Supporting Information

$Cu(OAc)_2$-Catalyzed Three-Component Cycloaddition of Malonates, Nitrosoarenes and Alkenes: Access to Isoxazolidines

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1. General

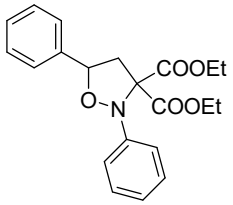
Unless otherwise indicated, all reagents were purchased from commercial sources and used without further purification. And deuterated solvents were purchased from Aldrich. Refinement of the mixed system through column chromatography which was performed on silica gel (200–300 mesh) with petroleum ether (solvent A)/ethyl acetate (solvent B) gradients as elution. In addition, all yields were referred to isolated yields (average of two runs) of compounds unless otherwise specified. The known compounds were partly characterized by melting points (for solid samples), ^{1}H NMR, and compared to authentic samples or the literature data. Melting points were measured with a RD-II digital melting point apparatus and were uncorrected. ^{1}H NMR data were acquired at 300 K on a Bruker Advance 600 MHz or 400 MHz spectrometer and ^{13}C NMR data were acquired at 300 K on a Bruker Advance 150 MHz or 100 MHz spectrometer using $CDCl_3$ as a solvent. Chemical shifts are reported in ppm from tetramethylsilane with the solvent $CDCl_3$ resonance as the internal standard ($CDCl_3$ δ = 7.26, 77.0). Spectra are reported as follows: chemical shift (δ = ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz), integration, and assignment.

2. General procedure for cycloaddition of malonates, nitrosoarenes and alkenes

To a tube equipped with a magnetic stir bar was added nitrosoarene **1** (0.24 mmol, 1.2 equiv), $Cu(OAc)_2$ (3.0 mg, 8.0 mol%), malonate **2** (0.24 mmol, 1.2 equiv) and CH_3CN (1.0 mL) in turn. The reaction system was then heated to 80 ^{o}C (oil bath) and stirred for 8 h. Subsequently, alkene **3** (0.2 mmol) was added and the reaction system was stirred until alkene **3** was completely consumed as determined by TLC. At last, the reaction mixture was purified by silica gel column chromatography to afford the desired pure cycloaddition product **4**.

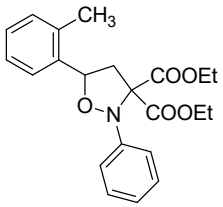
3. Characterization data for the cycloaddition products 4

Diethyl 2,5-diphenylisoxazolidine-3,3-dicarboxylate (4aaa) [lit 1]



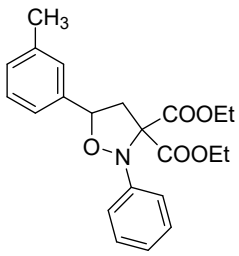
yellow oil, yield: 95%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 400 MHz), δ 7.57 (d, J = 6.8 Hz, 2H), 7.43−7.33 (m, 5H), 7.26 (t, J = 7.2 Hz, 2H), 7.04 (t, J = 7.6 Hz, 1H), 5.37 (dd, J = 9.6, 6.8 Hz, 1H), 4.24 (q, J = 7.2 Hz, 2H), 4.07−3.98 (m, 1H), 3.97−3.88 (m, 1H), 3.27−3.11 (m, 2H), 1.2 (t, J = 7.2 Hz, 3H), 1.02 (t, J = 7.2 Hz, 3H) ppm.

Diethyl 2-phenyl-5-(*o*-tolyl)isoxazolidine-3,3-dicarboxylate (4aab) [lit 1]



yellow oil, yield: 80%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 400 MHz), δ 7.76−7.58 (m, 2H), 7.55 (d, J = 8.8 Hz, 1H), 7.45−7.33 (m, 1H), 7.30−7.14 (m, 5H), 5.64 (dd, J = 9.6, 6.4 Hz, 1H), 4.31−4.17 (m, 2H), 4.13−4.00 (m, 1H), 3.99−3.89 (m, 1H), 3.31 (dd, J = 12.8, 6.0 Hz, 1H), 3.12−2.98 (m, 1H), 2.39 (s, 3H), 1.23 (t, J = 7.2 Hz, 3H), 1.10 (t, J = 7.2 Hz, 3H) ppm.

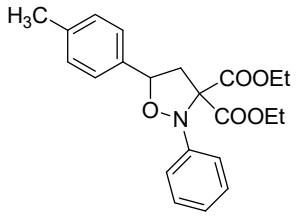
Diethyl 2-phenyl-5-(*m*-tolyl)isoxazolidine-3,3-dicarboxylate (4aac) [lit 1]



yellow oil, yield: 83%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 600 MHz), δ 7.38−7.33 (m, 4H), 7.29 (t, J = 7.8 Hz, 1H), 7.25−7.24 (m, 2H), 7.17 (d, J = 7.2 Hz, 1H), 7.03 (t, J = 7.2 Hz, 1H), 5.31 (dd, J = 9.6, 6.0 Hz, 1H), 4.20 (q, J = 7.2 Hz, 2H), 4.05−4.01 (m, 1H), 3.97−3.92 (m, 1H), 3.22 (dd, J =

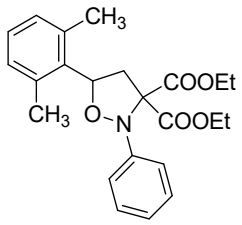
12.6, 6.0 Hz, 1H), 3.14 (dd, *J* = 12.6, 10.2 Hz, 1H), 2.40 (s, 3H), 1.19 (t, *J* = 7.2 Hz, 3H), 1.04 (t, *J* = 7.2 Hz, 3H) ppm.

Diethyl 2-phenyl-5-(*p*-tolyl)isoxazolidine-3,3-dicarboxylate (4aad) [lit 1]



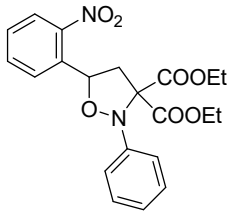
yellow oil, yield: 84%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 400 MHz), δ 7.47 (d, *J* = 8.0 Hz, 2H), 7.39 (dd, *J* = 9.6, 0.8 Hz, 2H), 7.29−7.15 (m, 4H), 7.02 (t, *J* = 7.2 Hz, 1H), 5.3 (dd, *J* = 9.2, 6.0 Hz, 1H), 4.24 (q, *J* = 7.2 Hz, 2H), 4.07−3.97 (m, 1H), 3.96−3.88 (m, 1H), 3.24−3.10 (m, 2H), 2.37−2.34 (s, 3H), 1.20 (t, *J* = 7.2 Hz, 3H), 1.05 (t, *J* = 6.8 Hz, 3H) ppm.

Diethyl 5-(2,6-dimethylphenyl)-2-phenylisoxazolidine-3,3-dicarboxylate (4aae) [lit 1]



yellow oil, yield: 86%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 400 MHz), δ 7.52 (s, 1H), 7.40 (dd, *J* = 2.4, 1.2 Hz, 2H), 7.30−7.23 (m, 2H), 7.09−7.00 (m, 3H), 5.57 (q, *J* = 6.0 Hz, 1H), 4.24−4.14 (m, 2H), 4.10−4.01 (m, 1H), 4.00−3.92 (m, 1H), 3.26 (dd, *J* = 6.8, 5.6 Hz, 1H), 3.05 (dd, *J* = 10.0, 2.8 Hz, 1H), 2.38 (s, 6H), 1.20 (t, *J* = 7.2 Hz, 3H), 1.06 (t, *J* = 7.2 Hz, 3H) ppm.

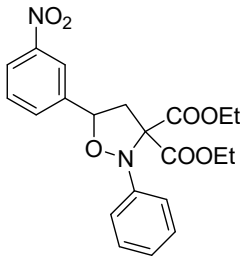
Diethyl 5-(2-nitrophenyl)-2-phenylisoxazolidine-3,3-dicarboxylate (4aaf) [lit 1]



white solid, mp: 74–77 °C, yield: 87%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 600 MHz), δ 7.69 (t, *J* = 8.0 Hz, 1H), 7.47 (t, *J* = 8.0 Hz, 1H), 7.45 (d, *J* = 8.0 Hz, 2H), 7.33 (dd, *J* = 16.0, 7.6 Hz, 2H), 7.09 (t, *J* = 9.6 Hz, 1H), 5.96

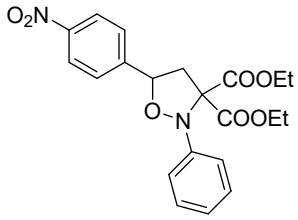
(t, *J* = 7.2 Hz, 1H), 4.12−3.98 (m, 4H), 3.78 (dd, *J* = 12.8, 7.6 Hz, 1H), 2.96 (dd, *J* = 12.8, 7.2 Hz, 1H), 1.07 (t, *J* = 7.2 Hz, 6H) ppm.

Diethyl 5-(3-nitrophenyl)-2-phenylisoxazolidine-3,3-dicarboxylate (4aag) [lit 1]



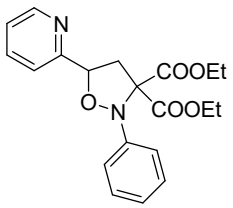
white solid, mp: 94–96 °C, yield: 94%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 600 MHz), δ 8.42 (s, 1H), 8.24−8.19 (m, 1H), 7.94 (d, *J* = 8.0 Hz, 1H), 7.63 (t, *J* = 8.0 Hz, 1H), 7.44−7.36 (m, 2H), 7.28 (t, *J* = 7.2 Hz, 2H), 7.12−7.05 (m, 1H), 5.50 (dd, *J* = 8.8, 7.2 Hz, 1H), 4.23−4.11 (m, 2H), 4.10−4.01 (m, 1H), 4.00−3.91 (m, 1H), 3.39 (dd, *J* = 12.8, 6.8 Hz, 1H), 3.17 (dd, *J* = 12.8, 6.8 Hz, 1H), 3.17 (dd, *J* = 12.8, 8.4 Hz, 1H), 1.16 (t, *J* = 7.2 Hz, 3H), 1.04 (t, *J*= 7.2 Hz, 3H) ppm.

Diethyl 5-(4-nitrophenyl)-2-phenylisoxazolidine-3,3-dicarboxylate (4aah) [lit 1]



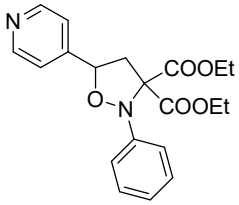
white solid, mp: 67–70 °C, yield: 96%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 600 MHz), δ 8.24 (d, *J* = 8.4 Hz, 2H), 7.71 (d, *J* = 8.4 Hz, 2H), 7.39 (d, *J* = 7.8 Hz, 2H), 7.28 (t, *J* = 7.8 Hz, 2H), 7.09 (t, *J* = 7.2 Hz, 1H), 5.45 (t, *J* = 7.2 Hz, 1H), 4.18−4.12 (m, 2H), 4.06−4.01 (m, 1H), 3.97−3.92 (m, 1H), 3.35 (dd, *J* = 12.6, 6.6 Hz, 1H), 3.07 (dd, *J* = 12.6, 8.4 Hz, 1H), 1.15 (t, *J* = 7.2 Hz, 3H), 1.02 (t, *J* = 7.2 Hz, 3H) ppm.

Diethyl 2-phenyl-5-(pyridin-2-yl)isoxazolidine-3,3-dicarboxylate (4aai) [lit 1]



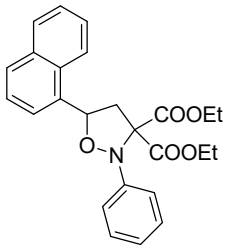
yellow oil, yield: 85%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 600 MHz), δ 8.48 (d, J = 4.2 Hz, 1H), 7.65−7.60 (m, 2H), 7.32 (d, J = 8.4 Hz, 2H), 7.19 (t, J = 7.8 Hz, 2H), 7.15−7.13 (m, 1H), 6.98 (t, J = 7.2 Hz, 1H), 5.43 (t, J = 7.2 Hz, 1H), 4.04−3.91 (m, 4H), 3.40 (dd, J = 13.2, 7.2 Hz, 1H), 3.22 (dd, J = 12.6, 7.2 Hz, 1H), 1.00−0.97 (m, 6H) ppm.

Diethyl 2-phenyl-5-(pyridin-4-yl)isoxazolidine-3,3-dicarboxylate (4aaj) [lit 1]



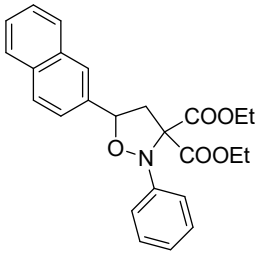
yellow oil, yield: 87%; TLC, R_f = 0.3 (PE:EtOAc = 3:1); ^{1}H NMR ($CDCl_3$, 600 MHz), δ 8.68 (s, 2H), 7.46 (s, 2H), 7.39 (d, J = 8.4 Hz, 2H), 7.28 (t, J = 7.8 Hz, 2H), 7.08 (t, J = 7.8 Hz, 1H), 5.35 (t, J = 7.8 Hz, 1H), 4.17−4.11 (m, 2H), 4.07−4.01 (m, 1H), 3.98−3.93 (m, 1H), 3.35 (dd, J = 13.2, 7.2 Hz, 1H), 3.06 (dd, J = 13.2, 8.4 Hz, 1H), 1.14 (t, J = 7.2 Hz, 3H), 1.03 (t, J = 7.2 Hz, 3H) ppm.

Diethyl 5-(naphthalen-1-yl)-2-phenylisoxazolidine-3,3-dicarboxylate (4aak) [lit 1]



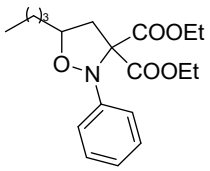
yellow oil, yield: 75%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 600 MHz), δ 8.10 (d, J = 8.4 Hz, 1H), 7.88 (t, J = 9.0 Hz, 2H), 7.83 (d, J = 7.8 Hz, 1H), 7.55−7.49 (m, 3H), 7.44 (d, J = 7.8 Hz, 2H), 7.28 (t, J = 7.8 Hz, 2H), 7.06 (t, J = 7.2 Hz, 1H), 6.10 (dd, J = 9.0, 6.0 Hz, 1H), 4.21 (q, J = 7.2 Hz, 2H), 4.04−4.01 (m, 1H), 3.98−3.95 (m, 1H), 3.51 (dd, J = 12.6, 6.0 Hz, 1H), 3.19 (dd, J = 12.6, 6.0 Hz, 1H), 1.20 (t, J = 7.2 Hz, 3H), 1.02 (t, J = 6.6 Hz, 3H) ppm.

Diethyl 5-(naphthalen-2-yl)-2-phenylisoxazolidine-3,3-dicarboxylate (4aal) [lit 1]



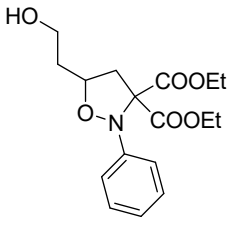
yellow oil, yield: 87%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 400 MHz), δ 7.97 (s, 1H), 7.92−7.82 (m, 3H), 7.74 (dd, J = 8.4, 1.6, Hz, 1H), 7.56−7.46 (m, 2H), 7.44 (d, J = 8.0 Hz, 2H), 7.32−7.24 (m, 2H), 7.05 (t, J = 7.2 Hz, 1H), 5.56 (dd, J = 9.6, 6.0 Hz, 1H), 4.26 (q, J = 7.2 Hz, 2H), 4.10−4.00 (m, 1H), 3.99−3.90 (m, 1H), 3.35−3.20 (m, 2H), 1.21 (t, J = 7.2 Hz, 3H), 1.04 (t, J = 7.2 Hz, 3H) ppm.

Diethyl 5-butyl-2-phenylisoxazolidine-3,3-dicarboxylate (4aam) [lit 1]



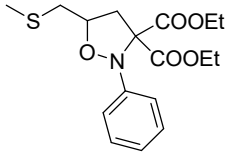
yellow oil, yield: 71%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 400 MHz), δ 7.31−7.25 (m, 2H), 7.22 (t, J = 7.2 Hz, 2H), 6.99 (t, J = 7.2 Hz, 1H), 4.36−4.27 (m, 1H), 4.18 (q, J = 7.2 Hz, 2H), 4.08−4.02 (m, 1H), 3.99−3.90 (m, 1H), 2.99 (dd, J = 12.4, 6.0 Hz, 1H), 2.74 (dd, J = 12.4, 9.2 Hz, 1H), 1.88−1.76 (m, 1H), 1.72−1.61 (m, 1H), 1.55−1.45 (m, 1H), 1.44−1.35 (m, 3H), 1.15 (t, J = 7.2 Hz, 3H), 1.04 (t, J = 7.2 Hz, 3H), 0.93 (t, J = 7.2 Hz, 3H) ppm.

Diethyl 5-(3-hydroxypropyl)-2-phenylisoxazolidine-3,3-dicarboxylate (4aan) [lit 1]



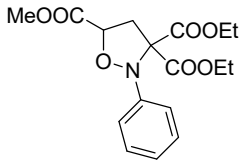
yellow oil, yield: 75%; TLC, R_f = 0.3 (PE:EtOAc = 5:1); ^{1}H NMR ($CDCl_3$, 400 MHz), δ 7.35−7.20 (m, 4H), 7.07−6.99 (m, 1H), 4.58−4.48 (m, 1H), 4.18−4.09 (m, 2H), 4.08−4.01 (m, 1H), 4.00−3.92 (m, 1H), 3.91 (dd, J = 7.2, 6.4 Hz, 2H), 3.08 (q, J = 6.4 Hz, 1H), 2.87 (q, J = 8.8 Hz,1H), 2.12−1.94 (m, 2H), 1.89 (t, J = 5.2 Hz, 1H), 1.11 (t, J = 7.2 Hz, 3H), 1.05 (t, J = 7.2 Hz, 3H) ppm.

Diethyl 5-((methylthio)methyl)-2-phenylisoxazolidine-3,3-dicarboxylate (4aao) [lit 1]



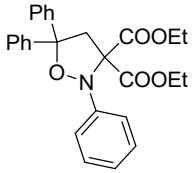
yellow oil, yield: 73%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 400 MHz), δ 7.38 (d, J = 8.8 Hz, 2H), 7.28 (s, 1H), 7.2 (d, J = 8.8 Hz, 2H), 4.61−4.48 (m, 1H), 4.20−4.01 (m, 4H), 3.14 (q, J = 6.4 Hz, 1H), 2.96−2.80 (m, 2H), 2.79−2.72 (m, 1H), 2.26−2.19 (s, 3H), 1.16 (q, J = 7.2 Hz, 6H) ppm.

3,3-diethyl 5-methyl 2-phenylisoxazolidine-3,3,5-tricarboxylate (4aap) [lit 1]



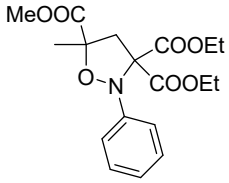
yellow oil, yield: 81%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 400 MHz), δ 7.43 (d, J = 8.8 Hz, 2H), 7.29−7.20 (m, 2H), 7.08 (t, J = 7.2 Hz, 1H), 4.91 (dd, J = 8.0, 5.6 Hz, 1H), 4.24−4.13 (m, 2H), 4.05−3.93 (m, 1H), 3.92−3.83 (m, 1H), 3.82 (s, 3H), 3.38−3.23 (m, 2H), 1.19 (t, J = 7.2 Hz, 3H), 0.96 (t, J = 7.2 Hz, 3H) ppm.

3-ethyl 4,5-dimethyl 2-phenylisoxazolidine-3,4,5-tricarboxylate (4aaq) [lit 1]



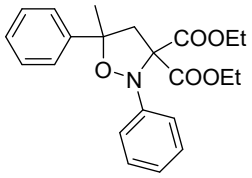
yellow oil, yield: 75%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 400 MHz), δ 7.53 (d, J = 7.2 Hz, 4H), 7.32 (t, J = 7.6 Hz, 6H), 7.28−7.2 (m, 4H), 7.00 (t, J = 7.2 Hz, 1H), 3.99−3.84 (m, 4H), 3.82 (s, 2H), 0.96 (t, J = 7.2 Hz, 6H) ppm.

3,3-diethyl 5-methyl 5-methyl-2-phenylisoxazolidine-3,3,5-tricarboxylate (4aar) [lit 1]



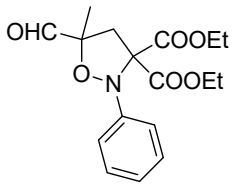
yellow oil, yield: 70%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 400 MHz), δ 7.39−7.33 (m, 2H), 7.27−7.20 (m, 2H), 7.07−7.02 (m, 1H), 4.31 (q, J = 7.2 Hz, 2H), 3.93−3.83 (m, 1H), 3.81−3.75 (s, 3H), 3.75−3.68 (m, 1H), 3.55 (d, J = 12.8 Hz, 1H), 3.05 (d, J = 12.8 Hz, 1H), 1.71 (s, 3H), 1.26 (q, J = 7.2 Hz, 3H), 0.86 (q, J = 7.2 Hz, 3H) ppm.

Diethyl 5-methyl-2,5-diphenylisoxazolidine-3,3-dicarboxylate (4aas) [lit 1]



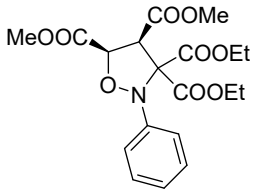
yellow oil, yield: 73%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 600 MHz), δ 7.48 (d, J = 7.2 Hz, 2H), 7.34−7.31 (m, 4H), 7.26−7.22 (m, 3H), 7.00 (t, J = 7.2 Hz, 1H), 4.06−4.00 (m, 2H), 3.94−3.86 (m, 2H), 3.45 (d, J = 12.6 Hz, 1H), 3.15 (d, J = 12.6 Hz, 1H), 1.74 (s, 3H), 1.04 (t, J = 7.2 Hz, 3H), 0.95 (t, J = 7.2 Hz, 3H) ppm.

Diethyl 5-formyl-5-methyl-2-phenylisoxazolidine-3,3-dicarboxylate (4aat) [lit 1]



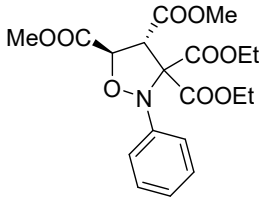
colourless oil, yield: 62%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 400 MHz), δ 9.71 (d, J = 0.4 Hz, 1H), 7.42 (dd, J = 8.8, 1.2 Hz, 2H), 7.30−7.24 (m, 3H), 7.10 (t, J = 7.2 Hz, 1H), 4.33−4.21 (m, 2H), 3.93−3.82 (m, 1H), 3.76−3.64 (m, 1H), 3.20 (d, J = 12.8 Hz, 1H), 3.05 (dd, J = 12.8, 0.8 Hz, 1H), 1.52 (s, 3H), 1.27 (t, J = 7.2 Hz, 3H), 0.83 (t, J = 7.2 Hz, 3H) ppm.

(4*S*,5*R*)-3,3-diethyl 4,5-dimethyl 2-phenylisoxazolidine-3,3,4,5-tetracarboxylate (4aau) [lit 1]



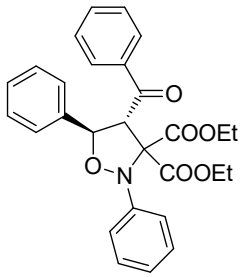
yellow oil, yield: 90%; TLC, R_f = 0.3 (PE:EtOAc = 5:1); ^{1}H NMR ($CDCl_3$, 600 MHz), δ 7.41 (d, J = 7.8 Hz, 2H), 7.26 (t, J = 7.8 Hz, 2H), 7.09 (t, J = 7.2 Hz, 1H), 5.24 (d, J = 7.8 Hz, 1H), 4.56 (d, J = 7.8 Hz, 1H), 4.21 (q, J = 7.2 Hz, 2H), 4.01−3.96 (m, 1H), 3.84−3.81 (m, 1H), 3.80 (s, 3H), 3.73 (s, 3H), 1.21 (t, J = 7.2 Hz, 3H), 0.94 (t, J = 7.2 Hz, 3H) ppm.

(4*S*, 5*S*)-3,3-diethyl-4,5-dimethyl-2-phenylisoxazolidine-3,3,4,5-tetracarboxylate (4aav) [lit 1]



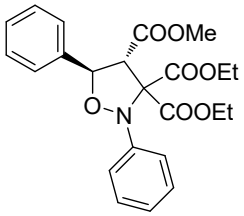
yellow oil, yield: 63%; TLC, R_f = 0.3 (PE:EtOAc = 5:1); ^{1}H NMR ($CDCl_3$, 600 MHz), δ 7.30 (d, J = 7.8 Hz, 2H), 7.25 (t, J = 7.8 Hz, 2H), 7.08 (t, J = 7.2 Hz, 1H), 5.16 (d, J = 6.6 Hz, 1H), 4.59 (d, J = 6.0 Hz, 1H), 4.23−4.17 (m, 1H), 4.12−4.07 (m, 1H), 4.02 (q, J = 7.2 Hz, 2H), 3.83 (s, 3H), 3.76 (s, 3H), 1.14 (t, J = 7.2 Hz, 3H), 1.02 (t, J = 7.2 Hz, 3H) ppm.

Diethyl 4-benzoyl-2,5-diphenylisoxazolidine-3,3-dicarboxylate (4aaw) [lit 1]



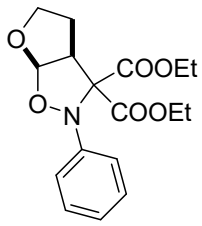
white solid (mp: 144–145 °C), yield: 61%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 400 MHz), δ 7.83 (d, J = 7.2 Hz, 2H), 7.61−7.45 (m, 5H), 7.40−7.27 (m, 7H), 7.14 (t, J = 7.2 Hz, 1H), 5.56 (s, 2H), 4.15−4.05 (m, 1H), 3.97−3.85 (m, 2H), 3.63−3.53 (m, 1H), 0.88 (t, J = 7.2 Hz, 3H), 0.79 (t, J = 7.2 Hz, 3H) ppm.

Triethyl 2,5-diphenylisoxazolidine-3,3,4-tricarboxylate (4aax) [lit 1]



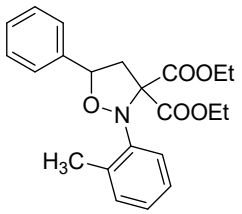
yellow oil, yield: 75%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 400 MHz), δ 7.61 (dd, J = 8.0, 2.0 Hz, 2H), 7.47−7.36 (m, 5H), 7.30−7.24 (m, 2H), 7.09 (t, J = 7.2 Hz, 1H), 5.47 (d, J = 9.2 Hz, 1H), 4.56 (d, J = 9.2 Hz, 1H), 4.33−4.22 (m, 1H), 4.21−4.10 (m, 1H), 4.05−3.95 (m, 1H), 3.82−3.72 (m, 1H), 3.70 (s, 3H), 1.21 (t, J = 7.2 Hz, 3H), 0.94 (t, J = 7.2 Hz, 3H) ppm.

Diethyl 2-phenyltetrahydrofuro[2,3-*d*]isoxazole-3,3(2*H*)-dicarboxylate (4aay) [lit 1]



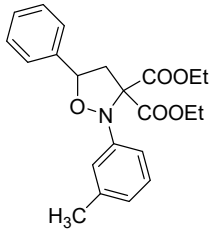
colourless oil, yield: 65%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 600 MHz), δ 7.46 (d, J = 8.0 Hz, 2H), 7.25 (d, J = 8.0 Hz, 2H), 7.10 (t, J = 7.2 Hz, 1H), 6.00 (d, J = 5.6 Hz, 1H), 4.40−4.31 (m, 1H), 4.30−4.19 (m, 2H), 4.04−3.97 (m, 1H), 3.95−3.84 (m, 2H), 2.17−2.05 (m, 1H), 1.97−1.89 (m, 1H), 1.29 (t, J = 7.2 Hz, 3H), 0.78 (t, J = 7.2 Hz, 3H) ppm.

Diethyl 5-phenyl-2-(*o*-tolyl)isoxazolidine-3,3-dicarboxylate (4baa) [lit 1]



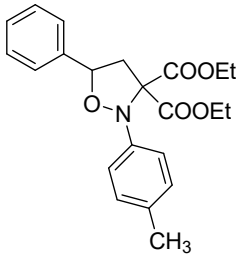
yellow oil, yield: 94%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 400 MHz), δ 7.49 (t, J = 7.2 Hz, 3H), 7.46 (s, 1H), 7.42−7.31 (m, 4H), 7.09 (dd, J = 8.4, 1.6 Hz, 1H). 5.43 (dd, J = 9.2, 6.4 Hz, 1H), 4.28−4.17 (m, 2H), 4.08−3.97 (m, 1H), 3.91−3.80 (m, 1H), 2.29−3.16 (m, 2H), 2.32 (s, 3H), 1.23 (t, J = 7.2 Hz, 3H), 1.06 (t, J = 7.2 Hz, 3H) ppm.

Diethyl 5-phenyl-2-(*m*-tolyl)isoxazolidine-3,3-dicarboxylate (4caa) [lit 1]



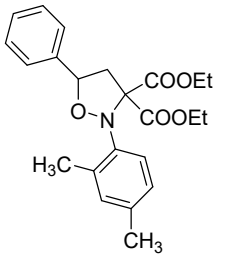
yellow oil, yield: 98%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 600 MHz), δ 7.55 (d, J = 7.2 Hz, 2H), 7.40 (t, J = 7.2 Hz, 2H), 7.35 (t, J = 7.2 Hz, 1H), 7.19−7.12 (m, 3H), 6.85 (d, J = 7.2 Hz, 1H), 5.34 (dd, J = 9.6, 6.0 Hz, 1H), 4.23−4.18 (m, 2H), 4.07−4.02 (m, 1H), 3.98−3.93 (m, 1H), 3.23 (dd, J = 13.2, 6.6 Hz, 1H), 3.14 (dd, J = 13.2, 9.0 Hz, 1H), 2.30 (s, 3H), 1.20 (t, J = 7.2 Hz, 3H), 1.04 (t, J = 7.2 Hz, 3H) ppm.

Diethyl 5-phenyl-2-(*p*-tolyl)isoxazolidine-3,3-dicarboxylate (4daa) [lit 1]



yellow oil, yield: 95%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 600 MHz), δ 7.55 (d, J = 7.2 Hz, 2H), 7.39 (t, J = 7.8 Hz, 2H), 7.35 (t, J = 7.2 Hz, 1H), 7.29 (d, J = 8.4 Hz, 2H), 7.06 (d, J = 8.4 Hz, 2H), 5.32 (dd, J = 9.6, 6.6 Hz, 1H), 4.23−4.18 (m, 2H), 4.04−3.98 (m, 1H), 3.94−3.89 (m, 1H), 3.21 (dd, J = 13.2, 6.6 Hz, 1H), 3.15 (dd, J = 13.2, 9.6 Hz, 1H), 2.28 (s, 3H), 1.21 (t, J = 7.2 Hz, 3H), 1.02 (t, J = 7.2 Hz, 3H) ppm.

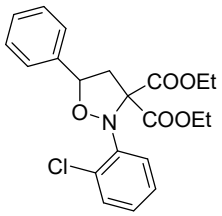
Diethyl 2-(2,4-dimethylphenyl)-5-phenylisoxazolidine-3,3-dicarboxylate (4eaa) [lit 1]



yellow oil, yield: 71%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 600 MHz), δ 7.49 (d, J = 7.2 Hz, 2H), 7.37 (t, J = 7.2 Hz, 2H),

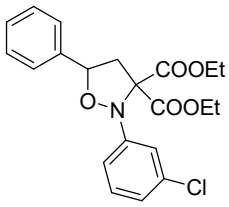
7.33−7.31 (m, 2H), 6.95 (s, 1H), 6.93 (d, J = 8.4 Hz, 1H), 5.32 (t, J = 7.8 Hz, 1H), 4.20−4.12 (m, 2H), 4.00−3.95 (m, 1H), 3.82−3.76 (m, 1H), 3.23 (d, J = 7.8 Hz, 2H), 2.43 (s, 3H), 2.26 (s, 3H), 1.17 (t, J = 7.2 Hz, 3H), 1.01 (t, J = 7.2 Hz, 3H) ppm.

Diethyl 2-(2-chlorophenyl)-5-phenylisoxazolidine-3,3-dicarboxylate (4faa) [lit 1]



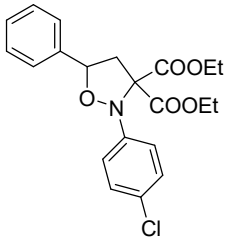
yellow oil, yield: 75%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 600 MHz), δ 7.62 (d, J = 8.4 Hz, 1H), 7.51 (d, J = 7.2 Hz, 2H), 7.39 (t, J = 7.2 Hz, 2H), 7.35 (t, J = 9.6 Hz, 2H), 7.22 (t, J = 7.8 Hz, 1H), 7.11 (t, J = 7.8 Hz, 1H), 5.43 (dd, J = 9.6, 5.4 Hz, 1H), 4.24−4.19 (m, 2H), 4.05−3.99 (m, 1H), 3.87−3.81 (m, 1H), 3.26 (dd, J = 12.6, 10.2 Hz, 1H), 3.18 (dd, J = 13.2, 6.0 Hz, 1H), 1.23 (t, J = 7.2 Hz, 3H), 1.05 (t, J = 7.2 Hz, 3H) ppm.

Diethyl 2-(3-chlorophenyl)-5-phenylisoxazolidine-3,3-dicarboxylate (4gaa) [lit 1]



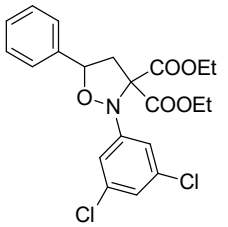
yellow oil, yield: 83%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 400 MHz), δ 7.53 (d, J = 8.4 Hz, 2H), 7.48 (d, J = 2.4 Hz, 2H), 7.45−7.42 (m, 1H), 7.41 (s, 1H), 7.40−7.35 (m, 2H), 7.13 (dd, J = 8.8, 2.4 Hz, 1H), 5.35 (dd, J = 9.6, 6.0 Hz, 1H), 4.28 (q, J = 7.2 Hz, 2H), 4.18−4.03 (m, 2H), 3.30 (dd, J = 12.8, 6.0 Hz, 1H), 3.16 (dd, J = 12.8, 9.6 Hz, 1H), 1.24 (t, J = 7.2 Hz, 3H), 1.11 (t, J = 7.2 Hz, 3H) ppm.

Diethyl 2-(4-chlorophenyl)-5-phenylisoxazolidine-3,3-dicarboxylate (4haa) [lit 1]



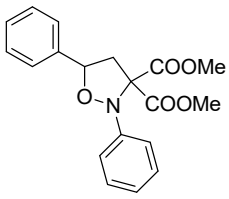
yellow oil, yield: 87%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 600 MHz), δ 7.53 (d, J = 7.2 Hz, 2H), 7.40 (t, J = 7.8 Hz, 2H), 7.37−7.31 (m, 3H), 7.22 (d, J = 9 Hz, 2H), 5.32 (dd, J = 9.6, 6.0 Hz, 1H), 4.22 (q, J = 7.2 Hz, 2H), 4.08−4.02 (m, 1H), 4.01−3.95 (m, 1H), 3.25 (dd, J = 12.6, 6.6 Hz, 1H), 3.15 (dd, J = 13.2, 9.6 Hz, 1H), 1.22 (t, J = 7.2 Hz, 3H), 1.06 (t, J = 7.2 Hz, 3H) ppm.

Diethyl 2-(3,5-dichlorophenyl)-5-phenylisoxazolidine-3,3-dicarboxylate (4iaa) [lit 1]



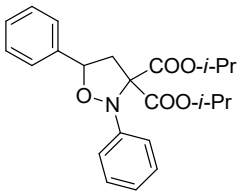
yellow oil, yield: 74%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 400 MHz), δ 7.52 (d, J = 6.8 Hz, 2H), 7.45−7.36 (m, 2H), 7.23 (d, J = 1.6 Hz, 2H), 6.98 (t, J = 1.6 Hz, 1H), 6.81−6.76 (m, 1H), 5.36 (dd, J = 9.6, 6.0 Hz, 1H), 4.31 (q, J = 7.2 Hz, 2H), 4.19−4.07 (m, 2H), 3.32 (dd, J = 12.8, 5.6 Hz, 1H), 3.15 (dd, J = 12.8, 9.6 Hz, 1H), 1.26 (t, J = 7.2 Hz, 3H), 1.15 (t, J = 7.2 Hz, 3H) ppm.

Dimethyl 2,5-diphenylisoxazolidine-3,3-dicarboxylate (4aba) [lit 1]



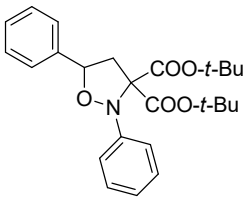
white solid, mp: 68–71 °C, yield: 97%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 600 MHz), δ 7.58 (dd, J = 8.4, 1.6 Hz, 2H), 7.44−7.37 (m, 3H), 7.36−7.32 (m, 2H), 7.30−7.23 (m, 2H), 7.05 (t, J = 7.2 Hz, 1H), 5.38 (dd, J = 9.6, 6.0 Hz, 1H), 3.75 (s, 3H), 3.54 (s, 3H), 3.29 (dd, J = 12.8, 6.4 Hz, 1H), 3.19 (dd, J = 12.8, 9.6 Hz, 1H) ppm.

Diisopropyl 2,5-diphenylisoxazolidine-3,3-dicarboxylate (4aca) [lit 1]



Yellow oil, yield: 94%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, J = 7.2 Hz, 2H), 7.45–7.32 (m, 5H), 7.28–7.20 (m, 2H), 7.06–6.95 (m, 1H), 5.37 (dd, J = 9.2, 6.4 Hz, 1H), 5.12–5.01 (m, 1H), 4.90–4.80 (m, 1H), 3.25–3.10 (m, 2H), 1.22 (q, J = 3.2 Hz, 6H), 1.10 (d, J = 6.4 Hz, 3H), 0.97 (d, J = 6.4 Hz, 3H) ppm.

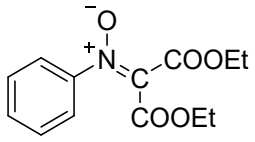
Di-*tert*-butyl 2,5-diphenylisoxazolidine-3,3-dicarboxylate (4ada) [lit 1]



white solid, mp: 76–80 °C, yield: 94%; TLC, R_f = 0.3 (PE:EtOAc = 20:1); ^{1}H NMR ($CDCl_3$, 400 MHz), δ 7.58 (d, J = 6.8 Hz, 2H), 7.45−7.36 (m, 5H), 7.29 (dd, J = 7.2, 2.8 Hz, 2H), 7.02 (t, J = 7.2 Hz, 1H), 6.36 (dd, J = 9.6, 6.8 Hz, 1H), 3.19−3.06 (m, 2H), 1.43 (s, 9 H), 1.26 (s, 9H) ppm.

4. Characterization data for the the intermediate 5a

1,3-diethoxy-1,3-dioxo-*N*-phenylpropan-2-imine oxide

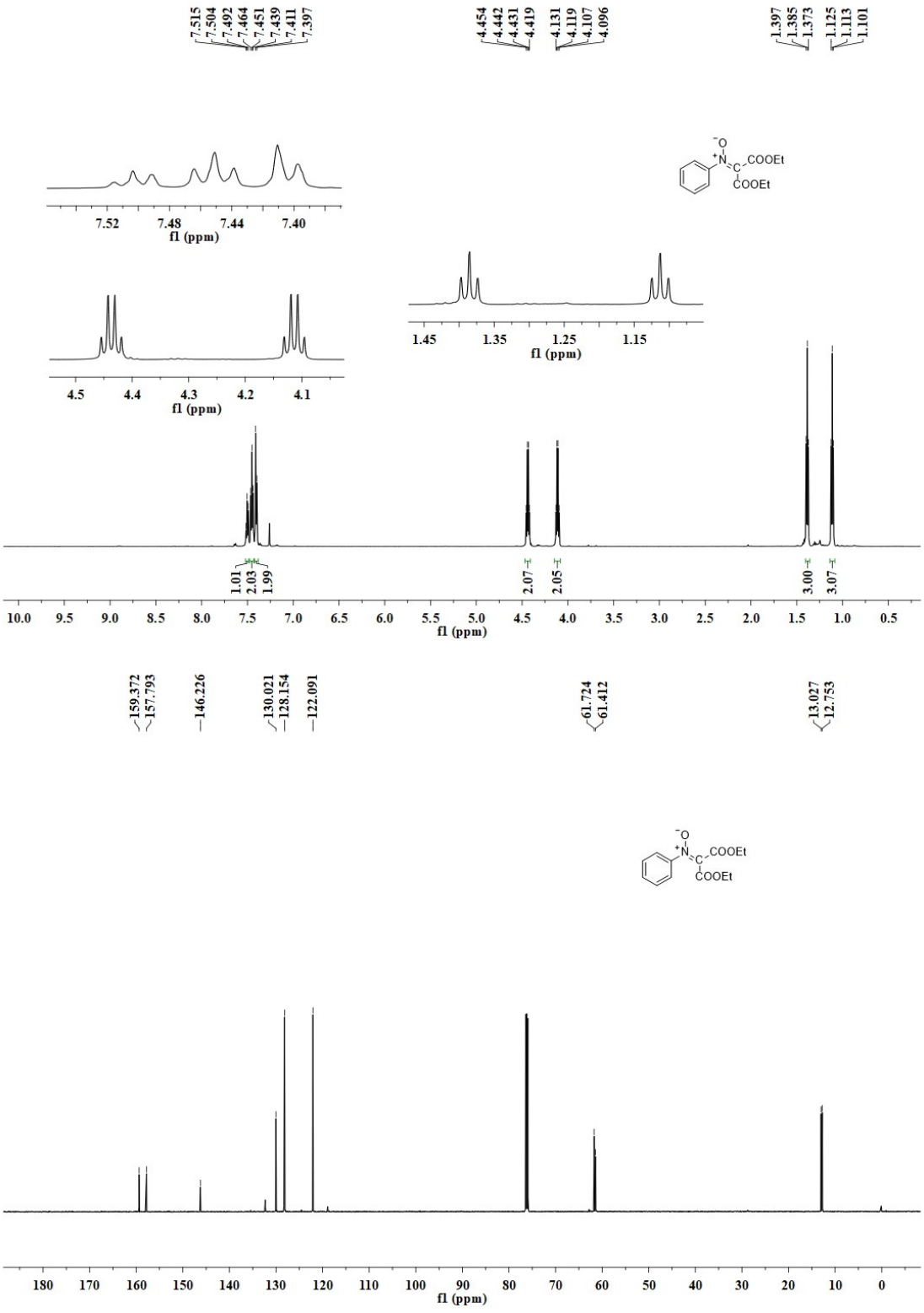


Yellow oil, yield: 90%; column chromatography eluent, petroleum ether/EtOAc = 10:1; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.50 (t, J = 6.6 Hz, 1H), 7.45 (t, J = 7.8 Hz, 2H), 7.40 (d, J = 8.4 Hz, 2H), 4.44 (q, J = 7.2 Hz, 2H), 4.11 (q, J = 7.2 Hz, 2H), 1.39 (t, J = 7.2 Hz, 3H), 1.11 (t, J = 7.2 Hz, 3H) ppm; ^{13}C{^{1}H} NMR (150MHz, $CDCl_3$) δ 159.3, 157.7, 146.2, 130.0, 128.1, 122.0, 61.7, 61.4, 13.0, 12.7 ppm; **HRMS** (ESI) *m*/*z*: [M + Na] $^+$ calcd for $C_{13}H_{15}NNaO_5^+$, 288.0842; found, 288.0848.

5. References

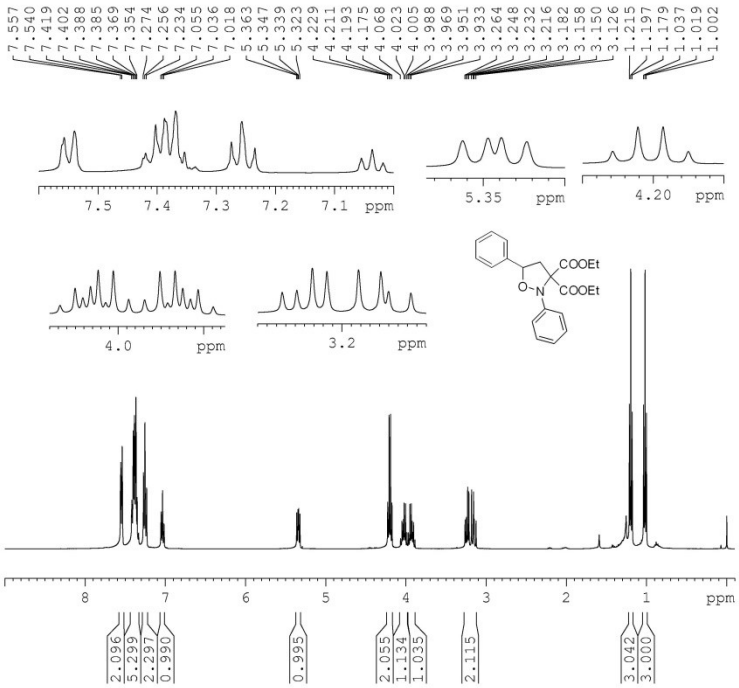
1) Li, X.; Zheng, L.; Gong, X.; Chang, H.; Gao, W.; Wei, W. *J. Org. Chem.* **2021**, *86*, 1096.

6. ^{1}H NMR and ^{13}C NMR spectra for the intermediate 5a



7. ^{1}H NMR and ^{13}C NMR spectra and NOESY for products 4

4aaa



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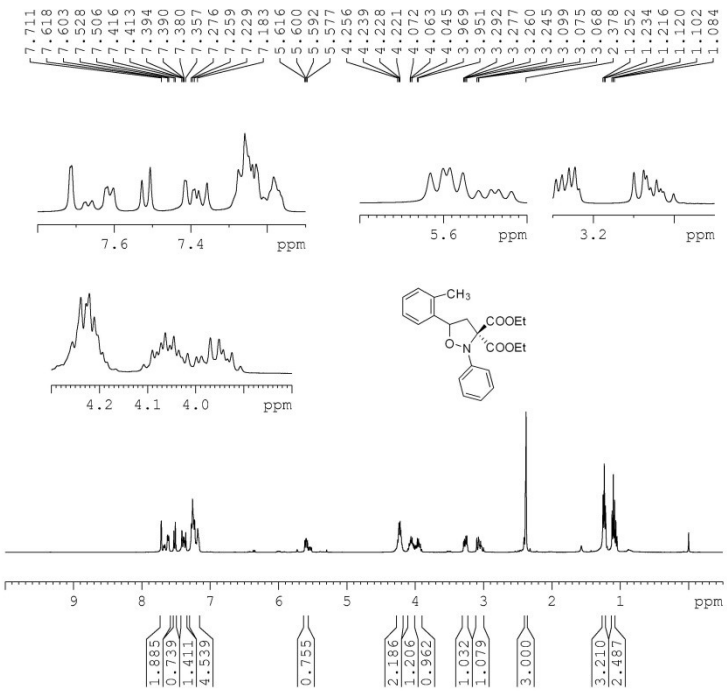
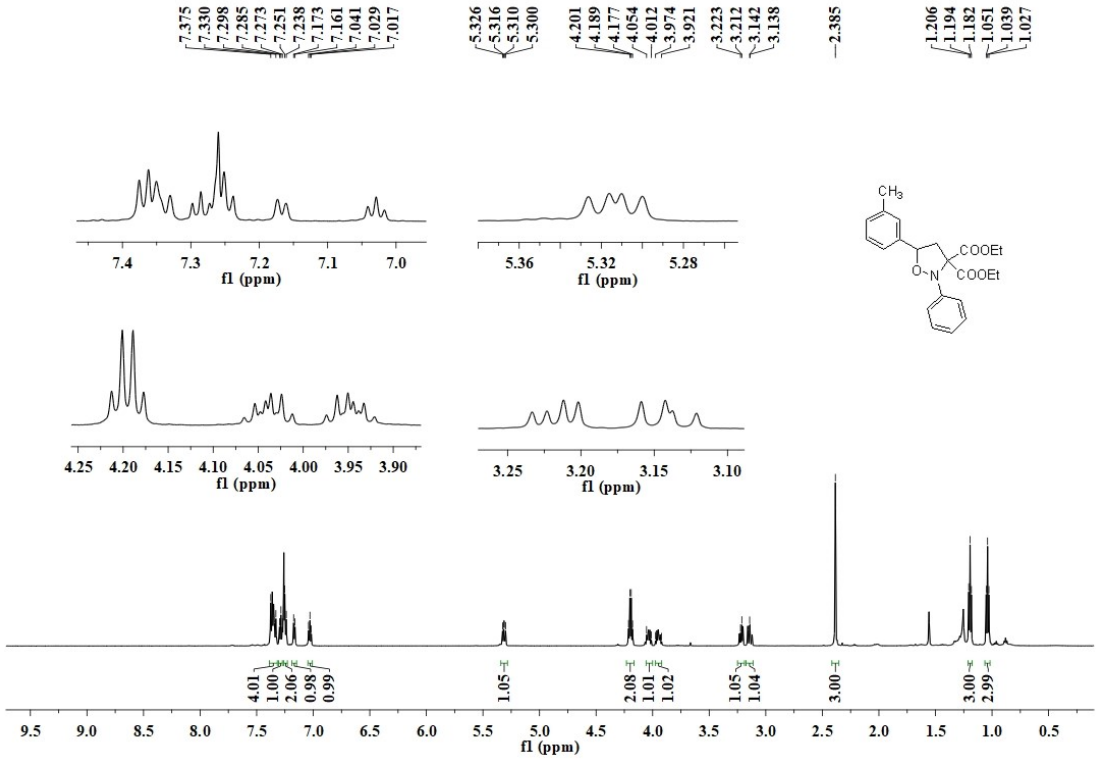
LB	0.30
GB	0
PC	1.00

4aab

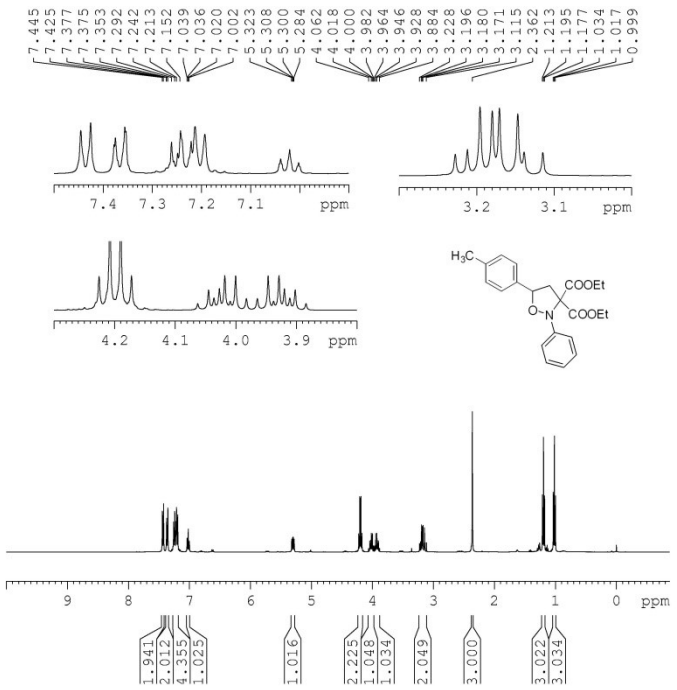


NAME	2018-12-03 tyut
EXPNO	33
PROCNO	1
Date_	20181203
Time	17.07
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8012.820
FIDRES	0.122266
AQ	4.0894966
RG	67.58
DW	62.400
DE	6.50
TE	296.0
D1	1.00000000
TD0	1
========	CHANNEL f1 ====
SFO1	400.1324710
NUC1	1H
P1	9.70
SI	65536
SF	400.1300102
WDW	EM
SSB	0
LB	0.30
GB	0
PC	1.00

4aac



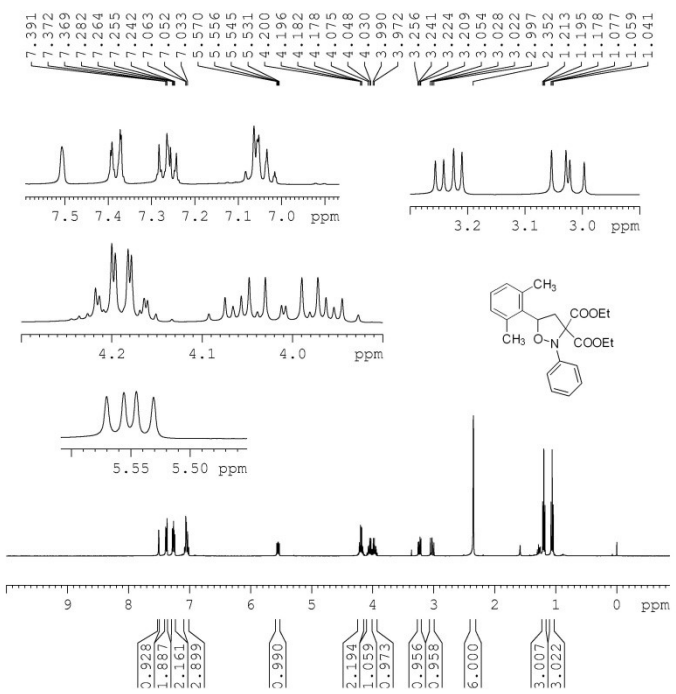
4aad



BRUKER

NAME	2018-10-28 tyut-1
EXPNO	4
PROCNO	1
Date_	20181026
Time	17.51
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 se
RG	34.32
DW	62.400 us
DE	6.50 us
TE	296.4 K
D1	1.00000000 se
TD0	1
========	CHANNEL f1 ======
SFO1	400.1324710 MH
NUC1	1H
P1	9.70 us
SI	65536
SF	400.1300145 MH
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

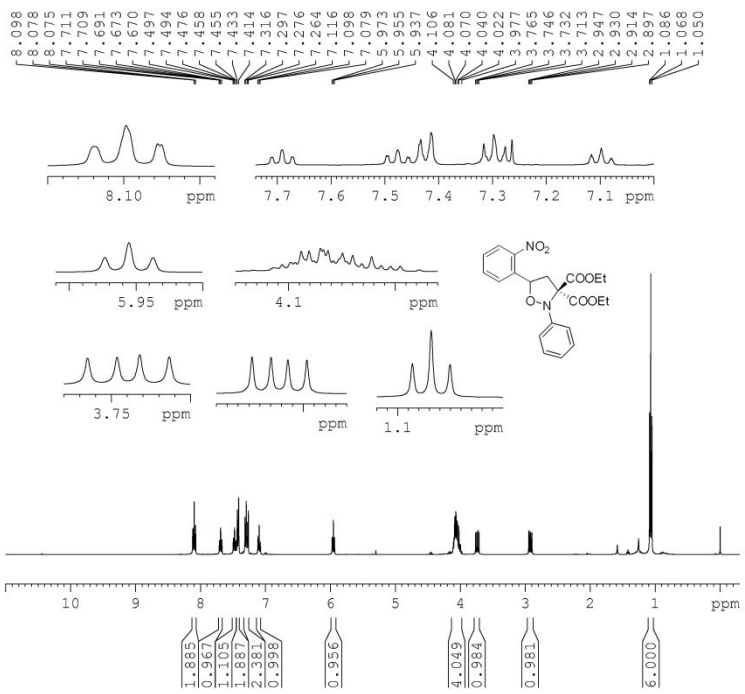
4aae



```
NAME        2018-10-12 tyut-1
EXPNO                      1
PROCNO                     1
Date_               20181012
Time                   14.50
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        16
DS                         2
SWH                8012.820 Hz
FIDRES             0.122266 Hz
AQ                 4.0894966 se
RG                     54.19
DW                    62.400 us
DE                     6.50 us
TE                    295.2 K
D1              1.00000000 se
TD0                        1

======== CHANNEL f1 ======
SFO1          400.1324710 MH
NUC1                    1H
P1                    9.70 us
SI                   65536
SF            400.1300116 MH
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

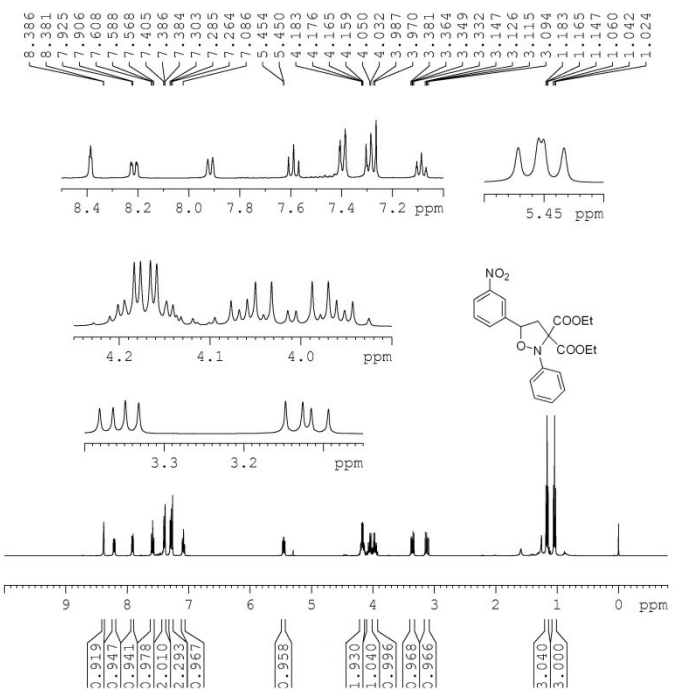
4aaf



```
NAME        2018-12-17 tyut
EXPNO                     35
PROCNO                     1
Date_               20181218
Time                    7.11
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        16
DS                         2
SWH                8012.820
FIDRES             0.122266
AQ                 4.0894966
RG                     60.71
DW                    62.400
DE                     6.50
TE                    293.3
D1              1.00000000
TD0                        1

======== CHANNEL f1 ====
SFO1          400.1324710
NUC1                    1H
P1                    9.70
SI                   65536
SF            400.1300085
WDW                    EM
SSB                     0
LB                    0.30
GB                      0
PC                   1.00
```

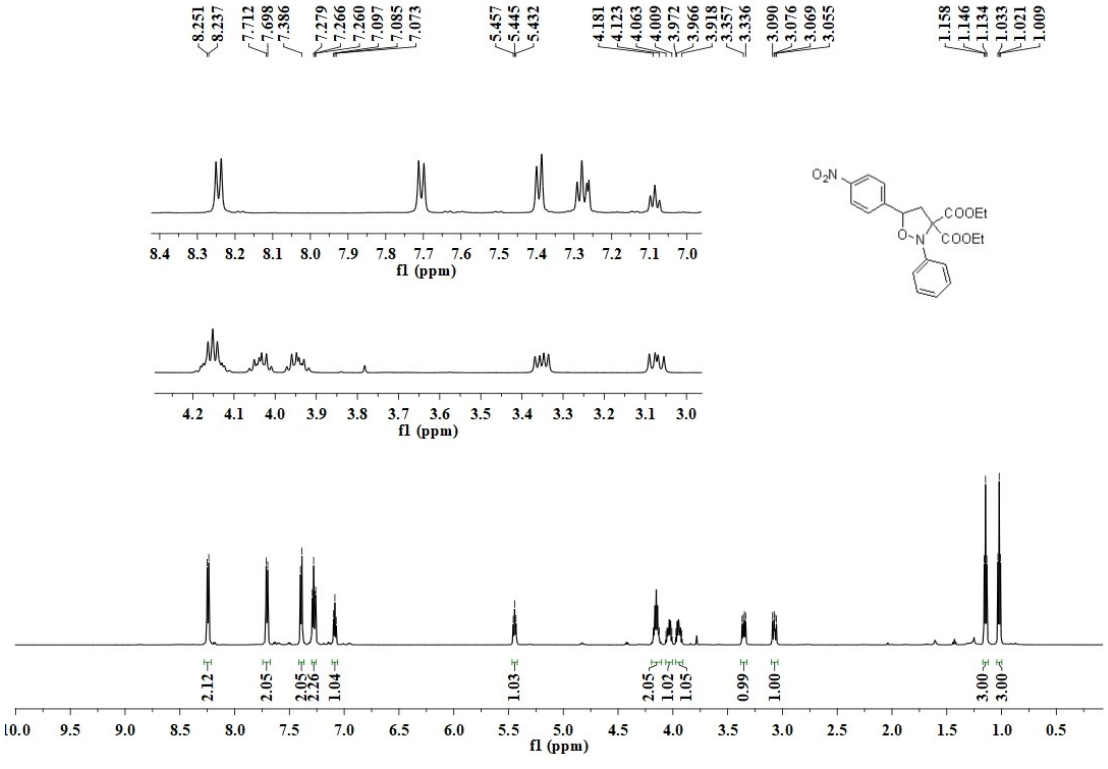
4aag



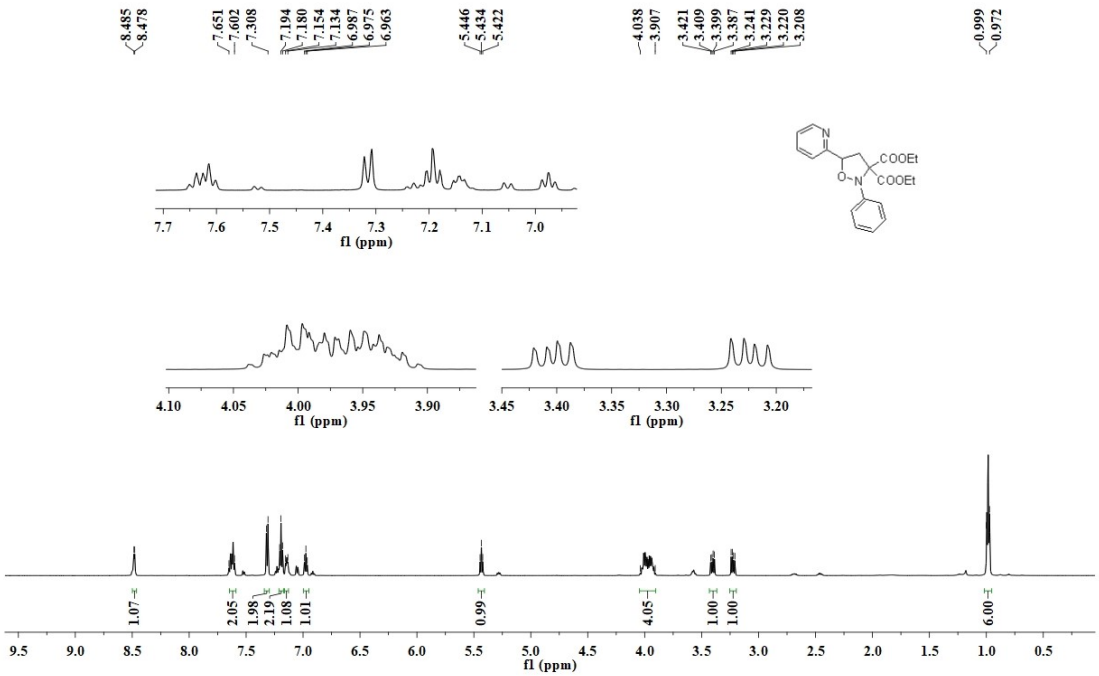
```
NAME        2018-11-06 tyut-1
EXPNO                      9
PROCNO                     1
Date_               20181106
Time                  22.54
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894966 se
RG                    67.58
DW                  62.400 us
DE                    6.50 us
TE                   295.5 K
D1              1.00000000 se
TD0                       1

======== CHANNEL f1 ======
SFO1          400.1324710 MH
NUC1                    1H
P1                    9.70 us
SI                    65536
SF            400.1300082 MH
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

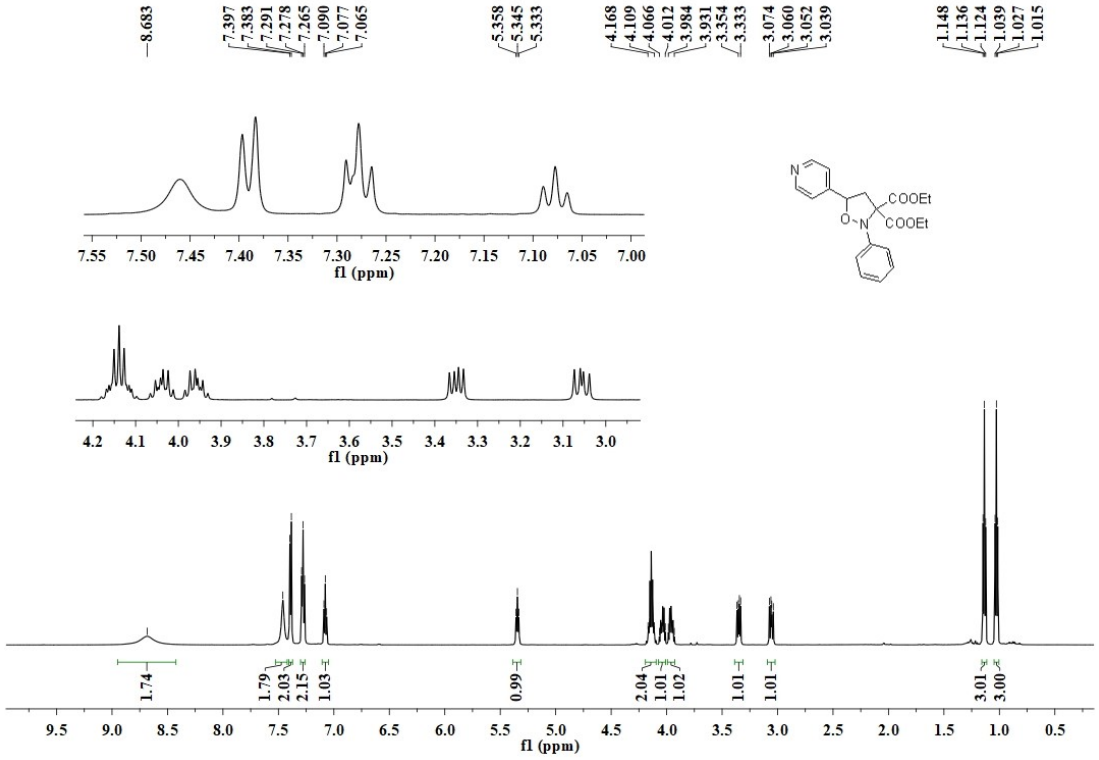
4aah



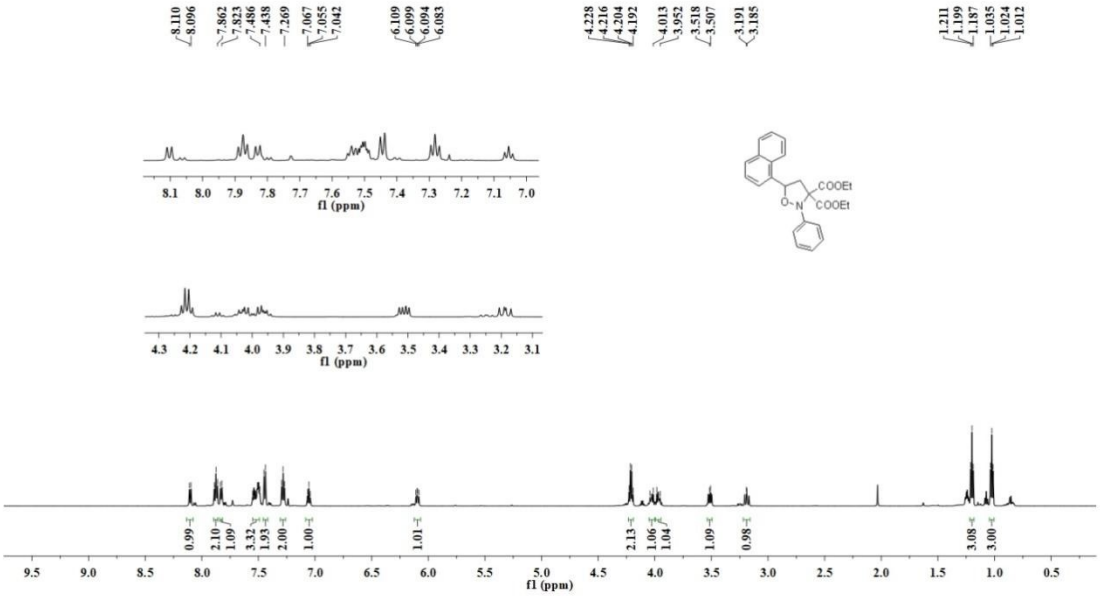
4aai


8.485
8.478
7.651
7.602
7.308
7.194
7.180
7.154
7.134
6.987
6.975
6.963
5.446
5.434
5.422
4.038
3.907
3.421
3.409
3.399
3.387
3.241
3.229
3.220
3.208
0.999
0.972
COOEt
COOEt
f1 (ppm)
1.07
2.05
1.98
2.19
1.08
1.01
0.99
4.05
1.00
1.00
6.00

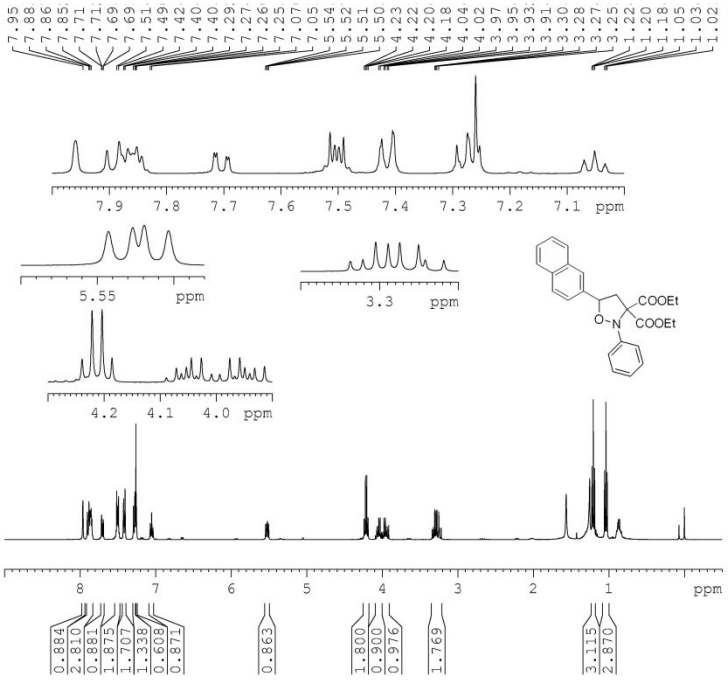
4aaj


8.683
7.397
7.383
7.291
7.278
7.265
7.090
7.077
7.065
5.358
5.345
5.333
4.168
4.109
4.066
4.012
3.984
3.931
3.354
3.333
3.074
3.060
3.052
3.039
1.148
1.136
1.124
1.039
1.027
1.015
COOEt
COOEt
f1 (ppm)
1.74
1.79
2.03
2.15
1.03
0.99
2.04
1.01
1.02
1.01
1.01
3.01
3.00

4aak



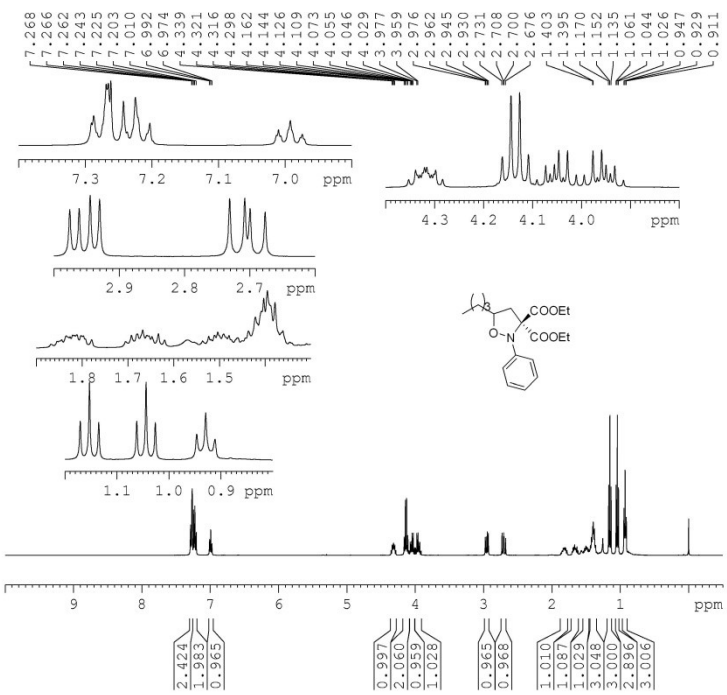
4aal



BRUKER

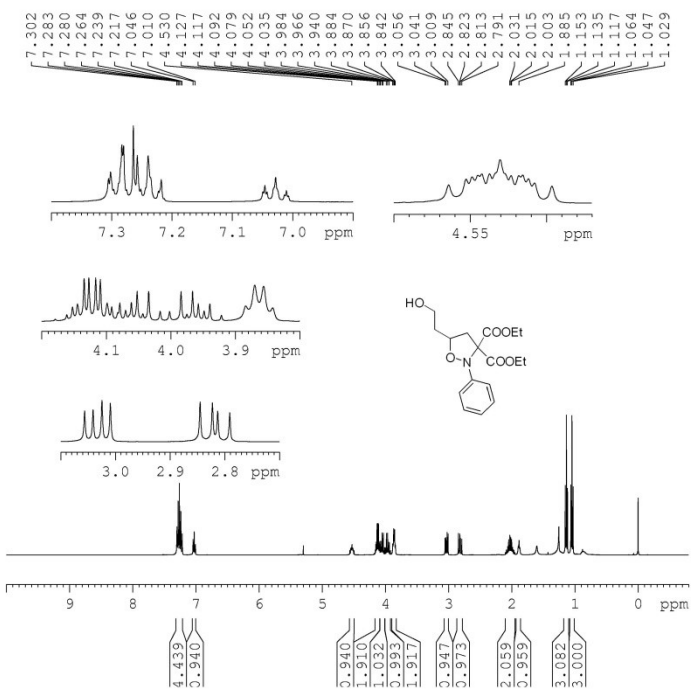
NAME	2018-11-04 tyut
EXPNO	6
PROCNO	1
Date_	20181105
Time	9.02
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8012.820
FIDRES	0.122266
AQ	4.0894966
RG	94.93
DW	62.400
DE	6.50
TE	295.3
D1	1.00000000
TD0	1
======== CHANNEL f1 ====	
SFO1	400.1324710
NUC1	1H
P1	9.70
SI	65536
SF	400.1300103
WDW	EM
SSB	0
LB	0.30
GB	0
PC	1.00

4aam



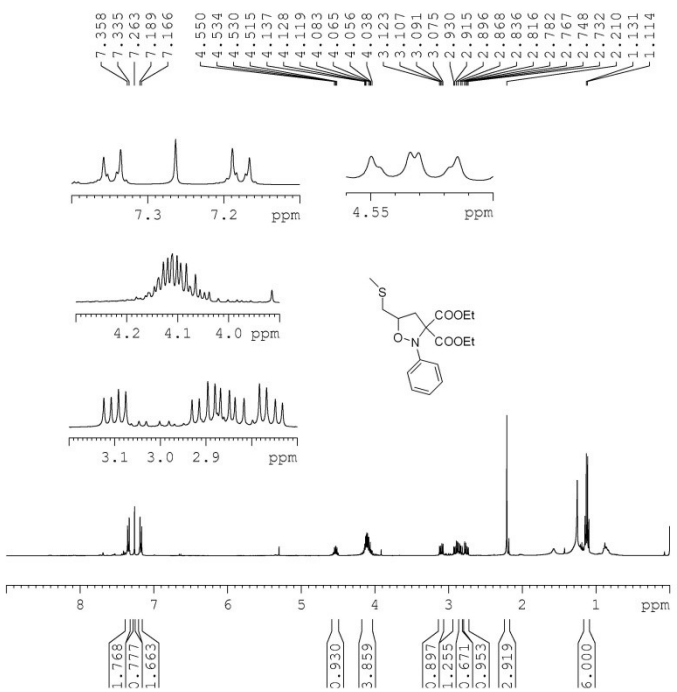
NAME	2018-11-29 tyut
EXPNO	32
PROCNO	1
Date_	20181129
Time	18.36
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8012.820
FIDRES	0.122266
AQ	4.0894966
RG	67.58
DW	62.400
DE	6.50
TE	297.4
D1	1.00000000
TD0	1
======== CHANNEL f1 ====	
SFO1	400.1324710
NUC1	1H
P1	9.70
SI	65536
SF	400.1300092
WDW	EM
SSB	0
LB	0.30
GB	0
PC	1.00

4aan



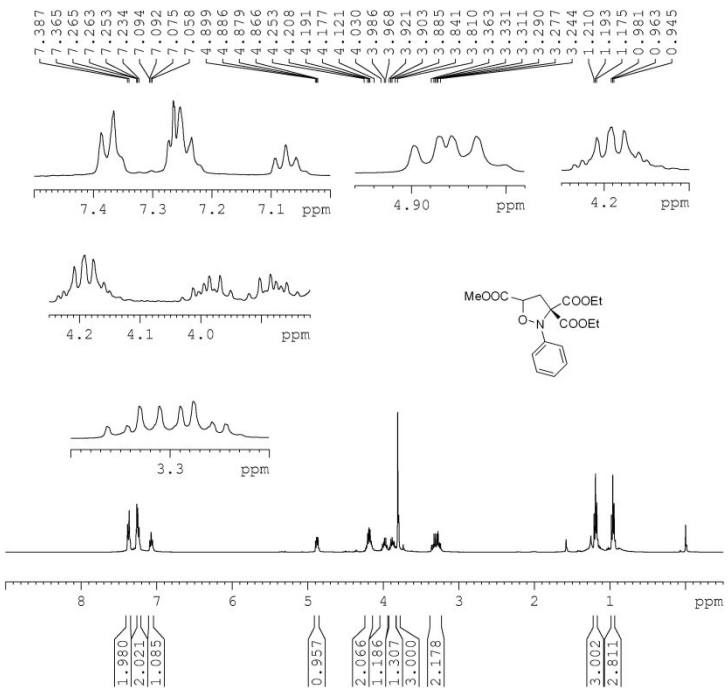
NAME	2018-11-06 tyut-1
EXPNO	8
PROCNO	1
Date_	20181106
Time	23.03
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 se
RG	74.25
DW	62.400 us
DE	6.50 us
TE	295.5 K
D1	1.00000000 se
TD0	1
======== CHANNEL f1 ======	
SFO1	400.1324710 MH
NUC1	1H
P1	9.70 us
SI	65536
SF	400.1300084 MH
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

4aao



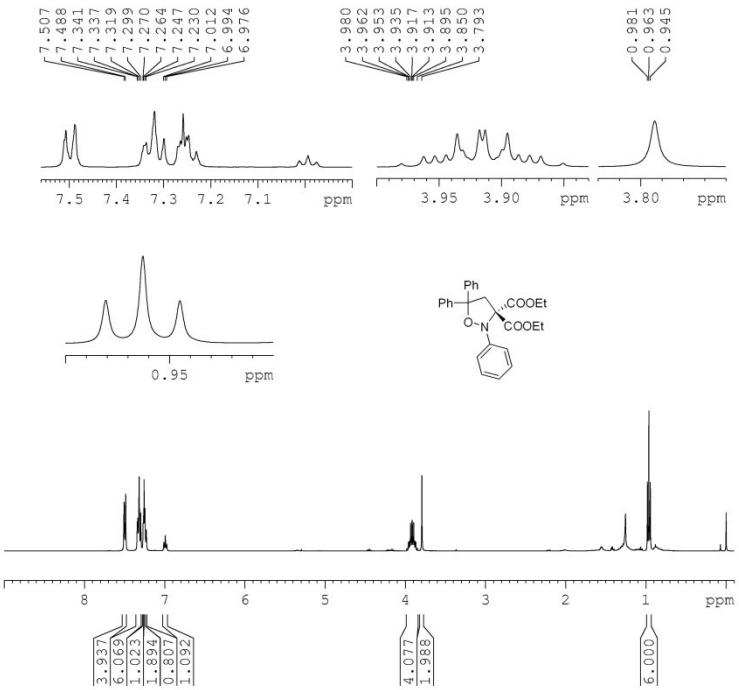
NAME	2018-11-06 tyut-1
EXPNO	11
PROCNO	1
Date_	20181106
Time	23.11
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 se
RG	74.25
DW	62.400 us
DE	6.50 us
TE	295.4 K
D1	1.00000000 se
TD0	1
======== CHANNEL f1 ======	
SFO1	400.1324710 MH
NUC1	1H
P1	9.70 us
SI	65536
SF	400.1300086 MH
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

4aap



NAME	2018-12-28 tyut
EXPNO	18
PROCNO	1
Date_	20181229
Time	22.19
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8012.820
FIDRES	0.122266
AQ	4.0894966
RG	74.25
DW	62.400
DE	6.50
TE	292.1
D1	1.00000000
TD0	1
======== CHANNEL f1 ====	
SFO1	400.1324710
NUC1	1H
P1	9.70
SI	65536
SF	400.1300089
WDW	EM
SSB	0
LB	0.30
GB	0
PC	1.00

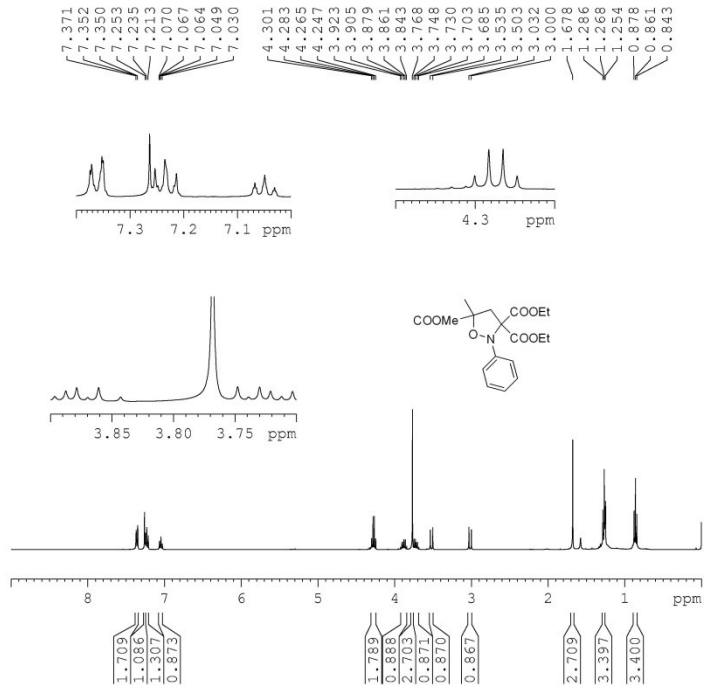
4aaq



```
NAME          2019-02-25 tyut
EXPNO                   10
PROCNO                   1
Date_             20190225
Time                17.04
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8012.820
FIDRES           0.122266
AQ               4.0894966
RG                  87.46
DW                  62.400
DE                    6.50
TE                  298.3
D1               1.00000000
TD0                     1

======== CHANNEL f1 ====
SFO1          400.1324710
NUC1                   1H
P1                   9.59
SI                  65536
SF            400.1300106
WDW                    EM
SSB                     0
LB                   0.30
GB                      0
PC                   1.00
```

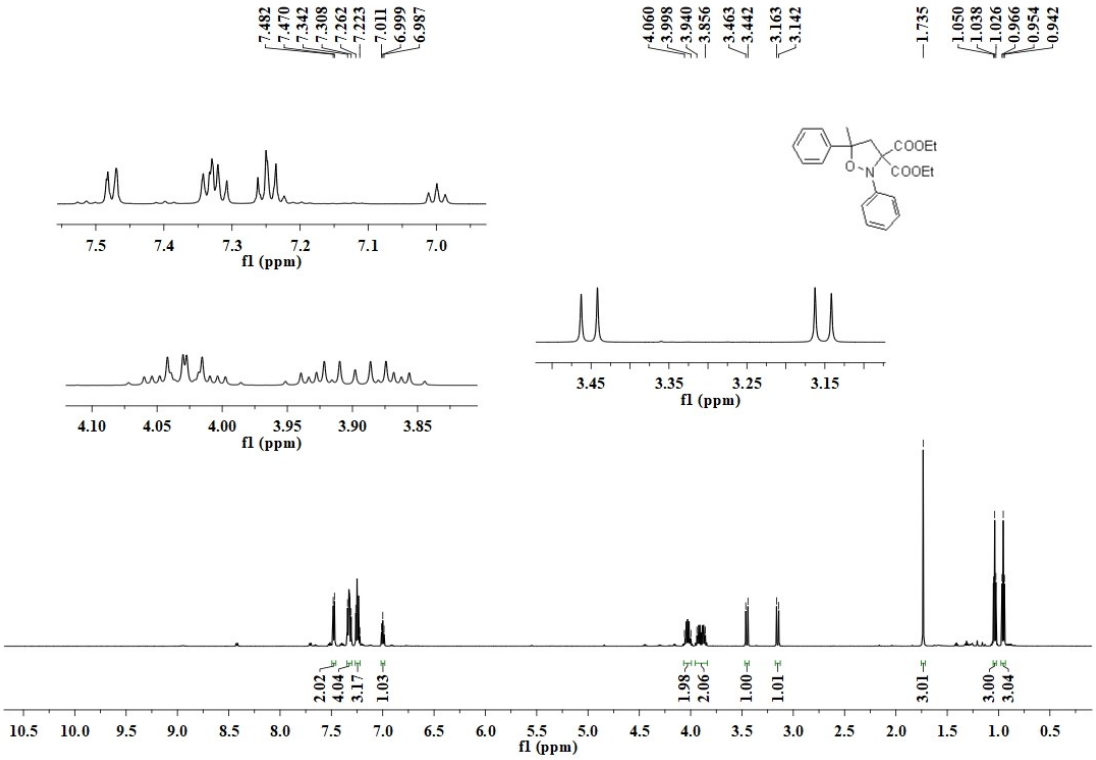
4aar



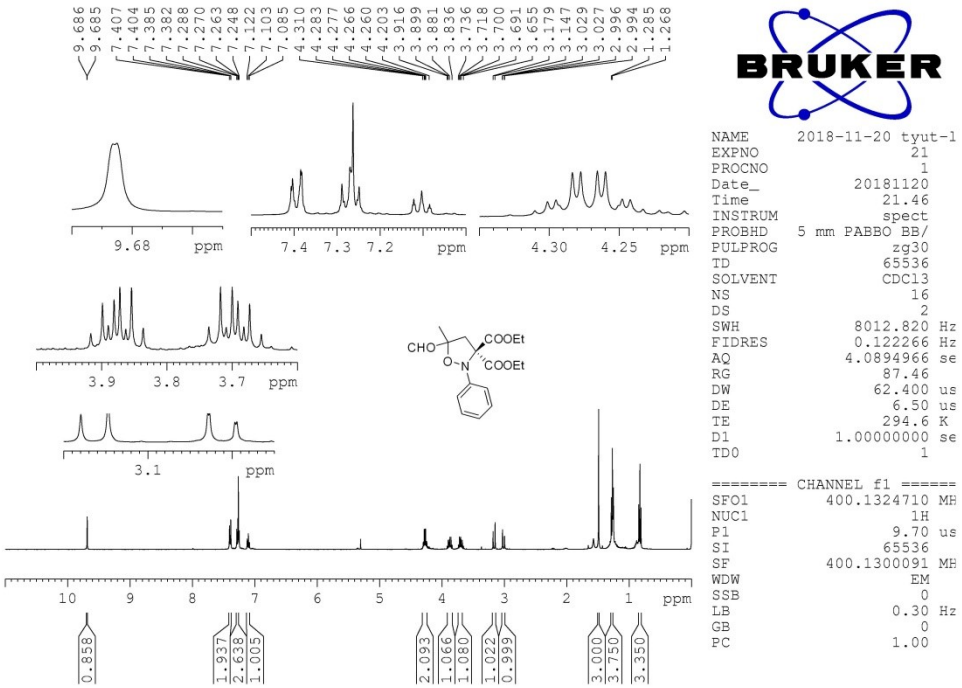
```
NAME          2018-11-12 tyut-1
EXPNO                   14
PROCNO                   1
Date_             20181112
Time                22.14
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894966 se
RG                  74.25
DW                  62.400 us
DE                    6.50 us
TE                  -73.5 K
D1               1.00000000 se
TD0                     1

======== CHANNEL f1 ======
SFO1          400.1324710 MH
NUC1                   1H
P1                   9.70 us
SI                  65536
SF            400.1300087 MH
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

4aas



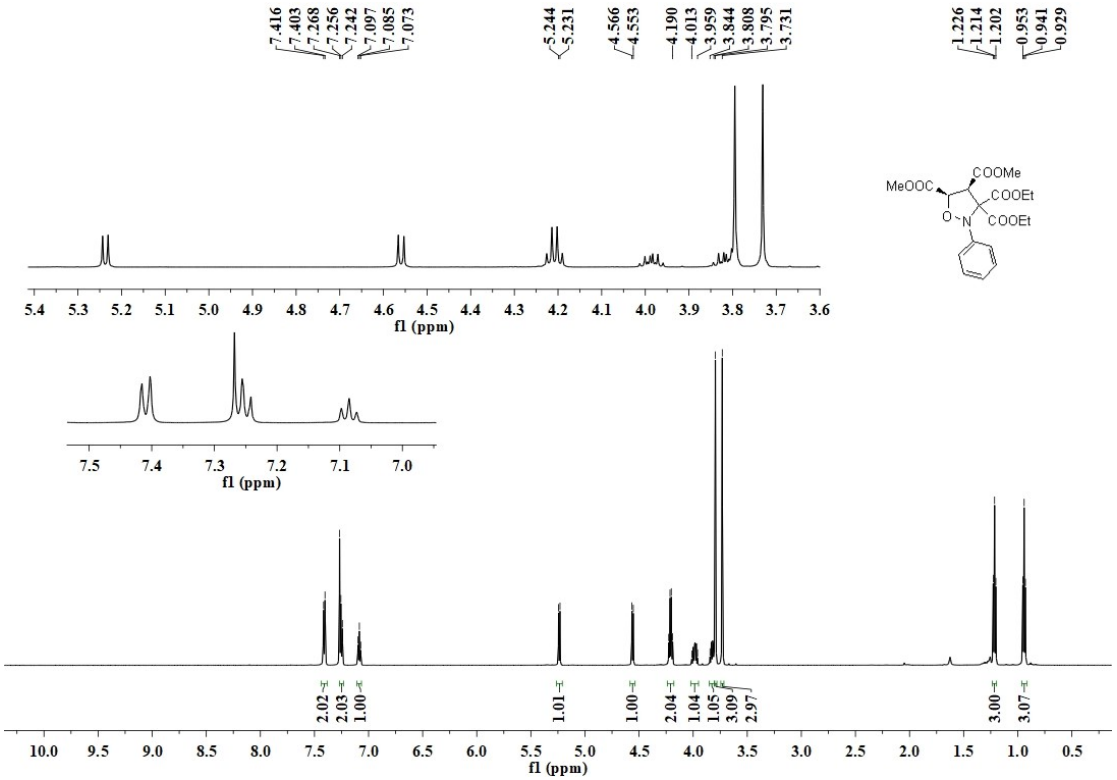
4aat

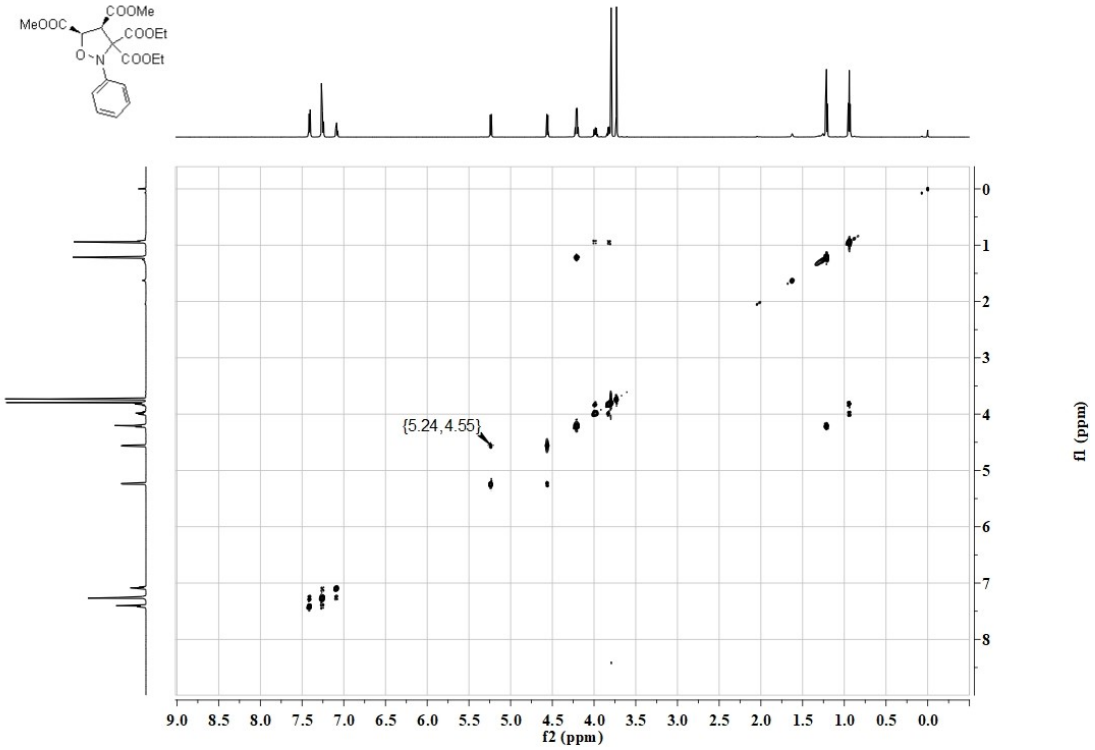


BRUKER

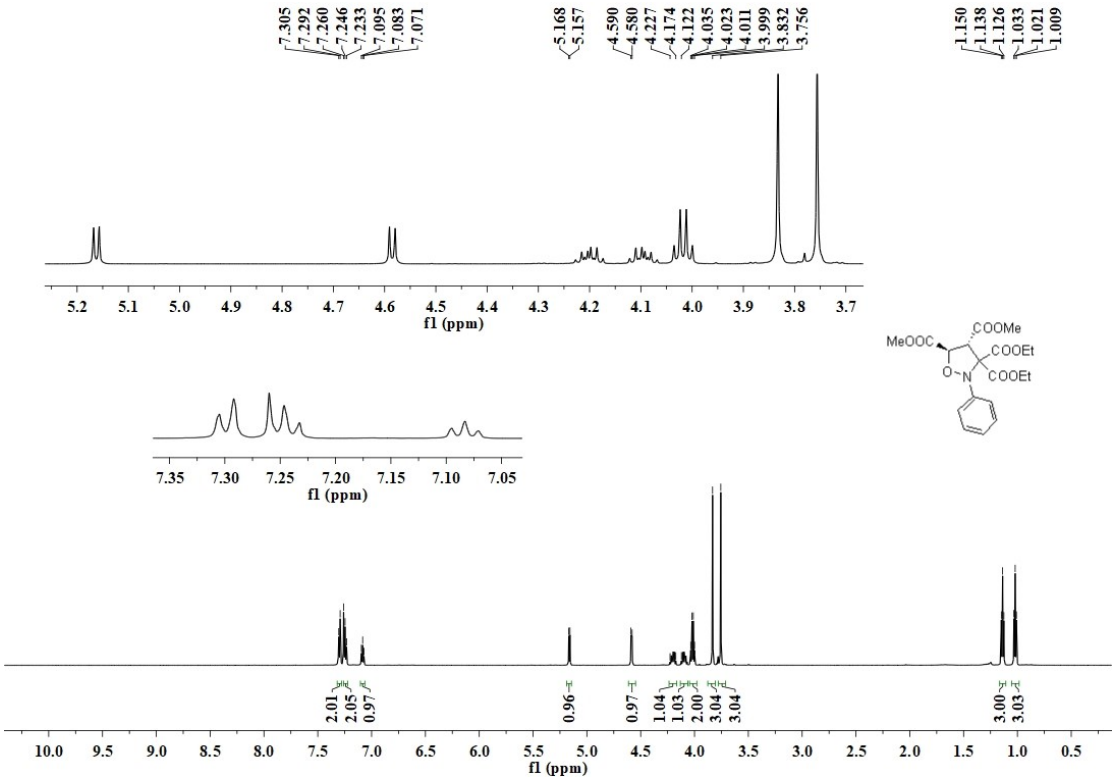
NAME	2018-11-20 tyut-1
EXPNO	21
PROCNO	1
Date_	20181120
Time	21.46
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 se
RG	87.46
DW	62.400 us
DE	6.50 us
TE	294.6 K
D1	1.00000000 se
TD0	1
========	CHANNEL f1 ======
SFO1	400.1324710 MH
NUC1	1H
P1	9.70 us
SI	65536
SF	400.1300091 MH
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

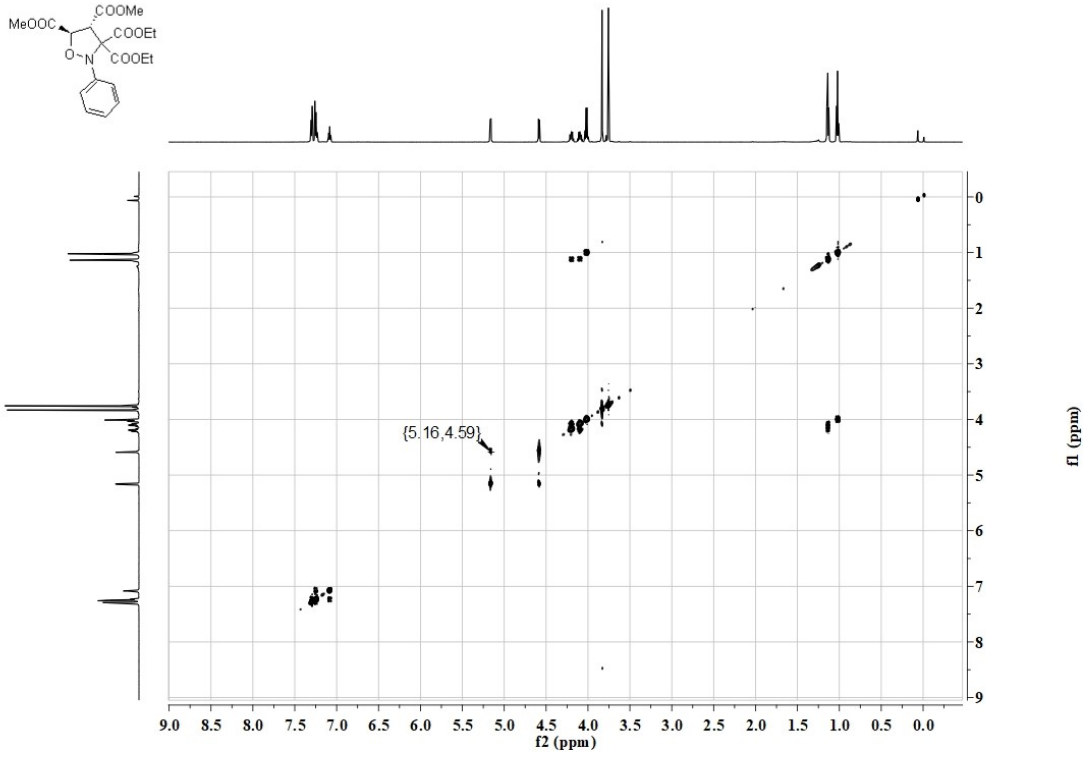
4aau


7.416
7.403
7.268
7.256
7.242
7.097
7.085
7.073
5.244
5.231
4.566
4.553
4.190
4.013
3.959
3.844
3.808
3.795
3.731
1.226
1.214
1.202
0.953
0.941
0.929
COOMe
MeOOC
COOEt
COOEt
fl (ppm)
2.02
2.03
1.00
1.01
1.00
2.04
1.04
1.05
3.09
2.97
3.00
3.07

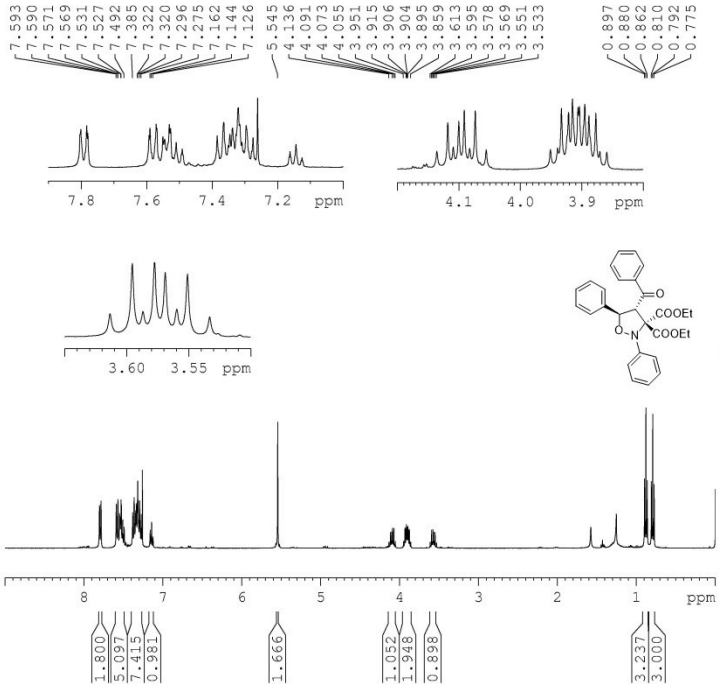

COOMe
MeOOC
COOEt
COOEt
{5.24,4.55}
f2 (ppm)
fl (ppm)

4aav


7.305
7.292
7.260
7.246
7.233
7.095
7.083
7.071
5.168
5.157
4.590
4.580
4.227
4.174
4.122
4.035
4.023
4.011
3.999
3.832
3.756
1.150
1.138
1.126
1.033
1.021
1.009
f1 (ppm)
COOMe
COOEt
COOEt
MeOOC
2.01
2.05
0.97
0.96
0.97
1.04
1.03
2.00
3.04
3.04
3.00
3.03

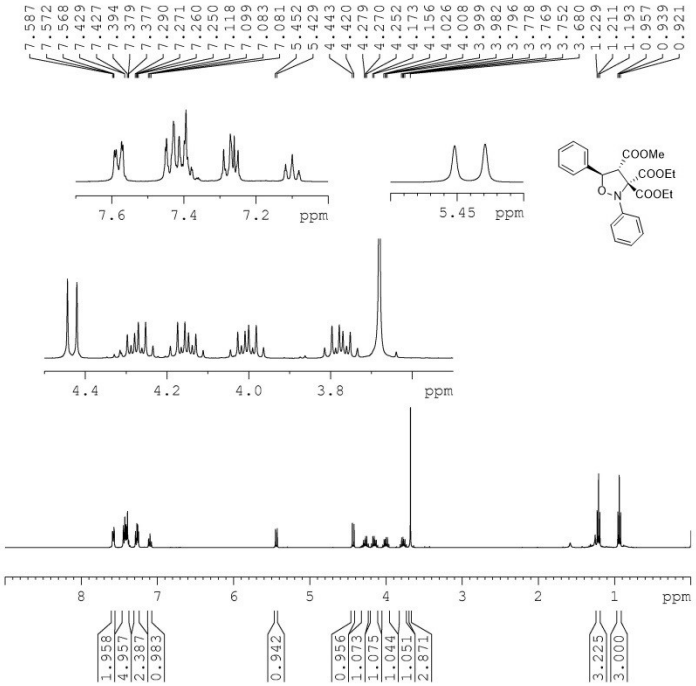

COOMe
COOEt
COOEt
MeOOC
{5.16,4.59}
f2 (ppm)
f1 (ppm)

4aaw



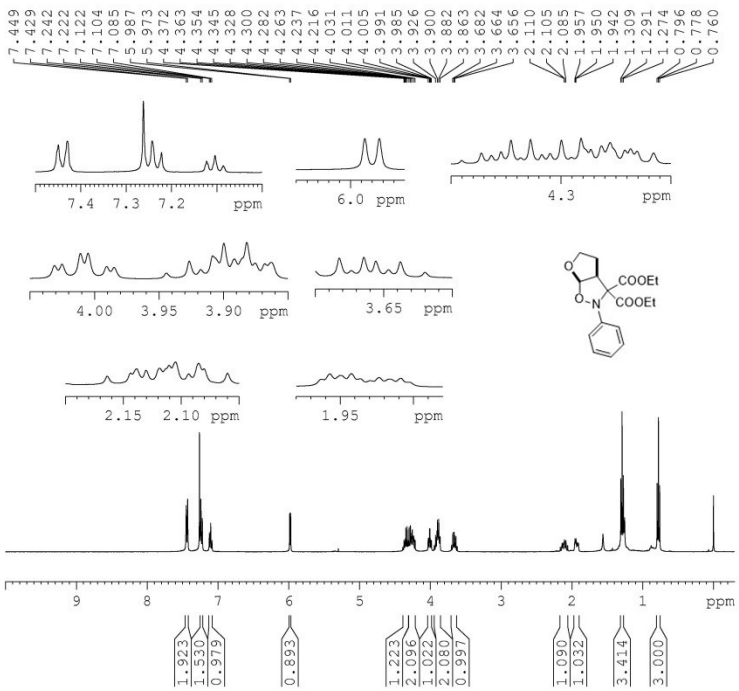
NAME	2018-11-20 tyut
EXPNO	20
PROCNO	1
Date_	20181120
Time	21.42
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8012.820
FIDRES	0.122266
AQ	4.0894966
RG	74.25
DW	62.400
DE	6.50
TE	294.6
D1	1.00000000
TD0	1
======== CHANNEL f1 ====	
SFO1	400.1324710
NUC1	1H
P1	9.70
SI	65536
SF	400.1300096
WDW	EM
SSB	0
LB	0.30
GB	0
PC	1.00

4aax



NAME	2018-11-14 tyut-1
EXPNO	16
PROCNO	1
Date_	20181114
Time	17.25
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 se
RG	67.58
DW	62.400 us
DE	6.50 us
TE	296.0 K
D1	1.00000000 se
TD0	1
======== CHANNEL f1 ======	
SFO1	400.1324710 MH
NUC1	1H
P1	9.70 us
SI	65536
SF	400.1300098 MH
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

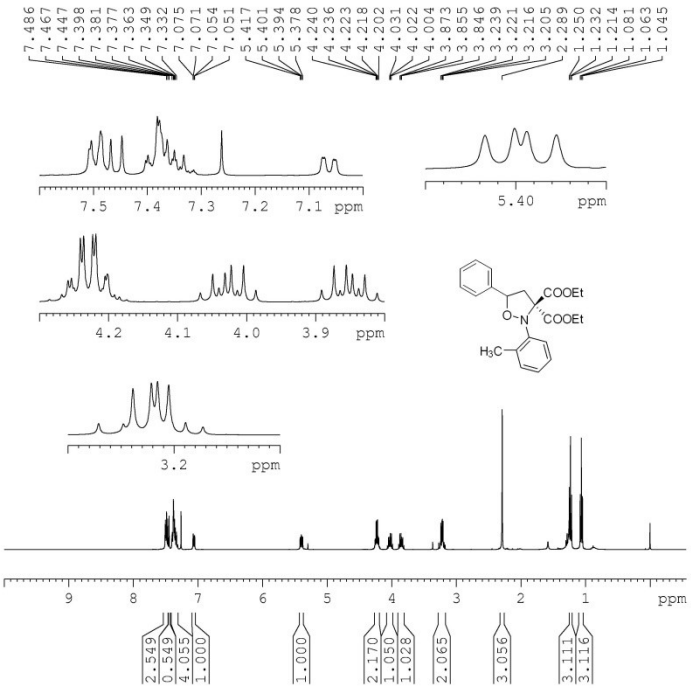
4aay




```
NAME          2018-11-29 tyut
EXPNO                     31
PROCNO                     1
Date_              20181129
Time                  18.32
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        16
DS                         2
SWH                8012.820
FIDRES            0.122266
AQ               4.0894966
RG                    94.93
DW                    62.400
DE                      6.50
TE                     297.4
D1               1.00000000
TD0                        1

======== CHANNEL f1 ====
SFO1           400.1324710
NUC1                    1H
P1                    9.70
SI                   65536
SF             400.1300093
WDW                    EM
SSB                     0
LB                   0.30
GB                      0
PC                   1.00
```

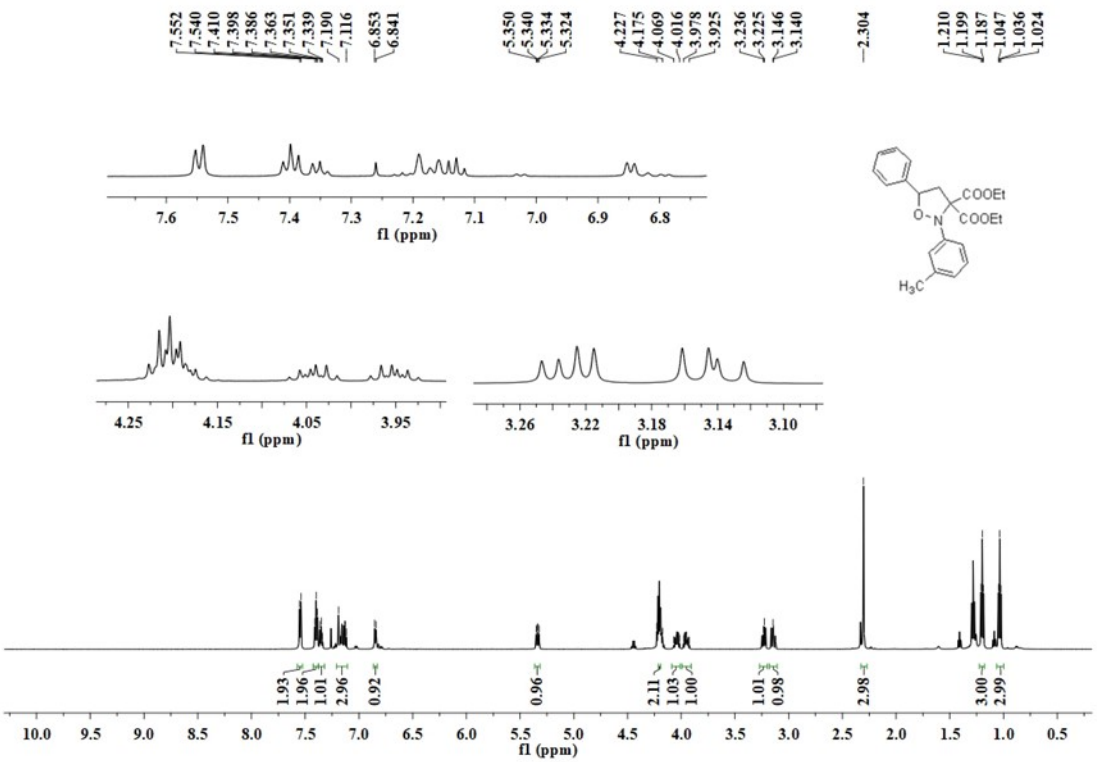
4baa



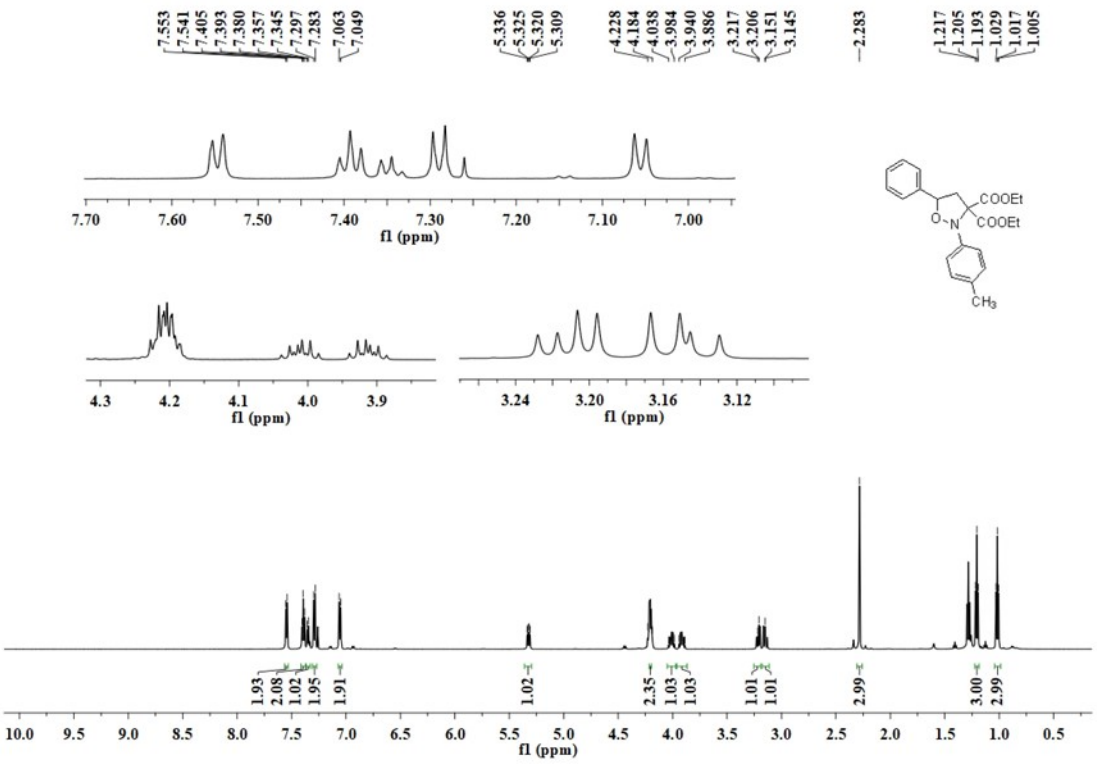

```
NAME          2018-11-20 tyut-1
EXPNO                     23
PROCNO                     1
Date_              20181120
Time                  21.54
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        16
DS                         2
SWH                8012.820 Hz
FIDRES            0.122266 Hz
AQ               4.0894966 se
RG                    67.58
DW                    62.400 us
DE                     6.50 us
TE                    294.6 K
D1               1.00000000 se
TD0                        1

======== CHANNEL f1 ======
SFO1           400.1324710 MH
NUC1                    1H
P1                    9.70 us
SI                   65536
SF             400.1300095 MH
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

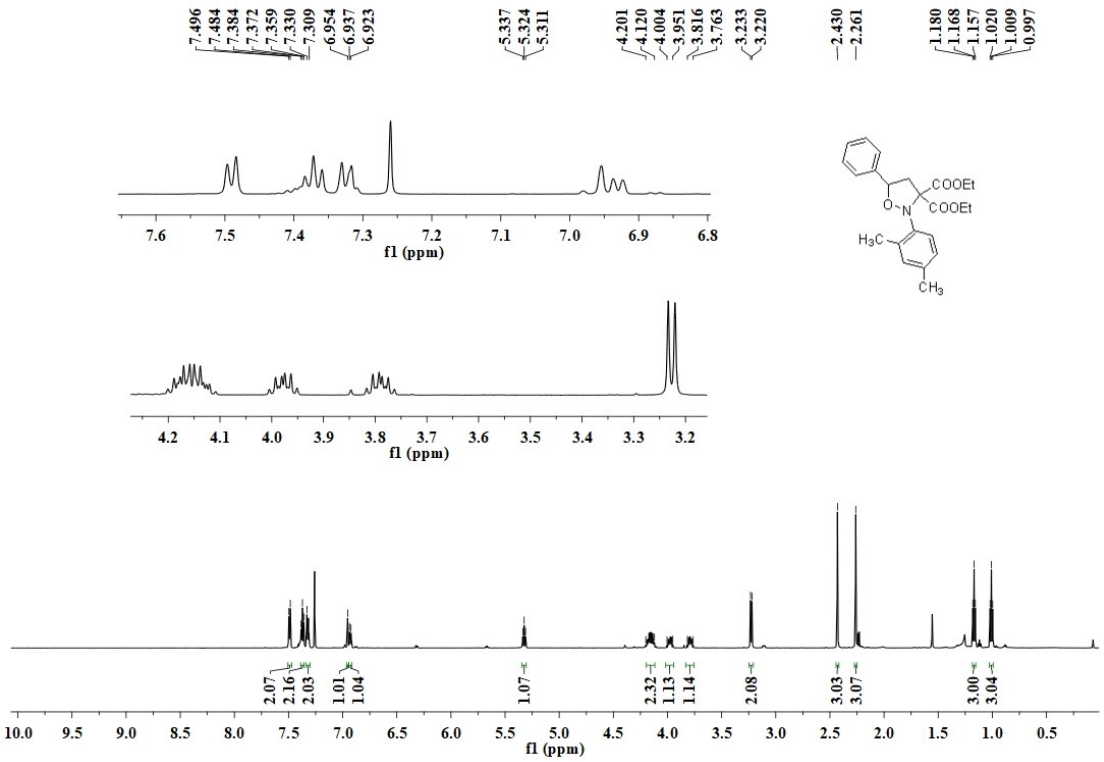
4caa


7.552
7.540
7.410
7.398
7.386
7.363
7.351
7.339
7.190
7.116
6.853
6.841
5.350
5.340
5.334
5.324
4.227
4.175
4.069
4.016
3.978
3.925
3.236
3.225
3.146
3.140
2.304
1.210
1.199
1.187
1.047
1.036
1.024
f1 (ppm)
COOEt
COOEt
H3C
1.93
1.96
1.01
2.96
0.92
0.96
2.11
1.03
1.00
1.01
0.98
2.98
3.00
2.99

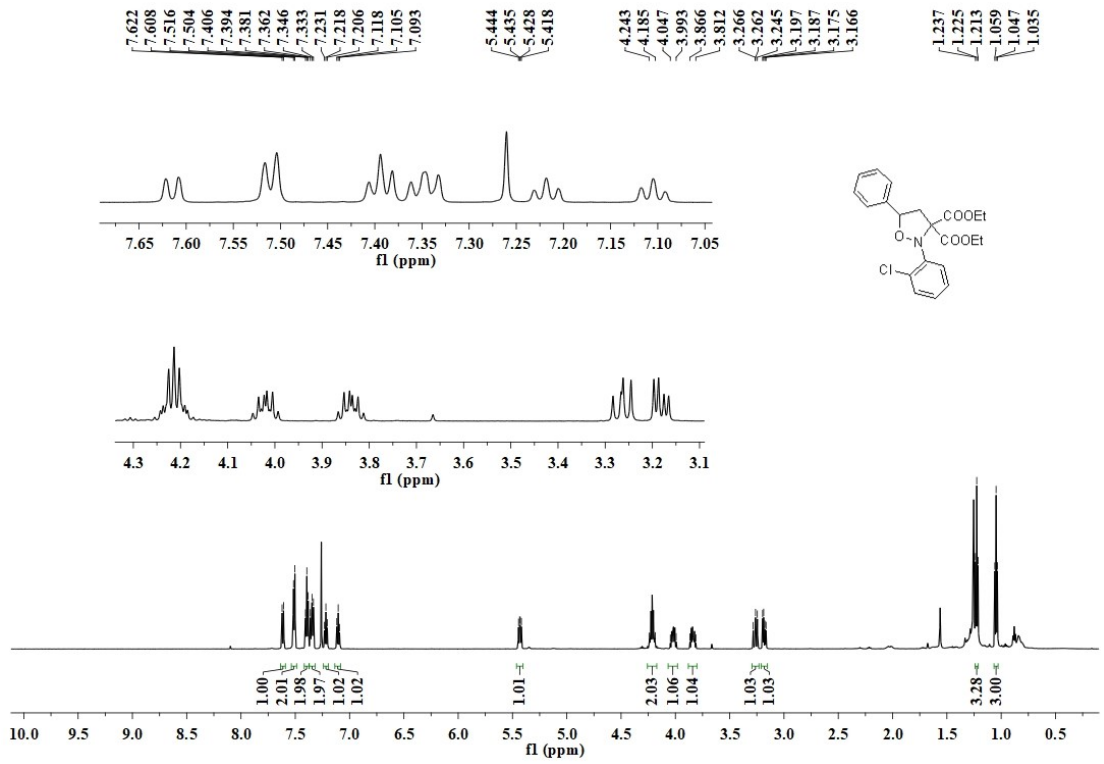
4daa


7.553
7.541
7.405
7.393
7.380
7.357
7.345
7.297
7.283
7.063
7.049
5.336
5.325
5.320
5.309
4.228
4.184
4.038
3.984
3.940
3.886
3.217
3.206
3.151
3.145
2.283
1.217
1.205
1.193
1.029
1.017
1.005
f1 (ppm)
COOEt
COOEt
CH3
1.93
2.08
1.02
1.95
1.91
1.02
2.35
1.03
1.03
1.01
1.01
2.99
3.00
2.99

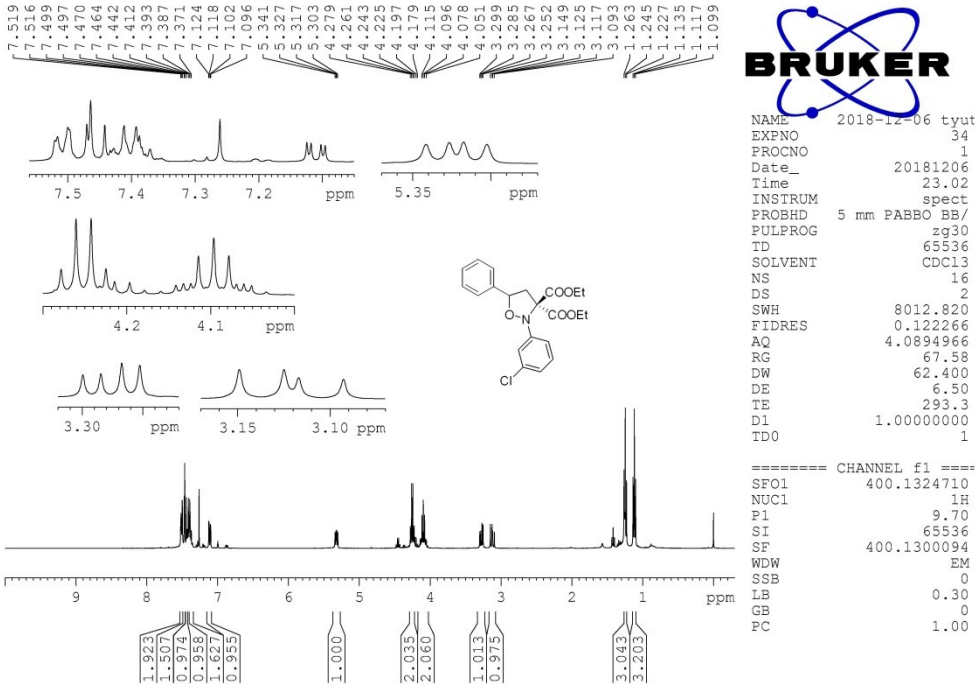
4eaa


7.496
7.484
7.384
7.372
7.359
7.330
7.309
6.954
6.937
6.923
5.337
5.324
5.311
4.201
4.120
4.004
3.951
3.816
3.763
3.233
3.220
2.430
2.261
1.180
1.168
1.157
1.020
1.009
0.997
COOEt
COOEt
H3C
CH3
f1 (ppm)
2.07
2.16
2.03
1.01
1.04
1.07
2.32
1.13
1.14
2.08
3.03
3.07
3.00
3.04

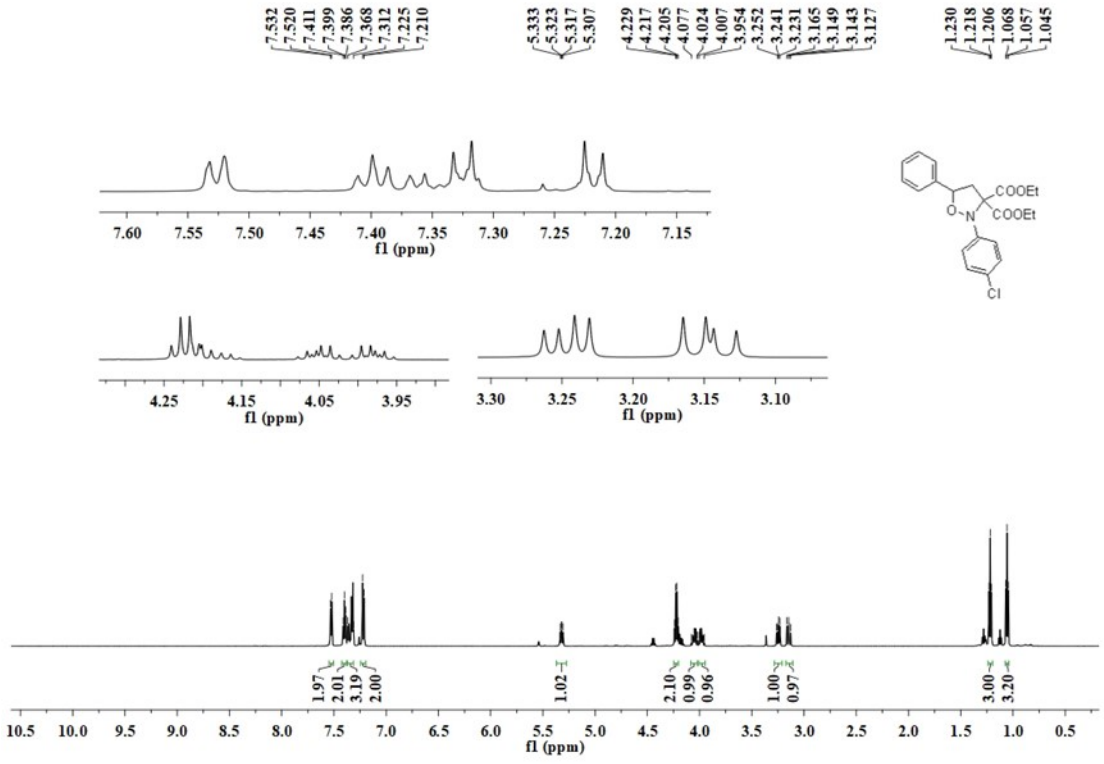
4faa


7.622
7.608
7.516
7.504
7.406
7.394
7.381
7.362
7.346
7.333
7.231
7.218
7.206
7.118
7.105
7.093
5.444
5.435
5.428
5.418
4.243
4.185
4.047
3.993
3.866
3.812
3.266
3.262
3.245
3.197
3.187
3.175
3.166
1.237
1.225
1.213
1.059
1.047
1.035
COOEt
COOEt
Cl
f1 (ppm)
1.00
2.01
1.98
1.97
1.02
1.02
1.01
2.03
1.06
1.04
1.03
1.03
3.28
3.00

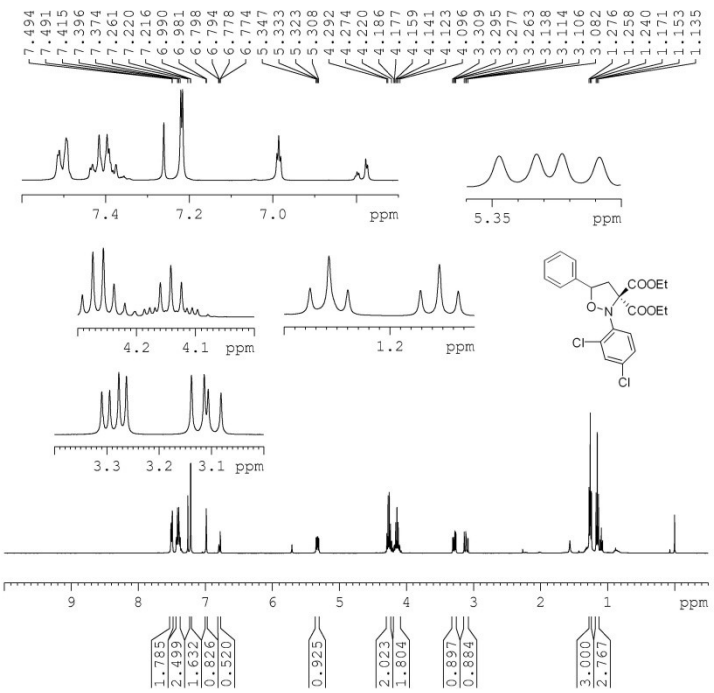
4gaa


7.519
7.516
7.499
7.497
7.470
7.464
7.442
7.412
7.393
7.387
7.371
7.124
7.118
7.102
7.096
5.341
5.327
5.317
5.303
4.279
4.261
4.243
4.225
4.197
4.179
4.115
4.096
4.078
4.051
3.299
3.285
3.267
3.252
3.149
3.125
3.117
3.093
1.263
1.245
1.227
1.135
1.117
1.099
BRUKER
NAME 2018-12-06 tyut
EXPNO 34
PROCNO 1
Date_ 20181206
Time 23.02
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820
FIDRES 0.122266
AQ 4.0894966
RG 67.58
DW 62.400
DE 6.50
TE 293.3
D1 1.00000000
TD0 1
======== CHANNEL f1 ====
SFO1 400.1324710
NUC1 1H
P1 9.70
SI 65536
SF 400.1300094
WDW EM
SSB 0
LB 0.30
GB 0
PC 1.00
COOEt
COOEt
Cl
ppm
1.923
1.507
0.974
0.958
1.627
0.955
1.000
2.035
2.060
1.013
0.975
3.043
3.203

4haa


7.532
7.520
7.411
7.399
7.386
7.368
7.312
7.225
7.210
5.333
5.323
5.317
5.307
4.229
4.217
4.205
4.077
4.024
4.007
3.954
3.252
3.241
3.231
3.165
3.149
3.143
3.127
1.230
1.218
1.206
1.068
1.057
1.045
COOEt
COOEt
Cl
f1 (ppm)
1.97
2.01
3.19
2.00
1.02
2.10
0.99
0.96
1.00
0.97
3.00
3.20

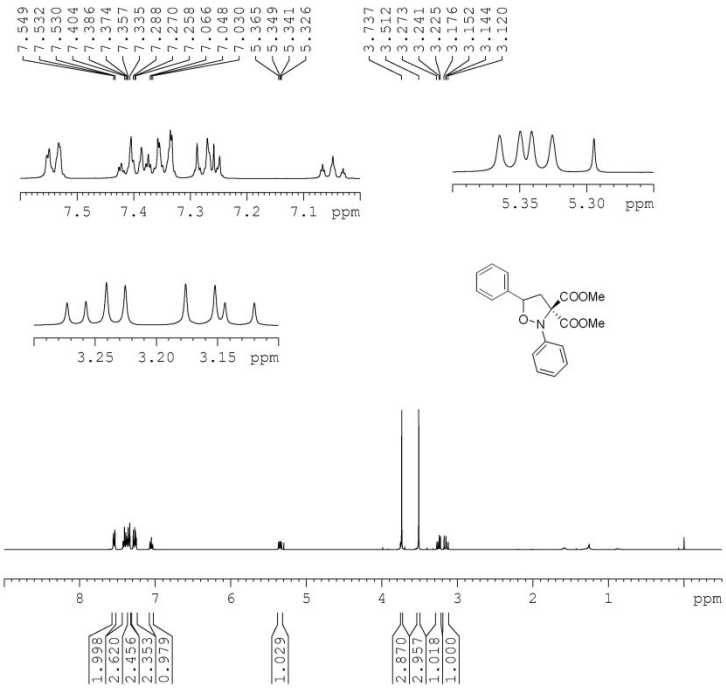
4iaa



```
NAME          2018-11-27 tyut
EXPNO                   29
PROCNO                   1
Date_             20181127
Time                 17.57
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH               8012.820
FIDRES            0.122266
AQ                4.0894966
RG                    87.46
DW                   62.400
DE                     6.50
TE                    294.1
D1              1.00000000
TD0                     1

======== CHANNEL f1 ====
SFO1           400.1324710
NUC1                    1H
P1                    9.70
SI                   65536
SF             400.1300095
WDW                    EM
SSB                     0
LB                   0.30
GB                      0
PC                   1.00
```

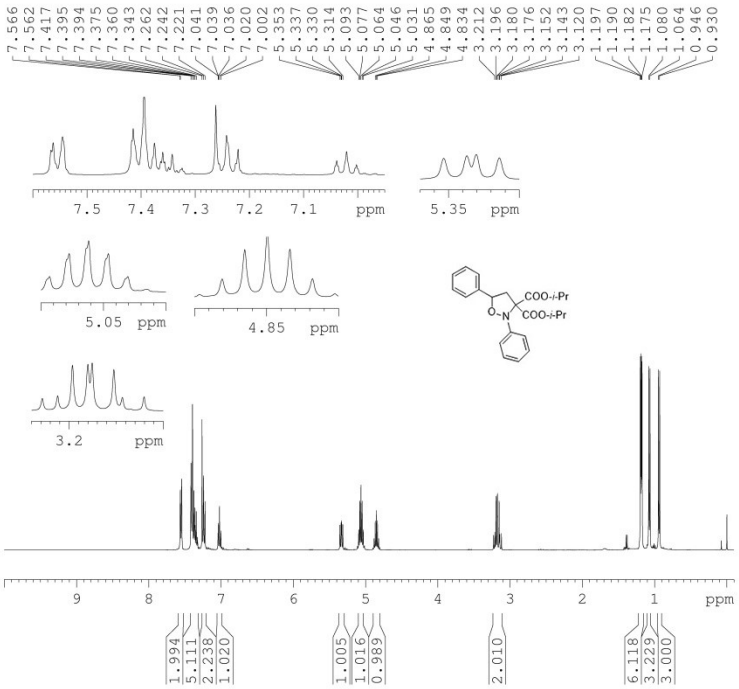
4aba



```
NAME          2018-11-26 tyut
EXPNO                   26
PROCNO                   1
Date_             20181126
Time                 22.33
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH               8012.820
FIDRES            0.122266
AQ                4.0894966
RG                    67.58
DW                   62.400
DE                     6.50
TE                    294.1
D1              1.00000000
TD0                     1

======== CHANNEL f1 ====
SFO1           400.1324710
NUC1                    1H
P1                    9.70
SI                   65536
SF             400.1300107
WDW                    EM
SSB                     0
LB                   0.30
GB                      0
PC                   1.00
```

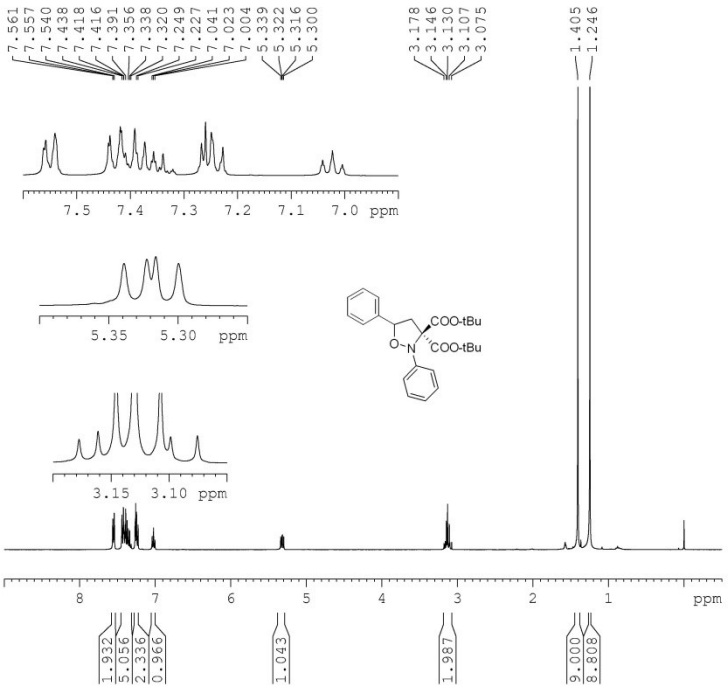
4aca



BRUKER

NAME	20191221-13
EXPNO	1
PROCNO	1
Date_	20191221
Time	16.30
INSTRUM	spect
PROBHD	Z116098_0711 (
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8012.820
FIDRES	0.244532
AQ	4.0894966
RG	32.73
DW	62.400
DE	6.50
TE	294.8
D1	1.00000000
TD0	1
SFO1	400.1324708
NUC1	1H
P1	9.76
SI	65536
SF	400.1300084
WDW	EM
SSB	0
LB	0.30
GB	0
PC	1.00

4ada



BRUKER

NAME	2018-11-27 tyut
EXPNO	28
PROCNO	1
Date_	20181127
Time	17.53
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8012.820
FIDRES	0.122266
AQ	4.0894966
RG	67.58
DW	62.400
DE	6.50
TE	294.1
D1	1.00000000
TD0	1
======== CHANNEL f1 ====	
SFO1	400.1324710
NUC1	1H
P1	9.70
SI	65536
SF	400.1300099
WDW	EM
SSB	0
LB	0.30
GB	0
PC	1.00