Electronic Supplementary Material (ESI) for Green Chemistry.

Chemical Fixation of Carbon Dioxide by Copper Catalyzed Multicomponent Reactions for Oxazolidinedione Syntheses

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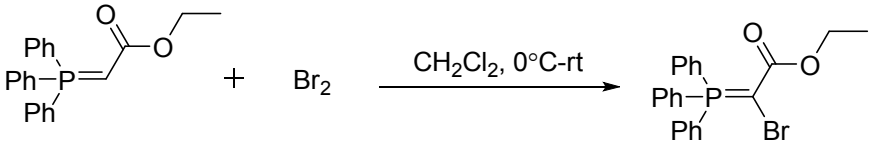
S1. Experimental

S1.1. General Considerations.

Common organic solvents were purchased from Daejung Chemicals, Korea. Unless otherwise specified all reagents and chemicals were purchased from Sigma Aldrich and/or Alfa Aesar, and used without further purification. GC/MS spectrum was recorded by Agilent 5975C GC/MSD System (Agilent Tech., USA/Germany). ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker 600MHz. The compounds were fully characterized by their Mass-spectra, ^{1}H, and ^{13}C NMR data. Reactions were performed with continuous magnetic stirring, under atmosphere of nitrogen or carbon dioxide, unless otherwise stated and all glassware was dried in an oven. Thin Layer Chromatography (TLC) analysis was carried out on Merck Kieselgel 60 PF254 pre-coated aluminium backed sheets and visualized either by UV fluorescence (254 nm) and/or by staining with potassium permanganate ($KMnO_4$) or vanillin.

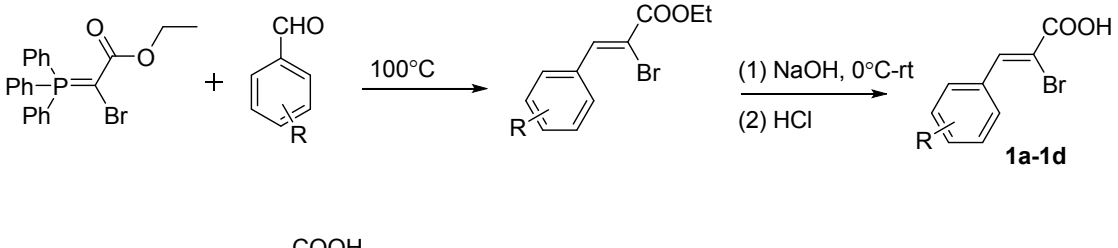
S1.2. Synthesis procedure.

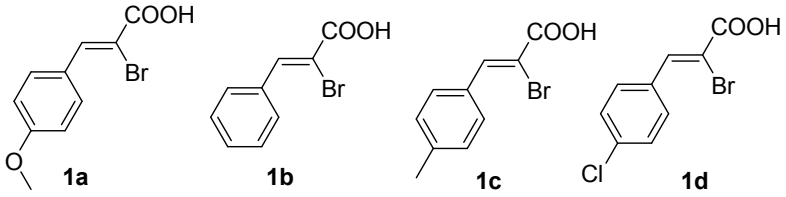
S1.2.1. Synthesis of bromocarbethoxymethylenetriphenylphosphorane.[1]



Carboethoxymethylidenetriphenyl-phosphorane (40 mmol, 13.9 g) was dissolved in CH_2Cl_2 (75 mL) and the solution was cooled to 5°C in ice-water bath. A solution of bromine (40 mmol, 6.4g) in CH_2Cl_2 (20 mL) was slowly added dropwise, and the batch was stirred overnight. The organic phase was washed with water (30 mL), and then twice with $NaHCO_3$ solution (50 mL) until HBr was neutralized. The CH_2Cl_2phase was dried over Na_2SO_4 and concentrated in vacuum. The residue was recrystallized from acetone/n-hexane (2:1) (27 mL). The crystals were dried in vacuum to afford bromocarbethoxymethylenetriphenylphosphorane as a yellow solid, yield 73% (12.5 g).

S1.2.2. Synthesis of 2-bromo-3-alkylacrylic acids (1a-1d).[1]



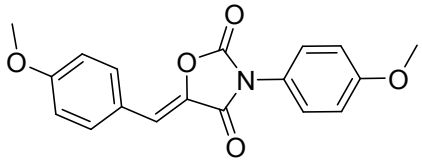


A mixture of aldehyde (20 mmol) and bromocarbethoxymethylenetriphenylphosphorane (20 mmol, 8.5 g) was added to a two-neck round bottom flask with a magnetic stirrer under

nitrogen atmosphere. The mixture was heated to 100 °C to form a homogeneous melt and the ensuing mixture was kept at 100 °C for 8 h. After cooling to room temperature, the mixture was subjected to column chromatography on silica gel to get ethyl 2-bromo-3-ethylacrylate Compound a: colorless liquid, yield 67% (3.4 g); Compound b: colorless liquid, 70% (3.8 g); Compound c: colorless liquid, 85% (4.8 g); Compound d: colorless liquid, 80% (4.6 g); Ethyl 2-bromo-3-alkylacrylate (10 mmol) was dissolved in CH_2Cl_2/CH_3OH (9:1) (100 mL), and the solution was cooled to 0 °C in ice-water bath. NaOH (20 mmol, 8.0 g) was added, and the mixture was stirred for 12 h at room temperature. The solvents were then removed under vacuum, the residue was diluted with water, and the aqueous solution was extracted with diethyl ether in order to remove the remaining ester. The aqueous phase was then cooled, acidified to pH 2-3 with dilute HCl, and extracted with Et_2O. The combined organic layer was dried over Na_2SO_4, and the solvent was removed to afford 2-bromo-3-phenylacrylic acid (**1a-1d**) with 100% Z-form. Compound (Z)-2-bromo-3-(4-methoxyphenyl)acrylic acid (**1a**): white solid, yield 74% (1.7 g); (Z)-2-bromo-3-phenylacrylic acid (**1b**): white solid, 82% (2.0 g); (Z)-2-bromo-3-p-tolylacrylic acid(**1c**): white solid,84% (2.2 g); (Z)-2-bromo-3-(4-chlorophenyl)acrylic acid (**1d**): white solid, 79% (2.1 g).

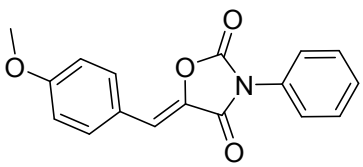
S1.3. General Synthetic Procedure for 3aa'-3de'. To a solution of a 2-bromo-3-phenylacrylic acid (0.5 mmol), amine (0.6 mmol), Cu_2O (1.0 mol%) and DMF (2 mL) in a Schlenk flask was added Cs_2CO_3 (1.0 mmol, 2 eq.). The inside of the reaction container was purged with CO_2 by a balloon three times (~1.0 atm). The reaction mixture was stirred at 80 °C for 12 h. Aqueous solution of $NaHCO_3$ was added to reaction mixture and the water layer was separated with separatory funnel using $CHCl_3$. The combined organic layer was dried over anhydrous Na_2SO_4, concentrated under reduced pressure. The pure corresponding oxazolidinone was obtained with no further purification.

*S1.3.1. (Z)-5-(4-Methoxybenzylidene)-3-(4-methoxyphenyl)oxazolidine-2,4-dione (**3aa'**).*



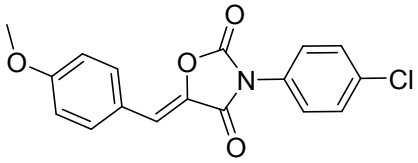
Yield 263.2 mg (81%); physical state: solid; color: white; mp = 197-199 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 3.84 (s, 3H, -OCH_3), 3.87 (s, 3H, -OCH_3), 6.85 (s, 1H), 6.96 (d, *J* = 9.0Hz, 2H), 7.0 (d, *J* = 7.2Hz, 2H), 7.39 (d, *J* = 7.2Hz, 2H), 7.76 (d, *J* = 9.0Hz, 2H); ^{13}C NMR (125MHz, $CDCl_3$): δ 55.4, 55.5, 114.3, 114.6, 114.7, 123.2, 123.4, 126.9, 133.1, 136.6, 151.4, 159.7, 161.57, 161.58 ; Anal. Calcd for $C_{18}H_{15}NO_5$: C, 66.46; H, 4.65; N, 4.31. Found: C, 66.39; H, 4.61; N, 4.26; Mass (EI): *m/z* = 325 (M^+). Anal. Calcd. for $C_{18}H_{15}NO_5$: C, 66.46; H, 4.65; N, 4.31; Found: C, 66.42; H, 4.68; N, 4.35.

*S1.3.2. (Z)-5-(4-Methoxybenzylidene)-3-phenyloxazolidine-2,4-dione (**3ab'**).*



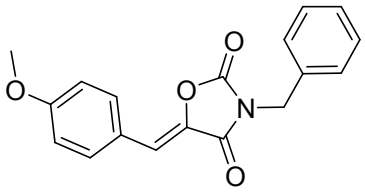
Yield 212.2 mg (72%); physical state: solid; color: light yellow; mp = 163-164°C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 3.90 (s, 3H, -OCH_3), 6.90 (s, 1H), 7.00 (d, J = 8.4Hz, 2H), 7.47-7.55 (m, 5H), 7.80 (d, J = 9.0Hz, 2H); ^{13}C NMR (125MHz, $CDCl_3$): δ 55.4, 114.4, 114.6, 123.4, 125.4, 128.9, 129.4, 130.8, 133.2, 135.5, 151.1, 161.3, 161.6; Mass (EI): m/z = 295 (M^+); Anal. Calcd. for $C_{17}H_{13}NO_4$: C, 69.15; H, 4.44; N, 4.74; Found: C, 69.09; H, 4.46; N, 4.77.

*S1.3.3. (Z)-3-(4-chlorophenyl)-5-(4-methoxybenzylidene)oxazolidine-2,4-dione (**3ac'**).*



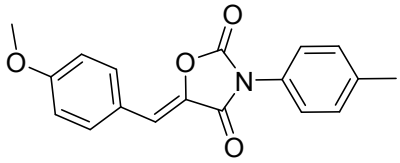
Yield 223.0 mg (68%); physical state: solid; yellow; mp = 187-189 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 3.90 (s, 3H, -OCH_3), 6.90 (s, 1H), 7.00 (d, J = 8.4Hz, 2H), 7.52-7.54 (m, 4H), 7.79 (d, J = 8.4Hz, 2H); ^{13}C NMR (125MHz, $CDCl_3$): δ 55.4, 114.7, 114.9, 123.3, 126.5, 129.5, 133.2, 134.6, 135.2, 150.7, 160.9, 161.7; Mass (EI): m/z = 329 (M^+); Anal. Calcd for $C_{17}H_{12}ClNO_4$: C, 61.92; H, 3.67; N, 4.25. Found: C, 61.89; H, 3.64; N, 4.23.

*S1.3.4. (Z)-3-Benzyl-5-(4-methoxybenzylidene)oxazolidine-2,4-dione (**3ad'**).* [2]



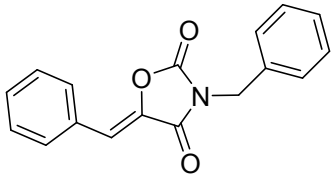
Yield 255.0 mg (83%); physical state: solid; color: white; mp = 117-118°C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 3.84 (s, 3H, -OCH_3), 4.77 (s, 2H, -NCH_2), 6.72 (s, 1H), 6.91 (d, J = 9.0Hz, 2H), 7.31-7.37 (m, 3H), 7.43-7.46 (m, 2H), 7.68 (d, J = 9.0Hz, 2H); ^{13}C NMR (125MHz, $CDCl_3$): δ 43.6, 55.3, 113.8, 114.5, 123.3, 128.4, 128.7, 128.8, 133.0, 134.5, 135.9, 152.1, 161.3, 162.1; Mass (EI): m/z = 309 (M^+).

*S1.3.5. (Z)-5-(4-Methoxybenzylidene)-3-p-tolyloxazolidine-2,4-dione (**3ae'**).*



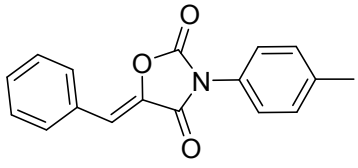
Yield 240.0 mg (78%); physical state: solid; color: light yellow; mp = 185-187 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 2.44 (s, 3H, -NCH_3), 3.90 (s, 3H, -OCH_3), 6.87 (s, 1H), 6.99 (d, *J* = 9.0Hz, 2H), 7.33 (d, *J* = 8.4Hz, 2H), 7.40 (d, *J* = 8.4Hz, 2H), 7.79 (d, *J* = 8.4Hz, 2H); ^{13}C NMR (125MHz, $CDCl_3$): δ 21.1, 55.4, 114.2, 114.6, 123.5, 125.3, 128.2, 129.9, 133.0, 135.7, 139.0, 151.1, 161.3, 161.6; Mass (EI): *m/z* = 309 (M^+); Anal. Calcd for $C_{18}H_{15}NO_4$: C, 69.89; H, 4.89; N, 4.53. Found: C, 69.85; H, 4.88; N, 4.53.

*S1.3.6. (Z)-3-Benzyl-5-benzylideneoxazolidine-2,4-dione (**3bd'**).* [2]



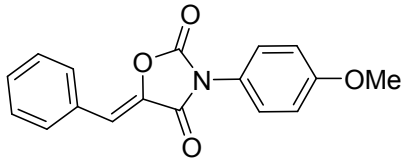
Yield 220.0 mg (79%); physical state: solid; color: white; mp = 159-160°C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 4.79 (s, 2H, -NCH_2), 6.77 (s, 1H), 7.35-7.48 (m, 8H), 7.72-7.76 (m, 2H); ^{13}C NMR (125MHz, $CDCl_3$): δ 43.7, 113.7, 128.5, 128.84, 128.87, 128.9, 130.4, 130.5, 131.0, 134.3, 137.4, 151.9, 161.9; Mass (EI): *m/z* = 279 (M^+).

*S1.3.7. (Z)-5-Benzylidene-3-p-tolyloxazolidine-2,4-dione (**3be'**).*



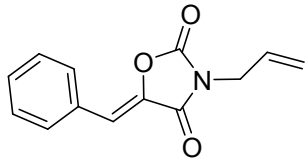
Yield 178.2 mg (71%); physical state: solid; color: white; mp = 177-178°C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 2.44 (s, 3H), 6.92 (s, 1H), 7.34 (d, *J* = 7.8Hz, 2H), 7.40 (d, *J* = 8.4Hz, 2H), 7.48-7.52 (m, 3H), 7.83 (d, *J* = 7.2Hz, 2H); ^{13}C NMR (125MHz, $CDCl_3$): δ 21.2, 114.2, 125.3, 127.9, 129.1, 130.0, 130.6, 130.7, 131.2, 137.2, 139.2, 151.0, 161.3; Mass (EI): *m/z* = 279 (M^+); Anal. Calcd for $C_{17}H_{13}NO_3$: C, 73.11; H, 4.69; N, 5.02. Found: C, 73.15; H, 4.77; N, 5.08.

*S1.3.8. (Z)-5-Benzylidene-3-(4-methoxyphenyl)oxazolidine-2,4-dione (**3ba'**).*



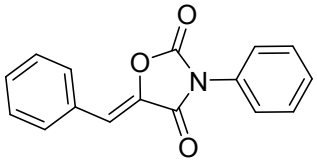
Yield 215.4 mg (73%); physical state: solid; color: white; mp = 192-193 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 3.84 (s, 3H), 6.86 (s, 1H), 7.01 (d, *J* = 8.4Hz, 2H), 7.39-7.47 (m, 5H), 7.79 (d, *J* = 7.2Hz, 2H); ^{13}C NMR (125MHz, $CDCl_3$): δ 55.5, 113.4, 114.5, 123.2, 127.1, 129.0, 130.4, 130.8, 130.9, 131.0, 137.4, 151.0, 159.8, 161.3; Mass (EI): *m/z* = 295 (M^+); Anal. Calcd for $C_{17}H_{13}NO_4$: C, 69.15; H, 4.44; N, 4.74. Found: C, 69.11; H, 4.45; N, 4.77.

*S1.3.9. (Z)-3-Allyl-5-benzylideneoxazolidine-2,4-dione (**3bg'**).*[2]



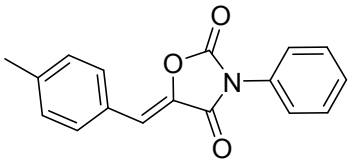
Yield 164.0 mg (72%); physical state: solid; color: white; mp = 80-81°C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 4.24 (d, J = 6.0Hz, 2H) 5.28-5.37 (m, 2H), 5.80-5.90 (m, 1H), 6.77 (s, 1H), 7.41-7.47 (m, 3H), 7.74-7.77 (m, 2H); ^{13}C NMR (125MHz, $CDCl_3$): δ 42.1, 113.6, 119.5, 128.9, 129.4, 130.4, 130.5, 131.0, 137.3, 151.7, 161.8; Mass (EI): *m/z* = 229 (M^+).

*S1.3.10. (Z)-5-Benzylidene-3-phenyloxazolidine-2,4-dione (**3bb'**).*



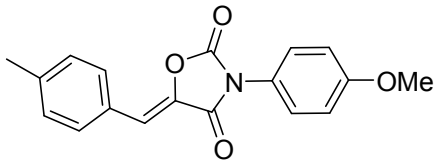
Yield 206.3 mg (78%); physical state: solid; color: white; mp = 183-185°C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 6.91 (s, 1H), 7.43-7.48 (m, 4H), 7.51-7.54 (m, 4H), 7.81 (d, *J* = 9.0Hz, 2H); ^{13}C NMR (125MHz, $CDCl_3$): δ 114.4, 125.4, 129.0, 129.1, 129.4, 130.7, 131.2, 137.0, 150.9, 161.1; Mass (EI): *m/z* = 265 (M^+); Anal. Calcd for $C_{16}H_{11}NO_3$: C, 72.45; H, 4.18; N, 5.28. Found: C, 72.41; H, 4.18; N, 5.25.

*S1.3.11. (Z)-5-(4-Methylbenzylidene)-3-phenyloxazolidine-2,4-dione (**3cb'**).*



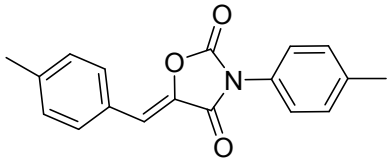
Yield 234.4 mg (84%); physical state: solid; color: white; mp = 181-182 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 2.38 (s, 3H), 6.85 (s, 1H), 7.23 (d, *J* = 7.8Hz, 2H), 7.42 (m, 1H), 7.47-7.49 (m, 4H), 7.67 (d, *J* = 7.8Hz, 2H); ^{13}C NMR (125MHz, $CDCl_3$): δ 21.6, 114.5, 125.4, 127.9, 128.9, 129.3, 129.8, 130.6, 131.2, 136.4, 141.4, 150.9, 161.2; Mass (EI): *m/z* = 279 (M^+); Anal. Calcd for $C_{17}H_{13}NO_3$: C, 73.11; H, 4.69; N, 5.02. Found: C, 73.08; H, 4.72; N, 4.98.

*S1.3.12. (Z)-3-(4-Methoxyphenyl)-5-(4-methylbenzylidene)oxazolidine-2,4-dione (**3ca'**).*



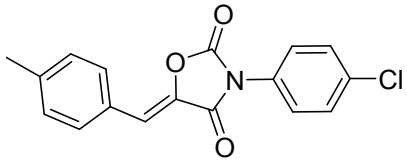
Yield 166.0 mg (54%); physical state: solid; color: light yellow; mp = 204-205 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 2.41 (s, 3H, -NCH_3), 3.84 (s, 3H, -OCH_3), 6.86 (s, 1H), 7.01 (d, *J* = 9.0Hz, 2H), 7.25 (d, *J* = 9.0Hz, 2H), 7.39 (d, *J* = 9.0Hz, 2H), 7.69 (d, *J* = 8.4Hz, 2H); ^{13}C NMR (125MHz, $CDCl_3$): δ 21.6, 55.5, 114.2, 114.7, 123.2, 126.9, 127.9, 129.8, 131.2, 136.6, 141.3, 151.3, 159.8, 161.5; Mass (EI): *m/z* = 309 (M^+); Anal. Calcd for $C_{18}H_{15}NO_4$: C, 69.89; H, 4.89; N, 4.53. Found: C, 69.97; H, 4.84; N, 4.55.

*S1.3.13. (Z)-5-(4-methylbenzylidene)-3-p-tolyloxazolidine-2,4-dione (**3ce'**).*



Yield 225.0 mg (77%); physical state: solid; color: white; ^{1}H NMR (600 MHz, $CDCl_3$) δ 2.44 (s, 6H, Ar-CH_3x2), 6.90 (s, 1H), 7.29 (d, *J* = 7.8Hz, 2H), 7.35 (d, *J* = 8.4Hz, 2H), 7.40 (d, *J* = 8.4Hz, 2H), 7.73 (d, *J* = 7.8Hz, 2H); ^{13}C NMR (125MHz, $CDCl_3$): δ 21.23, 21.65, 114.4, 125.3, 128.01, 128.04, 129.88, 130.04, 131.2, 136.5, 139.1, 141.3, 151.1, 161.4; Mass (EI): *m/z* = 293 (M^+); Anal. Calcd for $C_{18}H_{15}NO_3$: C, 73.71; H, 5.15; N, 4.78. Found: C, 73.75; H, 5.13; N, 4.79.

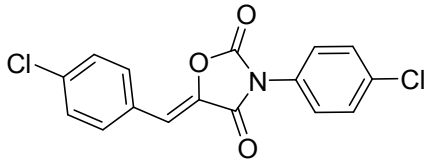
*S1.3.14. (Z)-3-(4-Chlorophenyl)-5-(4-methylbenzylidene)oxazolidine-2,4-dione (**3cc'**).*



Yield 256.0 mg (73%); physical state: solid; color: white shining crystal; mp = 192-193 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 2.34 (s, 3H), 6.80 (s, 1H), 7.21 (d, *J* = 5.4Hz, 2H), 7.44 (m, 4H), 7.64-7.65 (m, 1H), 7.80 (m, 1H); ^{13}C NMR (125MHz, $CDCl_3$): δ 20.9, 112.9, 126.7, 127.4, 128.7, 129.0,

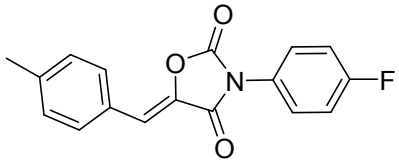
129.2, 130.3, 130.4, 133.5, 136.2, 140.3, 150.0, 160.3; Anal. Calcd for $C_{17}H_{12}ClNO_3$: C, 65.08; H, 3.86; N, 4.46. Found: C, 65.19; H, 3.73; N, 4.49; Mass (EI): *m/z* = 313 (M^+).

*S1.3.15. (Z)-5-(4-chlorobenzylidene)-3-(4-chlorophenyl)oxazolidine-2,4-dione (**3dc'**).*



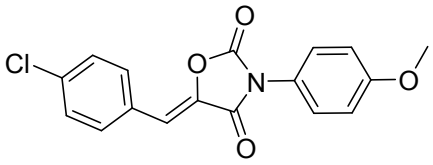
Yield 237.0 mg (71%); physical state: solid; color: light yellow; mp = 163-164°C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 6.88 (s, 1H), 7.44 (d, *J* = 8.4Hz, 2H), 7.49-7.53 (m, 4H), 7.77 (d, *J* = 8.4Hz, 2H); ^{13}C NMR (125MHz, $CDCl_3$): δ 112.2, 126.8, 129.1, 129.20, 129.26, 132.12, 132.19, 134.3, 136.1, 137.3, 150.2, 160.5; Mass (EI): *m/z* = 334 (M^+); Anal. Calcd for $C_{16}H_9Cl_2NO_3$: C, 57.51; H, 2.71; N, 4.19; Found: C, 57.48; H, 2.71; N, 4.23.

*S1.3.16. (Z)-3-(4-fluorophenyl)-5-(4-methylbenzylidene)oxazolidine-2,4-dione (**3cf'**).*



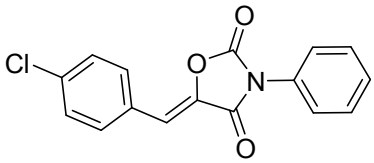
Yield 181.0 mg (58%); physical state: solid; mp = 154-155 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 2.41 (s, 3H), 6.87 (s, 1H), 7.21 (t, *J* = 9.0Hz, 2H), 7.27 (d, *J* = 7.8Hz, 2H), 7.52-7.54 (m, 2H), 7.70 (d, *J* = 8.4Hz, 2H); ^{13}C NMR (125MHz, $CDCl_3$): δ 21.5, 114.2, 116.2, 116.3, 126.8, 127.7, 127.9, 129.8, 131.11, 131.18, 136.5, 141.2, 150.8, 161.1, 161.3, 163.0; Mass (EI): *m/z* = 297 (M^+); Anal. Calcd for $C_{17}H_{12}FNO_3$: C, 68.68; H, 4.07; N, 4.71. Found: C, 68.72; H, 4.08; N, 4.63.

*S1.3.17. (Z)-5-(4-Chlorobenzylidene)-3-(4-methoxyphenyl)oxazolidine-2,4-dione (**3da'**).*



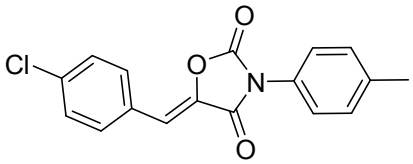
Yield 233.2 mg (80%); physical state: solid; color: white; mp = 203-205 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 3.81 (s, 3H, -OCH_3), 6.98 (s, 1H), 7.08 (d, *J* = 9.6Hz, 2H), 7.40 (d, *J* = 9.0Hz, 2H), 7.59 (d, *J* = 8.4Hz, 2H), 7.86 (d, *J* = 9.0Hz, 2H); ^{13}C NMR (125MHz, $CDCl_3$): δ 60.6, 115.0, 119.5, 128.6, 133.2, 133.3, 134.4, 134.5, 134.5, 135.4, 137.4, 139.8, 143.8, 156.3, 164.6, 166.7; Anal. Calcd for $C_{17}H_{12}ClNO_4$: C, 61.92; H, 3.67; N, 4.25. Found: C, 61.99; H, 3.64; N, 4.13; Mass (EI): *m/z* = 329 (M^+).

*S1.3.18. (Z)-5-(4-Chlorobenzylidene)-3-phenyloxazolidine-2,4-dione (**3db'**).*



Yield 245.0 mg (82%); physical state: solid; color: light yellow; mp = 172-173 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 6.83 (s, 1H), 7.41-7.43 (m, 3H), 7.47-7.51 (m, 4H), 7.72 (d, *J* = 7.2Hz, 2H); ^{13}C NMR (125MHz, $CDCl_3$): δ 112.8, 125.4, 129.0, 129.1, 129.41, 129.44, 130.4, 132.3, 136.7, 137.3, 150.7, 160.9; Mass (EI): *m/z* = 299 (M^+); Anal. Calcd for $C_{16}H_{10}ClNO_3$: C, 64.12; H, 3.36; N, 4.67. Found: C, 64.16; H, 3.38; N, 4.53.

*S1.3.19. (Z)-5-(4-Chlorobenzylidene)-3-p-tolyloxazolidine-2,4-dione (**3de'**).*



Yield 253.0 mg (81%); physical state: solid; color: white; mp = 187-188°C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 2.41 (s, 3H), 6.83 (s, 1H), 7.31 (d, *J* = 7.8Hz, 2H), 7.36 (d, *J* = 8.4Hz, 2H), 7.42 (d, *J* = 8.4Hz, 2H), 7.73 (d, *J* = 8.4Hz, 2H); ^{13}C NMR (125MHz, $CDCl_3$): δ 21.2, 112.7, 125.2, 127.8, 129.2, 129.4, 130.0, 132.3,136.7, 137.4, 139.3, 150.8, 161.1; Anal. Calcd for $C_{17}H_{12}ClNO_3$: C, 65.08; H, 3.86; N, 4.46. Found: C, 65.15; H, 3.78; N, 4.41; Mass (EI): *m/z* = 313 (M^+).

S1.4. Crystallographic data collection and refinement of the structures. The diffraction data of oxazolidinone **3aa'** was measured at 173 K with Mo Kα radiation on an X-ray diffraction camera system using a Bruker SMART CCD equipped with a graphite crystal incident beam monochromator. The SMART and SAINT software packages were used for data collection and integration, respectively. The collected data were corrected for absorbance using SADABS, based on the Laue symmetry, using equivalent reflections. The ADSC Q210 ADX program was used for data collection, and HKL300022 was used for cell refinement, reduction, and absorption correction. The crystal structures were solved by the direct method and were refined by full-matrix least-squares calculations using the SHELXTL program package.[3] Crystallization of compound **3aa'** with benzene solvent led to formation of crystal. Single crystal X-ray structure analysis reveals that compound **3aa'** crystalized in the orthorhombic Pbca space group.

Crystallographic and structure refinement parameter for oxazolidinone 3aa'.

	3aa'
CCDC No.	1014398
Formulae	$C_{18}\ H_{15}\ N\ O_5$
Formula. wt.	325.31
Crystal system	orthorhombic
Space group	Pbca
a (Å)	12.291 (3)
b (Å)	7.4147 (15)
c (Å)	34.667 (7)
α (°)	90.00
β (°)	90.00
γ (°)	90.00
V (Å^3)	3159.3 (11)
Z	8
density/Mg m^{-3}	1.368
abs. Coeff. /mm^{-1}	0.101
F(000)	1360
total no. of reflections	28515
Reflections, *I > 2σ(I)*	1860
Max. (2θ°)	50.00
ranges (h, k, l)	-12 ≤ h ≤ 15

	-9 ≤ k ≤ 9
	-44 ≤ l ≤ 44
Complete to 2θ (%)	99.6
data/ restraints/parameters	3606/ 0 / 219
GOF (F^2)	1.016
R indices [$I > 2\sigma(I)$]	0.0506
R indices (all data)	0.1129

Crystallographic parameters of **3aa'**

S1.5. Gas-chromatography/MS Spectrum data:

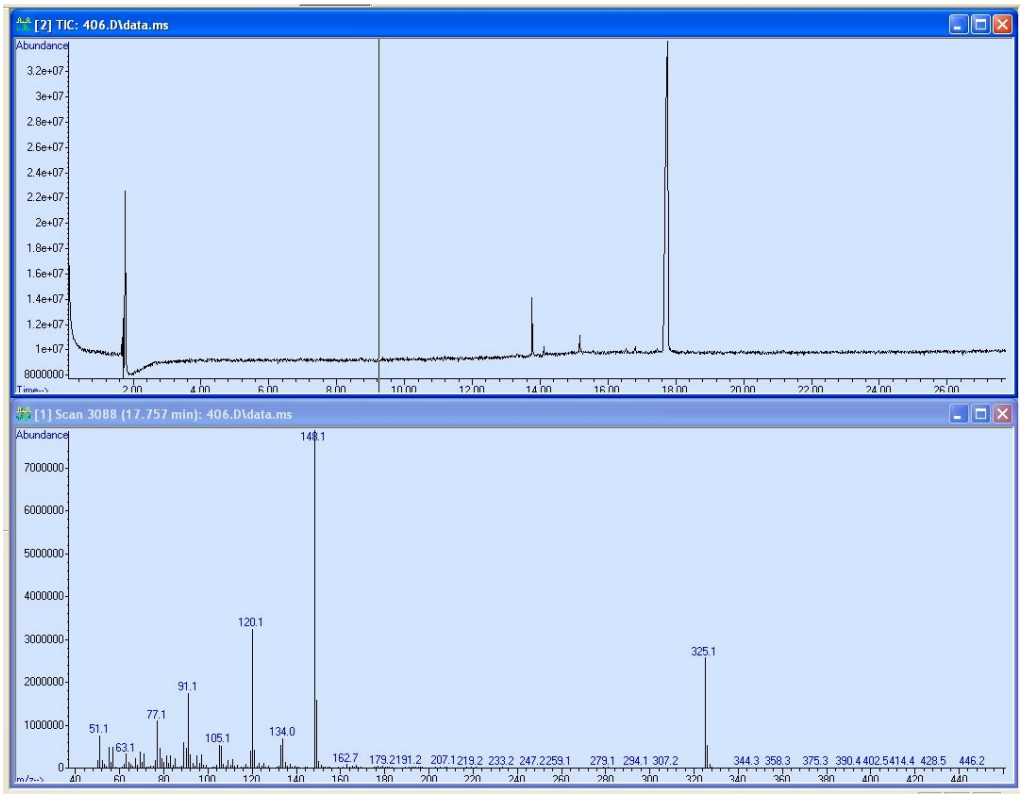


Figure S1. GC-MS spectra for the oxazolidinone **3aa'**.

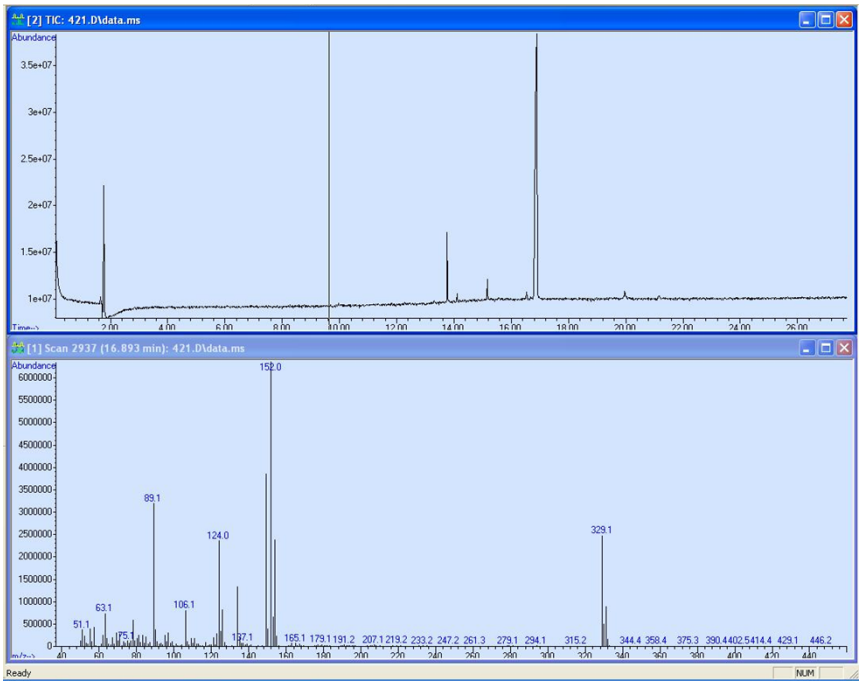
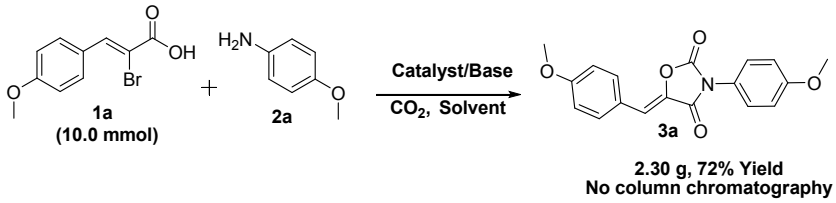


Figure S2. GC-MS spectra of oxazolidinone **3aa'** synthesised by labled $C^{18}O_2$.



Scheme S1. Gram-scale synthesis of oxazolidinone **3aa'**.

2. References

1. X. Gong, H. Yang, H. Liu, Y. Jiang, Y. Zhao, H. Fu, *Org. Lett.*, 2010, **12**, 3128.
2. G. Chen, C. Fu, S. Ma, *Org. Biomol. Chem.* 2011**, 9**, 105-110.
3. D. Kim, X. Liu, M. Oh, X. Song, Y. Zou, D. Singh, K. S. Kim, M. S. Lah, *CrystEngComm* 2014**, 16**, 6391-6397.

Copies of NMR spectra of oxazolidinone compound:

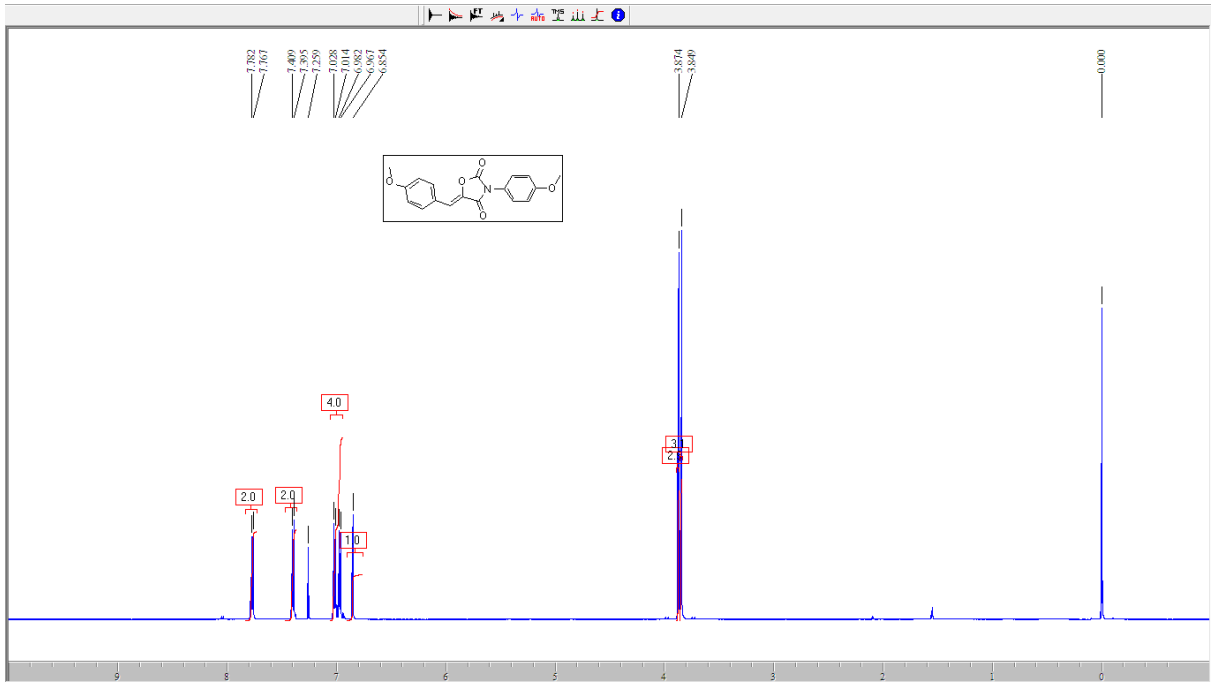


Figure S3: ^{1}H NMR spectra of compound 3aa'.

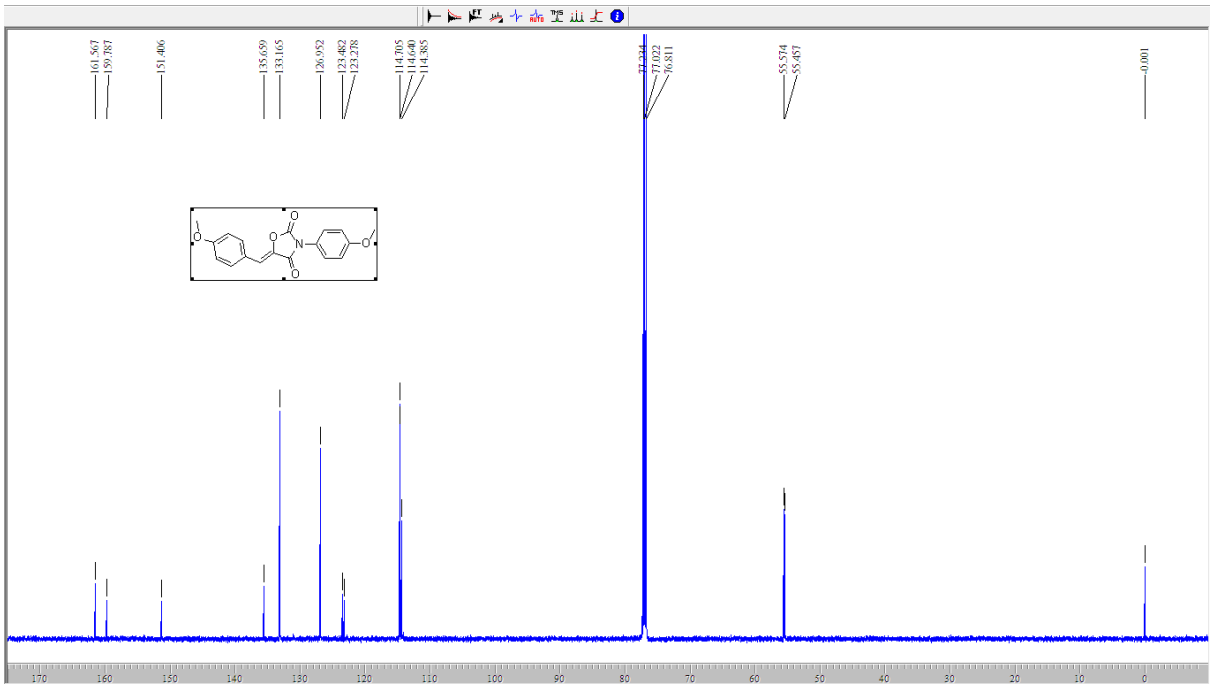


Figure S4: ^{13}C NMR spectra of compound 3aa'.

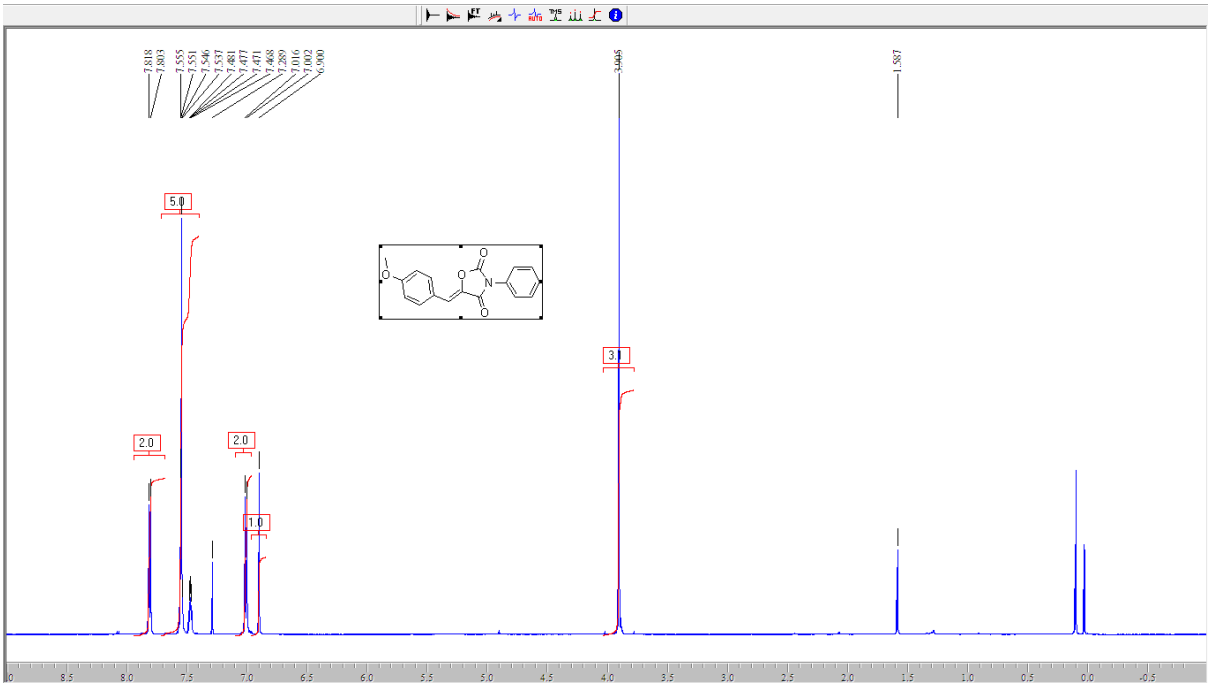


Figure S5: ^{1}H NMR spectra of compound 3ab'.

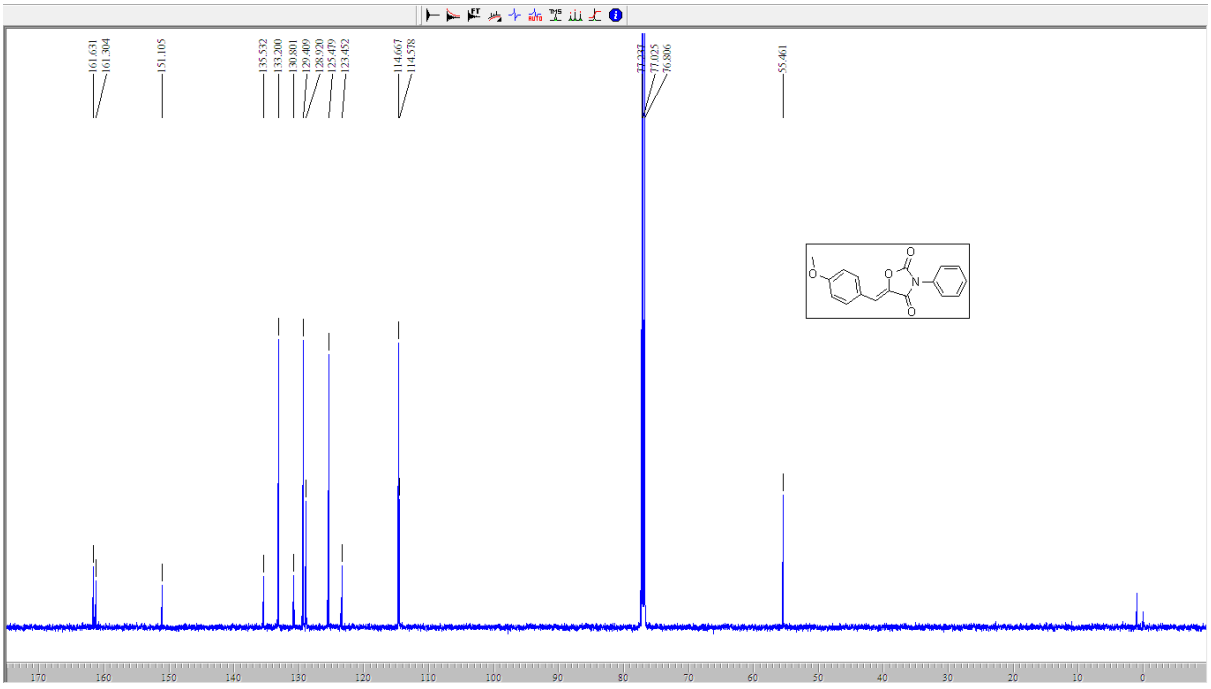


Figure S6: ^{1}H NMR spectra of compound 3ab'.

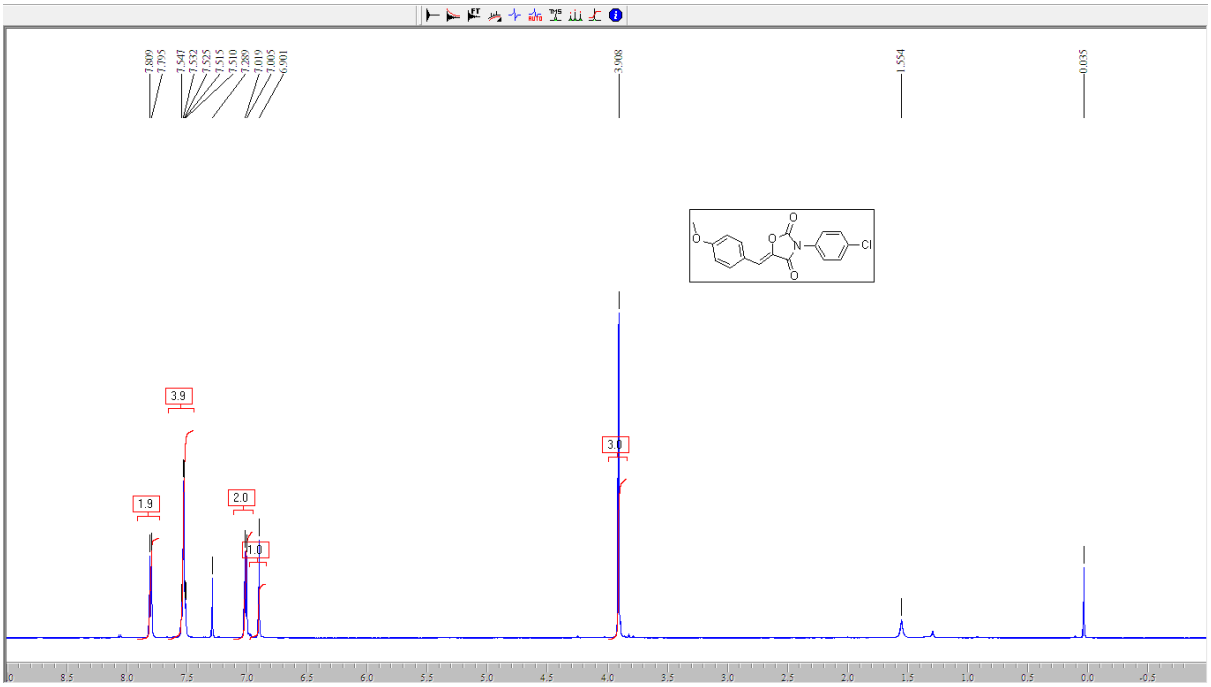


Figure S7: ^{1}H NMR spectra of compound 3ac'.

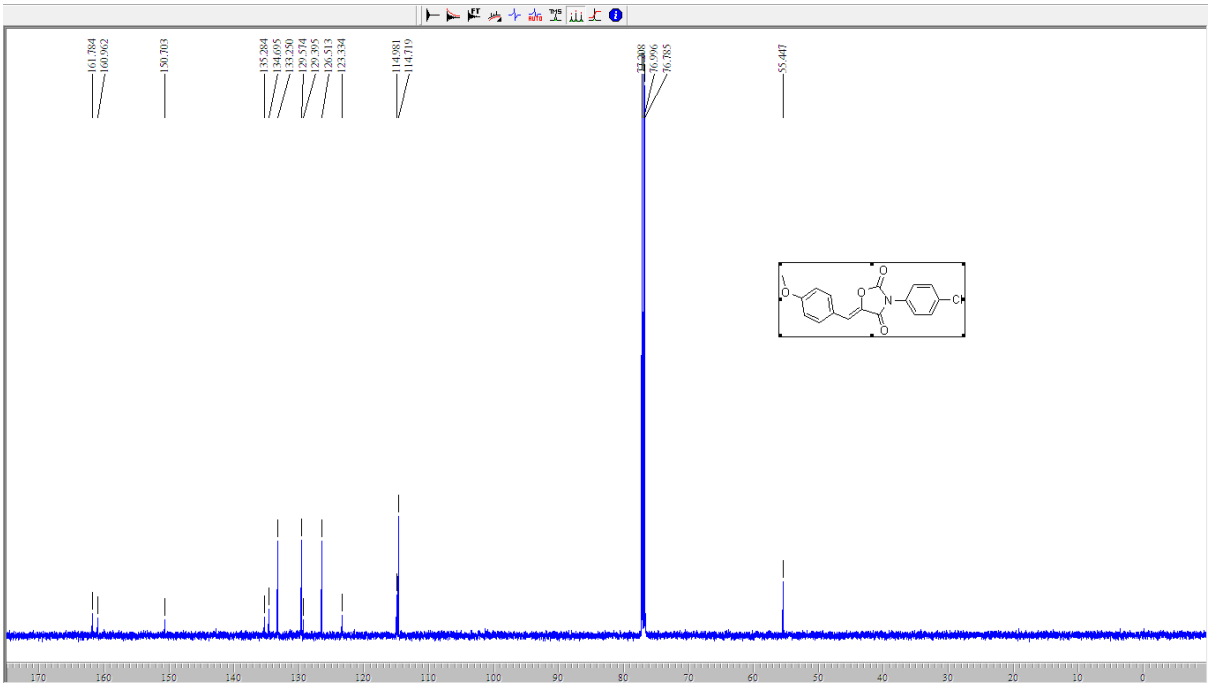


Figure S8: ^{13}C NMR spectra of compound 3ac'.

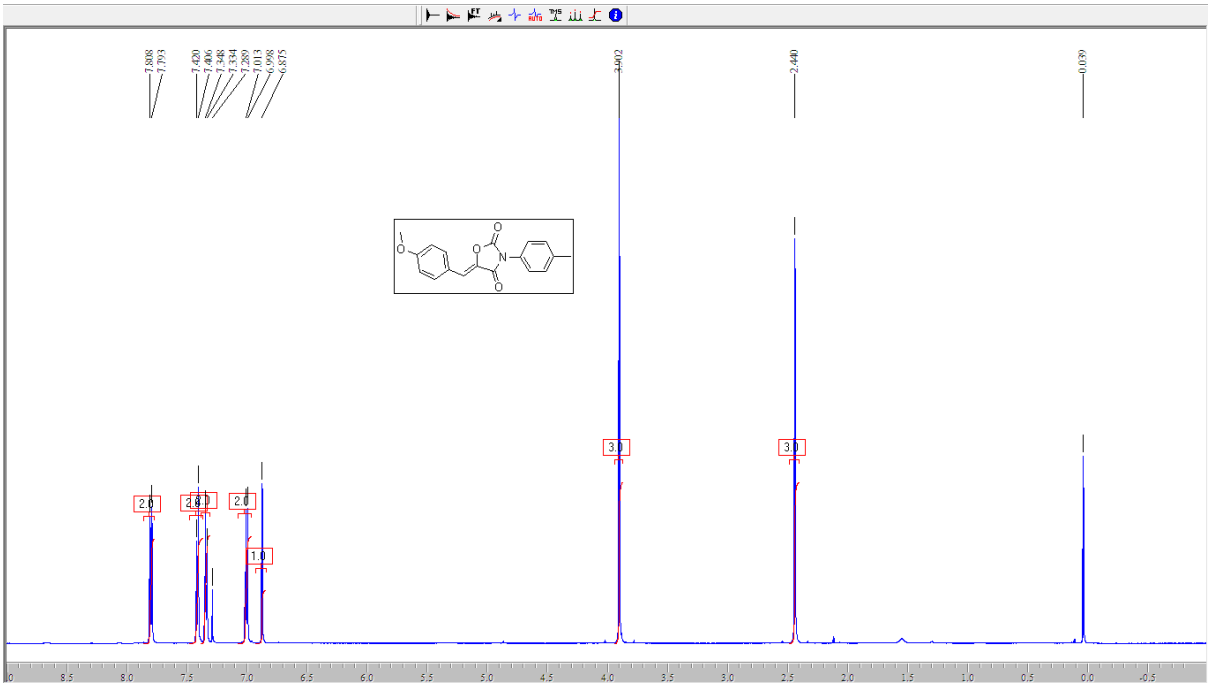


Figure S9: ^{1}H NMR spectra of compound 3ae'.

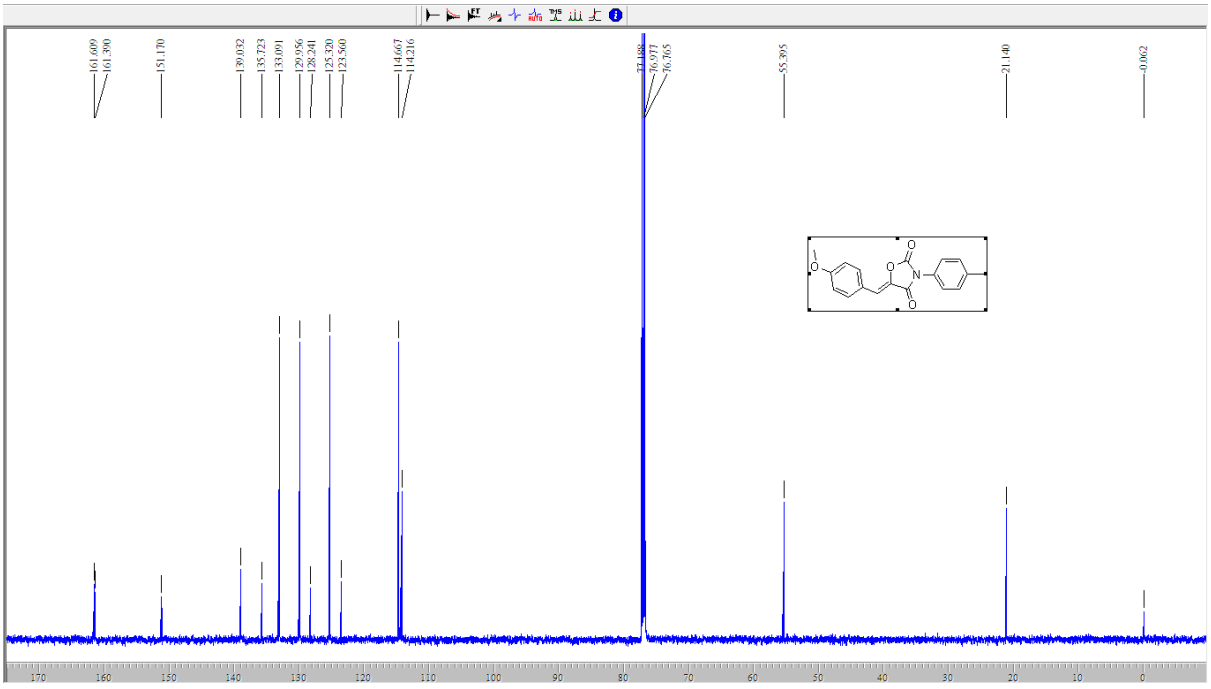


Figure S10: ^{13}C NMR spectra of compound 3ae'.

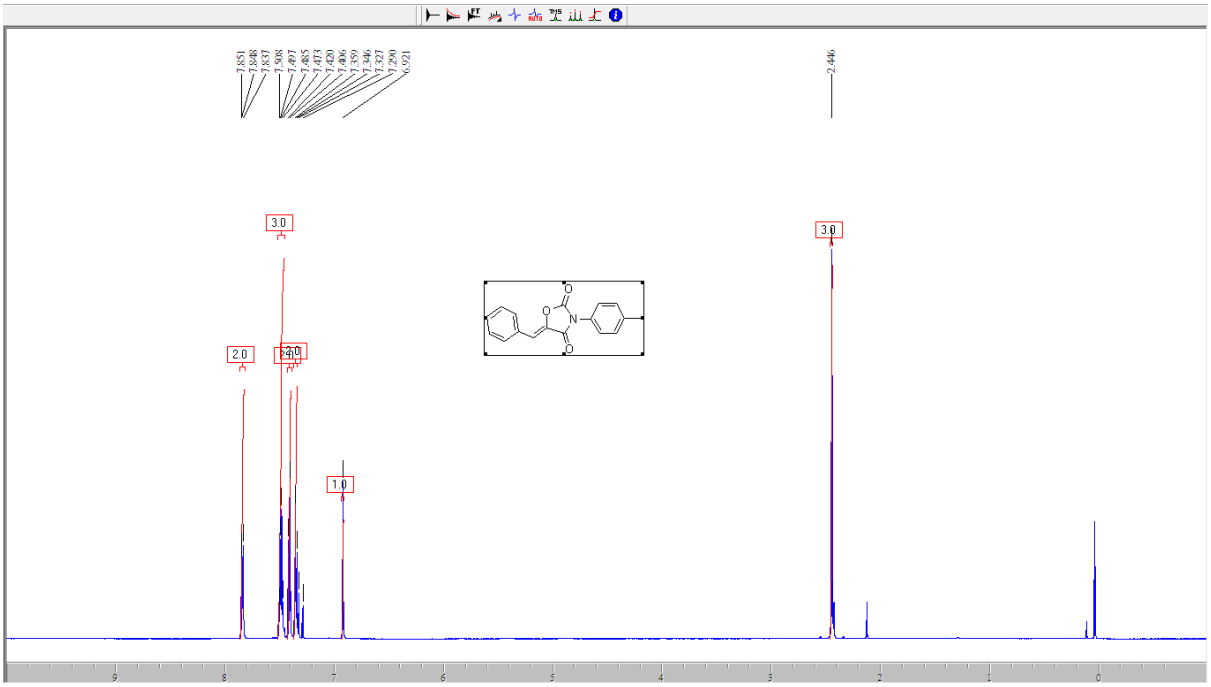


Figure S11: ^{1}H NMR spectra of compound 3be'.

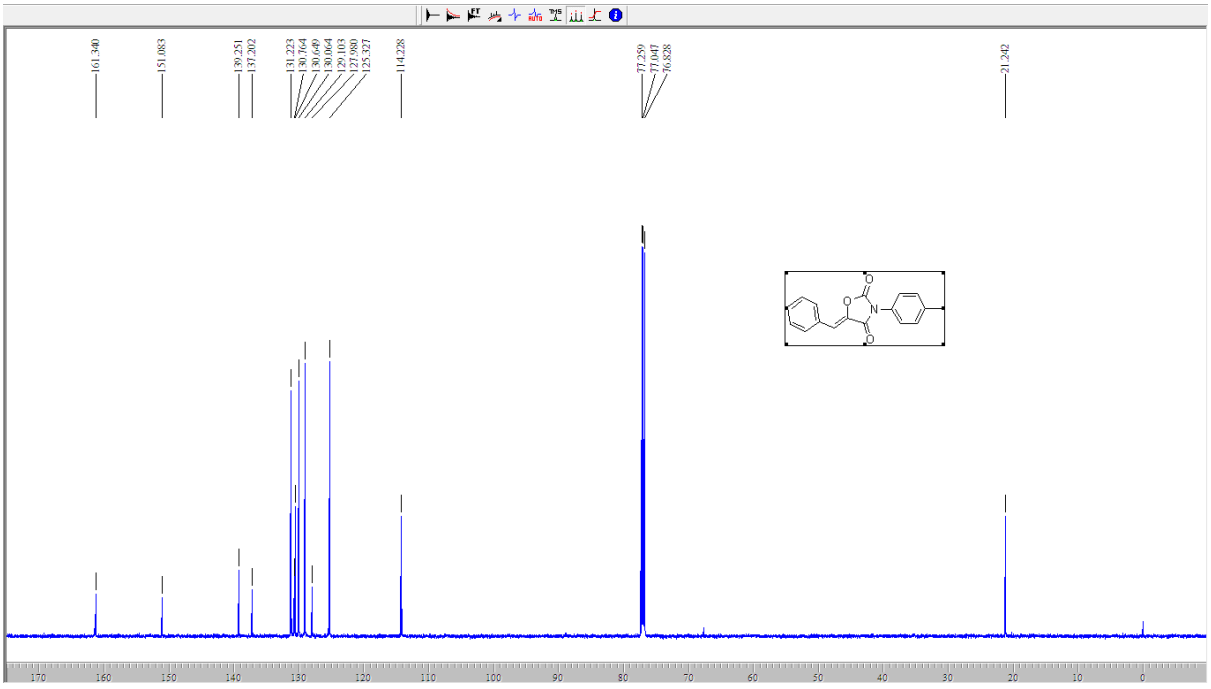


Figure S12: ^{1}H NMR spectra of compound 3be'.

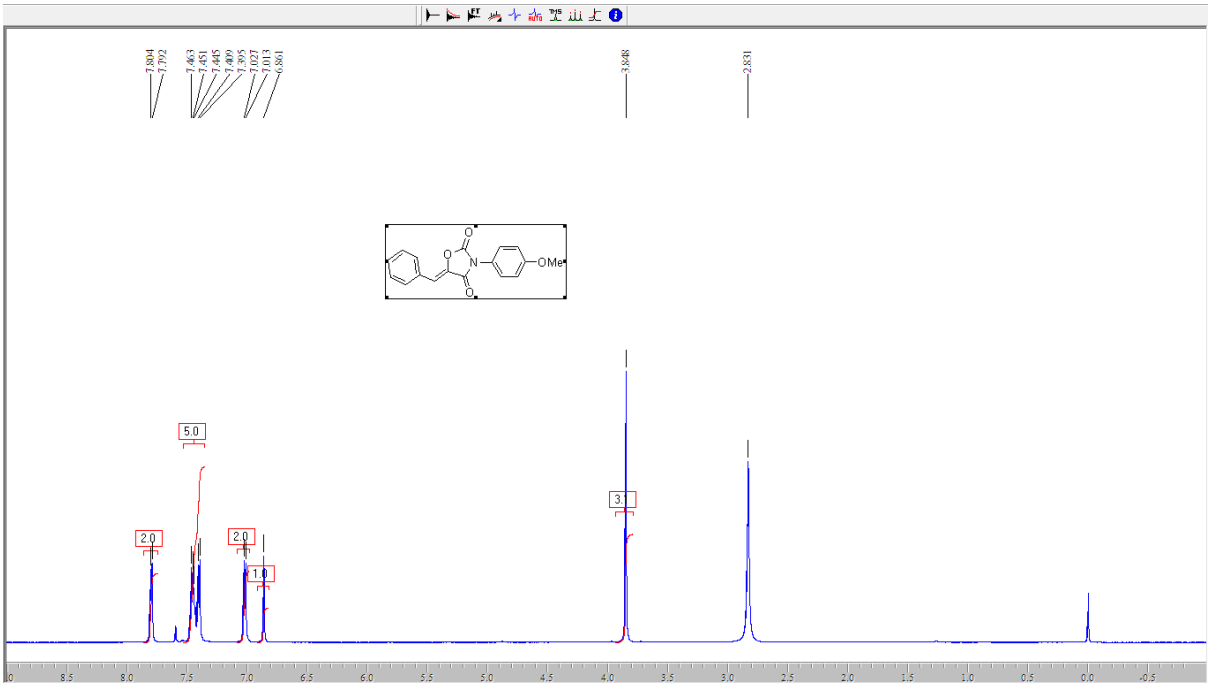


Figure S13: ^{1}H NMR spectra of compound 3ba'.

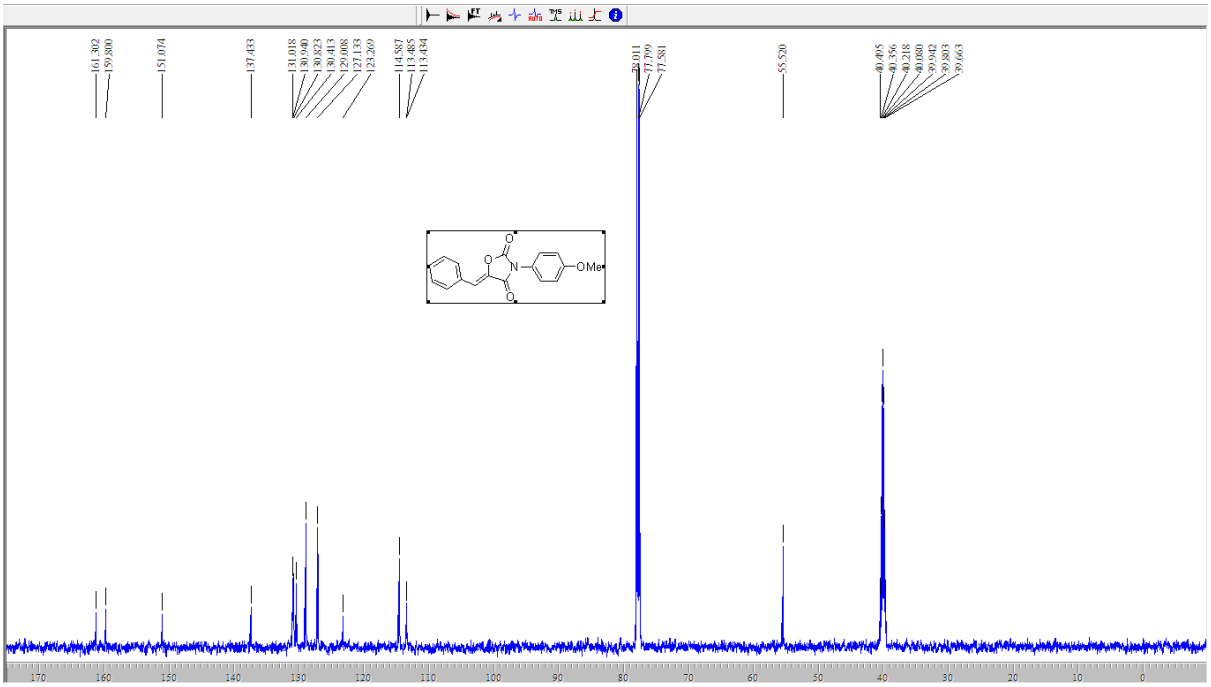


Figure S14: ^{13}C NMR spectra of compound 3ba'.

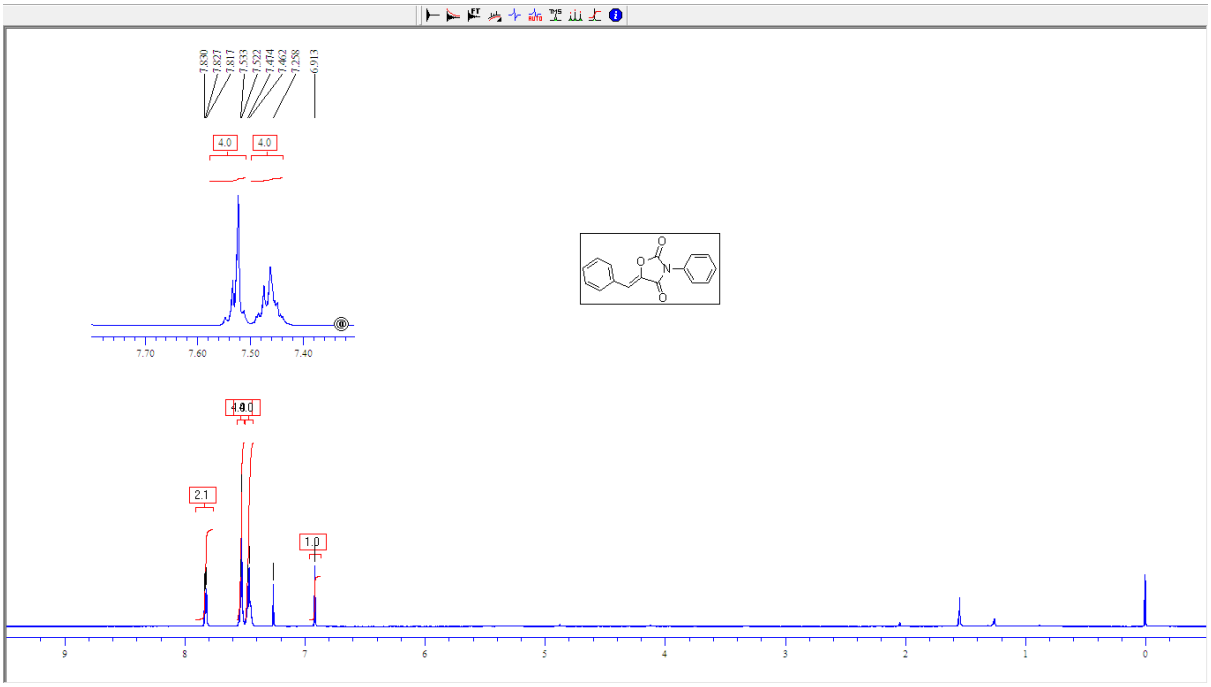


Figure S15: ^{1}H NMR spectra of compound 3bb'.

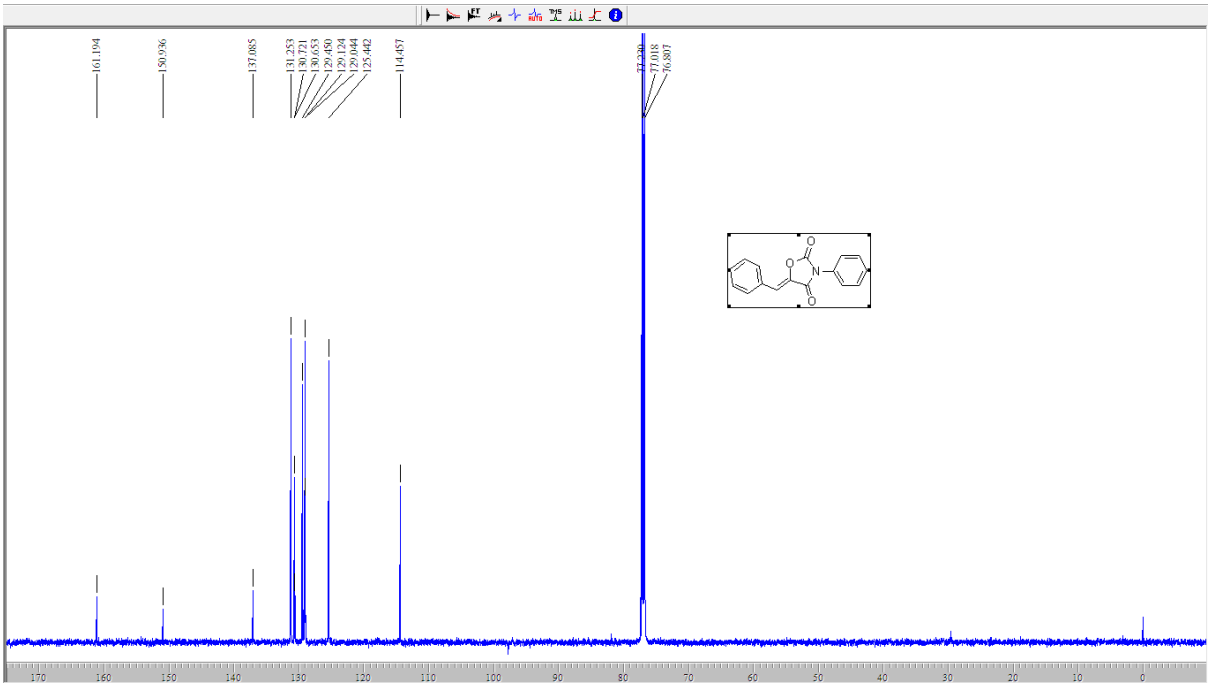


Figure S16: ^{13}C NMR spectra of compound 3bb'.

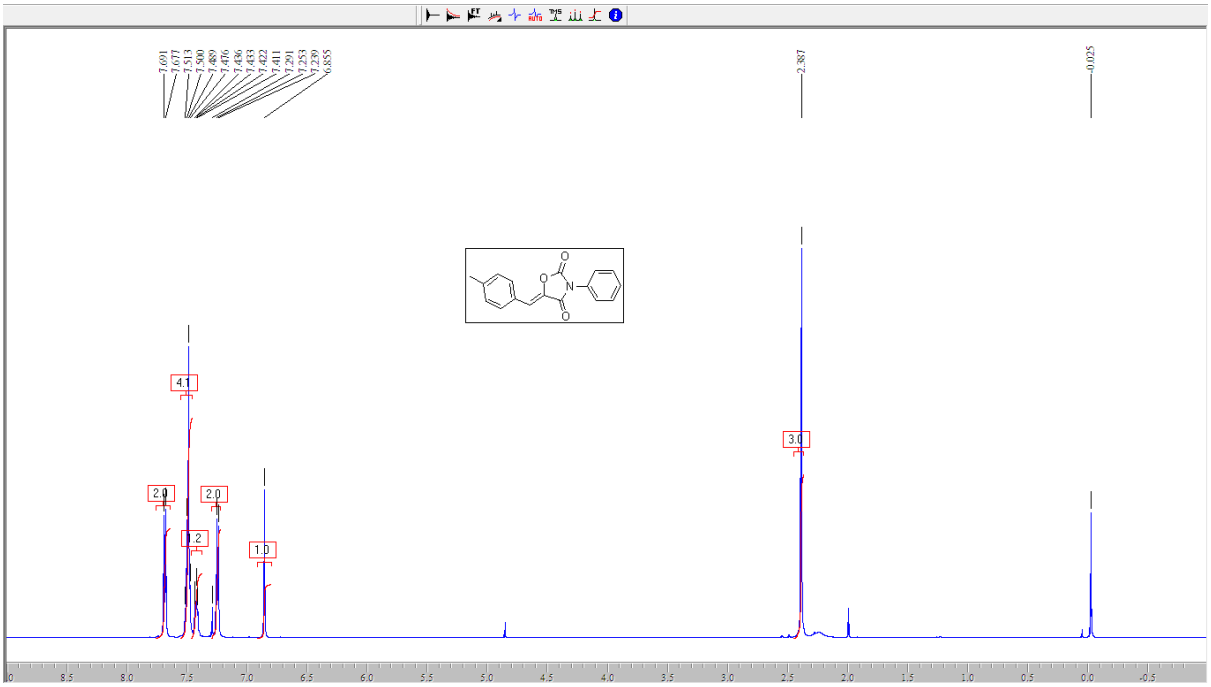


Figure S17: ^{1}H NMR spectra of compound 3cb'.

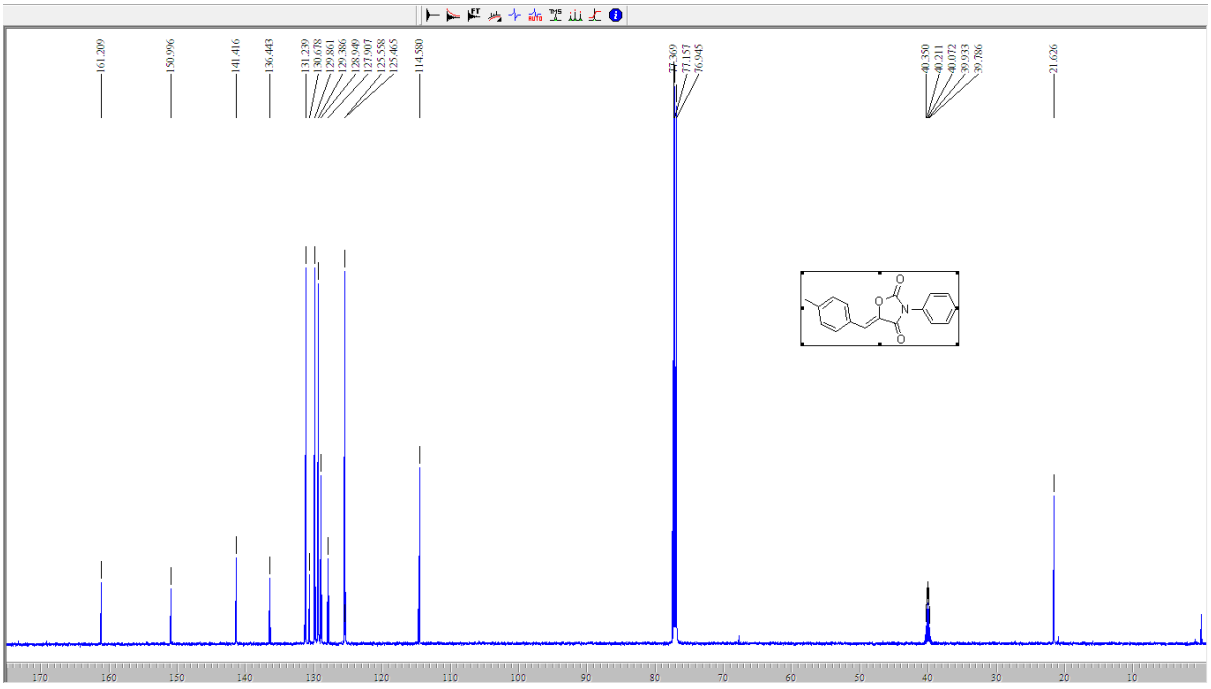


Figure S18: ^{13}C NMR spectra of compound 3cb'.

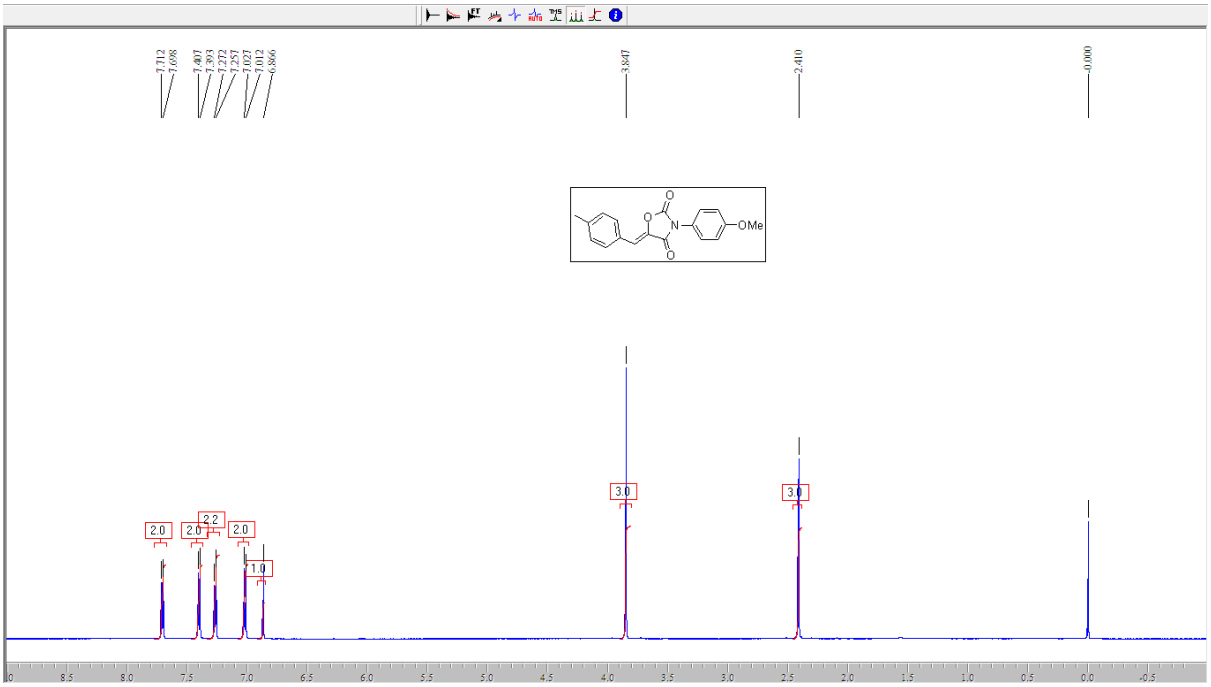


Figure S19: ^{1}H NMR spectra of compound 3ca'.

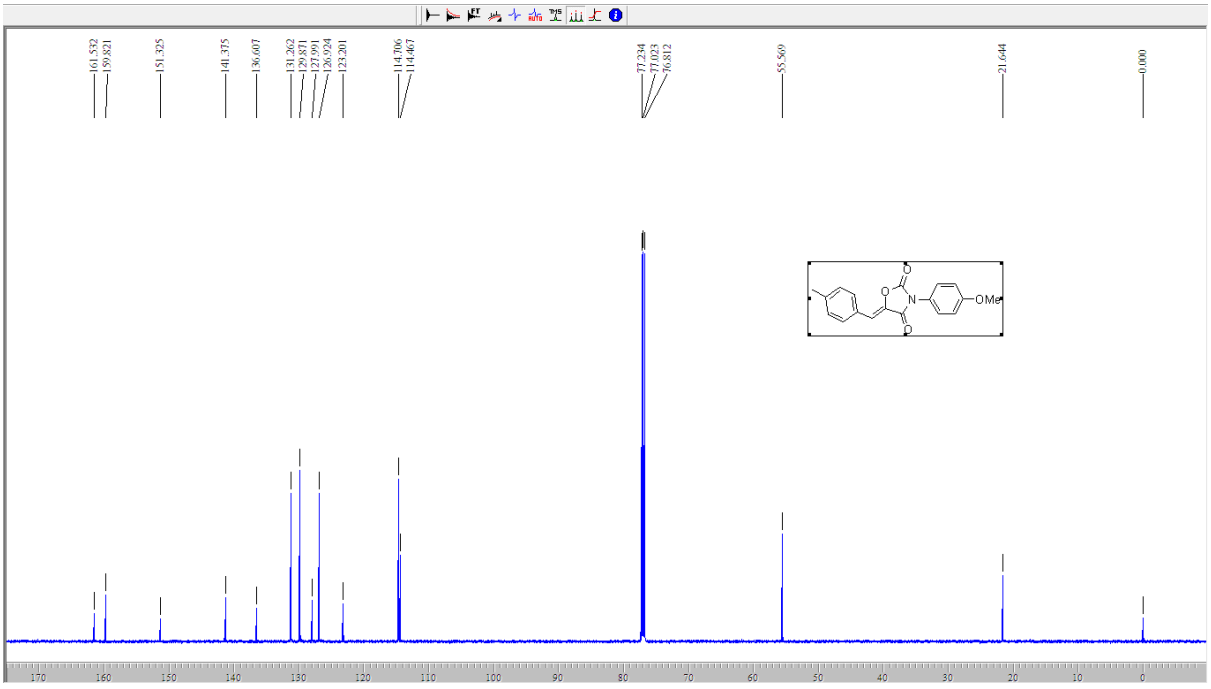


Figure S20: ^{13}C NMR spectra of compound 3ca'.

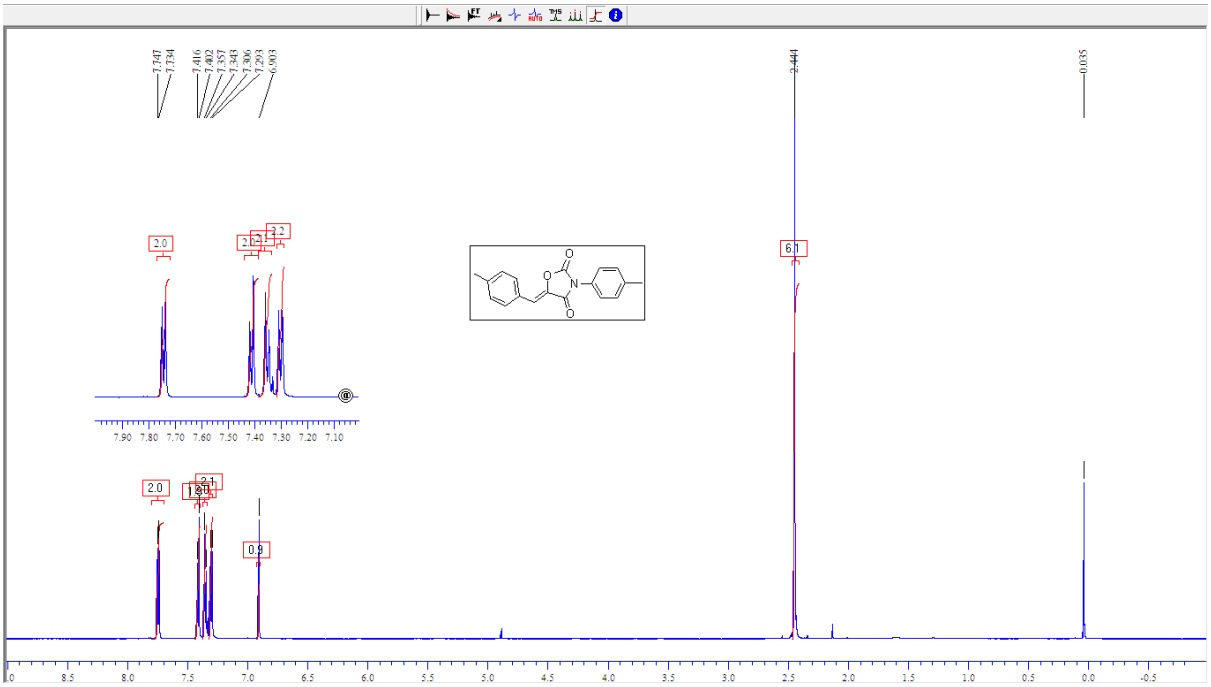


Figure S21: ^{1}H NMR spectra of compound 3ce'.

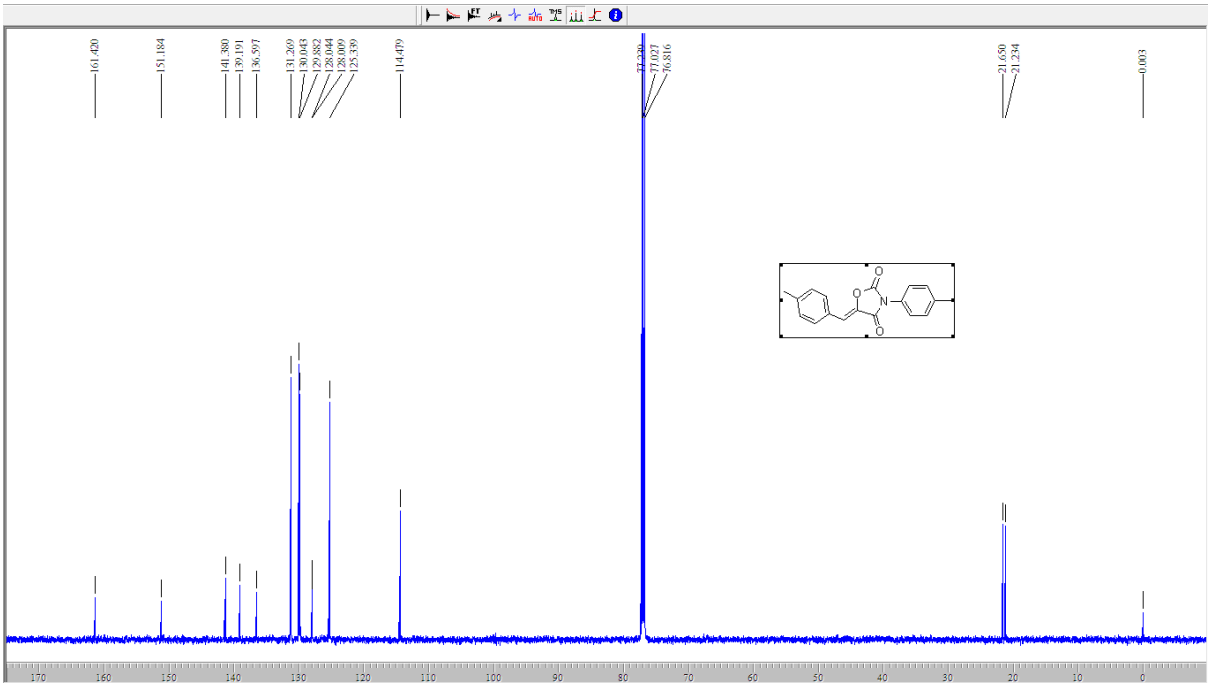


Figure S22: ^{13}C NMR spectra of compound 3ce'.

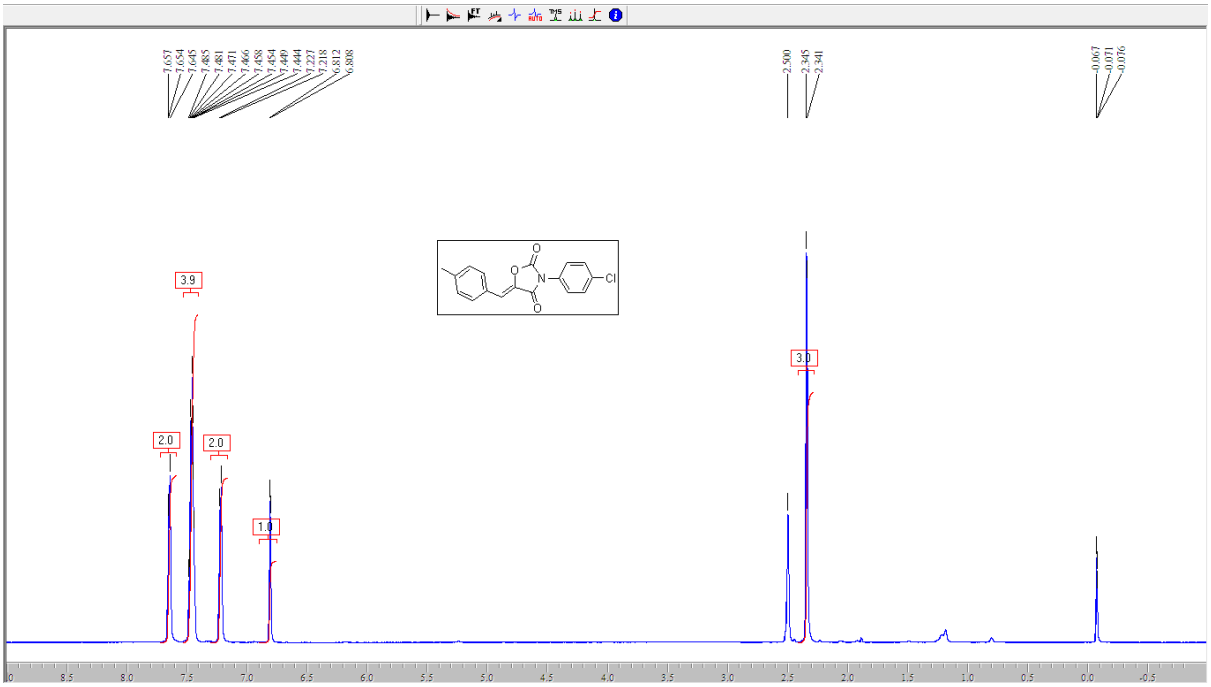


Figure S23: ^{1}H NMR spectra of compound 3cc'.

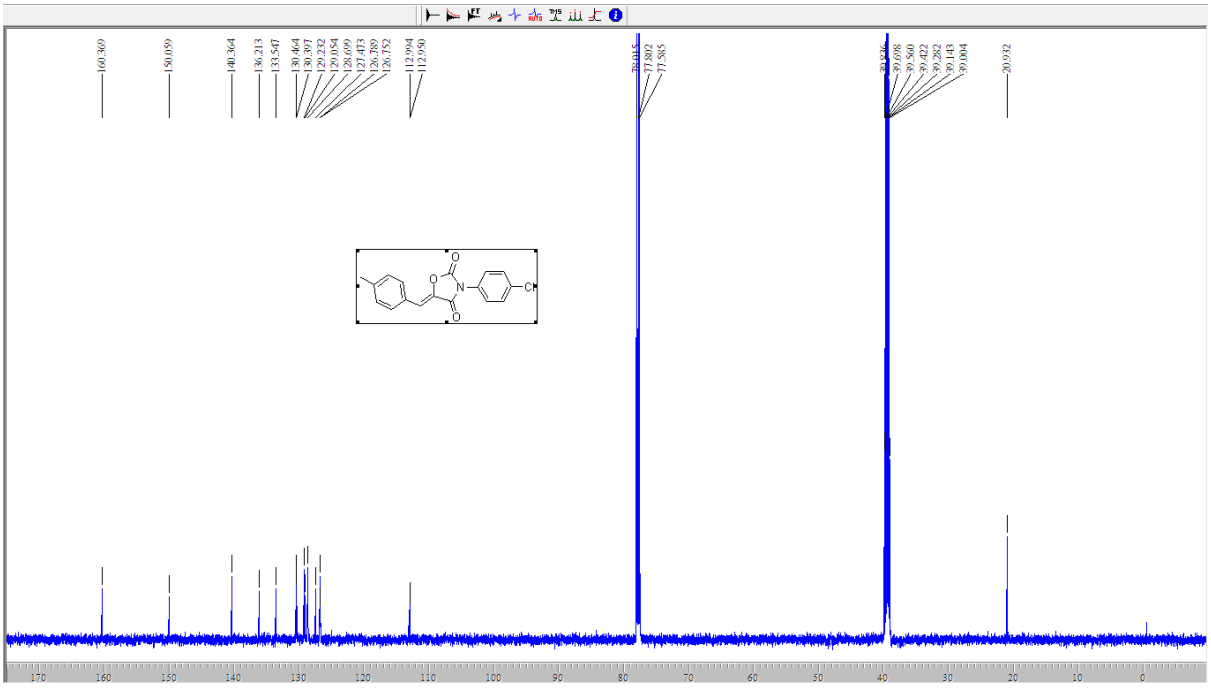


Figure S24: ^{13}C NMR spectra of compound 3cc'.

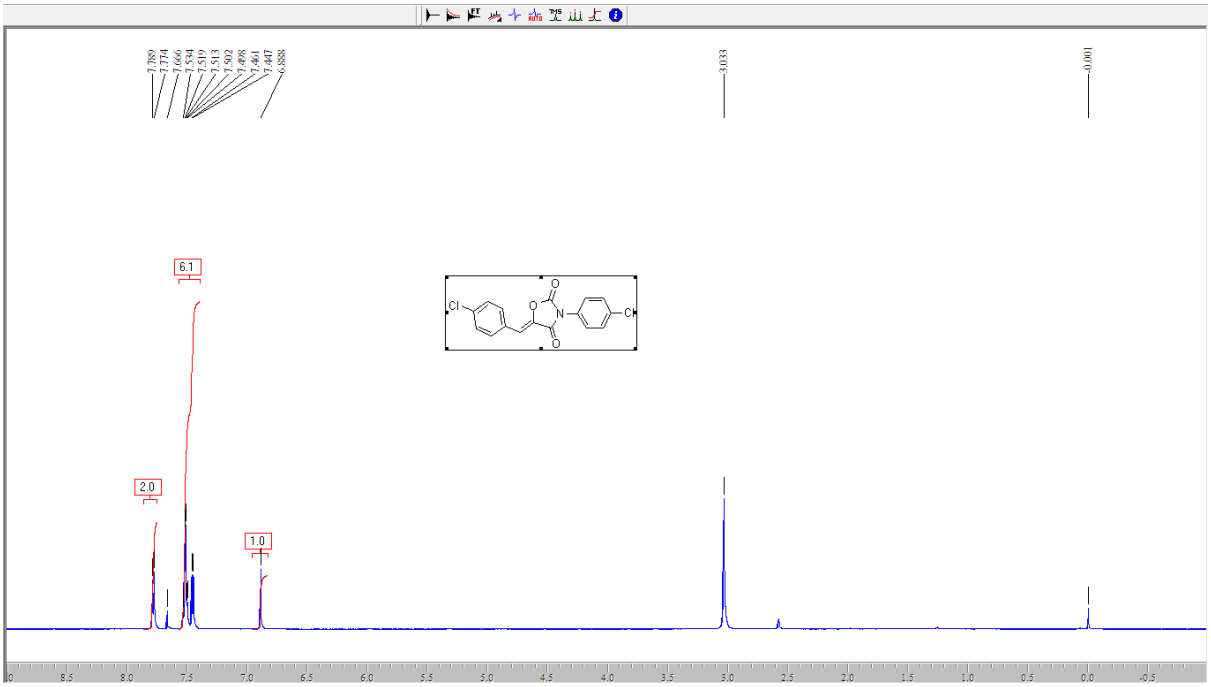


Figure S25: ^{1}H NMR spectra of compound 3dc'.

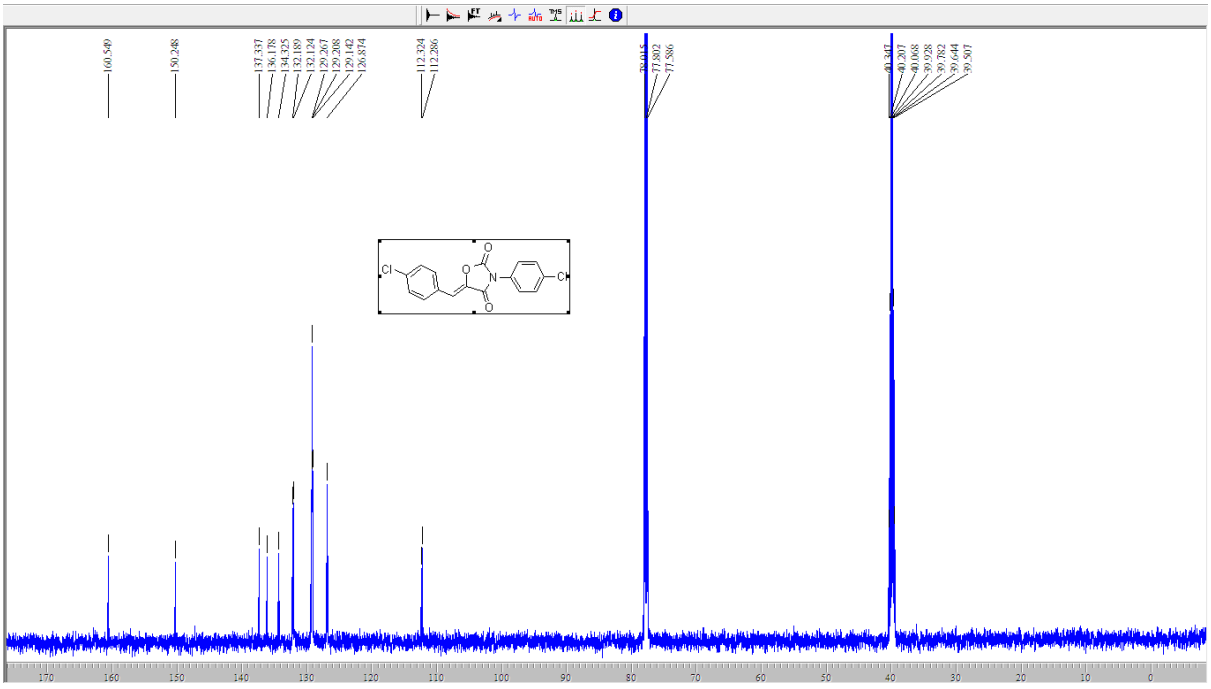


Figure S26: ^{13}C NMR spectra of compound 3dc'.

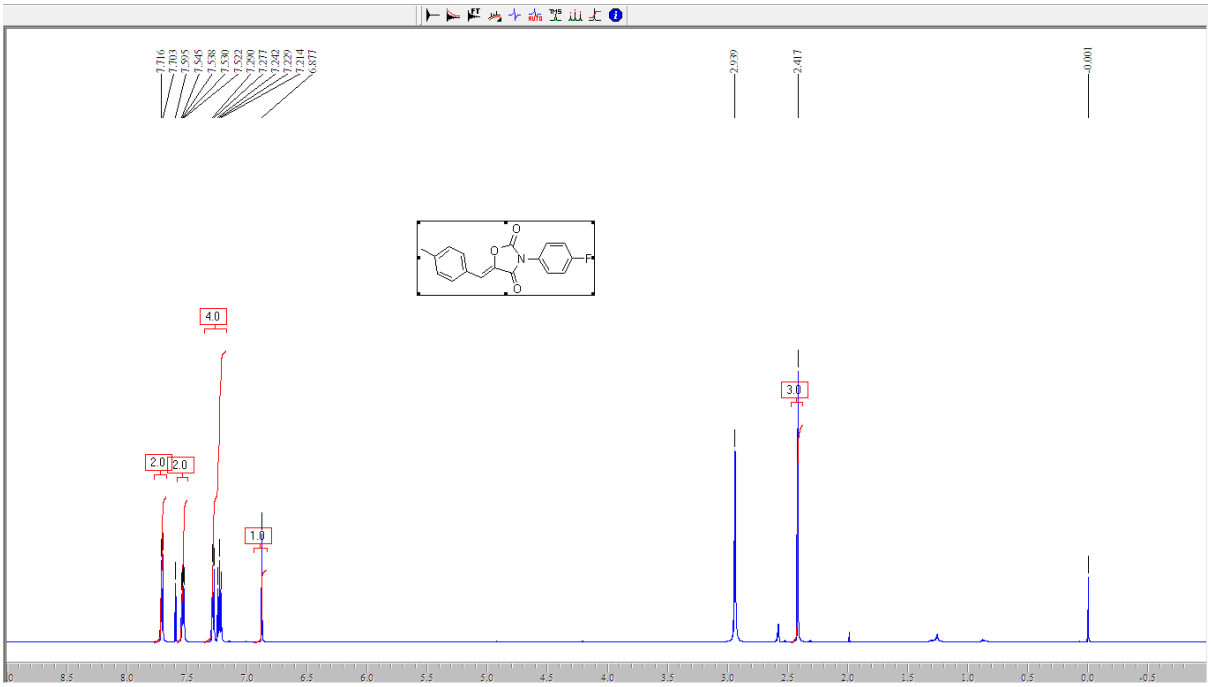


Figure S27: ^{1}H NMR spectra of compound 3cf'.

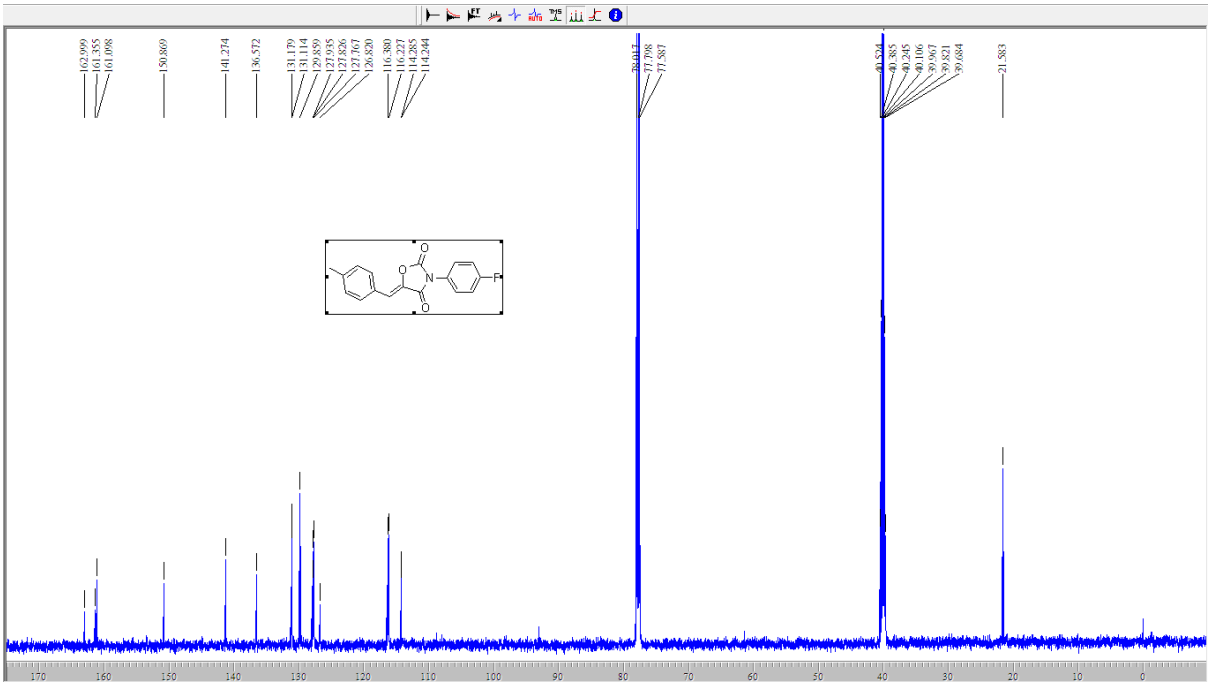


Figure S28: ^{13}C NMR spectra of compound 3cf'.

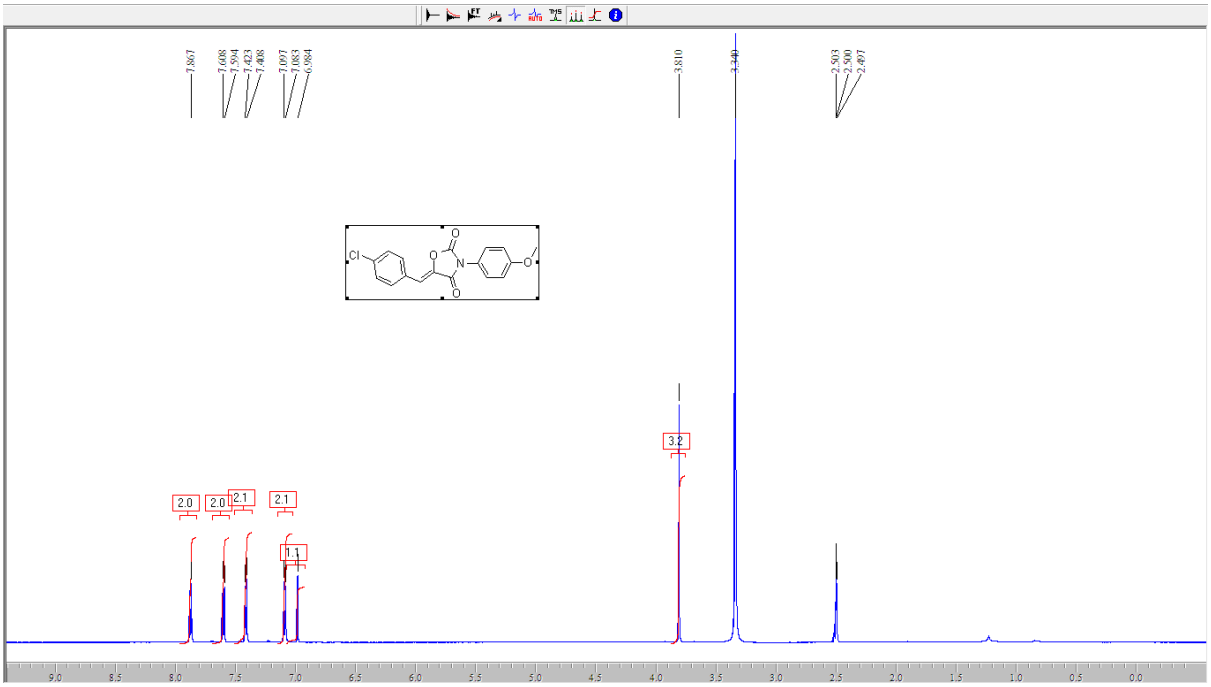


Figure S29: ^{1}H NMR spectra of compound 3da'.

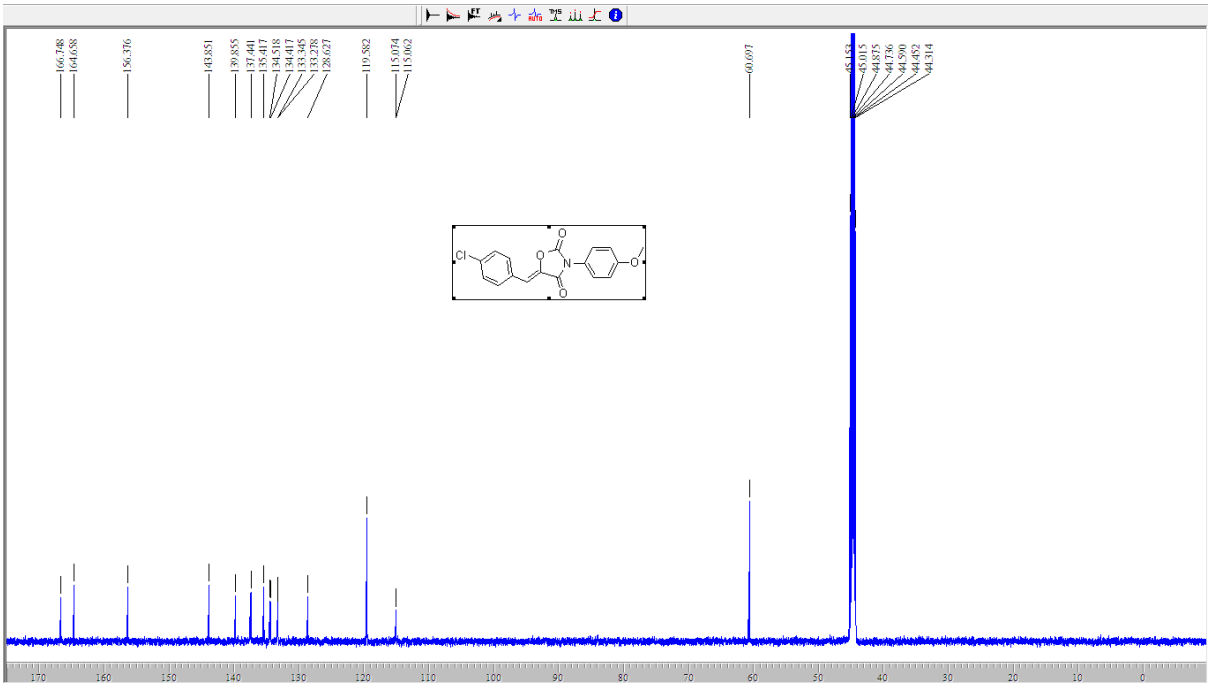


Figure S30: ^{13}C NMR spectra of compound 3da'.

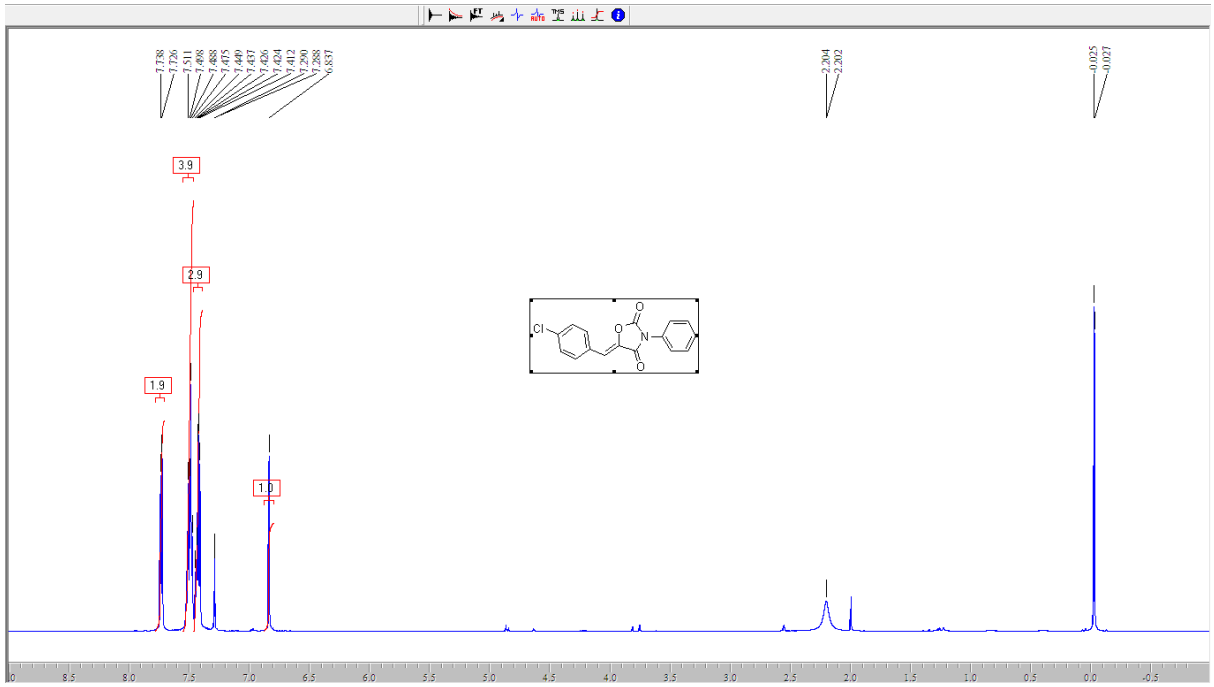


Figure S31: ^{1}H NMR spectra of compound 3db'.

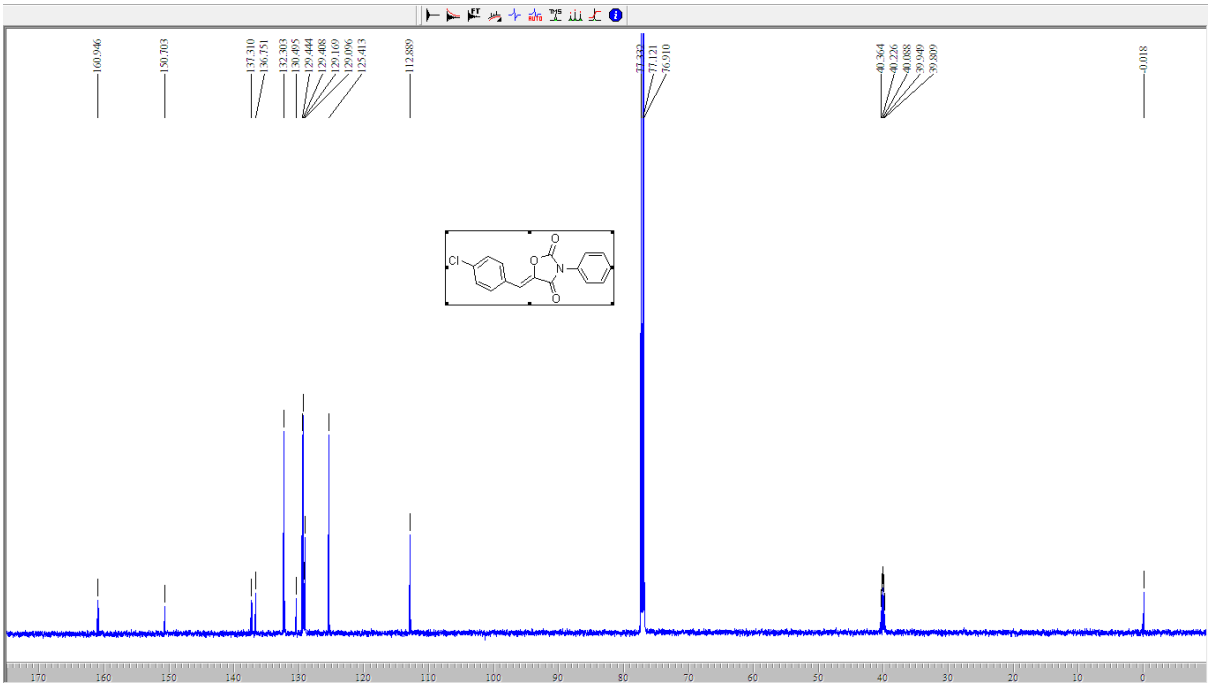


Figure S32: ^{1}H NMR spectra of compound 3db'.

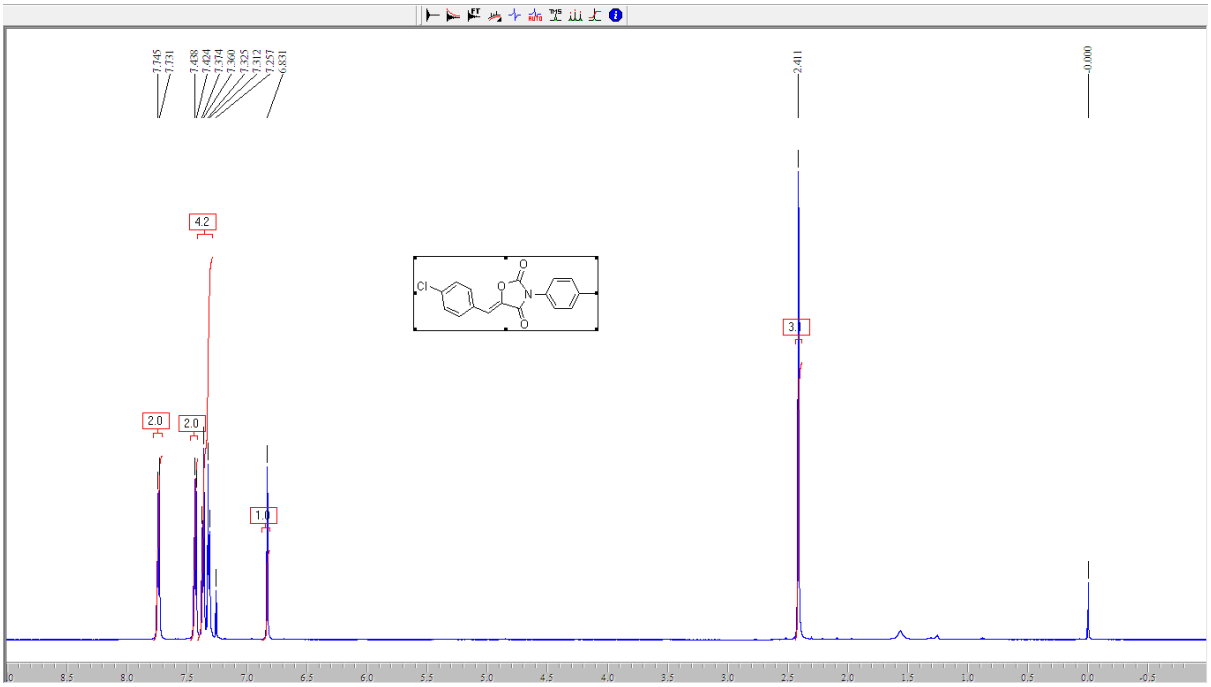


Figure S33: ^{1}H NMR spectra of compound 3de'.

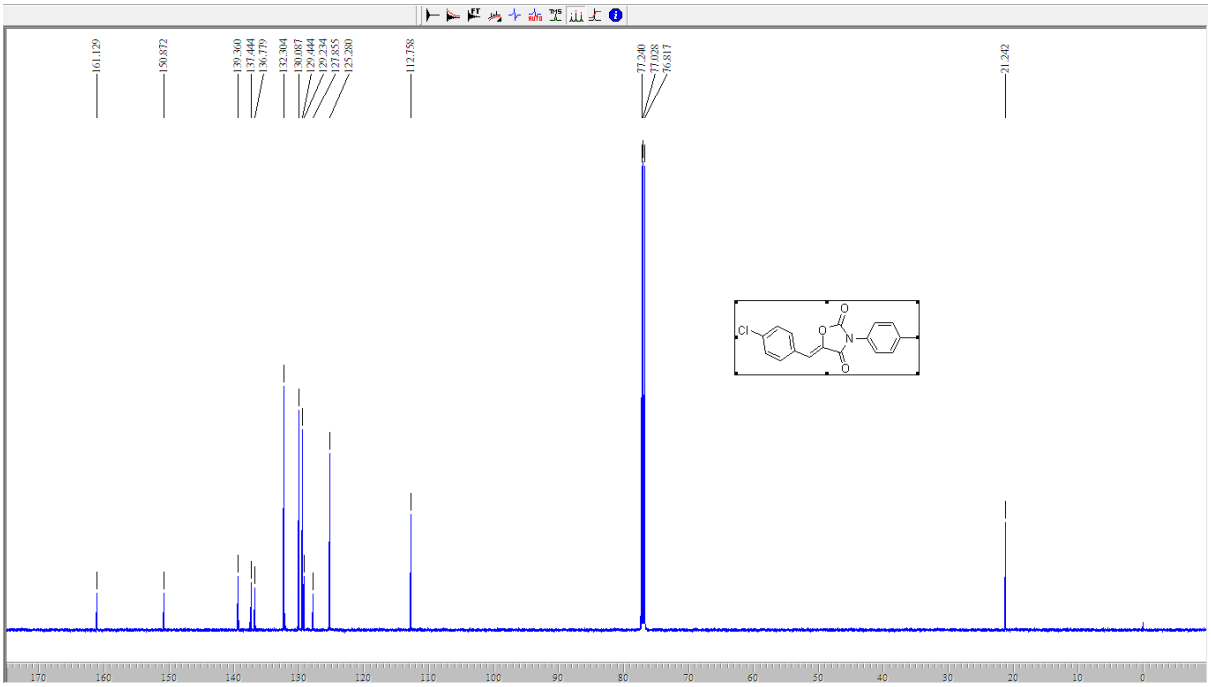


Figure S34: ^{13}C NMR spectra of compound 3de'.

Copies of IR spectra of oxazolidinone compound:

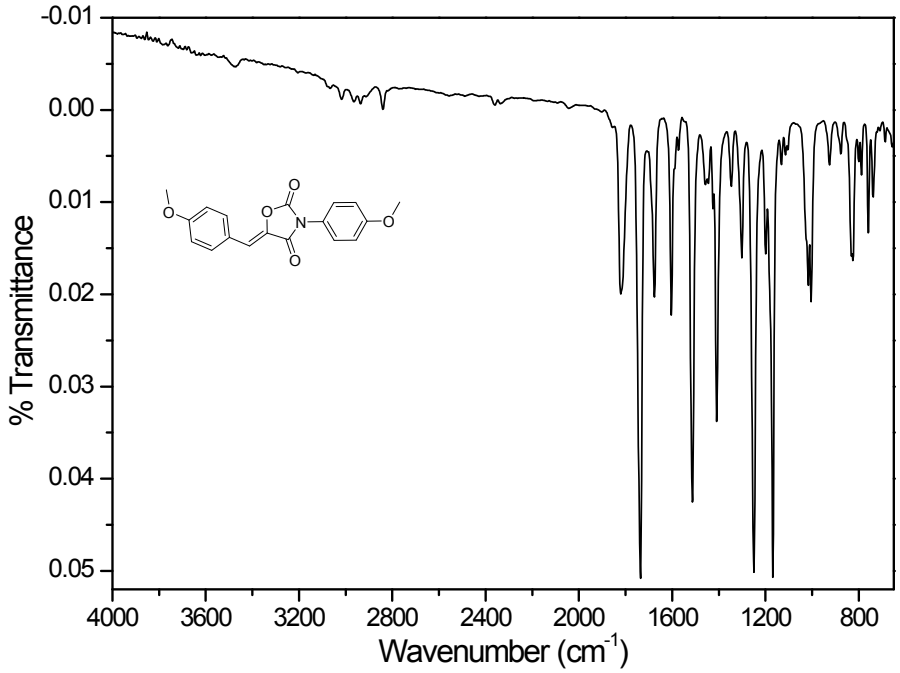


Figure S35: IR spectra of compound 3aa'.

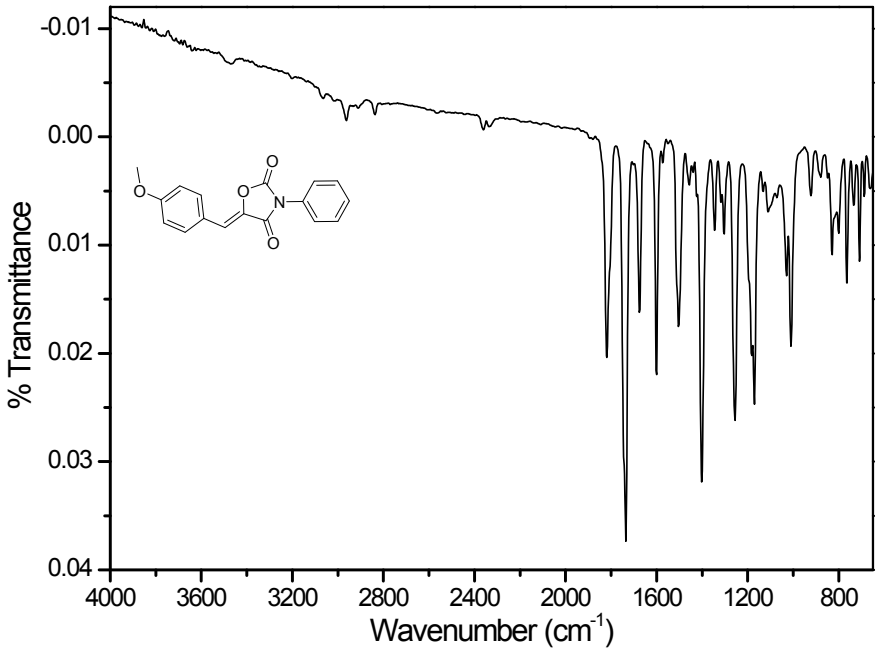


Figure S36: IR spectra of compound 3ab'.

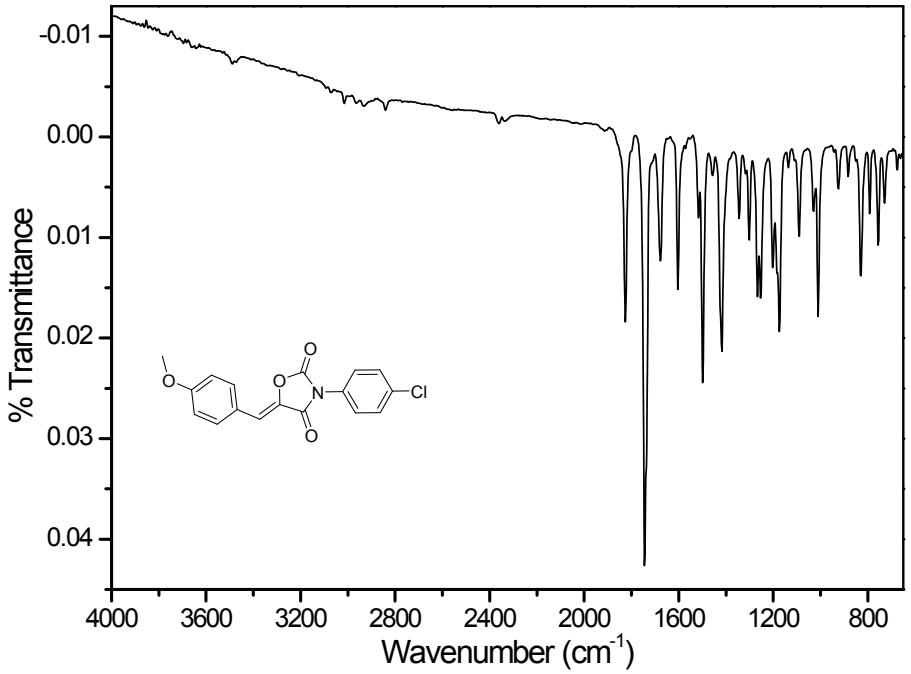


Figure S37: IR spectra of compound 3ac'.

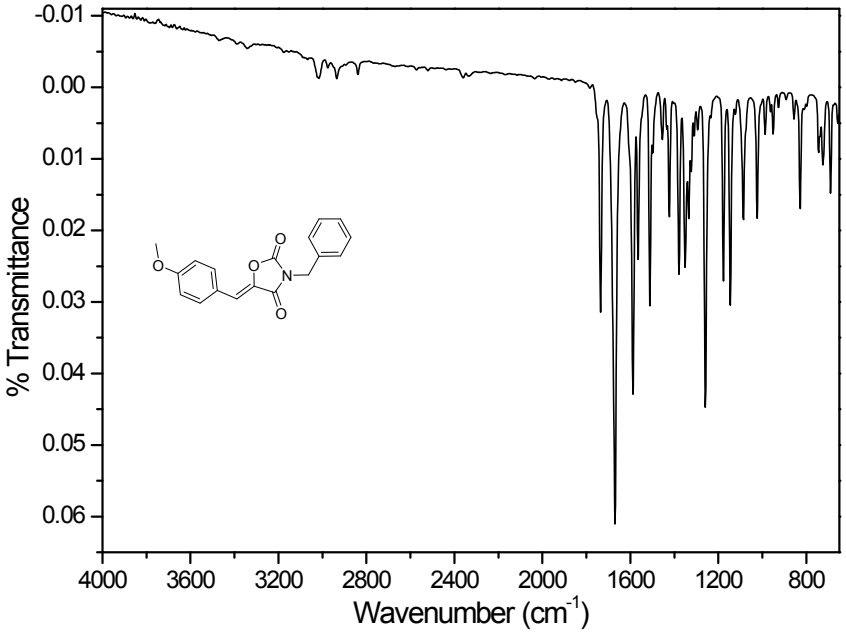


Figure S38: IR spectra of compound 3ad'.

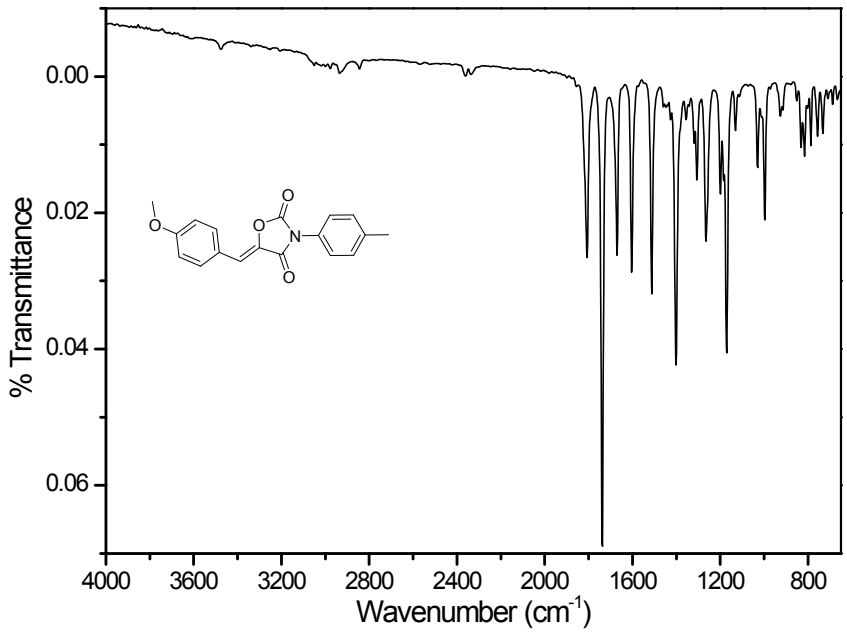


Figure S39: IR spectra of compound 3ae'.

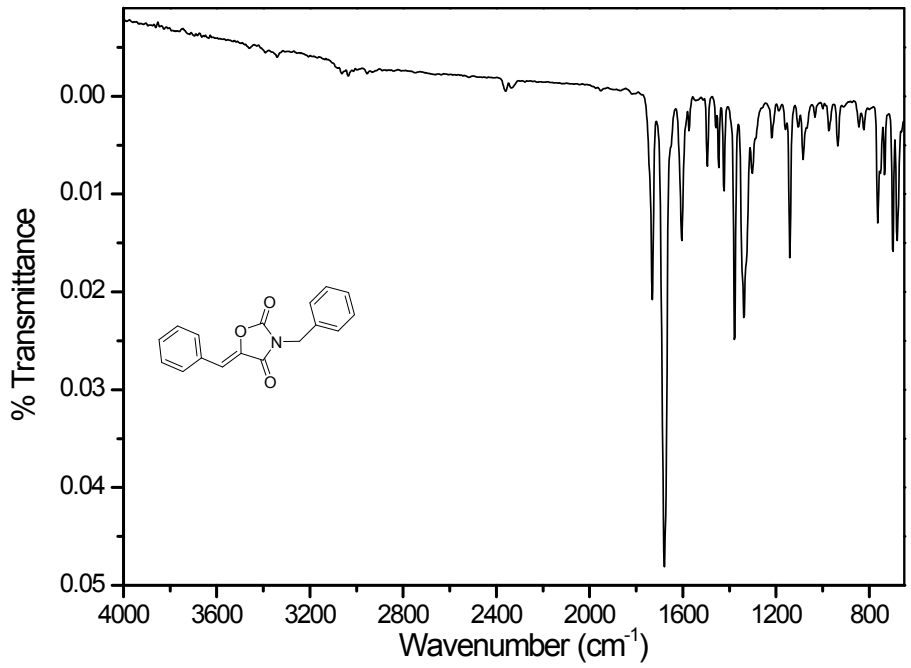


Figure S40: IR spectra of compound 3bd'.

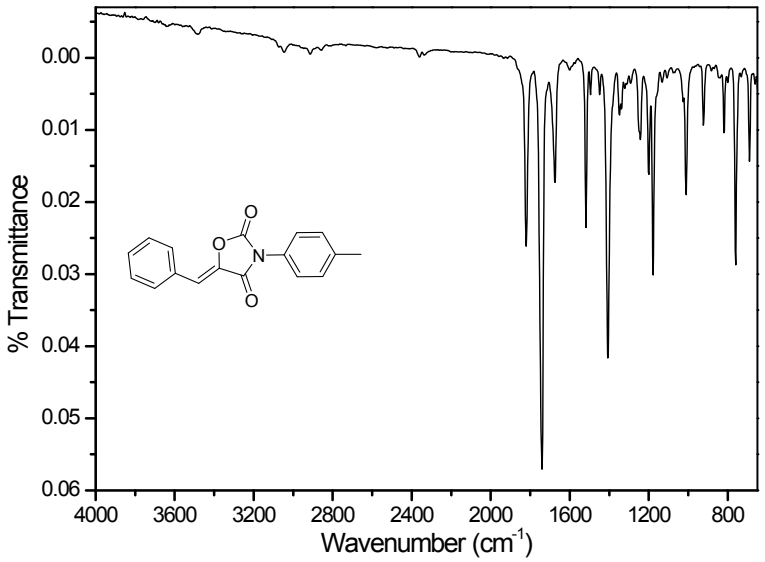


Figure S41: IR spectra of compound 3be'.

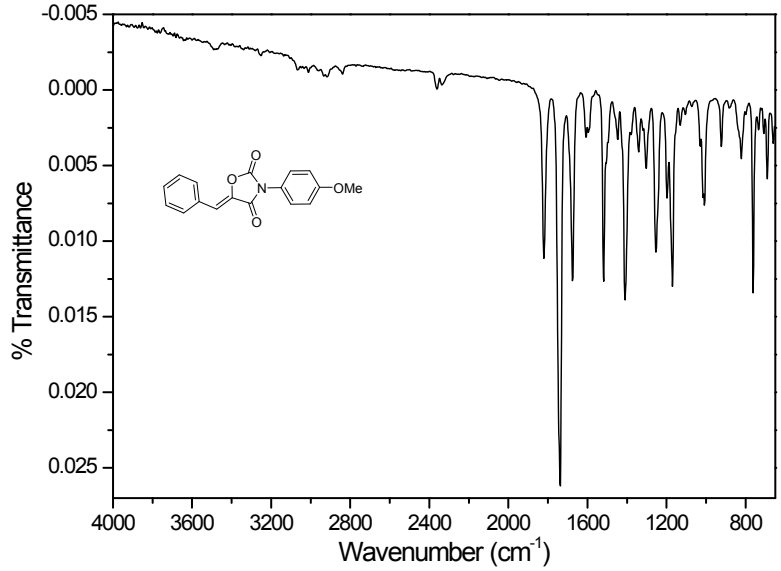


Figure S42: IR spectra of compound 3ba'.

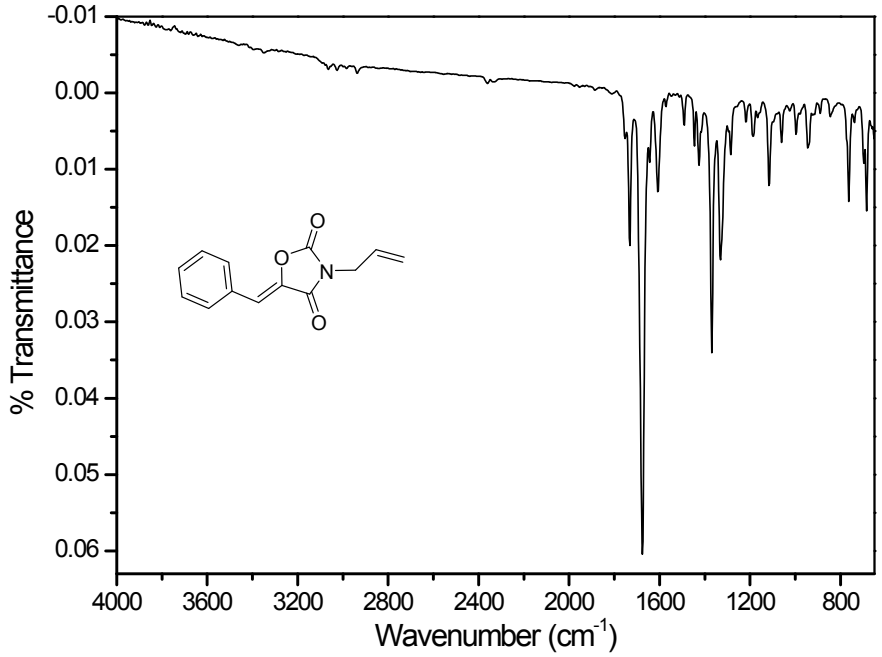


Figure S43: IR spectra of compound 3bg'.

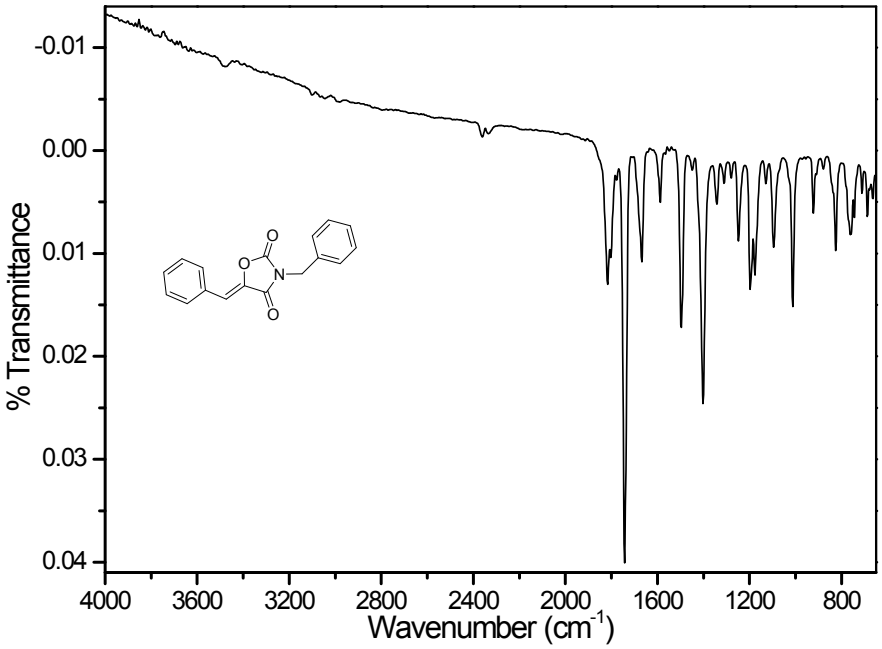


Figure S44: IR spectra of compound 3bb'.

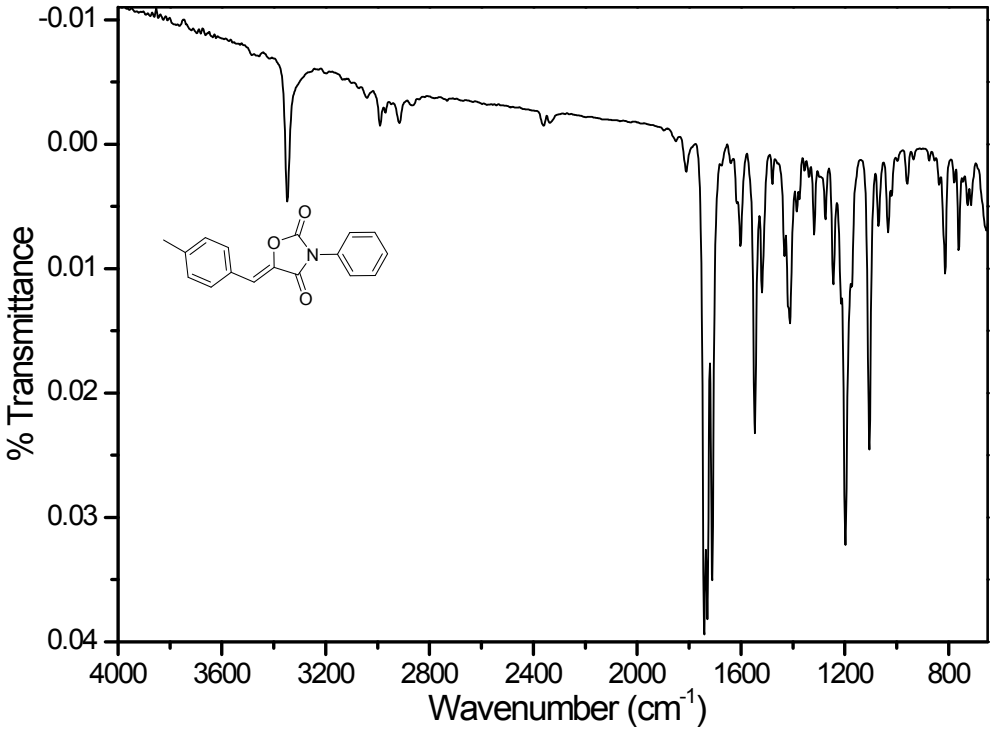


Figure S45: IR spectra of compound 3cb'.

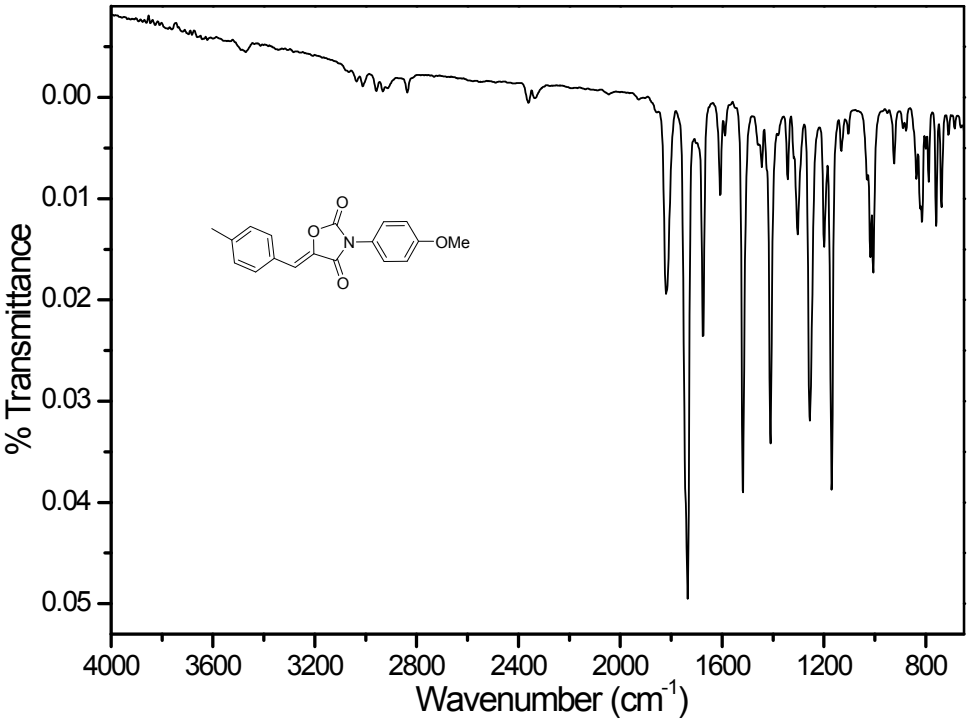


Figure S46: IR spectra of compound 3ca'.

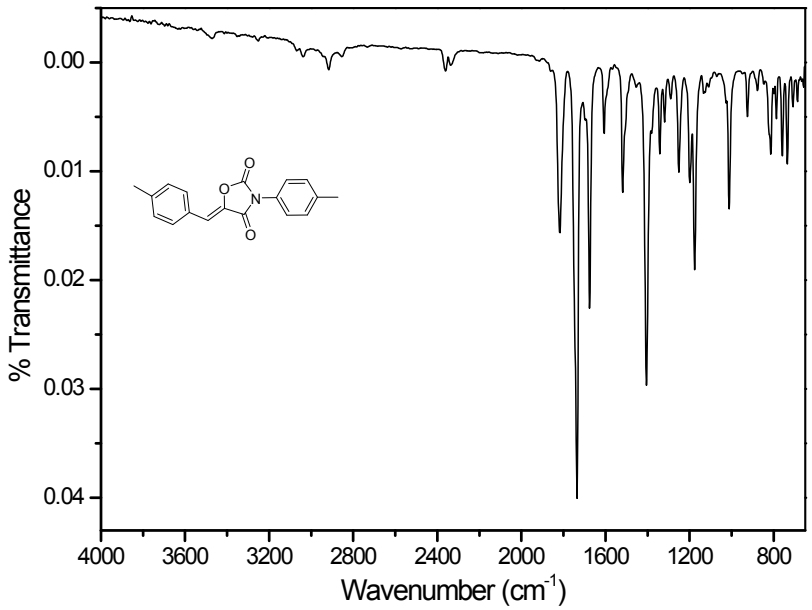


Figure S47: IR spectra of compound 3ce'.

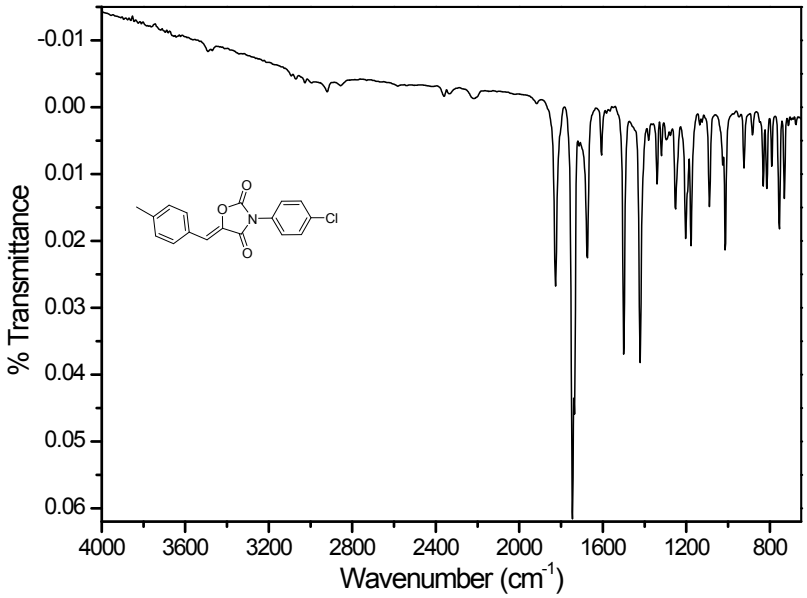


Figure S48: IR spectra of compound 3cc'.

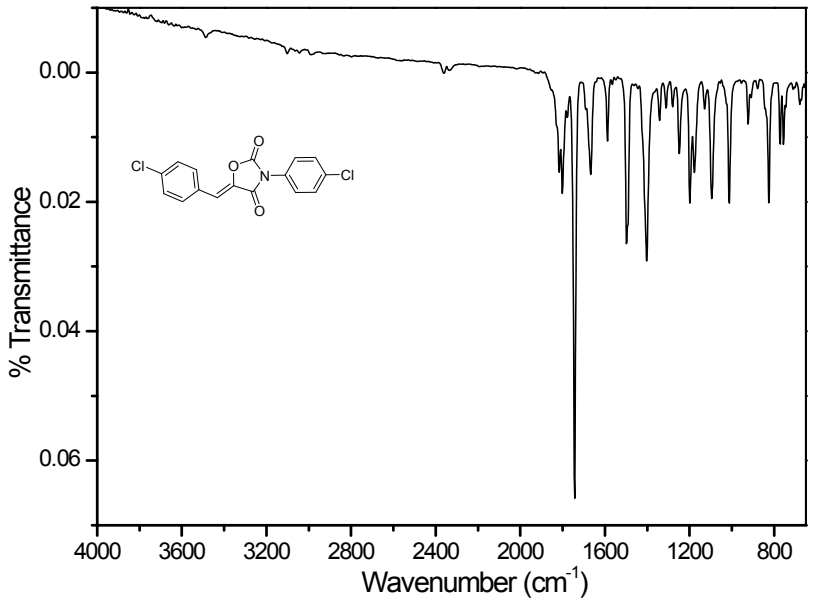


Figure S49: IR spectra of compound 3dc'.

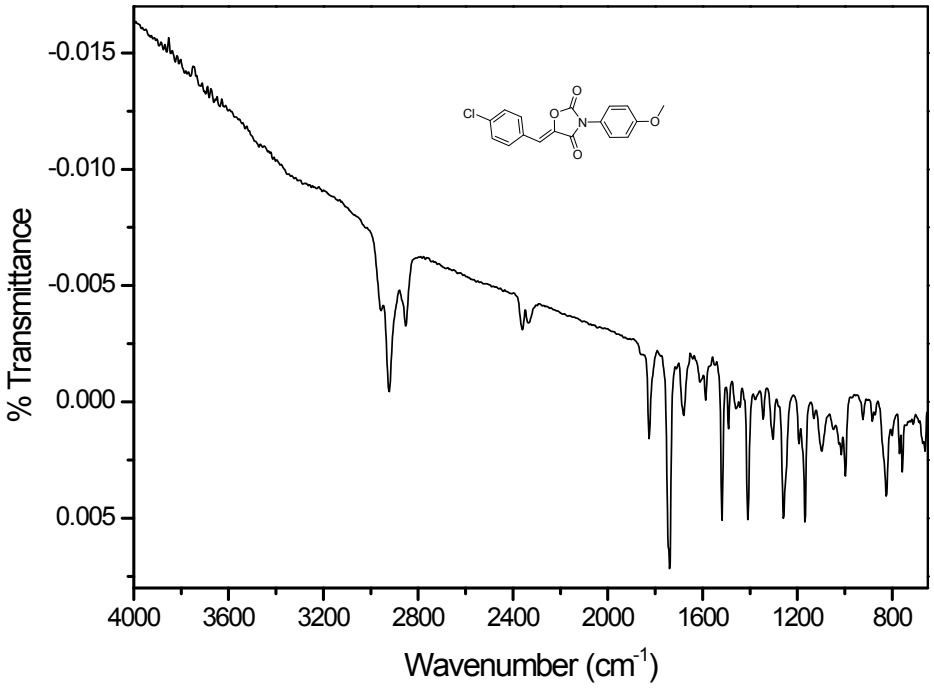


Figure S50: IR spectra of compound 3da'.

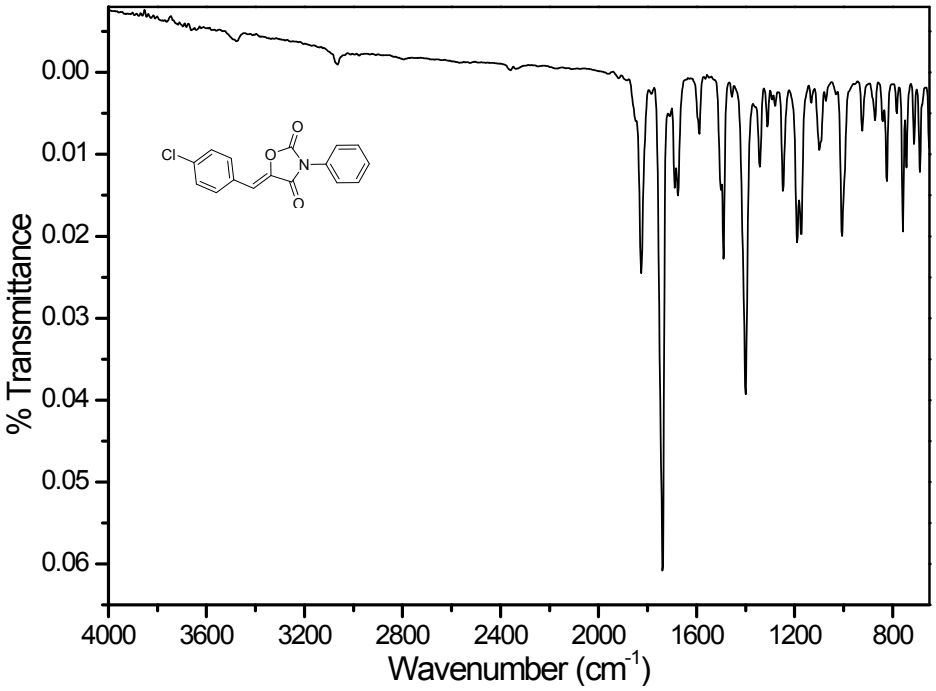


Figure S51: IR spectra of compound 3db'.

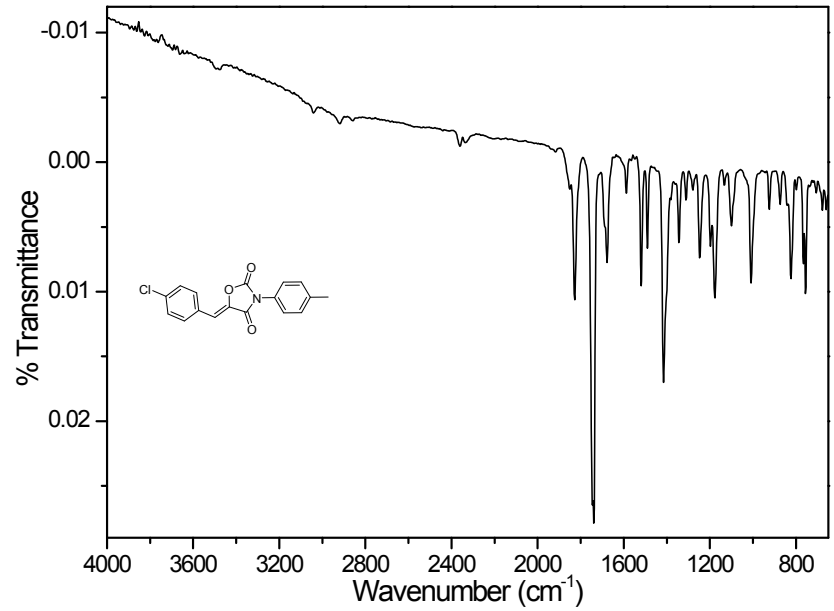


Figure S52: IR spectra of compound 3de'.