

Boulton–Katritzky rearrangement of 5-substituted phenyl-3-[2-(morpholin-1-yl)ethyl]-1,2,4-oxadiazoles as a synthetic path to spiropyrazoline benzoates and chloride with antitubercular properties

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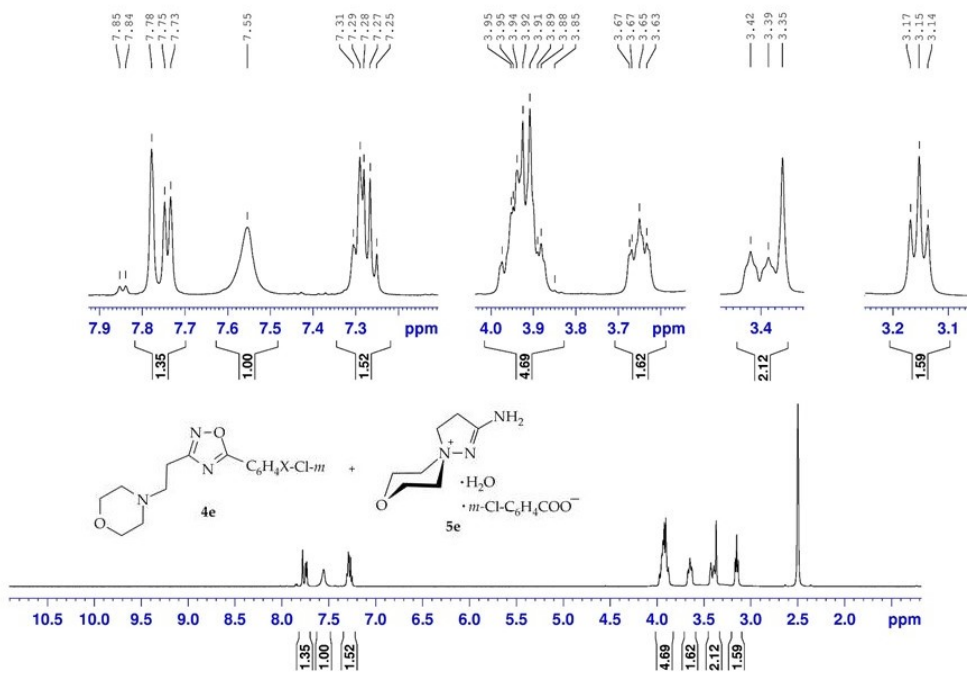
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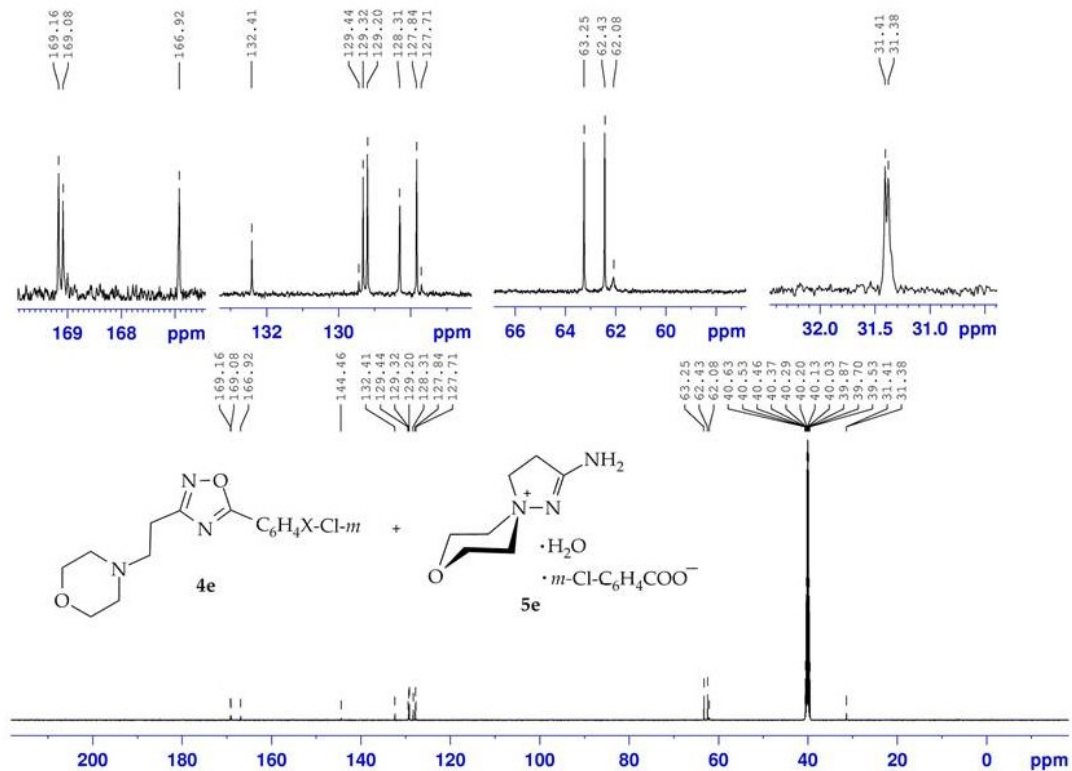
Table S1. Experimental details and crystallographic information for **5c-e**, **6**.

	5c ·H ₂ O	5d	5e ·H ₂ O	6 ·H ₂ O
Formula	C ₁₄ H ₂₁ N ₃ O ₄	C ₁₄ H ₁₈ BrN ₃ O ₃	C ₁₄ H ₂₀ ClN ₃ O ₄	C ₇ H ₁₆ ClN ₃ O ₂
Formula weight	295.34	356.22	329.78	209.68
Space group	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁	<i>C</i> 2/ <i>c</i>	<i>P</i> 2 ₁ / <i>c</i>
a (Å)	7.4202(6)	12.9674(11)	11.0930(7)	7.9085(4)
b (Å)	7.8105(6)	8.2138(7)	10.8351(7)	15.5190(7)
c (Å)	26.369(2)	14.9276(12)	26.8924(16)	9.2443(4)
β (°)	93.132(2)	106.429(2)	98.765(1)	114.271(1)
V (Å ³)	1525.9(2)	1525.0(2)	3194.6(3)	1034.29(8)
Z	4	4	8	4
μ (mm ⁻¹)	0.095	2.709	0.261	0.345
d _{calc} (g cm ⁻³)	1.286	1.551	1.371	1.347
F(000)	632	728	1392	448
No. of measured rfls.	12067	27516	22187	13144
No. of independent rfls. (R _{int})	3301 (0.0265)	13586 (0.044)	5122 (0.025)	3014 (0.024)
No. of observed rfls. [I > 2σ(I)]	2892	9578	4656	2721
No. of parameters	206	379	215	134
Goodness-of-fit	1.03	0.99	1.08	1.03
R ₁ [I > 2σ(I)]	0.038	0.045	0.036	0.035
wR ₂ [all data]	0.099	0.105	0.091	0.085
ΔQ _{max} , ΔQ _{min} (eÅ ⁻³)	0.71, -0.21	1.49, -0.86	0.45, -0.35	0.39, -0.21

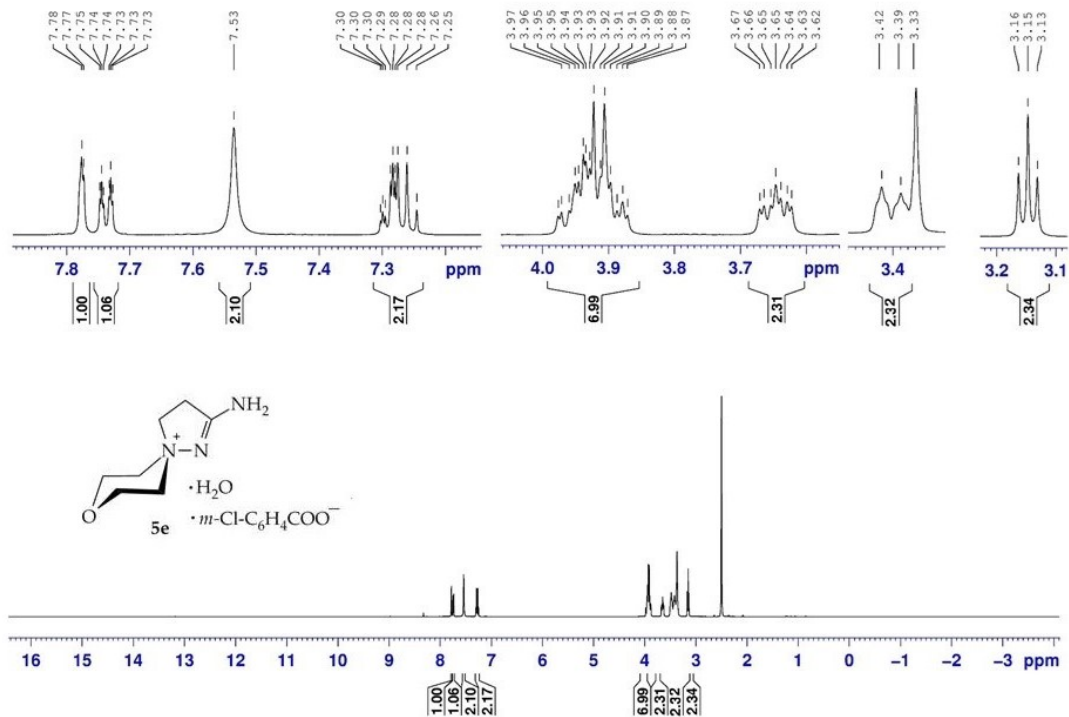
Avance III 500 ^1H NMR **4e+5e** in DMSO-d_6



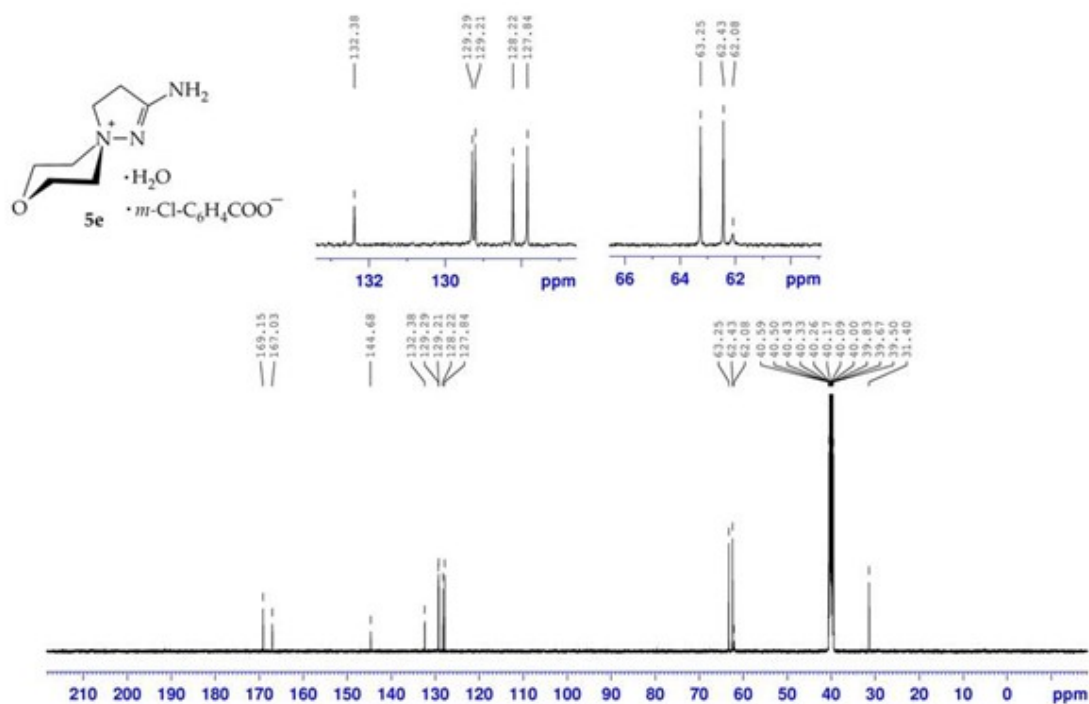
Avance III 500 ^{13}C NMR **4e** + **5e** in DMSO-d_6



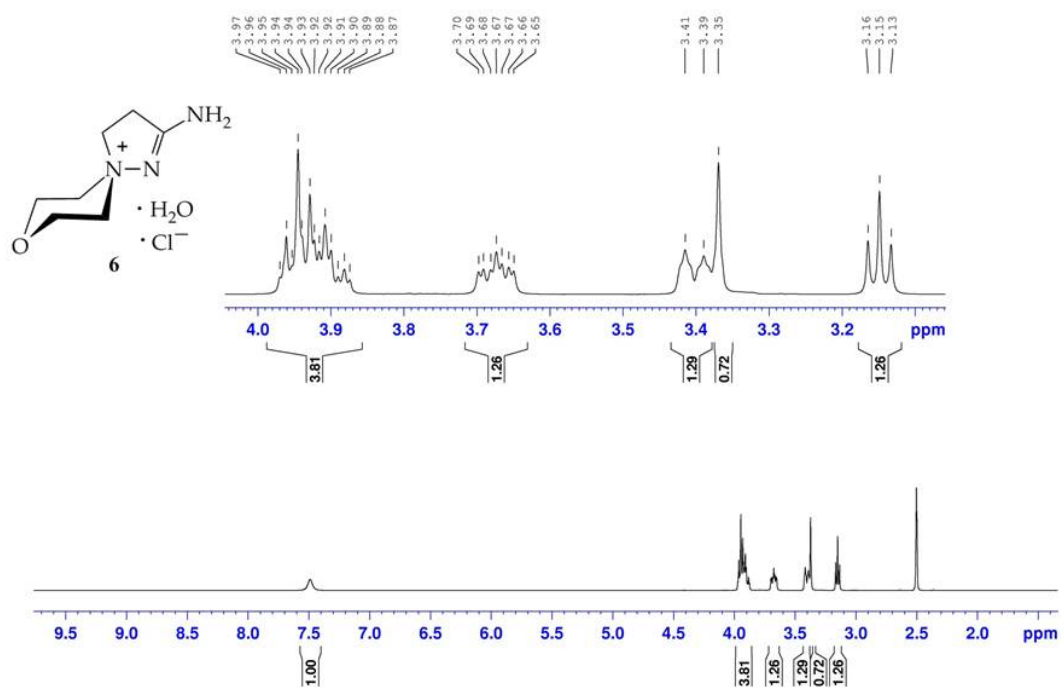
Avance III 500 ^1H NMR **5e** in DMSO-d_6



Avance III 500 ^{13}C NMR **5e** in DMSO- d_6



Avance III 500 ^1H NMR **6** in DMSO- d_6



Avance III 500 ^{13}C NMR 6 in DMSO- d_6

