

Access and Modulation of Substituted Pyrrolo[3,4-*c*]pyrazole-4,6-(2*H*,5*H*)-diones

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Figure S1: Ethyl 5-hydroxy-1-(p-tolyl)-1H-pyrazole-3-carboxylate (1)

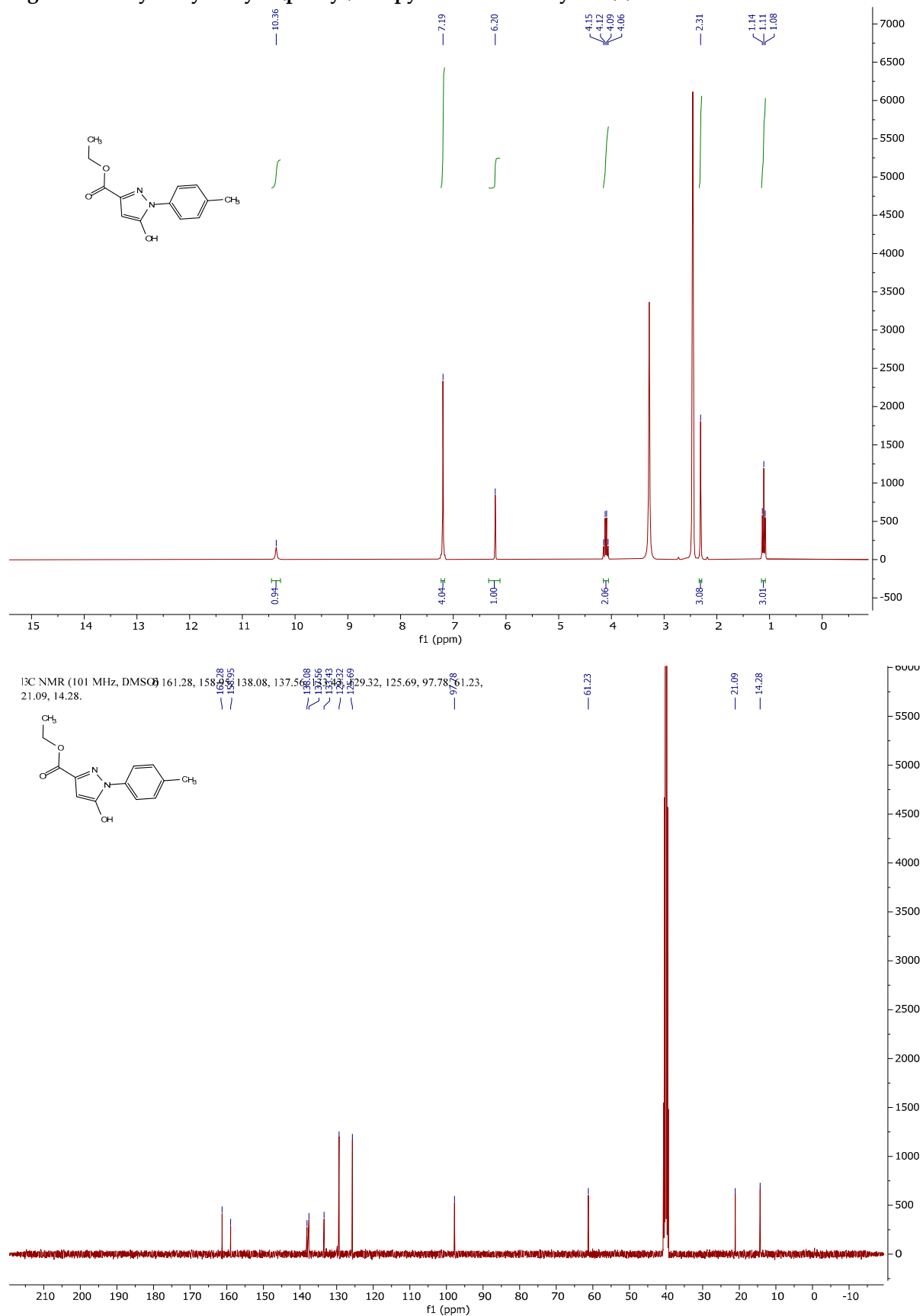


Figure S2: Ethyl 5-hydroxy-1-(4-nitrophenyl)-1H-pyrazole-3-carboxylate (2)

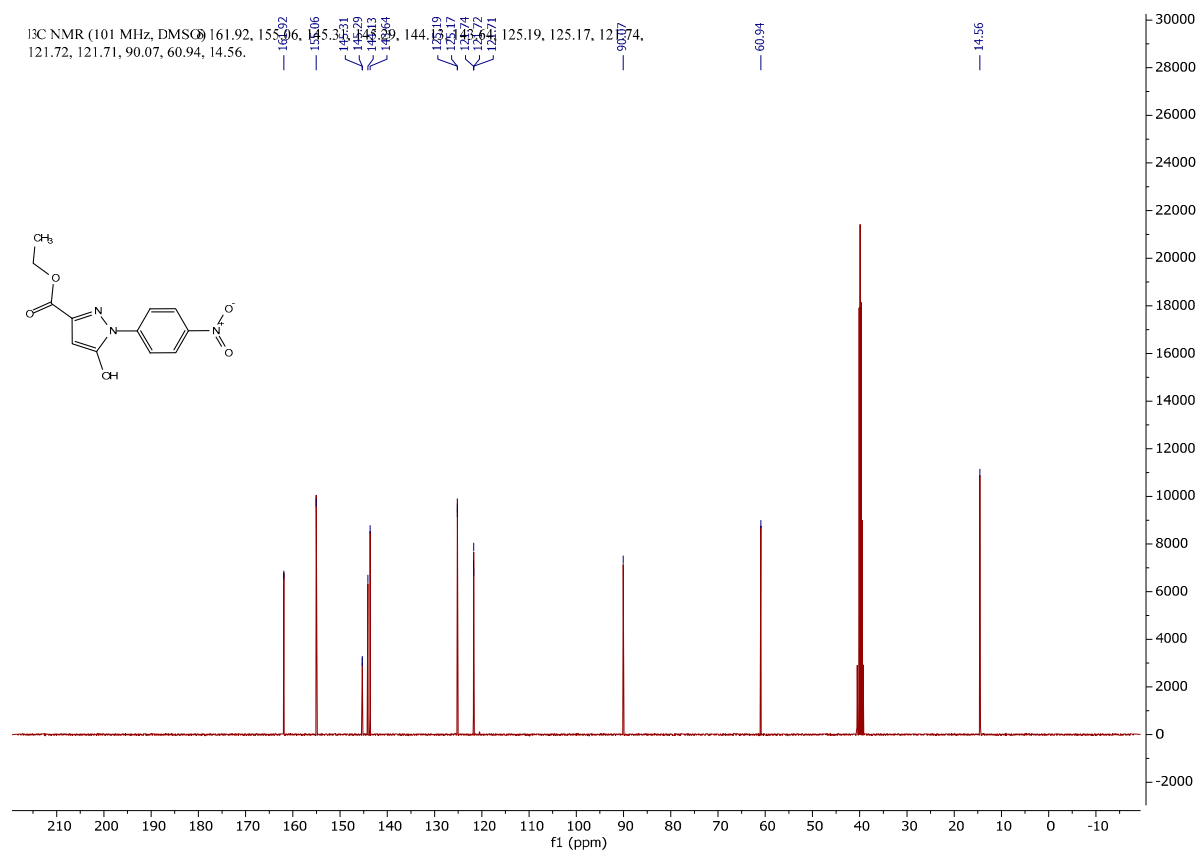
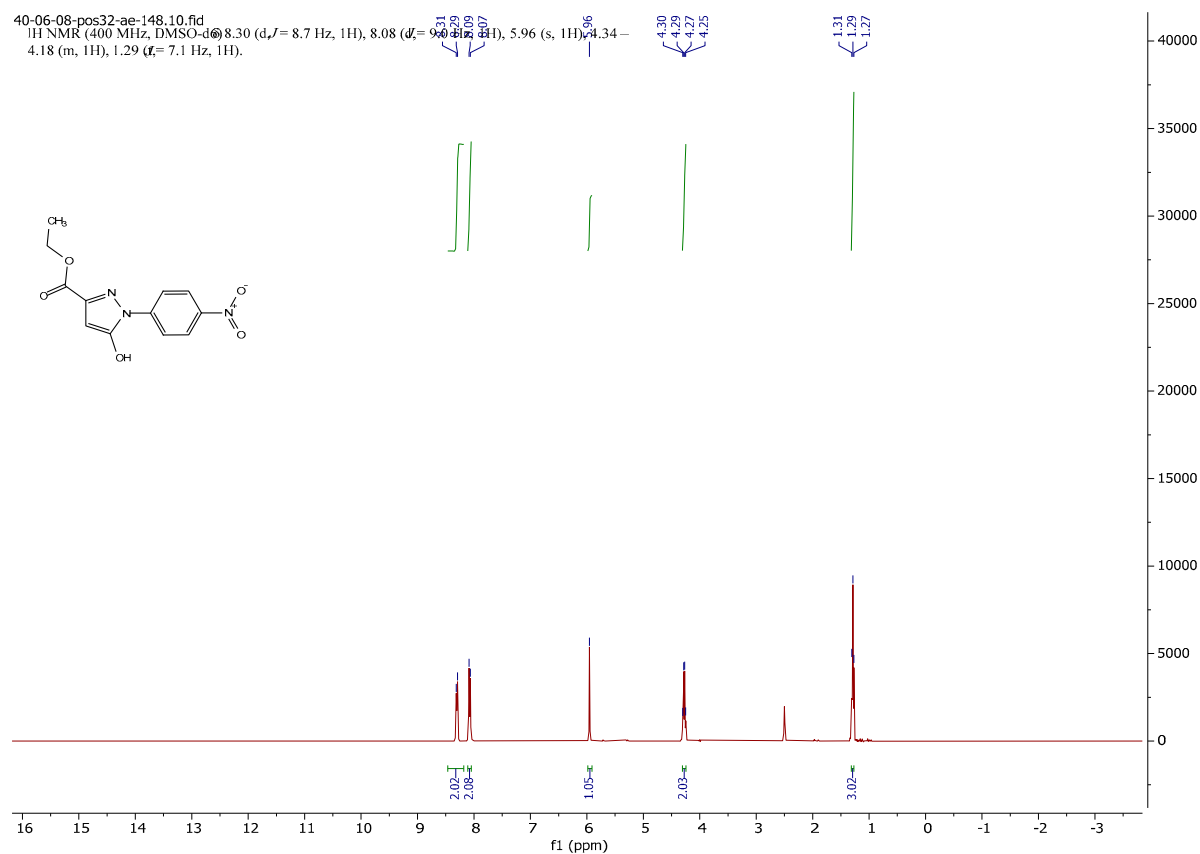


Figure S3: Ethyl 5-chloro-4-formyl-1-(p-tolyl)-1H-pyrazole-3-carboxylate (3)

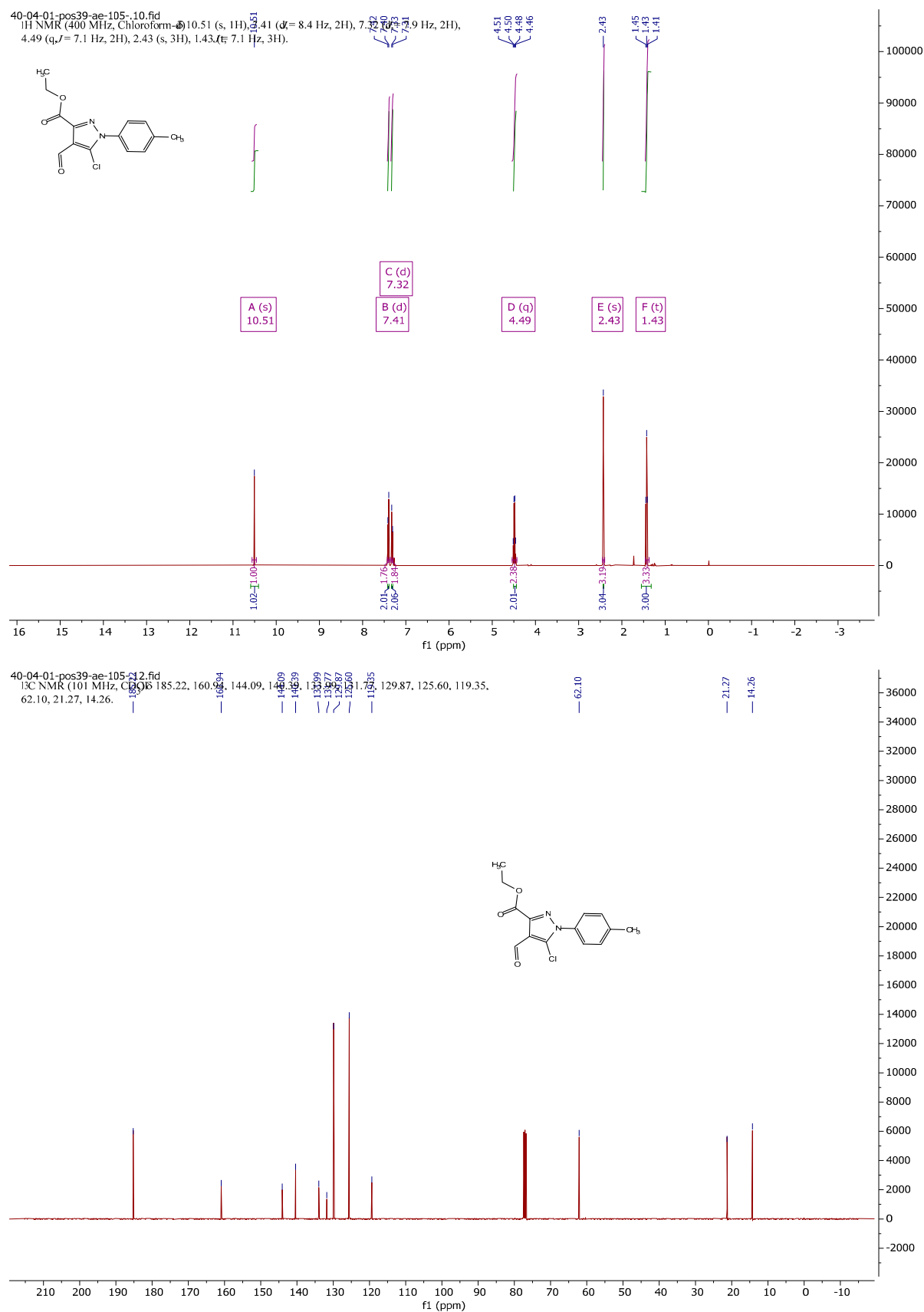


Figure S4: Ethyl 5-chloro-4-formyl-1-(4-nitrophenyl)-1H-pyrazole-3-carboxylate (4)

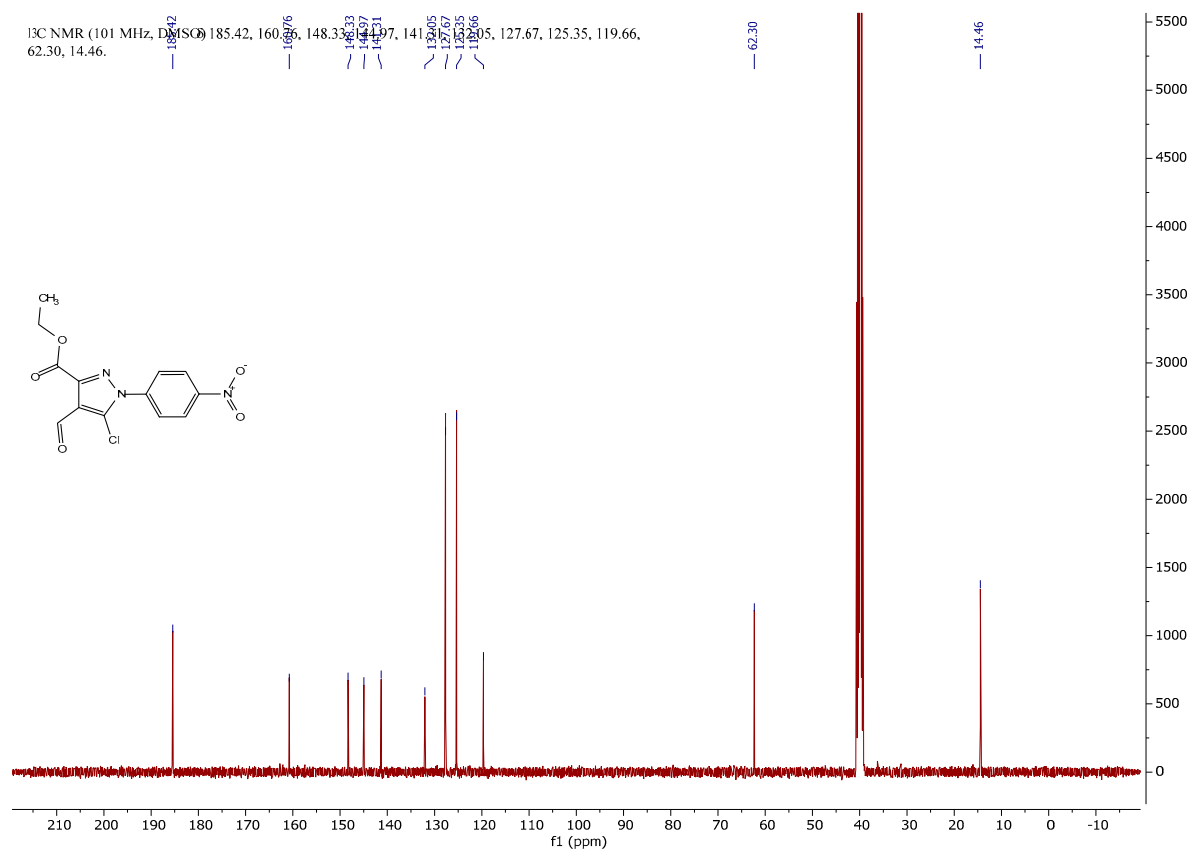
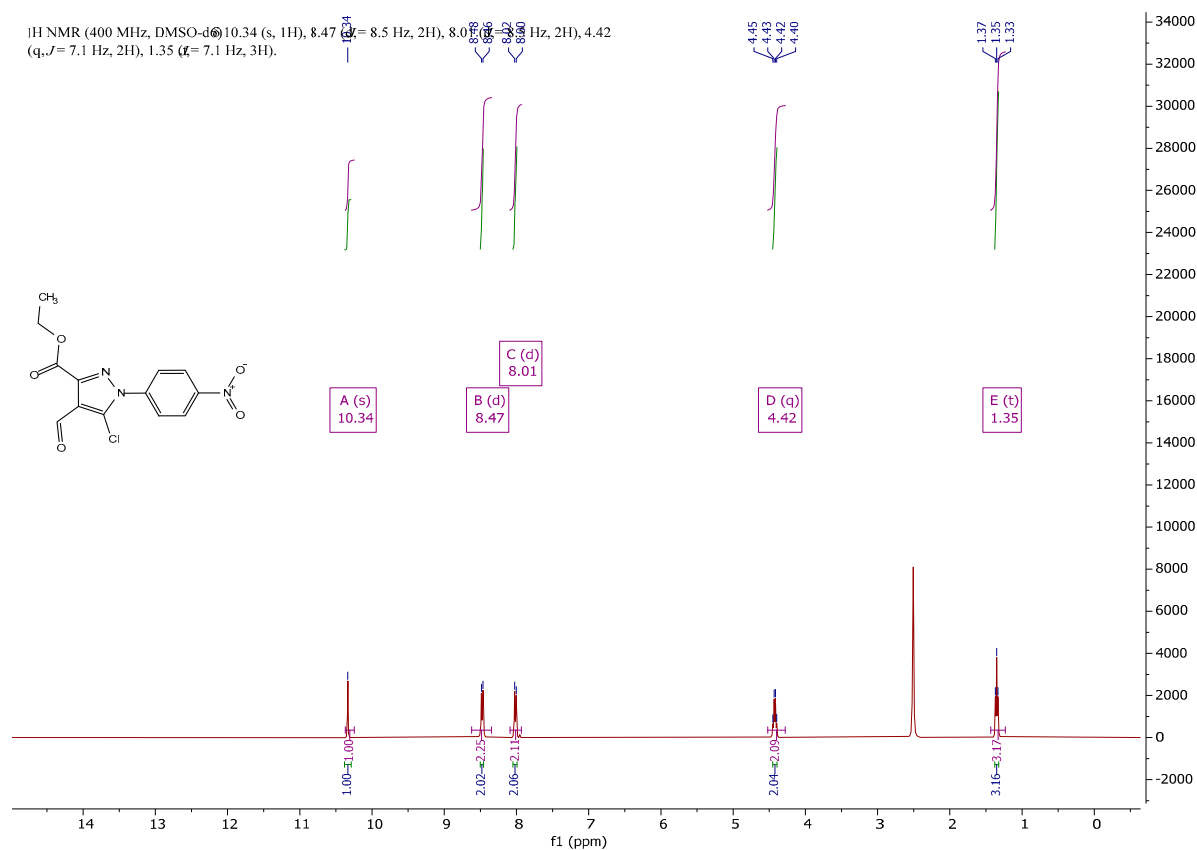


Figure S5: 5-Chloro-3-(ethoxycarbonyl)-1-(p-tolyl)-1H-pyrazole-4-carboxylic acid (5)

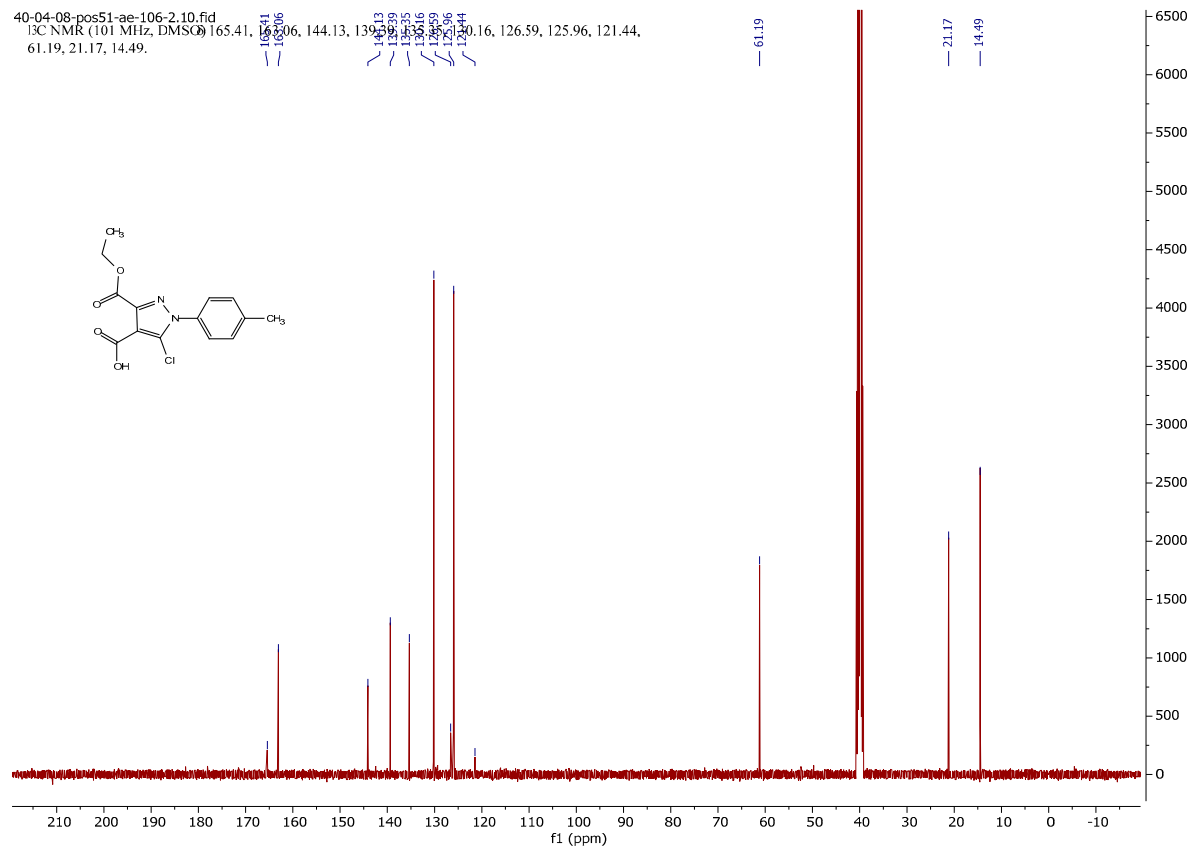
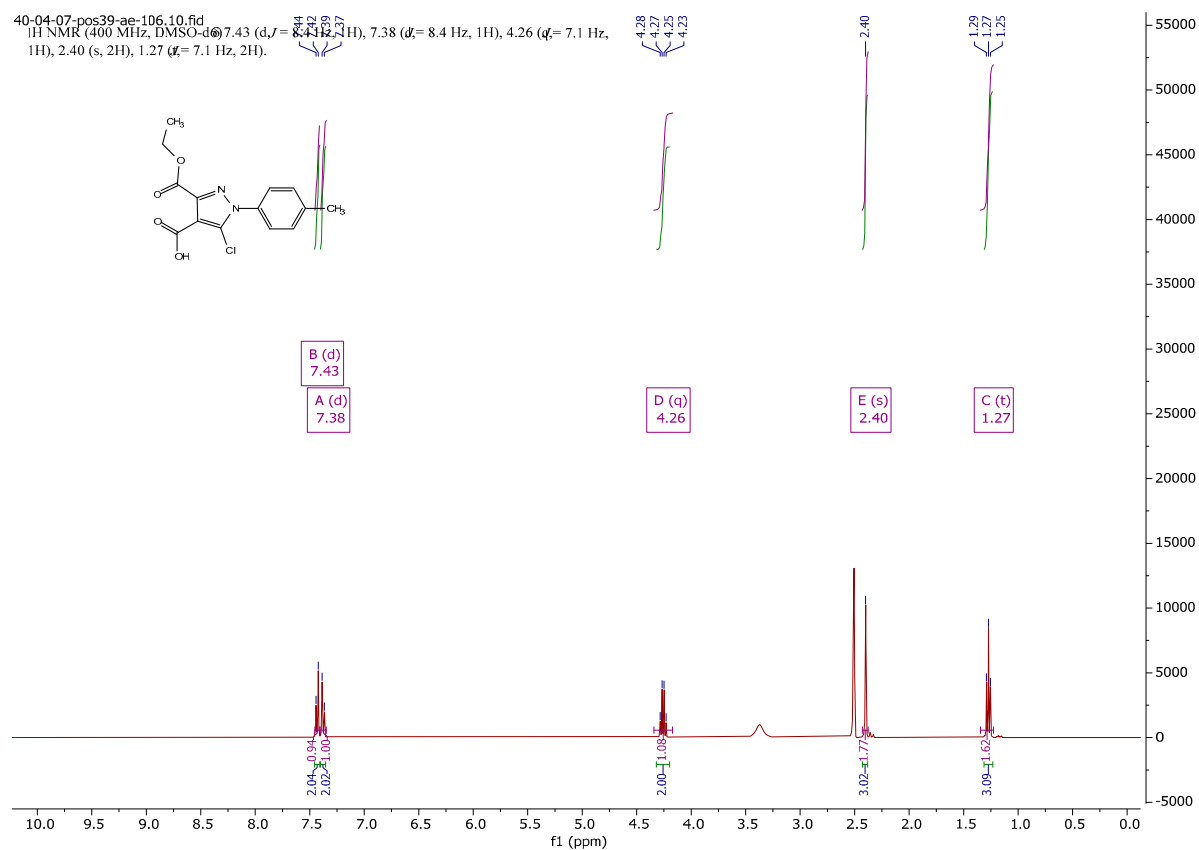


Figure S6: 5-Chloro-3-(ethoxycarbonyl)-1-(4-nitrophenyl)-1H-pyrazole-4-carboxylic acid (6)

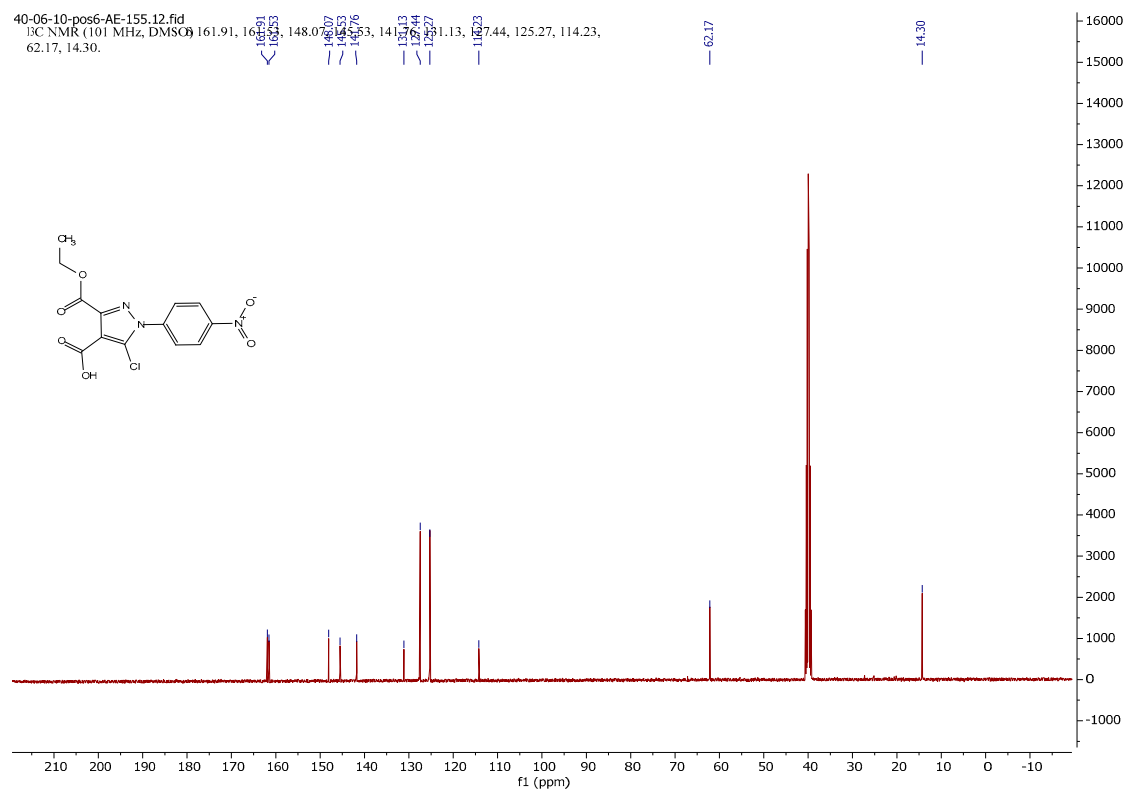
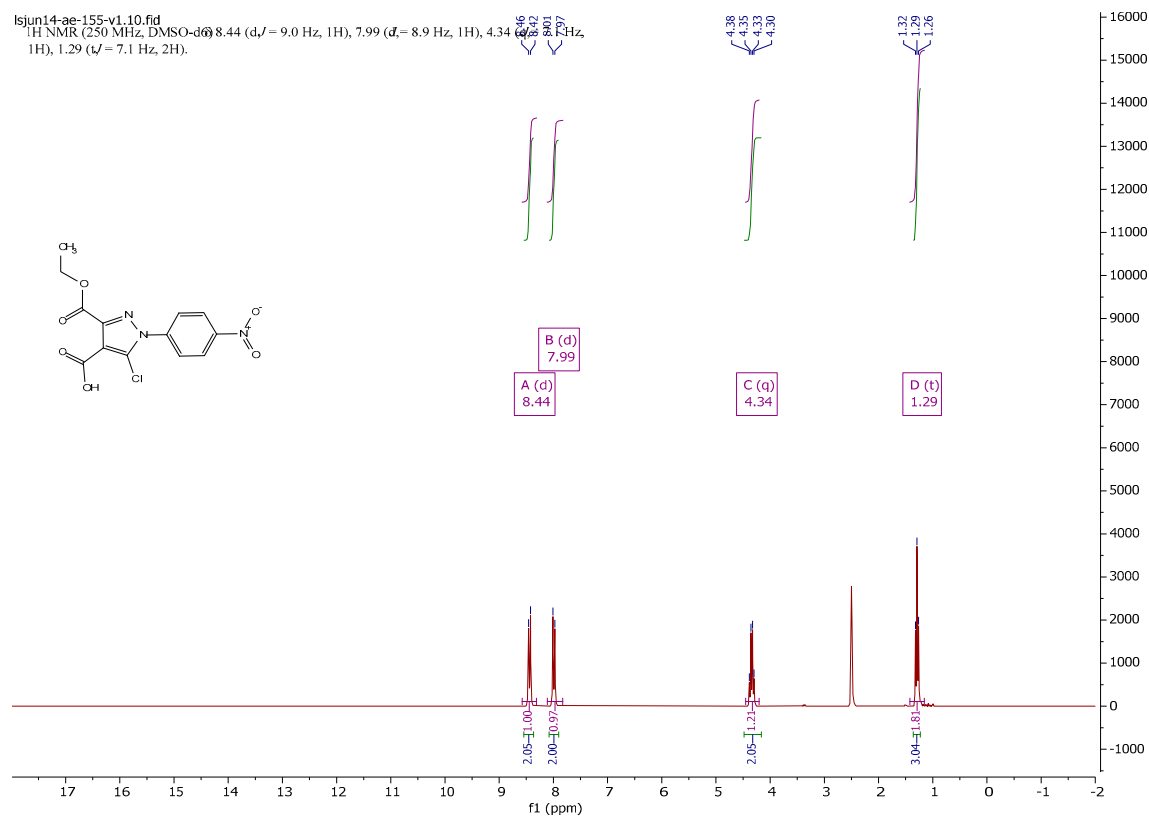


Figure S7: Ethyl 5-chloro-4-(methylcarbamoyl)-1-(p-tolyl)-1H-pyrazole-3-carboxylate (7)

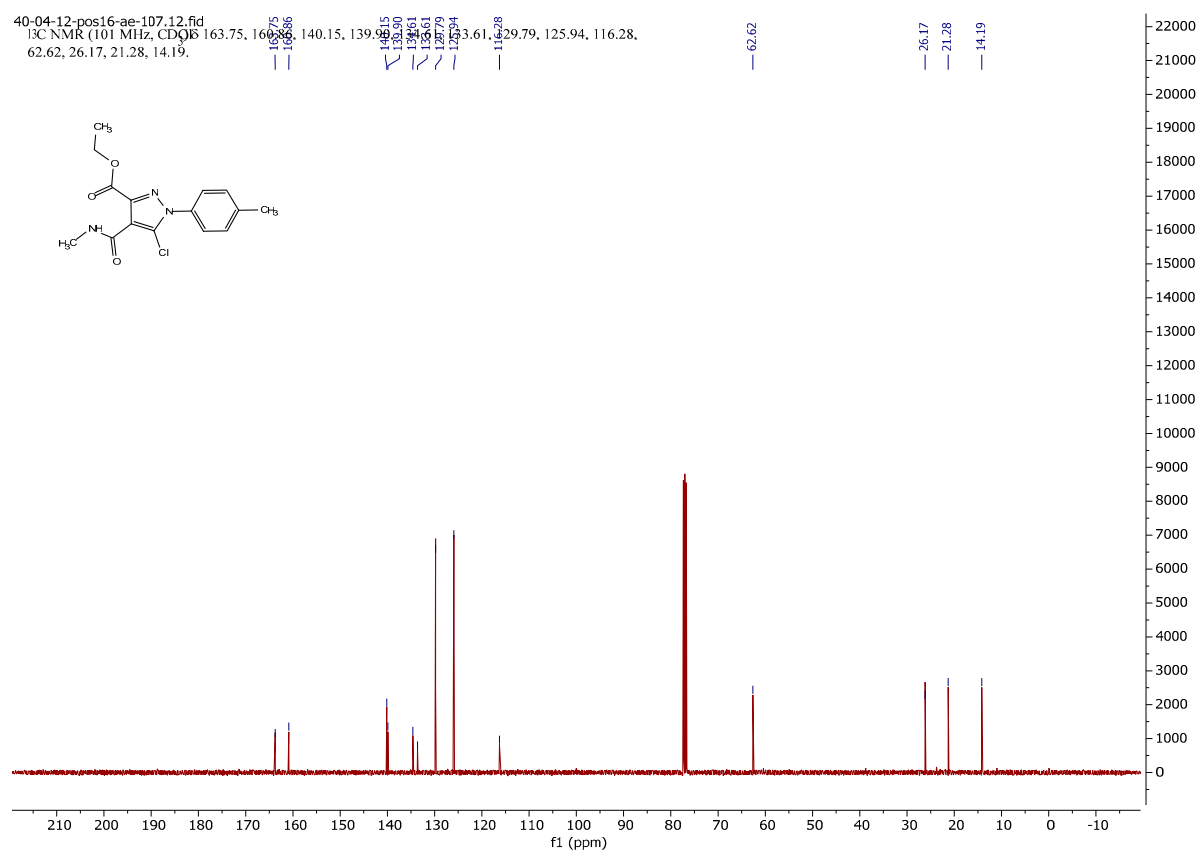
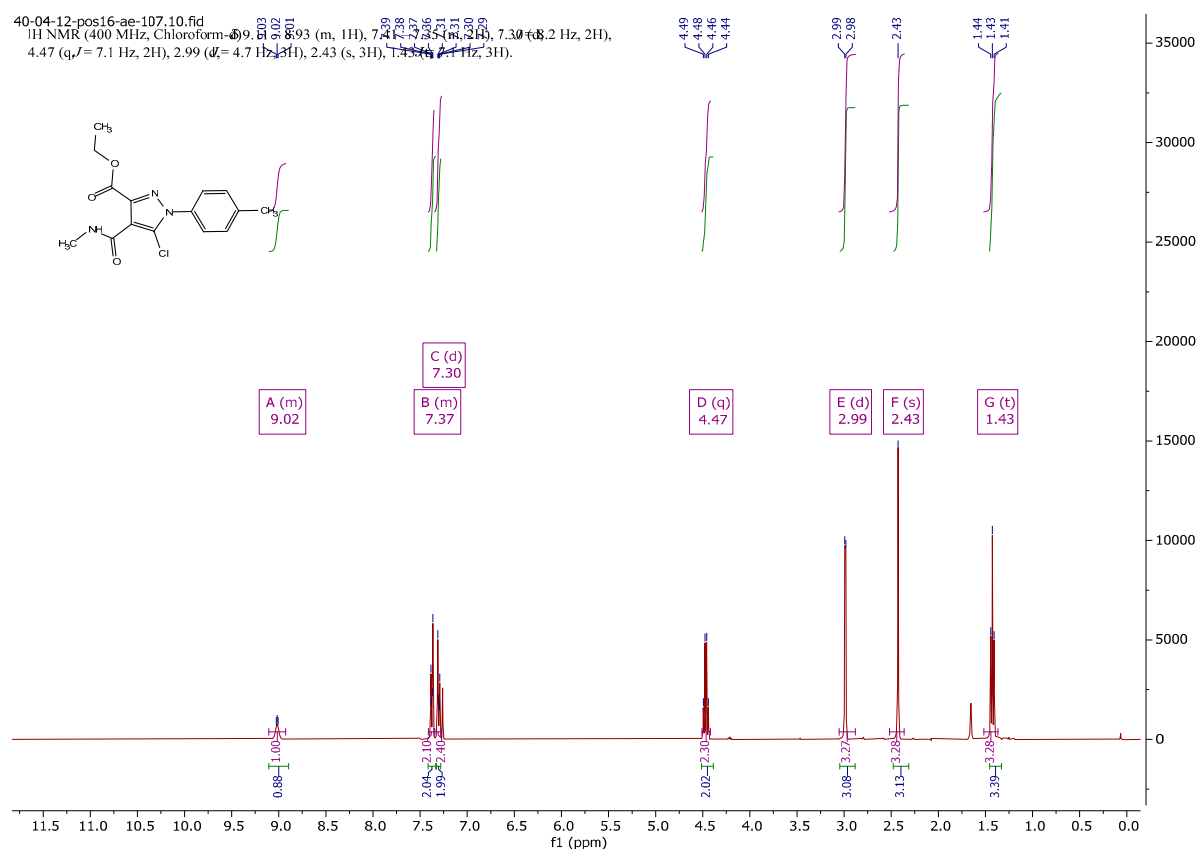


Figure S8: Ethyl 5-chloro-4-[(4-methoxyphenyl)methylcarbamoyl]-1-(p-tolyl)-1H-pyrazole-3-carboxylate (8)

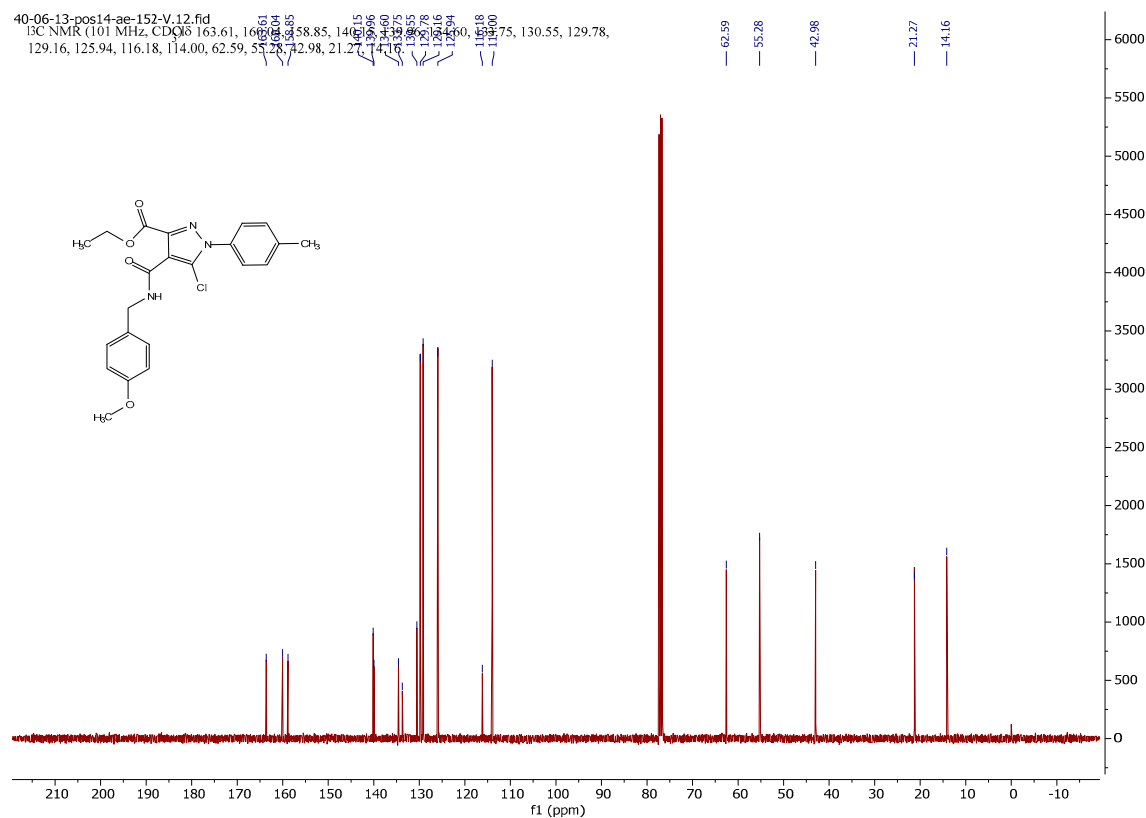
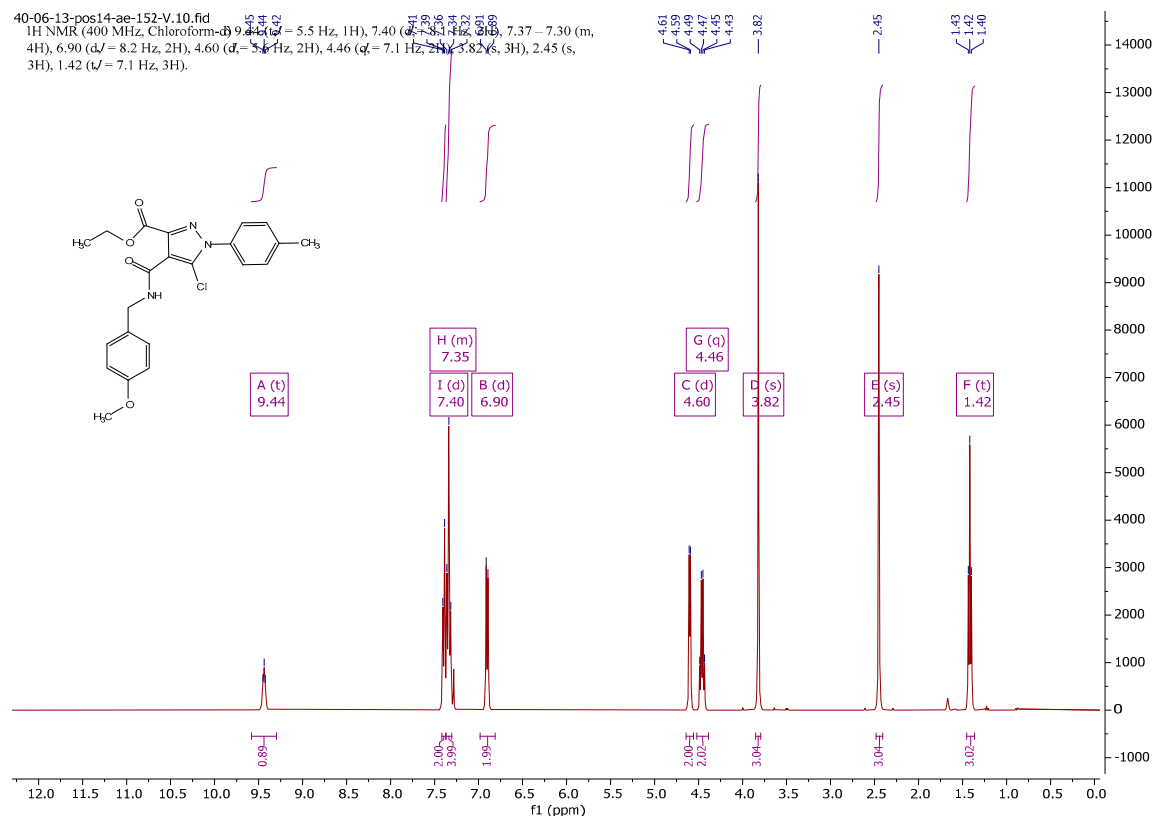
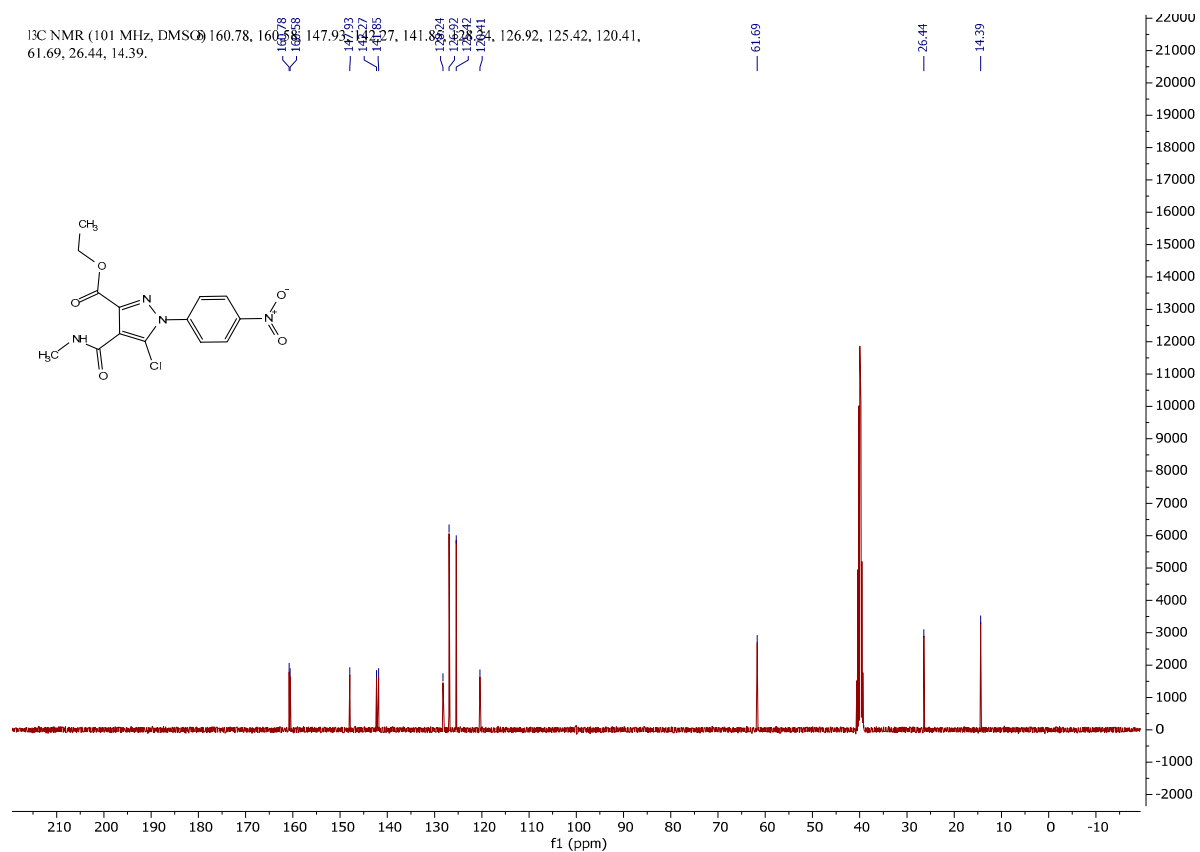
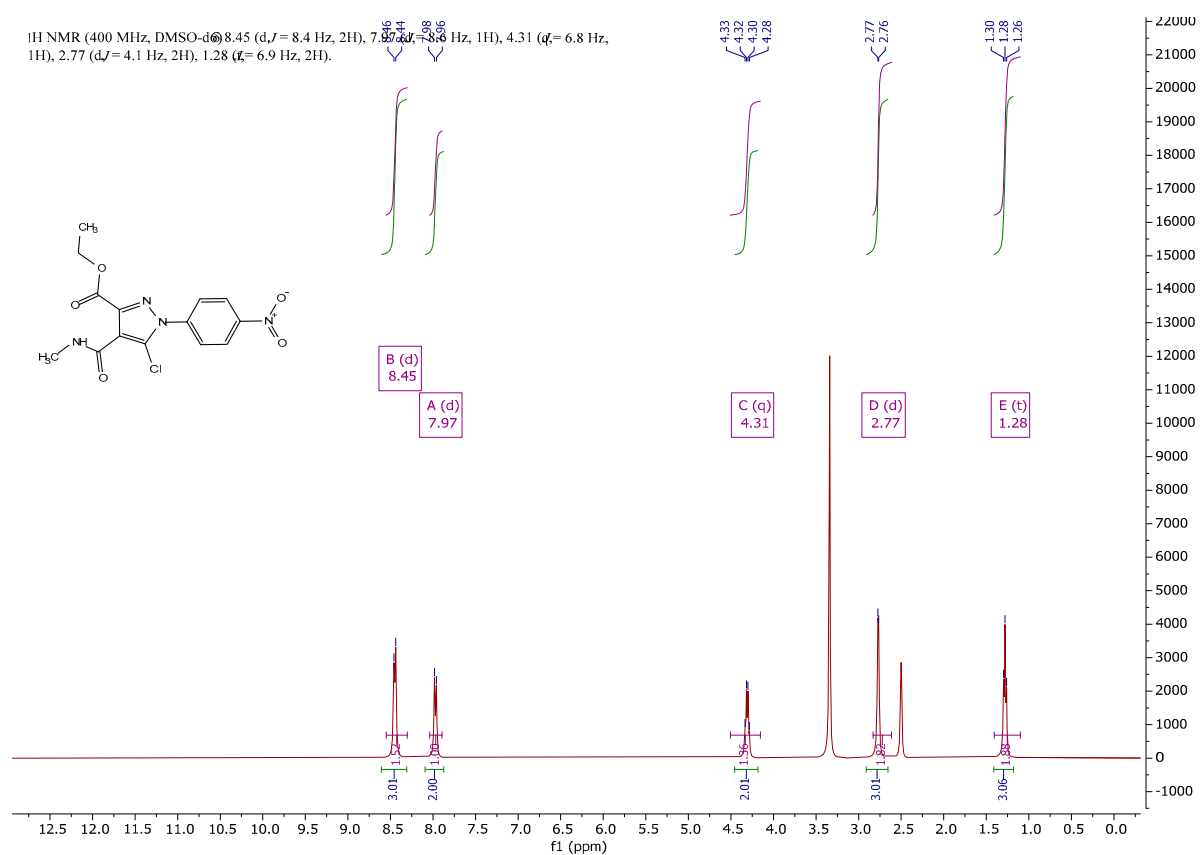


Figure S9: Ethyl 5-chloro-4-(methylcarbamoyl)-1-(4-nitrophenyl)-1H-pyrazole-3-carboxylate (9)

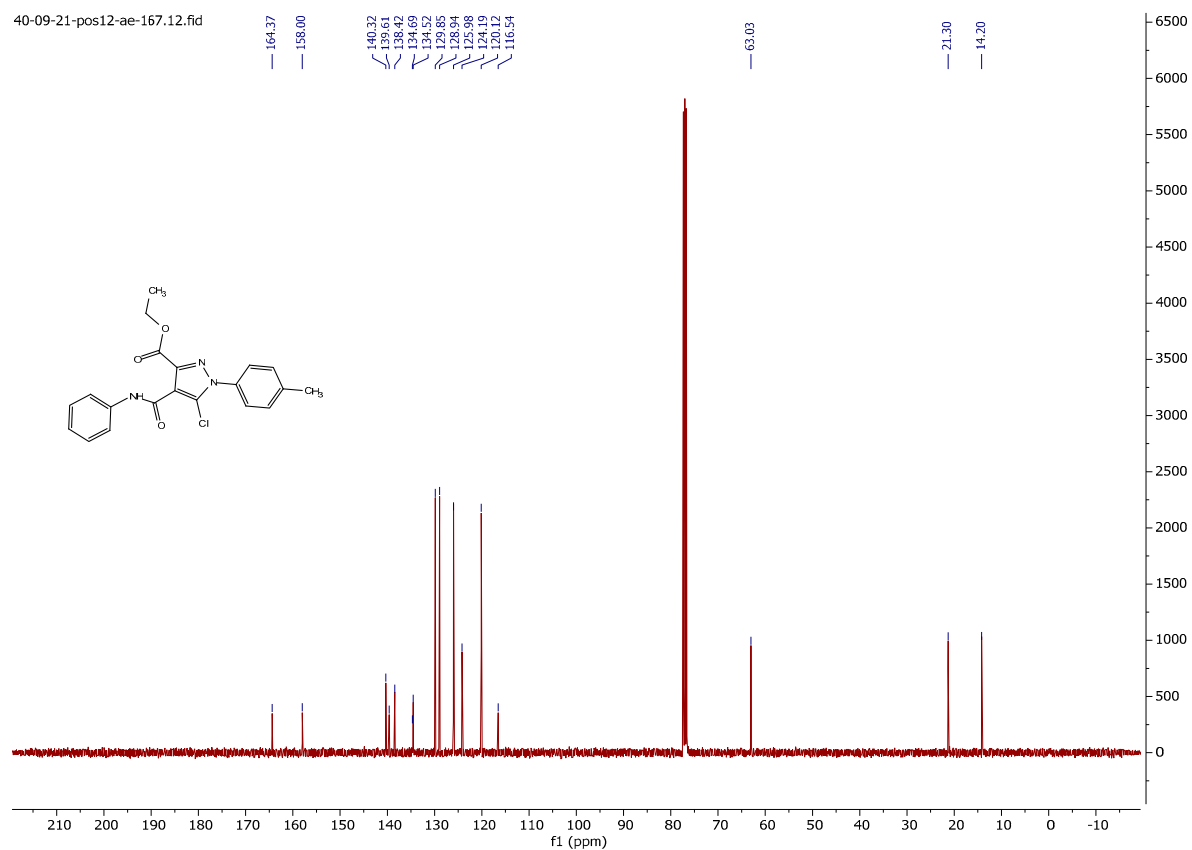


40-09-21-pos12-ae-157.10.fid

Chemical structure: COC(=O)c1nc(NC(=O)c2ccccc2)c(Cl)n1-c3ccc(C)cc3

¹H NMR spectrum (ppm):

- 11.11 (s, 1H)
- 7.79, 7.77, 7.74, 7.42, 7.40, 7.36, 7.34, 7.32, 7.15, 7.13, 7.11 (m, 7H)
- 4.57, 4.55, 4.53, 4.52 (s, 3H)
- 2.45 (s, 3H)
- 1.48, 1.46, 1.45 (s, 3H)



40-06-15-pos47-ae-109.10.fid

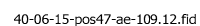
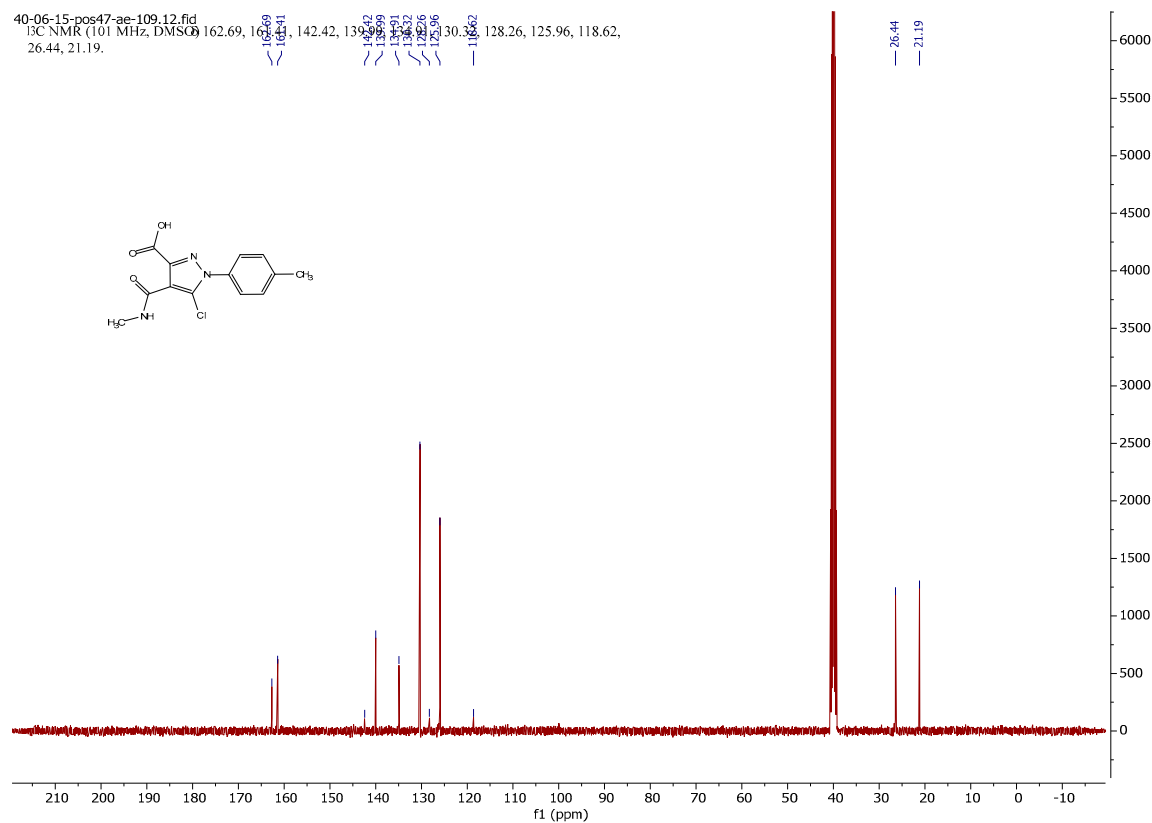
¹³C NMR (101 MHz, DMSO-*d*₆) δ 26.44, 21.19.

Figure S12: 5-Chloro-4-((4-methoxybenzyl)carbamoyl)-1-(p-tolyl)-1H-pyrazole-3-carboxylic acid (12)

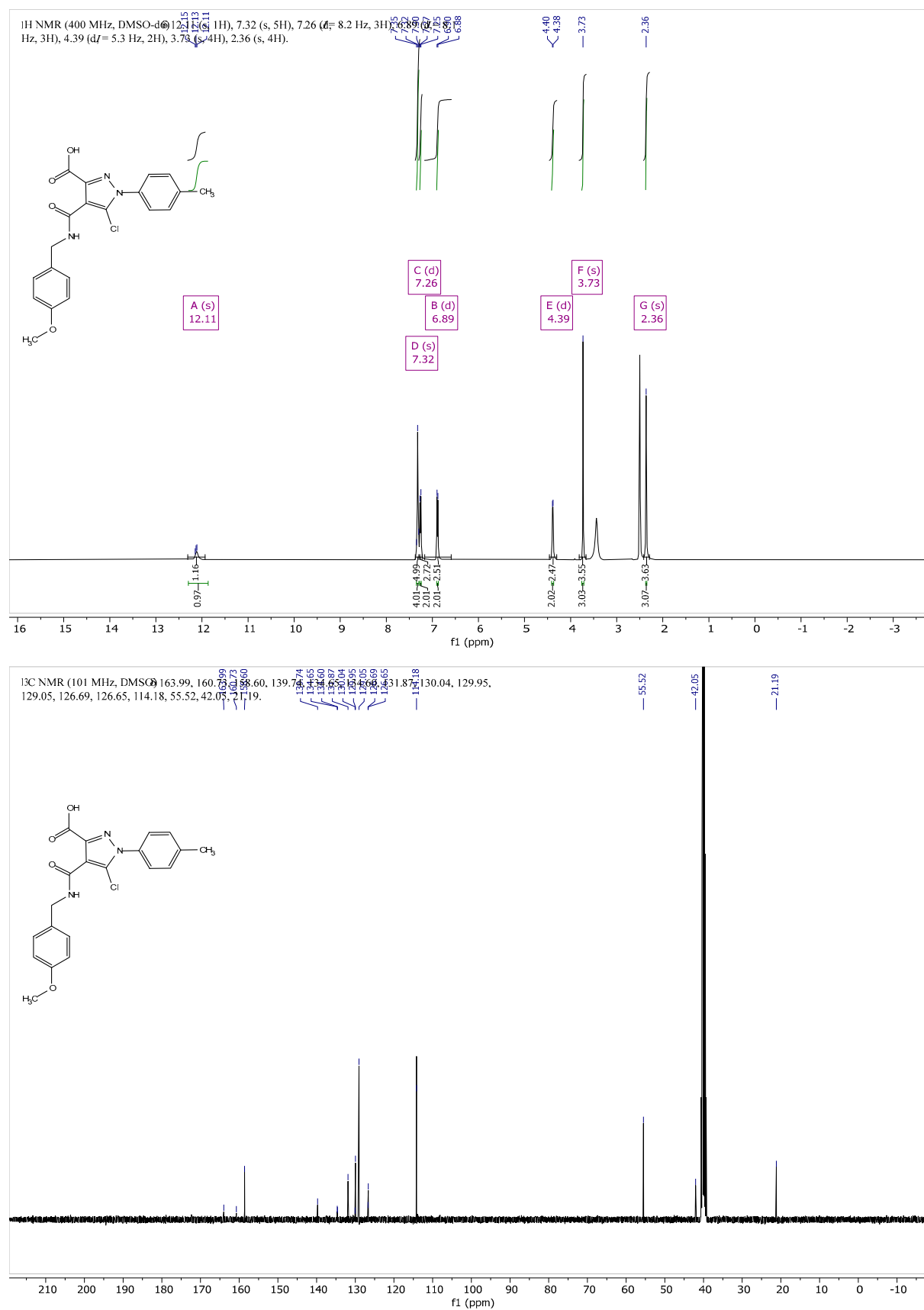


Figure S13: 5-Chloro-4-(methylcarbamoyl)-1-(4-nitrophenyl)-1H-pyrazole-3-carboxylic acid (13)

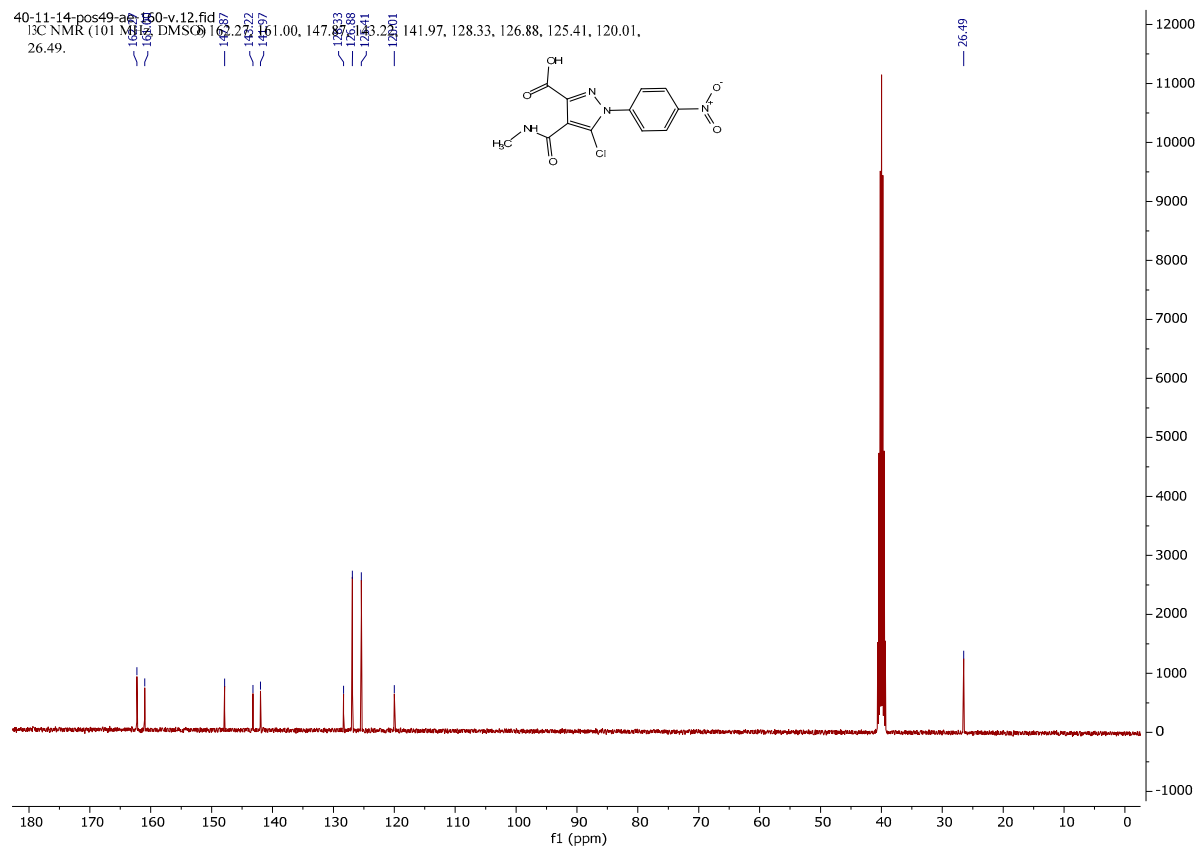
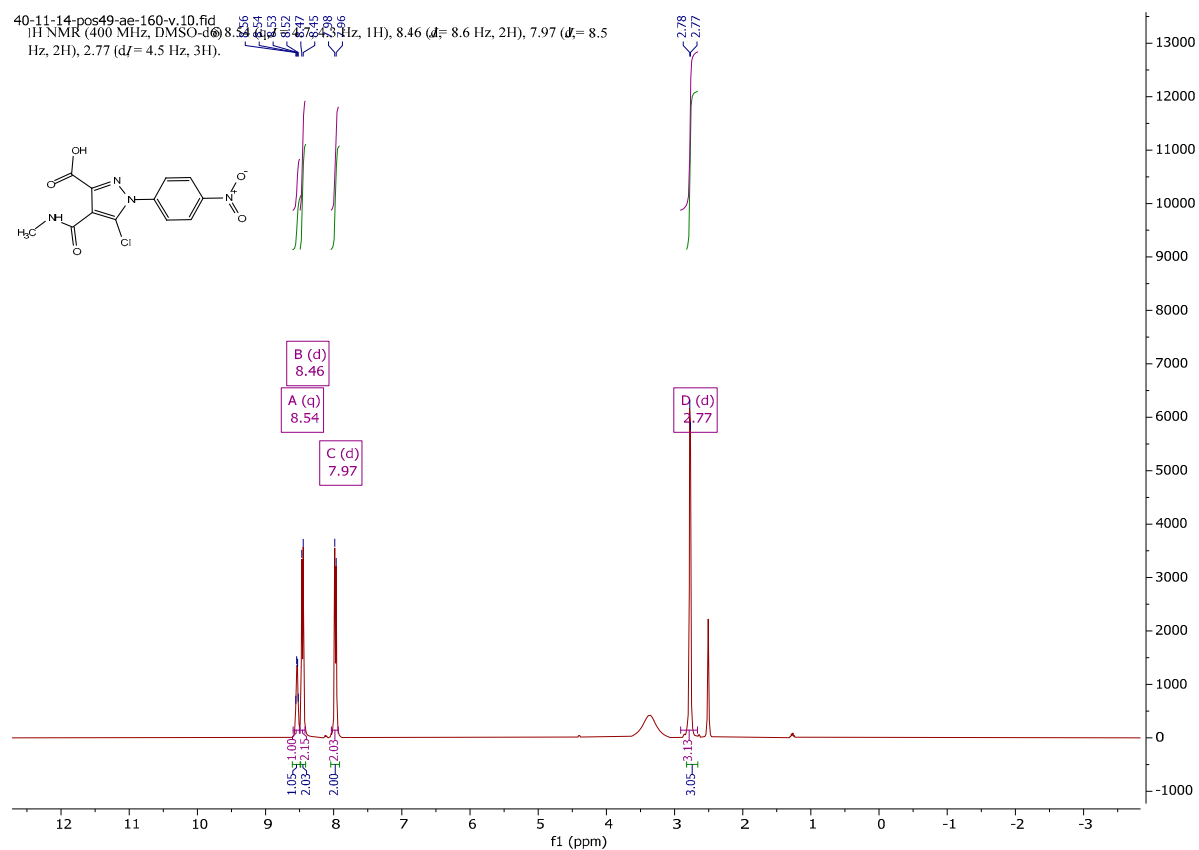


Figure S14: 5-Chloro-4-(phenylcarbamoyl)-1-(p-tolyl)-1H-pyrazole-3-carboxylic acid (14)

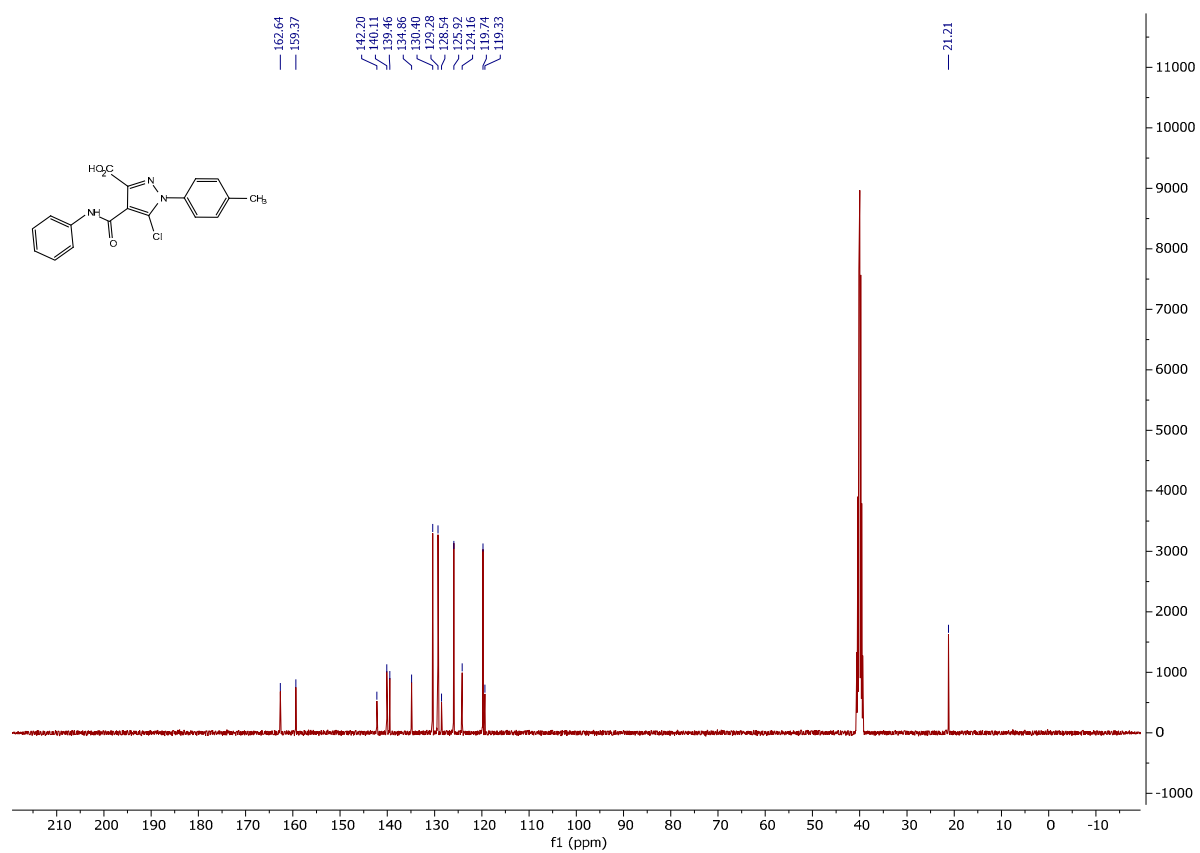
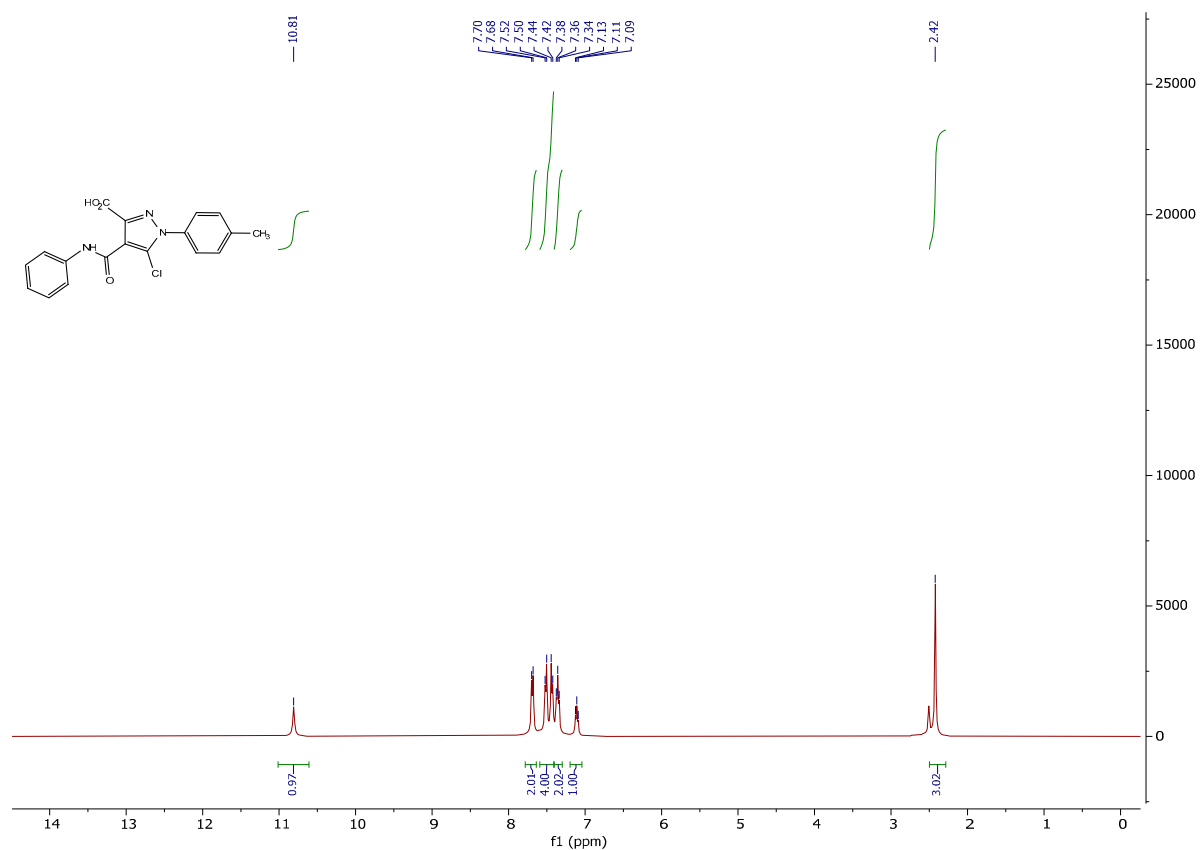


Figure S15: 3-Chloro-5-methyl-2-(p-tolyl)pyrrolo[3,4-c]pyrazole-4,6-(2*H*,5*H*)-dione (15)

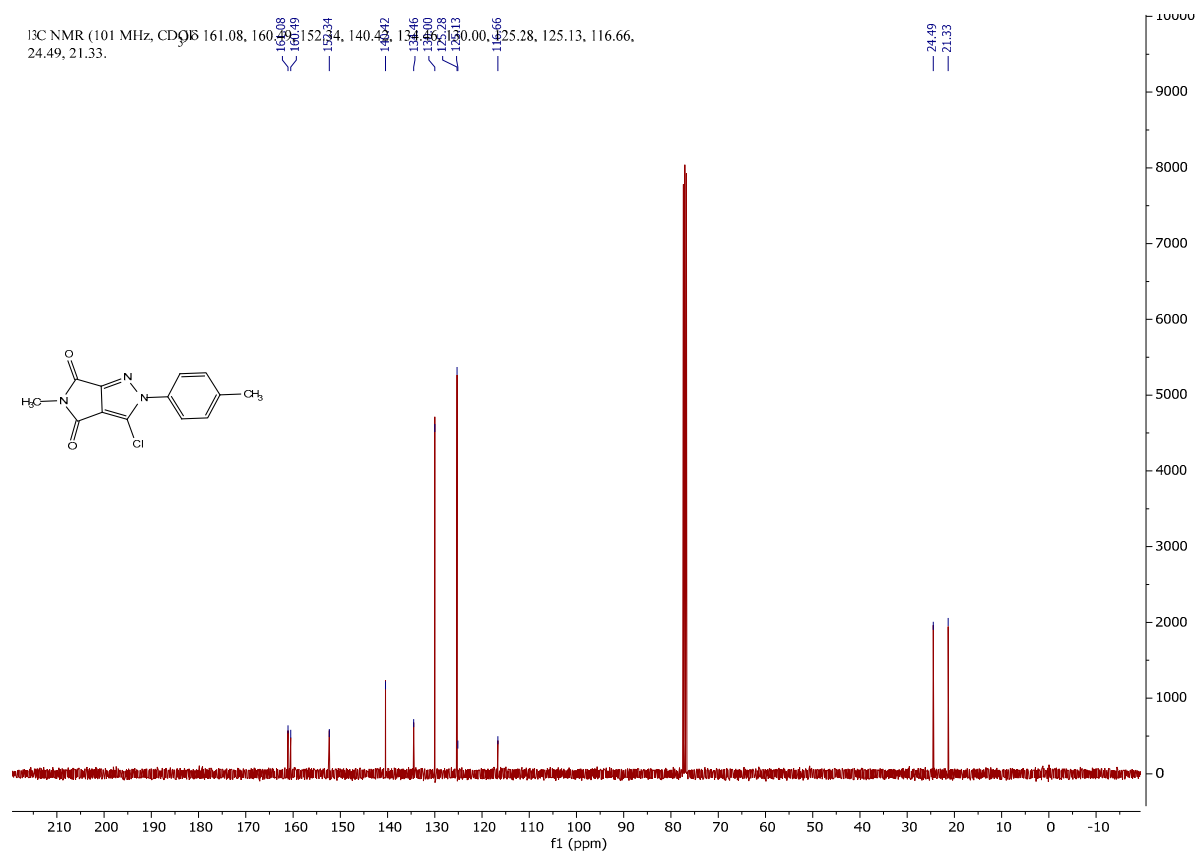
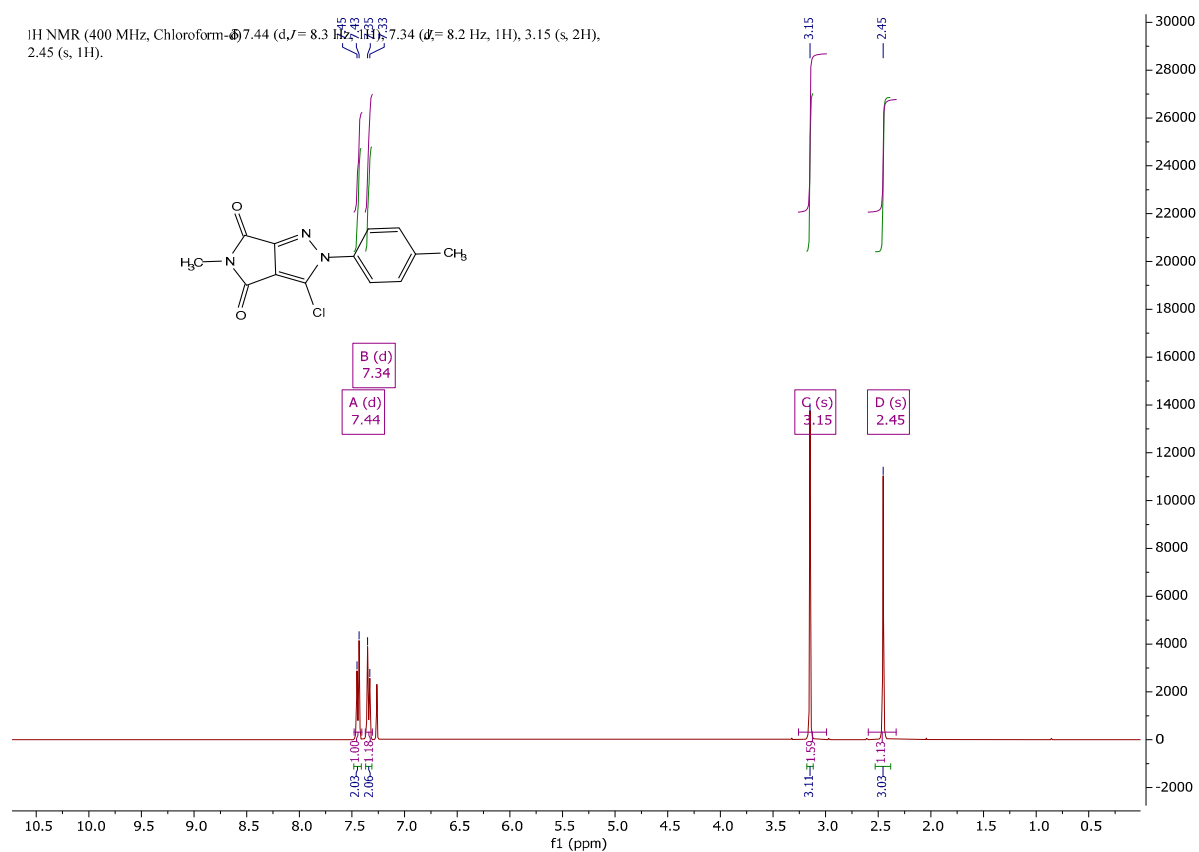


Figure S16: 3-Chloro-5-(4-methoxybenzyl)-2-(p-tolyl)pyrrolo[3,4-c]pyrazole-4,6-(2*H*,5*H*)-dione (16)

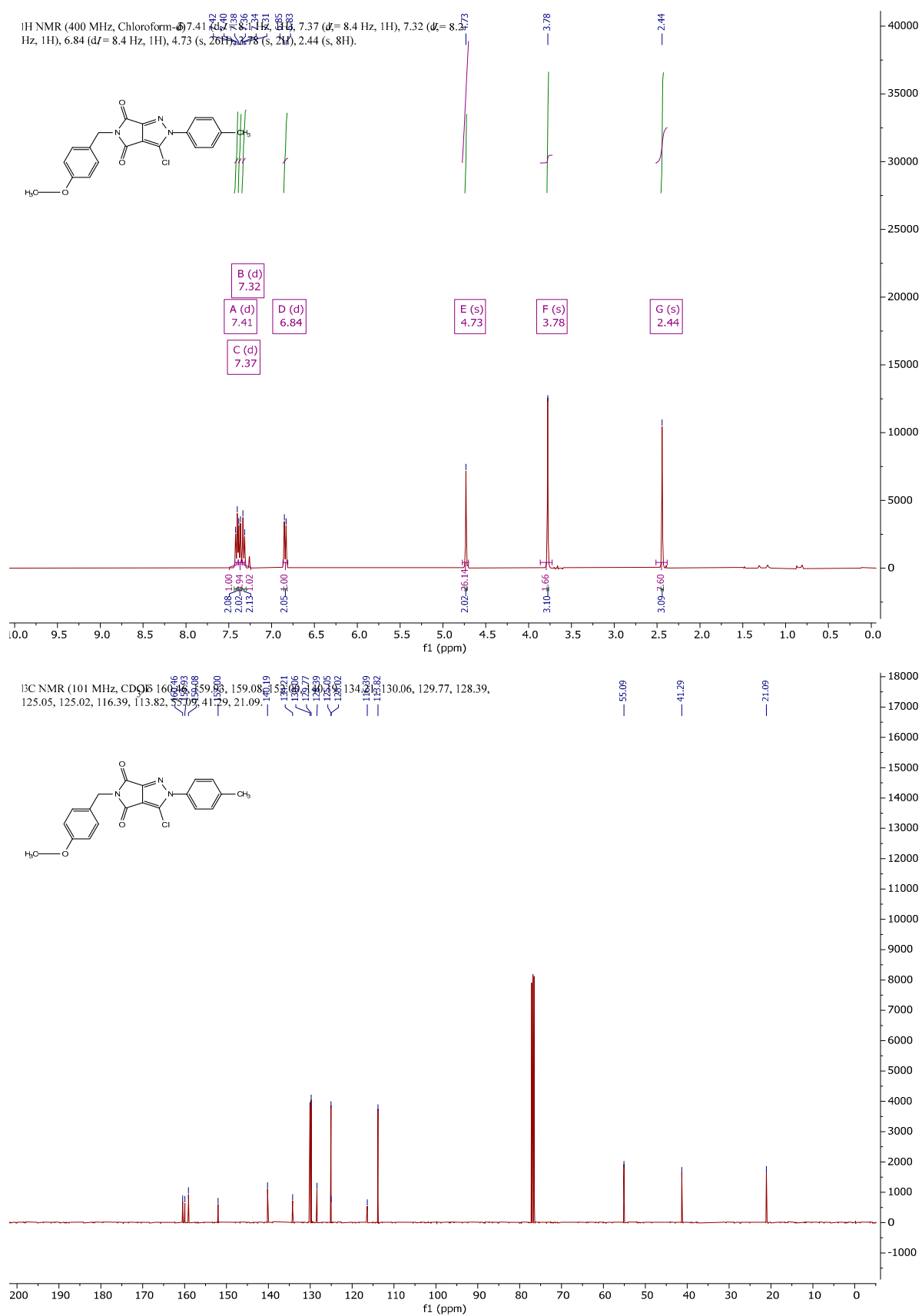


Figure S17: 3-Chloro-5-methyl-2-(4-nitrophenyl)pyrrolo[3,4-c]pyrazole-4,6-(2*H*,5*H*)-dione (17)

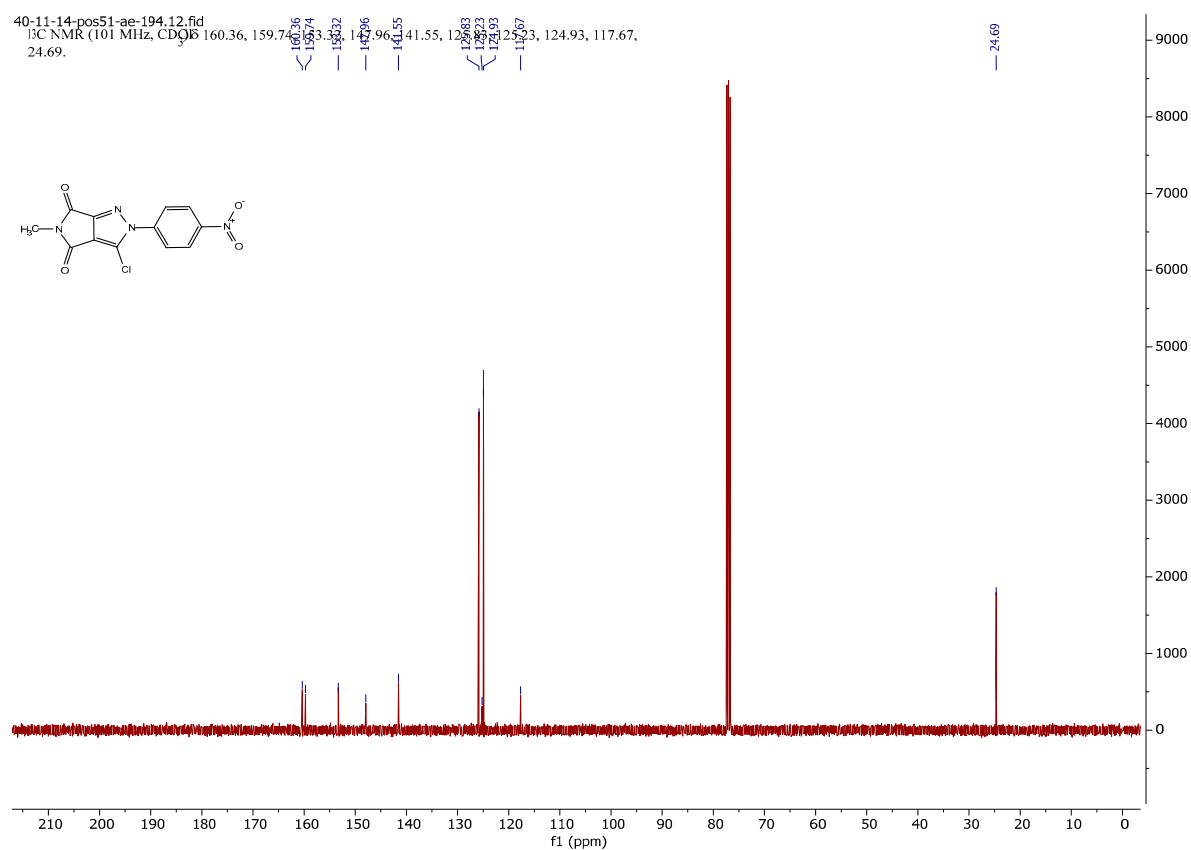
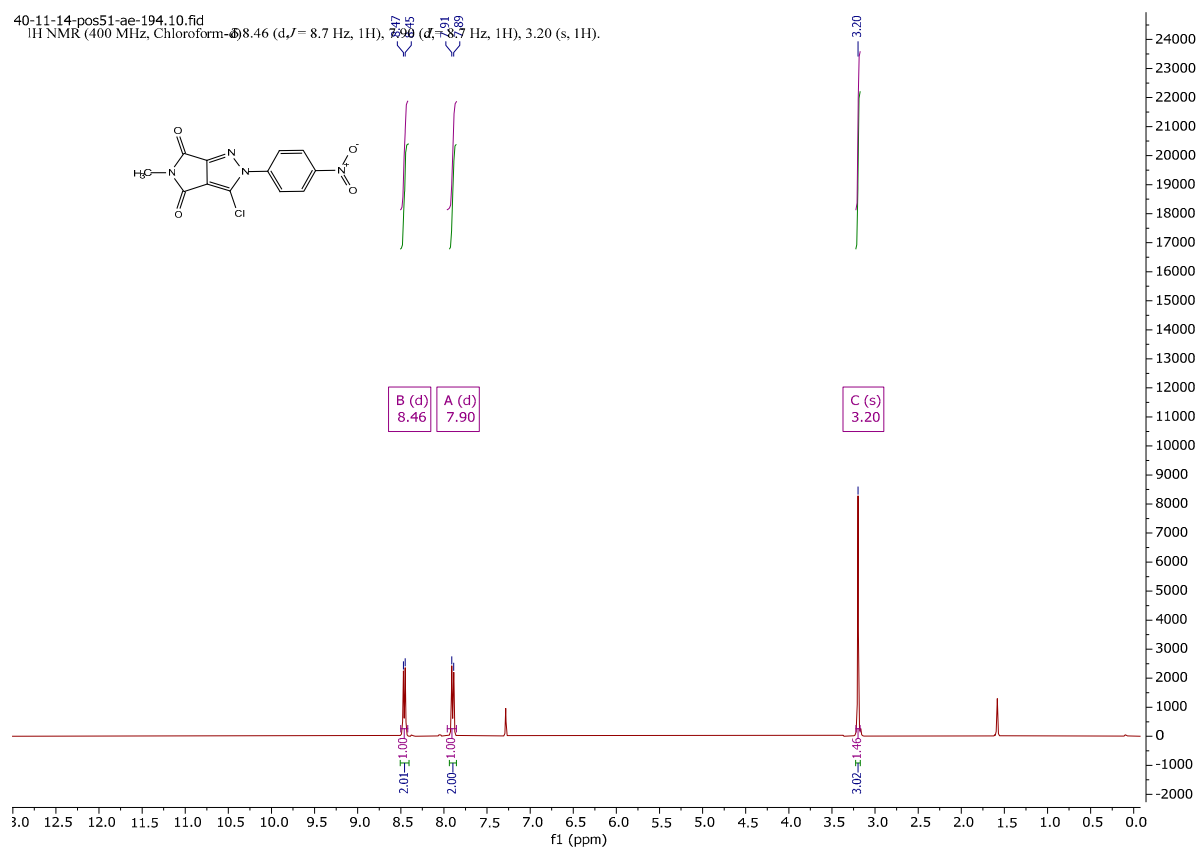


Figure S18: 5-Methyl-2,3-di-p-tolylpyrrolo[3,4-c]pyrazole-4,6-(2H,5H)-dione (19)

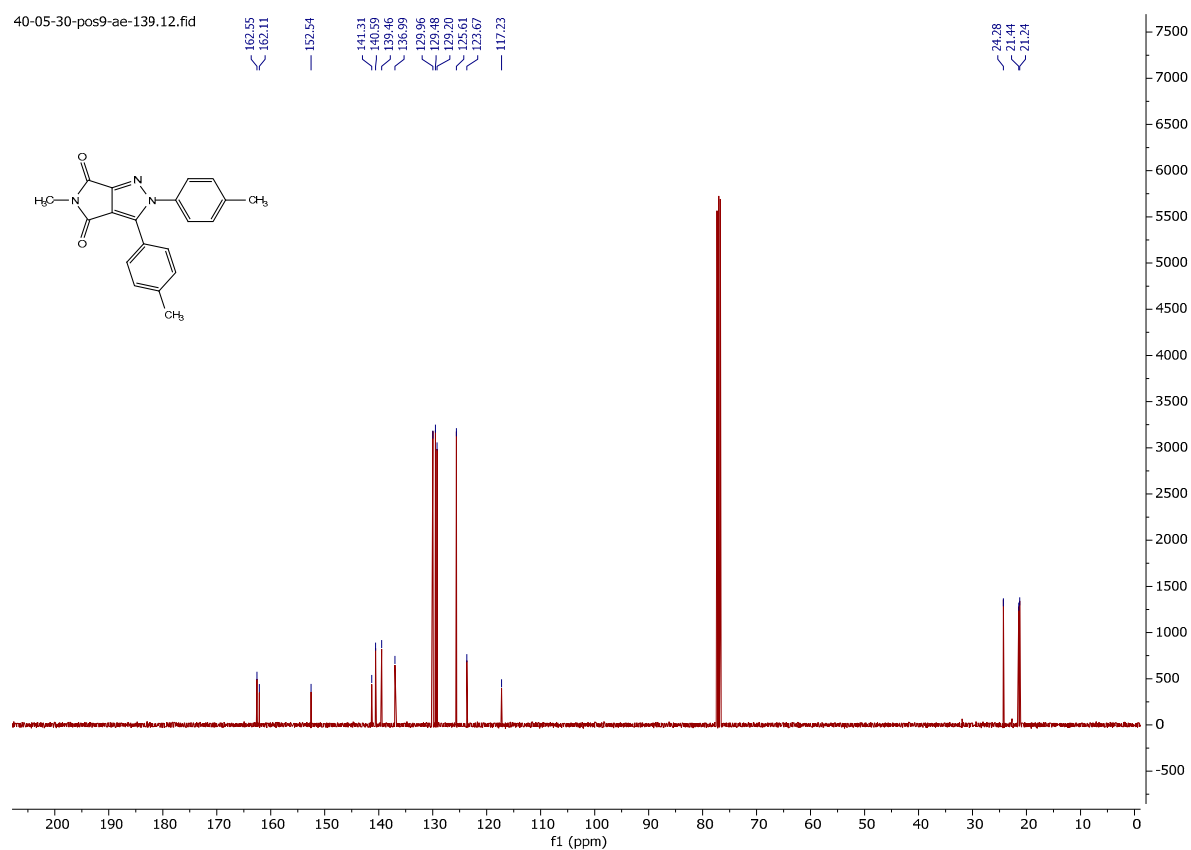
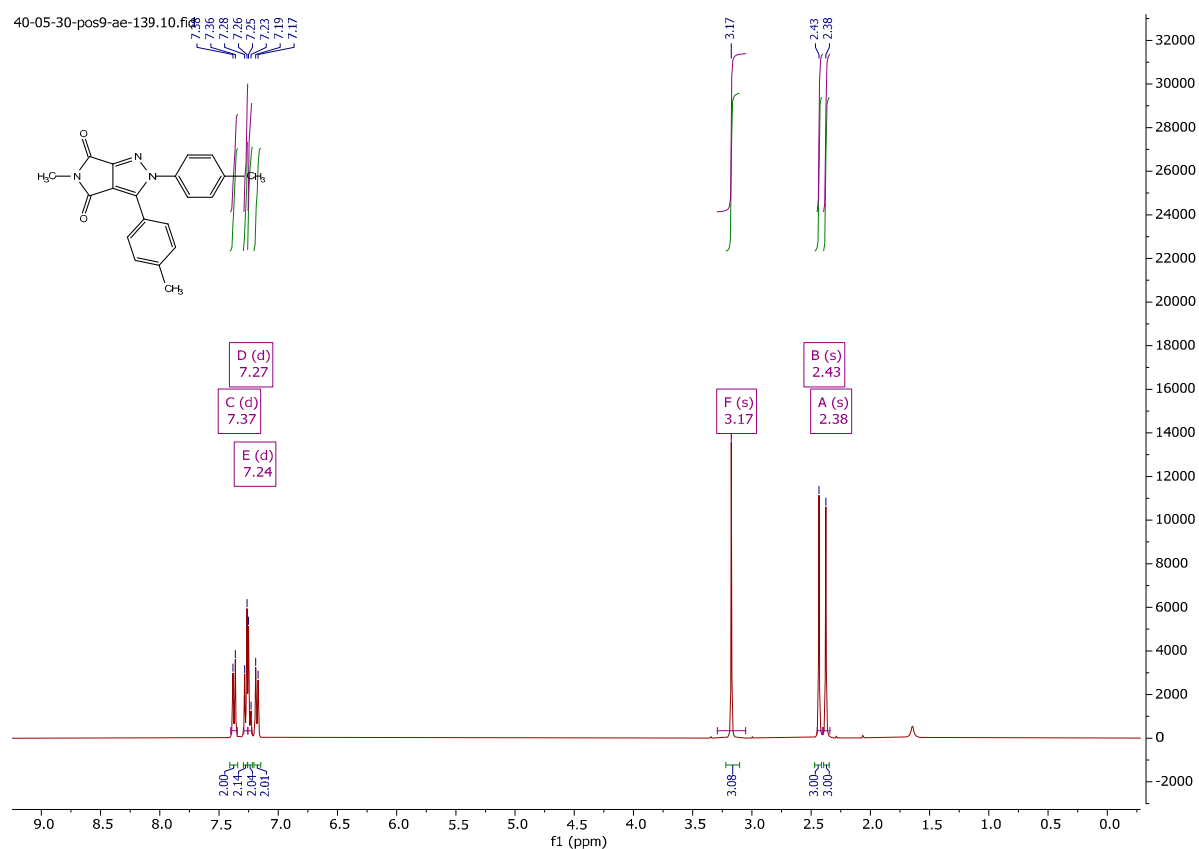


Figure S19: 3-(4-Methoxyphenyl)-5-methyl-2-(p-tolyl)pyrrolo[3,4-c]pyrazole-4,6-(2*H*,5*H*)-dione (20)

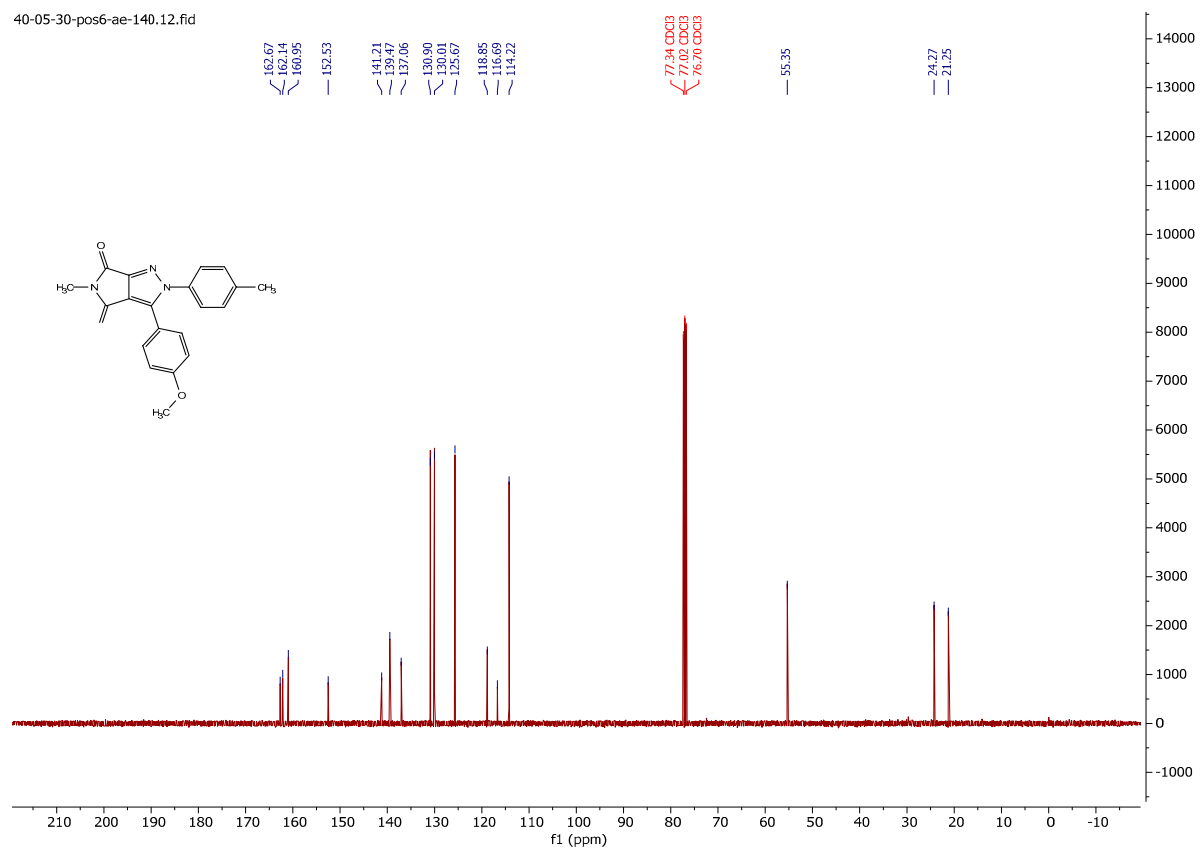
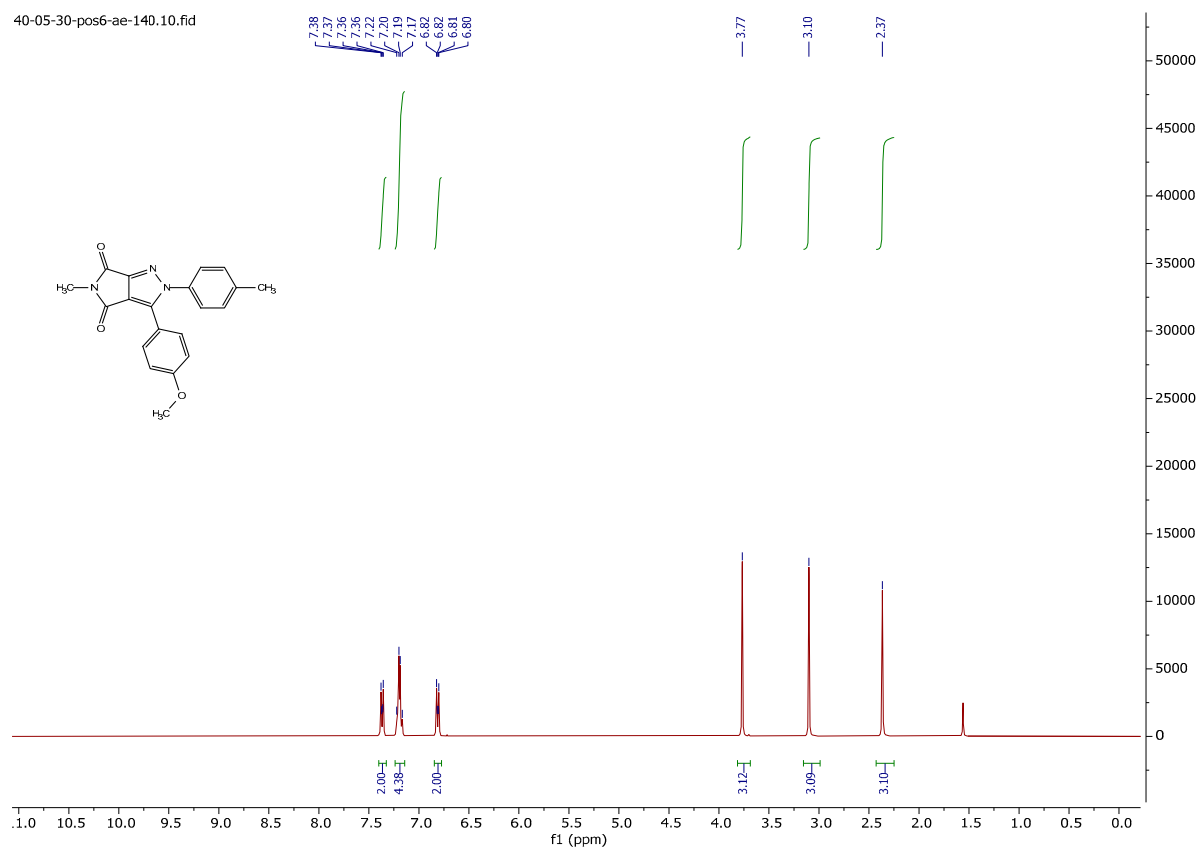


Figure S20: 3-(3-Methoxyphenyl)-5-methyl-2-(p-tolyl)pyrrolo[3,4-c]pyrazole-4,6-(2H,5H)-dione (21)

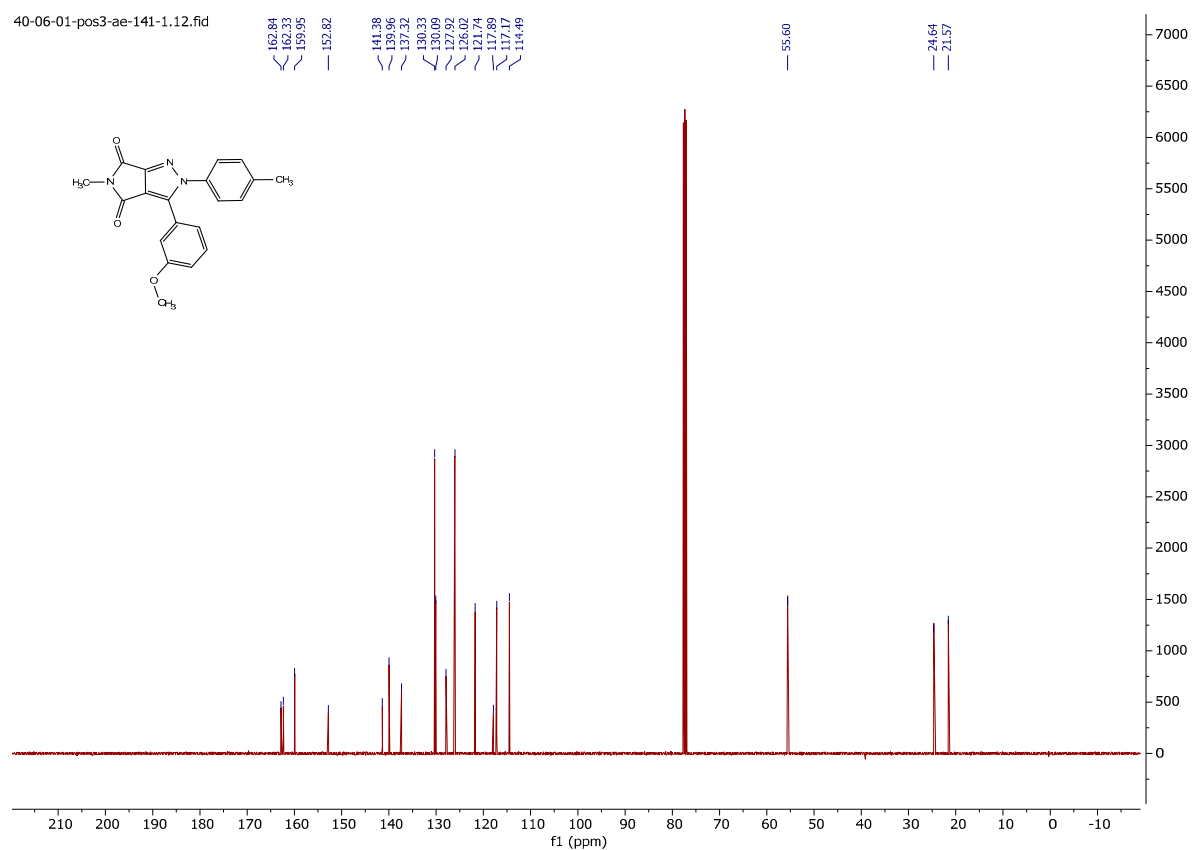
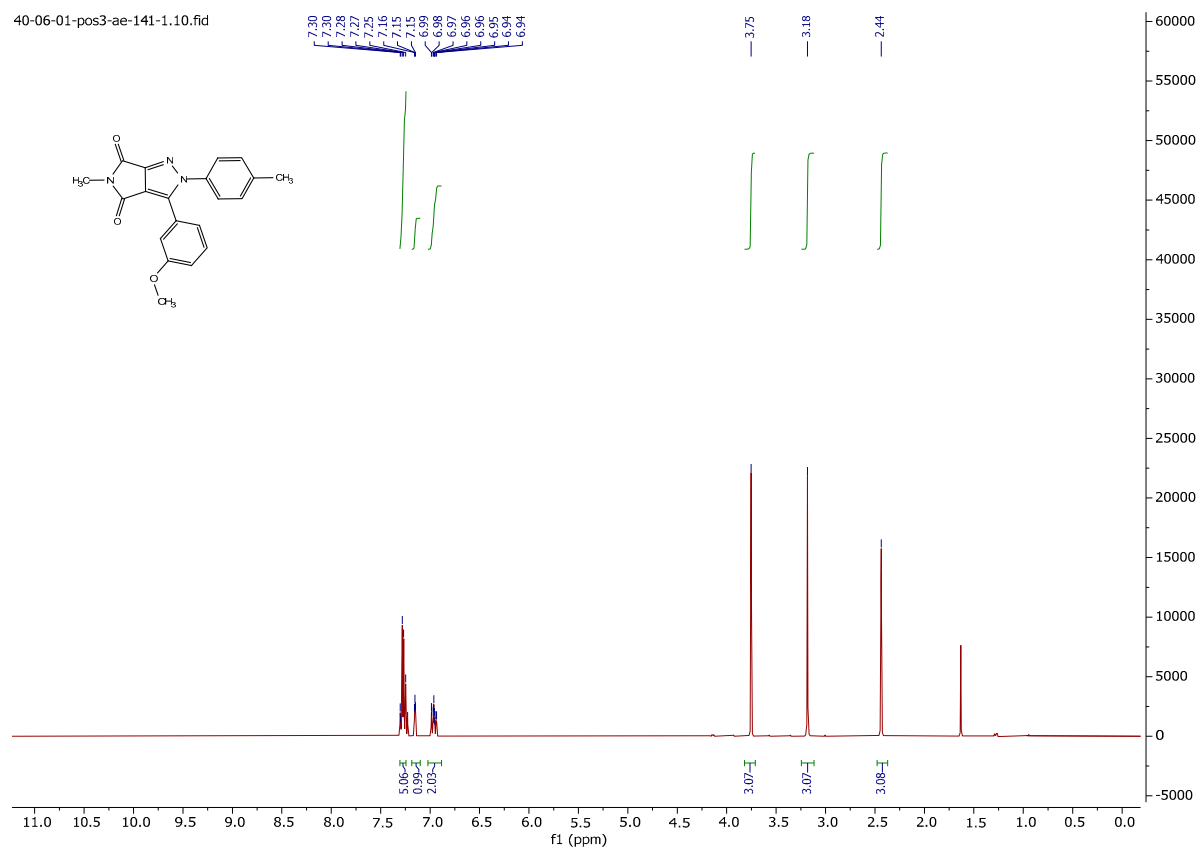


Figure S21:3-(4-Fluorophenyl)-5-methyl-2-(p-tolyl)pyrrolo[3,4-c]pyrazole-4,6-(2H,5H)-dione (23)

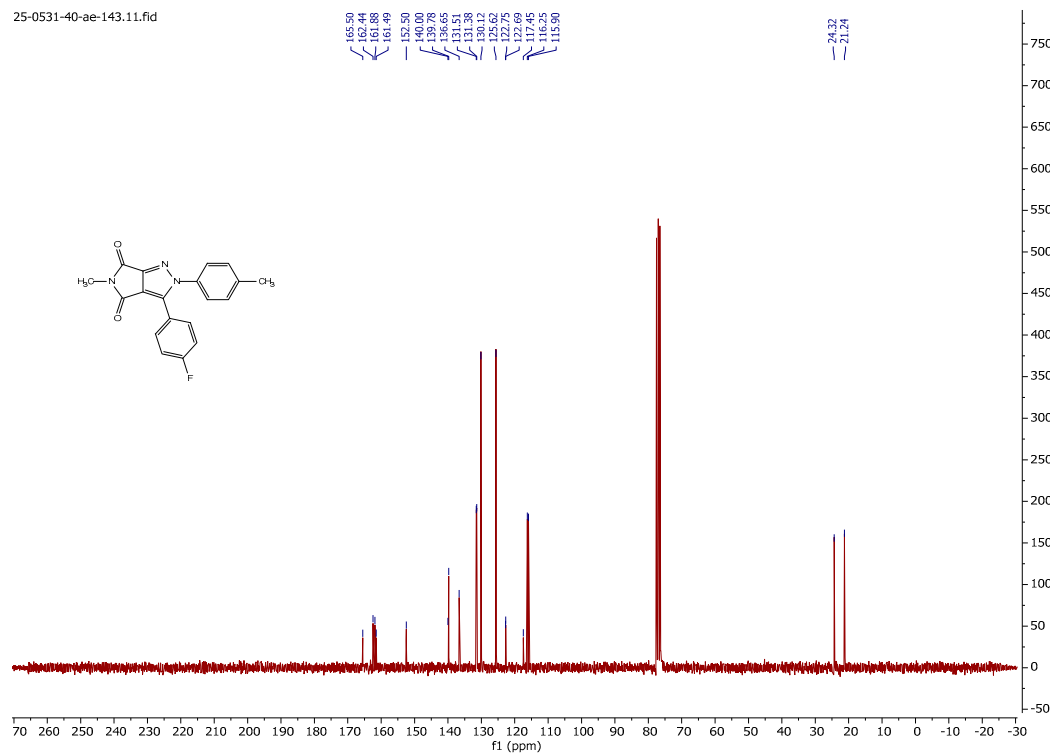
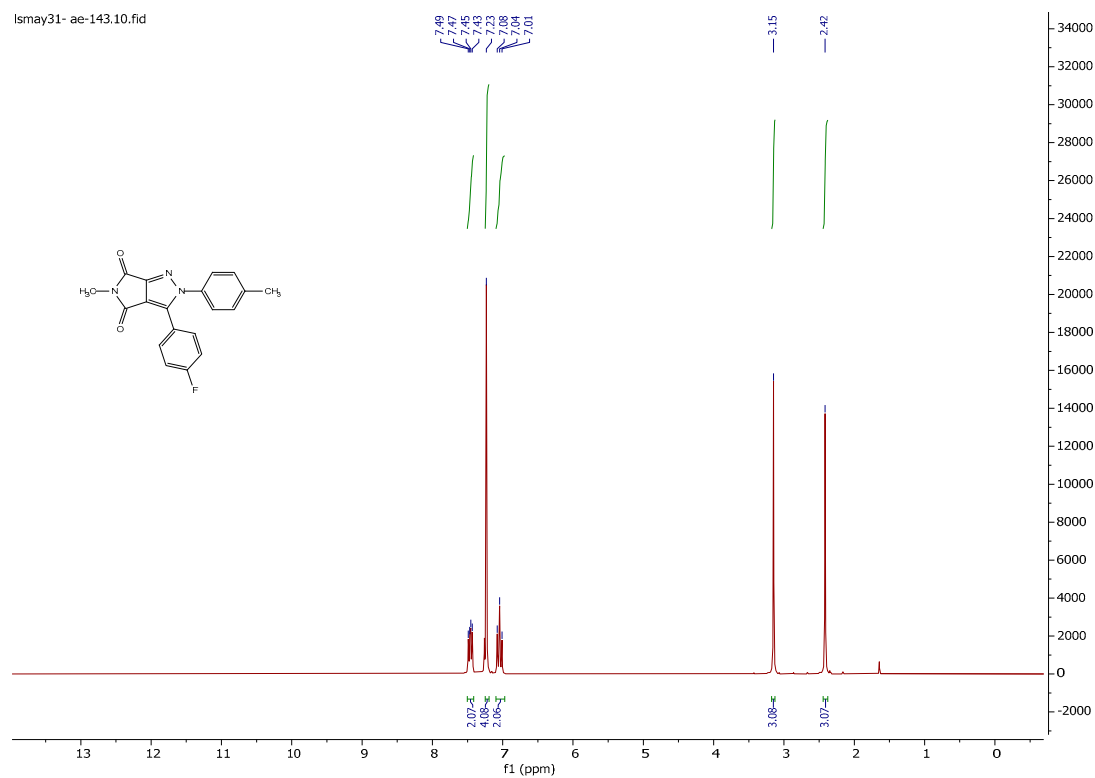


Figure S22:3-(4-Cyanophenyl)-5-methyl-2-(p-tolyl)pyrrolo[3,4-c]pyrazole-4,6-(2*H*,5*H*)-dione (24)

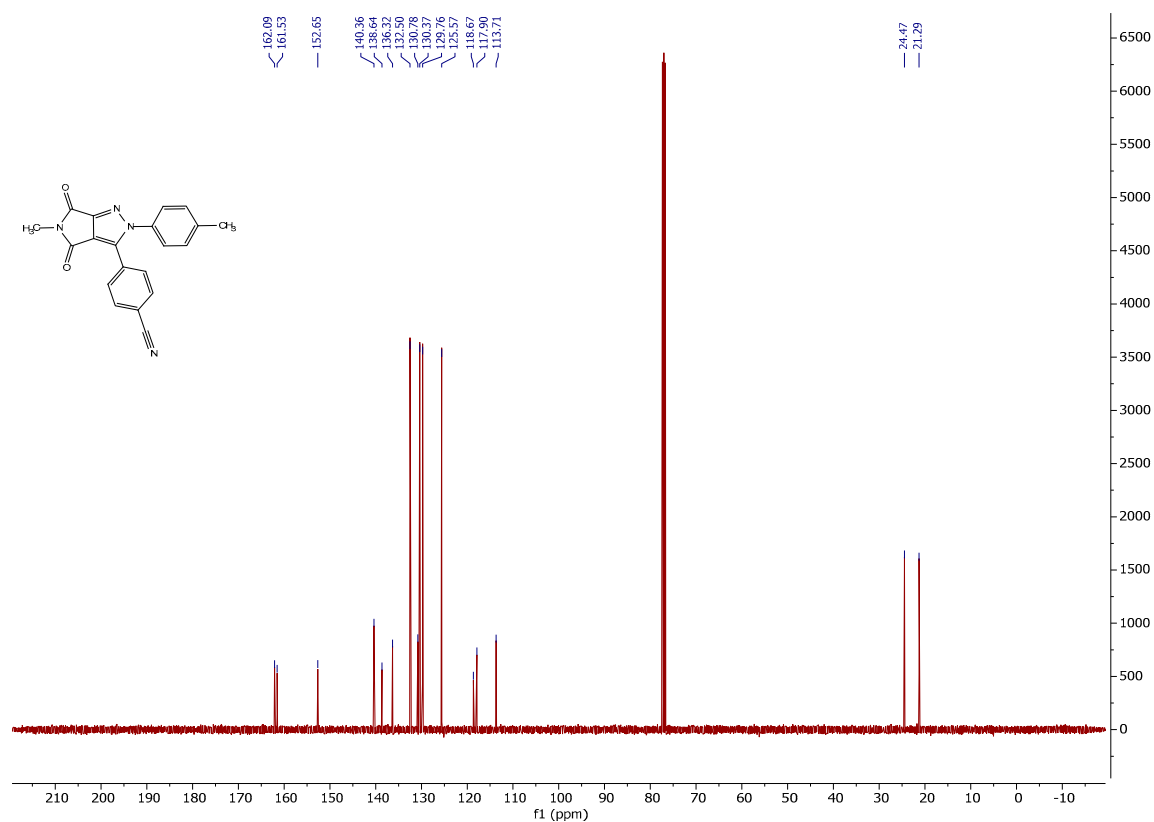
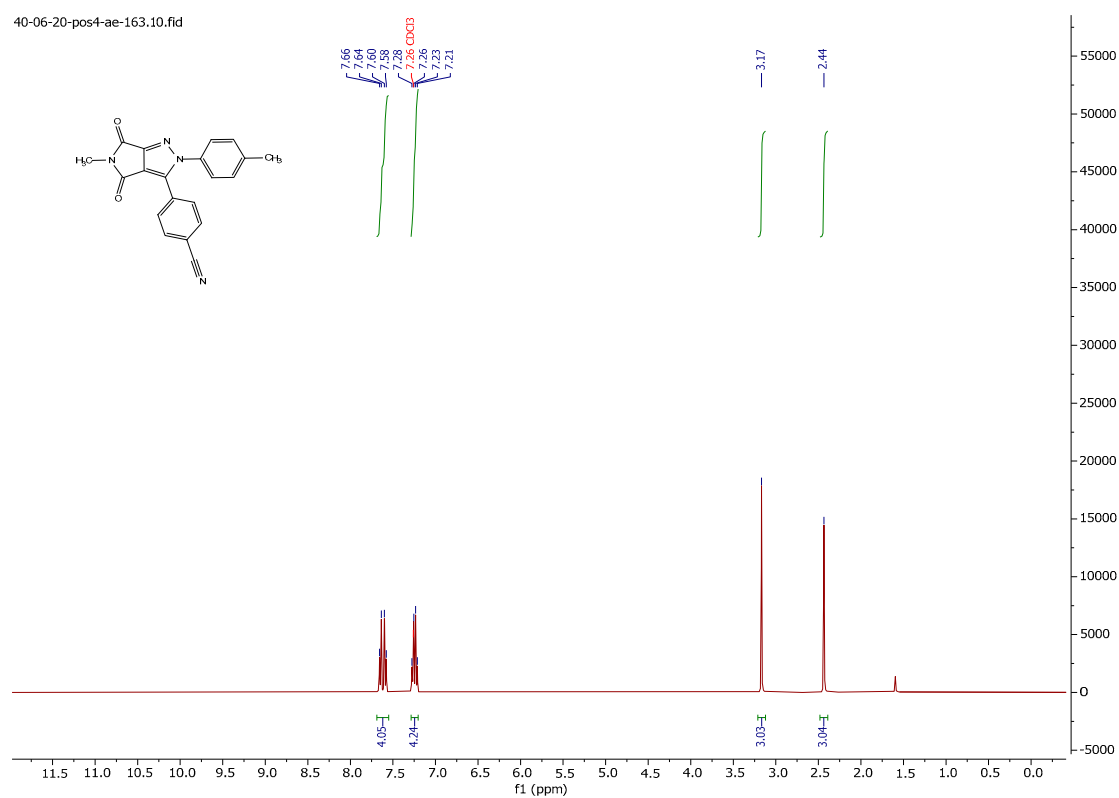


Figure S23:3-(Furan-2-yl)-5-methyl-2-(p-tolyl)pyrrolo[3,4-c]pyrazole-4,6-(2*H*,5*H*)-dione (25)

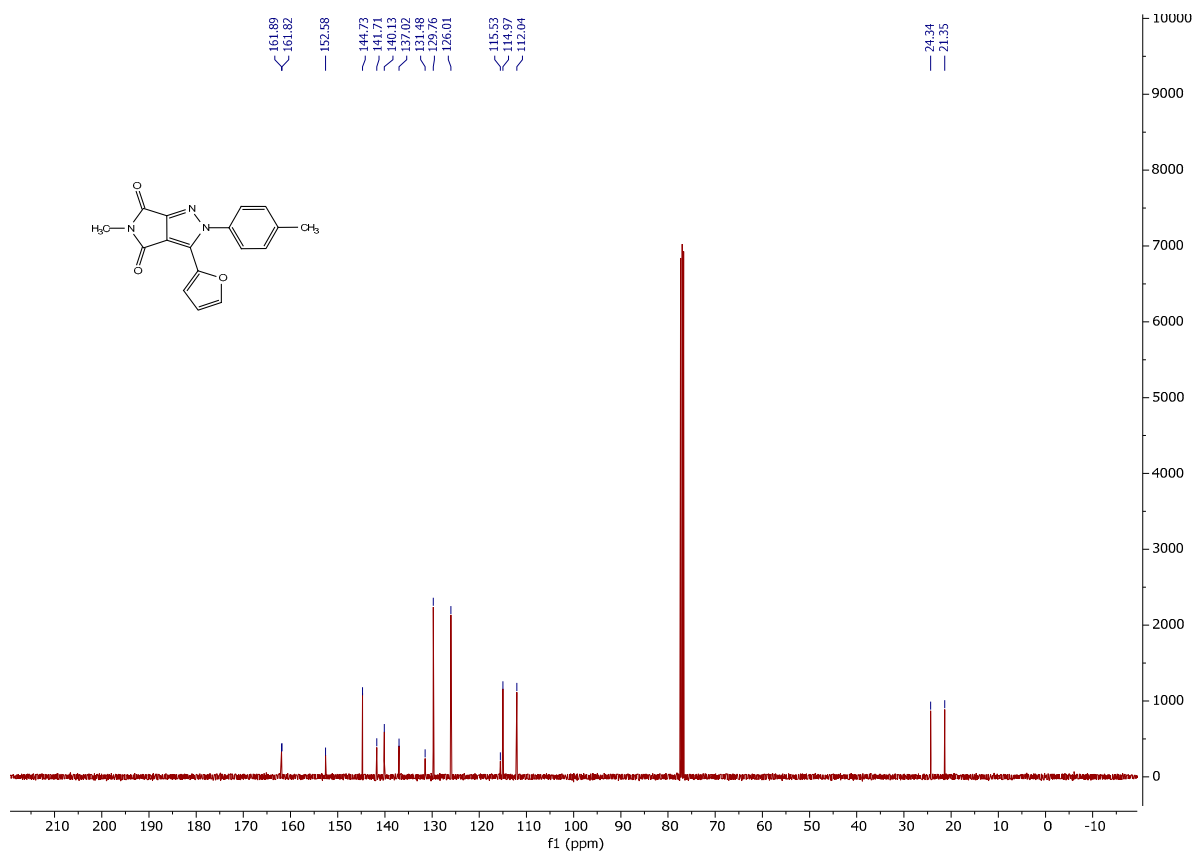
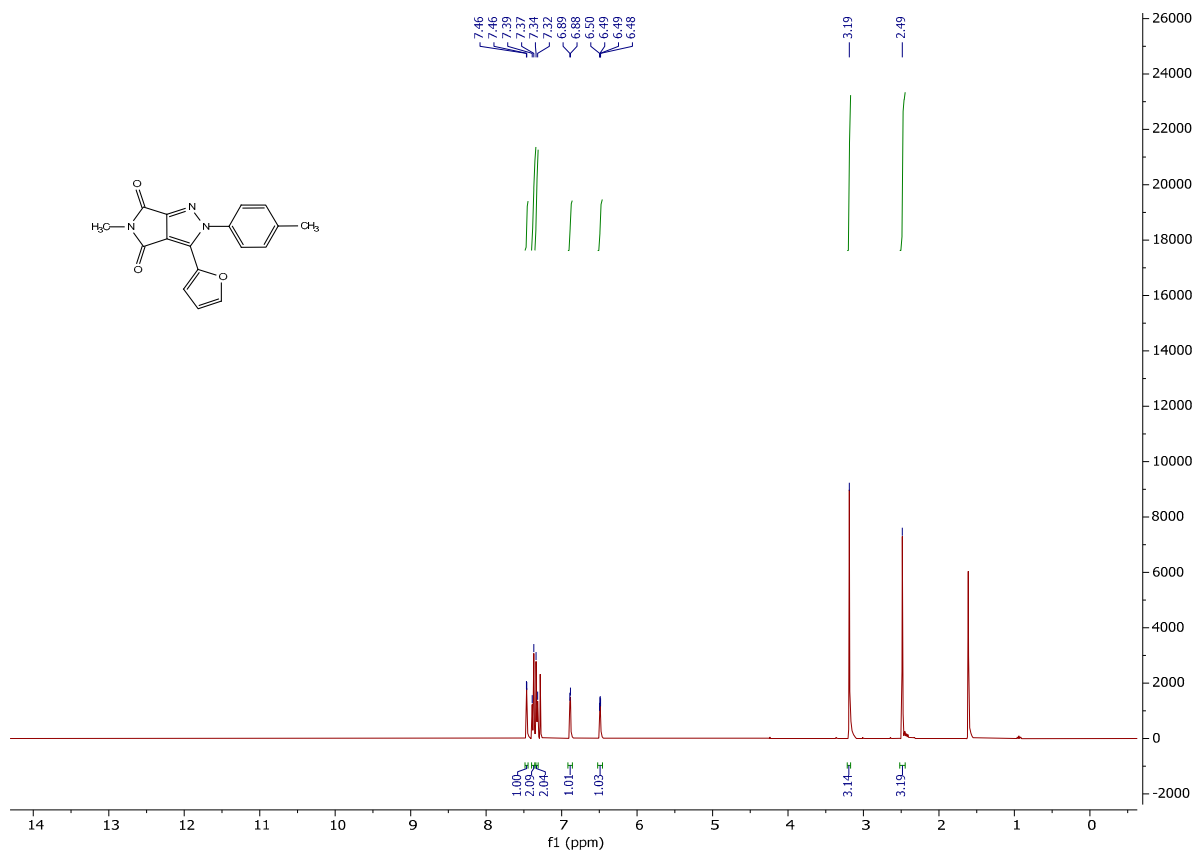
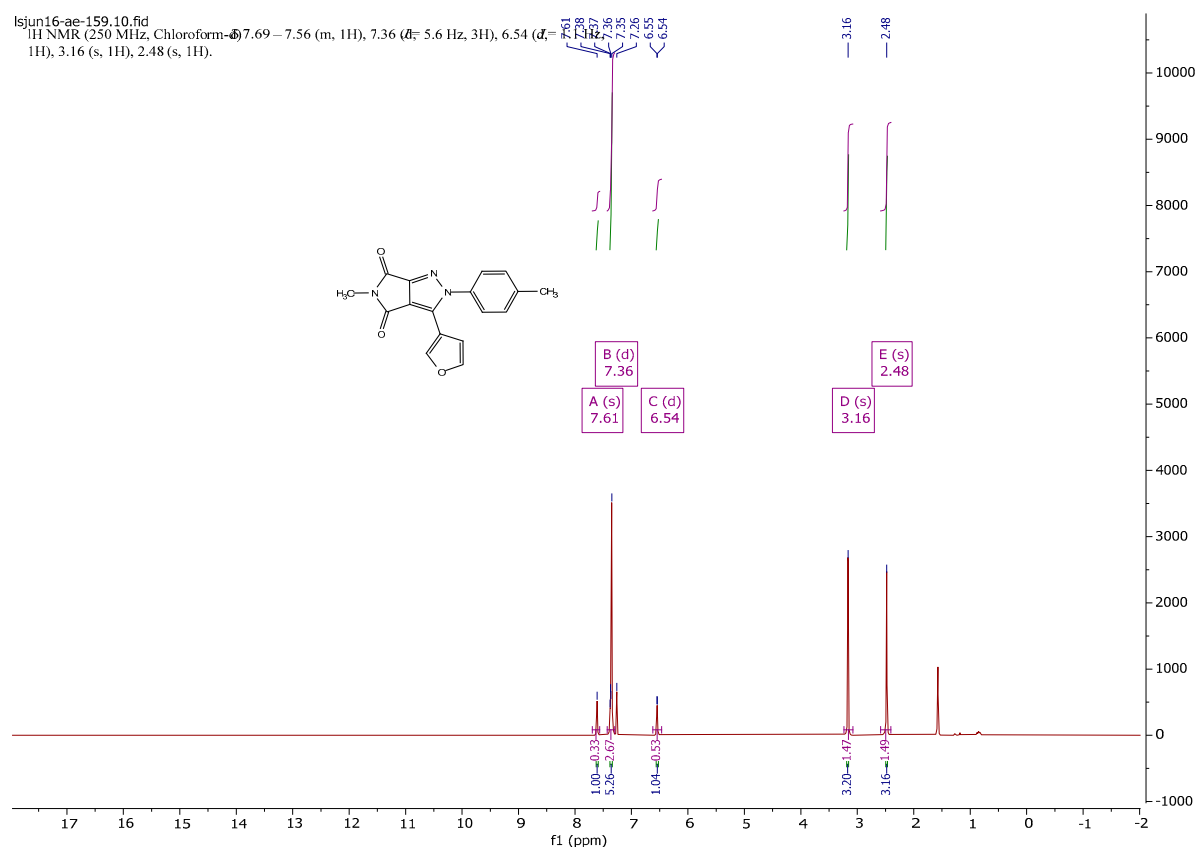


Figure S24:3-(Furan-3-yl) -5-methyl-2-(p-tolyl)pyrrolo[3,4-c]pyrazole-4,6-(2H,5H)-dione (26)

lsjun16-ae-159.10.fid

¹H NMR (250 MHz, Chloroform-d) 7.69–7.56 (m, 1H), 7.36 (d, *d* = 5.6 Hz, 3H), 6.54 (d, *d* = 5.6 Hz, 3H), 3.16 (s, 1H), 2.48 (s, 1H).



40-06-16-pos56-ae-159.12.fid

¹³C NMR (101 MHz, CDCl₃) 162.53, 162.06, 152.38, 149.80, 149.52, 149.21, 148.99, 134.55, 130.27, 126.41, 116.13, 113.56, 109.58, 24.30, 21.38.

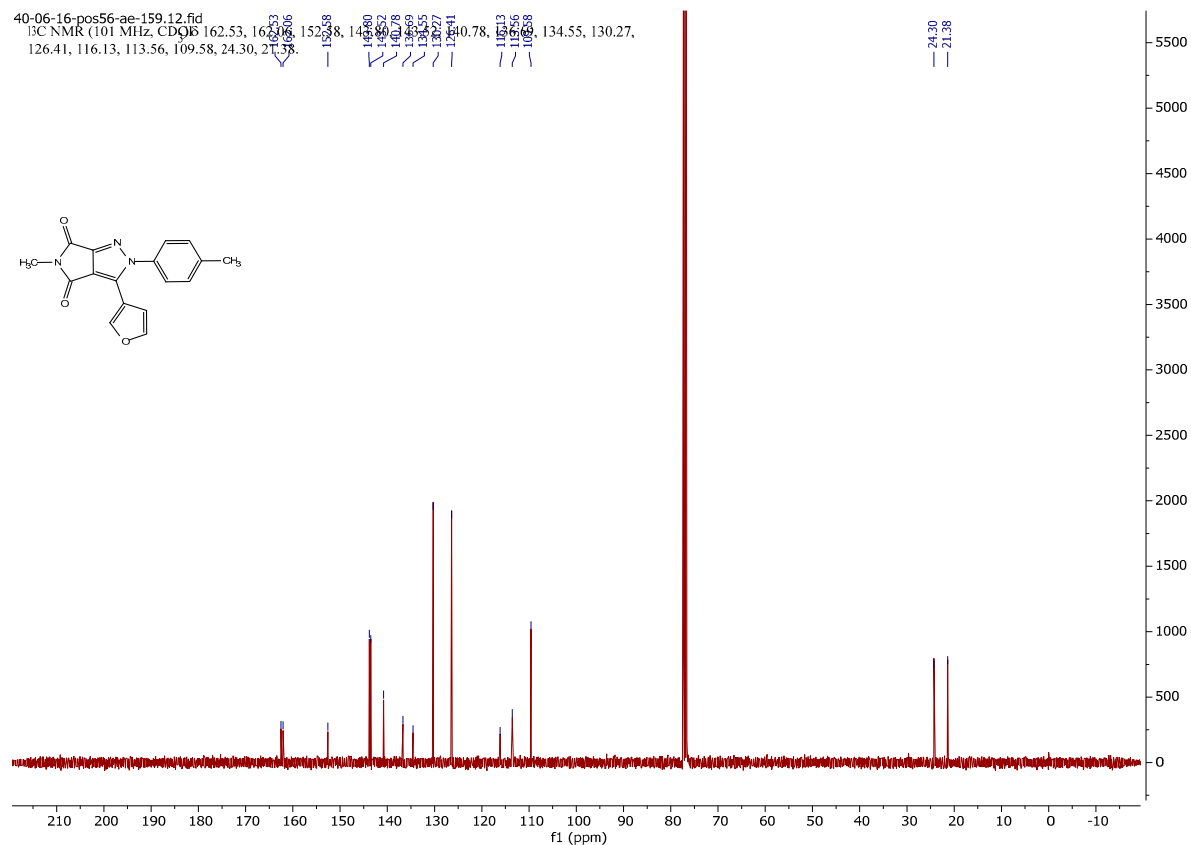


Figure S25: 5-Methyl-3-(thiophen-3-yl)-2-(p-tolyl)pyrrolo[3,4-c]pyrazole-4,6-(2H,5H)-dione (27)

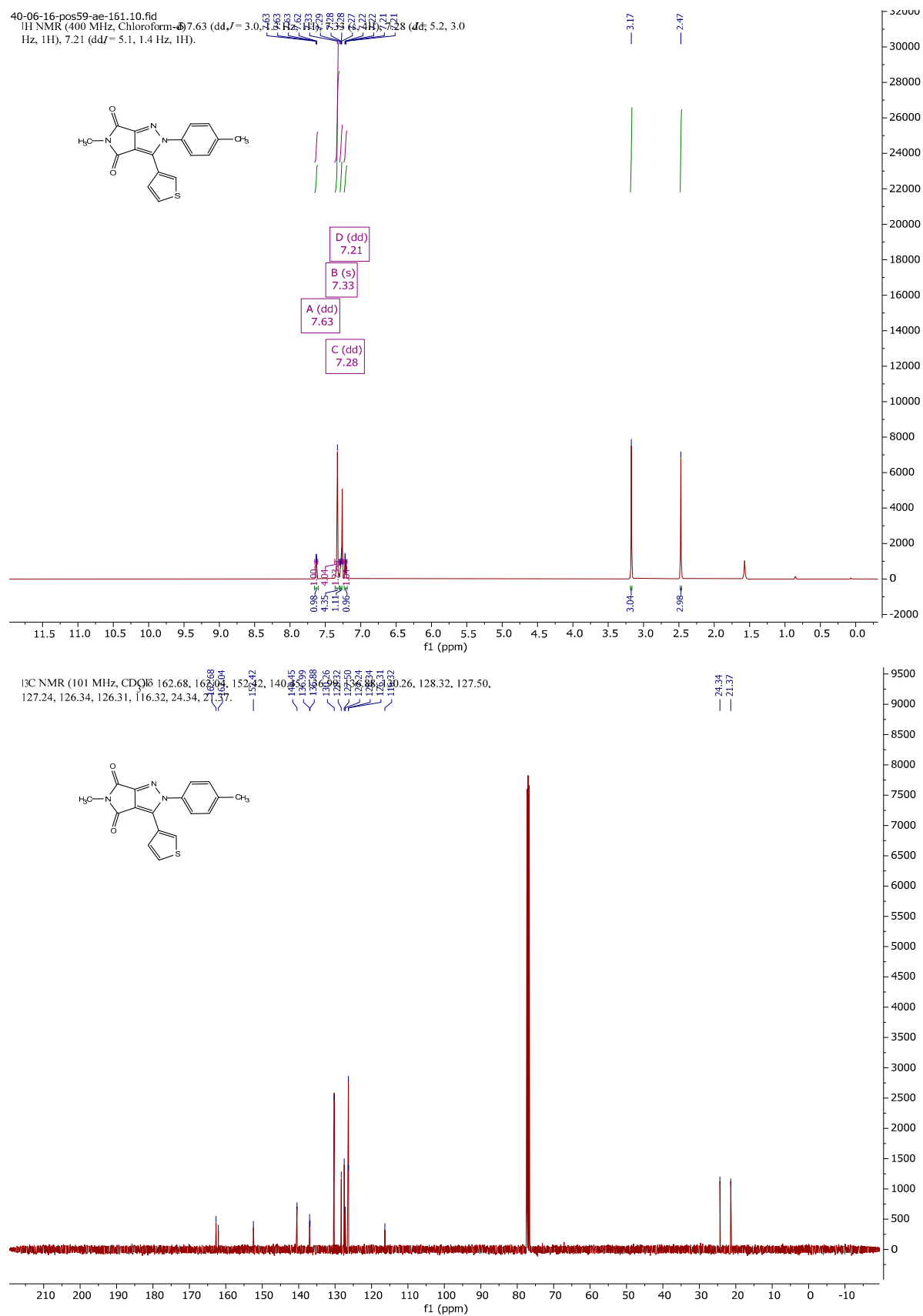


Figure S26: 5-(4-Methoxybenzyl)-2,3-di-p-tolylpyrrolo[3,4-c]pyrazole-4,6-(2*H*,5*H*)-dione (29)

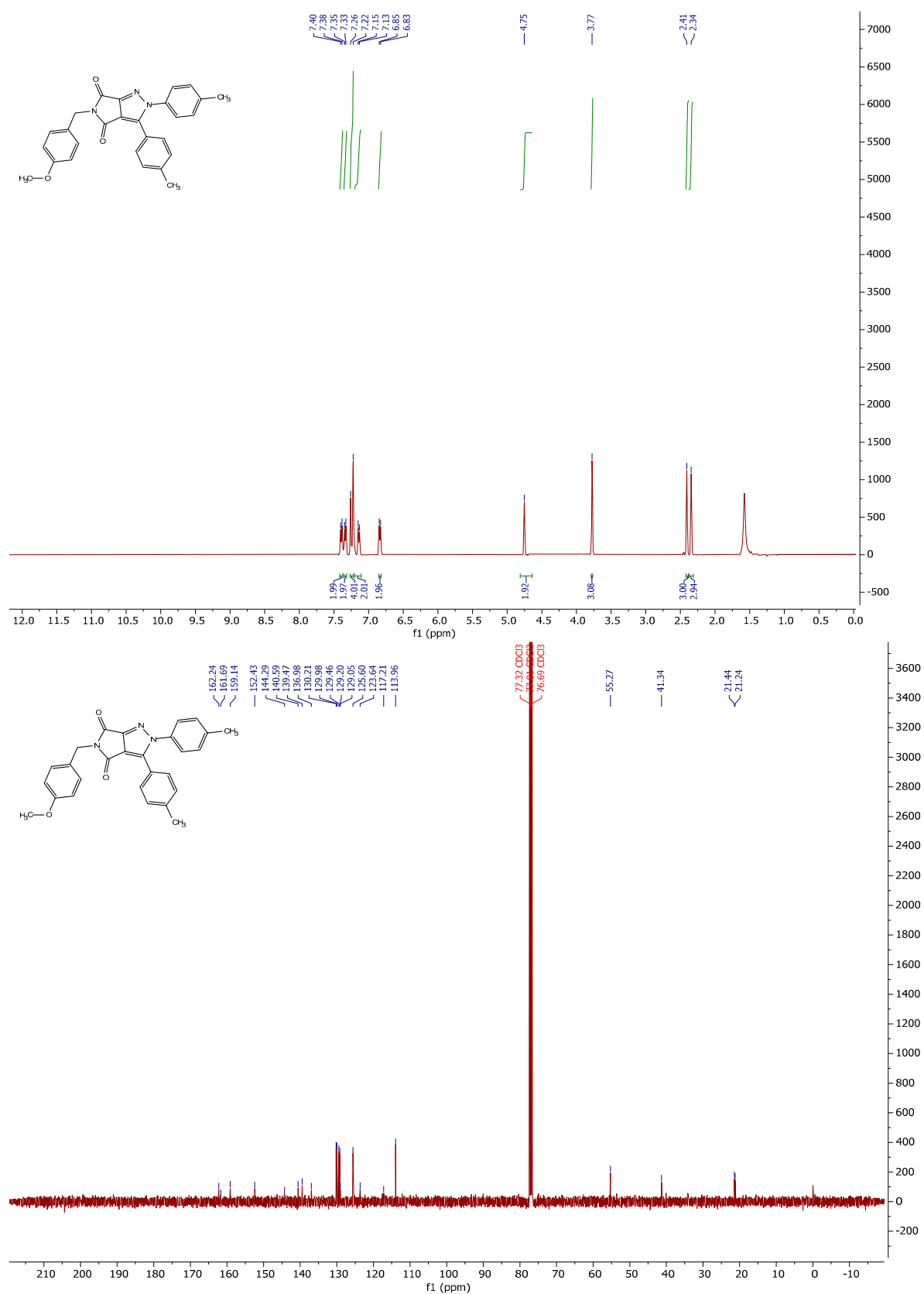


Figure S27: 5-Methyl-2-(4-nitrophenyl)-3-(p-tolyl)pyrrolo[3,4-c]pyrazole-4,6-(2*H*,5*H*)-dione (30)

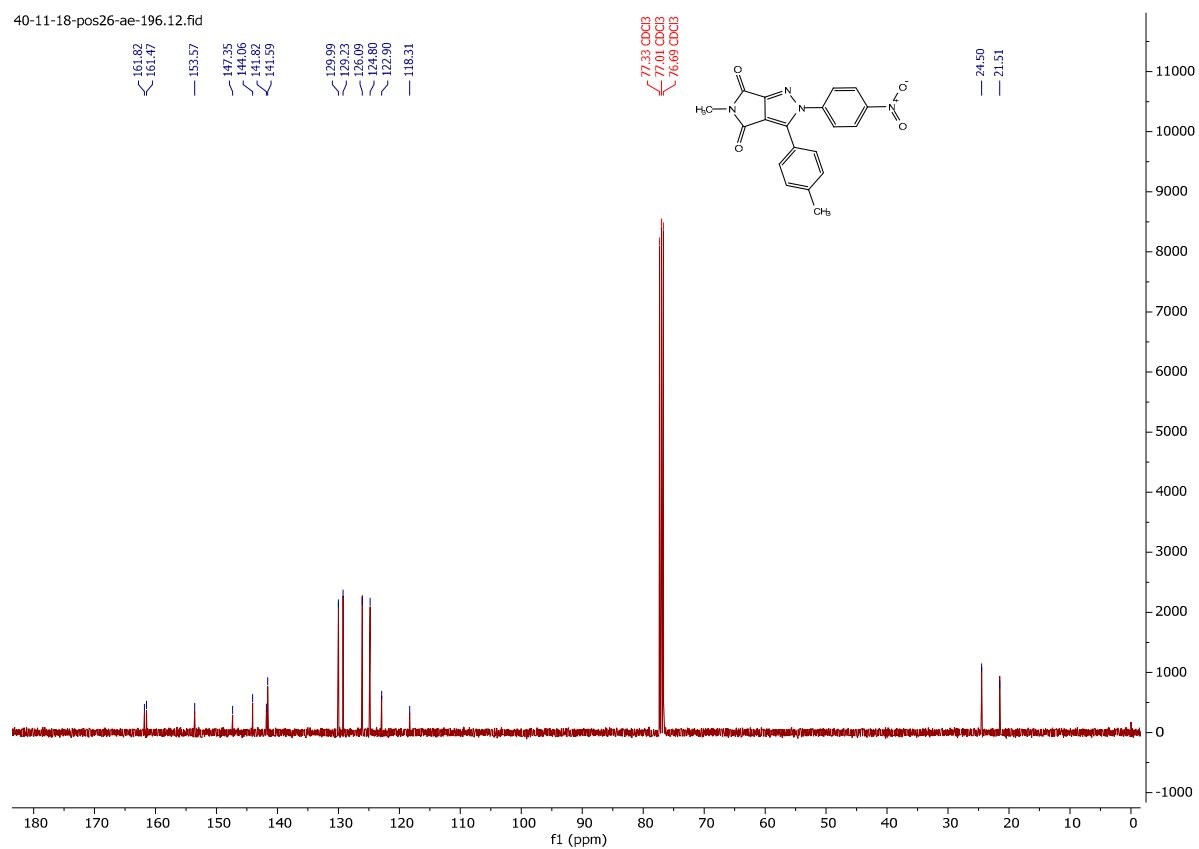
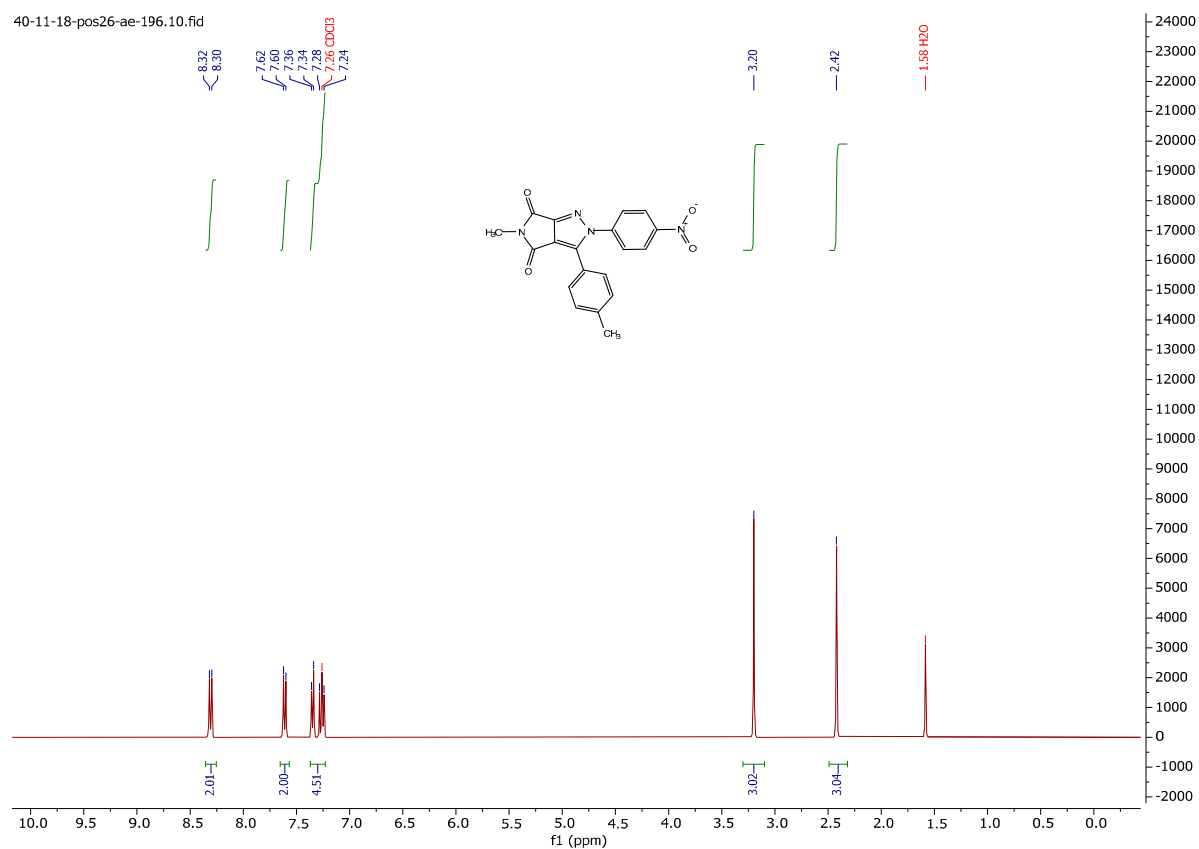


Figure S28: 5-Methyl-3-(phenylamino)-2-(p-tolyl)pyrrolo[3,4-c]pyrazole-4,6-(2H,5H)-dione (31)

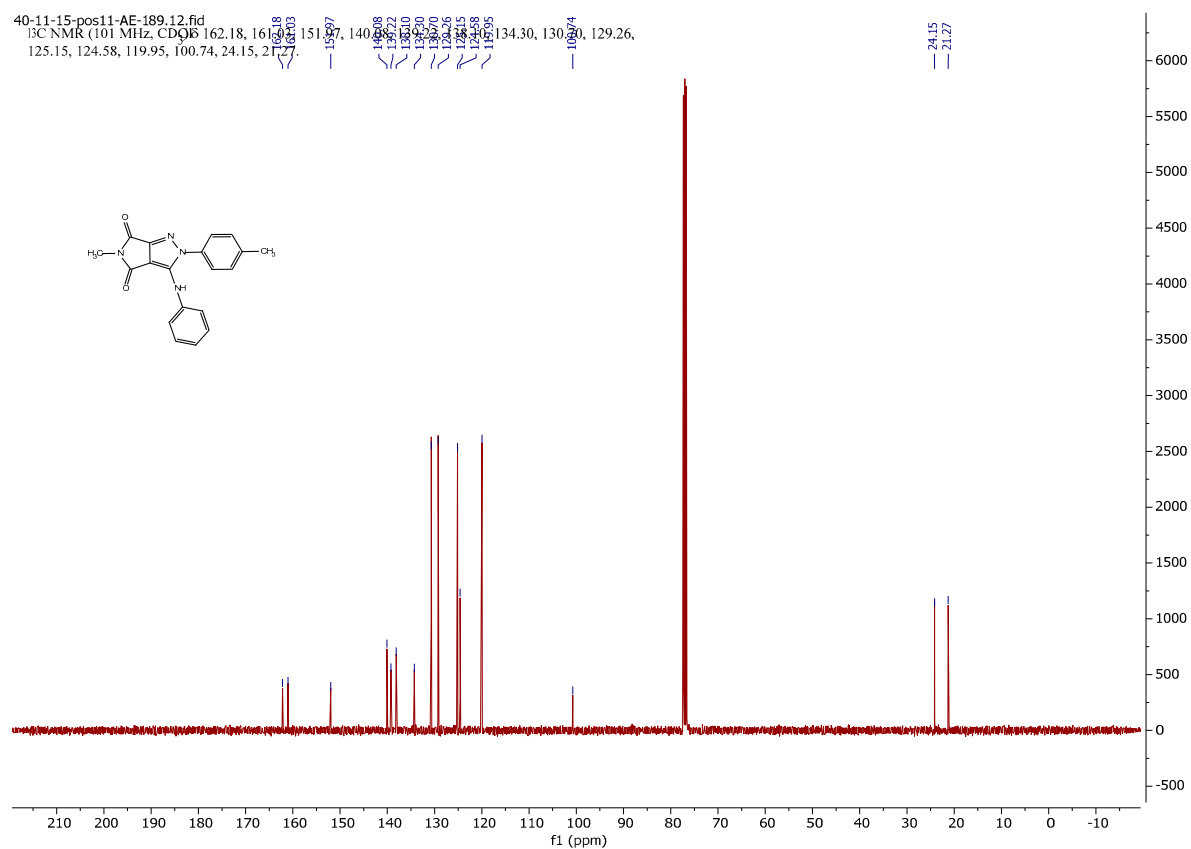
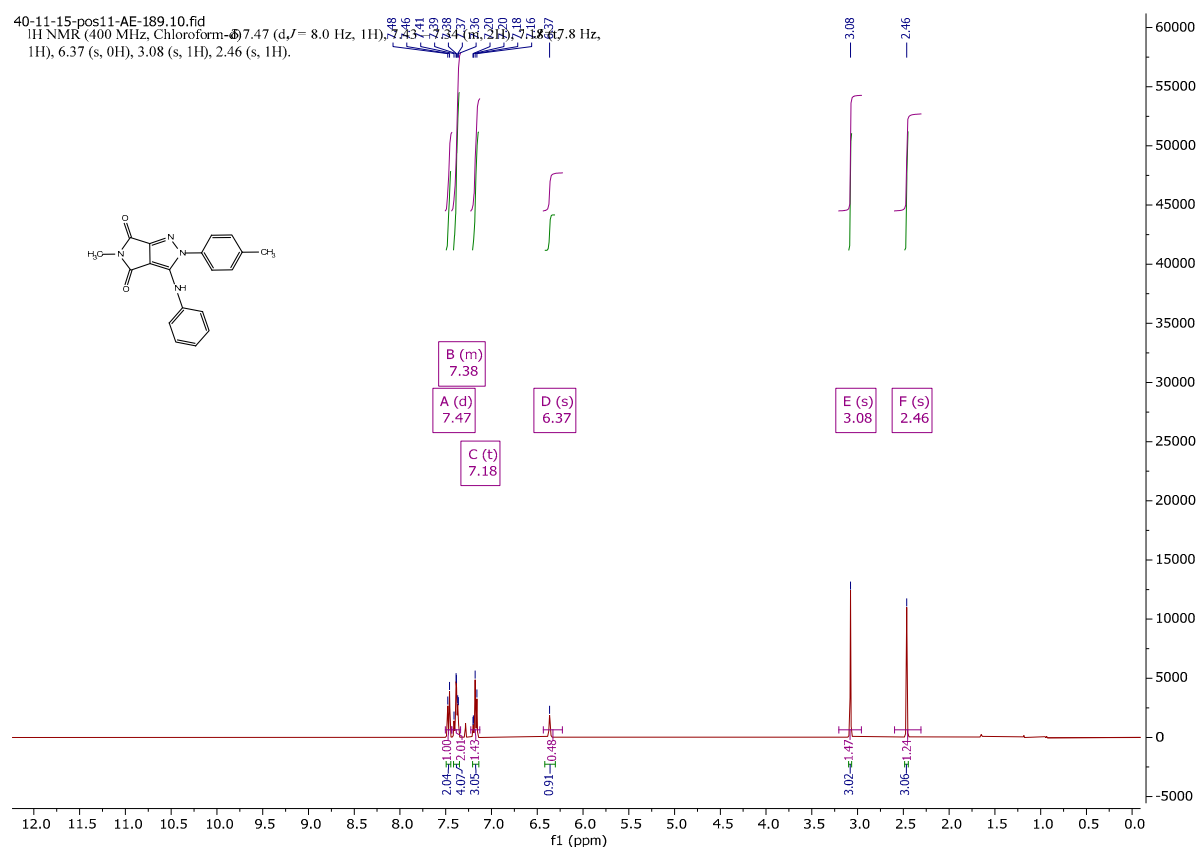
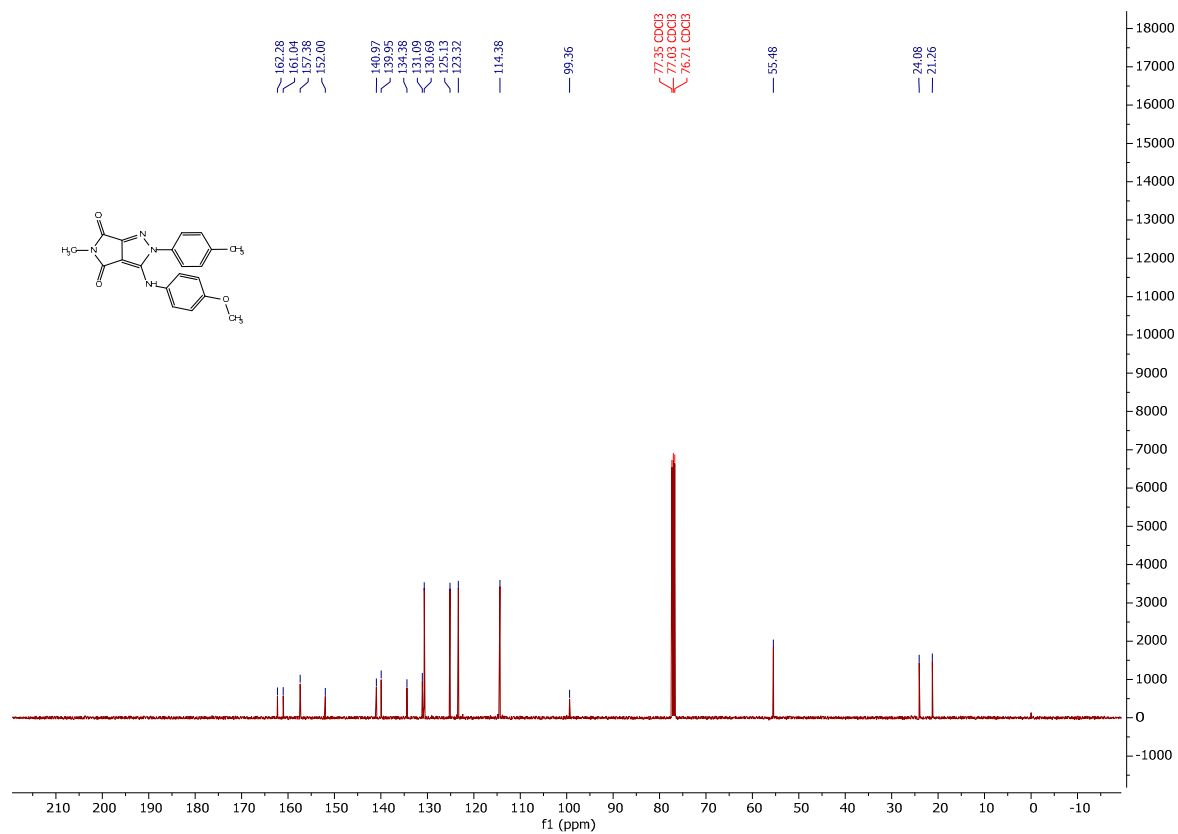
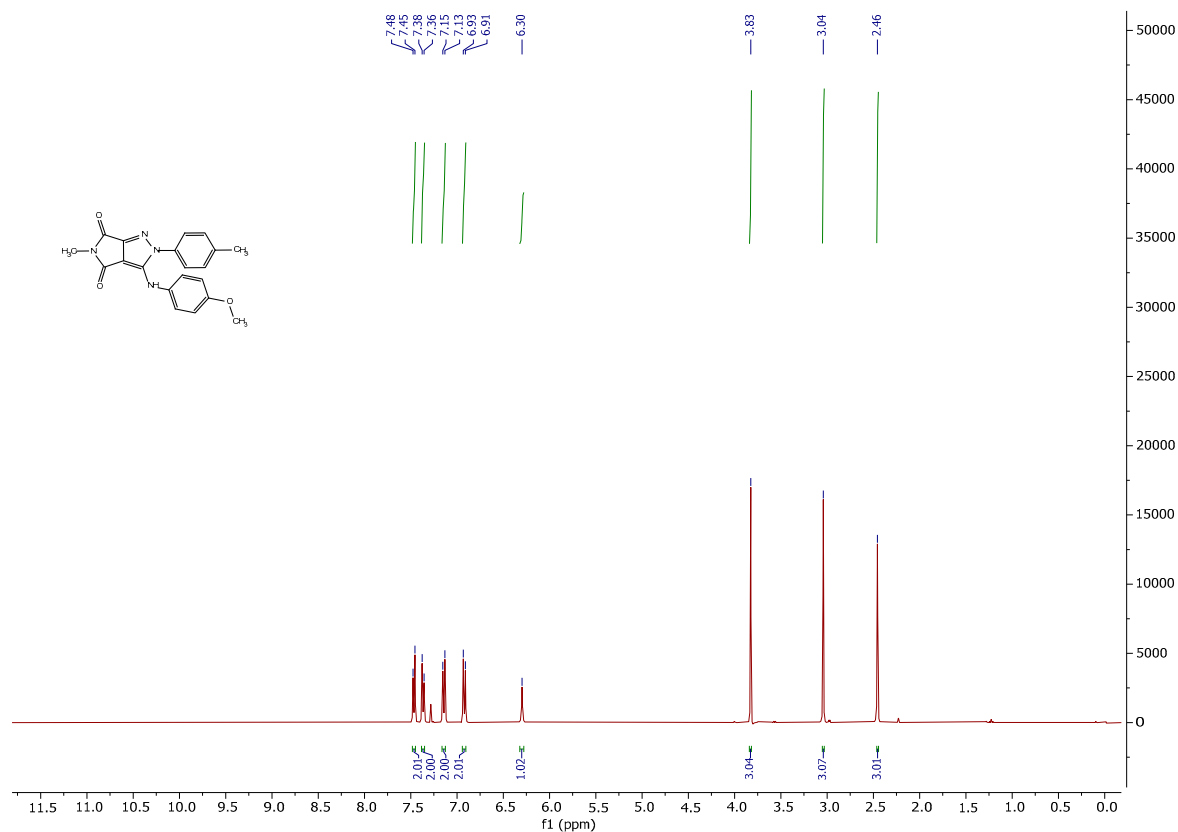


Figure S29: 3-((4-Methoxyphenyl)amino)-5-methyl-2-(p-tolyl)pyrrolo[3,4-c]pyrazole-4,6-(2H,5H)-dione (32)



¹H NMR (400 MHz, Chloroform-d) δ 7.46 (d, J = 7.8 Hz, 1H), 7.37 (d, J = 7.7 Hz, 1H), 7.33 (s, 1H), 7.26 (t, 1H), 7.22 (t, 1H), 7.17 (t, 1H), 7.04 (s, 1H), 6.77 (s, 0H), 6.70 (s, 1H), 6.39 (s, 0H), 3.83 (s, 1H), 3.09 (s, 1H), 2.46 (s, 1H).

Chemical structure of compound 10: COc1ccc(Nc2c(=O)n(C)nc2-c3ccccc3OC)nn1

Peak Label	Chemical Shift δ (ppm)	Integration
H (d)	7.37	1.12
E (s)	6.77	1.06
G (t)	7.26	1.03
D (s)	6.39	1.08
I (d)	7.46	1.00
F (t)	6.70	1.26
A (s)	3.83	1.00
B (s)	3.09	1.08
C (s)	2.46	1.21

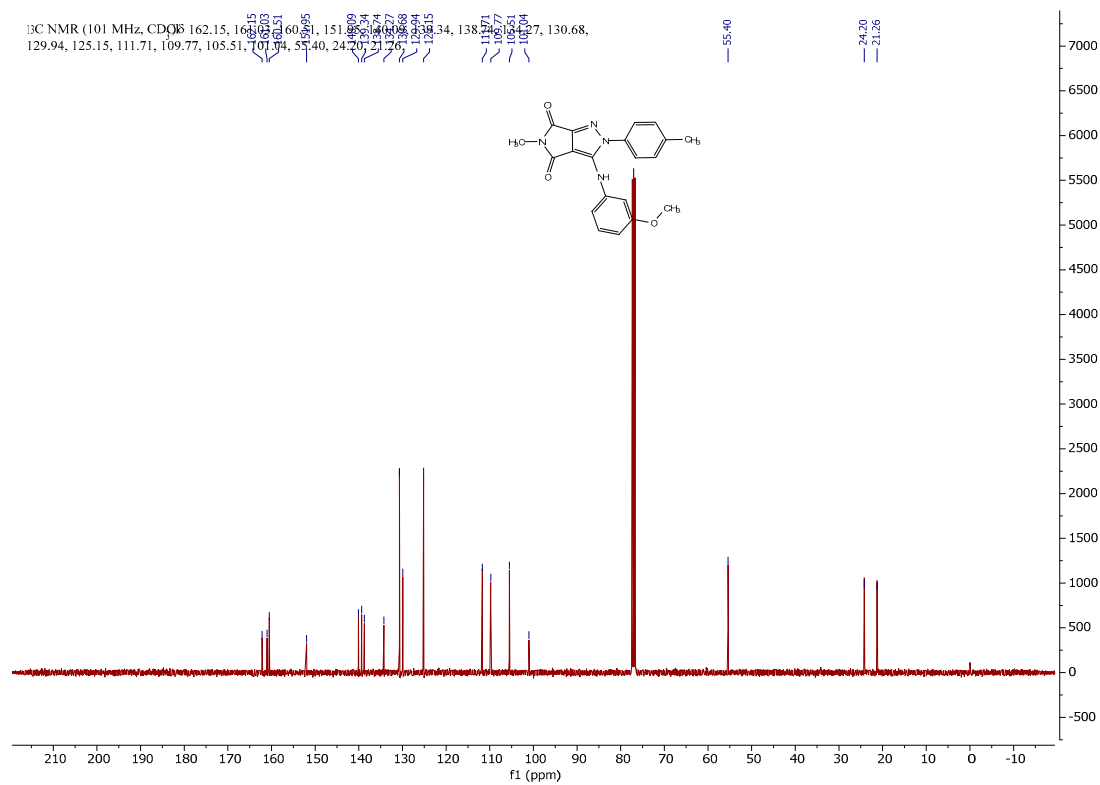


Figure S31: 3-((2-Methoxyphenyl)amino)-5-methyl-2-(p-tolyl)pyrrolo[3,4-c]pyrazole-4,6-(2*H*,5*H*)-dione (34)

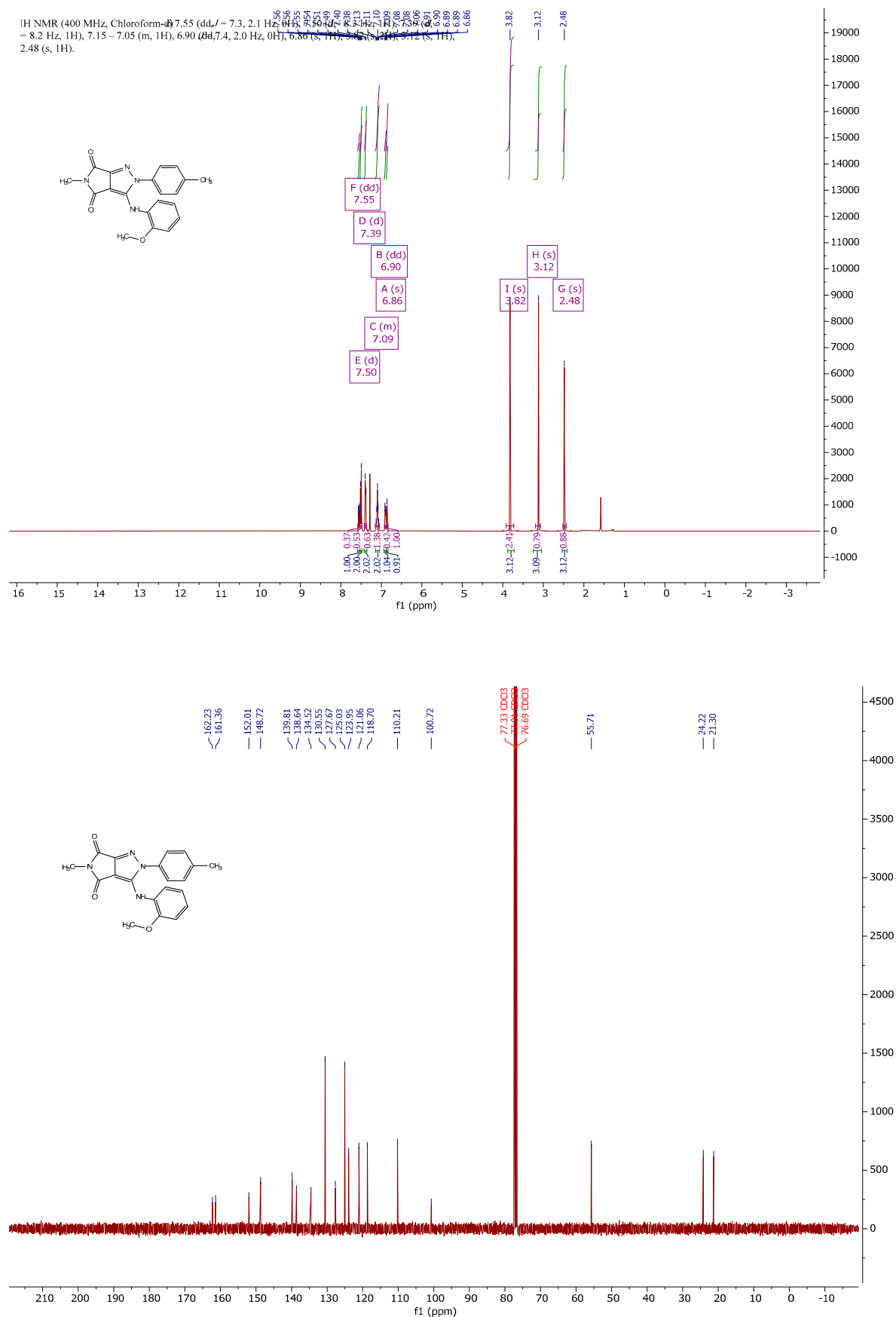


Figure S32: 5-Methyl-2-(p-tolyl)-3-((4-(trifluoromethyl)phenyl)amino)pyrrolo[3,4-c]pyrazole-4,6-(2*H*,5*H*)-dione (35)

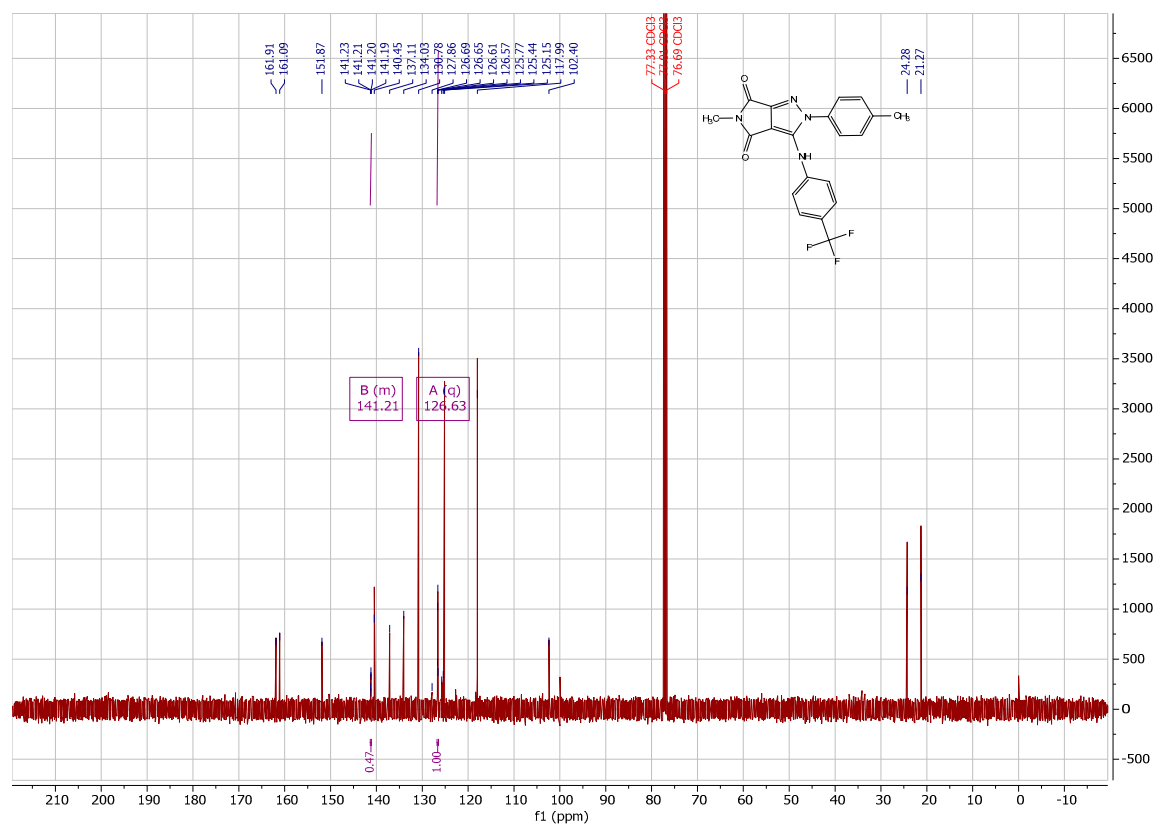
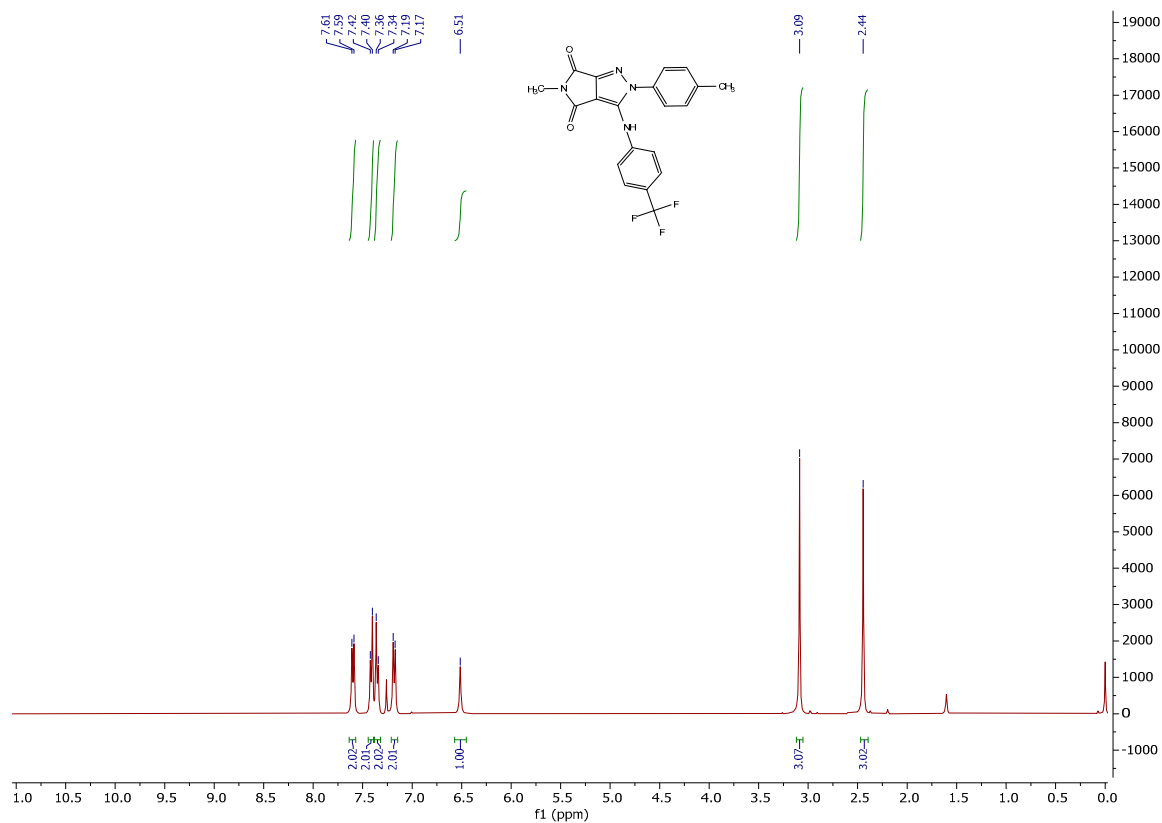


Figure S33: 5-(4-Methoxybenzyl)-3-(anilino)-2-(p-tolyl)pyrrolo[3,4-c]pyrazole-4,6-(2H,5H)-dione (39)

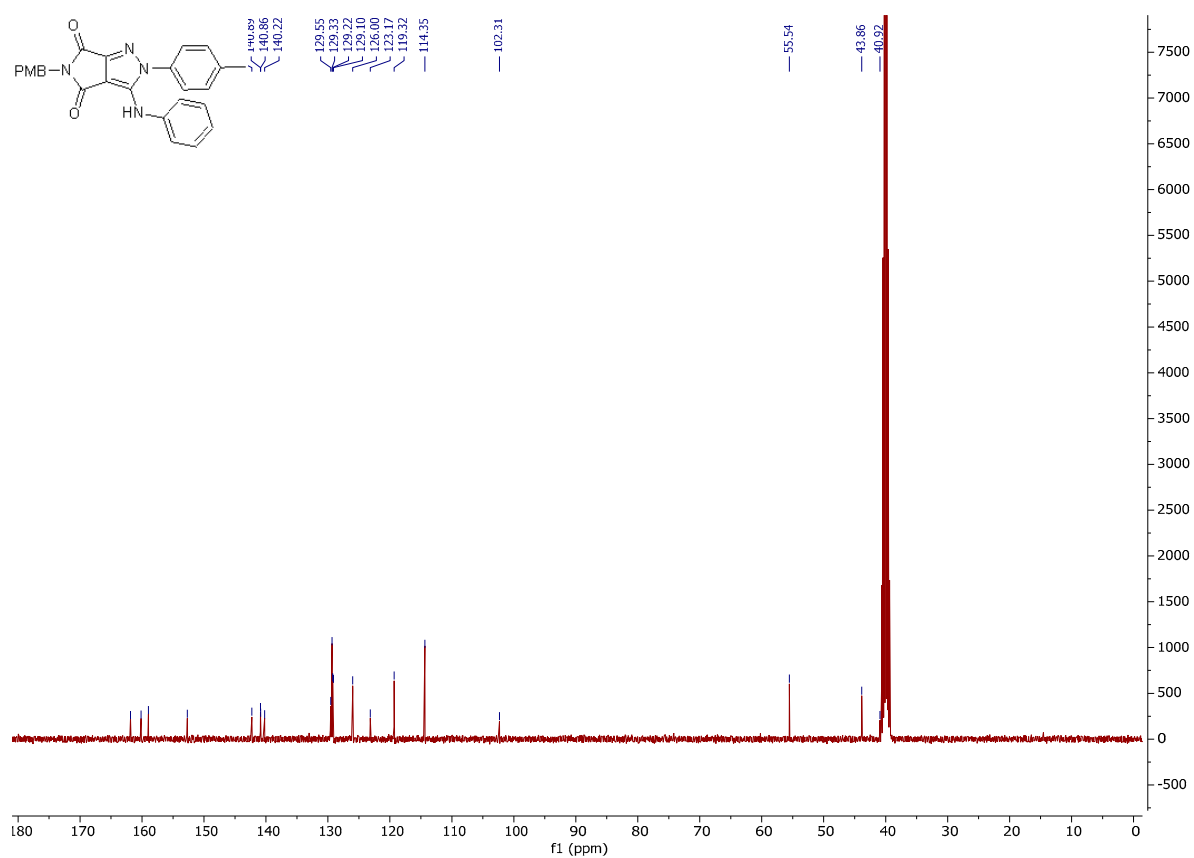
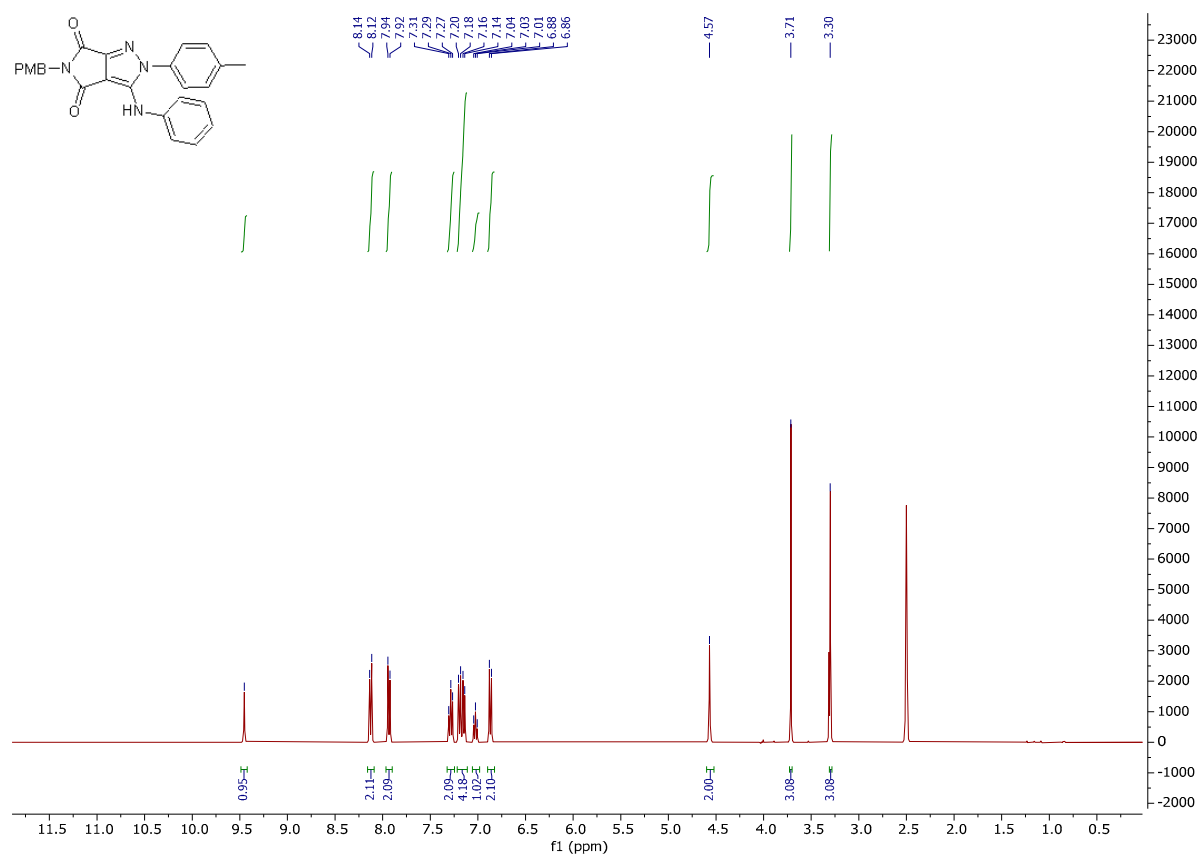


Figure S34: 5-Methyl-2-(4-nitrophenyl)-3-(phenylamino)pyrrolo[3,4-c]pyrazole-4,6-(2*H*,5*H*)-dione
(40)

