

Supporting Information

Brønsted acid-catalyzed multicomponent reaction for the synthesis of highly functionalized γ -lactam derivatives.

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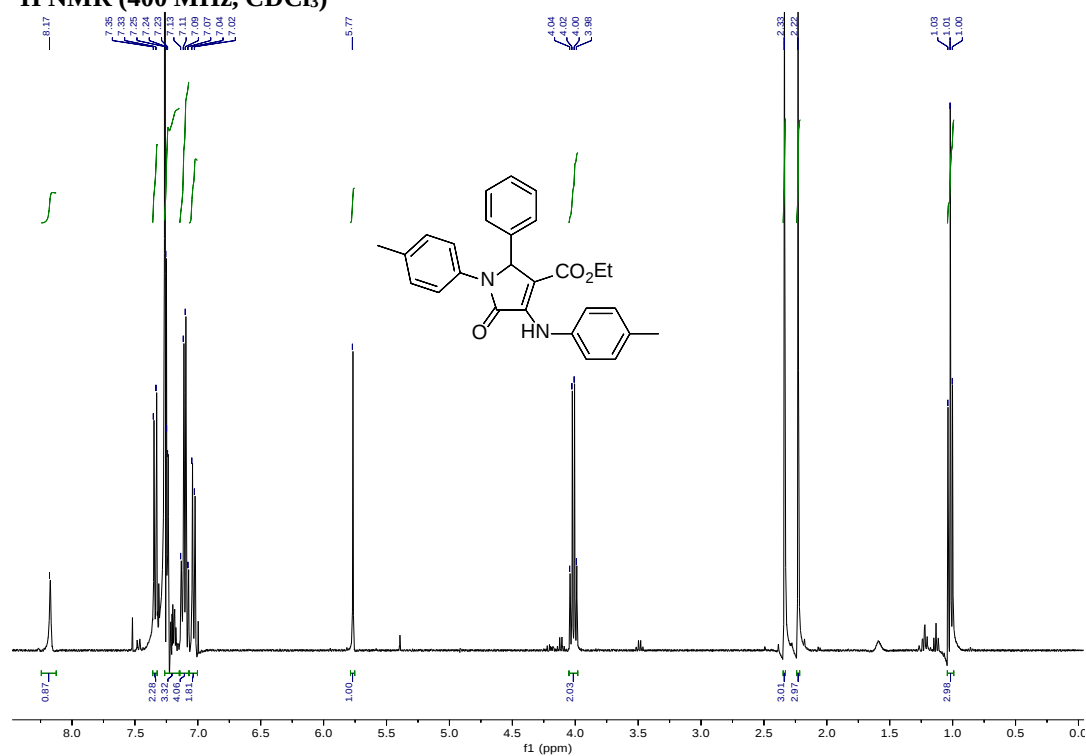
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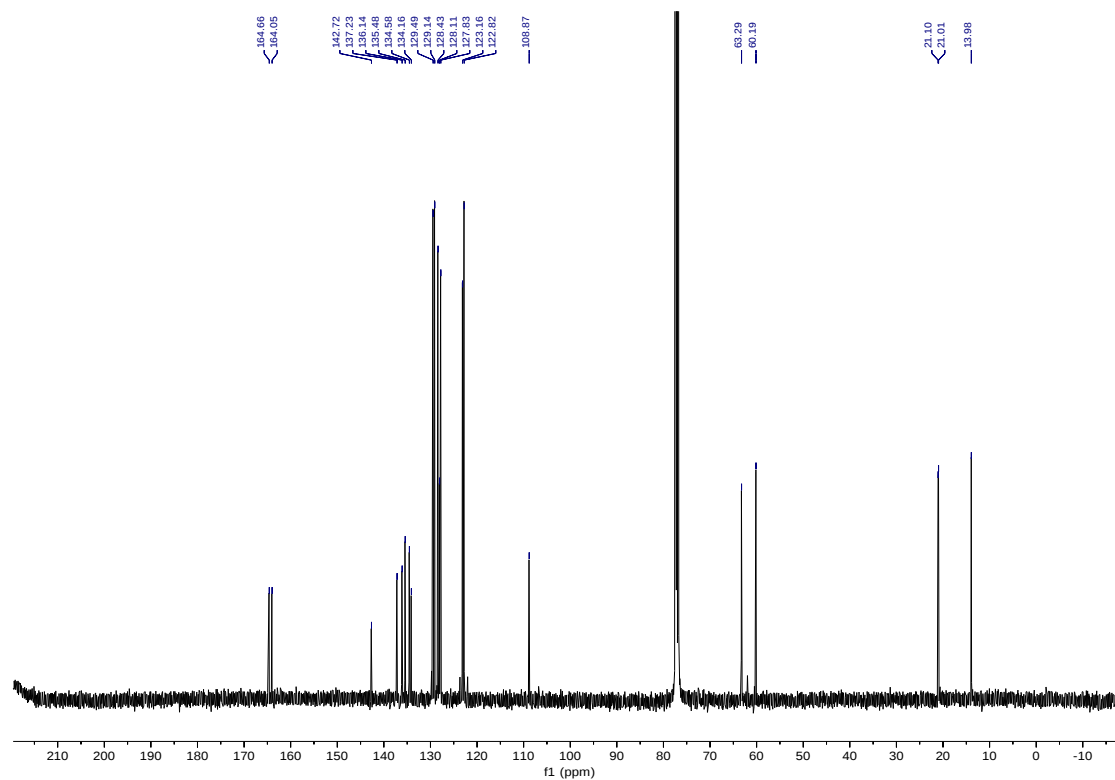
1. ^1H and ^{13}C NMR spectra of compounds 10, 11, 12 and 16.

Ethyl 5-oxo-2-phenyl-1-(p-tolyl)-4-(p-tolylamino)-2,5-dihydro-1H-pyrrole-3-carboxylate. (10a).

^1H NMR (400 MHz, CDCl_3)

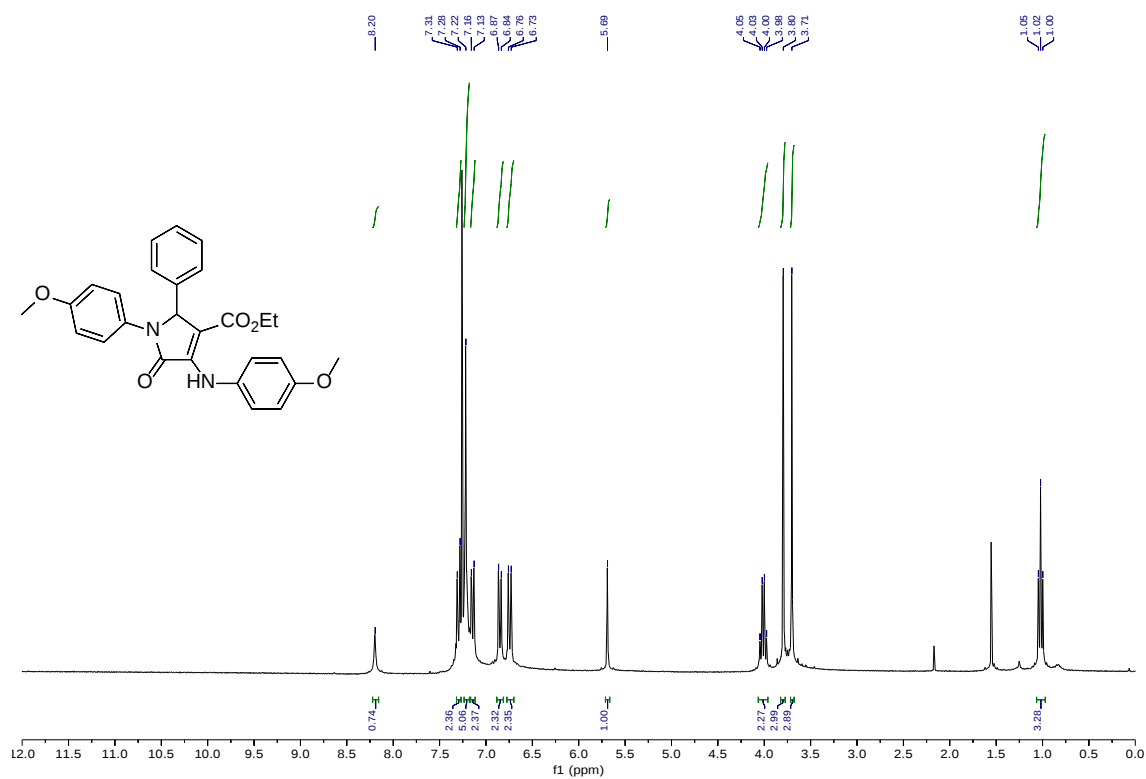


^{13}C NMR (101 MHz, CDCl_3)

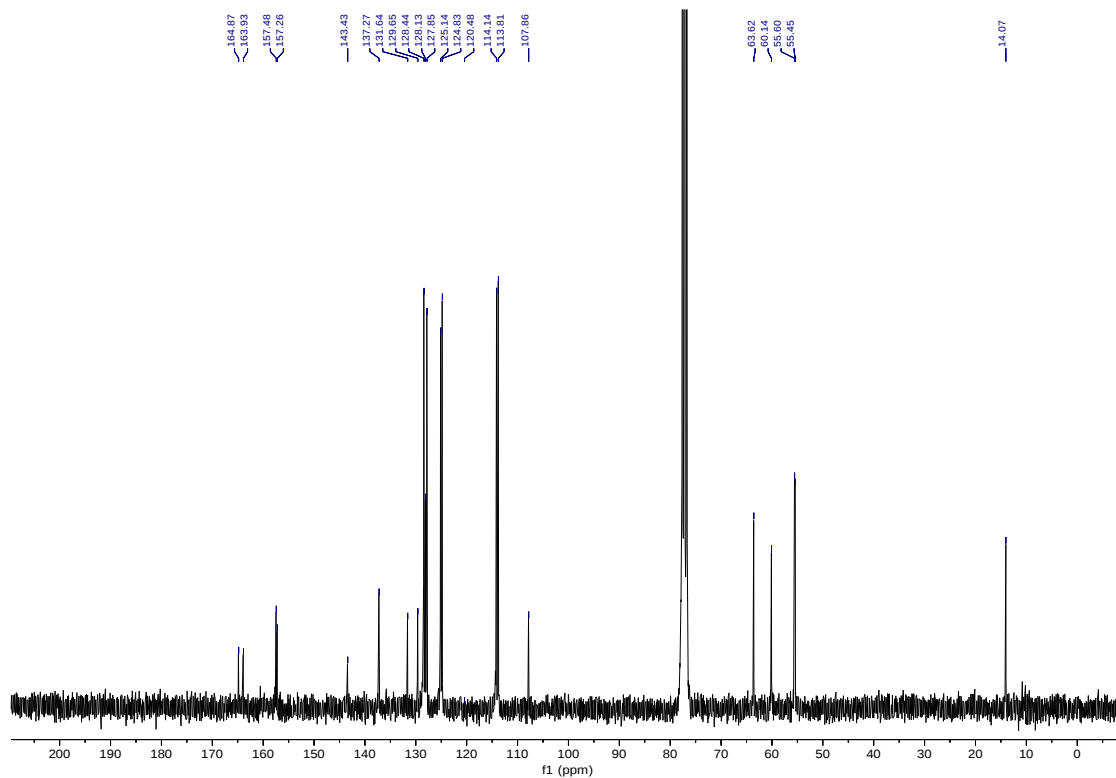


Ethyl 1-(4-methoxyphenyl)-4-((4-methoxyphenyl)amino)-5-oxo-2-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (10b).

¹H NMR (300 MHz, CDCl₃)

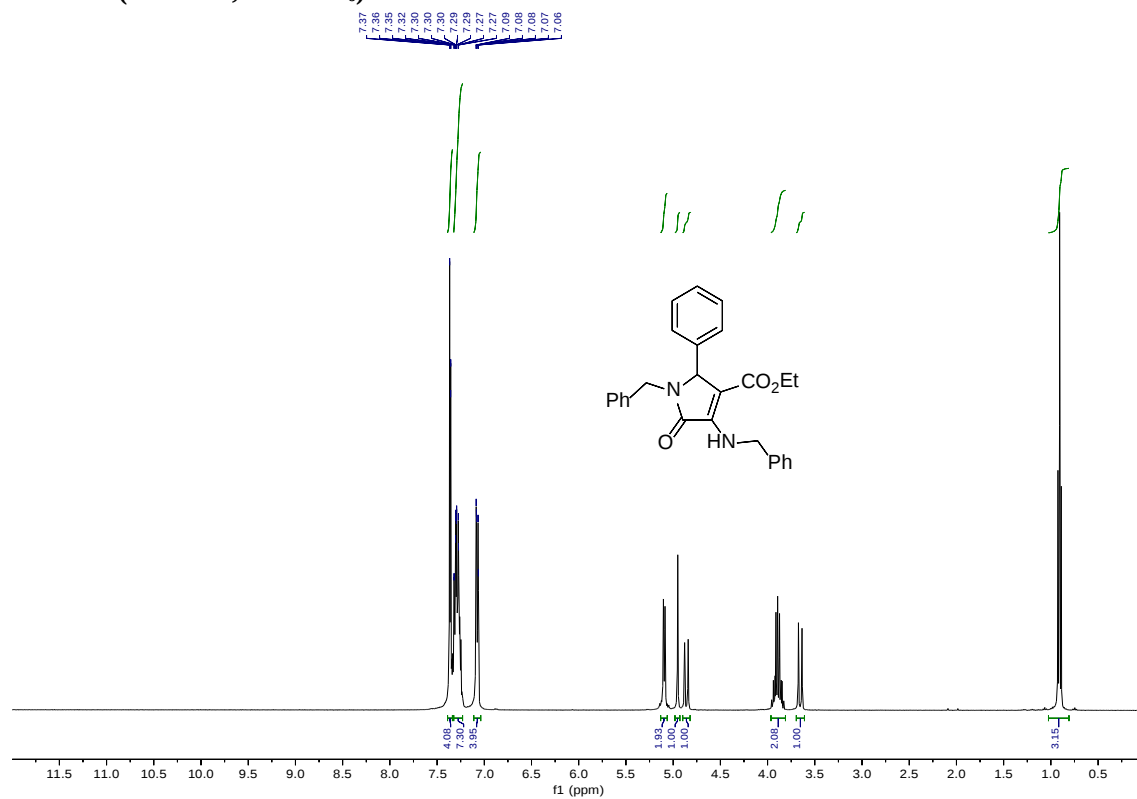


¹³C NMR (75 MHz, CDCl₃)

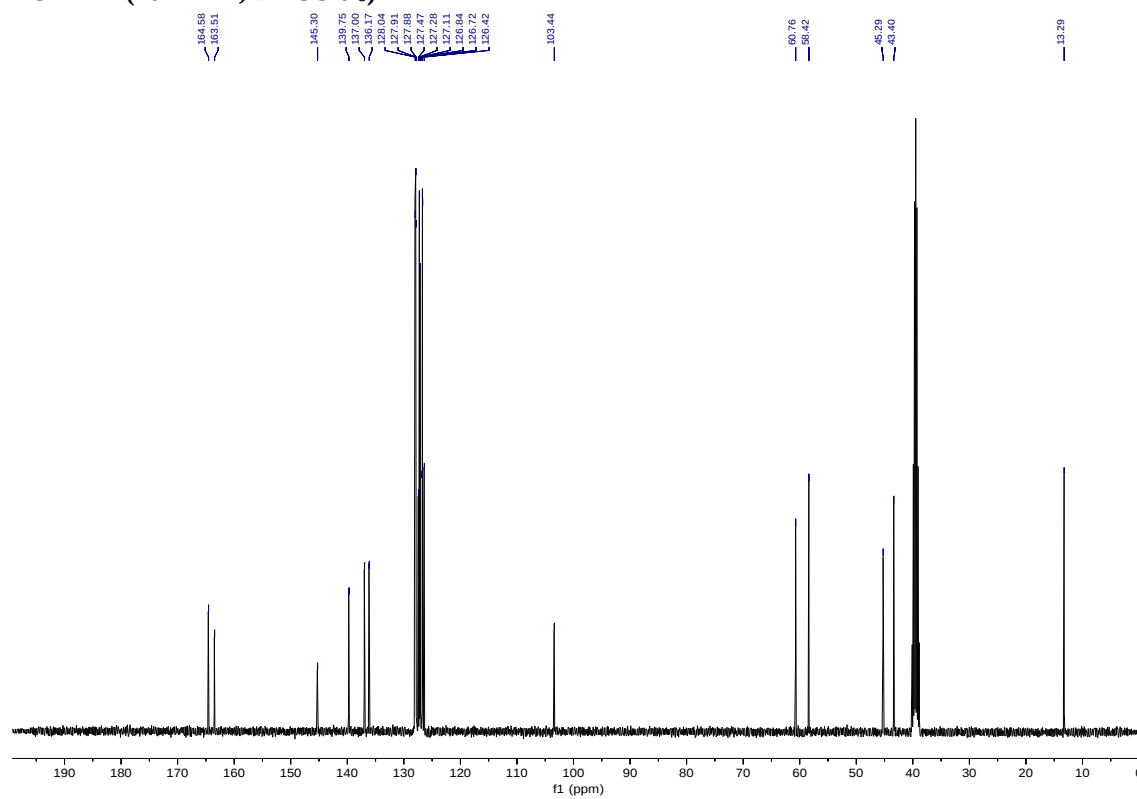


Ethyl 1-benzyl-4-(benzylamino)-5-oxo-2-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (10c).

¹H NMR (400 MHz, DMSO-*d*₆)

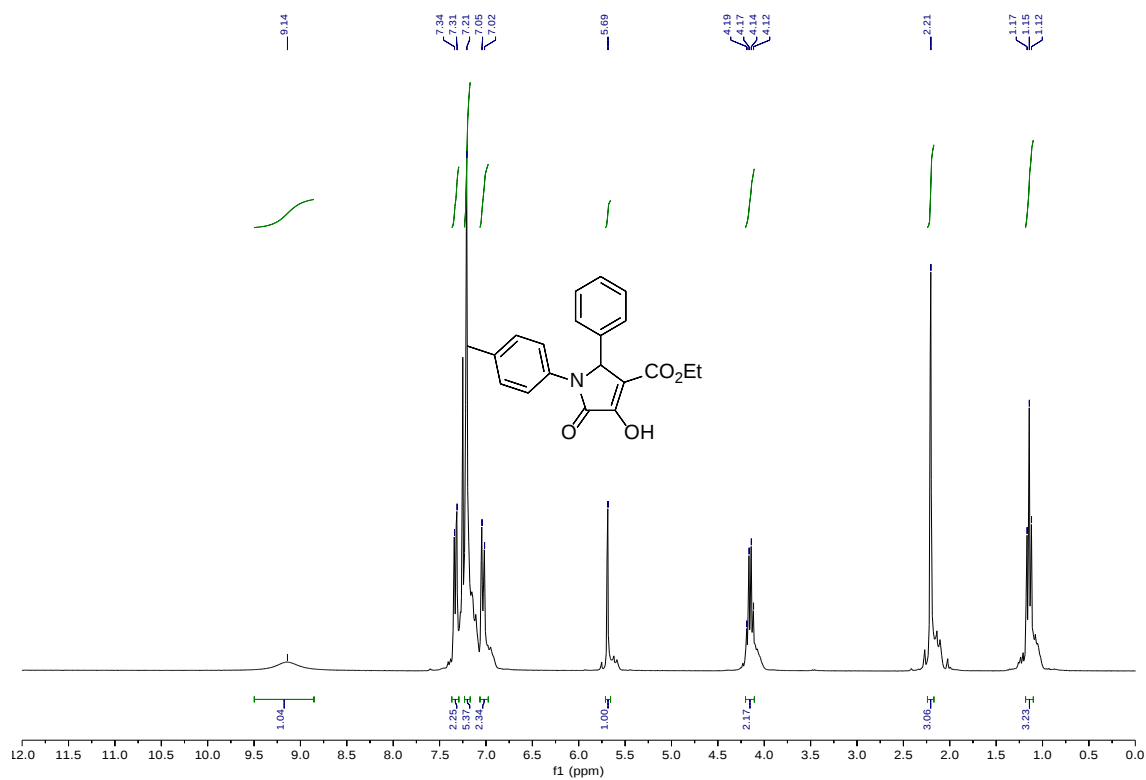


¹³C NMR (101 MHz, DMSO *d*₆)

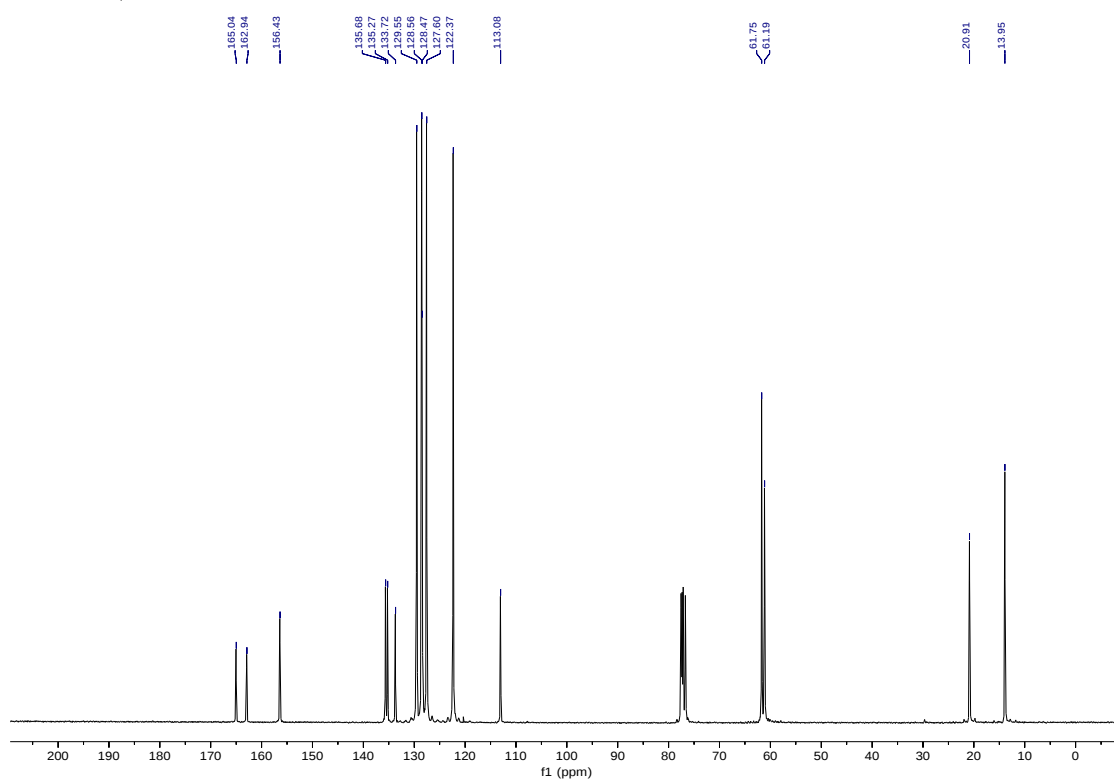


Ethyl 4-hydroxy-5-oxo-2-phenyl-1-(p-tolyl)-2,5-dihydro-1H-pyrrole-3-carboxylate.
(11a).

¹H NMR (300 MHz, CDCl₃)

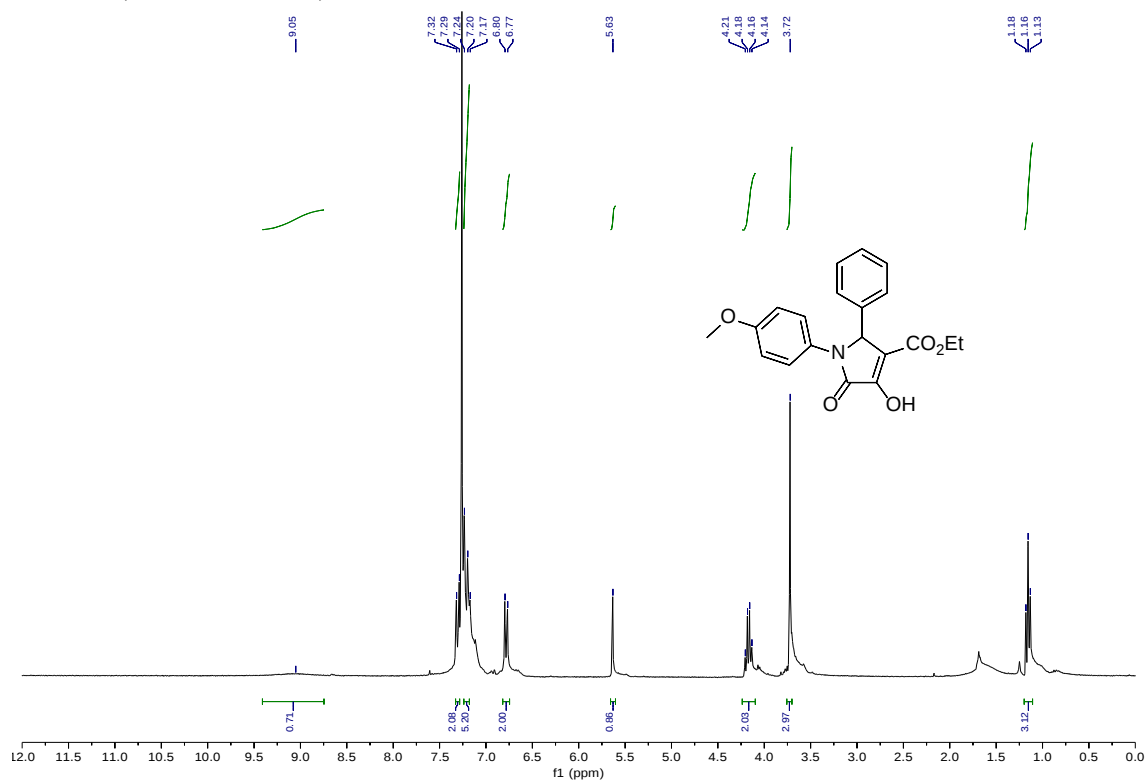


¹³C NMR (75 MHz, CDCl₃)

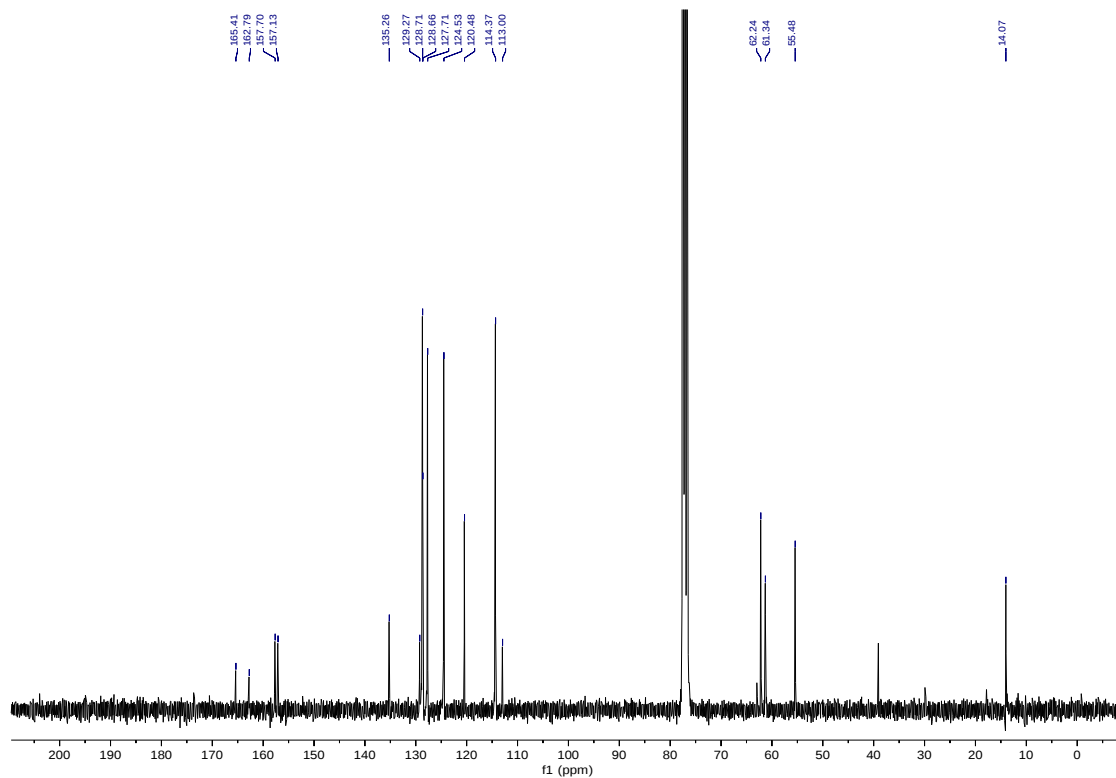


Ethyl 4-hydroxy-1-(4-methoxyphenyl)-5-oxo-2-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate. (11b).

¹H NMR (300 MHz, CDCl₃)

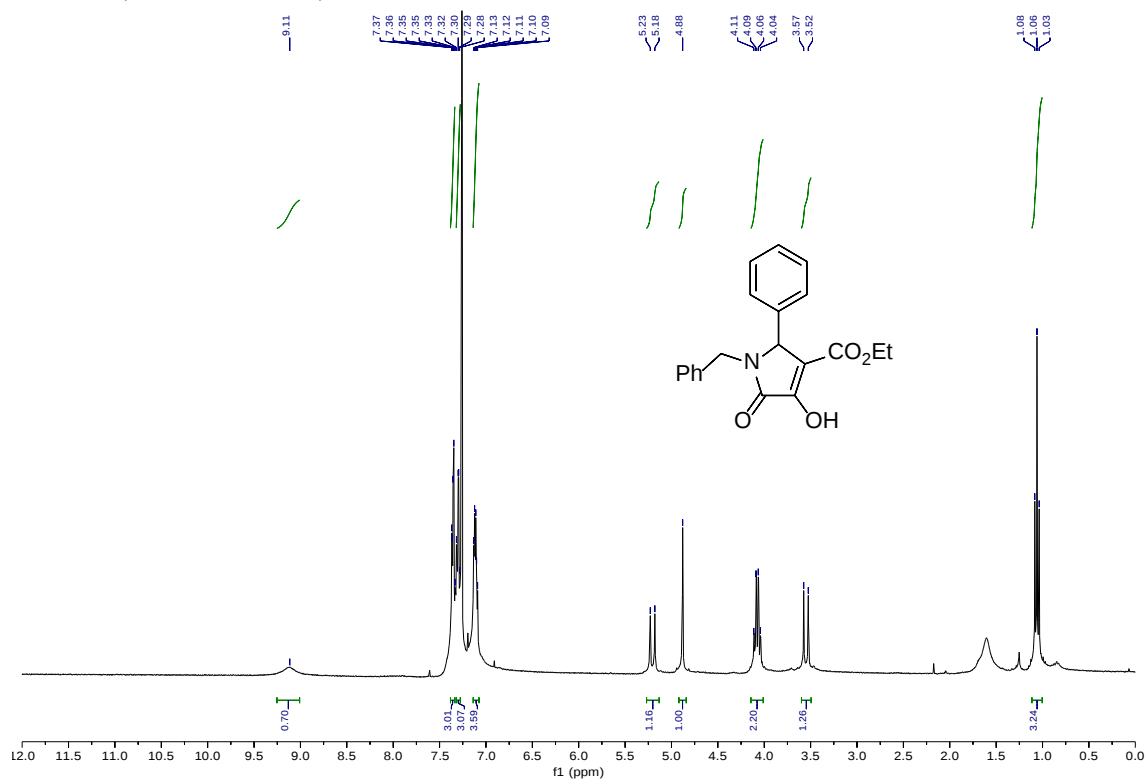


¹³C NMR (75 MHz, CDCl₃)

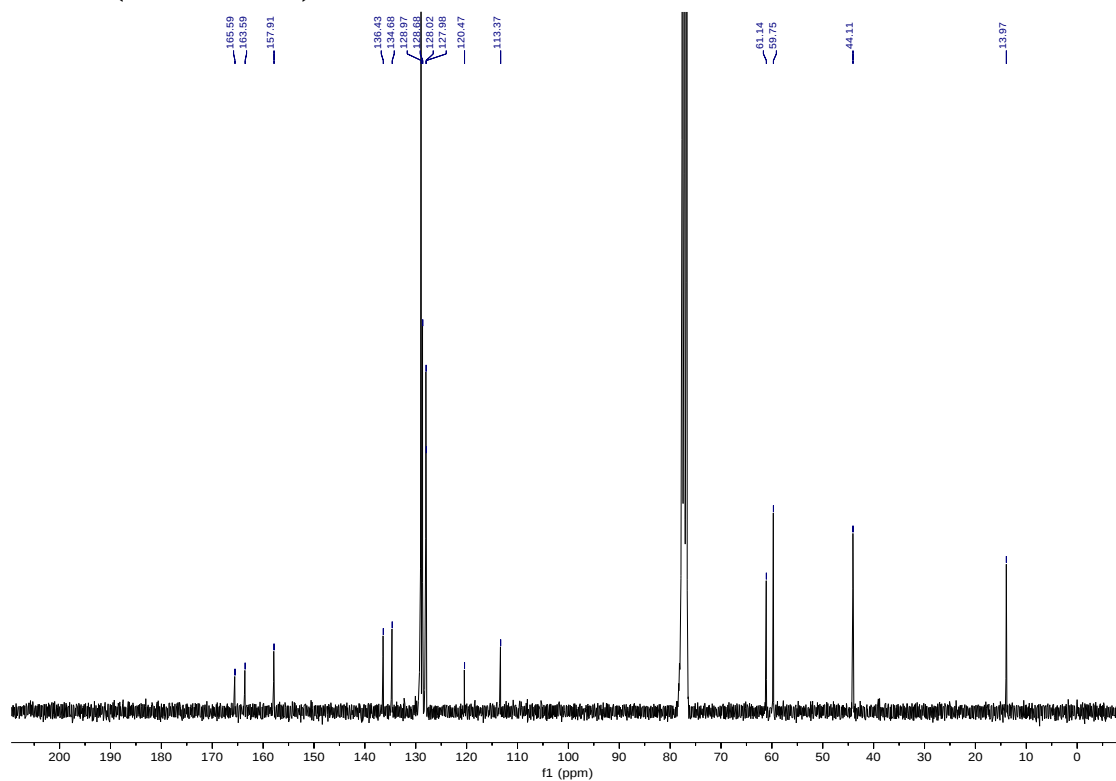


Ethyl 1-benzyl-4-hydroxy-5-oxo-2-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate.
(11c).

^1H NMR (300 MHz, CDCl_3)

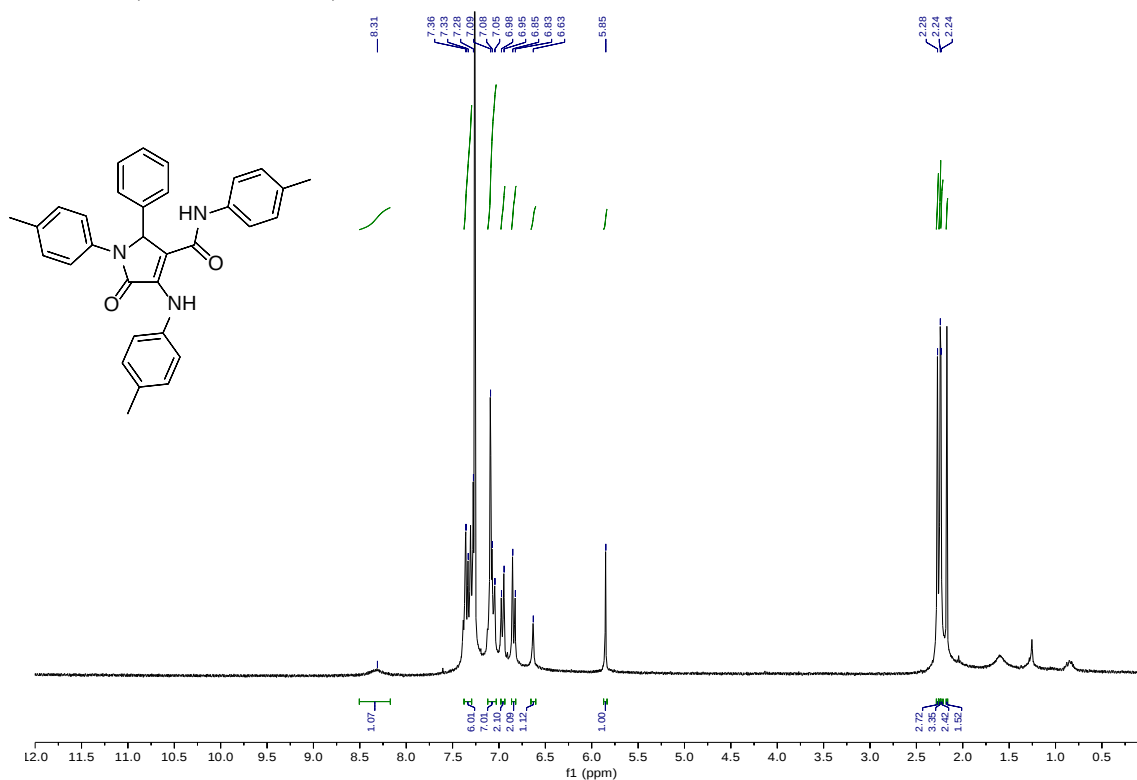


^{13}C NMR (75 MHz, CDCl_3)

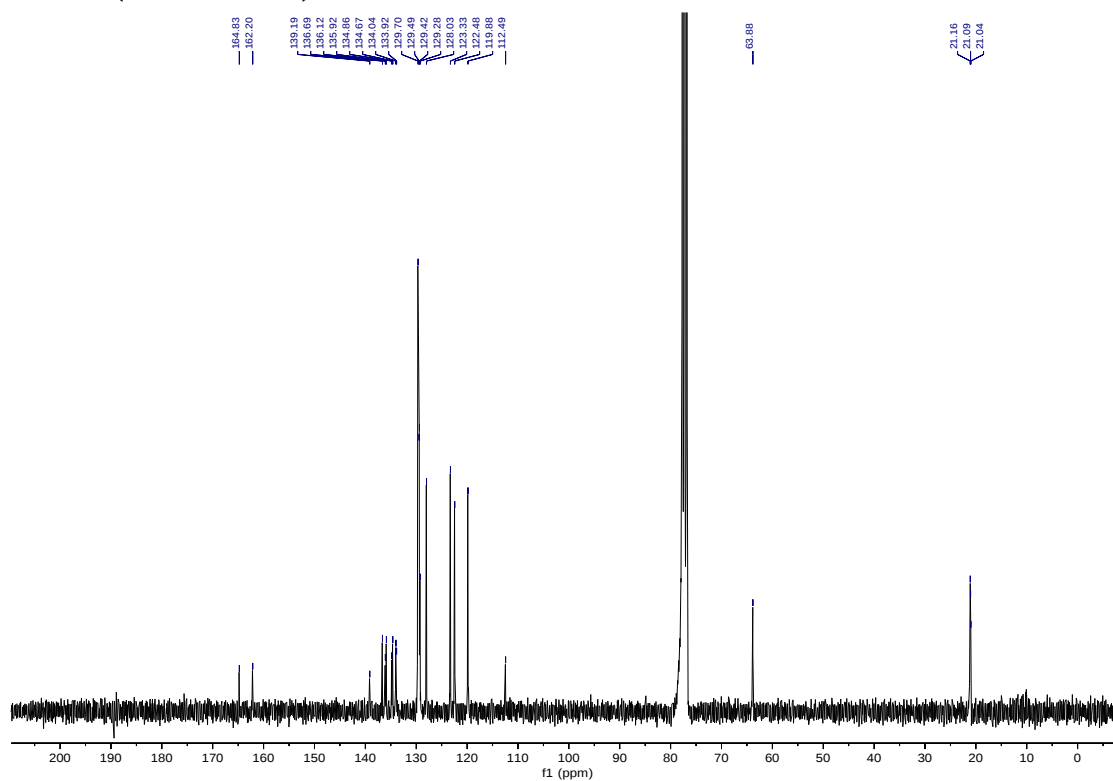


5-oxo-2-phenyl-N,1-di-p-tolyl-4-(p-tolylamino)-2,5-dihydro-1H-pyrrole-3-carboxamide (12a).

¹H NMR (300 MHz, CDCl₃)

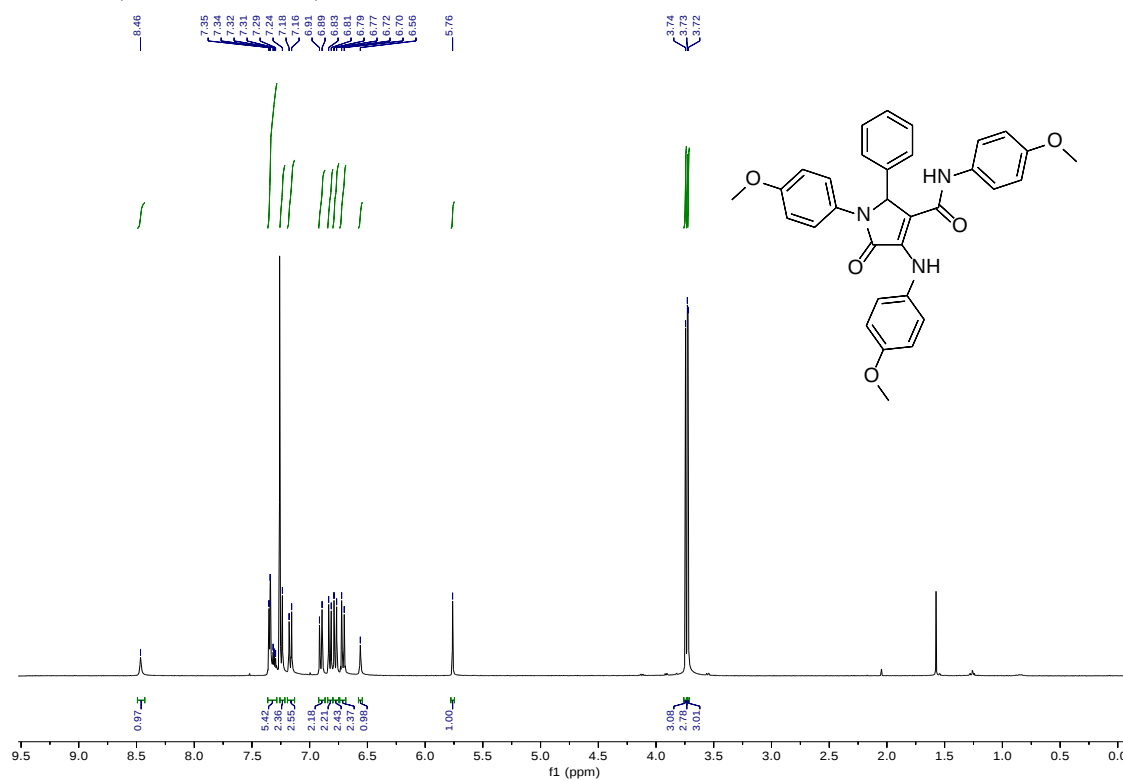


¹³C NMR (75 MHz, CDCl₃)

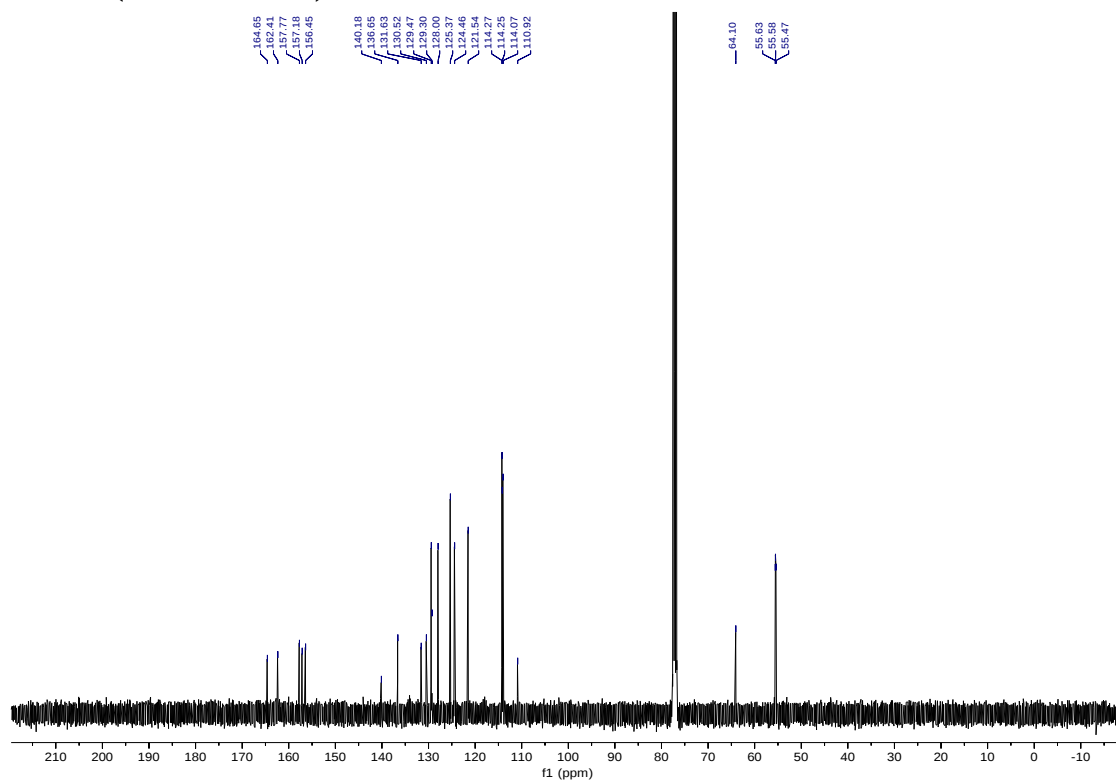


N,1-bis(4-methoxyphenyl)-4-((4-methoxyphenyl)amino)-5-oxo-2-phenyl-2,5-dihydro-1H-pyrrole-3-carboxamide. (12b).

¹H NMR (400 MHz, CDCl₃)

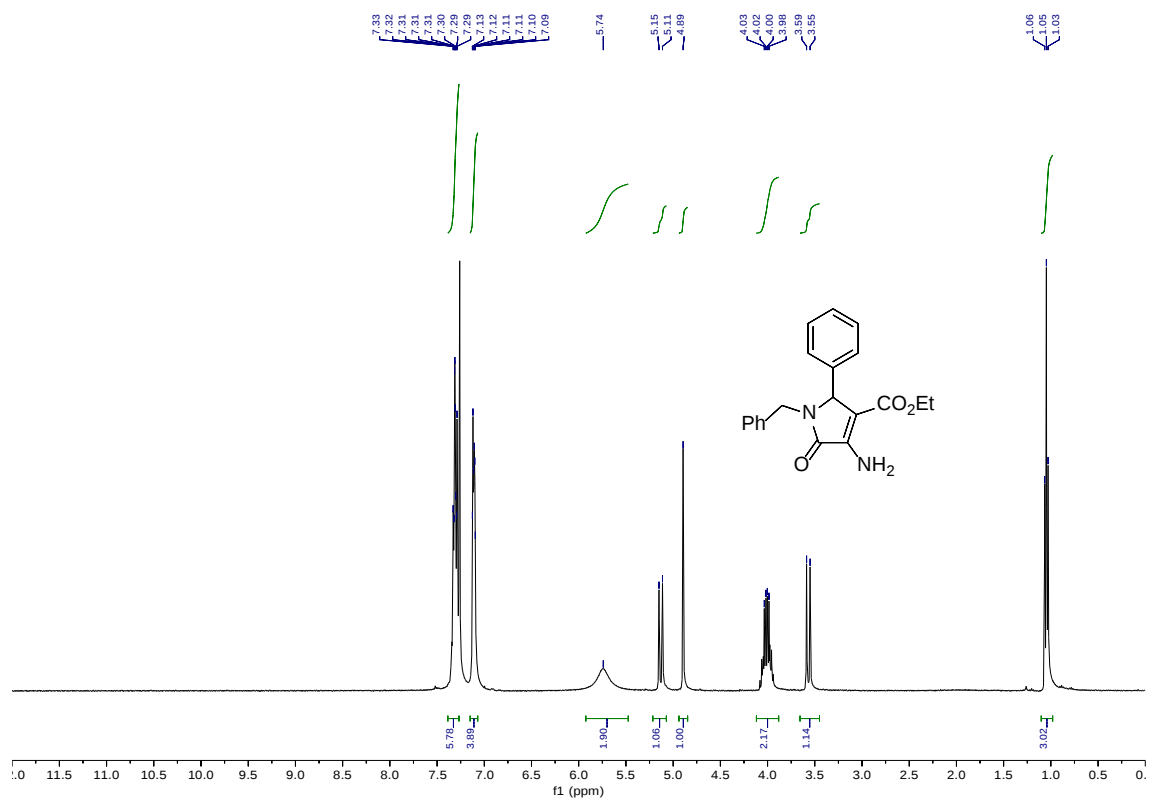


¹³C NMR (101 MHz, CDCl₃)

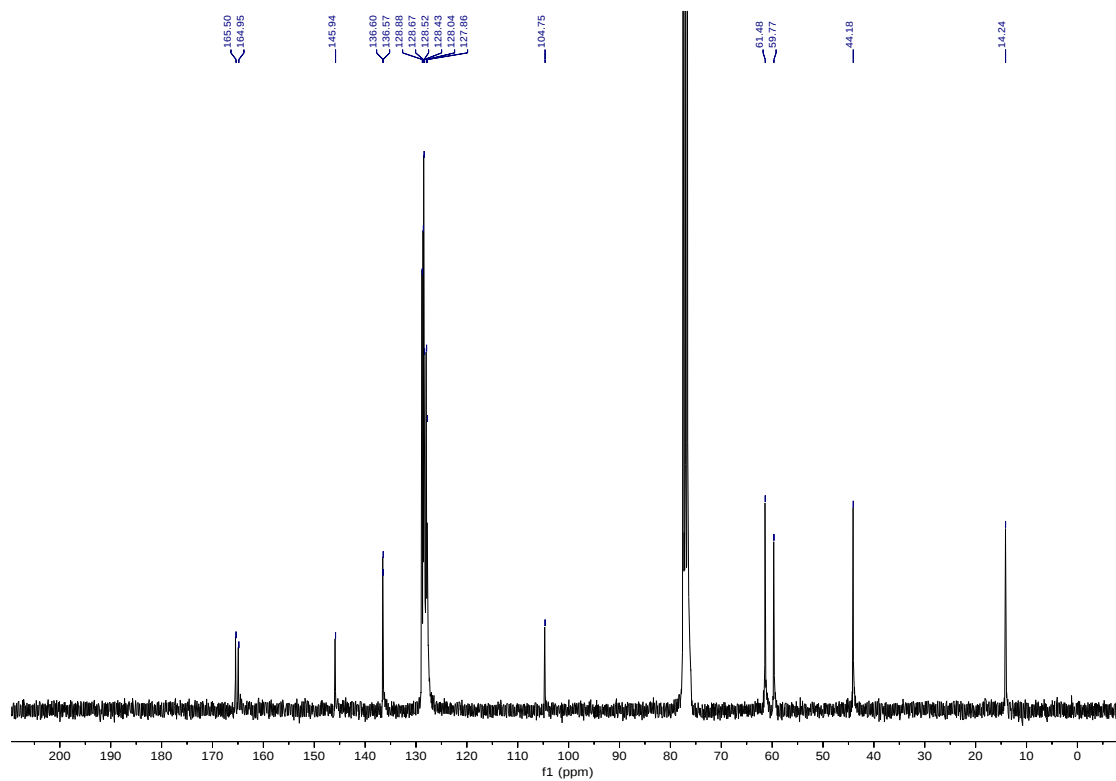


Ethyl 4-amino-1-benzyl-5-oxo-2-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (16).

¹H NMR (400 MHz, CDCl₃)



¹³C NMR (75 MHz, CDCl₃)



2. Crystal structure determination for compound 11a.

Thermal ellipsoid plot/ORTEP for compound 11a (50% contour probability level).

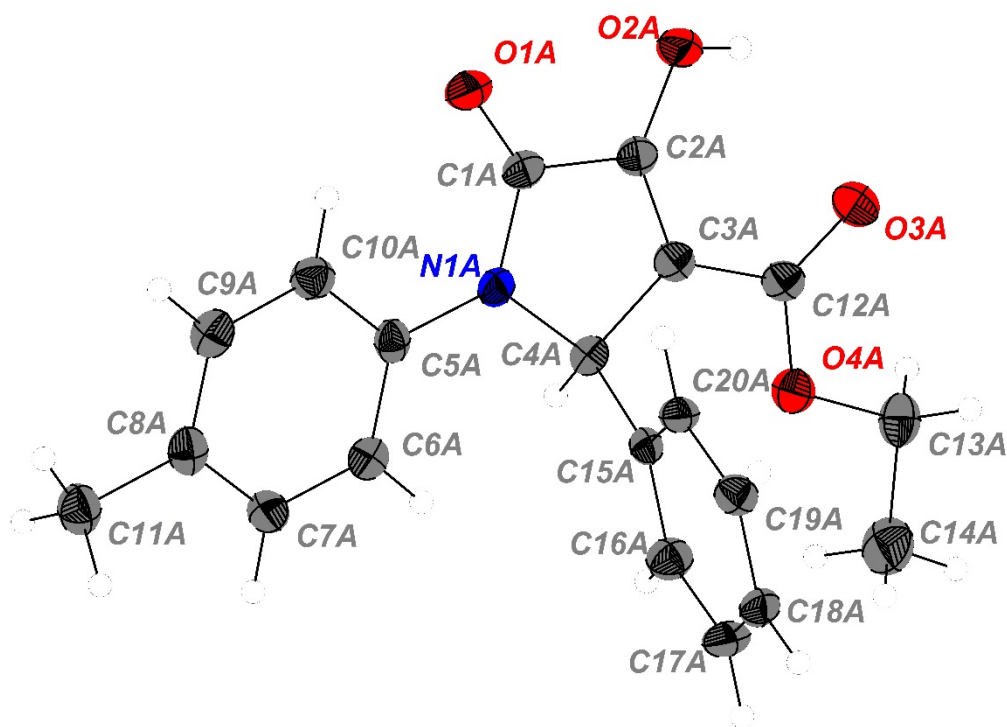


Table. Crystal data and structure refinement for 11a.

Identification code	a20180048_EM336OH
Empirical formula	C ₂₀ H ₁₉ NO ₄
Formula weight	3376.36
Temperature/K	149.99(10)
Crystal system	triclinic
Space group	P1
a/Å	9.8131(3)
b/Å	16.1669(7)
c/Å	17.7028(7)
α /°	114.324(4)
β /°	90.139(3)
γ /°	100.214(3)
Volume/Å ³	2509.70(17)
Z	6
ρ calcg/cm ³	1.339
μ /mm ⁻¹	0.765
F(000)	1068.0
Crystal size/mm ³	0.257 × 0.12 × 0.052
Radiation	CuK α (λ = 1.54184)
2 θ range for data collection/°	9.19 to 137.994
Index ranges	-9 ≤ h ≤ 11, -19 ≤ k ≤ 19, -21 ≤ l ≤ 21
Reflections collected	18227

Independent reflections	9284 [$R_{\text{int}} = 0.0487$, $R_{\text{sigma}} = 0.0647$]
Data/restraints/parameters	9284/0/685
Goodness-of-fit on F^2	1.039
Final R indexes [$I \geq 2 \sigma(I)$]	$R_1 = 0.0447$, $wR_2 = 0.1034$
Final R indexes [all data]	$R_1 = 0.0662$, $wR_2 = 0.1148$
Largest diff. peak/hole / $e \text{ \AA}^{-3}$	0.45/-0.21