Supporting Information

N-Alkyl Nitrones as Substrates for Access to *N*-Aryl Isoxazolidines *via* Catalyst-Free One-Pot Three-Component Reaction with Nitroso Compounds and Olefins

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1. General

Unless otherwise indicated, all reagents were purchased from commercial sources and used without further purification unless otherwise stated. And deuterated solvents were purchased from Sigma−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. All compounds were characterized by ^{1}H NMR, ^{13}C NMR, HRMS, and compared to the literature data. ^{1}H NMR data were acquired at 300 K on a Bruker Advance 400 MHz spectrometer using $CDCl_3$ as solvent. Chemical shifts are reported in ppm from tetramethylsilane with the solvent $CDCl_3$ resonance as the internal standard ($CDCl_3$ = 7.26). 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. ^{13}C NMR data were collected at 100 MHz with complete proton decoupling. The chemical shifts are reported in ppm downfield to the central $CDCl_3$ resonance (δ = 77.16). High-resolution mass spectra were performed on a micrOTOF-Q II instrument with an ESI source. Melting points were measured with a RD-II melting point apparatus and are uncorrected.

2. General procedures

2.1 General procedure for the construction of diverse *N*-aryl isoxazolidines 4

To a reaction system of nitrosobenzene **1a** (21.6 mg, 0.2 mmol) and (*Z*)-*N*-benzylidenemethanamine oxide **2a** (27.3 mg, 0.2 mmol, 1.0 equiv) in 1.0 mL of PhMe was added styrene **3a** (23.4 uL, 0.2 mmol, 1.0 equiv). Subsequently, the resultant solution was stirred under air atmosphere at 100 ^{o}C (oil bath) for 15 h. Finally, the reaction mixture was purified by silica gel column chromatography to achieve the corresponding cycloaddition products **4aaa** (major) and **4a'a'a'** (minor) (58.6 mg, 97% isolated total yield, 6:1 dr).

2.2 Operational procedure for 5.0 mmol-scale preparation of 4aaa and 4a'a'a'

The reaction system of nitrosobenzene **1a** (0.54 g, 5.0 mmol), (*Z*)-*N*-benzylidenemethanamine oxide **2a** (0.683 g, 5.0 mmol, 1.0 equiv) and styrene **3a** (0.585 mL, 5 mmol, 1.0 equiv) in 20.0 mL of PhMe was stirred at 100 ^{o}C (oil bath)

for 18 h. At last, the reaction mixture was concentrated in vacuum and purified by silica gel column chromatography to give the desired products **4aaa** (major) and **4a'a'a'** (minor) (1.40 g, 93% isolated total yield, 6:1 dr).

2.3 Operational procedure for the synthesis of 4aaa and 4a'a'a' using *N*-alkyl nitrones as starting materials

To a reaction system of nitrosobenzene **1a** (21.6 mg, 0.2 mmol) and *N*-alkyl nitrone **2** (0.2 mmol, 1.0 equiv) in 1.0 mL of PhMe was added styrene **3a** (23.4 uL, 0.2 mmol, 1.0 equiv). Subsequently, the resultant solution was stirred under air atmosphere at 100 ^{o}C (oil bath) for 15 h. Finally, the reaction mixture was purified by silica gel column chromatography to achieve the corresponding cycloaddition products **4aaa** (major) and **4a'a'a'** (minor) (6:1 dr).

2.4 Operational procedure for the synthesis of *N*-alkyl nitrones

To a stirred solution of *N*-methylhydroxylamine hydrochloride (1.20 g, 13.6 mmol), sodium carbonate (1.45 g, 13.6 mmol) and magnesium sulfate (1.5 g, 12.1 mmol) in CH_2Cl_2 (15 mL) was added benzaldehyde (0.5 mL , 5.0 mmol) at room temperature. The reaction mixture was then stirred for 24 h at room temperature. Next, the resulting mixture was filtered and washed using EtOAc (20 mL×3). Combined organic extracts were dried with anhydrous Na_2SO_4, and the solvents were evaporated *in vacuo*. The residue was purified by flash chromatography over silica gel using petroleum ether/ethyl acetate (5:1, v/v) to afford the corresponding *N*-methylnitrone.

2.5 The procedure for the preparation of nitrone 6a

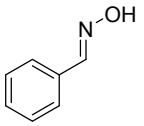
The reaction system of nitrosobenzene **1a** (21.6 mg, 0.2 mmol) and (*Z*)-*N*-benzylidenemethanamine oxide **2a** (27.3 mg, 0.2 mmol, 1.0 equiv) in 1.0 mL of PhMe was stirred under air atmosphere at 100 ^{o}C (oil bath) for 15 h. Finally, the reaction mixture was purified by silica gel column chromatography to give the corresponding nitrone **6a** (35.9 mg, 91% yield).

2.6 The procedure for the reaction of nitrone 6a with styrene 3a

To a reaction system of nitrone **6a** (39.4 mg, 0.2 mmol) in 1.0 mL of PhMe was added styrene **3a** (23.4 uL, 0.2 mmol, 1.0 equiv). Then, the resultant solution was stirred under air atmosphere at 100 ^{o}C (oil bath) for 15 h. Finally, the reaction mixture was purified by silica gel column chromatography to provide the corresponding

cycloaddition products **4aaa** (major) and **4a'a'a'** (minor) (58.6 mg, 97% isolated total yield, 6:1 dr).

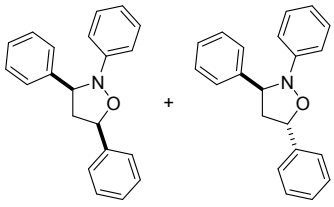
3. Characterization data for (*E*)-benzaldehyde oxime E



Yellow oil; Silica gel TLC R_f = 0.25 (PE:EA = 8:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.77 (s, 1H), 8.17−8.16 (m, 1H), 7.60−7.56 (m, 2H), 7.41−7.39 (m, 3H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 150.5, 132.0, 130.2, 128.9, 127.2 ppm.

4. Characterization data for all products 4

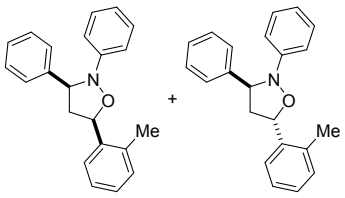
2,3,5-triphenylisoxazolidine (4aaa + 4a'a'a')[lit 1]



(*cis* + *trans*)

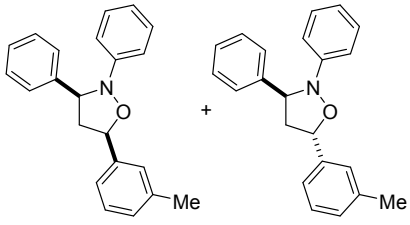
Dark yellow oil, 58.5 mg, 97% yield, dr = 6:1; Silica gel TLC R_f = 0.40 (PE:EA = 50:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.55−7.53 (m, 2H), 7.43−7.41 (m, 2H), 7.40−7.34 (m, 4H), 7.33−7.30 (m, 2H), 7.29−7.22 (m, 3H), 7.21−7.17 (m, 0.44H), 7.07−7.04 (m, 2H), 7.01−6.99 (m, 0.39H), 6.95−6.90 (m, 1H), 5.37 (q, J = 8.0 Hz, 0.18H), 5.18 (dd, J = 6.0, 4.0 Hz, 0.18H), 4.93 (t, J = 8.0 Hz, 1H), 4.70 (dd, J = 6.0, 4.0 Hz, 0.17H), 3.19 (ddd, J = 12.0, 8.0, 4.0 Hz, 1H), 2.81−2.74 (m, 0.17H), 2.68−2.62 (m, 0.17H), 2.50 (ddd, J = 22.0, 8.2, 2.0 Hz, 1H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 152.7, 150.6, 143.0, 142.3, 139.1, 137.9, 129.1, 129.0, 128.9, 128.8, 128.7, 128.5, 128.3, 127.4, 126.9, 126.4, 123.3, 122.0, 121.5, 116.0, 114.0, 80.7, 78.9, 77.5, 77.2, 76.8, 71.6, 69.8, 48.9, 47.4 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{21}H_{19}NNaO^+$, 324.1359; found, 324.1360.

2,3-diphenyl-5-(o-tolyl)isoxazolidine (4aab + 4a'a'b')


(*cis* + *trans*)

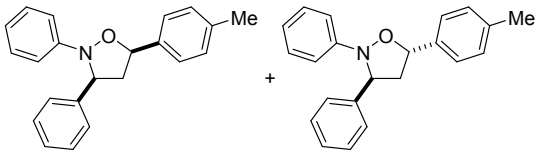
Yellow oil, 55.5 mg, 88% yield, dr = 6:1; Silica gel TLC R_f = 0.40 (PE:EA = 30:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.32−8.29 (m, 0.16H), 8.21−8.15 (m, 0.18H), 7.63−7.59 (m, 1H), 7.55−7.45 (m, 3H), 7.39−7.35 (m, 2H), 7.30−7.14 (m, 7H), 7.08−7.05 (m, 2H), 7.02−6.99 (m, 0.40H), 6.96−6.91 (m, 1H), 5.61−5.55 (m, 0.17H), 5.37−5.33 (m, 1H), 4.95−4.90 (m, 1H), 4.64−4.60 (m, 0.17H), 3.23−3.16 (m, 1H), 2.76−2.65 (m, 0.42H), 2.43−2.38 (m, 1H), 2.34 (s, 0.62H), 2.33 (s, 3H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 152.6, 150.4, 142.9, 142.3, 137.6, 136.3, 135.6, 135.4, 131.7, 130.6, 130.5, 129.7, 128.9, 128.6, 127.8, 127.5, 127.0, 126.3, 125.6, 125.5, 122.4, 122.1, 121.4, 116.3, 115.1, 114.0, 77.5, 77.2, 76.8, 75.8, 71.6, 69.7, 47.6, 46.6, 19.6, 19.5 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{22}H_{21}NNaO^+$, 338.1515; found, 338.1520.

2,3-diphenyl-5-(m-tolyl)isoxazolidine (4aac + 4a'a'c')


(*cis* + *trans*)

Yellow oil, 56.1 mg, 89% yield, dr = 6:1; Silica gel TLC R_f = 0.40 (PE:EA = 30:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.56−7.54 (m, 2.30H), 7.40−7.36 (m, 2.39H), 7.31−7.19 (m, 7H), 7.14−7.12 (m, 1H), 7.07−7.04 (m, 2H), 7.02−6.99 (m, 0.36H), 6.95−6.91 (m, 1H), 5.35−5.30 (m, 0.17H), 5.15−5.10 (m, 1H), 4.93−4.89 (m, 1H), 4.70−4.65 (m, 0.16H), 3.18−3.11 (m, 1H), 2.82−2.74 (m, 0.16H), 2.67−2.60 (m, 0.16H), 2.51−2.43 (m, 1H), 2.34 (s, 0.53H), 2.33 (s, 3H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 152.8, 143.0, 142.4, 139.0, 138.4, 138.3, 137.7, 129.3, 129.1, 129.0, 128.9, 128.7, 128.6, 127.6, 127.4, 126.9, 126.4, 124.1, 124.0, 122.0, 121.4, 116.0, 114.0, 80.8, 79.0, 77.5, 77.2, 76.8, 71.2, 69.8, 71.7, 69.8, 48.8, 47.4, 21.5 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{22}H_{21}NNaO^+$, 338.1515; found, 338.1518.

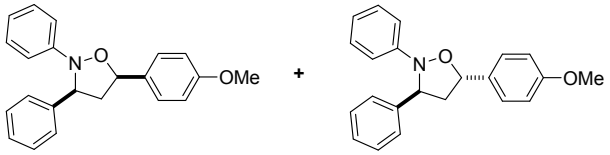
2,3-diphenyl-5-(p-tolyl)isoxazolidine (4aad + 4a'a'd')


(*cis* + *trans*)

Yellow solid, 59.3 mg, 94% yield, dr = 7:1; mp 86−88 ^{o}C; Silica gel TLC R_f = 0.40

(PE:EA = 30:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.56−7.53 (m, 2H), 7.40−7.37 (m, 2H), 7.26−7.22 (m, 2H), 7.18−7.15 (m, 2H), 7.06−6.98 (m, 2H), 6.94−6.90 (m, 1H), 5.33−5.30 (m, 0.14H), 5.14−5.10 (m, 1H), 4.92 (t, J = 8.0 Hz, 1H), 4.69−4.66 (m, 0.13H), 3.16−3.10 (m, 1H), 2.80−2.73 (m, 0.13H), 2.64−2.58 (m, 0.13H), 2.45−2.41 (m, 1H), 2.33 (s, 3H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 152.8, 150.7, 143.1, 142.4, 138.3, 138.1, 135.9, 134.7, 129.4, 128.9, 128.9, 128.6, 127.0, 126.9, 126.8, 126.4, 125.6, 121.9, 121.4, 115.9, 114.0, 80.7, 77.5, 77.2, 76.8, 71.7, 69.9, 48.8, 47.3, 22.0, 21.3 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{22}H_{21}NNaO^+$, 338.1515; found, 338.1522.

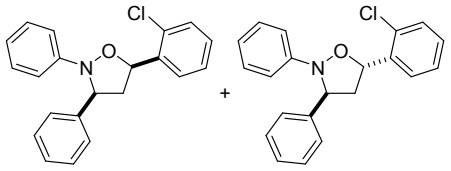
5-(4-methoxyphenyl)-2,3-diphenylisoxazolidine (4aae + 4a'a'e')



(*cis* + *trans*)

Yellow solid, 60.3 mg, 91% yield, dr = 7:1; mp 76−78 °C; Silica gel TLC R_f = 0.30 (PE:EA = 50:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.62−7.61 (m, 2H), 7.46−7.42 (m, 4H), 7.37−7.31 (m, 2H), 7.10−7.09 (m, 1H), 7.05−6.94 (m, 3H), 5.19−5.15 (m, 1H), 5.38−5.34 (m, 0.14H), 5.19−5.15 (m, 1H), 4.99−4.95 (m, 1H), 4.77−4.73 (m, 0.12H), 3.84 (s, 3H), 3.19−3.14 (m, 1H), 2.88−2.79 (m, 0.13H), 2.68−2.62 (m, 0.15H), 2.55−2.47 (m, 1H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 159.8, 159.7, 152.8, 150.7, 143.2, 142.5, 129.1, 128.6, 128.4, 127.4, 126.4, 121.4, 115.9, 114.1, 113.9, 80.5, 78.7, 77.5, 77.4, 77.2, 76.8, 71.9, 70.0, 55.4, 48.6, 47.1 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{22}H_{21}NNaO_2^+$, 354.1465; found, 354.1466.

5-(2-chlorophenyl)-2,3-diphenylisoxazolidine (4aaf + 4a'a'f')

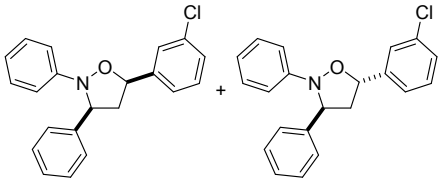


(*cis* + *trans*)

Yellow oil, 60.3 mg, 90% yield, dr = 6:1; Silica gel TLC R_f = 0.40 (PE:EA = 30:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.32−8.29 (m, 1H), 8.23−8.15 (m, 1H), 7.92−7.90 (m, 0.17H), 7.74 (d, J = 4.0 Hz, 0.44H), 7.72 (d, J = 4.0 Hz, 0.47H), 7.53−7.47 (m, 4H), 7.40−7.19 (m, 12H), 7.09−7.06 (m, 2H), 6.98−6.94 (m, 1H), 5.76 (t, J = 8.0 Hz, 0.16H), 5.58−5.51 (m, 1H), 5.35−5.31 (m, 0.16H), 4.91 (t, J = 4.0 Hz, 1H), 4.59−4.55 (m, 0.16H), 3.60−3.52 (m, 0.17H), 3.42 (ddd, J = 12.0, 8.0, 4.0 Hz, 1H), 2.96−2.90 (m, 0.16H), 2.70−2.63 (m, 0.16H), 2.34 (ddd, J = 16.0, 6.0, 4.0 Hz, 1H), 2.15−2.08 (m, 0.18H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 152.1, 151.7, 144.1, 142.5, 141.6, 140.5, 138.2, 137.2, 136.8, 132.4, 132.0, 131.7, 129.6, 129.6, 129.5, 129.4,

129.3, 129.1, 128.9, 128.8, 128.7, 128.6, 127.9, 127.8, 127.6, 127.5, 127.2, 127.1, 127.0, 126.9, 126.9, 126.5, 125.7, 122.5, 122.3, 121.9, 116.4, 114.6, 114.2, 77.5, 77.2, 76.8, 71.4, 68.9, 68.5, 47.5, 47.1, 45.8 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{21}H_{18}ClNNaO^+$, 358.0969; found, 358.0972.

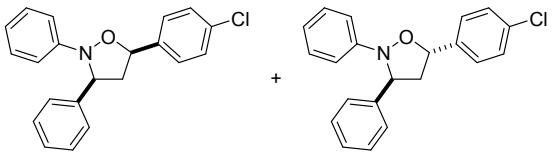
5-(3-chlorophenyl)-2,3-diphenylisoxazolidine (4aag + 4a'a'g')



(*cis* + *trans*)

Yellow oil, 62.3 mg, 93% yield, dr = 2:1; Silica gel TLC R_f = 0.40 (PE:EA = 30:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.29−8.27 (m, 1H), 8.17−8.15 (m, 1H), 7.73−7.71 (m, 0.48H), 7.51−7.40 (m, 7H), 7.57−7.28 (m, 6H), 7.26−7.14 (m, 10H), 7.12−6.97 (m, 4H), 6.94−6.91 (m, 2H), 5.74−5.71 (m, 0.07H), 5.57−5.49 (m, 0.63H), 5.34−5.27 (m, 0.22H), 5.11−5.05 (m, 1H), 4.87−4.80 (m, 1.50H), 4.66−4.62 (m, 0.17H), 4.57−4.52 (m, 0.09H), 3.64−3.49 (m, 0.36H), 3.38−3.32 (m, 0.47H), 3.14−3.06 (m, 1H), 2.93−2.87 (m, 0.07H), 2.82−2.58 (m, 0.50H), 2.41−2.24 (m, 1.53H), 2.17−2.07 (m, 0.18H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 152.3, 152.1, 144.0, 142.5, 142.4, 140.4, 137.2, 134.6, 134.5, 132.3, 132.0, 131.7, 129.9, 129.8, 129.7, 129.1, 128.9, 128.8, 128.7, 127.7, 127.4, 127.2, 126.8, 126.4, 126.3, 125.6, 124.9, 124.8, 124.4, 122.4, 121.8, 121.7, 116.3, 116.0, 115.2, 114.5, 114.1, 114.0, 79.7, 77.2, 76.8, 75.7, 75.6, 71.4, 71.3, 70.8, 69.5, 68.8, 68.4, 53.6, 48.6, 47.4, 47.3, 35.9 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{21}H_{18}ClNNaO^+$, 358.0969; found, 358.0971.

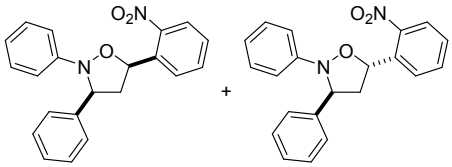
5-(4-chlorophenyl)-2,3-diphenylisoxazolidine (4aah + 4a'a'h')



(*cis* + *trans*)

Yellow oil, 63.7 mg, 95% yield, dr = 7:1; Silica gel TLC R_f = 0.40 (PE:EA = 30:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.52−7.50 (m, 2H), 7.40−7.28 (m, 8H), 7.26−7.22 (m, 2H), 7.04−7.02 (m, 2H), 6.95−6.92 (m, 1H), 5.32−5.28 (m, 0.15H), 5.15 (dd, J = 10.0, 4.0 Hz, 1H), 4.91 (t, J = 8.0 Hz, 1H), 4.68 (dd, J = 8.0, 4.0 Hz, 0.15H), 3.17−3.11 (m, 1H), 2.75−2.61(m, 0.31H), 2.43−2.36 (m, 1H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 152.4, 150.5, 142.7, 142.0, 137.7, 136.7, 134.1, 134.0, 129.1, 129.0, 128.8, 128.7, 128.3, 128.2, 127.7, 127.5, 126.8, 126.3, 122.4, 122.1, 121.7, 115.9, 114.1, 79.8, 77.5, 77.2, 76.8, 71.5, 69.7, 48.7, 47.3 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{21}H_{18}ClNNaO^+$, 358.0969; found, 358.0964.

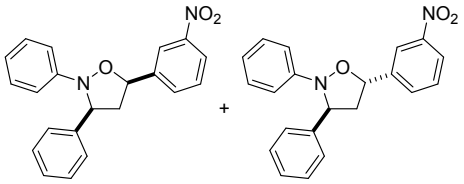
5-(2-nitrophenyl)-2,3-diphenylisoxazolidine (4aai + 4a'a'i')



(*cis* + *trans*)

Yellow oil, 25.6 mg, 37% yield, dr = 7:1; Silica gel TLC R_f = 0.20 (PE:EA = 20:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.10−8.08 (m, 1H), 8.05−8.02 (m, 1H), 7.67−7.60 (m, 1H), 7.47−7.41 (m, 3H), 7.35−7.31 (m, 2H), 7.29−7.13 (m, 4H), 7.13−6.87 (m, 4H), 6.00 (t, *J* = 8.0 Hz, 0.15H), 5.87 (t, *J* = 8.0 Hz, 1H), 4.84 (t, *J* = 8.0 Hz, 1H), 4.61 (dd, *J* = 8.0, 4.0 Hz, 0.15H), 3.63 (ddd, *J* = 16.0, 6.0, 4.0 Hz, 1H), 3.17−3.10 (m, 0.15H), 2.75−2.68 (m, 0.15H), 2.34 (dt, *J* = 12.8, 8.0 Hz, 1H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 151.2, 149.4, 147.5, 141.8, 140.9, 137.3, 137.2, 134.1, 134.0, 129.0, 128.7, 128.5, 128.4, 127.6, 127.2, 126.6, 124.9, 124.8, 122.5, 116.6, 115.3, 77.5, 77.2, 76.8, 75.9, 75.0, 70.9, 68.5, 48.7, 48.2 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{21}H_{18}N_2NaO_3^+$, 369.1210; found, 369.1216.

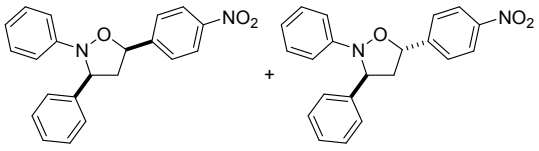
5-(3-nitrophenyl)-2,3-diphenylisoxazolidine (4aaj + 4a'a'j')



(*cis* + *trans*)

Yellow oil, 58.9 mg, 85% yield, dr = 7:1; Silica gel TLC R_f = 0.20 (PE:EA = 20:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.29−8.26 (m, 1H), 8.17−8.13 (m, 1H), 7.77−7.74 (m, 1H), 7.54−7.45 (m, 4H), 7.40−7.36 (m, 2H), 7.32−7.19 (m, 4H), 7.07−7.05 (m, 2H), 7.01−6.94 (m, 1H), 5.46 (t, *J* = 8.0 Hz, 0.16H), 5.31−5.26 (m, 1H), 4.95 (t, *J* = 8.0 Hz, 1H), 4.73 (t, *J* = 8.0 Hz, 0.15H), 2.29−2.23 (m, 1H), 2.78−2.75 (m, 0.29H), 2.49−2.41 (m, 1H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 151.5, 149.7, 148.0, 141.6, 141.2, 141.1, 140.7, 132.4, 128.7, 128.6, 128.4, 127.5, 127.3, 126.4, 125.9, 122.8, 122.1, 121.7, 121.4, 121.2, 115.7, 114.0, 78.7, 77.1, 76.7, 76.4, 70.9, 48.1, 46.9 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{21}H_{18}N_2NaO_3^+$, 369.1210; found, 369.1205.

5-(4-nitrophenyl)-2,3-diphenylisoxazolidine (4aak + 4a'a'k')

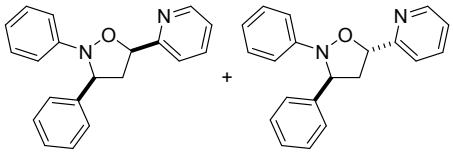


(*cis* + *trans*)

Dark yellow oil, 64.4 mg, 93% yield, dr = 5:1; Silica gel TLC R_f = 0.20 (PE:EA = 30:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.21−8.17 (m, 2H), 7.59−7.48 (m, 5H), 7.41−7.14 (m, 7H), 7.07−7.04 (m, 2H), 7.01−6.95 (m, 1H), 5.47 (t, *J* = 8.0 Hz, 0.19H),

5.32 (dd, J = 10.0, 4.0 Hz, 1H), 4.93 (t, J = 8.0 Hz, 1H), 4.71 (dd, J = 8.0, 4.0 Hz, 1H), 3.30−3.23 (m, 1H), 2.81−2.69 (m, 0.4H), 2.45−2.38 (m, 1H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 151.7, 150.1, 147.7, 147.0, 146.5, 142.0, 141.4, 129.1, 129.0, 129.0, 128.8, 127.9, 127.7, 127.4, 127.3, 126.8, 126.4, 123.9, 123.8, 122.5, 122.2, 116.1, 114.5, 79.0, 77.5, 77.2, 76.8, 71.2, 69.3, 48.6, 47.4 ppm; **HRMS** (ESI) *m/z*: [M + Na]$^+$ calcd for $C_{21}H_{18}N_2NaO_3^+$, 369.1210; found, 369.1209.

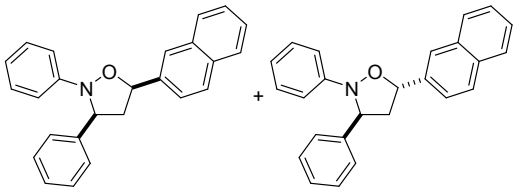
2,3-diphenyl-5-(pyridin-2-yl)isoxazolidine (4aal + 4a'a'l')



(*cis* + *trans*)

Yellow oil, 35.7 mg, 59% yield, dr = 2:1; Silica gel TLC R_f = 0.30 (PE:EA = 30:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.55−8.52 (m, 1H), 7.70−7.60 (m, 3H), 7.56−7.43 (m, 4H), 7.38−7.30 (m, 4H), 7.29−7.23 (m, 4H), 7.20−7.16 (m, 2H), 7.11−7.07 (m, 2H), 7.01−6.87 (m, 3H), 5.51 (t, J = 8.0 Hz, 0.61H), 5.39−5.35 (m, 1H), 4.86 (t, J = 8.0 Hz, 1H), 4.68−4.65 (m, 0.61H), 3.35−3.28 (m, 1H), 3.09−3.02 (m, 0.60H), 2.86−2.80 (m, 0.61H), 2.67−2.60 (m, 1H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 159.3, 159.2, 151.9, 150.5, 149.3, 149.1, 142.3, 141.6, 136.9, 136.8, 129.0, 128.9, 128.8, 128.6, 127.7, 127.4, 126.9, 126.5, 122.9, 122.0, 121.9, 121.4, 120.8, 116.1, 114.8, 80.6, 79.7, 77.5, 77.2, 76.8, 71.1, 68.9, 46.9, 45.8 ppm; **HRMS** (ESI) *m/z*: [M + Na]$^+$ calcd for $C_{20}H_{18}N_2NaO^+$, 325.1311; found, 325.1316.

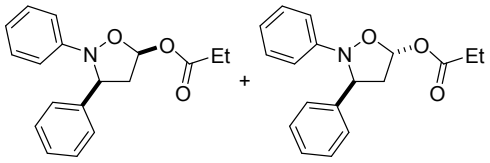
5-(naphthalen-2-yl)-2,3-diphenylisoxazolidine (4aam + 4a'a'm')



(*cis* + *trans*)

Yellow solid, 56.9 mg, 81% yield, dr = 3:1; mp 97−99 ^{o}C; Silica gel TLC R_f = 0.30 (PE:EA = 50:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.04−7.86 (m, 6H), 7.65−7.51 (m, 7H), 7.48−7.44 (m, 2H), 7.38−7.32 (m, 3H), 7.21−7.10 (m, 3H), 7.04−7.00 (m, 1H), 5.60−5.56 (m, 0.16H), 5.45−5.37 (m, 1.16H), 5.19−5.15 (m, 0.11H), 5.04 (t, J = 8.0 Hz, 1H), 4.82−4.78 (m, 0.16H), 3.37−3.24 (m, 1.14H), 2.97−2.89 (m, 0.18H), 2.81−2.58 (m, 1.30H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 152.7, 150.7, 142.9, 142.3, 136.5, 134.7, 133.3, 131.7, 129.0, 128.1, 127.7, 127.2, 126.4, 126.3, 126.0, 124.9, 122.5, 122.1, 116.0, 114.1, 80.9, 80.8, 79.1, 77.5, 77.2, 76.8, 72.0, 71.7, 69.9, 48.8, 47.4 ppm; **HRMS** (ESI) *m/z*: [M + Na]$^+$ calcd for $C_{25}H_{21}NNaO^+$, 374.1515; found, 374.1517.

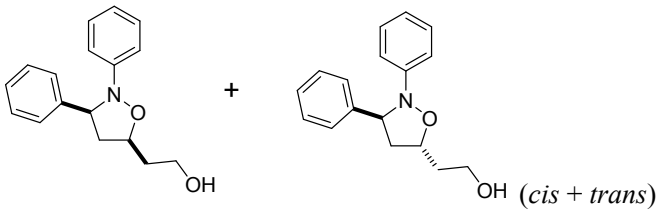
2,3-diphenylisoxazolidin-5-yl propionate (4aan + 4a'a'n')



(*cis* + *trans*)

Yellow oil, 47.0 mg, 79% yield, dr = 10:1; Silica gel TLC R_f = 0.30 (PE:EA = 40:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.54−7.51 (m, 2H), 7.42−7.30 (m, 3H), 7.22−7.17 (m, 2H), 7.01−6.95 (m, 3H), 6.61−6.59 (m, 1H), 4.81−4.77 (m, 0.09H), 4.44 (dd, *J* = 10.0, 8.0 Hz, 1H), 3.21−3.14 (m, 1H), 2.92−2.87 (m, 0.08H), 2.65−2.58 (m, 0.10H), 2.54 (ddd, *J* = 12.0, 6.4, 1.6 Hz, 1H), 2.46−2.32 (m, 2H), 2.23−2.06 (m, 0.20H), 1.16 (t, *J* = 8.0 Hz, 1H), 1.02−0.99 (m, 0.26H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 174.0, 149.8, 140.7, 129.0, 128.7, 128.0, 127.3, 123.4, 117.0, 114.2, 94.6, 77.5, 77.2, 76.8, 69.3, 46.1, 27.9 ppm; **HRMS** (ESI) *m/z*: [M + Na]$^+$ calcd for $C_{18}H_{19}NNaO_3^+$, 320.1257; found, 320.1255.

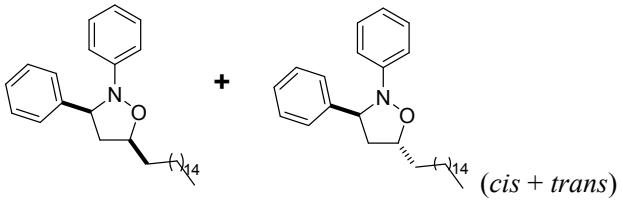
2-(2,3-diphenylisoxazolidin-5-yl)ethan-1-ol (4aao + 4a'a'o')



(*cis* + *trans*)

Yellow oil, 19.0 mg, 35% yield, dr = 7:1; Silica gel TLC R_f = 0.20 (PE:EA = 3:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.42−7.40 (m, 2H), 7.32−7.28 (m, 2H), 7.23−7.21 (m, 1H), 7.19−7.16 (m, 2H), 6.91−6.89 (m, 2H), 6.87−6.83 (m, 1H), 4.68 (t, *J* = 8.0 Hz, 1H), 4.34−4.27 (m, 1.03H), 3.80−3.76 (m, 2.13H), 2.86 (ddd, *J* = 16.0, 8.0, 8.0 Hz, 1.03H), 2.06 (ddd, *J* = 18.0, 7.0, 2.4 Hz, 1.11H), 1.97−1.84 (m, 3.20H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 151.3, 141.8, 128.2, 128.1, 127.9, 127.8, 127.7, 127.5, 126.4, 126.3, 125.6, 125.1, 120.8, 120.7, 120.4, 114.4, 113.0, 74.9, 69.8, 68.2, 59.5, 59.4, 58.5, 45.1, 43.4, 35.4, 34.6 ppm; **HRMS** (ESI) *m/z*: [M + Na]$^+$ calcd for $C_{16}H_{17}NNaO_2^+$, 278.1151; found 278.1155.

5-hexadecyl-2,3-diphenylisoxazolidine (4aap + 4a'a'p')

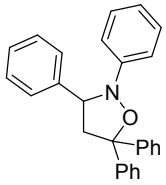


(*cis* + *trans*)

Yellow solid, 57.6 mg, 64% yield, dr = 10:1; mp 108−110 °C; Silica gel TLC R_f = 0.30 (PE:EA = 60:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.49−7.48 (m, 2H), 7.38−7.34 (m, 2H), 7.28−7.26 (m, 1H), 7.25−7.20 (m, 2H), 6.99−6.96 (m, 2H), 6.91−6.88 (m,

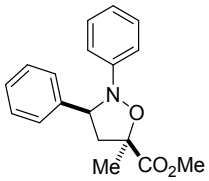
1H), 4.74 (t, *J* = 8.0 Hz, 1H), 4.56−4.53 (m, 0.10H), 4.35−4.27 (m, 0.11H), 4.17−4.05 (m, 1H), 2.89−2.83 (m, 1H), 2.44−2.31 (m, 0.19H), 2.06−1.99 (m, 1H), 1.82−1.73 (m, 1.11H), 1.66−1.57 (m, 1.11H), 1.55−1.47 (m, 1.14H), 1.35−1.26 (m, 29.94H), 0.88 (t, *J* = 8.0 Hz, 3.38H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 153.0, 143.5, 131.7, 128.9, 127.4, 125.7, 122.5, 121.5, 121.1, 115.3, 113.9, 79.2, 77.9, 71.2, 69.5, 46.7, 32.9, 32.1, 29.8, 29.7, 29.7, 29.5, 26.7, 26.6, 22.8, 14.3 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{31}H_{47}NNaO^+$, 472.3550; found 472.3547.

2,3,5,5-tetraphenylisoxazolidine (4aaq)



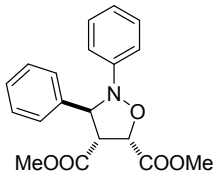
Yellow oil, 46.0 mg, 61% yield; Silica gel TLC R_f = 0.30 (PE:EA = 30:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.54−7.50 (m, 2H), 7.48−7.45 (m, 2H), 7.34−7.28 (m, 3H), 7.27−7.25 (m, 6H), 7.23−7.20 (m, 2H), 7.18−7.14 (m, 2H), 7.00−6.98 (m, 2H), 6.90−6.86 (m, 1H), 4.65 (t, *J* = 8.0 Hz, 1H), 3.56 (dd, *J* = 12.0, 8.0 Hz, 1H), 3.20 (dd, *J* = 12.0, 8.0 Hz, 1H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 150.3, 144.8, 144.1, 141.4, 129.0, 128.6, 128.3, 128.3, 127.6, 127.5, 127.3, 127.0, 126.5, 126.3, 121.5, 115.7, 87.1, 77.5, 77.2, 76.8, 69.0, 53.3 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{27}H_{23}NNaO^+$, 400.1672; found, 400.1676.

methyl 5-methyl-2,3-diphenylisoxazolidine-5-carboxylate (4aar)



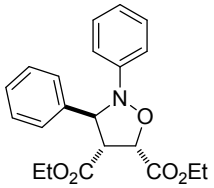
Yellow oil, 58.0 mg, 98% yield, dr = 7:1; Silica gel TLC R_f = 0.27 (PE:EA = 30:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.39−7.37 (m, 2H), 7.29−7.25 (m, 2H), 7.21−7.17 (m, 1H), 7.10−7.05 (m, 2H), 6.87−6.84 (m, 2H), 6.80−6.76 (m, 1H), 4.70 (t, *J* = 8.0 Hz, 1H), 4.39−4.35 (m, 0.15H), 3.68 (s, 0.44H), 3.49 (s, 3H), 3.28 (dd, *J* = 12.0, 8.0 Hz, 1H), 2.95 (dd, *J* = 12.0, 8.0 Hz, 0.14H), 2.60 (dd, *J* = 12.0, 8.0 Hz, 0.15H), 2.25 (dd, *J* = 12.0, 8.0 Hz, 1H), 1.56 (s, 3H), 1.54 (s, 0.46H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 174.7, 173.5, 151.3, 149.8, 141.2, 140.7, 129.0, 128.9, 128.8, 128.6, 128.5, 127.8, 127.7, 127.1, 126.7, 122.9, 121.5, 117.1, 114.7, 83.4, 82.0, 69.7, 52.7, 52.4, 49.8, 49.1, 23.1, 22.5 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{18}H_{19}NNaO_3^+$, 320.1257; found 320.1261.

dimethyl-2,3-diphenylisoxazolidine-4,5-dicarboxylate (4aas)



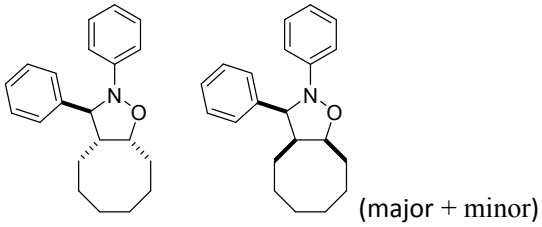
Dark yellow oil, 46.4 mg, 68% yield; Silica gel TLC R_f = 0.30 (PE:EA = 20:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.60−7.55 (m, 2H), 7.41−7.31 (m, 2H), 7.22−7.18 (m, 2H), 7.02−6.94 (m, 3H), 5.08 (d, J = 8.0 Hz, 1H), 5.00 (d, J = 8.0 Hz, 1H), 3.88 (t, J = 8.0 Hz, 1H), 3.68 (s, 3H), 3.67 (s, 3H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 169.1, 168.9, 149.9, 139.1, 129.0, 128.5, 128.3, 127.2, 122.8, 116.1, 77.4, 77.2, 76.8, 71.2，60.0，52.5，52.4 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{19}H_{19}NNaO_5^+$, 364.1155; found, 364.1157.

diethyl 2,3-diphenylisoxazolidine-4,5-dicarboxylate (4aat)



Yellow oil, 52.6 mg, 71% yield; Silica gel TLC R_f = 0.22 (PE:EA = 30:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.58−7.56 (m, 2H), 7.39−7.36 (m, 2H), 7.33−7.29 (m, 1H), 7.20−7.15 (m, 2H), 6.99−6.96 (m, 2H), 6.94−6.90 (m, 1H), 5.03 (s, 1H), 5.01 (s, 1H), 4.11−4.00 (m, 4H), 3.83 (t, J = 8.0 Hz, 1H), 1.19 (t, J = 8.0 Hz, 1H), 1.13 (t, J = 8.0 Hz, 1H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 168.4, 168.4, 150.5, 139.5, 128.4, 128.1, 127.1, 122.4, 115.5, 77.5, 71.0, 61.5, 61.4, 60.1, 13.9, 13.7 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{21}H_{23}NNaO_5^+$, 392.1468; found 392.1473.

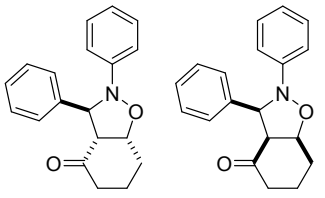
2,3-diphenyldecahydrocycloocta[*d*]isoxazole (4aau)



Yellow oil, 49.3 mg, 80% yield, dr = 3:1; Silica gel TLC R_f = 0.47 (PE:EA = 50:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.48−7.46 (m, 2.66H), 7.38−7.32 (m, 2.85H), 7.28−7.22 (m, 3.40H), 7.14−7.09 (m, 0.71H), 7.06−7.04 (m, 2H), 6.94−6.87 (m, 2H), 4.83 (d, J = 8.0 Hz, 1H), 4.50−4.45 (m, 0.34H), 4.41−4.36 (m, 1H), 3.81 (d, J = 8.0 Hz, 0.33H), 2.69−2.63 (m, 1H), 2.56−2.50 (m, 0.34H), 1.96−1.80 (m, 1.4H), 1.79−1.72 (m, 3.8H), 1.59−1.48 (m, 3.8H), 1.41−1.33 (m, 2H), 1.30−1.17 (m, 5H)

ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 152.2, 151.1, 141.5, 139.8, 128.9, 128.9, 128.5, 128.3, 128.2, 127.8, 127.5, 127.2, 122.0, 121.5, 116.4, 114.5, 82.0, 81.9, 78.1, 75.8, 57.4, 49.1, 29.9, 29.3, 28.5, 28.1, 27.7, 27.3, 25.7, 25.6, 25.5, 25.5, 25.3, 23.8 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{21}H_{25}NNaO^+$, 330.1828; found 330.1833.

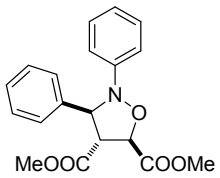
2,3-diphenylhexahydrobenzo[d]isoxazol-4(2H)-one (4aav)



(major + minor)

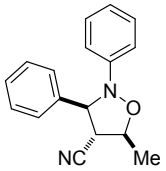
Yellow oil, 38.1 mg, 65% yield, dr = 5:1; Silica gel TLC R_f = 0.22 (PE:EA = 20:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.55−7.53 (m, 0.42H), 7.49−7.48 (m, 2H), 7.38−7.32 (m, 2.44H), 7.30−7.25 (m, 3H), 7.19−7.15 (m, 0.45H), 7.09−7.07 (m, 2H), 7.01−6.97 (m, 1H), 6.90−6.87 (m, 0.65H), 5.24 (d, *J* = 8.0 Hz, 1H), 5.20 (d, *J* = 4.0 Hz, 0.20H), 4.85−4.83 (m, 0.21H), 3.53 (t, *J* = 8.0 Hz, 1H), 3.01−2.99 (m, 0.21H), 2.53−2.50 (m, 0.21H), 2.33−2.26 (m, 0.44H), 2.11−2.03 (m, 1.3H), 2.01−1.94 (m, 1.43H), 1.86−1.76 (m, 2H), 1.52−1.44 (m, 1.23H), 1.35−1.27 (m, 1.28H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 209.7, 207.4, 150.6, 150.4, 142.4, 138.0, 129.1, 129.0, 128.6, 128.5, 127.9, 127.7, 127.6, 126.7, 122.6, 121.7, 115.0, 114.8, 77.5, 72.1, 69.6, 64.2, 60.0, 40.8, 40.4, 27.4, 25.7, 20.5, 18.5 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{19}H_{19}NNaO_2^+$, 316.1308; found 316.1314.

dimethyl-2,3-diphenylisoxazolidine-4,5-dicarboxylate (4aaw)



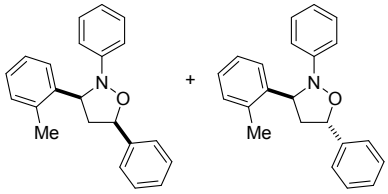
Dark yellow oil, 47.1 mg, 69% yield; Silica gel TLC R_f = 0.30 (PE:EA = 20:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.49−7.46 (m, 2H), 7.40−7.30 (m, 3H), 7.23−7.18 (m, 2H), 7.02−6.98 (m, 3H), 5.14 (d, *J* = 8.0 Hz, 1H), 4.77 (d, *J* = 8.0 Hz, 1H), 4.05 (dd, *J* = 6.0, 4.0 Hz, 1H), 3.85 (s, 3H), 3.73 (s, 3H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 171.1, 170.6, 148.9, 139.1, 129.1, 128.8, 128.3, 127.3, 123.8, 117.4, 77.7，77.5, 77.2, 76.8, 73.0，60.5，53.0，52.9 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{19}H_{19}NNaO_5^+$, 364.1155; found, 364.1155.

5-methyl-2,3-diphenylisoxazolidine-4-carbonitrile (4aax)



Yellow oil, 13.8 mg, 26% yield; Silica gel TLC R_f = 0.30 (PE:EA = 10:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.58−7.56 (m, 2H), 7.45−7.41 (m, 2H), 7.39−7.35 (m, 1H), 7.30−7.25 (m, 2H), 7.01−6.99 (m, 1H), 6.96−6.94 (m, 2H), 4.98 (d, J = 8.0 Hz, 1H), 4.51−4.44 (m, 1H), 3.14 (dd, J = 8.0, 8.0 Hz, 1H), 1.56 (d, J = 8.0 Hz, 3H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 151.1, 139.4, 129.5, 129.4, 128.8, 126.2, 122.6, 117.3, 114.1, 78.1, 74.7, 50.3, 16.7 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{17}H_{16}N_2NaO^+$, 287.1155; found 287.1159.

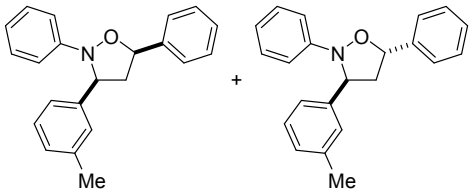
2,5-diphenyl-3-(o-tolyl)isoxazolidine (4aba + 4a'b'a')



(*cis* + *trans*)

Yellow oil, 55.5 mg, 88% yield, dr = 5:1; Silica gel TLC R_f = 0.40 (PE:EA = 30:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.88−7.82 (m, 1H), 7.43−7.42 (m, 2H), 7.36−7.30 (m, 4H), 7.28−7.18 (m, 6H), 7.03−7.00 (m, 2H), 6.96−6.91 (m, 2H), 5.37−5.35 (m, 0.21H), 5.21−5.16 (m, 1H), 5.11−5.06 (m, 1H), 4.86−4.83 (m, 0.21H), 3.25−3.18 (m, 1H), 2.86−2.77 (m, 0.20H), 2.52−2.47 (m, 0.20H), 2.41−2.40 (m, 3H), 2.37−2.36 (m, 0.63H), 2.33−2.25 (m, 1H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 152.7, 150.7, 141.0, 140.6, 138.9, 137.9, 134.3, 133.9, 130.7, 130.6, 129.2, 128.7, 128.5, 127.2, 127.1, 126.9, 126.8, 126.6, 126.3, 121.8, 121.3, 115.6, 113.8, 80.7, 77.5, 77.2, 76.8, 69.3, 66.9, 47.5, 45.9, 19.71, 19.6 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{22}H_{21}NNaO^+$, 338.1515; found, 338.1517.

2,5-diphenyl-3-(m-tolyl)isoxazolidine (4aca + 4a'c'a')

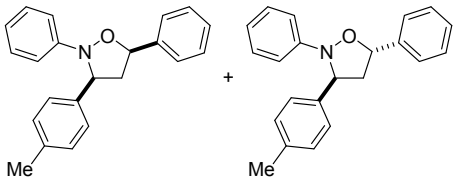


(*cis* + *trans*)

Yellow oil, 56.1 mg, 89% yield, dr = 7:1; Silica gel TLC R_f = 0.40 (PE:EA = 30:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.44−7.42 (m, 2H), 7.39−7.36 (m, 6H), 7.29−7.23 (m, 3H), 7.21−7.13 (m, 1H), 7.11−7.05 (m, 3H), 7.00−6.91 (m, 1H), 5.35−5.33 (m, 0.16H), 5.17−5.12 (m, 1H), 4.91−4.85 (m, 1H), 4.67−4.63 (m, 0.15H), 3.18−3.11 (m, 1H), 2.80−2.72 (m, 0.17H), 2.67−2.61 (m, 0.17H), 2.50−2.42 (m, 1H), 2.37 (s, 0.42H),

2.36 (s, 3H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 152.8, 150.7, 142.9, 142.4, 139.1, 138.7, 138.6, 137.9, 129.1, 128.8, 128.7, 128.5, 128.4, 128.2, 127.4, 127.0, 126.9, 126.4, 123.9, 123.4, 122.4, 121.9, 121.4, 115.9, 114.0, 80.7, 77.2, 76.8, 71.4, 69.8, 48.9, 47.4, 21.6 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{22}H_{21}NNaO^+$, 338.1515; found, 338.1516.

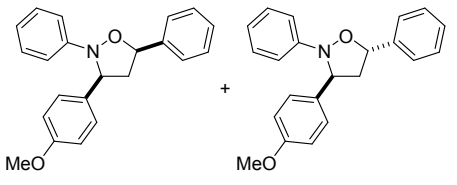
2,5-diphenyl-3-(p-tolyl)isoxazolidine (4ada + 4a'd'a')



(*cis* + *trans*)

Yellow oil, 58.0 mg, 92% yield, dr = 5:1; Silica gel TLC R_f = 0.40 (PE:EA = 30:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.44−7.42 (m, 5H), 7.34−7.30 (m, 3H), 7.26−7.16 (m, 5H), 7.07−7.00 (m, 2H), 6.94−6.90 (m, 1H), 5.37−5.33 (m, 0.19H), 5.16−5.12 (m, 1H), 4.88−4.85 (m, 1H), 4.66−4.62 (m, 0.19H), 3.16−3.10 (m, 1H), 2.80−2.71 (m, 0.18H), 2.66−2.60 (m, 0.19H), 2.49−2.40 (m, 1H), 2.36−2.32 (m, 1H), 2.35 (s, 0.63H), 2.34 (s, 3H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 152.8, 150.7, 140.0, 139.2, 138.0, 137.3, 137.1, 129.6, 129.6, 128.8, 128.7, 128.6, 128.6, 128.4, 128.2, 127.0, 126.8, 126.3, 121.9, 121.4, 116.0, 114.1, 80.6, 77.5, 77.2, 76.8, 71.5, 69.5, 49.0, 47.5, 21.1 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{22}H_{21}NNaO^+$, 338.1515; found, 338.1511.

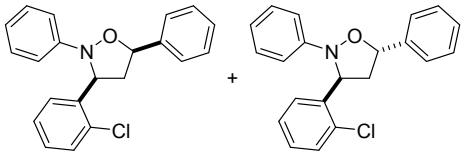
3-(4-methoxyphenyl)-2,5-diphenylisoxazolidine (4aea + 4a'e'a')



(*cis* + *trans*)

Yellow oil, 57.6 mg, 87% yield, dr = 3:1; Silica gel TLC R_f = 0.30 (PE:EA = 50:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.48−7.43 (m, 5H), 7.39−7.30 (m, 4H), 7.28−7.18 (m, 3H), 7.07−7.05 (m, 2H), 6.96−6.91 (m, 4H), 5.39 (dd, *J* = 6.0, 4.0 Hz, 0.31H), 5.19 (dd, *J* = 10.0, 4.0 Hz, 1H), 4.89 (t, *J* = 8.0 Hz, 1H), 4.64 (dd, *J* = 8.0, 4.0 Hz, 0.26H), 3.83 (s, 0.65H), 3.82 (s, 3H), 3.18−3.12 (m, 1H), 2.80−2.72 (m, 0.28H), 2.68−2.62 (m, 0.28H), 2.50−2.42 (m, 1H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 159.0, 152.7, 138.1, 135.0, 129.1, 128.7, 128.6, 128.5, 128.3, 128.1, 127.6, 127.0, 126.9, 122.1, 121.5, 116.2, 114.4, 114.3, 114.2, 80.7, 78.9, 77.5, 77.2, 76.8, 71.3, 69.5, 55.5, 49.0, 47.6 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{22}H_{21}NNaO_2^+$, 354.1465; found, 354.1466.

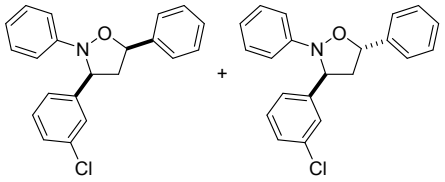
3-(2-chlorophenyl)-2,5-diphenylisoxazolidine (4afa + 4a'f'a')



(*cis* + *trans*)

Yellow oil, 61.0 mg, 91% yield, dr = 9:1; Silica gel TLC R_f = 0.40 (PE:EA = 50:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.97−7.95 (m, 1H), 7.39−7.31 (m, 3H), 7.35−7.33 (m, 2H), 7.31−7.29 (m, 3H), 7.28−7.19 (m, 3H), 7.06−7.03 (m, 2H), 6.98−6.93 (m, 1H), 5.35 (t, *J* = 8.0 Hz, 1H), 5.27−5.24 (m, 0.11H), 5.20 (dd, *J* = 10.0, 8.0 Hz, 1H), 5.14−5.12 (m, 0.11H), 3.40 (ddd, *J* = 16.0, 6.0, 4.0 Hz, 1H), 2.92−2.84 (m, 0.11H), 2.58−2.52 (m, 0.11H), 2.30 (ddd, *J* = 16.0, 6.0, 4.0 Hz, 1H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 152.1, 150.5, 140.7, 139.8, 138.4, 137.7, 132.1, 131.9, 129.5, 129.2, 128.8, 128.7, 128.6, 128.5, 128.4, 128.0, 127.5, 127.0, 121.8, 121.6, 115.5, 113.8, 80.7, 78.9, 77.5, 77.2, 76.8, 68.7, 66.9, 47.1, 45.2 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{21}H_{18}ClNNaO^+$, 358.0969; found, 358.0969.

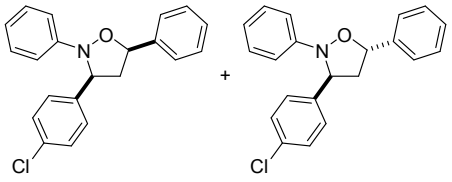
3-(3-chlorophenyl)-2,5-diphenylisoxazolidine (4aga + 4a'g'a')



(*cis* + *trans*)

Yellow solid, 63.0 mg, 94% yield, dr = 7:1; mp 76−78 °C; Silica gel TLC R_f = 0.40 (PE:EA = 50:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.59−7.56 (m, 1H), 7.50−7.40 (m, 4H), 7.38−7.25 (m, 8H), 7.24−7.21 (m, 1H), 7.07−7.02 (m, 2H), 7.00−6.93 (m, 1H), 5.38−5.31 (m, 0.18H), 5.19−5.14 (m, 1H), 4.94−4.88 (m, 1H), 4.68−4.65 (m, 0.15H), 3.21−3.14 (m, 1H), 2,82−2.74 (m, 0.16H), 2.64−2.59 (m, 0.15H), 2.46−2.39 (m, 1H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 152.3, 145.2, 144.6, 137.6, 134.8, 130.3, 130.2, 128.9, 128.6, 127.5, 126.5, 124.5, 122.5, 122.2, 121.7, 121.5, 115.9, 114.0, 113.9, 80.7, 77.5, 77.2, 76.8, 71.7, 71.0, 69.2, 48.9, 48.6, 47.1 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{21}H_{18}ClNNaO^+$, 358.0969; found, 358.0975.

3-(4-chlorophenyl)-2,5-diphenylisoxazolidine (4aha + 4a'h'a')

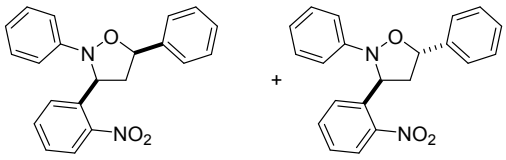


(*cis* + *trans*)

Yellow oil, 63.6 mg, 95% yield, dr = 7:1; Silica gel TLC R_f = 0.40 (PE:EA = 50:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.49−7.46 (m, 2H), 7.43−7.31 (m, 8H), 7.29−7.18 (m, 3H), 7.05−7.02 (m, 2H), 6.97−6.93 (m, 1H), 5.34−5.30 (m, 0.15H), 5.18−5.14 (m,

1H), 4.91 (t, J = 8.0 Hz, 1H), 4.67−4.63 (m, 0.14H), 3.19−3.13 (m, 1H), 2.81−2.74 (m, 0.14H), 2.63−2.57 (m, 0.15H), 2.44−2.36 (m, 1H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 152.3, 141.6, 138.9, 137.7, 133.1, 129.2, 129.1, 128.7, 128.6, 127.8, 126.9, 126.8, 122.3, 121.7, 116.0, 114.0, 80.7, 78.9, 77.5, 77.2, 76.8, 70.9, 69.2, 48.6, 47.2 ppm; **HRMS** (ESI) *m/z*: [M + Na]$^+$ calcd for $C_{21}H_{18}ClNNaO^+$, 358.0969; found, 358.0973.

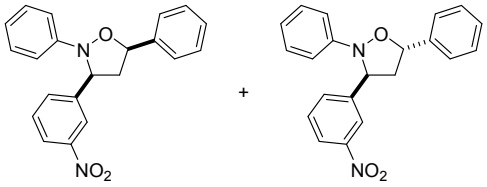
3-(2-nitrophenyl)-2,5-diphenylisoxazolidine (4aia + 4a'i'a')



(*cis* + *trans*)

Yellow oil, 66.5 mg, 96% yield, dr = 9:1; Silica gel TLC R_f = 0.20 (PE:EA = 30:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.29−8.26 (m, 1H), 8.08−8.04 (m, 1H), 7.71−7.66 (m, 1H), 7.47−7.42 (m, 1H), 7.36−7.19 (m, 8H), 7.04−7.02 (m, 2H), 6.98−6.92 (m, 1H), 5.46−5.43 (m, 0.11H), 5.23−5.19 (m, 1H), 3.52−3.45 (m, 1H), 3.08−3.00 (m, 0.11H), 2.59−2.53 (m, 0.10H), 2.30−2.22 (m, 1H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 151.5, 150.2, 147.3, 139.3, 138.0, 137.9, 137.5, 134.4, 134.2, 129.4, 128.9, 128.7, 128.6, 128.3, 127.0, 125.3, 125.0, 122.1, 121.8, 115.4, 113.7, 80.6, 79.1, 77.5, 77.2, 76.8, 68.2, 66.4, 47.8, 45.9 ppm; **HRMS** (ESI) *m/z*: [M + Na]$^+$ calcd for $C_{21}H_{18}N_2NaO_3^+$, 369.1210; found, 369.1204.

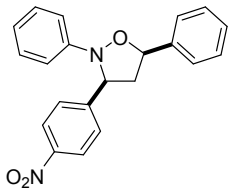
3-(3-nitrophenyl)-2,5-diphenylisoxazolidine (4aja + 4a'j'a')



(*cis* + *trans*)

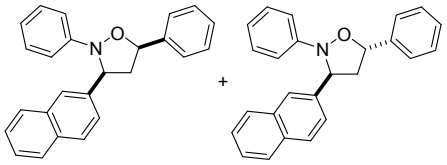
Yellow oil, 66.5 mg, 96% yield, dr = 9:1; Silica gel TLC R_f = 0.20 (PE:EA = 20:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.43−8.39 (m, 1H), 8.18−8.13 (m, 1H), 7.93−7.90 (m, 1H), 7.59−7.53 (m, 1H), 7.44−7.32 (m, 5H), 7.32−7.20 (m, 3H), 7.06−7.03 (m, 2H), 7.00−6.94 (m, 1H), 5.35−5.32 (m, 0.12H), 5.23 (dd, J = 10.0, 4.0 Hz, 1H), 5.07 (t, J = 8.0 Hz, 1H), 5.84−4.80 (m, 0.11H), 3.30−3.23 (m, 1H), 2.90−2.82 (m, 0.11H), 2.67−2.62 (m, 0.12H), 2.46−2.39 (m, 1H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 151.8, 150.0, 148.7, 145.4, 144.5, 138.4, 137.3, 133.1, 132.6, 130.0, 129.3, 128.8, 128.7, 126.8, 122.8, 122.5, 122.0, 121.9, 121.5, 116.0, 113.9, 80.8, 79.0, 77.5, 77.2, 76.8, 70.5, 68.9, 48.2, 46.7 ppm; **HRMS** (ESI) *m/z*: [M + Na]$^+$ calcd for $C_{21}H_{18}N_2NaO_3^+$, 369.1210; found, 369.1205.

3-(4-nitrophenyl)-2,5-diphenylisoxazolidine (4aka)



Yellow solid, 67.9 mg, 98% yield, dr > 99:1; mp 106−108 °C; Silica gel TLC R_f = 0.20 (PE:EA = 20:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.28−8.25 (m, 2H), 7.76−7.74 (m, 2H), 7.42−7.30 (m, 7H), 7.08−6.98 (m, 3H), 5.26−5.22 (m, 1H), 5.10 (t, J = 8.0 Hz, 1H), 5.32−5.26 (m, 1H), 2.48−2.41 (m, 1H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 151.8, 150.6, 147.3, 137.3, 129.3, 128.8, 128.7, 127.3, 126.9, 124.3, 122.0, 113.9, 80.7, 77.5, 77.2, 76.8, 70.6, 48.1 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{21}H_{18}N_2NaO_3^+$, 369.1210; found, 369.1214.

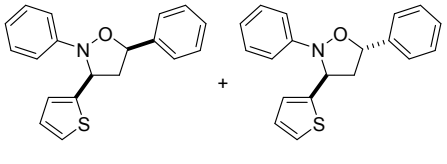
3-(naphthalen-2-yl)-2,5-diphenylisoxazolidine (4ala + 4a'l'a')



(*cis* + *trans*)

Yellow solid, 60.4 mg, 86% yield, dr = 3:1; mp 134−136 °C; Silica gel TLC R_f = 0.30 (PE:EA = 30:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.32−8.30 (m, 0.13H), 8.18−8.03 (m, 3H), 7.94−7.92 (m, 1H), 7.85−7.81 (m, 1H), 7.56−7.45 (m, 5H), 7.46−7.36 (m, 3H), 7.35−7.24 (m, 6H), 7.22−7.18 (m, 1H), 7.11−7.07 (m, 2H), 7.01−7.93 (m, 2H), 5.63 (t, J = 8.0 Hz, 1H), 5.45 (dd, J = 12.0, 4.0 Hz, 0.39H), 5.36−5.28 (m, 1.53H), 3.46−3.40 (m, 1H), 3.03−2.95 (m, 0.39H), 2.67−2.64 (m, 0.39H), 2.51−2.44 (m, 1H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 152.7, 138.5, 138.2, 137.8, 134.2, 130.2, 129.3, 129.2, 128.6, 128.0, 127.2, 126.9, 126.3, 126.0, 125.8, 125.7, 124.3, 123.7, 123.2, 123.1, 121.7, 121.4, 115.5, 113.9, 80.8, 79.0, 77.5, 77.4, 77.2, 76.8, 69.6, 67.0, 48.0, 46.2 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{25}H_{21}NNaO^+$, 374.1515; found, 374.1515.

2,5-diphenyl-3-(thiophen-2-yl)isoxazolidine (4ama + 4a'm'a')

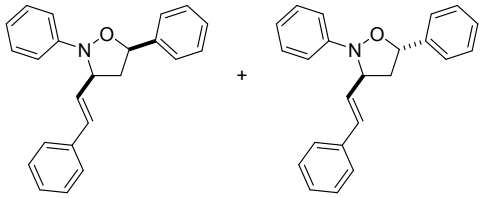


(*cis* + *trans*)

Yellow oil, 26.4 mg, 43% yield, dr = 3:1; Silica gel TLC R_f = 0.30 (PE:EA = 30:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.33−8.30 (m, 0.4H), 8.20−8.15 (m, 0.4H), 7.57−7.48 (m, 1H), 7.47−7.41 (m, 3H), 7.40−7.32 (m, 4H), 7.32−7.23 (m, 4H), 7.15−7.12 (m, 2H), 7.10−7.05 (m, 2H), 7.03−6.96 (m, 2H), 5.42−5.38 (m, 0.28H), 5.22−5.16 (m, 2.11H), 4.99−4.95 (m, 0.31H), 3.21−3.15 (m, 1H), 2.79−2.72 (m, 0.51H), 2.63−2.56

(m, 1H), 2.51−2.44 (m, 0.15H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 151.7, 147.3, 138.0, 131.7, 129.1, 128.7, 128.4, 126.9, 124.9, 123.9, 122.5, 122.1, 116.3, 114.5, 114.1, 80.8, 78.9, 77.5, 77.2, 76.8, 67.9, 66.5, 48.1, 47.2 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{19}H_{17}NNaOS^+$, 330.0923; found, 330.0925.

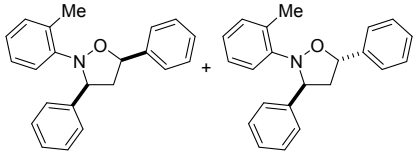
2,5-diphenyl-3-((E)-styryl)isoxazolidine (4ana + 4a'n'a')



(*cis* + *trans*)

Yellow oil, 53.0 mg, 81% yield, dr = 8:1; Silica gel TLC R_f = 0.30 (PE:EA = 30:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.49−7.45 (m, 2H), 7.43−7.39 (m, 3H), 7.37−7.35 (m, 2H), 7.34−7.31 (m, 3H), 7.30−7.28 (m, 2H), 7.26−7.23 (m, 2H), 7.19−7.14 (m, 2H), 7.00−6.94 (m, 1H), 6.77 (s, 0.39H), 6.73 (s, 0.53H), 6.49−6.43 (m, 1H), 5.33 (t, *J* = 8.0 Hz, 0.13H), 5.12 (dd, *J* = 10.0, 4.0 Hz, 1H), 4.54−4.48 (m, 1H), 4.36−4.28 (m, 0.14H), 2.97−2.90 (m, 1H), 2.62−2.58 (m, 0.26H), 2.38−2.31 (m, 1H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 152.5, 150.6, 139.4, 138.2, 136.7, 136.6, 131.8, 131.7, 130.5, 128.7, 128.2, 127.8, 126.6, 125.6, 122.4, 121.7, 116.4, 114.4, 80.0, 78.9, 77.5, 77.2, 76.8, 70.2, 68.7, 45.9, 44.7 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{23}H_{21}NNaO^+$, 350.1515; found, 350.1512.

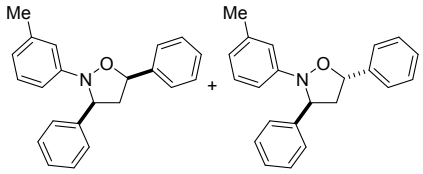
3,5-diphenyl-2-(o-tolyl)isoxazolidine (4baa + 4b'a'a')



(*cis* + *trans*)

Yellow oil, 50.4 mg, 80% yield, dr = 2:1; Silica gel TLC R_f = 0.40 (PE:EA = 30:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.51−7.47 (m, 4H), 7.44−7.38 (m, 4H), 7.37−7.22 (m, 9H), 7.19−7.15 (m, 1H), 7.12−7.08 (m, 2H), 7.02−6.98 (m, 1H), 5.50 (t, *J* = 8.0 Hz, 1H), 5.35 (t, *J* = 8.0 Hz, 0.46H), 4.82 (t, *J* = 8.0 Hz, 1H), 4.70−4.67 (m, 0.42H), 3.30−3.23 (m, 1H), 2.84−2.71 (m, 0.88H), 2.56−2.49 (m, 1H), 2.16 (s, 1.2H), 2.14 (s, 3H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 149.0, 141.7, 140.7, 131.4, 131.1, 128.7, 128.6, 128.0, 127.4, 127.3, 126.9, 126.4, 126.2, 124.5, 117.7, 80.4, 79.2, 77.5, 77.2, 76.8, 70.0, 69.5, 48.1, 45.6, 19.6, 18.8 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{22}H_{21}NNaO^+$, 338.1515; found, 338.1518.

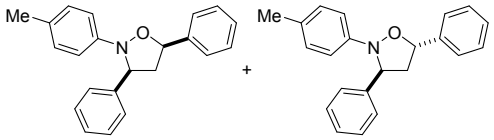
3,5-diphenyl-2-(m-tolyl)isoxazolidine (4caa + 4c'a'a')



(*cis* + *trans*)

Yellow oil, 55.5 mg, 88% yield, dr = 5:1; Silica gel TLC R_f = 0.40 (PE:EA = 30:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.17−8.03 (m, 0.27H), 7.62−7.60 (m, 2H), 7.51−7.33 (m, 10H), 7.22−7.18 (m, 1H), 7.15−7.11 (m, 0.23H), 6.97−6.96 (m, 1H), 6.92−6.90 (m, 1H), 6.83−6.81 (m, 1H), 5.42−5.38 (m, 0.20H), 5.25−5.21 (m, 1H), 5.00−4.97 (m, 1H), 4.77−4.74 (m, 0.19H), 3.27−3.20 (m, 1H), 2.88−2.80 (m, 0.19H), 2.55−2.48 (m, 1H), 2.37−2.32 (m, 3.65H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 152.7, 150.6, 143.2, 142.4, 139.1, 139.0, 138.5, 138.0, 128.6, 128.6, 128.5, 128.3, 127.4, 126.9, 126.4, 122.9, 122.6, 122.3, 116.8, 114.6, 113.0, 111.1, 80.7, 78.9, 77.5, 77.2, 76.8, 71.5, 69.8, 48.9, 47.3, 21.8, 21.7 ppm; **HRMS** (ESI) *m/z*: [M + Na]$^+$ calcd for $C_{22}H_{21}NNaO^+$, 338.1515; found, 338.1517.

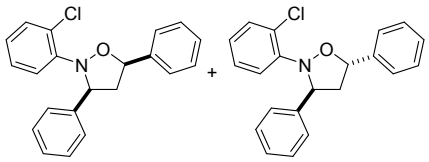
3,5-diphenyl-2-(p-tolyl)isoxazolidine (4daa + 4d'a'a')



(*cis* + *trans*)

Yellow oil, 58.6 mg, 93% yield, dr = 2:1; Silica gel TLC R_f = 0.40 (PE:EA = 30:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.56−7.51 (m, 4H), 7.49−7.42 (m, 4H), 7.39−7.27 (m, 8H), 7.24−7.20 (m, 1H), 7.16−7.13 (m, 2H), 7.07−7.03 (m, 1H), 5.54 (t, *J* = 8.0 Hz, 1H), 5.40 (t, *J* = 8.0 Hz, 0.47H), 4.86 (t, *J* = 8.0 Hz, 1H), 4.75−4.71 (m, 0.44H), 3.33−3.26 (m, 1H), 2.89−2.75 (m, 0.94H), 2.60−2.53 (m, 1H), 2.21 (s, 1.33H), 2.19 (s, 3H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 148.9, 147.9, 141.7, 140.7, 140.3, 139.8, 133.0, 131.4, 131.1, 130.8, 128.7, 128.6, 128.5, 128.1, 127.9, 127.4, 127.3, 126.8, 126.3, 126.2, 125.2, 124.5, 119.7, 117.7, 80.4, 79.2, 77.5, 77.2, 76.8, 69.9, 69.5, 48.1, 45.6, 19.6, 18.8 ppm; **HRMS** (ESI) *m/z*: [M + Na]$^+$ calcd for $C_{22}H_{21}NNaO^+$, 338.1515; found, 338.1520.

2-(2-chlorophenyl)-3,5-diphenylisoxazolidine (4eaa + 4e'a'a')

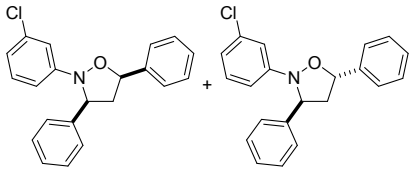


(*cis* + *trans*)

Yellow oil, 51.6 mg, 77% yield, dr = 3:1; Silica gel TLC R_f = 0.40 (PE:EA = 30:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.01−7.99 (m, 0.09H), 7.75−7.72 (m, 0.1H), 7.59−7.57 (m, 0.67H), 7.52−7.46 (m, 4H), 7.43−7.25 (m, 11H), 7.23−7.17 (m, 2H),

7.13−7.09 (m, 0.35H), 6.97−6.93 (m, 1H), 5.51 (t, *J* = 8.0 Hz, 1H), 5.27−5.20 (m, 1.33H), 5.09−5.07 (m, 0.28H), 3.27−3.19 (m, 1H), 2.81−2.67 (m, 0.60H), 2.51−2.45 (m, 1H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 148.0, 147.8, 142.7, 140.5, 139.1, 131.2, 130.8, 130.4, 130.3, 128.7, 128.6, 128.5, 128.4, 128.2, 127.4, 127.3, 127.1, 127.0, 126.9, 126.9, 126.7, 124.9, 124.2, 123.5, 120.6, 118.1, 81.0, 79.8, 77.5, 77.2, 76.8, 69.8, 69.6, 47.0, 42.7 ppm; **HRMS** (ESI) *m/z*: [M + Na]$^+$ calcd for $C_{21}H_{18}ClNNaO^+$, 358.0969; found, 358.0974.

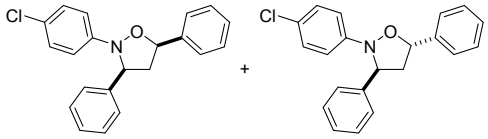
2-(3-chlorophenyl)-3,5-diphenylisoxazolidine (4faa + 4f'a'a')



(*cis* + *trans*)

Yellow oil, 55.6 mg, 83% yield, dr = 5:1; Silica gel TLC R_f = 0.40 (PE:EA = 30:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.35−8.34 (m, 0.18H), 8.31−8.29 (m, 0.17H), 8.24−8.23 (m, 0.10H), 8.22−8.21 (m, 0.09H), 8.04−8.03 (m, 0.10H), 8.02−8.01 (m, 0.09H), 7.56−7.55 (m, 2H), 7.48−7.32 (m, 10H), 7.20−7.15 (m, 1H), 7.13−7.12 (m, 1H), 7.10−7.08 (m, 0.39H), 6.94−6.87 (m, 2H), 6.80−6.77 (m, 0.22H), 5.40−5.36 (m, 0.23H), 5.19 (dd, *J* = 10.0, 8.0 Hz, 1H), 4.93 (t, *J* = 8.0 Hz, 1H), 4.74−4.71 (m, 0.21H), 3.25−3.19 (m, 1H), 2.87−2.80 (m, 0.22H), 2.71−2.65 (m, 0.22H), 2.54−2.46 (m, 1H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 153.9, 151.7, 142.5, 141.9, 138.6, 137.4, 135.0, 134.5, 132.2, 130.2, 130.1, 130.0, 129.9, 129.1, 128.7, 127.7, 126.9, 126.3, 125.5, 124.2, 123.0, 121.7, 121.3, 120.8, 115.8, 114.0, 113.7, 112.1, 81.0, 77.5, 77.2, 76.8, 71.5, 69.6, 48.9, 47.2 ppm; **HRMS** (ESI) *m/z*: [M + Na]$^+$ calcd for $C_{21}H_{18}ClNNaO^+$, 358.0969; found, 358.0968.

2-(4-chlorophenyl)-3,5-diphenylisoxazolidine (4gaa + 4g'a'a')

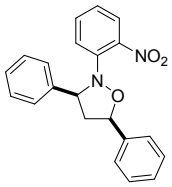


(*cis* + *trans*)

Yellow oil, 61.0 mg, 91% yield, dr = 5:1; Silica gel TLC R_f = 0.40 (PE:EA = 30:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.53−7.51 (m, 3H), 7.44−7.28 (m, 10H), 7.24−7.22 (m, 2H), 7.01−6.99 (m, 2H), 5.41−5.38 (m, 0.21H), 5.19 (dd, *J* = 6.0, 4.0 Hz, 1H), 4.89 (t, *J* = 8.0 Hz, 1H), 4.67 (dd, *J* = 8.0, 4.0 Hz, 0.18H), 3.25−3.18 (m, 1H), 2.87−2.80 (m, 0.2H), 2.74−2.68 (m, 0.2H), 2.55−2.47 (m, 1H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 151.2, 149.1, 142.4, 141.8, 138.9, 137.6, 129.1, 129.0, 128.8, 128.6, 127.7, 126.9, 126.8, 126.4, 126.3, 117.3, 115.4, 80.8, 77.5, 77.2, 76.8, 71.8, 69.9, 49.0, 47.4 ppm; **HRMS** (ESI) *m/z*: [M + Na]$^+$ calcd for $C_{21}H_{18}ClNNaO^+$, 358.0969; found,

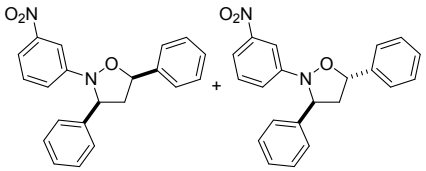
358.0965.

2-(2-nitrophenyl)-3,5-diphenylisoxazolidine (4haa)



Yellow oil, 40.8 mg, 59% yield, dr > 99:1; Silica gel TLC R_f = 0.20 (PE:EA = 30:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.67−7.65 (m, 1H), 7.45−7.31 (m, 12H), 7.03−6.99 (m, 1H), 5.31 (q, J = 8.0 Hz, 1H), 5.02 (t, J = 4.0 Hz, 1H), 3.28 (ddd, J = 12.0, 8.0, 4.0 Hz, 1H), 2.56 (ddd, J = 16.0, 6.0, 4.0 Hz, 1H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 143.7, 140.8, 139.6, 137.7, 132.8, 128.8, 128.7, 127.8, 126.9, 126.6, 125.4, 122.1, 117.9, 80.9, 77.5, 77.2, 76.8, 70.1, 47.9 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{21}H_{18}N_2NaO_3^+$, 369.1210; found, 369.1216.

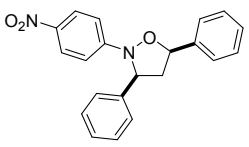
2-(3-nitrophenyl)-3,5-diphenylisoxazolidine (4iaa + 4i'a'a')



(*cis* + *trans*)

Yellow oil, 49.2 mg, 71% yield, dr = 4:1; Silica gel TLC R_f = 0.20 (PE:EA = 30:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.93 (t, J = 2.0 Hz, 1H), 7.88 (t, J = 4.0 Hz, 0.14H), 7.79−7.78 (m, 0.48H), 7.76−7.75 (m, 0.63H), 7.74−7.73 (m, 0.14H), 7.57−7.50 (m, 3H), 7.48−7.27 (m, 13H), 7.19−7.18 (m, 0.14H), 7.17−7.16 (m, 0.14H), 5.45−5.42 (m, 0.25H), 5.20 (dd, J = 12.0, 4.0 Hz, 1H), 4.96 (t, J = 8.0 Hz, 1H), 4.80 (dd, J = 8.0, 4.0 Hz, 0.25H), 3.29−3.22 (m, 1H), 2.93−2.85 (m, 0.26H), 2.73−2.71 (m, 0.28H), 2.60−2.52 (m, 1H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 153.4, 151.2, 149.1, 141.8, 141.4, 138.3, 137.1, 129.9, 129.3, 129.2, 128.8, 128.6, 128.2, 128.0, 127.0, 126.8, 126.7, 126.3, 121.0, 119.7, 116.1, 116.0, 110.1, 108.5, 81.3, 79.4, 77.5, 77.2, 76.8, 71.5, 69.5, 49.0, 47.2 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{21}H_{18}N_2NaO_3^+$, 369.1210; found, 369.1214.

2-(4-nitrophenyl)-3,5-diphenylisoxazolidine (4jaa)

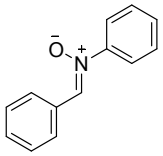


Yellow oil, 6.2 mg, 9% yield, dr > 99:1; Silica gel TLC R_f = 0.20 (PE:EA = 30:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.14−8.10 (m, 2H), 7.53−7.51 (m, 2H), 7.48−7.38 (m,

7H), 7.37−7.33 (m, 1H), 7.01−6.97 (m, 2H), 5.16 (dd, *J* = 12.0, 4.0 Hz, 1H), 5.04 (t, *J* = 8.0 Hz, 1H), 3.31−3.25 (m, 1H), 2.59−2.51 (m, 1H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 156.3, 141.4, 141.0, 136.4, 129.3, 129.1, 128.9, 128.1, 127.0, 126.0, 125.7, 112.3, 81.8, 77.5, 77.2, 76.8, 70.1, 48.8 ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{21}H_{18}N_2NaO_3^+$, 369.1210; found, 369.1211.

5. Characterization data for nitrone intermediate 6a

(*Z*)-*N*-benzylideneaniline oxide

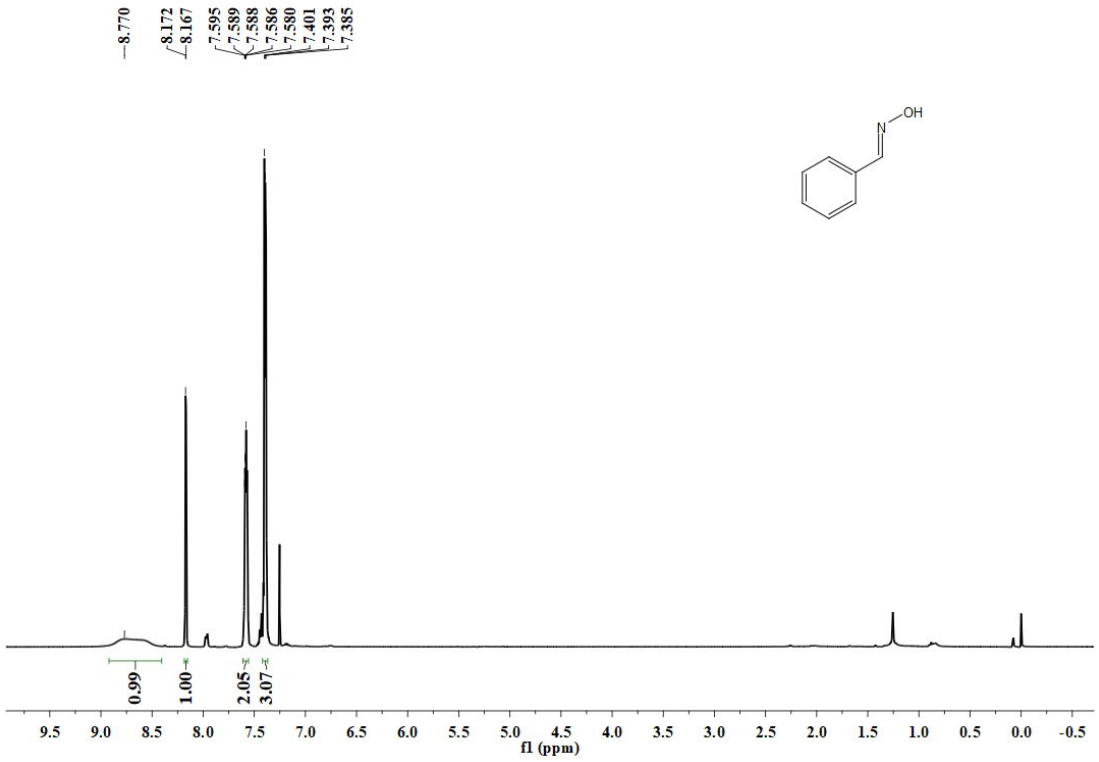


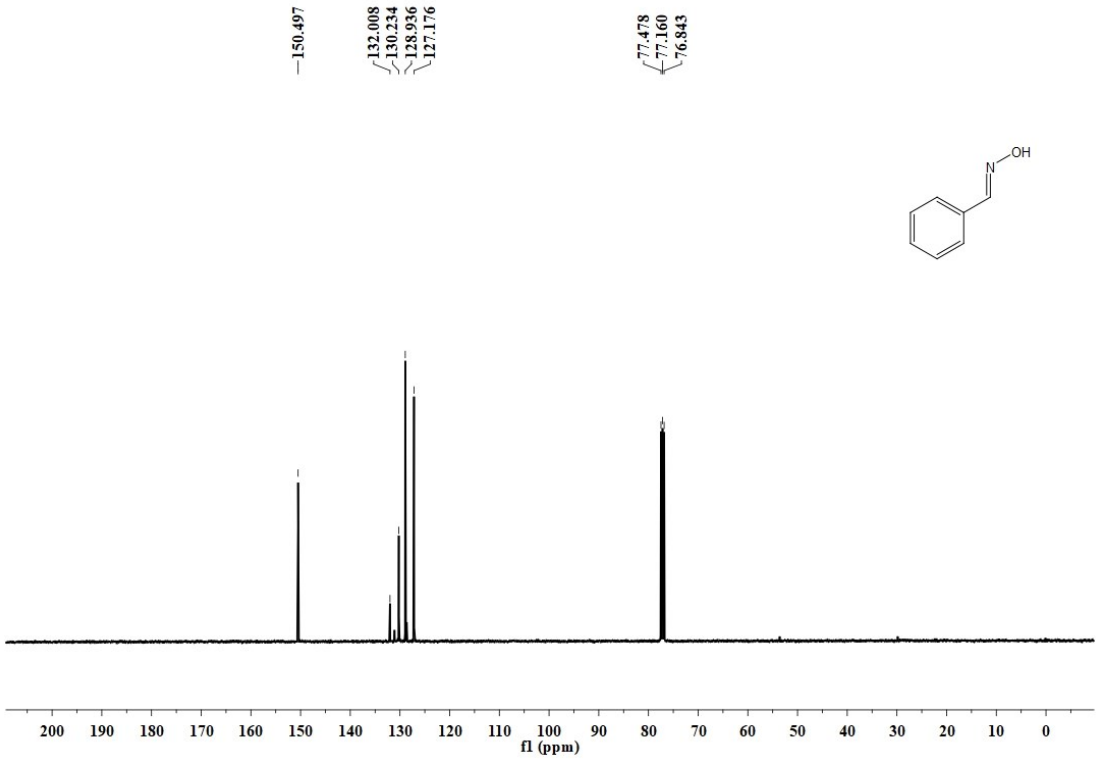
White solid, mp 104-106 °C; **^{1}H NMR**(400 MHz, $CDCl_3$) δ 8.41–8.39 (m, 2H), 7.93 (s, 1H), 7.79–7.76 (m, 2H), 7.50–7.47 (m, 6H); **HRMS** (ESI) m/z $[M + H]^+$ Calcd for $C_{13}H_{12}NO^+$ 198.0913; found 198.0920.

6. References

1. Simonsen, K. B.; Bayón, P.; Hazell, R. G.; Gothelf, K. V.; Jørgensen, K. A. Catalytic Enantioselective Inverse-Electron Demand 1,3-Dipolar Cycloaddition Reactions of Nitrones with Alkenes. *J. Am. Chem. Soc.* **1999**, *121*, 3845.

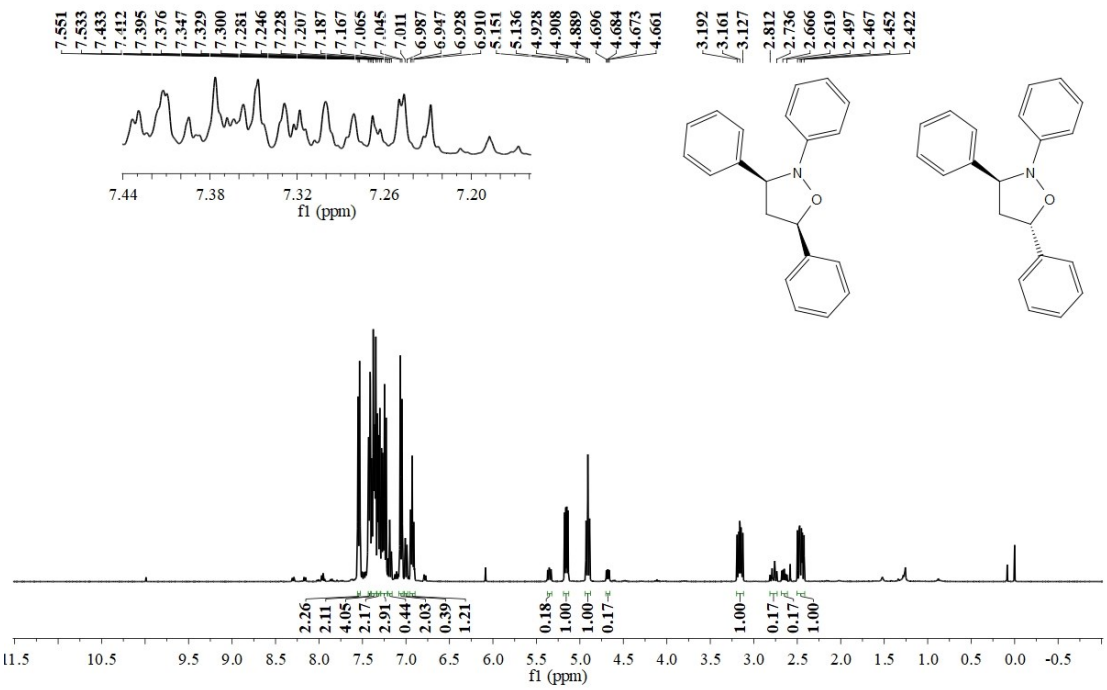
7. ^{1}H NMR and ^{13}C NMR spectra for (*E*)-benzaldehyde oxime E

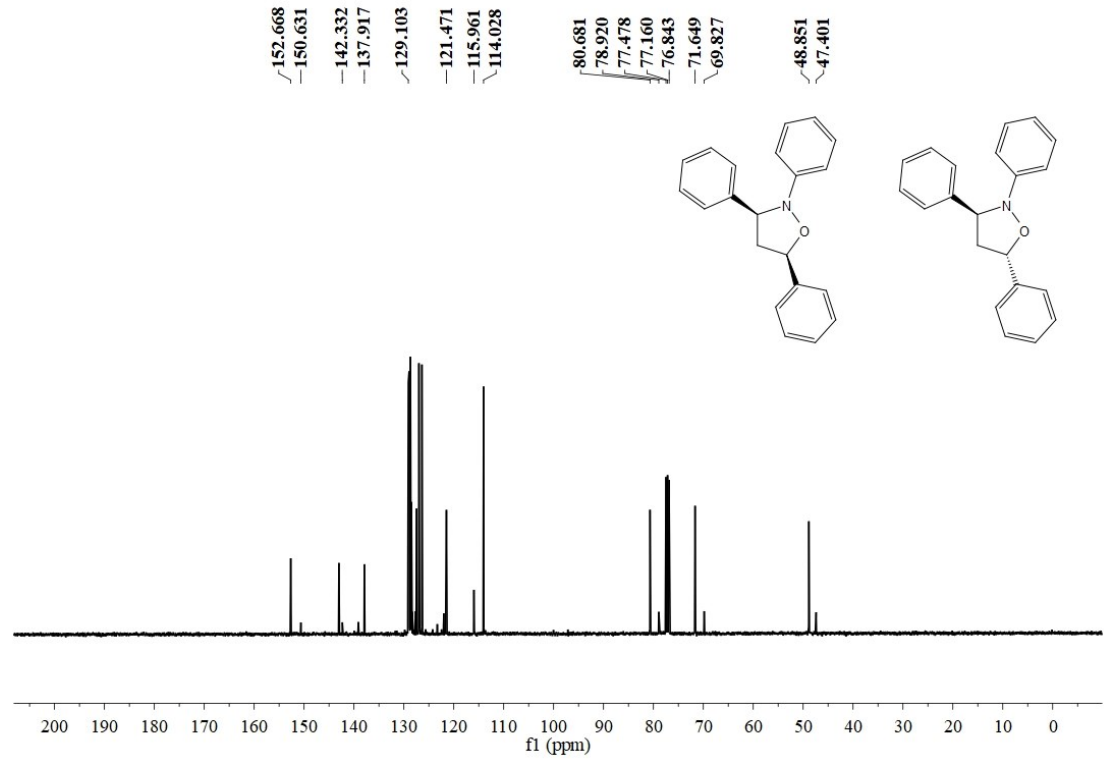




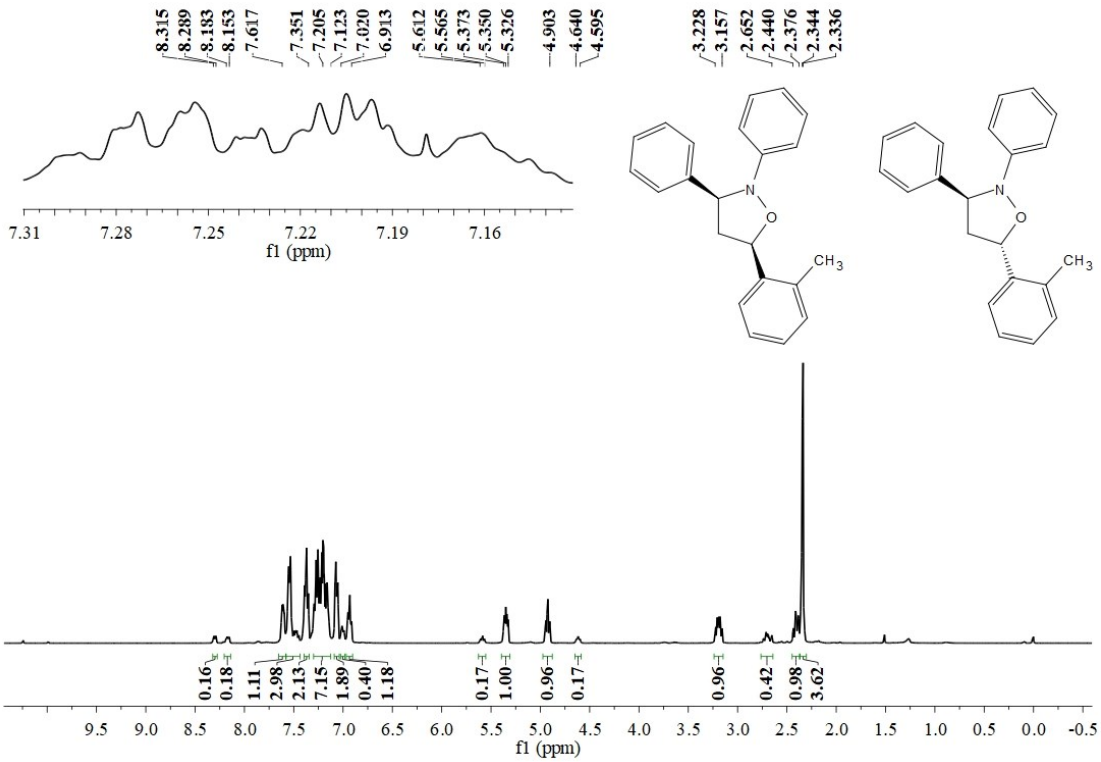
8. ^{1}H NMR and ^{13}C NMR spectra for products 4

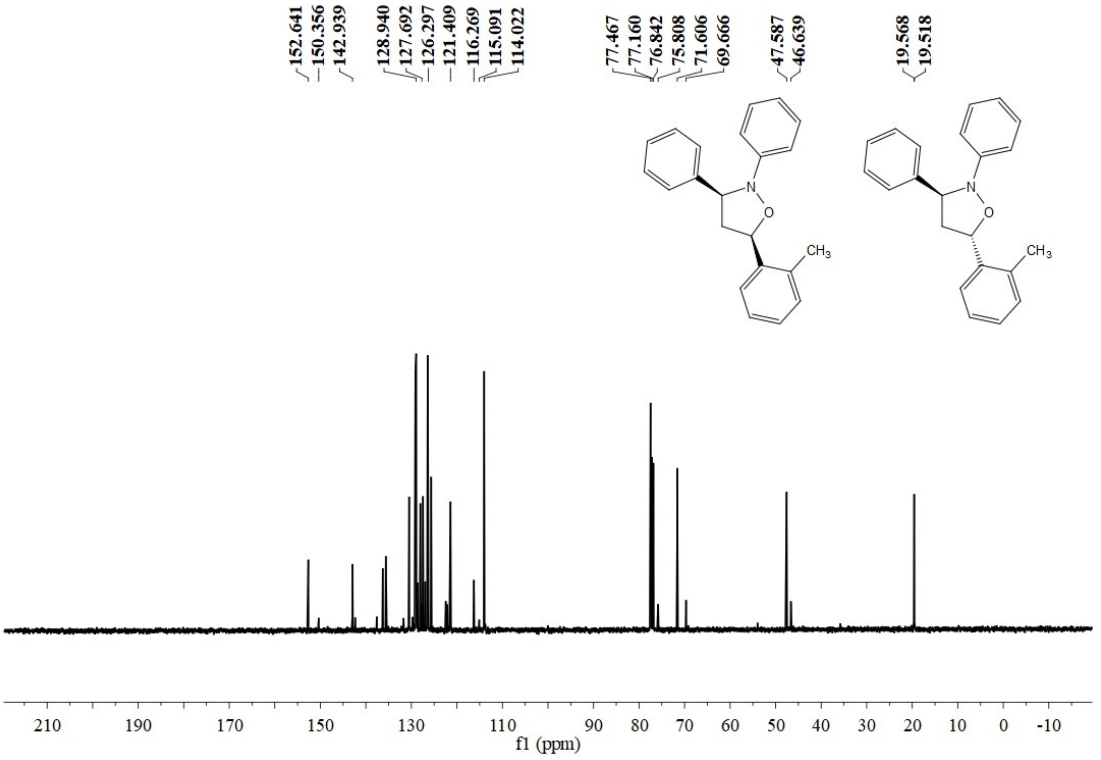
4aaa + 4a'a'a'



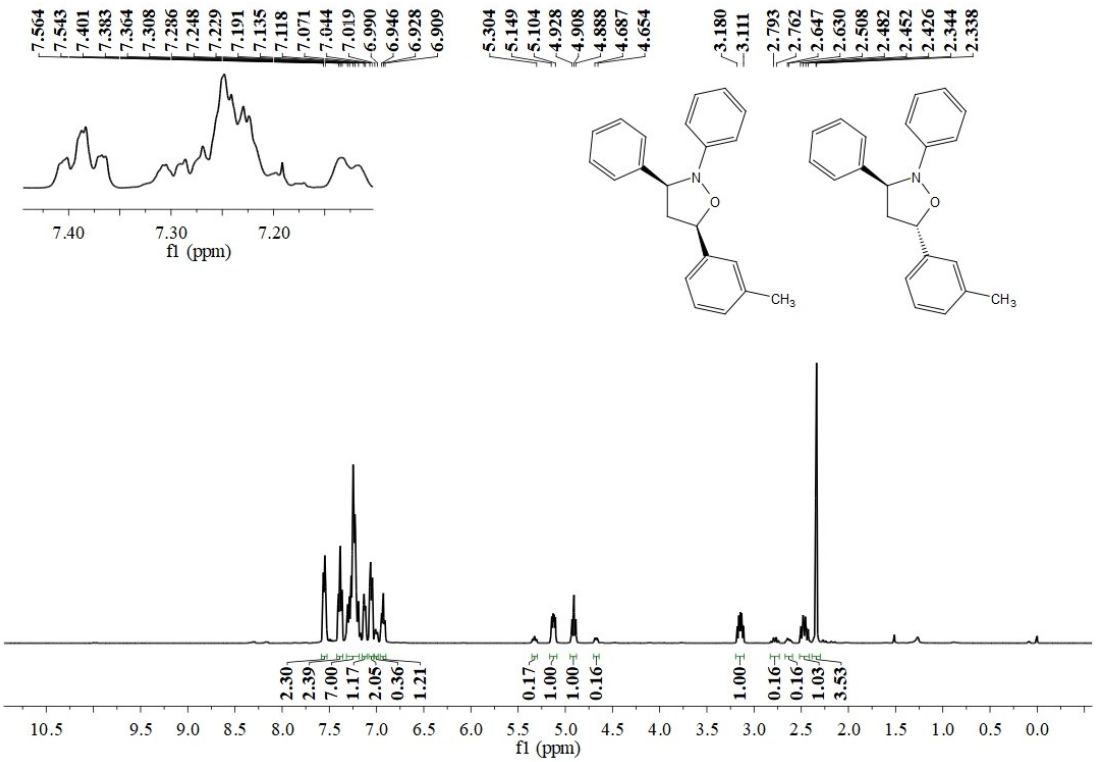


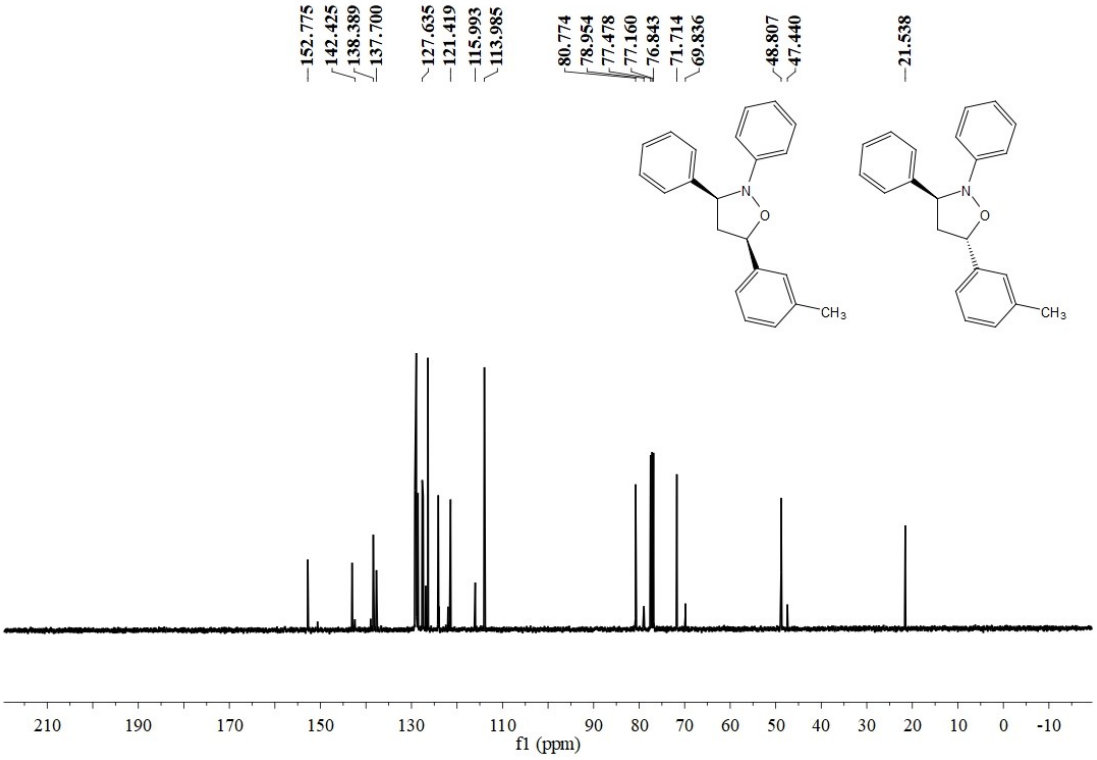
4aab + 4a'a'b'


8.315
8.289
8.183
8.153
7.617
7.351
7.205
7.123
7.020
6.913
5.612
5.565
5.373
5.350
5.326
4.903
4.640
4.595
3.228
3.157
2.652
2.440
2.376
2.344
2.336
7.31
7.28
7.25
7.22
7.19
7.16
f1 (ppm)
CH3
0.16
0.18
1.11
2.98
2.13
7.15
1.89
0.40
1.18
0.17
1.00
0.96
0.17
0.96
0.42
0.98
3.62
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

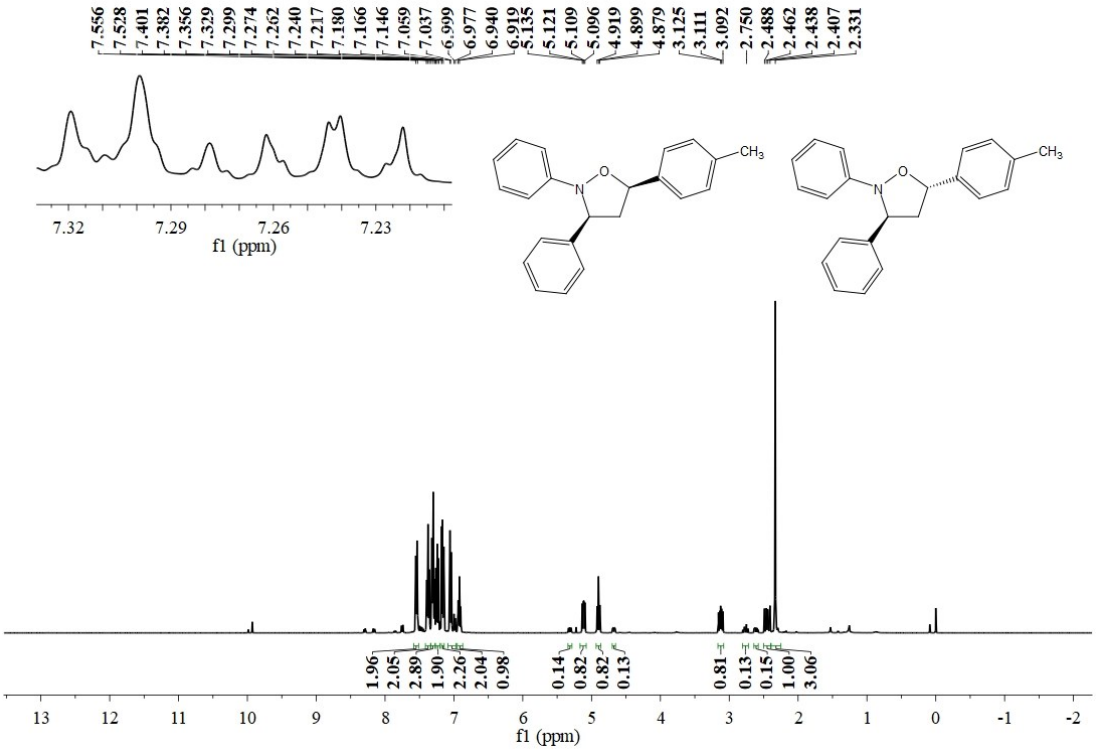

152.641
150.356
142.939
128.940
127.692
126.297
121.409
116.269
115.091
114.022
77.467
77.160
76.842
75.808
71.606
69.666
47.587
46.639
19.568
19.518
CH3
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

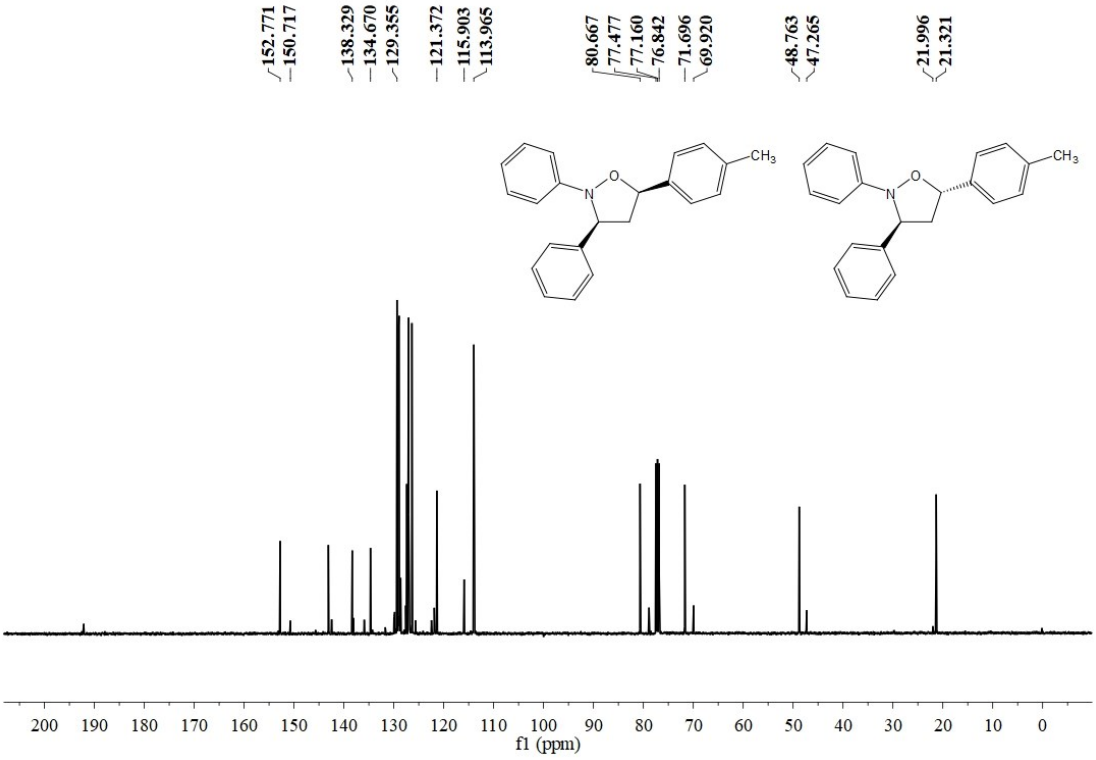
4aac + 4a'a'c'


7.564
7.543
7.401
7.383
7.364
7.308
7.286
7.248
7.229
7.191
7.135
7.118
7.071
7.044
7.019
6.990
6.946
6.928
6.909
5.304
5.149
5.104
4.928
4.908
4.888
4.687
4.654
3.180
3.111
2.793
2.762
2.647
2.630
2.508
2.482
2.452
2.426
2.344
2.338
7.40
7.30
7.20
f1 (ppm)
CH3
CH3
2.30
2.39
7.00
1.17
2.05
0.36
1.21
0.17
1.00
1.00
0.16
1.00
0.16
0.16
1.03
3.53
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

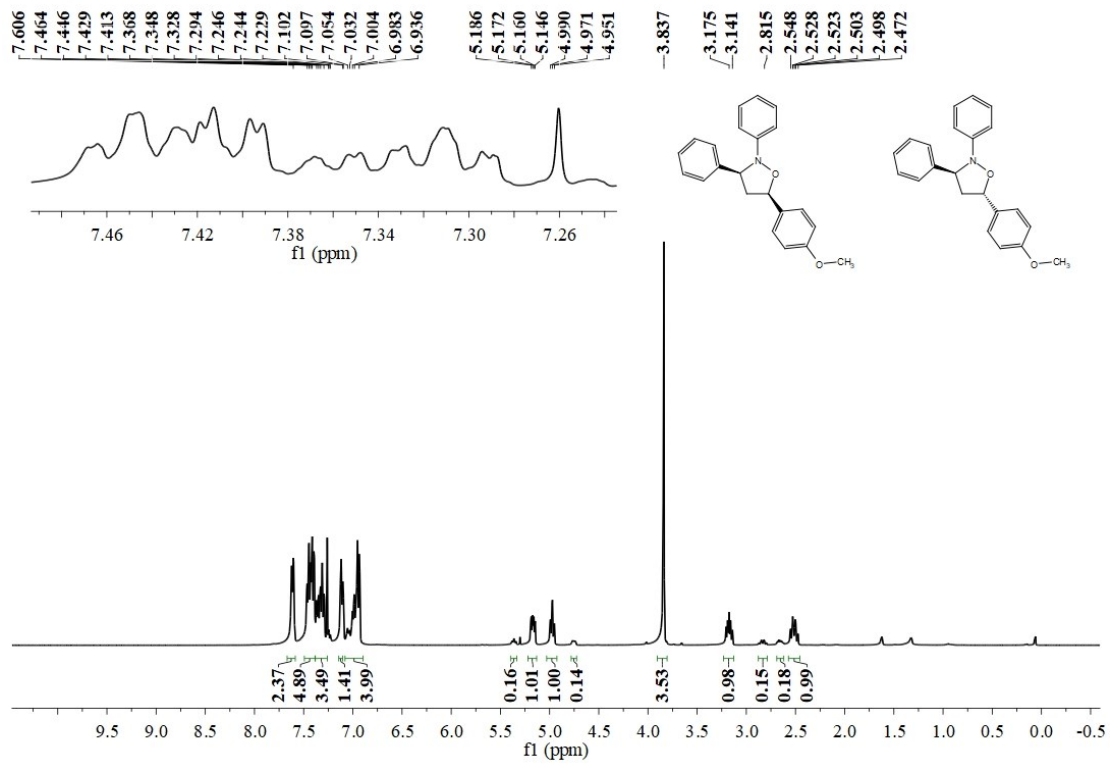

152.775
142.425
138.389
137.700
127.635
121.419
115.993
113.985
80.774
78.954
77.478
77.160
76.843
71.714
69.836
48.807
47.440
21.538
CH3
CH3
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

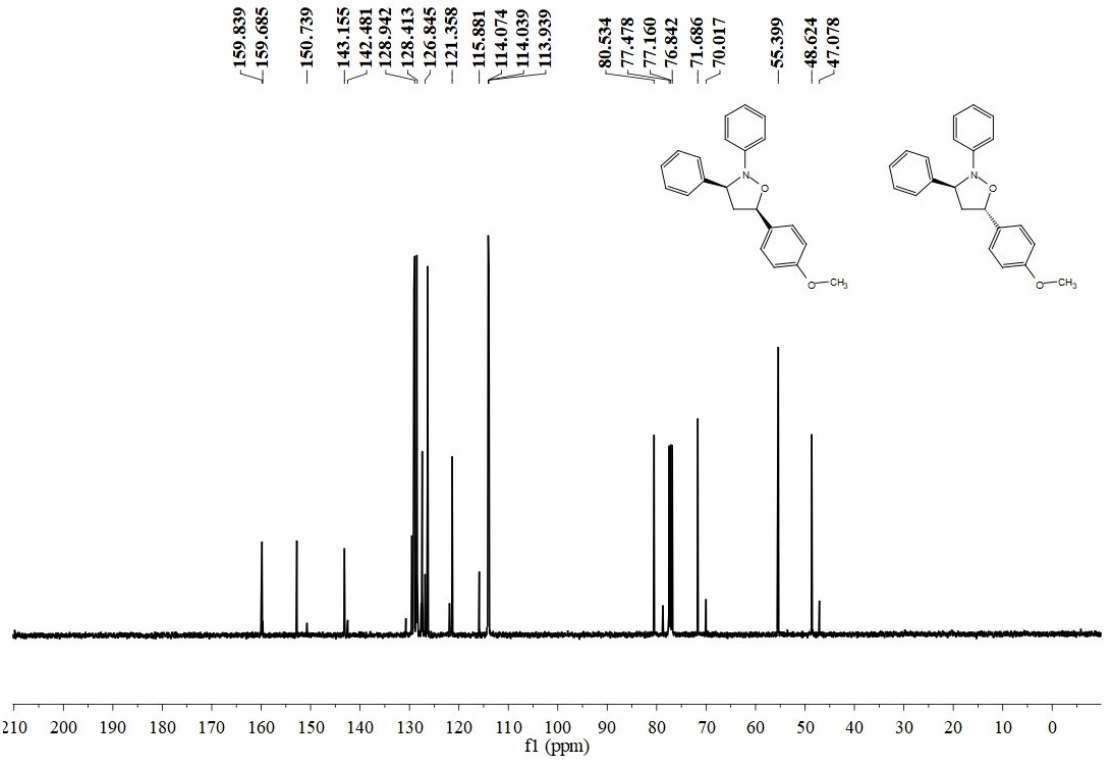
4aad + 4a'a'd'


7.556
7.528
7.401
7.382
7.356
7.329
7.299
7.274
7.262
7.240
7.217
7.180
7.166
7.146
7.059
7.037
6.999
6.977
6.940
6.919
5.135
5.121
5.109
5.096
4.919
4.899
4.879
3.125
3.111
3.092
2.750
2.488
2.462
2.438
2.407
2.331
7.32
7.29
7.26
7.23
f1 (ppm)
CH3
1.96
2.05
2.89
1.90
2.26
2.04
0.98
0.14
0.82
0.82
0.13
0.81
0.13
0.15
1.00
3.06
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)

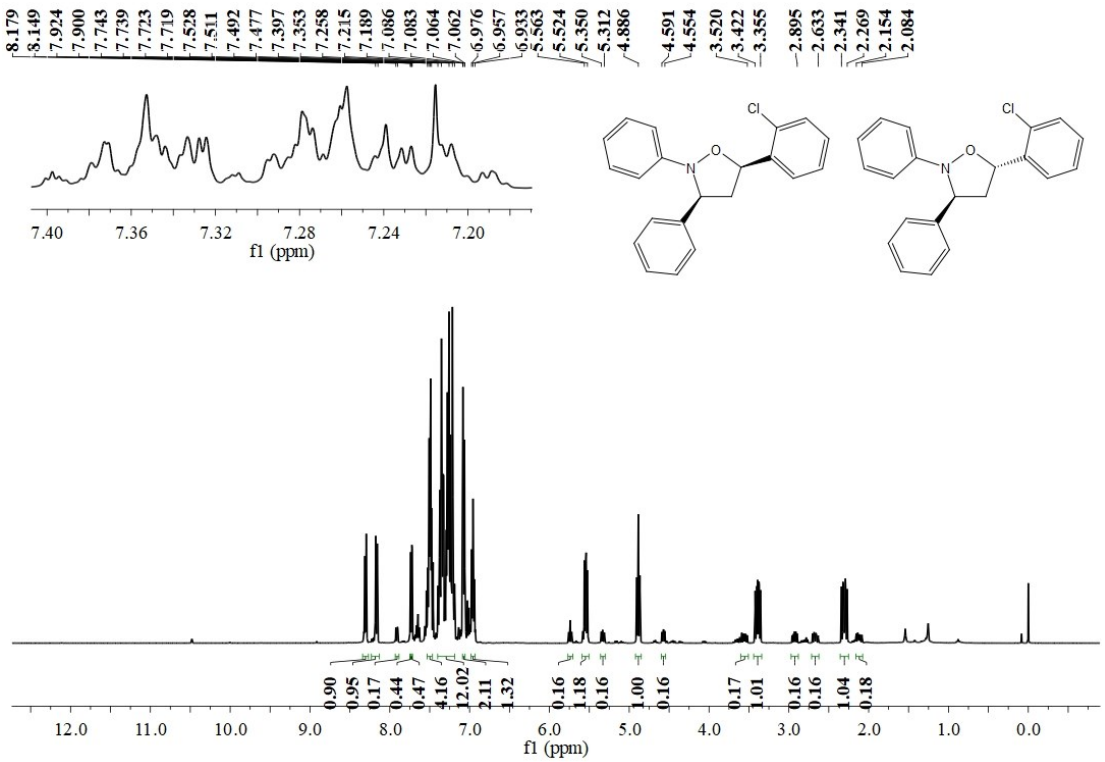

152.771
150.717
138.329
134.670
129.355
121.372
115.903
113.965
80.667
77.477
77.160
76.842
71.696
69.920
48.763
47.265
21.996
21.321
CH3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

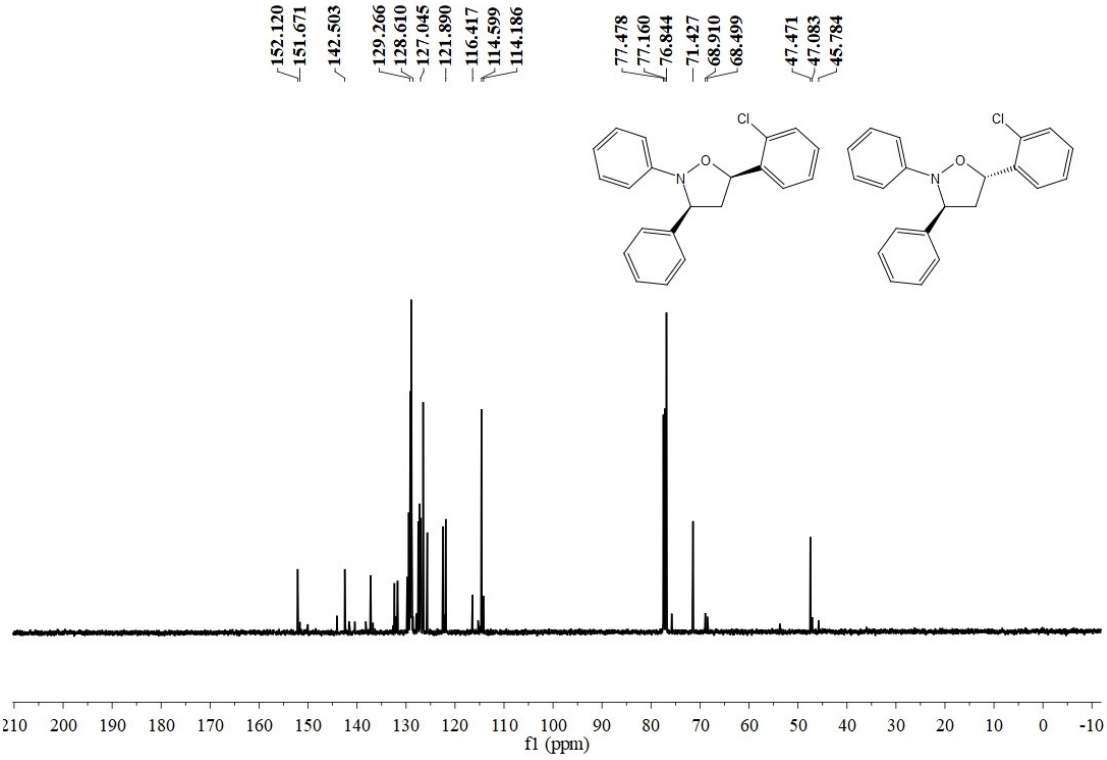
4aae + 4a'a'e'


7.606
7.464
7.446
7.429
7.413
7.368
7.348
7.328
7.294
7.246
7.244
7.229
7.102
7.097
7.054
7.032
7.004
6.983
6.936
5.186
5.172
5.160
5.146
4.990
4.971
4.951
3.837
3.175
3.141
2.815
2.548
2.528
2.523
2.503
2.498
2.472
f1 (ppm)
2.37
4.89
3.49
1.41
3.99
0.16
1.01
1.00
0.14
3.53
0.98
0.15
0.18
0.99
f1 (ppm)

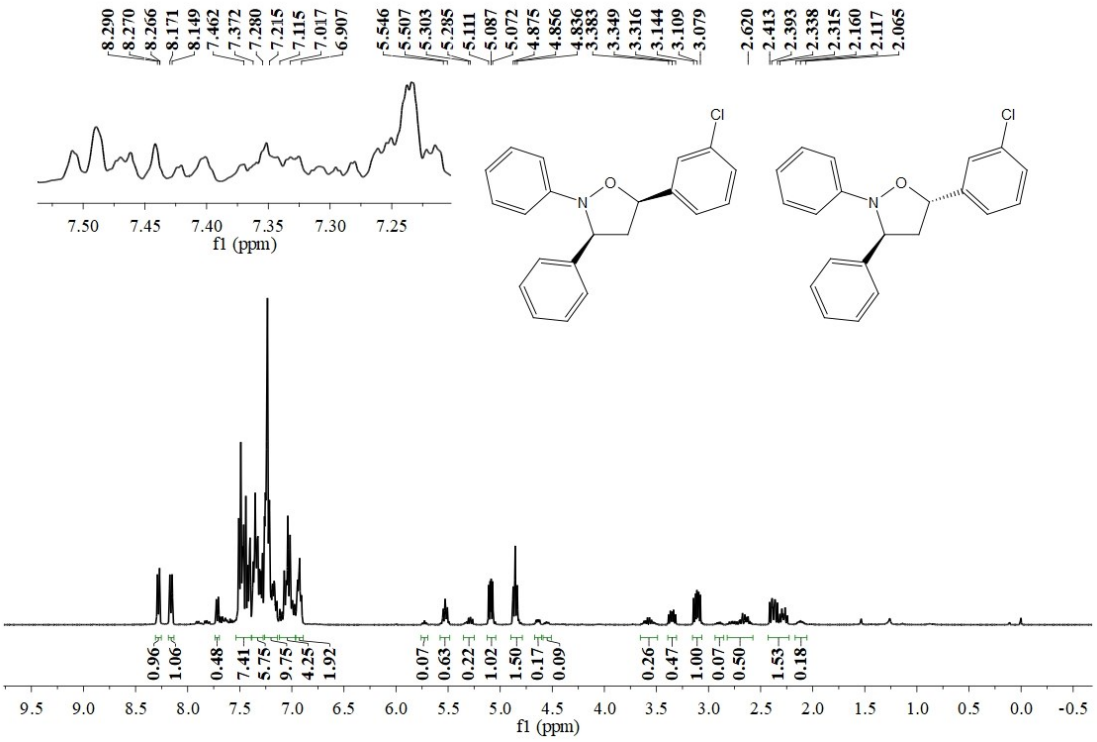

159.839
159.685
150.739
143.155
142.481
128.942
128.413
126.845
121.358
115.881
114.074
114.039
113.939
80.534
77.478
77.160
76.842
71.686
70.017
55.399
48.624
47.078
f1 (ppm)

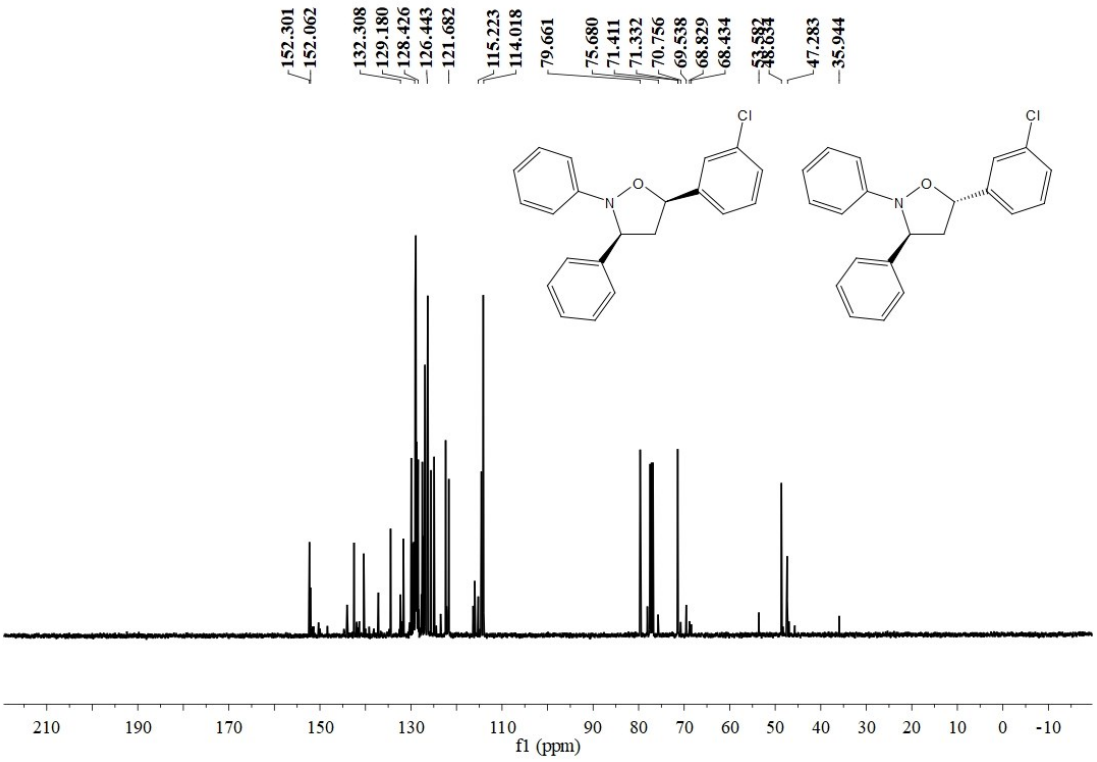
4aaf + 4a'a'f'


8.179
8.149
7.924
7.900
7.743
7.739
7.723
7.719
7.528
7.511
7.492
7.477
7.397
7.353
7.258
7.215
7.189
7.086
7.083
7.064
7.062
6.976
6.957
6.933
5.563
5.524
5.350
5.312
4.886
4.591
4.554
3.520
3.422
3.355
2.895
2.633
2.341
2.269
2.154
2.084
Cl
Cl
7.40
7.36
7.32
7.28
7.24
7.20
f1 (ppm)
0.90
0.95
0.17
0.44
0.47
4.16
12.02
2.11
4.32
0.16
1.18
0.16
1.00
0.16
0.17
1.01
0.16
0.16
1.04
0.18
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

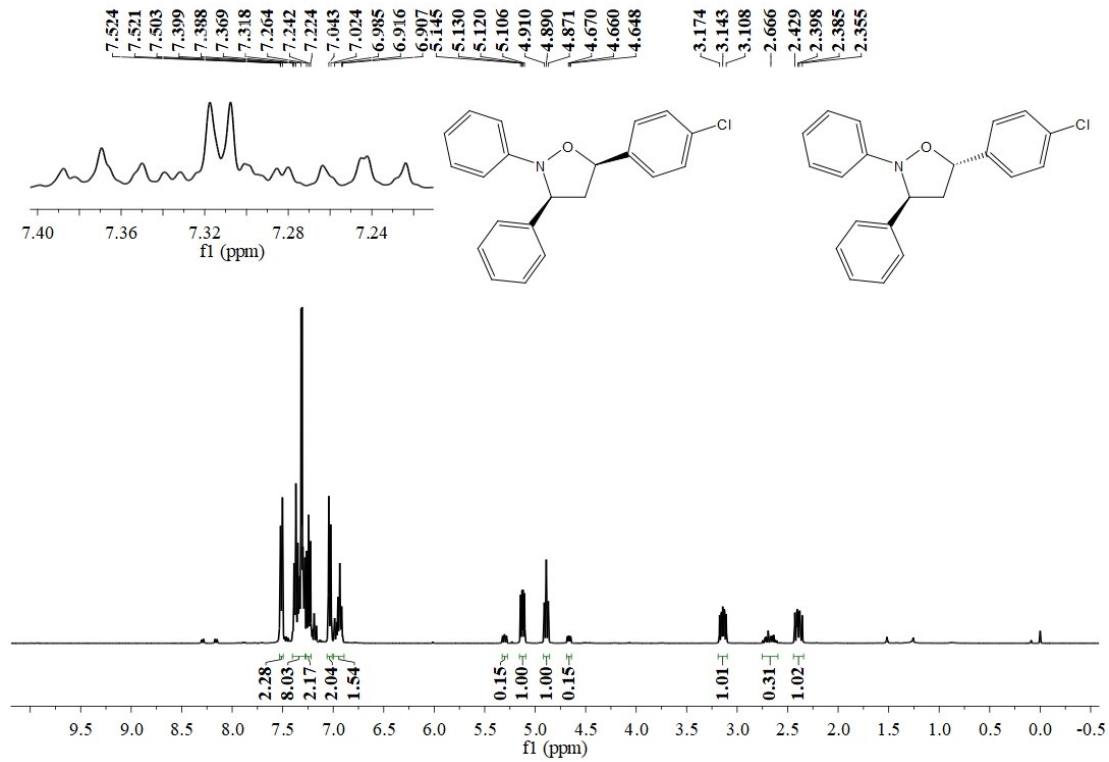

152.120
151.671
142.503
129.266
128.610
127.045
121.890
116.417
114.599
114.186
77.478
77.160
76.844
71.427
68.910
68.499
47.471
47.083
45.784
Cl
Cl
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

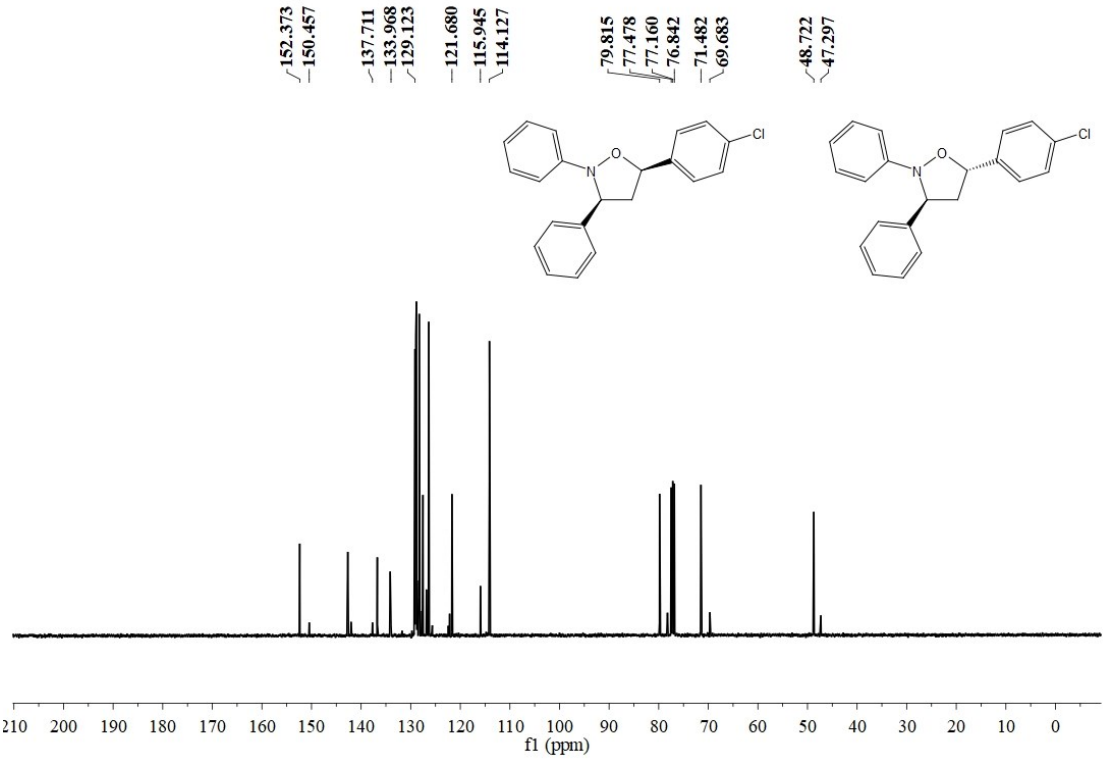
4aag + 4a'a'g'


8.290
8.270
8.266
8.171
8.149
7.462
7.372
7.280
7.215
7.115
7.017
6.907
5.546
5.507
5.303
5.285
5.111
5.087
5.072
4.875
4.856
4.836
3.383
3.349
3.316
3.144
3.109
3.079
2.620
2.413
2.393
2.338
2.315
2.160
2.117
2.065
Cl
N
O
f1 (ppm)
0.96
1.06
0.48
7.41
5.75
9.75
4.25
1.92
0.07
0.63
0.22
1.02
1.50
0.17
0.09
0.26
0.47
1.00
0.07
0.50
1.53
0.18

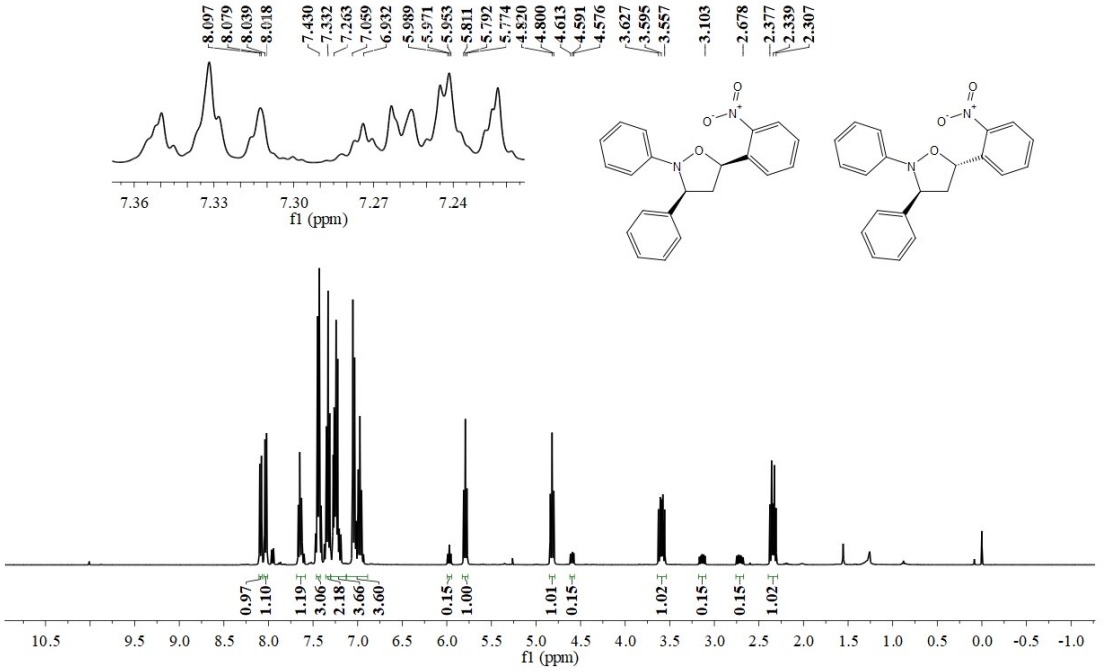

152.301
152.062
132.308
129.180
128.426
126.443
121.682
115.223
114.018
79.661
75.680
71.411
71.332
70.756
69.538
68.829
68.434
53.582
38.634
47.283
35.944
Cl
N
O
f1 (ppm)

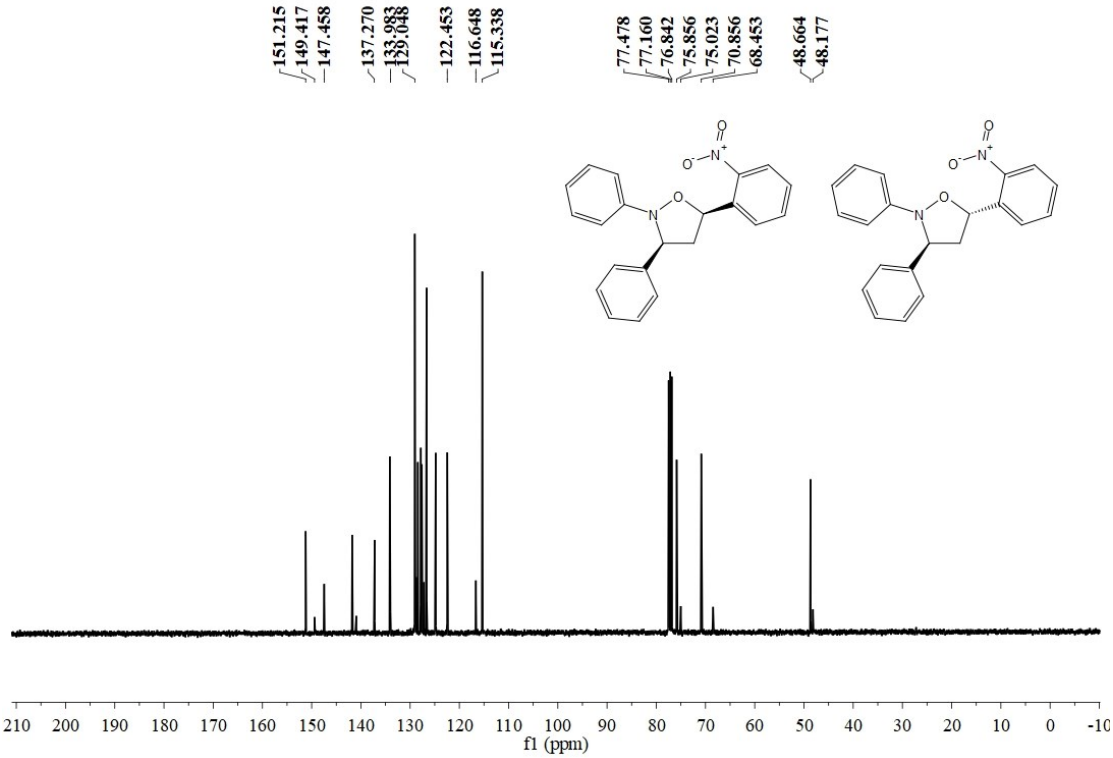
4aah + 4a'a'h'


7.524
7.521
7.503
7.399
7.388
7.369
7.318
7.264
7.242
7.224
7.043
7.024
6.985
6.916
6.907
5.145
5.130
5.120
5.106
4.910
4.890
4.871
4.670
4.660
4.648
3.174
3.143
3.108
2.666
2.429
2.398
2.385
2.355
Cl
Cl
7.40
7.36
7.32
7.28
7.24
f1 (ppm)
2.28
8.03
2.17
2.04
1.54
0.15
1.00
1.00
0.15
1.01
0.31
1.02
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

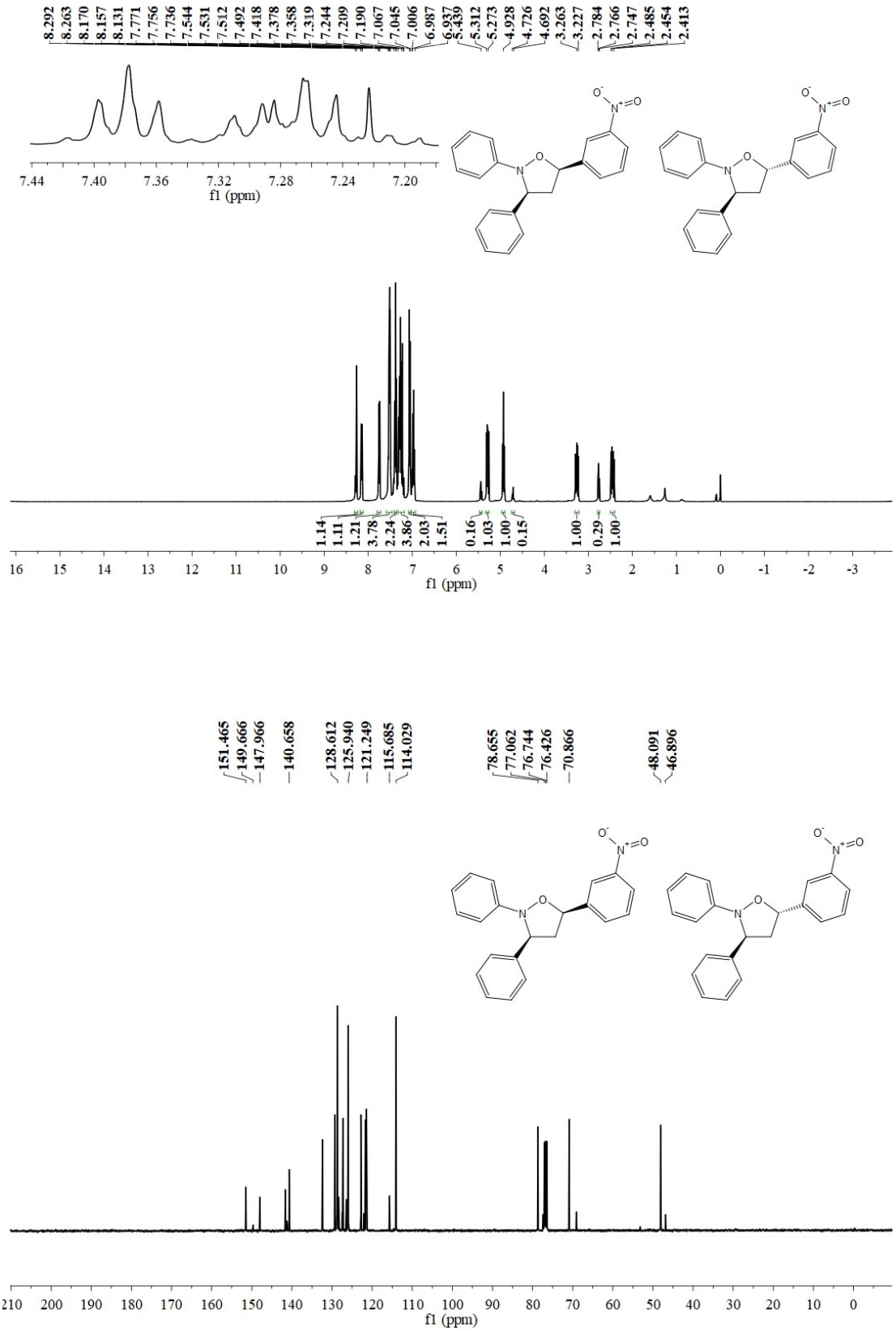

152.373
150.457
137.711
133.968
129.123
121.680
115.945
114.127
79.815
77.478
77.160
76.842
71.482
69.683
48.722
47.297
Cl
Cl
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

4aai + 4a'a'i'

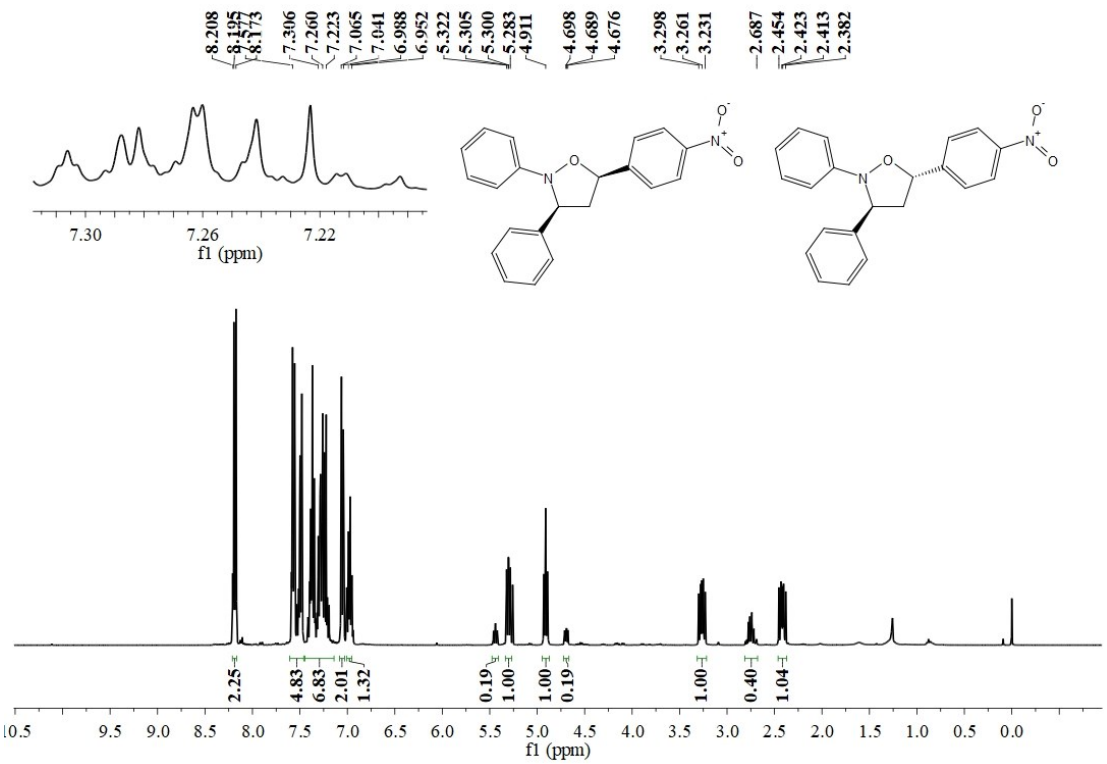

8.097
8.079
8.039
8.018
7.430
7.332
7.263
7.059
6.932
5.989
5.971
5.953
5.811
5.792
5.774
4.820
4.800
4.613
4.591
4.576
3.627
3.595
3.557
3.103
2.678
2.377
2.339
2.307
7.36
7.33
7.30
7.27
7.24
f1 (ppm)
0.97
1.10
1.19
3.06
2.18
3.66
3.60
0.15
1.00
1.01
0.15
1.02
0.15
0.15
1.02
f1 (ppm)

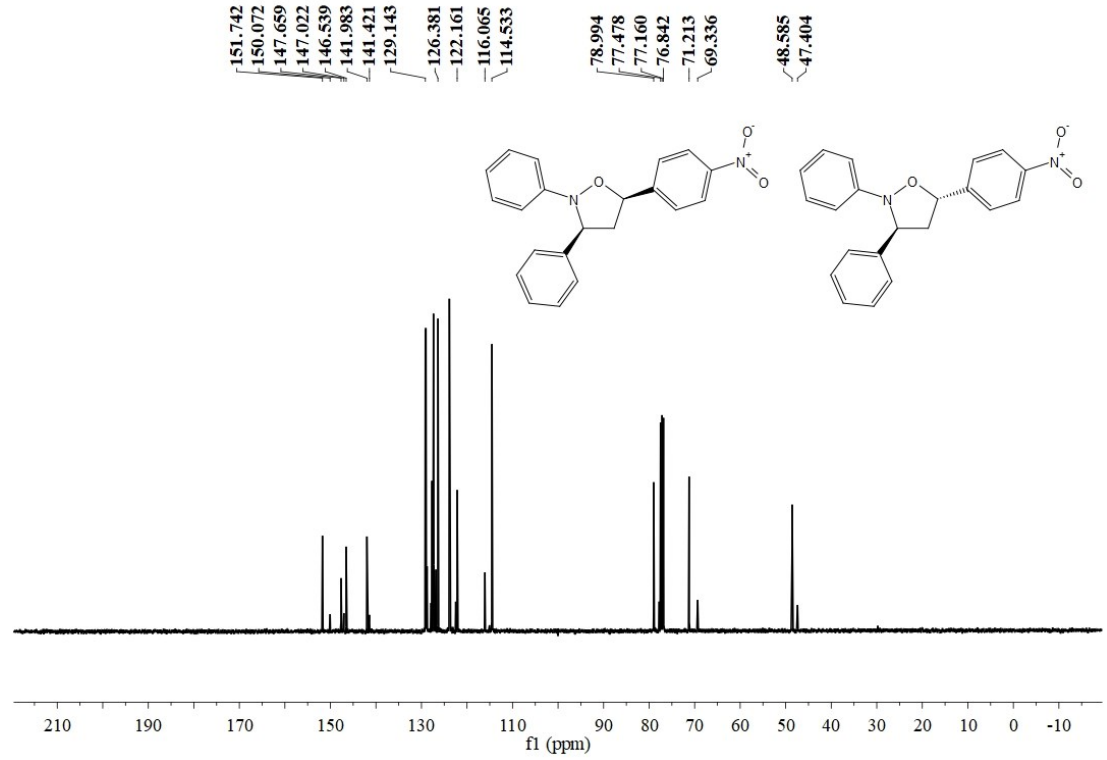

151.215
149.417
147.458
137.270
133.983
129.048
122.453
116.648
115.338
77.478
77.160
76.842
75.856
75.023
70.856
68.453
48.664
48.177
f1 (ppm)

4aaj + 4a'a'j'

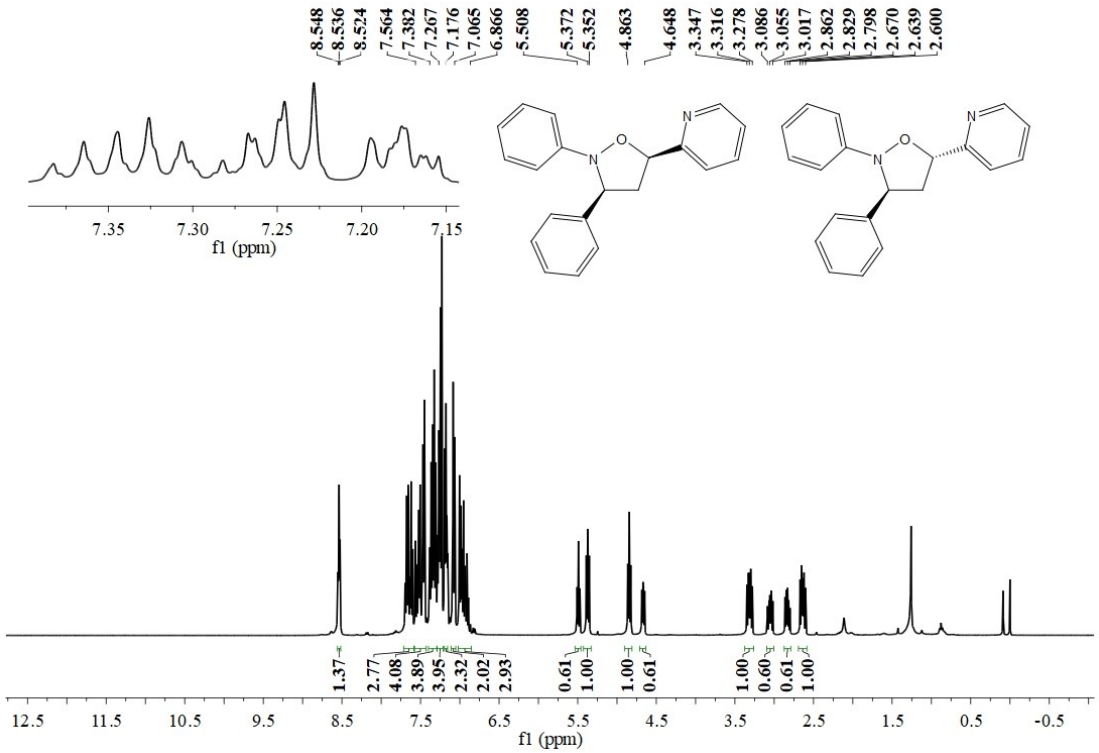

8.292
8.263
8.170
8.157
8.131
7.771
7.756
7.736
7.544
7.531
7.512
7.492
7.418
7.378
7.358
7.319
7.244
7.209
7.190
7.067
7.045
7.006
6.987
6.937
5.439
5.312
5.273
4.928
4.726
4.692
3.263
3.227
2.784
2.766
2.747
2.485
2.454
2.413
7.44
7.40
7.36
7.32
7.28
7.24
7.20
f1 (ppm)
1.14
1.11
1.21
3.78
2.24
3.86
2.03
1.51
0.16
1.03
1.00
0.15
1.00
0.29
1.00
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)
151.465
149.666
147.966
140.658
128.612
125.940
121.249
115.685
114.029
78.655
77.062
76.744
76.426
70.866
48.091
46.896
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

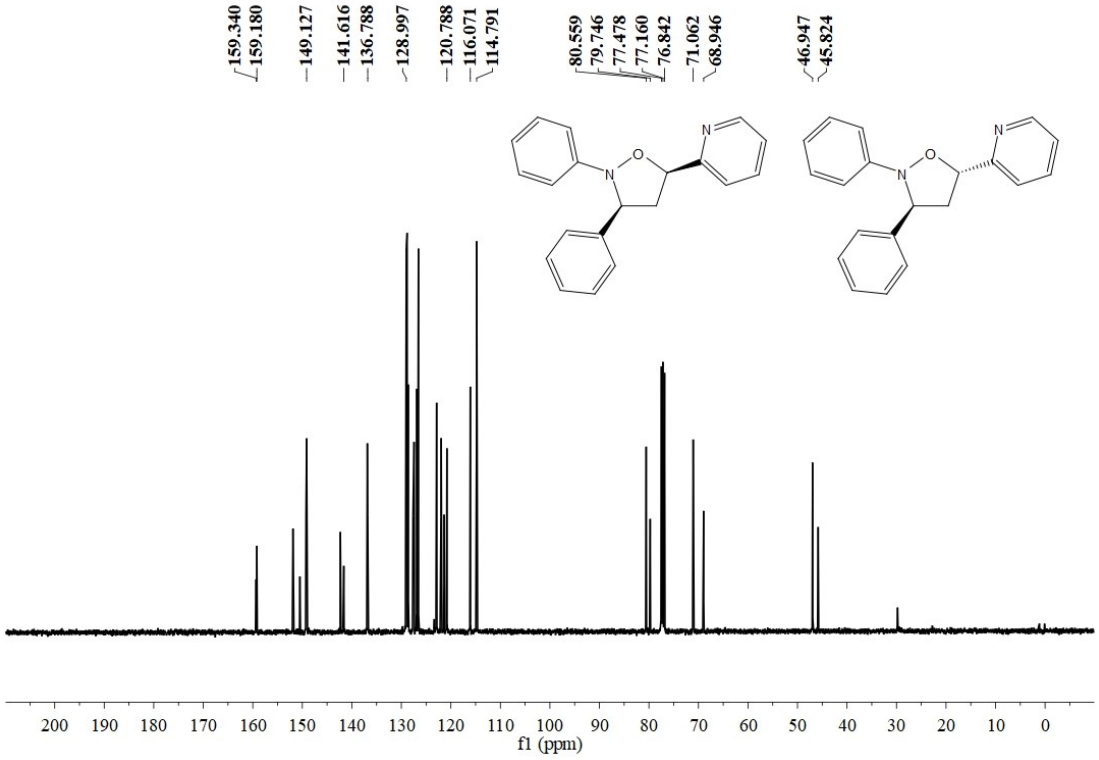
4aak + 4a'a'k'


8.208
8.195
8.177
8.173
7.306
7.260
7.223
7.065
7.041
6.988
6.952
5.322
5.305
5.300
5.283
4.911
4.698
4.689
4.676
3.298
3.261
3.231
2.687
2.454
2.423
2.413
2.382
7.30
7.26
7.22
f1 (ppm)
2.25
4.83
6.83
2.01
1.32
0.19
1.00
1.00
0.19
1.00
0.40
1.04
f1 (ppm)

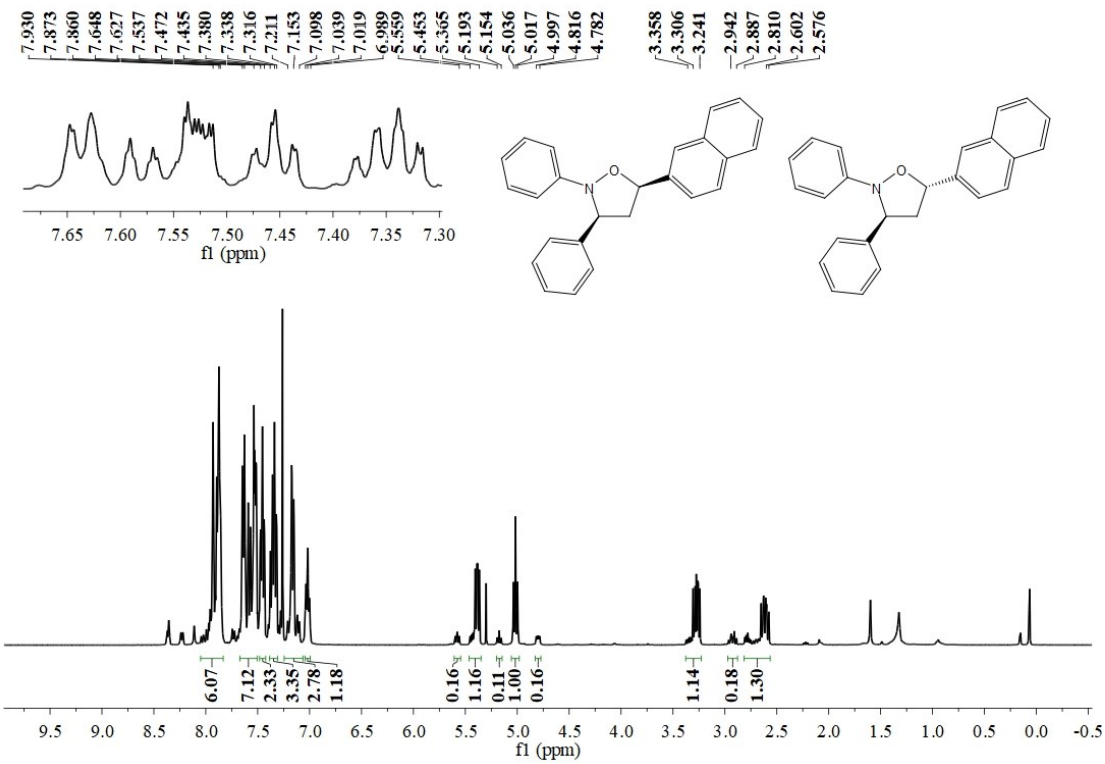

151.742
150.072
147.659
147.022
146.539
141.983
141.421
129.143
126.381
122.161
116.065
114.533
78.994
77.478
77.160
76.842
71.213
69.336
48.585
47.404
f1 (ppm)

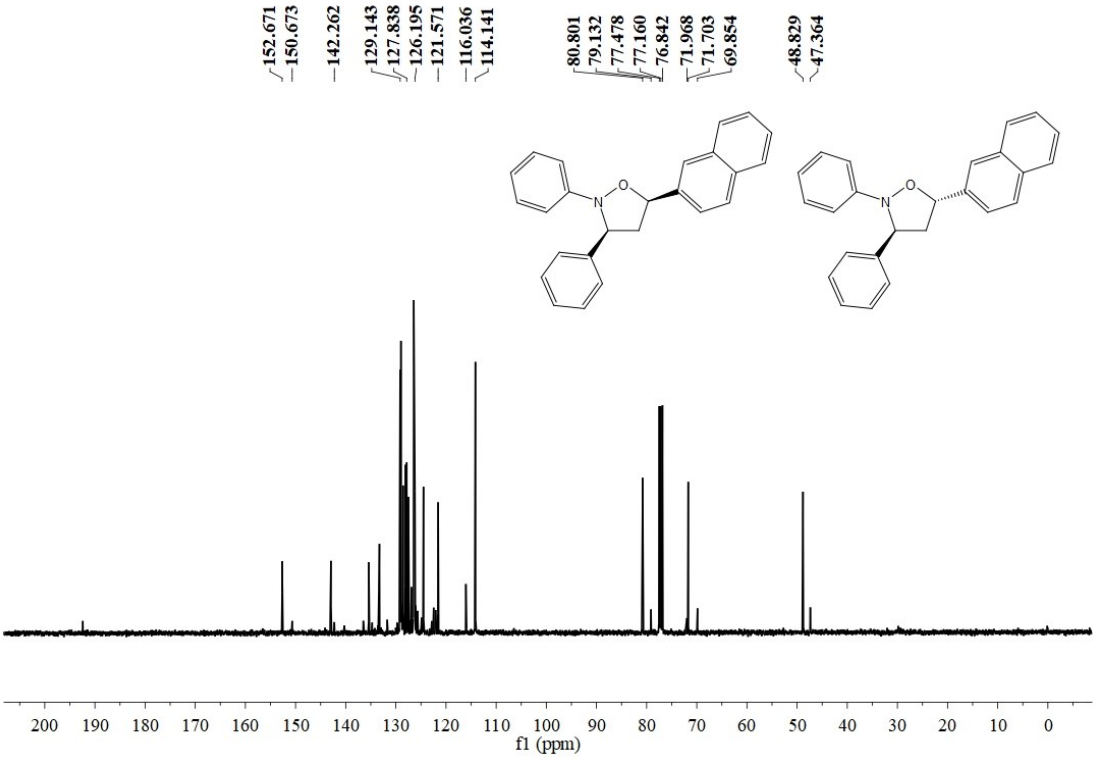
4aal + 4a'a'l'


8.548
8.536
8.524
7.564
7.382
7.267
7.176
7.065
6.866
5.508
5.372
5.352
4.863
4.648
3.347
3.316
3.278
3.086
3.055
3.017
2.862
2.829
2.798
2.670
2.639
2.600
7.35
7.30
7.25
7.20
7.15
f1 (ppm)
1.37
2.77
4.08
3.89
3.95
2.32
2.02
2.93
0.61
1.00
1.00
0.61
1.00
0.60
0.61
1.00
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

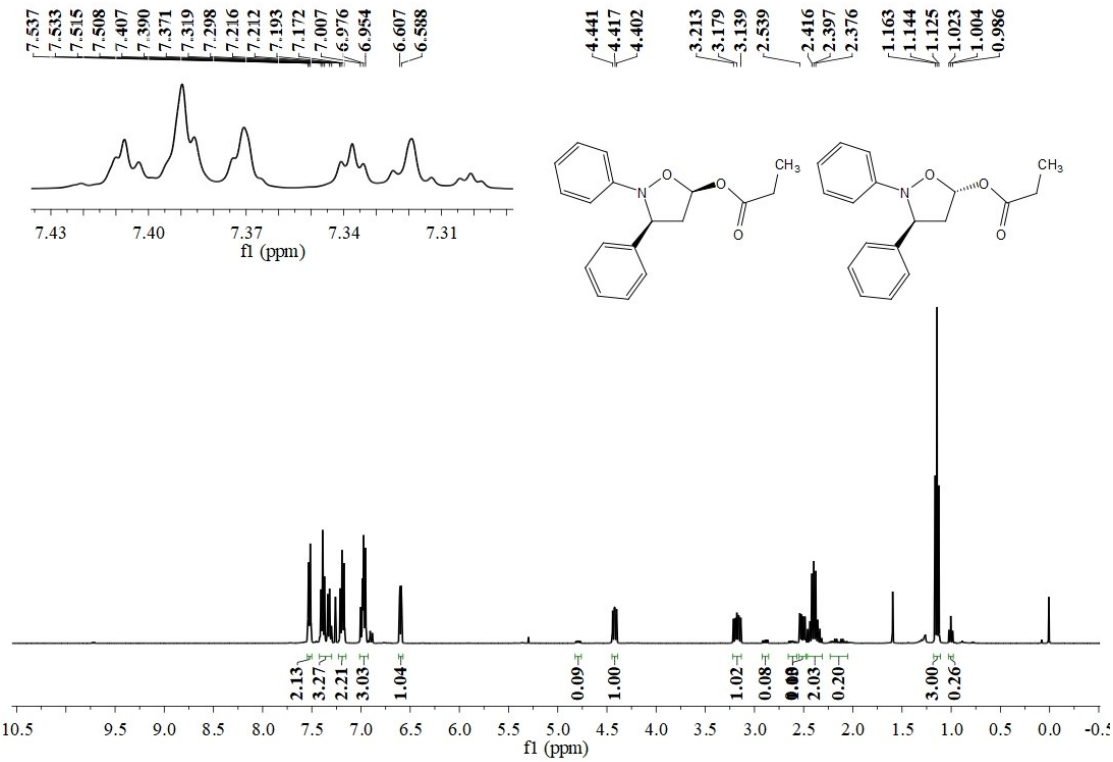

159.340
159.180
149.127
141.616
136.788
128.997
120.788
116.071
114.791
80.559
79.746
77.478
77.160
76.842
71.062
68.946
46.947
45.824
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

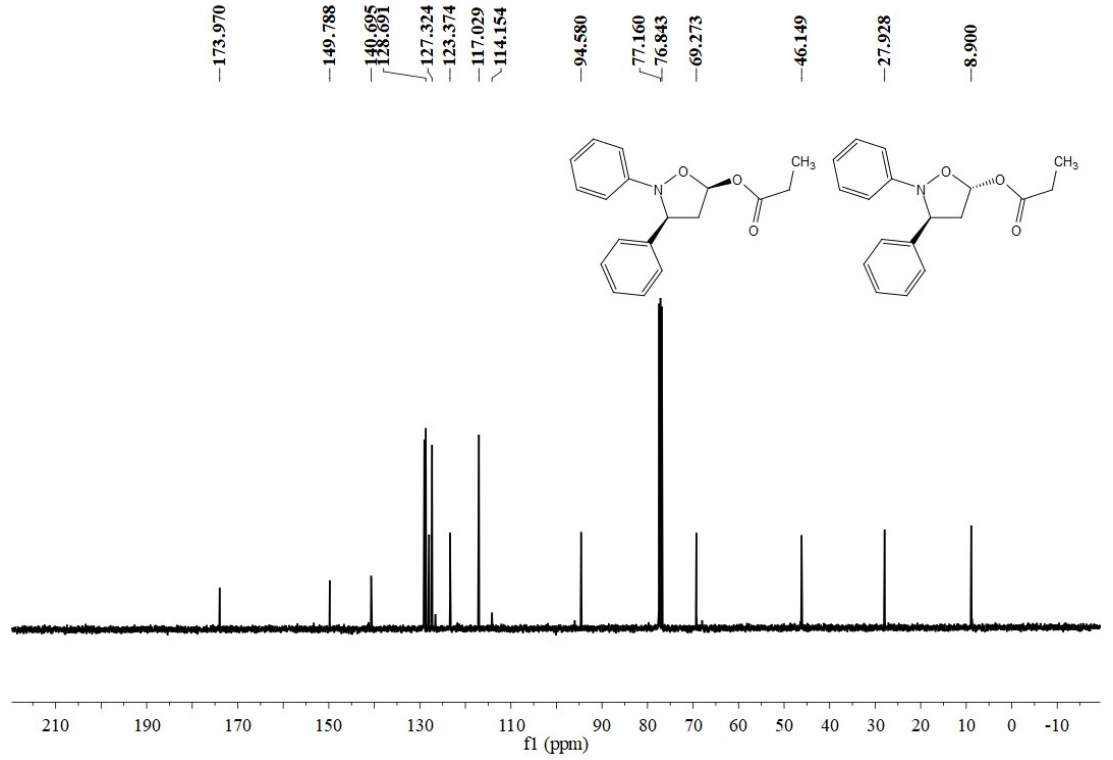
4aam + 4a'a'm'


7.930
7.873
7.860
7.648
7.627
7.537
7.472
7.435
7.380
7.338
7.316
7.211
7.153
7.098
7.039
7.019
6.989
5.559
5.453
5.365
5.193
5.154
5.036
5.017
4.997
4.816
4.782
3.358
3.306
3.241
2.942
2.887
2.810
2.602
2.576
7.65 7.60 7.55 7.50 7.45 7.40 7.35 7.30
f1 (ppm)
6.07
7.12
2.33
3.35
2.78
1.18
0.16
1.16
0.11
1.00
0.16
1.14
0.18
1.30
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

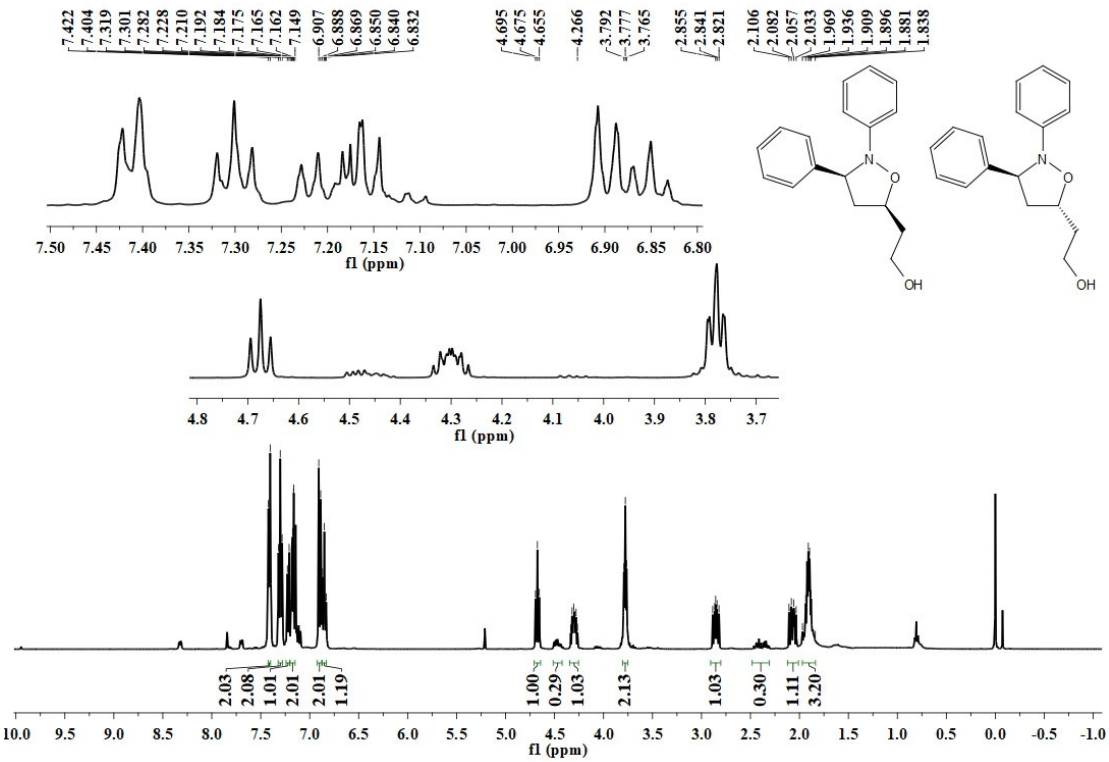

152.671
150.673
142.262
129.143
127.838
126.195
121.571
116.036
114.141
80.801
79.132
77.478
77.160
76.842
71.968
71.703
69.854
48.829
47.364
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

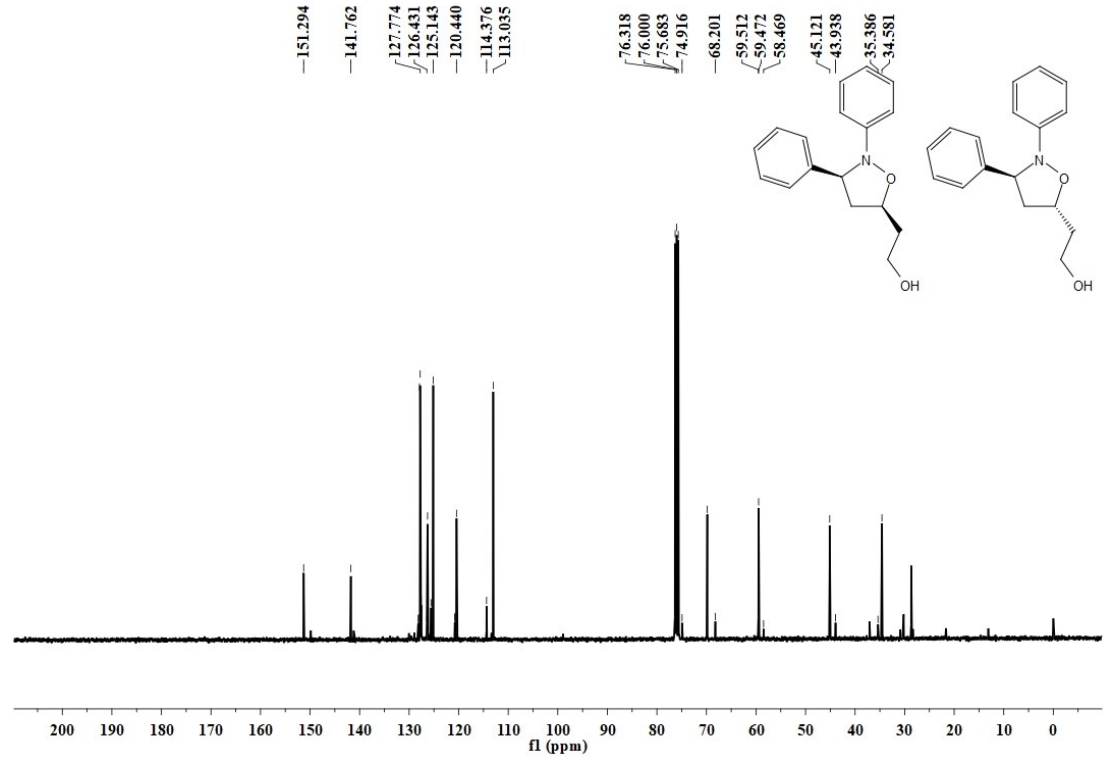
4aan + 4a'a'n'


7.537
7.533
7.515
7.508
7.407
7.390
7.371
7.319
7.298
7.216
7.212
7.193
7.172
7.007
6.976
6.954
6.607
6.588
4.441
4.417
4.402
3.213
3.179
3.139
2.539
2.416
2.397
2.376
1.163
1.144
1.125
1.023
1.004
0.986
7.43
7.40
7.37
7.34
7.31
f1 (ppm)
CH3
2.13
3.27
2.21
3.03
1.04
0.09
1.00
1.02
0.08
2.03
0.20
3.00
0.26
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

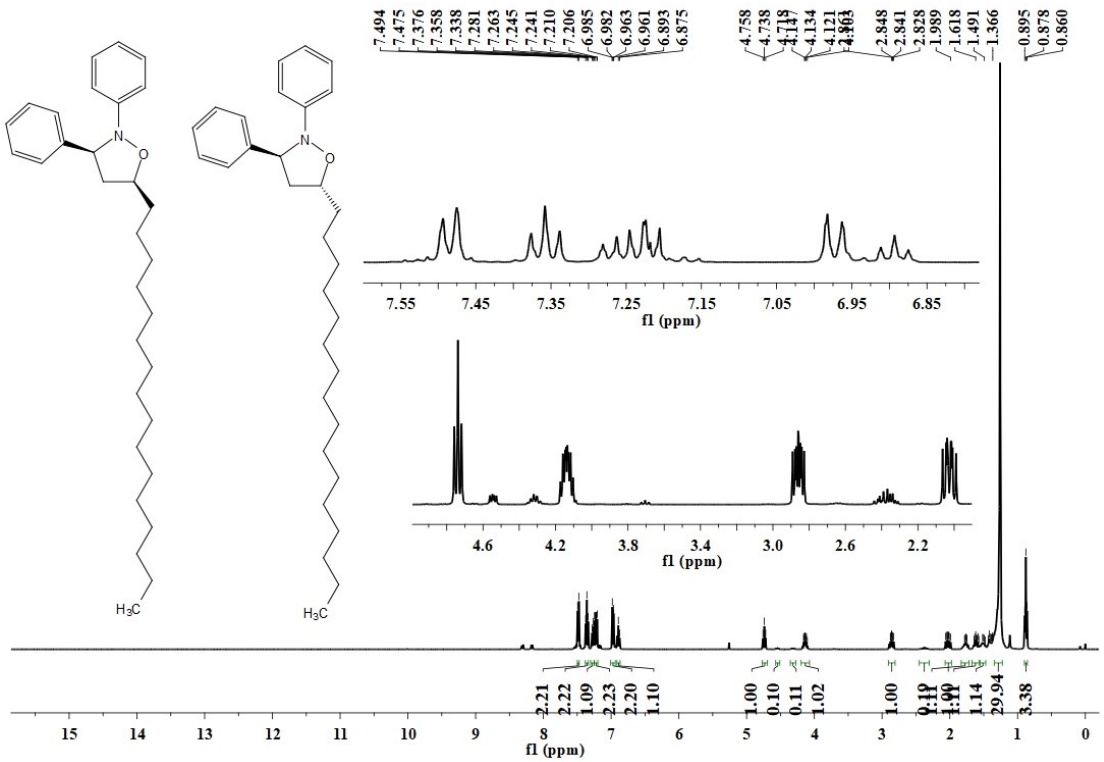

173.970
149.788
140.695
128.691
127.324
123.374
117.029
114.154
94.580
77.160
76.843
69.273
46.149
27.928
8.900
CH3
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

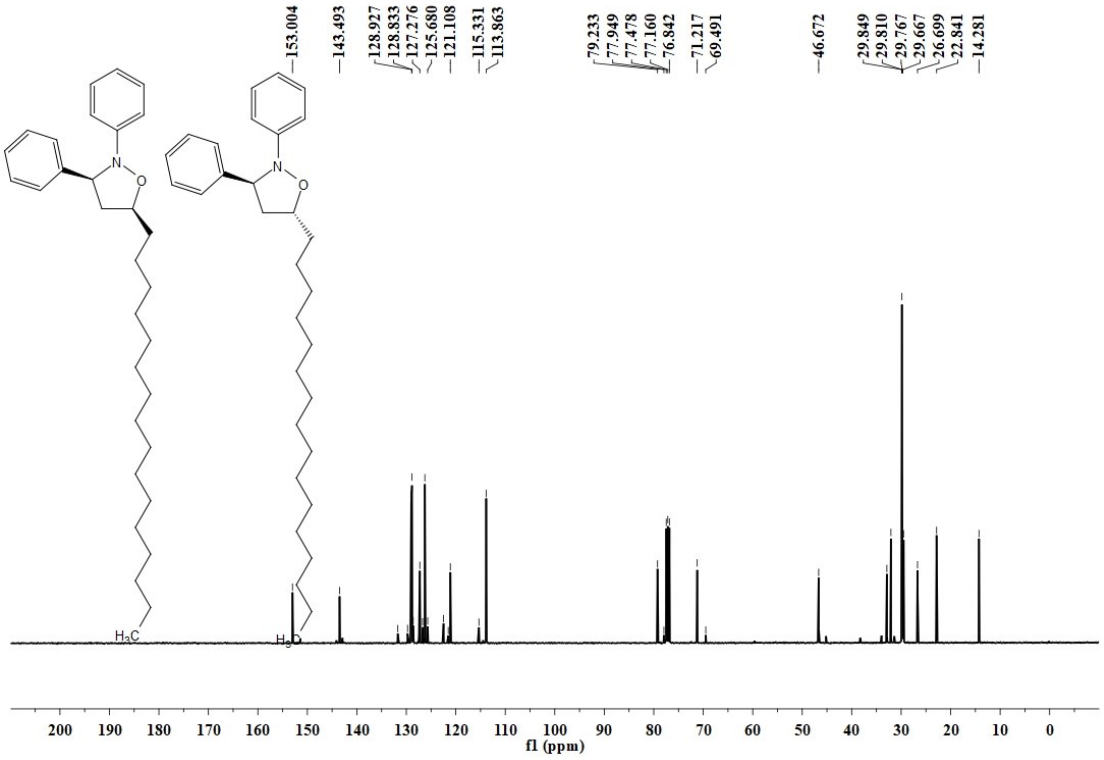
4aao + 4a'a'o'


7.422
7.404
7.319
7.301
7.282
7.228
7.210
7.192
7.184
7.175
7.165
7.162
7.149
6.907
6.888
6.869
6.850
6.840
6.832
4.695
4.675
4.655
4.266
3.792
3.777
3.765
2.855
2.841
2.821
2.106
2.082
2.057
2.033
1.969
1.936
1.909
1.896
1.881
1.838
fl (ppm)
OH
OH
2.03
2.08
1.01
2.01
2.01
1.19
1.00
0.29
1.03
2.13
1.03
0.30
1.11
3.20
fl (ppm)

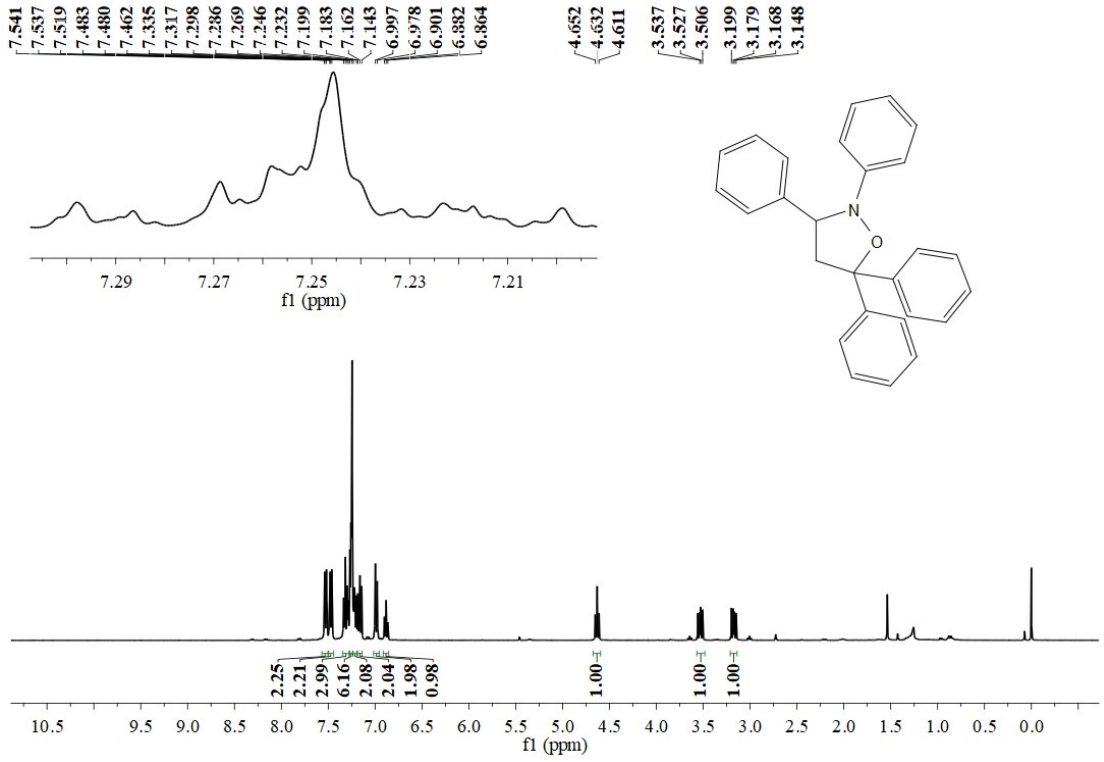

151.294
141.762
127.774
126.431
125.143
120.440
114.376
113.035
76.318
76.000
75.683
74.916
68.201
59.512
59.472
58.469
45.121
43.938
35.386
34.581
OH
OH
fl (ppm)

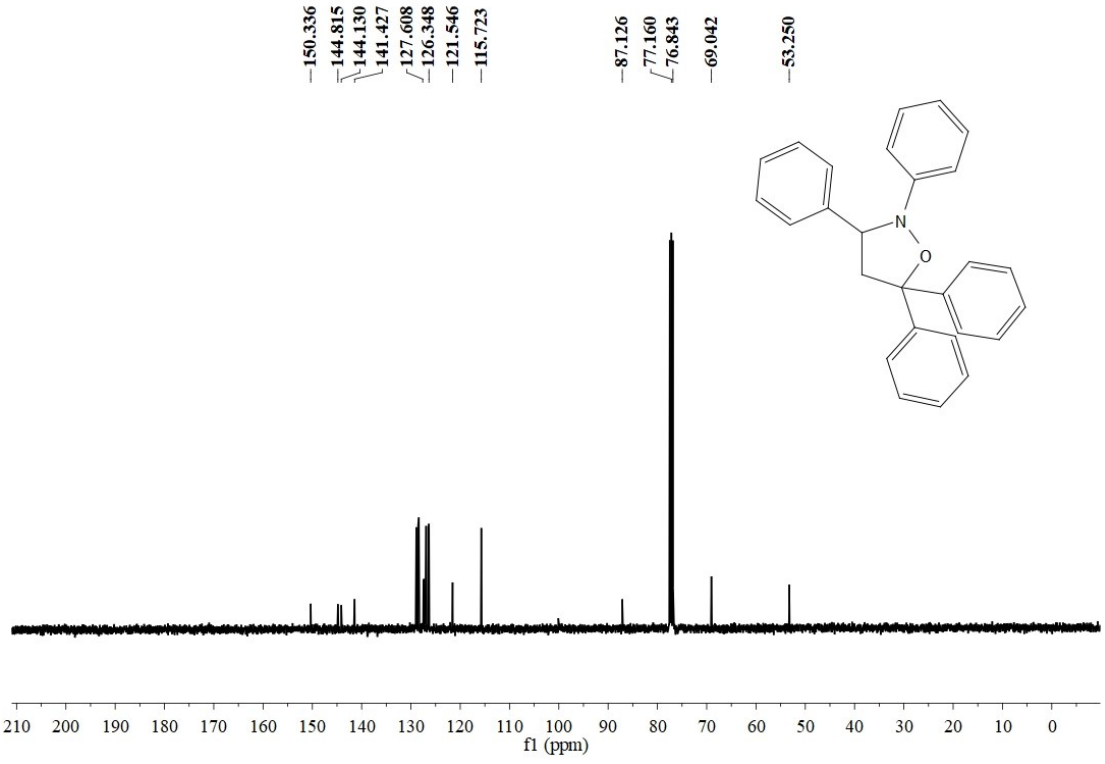
4aap + 4a'a'p'


7.494
7.475
7.376
7.358
7.338
7.281
7.263
7.245
7.241
7.210
7.206
6.985
6.982
6.963
6.961
6.893
6.875
4.758
4.738
4.134
4.121
2.848
2.841
2.828
1.989
1.618
1.491
1.366
0.895
0.878
0.860
fl (ppm)
fl (ppm)
fl (ppm)

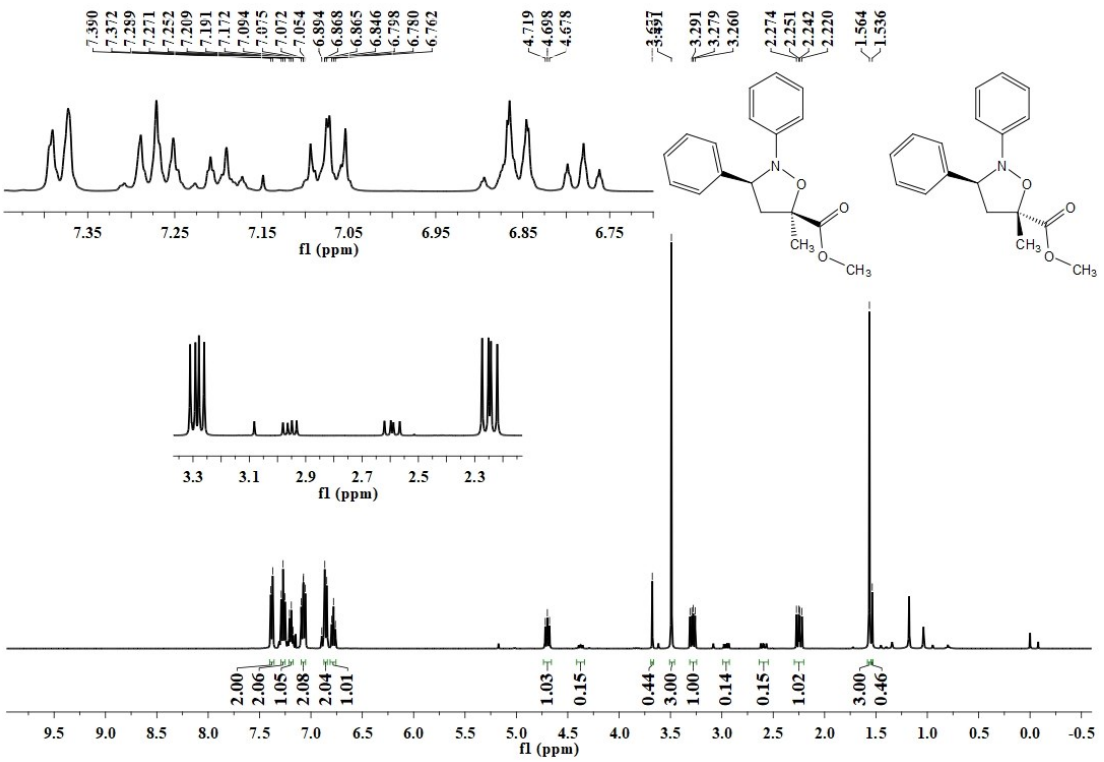

153.004
143.493
128.927
128.833
127.276
125.680
121.108
115.331
113.863
79.233
77.949
77.478
77.160
76.842
71.217
69.491
46.672
29.849
29.810
29.767
29.667
26.699
22.841
14.281
fl (ppm)

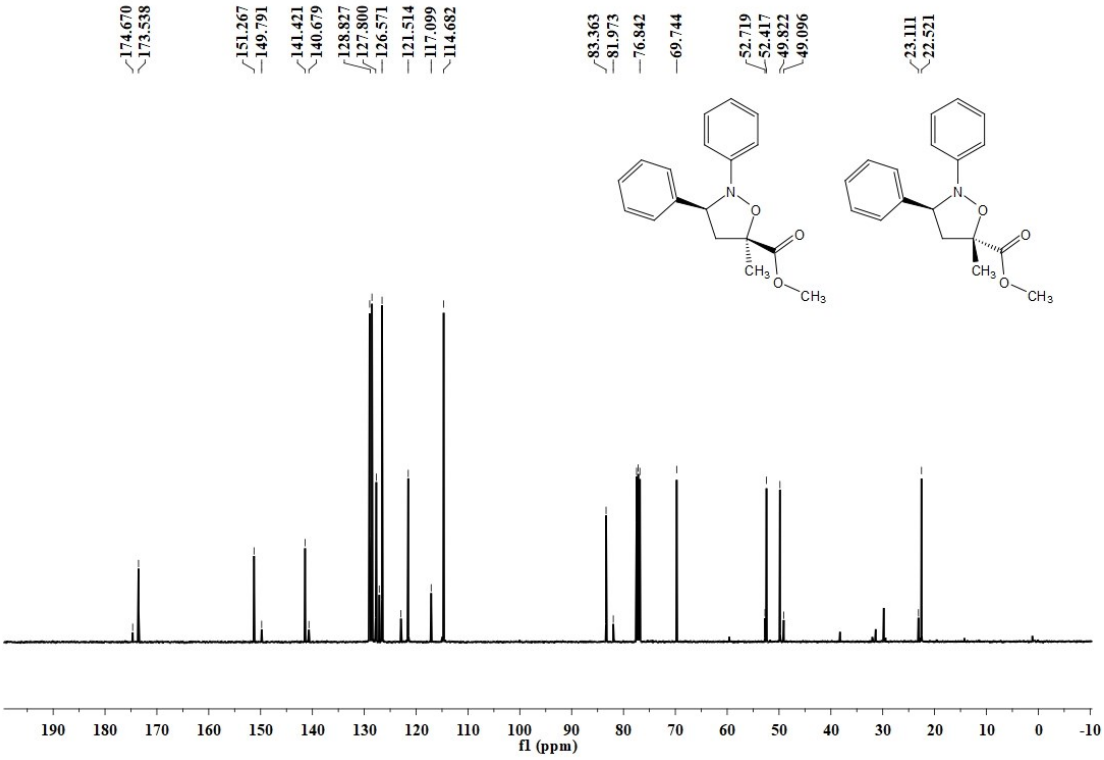
4aaq


7.541
7.537
7.519
7.483
7.480
7.462
7.335
7.317
7.298
7.286
7.269
7.246
7.232
7.199
7.183
7.162
7.143
6.997
6.978
6.901
6.882
6.864
4.652
4.632
4.611
3.537
3.527
3.506
3.199
3.179
3.168
3.148
7.29
7.27
7.25
7.23
7.21
f1 (ppm)
N
O
2.25
2.21
2.99
6.16
2.08
2.04
1.98
0.98
1.00
1.00
1.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

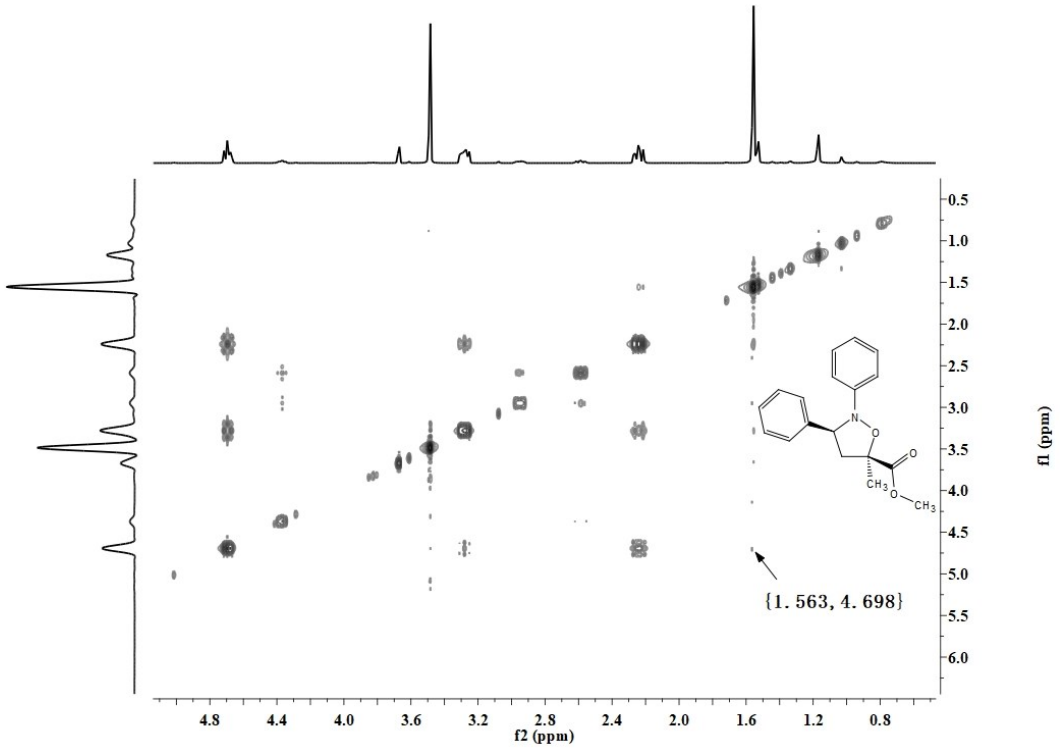

150.336
144.815
144.130
141.427
127.608
126.348
121.546
115.723
87.126
77.160
76.843
69.042
53.250
N
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

4aar

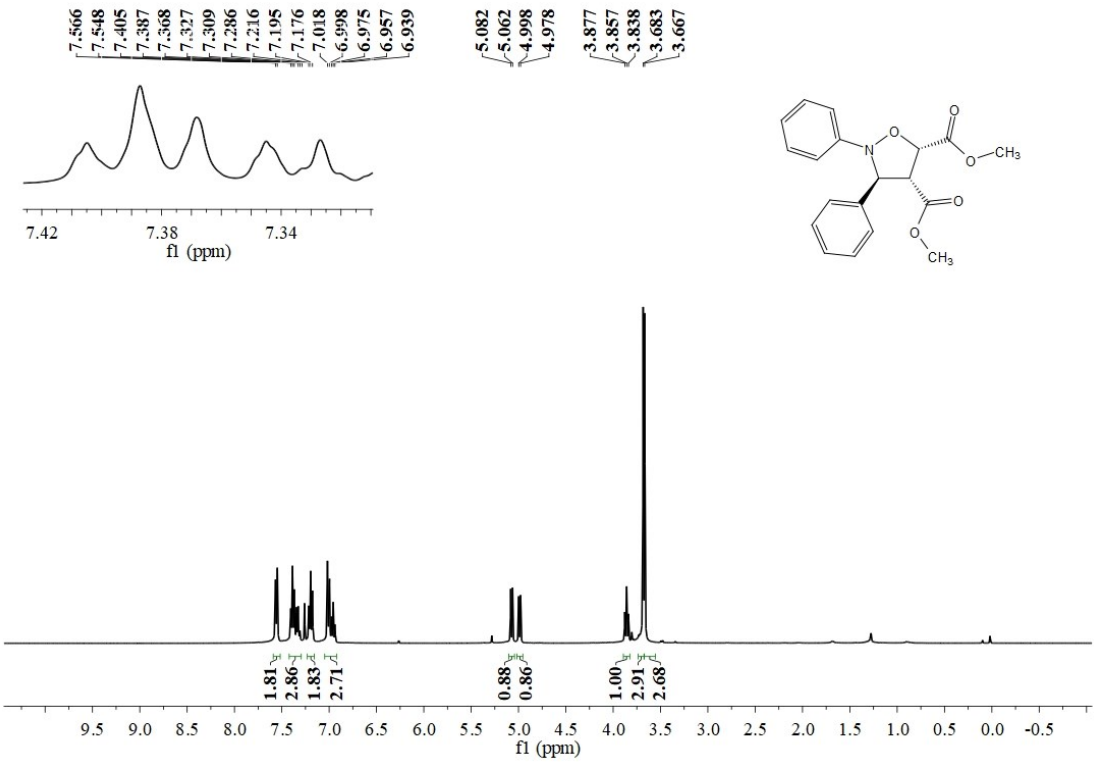

7.390
7.372
7.289
7.271
7.252
7.209
7.191
7.172
7.094
7.075
7.072
7.054
6.894
6.868
6.865
6.846
6.798
6.780
6.762
4.719
4.698
4.678
3.677
3.651
3.291
3.279
3.260
2.274
2.251
2.242
2.220
1.564
1.536
fl (ppm)
2.00
2.06
1.05
2.08
2.04
1.01
1.03
0.15
0.44
3.00
1.00
0.14
0.15
1.02
3.00
0.46

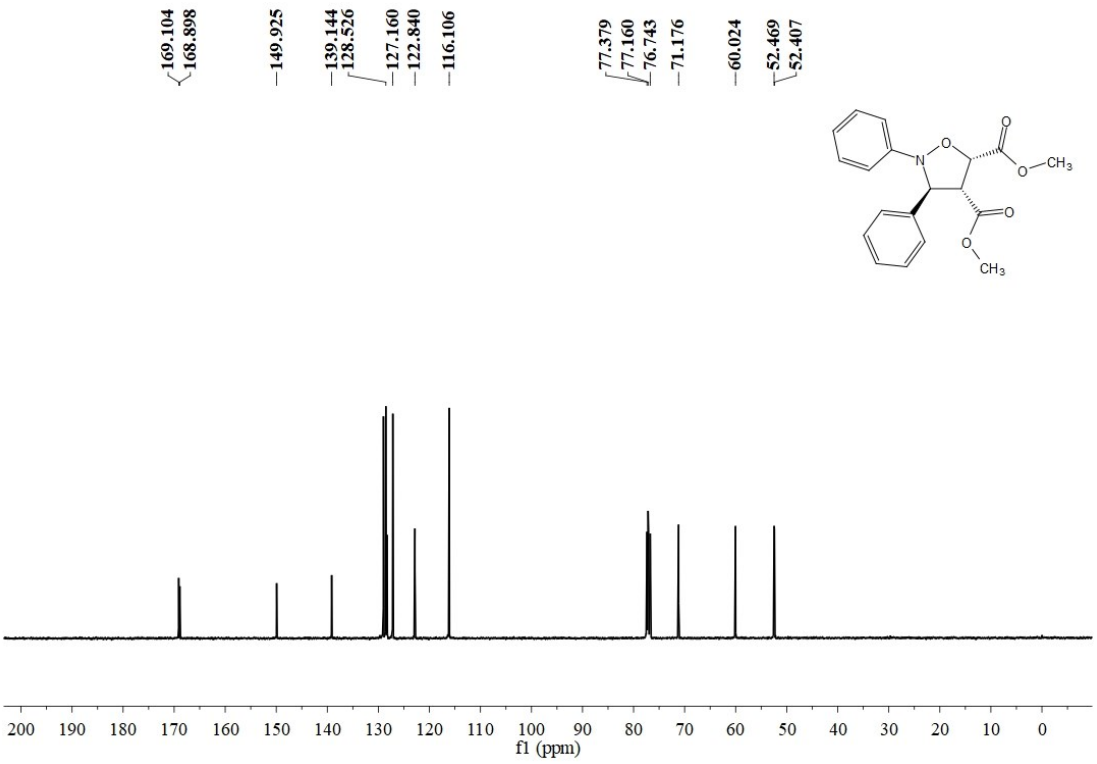

174.670
173.538
151.267
149.791
141.421
140.679
128.827
127.800
126.571
121.514
117.099
114.682
83.363
81.973
76.842
69.744
52.719
52.417
49.822
49.096
23.111
22.521
fl (ppm)

Confirmation of relative configuration of 4aar via nuclear overhauser effect spectroscopy (NOESY)

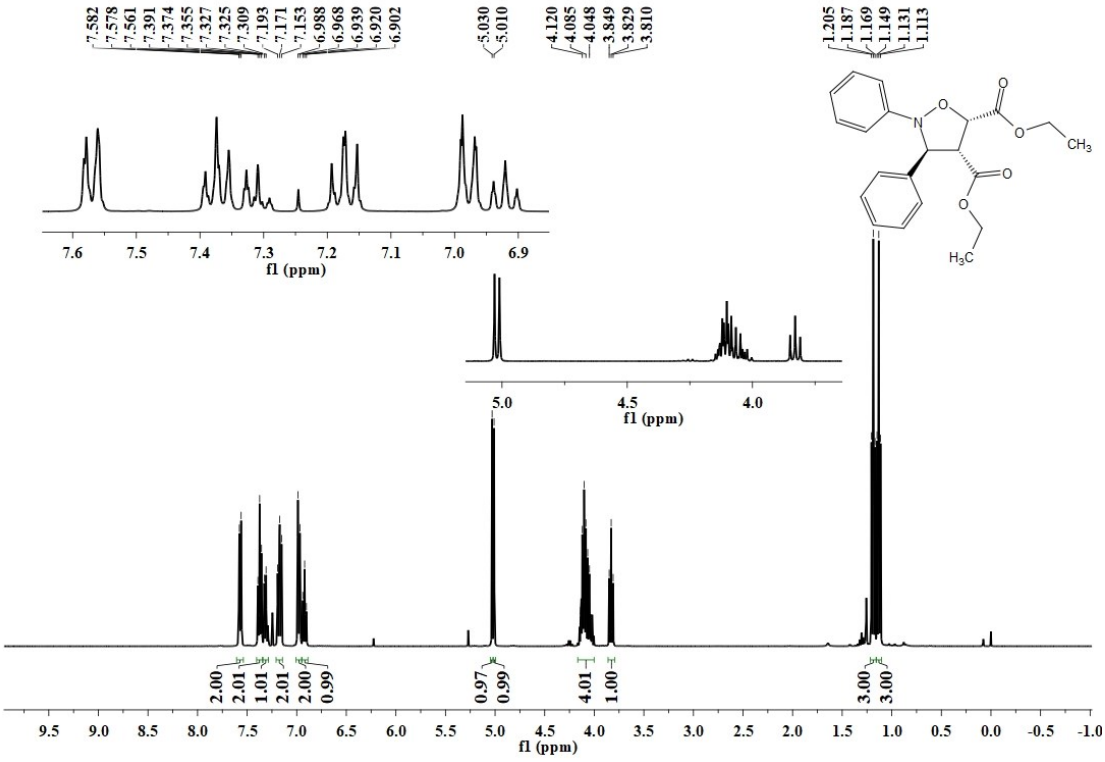


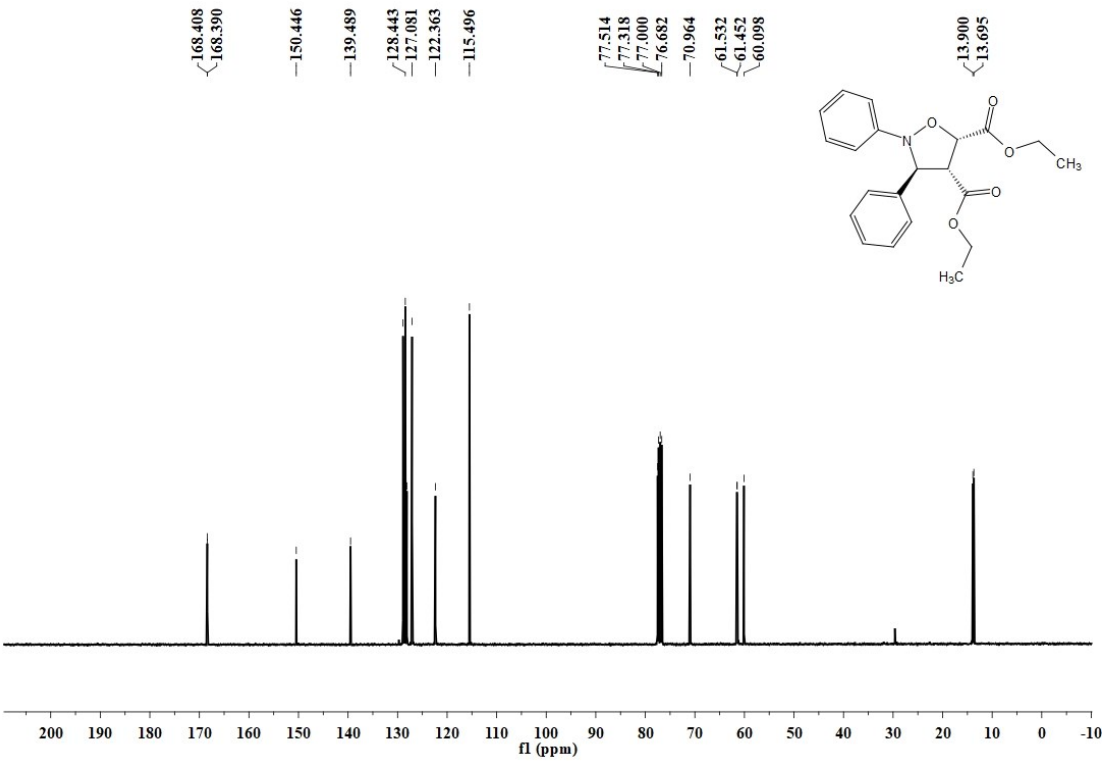
4aas


7.566
7.548
7.405
7.387
7.368
7.327
7.309
7.286
7.216
7.195
7.176
7.018
6.998
6.975
6.957
6.939
5.082
5.062
4.998
4.978
3.877
3.857
3.838
3.683
3.667
7.42
7.38
7.34
f1 (ppm)
1.81
2.86
1.83
2.71
0.88
0.86
1.00
2.91
2.68
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

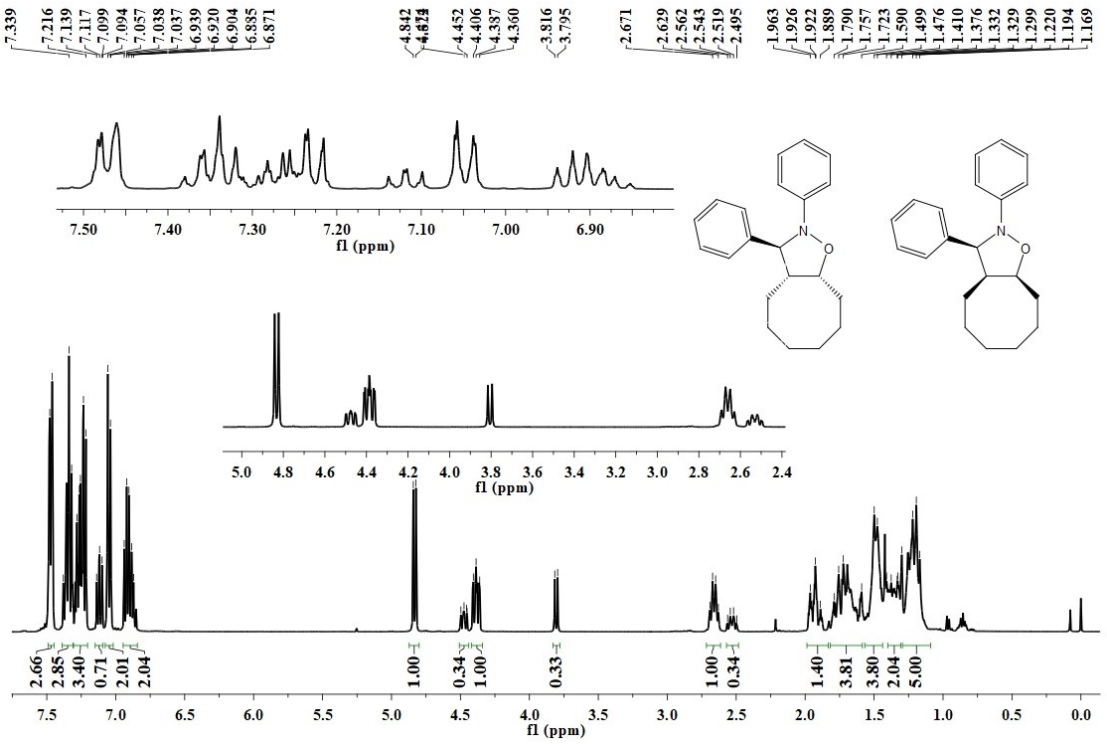

169.104
168.898
149.925
139.144
128.526
127.160
122.840
116.106
77.379
77.160
76.743
71.176
60.024
52.469
52.407
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

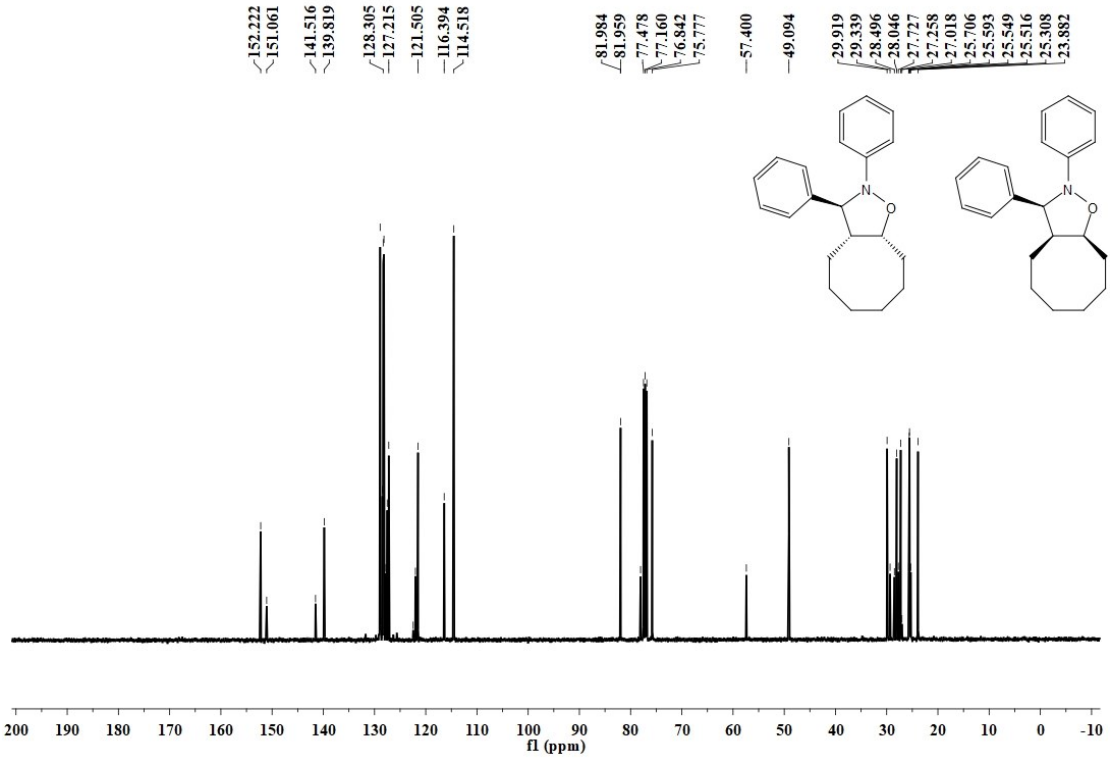
4aat


7.582
7.578
7.561
7.391
7.374
7.355
7.327
7.325
7.309
7.193
7.171
7.153
6.988
6.968
6.939
6.920
6.902
5.030
5.010
4.120
4.085
4.048
3.849
3.829
3.810
1.205
1.187
1.169
1.149
1.131
1.113
f1 (ppm)
2.00
2.01
1.01
2.01
2.00
0.99
0.97
0.99
4.01
1.00
3.00
3.00

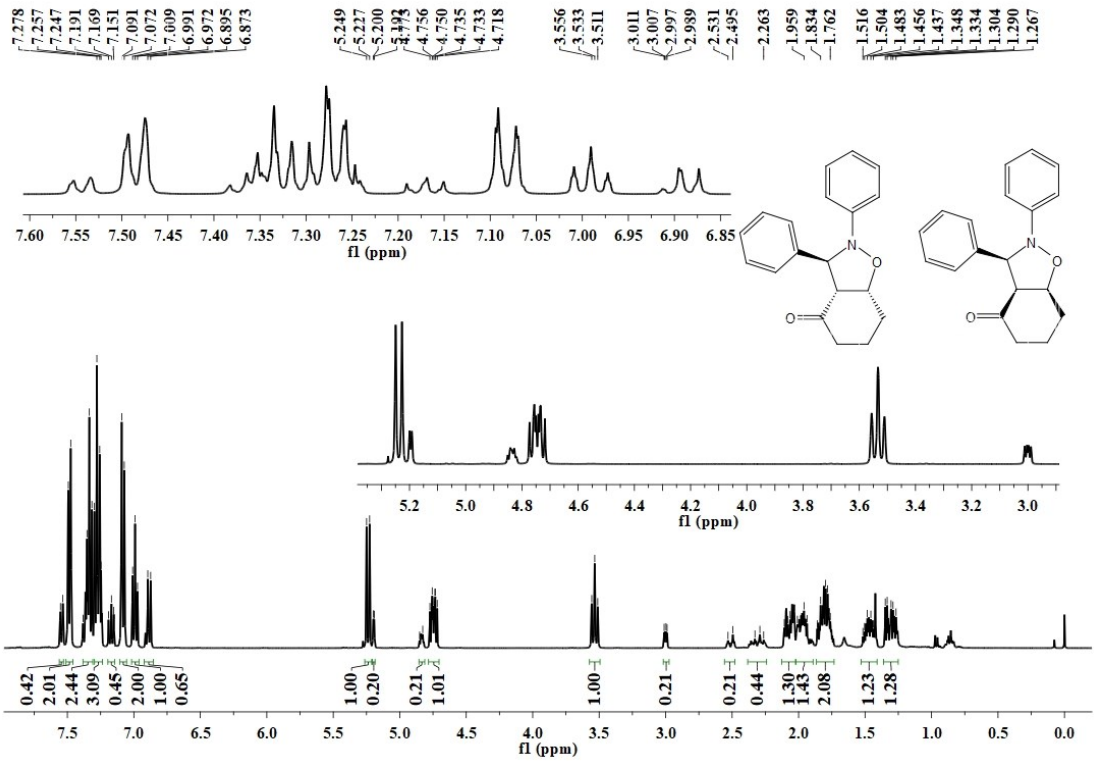

168.408
168.390
150.446
139.489
128.443
127.081
122.363
115.496
77.514
77.318
77.000
76.682
70.964
61.532
61.452
60.098
13.900
13.695
f1 (ppm)

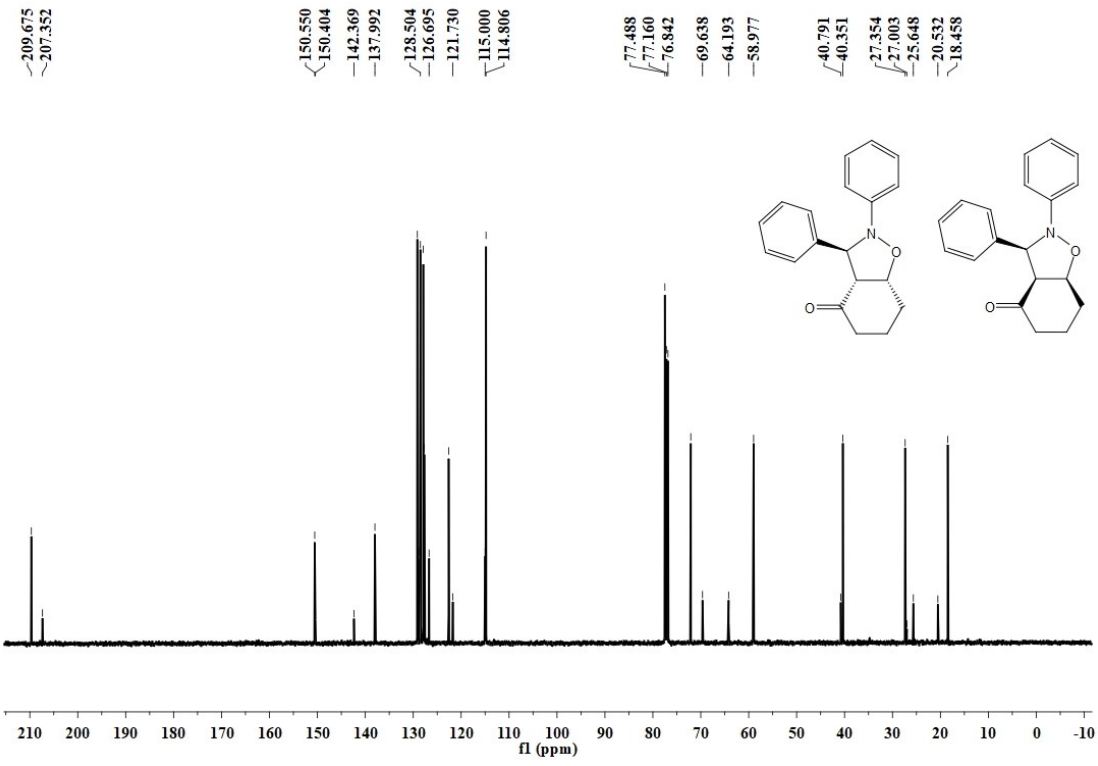
4aau


7.339
7.216
7.139
7.117
7.099
7.094
7.057
7.038
7.037
6.939
6.920
6.904
6.885
6.871
4.842
4.824
4.452
4.406
4.387
4.360
3.816
3.795
2.671
2.629
2.562
2.543
2.519
2.495
1.963
1.926
1.922
1.889
1.790
1.757
1.723
1.590
1.499
1.476
1.410
1.376
1.332
1.329
1.299
1.220
1.194
1.169
f1 (ppm)
2.66
2.85
3.40
0.71
2.01
2.04
1.00
0.34
1.00
0.33
1.00
0.34
1.40
3.81
3.80
2.04
5.00

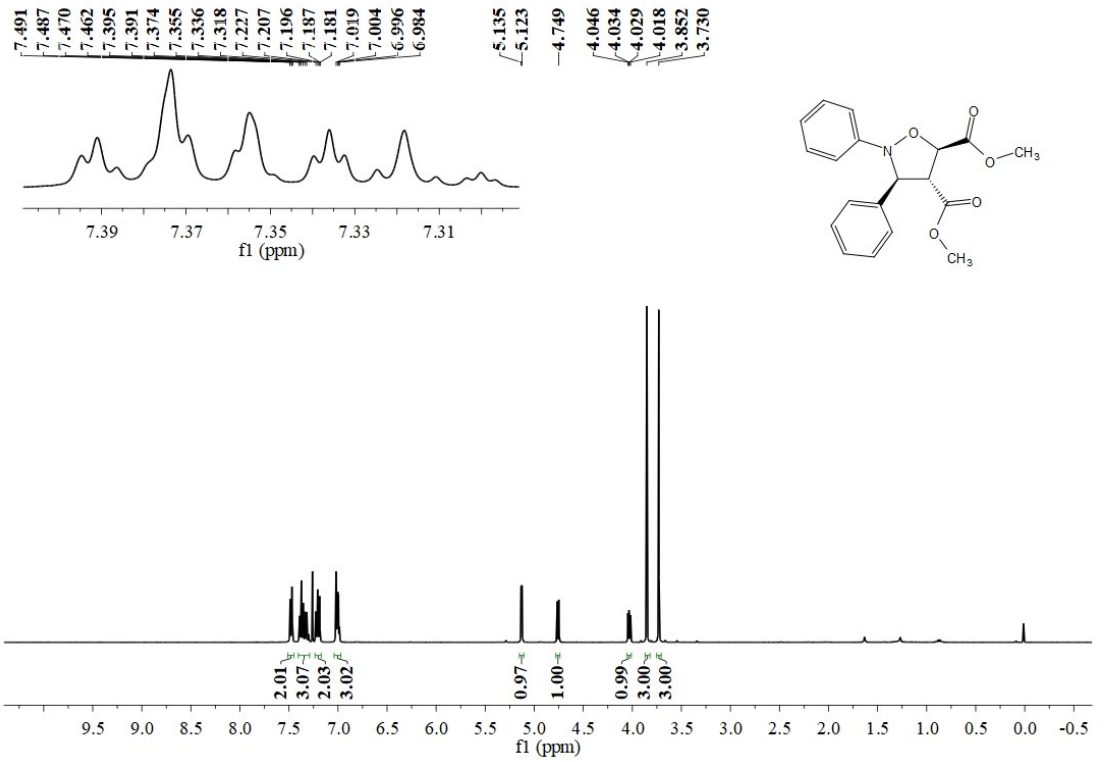

152.222
151.061
141.516
139.819
128.305
127.215
121.505
116.394
114.518
81.984
81.959
77.478
77.160
76.842
75.777
57.400
49.094
29.919
29.339
28.496
28.046
27.727
27.258
27.018
25.706
25.593
25.549
25.516
25.308
23.882
f1 (ppm)

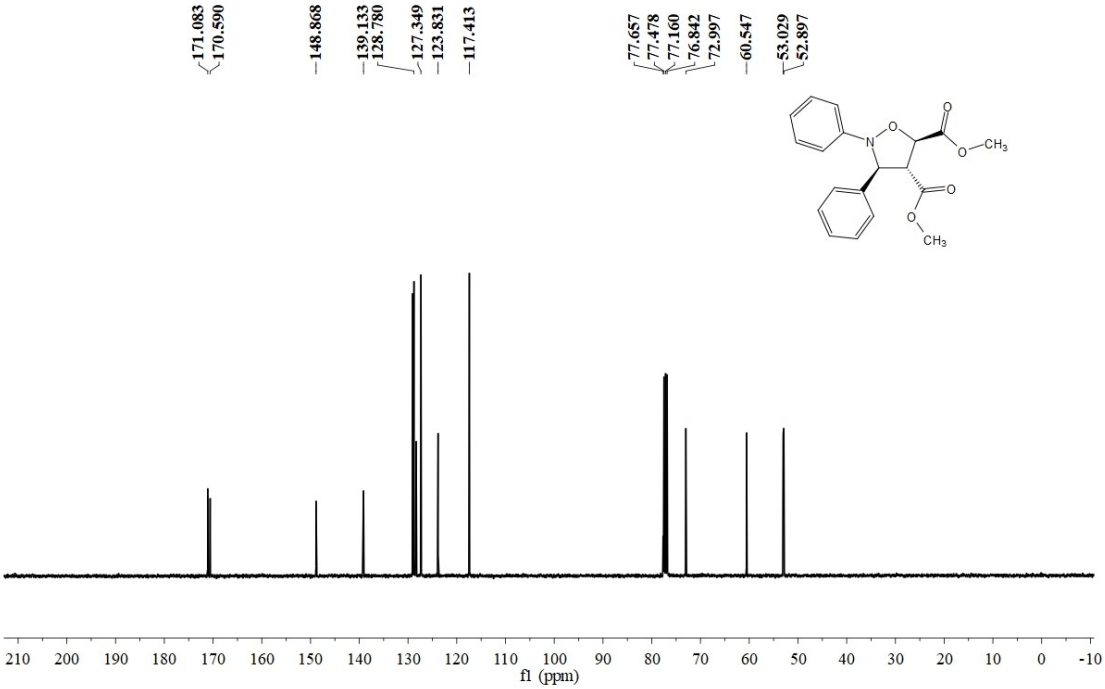
4aav



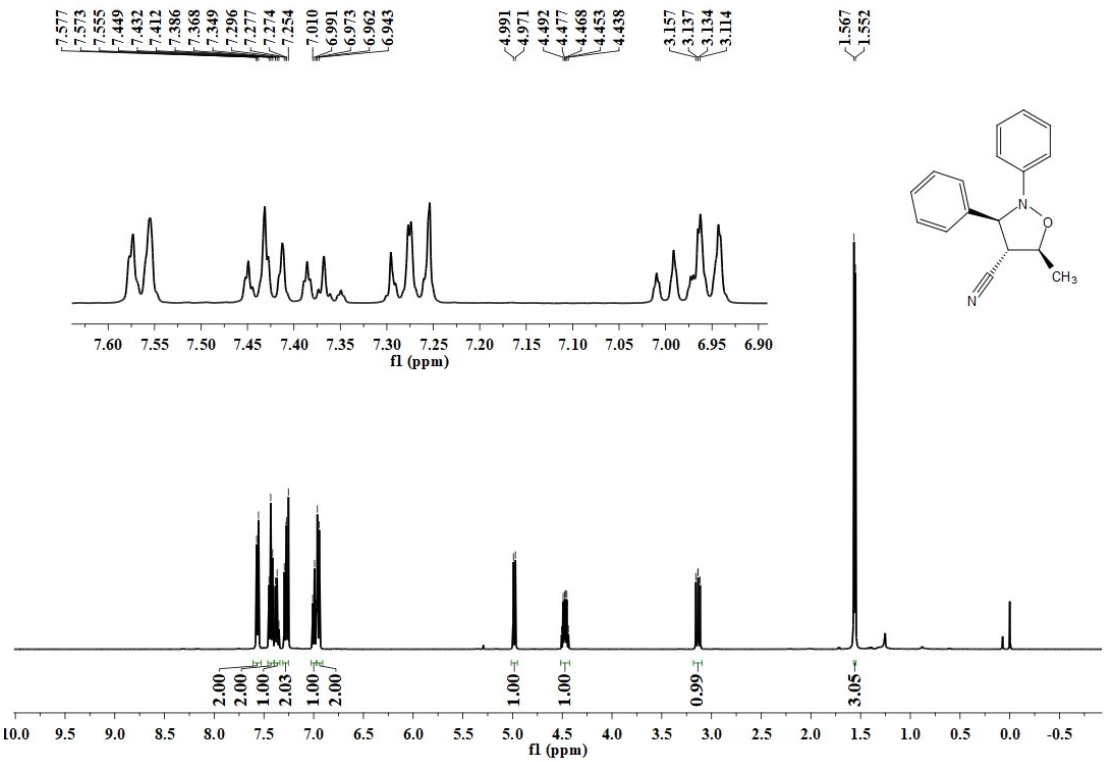


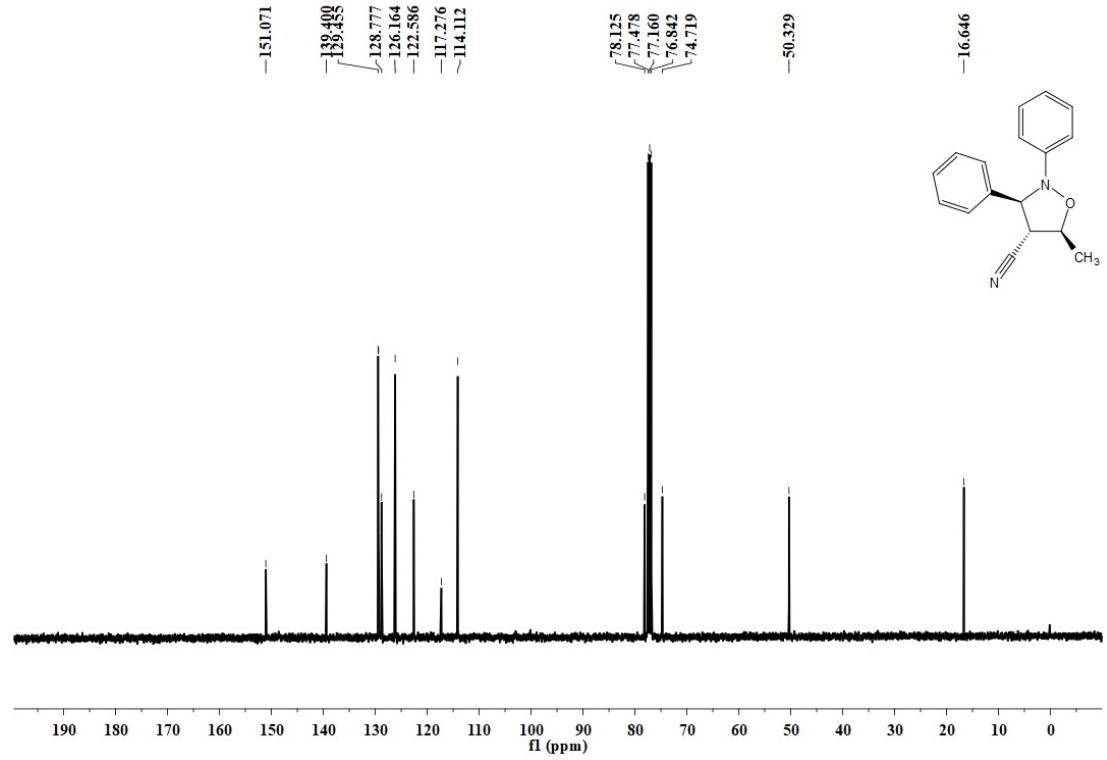
4aaw


7.491
7.487
7.470
7.462
7.395
7.391
7.374
7.355
7.336
7.318
7.227
7.207
7.196
7.187
7.181
7.019
7.004
6.996
6.984
5.135
5.123
4.749
4.046
4.034
4.029
4.018
3.852
3.730
7.39
7.37
7.35
7.33
7.31
f1 (ppm)
2.01
3.07
2.03
3.02
0.97
1.00
0.99
3.00
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

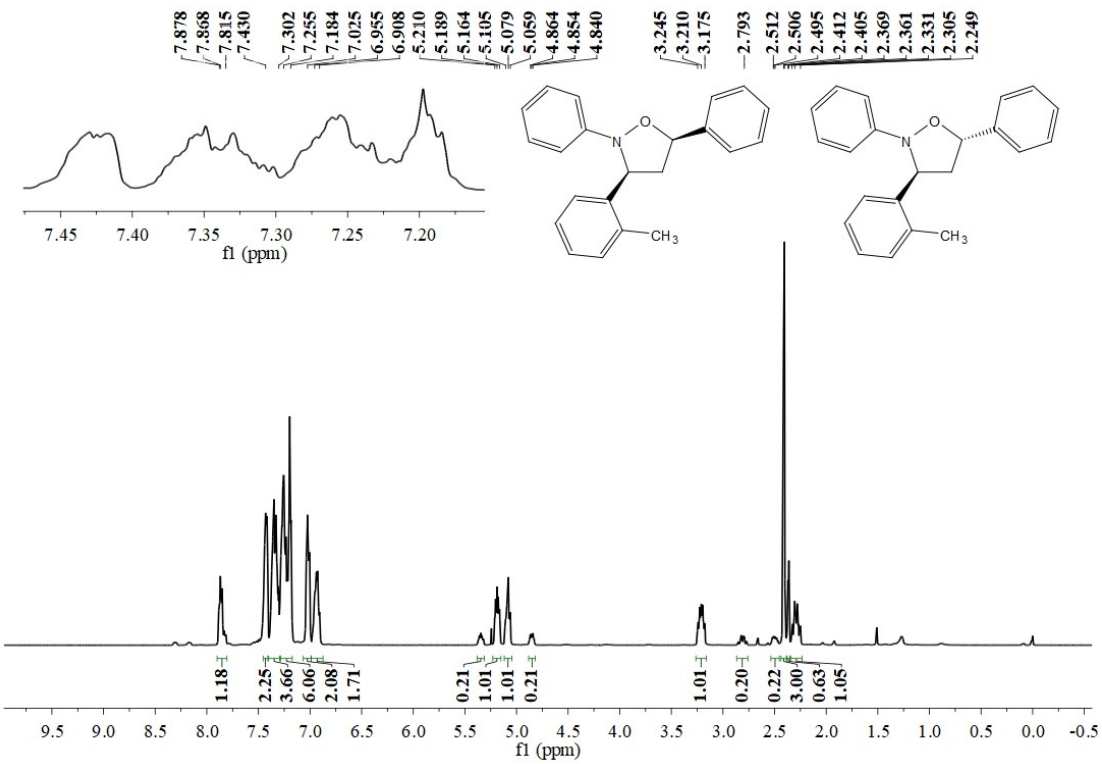

171.083
170.590
148.868
139.133
128.780
127.349
123.831
117.413
77.657
77.478
77.160
76.842
72.997
60.547
53.029
52.897
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

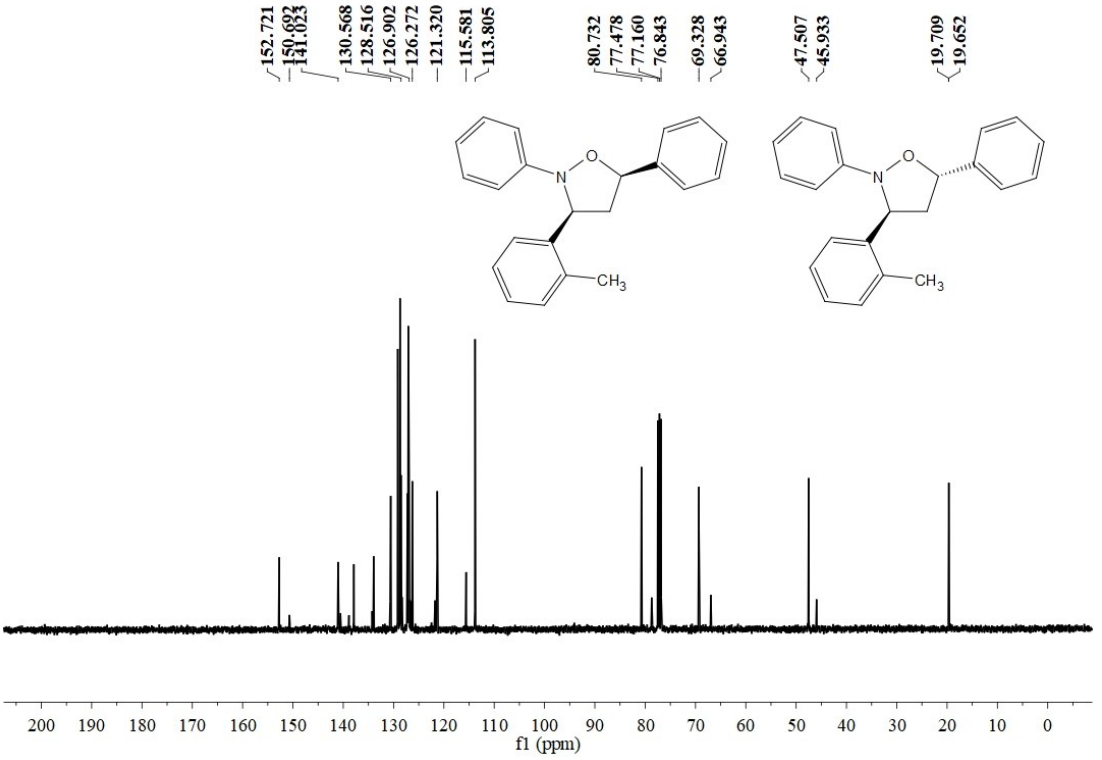
4aax


7.577
7.573
7.555
7.449
7.432
7.412
7.386
7.368
7.349
7.296
7.277
7.274
7.254
7.010
6.991
6.973
6.962
6.943
4.991
4.971
4.492
4.477
4.468
4.453
4.438
3.157
3.137
3.134
3.114
1.567
1.552
2.00
2.00
1.00
2.03
1.00
2.00
1.00
1.00
0.99
3.05
f1 (ppm)
CH3
N
O

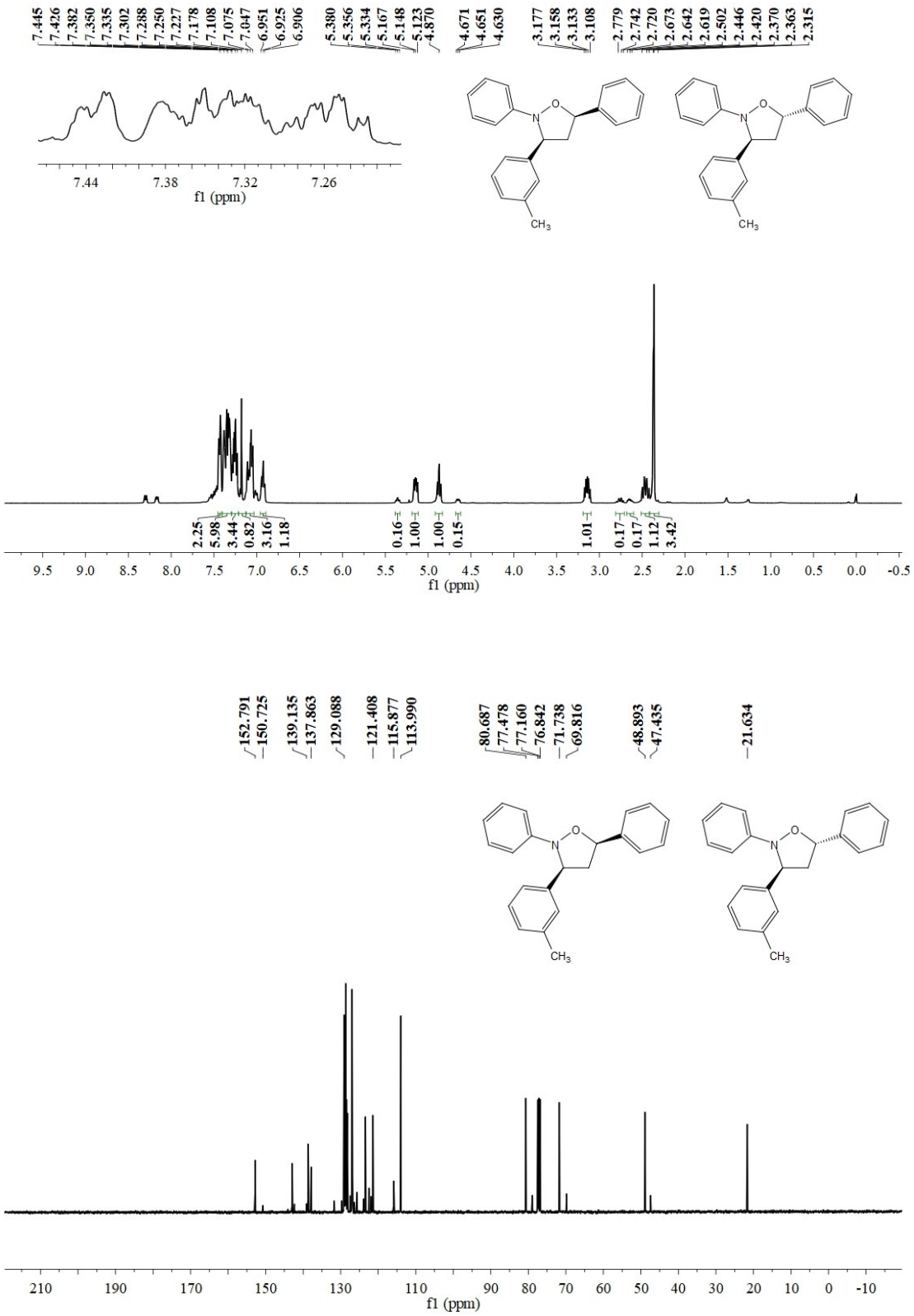

151.071
139.400
139.455
129.455
128.777
126.164
122.586
117.276
114.112
78.125
77.478
77.160
76.842
74.719
50.329
16.646
f1 (ppm)
CH3
N
O

4aba + 4a'b'a'

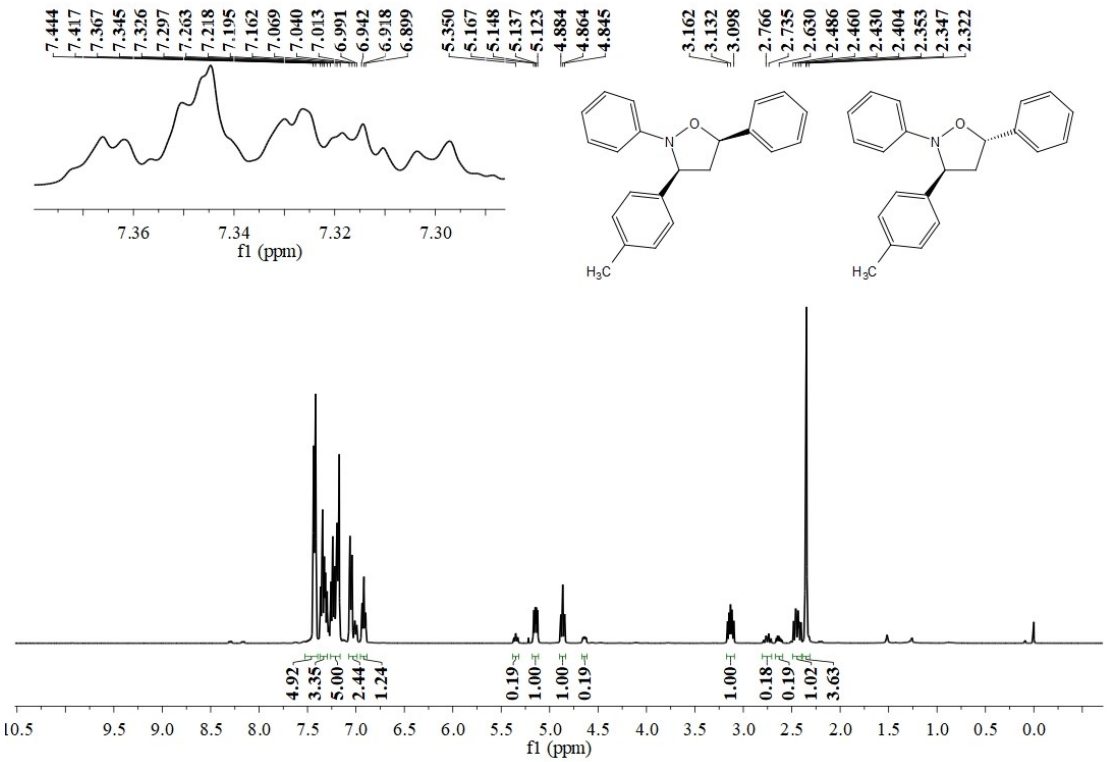

7.878
7.868
7.815
7.430
7.302
7.255
7.184
7.025
6.955
6.908
5.210
5.189
5.164
5.105
5.079
5.059
4.864
4.854
4.840
3.245
3.210
3.175
2.793
2.512
2.506
2.495
2.412
2.405
2.369
2.361
2.331
2.305
2.249
CH3
CH3
f1 (ppm)
1.18
2.25
3.66
6.06
2.08
1.71
0.21
1.01
1.01
0.21
1.01
0.20
0.22
3.00
0.63
1.05
f1 (ppm)

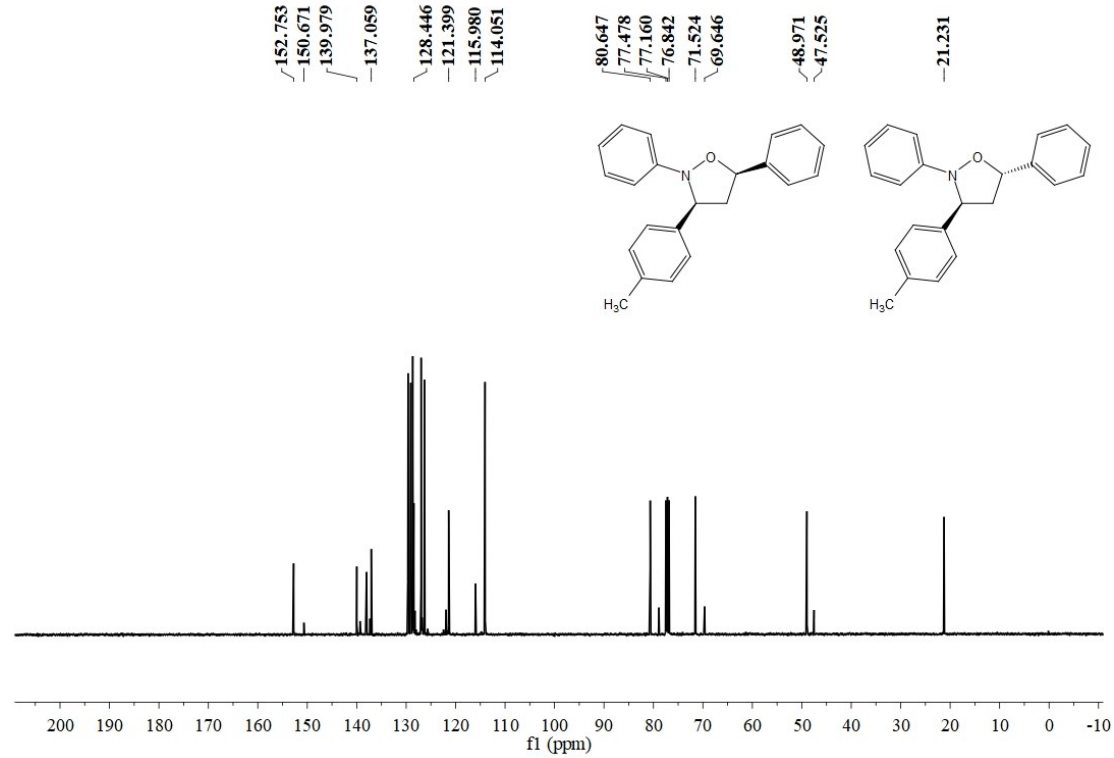

152.721
150.683
141.023
130.568
128.516
126.902
126.272
121.320
115.581
113.805
80.732
77.478
77.160
76.843
69.328
66.943
47.507
45.933
19.709
19.652
CH3
CH3
f1 (ppm)

4aca + 4a'c'a'

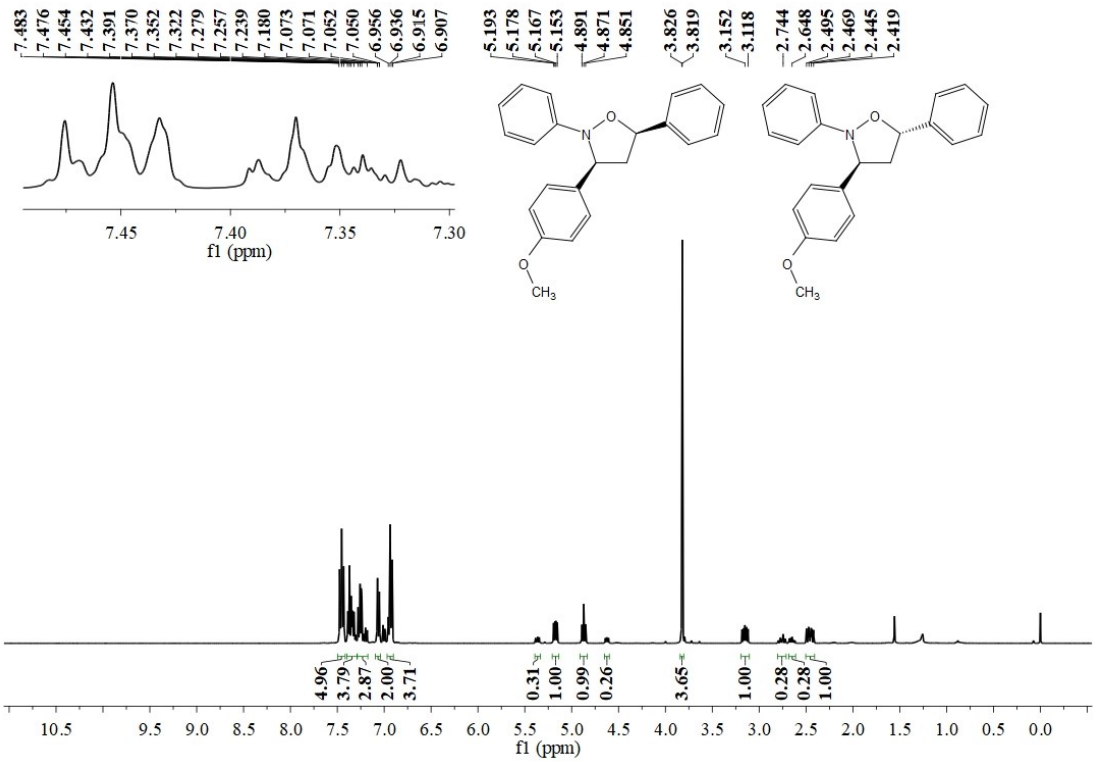

7.445
7.426
7.382
7.350
7.335
7.302
7.288
7.250
7.227
7.178
7.108
7.075
7.047
6.951
6.925
6.906
5.380
5.356
5.334
5.167
5.148
5.123
4.870
4.671
4.651
4.630
3.177
3.158
3.133
3.108
2.779
2.742
2.720
2.673
2.642
2.619
2.502
2.446
2.420
2.370
2.363
2.315
7.44
7.38
7.32
7.26
f1 (ppm)
CH3
CH3
2.25
5.98
3.44
0.82
3.16
1.18
0.16
1.00
1.00
0.15
1.01
0.17
0.17
1.12
3.42
f1 (ppm)
152.791
150.725
139.135
137.863
129.088
121.408
115.877
113.990
80.687
77.478
77.160
76.842
71.738
69.816
48.893
47.435
21.634
CH3
CH3
f1 (ppm)

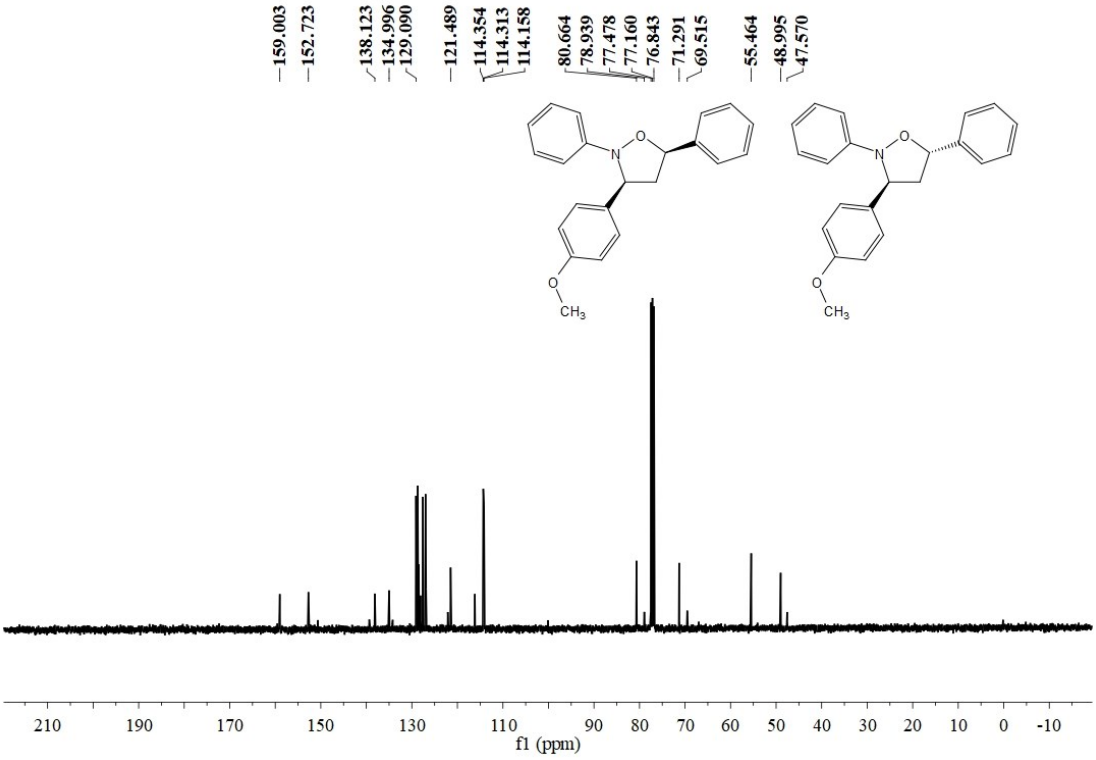
4ada + 4a'd'a'


7.444
7.417
7.367
7.345
7.326
7.297
7.263
7.218
7.195
7.162
7.069
7.040
7.013
6.991
6.942
6.918
6.899
5.350
5.167
5.148
5.137
5.123
4.884
4.864
4.845
3.162
3.132
3.098
2.766
2.735
2.630
2.486
2.460
2.430
2.404
2.353
2.347
2.322
7.36
7.34
7.32
7.30
f1 (ppm)
H3C
4.92
3.35
5.00
2.44
1.24
0.19
1.00
1.00
0.19
1.00
0.18
0.19
1.02
3.63
f1 (ppm)

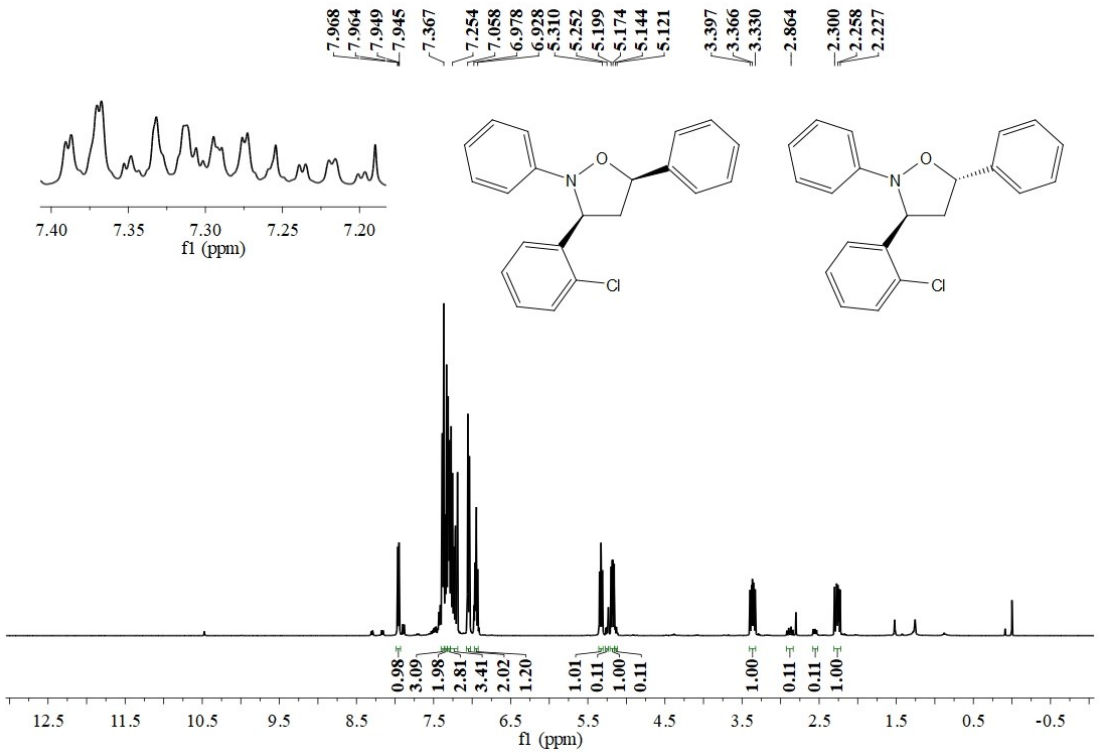

152.753
150.671
139.979
137.059
128.446
121.399
115.980
114.051
80.647
77.478
77.160
76.842
71.524
69.646
48.971
47.525
21.231
H3C
f1 (ppm)

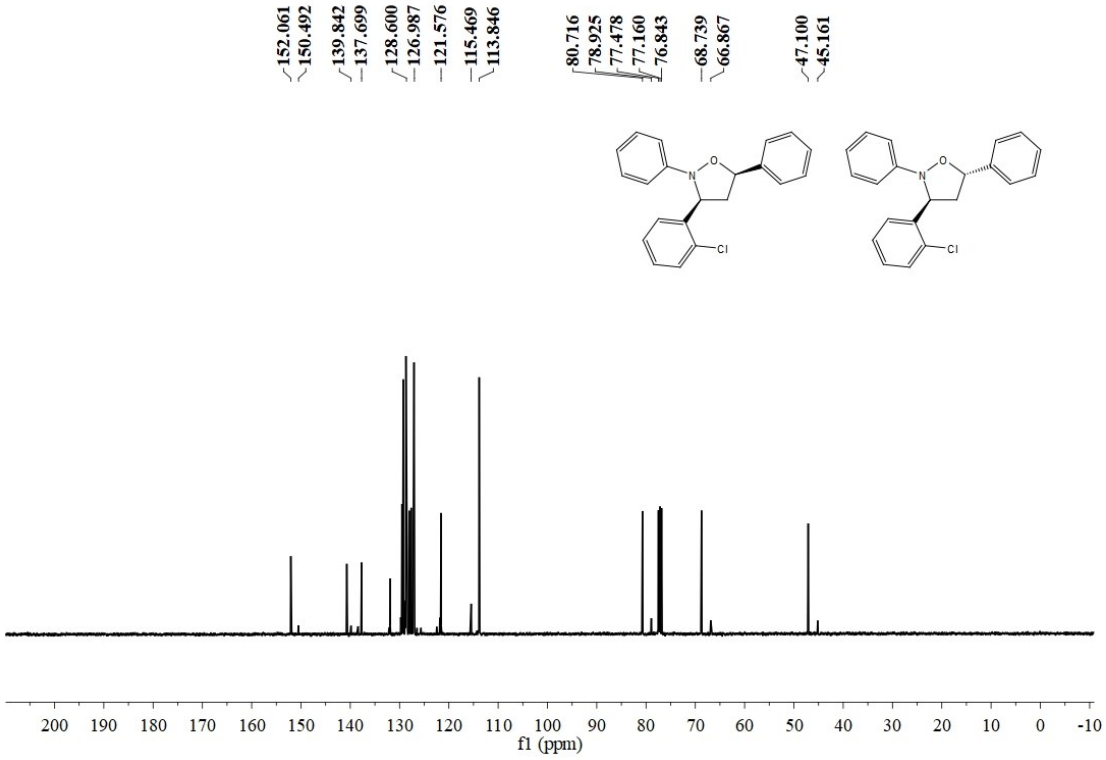
4aea + 4a'e'a'


7.483
7.476
7.454
7.432
7.391
7.370
7.352
7.322
7.279
7.257
7.239
7.180
7.073
7.071
7.052
7.050
6.956
6.936
6.915
6.907
5.193
5.178
5.167
5.153
4.891
4.871
4.851
3.826
3.819
3.152
3.118
2.744
2.648
2.495
2.469
2.445
2.419
7.45
7.40
7.35
7.30
f1 (ppm)
O
CH3
4.96
3.79
2.87
2.00
3.71
0.31
1.00
0.99
0.26
3.65
1.00
0.28
0.28
1.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

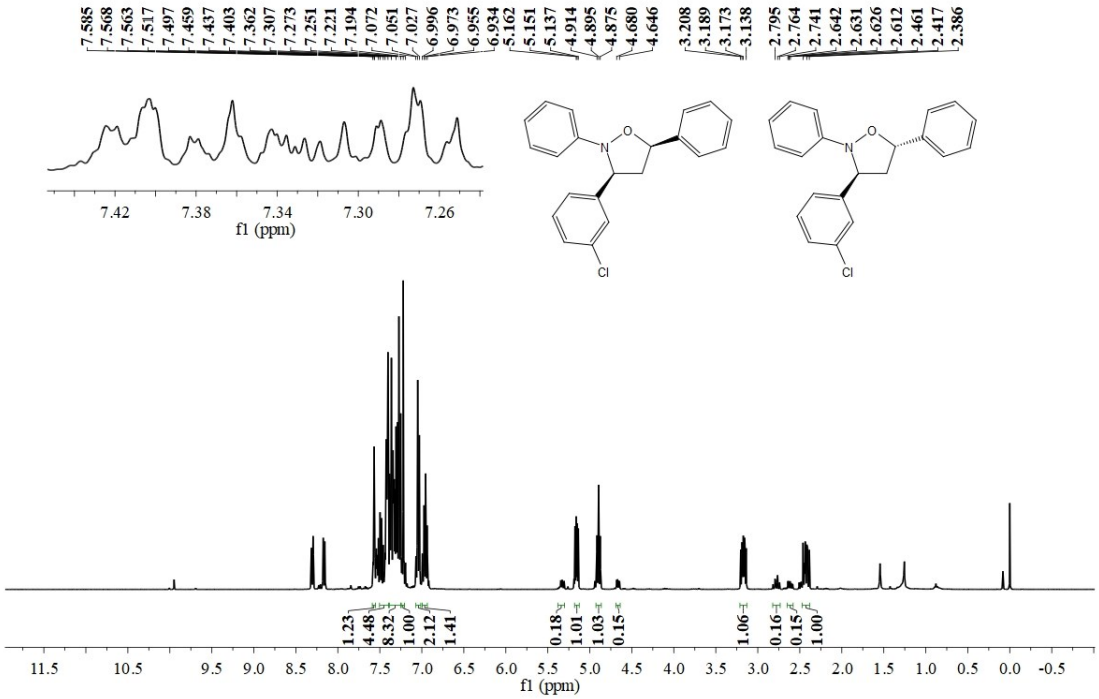

159.003
152.723
138.123
134.996
129.090
121.489
114.354
114.313
114.158
80.664
78.939
77.478
77.160
76.843
71.291
69.515
55.464
48.995
47.570
O
CH3
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

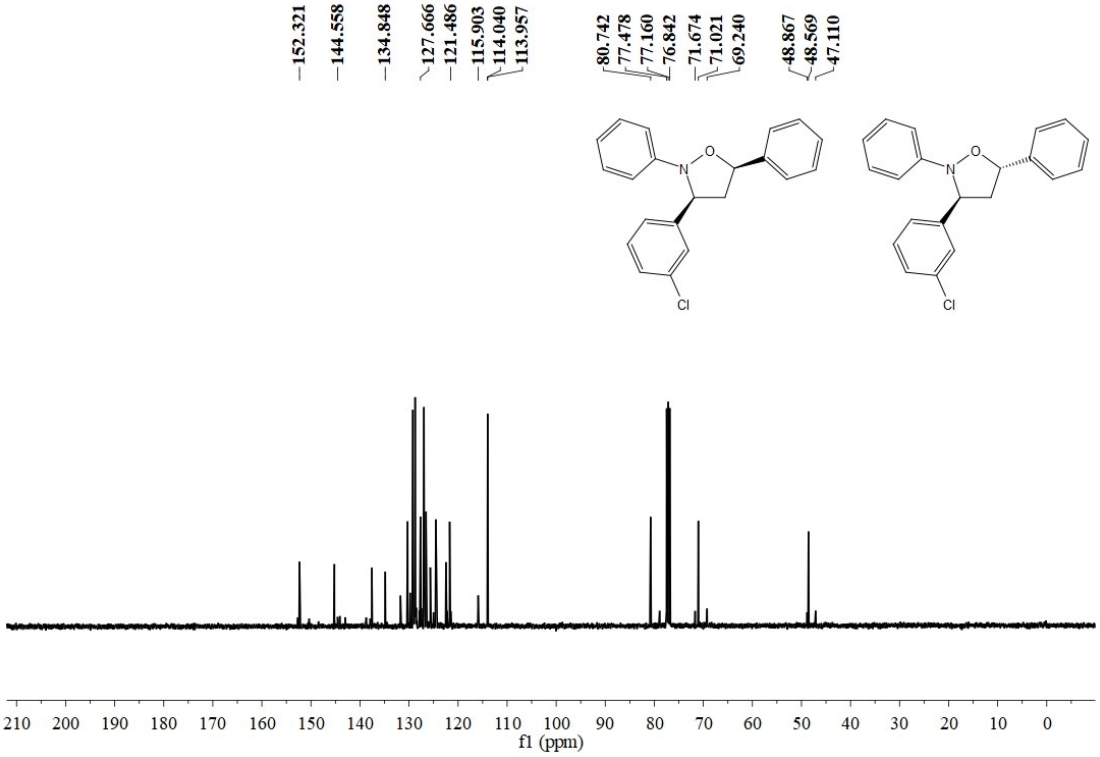
4afa + 4a'f'a'


7.968
7.964
7.949
7.945
7.367
7.254
7.058
6.978
6.928
5.310
5.252
5.199
5.174
5.144
5.121
3.397
3.366
3.330
2.864
2.300
2.258
2.227
7.40
7.35
7.30
7.25
7.20
f1 (ppm)
N
O
Cl
0.98
3.09
1.98
2.81
3.41
2.02
1.20
1.01
0.11
1.00
0.11
1.00
0.11
0.11
1.00
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

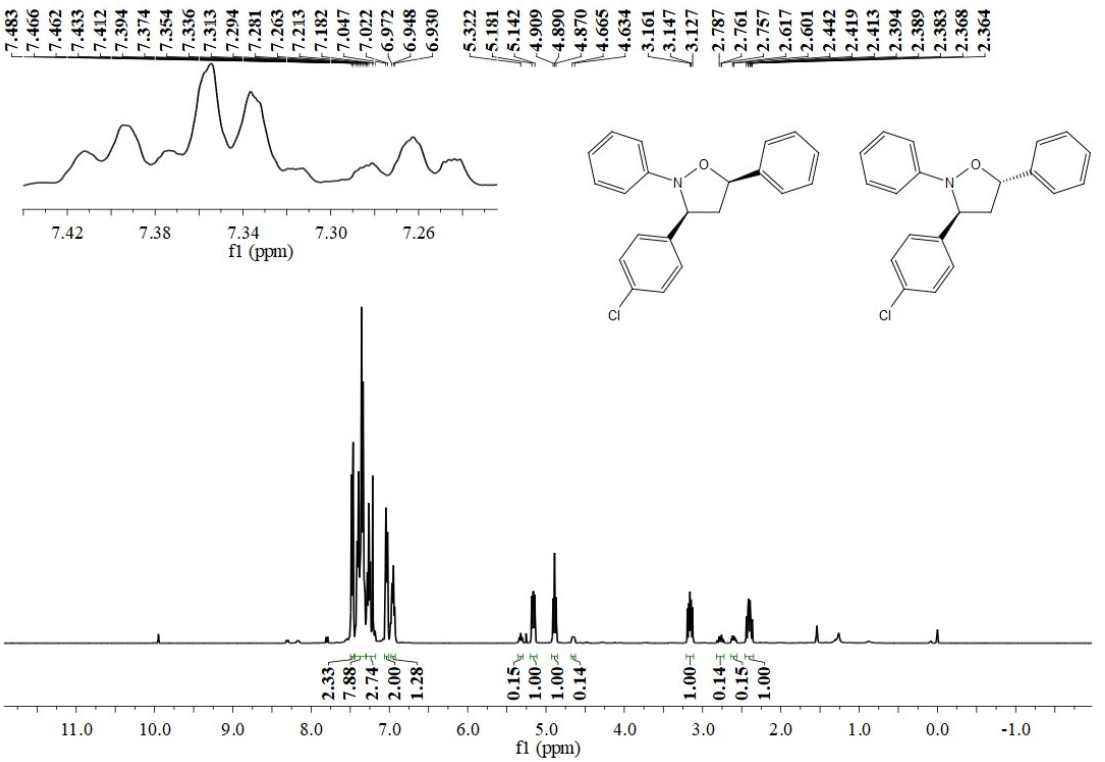

152.061
150.492
139.842
137.699
128.600
126.987
121.576
115.469
113.846
80.716
78.925
77.478
77.160
76.843
68.739
66.867
47.100
45.161
N
O
Cl
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

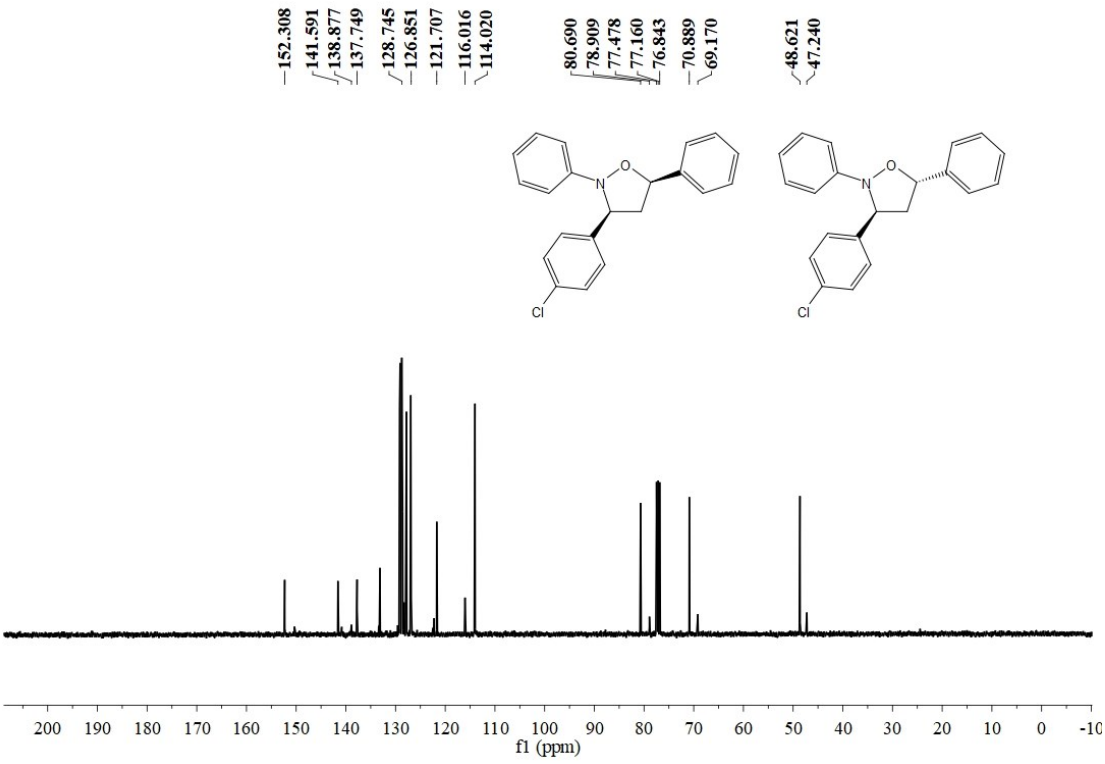
4aga + 4a'g'a'


7.585
7.568
7.563
7.517
7.497
7.459
7.437
7.403
7.362
7.307
7.273
7.251
7.221
7.194
7.072
7.051
7.027
6.996
6.973
6.955
6.934
5.162
5.151
5.137
4.914
4.895
4.875
4.680
4.646
3.208
3.189
3.173
3.138
2.795
2.764
2.741
2.642
2.631
2.626
2.612
2.461
2.417
2.386
7.42
7.38
7.34
7.30
7.26
f1 (ppm)
Cl
Cl
1.23
4.48
8.32
1.00
2.12
1.41
0.18
1.01
1.03
0.15
1.06
0.16
0.15
1.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

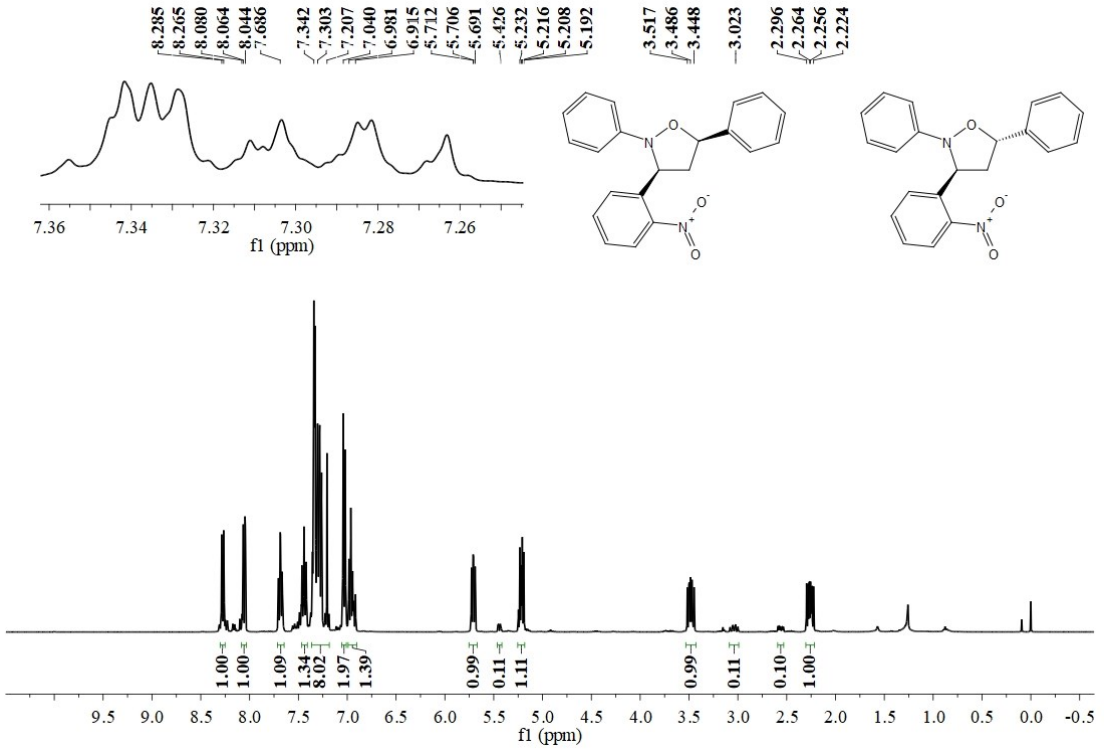

152.321
144.558
134.848
127.666
121.486
115.903
114.040
113.957
80.742
77.478
77.160
76.842
71.674
71.021
69.240
48.867
48.569
47.110
Cl
Cl
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

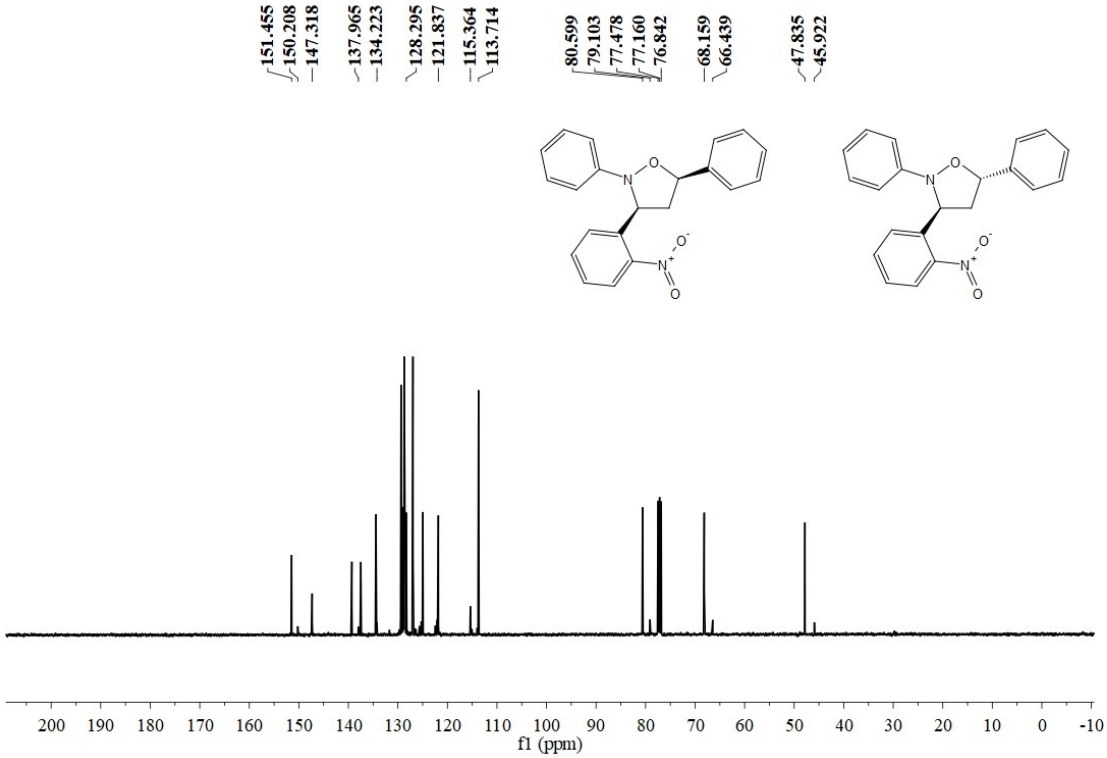
4aha + 4a'h'a'


7.483
7.466
7.462
7.433
7.412
7.394
7.374
7.354
7.336
7.313
7.294
7.281
7.263
7.213
7.182
7.047
7.022
6.972
6.948
6.930
5.322
5.181
5.142
4.909
4.890
4.870
4.665
4.634
3.161
3.147
3.127
2.787
2.761
2.757
2.617
2.601
2.442
2.419
2.413
2.394
2.389
2.383
2.368
2.364
7.42
7.38
7.34
7.30
7.26
f1 (ppm)
N
O
Cl
2.33
7.88
2.74
2.00
1.28
0.15
1.00
1.00
0.14
1.00
0.14
0.15
1.00
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)

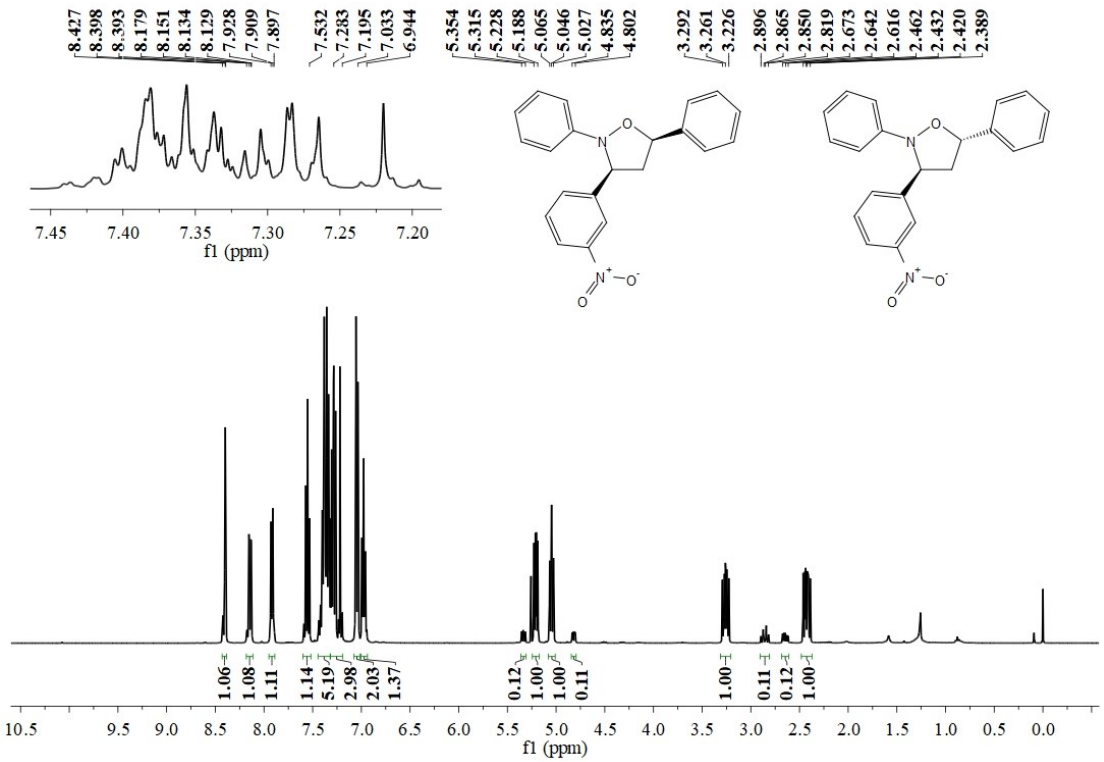

152.308
141.591
138.877
137.749
128.745
126.851
121.707
116.016
114.020
80.690
78.909
77.478
77.160
76.843
70.889
69.170
48.621
47.240
N
O
Cl
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

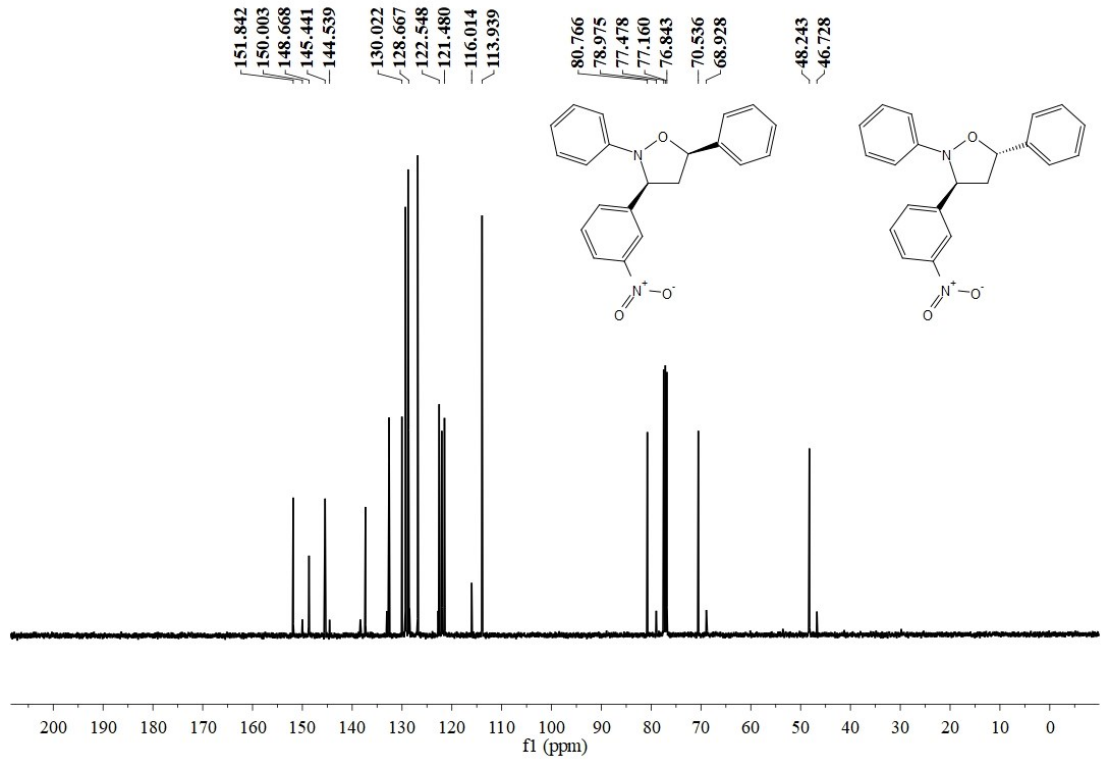
4aia + 4a'i'a'


8.285
8.265
8.080
8.064
8.044
7.686
7.342
7.303
7.207
7.040
6.981
6.915
5.712
5.706
5.691
5.426
5.232
5.216
5.208
5.192
3.517
3.486
3.448
3.023
2.296
2.264
2.256
2.224
7.36
7.34
7.32
7.30
7.28
7.26
f1 (ppm)
1.00
1.00
1.09
1.34
8.02
1.97
1.39
0.99
0.11
1.11
0.99
0.11
0.10
1.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

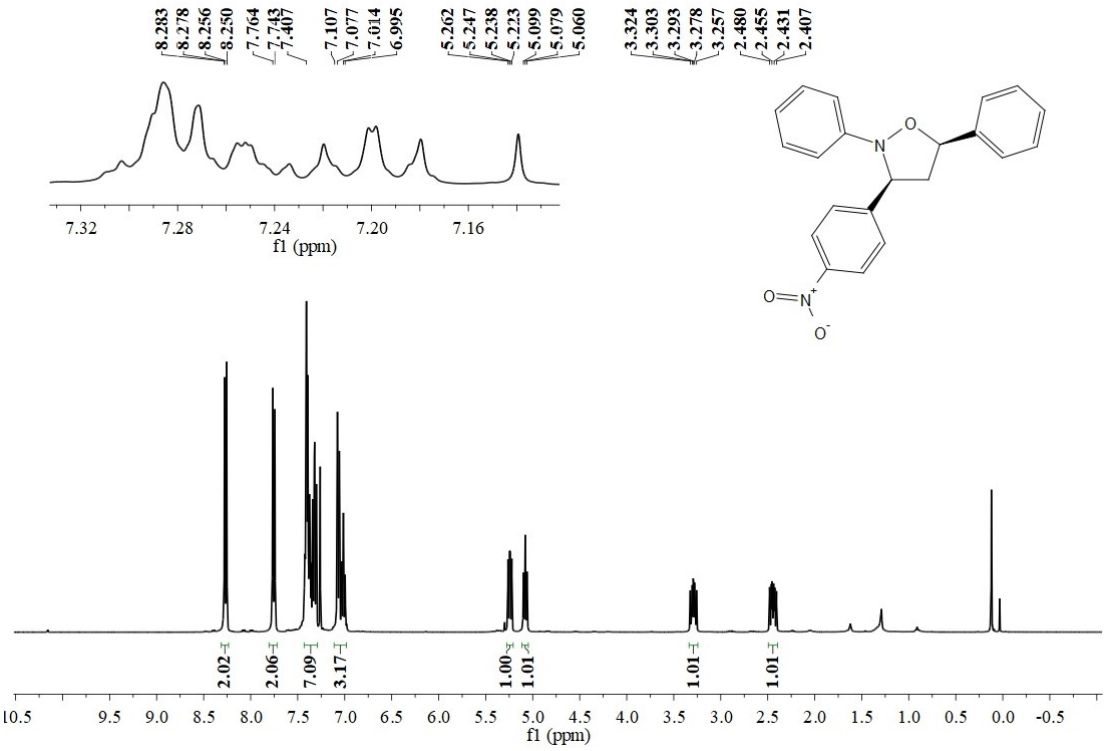

151.455
150.208
147.318
137.965
134.223
128.295
121.837
115.364
113.714
80.599
79.103
77.478
77.160
76.842
68.159
66.439
47.835
45.922
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

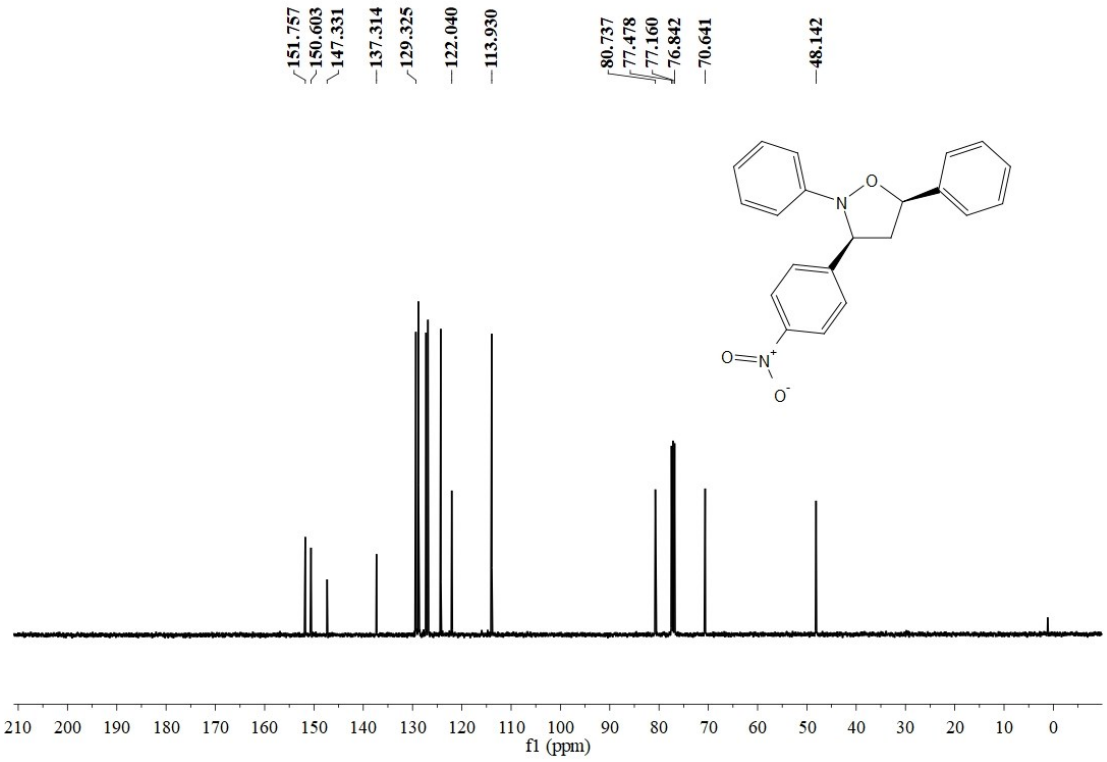
4aja + 4a'j'a'


8.427
8.398
8.393
8.179
8.151
8.134
8.129
7.928
7.909
7.897
7.532
7.283
7.195
7.033
6.944
5.354
5.315
5.228
5.188
5.065
5.046
5.027
4.835
4.802
3.292
3.261
3.226
2.896
2.865
2.850
2.819
2.673
2.642
2.616
2.462
2.432
2.420
2.389
f1 (ppm)
1.06
1.08
1.11
1.14
5.19
2.98
2.03
1.37
0.12
1.00
1.00
0.11
1.00
0.11
0.12
1.00

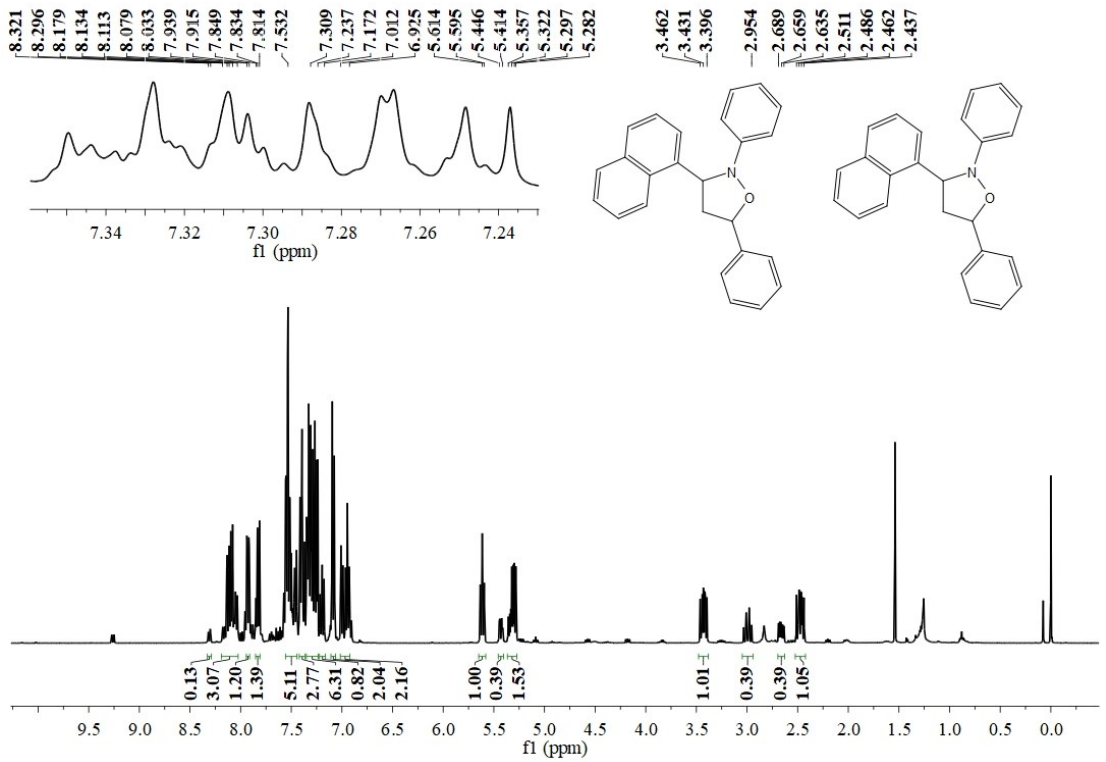

151.842
150.003
148.668
145.441
144.539
130.022
128.667
122.548
121.480
116.014
113.939
80.766
78.975
77.478
77.160
76.843
70.536
68.928
48.243
46.728
f1 (ppm)

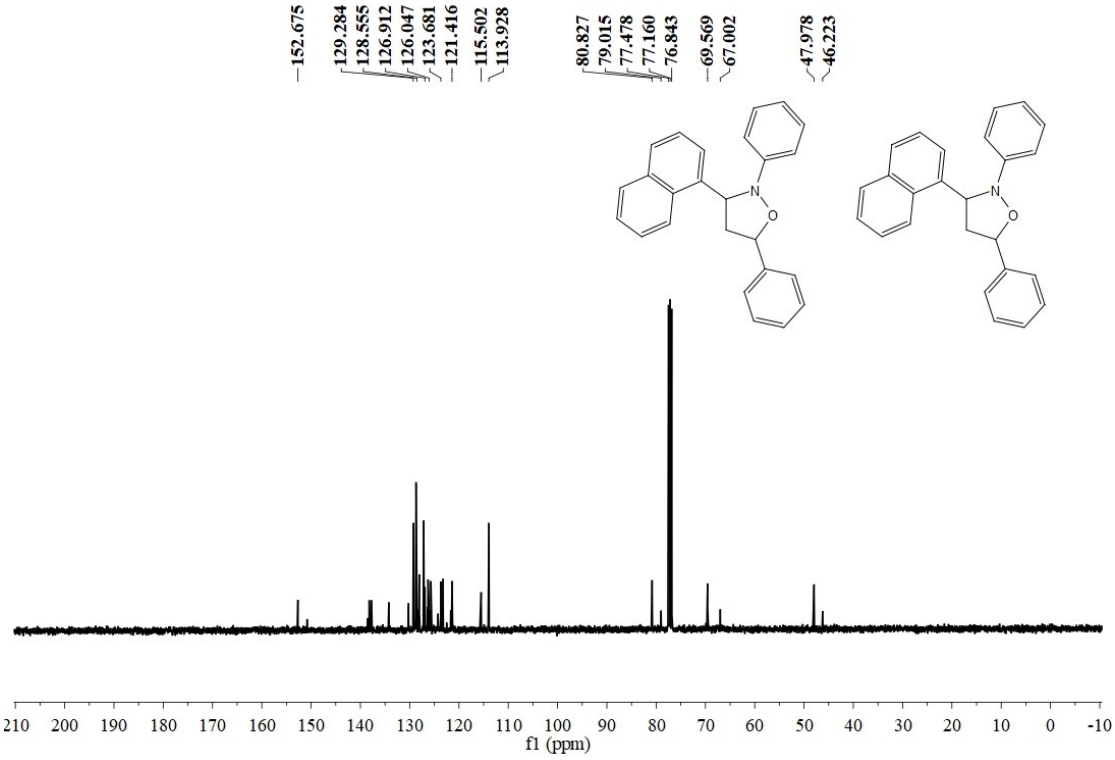
4aka


8.283
8.278
8.256
8.250
7.764
7.743
7.407
7.107
7.077
7.014
6.995
5.262
5.247
5.238
5.223
5.099
5.079
5.060
3.324
3.303
3.293
3.278
3.257
2.480
2.455
2.431
2.407
7.32
7.28
7.24
7.20
7.16
f1 (ppm)
2.02
2.06
7.09
3.17
1.00
1.01
1.01
1.01
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

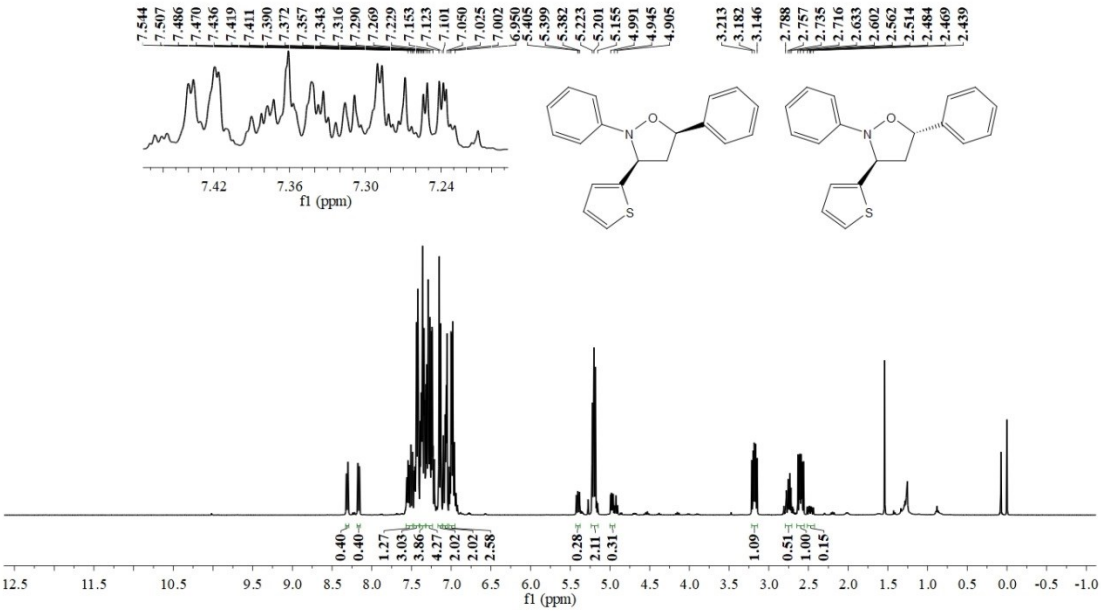

151.757
150.603
147.331
137.314
129.325
122.040
113.930
80.737
77.478
77.160
76.842
70.641
48.142
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

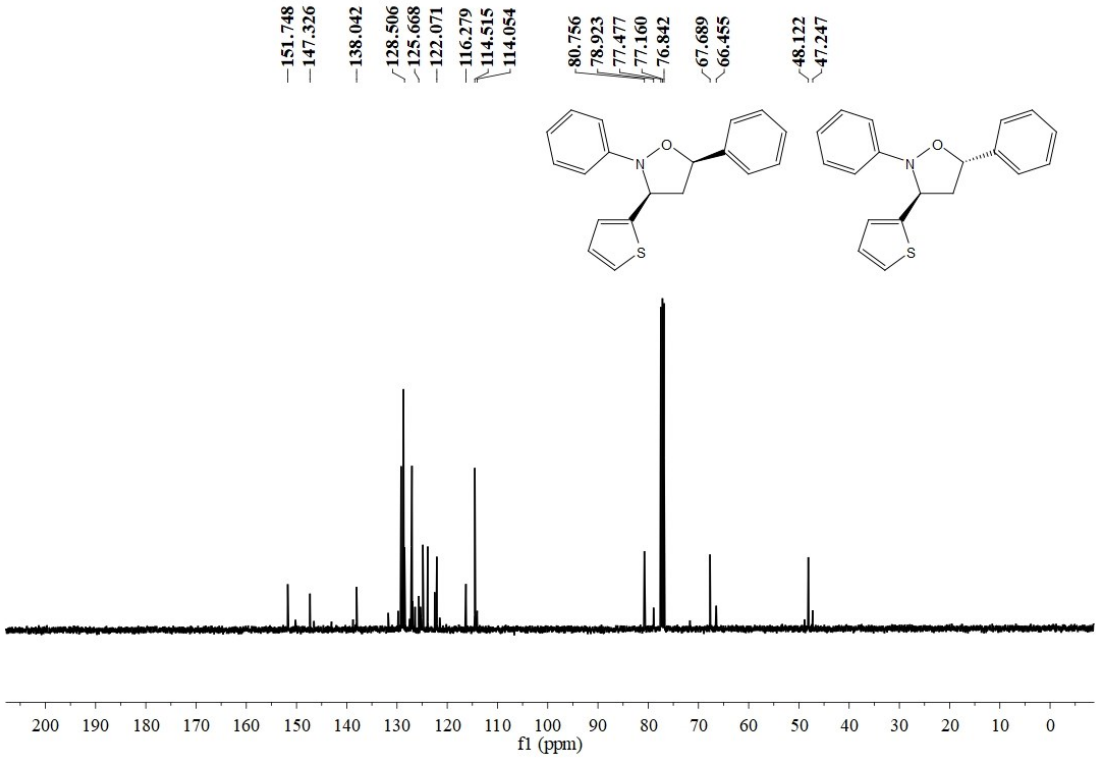
4ala + 4a'l'a'


8.321
8.296
8.179
8.134
8.113
8.079
8.033
7.939
7.915
7.849
7.834
7.814
7.532
7.309
7.237
7.172
7.012
6.925
5.614
5.595
5.446
5.414
5.357
5.322
5.297
5.282
3.462
3.431
3.396
2.954
2.689
2.659
2.635
2.511
2.486
2.462
2.437
7.34
7.32
7.30
7.28
7.26
7.24
f1 (ppm)
0.13
3.07
1.20
1.39
5.11
2.77
6.31
0.82
2.04
2.16
1.00
0.39
1.53
1.01
0.39
0.39
1.05
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

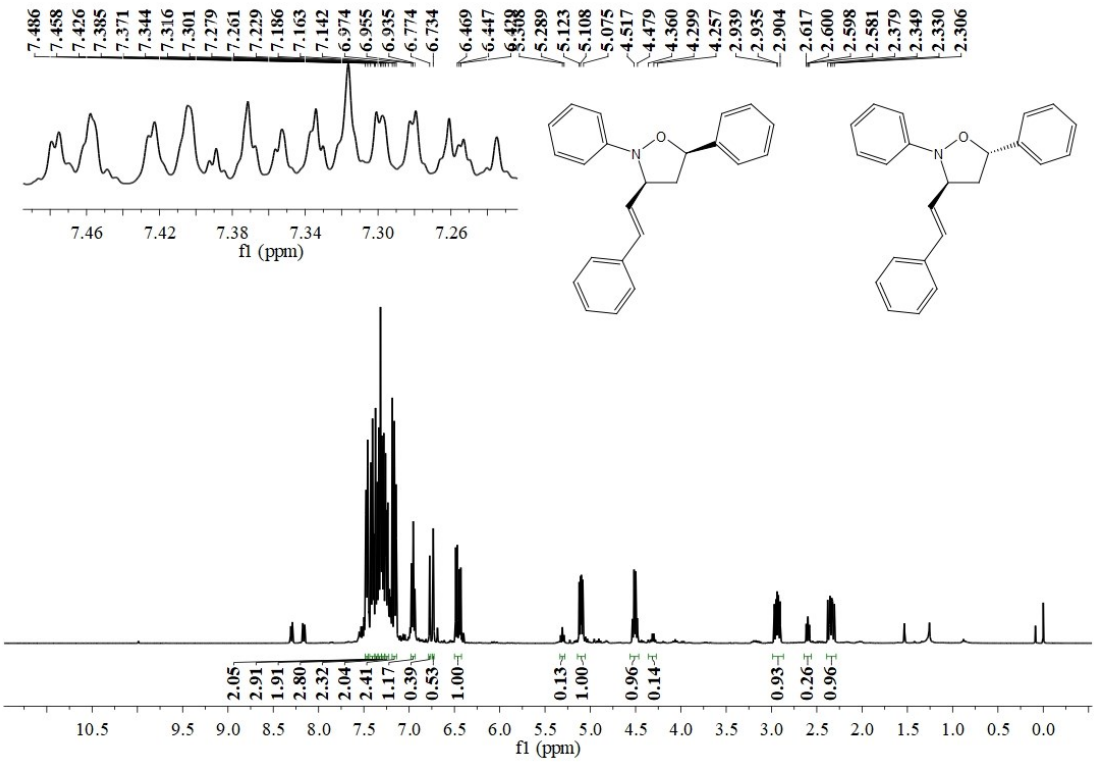

152.675
129.284
128.555
126.912
126.047
123.681
121.416
115.502
113.928
80.827
79.015
77.478
77.160
76.843
69.569
67.002
47.978
46.223
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

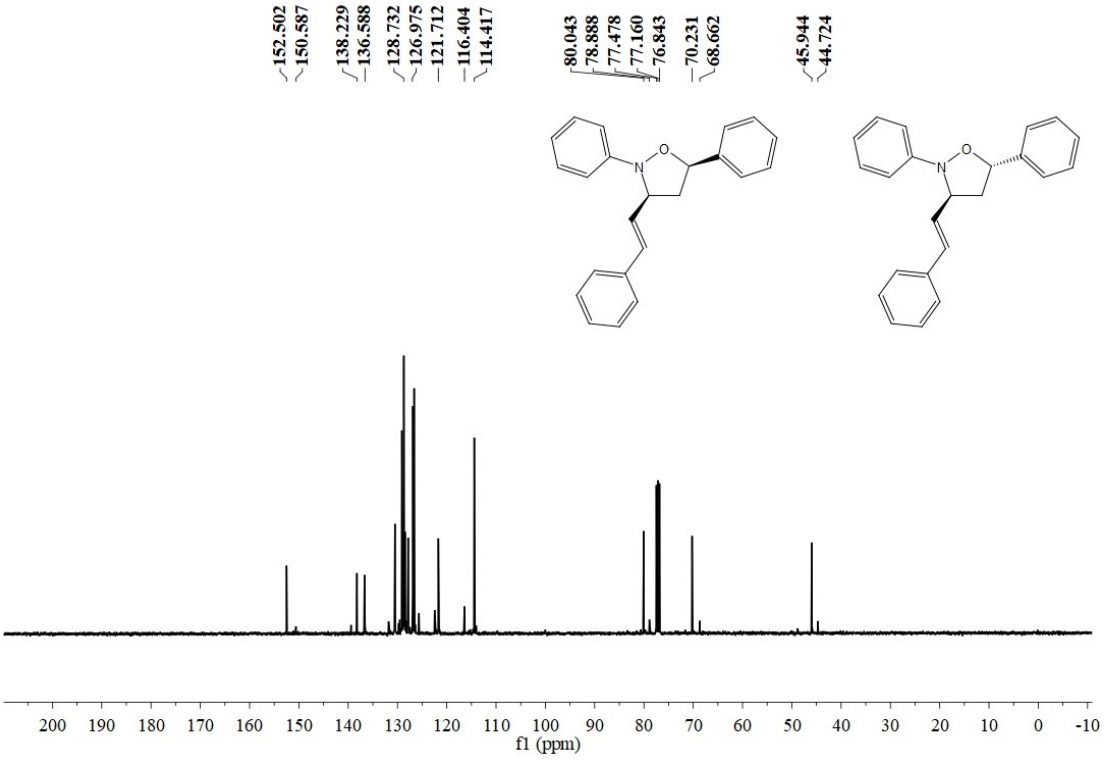
4ama + 4a'm'a'


7.544
7.507
7.486
7.470
7.436
7.419
7.411
7.390
7.372
7.357
7.343
7.316
7.290
7.269
7.229
7.153
7.123
7.101
7.050
7.025
7.002
6.950
5.405
5.399
5.382
5.223
5.201
5.155
4.991
4.945
4.905
3.213
3.182
3.146
2.788
2.757
2.735
2.716
2.633
2.602
2.562
2.514
2.484
2.469
2.439
7.42
7.36
7.30
7.24
f1 (ppm)
0.40
0.40
1.27
3.03
3.86
4.27
2.02
2.02
2.58
0.28
2.11
0.31
1.09
0.51
1.00
0.15
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

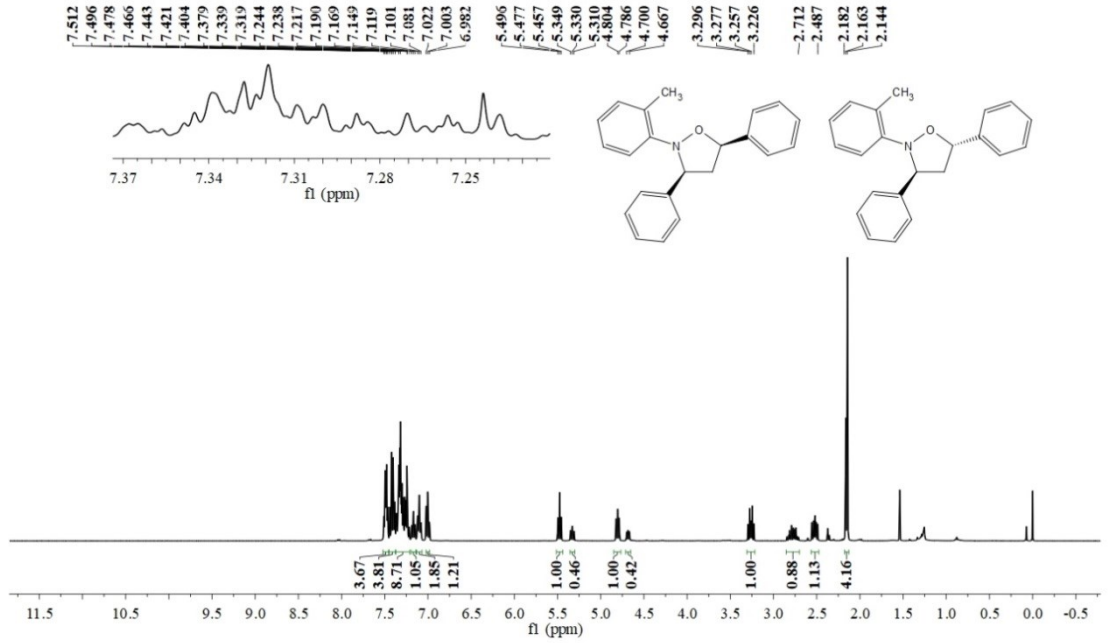

151.748
147.326
138.042
128.506
125.668
122.071
116.279
114.515
114.054
80.756
78.923
77.477
77.160
76.842
67.689
66.455
48.122
47.247
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

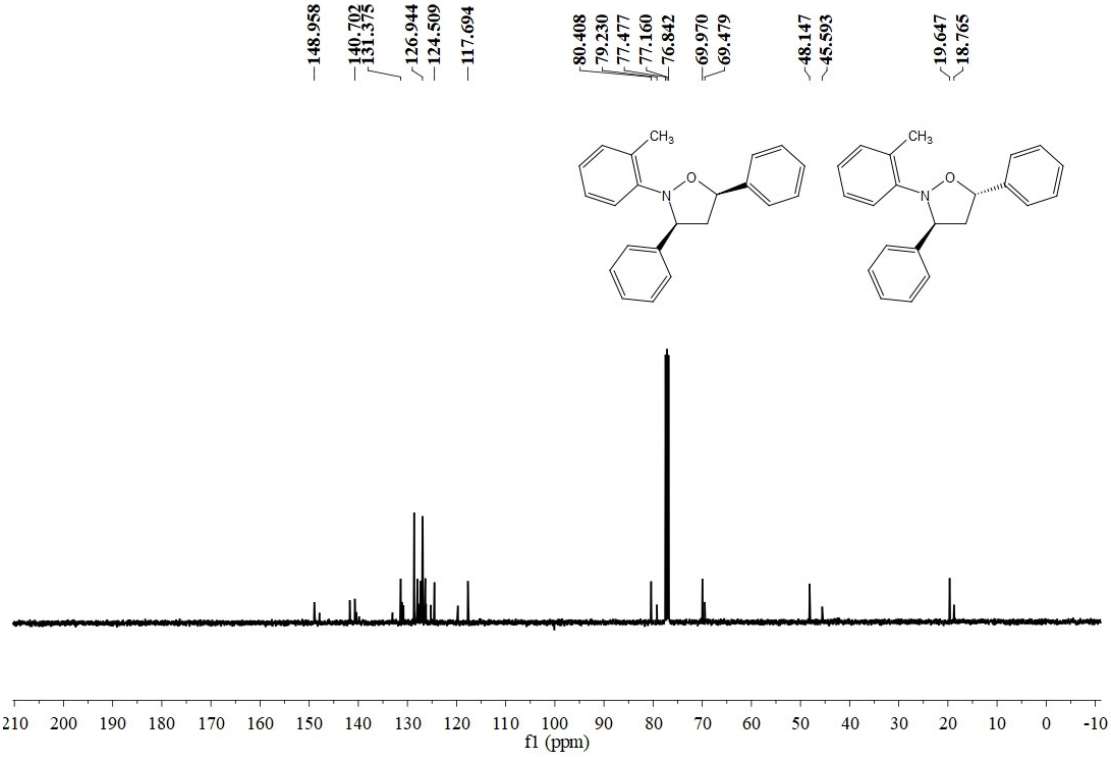
4ana + 4a'n'a'


7.486 7.458 7.426 7.385 7.371 7.344 7.316 7.301 7.279 7.261 7.229 7.186 7.163 7.142 6.974 6.955 6.935 6.774 6.734
6.469 6.447 6.428 6.408 5.289 5.123 5.108 5.075 4.517 4.479 4.360 4.299 4.257 2.939 2.935 2.904
2.617 2.600 2.598 2.581 2.379 2.349 2.330 2.306
7.46 7.42 7.38 7.34 7.30 7.26
f1 (ppm)
2.05 2.91 1.91 2.80 2.32 2.04 2.41 1.17 0.39 0.53 1.00 0.13 1.00 0.96 0.14 0.93 0.26 0.96
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

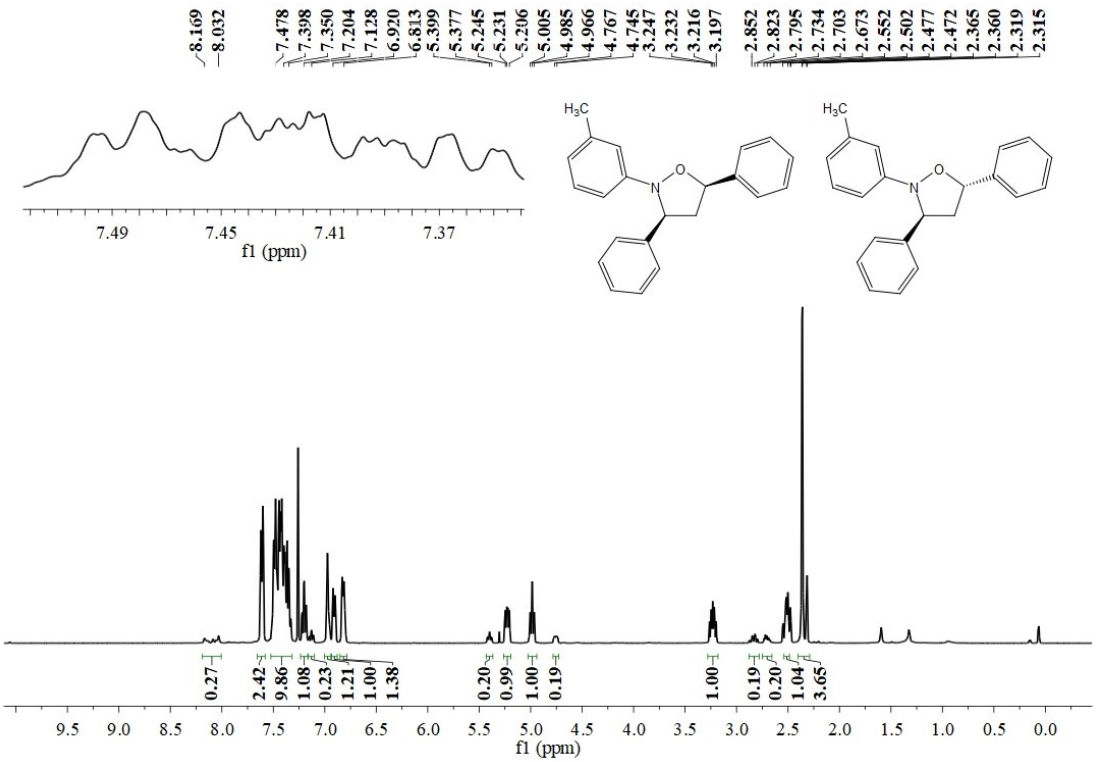

152.502 150.587 138.229 136.588 128.732 126.975 121.712 116.404 114.417
80.043 78.888 77.478 77.160 76.843 70.231 68.662
45.944 44.724
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

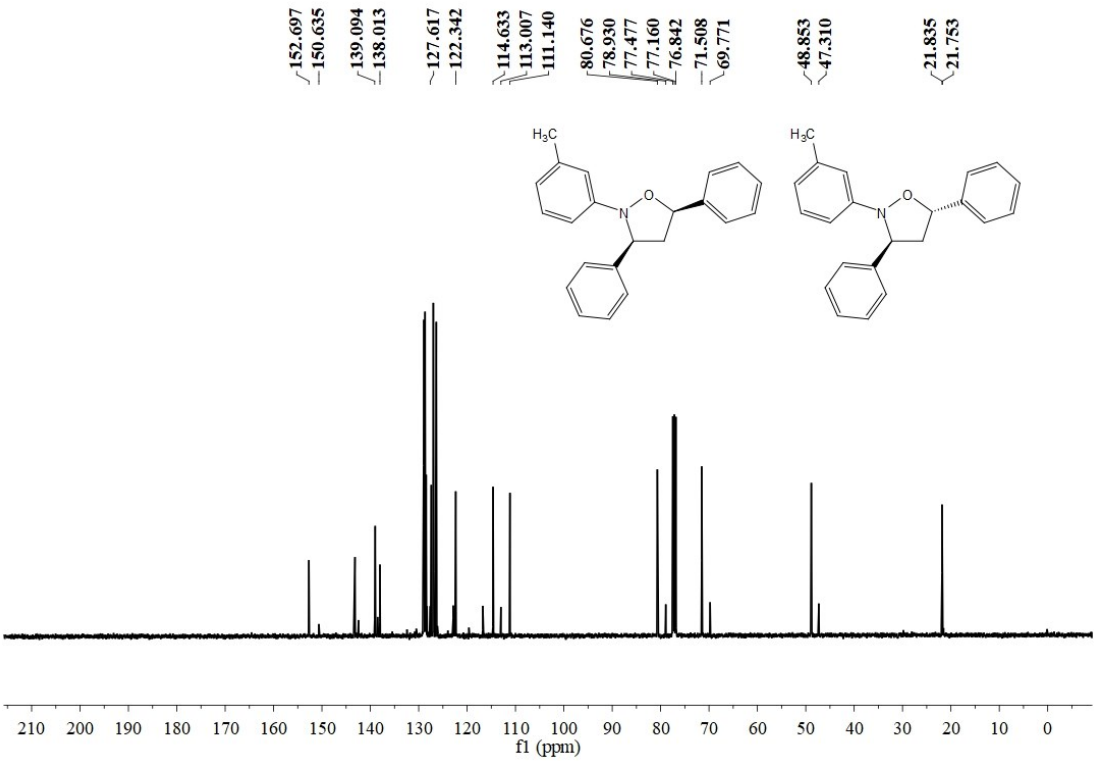
4baa + 4b'a'a'


7.512
7.496
7.478
7.466
7.443
7.421
7.404
7.379
7.339
7.319
7.244
7.238
7.217
7.190
7.169
7.149
7.119
7.101
7.081
7.022
7.003
6.982
5.496
5.477
5.457
5.349
5.330
5.310
4.804
4.786
4.700
4.667
3.296
3.277
3.257
3.226
2.712
2.487
2.182
2.163
2.144
CH3
7.37
7.34
7.31
7.28
7.25
f1 (ppm)
3.67
3.81
8.71
1.05
1.85
1.21
1.00
0.46
1.00
0.42
1.00
0.88
1.13
4.16
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

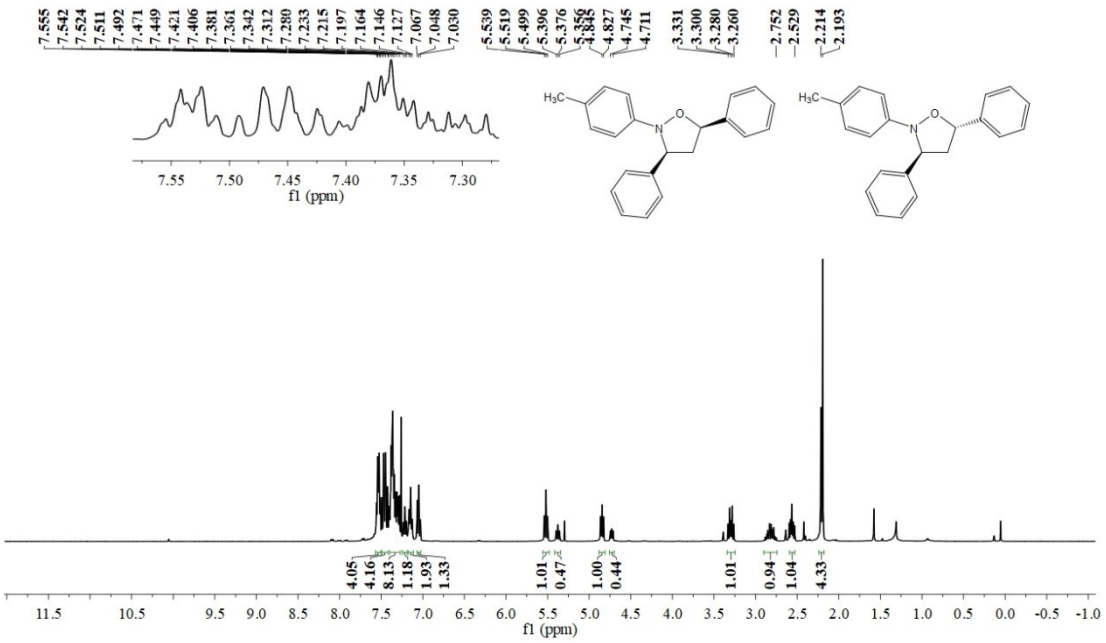

148.958
140.702
131.375
126.944
124.509
117.694
80.408
79.230
77.477
77.160
76.842
69.970
69.479
48.147
45.593
19.647
18.765
CH3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

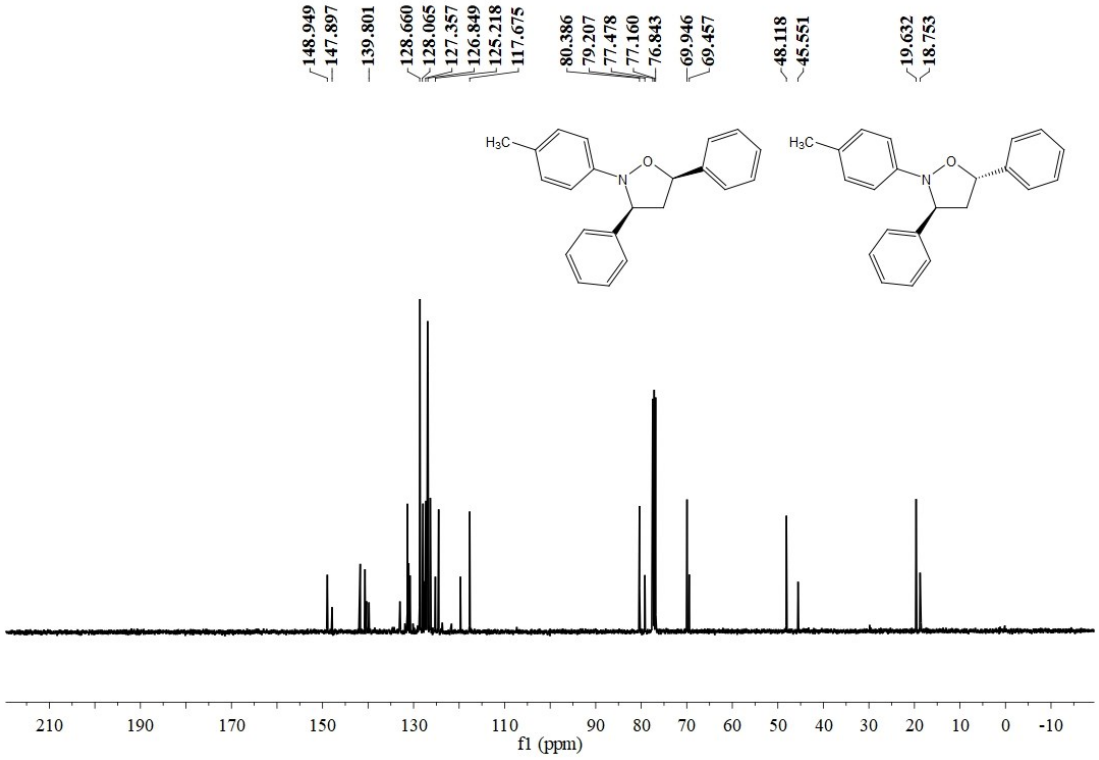
4caa + 4c'a'a'


8.169
8.032
7.478
7.398
7.350
7.204
7.128
6.920
6.813
5.399
5.377
5.245
5.231
5.206
5.005
4.985
4.966
4.767
4.745
3.247
3.232
3.216
3.197
2.852
2.823
2.795
2.734
2.703
2.673
2.552
2.502
2.477
2.472
2.365
2.360
2.319
2.315
H3C
H3C
7.49
7.45
7.41
7.37
f1 (ppm)
0.27
2.42
9.86
1.08
0.23
1.21
1.00
1.38
0.20
0.99
1.00
0.19
1.00
0.19
0.20
1.04
3.65
f1 (ppm)

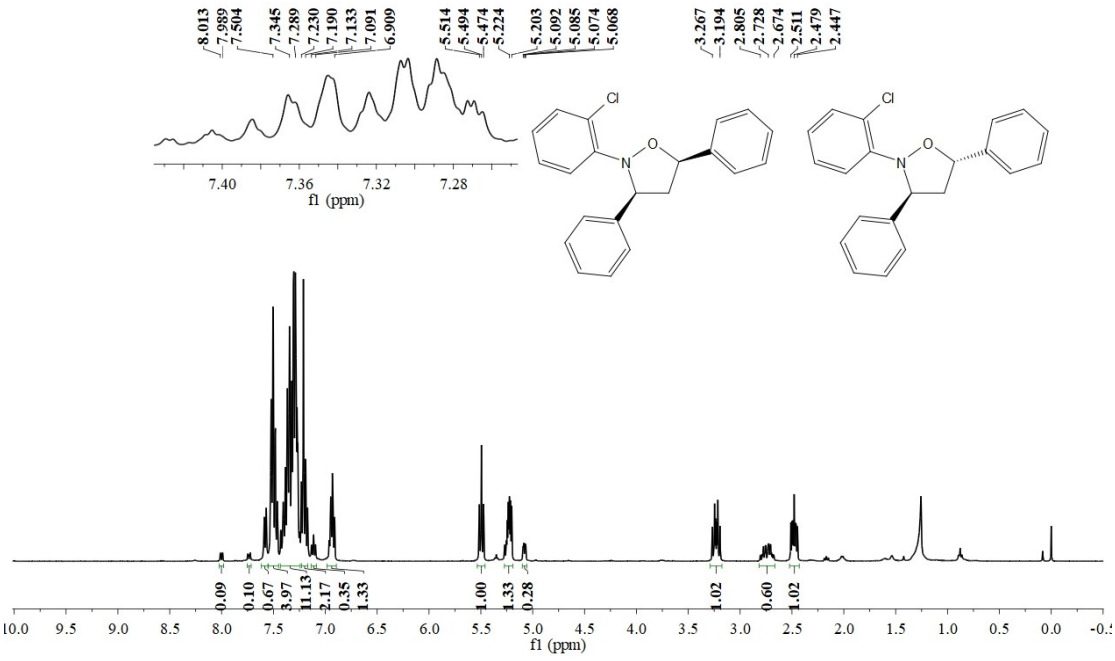

152.697
150.635
139.094
138.013
127.617
122.342
114.633
113.007
111.140
80.676
78.930
77.477
77.160
76.842
71.508
69.771
48.853
47.310
21.835
21.753
H3C
H3C
f1 (ppm)

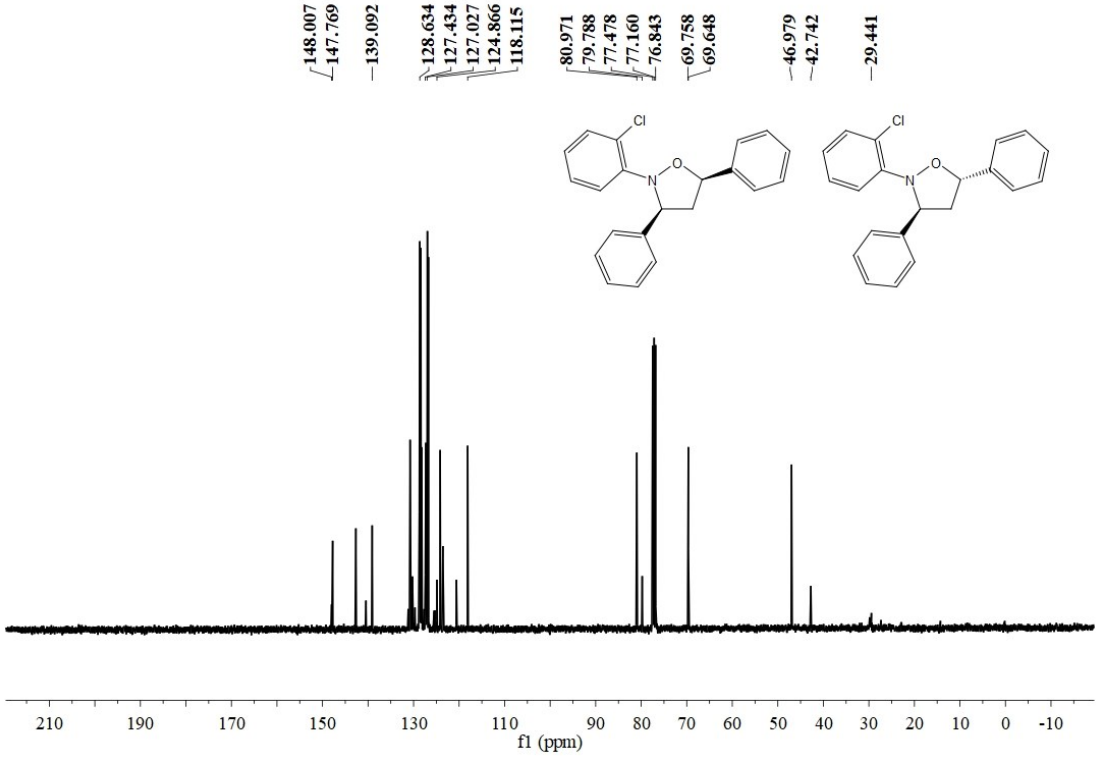
4daa + 4d'a'a'


7.555
7.542
7.524
7.511
7.492
7.471
7.449
7.421
7.406
7.381
7.361
7.342
7.312
7.280
7.233
7.215
7.197
7.164
7.146
7.127
7.067
7.048
7.030
5.539
5.519
5.499
5.396
5.376
4.827
4.745
4.711
3.331
3.300
3.280
3.260
2.752
2.529
2.214
2.193
H3C
N
O
7.55 7.50 7.45 7.40 7.35 7.30
f1 (ppm)
4.05
4.16
8.13
1.18
1.93
1.33
1.01
0.47
1.00
0.44
1.01
0.94
1.04
4.33
11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

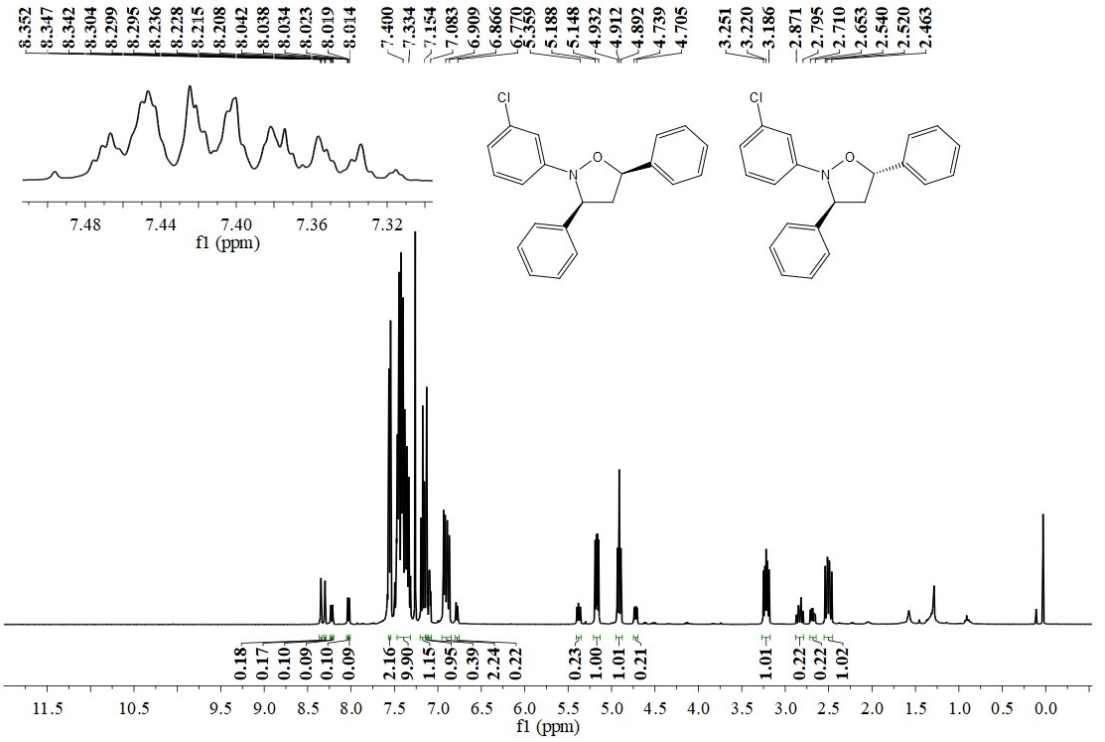

148.949
147.897
139.801
128.660
128.065
127.357
126.849
125.218
117.675
80.386
79.207
77.478
77.160
76.843
69.946
69.457
48.118
45.551
19.632
18.753
H3C
N
O
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

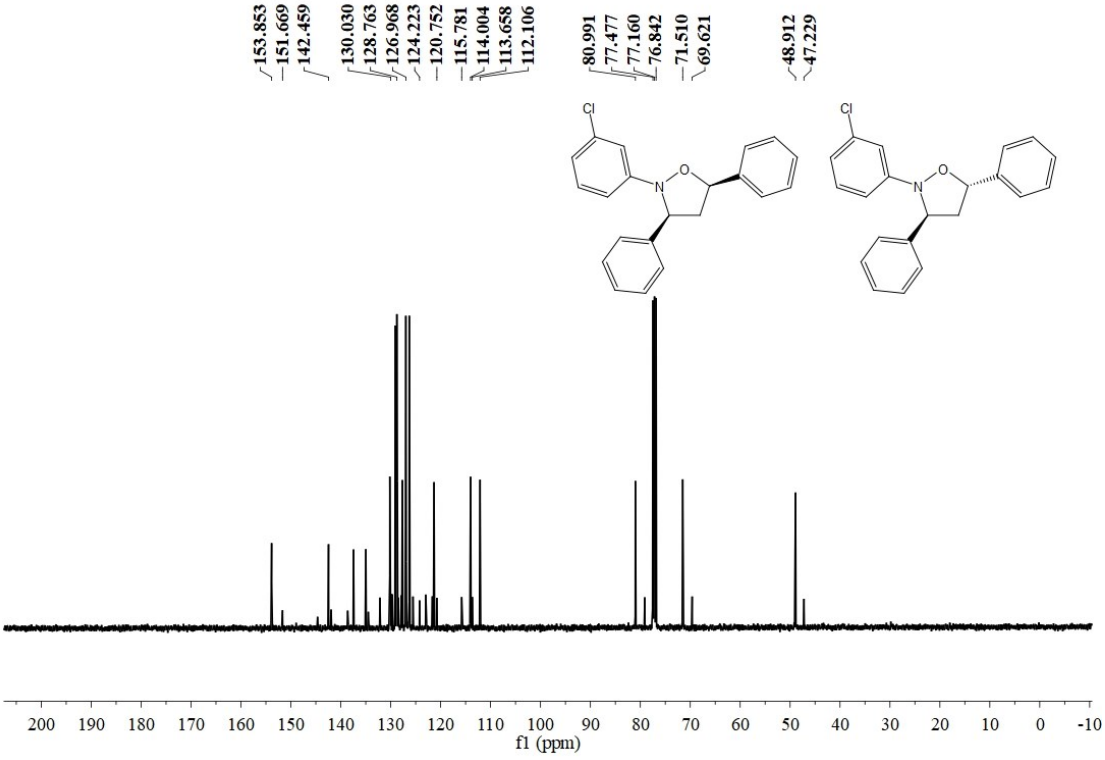
4eaa + 4e'a'a'


8.013
7.989
7.504
7.345
7.289
7.230
7.190
7.133
7.091
6.909
5.514
5.494
5.474
5.224
5.203
5.092
5.085
5.074
5.068
3.267
3.194
2.805
2.728
2.674
2.511
2.479
2.447
Cl
N
O
7.40
7.36
7.32
7.28
f1 (ppm)
0.09
0.10
0.67
3.97
11.13
2.17
0.35
1.33
1.00
1.33
0.28
1.02
0.60
1.02
f1 (ppm)

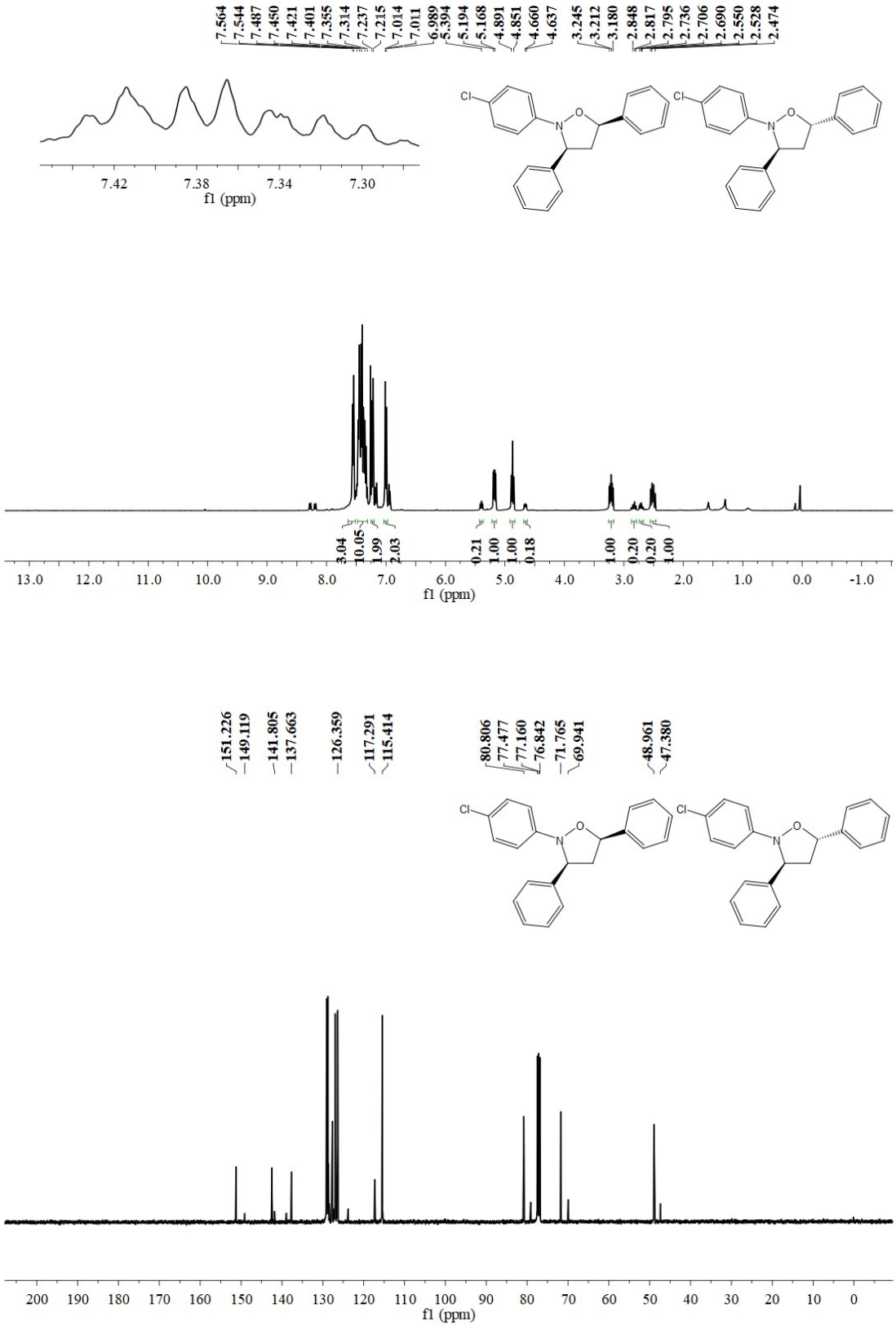

148.007
147.769
139.092
128.634
127.434
127.027
124.866
118.115
80.971
79.788
77.478
77.160
76.843
69.758
69.648
46.979
42.742
29.441
Cl
N
O
f1 (ppm)

4faa + 4f'a'a'

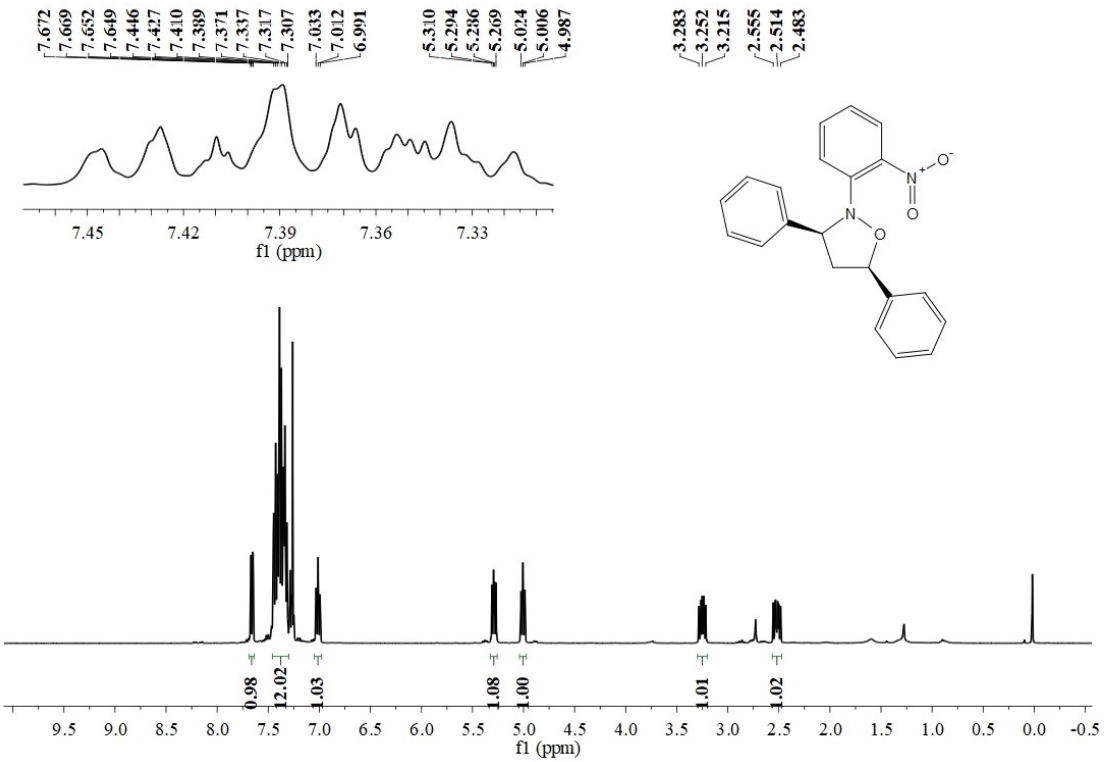

8.352
8.347
8.342
8.304
8.299
8.295
8.236
8.228
8.215
8.208
8.042
8.038
8.034
8.023
8.019
8.014
7.400
7.334
7.154
7.083
6.909
6.866
6.770
5.359
5.188
5.148
4.932
4.912
4.892
4.739
4.705
3.251
3.220
3.186
2.871
2.795
2.710
2.653
2.540
2.520
2.463
Cl
N
O
7.48
7.44
7.40
7.36
7.32
f1 (ppm)
0.18
0.17
0.10
0.09
0.10
0.09
2.16
9.90
1.15
0.95
0.39
2.24
0.22
0.23
1.00
1.01
0.21
1.01
0.22
0.22
1.02
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

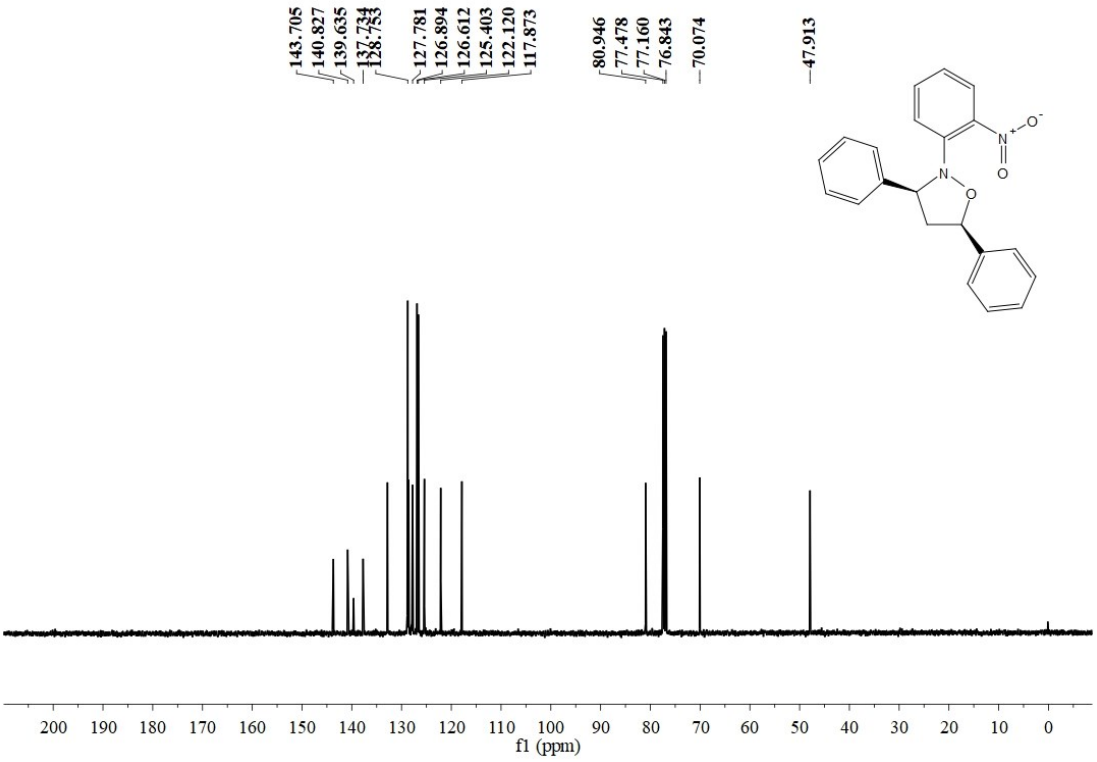

153.853
151.669
142.459
130.030
128.763
126.968
124.223
120.752
115.781
114.004
113.658
112.106
80.991
77.477
77.160
76.842
71.510
69.621
48.912
47.229
Cl
N
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

4gaa + 4g'a'a'

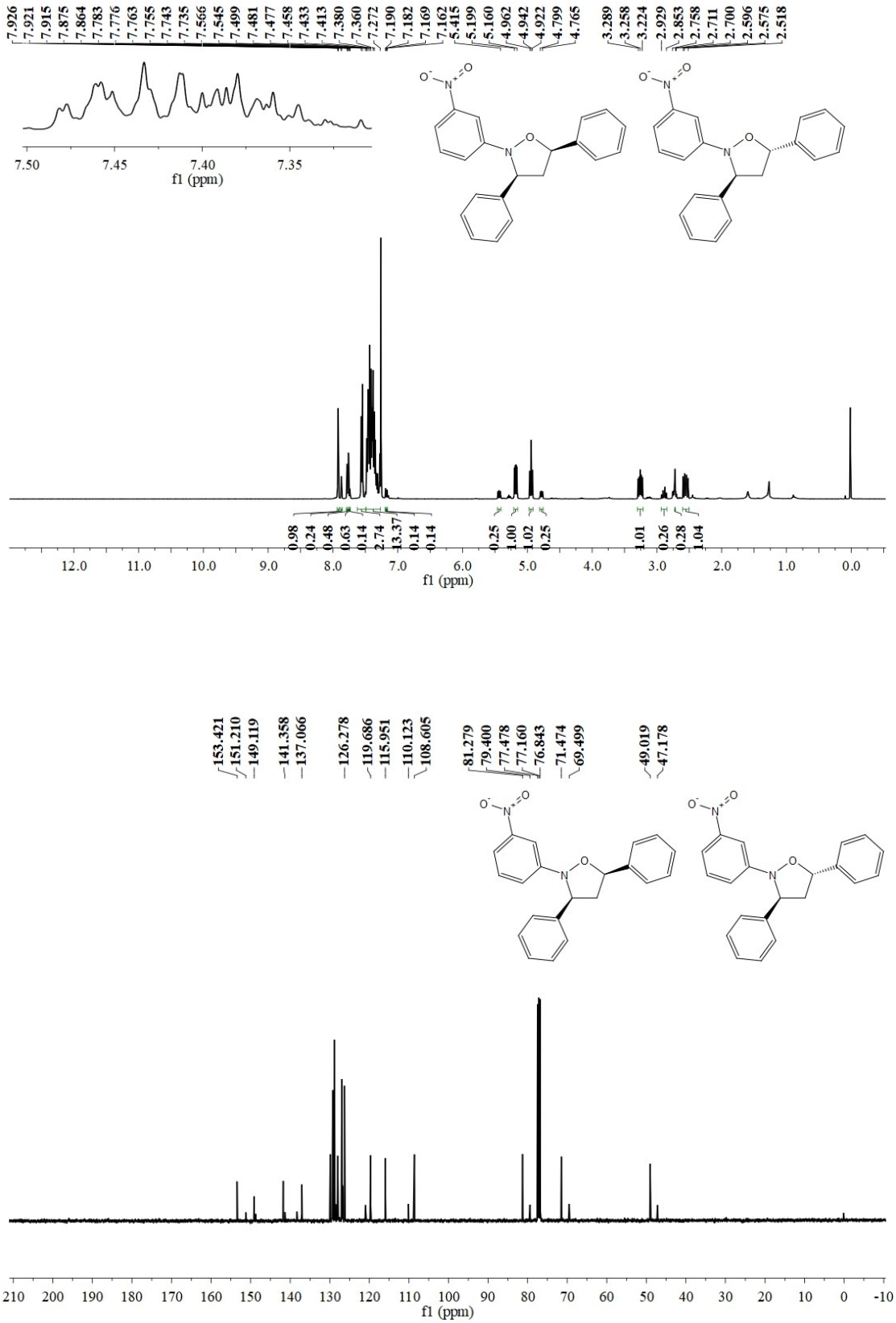

7.564
7.544
7.487
7.450
7.421
7.401
7.355
7.314
7.237
7.215
7.014
7.011
6.989
5.394
5.194
5.168
4.891
4.851
4.660
4.637
3.245
3.212
3.180
2.848
2.817
2.795
2.736
2.706
2.690
2.550
2.528
2.474
Cl
N
O
7.42
7.38
7.34
7.30
f1 (ppm)
3.04
10.05
1.99
2.03
0.21
1.00
1.00
0.18
1.00
0.20
0.20
1.00
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)
151.226
149.119
141.805
137.663
126.359
117.291
115.414
80.806
77.477
77.160
76.842
71.765
69.941
48.961
47.380
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

4haa + 4h'a'a'

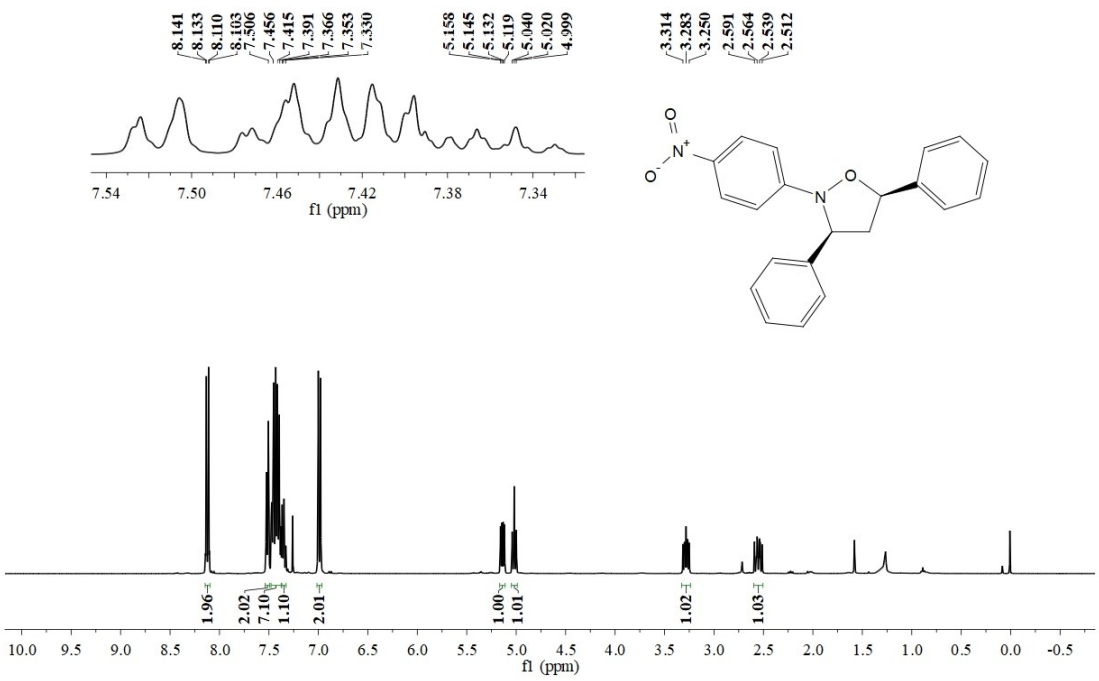

7.672
7.669
7.652
7.649
7.446
7.427
7.410
7.389
7.371
7.337
7.317
7.307
7.033
7.012
6.991
5.310
5.294
5.286
5.269
5.024
5.006
4.987
3.283
3.252
3.215
2.555
2.514
2.483
7.45
7.42
7.39
7.36
7.33
f1 (ppm)
0.98
12.02
1.03
1.08
1.00
1.01
1.02
f1 (ppm)

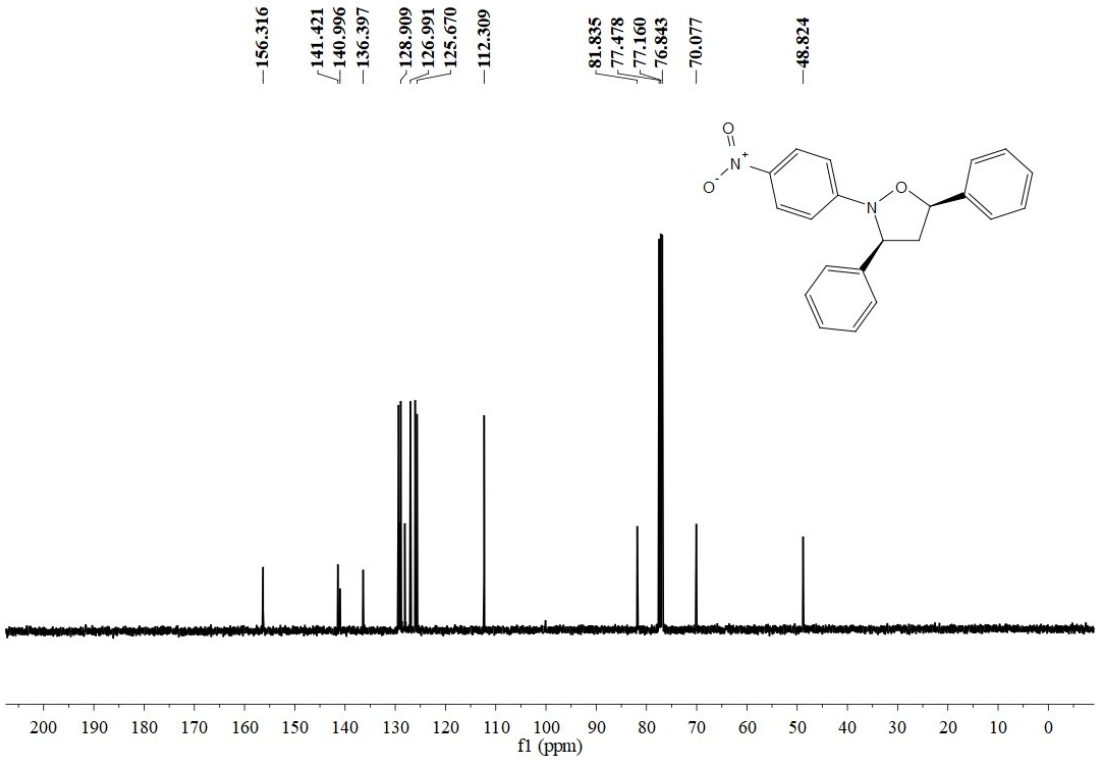

143.705
140.827
139.635
137.734
128.753
127.781
126.894
126.612
125.403
122.120
117.873
80.946
77.478
77.160
76.843
70.074
47.913
f1 (ppm)

4iaa + 4i'a'a'


7.926
7.921
7.915
7.875
7.864
7.783
7.776
7.763
7.755
7.743
7.735
7.566
7.545
7.499
7.481
7.477
7.458
7.433
7.413
7.380
7.360
7.272
7.190
7.182
7.169
7.162
5.415
5.199
5.160
4.962
4.942
4.922
4.799
4.765
3.289
3.258
3.224
2.929
2.853
2.758
2.711
2.700
2.596
2.575
2.518
7.50
7.45
7.40
7.35
f1 (ppm)
0.98
0.24
0.48
0.63
0.14
2.74
13.37
0.14
0.14
0.25
1.00
1.02
0.25
1.01
0.26
0.28
1.04
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)
153.421
151.210
149.119
141.358
137.066
126.278
119.686
115.951
110.123
108.605
81.279
79.400
77.478
77.160
76.843
71.474
69.499
49.019
47.178
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

4jaa


8.141
8.133
8.110
8.103
7.506
7.456
7.415
7.391
7.366
7.353
7.330
5.158
5.145
5.132
5.119
5.040
5.020
4.999
3.314
3.283
3.250
2.591
2.564
2.539
2.512
1.96
2.02
7.10
1.10
2.01
1.00
1.01
1.02
1.03
f1 (ppm)


156.316
141.421
140.996
136.397
128.909
126.991
125.670
112.309
81.835
77.478
77.160
76.843
70.077
48.824
f1 (ppm)

9. ^{1}H NMR spectra for nitrone intermediate 6a