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# **Supporting Information**

# Synthesis, characterization and biological activities of 3-aryl-1,4-naphthoquinones – Green palladium-catalysed Suzuki cross couplings

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# IV, <sup>1</sup>H and <sup>13</sup>C NMR Spectra of the Products

#### 2-Hydroxy-3-iodonaphthalene-1,4-dione (6)



Figure S1 - Infrared spectrum of 2-hydroxy-3-iodonaphthalene-1,4-dione (6)



Figure S2 - <sup>1</sup>H NMR Spectra of 2-hydroxy-3-iodonaphthalene-1,4-dione (6)



Figure S3 - <sup>13</sup>C NMR Spectra of 2-hydroxy-3-iodonaphthalene-1,4-dione (6)



2-Amino-3-iodonaphthalene-1,4-dione (7)

Figure S4 - Infrared spectrum of 2-amino-3-iodonaphthalene-1,4-dione (7)



Figure S5 - <sup>1</sup>H NMR Spectra of 2-amino-3-iodonaphthalene-1,4-dione (7)



Figure S6 - <sup>13</sup>C NMR Spectra of 2-amino-3-iodonaphthalene-1,4-dione (7)

# 2-Bromo-3-hydroxynaphthalene-1,4-dione (8)



## Agilent Resolutions Pro

Figure S7 - Infrared spectrum of 2-bromo-3-hydroxynaphthalene-1,4-dione (8)



Figure S8 - <sup>1</sup>H NMR Spectra of 2-bromo-3-hydroxynaphthalene-1,4-dione (8)



Figure S9 - <sup>13</sup>C NMR Spectra of 2-bromo-3-hydroxynaphthalene-1,4-dione (8)



2-Hydroxi-3-phenylnaphthalene-1,4-dione (10a)





Figure S11 – <sup>1</sup>H NMR Spectrum of 2-hydroxi-3-phenylnaphthalene-1,4-dione (10a)



7.63 7.62 7.61 7.60 7.59 7.58 7.57 7.56 7.55 7.54 7.53 7.52 7.51 7.50 7.49 7.48 7.47 7.46 7.45 7.44 7.43 7.42 7.41 7.40 7.39 7.38 f1 (pm)





Figure S13 <sup>13</sup>C NMR Spectra of 2-hydroxi-3-phenylnaphthalene-1,4-dione (10a)

#### 2-(4-Fluorophenyl)-3-phenylnaphthalene-1,4-dione (10b)





Figure S14 Infrared spectrum of 2-(4-fluorophenyl)-3-phenylnaphthalene-1,4-dione (10b)





Figure S15 - <sup>1</sup>H NMR Spectra of 2-(4-fluorophenyl)-3-phenylnaphthalene-1,4-dione (10b)



Figure S16 - <sup>13</sup>C NMR Spectra of 2-(4-fluorophenyl)-3-phenylnaphthalene-1,4-dione (10b)



2-(3-Fluorophenyl)-3-phenylnaphthalene-1,4-dione (10c)

Figure S17 Infrared spectrum of 2-(3-fluorophenyl)-3-phenylnaphthalene-1,4-dione (10c)





Figure S18 - <sup>1</sup>H NMR Spectra of 2-(3-fluorophenyl)-3-phenylnaphthalene-1,4-dione (10c)



Figure S19 - <sup>13</sup>C NMR Spectra of 2-(3-fluorophenyl)-3-phenylnaphthalene-1,4-dione (10c)



2-Hydroxy-3-(thiophen-2-yl)naphthalene-1,4-dione (10d)

Figure S20 - Infrared spectrum of 2-hydroxy-3-(thiophen-2-yl)naphthalene-1,4-dione (10d)





Figure S21 - <sup>1</sup>H NMR Spectra of 2-hydroxy-3-(thiophen-2-yl)naphthalene-1,4-dione (10d)



Figure S22 - <sup>13</sup>C NMR Spectra of 2-hydroxy-3-(thiophen-2-yl)naphthalene-1,4-dione (10d)



2-Hydroxy-3-(thiophen-3-yl)naphthalene-1,4-dione (10e)

Figure S23 - Infrared spectrum of 2-hydroxy-3-(thiophen-3-yl)naphthalene-1,4-dione (10e)





Figure S24 - <sup>1</sup>H NMR Spectra of 2-hydroxy-3-(thiophen-3-yl)naphthalene-1,4-dione (10e)



Figure S25 - <sup>13</sup>C NMR Spectra of 2-hydroxy-3-(thiophen-3-yl)naphthalene-1,4-dione (10e)



3-(3-Hydroxy-1,4-dioxo-1,4-dhydronaphthalen-2-yl)benzaldehyde (10f)

Figure S26 - Infrared spectrum of 3-(3-Hydroxy-1,4-dioxo-1,4-dhydronaphthalen-2-yl)benzaldehyde (10f)





Figure S27 - <sup>1</sup>H NMR Spectra of of 3-(3-Hydroxy-1,4-dioxo-1,4-dhydronaphthalen-2-yl)benzaldehyde



Figure S28<sup>13</sup>C NMR Spectra of of 3-(3-Hydroxy-1,4-dioxo-1,4-dhydronaphthalen-2-yl)benzaldehyde (10f)



4-(3-hydroxy-1,4-dioxo-1,4-dihydronaphthalen-2-yl)benzaldehyde (10g)

Figure S29 - Infrared spectrum of 4-(3-hydroxy-1,4-dioxo-1,4-dihydronaphthalen-2-yl)benzaldehyde



8.10 8.06 8.02



Figure S30 - <sup>1</sup>H NMR Spectra of 4-(3-hydroxy-1,4-dioxo-1,4-dihydronaphthalen-2-yl)benzaldehyde (10g)



Figure S31 - <sup>13</sup>C NMR Spectra of of 4-(3-hydroxy-1,4-dioxo-1,4-dihydronaphthalen-2-yl)benzaldehyde



2-Hydroxy-3-(4-methoxyphenyl)naphthalene-1,4-dione (10h)

Figure S32 Infrared spectrum of 2-hydroxy-3-(4-methoxyphenyl)naphthalene-1,4-dione (10h)





Figure S33 - <sup>1</sup>H NMR Spectra of 2-hydroxy-3-(4-methoxyphenyl)naphthalene-1,4-dione (10h)



Figure S34 - <sup>1</sup>H NMR Spectra of 2-hydroxy-3-(4-methoxyphenyl)naphthalene-1,4-dione (10h)



2-Hydroxy-3-(3-methoxyphenyl)naphthalene-1,4-dione (10i)

Figure S35 - Infrared spectrum of 2-hydroxy-3-(3-methoxyphenyl)naphthalene-1,4-dione (10i)





Figure S36 - <sup>1</sup>H NMR Spectra of 2-hydroxy-3-(3-methoxyphenyl)naphthalene-1,4-dione (10i)



Figure S37 - <sup>13</sup>C NMR Spectra of 2-hydroxy-3-(3-methoxyphenyl)naphthalene-1,4-dione (10i)



4-(3-Hydroxy-1,4-dioxo-1,4-dihydronaphthalen-2-yl)benzonitrile (10j)

Figure S38 - Infrared spectrum of 4-(3-Hydroxy-1,4-dioxo-1,4-dihydronaphthalen-2-yl)benzonitrile (10j)





Figure S39 - <sup>1</sup>H NMR Spectra of 4-(3-Hydroxy-1,4-dioxo-1,4-dihydronaphthalen-2-yl)benzonitrile (10j)



Figure S40 - <sup>13</sup>C NMR Spectra of 4-(1,4-diihydro-2-hidroxy-1,4-dioxonphtalen-3-yl)benzonitrile (10j)





Figure S41 - Infrared spectrum of 2-Hydroxy-3-(*p*-tolyl)naphthalene-1,4-dione (10k)





Figure S42 - <sup>1</sup>H NMR Spectra of 2-Hydroxy-3-(*p*-tolyl)naphthalene-1,4-dione (10k)



Figure S43 - <sup>13</sup>C NMR Spectra of 2-Hydroxy-3-(*p*-tolyl)naphthalene-1,4-dione (10k)

![](_page_33_Figure_2.jpeg)

2-Amino-3-phenylnaphthalene-1,4-dione (11)

Figure S44 - Infrared spectrum of 2-amino-3-phenylnaphthalene-1,4-dione (11)

![](_page_34_Figure_0.jpeg)

![](_page_35_Figure_0.jpeg)

Figure S45 - <sup>1</sup>H NMR Spectra of 2-amino-3-phenylnaphthalene-1,4-dione (11)

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Figure S46 - <sup>13</sup>C NMR Spectra of 2-amino-3-phenylnaphthalene-1,4-dione (11)