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**Electronic Supplementary Information** 

# Investigation of the *In Vitro* Anticancer Potential of Bis(imino)acenaphthene-*N*-Heterocyclic Carbene Transition Metal Complexes Revealed TrxR Inhibition and Triggering of Immunogenic Cell Death (ICD) for Allyl Palladates

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#### NMR spectra



220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



<sup>1</sup>H NMR and <sup>13</sup>C {<sup>1</sup>H} NMR for 3a



<sup>1</sup>H NMR and <sup>13</sup>C {<sup>1</sup>H} NMR for 3b



z20 z10 z00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



#### <sup>1</sup>H NMR and <sup>13</sup>C {<sup>1</sup>H} NMR for 4b





<sup>1</sup>H NMR and <sup>13</sup>C {<sup>1</sup>H} NMR for 4c



190 185 180 175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 ppm

<sup>1</sup>H NMR and <sup>13</sup>C {<sup>1</sup>H} NMR for 5a



200 190 ppm . 170 140 130 . 70 



<sup>1</sup>H NMR and <sup>13</sup>C {<sup>1</sup>H} NMR for 5c



## Examples of NMR Spectra in DMSO-d<sup>6</sup>/D<sub>2</sub>O (1:1) for stability studies

<sup>1</sup>H NMR of 2b in DMSO-d<sup>6</sup>/D<sub>2</sub>O (1:1) (t = 0 and 48h)



12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 f1 (ppm)





12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 f1 (ppm)

### Examples of UV-Vis spectra in aqueous solution at different pH

UV-Vis spectra of 2a ( $5 \cdot 10^{-5}$  M) in phosphate buffer solution (pH = 7.2) with 10% of DMSO (t = 0 and 48h)









UV-Vis spectra of 2b ( $5 \cdot 10^{-5}$  M) in phosphate buffer solution (pH = 6) with 10% of DMSO (t = 0 and 48h)



UV-Vis spectra of 2b ( $5 \cdot 10^{-5}$  M) in phosphate buffer solution (pH = 8) with 10% of DMSO (t = 0 and 48h)