

Supporting Information

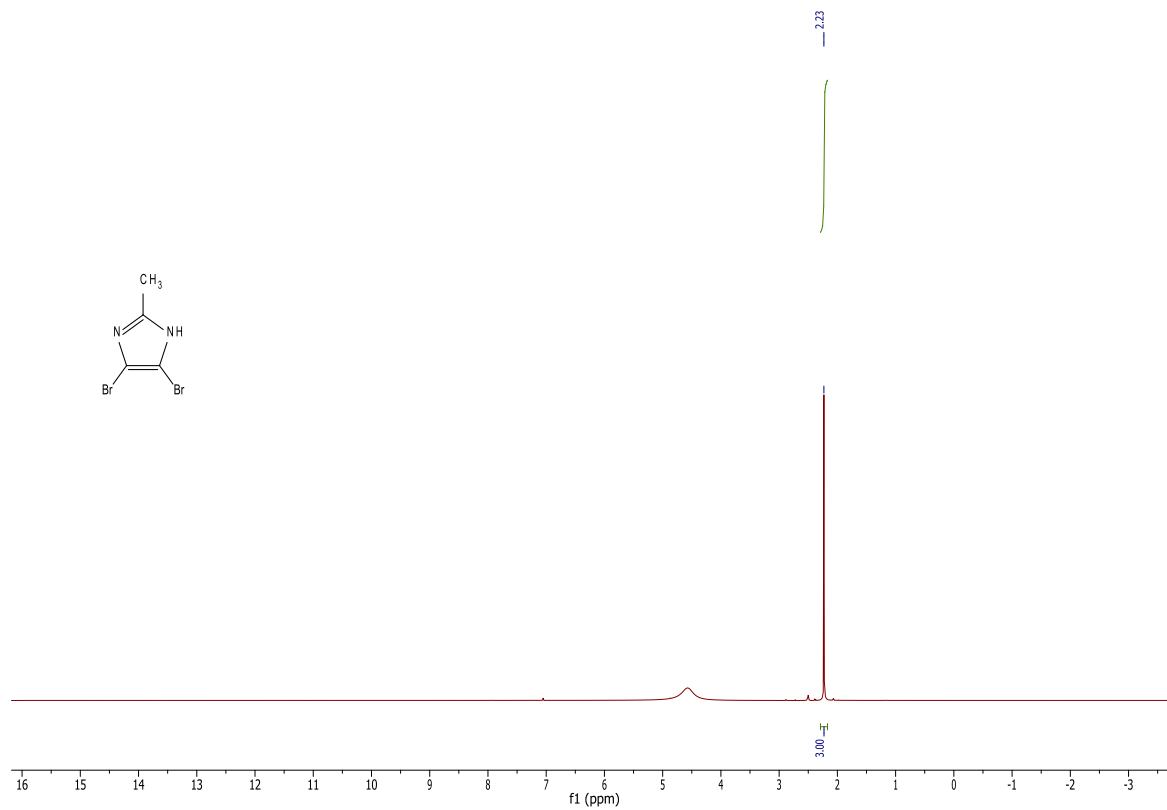
**A new synthetic approach to the imidazo[1,5-*a*]imidazol-2-one scaffold
and effective functionalization through Suzuki-Miyaura cross coupling
reactions**

M. Loubidi,^{a,b} C. Pillard,^c A. El Hakmaoui,^b P. Bernard,^c M. Akssira,^{*b} and G. Guillaumet.^{*a}

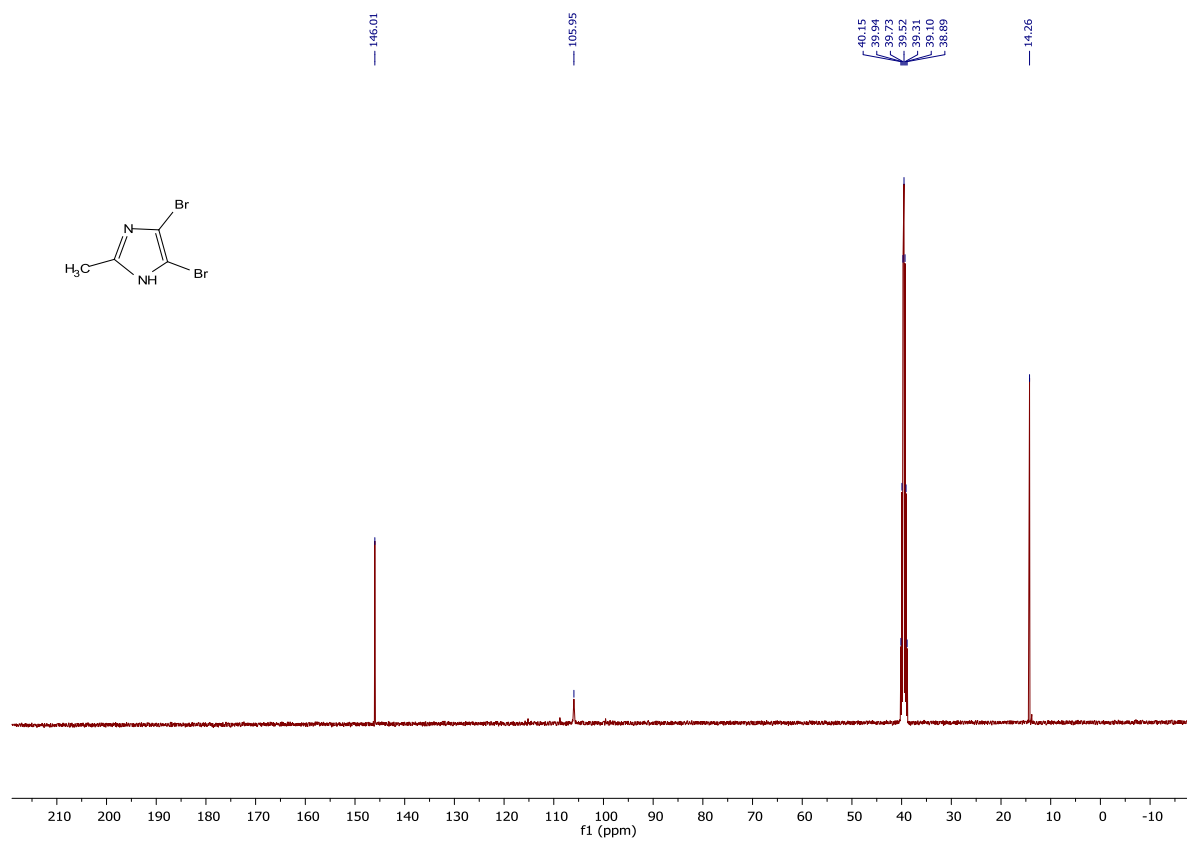
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4,5-Dibromo-2-methyl-1H-imidazole (2)

^1H NMR (400 MHz, DMSO-d_6): δ

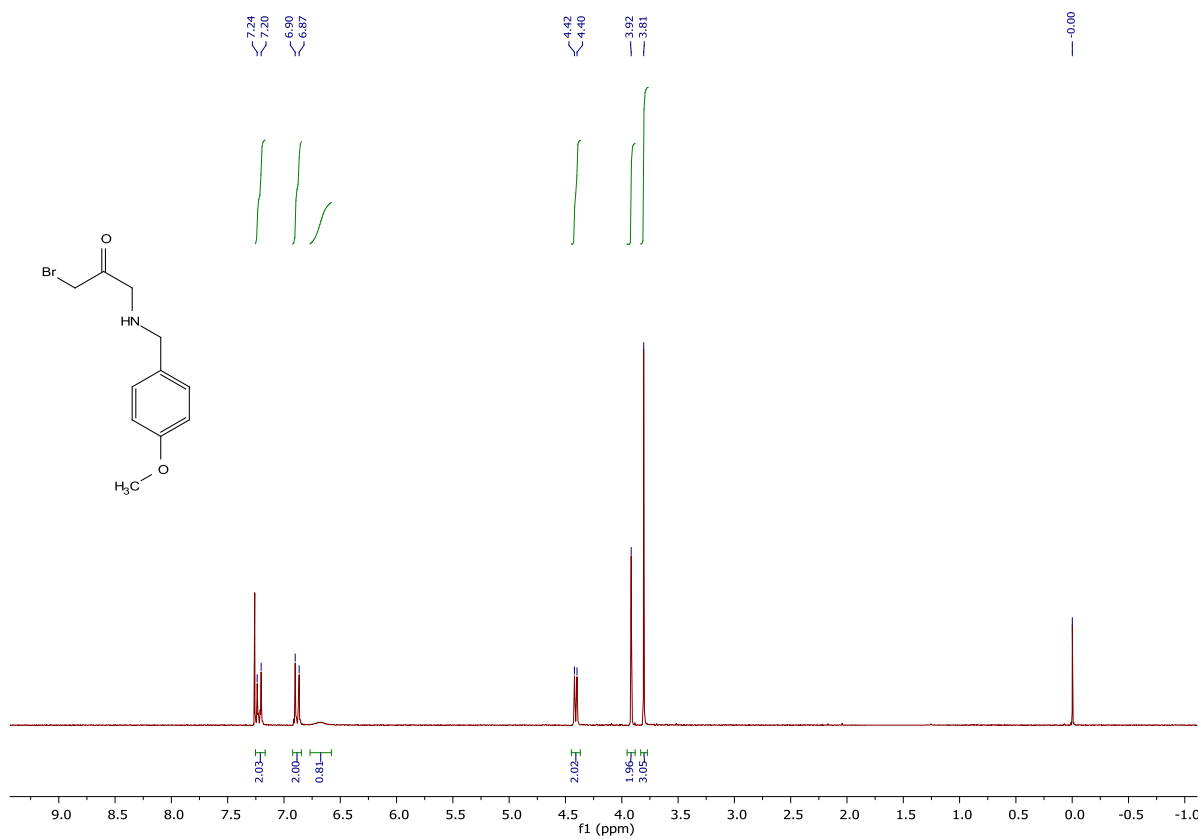


^{13}C NMR (101 MHz, DMSO-d_6): δ

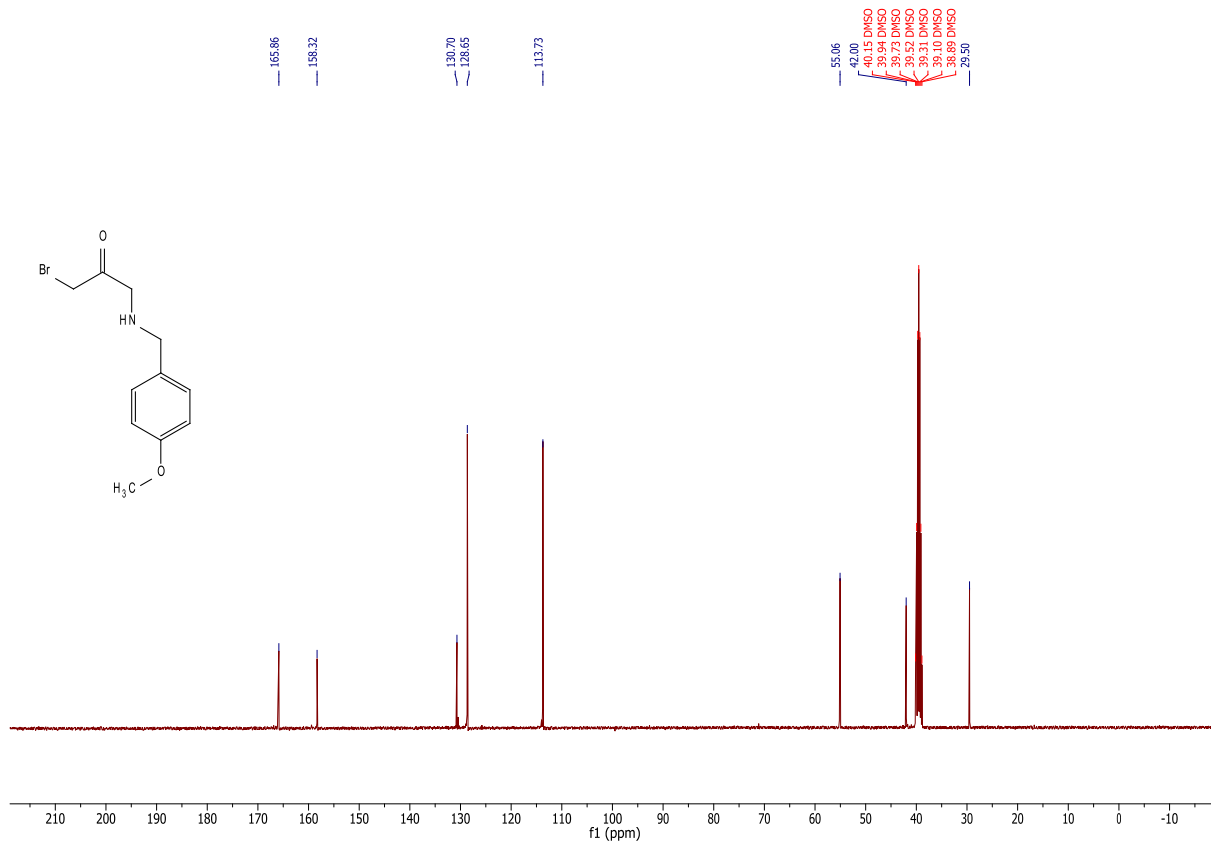


2-Bromo-*N*-(4-methoxybenzyl)acetamide (4)

^1H NMR (400 MHz, CDCl_3): δ

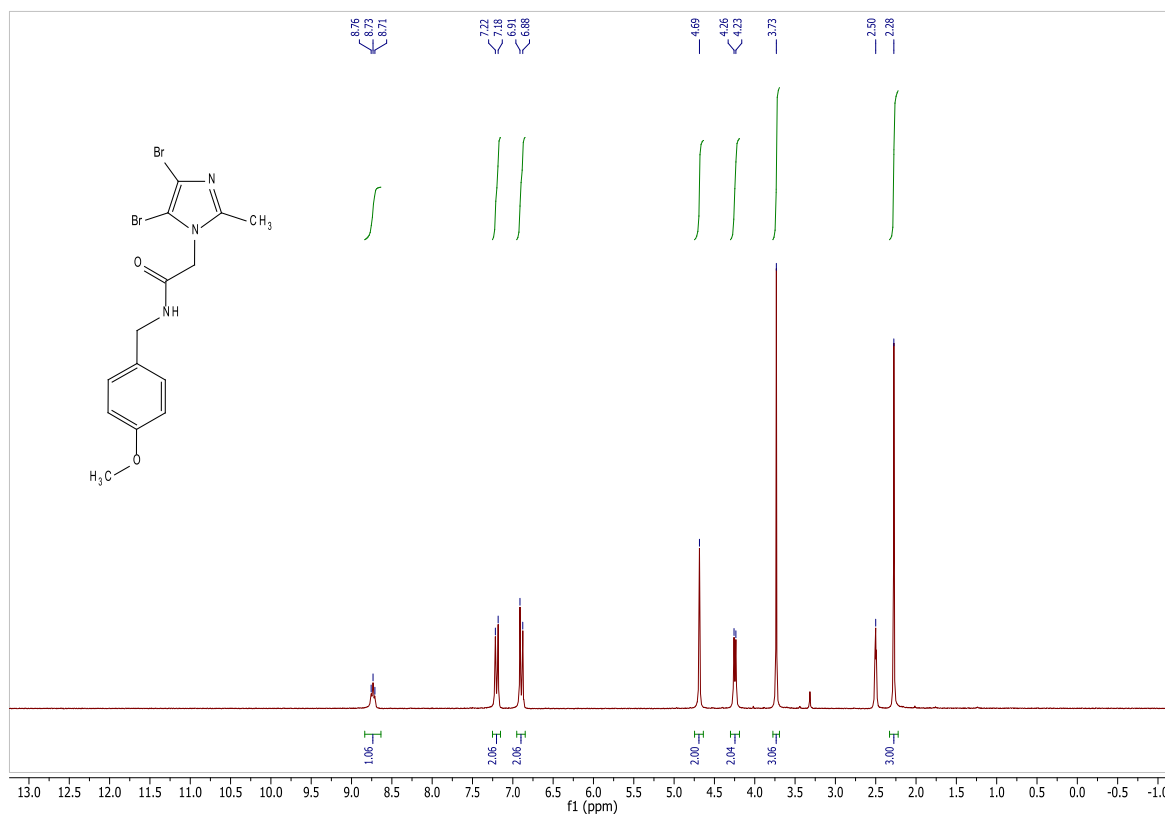


^{13}C NMR (101 MHz, DMSO): δ

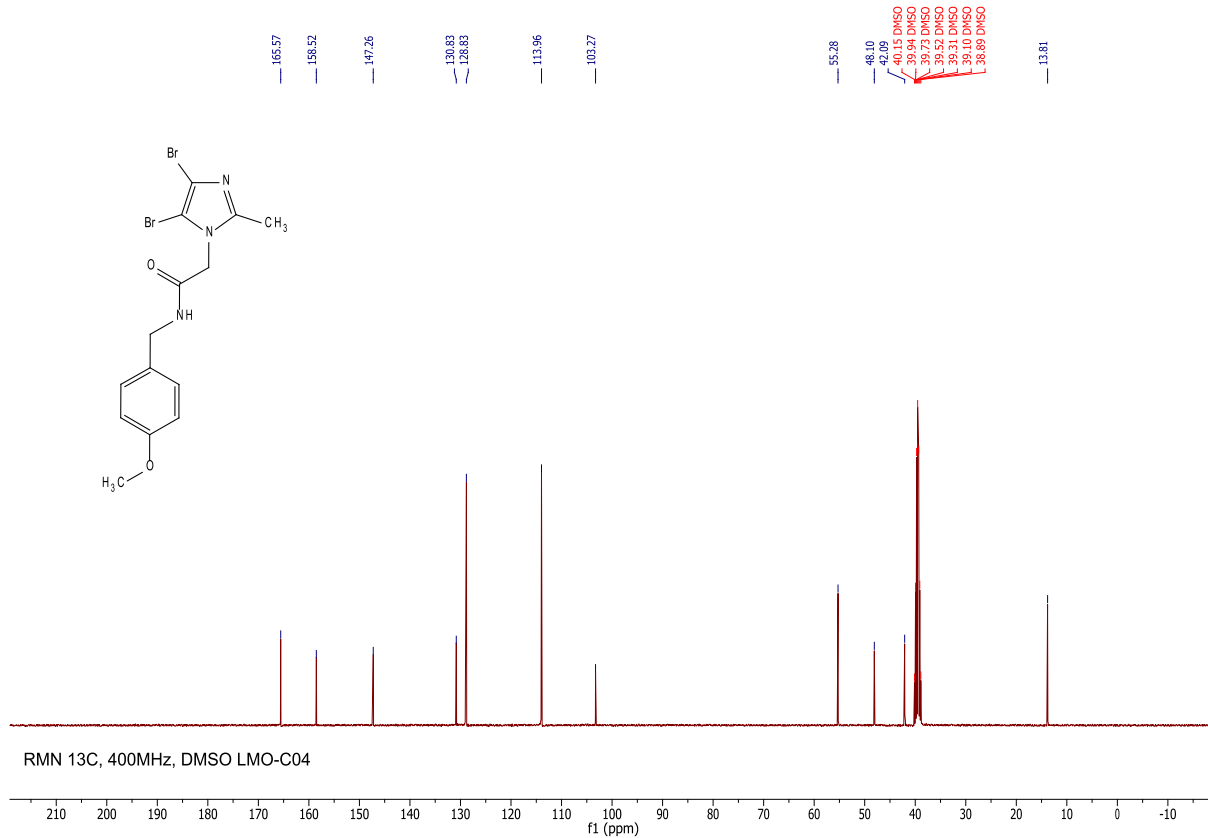


2-(4,5-Dibromo-2-methyl-1H-imidazol-1-yl)-N-(4-methoxybenzyl) acetamide (5).

¹H NMR (250 MHz, DMSO-d₆): δ



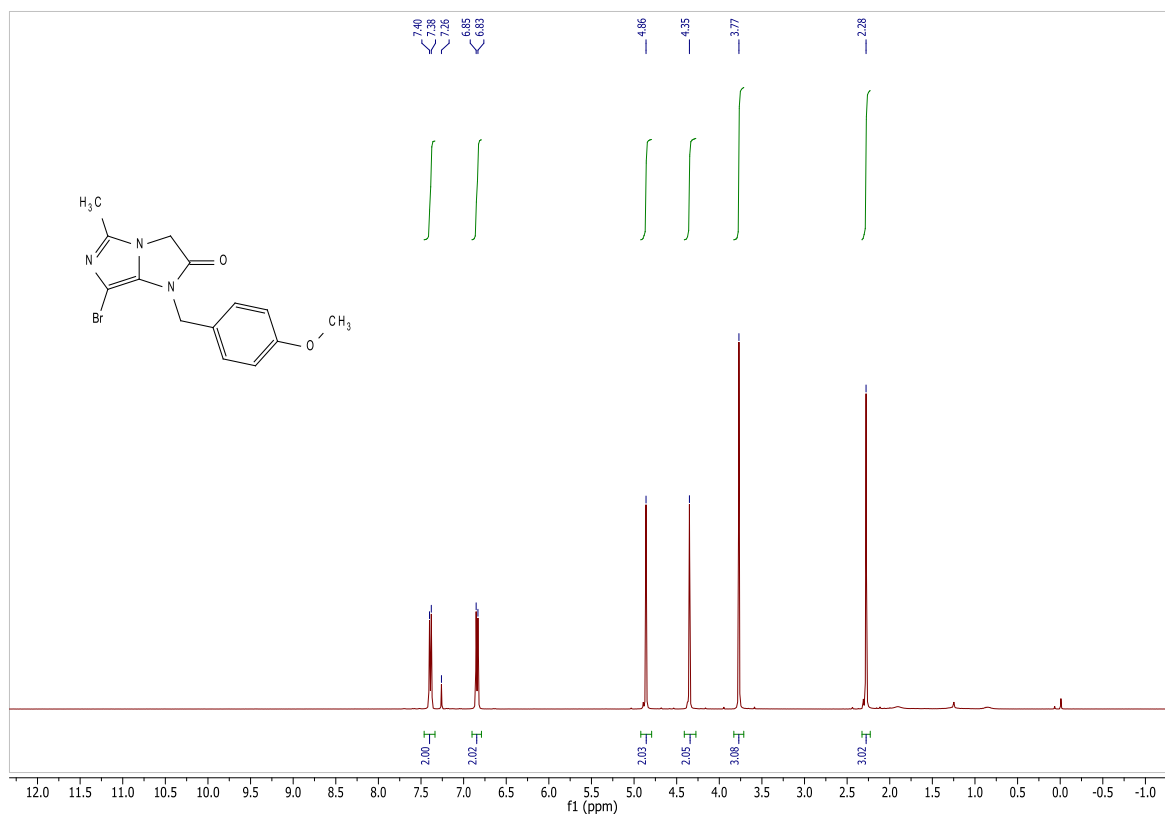
¹³C NMR (101 MHz, DMSO-d₆): δ



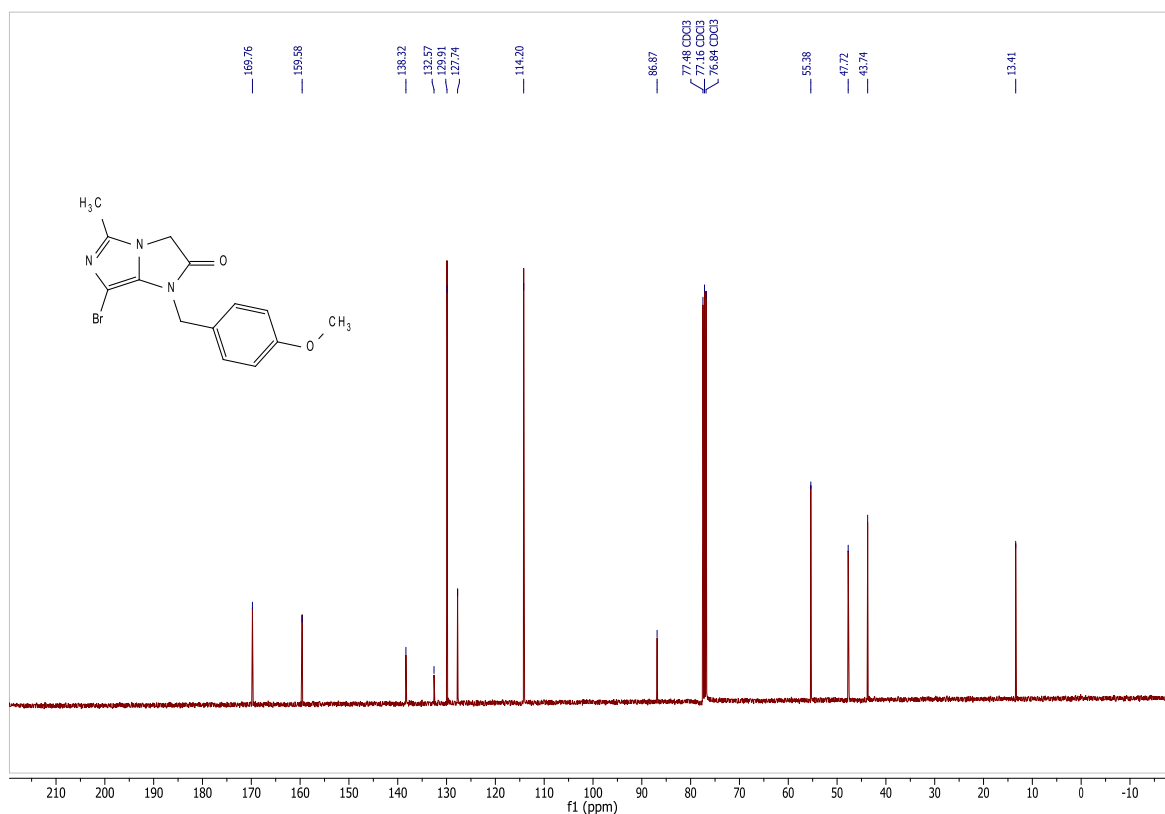
RMN 13C, 400MHz, DMSO LMO-C04

7-Bromo-1-(4-methoxybenzyl)-5-methyl-1H-imidazo[1,5-a]imidazol-2(3H)-one (6).

^1H NMR (400 MHz, CDCl_3): δ

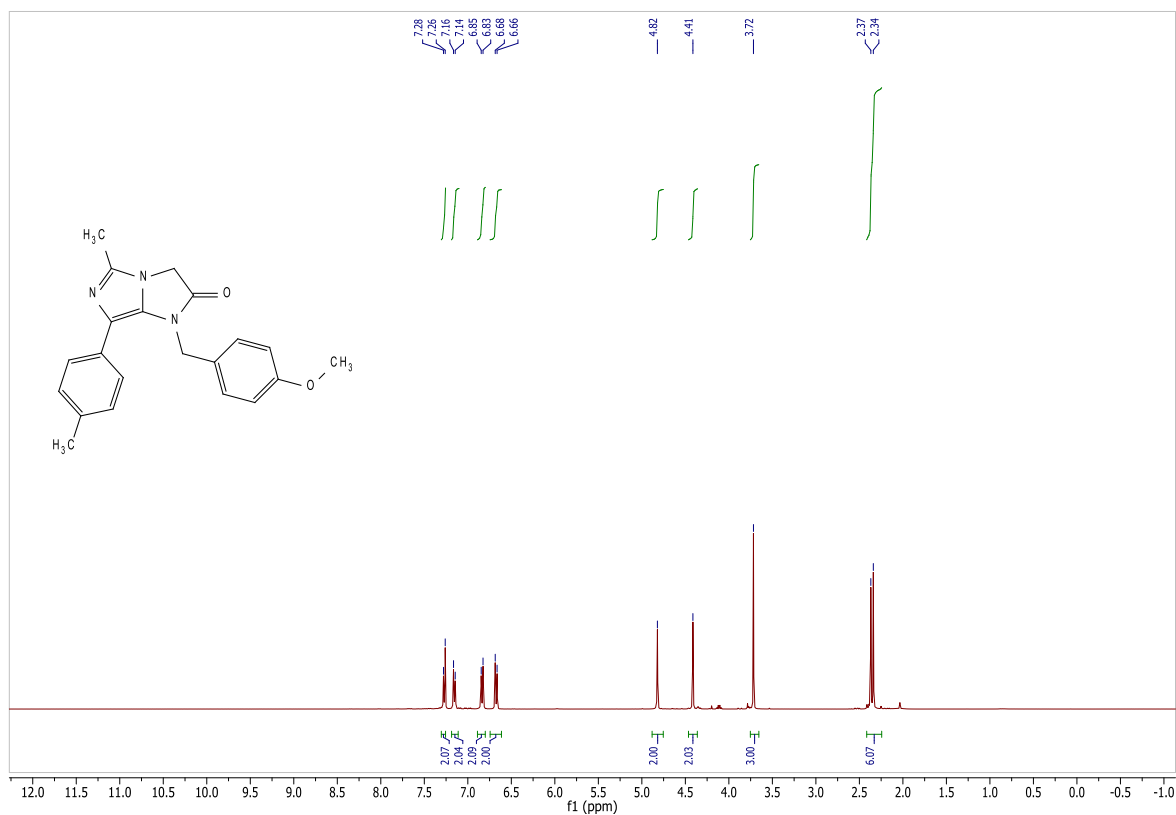


^{13}C NMR (101 MHz, CDCl_3): δ

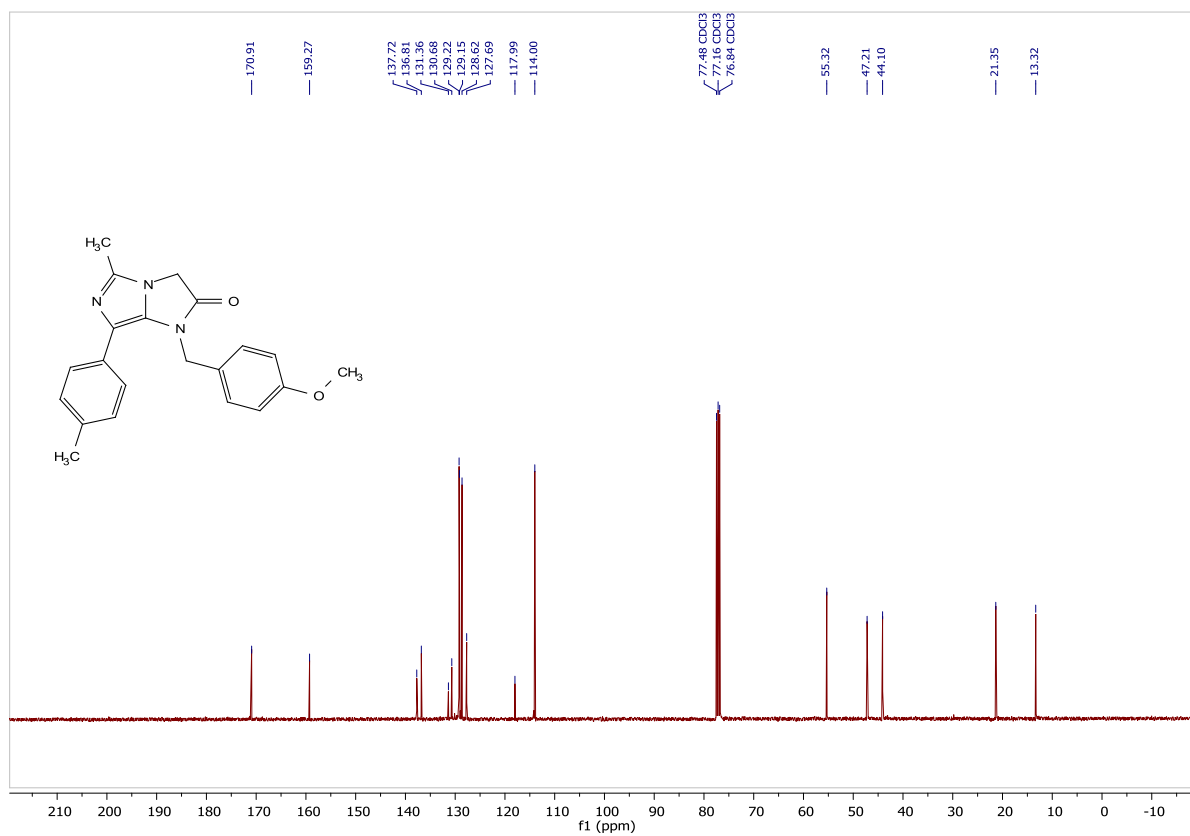


1-(4-Methoxybenzyl)-5-methyl-7-(p-tolyl)-1H-imidazo[1,5-a]imidazol-2(3H)-one (7).

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ

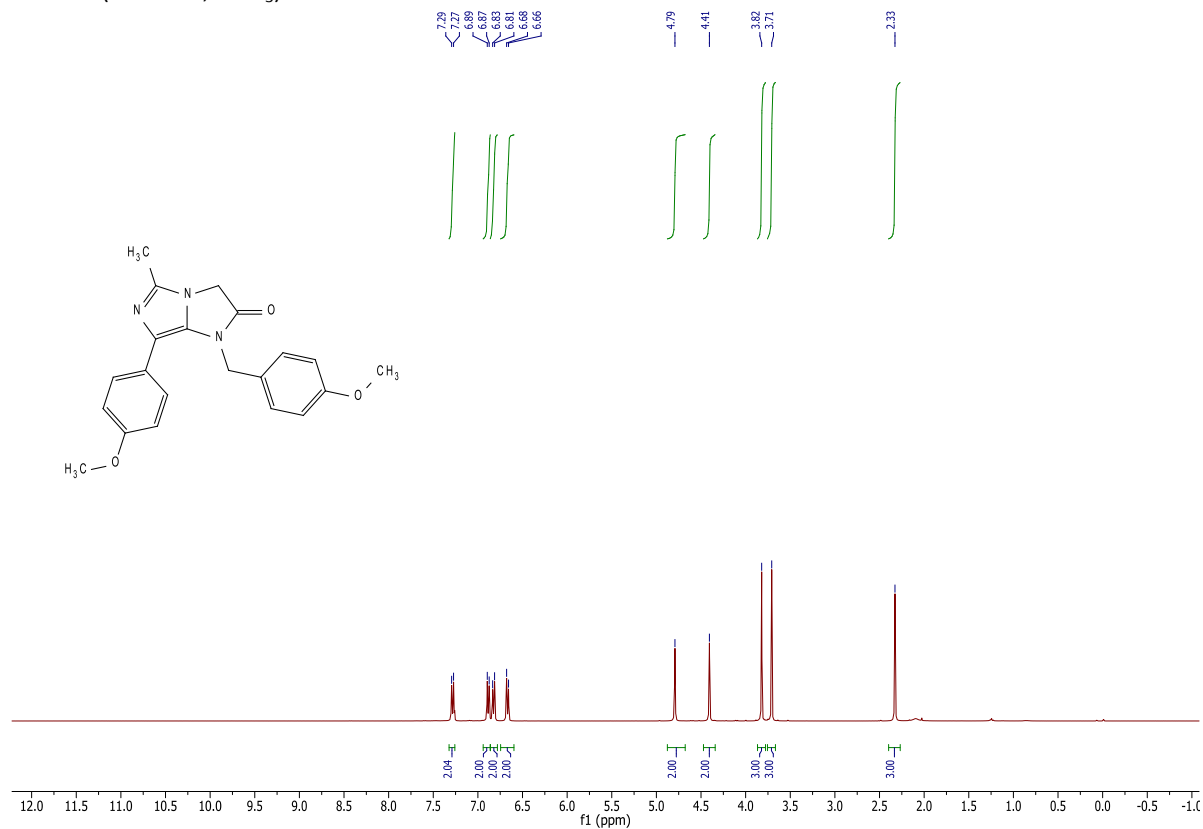


$^1\text{H NMR}$ (400 MHz, CDCl_3): δ

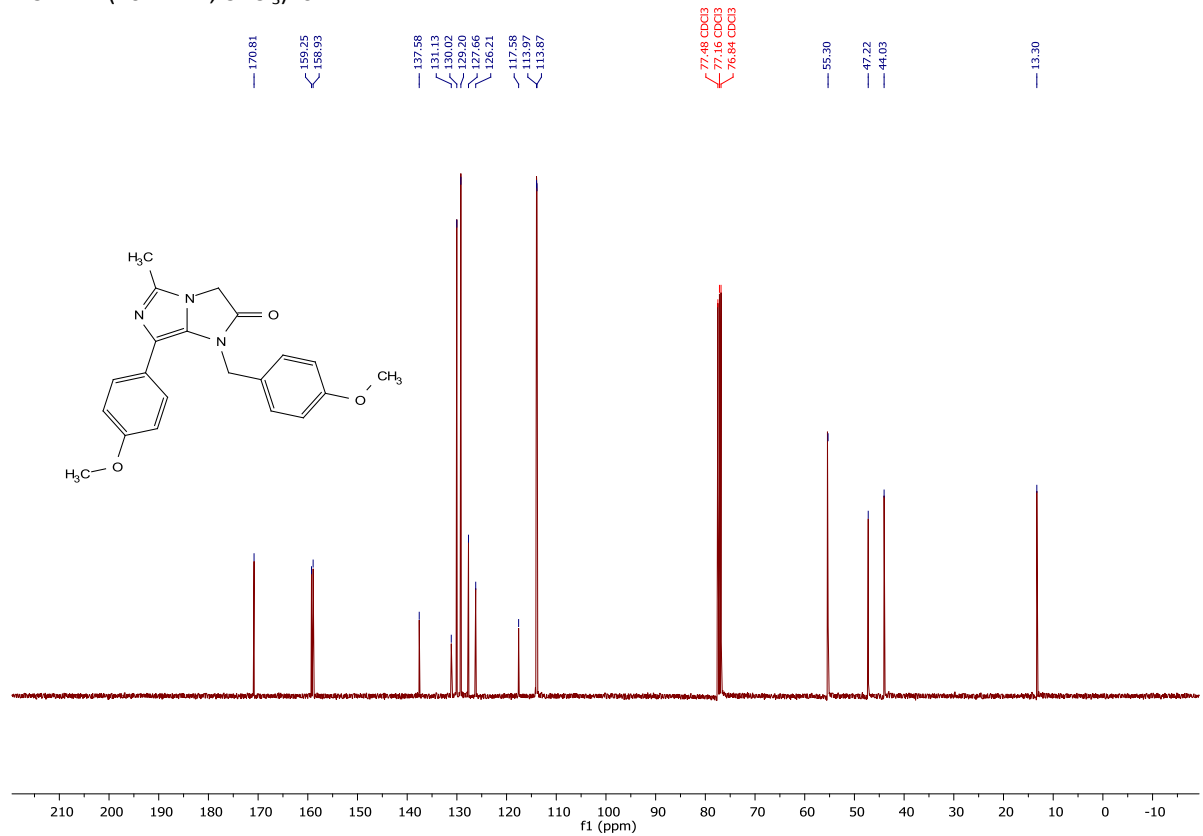


1-(4-Methoxybenzyl)-7-(4-methoxyphenyl)-5-methyl-1H-imidazo[1,5-a]imidazol-2(3H)-one. (8)

^1H NMR (400 MHz, CDCl_3): δ

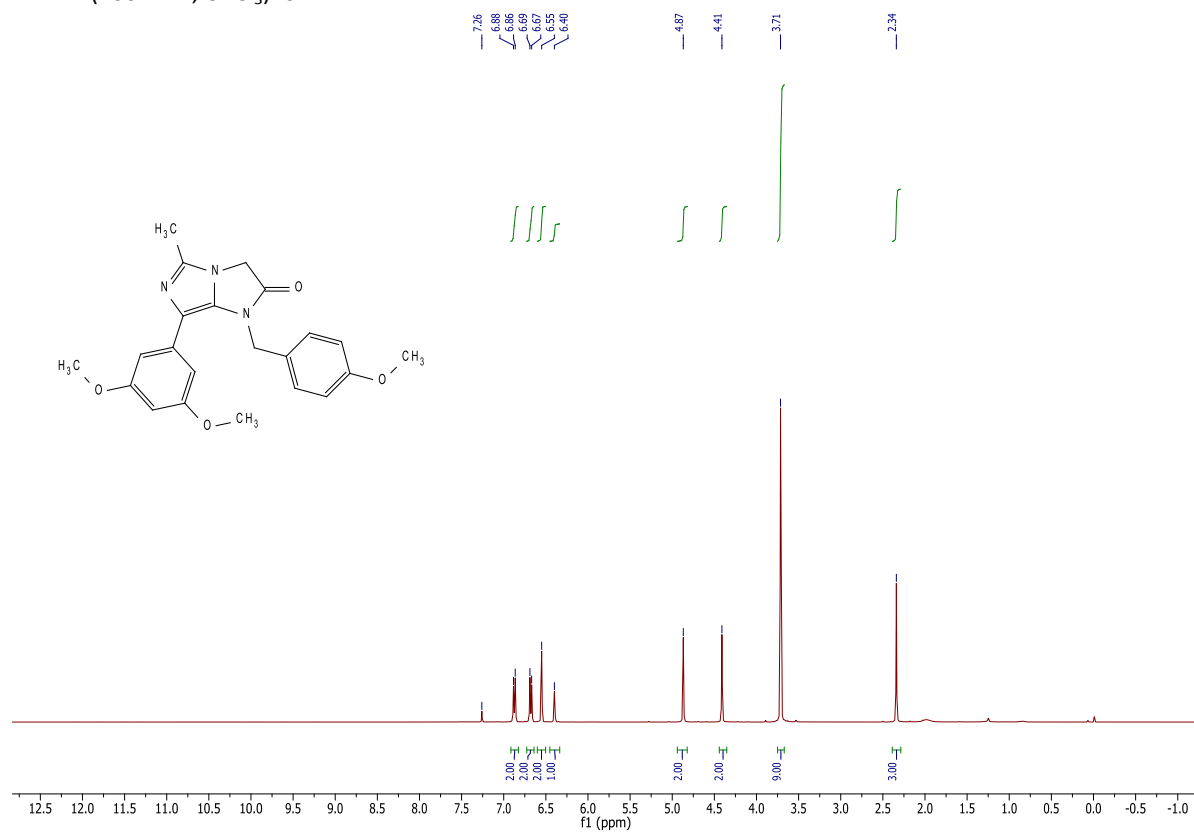


^{13}C NMR (101 MHz, CDCl_3): δ

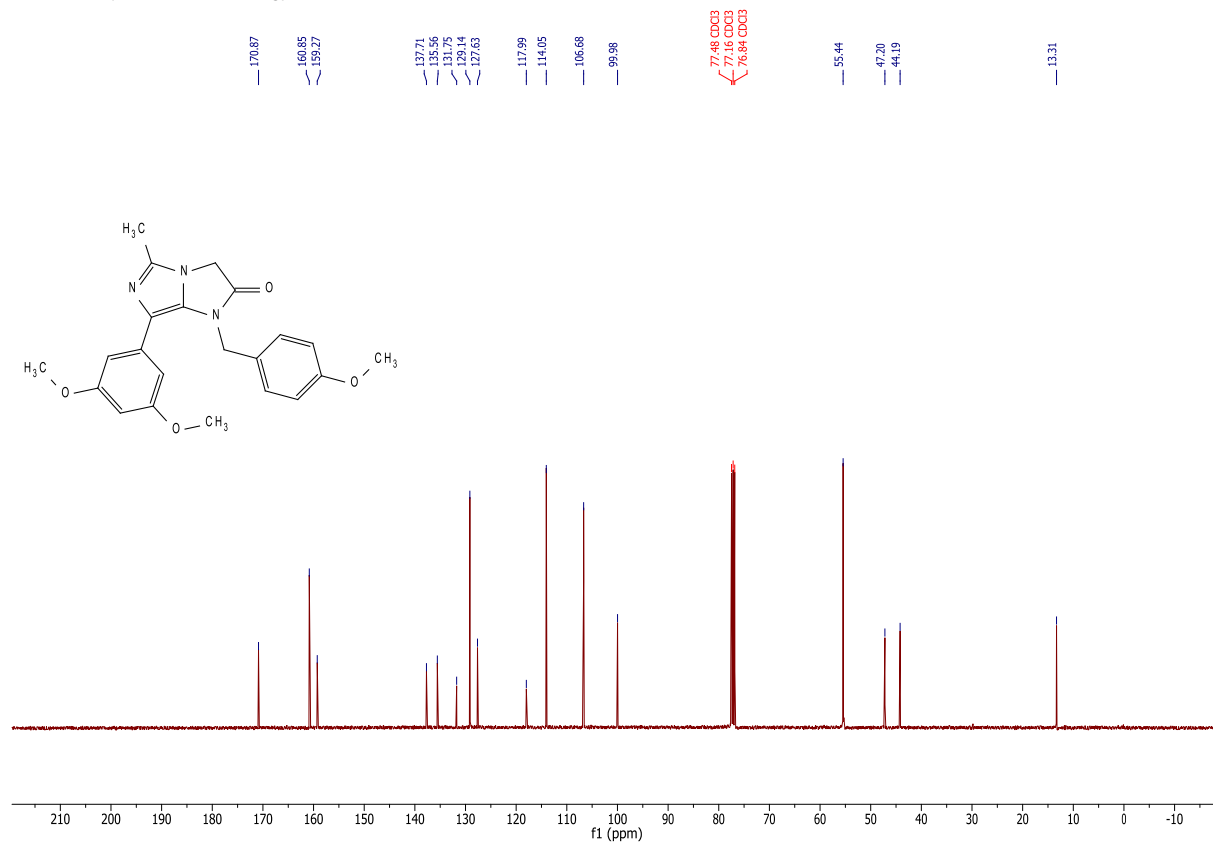


7-(3,5-Dimethoxyphenyl)-1-(4-methoxybenzyl)-5-methyl-1H-imidazo[1,5-a]imidazol-2(3H)-one (9).

^1H NMR (400 MHz, CDCl_3): δ

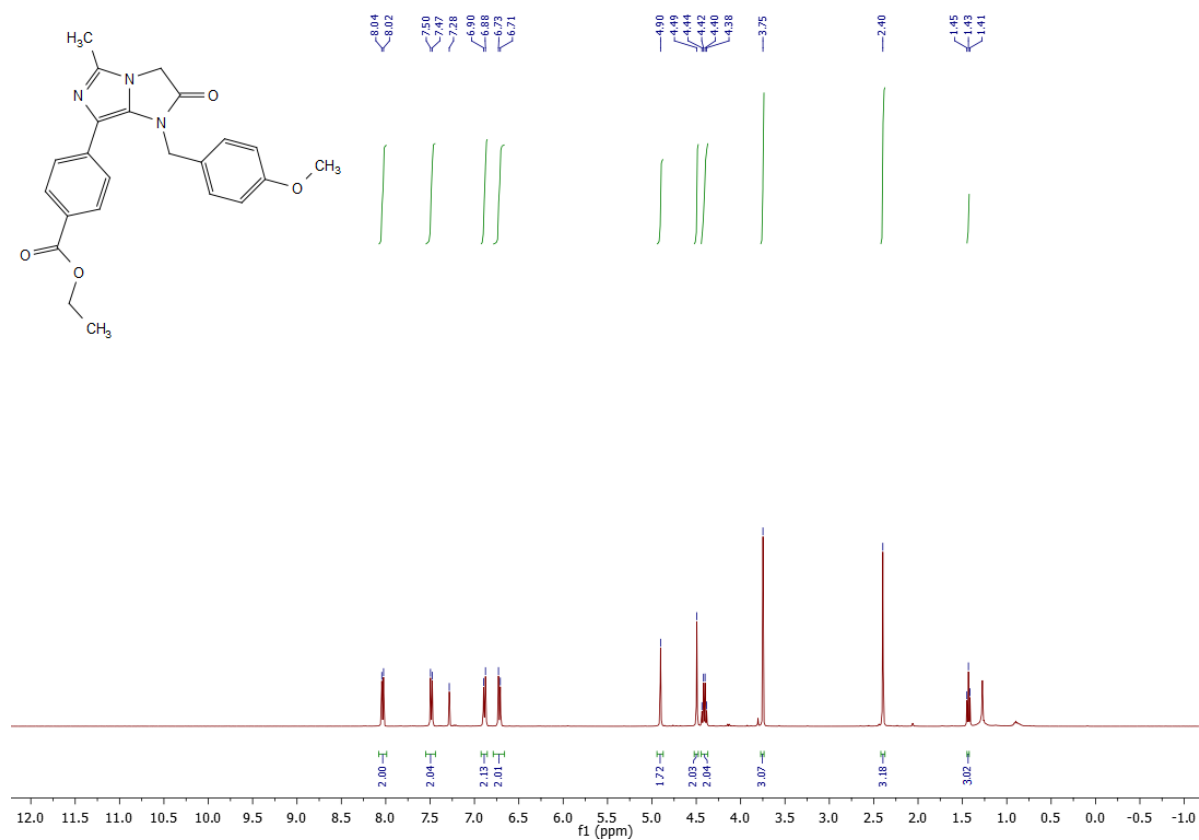


^{13}C NMR (101 MHz, CDCl_3): δ

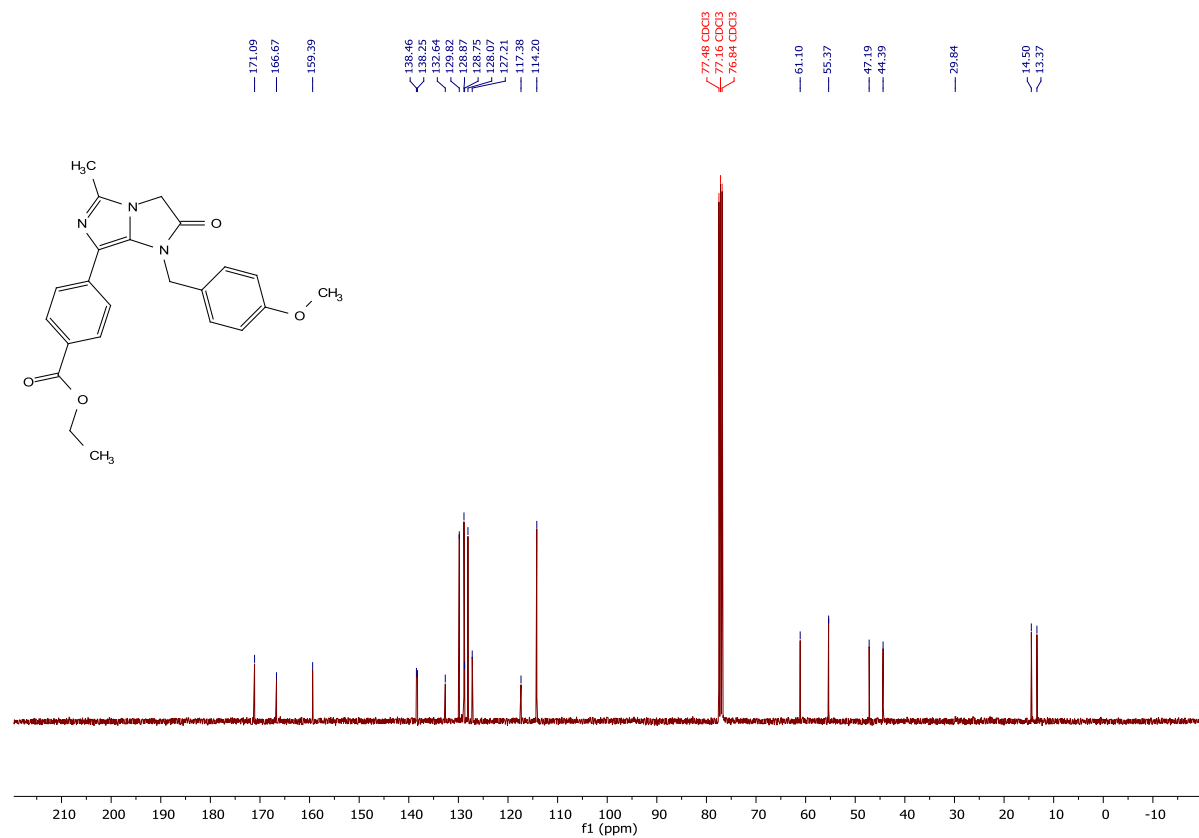


Ethyl 4-(1-(4-methoxybenzyl)-5-methyl-2-oxo-2,3-dihydro-1H-imidazo[1,5-a]imidazol-7-yl)benzoate (10).

^1H NMR (400 MHz, CDCl_3): δ

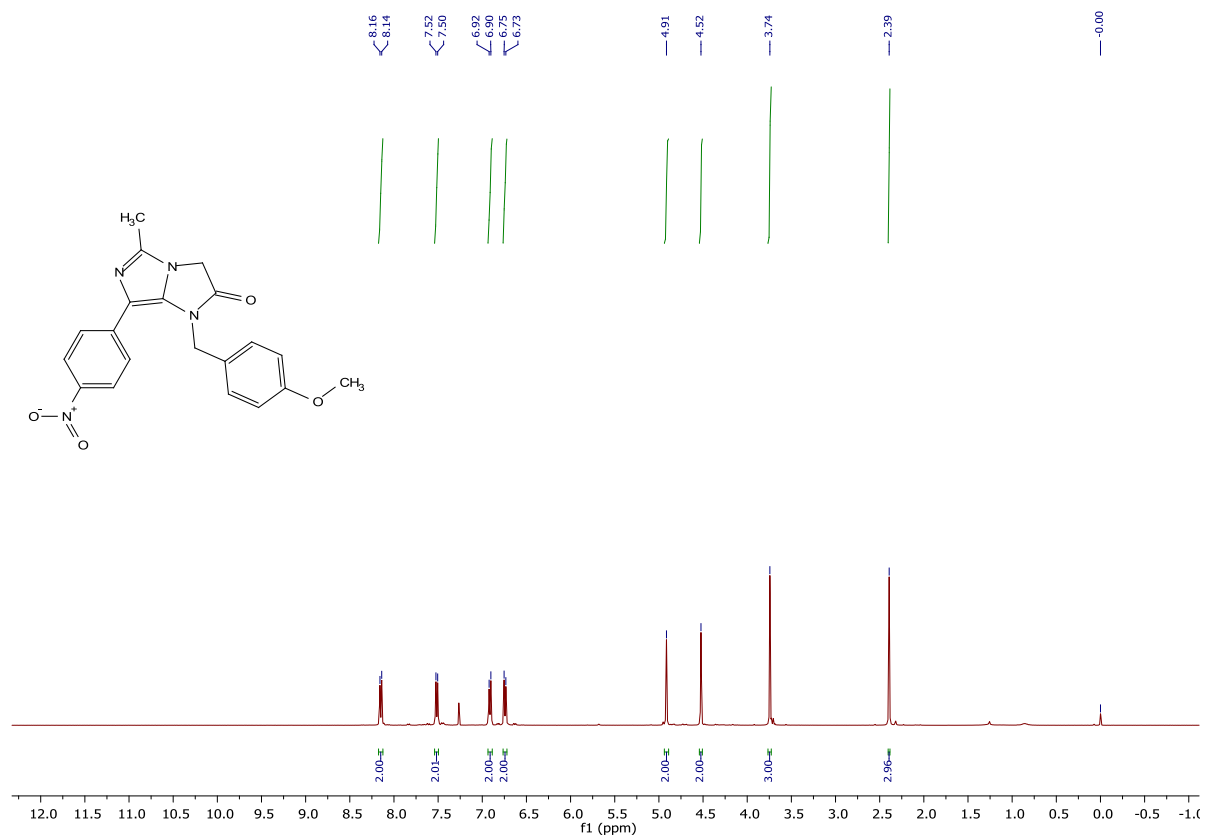


^{13}C NMR (101 MHz, CDCl_3): δ

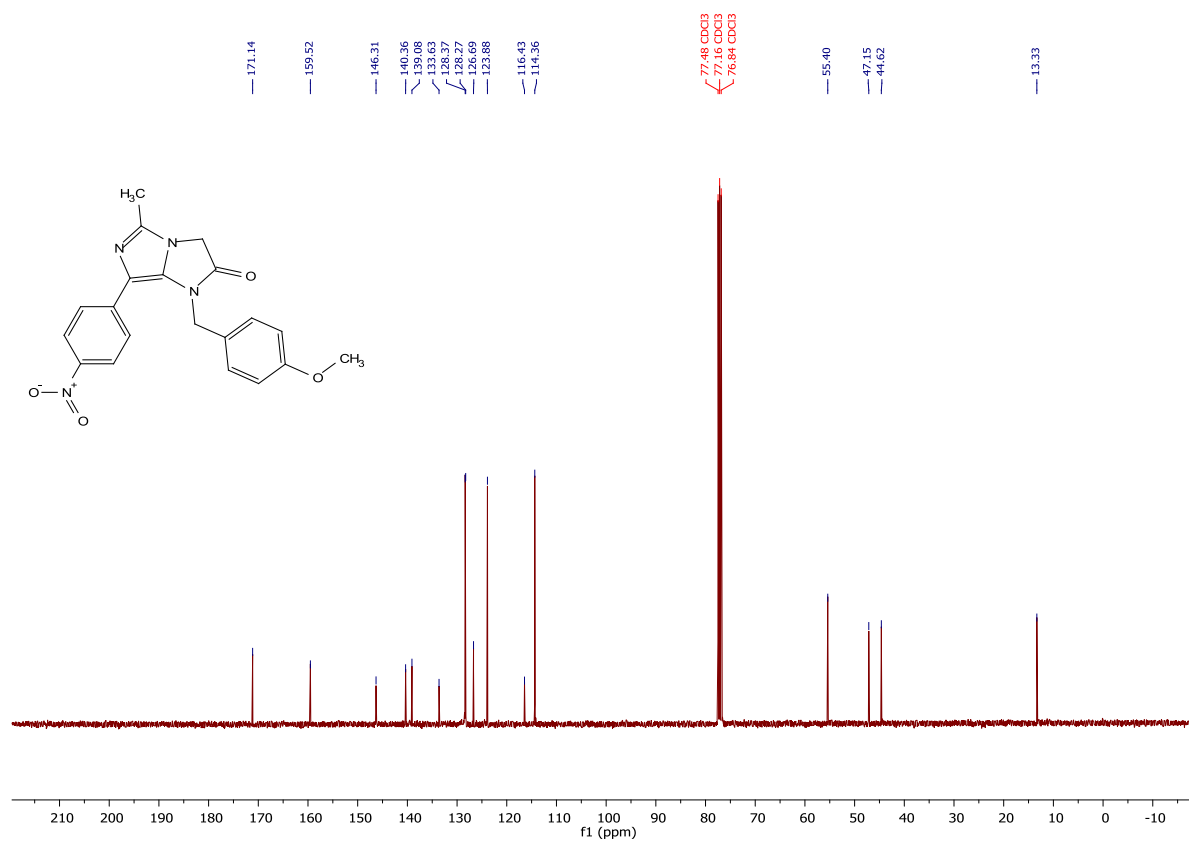


1-(4-Methoxybenzyl)-5-methyl-7-(4-nitrophenyl)-1H-imidazo[1,5-a]imidazol-2(3H)-one (11).

^1H NMR (400 MHz, CDCl_3): δ

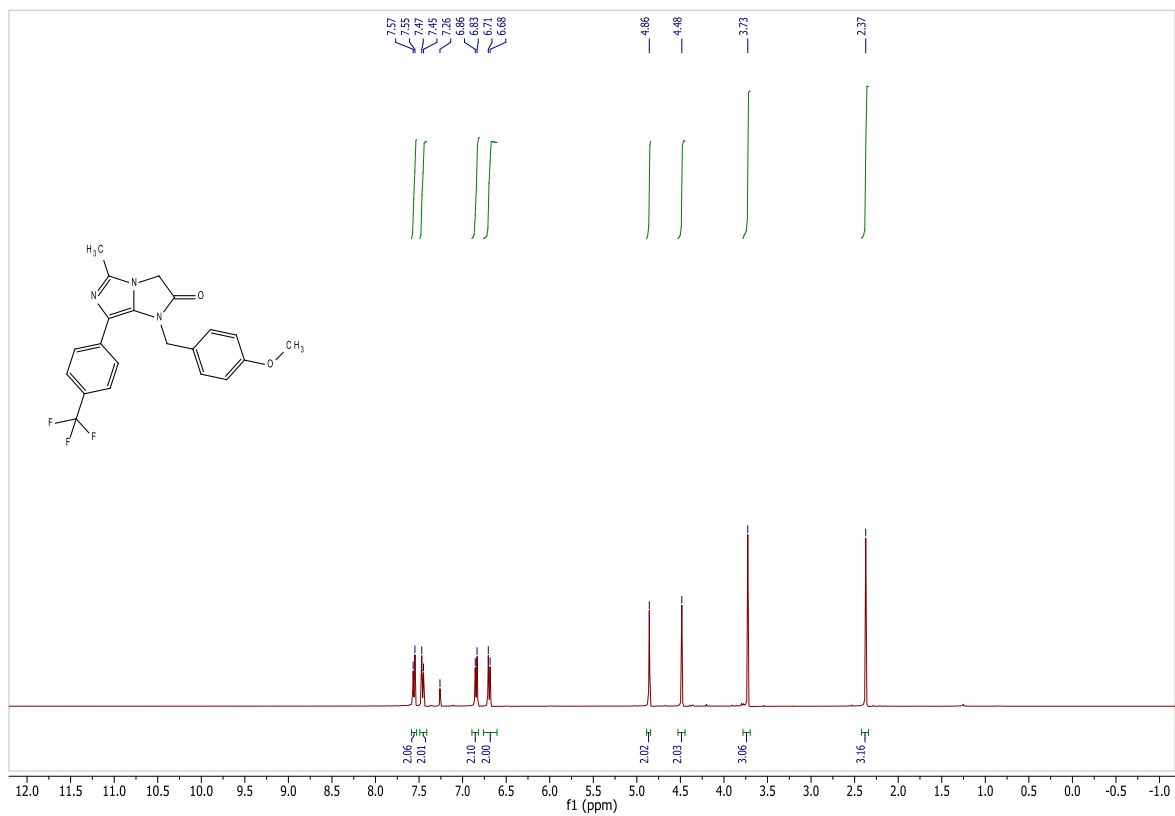


^{13}C NMR (101 MHz, CDCl_3): δ

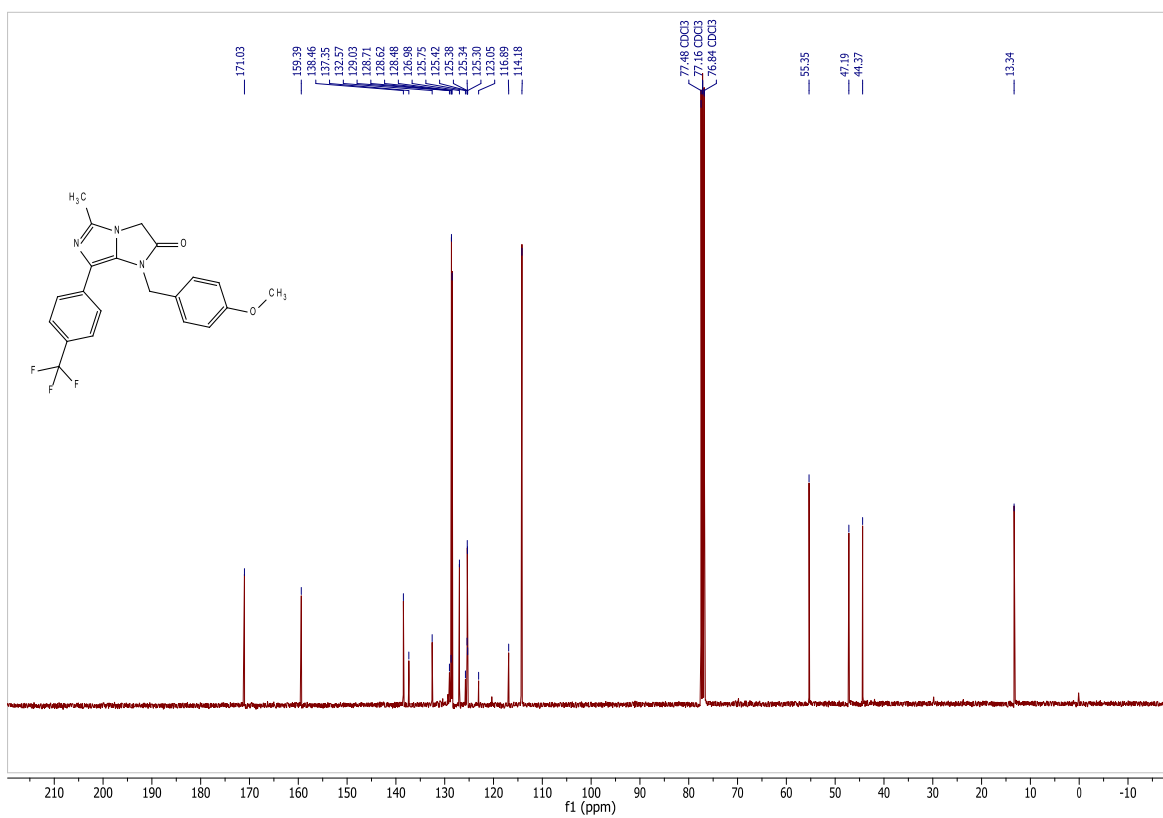


1-(4-Methoxybenzyl)-5-methyl-7-(4-(trifluoromethyl)phenyl)-1H-imidazo[1,5-a]imidazol-2(3H)-one (12).

^1H NMR (400 MHz, CDCl_3): δ

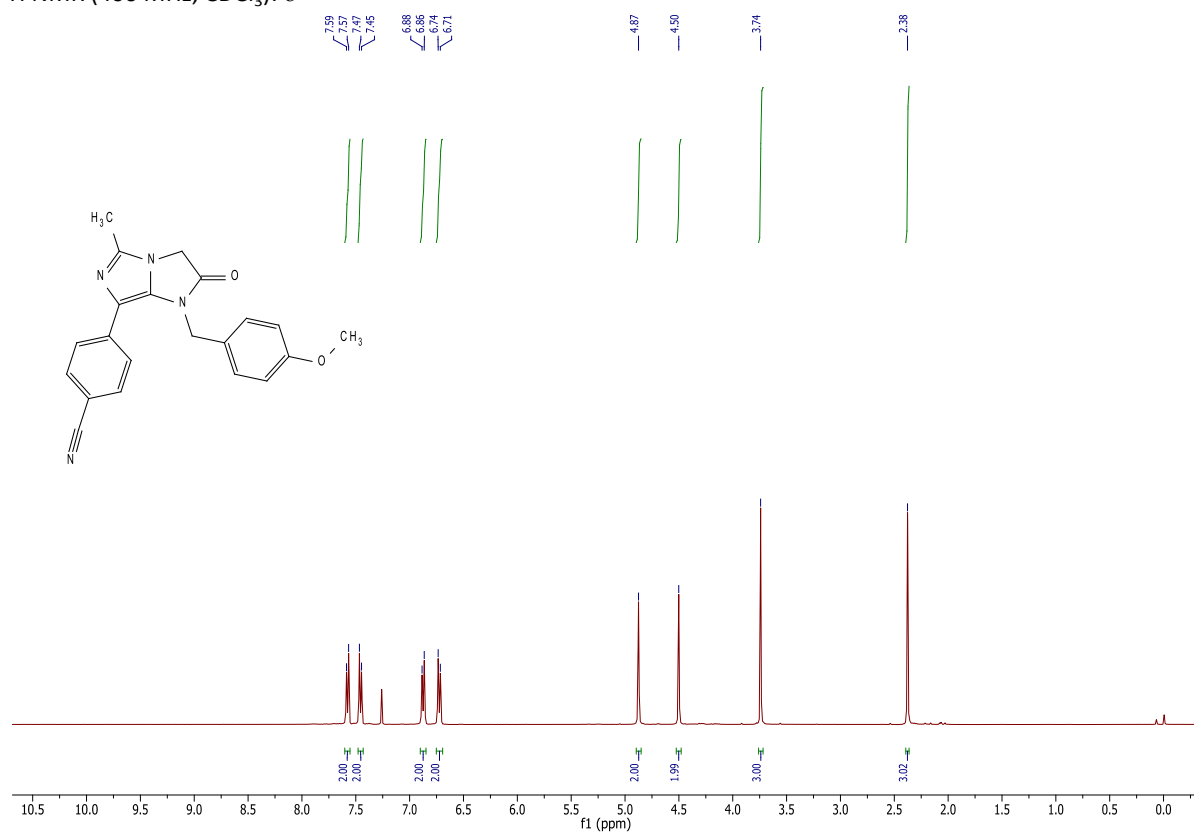


^{13}C NMR (101 MHz, CDCl_3): δ

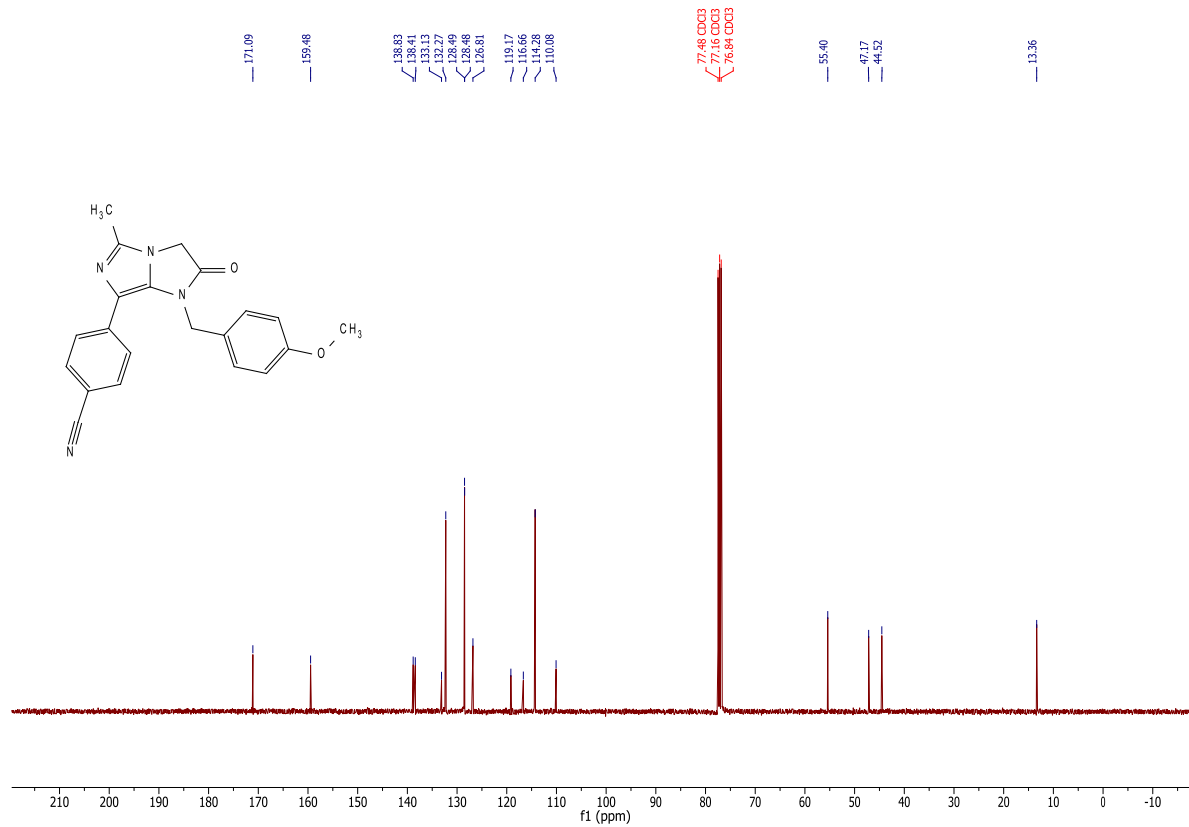


4-(1-(4-Methoxybenzyl)-5-methyl-2-oxo-2,3-dihydro-1H-imidazo[1,5-a]imidazol-7-yl)benzonitrile (13).

^1H NMR (400 MHz, CDCl_3): δ

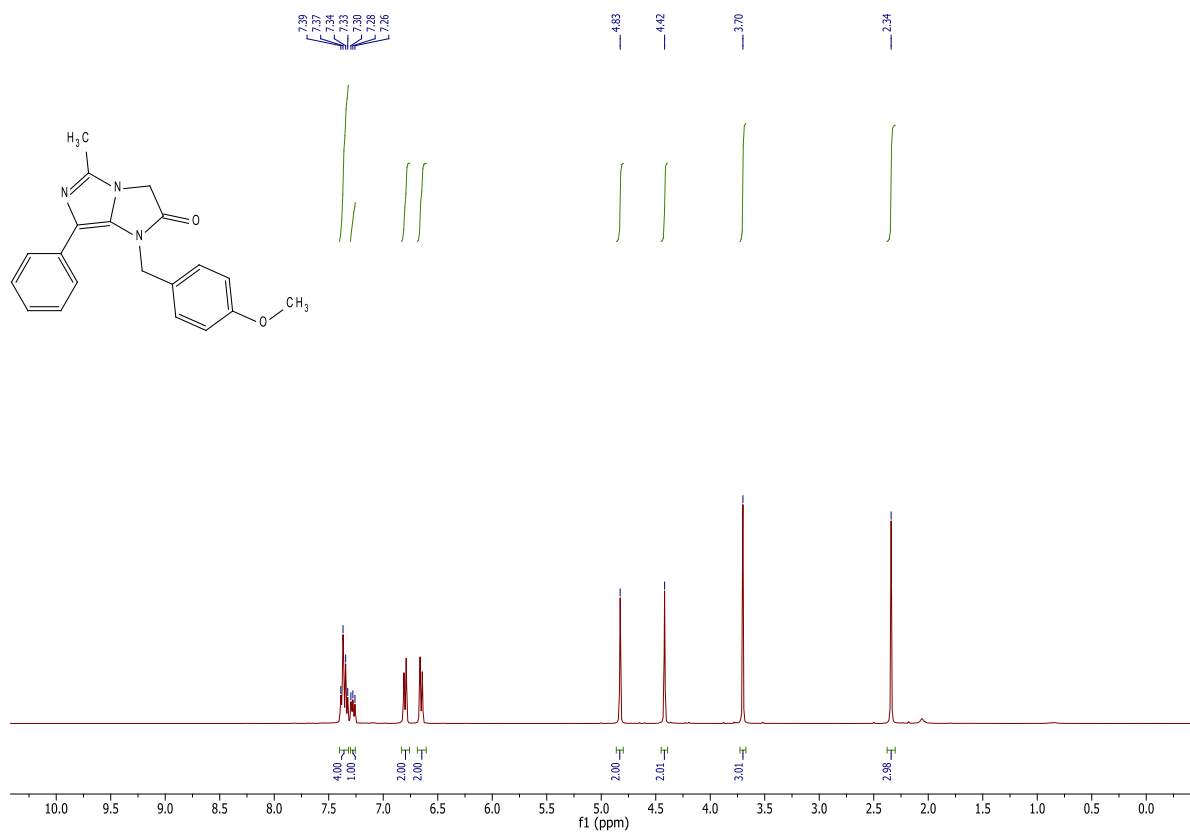


^{13}C NMR (101 MHz, CDCl_3): δ

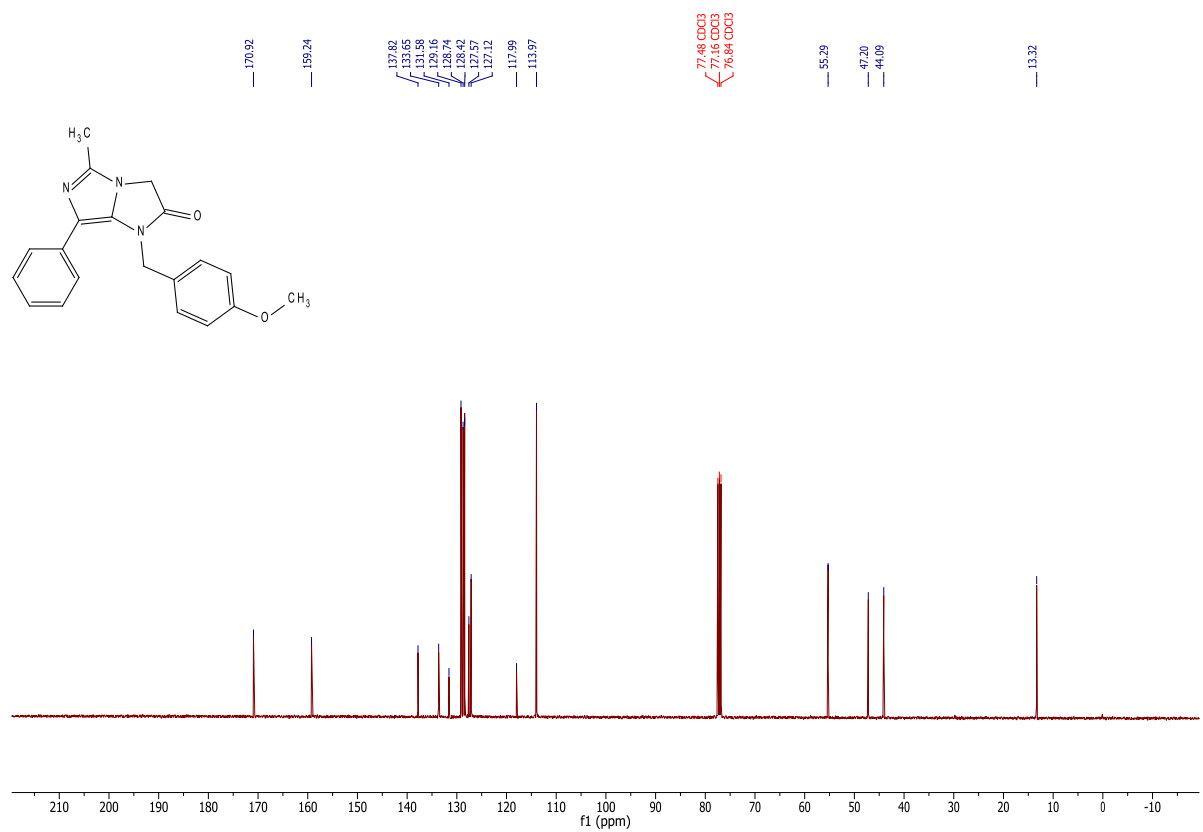


1-(4-Methoxybenzyl)-5-methyl-7-phenyl-1H-imidazo[1,5-a]imidazol-2(3H)-one (14).

^1H NMR (400 MHz, CDCl_3): δ

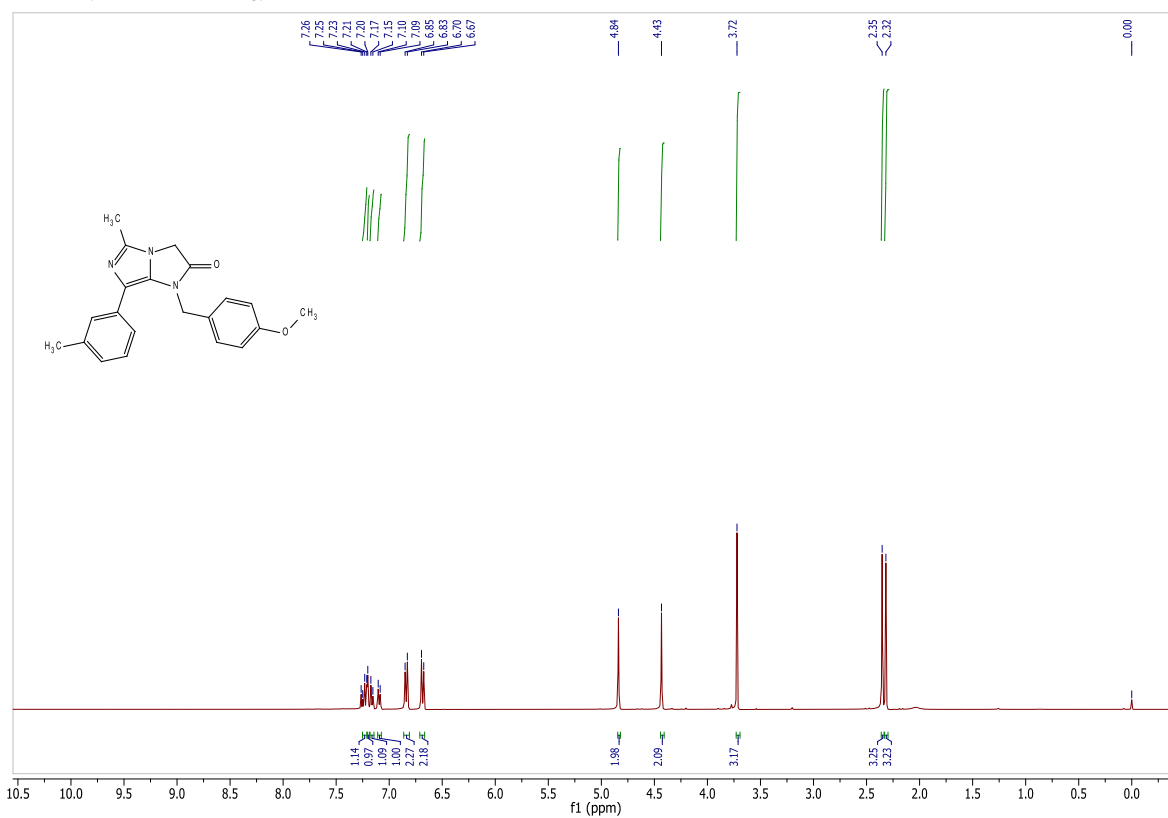


^{13}C NMR (101 MHz, CDCl_3): δ

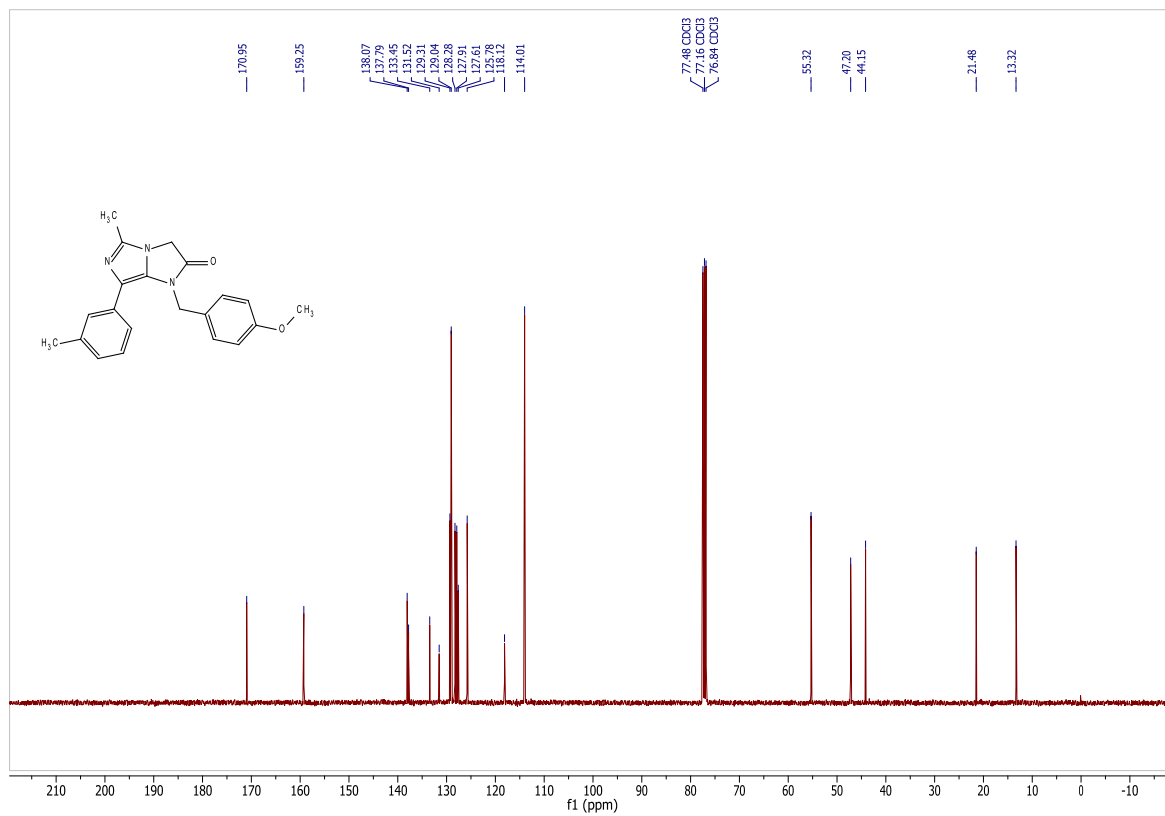


1-(4-Methoxybenzyl)-5-methyl-7-(m-tolyl)-1H-imidazo[1,5-a]imidazol-2(3H)-one (15).

^1H NMR (400 MHz, CDCl_3): δ

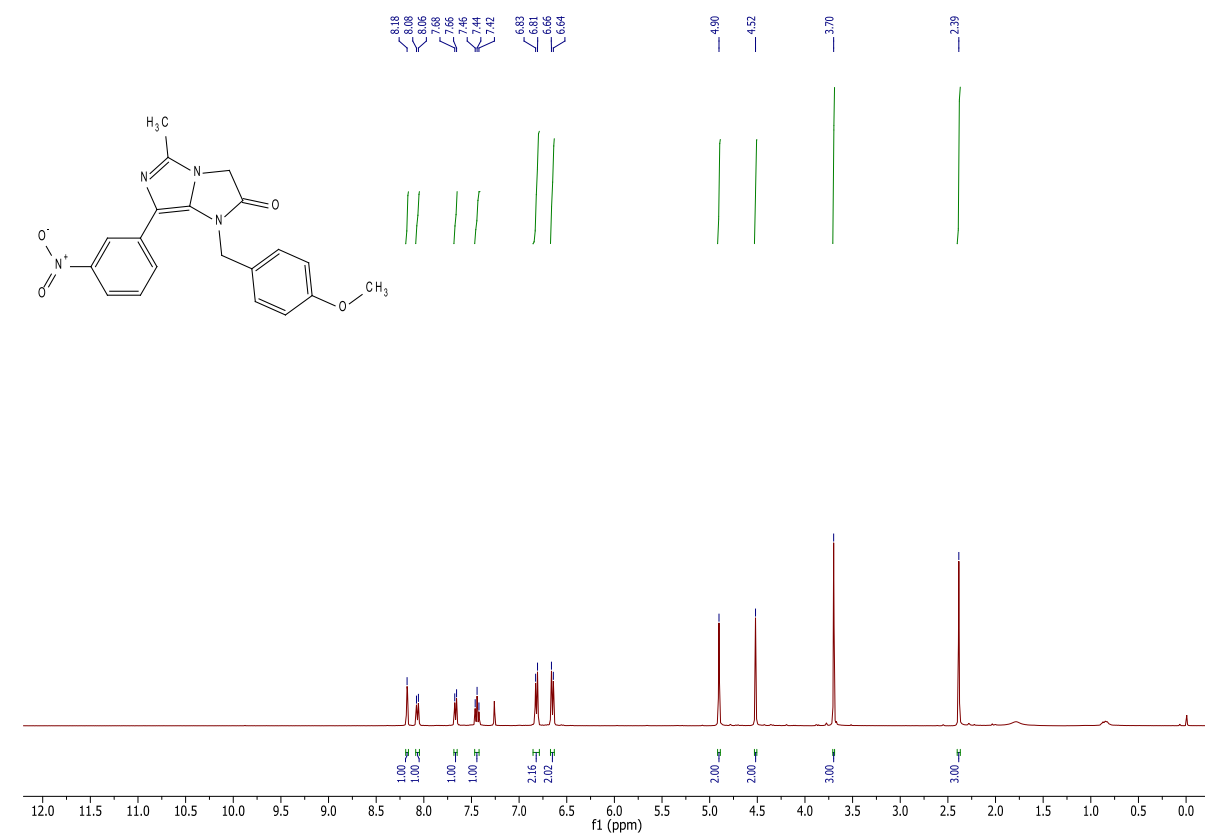


^{13}C NMR (101 MHz, CDCl_3): δ

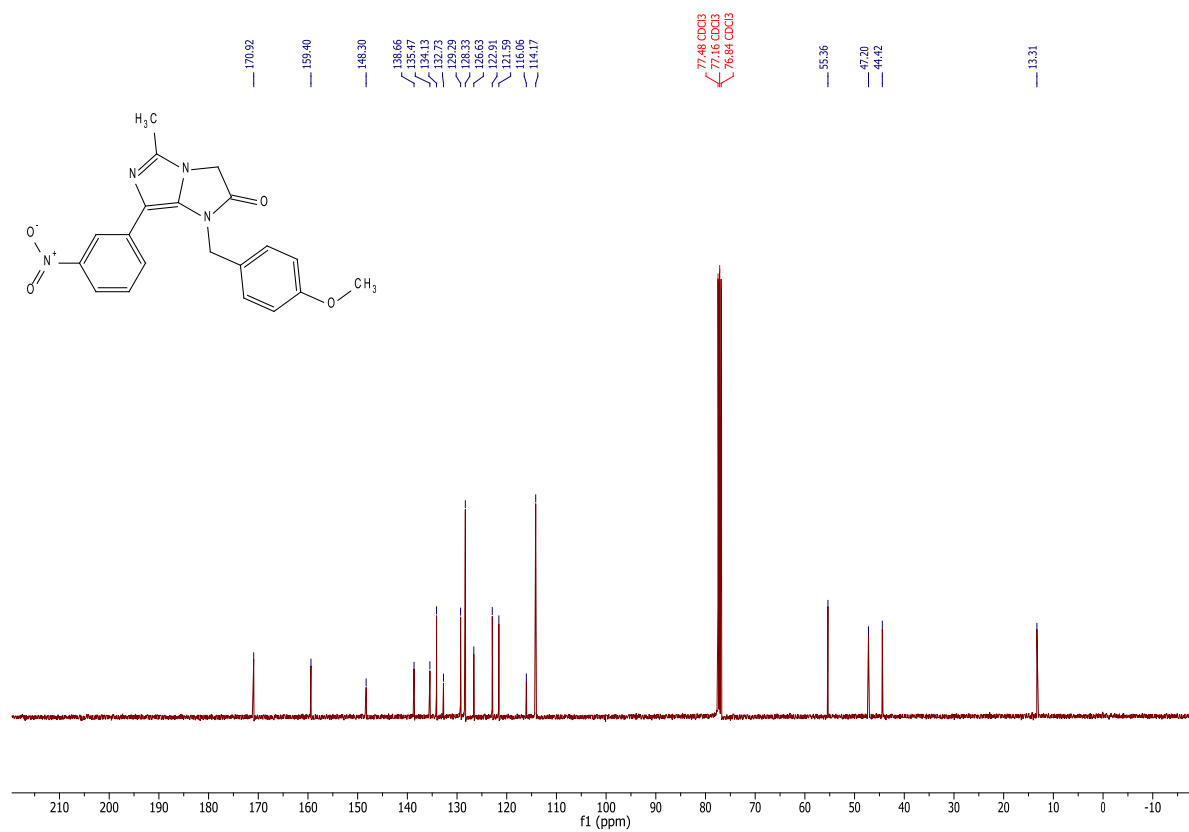


1-(4-Methoxybenzyl)-5-methyl-7-(3-nitrophenyl)-1H-imidazo[1,5-a]imidazol-2(3H)-one (16).

^1H NMR (400 MHz, CDCl_3): δ

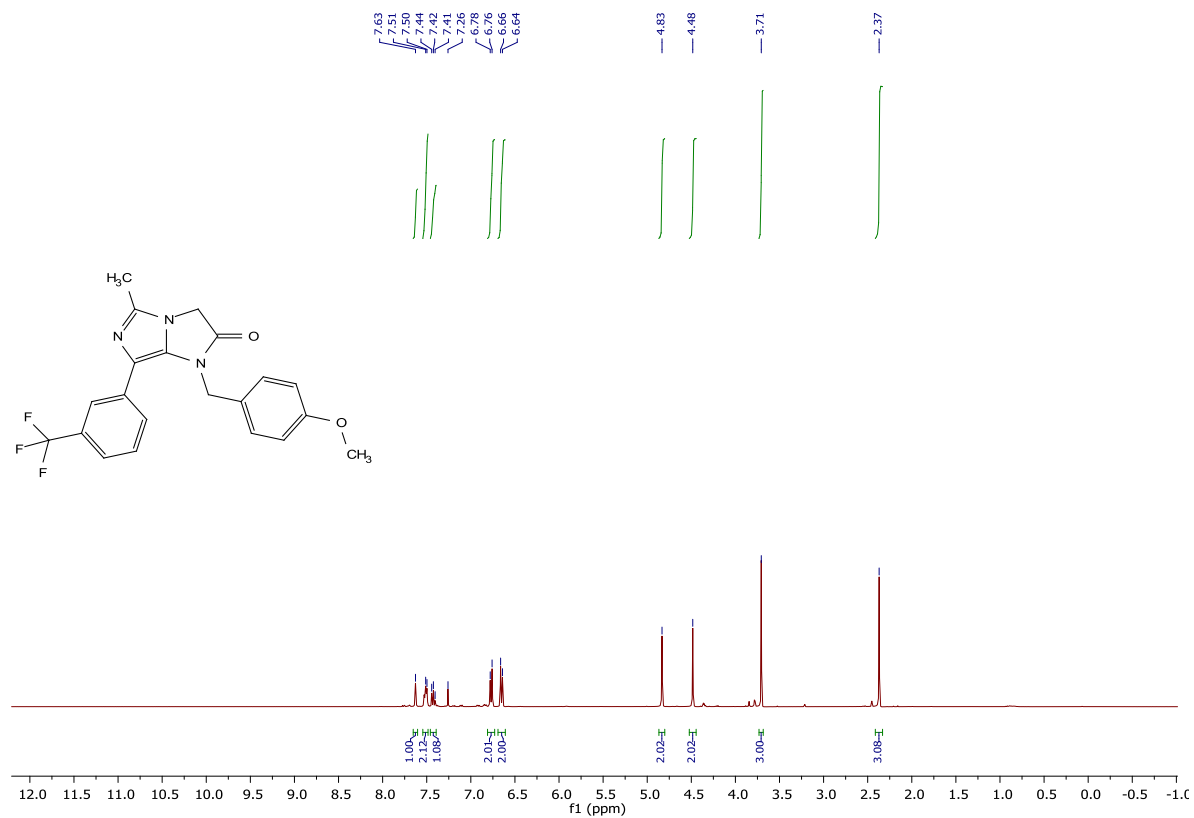


^{13}C NMR (101 MHz, CDCl_3): δ

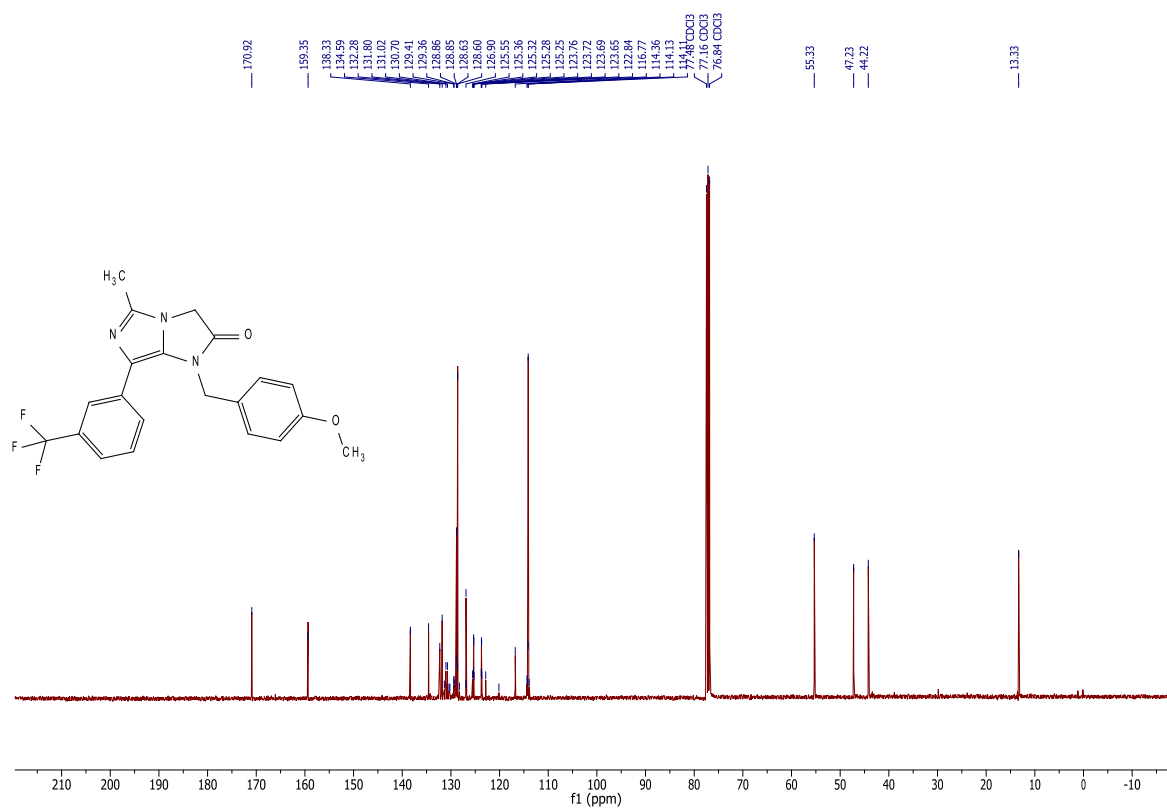


1-(4-Methoxybenzyl)-5-methyl-7-(3-(trifluoromethyl)phenyl)-1H-imidazo[1,5-a]imidazol-2(3H)-one (17).

^1H NMR (400 MHz, CDCl_3): δ

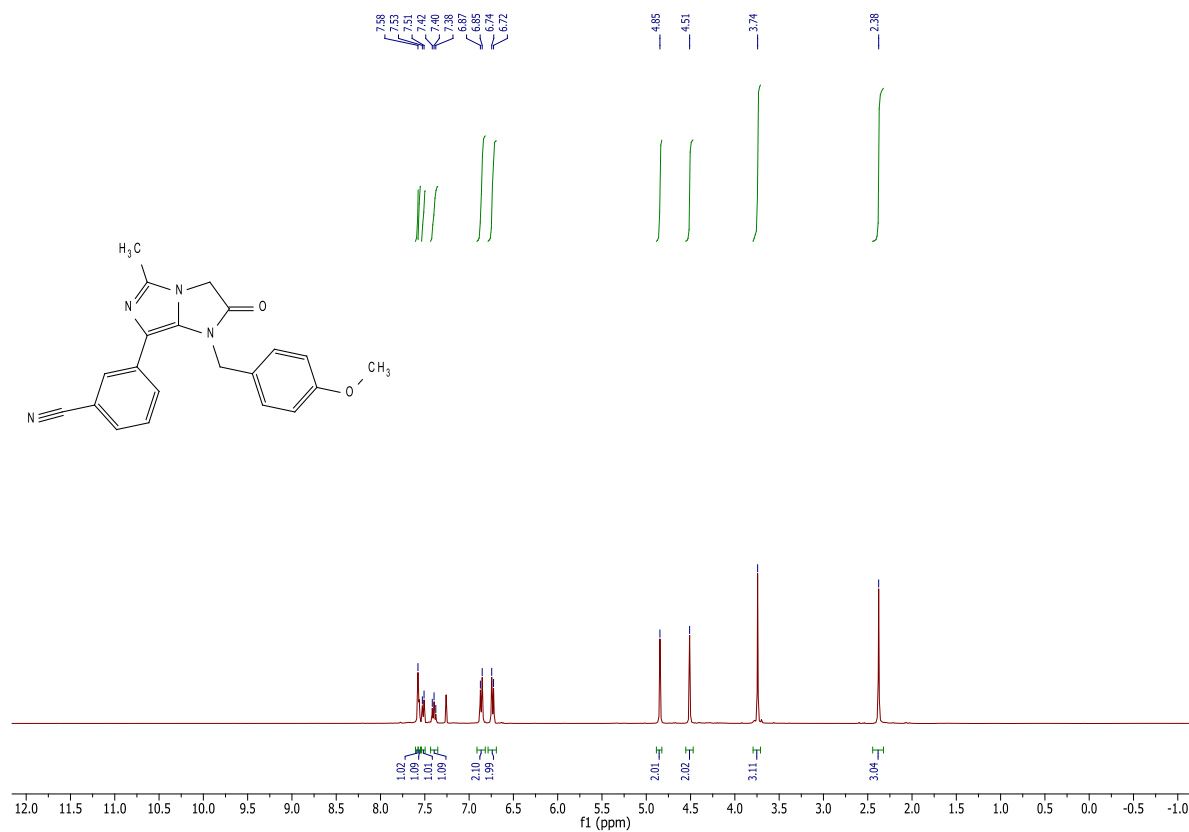


^{13}C NMR (101 MHz, CDCl_3): δ

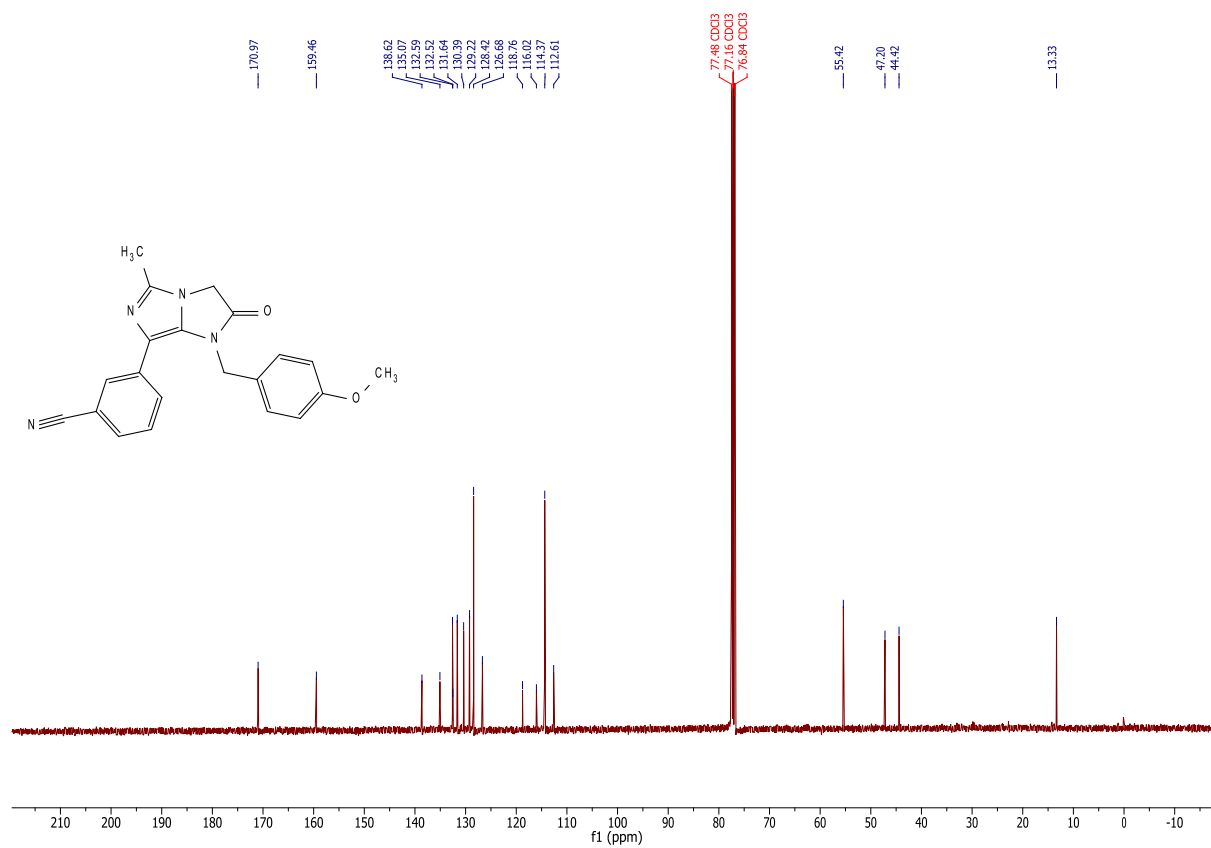


3-(1-(4-Methoxybenzyl)-5-methyl-2-oxo-2,3-dihydro-1H-imidazo[1,5-a]imidazol-7-yl)benzotrile (18).

^1H NMR (400 MHz, CDCl_3): δ

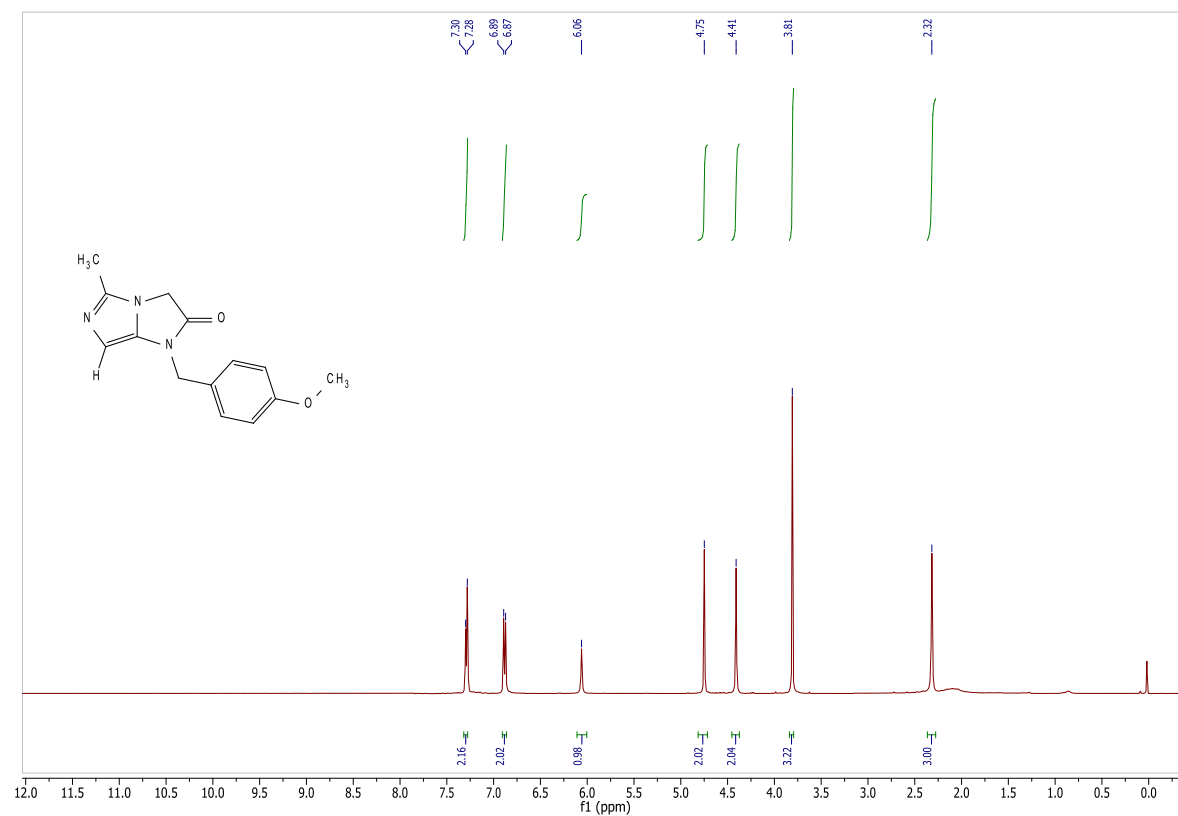


^{13}C NMR (101 MHz, CDCl_3): δ

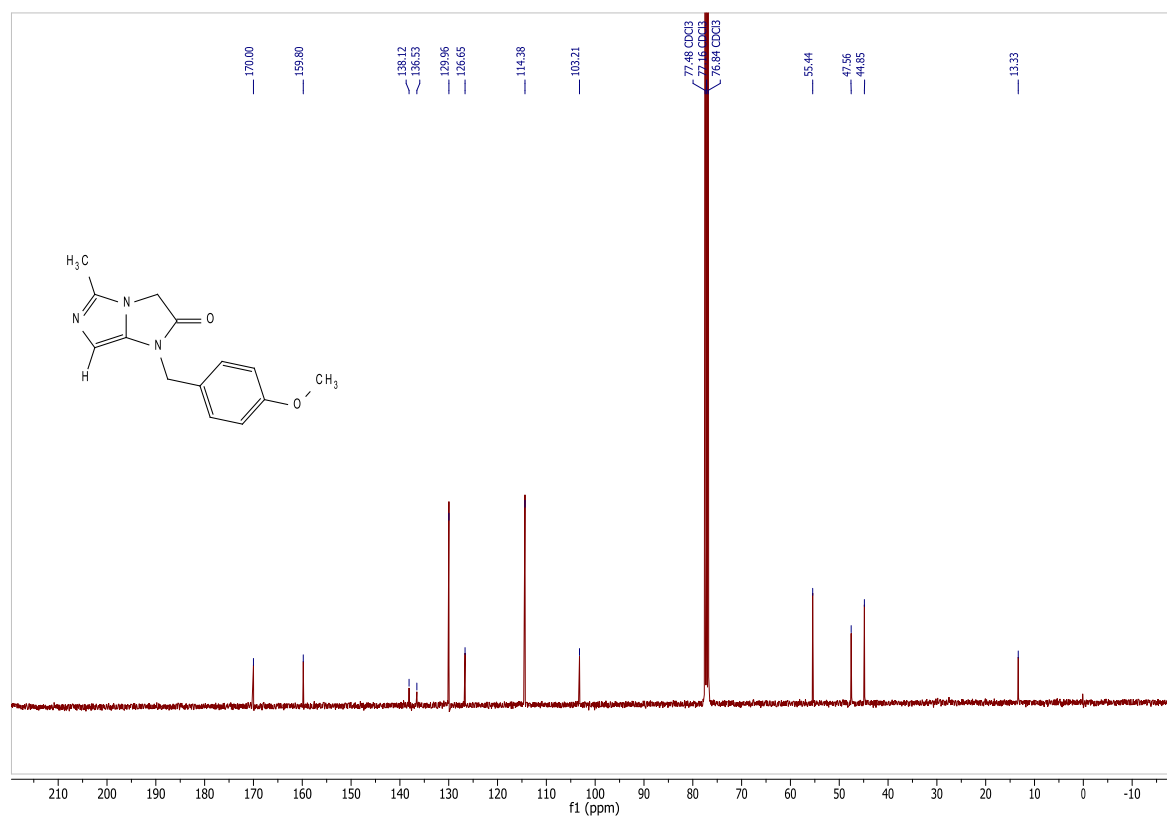


1-(4-Methoxybenzyl)-5-methyl-1H-imidazo[1,5-a]imidazol-2(3H)-one (19).

^1H NMR (400 MHz, CDCl_3): δ

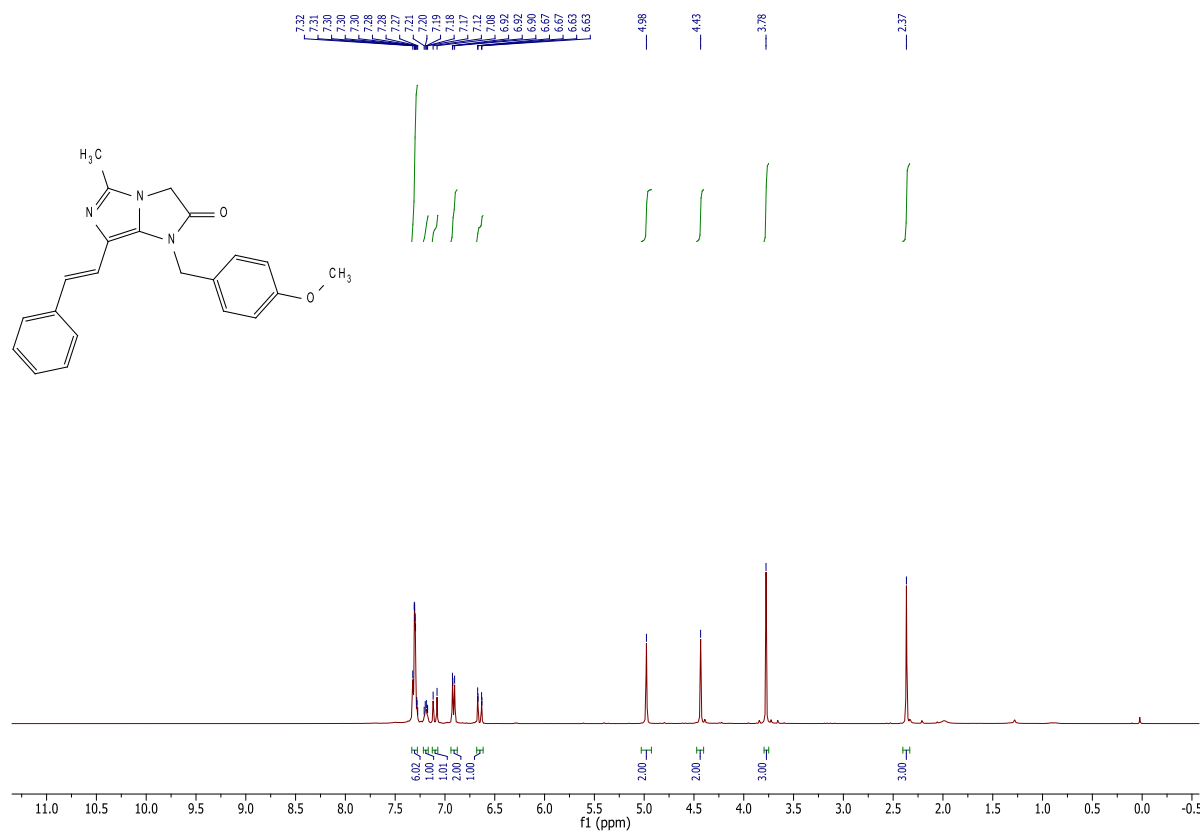


^{13}C NMR (101 MHz, CDCl_3): δ

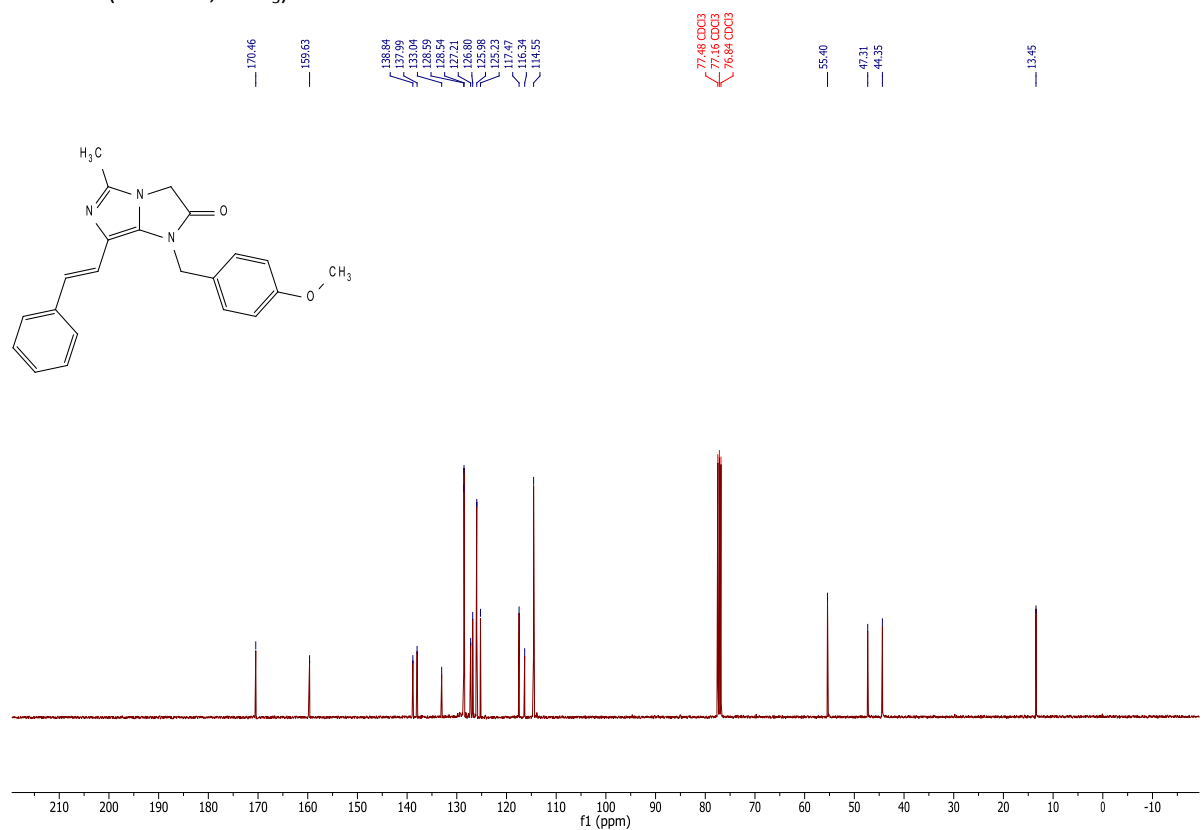


(E)-1-(4-Methoxybenzyl)-5-methyl-7-styryl-1H-imidazo[1,5-a]imidazol-2(3H)-one (20).

^1H NMR (400 MHz, CDCl_3): δ

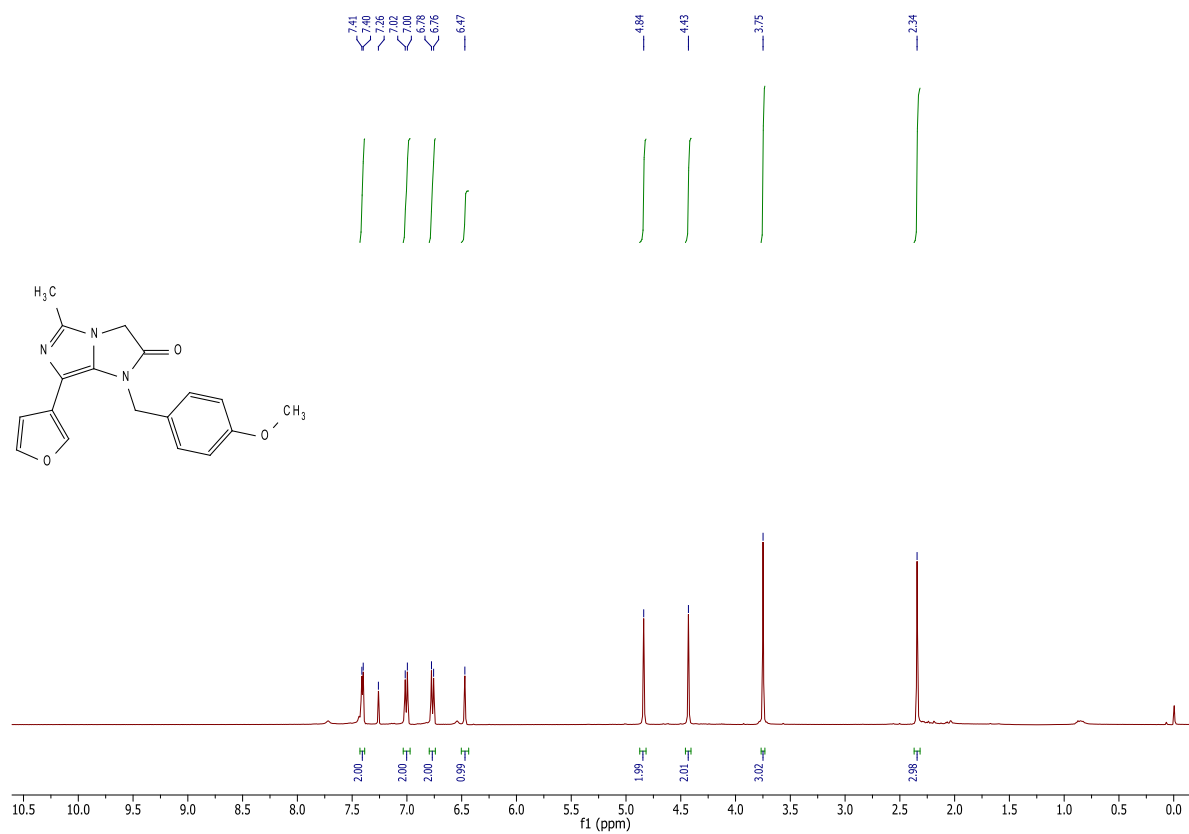


^{13}C NMR (101 MHz, CDCl_3): δ

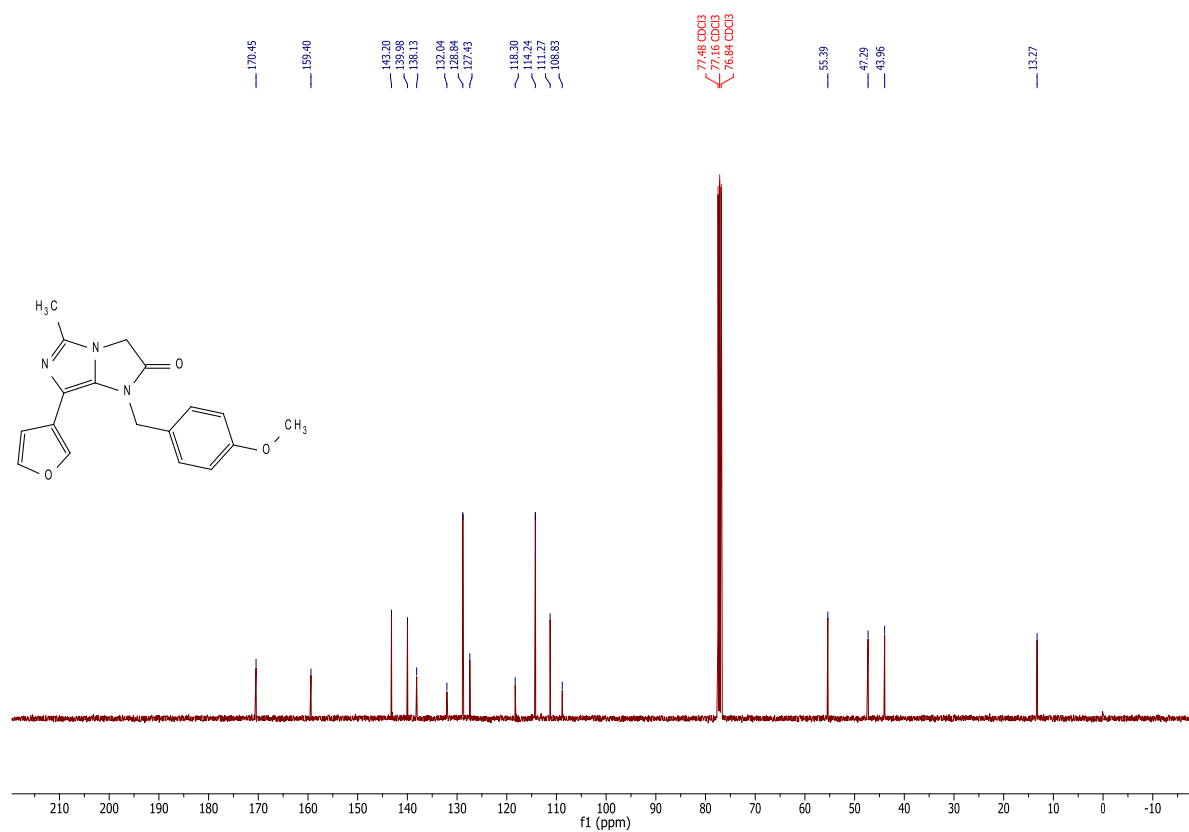


7-(Furan-3-yl)-1-(4-methoxybenzyl)-5-methyl-1H-imidazo[1,5-a]imidazol-2(3H)-one (21).

^1H NMR (400 MHz, CDCl_3): δ

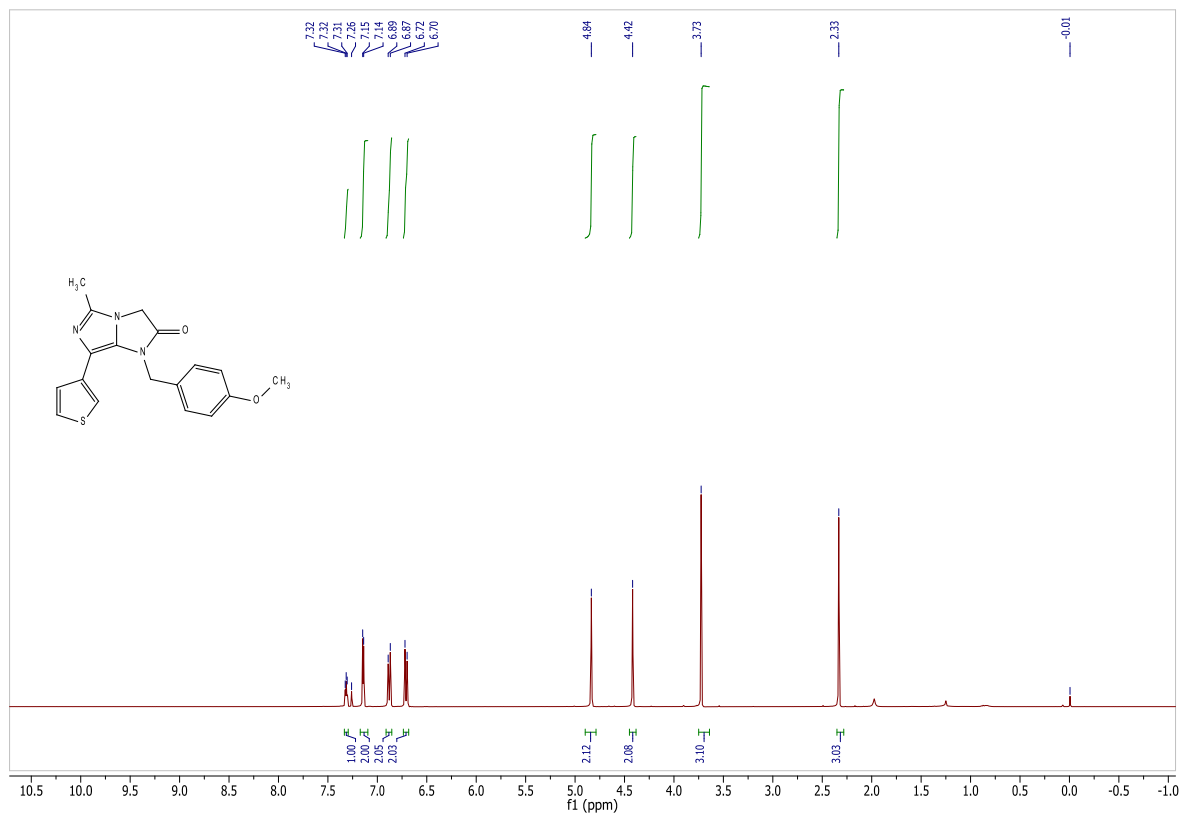


^{13}C NMR (101 MHz, CDCl_3): δ



1-(4-Methoxybenzyl)-5-methyl-7-(thiophen-3-yl)-1H-imidazo[1,5-a]imidazol-2(3H)-one (22).

^1H NMR (400 MHz, CDCl_3): δ



^{13}C NMR (101 MHz, CDCl_3): δ

