Chemistry of Heterocyclic Compounds **2019**, *55*(8), 000-000

STRATEGY FOR THE PALLADIUM(II)-CATALYZED OXIDATIVE C–H/N–H CROSS-COUPLING OF 2*H*-IMIDAZOLE 1-OXIDE WITH AZOLES IN THE DESIGN OF NOVEL BIHETEROCYCLIC SYSTEMS

SUPPLEMENTARY INFORMATION

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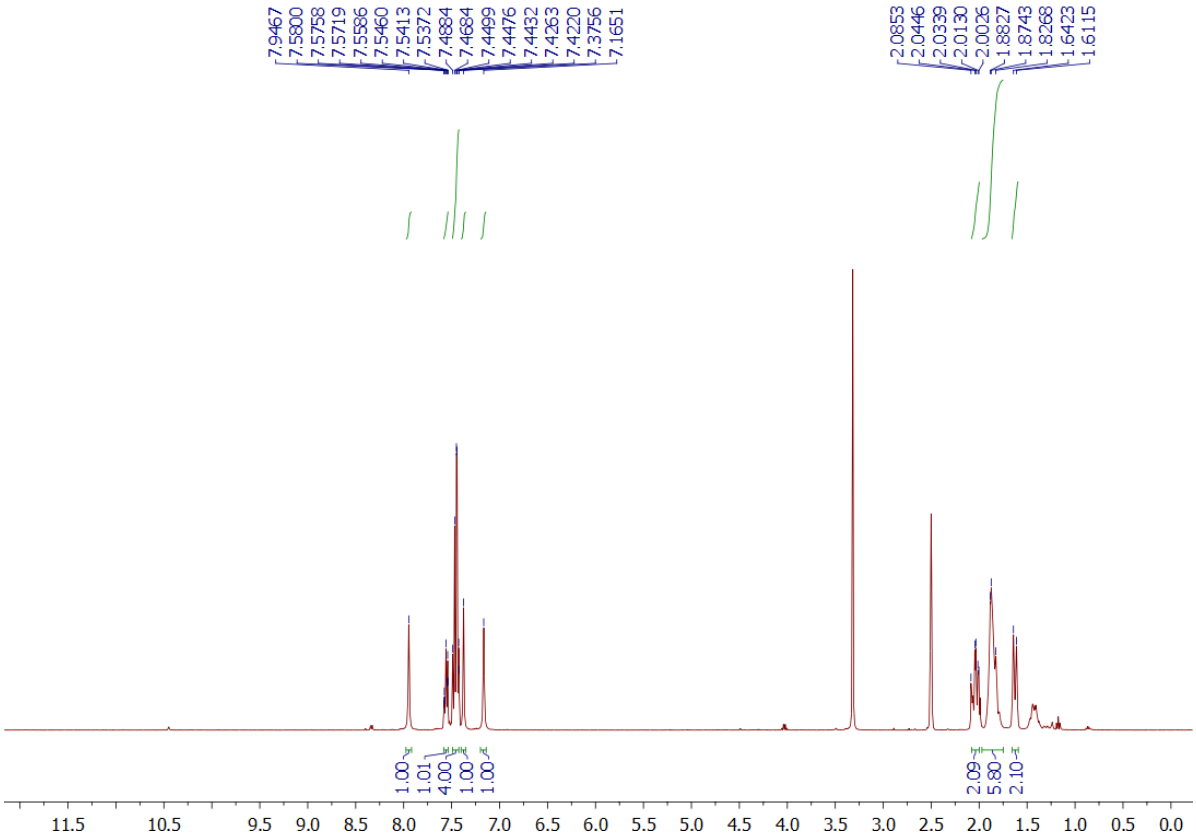

Fig. S1. ^{1}H NMR spectra (DMSO-d_6, 400 MHz) of 2-(1*H*-imidazol-1-yl)-3-phenyl-1,4-diazaspiro[4.5]deca-1,3-diene 1-oxide (**3**)

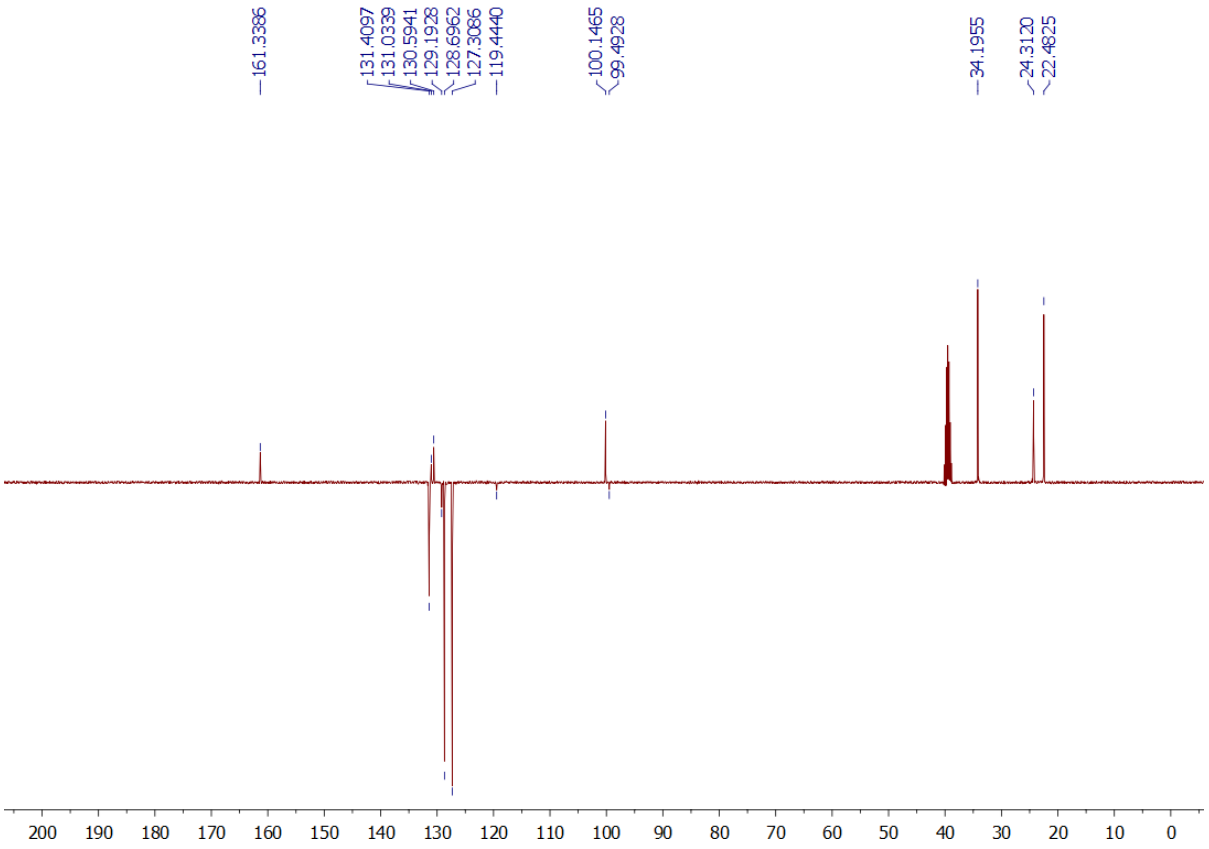

Fig. S2. ^{13}C NMR spectra (APT, DMSO-d_6, 100 MHz) of 2-(1*H*-imidazol-1-yl)-3-phenyl-1,4-diazaspiro[4.5]deca-1,3-diene 1-oxide (3)

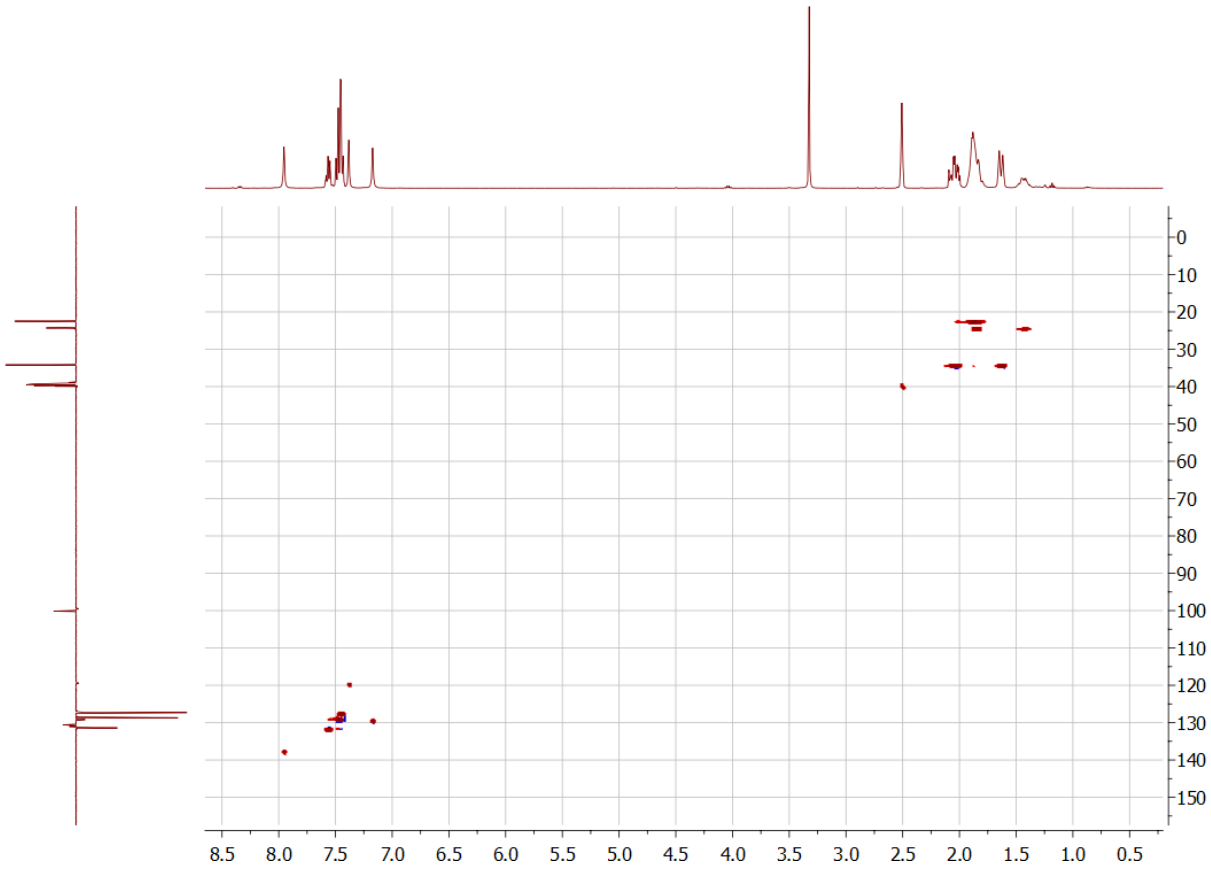

Fig. S3. ^{1}H–^{13}C HSQC spectra of 2-(1*H*-imidazol-1-yl)-3-phenyl-1,4-diazaspiro[4.5]deca-1,3-diene 1-oxide (3)

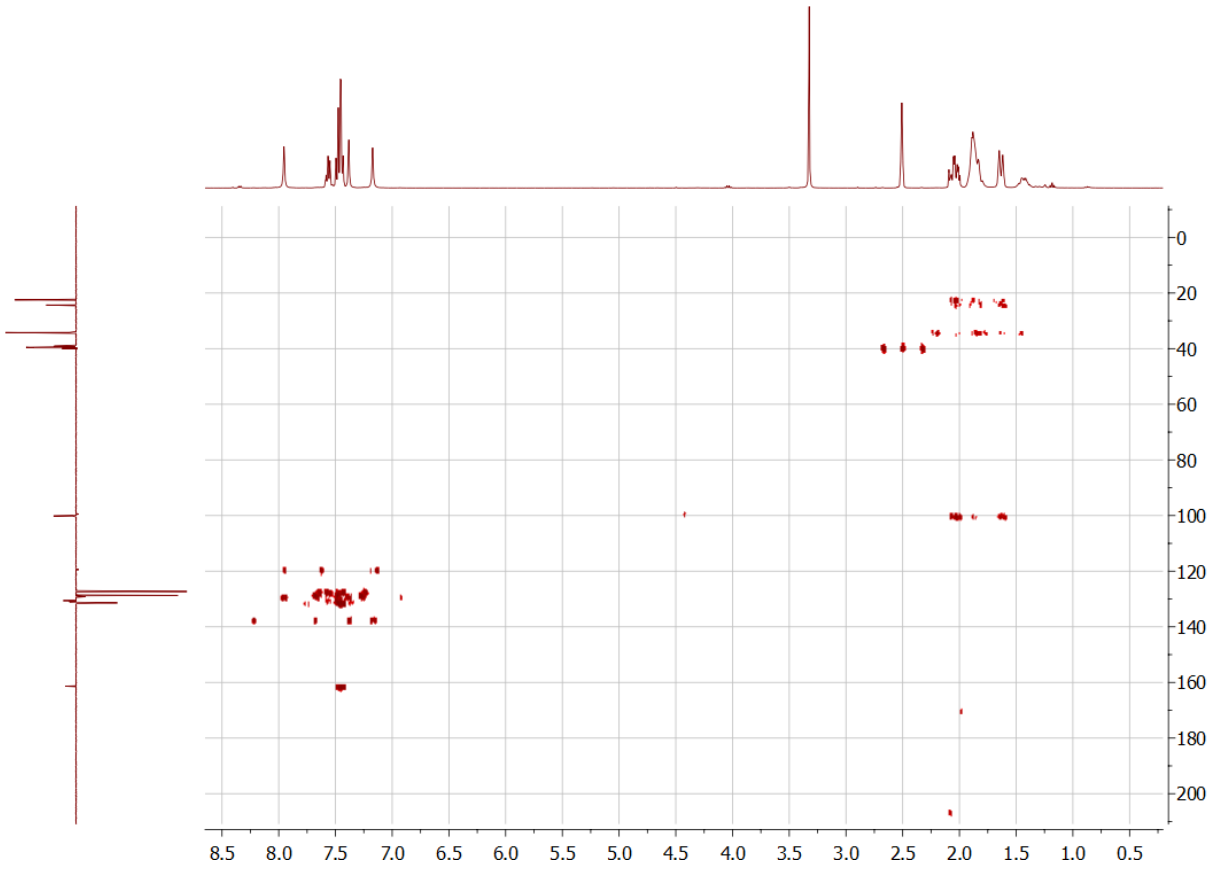

Fig. S4. $^{1}H–^{13}C$ HMBC spectra of 2-(1*H*-imidazol-1-yl)-3-phenyl-1,4-diazaspiro[4.5]deca-1,3-diene 1-oxide (3)

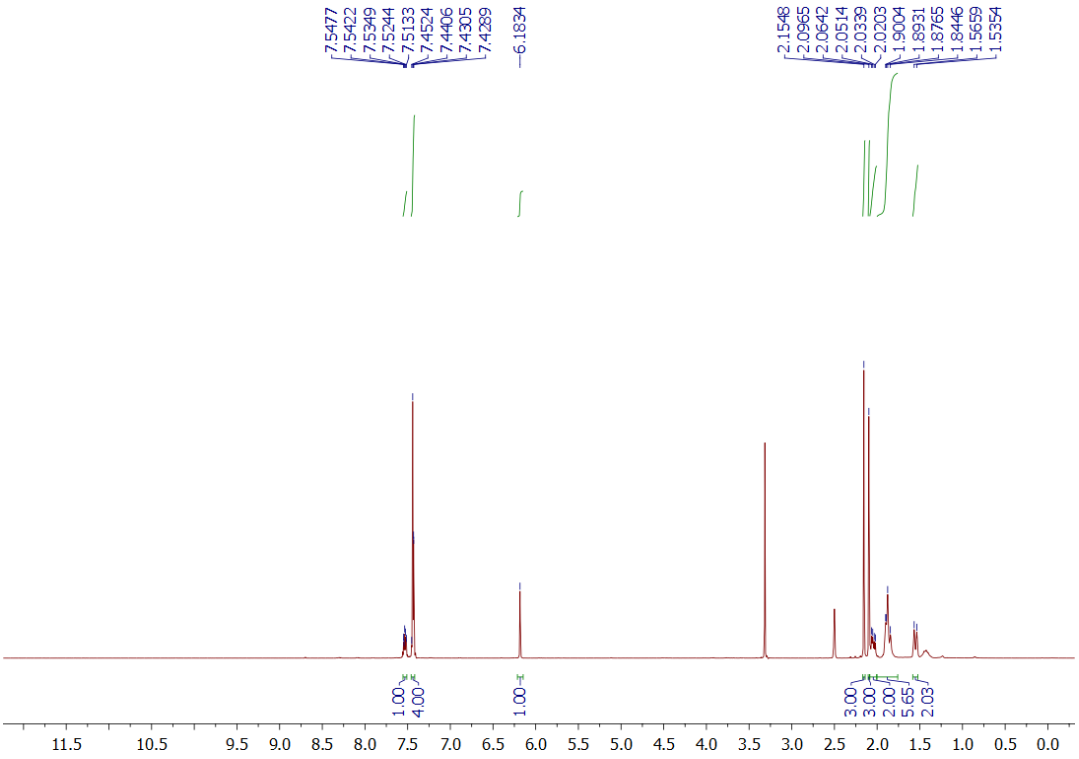

Fig. S5. ^{1}H NMR spectra (DMSO-d_6, 400 MHz) of 2-(3,5-dimethyl-1*H*-pyrazol-1-yl)-3-phenyl-1,4-diazaspiro[4.5]deca-1,3-diene 1-oxide (5)

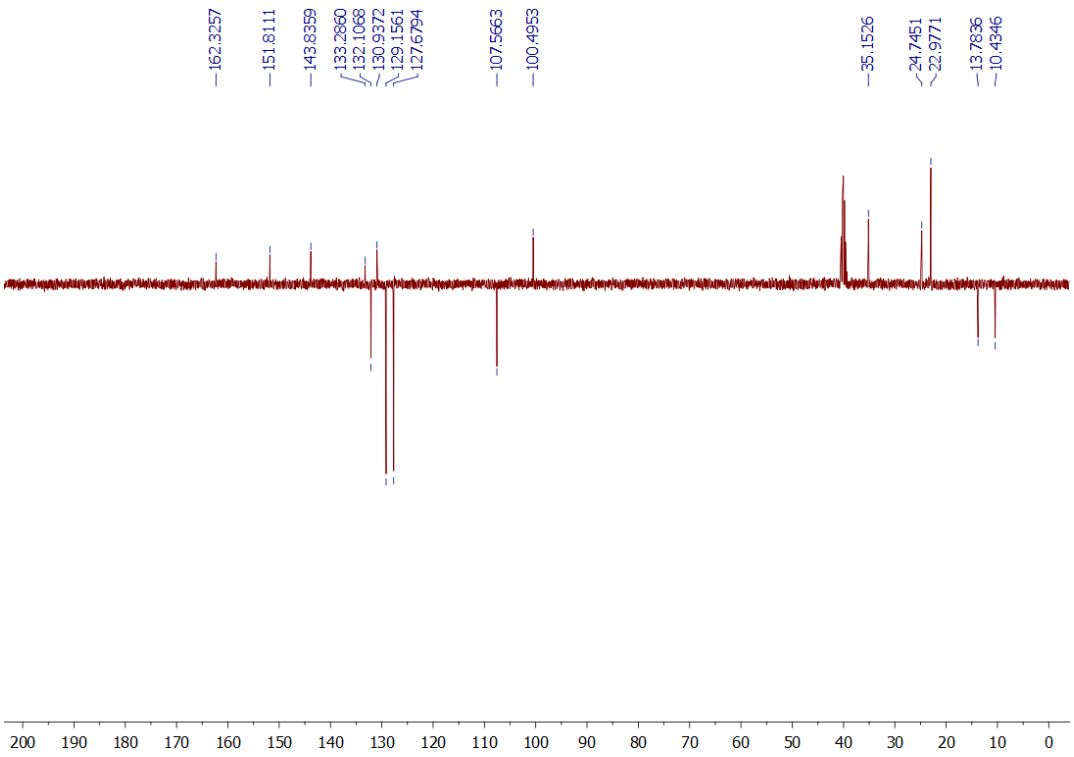

Fig. S6. ^{13}C NMR spectra (APT, DMSO-d_6, 100 MHz) of 2-(3,5-dimethyl-1*H*-pyrazol-1-yl)-3-phenyl-1,4-diazaspiro[4.5]deca-1,3-diene 1-oxide (5)

X-Ray Analysis Data

The crystallographic data and basic refinement parameters for 2-(1*H*-imidazol-1-yl)-3-phenyl-1,4-diazaspiro[4.5]deca-1,3-diene 1-oxide **3** are shown in Table S1.

Table S1. X-ray analysis data and basic refinement parameters for **3**

Parameter	3
Molecular formula	$C_{17}H_{18}N_4O$
Molecular weight	294.35
T/K	295(2)
λ/Å	1.54184
Syngony	orthorombic
Space group	P2(1)2(1)2(1)
a/Å	7.102(6)
b/Å	11.937(11)
c/Å	17.074(12)
α/deg	90.00
β/deg	90.00
γ/deg	90.00
V/Å^3	1448(2)
Z	4
d_{calc}/g·cm^{-3}	1.351
μ/mm^{-1}	0.701
F(000)	624
Crystal size/mm	0.25×0.12×0.04
2θ-Scan range/deg	3.201–65.46
Completeness based on $2\theta_{max}$	0.976
Completeness based on 2θ = 52°	0.976
hkl ranges	$-8 < h < 8$ $-12 < k < 14$ $-19 < l < 20$
Total number of reflections	11457
Number of independent reflections	2468
Number of reflections with $I > 2\sigma(I)$	7756
Number of refined parameters	212
Absorption correction	multi-scan
GOOF (based on F^2)	1.000
R factors (based on reflections with $I > 2\sigma(I)$)	
R_1	0.0295
wR^2	0.0784
R factors (based on all reflections)	
R_1	0.0326
wR^2	0.0800
$\Delta\rho_{max}$ / $\Delta\rho_{min}$, eÅ^{-3}	0.127 / –0.118

Crystallographic data (excluding structure factors) for the structure 2-(1*H*-imidazol-1-yl)-3-phenyl-1,4-diazaspiro[4.5]deca-1,3-diene 1-oxide **3** in this paper has been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC 1908421. Copies of the data can be obtained, free of charge, on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK, (fax: +44 (0)1223 336033 or e-mail: deposit@ccdc.cam.ac.uk)