

Supporting Information

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Design, synthesis, *in silico* and biological evaluation of biotin-pyrazole derivatives as cytotoxic agent

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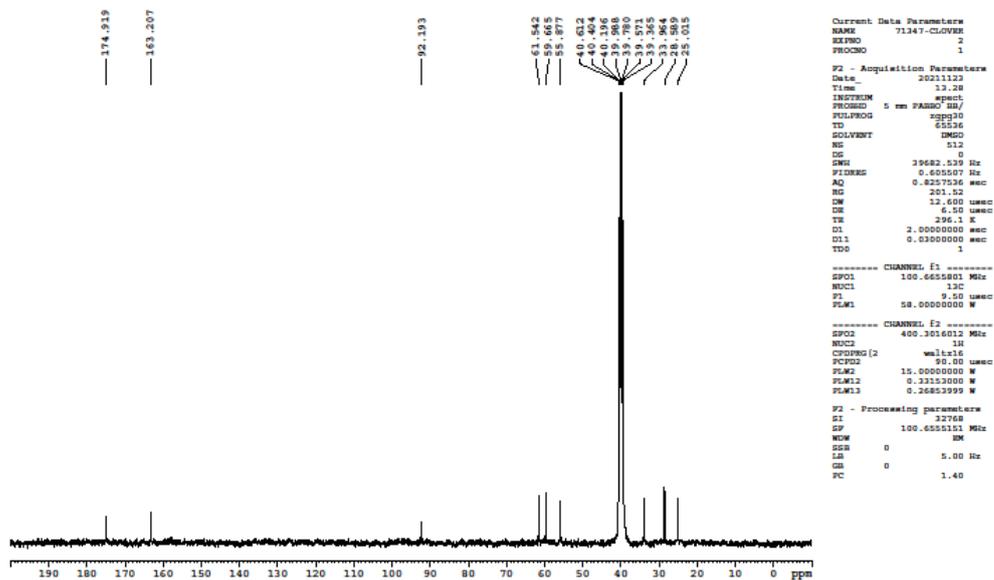


Figure S2: ^{13}C -NMR (400 MHz, DMSO-*d*₆) Spectrum of **2** ((3a*S*,4*S*,6a*R*)-4-(5-(4-bromo-1*H*-pyrazol-1-yl)-5-oxopentyl)tetrahydro-1*H*-thieno[3,4-*d*]imidazol-2(3*H*)-one)

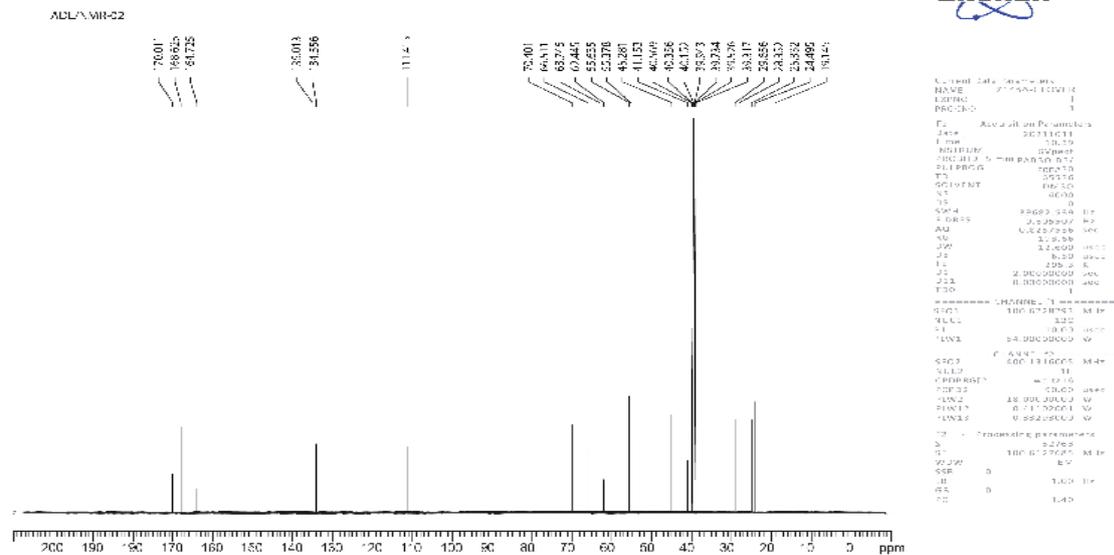


Figure S4: ^{13}C -NMR (400 MHz, DMSO-*d*₆) Spectrum of **3a** ((3*a*S,4*S*,6*a*R)-4-(5-(4-(3-methylmorpholine-4-carbonyl)-1*H*-pyrazol-1-yl)-5-oxopentyl)tetrahydro-1*H*-thieno[3,4-*d*]imidazol-2(3*H*)-one)

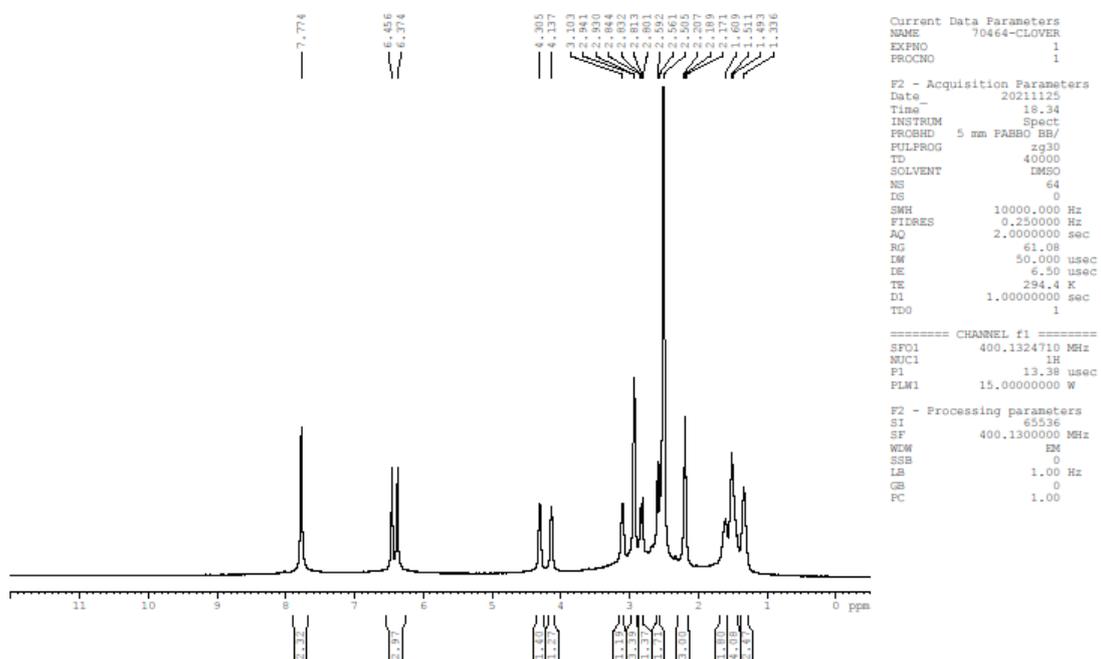


Figure S5: $^1\text{H-NMR}$ (400 MHz, $\text{DMSO-}d_6$) Spectrum of **3b** ((3aS,4S,6aR)-4-(5-oxo-5-(4-(thiomorpholine-4-carbonyl)-1H-pyrazol-1-yl) pentyl) tetra hydro-1H-thieno[3,4-d]imidazol-2(3H)-one)

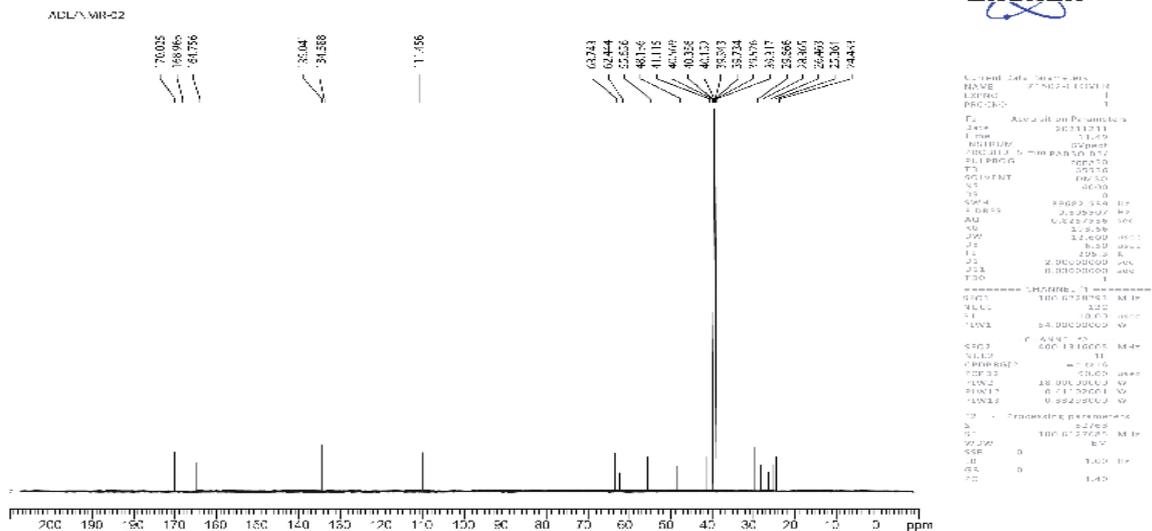


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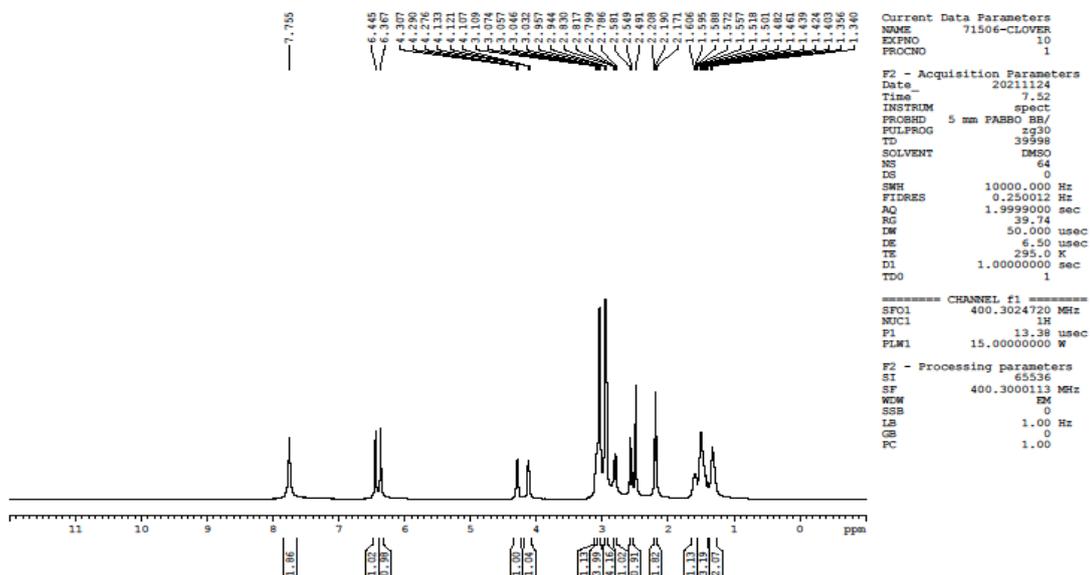


Figure S7: $^1\text{H-NMR}$ (400 MHz, $\text{DMSO-}d_6$) Spectrum of **3c** ((3aS,4S,6aR)-4-(5-(4-(1,1-dioxidothiomorpholine-4-carbonyl)-1H-pyrazol-1-yl)-5-oxo pentyl)tetrahydro-1H-thieno[3,4-d]imidazol-2(3H)-one)

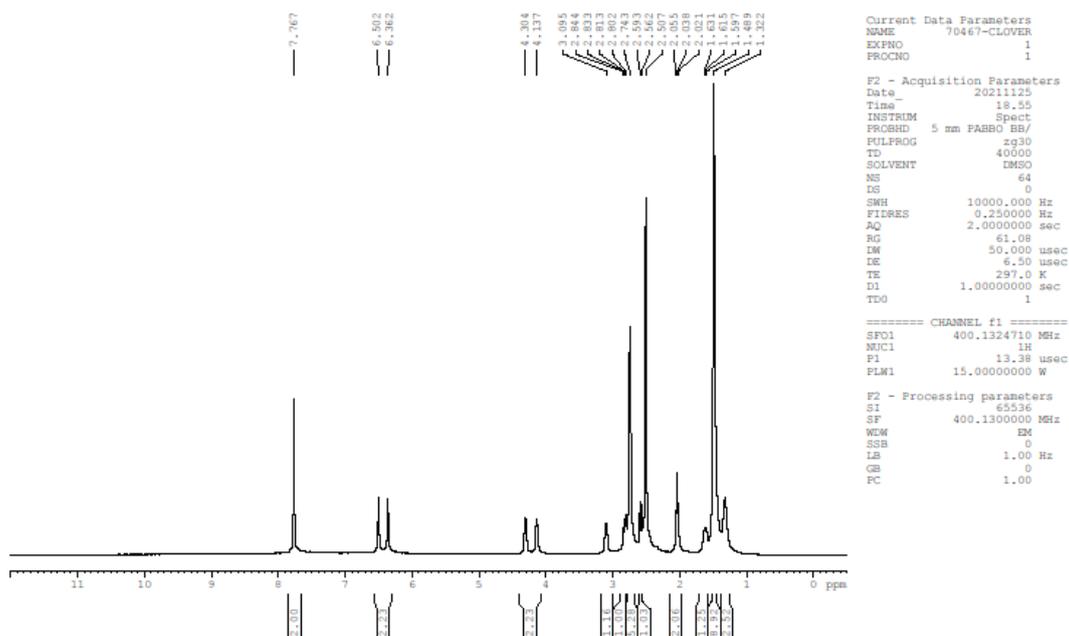


Figure S9: $^1\text{H-NMR}$ (400 MHz, $\text{DMSO-}d_6$) Spectrum of **3d** ((3a*S*,4*S*,6a*R*)-4-(5-oxo-5-(4-(piperidine-1-carbonyl)-1*H*-pyrazol-1-yl)pentyl)tetrahydro-1*H*-thieno[3,4-*d*]imidazol-2(3*H*)-one)

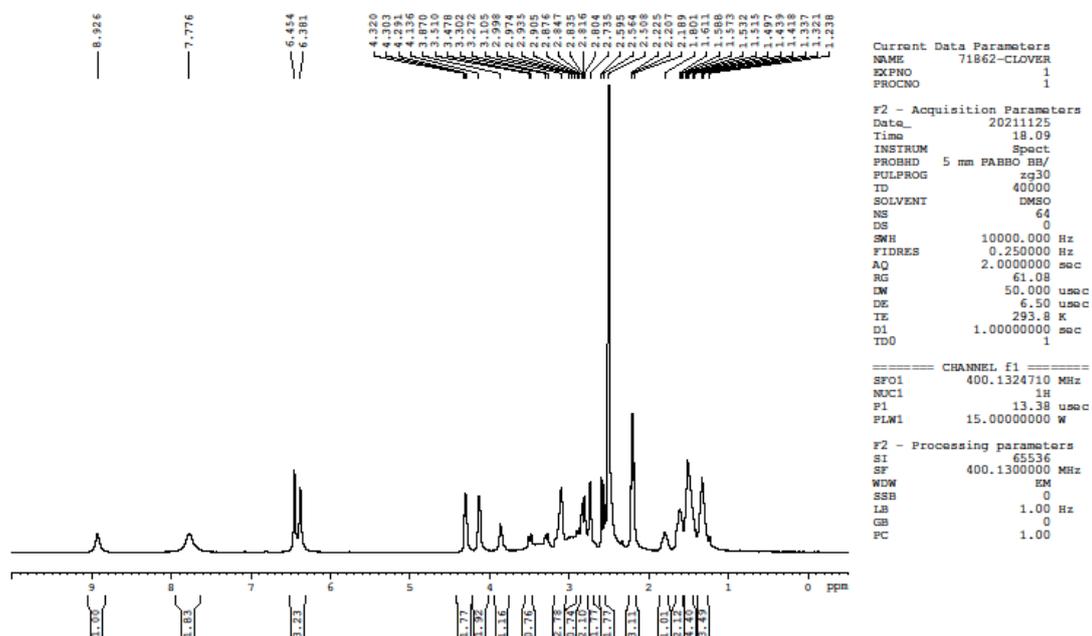


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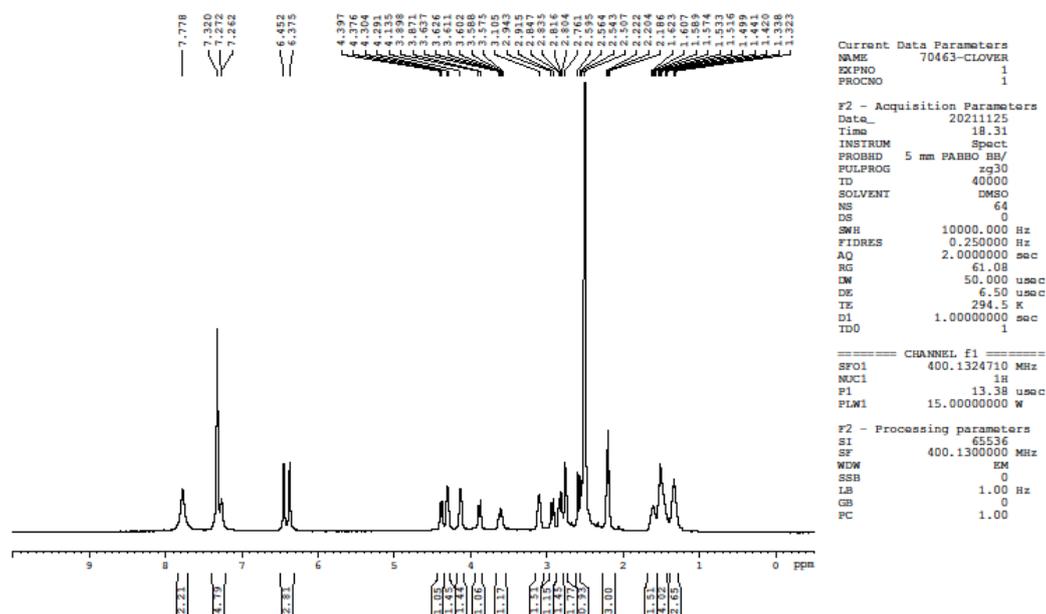


Figure S13: $^1\text{H-NMR}$ (400 MHz, $\text{DMSO-}d_6$) Spectrum of **3f** ((3*a*S,4*S*,6*a*R)-4-(5-oxo-5-(4-(2-phenylmorpholine-4-carbonyl)-1*H*-pyrazol-1-yl)pentyl)tetrahydro-1*H*-thieno[3,4-*d*]imidazol-2(3*H*)-one)

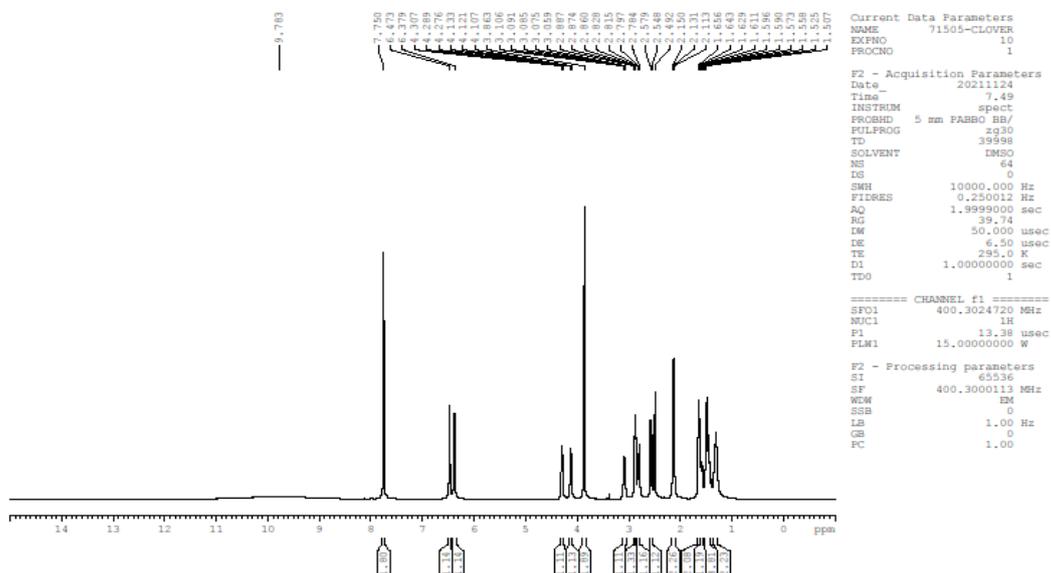


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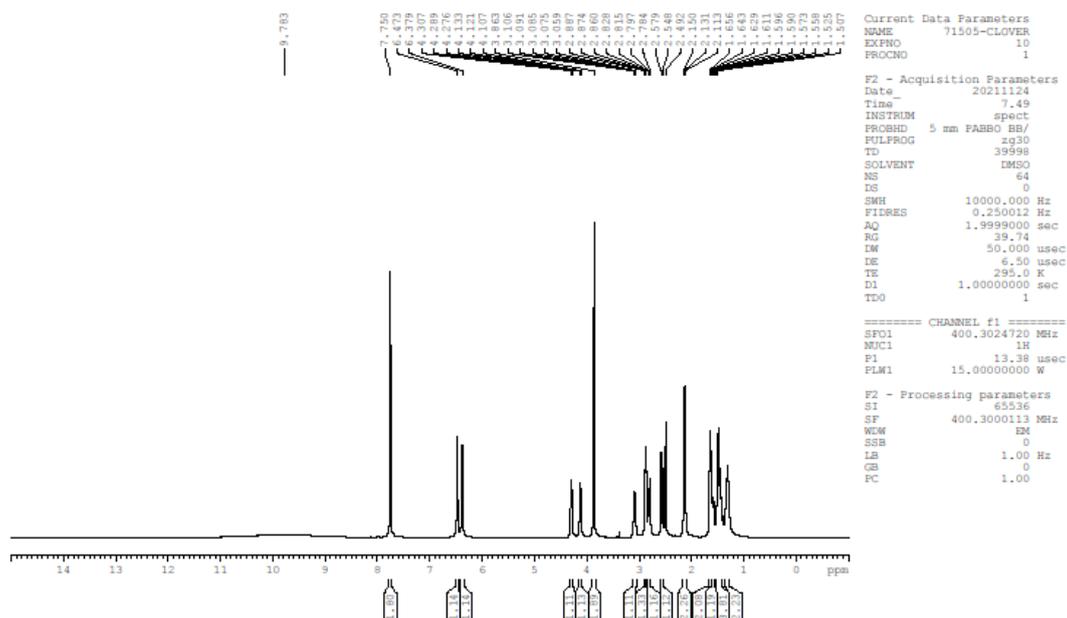


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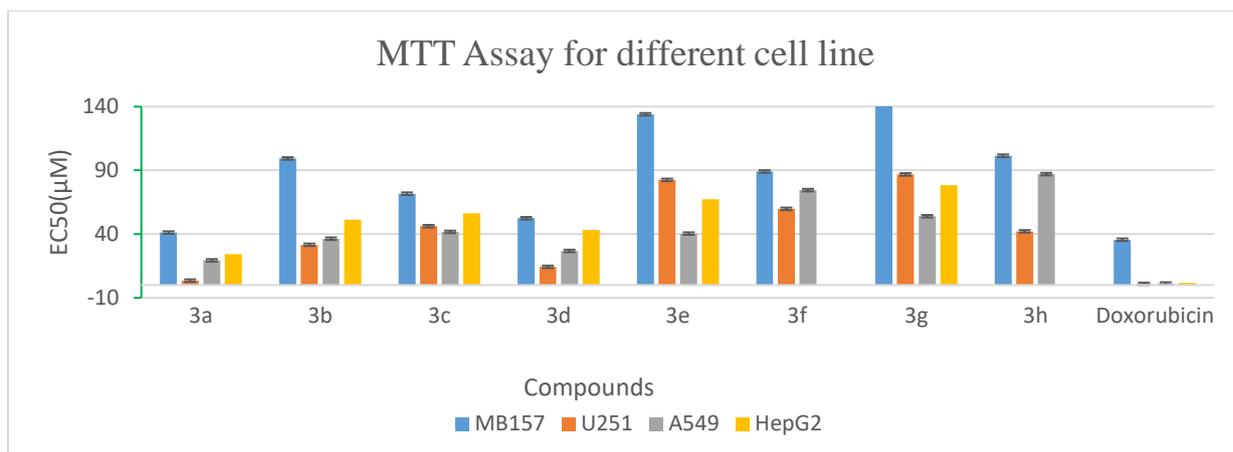


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