925064,2.8712598944,2.7956358051
C,0,-2.669513212,1.5751391431,3.8341275321
H,0,-1.0265525684,0.8247794579,2.6534076423
C,0,-5.3518062338,4.15143307,0.5401280007
H,0,-3.7501182151,3.3512330407,-0.5834600576
C,0,-5.4462344657,3.6201089922,2.8941554451
H,0,-2.3122384919,1.0952924458,4.7444449623
C,0,-5.9928874407,4.2532650378,1.8018459459
H,0,-5.9221914836,3.6757891616,3.8684565919
H,0,-6.9126760282,4.8163057739,1.9115201619
N,0,-1.1687069687,0.5033098914,-0.0791161862
O,0,-5.8222131536,4.7361186707,-0.5964329565
C,0,-7.0056487021,5.523266288,-0.526682489
H,0,-7.1691652275,5.9012977692,-1.5380274787
H,0,-7.8753695731,4.9259740563,-0.2243299507

H,0,-6.8885108612,6.3731628463,0.1580106306
N,0,-3.7805202939,2.2746554297,3.9303146762
H,0,-0.5842143813,0.0255649685,0.6218855291
C,0,-1.8151281506,-0.3016290646,-0.9726890787
N,0,-1.4872954964,-1.6101127729,-0.8452678739
H,0,-0.8390839205,-1.8482114907,-0.0950128239
S,0,-2.8919340254,0.3026863385,-2.1534318589
O,0,3.1485464745,-1.3927646652,-0.9511490185
O,0,2.3420905723,0.46812658,-1.9477514317
O,0,6.6577170997,1.476533188,-1.589036167
O,0,4.7187760575,2.4233312483,-2.2770548609
C,0,5.3138847715,1.4727563799,-1.7873551182
C,0,3.3075590156,-0.1283750341,-1.4913519166
C,0,4.714565739,0.2179828318,-1.3485649714
C,0,5.3262136192,-0.8411989964,-0.6972043817
C,0,4.3489774921,-1.8070848797,-0.3626654603
C,0,4.5462847079,-3.2974340449,-0.3479184531
C,0,7.3560745209,2.6776346357,-1.9838088712
C,0,8.8282709594,2.4691631495,-1.6893156292
H,0,6.3739519143,-0.9176689116,-0.4370224945
H,0,3.7049914126,-3.7649585401,0.1789649978
H,0,7.1781028667,2.860722305,-3.0485905021
H,0,6.9472380058,3.5282813072,-1.4279625291
H,0,8.9960404056,2.2832269847,-0.6228587594
H,0,9.3922731503,3.3648650902,-1.9734541583
H,0,9.2273931753,1.6204150239,-2.2548947638
H,0,5.4496346059,-3.5171405121,0.2306996792
C,0,3.9231318366,-1.276217575,1.7196662683
H,0,4.0905222922,-0.221130068,1.5323177853
C,0,2.567053183,-1.6197197164,1.8755506238
H,0,2.2039899208,-2.5823830701,2.2025734639
C,0,4.9858911371,-1.9455483674,2.4977350456
C,0,6.213536926,-1.2822809126,2.682190544
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C,0,7.2418381831,-1.8614495359,3.4212451476
H,0,6.3532343629,-0.2966443313,2.244360981
C,0,5.8572465248,-3.7971169283,3.8186817245
H,0,3.8896189768,-3.7533208851,2.972305769
C,0,7.0691528018,-3.1253636539,3.9910783648
H,0,8.177503434,-1.3250182724,3.5557684318
H,0,5.7107440614,-4.7780889434,4.2630734789
H,0,7.8700366507,-3.5806149212,4.5673222126
N,0,1.5724014904,-0.7592828491,1.5297300714

O,0,1.8078590432,0.4236428648,1.134419484
O,0,0.3563842888,-1.1582654771,1.6547741562
H,0,1.016629821,1.4702713156,-0.7429610349
C,0,-2.003309524,-2.738370454,-1.6265295883
H,0,-2.7610437374,-2.3250962895,-2.2885613344
C,0,-0.9090165105,-3.3918072466,-2.5439842912
C,0,0.3849950107,-3.7469929365,-1.7864078683
H,0,0.8805348529,-2.8540259319,-1.3903646422
H,0,0.1904441626,-4.4360837631,-0.9630266964
H,0,1.0908508983,-4.221500191,-2.4801094536
C,0,-0.5577481363,-2.3869810341,-3.6593509407
H,0,-1.4340134889,-2.1187943354,-4.2612891398
H,0,-0.130643956,-1.463863676,-3.255551426
H,0,0.1890201109,-2.8253376249,-4.3333491109
C,0,-1.4916694959,-4.6626284562,-3.1917537225
H,0,-2.4062918723,-4.4471748598,-3.7576350289
H,0,-0.767185823,-5.0885637998,-3.8966175978
H,0,-1.7180948915,-5.4302971768,-2.4455079869
C,0,-2.6357922549,-3.7148740173,-0.5970541196
O,0,-1.91789816,-4.5257019417,-0.0018838001
N,0,-3.9714250272,-3.6292889368,-0.3070404727
C,0,-4.4678727518,-4.5282374049,0.7511603388
H,0,-5.559707022,-4.5481925498,0.6713045069
H,0,-4.1024540026,-5.5380769103,0.5419675998
C,0,-4.9522566288,-2.7023554187,-0.8913399203
H,0,-5.4797298423,-2.2184114867,-0.0611767436
H,0,-4.4361746402,-1.9014207417,-1.4227557774
C,0,-4.0667499057,-4.1416759877,2.1903709123
H,0,-2.973032381,-4.1758403185,2.2382522126
C,0,-4.62224752,-5.1929798958,3.1610299122
H,0,-4.2703681741,-6.2010795154,2.9091757101
H,0,-4.3097462174,-4.9803706685,4.1903225472
H,0,-5.72098685,-5.2098367494,3.148175821
C,0,-4.5229054975,-2.7314745859,2.5844779764
H,0,-4.0912203645,-1.9650656827,1.9312906672
H,0,-5.6168120031,-2.633828691,2.5496962312
H,0,-4.2076656076,-2.4977563693,3.6088215721
C,0,-5.9949922059,-3.3547629239,-1.8254099209
H,0,-6.5112062539,-4.1484690599,-1.265469958
C,0,-7.0412440137,-2.301541044,-2.2171825007
H,0,-6.5821231445,-1.4760789606,-2.7760934085
H,0,-7.8208348822,-2.7395210335,-2.8518221144
H,0,-7.53278143,-1.8716158045,-1.3355476567

C,0,-5.3591405545,-3.9938285913,-3.0639857986
H,0,-4.6212453806,-4.7545718701,-2.7884361506
H,0,-6.1202911829,-4.4820781211,-3.684721366
H,0,-4.8596424764,-3.2410514344,-3.6875770937
C,0,4.6665899712,-3.9098468482,-1.7529965053
H,0,4.7905857235,-4.9970762473,-1.6846510512
H,0,3.7708137076,-3.7097559457,-2.3494540703
H,0,5.530957796,-3.5045033387,-2.2916083084

ee-TS-CCAttack-Pap

E(RB3LYP)= -3353.32782763 Hartree

Sum of electronic and thermal Free Energies= -3352.239720 Hartree

C,0,0.0729063127,-2.5141046958,-0.1926757531
C,0,0.0425369427,-4.8560675204,-1.1655470342
C,0,0.4029787842,-4.0089056754,0.0702001848
H,0,-0.7137107505,-2.1600488539,0.4775427724
H,0,1.4694859103,-4.1272381653,0.2844951467
H,0,-0.1331783986,-4.3586540177,0.9568785828
C,0,0.3738621699,-2.870334305,-2.6755971103
H,0,-0.2002019393,-2.7830487701,-3.5998420354
H,0,1.1984030387,-2.1566266438,-2.7276088347
C,0,0.8281275984,-4.3169770937,-2.3776993258
H,0,0.6587606813,-4.9494554707,-3.2551271302
H,0,1.9021310191,-4.3427253597,-2.1654286096
H,0,0.3040098409,-5.9027531525,-0.9841728302
C,0,-1.4755985065,-4.7499301295,-1.483371496
H,0,-1.6403748302,-5.2221796594,-2.4591082853
C,0,-1.819424962,-3.2401410375,-1.5937749699
H,0,-2.3409947063,-2.9833082849,-2.5155392112
H,0,-2.4215399377,-2.8905521222,-0.7513788106
N,0,-0.553535607,-2.4187352379,-1.574123925
C,0,-2.3566500291,-5.4447002734,-0.47785557
H,0,-2.3400204813,-5.0461747651,0.5378893471
C,0,-3.1341138669,-6.4926209545,-0.7520424826
H,0,-3.7435616109,-6.9661521419,0.0135808498
H,0,-3.1910340448,-6.9216244464,-1.7510942579
C,0,1.2933470063,-1.5743950965,-0.0585434616
H,0,2.1021029076,-1.9281388306,-0.695226517
C,0,1.7591870409,-1.559507017,1.4037032147
C,0,3.0162384304,-2.114532164,1.8177396292
C,0,0.9451276512,-1.0076153307,2.3718730391
C,0,3.9646489338,-2.6974118149,0.9428802475
C,0,3.315430142,-2.0753623096,3.2241001334

C,0,1.3504893234,-1.0101360178,3.7271989251
H,0,-0.0164847445,-0.5715693963,2.1159980668
C,0,5.1493783155,-3.2321893439,1.4223093067
H,0,3.8128190509,-2.7057638642,-0.1299321818
C,0,4.536026245,-2.6322191616,3.6801822387
H,0,0.6966715734,-0.5710461114,4.4797292442
C,0,5.4372985447,-3.2031939284,2.8114403718
H,0,4.7368073882,-2.5914031119,4.7464158651
H,0,6.3625496627,-3.618891487,3.1937424557
N,0,0.9477985968,-0.2467380502,-0.5444000721
O,0,5.9857584947,-3.7671335954,0.4892604941
C,0,7.2426446171,-4.2815563708,0.91334626
H,0,7.7466893054,-4.6198969419,0.0055004784
H,0,7.8562001283,-3.5096217575,1.3947483903
H,0,7.1250253516,-5.1345066751,1.5942813098
N,0,2.4826223679,-1.5276471335,4.1558961688
H,0,0.1525594649,0.2113839759,-0.092162528
C,0,1.7897097152,0.5577494028,-1.2644517702
N,0,1.4007558863,1.850868949,-1.3075361302
H,0,0.5439036096,2.0928671463,-0.8094078403
S,0,3.170835312,-0.0593757006,-2.0613445473
O,0,-2.9757565727,2.5697445016,-0.4735126608
O,0,-1.2379136163,1.3317005052,0.2543190745
O,0,-4.6658865973,-0.874572213,2.0165489301
O,0,-2.4605767089,-1.178218049,1.6174342615
C,0,-3.4732811565,-0.497534113,1.4975571214
C,0,-2.455634736,1.491631461,0.1903350867
C,0,-3.5757063669,0.7704125297,0.7831927112
C,0,-4.7204632887,1.4827195459,0.4827895073
C,0,-4.3820661367,2.5030572576,-0.4439491147
C,0,-5.0453794828,3.8520282301,-0.5574738762
C,0,-4.6878880219,-2.123845159,2.7433584883
C,0,-6.1152212896,-2.3687971699,3.1898051444
H,0,-5.7302089697,1.2322719017,0.7774182449
H,0,-4.7123841691,4.3360544225,-1.4837411304
H,0,-4.323945889,-2.9244056509,2.0904137912
H,0,-4.0027195042,-2.0515612465,3.59448644
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H,0,-6.1689016083,-3.3070968274,3.7532717832
H,0,-6.7910105763,-2.4462564007,2.3311874153
H,0,-6.12540097,3.6930438933,-0.6502760793
C,0,-4.7268087585,1.530528797,-2.2213738076
H,0,-4.3784653728,2.3887892586,-2.7912128671

C,0,-3.84565999,0.4277150955,-2.3075521234
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C,0,-6.1971485079,1.3075799401,-2.3052039039
C,0,-6.9903143764,2.2303185789,-3.0078018005
C,0,-6.8345610168,0.1949106369,-1.7274269014
C,0,-8.3686148297,2.0504265446,-3.1318677257
H,0,-6.5168081981,3.0909852754,-3.4733893558
C,0,-8.2105963393,0.0143765846,-1.8506433185
H,0,-6.252660329,-0.5331303524,-1.1687571069
C,0,-8.9855683257,0.9412925508,-2.5532594617
H,0,-8.9578903884,2.7773235342,-3.684870178
H,0,-8.6810376651,-0.8535592674,-1.3954744948
H,0,-10.0585083972,0.797869025,-2.6482954494
N,0,-2.5963733173,0.549908488,-2.8646655438
O,0,-2.1924829499,1.6316703653,-3.3412120821
O,0,-1.8627711752,-0.5014162035,-2.9284562624
H,0,-0.8419401624,-1.4401672482,-1.7895408045
C,0,2.1062889711,2.9606357047,-1.9596867219
H,0,2.9977236091,2.5243313066,-2.4046691123
C,0,1.2872241137,3.5957194183,-3.1386497311
C,0,-0.0966950565,4.1357119536,-2.7285508183
H,0,-0.7264827185,3.362637784,-2.2794557371
H,0,-0.0141450169,4.9685297927,-2.0293270447
H,0,-0.6236991857,4.4807484921,-3.6274599683
C,0,1.0872263853,2.5080648966,-4.2147533277
H,0,2.0388419957,2.0602265616,-4.5253486114
H,0,0.4215679813,1.7125265768,-3.8674117651
H,0,0.618969374,2.9513447137,-5.1024353872
C,0,2.1186219229,4.7450831782,-3.7397644587
H,0,3.0895672603,4.3968677646,-4.1124897037
H,0,1.5833805249,5.1878942761,-4.588503853
H,0,2.2935137802,5.5450958168,-3.0116362385
C,0,2.4750942243,3.9596921835,-0.8282875996
O,0,1.6147484218,4.7355224139,-0.4013800566
N,0,3.725542053,3.9406809063,-0.2641506972
C,0,3.9375813001,4.8693380618,0.8620341834
H,0,5.018705201,4.9569249808,1.0108109167
H,0,3.5634845635,5.8536730138,0.5660657073
C,0,4.842154281,3.0395326526,-0.5863098669
H,0,5.1665099091,2.5727734387,0.3512608009
H,0,4.4864550211,2.222479141,-1.2152172785
C,0,3.2690485921,4.4664772667,2.193880772
H,0,2.1901018305,4.4239143011,2.0103801401

C,0,3.5339803299,5.5632044888,3.2343045627
H,0,3.1752160736,6.5409383314,2.8893404322
H,0,3.0257331268,5.3387194612,4.1796563458
H,0,4.6067556257,5.6585556159,3.4525885139
C,0,3.7265792945,3.0968803048,2.7095780175
H,0,3.4957493982,2.2951468895,1.999619545
H,0,4.8074940561,3.0782314751,2.9061959611
H,0,3.2203813387,2.8496338691,3.650854892
C,0,6.0652281202,3.7121366925,-1.2480099558
H,0,6.3892922437,4.5462726292,-0.6088901531
C,0,7.2179331498,2.6997417178,-1.3108437102
H,0,6.9489485624,1.8276085069,-1.9205915383
H,0,8.1129121768,3.151586905,-1.7548022587
H,0,7.4897132375,2.3346930424,-0.3126613167
C,0,5.7512064472,4.2809881702,-2.6348748637
H,0,4.9375139561,5.0122685699,-2.5962293329
H,0,6.6291247724,4.786670111,-3.0555993087
H,0,5.4634618706,3.4855323269,-3.334632761
C,0,-4.7502478136,4.7777112682,0.6324913563
H,0,-3.6748490929,4.955413236,0.7351404948
H,0,-5.2401493468,5.7484707219,0.492784111
H,0,-5.1145156225,4.3473934237,1.5726431425

ee-TS-CCAttack-Tak

E(RB3LYP)= -3353.33486421 Hartree

Sum of electronic and thermal Free Energies= -3352.247608 Hartree

C,0,1.4509930501,2.6471573275,-0.4085281142
C,0,2.3725234135,4.8067187595,0.553878078
C,0,2.457558893,3.8116162821,-0.6195891531
H,0,0.7012312113,2.6134078155,-1.2018558767
H,0,3.4767580102,3.4189237602,-0.6813545933
H,0,2.259508903,4.3105816848,-1.5725063045
C,0,1.4885702173,3.0150769284,2.0862654552
H,0,0.8122051535,3.2935071585,2.8970771232
H,0,1.8538592819,2.006562526,2.2874047192
C,0,2.6227202435,4.0421525084,1.8688840423
H,0,2.6629921262,4.7375689222,2.7136612753
H,0,3.5919567185,3.5341165012,1.8257775593
H,0,3.1234820472,5.5921867164,0.42720386
C,0,0.9584486459,5.445731416,0.6284991605
H,0,0.8938837821,5.9913245234,1.5775975188
C,0,-0.0681869068,4.2823025785,0.6489372609
H,0,-0.7873177141,4.3719435338,1.4641046058

H,0,-0.6303941202,4.1954913178,-0.2823232028
N,0,0.6406956047,2.9623020083,0.8408171422
C,0,0.6634254131,6.4176733739,-0.4839885103
H,0,0.6454065475,6.006908439,-1.4944235304
C,0,0.4231960425,7.7173831389,-0.3082462283
H,0,0.2211160256,8.3776490037,-1.1478507491
H,0,0.4177688617,8.1740462148,0.6801645467
C,0,2.1299325282,1.2579087961,-0.3211547497
H,0,2.8930031002,1.2722921474,0.4549830174
C,0,2.7768927257,0.9331707786,-1.67578602
C,0,4.199278161,0.8638809511,-1.8570484158
C,0,1.9728662823,0.7065475027,-2.7749659272
C,0,5.1528901393,1.053603694,-0.8275715636
C,0,4.6752331501,0.5887264443,-3.1864478332
C,0,2.5538560949,0.427548529,-4.0343511073
H,0,0.889097972,0.7390263445,-2.6963238404
C,0,6.512350359,0.9905322678,-1.0871028821
H,0,4.8509515989,1.2145774031,0.2004010463
C,0,6.0721825742,0.5306190053,-3.4163384649
H,0,1.9055741203,0.2495391986,-4.8915077042
C,0,6.9791602514,0.7293996964,-2.4010274684
H,0,6.4038889932,0.3210439341,-4.4286635313
H,0,8.0412374538,0.6777896315,-2.6110105396
N,0,1.1636559497,0.2486495064,0.0850837494
O,0,7.3352749333,1.1898440225,-0.0194527618
C,0,8.7416082861,1.0945210119,-0.2127447539
H,0,9.1878030484,1.26362928,0.7695833229
H,0,9.0361470804,0.0998876367,-0.5710799104
H,0,9.1111084815,1.8592713341,-0.9082894295
N,0,3.8509404968,0.3756113929,-4.2526749526
H,0,0.3682542642,0.0881079969,-0.5483098186
C,0,1.4209698968,-0.7573221967,0.9754659049
N,0,0.4783322265,-1.7271545211,0.9716265652
H,0,-0.2993079137,-1.609645333,0.3235215666
S,0,2.7809345968,-0.7509628195,2.011081735
O,0,-2.8985997472,2.7748081671,0.080111312
O,0,-1.6729425527,1.6679060774,1.6335309685
O,0,-5.7780643219,0.222050743,2.5447862912
O,0,-3.73591428,0.2839146388,3.529914761
C,0,-4.4741027455,0.6059110374,2.6170926735
C,0,-2.7818097632,1.9061791107,1.1504262259
C,0,-4.122014113,1.4650511628,1.4832803675
C,0,-4.9854091511,2.0736889771,0.5871583754

C,0,-4.2305066918,2.7986396057,-0.3579592425
C,0,-4.6363361605,4.0705015549,-1.0501902457
C,0,-6.2679736717,-0.5708602047,3.6472256198
C,0,-7.7308924716,-0.8669696311,3.3818599112
H,0,-6.0607936052,1.964056535,0.5618513096
H,0,-3.9384043795,4.2728755087,-1.8726864874
H,0,-5.675972843,-1.4890616409,3.7197323894
H,0,-6.128830995,-0.0123834494,4.5791183526
H,0,-8.3131175794,0.0578900082,3.3067549525
H,0,-8.142999137,-1.4655479871,4.2022002096
H,0,-7.8567360633,-1.4307169782,2.4511434074
H,0,-5.6215084725,3.9090254552,-1.5021773641
C,0,-4.1017049768,1.3487368302,-1.9819636877
H,0,-3.6042568113,2.1110790559,-2.5739980449
C,0,-3.253771329,0.3198998704,-1.5444988905
H,0,-3.5806186277,-0.6352961341,-1.1626404548
C,0,-5.4993872929,1.063522169,-2.3781320077
C,0,-6.0734823772,1.7935636687,-3.433609068
C,0,-6.2810036894,0.0730265158,-1.7543739827
C,0,-7.3795839411,1.5434250462,-3.855830538
H,0,-5.4815828339,2.5534139957,-3.9381699593
C,0,-7.5847116526,-0.1752803893,-2.1755515991
H,0,-5.8738364384,-0.4951025447,-0.9231722846
C,0,-8.1411564312,0.5576045714,-3.2283655024
H,0,-7.7982798651,2.1170503675,-4.6786363681
H,0,-8.1705516188,-0.9443459841,-1.6788675074
H,0,-9.1585553333,0.3596295823,-3.5548204577
N,0,-1.8919070457,0.4372971022,-1.6317312032
O,0,-1.3397040713,1.4796486958,-2.0804711564
O,0,-1.1798352251,-0.5627926302,-1.2771839797
H,0,-0.1203869311,2.2559123158,0.982490103
C,0,0.4480705899,-2.9540923273,1.7732929917
H,0,1.3736875273,-2.969210237,2.3448454011
C,0,-0.7315558095,-2.9619653779,2.8102537051
C,0,-2.0941293089,-2.6172000369,2.1776377334
H,0,-2.0940493794,-1.6079620424,1.7518304594
H,0,-2.3641951532,-3.3299248096,1.3967335403
H,0,-2.8679533949,-2.6291313995,2.9540004727
C,0,-0.4199991418,-1.9120531558,3.8956575019
H,0,0.5261492257,-2.1237517644,4.4079263028
H,0,-0.3627860183,-0.9025244546,3.4780503299
H,0,-1.2171615002,-1.9064156858,4.6486771707
C,0,-0.8080404787,-4.3488352414,3.4766304243

H,0,0.1379003543,-4.6170669517,3.9631540975
H,0,-1.582328567,-4.3463924634,4.2534630114
H,0,-1.0630418475,-5.1331092377,2.7573163426
C,0,0.398042704,-4.1219519773,0.7492102199
O,0,-0.6863005489,-4.4595220227,0.2629603429
N,0,1.5573533563,-4.7255368282,0.3387565771
C,0,1.4161487909,-5.7532521401,-0.7093611613
H,0,2.341570151,-6.3388590242,-0.7186224885
H,0,0.6023100507,-6.4242265825,-0.4194909137
C,0,2.9243258591,-4.4240966792,0.7864047314
H,0,3.5402628278,-4.2876345926,-0.1100162024
H,0,2.9398170156,-3.4655628363,1.3068145757
C,0,1.1353198995,-5.2118770869,-2.127166896
H,0,0.2108117458,-4.6272920178,-2.0694042111
C,0,0.8942089834,-6.3934488488,-3.0763755461
H,0,0.0650956794,-7.0235828107,-2.7318234165
H,0,0.6456886076,-6.0414348103,-4.0846764682
H,0,1.785719007,-7.030459854,-3.1606775132
C,0,2.2500312747,-4.3001617218,-2.6549810719
H,0,2.3973297293,-3.4220123748,-2.016615083
H,0,3.2080129934,-4.8332243205,-2.7303465647
H,0,2.0023711704,-3.9306563255,-3.6576309207
C,0,3.5784943222,-5.5066609502,1.6737537024
H,0,3.5777261234,-6.4546679954,1.116552427
C,0,5.0401584525,-5.1174728975,1.9354241468
H,0,5.1045057682,-4.1643375232,2.4757180902
H,0,5.5480884023,-5.8784595418,2.5396740322
H,0,5.6028351458,-5.0055609874,1.0001777127
C,0,2.8203450327,-5.732503792,2.985326498
H,0,1.778766547,-6.0164901484,2.8028437773
H,0,3.2842989205,-6.5366023707,3.5695718662
H,0,2.826262979,-4.8282706768,3.6075878606
C,0,-4.6882037975,5.2925439822,-0.1186315139
H,0,-3.711643825,5.4831876486,0.3397664223
H,0,-4.9774218541,6.1902519639,-0.6779588513
H,0,-5.4162728273,5.1468603084,0.6872771686

dr2-TS-CCAtack-Pap

E(RB3LYP)= -3353.33287147 Hartree

Sum of electronic and thermal Free Energies= -3352.243424 Hartree

C,0,0.566832394,2.3457346717,-0.1732366453
C,0,1.3760904462,4.3698600792,-1.4795262889
C,0,0.6054546187,3.9000948073,-0.2297693498

H,0,1.0832895201,1.9714709583,0.7114504581
H,0,-0.4114224501,4.3020842959,-0.2683572624
H,0,1.0597455091,4.297619768,0.6825287699
C,0,0.8435506602,2.2240498048,-2.6737895382
H,0,1.5439555254,1.8336569634,-3.4151400272
H,0,-0.1062936536,1.7021311942,-2.8052573787
C,0,0.7066088478,3.76217003,-2.7275375552
H,0,1.1749798868,4.1488138222,-3.638679048
H,0,-0.3492818763,4.0510941428,-2.7632448494
H,0,1.3555390121,5.4624500556,-1.5359961632
C,0,2.8493921036,3.8771361855,-1.4369949768
H,0,3.2882802708,4.0644321946,-2.4245434353
C,0,2.8113484999,2.346607334,-1.1864831693
H,0,3.4293236768,1.777092663,-1.8809676781
H,0,3.1315473248,2.0768867322,-0.1784537012
N,0,1.4020667661,1.8291329953,-1.3323818066
C,0,3.6990946185,4.5842185326,-0.4136485795
H,0,3.4008728585,4.4639480796,0.6291438682
C,0,4.7666841158,5.3298607733,-0.7003506903
H,0,5.3418699968,5.8257901056,0.0775302758
H,0,5.1101816705,5.4733529393,-1.723488106
C,0,-0.8733420737,1.7770859841,-0.1844522195
H,0,-1.4090914333,2.1724660527,-1.0451115468
C,0,-1.5986276273,2.2017026922,1.1025423502
C,0,-2.6961058683,3.1276591164,1.1034578443
C,0,-1.1927805712,1.6824857081,2.3149859242
C,0,-3.244192447,3.727870031,-0.0560185797
C,0,-3.2708964303,3.459621231,2.3798122362
C,0,-1.841590074,2.0727046463,3.5098563343
H,0,-0.3708465666,0.9756206579,2.3743978331
C,0,-4.2974929037,4.6237628282,0.0273530385
H,0,-2.8887742991,3.4704849804,-1.0463723283
C,0,-4.346458739,4.3807546878,2.4291342121
H,0,-1.5078183077,1.6536244081,4.458468536
C,0,-4.8542049881,4.9586950984,1.2884297762
H,0,-4.7597914752,4.6146728761,3.4055445999
H,0,-5.6789221547,5.6581666006,1.3617552279
N,0,-0.8733291827,0.3286331222,-0.3603922141
O,0,-4.7402117267,5.1382681094,-1.1544856437
C,0,-5.8835833675,5.9850723911,-1.1473363343
H,0,-6.0768850963,6.231007902,-2.1936660561
H,0,-6.7625437303,5.476881309,-0.7309711239
H,0,-5.700509248,6.9146796694,-0.5928221205

N,0,-2.8367243349,2.9329151495,3.5612480056
H,0,-0.3563456033,-0.2303822382,0.3225689757
C,0,-1.7816404515,-0.3393388358,-1.1364793093
N,0,-1.8301000822,-1.6716064733,-0.9081014909
H,0,-1.2078766386,-2.0401334937,-0.1856478
S,0,-2.7361488063,0.4591555189,-2.3122981687
O,0,1.6606068103,-3.6957926408,1.100774583
O,0,0.2326492465,-1.9307781693,1.1881087849
O,0,3.9203397281,-0.1495355269,2.8887722988
O,0,1.8914144415,0.5058917235,2.1386802354
C,0,2.7219282276,-0.3778389235,2.3104011214
C,0,1.3618513971,-2.3771208184,1.3769959007
C,0,2.5639756926,-1.7787371085,1.9385613016
C,0,3.5455124413,-2.7408815378,1.9241557447
C,0,3.0405798614,-3.905461911,1.2773586083
C,0,3.3837379183,-5.3140504737,1.6908552314
C,0,4.1997992354,1.2093183641,3.2926558451
C,0,5.5628681796,1.2191126371,3.9543073775
H,0,4.5679457378,-2.6214772717,2.2582028577
H,0,2.9888012754,-6.0141315041,0.947887762
H,0,4.1791543816,1.8552270602,2.4082751463
H,0,3.4125757027,1.5471072572,3.9743205155
H,0,5.578458277,0.5715692361,4.8374199513
H,0,5.8095145346,2.2382578662,4.2727829307
H,0,6.3395195834,0.8795035825,3.2608776152
H,0,4.4746782657,-5.4193878325,1.6699898441
C,0,3.8171323438,-3.4967955511,-0.6131442057
H,0,4.6964834666,-2.9227592353,-0.3363974567
C,0,2.813596307,-2.717153865,-1.247605229
H,0,1.9439766106,-3.1403221076,-1.7234854137
C,0,4.1511107573,-4.835945989,-1.1668406019
C,0,5.4879698554,-5.2676740187,-1.1470203249
C,0,3.1852312573,-5.6917934316,-1.7269795559
C,0,5.8539358434,-6.5036571911,-1.6795470524
H,0,6.2497164908,-4.6181494758,-0.7217919458
C,0,3.5505733246,-6.9275287947,-2.2571717674
H,0,2.1410379455,-5.3946325308,-1.7432451065
C,0,4.8858708441,-7.3393417974,-2.2378366328
H,0,6.8963127115,-6.8111276104,-1.6606871889
H,0,2.7879864535,-7.5724317498,-2.6859015688
H,0,5.1674284508,-8.3030807734,-2.6535417865
N,0,2.8261727321,-1.360144527,-1.257935719
O,0,3.7808917977,-0.6750671204,-0.7935194701

O,0,1.8145080694,-0.7774863571,-1.8145104538
H,0,1.4878995198,0.7696558938,-1.3311065139
C,0,-2.698374536,-2.6453788419,-1.5788536064
H,0,-3.3623142573,-2.0651173122,-2.2171384579
C,0,-1.9135032928,-3.6160710788,-2.5295890999
C,0,-0.8162228744,-4.433260945,-1.8196728488
H,0,-0.1365652595,-3.7903420326,-1.2507308572
H,0,-1.234655199,-5.1625983773,-1.1263465606
H,0,-0.2200805885,-4.9634306731,-2.5745091001
C,0,-1.2450171608,-2.7676037701,-3.6310370312
H,0,-1.9711573234,-2.1471187921,-4.1675061232
H,0,-0.4737805217,-2.106523207,-3.2215372223
H,0,-0.7605591631,-3.4271900793,-4.3621895819
C,0,-2.9218032359,-4.5772109331,-3.1877734079
H,0,-3.6888078872,-4.0336001757,-3.753296914
H,0,-2.4044271001,-5.2387647543,-3.893568044
H,0,-3.4201937534,-5.211213708,-2.447193592
C,0,-3.4999776949,-3.3657530565,-0.4576262535
O,0,-3.0349811327,-4.3734137645,0.0834470869
N,0,-4.6908171522,-2.8412101465,-0.0278062501
C,0,-5.3233209664,-3.5248268468,1.115009982
H,0,-6.3685360351,-3.2006063046,1.1518490758
H,0,-5.3161677551,-4.6004038871,0.9155402603
C,0,-5.39284928,-1.668749853,-0.5670279696
H,0,-5.6562063575,-1.0250516622,0.2803404004
H,0,-4.714066423,-1.0832168976,-1.1883348413
C,0,-4.6568977521,-3.2651161279,2.482223218
H,0,-3.6156890604,-3.5956515891,2.3992251649
C,0,-5.348575093,-4.12389905,3.5500332086
H,0,-5.3089126752,-5.1906503207,3.297371754
H,0,-4.8673378353,-3.9972116776,4.5271503539
H,0,-6.4057574646,-3.8469424324,3.6654093599
C,0,-4.6631287187,-1.783168558,2.8776187387
H,0,-4.1324852716,-1.1625078335,2.147196121
H,0,-5.6863291125,-1.3943650461,2.9753860804
H,0,-4.1661180743,-1.6390491133,3.8448832948
C,0,-6.6776233571,-1.989725658,-1.3629115459
H,0,-7.3460984109,-2.5735234976,-0.7135605101
C,0,-7.3950340825,-0.6777910855,-1.7111643619
H,0,-6.7736917039,-0.0441026398,-2.3567685654
H,0,-8.3337894578,-0.8738270553,-2.2430073895
H,0,-7.6370581415,-0.0982693112,-0.8116180073
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dr2-TS-CCAttack-Tak

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Sum of electronic and thermal Free Energies= -3352.242251 Hartree

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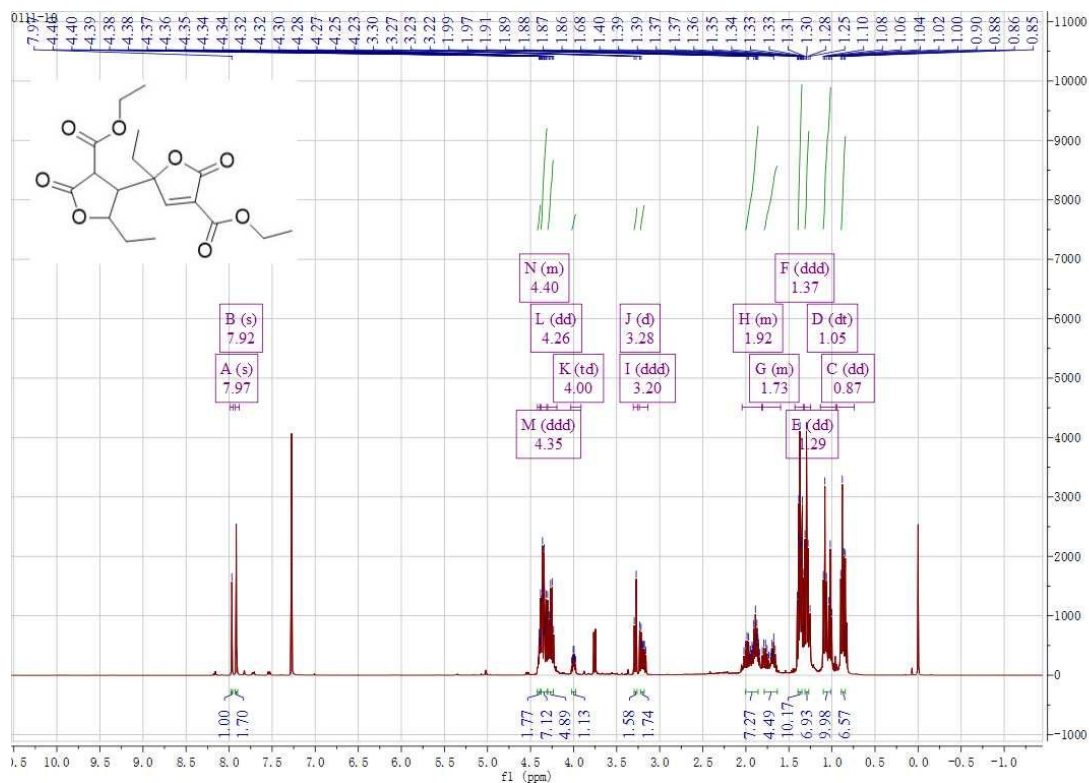
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4.3 References

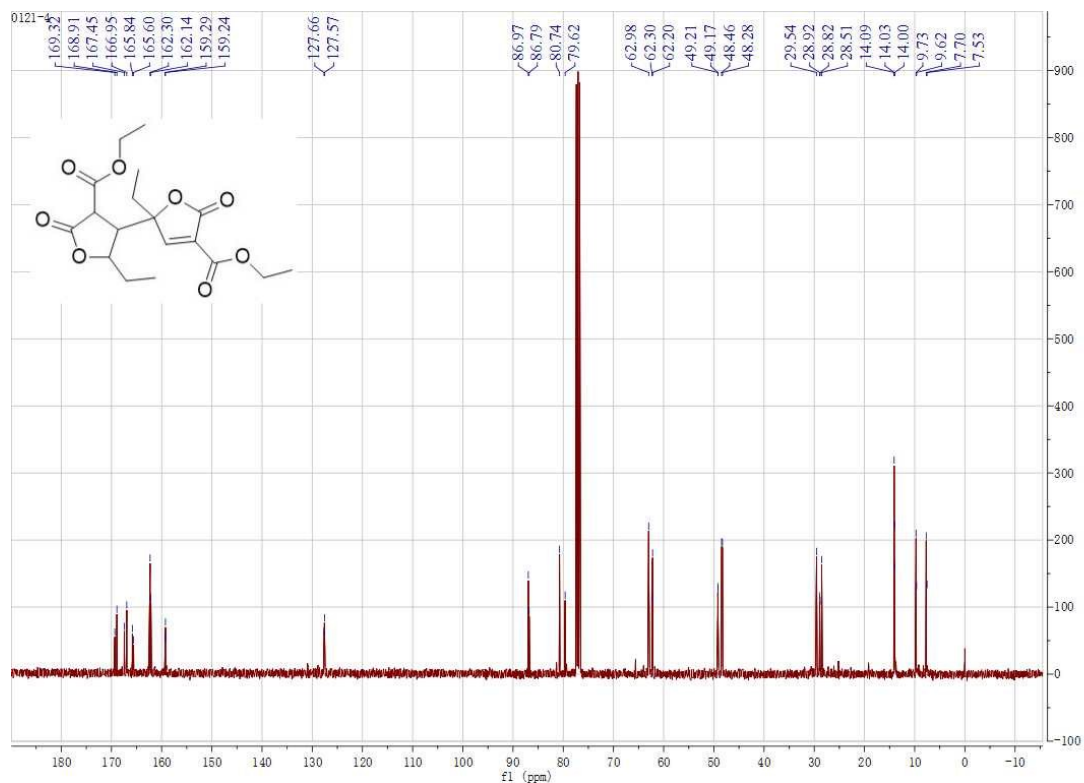
- [1] (a) P. Hohenberg and W. Kohn, *Phys. Rev. B*, 1964, **136**, 864; (b) W. Kohn and L. J. Sham, *Phys. Rev. A*, 1965, **140**, 1133.
- [2] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A., Jr. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian 09, revision A. 02; Gaussian, Inc.: Wallingford, CT. 2009.
- [3] (a) A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648; (b) C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785; (c) J. P. Perdew, K. Burke and Y. Wang, *Phys. Rev. B*, 1996, **54**, 16533.
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- [5] C. Legault, CYLview, 1.0b; Université de Sherbrooke: Quebec, Canada, 2009.

5. NMR Spectra for Product 1a-d, 3aa-3ba and 4aa.

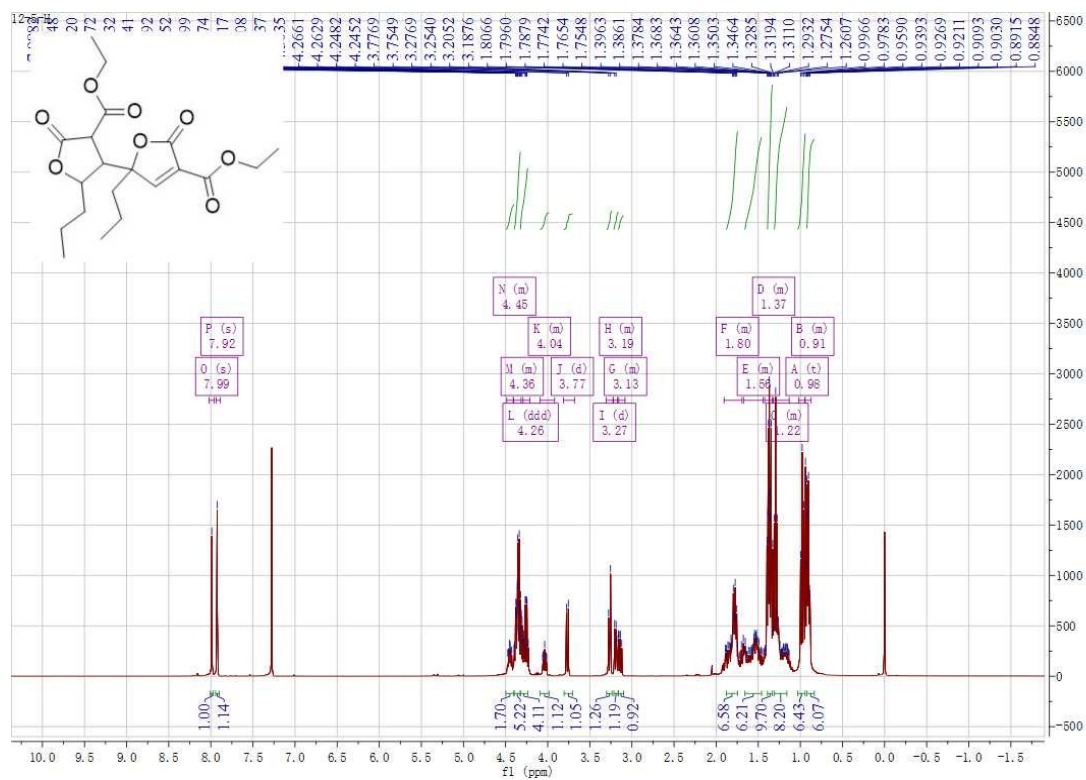
¹H NMR of product **1a** (400 MHz, CDCl₃)



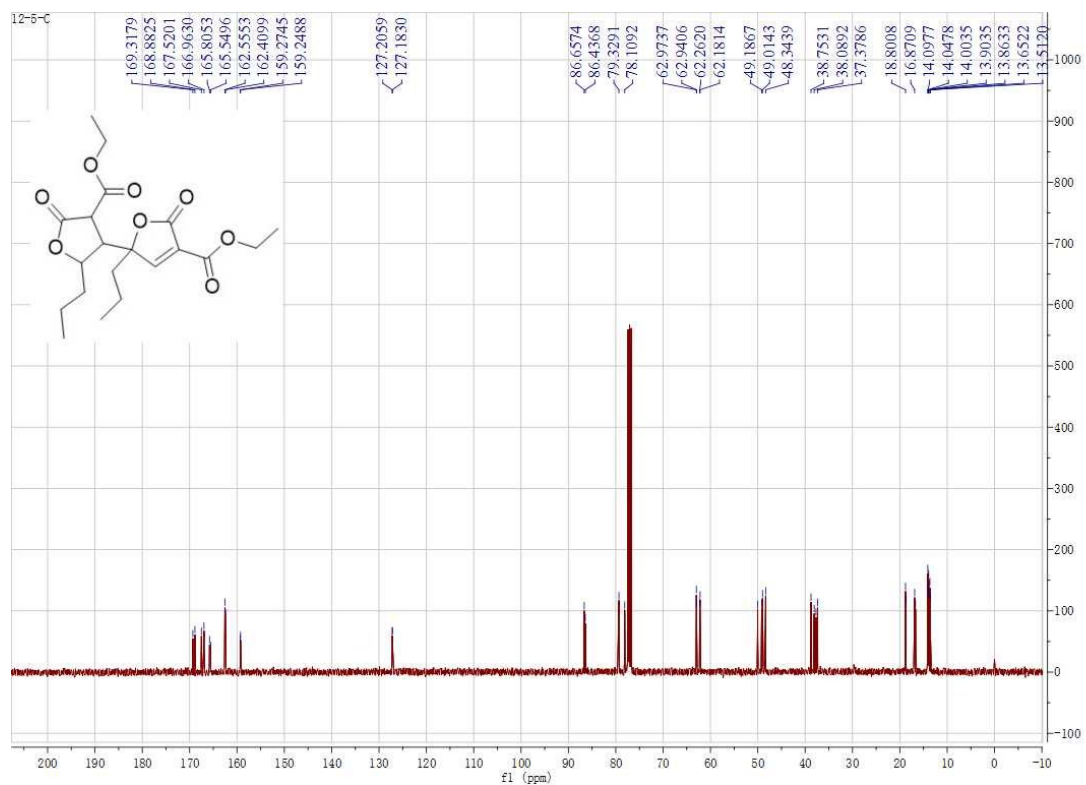
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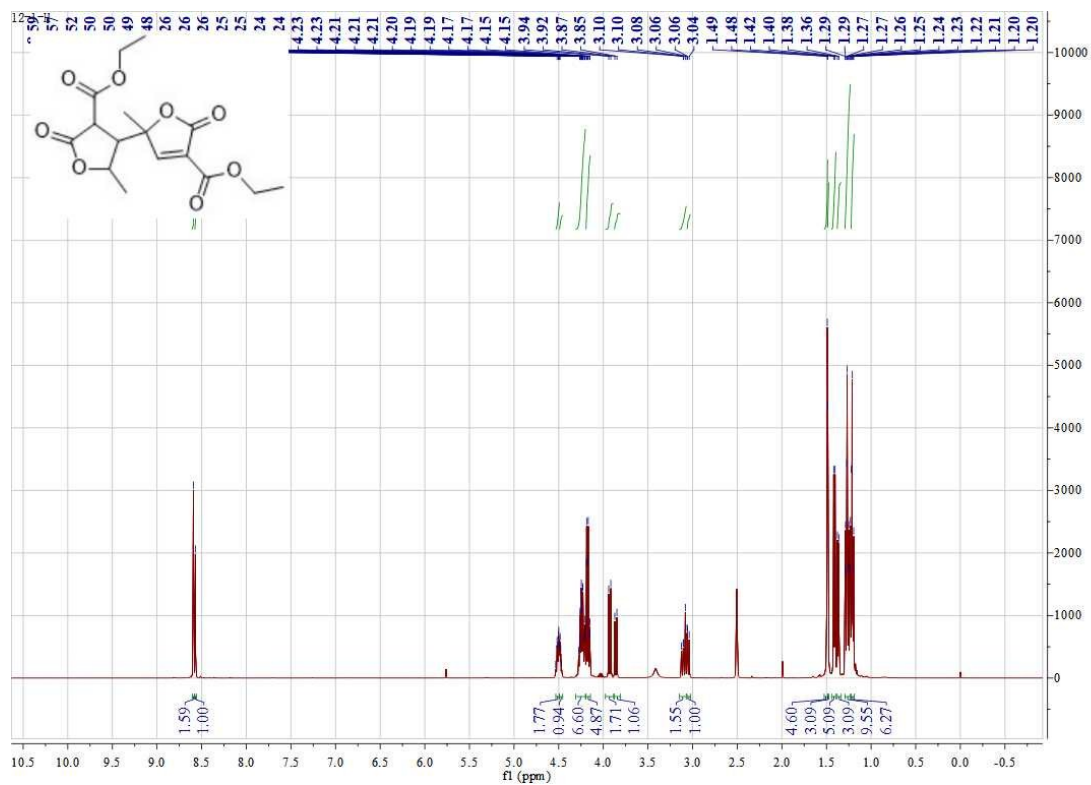
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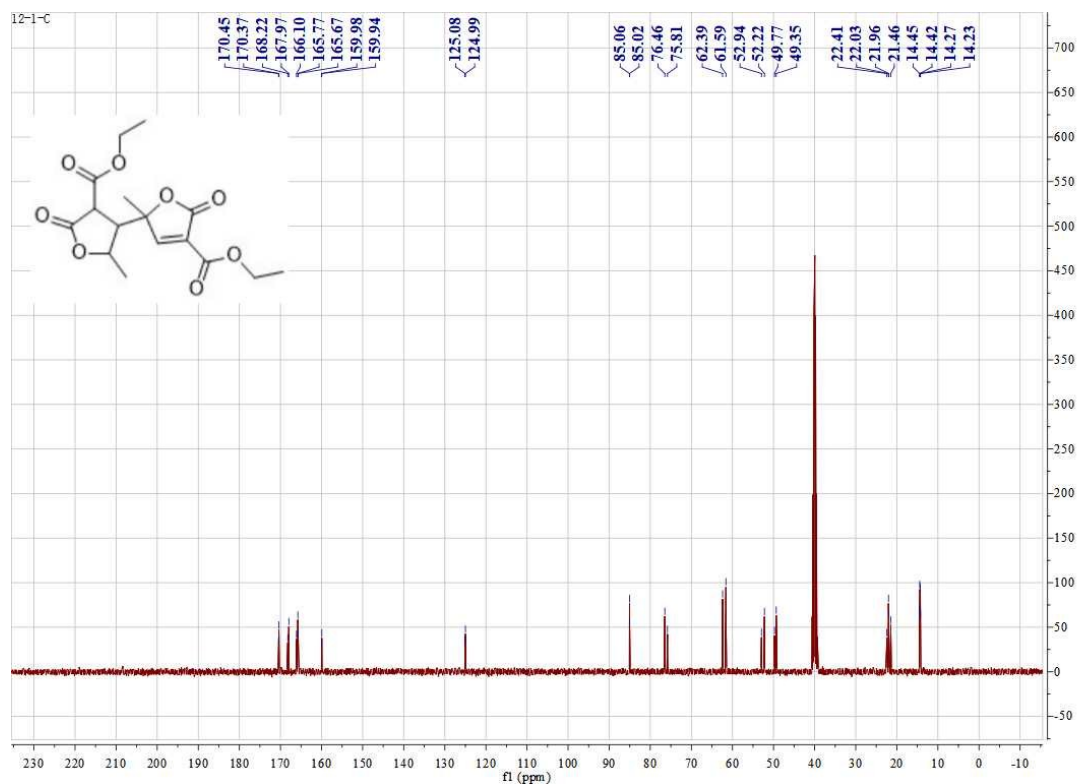
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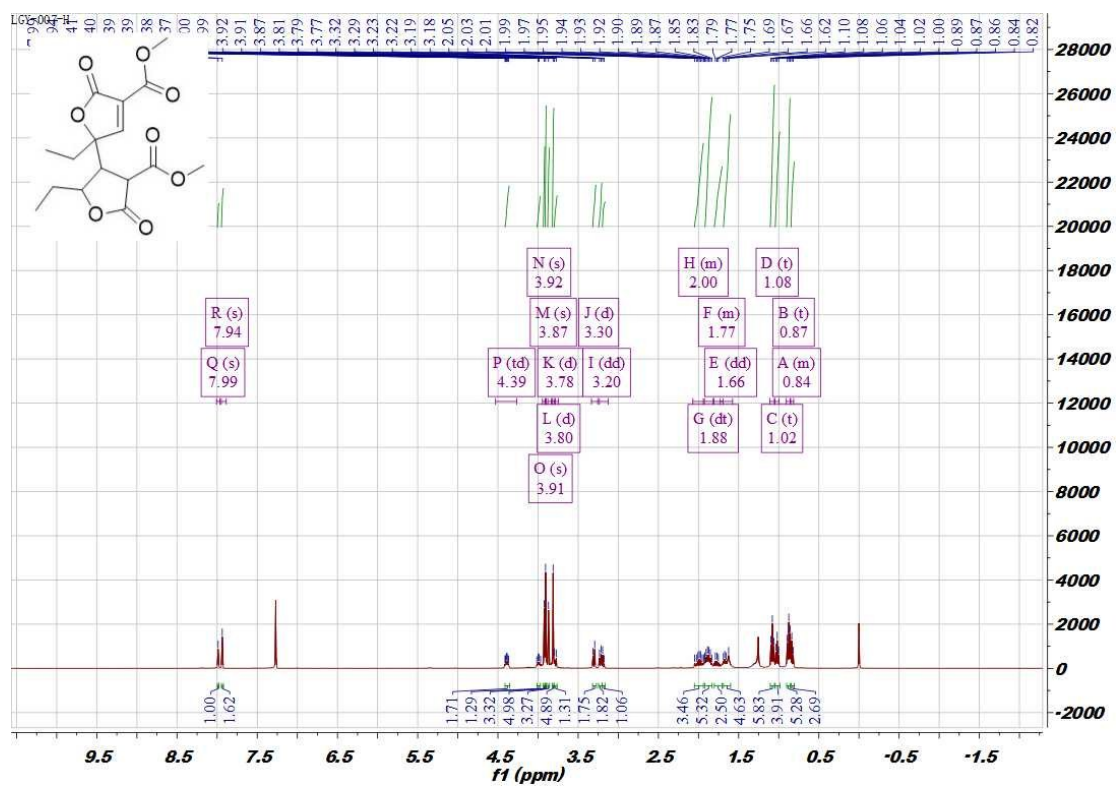
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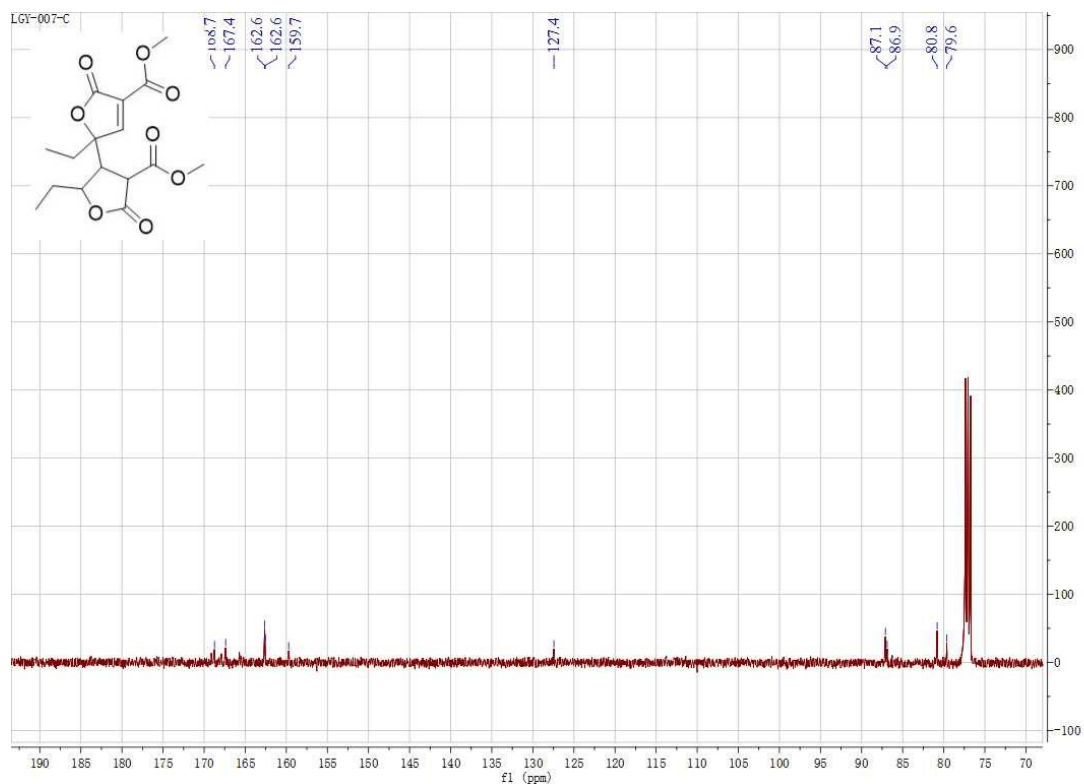
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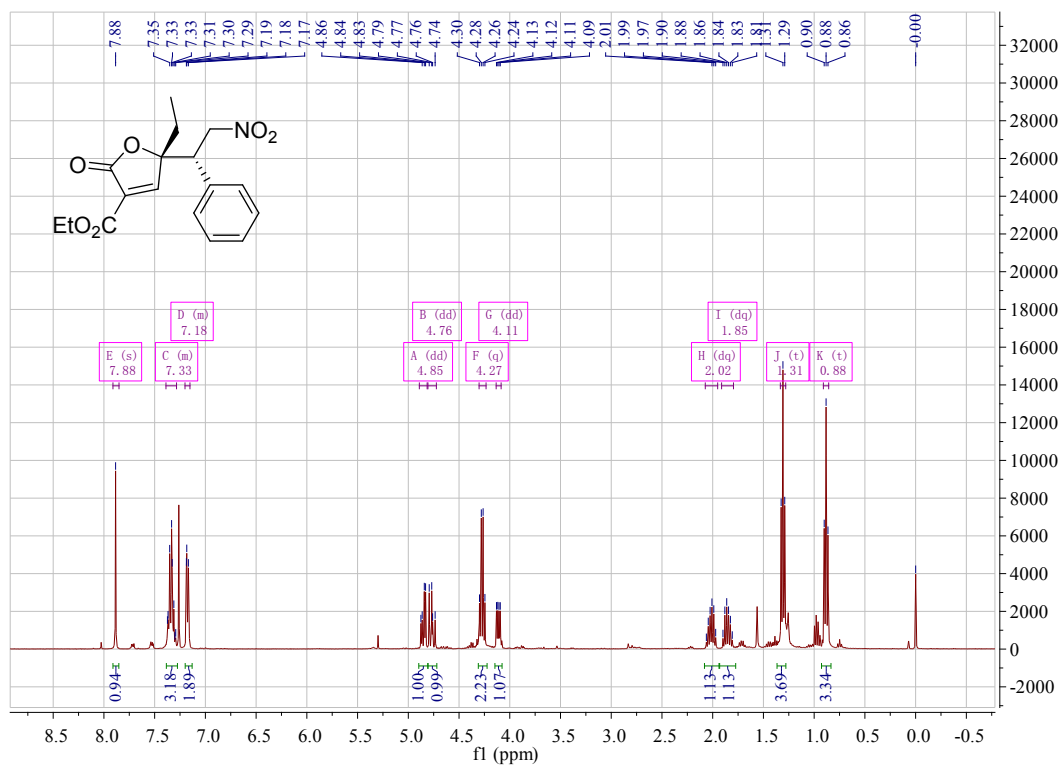
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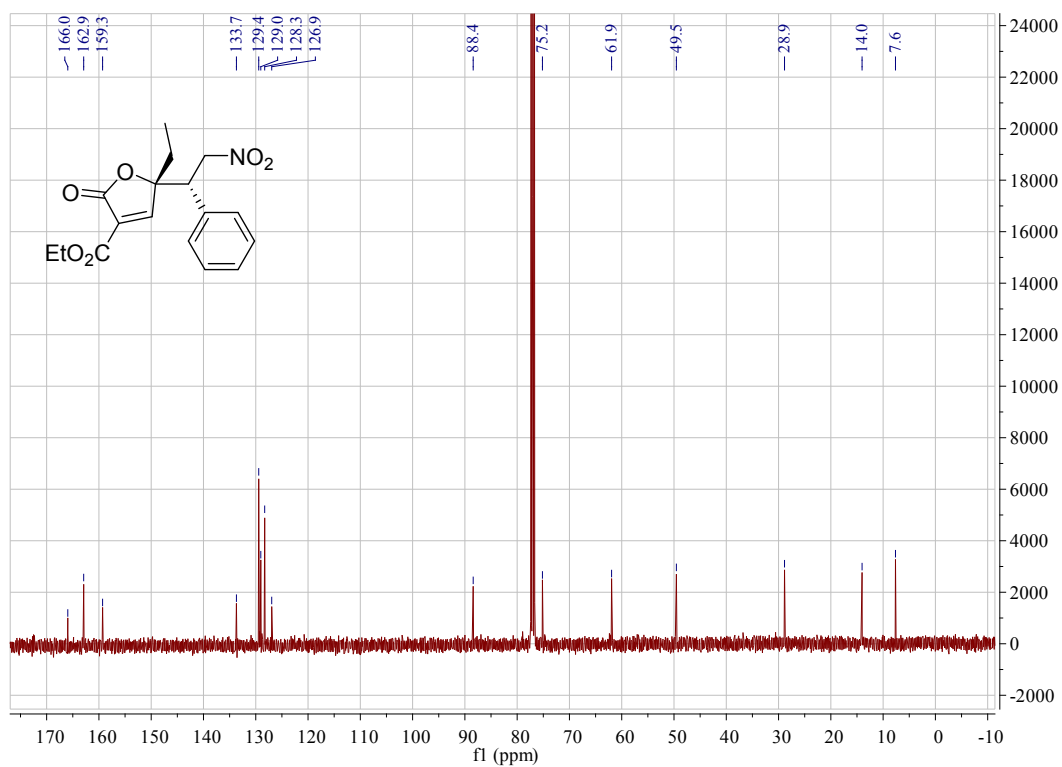
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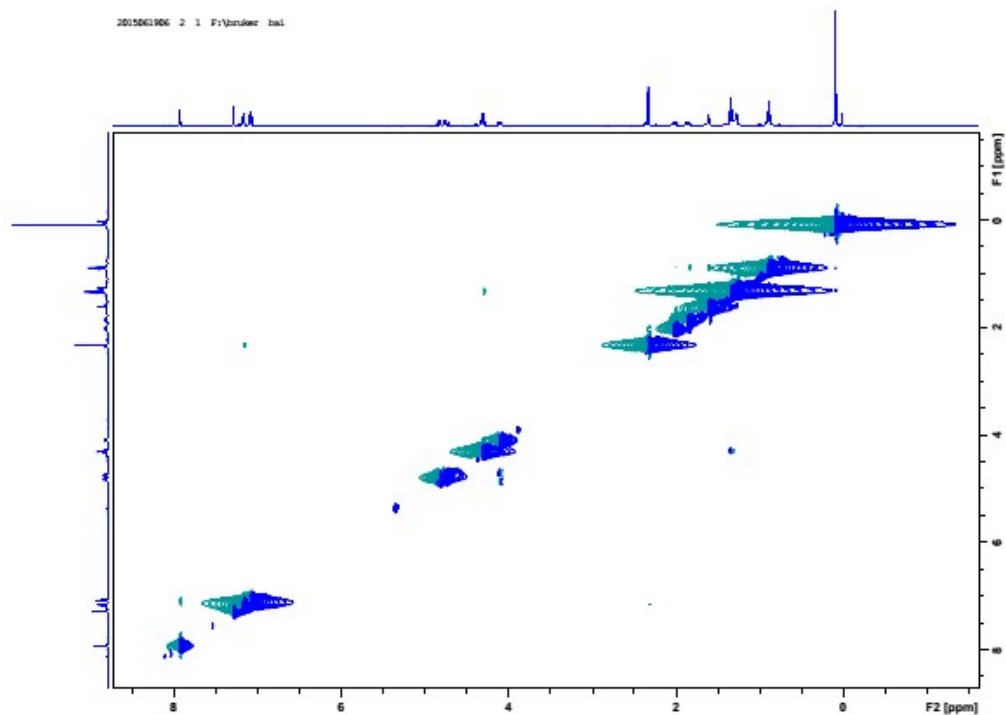
¹H NMR of product 3aa (400 MHz, CDCl₃)



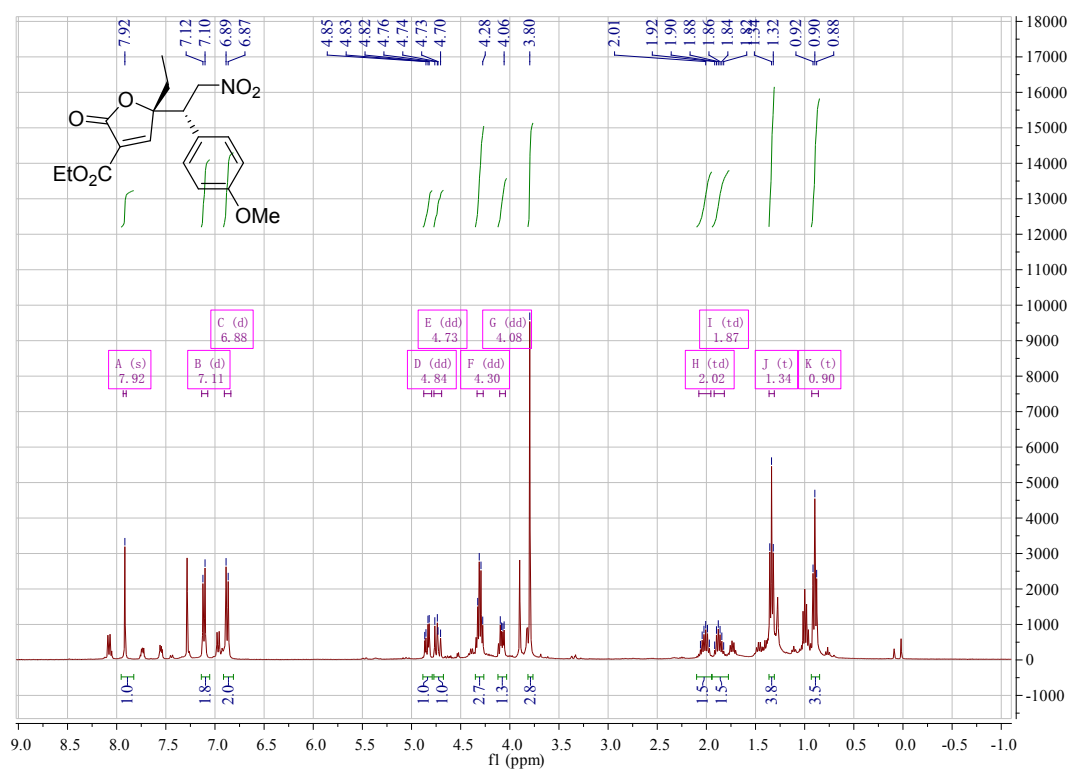
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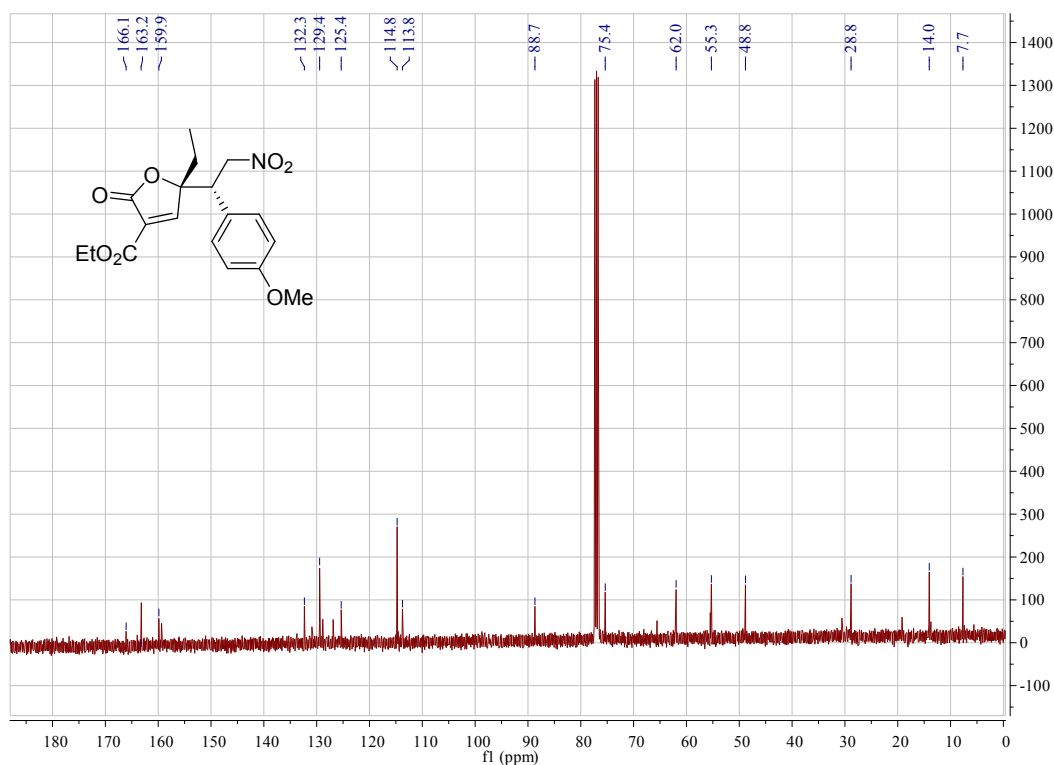
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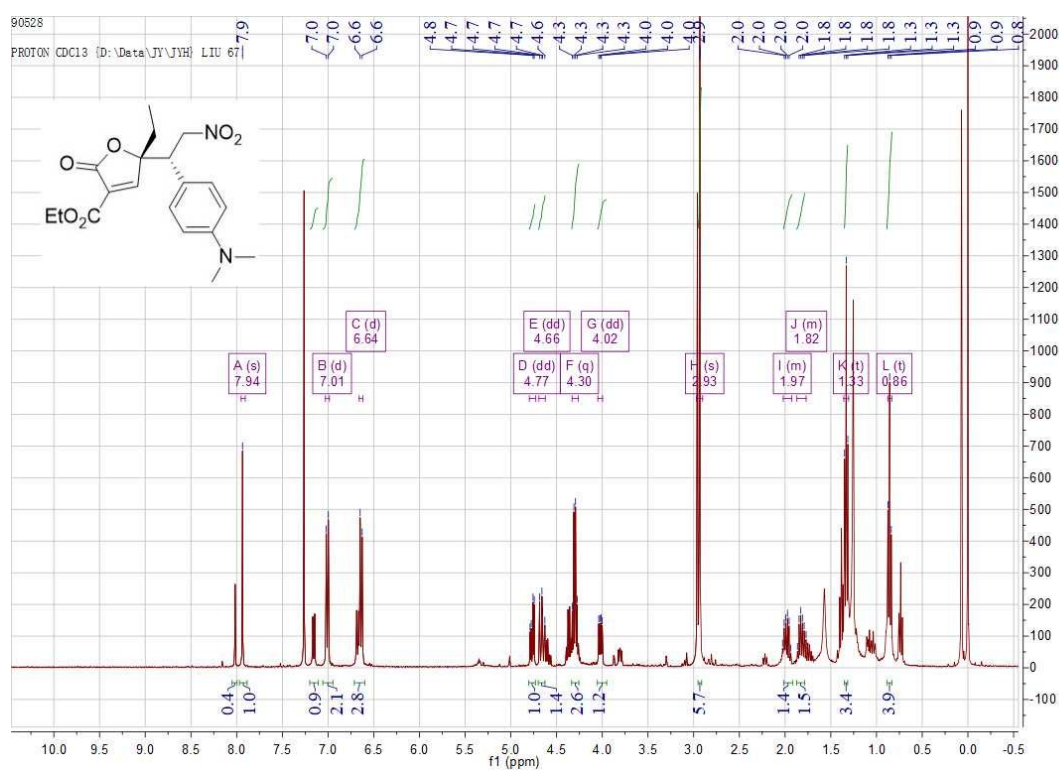
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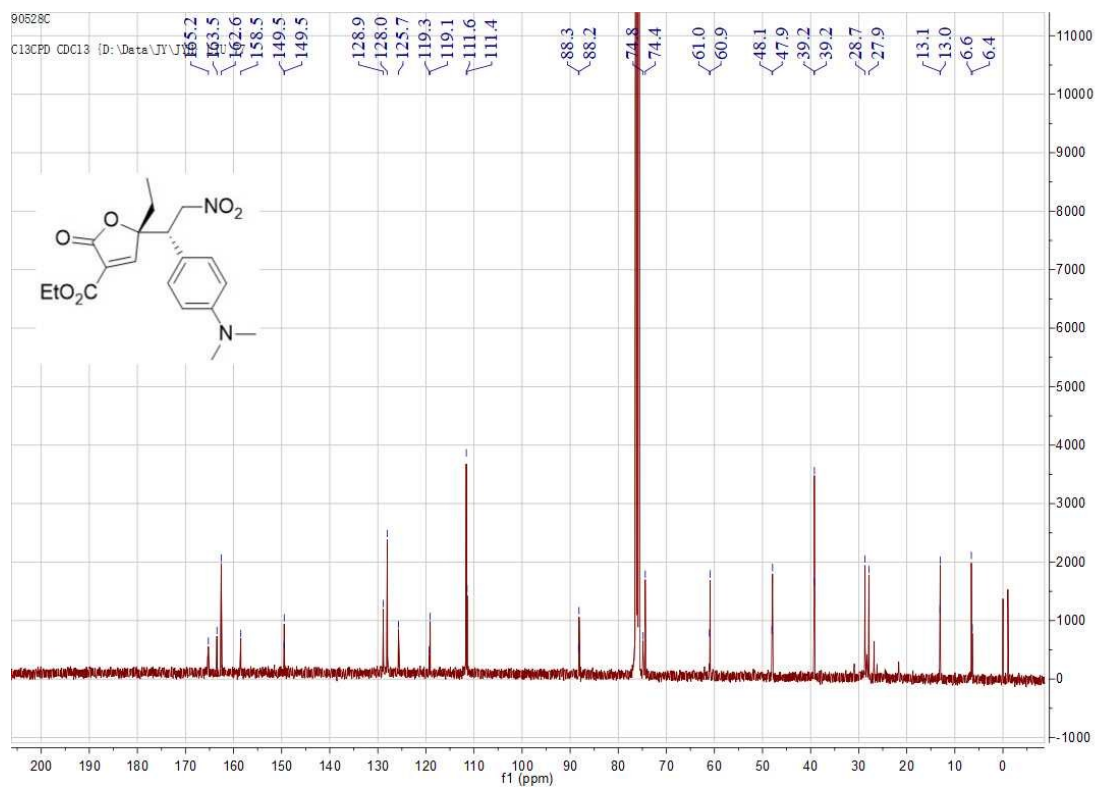
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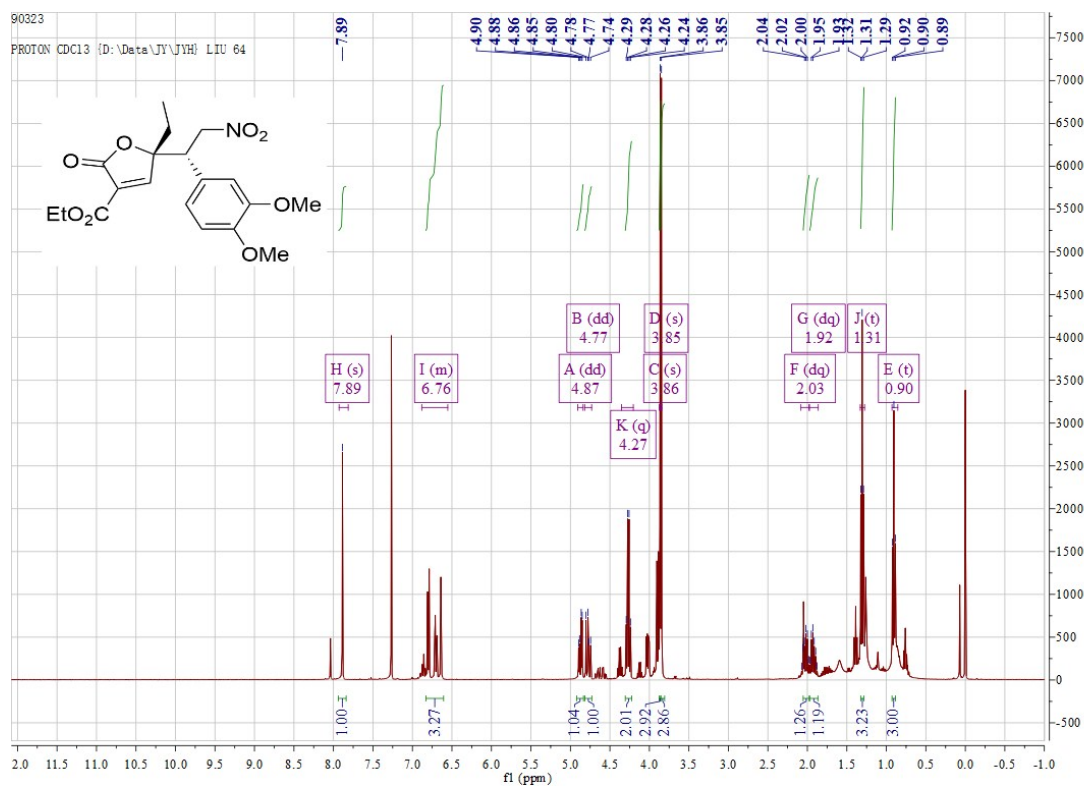
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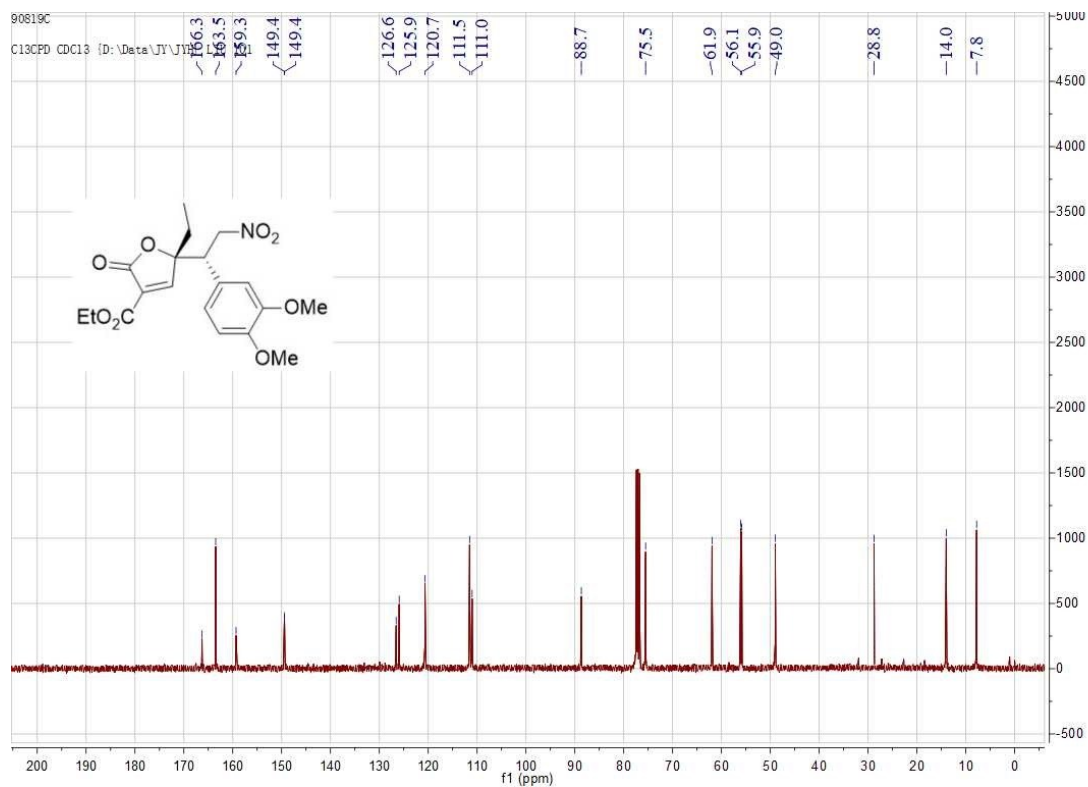
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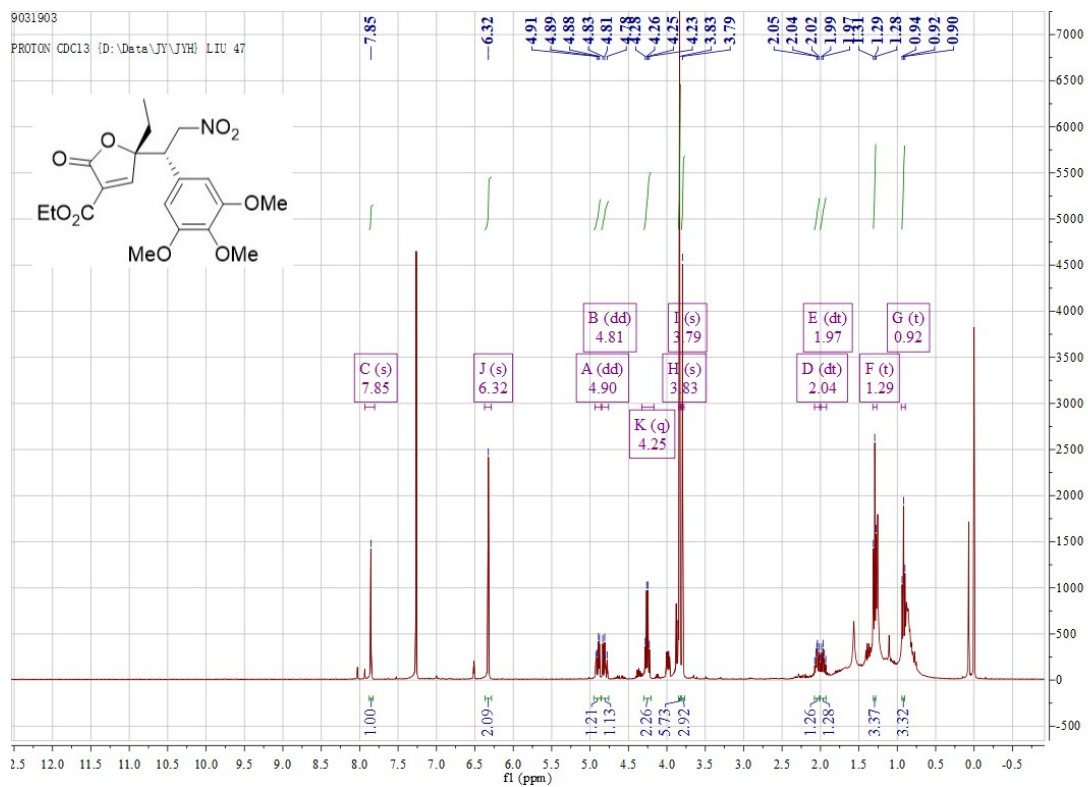
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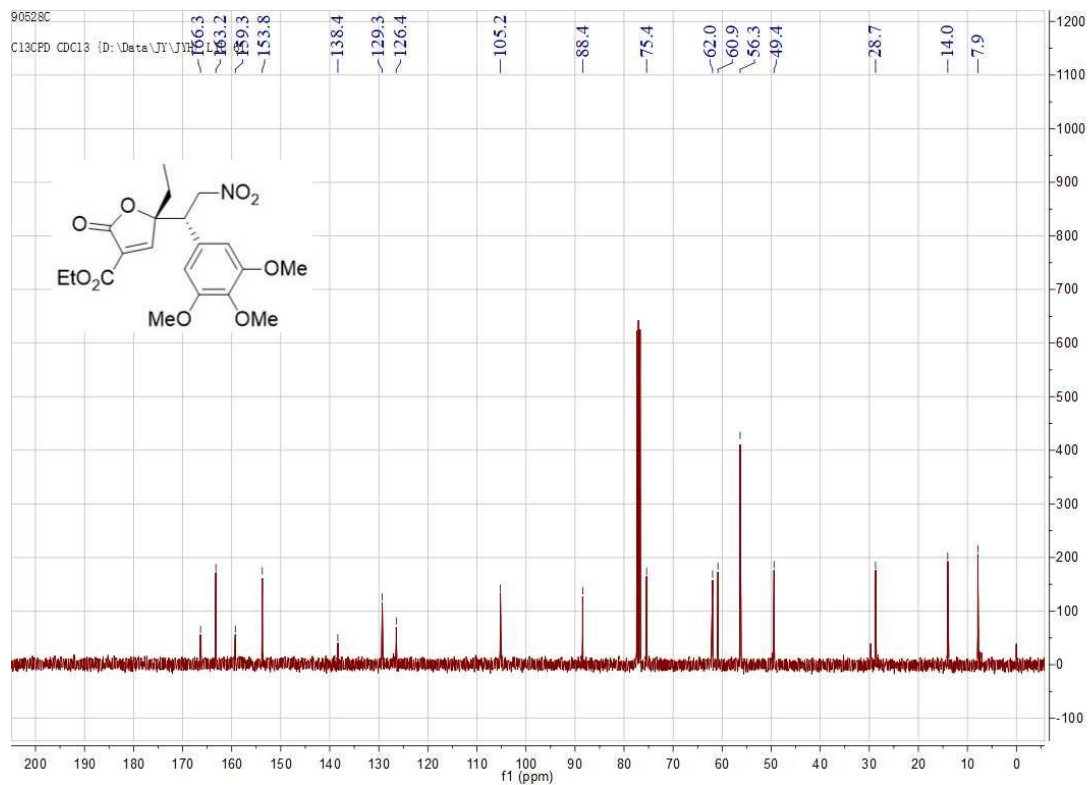
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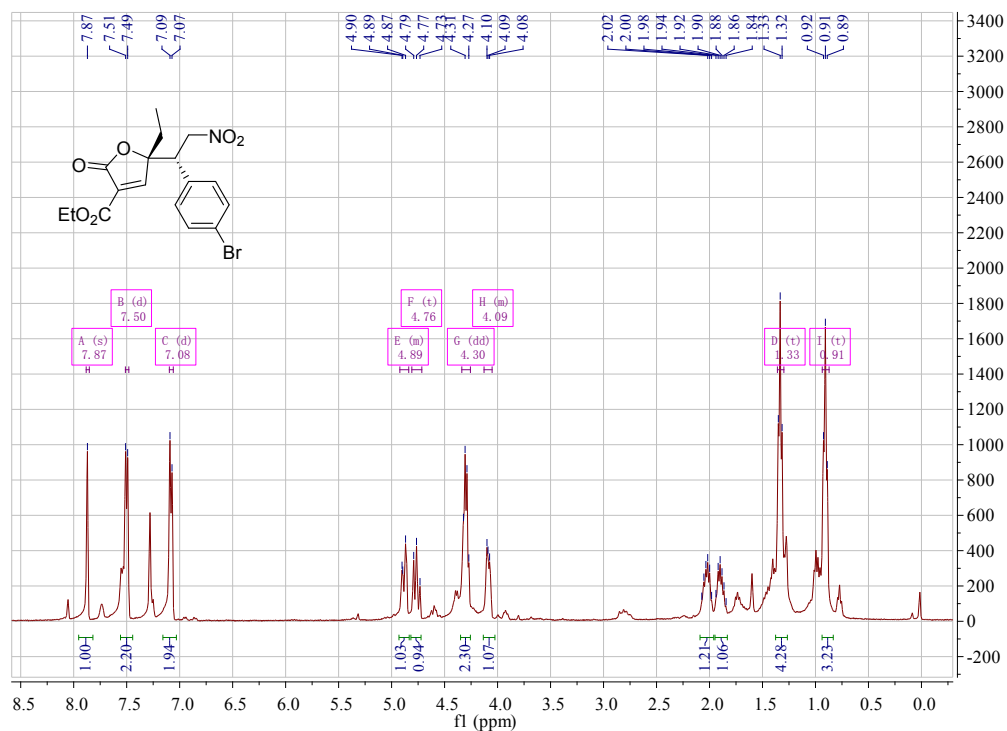
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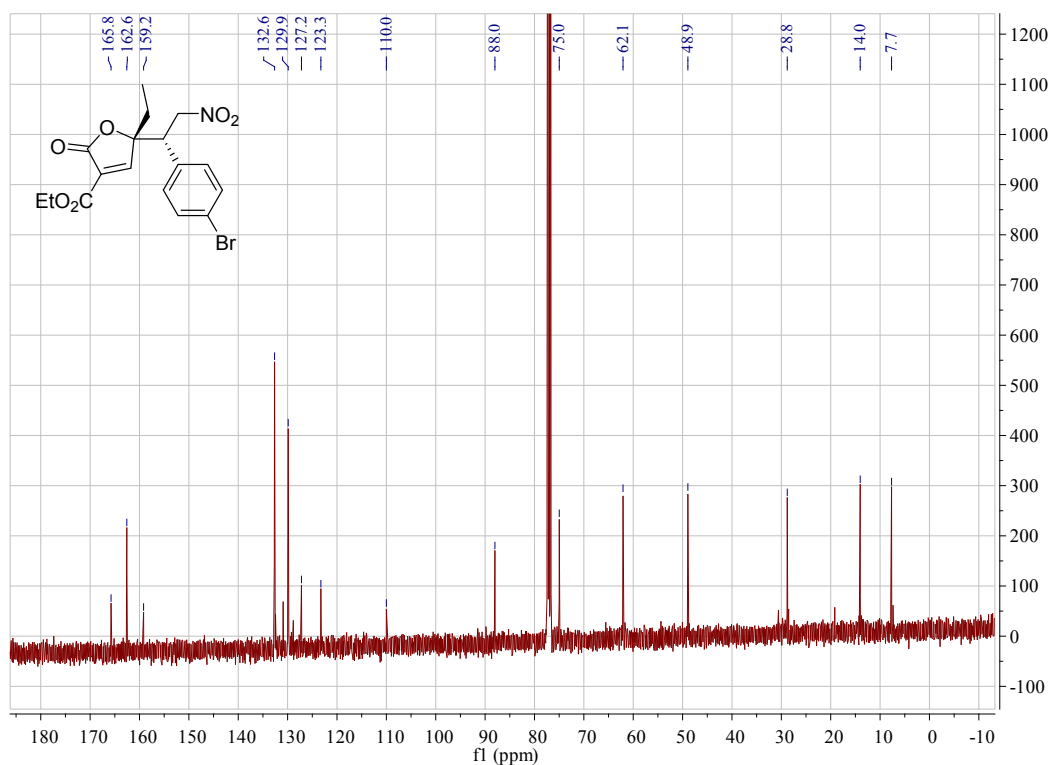
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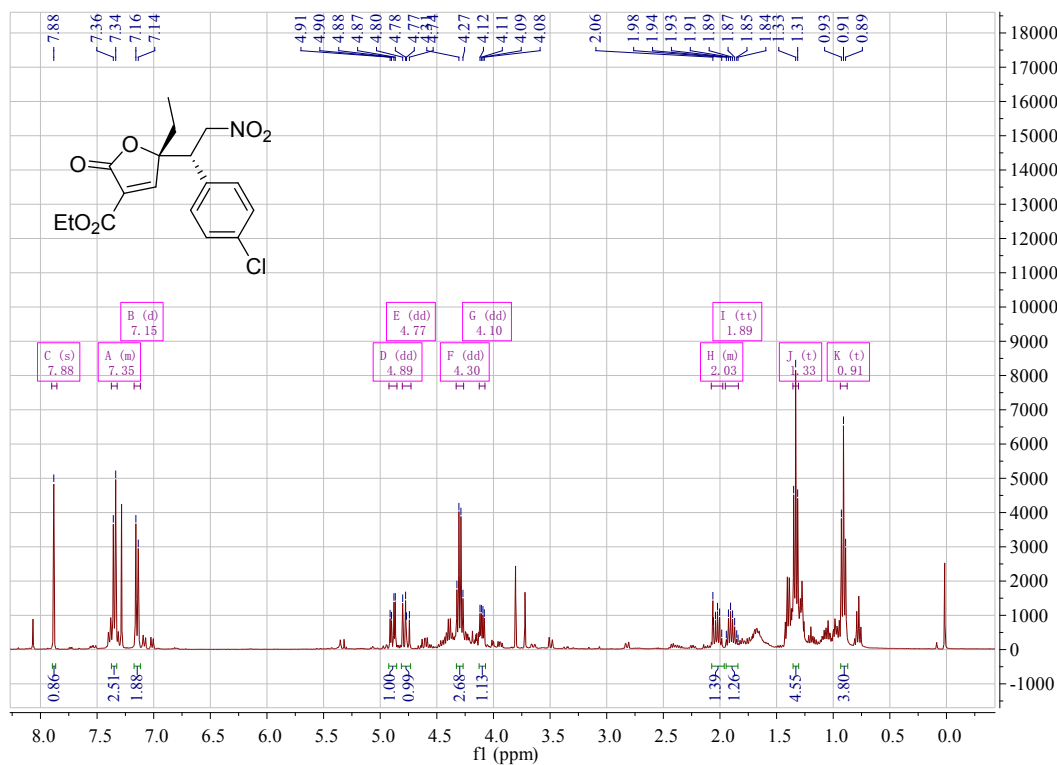
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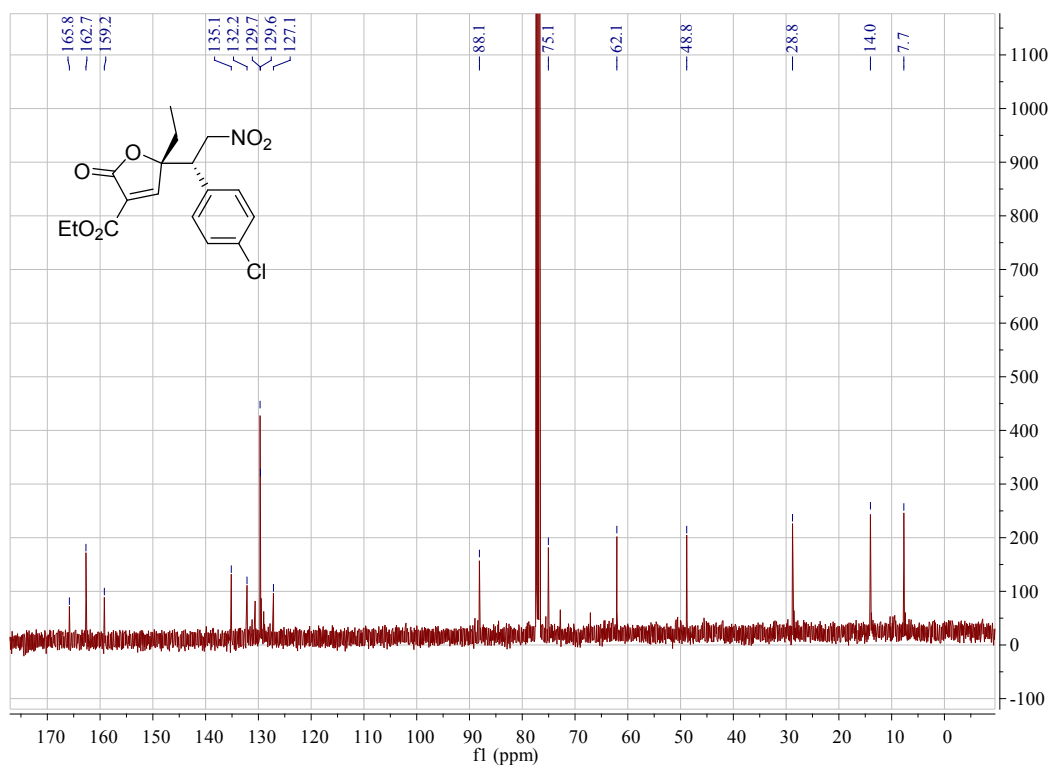
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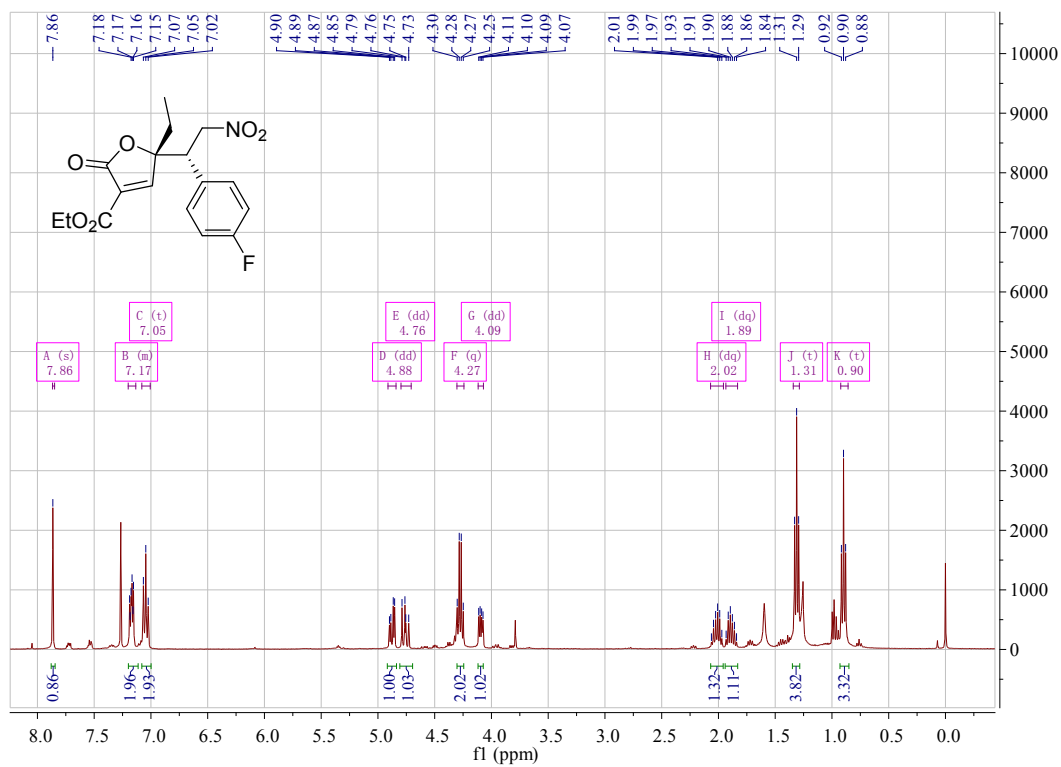
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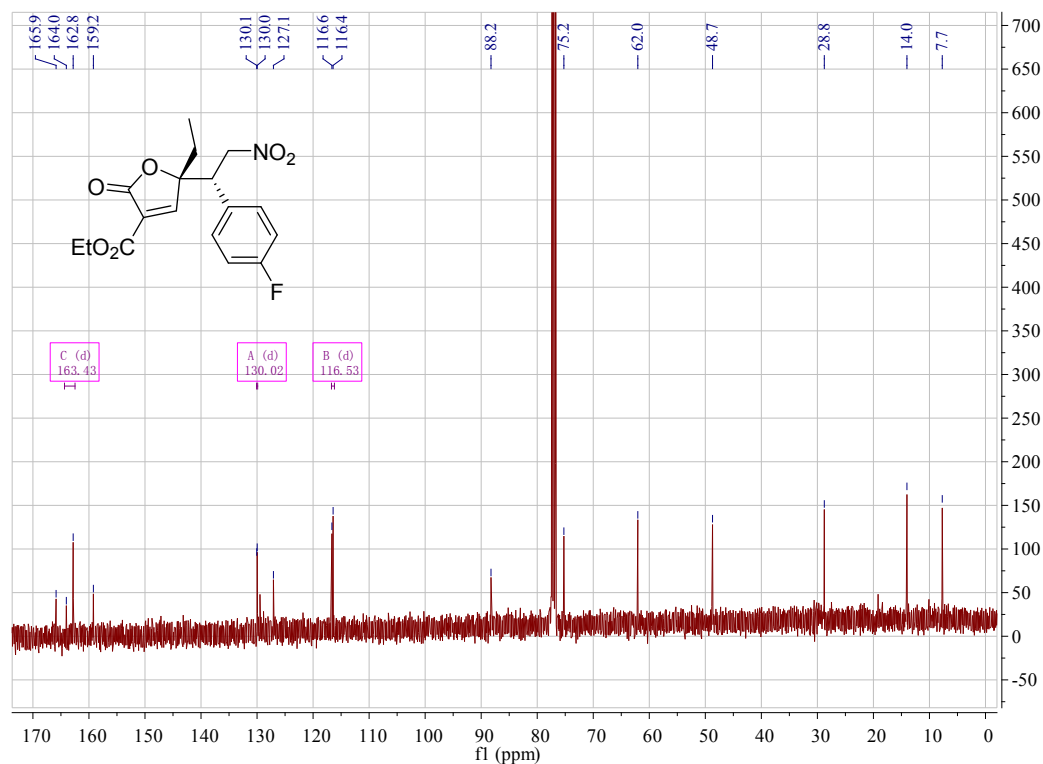
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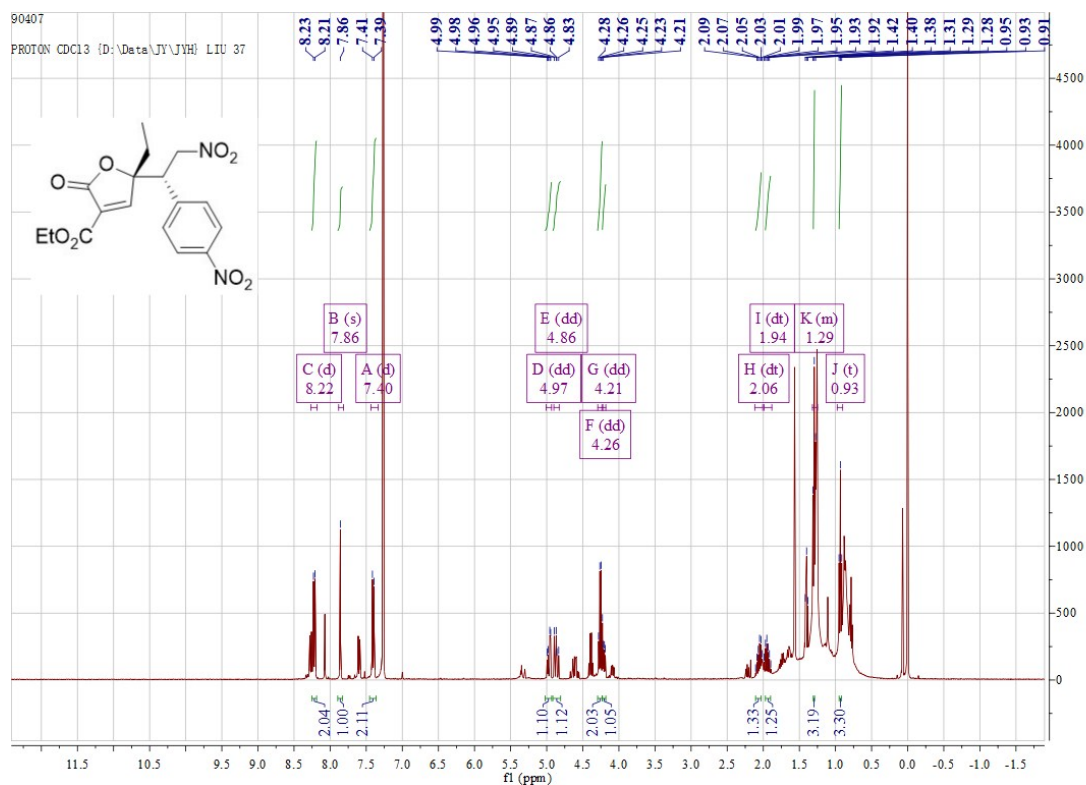
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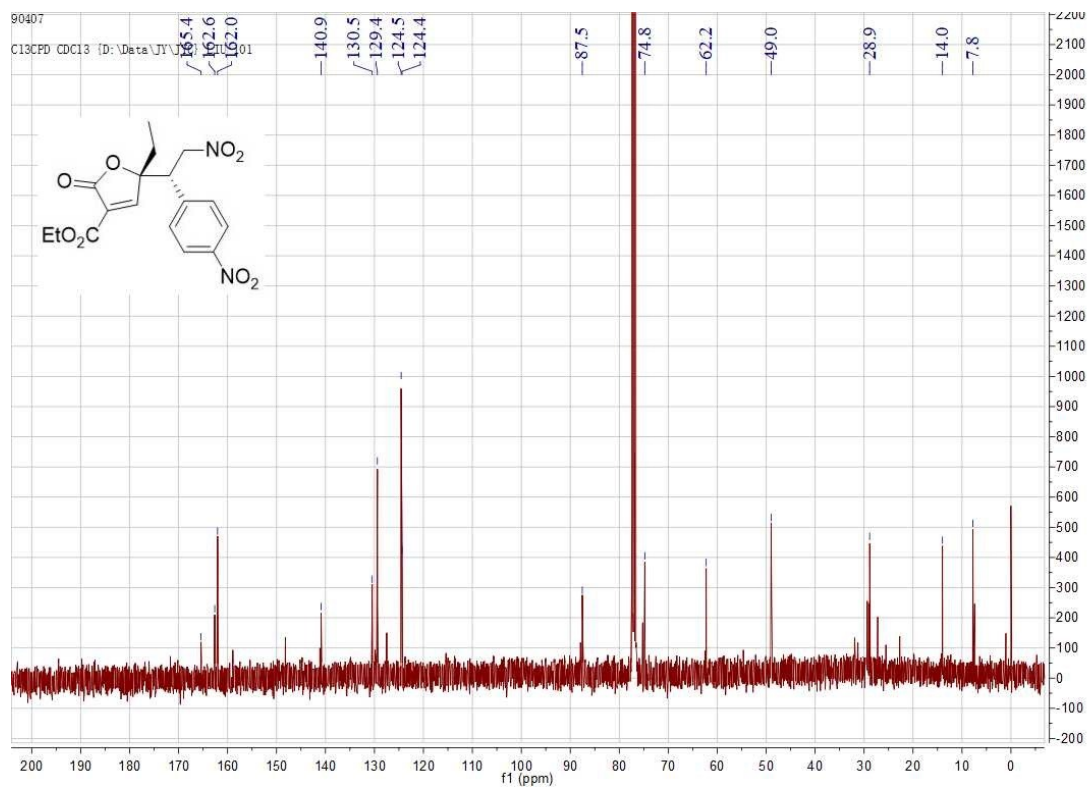
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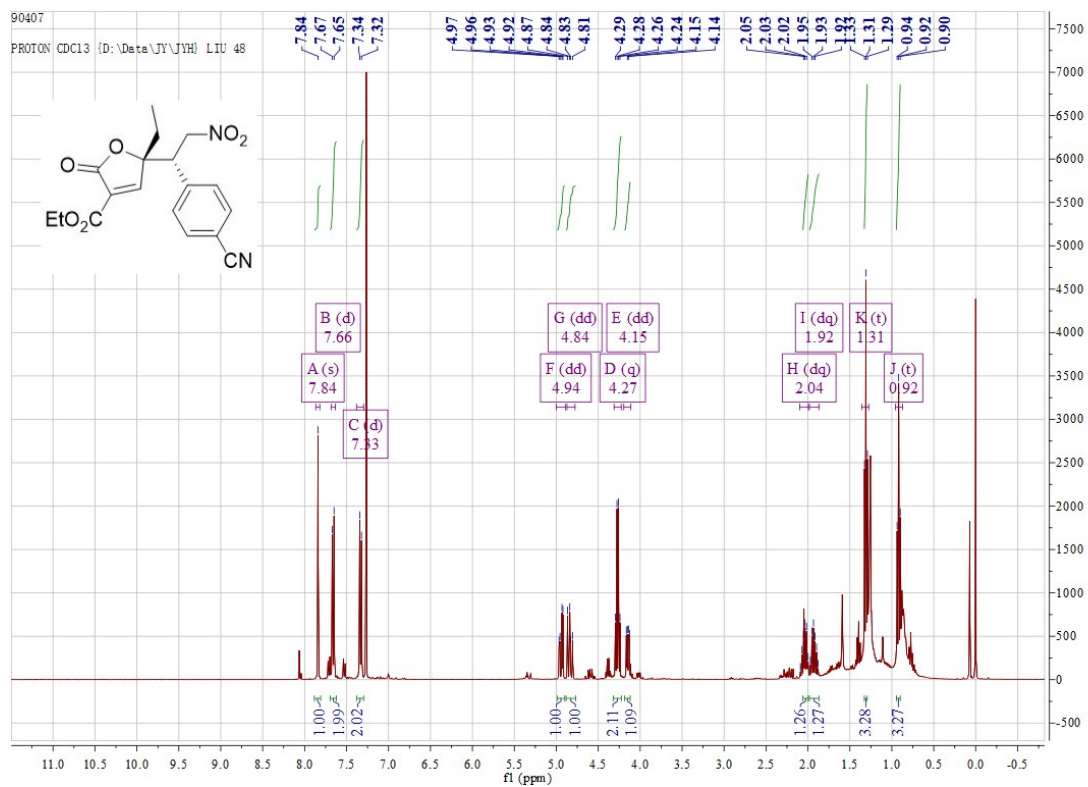
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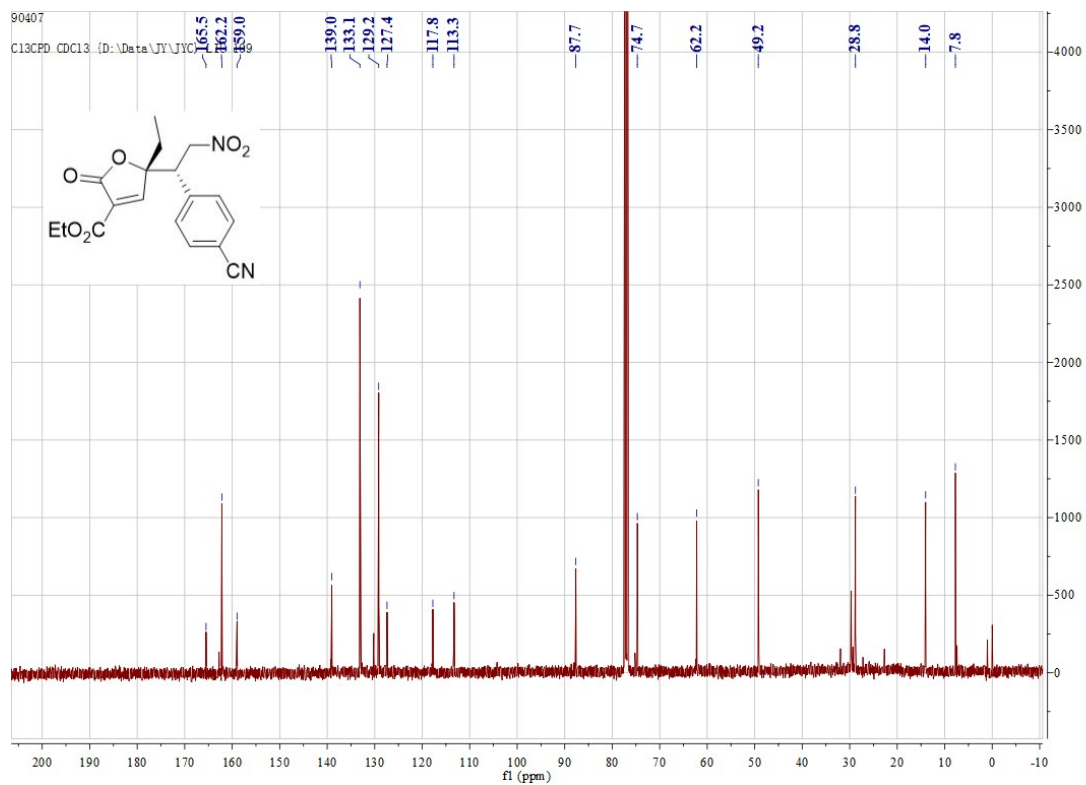
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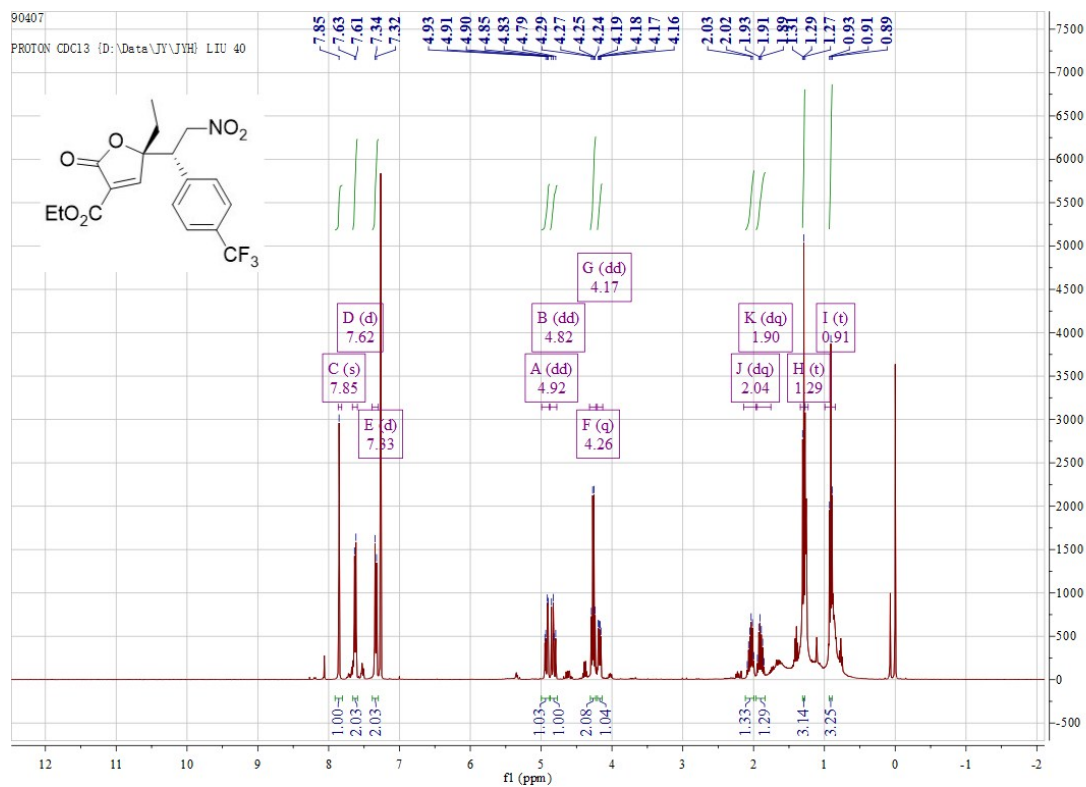
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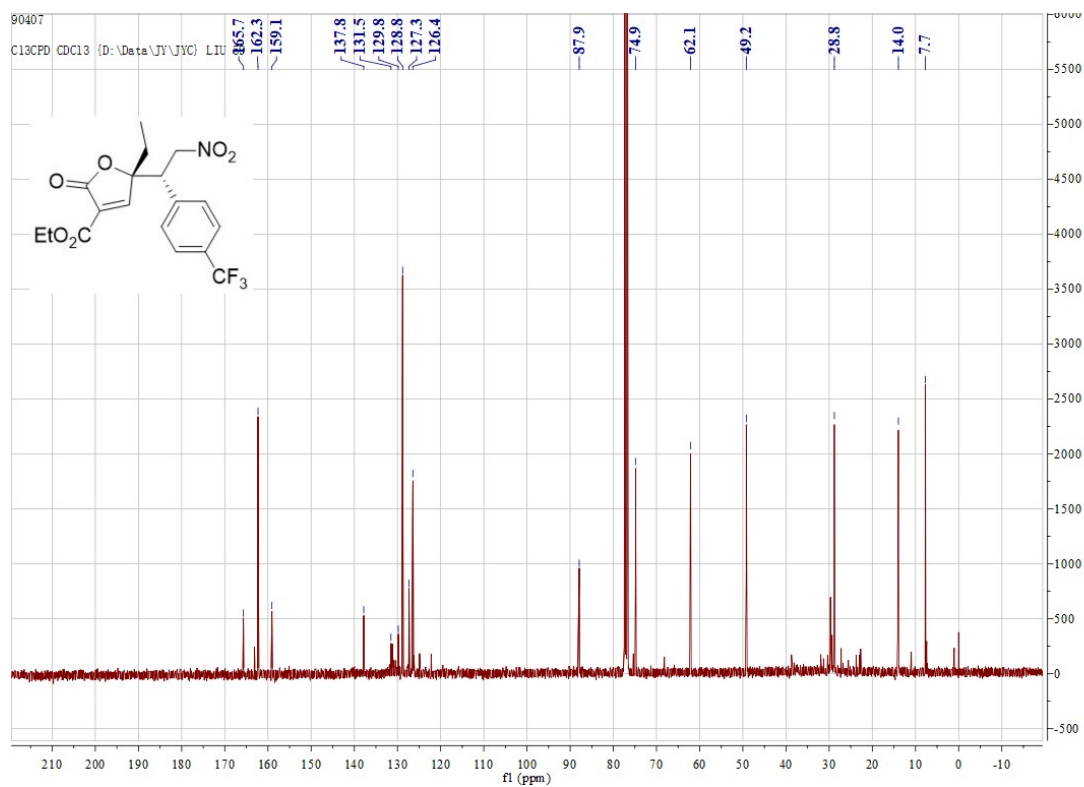
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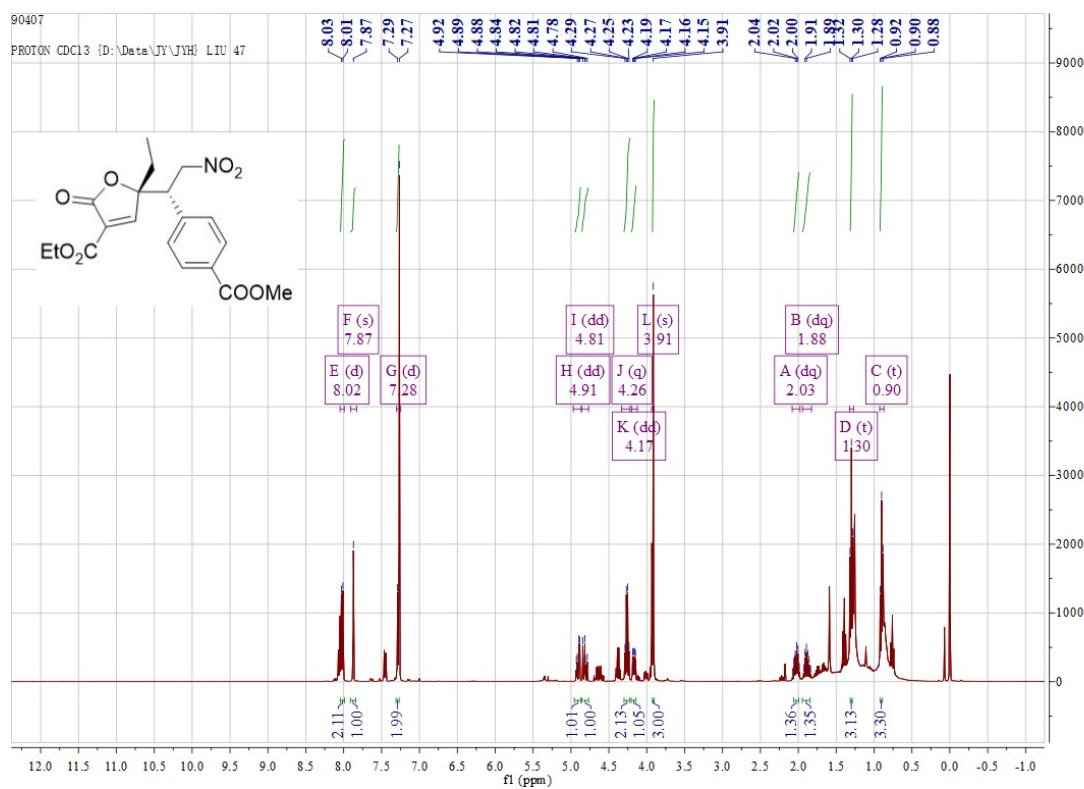
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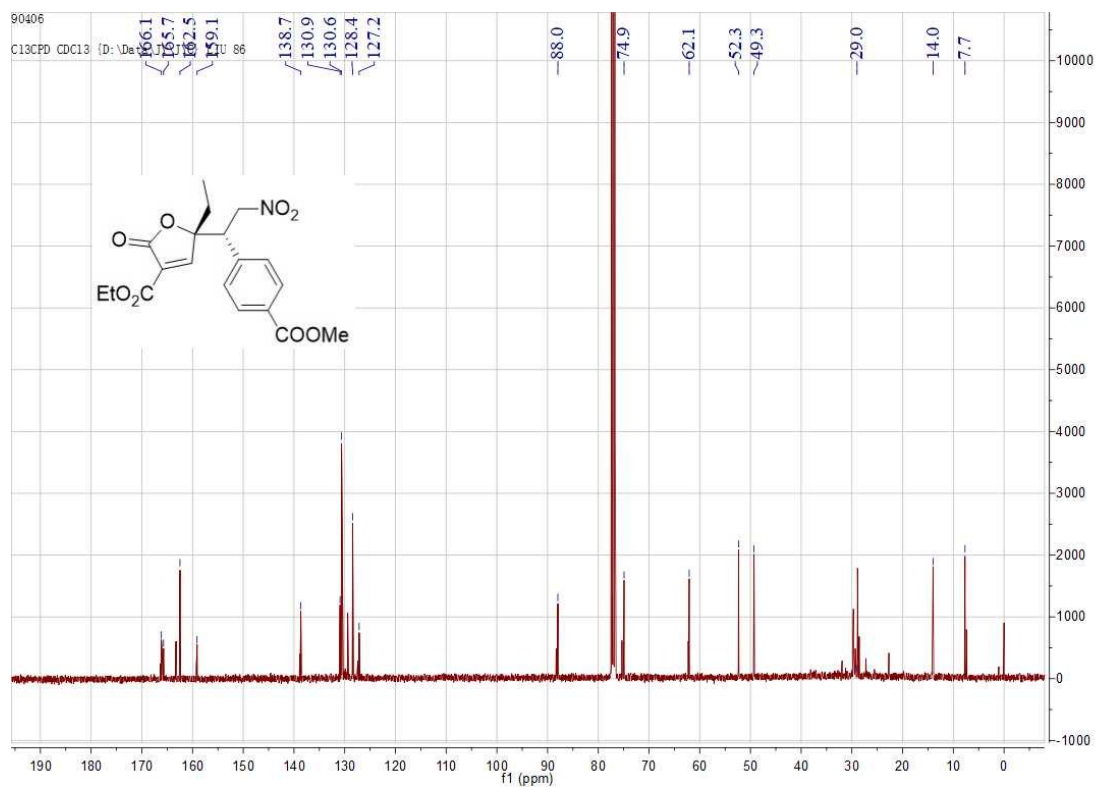
¹³C NMR of product **3a** (100 MHz, CDCl₃)



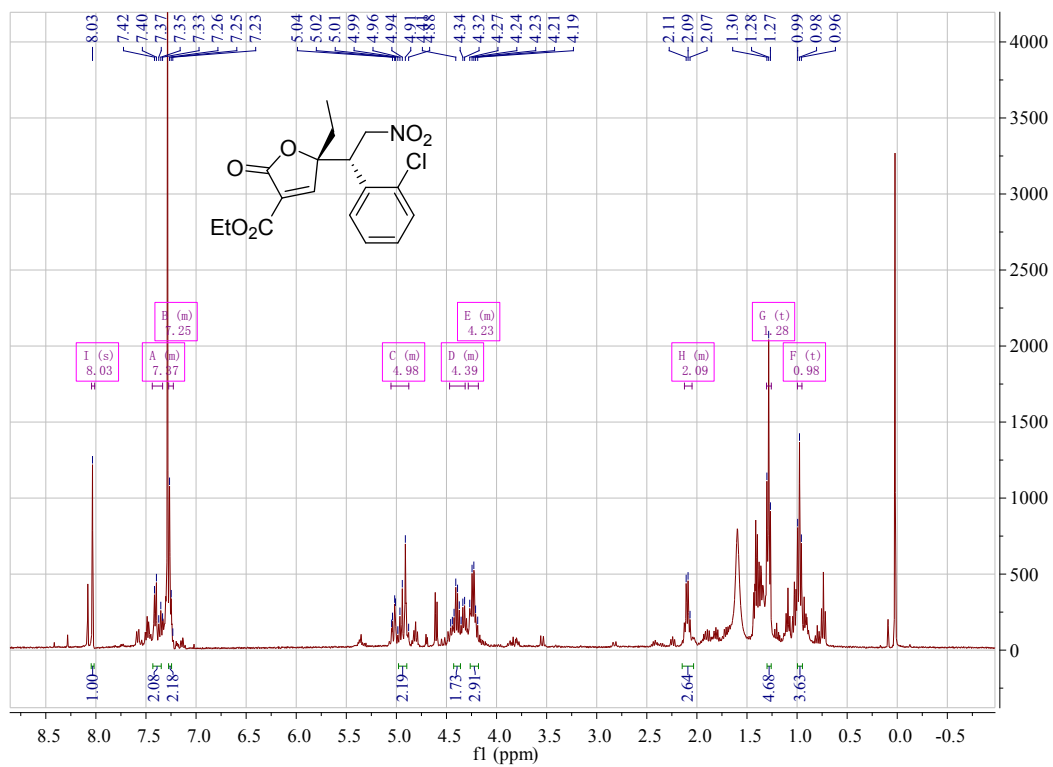
¹H NMR of product **3am** (400 MHz, CDCl₃)



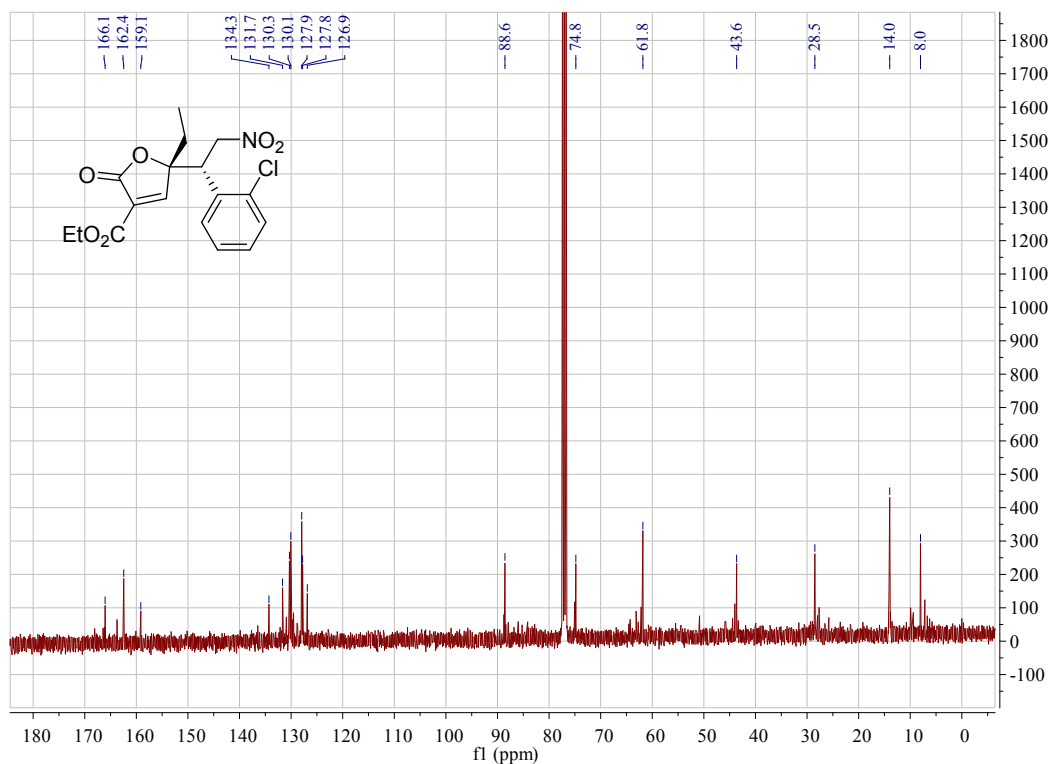
¹³C NMR of product **3am** (100 MHz, CDCl₃)



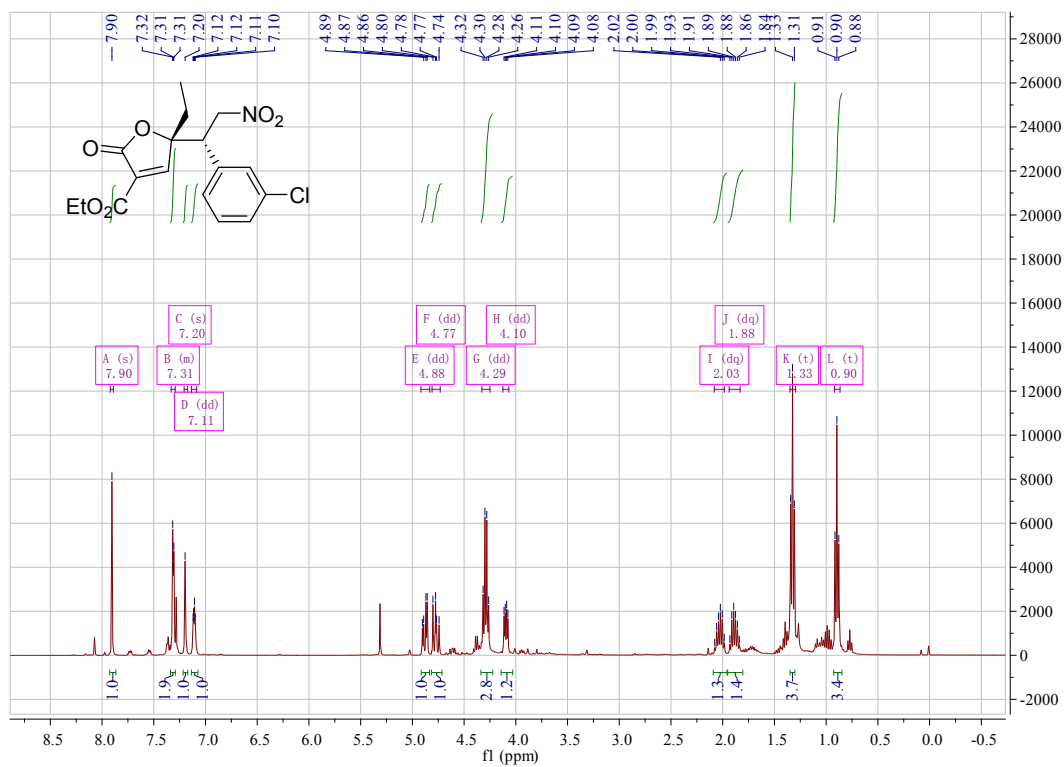
^1H NMR of product **3an** (400 MHz, CDCl_3)



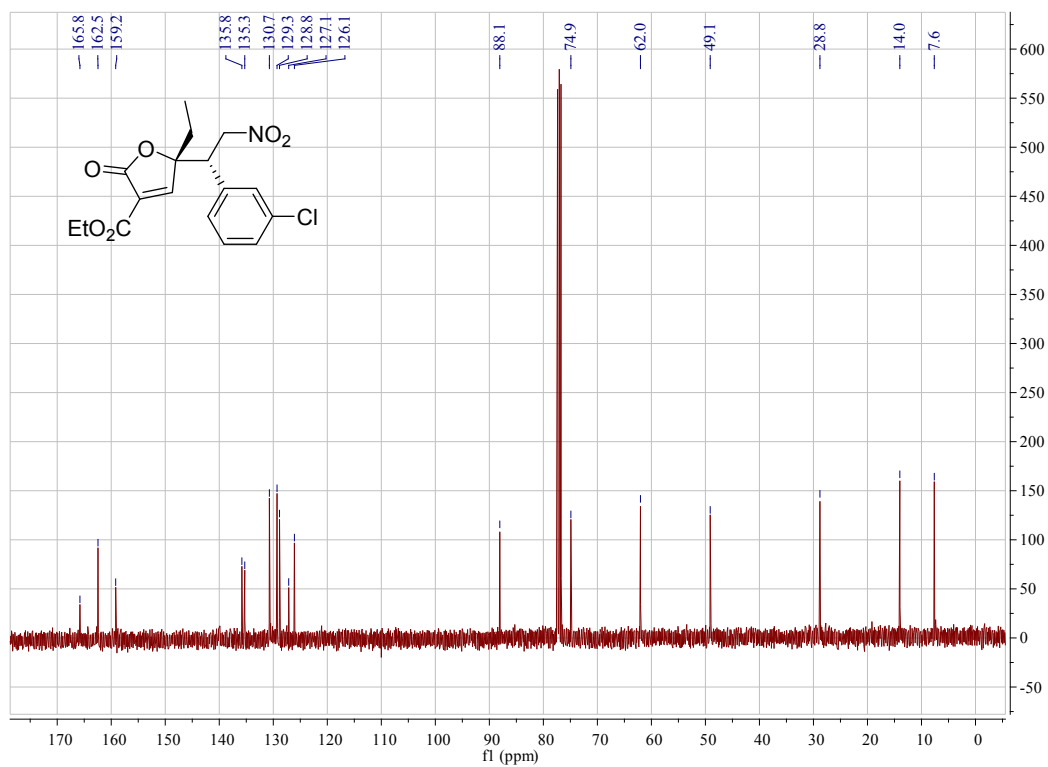
^{13}C NMR of product **3an** (100 MHz, CDCl_3)



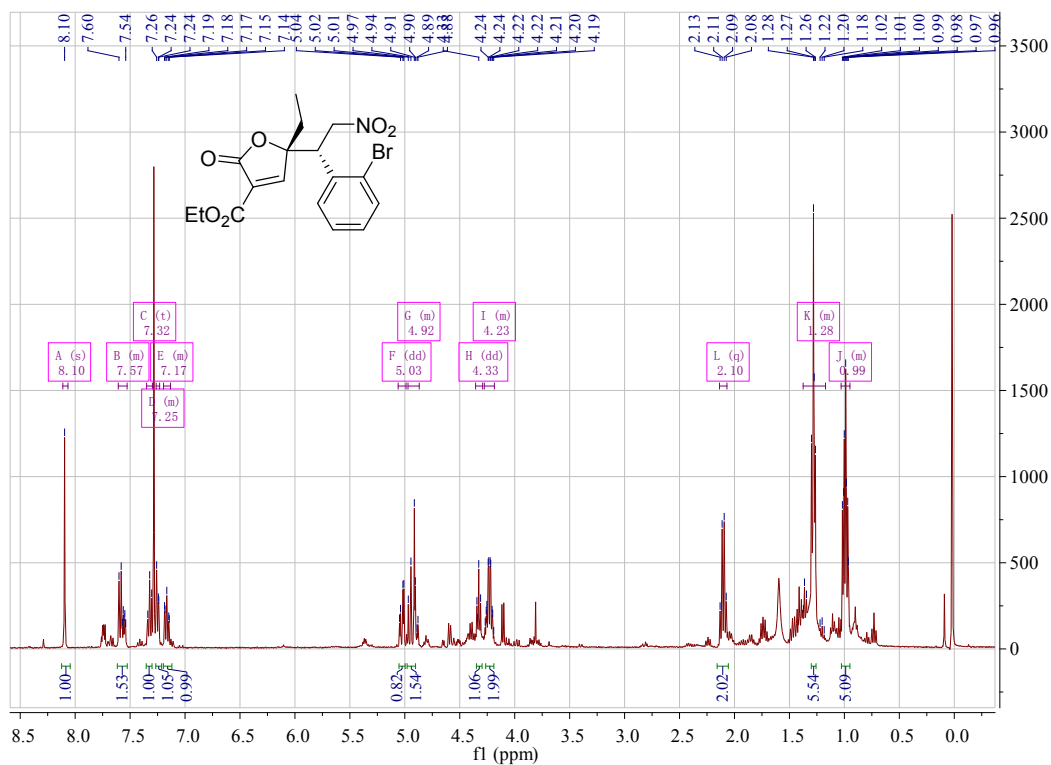
^1H NMR of product **3ao** (400 MHz, CDCl_3)



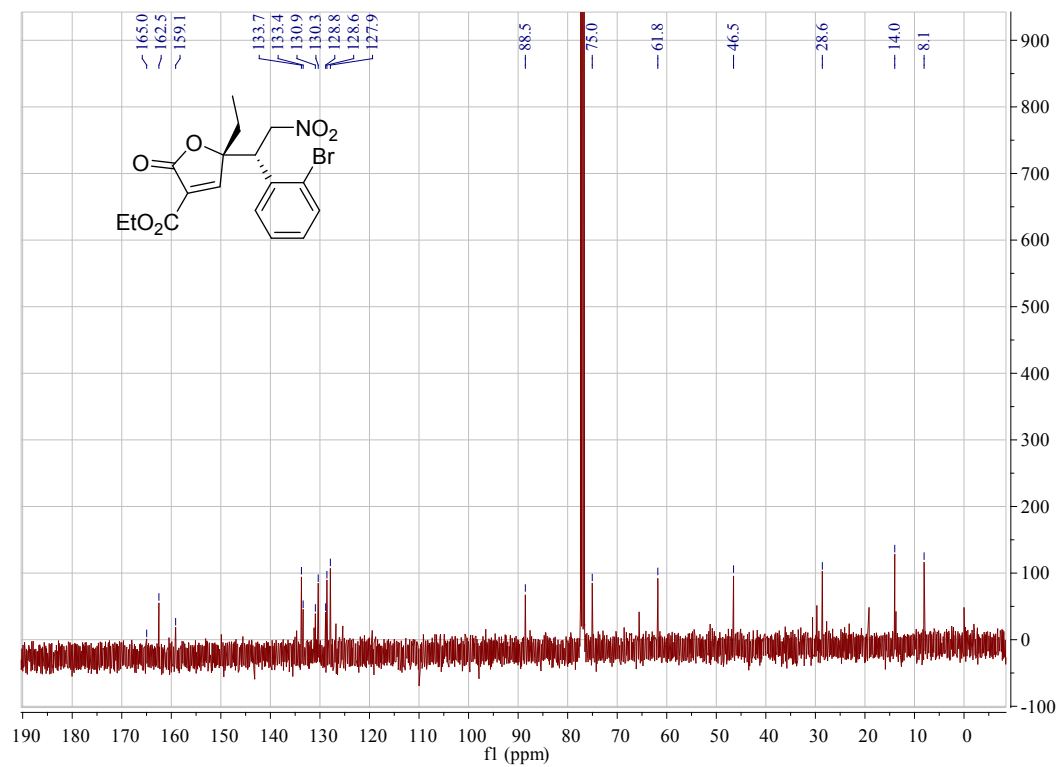
^{13}C NMR of product **3ao** (100 MHz, CDCl_3)



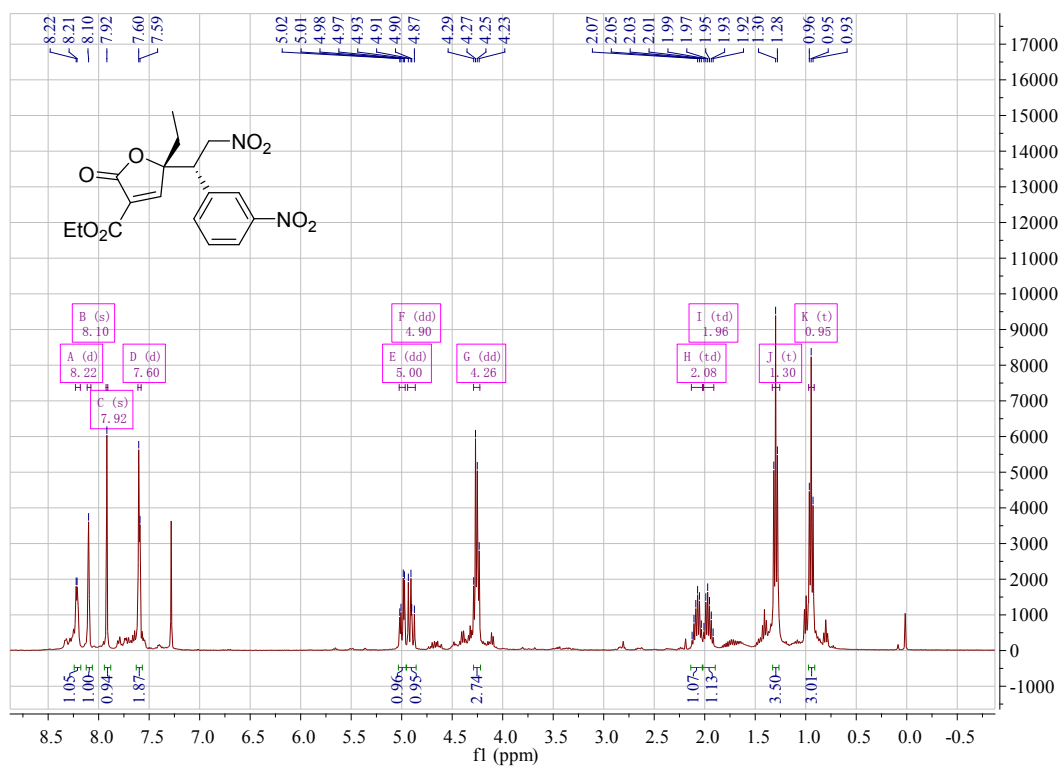
^1H NMR of product **3ap** (400 MHz, CDCl_3)



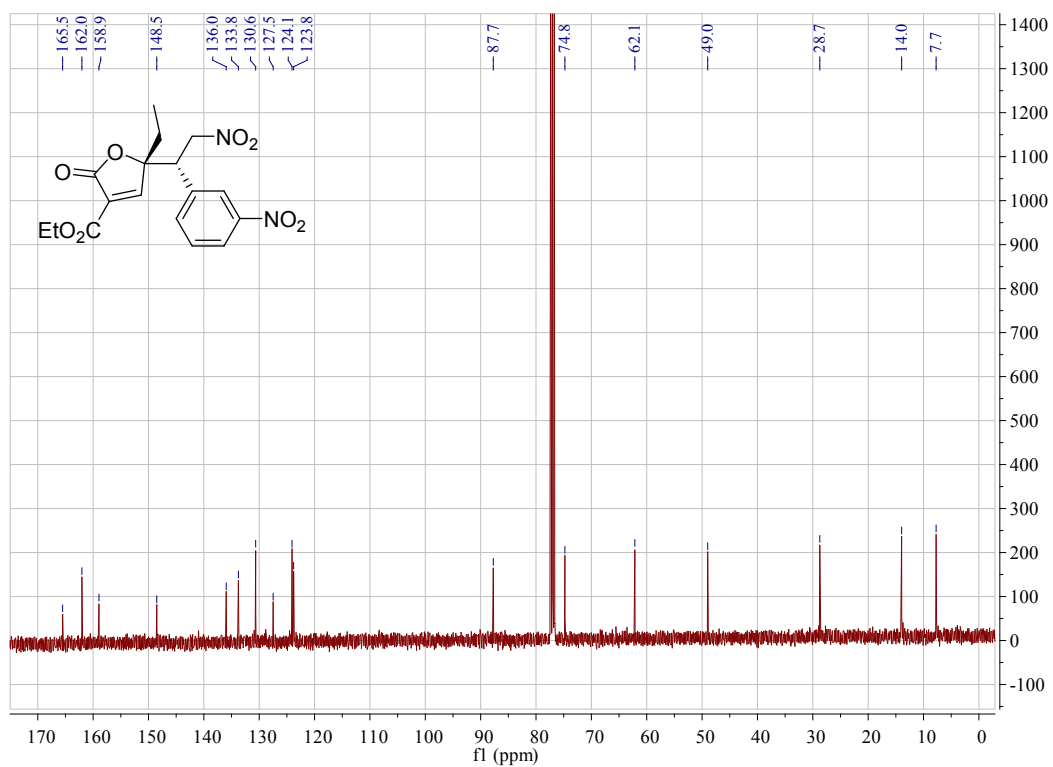
^{13}C NMR of product **3ap** (100 MHz, CDCl_3)



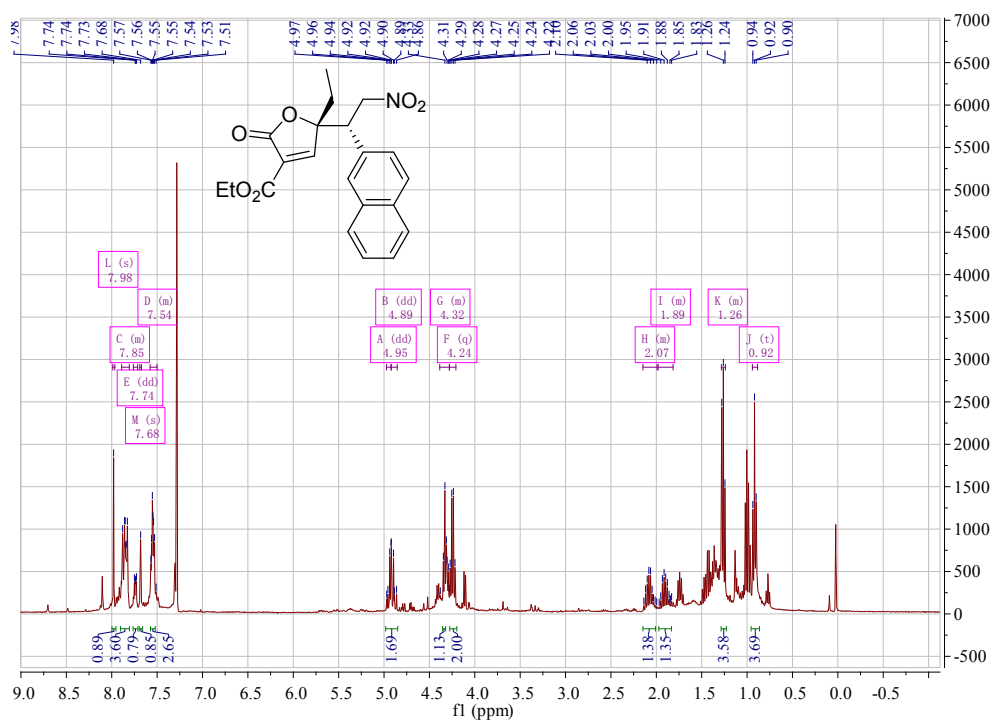
¹H NMR of product 3aq (400 MHz, CDCl₃)



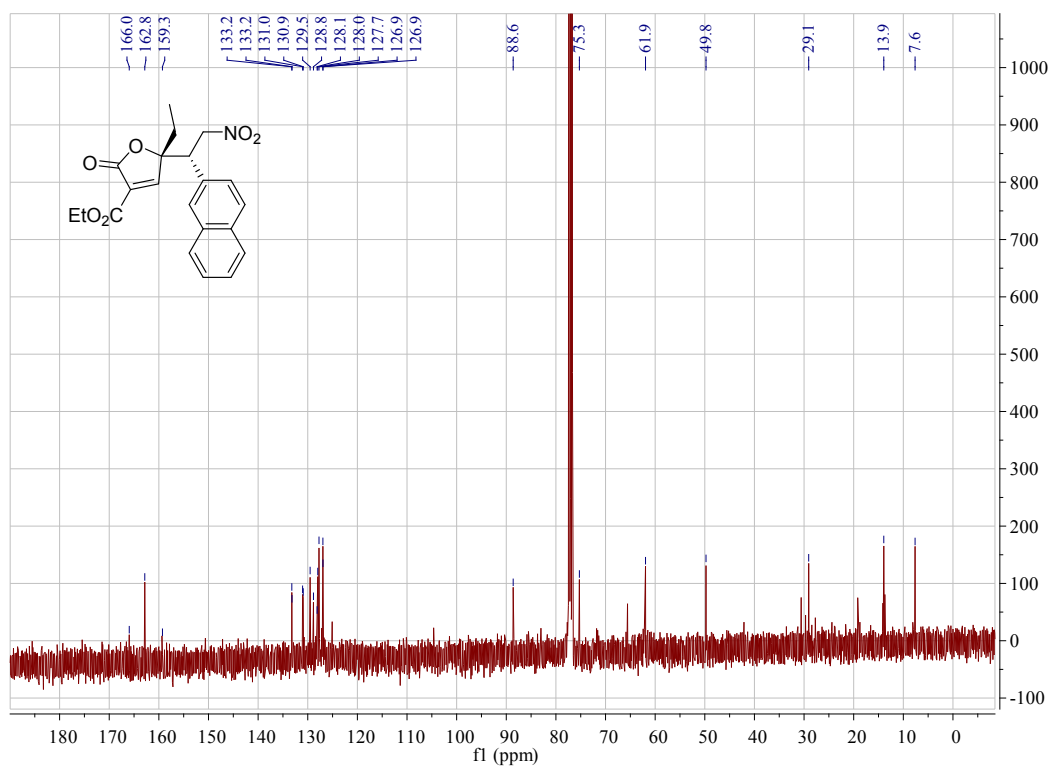
¹³C NMR of product 3aq (100 MHz, CDCl₃)



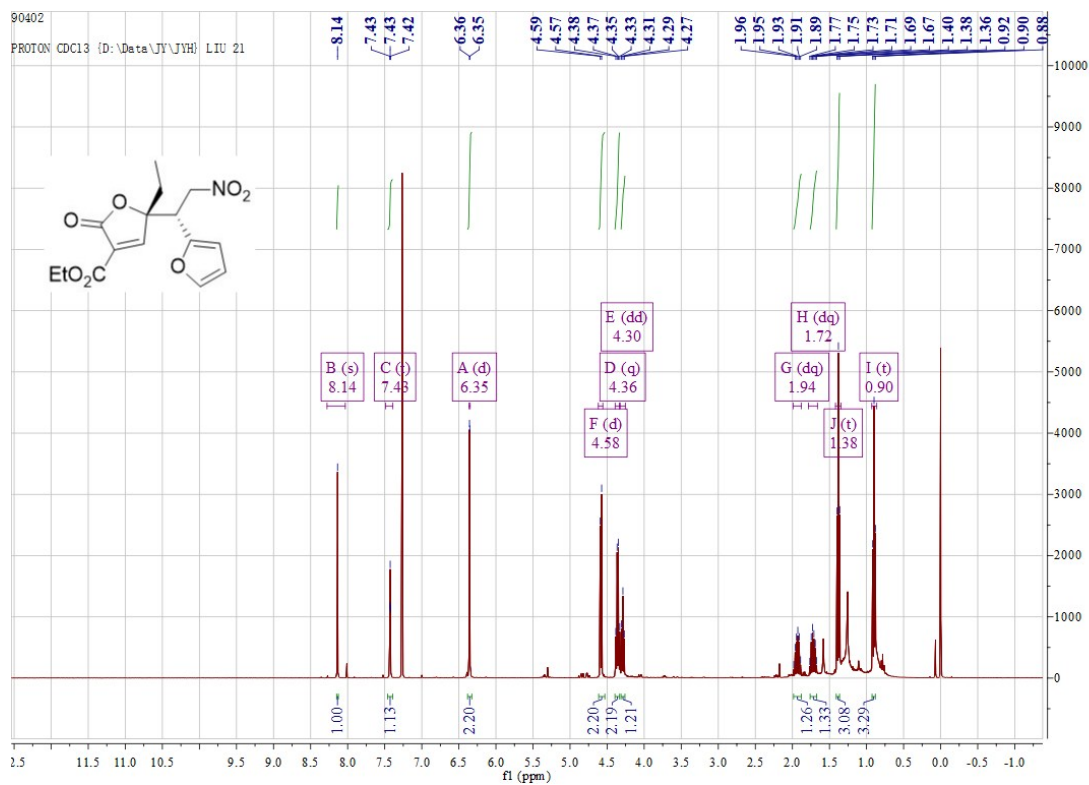
¹H NMR of product **3ar** (400 MHz, CDCl₃)



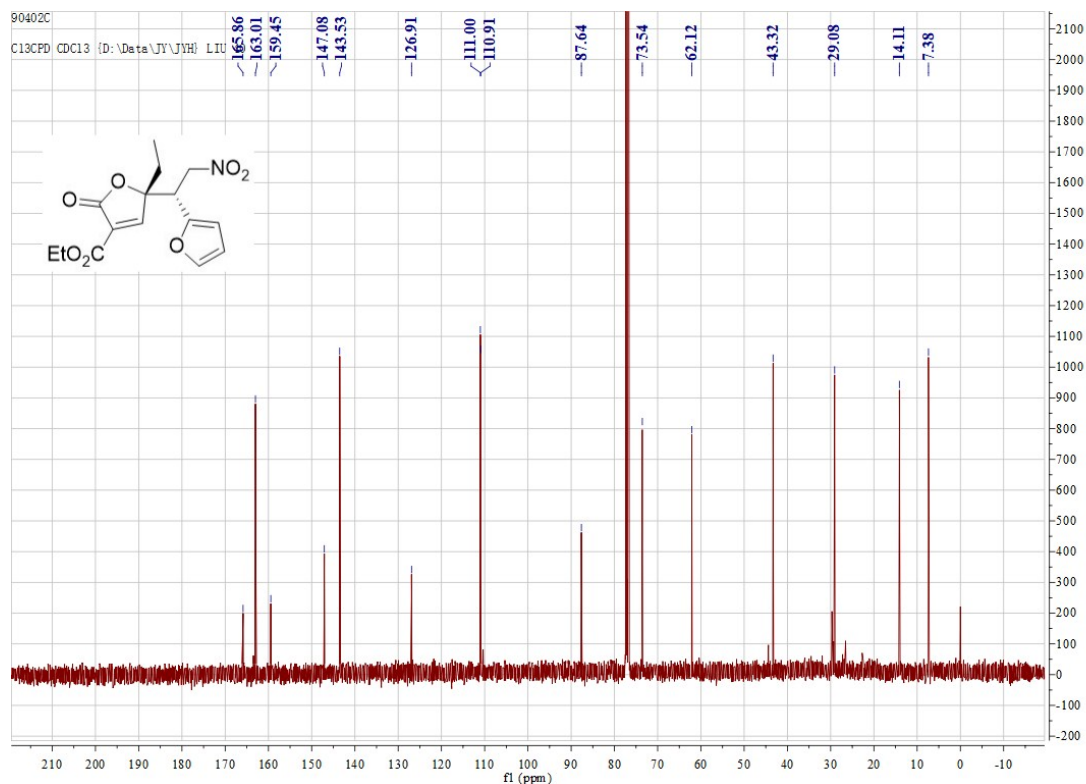
¹³C NMR of product 3ar (100 MHz, CDCl₃)



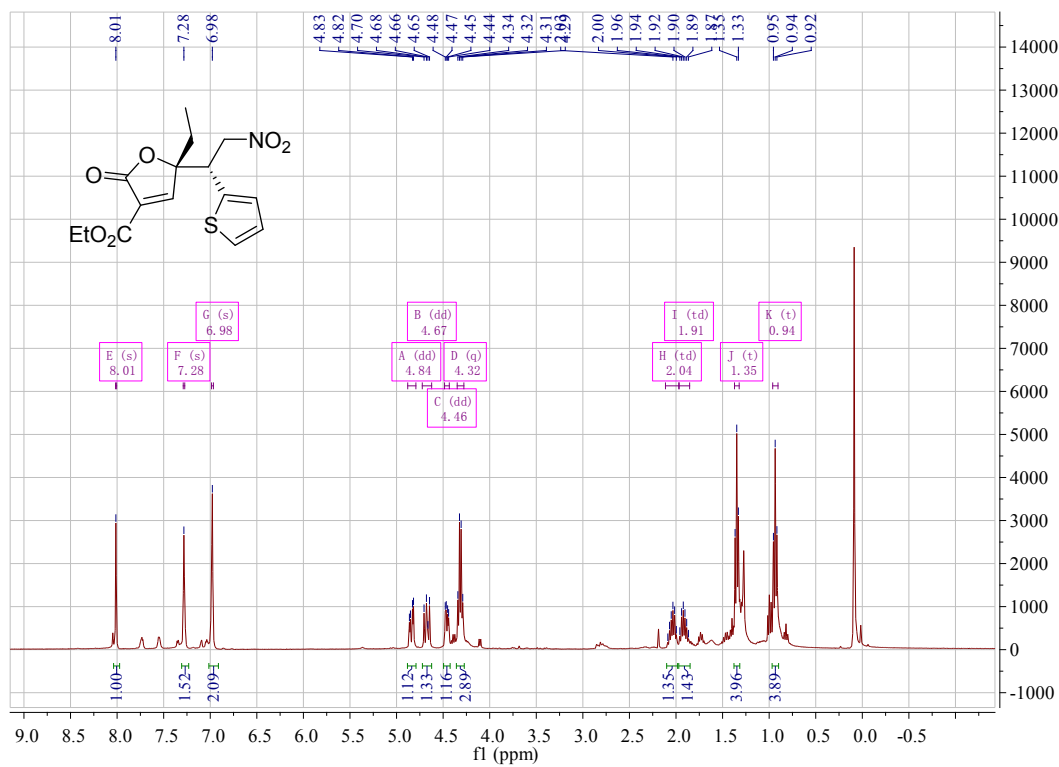
¹H NMR of product 3as (400 MHz, CDCl₃)



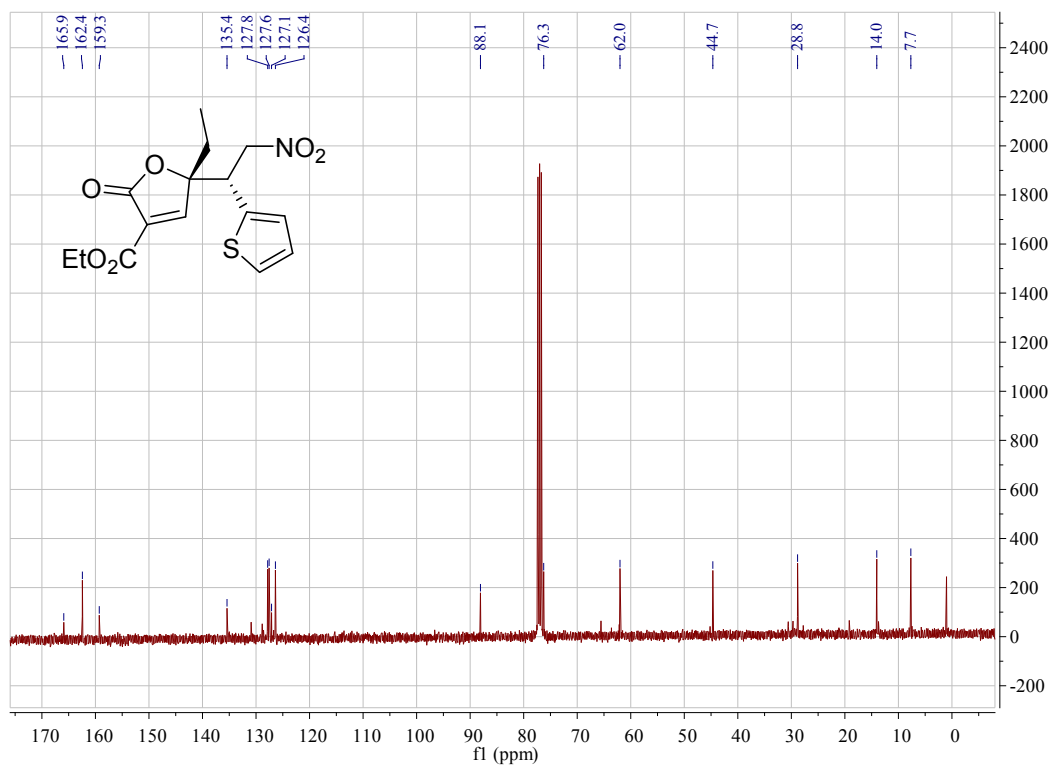
¹³C NMR of product **3as**(100 MHz, CDCl₃)



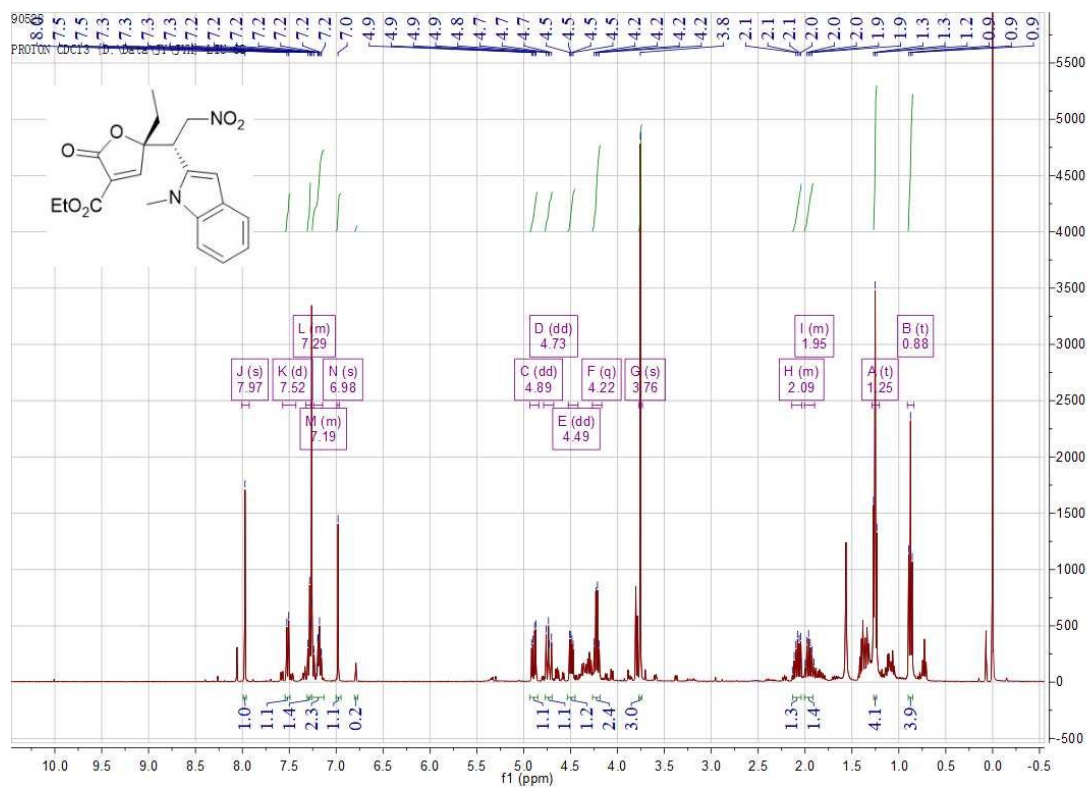
¹H NMR of product **3at** (400 MHz, CDCl₃)



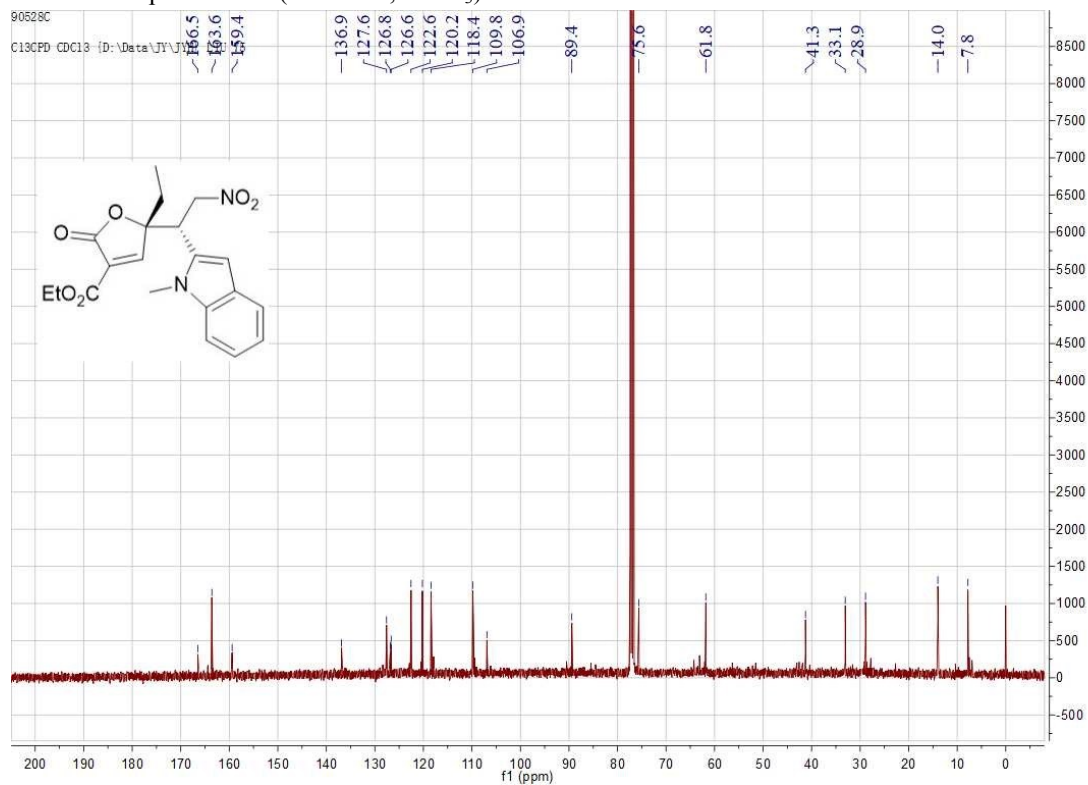
¹³C NMR of product 3at(100 MHz, CDCl₃)



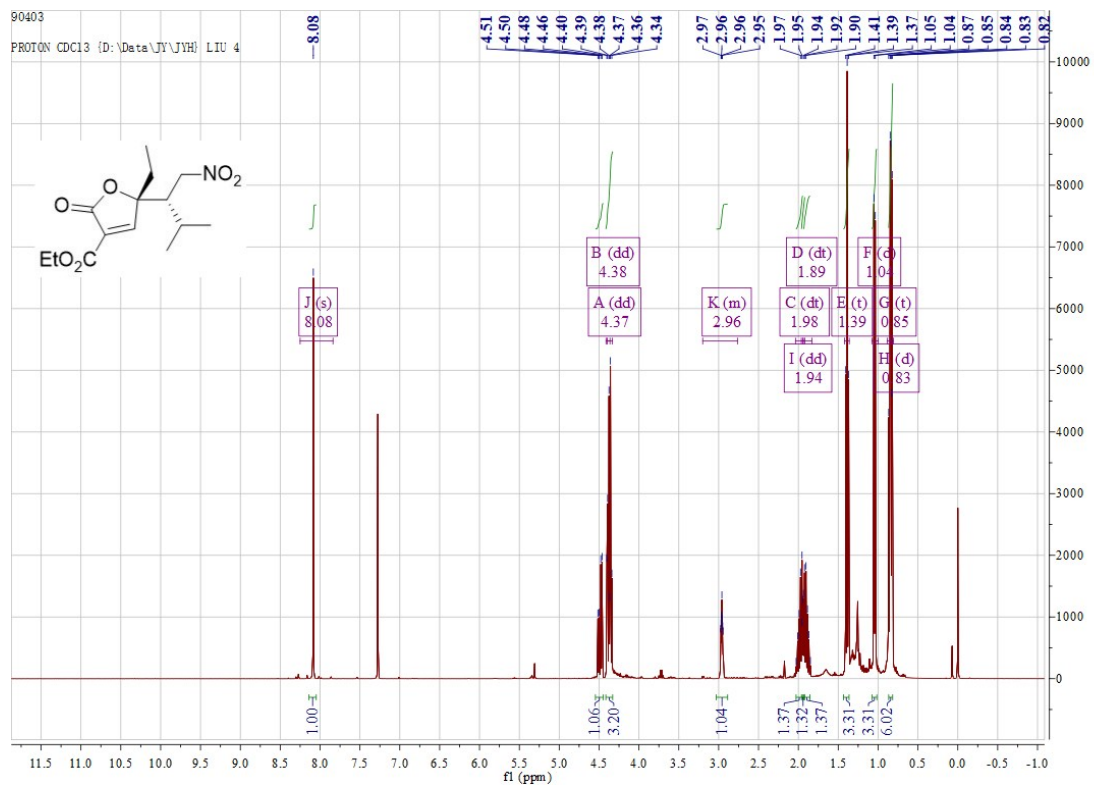
¹H NMR of product 3au (400 MHz, CDCl₃)



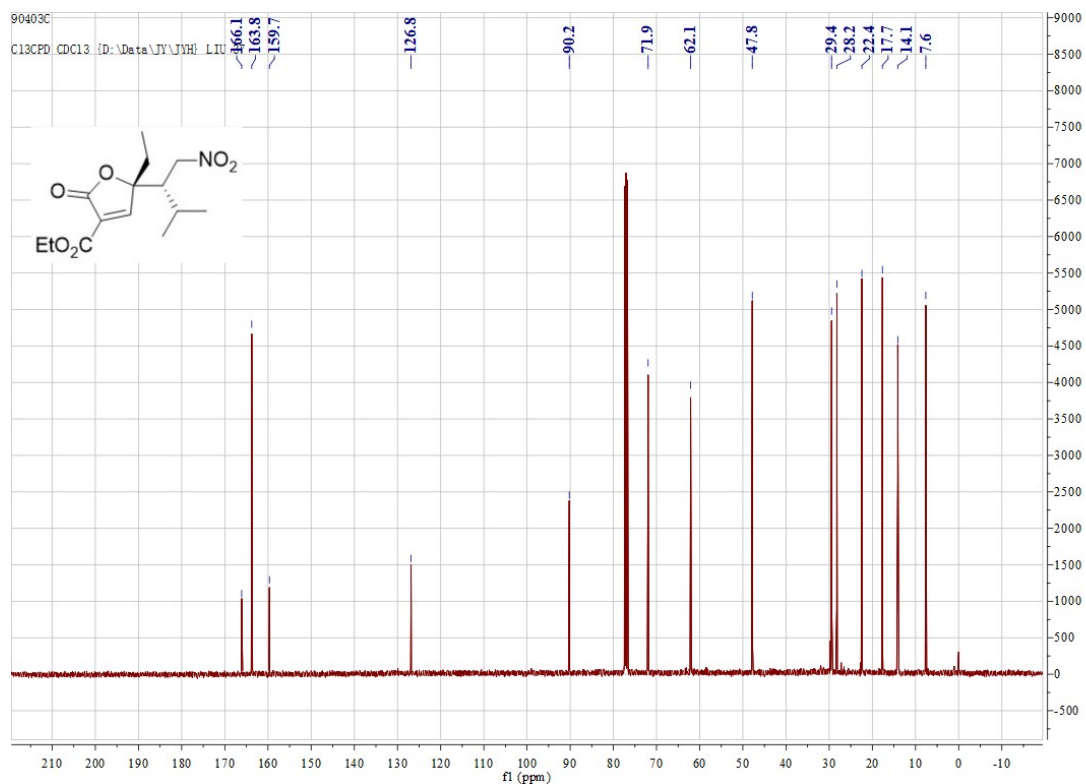
¹³C NMR of product **3au** (100 MHz, CDCl₃)



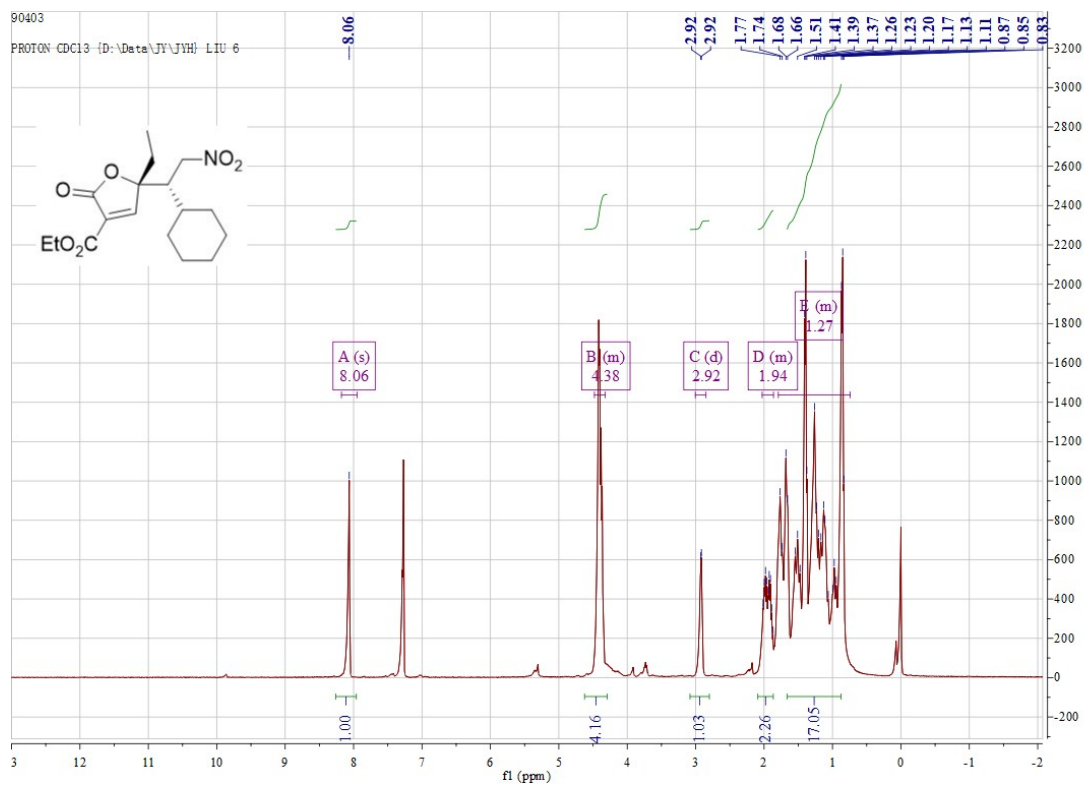
¹H NMR of product **3av** (400 MHz, CDCl₃)



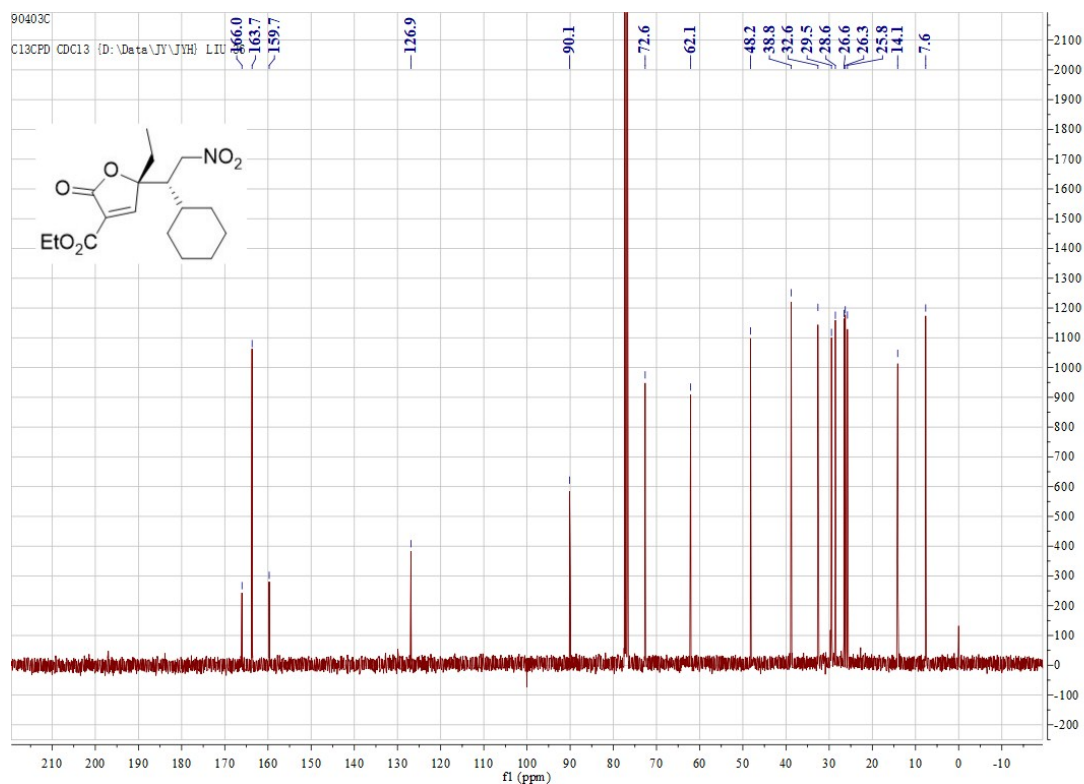
¹³C NMR of product **3aw**(100 MHz, CDCl₃)



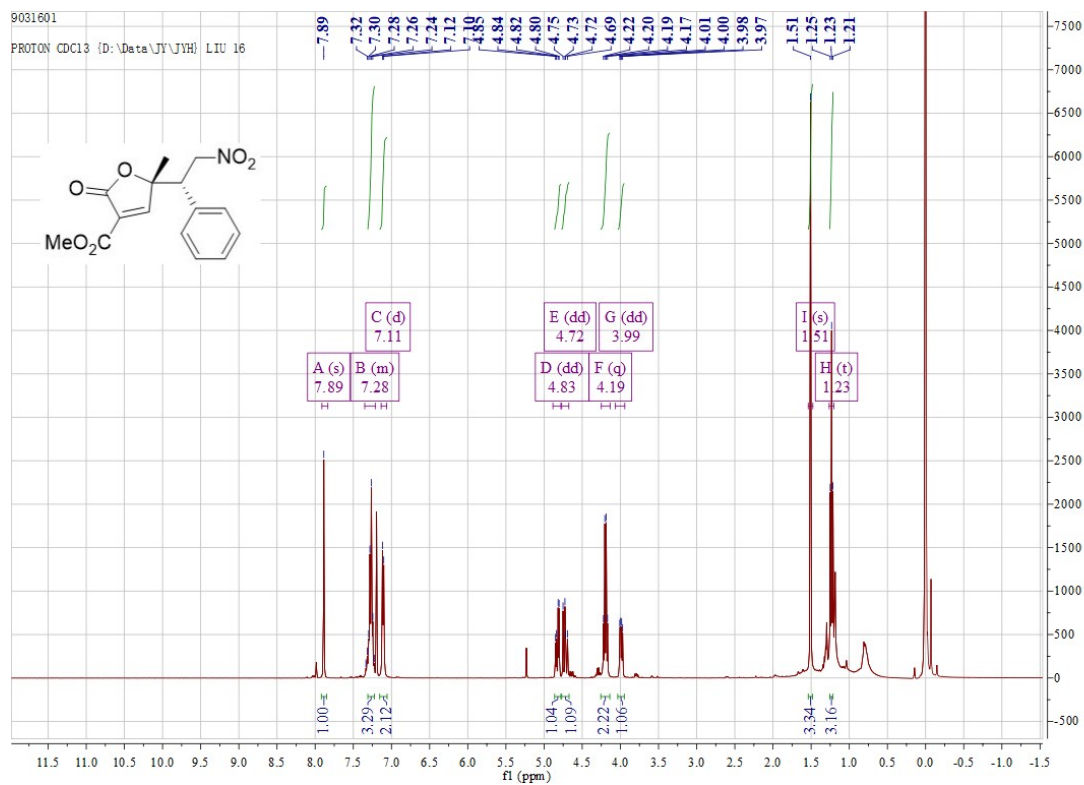
¹H NMR of product **3ax**(400 MHz, CDCl₃)



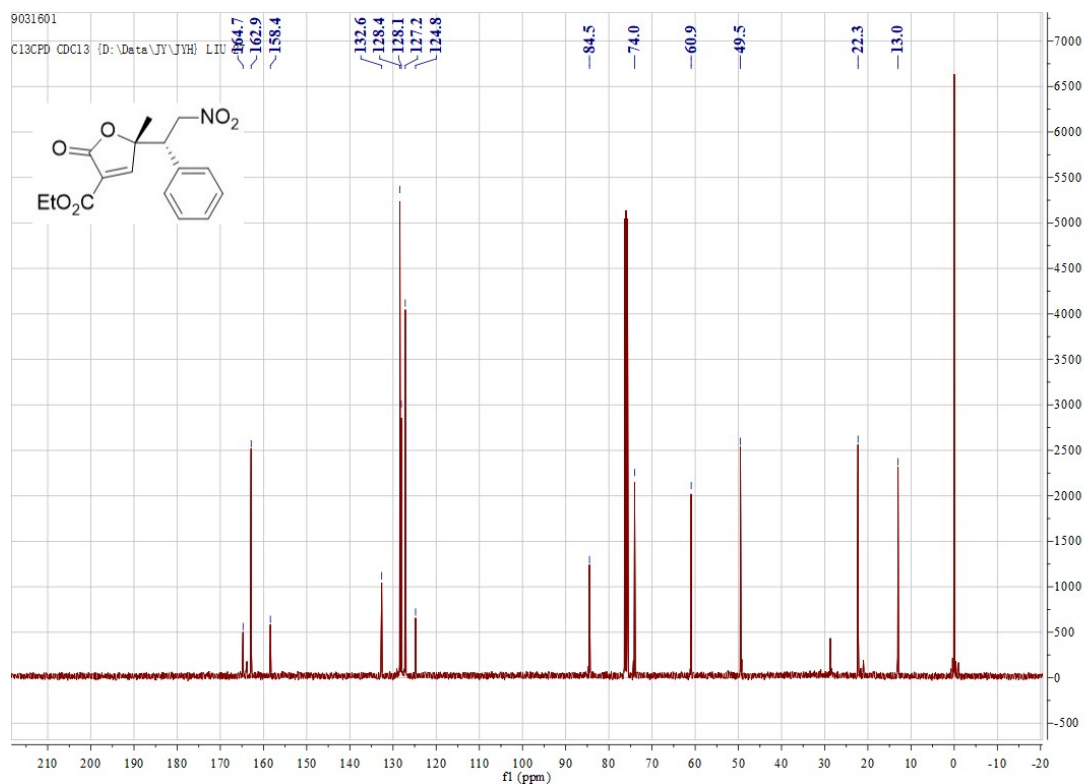
¹³C NMR of product **3ax**(100 MHz, CDCl₃)



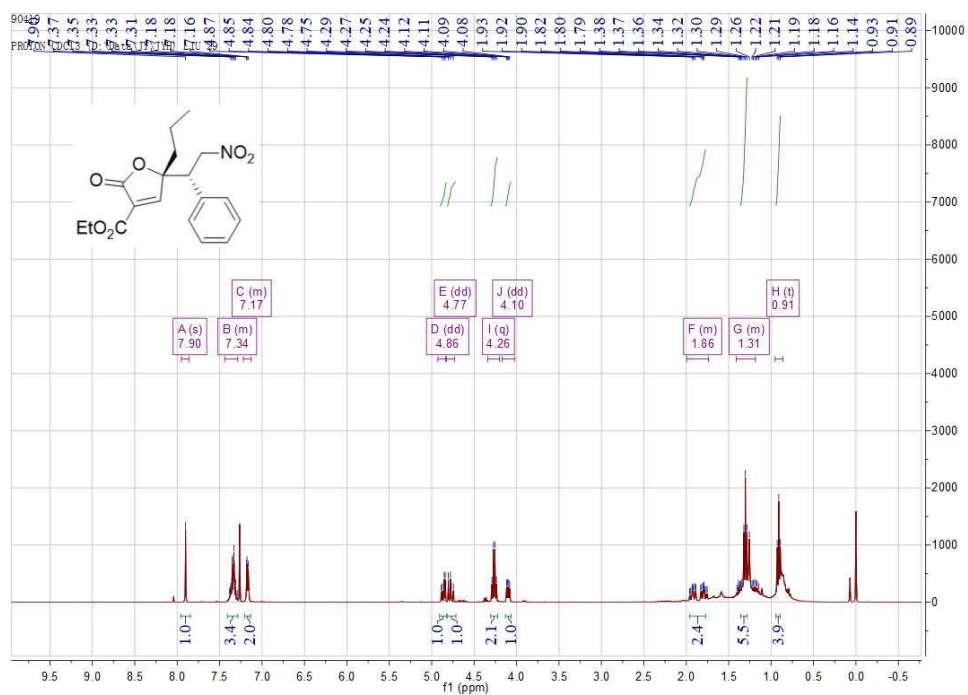
¹H NMR of product **3ay**(400 MHz, CDCl₃)



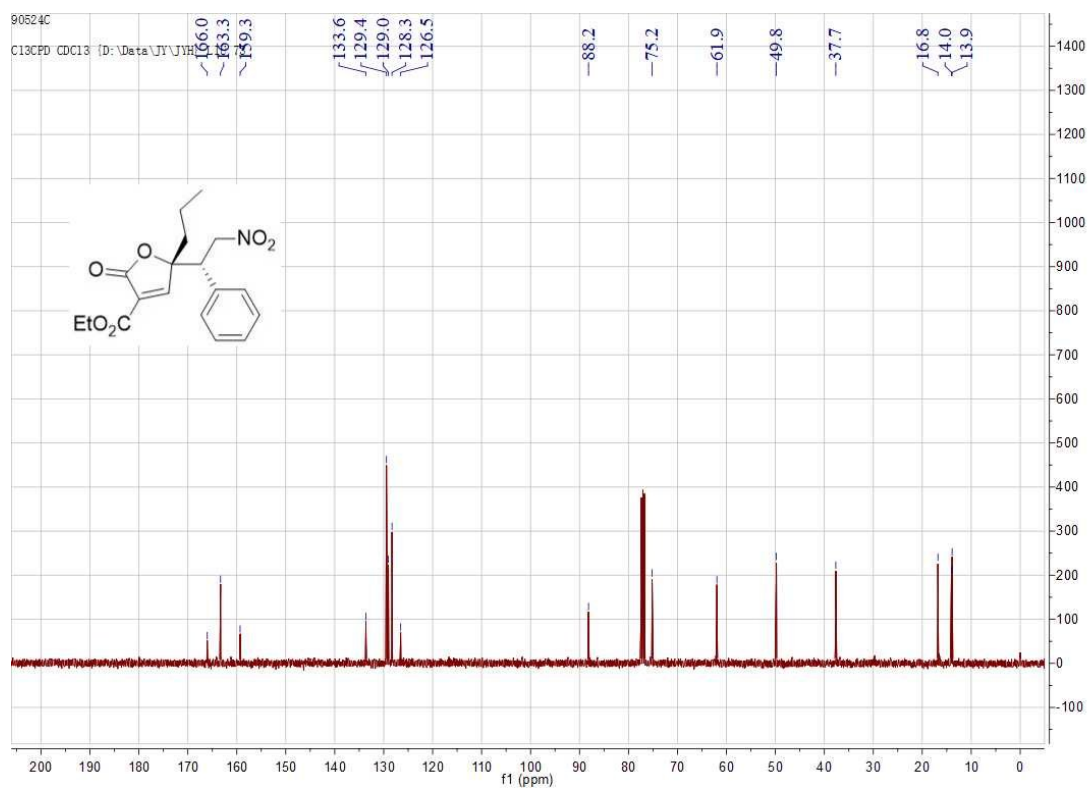
¹³C NMR of product **3ay**(100 MHz, CDCl₃)



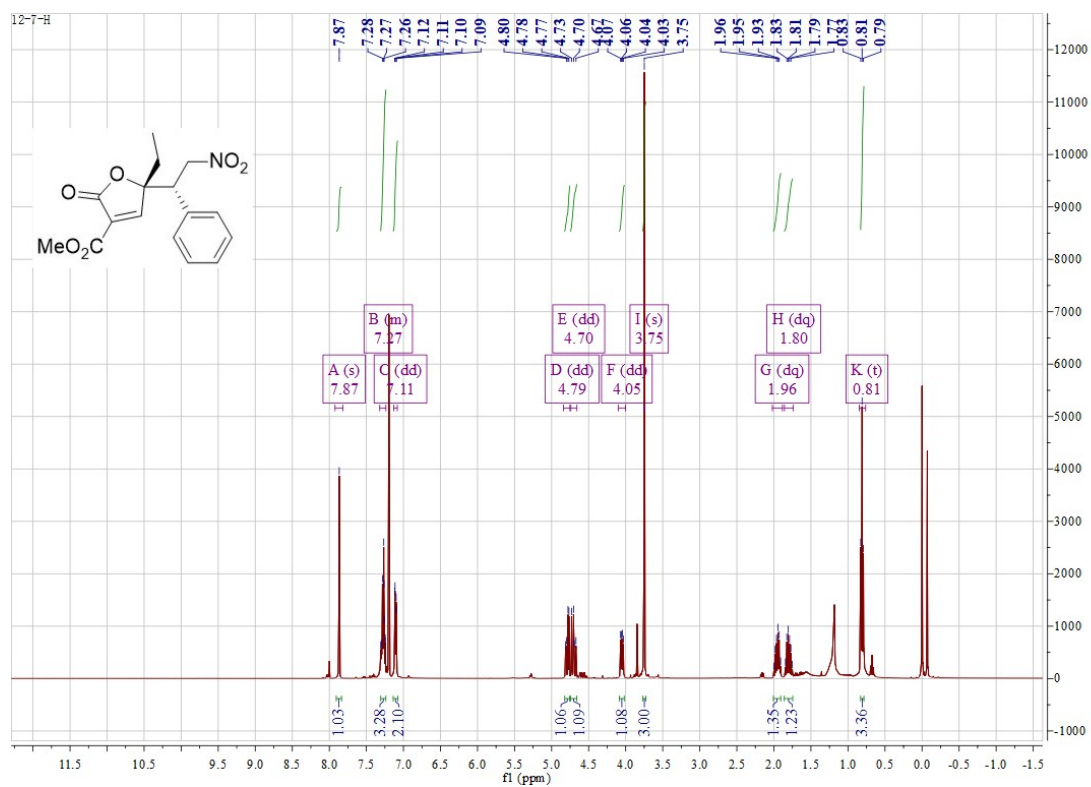
¹H NMR of product **3az**(400 MHz, CDCl₃)



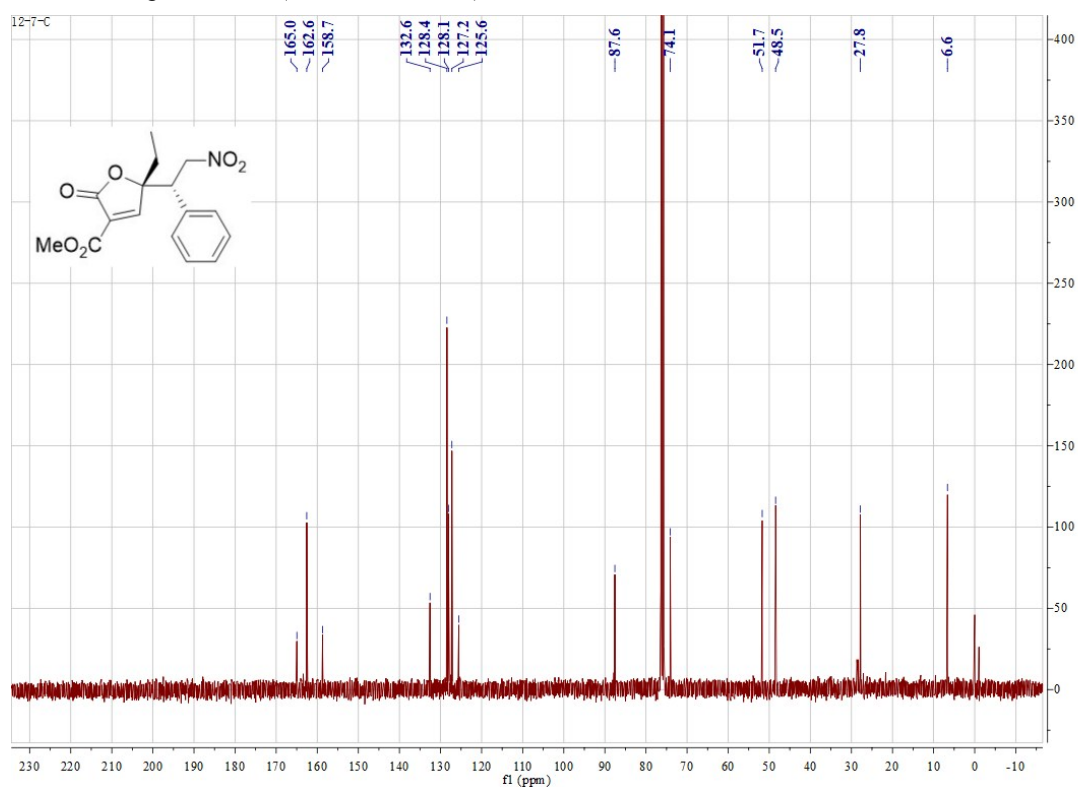
^{13}C NMR of product **3az** (100 MHz, CDCl_3)



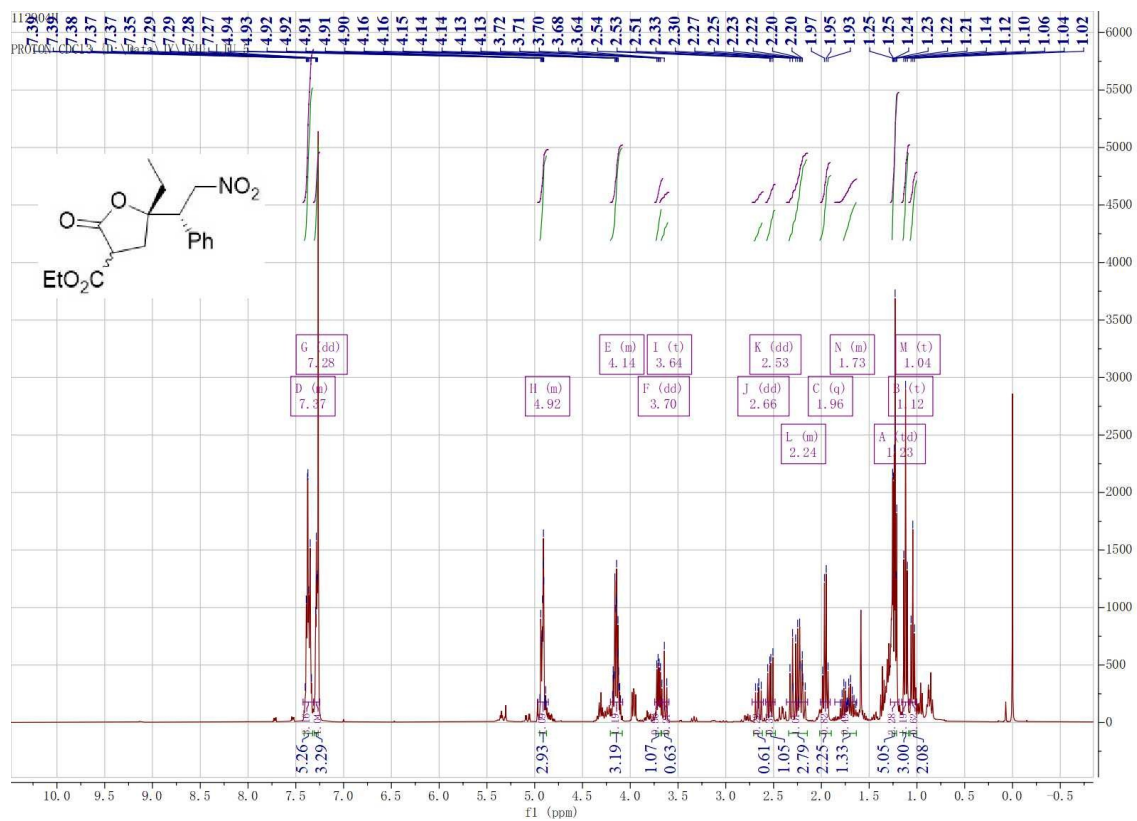
^1H NMR of product **3ba** (400 MHz, CDCl_3)



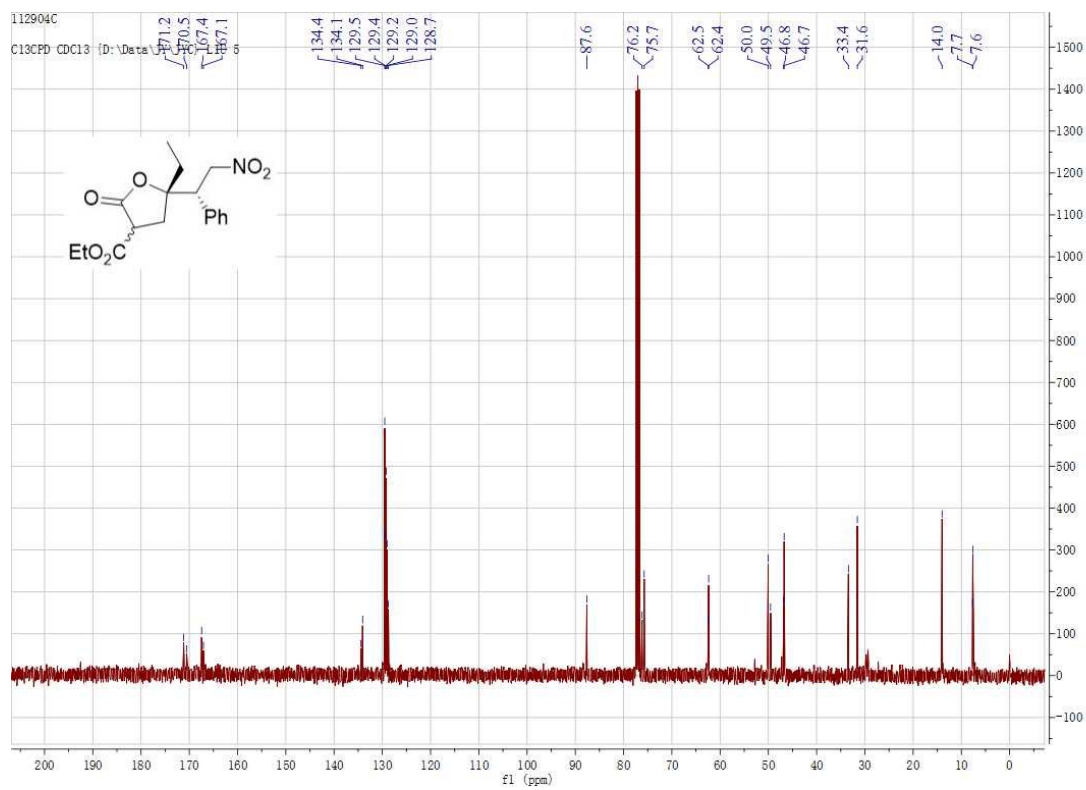
^{13}C NMR of product **3ba** (100 MHz, CDCl_3)



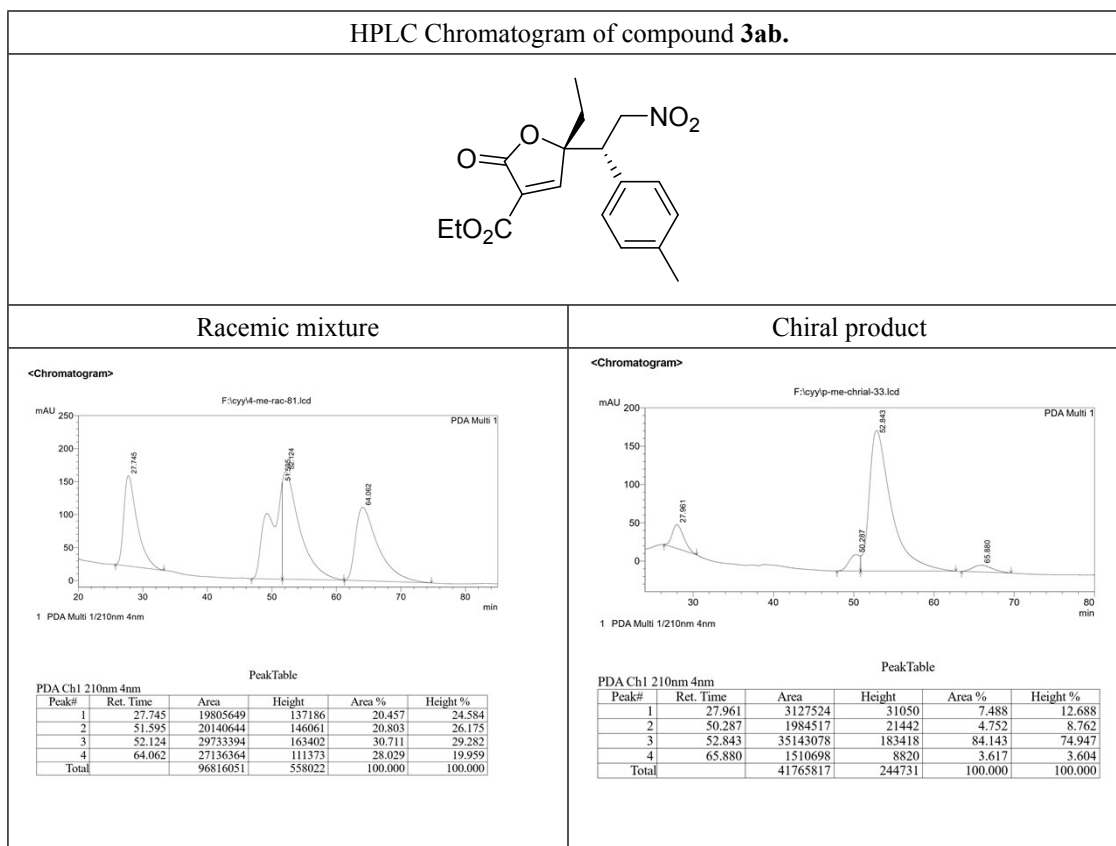
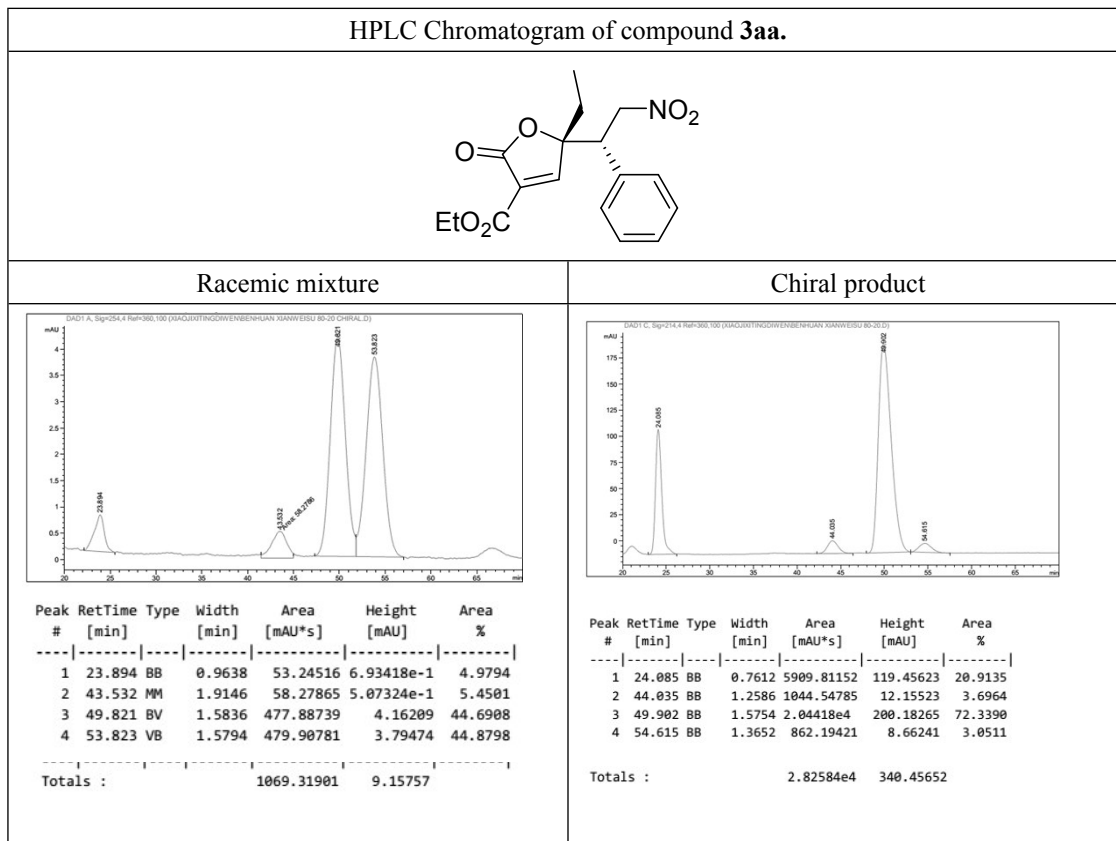
^1H NMR of product **4aa** (400 MHz, CDCl_3)



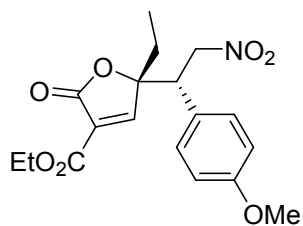
¹³C NMR of product 4aa (100 MHz, CDCl₃)



6. HPLC data for Product 3aa-3ba

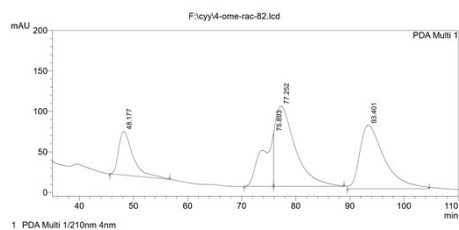


HPLC Chromatogram of compound 3ac.



Racemic mixture

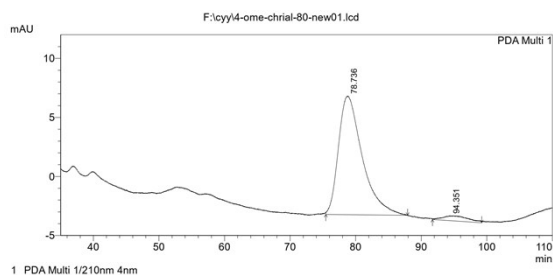
<Chromatogram>



Peak#	Ret. Time	Area	Height	Area %	Height %
1	48.177	9971147	54041	14.161	18.126
2	75.893	9693050	66025	13.766	22.145
3	77.252	25659588	99375	36.443	33.331
4	93.401	25087125	78706	35.630	26.398
Total		70410910	298147	100.000	100.000

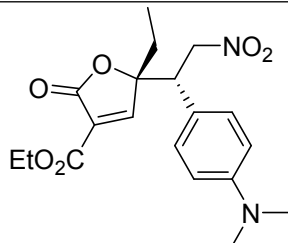
Chiral product

<Chromatogram>



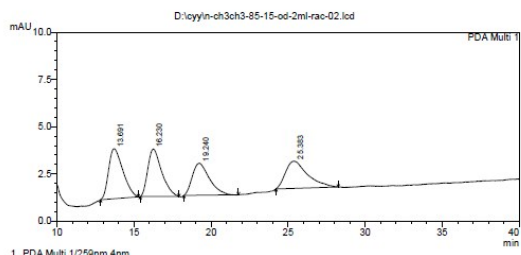
Peak#	Ret. Time	Area	Height	Area %	Height %
1	78.736	2534771	10062	95.650	95.980
2	94.351	115268	421	4.350	4.020
Total		2650039	10483	100.000	100.000

HPLC Chromatogram of compound 3ad.



Racemic mixture

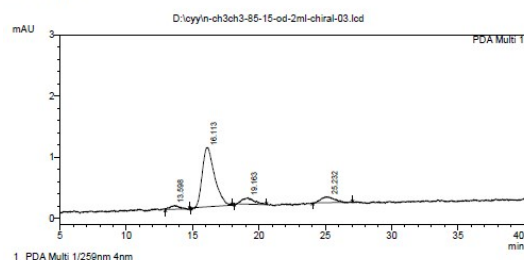
<Chromatogram>



Peak#	Ret. Time	Height	Area	Area %
1	13.691	3547	171140	32.350
2	16.220	3519	157837	26.146
3	19.240	1700	130598	21.894
4	23.383	1483	144565	28.370
Total		8315	603702	100.000

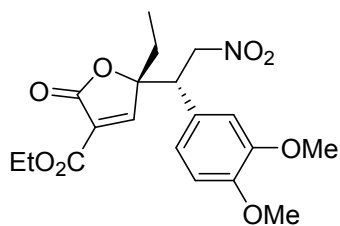
Chiral product

<Chromatogram>

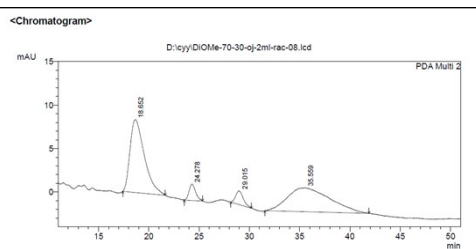


Peak#	Ret. Time	Height	Area	Area %
1	13.698	64	2968	3.760
2	16.113	958	62180	79.572
3	19.183	105	6445	8.348
4	23.322	101	6714	8.383
Total		1281	78151	100.000

HPLC Chromatogram of compound **3ac**.



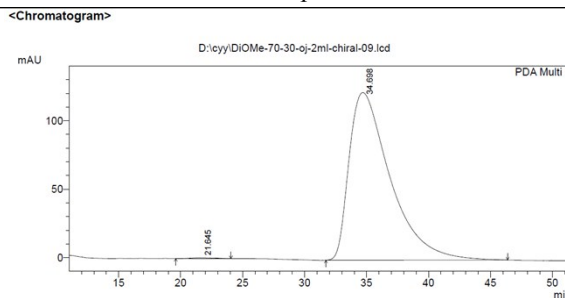
Racemic mixture



1 PDA Multi 2/210nm 4nm

PeakTable					
Peak#	Ret. Time	Height	Height %	Area	Area %
1	18.652	8386	57.290	831147	45.838
2	24.278	1899	12.973	86724	4.783
3	29.015	1589	10.855	83020	4.579
4	35.550	2764	18.882	812355	44.801
Total		14637	100.000	1813246	100.000

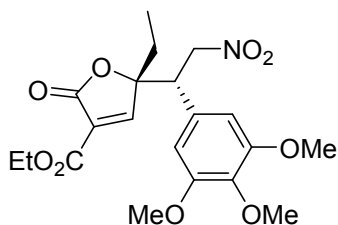
Chiral product



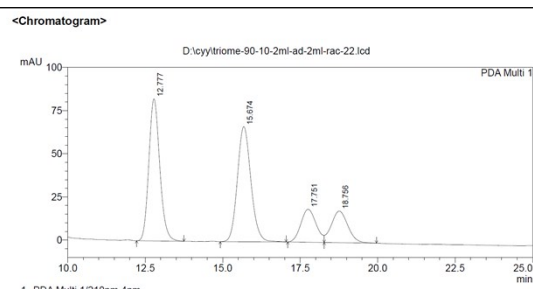
1 PDA Multi 1/210nm 4nm

PeakTable					
Peak#	Ret. Time	Height	Height %	Area	Area %
1	21.645	723	0.586	92164	0.324
2	34.698	122507	99.414	28312324	99.676
Total		123230	100.000	28404488	100.000

HPLC Chromatogram of compound **3af**.



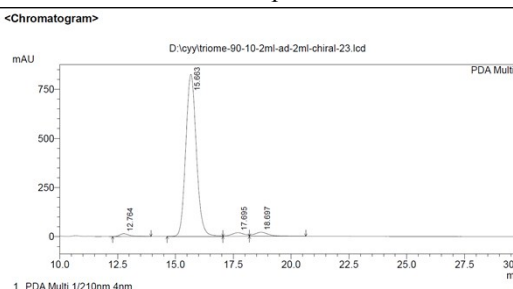
Racemic mixture



1 PDA Multi 1/210nm 4nm

PeakTable					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.777	2021573	82333	37.586	44.149
2	15.674	2025290	66710	37.655	35.772
3	17.751	652137	19126	12.125	10.256
4	18.756	679523	18320	12.634	9.824
Total		5378524	186489	100.000	100.000

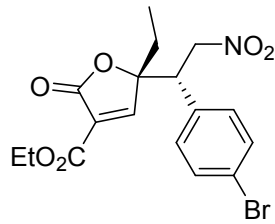
Chiral product



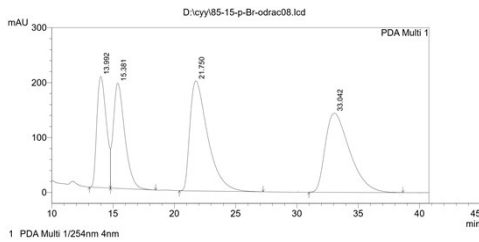
1 PDA Multi 1/210nm 4nm

PeakTable					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.764	413969	14444	1.465	1.644
2	15.663	26270312	825083	92.966	93.935
3	17.695	705226	18312	2.496	2.085
4	18.697	868390	20518	3.073	2.336
Total		28257896	878356	100.000	100.000

HPLC Chromatogram of compound **3ag**.

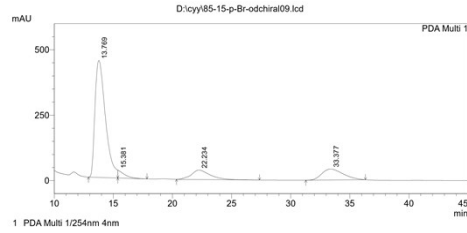


Racemic mixture



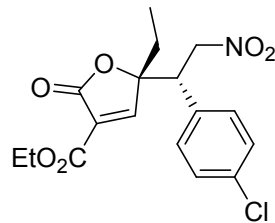
Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.992	10892646	202312	17.104	27.392
2	15.381	12517595	191749	19.655	25.962
3	21.750	20287894	200399	31.856	27.133
4	33.042	19987323	144112	31.384	19.512
Total		63685459	738573	100.000	100.000

Chiral product

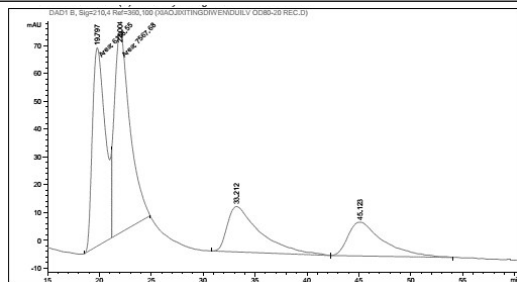


Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.769	27462001	446982	72.440	80.571
2	15.381	1147259	29932	3.026	5.395
3	22.234	4022017	35978	10.609	6.485
4	33.377	5278668	41876	13.924	7.548
Total		37909946	554767	100.000	100.000

HPLC Chromatogram of compound **3ah**.

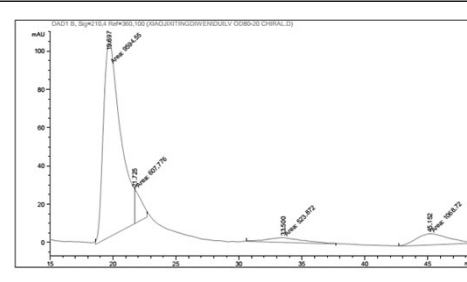


Racemic mixture



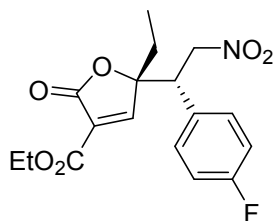
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.797	MF	1.4381	6158.54834	71.37608	30.5933
2	22.004	FM	1.7476	7567.68115	72.17051	37.5934
3	33.212	BB	3.0560	3561.46216	16.28172	17.6920
4	45.123	BB	3.4003	2842.66895	12.15551	14.1213
Totals :				2.01304e4	171.98383	

Chiral product

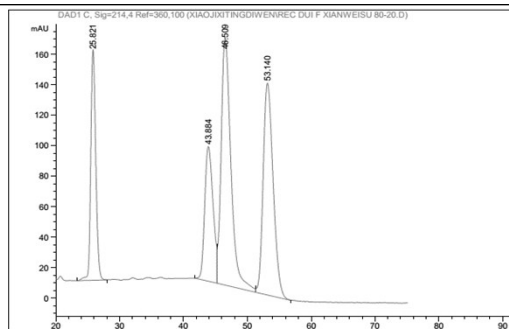


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.697	MF	1.5636	9594.54883	102.26734	81.3448
2	21.725	FM	0.5634	607.77557	17.97822	5.1529
3	33.500	MM	3.4467	523.87164	2.53319	4.4415
4	45.152	MM	3.0457	1068.72437	5.84825	9.0609
Totals :				1.17949e4	128.62700	

HPLC Chromatogram of compound 3ai.



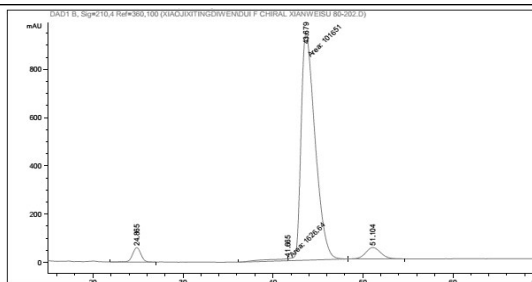
Racemic mixture



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	25.821	BB	0.8300	8124.75635	151.42014	16.7744
2	43.884	BV	1.4133	8021.56494	88.50935	16.5613
3	46.509	VV	1.5892	1.71977e4	162.70244	35.5064
4	53.140	VB	1.6823	1.50916e4	139.04182	31.1580

Totals : 4.84356e4 541.67374

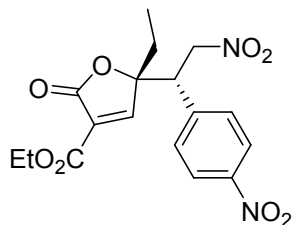
Chiral product



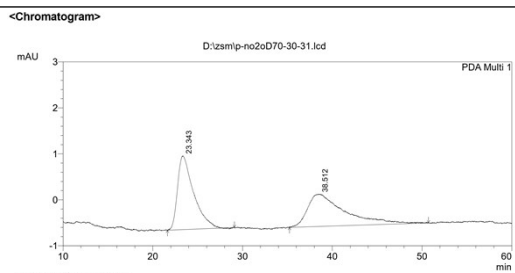
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	24.865	BV	1.0153	3966.48877	60.30684	3.5193
2	41.665	MF	3.0869	1626.64148	8.78236	1.4433
3	43.679	FM	1.8051	1.01651e5	938.57629	90.1917
4	51.104	BB	1.7986	5461.31543	46.89914	4.8457

Totals : 1.12705e5 1054.56463

HPLC Chromatogram of compound 3aj.



Racemic mixture

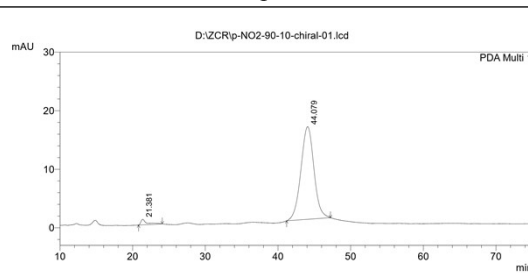


1 PDA Multi 1/254nm 4nm

PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	23.343	199346	1607	49.514	69.506
2	38.512	203262	705	50.486	30.494
Total		402608	2312	100.000	100.000

Chiral product

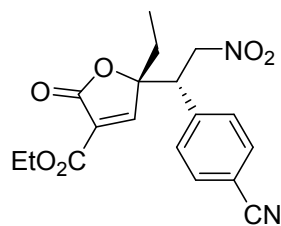


1 PDA Multi 1/254nm 4nm

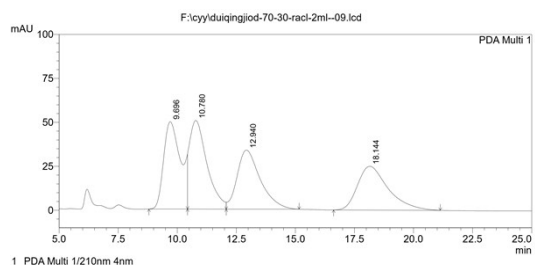
PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	21.381	57748	945	2.840	5.641
2	44.079	1975709	15815	97.160	94.359
Total		2033457	16760	100.000	100.000

HPLC Chromatogram of compound 3ak.

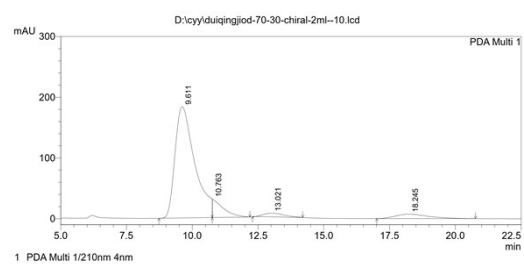


Racemic mixture



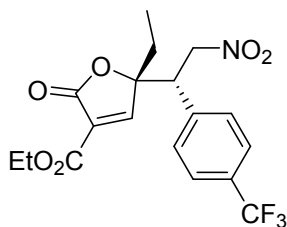
PeakTable					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.696	2482612	49691	25.790	31.325
2	10.780	2591066	50425	26.917	31.788
3	12.940	2301833	33603	23.912	21.183
4	18.144	2250581	24911	23.380	15.704
Total		9626092	158630	100.000	100.000

Chiral product

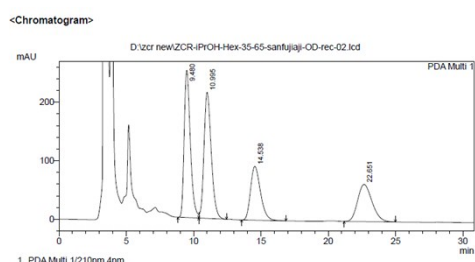


PeakTable					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.611	9519782	183261	83.914	80.702
2	10.763	848998	30449	7.484	13.408
3	13.021	328686	6060	2.897	2.668
4	18.245	647239	7316	5.705	3.222
Total		11344705	227085	100.000	100.000

HPLC Chromatogram of compound 3al.

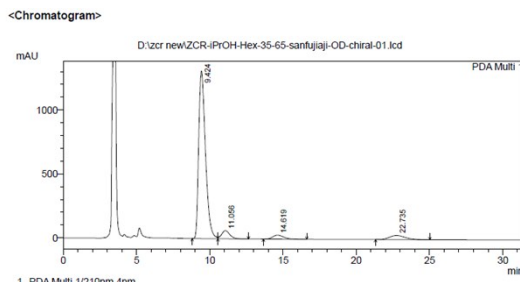


Racemic mixture



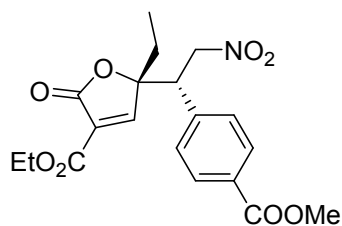
PeakTable					
Peak#	Ret. Time	Height	Height %	Area	Area %
1	9.480	251768	40.398	7999637	31.252
2	10.995	215806	34.638	8113271	31.696
3	14.538	92043	14.769	4742900	18.520
4	22.651	63597	10.205	4741298	18.523
Total		623213	100.000	25597106	100.000

Chiral product

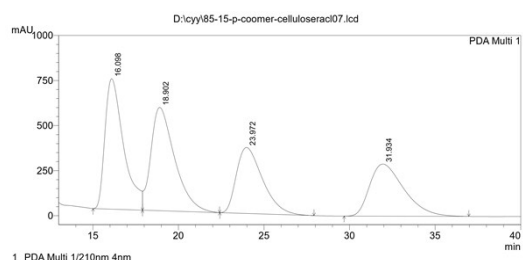


PeakTable					
Peak#	Ret. Time	Height	Height %	Area	Area %
1	9.424	1310396	91.175	42030523	86.688
2	11.056	63562	4.423	2447332	5.048
3	14.619	31190	2.170	1608512	3.318
4	22.735	32087	2.233	2398323	4.947
Total		1437235	100.000	48484690	100.000

HPLC Chromatogram of compound **3am**.

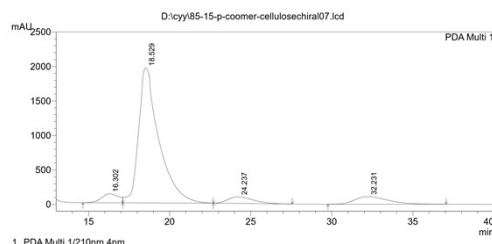


Racemic mixture



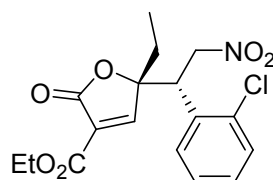
PeakTable					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	16.098	54746813	723621	28.897	37.072
2	18.902	55338636	572907	29.210	29.351
3	23.972	39053148	366046	20.614	18.753
4	31.934	40314996	289356	21.280	14.824
Total		189453593	1951930	100.000	100.000

Chiral product

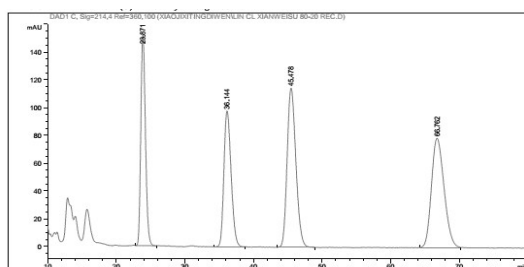


PeakTable					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	16.302	9625232	130123	4.658	5.671
2	18.529	171078073	1958635	82.798	85.361
3	24.237	10265756	95305	4.968	4.154
4	32.231	15652594	110456	7.575	4.814
Total		206621655	2294519	100.000	100.000

HPLC Chromatogram of compound **3an**.

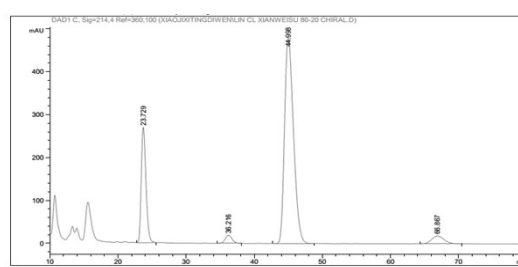


Racemic mixture



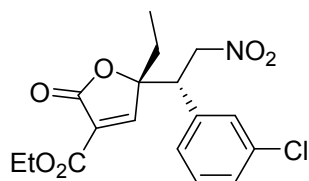
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.871	BB	0.7312	7117.37256	151.74356	20.6623
2	36.144	BB	1.1343	7166.87207	97.87418	20.8060
3	45.478	BB	1.3884	1.01502e4	114.69798	29.4669
4	66.762	BB	1.9483	1.00116e4	78.69189	29.0647
Totals :				3.44461e4	443.00762	

Chiral product

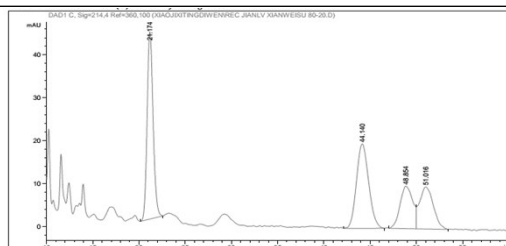


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.729	BB	0.7397	1.28250e4	269.27048	21.2625
2	36.216	BB	1.0977	1342.00146	18.60114	2.2249
3	44.998	BB	1.4167	4.38670e4	480.68463	72.7269
4	66.867	BB	1.8973	2283.44116	18.28034	3.7857
Totals :				6.03175e4	786.83658	

HPLC Chromatogram of compound **3ao**.



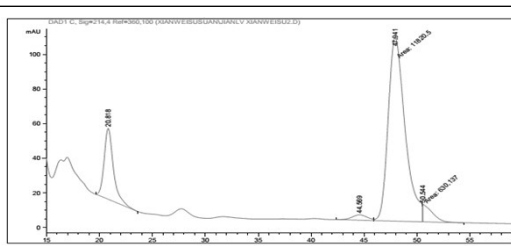
Racemic mixture



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.174	BB	0.6903	1951.04834	43.57805	34.0742
2	44.140	BB	1.4053	1809.18115	19.66584	31.5966
3	48.854	BV	1.2420	946.57367	9.91320	16.5315
4	51.016	VB	1.3897	1019.07312	9.79608	17.7977

Totals : 5725.87628 82.95316

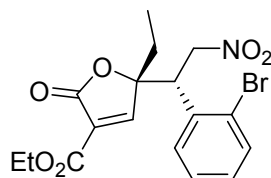
Chiral product



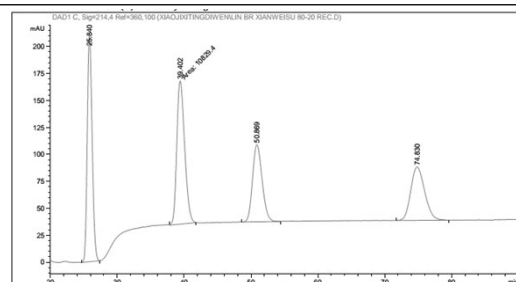
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.818	BB	0.9120	2495.36987	40.89043	16.3566
2	44.569	BV	1.3154	310.05273	3.06692	2.0323
3	47.941	MF	1.8630	1.18205e4	105.75022	77.4807
4	50.544	FM	1.0325	630.13696	10.17188	4.1304

Totals : 1.52560e4 159.87945

HPLC Chromatogram of compound **3ap**.



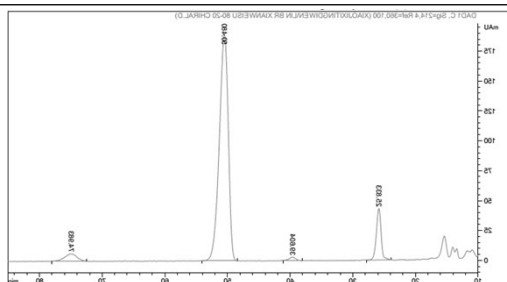
Racemic mixture



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	25.840	BB	0.7955	1.06789e4	209.19695	29.8559
2	39.402	MM	1.3584	1.08294e4	132.86803	30.2769
3	50.869	BB	1.5288	7113.67676	71.49628	19.8884
4	74.830	BB	2.1364	7145.96826	49.61184	19.9787

Totals : 3.57679e4 463.17309

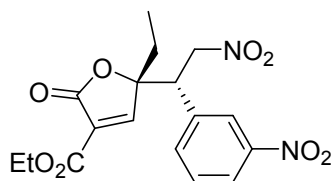
Chiral product



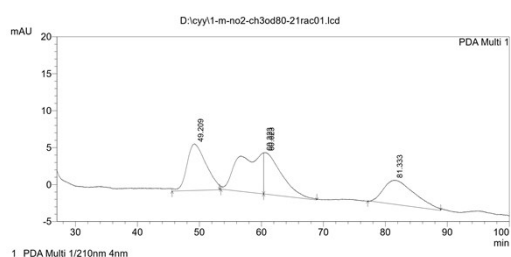
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	25.833	BB	0.8190	2286.86597	43.09853	10.2806
2	39.604	BB	1.0009	223.64978	2.98920	1.0054
3	50.480	BB	1.5733	1.88881e4	189.10185	84.9115
4	74.983	BB	1.6689	845.84320	6.07314	3.8025

Totals : 2.22445e4 241.26272

HPLC Chromatogram of compound **3aq**.

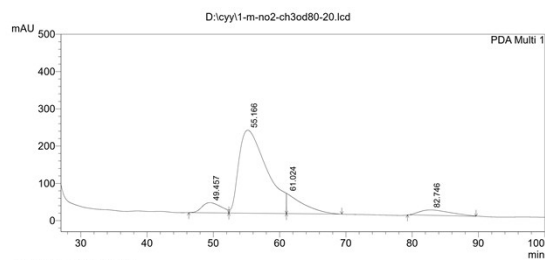


Racemic mixture



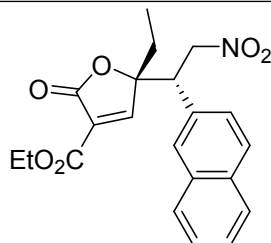
Peak Table					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	49.209	1349371	6306	26.508	30.321
2	60.623	1478843	5592	29.052	26.889
3	81.333	1127181	5641	22.143	27.123
4	82.746	1135084	3258	22.297	15.667
Total		5090359	20797	100.000	100.000

Chiral product

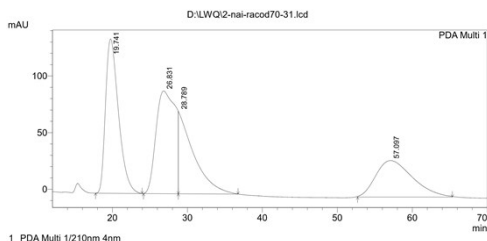


Peak Table					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	49.457	5347004	27198	6.328	8.526
2	55.166	65097615	222781	77.640	69.839
3	61.024	9232281	54484	10.926	17.080
4	82.746	4821146	14532	5.706	4.555
Total		84498047	318994	100.000	100.000

HPLC Chromatogram of compound **3ar**.

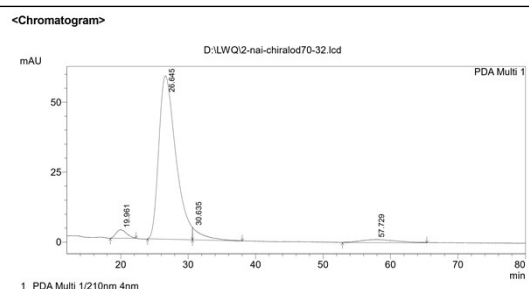


Racemic mixture



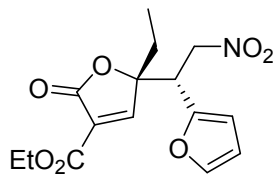
Peak Table					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	19.741	16400574	136279	30.429	41.037
2	26.831	16141935	90702	29.949	27.313
3	28.789	10333401	72834	19.172	21.932
4	57.097	11022093	32272	20.450	9.718
Total		53898002	332087	100.000	100.000

Chiral product

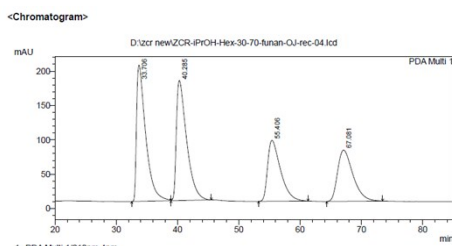


Peak Table					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	19.961	330810	3059	2.900	4.567
2	26.645	10183392	58353	89.283	87.120
3	30.635	459000	4432	4.024	6.616
4	57.729	432498	1136	3.792	1.696
Total		11405700	66980	100.000	100.000

HPLC Chromatogram of compound 3as.

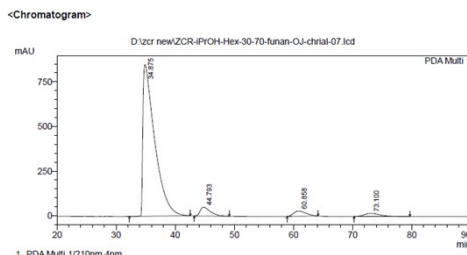


Racemic mixture



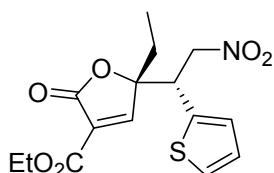
PeakTable					
Peak#	Ret. Time	Height	Height %	Area	Area %
1	33.706	199290	56.987	20629230	30.782
2	40.285	174660	32.580	20309644	30.305
3	55.406	88693	16.544	13066718	19.498
4	67.081	74457	13.889	13010893	19.414
Total		536100	100.000	67016485	100.000

Chiral product

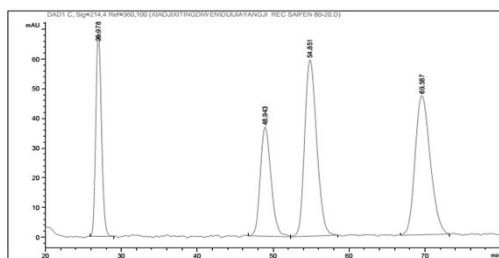


PeakTable					
Peak#	Ret. Time	Height	Height %	Area	Area %
1	34.875	847461	89.839	117968996	89.783
2	44.793	49054	5.200	5896596	4.488
3	60.858	29054	3.080	4204786	3.200
4	73.100	17747	1.881	3333286	2.529
Total		943317	100.000	131393664	100.000

HPLC Chromatogram of compound 3at.



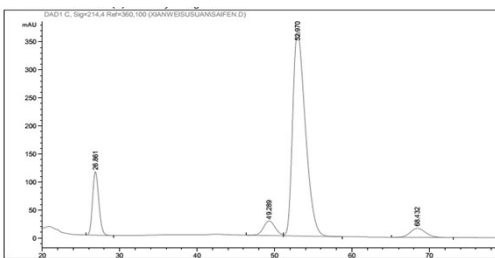
Racemic mixture



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	26.978	BB	0.8017	3571.58740	68.79678	17.6214
2	48.943	BB	1.5211	3635.08325	36.77727	17.9347
3	54.851	BB	1.6938	6564.95215	59.38007	32.3899
4	69.587	BB	2.1057	6496.86670	46.85364	32.0540

Totals : 2.02685e4 211.80776

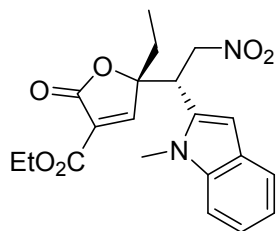
Chiral product



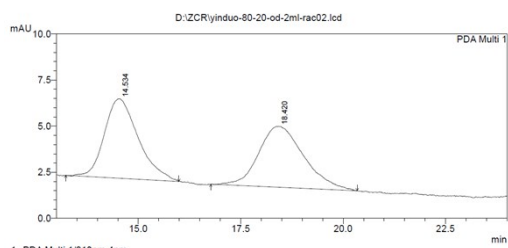
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	26.861	BB	0.8734	6349.53662	113.36591	11.9891
2	49.289	BV	1.6152	2745.04565	26.18110	5.1831
3	52.970	VB	1.7562	4.16301e4	364.56894	78.6052
4	68.432	BB	1.9916	2236.30420	16.22889	4.2226

Totals : 5.29610e4 520.34484

HPLC Chromatogram of compound **3au**.

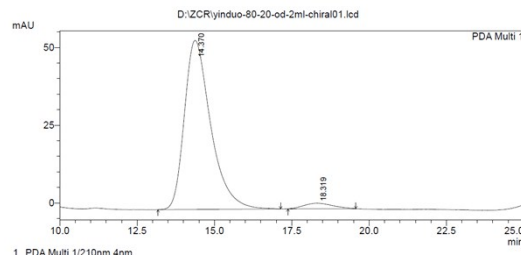


Racemic mixture



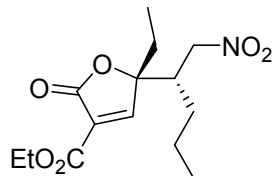
PeakTable					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.534	248252	4314	49.504	56.648
2	18.420	253224	3362	50.496	43.352
Total		501479	7616	100.000	100.000

Chiral product

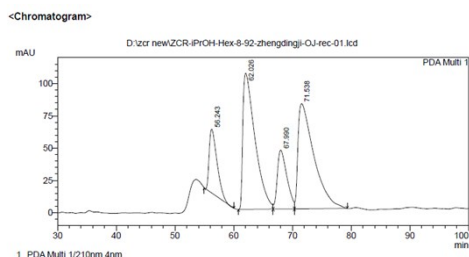


PeakTable					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.376	3230707	54307	96.535	96.590
2	18.319	116295	1799	3.475	3.201
Total		3347002	56196	100.000	100.000

HPLC Chromatogram of compound **3av**.

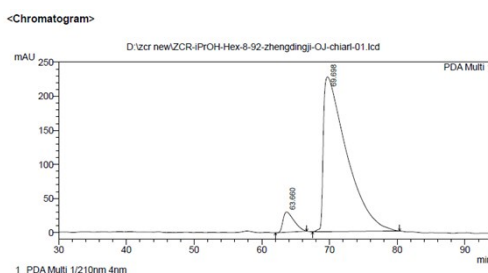


Racemic mixture



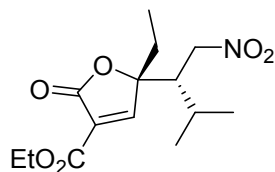
PeakTable					
Peak#	Ret. Time	Height	Height %	Area	Area %
1	56.243	49397	17.533	4594118	11.376
2	62.026	105330	37.382	15190830	37.617
3	67.990	45611	16.189	5169756	12.803
4	71.538	81413	28.896	15428060	38.205
Total		281741	100.000	40382764	100.000

Chiral product

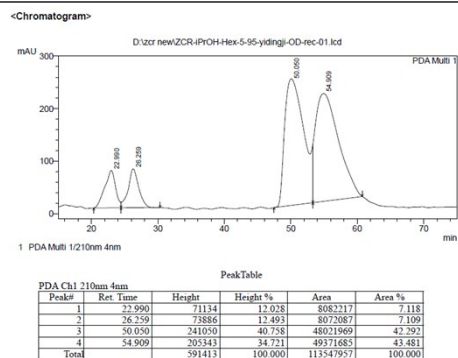


PeakTable					
Peak#	Ret. Time	Height	Height %	Area	Area %
1	68.660	29677	11.559	3345567	5.797
2	69.698	227065	88.441	54365414	94.203
Total		256742	100.000	57710981	100.000

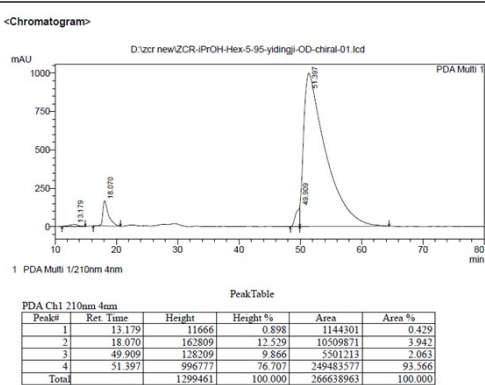
HPLC Chromatogram of compound **3aw**.



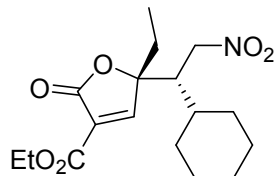
Racemic mixture



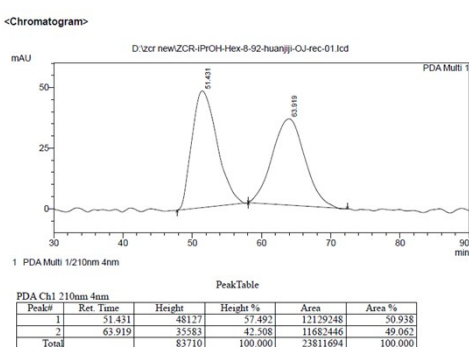
Chiral product



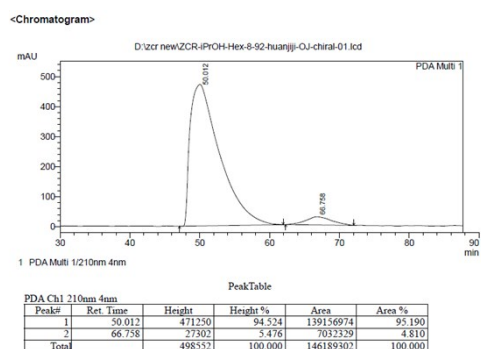
HPLC Chromatogram of compound **3ax**.



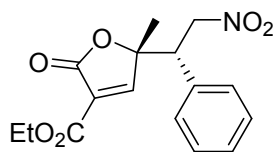
Racemic mixture



Chiral product

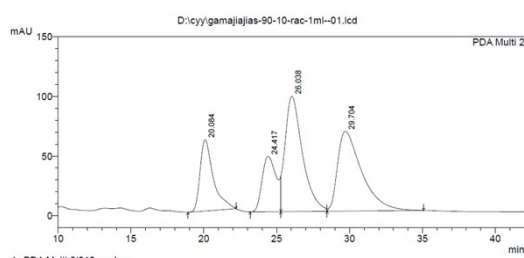


HPLC Chromatogram of compound **3ay**.



Racemic mixture

<Chromatogram>



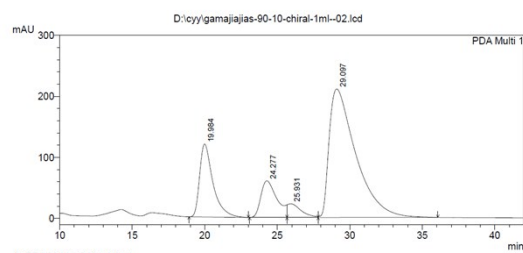
1 PDA Multi 2/210nm 4nm

PeakTable

Peak#	Ret. Time	Height	Height %	Area	Area %
1	20.084	59603	22.097	3793761	16.719
2	24.417	46473	17.229	3190948	14.063
3	26.038	96788	35.882	7987984	35.203
4	29.704	66873	24.792	7718325	34.015
Total		269737	100.000	22691018	100.000

Chiral product

<Chromatogram>

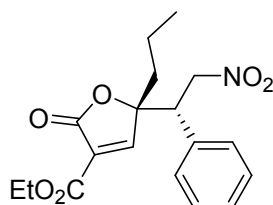


1 PDA Multi 1/210nm 4nm

PeakTable

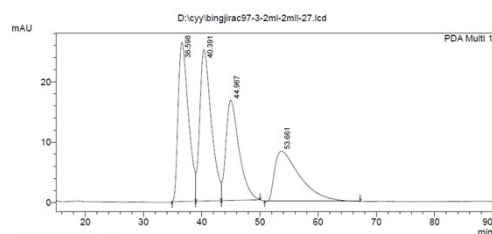
Peak#	Ret. Time	Height	Height %	Area	Area %
1	19.984	119595	28.985	7650140	18.860
2	24.277	60098	14.565	4613250	11.373
3	25.931	22461	5.443	1436642	3.542
4	29.097	210461	51.007	26863005	66.225
Total		412614	100.000	40563036	100.000

HPLC Chromatogram of compound **3az**.



Racemic mixture

<Chromatogram>



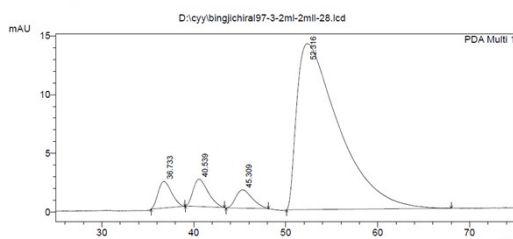
1 PDA Multi 1/254nm 4nm

PeakTable

Peak#	Ret. Time	Height	Height %	Area	Area %
1	36.598	26332	34.549	3223427	27.472
2	40.391	25075	32.900	3469679	29.571
3	44.967	16593	21.771	2614052	22.279
4	53.661	8217	10.780	2426131	20.677
Total		76217	100.000	11733289	100.000

Chiral product

<Chromatogram>



1 PDA Multi 1/254nm 4nm

PeakTable

Peak#	Ret. Time	Height	Height %	Area	Area %
1	36.733	2262	11.151	229534	4.419
2	40.539	2324	11.460	262461	5.053
3	45.309	1567	7.729	194402	3.743
4	52.316	14128	69.660	4507338	86.784
Total		20281	100.000	5193735	100.000

