Palladium-catalyzed C(sp$^2$)−H Olefination/Annulation Cascades of Aryl Carboxamides Assisted by N,S-bidentate Auxiliary

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1. NMR Spectra for All Compounds

$^1$H NMR: (E)-methyl-2-(2-(methylthio)phenyl)-3-oxoisoindolin-1-ylidene)acetate (3)

$^{13}$C NMR: (E)-methyl-2-(2-(methylthio)phenyl)-3-oxoisoindolin-1-ylidene)acetate (3)
$^1$H NMR:
(E)-methyl-2-(6-methyl-2-(2-(methylthio)phenyl)-3-oxoisooindolin-1-ylidene)acetate (4)

$^{13}$C NMR:
(E)-methyl-2-(6-methyl-2-(2-(methylthio)phenyl)-3-oxoisooindolin-1-ylidene)acetate (4)
$^1$H NMR:
(E)-methyl-2-(4-methyl-2-(2-(methylthio)phenyl)-3-oxoisooindolin-1-ylidene)acetate (5)

$^{13}$C NMR:
(E)-methyl-2-(4-methyl-2-(2-(methylthio)phenyl)-3-oxoisooindolin-1-ylidene)acetate (5)
$^1$H NMR:

(E)-methyl-2-(5-methyl-2-(2-(methylthio)phenyl)-3-oxoisooindolin-1-yldene)acetate (6)

$^{13}$C NMR:

(E)-methyl-2-(5-methyl-2-(2-(methylthio)phenyl)-3-oxoisooindolin-1-yldene)acetate (6)
^1H NMR:
(E)-methyl-2-(6-ethyl-2-(2-(methylthio)phenyl)-3-oxoisoindolin-1-ylidene)acetate (7)

^13C NMR:
(E)-methyl-2-(6-ethyl-2-(2-(methylthio)phenyl)-3-oxoisoindolin-1-ylidene)acetate (7)
$^1$H NMR:
(E)-methyl-2-(6-methoxy-2-(2-(methylthio)phenyl)-3-oxoisoindolin-1-ylidene)acetate (8)

$^{13}$C NMR:
(E)-methyl-2-(6-methoxy-2-(2-(methylthio)phenyl)-3-oxoisoindolin-1-ylidene)acetate (8)
$^1$H NMR:
(E)-methyl-2-(6-(2-(methylthio)phenyl)-7-oxo-6,7-dihydro-5H-[1,3]dioxolo[4,5-f]isoindol-5-ylidene)acetate (9)

$^{13}$C NMR:
(E)-methyl-2-(6-(2-(methylthio)phenyl)-7-oxo-6,7-dihydro-5H-[1,3]dioxolo[4,5-f]isoindol-5-ylidene)acetate (9)
$^1$H NMR:
(E)-methyl-2-(6-fluoro-2-(2-(methylthio)phenyl)-3-oxoisooindolin-1-ylidene)acetate (10)

$^{13}$C NMR:
(E)-methyl-2-(6-fluoro-2-(2-(methylthio)phenyl)-3-oxoisooindolin-1-ylidene)acetate (10)
$^1$H NMR:
(E)-methyl-2-(4-fluoro-2-(2-(methylthio)phenyl)-3-oxoisoindolin-1-ylidene)acetate (11)

$^{13}$C NMR:
(E)-methyl-2-(4-fluoro-2-(2-(methylthio)phenyl)-3-oxoisoindolin-1-ylidene)acetate (11)
$^1$H NMR:
(E)-methyl-2-(5-fluoro-2-(2-(methylthio)phenyl)-3-oxoisodolin-1-ylidene)acetate (12)

$^{13}$C NMR:
(E)-methyl-2-(5-fluoro-2-(2-(methylthio)phenyl)-3-oxoisodolin-1-ylidene)acetate (12)
$^1$H NMR:
(E)-methyl-2-(6-chloro-2-(2-(methylthio)phenyl)-3-oxoisooindolin-1-ylidene)acetate (13)

$^{13}$C NMR:
(E)-methyl-2-(6-chloro-2-(2-(methylthio)phenyl)-3-oxoisooindolin-1-ylidene)acetate (13)
$^1$H NMR:
(E)-methyl-2-(6-bromo-2-(2-(methylthio)phenyl)-3-oxoisindolin-1-ylidene)acetate (14)

$^{13}$C NMR:
(E)-methyl-2-(6-bromo-2-(2-(methylthio)phenyl)-3-oxoisindolin-1-ylidene)acetate (14)
$^1$H NMR:
(E)-methyl-2-(2-(methylthio)phenyl)-3-oxo-6-(trifluoromethyl)isoindolin-1-ylidene) acetate (15)

$^{13}$C NMR:
(E)-methyl-2-(2-(methylthio)phenyl)-3-oxo-6-(trifluoromethyl)isoindolin-1-ylidene) acetate (15)
$^1$H NMR:
(E)-methyl-2-(2-(methylthio)phenyl)-3-oxo-6-phenylisoindolin-1-ylidene)acetate (16)

$^{13}$C NMR:
(E)-methyl-2-(2-(methylthio)phenyl)-3-oxo-6-phenylisoindolin-1-ylidene)acetate (16)
$^1$H NMR:
(E)-methyl-2-(2-(methylthio)phenyl)-3-oxo-2,3-dihydro-1H-benzo[f]isoindol-1-yliden e)acetate (17)

$^{13}$C NMR:
(E)-methyl-2-(2-(methylthio)phenyl)-3-oxo-2,3-dihydro-1H-benzo[f]isoindol-1-yliden e)acetate (17)
^1H NMR:
(E)-methyl-2-(2-(4-methyl-2-(methylthio)phenyl)-3-oxoisooindolin-1-ylidene)acetate (18)

^13C NMR:
(E)-methyl-2-(2-(4-methyl-2-(methylthio)phenyl)-3-oxoisooindolin-1-ylidene)acetate (18)
$^1$H NMR:
(E)-methyl-2-(2-(4-ethoxy-2-(methylthio)phenyl)-3-oxoisooindolin-1-ylidene)acetate (19)

$^{13}$C NMR:
(E)-methyl-2-(2-(4-ethoxy-2-(methylthio)phenyl)-3-oxoisooindolin-1-ylidene)acetate (19)
$^1$H NMR:
(E)-methyl-2-(2-(4-chloro-2-(methylthio)phenyl)-3-oxoisooindolin-1-ylidene)acetate (20)

$^{13}$C NMR:
(E)-methyl-2-(2-(4-chloro-2-(methylthio)phenyl)-3-oxoisooindolin-1-ylidene)acetate (20)
\(^1\)H NMR:
(E)-methyl-2-(2-(2-(methylthio)-4-(trifluoromethyl)phenyl)-3-oxoisooindolin-1-ylidene) acetate (21)

\(^{13}\)C NMR:
(E)-methyl-2-(2-(2-(methylthio)-4-(trifluoromethyl)phenyl)-3-oxoisooindolin-1-ylidene) acetate (21)
$^1$H NMR: (E)-methyl-2-(2-(ethylthio)phenyl)-3-oxoisoindolin-1-ylidene)acetate (22)

$^{13}$C NMR: (E)-methyl-2-(2-(ethylthio)phenyl)-3-oxoisoindolin-1-ylidene)acetate (22)
\(^1\)H NMR: (E)-methyl-2-(2-(2-(cyclohexylthio)phenyl)-3-oxoisooindolin-1-ylidene)acetate (23)

\[^{13}\]C NMR: (E)-methyl-2-(2-(2-(cyclohexylthio)phenyl)-3-oxoisooindolin-1-ylidene)acetate (23)
$^1$H NMR: (E)-methyl-2-(3-oxo-2-(2-(phenylthio)phenyl)isoindolin-1-ylidene)acetate (24)

$^{13}$C NMR: (E)-methyl-2-(3-oxo-2-(2-(phenylthio)phenyl)isoindolin-1-ylidene)acetate (24)
2. X-Ray of compound 3

Figure 1. The crystal structure of 3

The displacement ellipsoids are drawn at the 30% probability level.

Single crystals suitable for X-ray analysis were obtained by slow evaporation of ethyl acetate solvent.

Supplementary crystallographic data was deposited at the Cambridge Crystallographic Data Centre (CCDC) under the number CCDC-1880824 (3) and can be obtained free of charge via www.ccdc.cam.ac.uk/data_request.cif