

Supporting Information

Visible Light Dye Photosensitised Oxidation of Pyrroles Using a Simple LED Photoreactor

1.1 General Experimental	2
1.2 Emission Spectra of LEDs/Absorbance Spectra of dye sensitisers	4
1.3 Photo of photo-oxidation apparatus	7
1.4 NMR spectra of new compounds produced by the photo-oxidation methodology	8

1.1 General Experimental

Nuclear Magnetic Resonance Spectroscopy

Proton (^1H) and carbon (^{13}C) nuclear magnetic resonance spectra were obtained on a Varian Mercury 2000 spectrometer operating at 300 MHz and 75 MHz respectively, or on a Bruker spectrometer operating at 400 MHz and 75 MHz respectively. Spectra were collected from samples dissolved in deuterated chloroform (CDCl_3), unless otherwise stated. Chemical shifts were recorded as δ values in parts per million (ppm) and referenced to the solvent used (in the case of CDCl_3 , chemical shifts respectively appear at 7.26 ppm and 77.16 ppm for ^1H and ^{13}C spectra). Coupling constants were recorded in J values in Hz. The following abbreviations were used to describe ^1H spectra peak splitting patterns; s = singlet, d = doublet, dd = doublet of doublets, ddd = doublet of doublet of doublets, dddd = doublet of doublet of doublet of doublets, t = triplet, dt = doublet of triplets, q = quartet, dq = doublet of quartets, bs = broad singlet and m = multiplet.

Infrared Spectroscopy

Infrared spectra were obtained on a Shimadzu FTIR 8400s spectrometer, using NaCl plates. Liquids and solids were recorded as thin films from either CDCl_3 or CH_2Cl_2 in cm^{-1} .

Mass Spectrometry

Mass spectrometry and High-Resolution mass spectrometry was performed on a Kratos Concept ISQ GC-MS instrument using electron impact mass spectrometry or by Liquid Secondary ion mass spectrometry with *m*-nitrobenzoic acid as the matrix; or by electrospray ionization by direct infusion into an LTQ-Orbitrap XL mass spectrometer using a syringe pump. Analytical analyses were performed by The Central Science Laboratory (CSL) at the University of Tasmania. The molecular ion and mass fragments are quoted, with relative intensities of the peaks referenced to the most intense taken as 100%.

UV-Vis Absorbance

UV-Vis absorbance spectra for dye-sensitisers were recorded on a Shimadzu UV-1800 UV-Vis spectrophotometer. Quartz spectrosil precision cell cuvettes were used for the analysis with a path length of 1 cm.

Column Chromatography

Merck flash grade silica (32-63 μm) was used for column and flash chromatography, which was performed according to the general method of Still *et al.* Automated gradient flash chromatography was performed using a REVELERIS® X2 Flash Chromatography System provided by Grace Materials Technology. The system used 40 μm silica cartridges.

Thin Layer Chromatography (TLC)

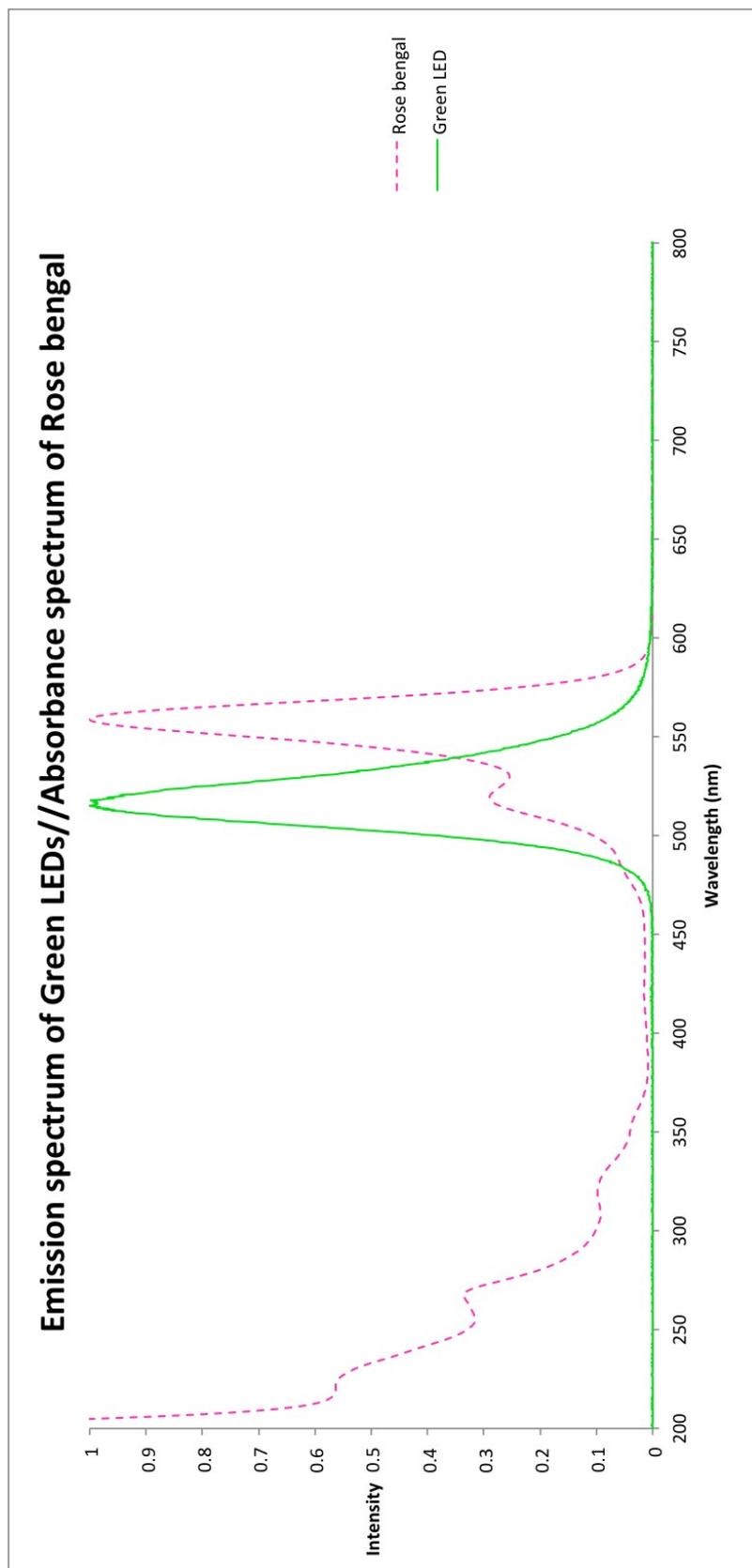
Merck silica gel 60 F254 aluminium backed sheets were used for analytical thin layer chromatography. TLC plates were visualised under a 254 nm UV lamp and/or by treatment with a phosphomolybdic acid (37.5 g), ceric sulfate (7.5 g), sulfuric acid (37.5 ml), water (720 ml) dip or a potassium permanganate dip (3 g KMnO_4 , 20 g K_2CO_3 , 5 ml 5% aqueous NaOH, 300 ml H_2O), followed by heating.

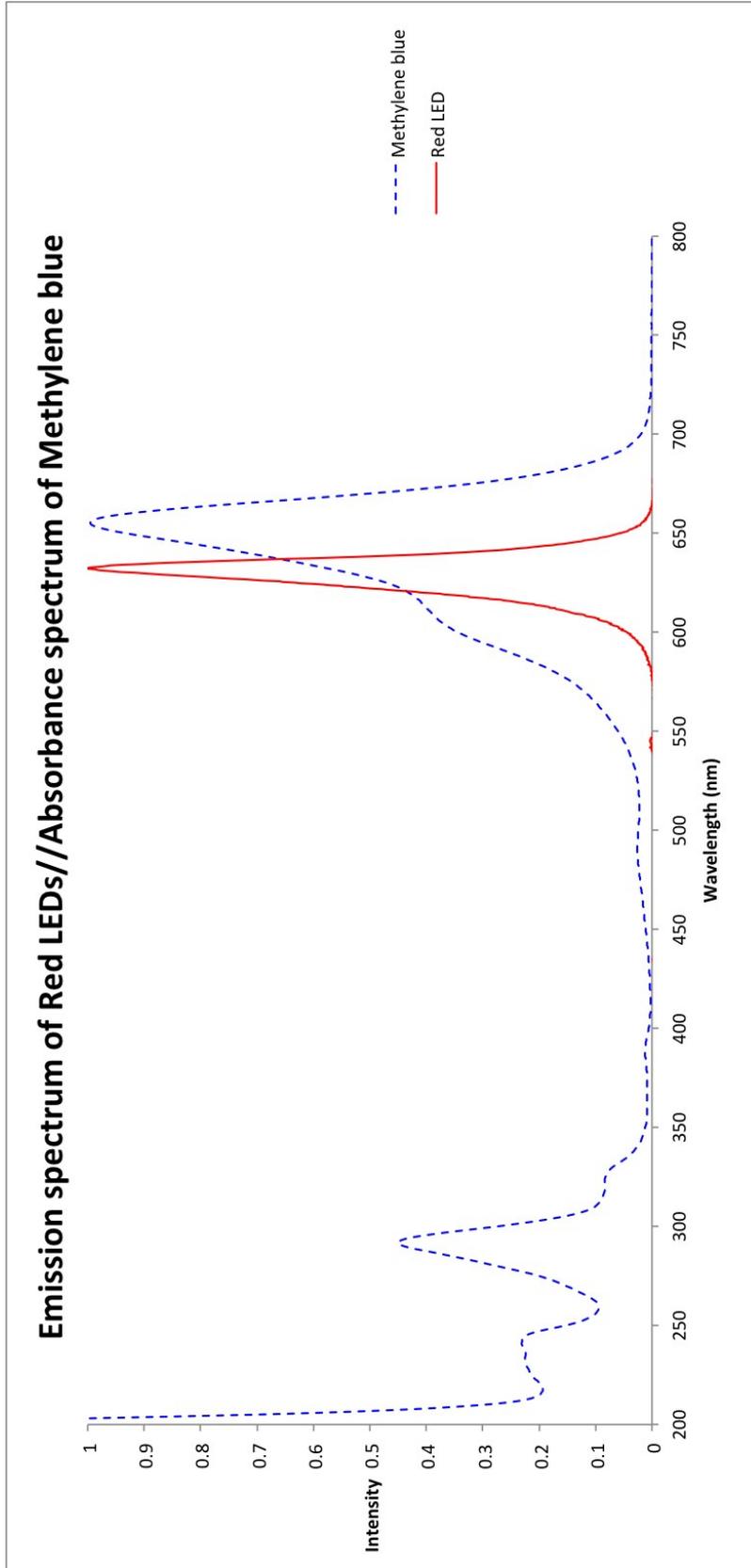
Solvents and Reagents

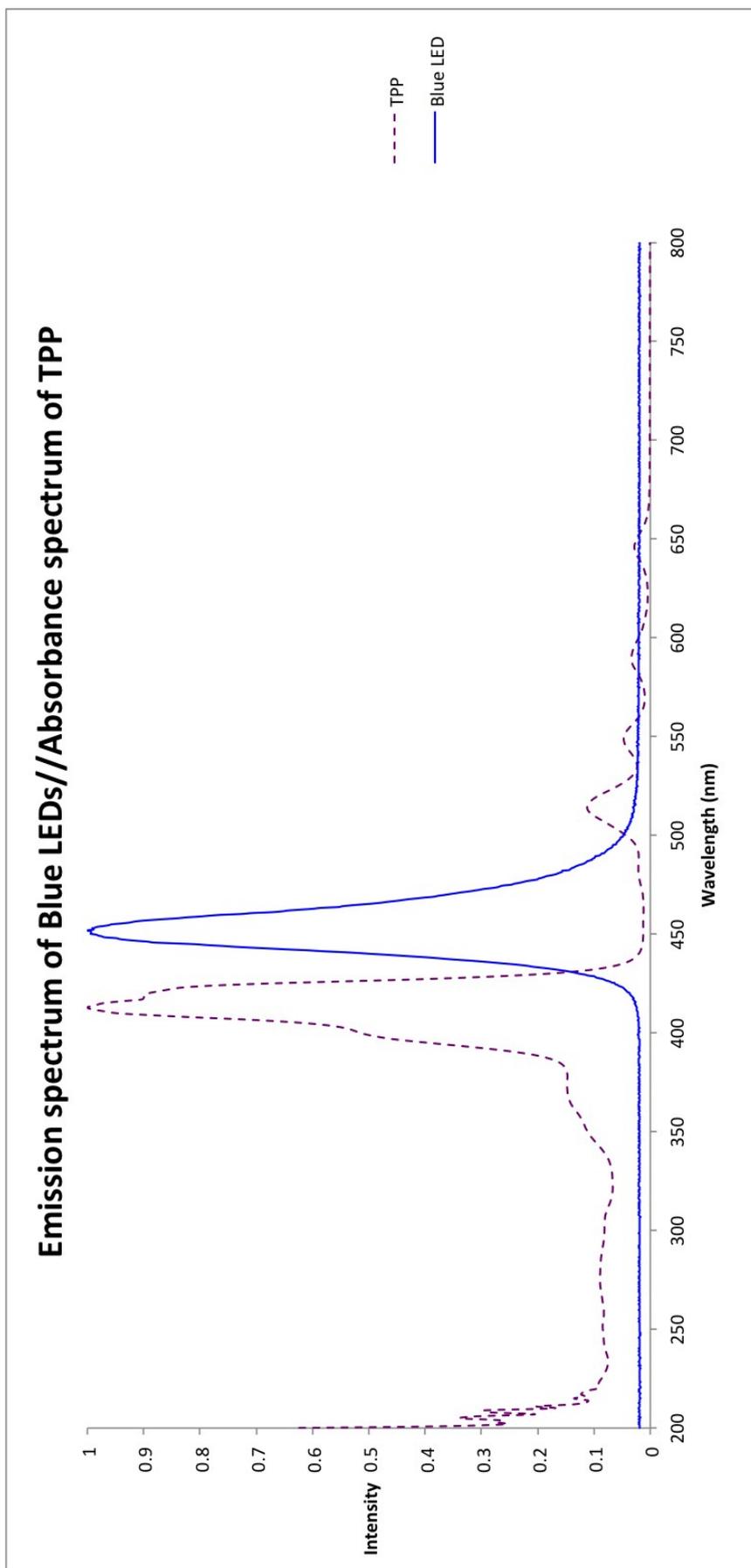
All solvents and reagents were purified by standard laboratory procedures. Anhydrous magnesium sulfate was used for drying organic extracts unless otherwise stated and solvents were removed under reduced pressure on a rotary evaporator.

1.2 Emission Spectra of LEDs/Absorbance Spectra of dye sensitisers

Green LED/ Rose Bengal







1.3 Photo of photo-oxidation apparatus

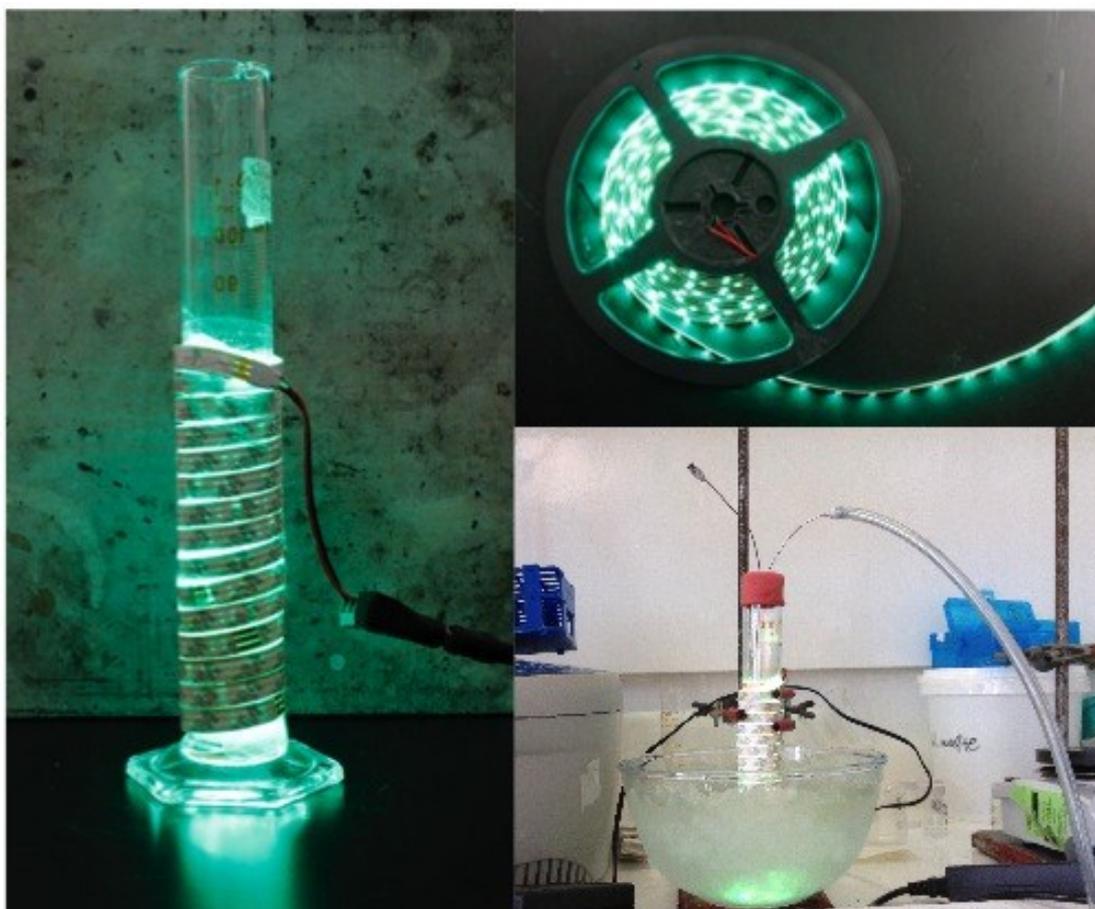
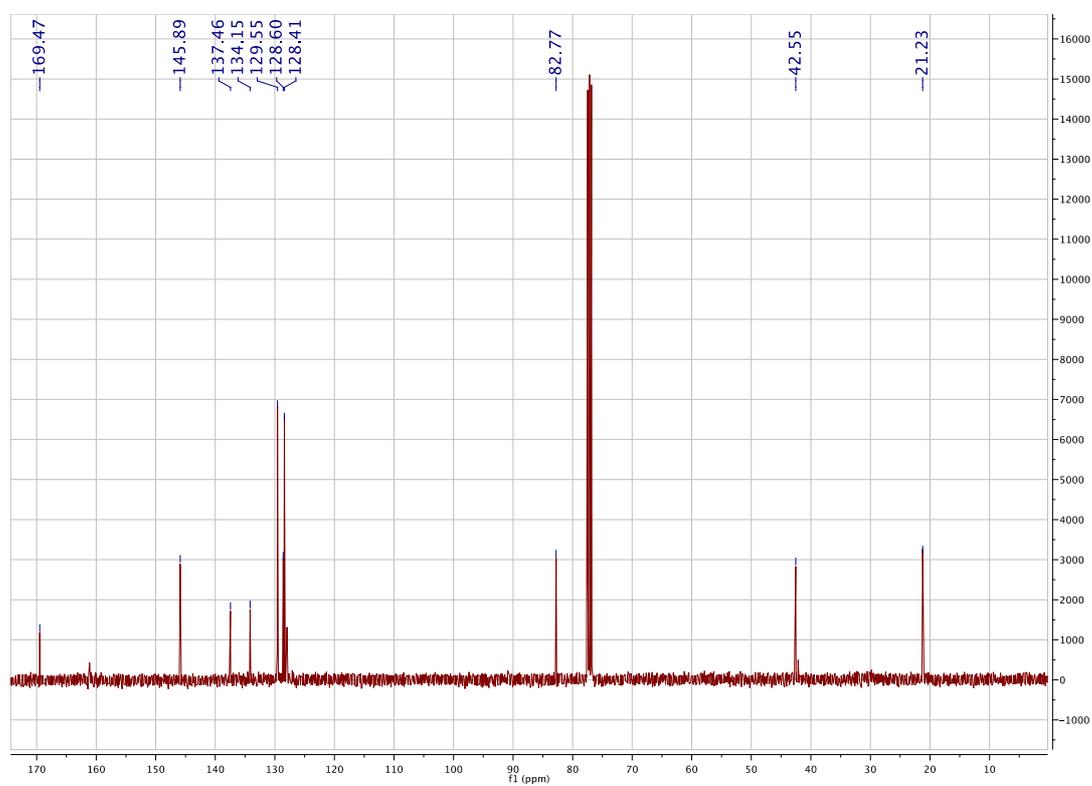
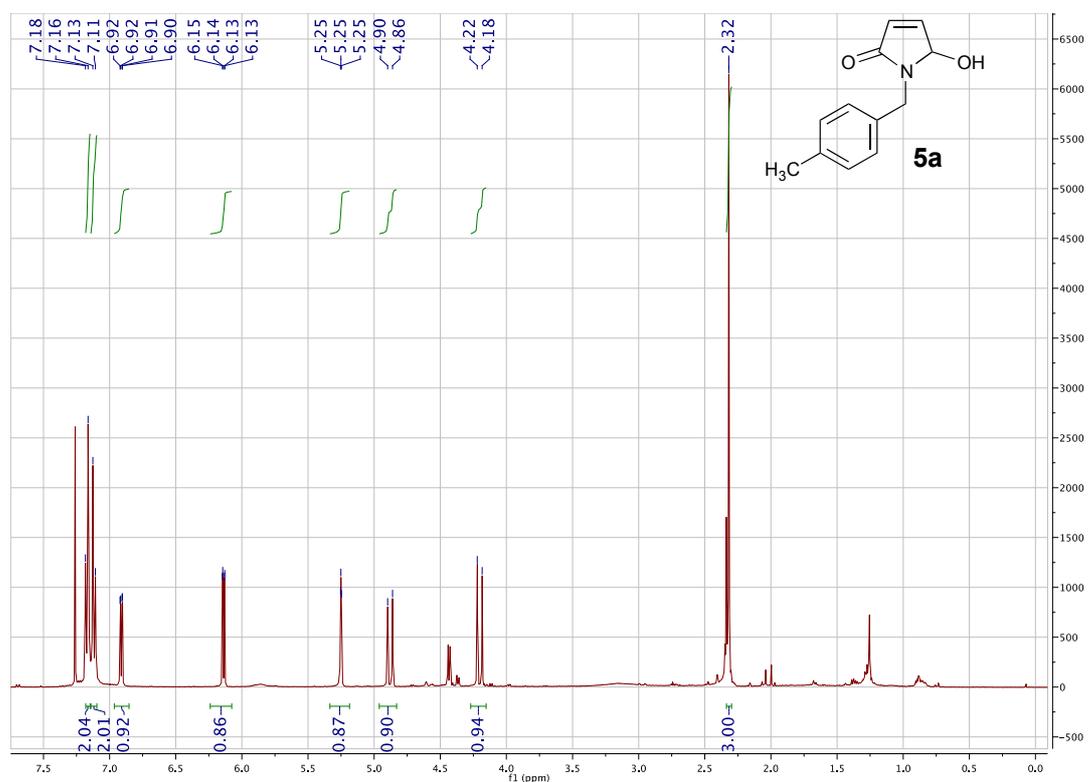


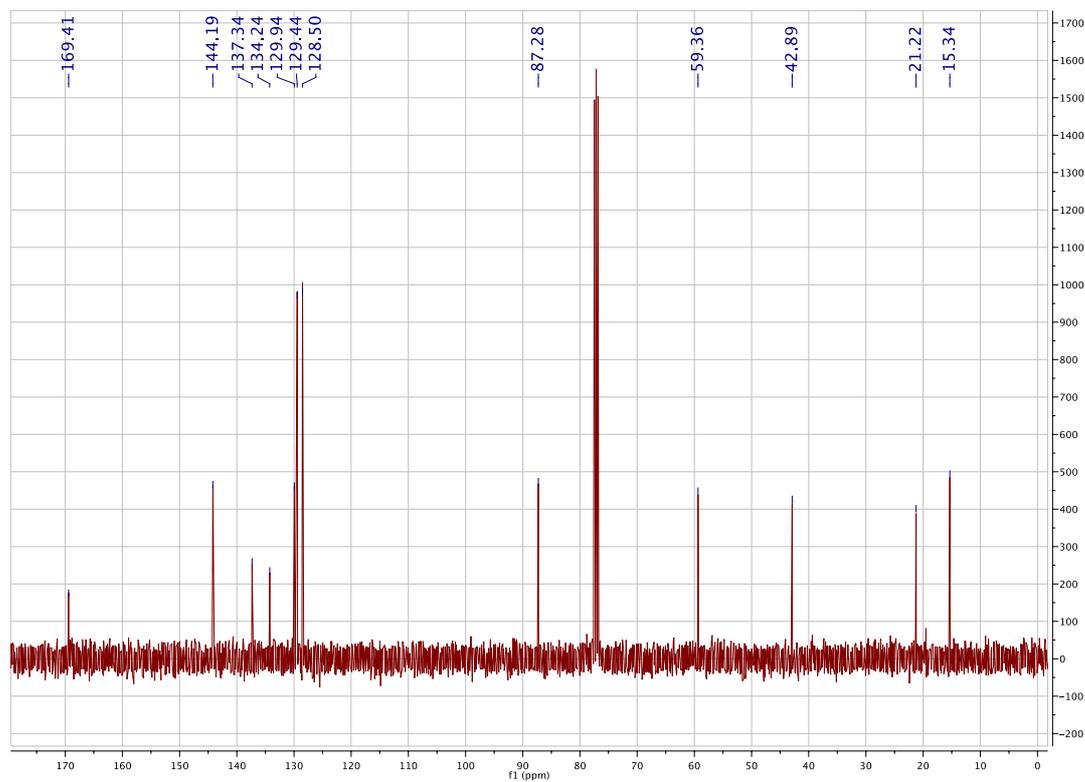
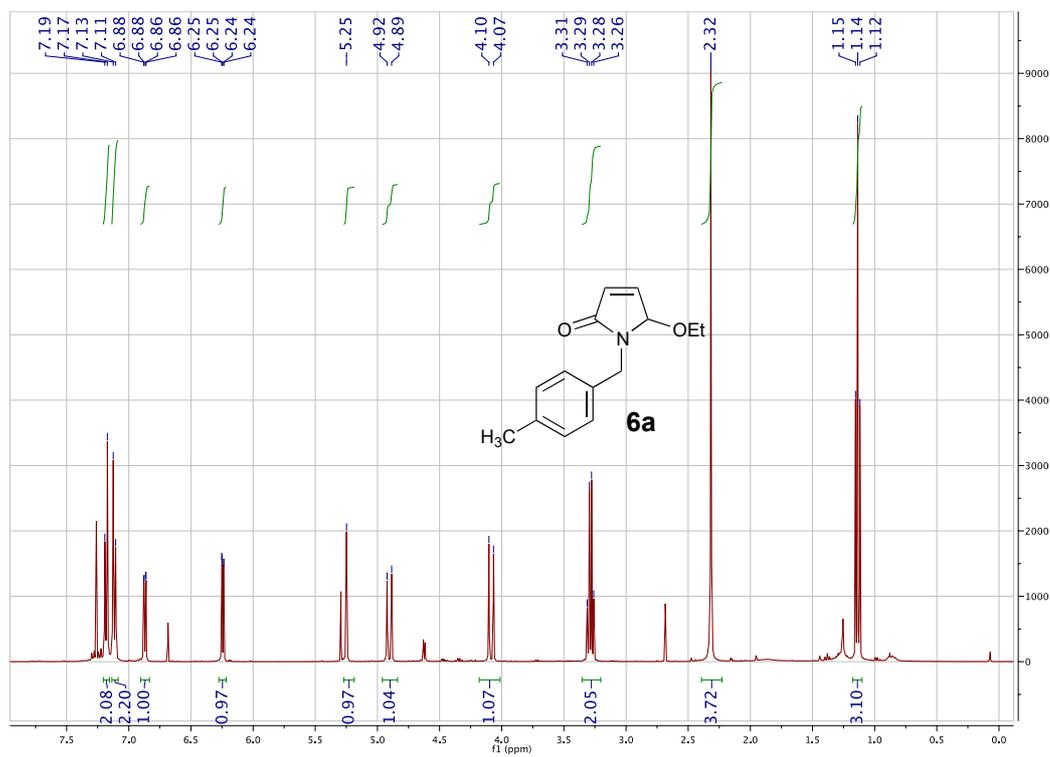
Figure S-1: *Left* – Photo of the green LED photoreactor described in the body of the main article; *Upper Right* – Photo of green LEDs used to construct the LED photo reactor; *Lower Right* – Photo of the green LED photoreactor during operation as described in the body of the main article.

1.4 NMR spectra of new compounds produced by the photo-oxidation methodology

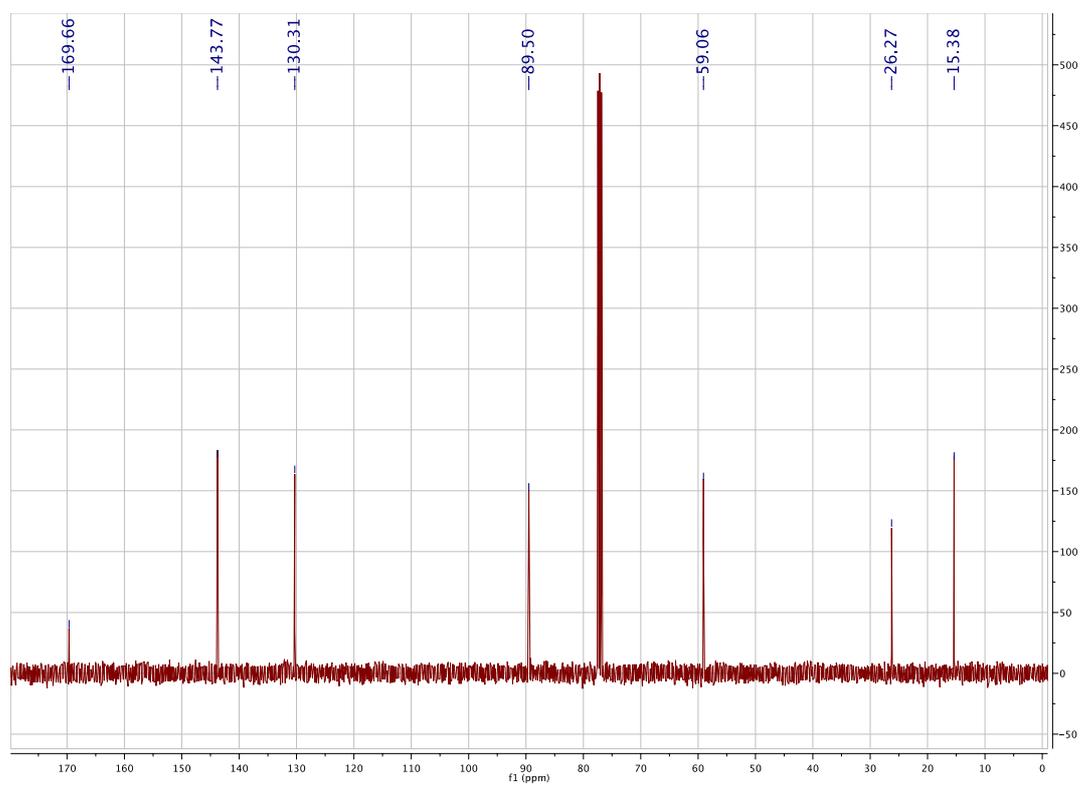
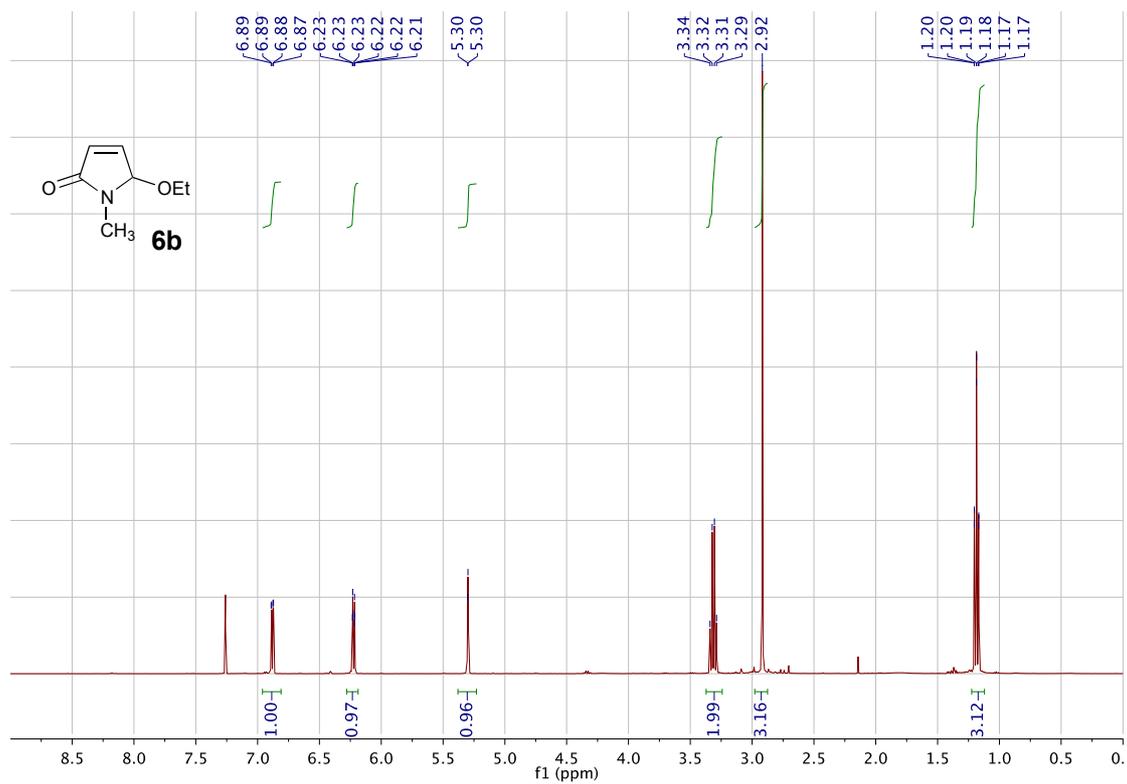
(±)-5-Hydroxy-1-(*p*-methylbenzyl)-pyrrolin-2-one (**5a**)



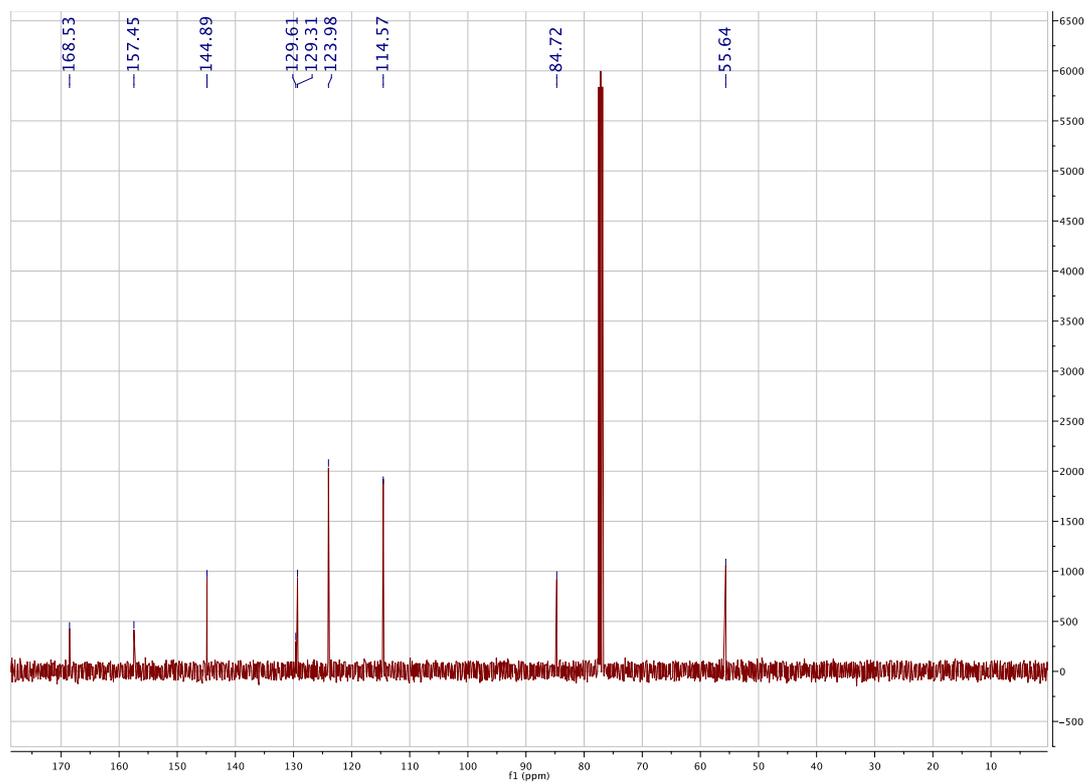
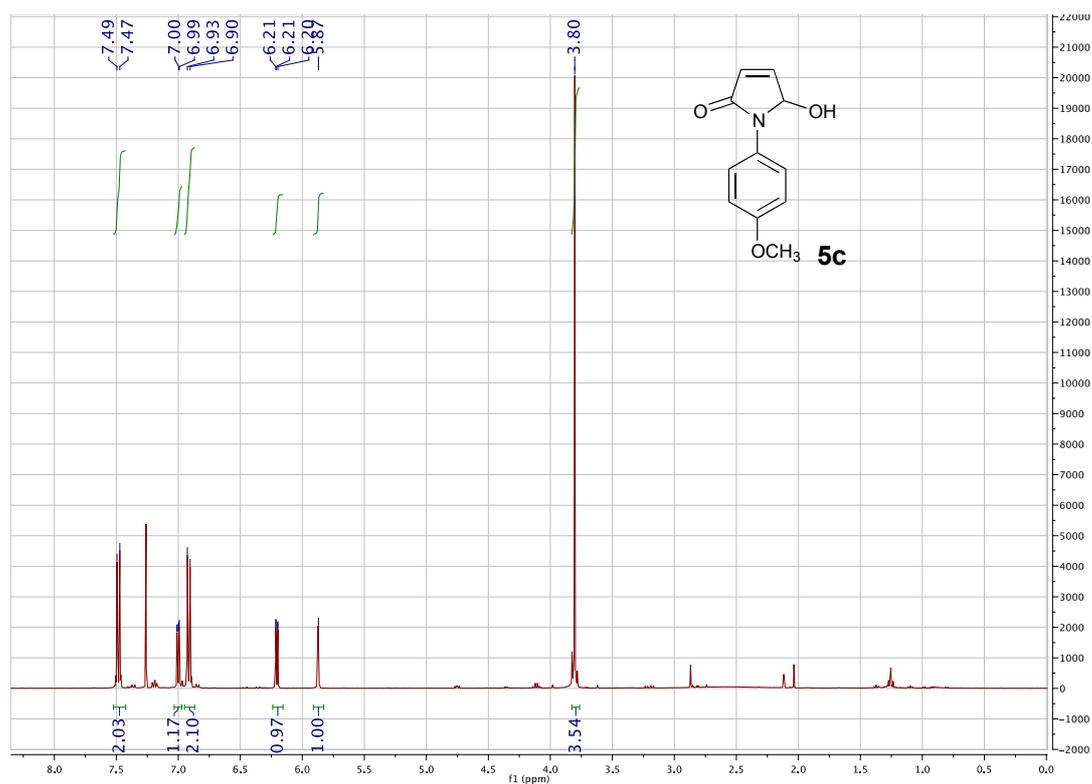
(±)-5-Ethoxy-1-(*p*-methylbenzyl)-pyrrolidin-2-one (6a)



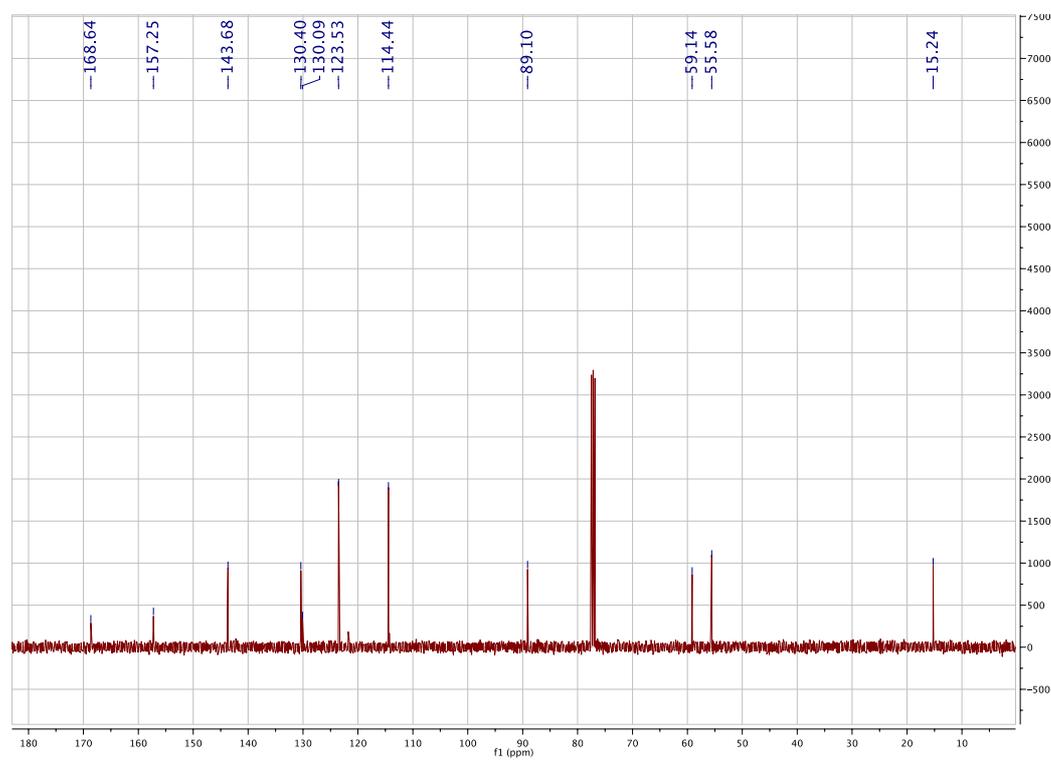
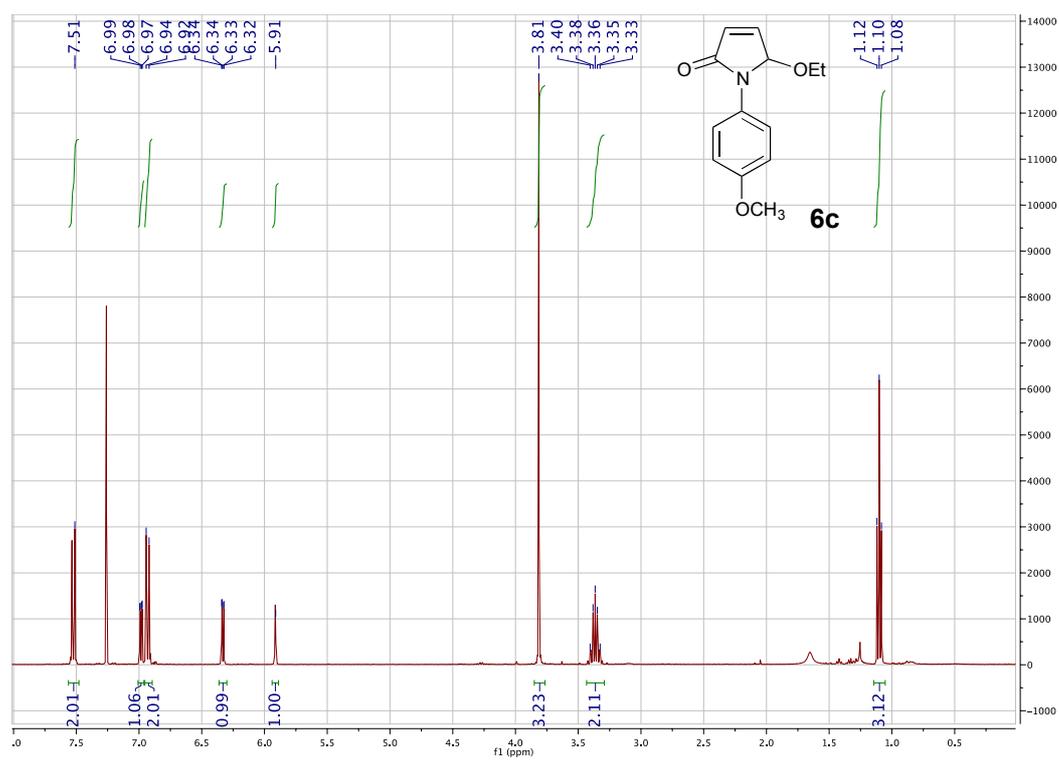
(±)-5-Ethoxy-1-methyl-pyrrolin-2-one (6b)



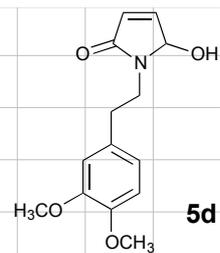
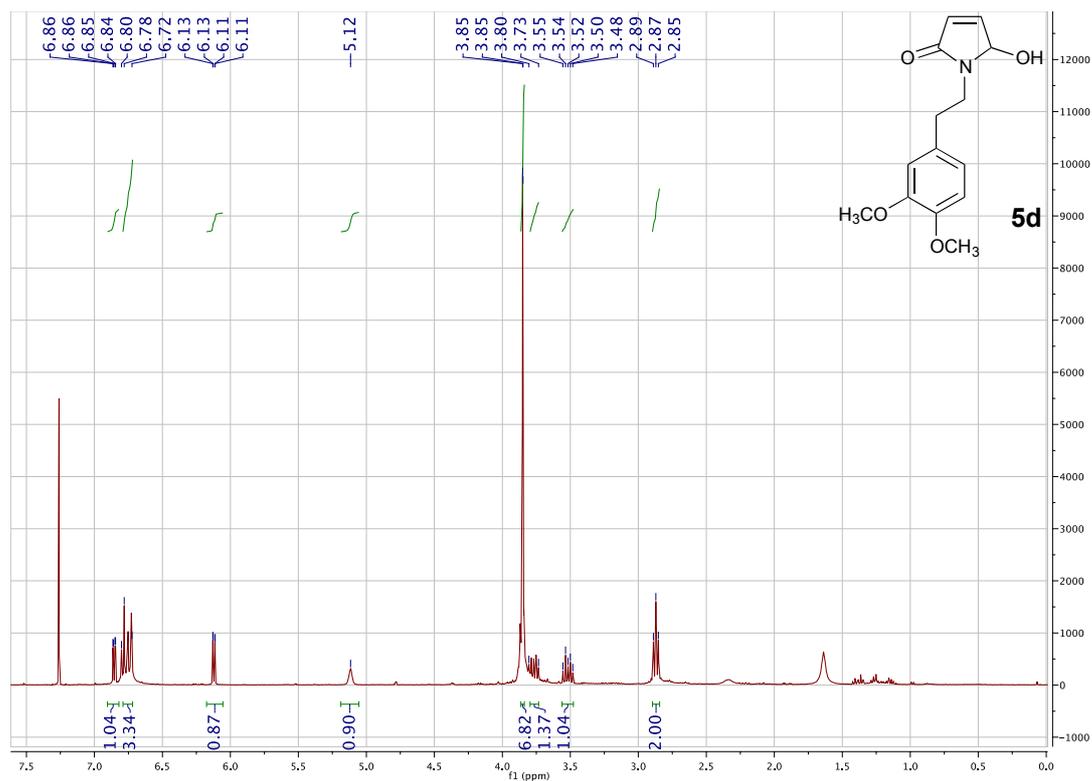
(±)-5-Hydroxy-1-(p-methoxyphenyl)-pyrrolin-2-one (5c)



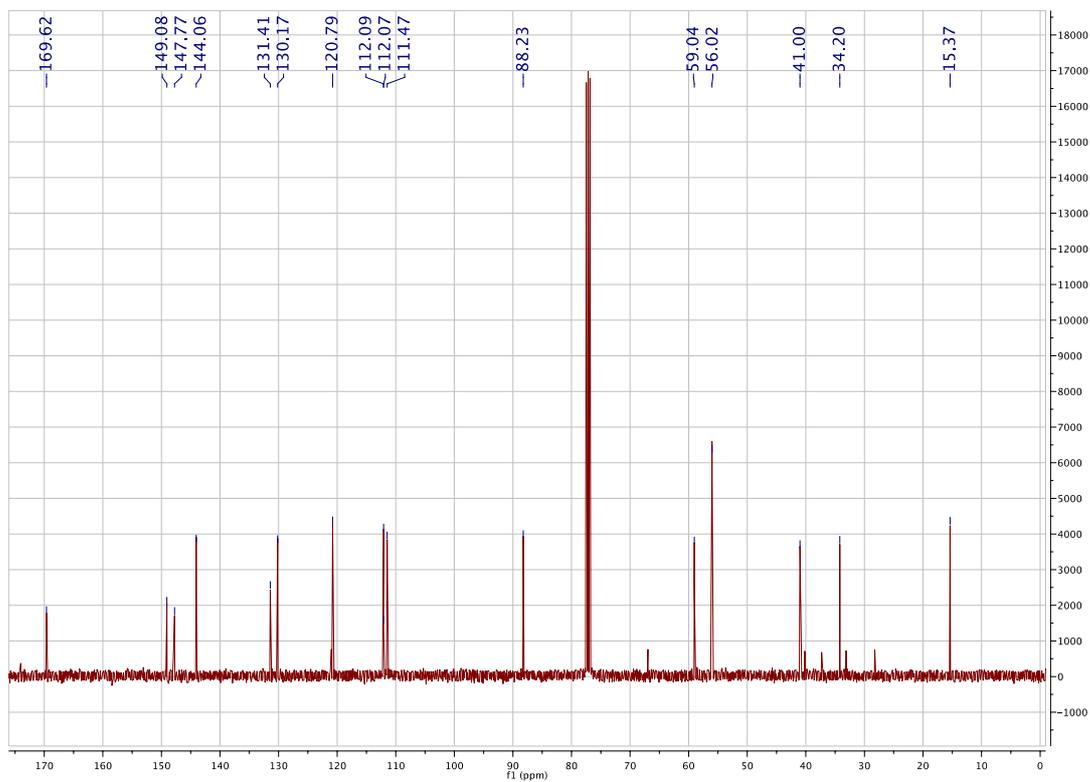
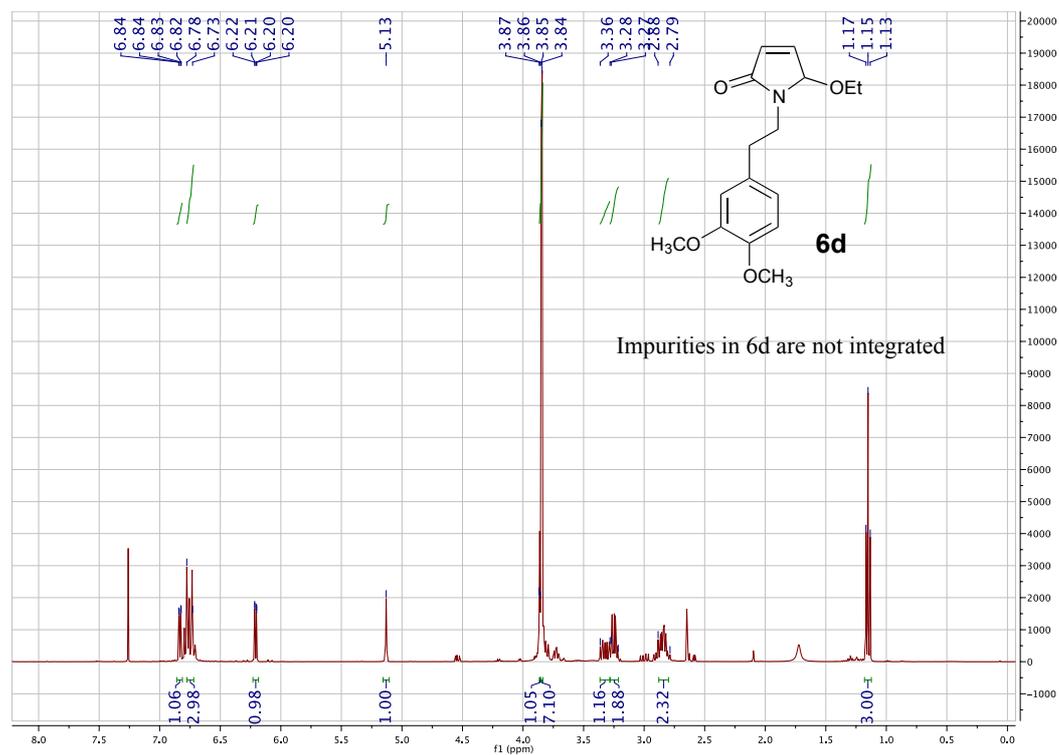
(±)-5-Ethoxy-1-(p-methoxyphenyl)-pyrrolin-2-one (6c).



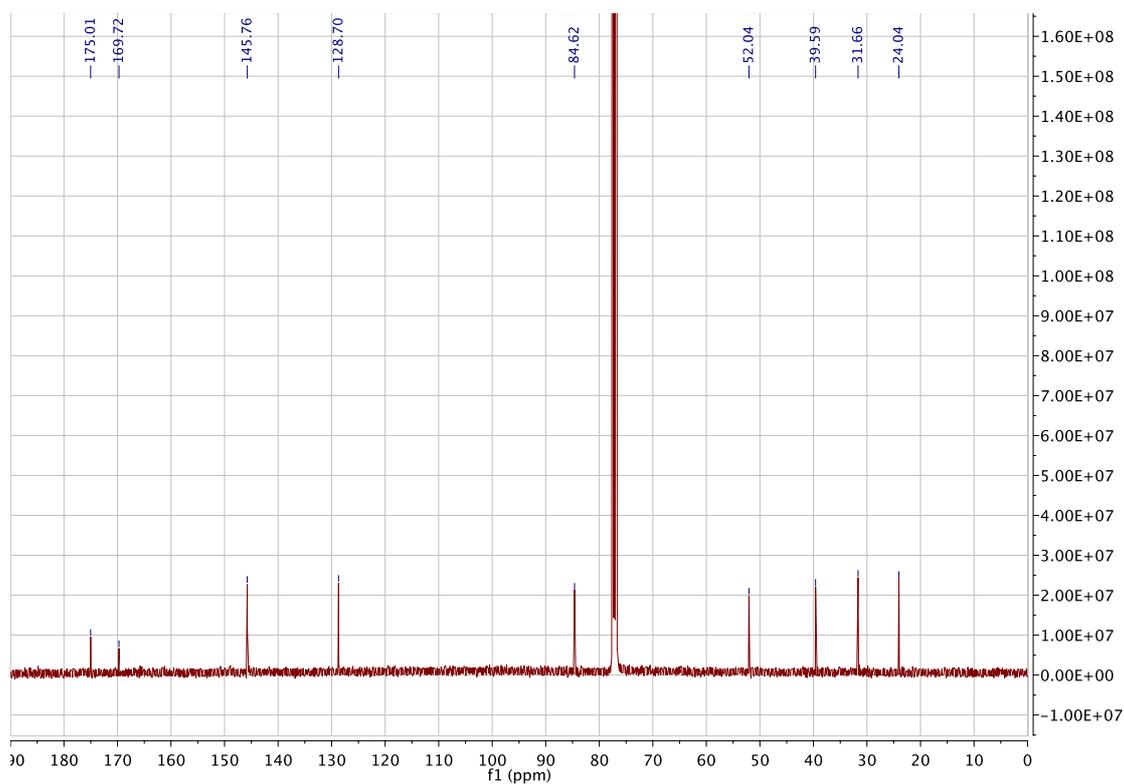
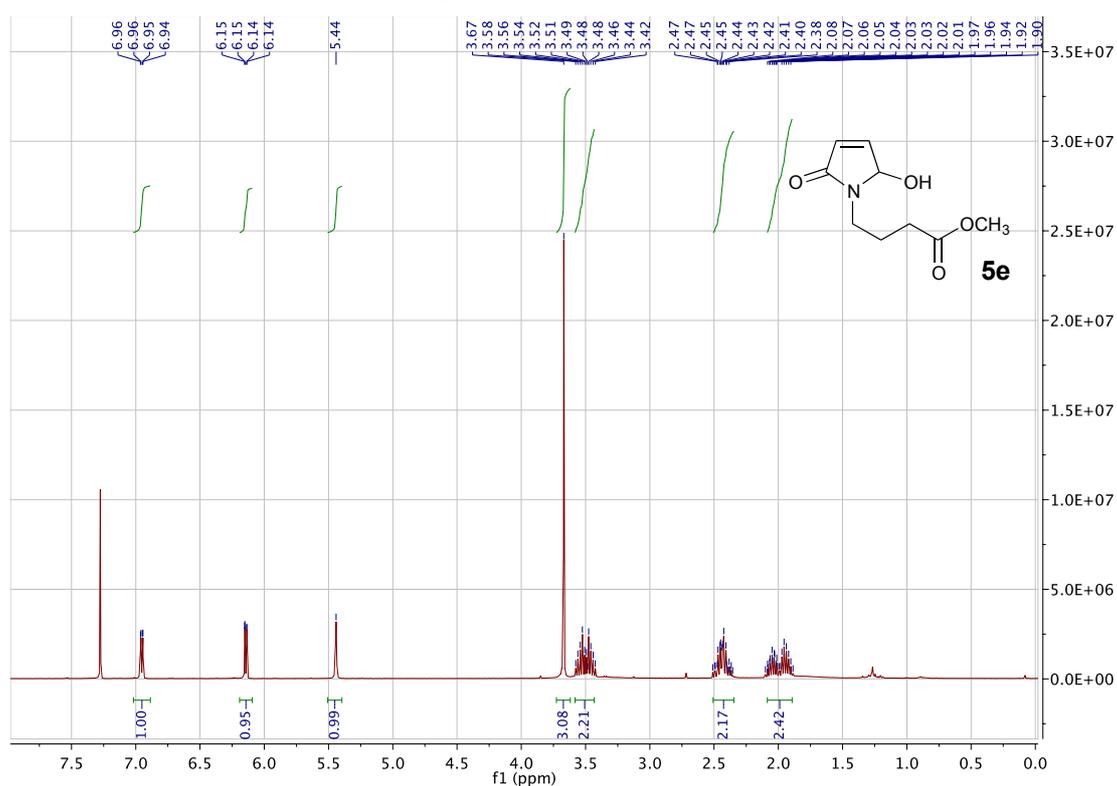
(±)-1-[2-(3,4-Dimethoxyphenyl)ethyl]-5-hydroxy-pyrrolin-2-one (5d)



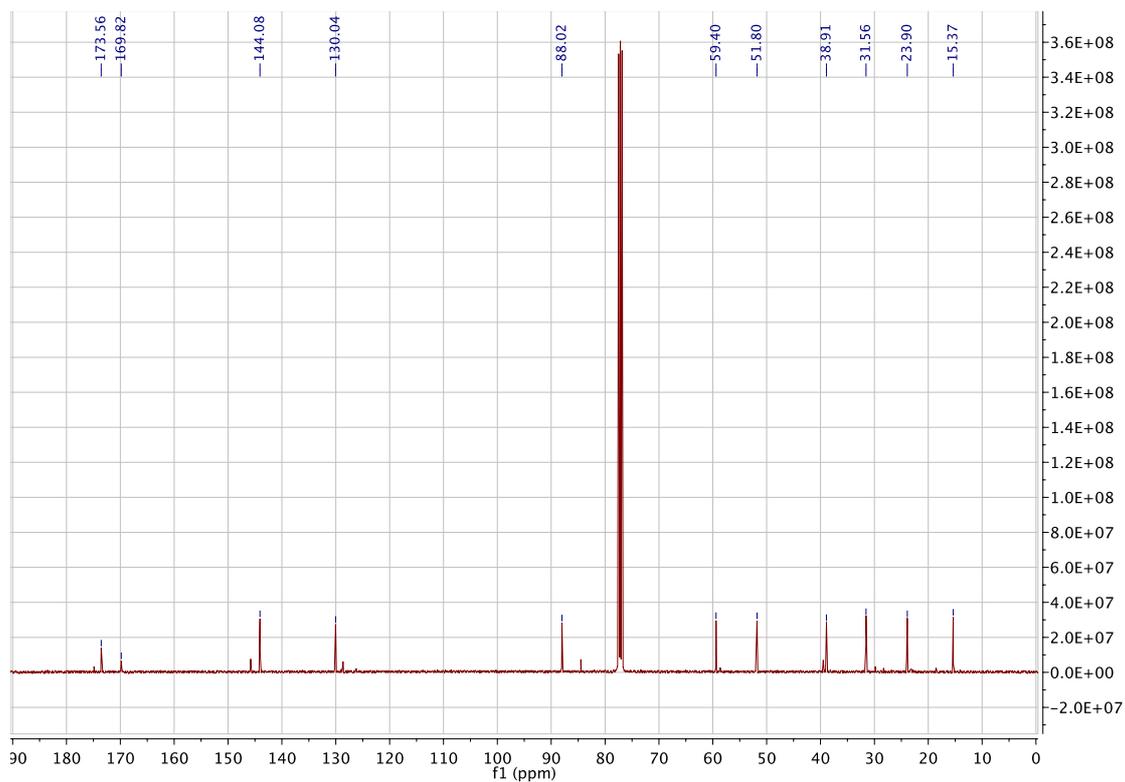
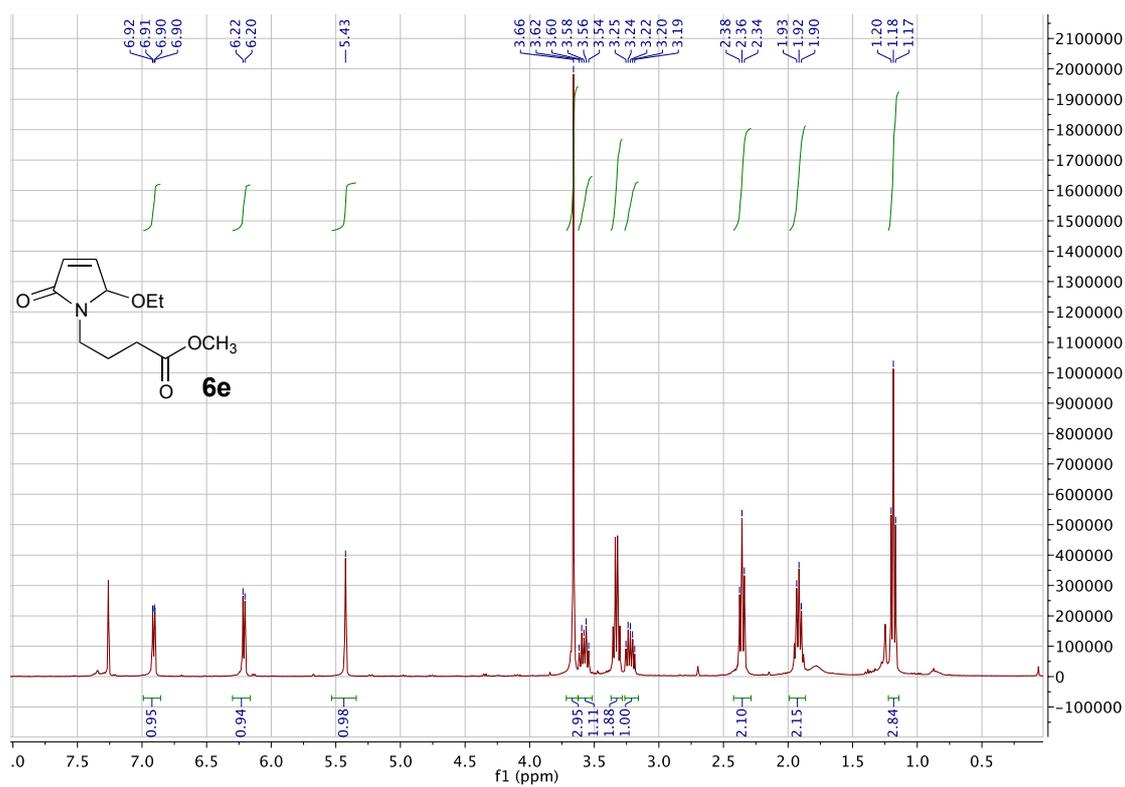
(±)-1-[2-(3,4-Dimethoxyphenyl)ethyl]-5-ethoxy-pyrrolin-2-one (6d)



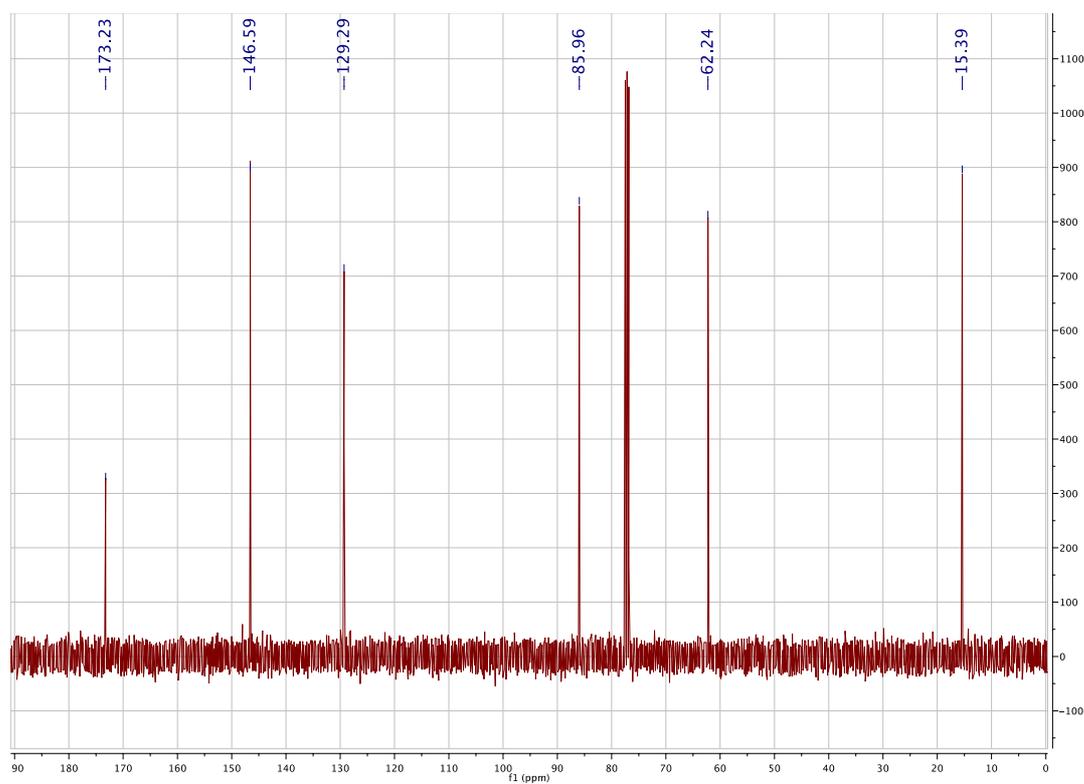
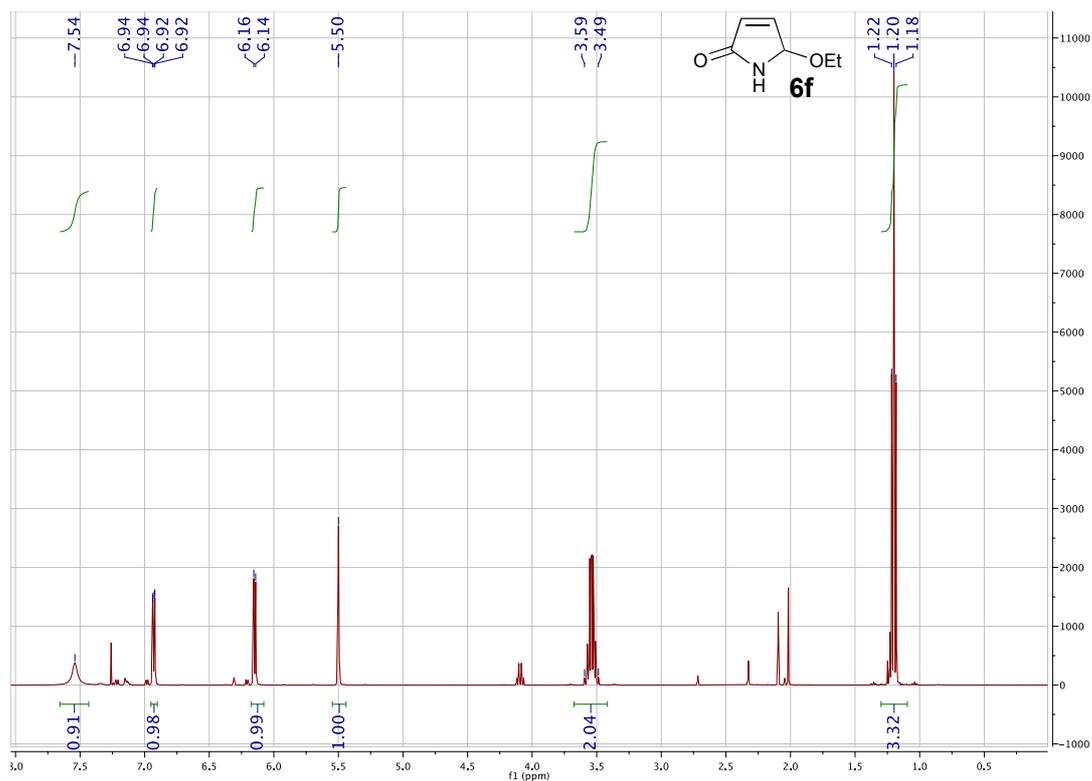
(±)-Methyl 4-(5-hydroxy-2-oxo-pyrrolin-1-yl)butyrate (5e)



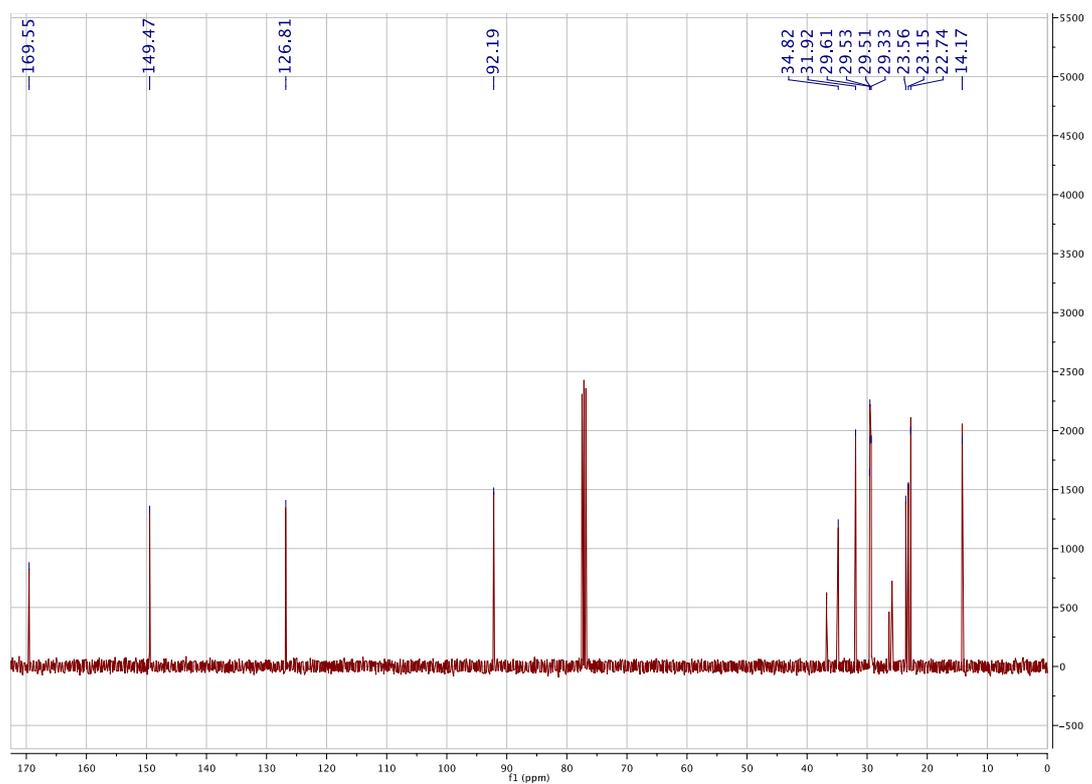
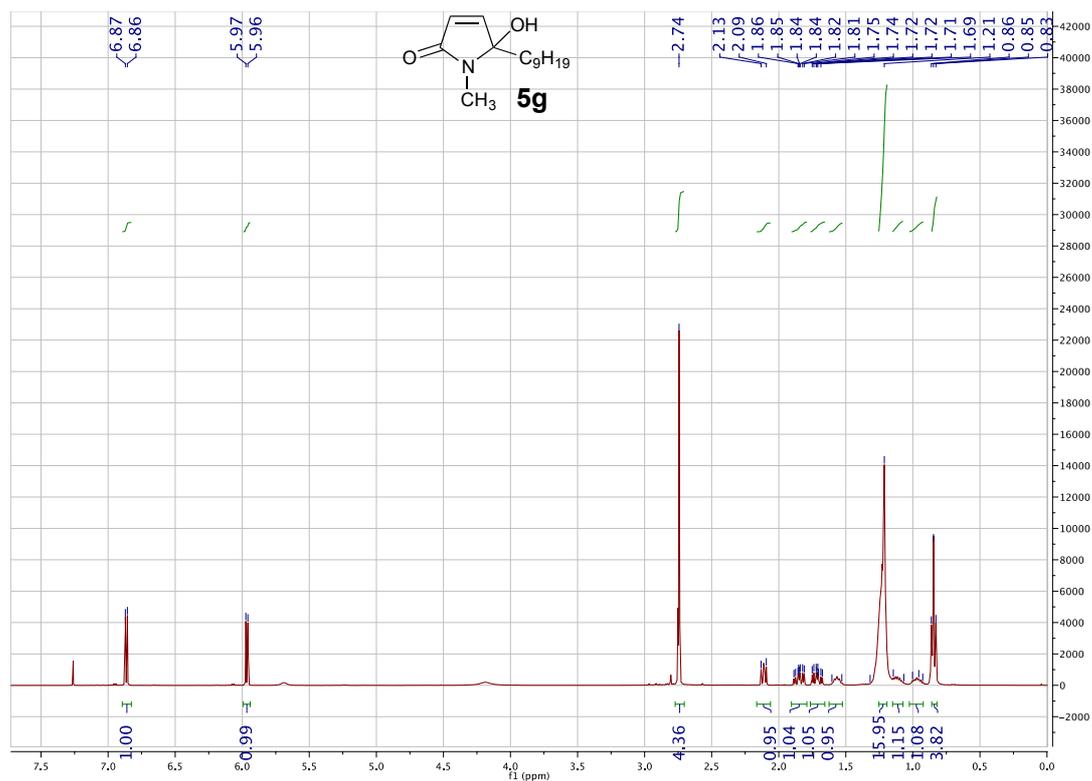
(±)-Methyl 4-(5-ethoxy-2-oxo-pyrrolin-1-yl)butyrate (6e)



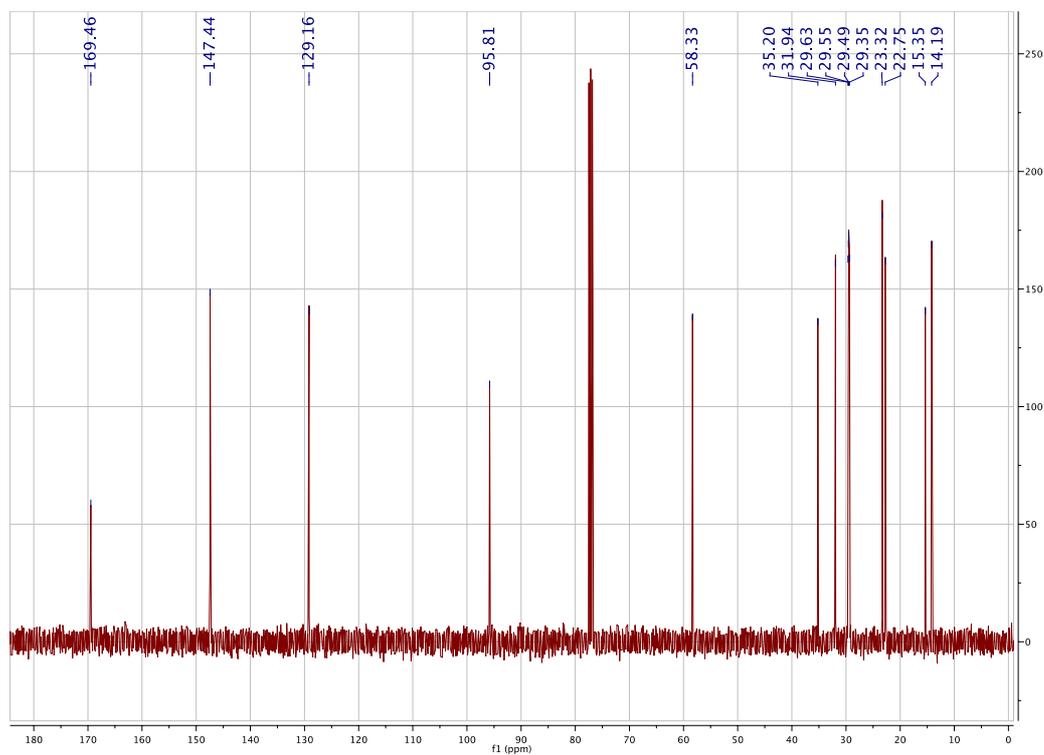
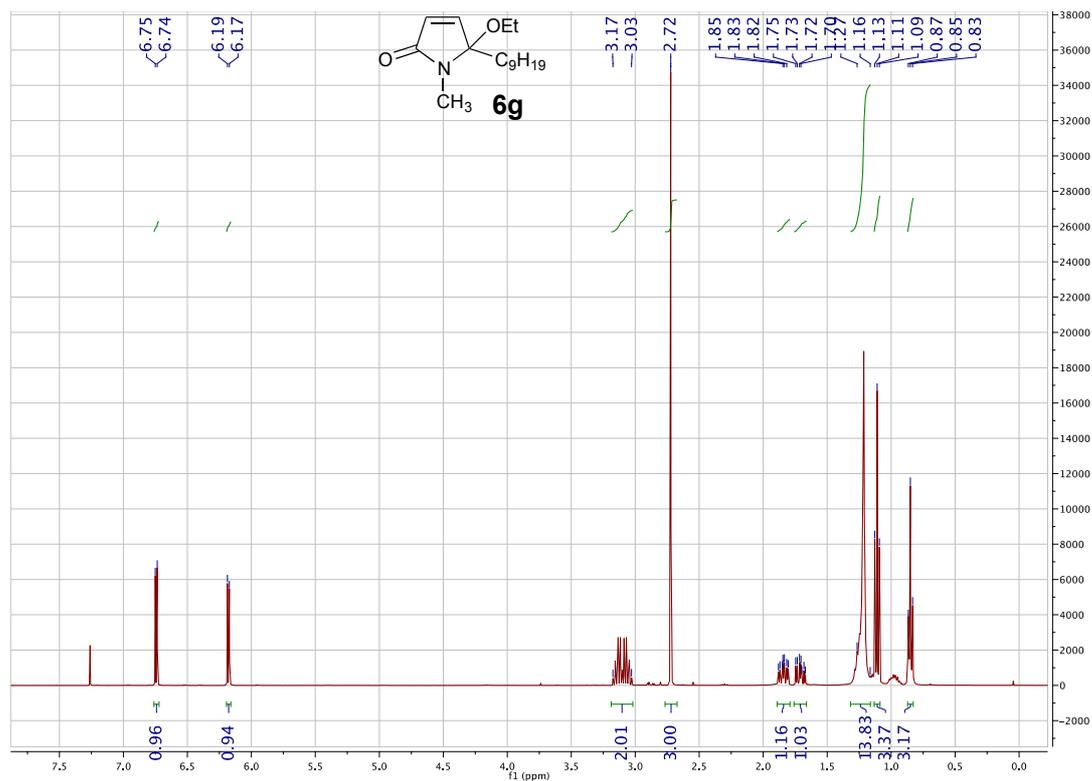
(±)-5-Ethoxy-pyrrolin-2-one (6f)



(±)-5-Hydroxy-1-methyl-5-nonyl-pyrrolidin-2-one (5g)



(±)-5-Ethoxy-1-methyl-5-nonyl-pyrrolidin-2-one (6g)



(±)-5-Benzyl-5-ethoxy-1-(*p*-tolylsulfonyl)-pyrrolin-2-one (6i)

