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Supplementary Information

Property-Based Design and Synthesis of New Chloroquine Hybrids via Simple Incorporation of 2-Imino-thiazolidin-4-one or 1*H*-Pyrrol-2,5-dione Fragments on the 4-Amino-7-chloroquinoline Side Chain

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N^1*-(7-Chloroquinolin-4-yl)-ethane-1,2-diamine (**8a**):* yellowish white solid, yield 75% from **6** and diamine **7a**; mp 143-145 °C; IR (KBr) ν_{max}/cm^{-1}: 3248$_{(N-H)}$, 2893$_{(CH2)}$, 1589$_{(N-H)}$, 1142$_{(C-N)}$; GC-MS: t_R = 22.13 min, MS (EI) *m/z* (%): 221 ($M^{+\bullet}$, 29), 192 (55), 191 (100), 179 (17), 163 (25), 156 (87), 155 (44), 128 (18).

N^1*-(7-Chloroquinolin-4-yl)-propane-1,3-diamine (**8b**):* yellowish white solid, yield 86% from **6** and diamine **7b**; mp 130-132 °C; IR (KBr) ν_{max}/cm^{-1}: 3278$_{(N-H)}$, 2871$_{(CH2)}$, 1589$_{(N-H)}$, 1141$_{(C-N)}$; GC-MS: t_R = 23.23 min, MS (EI) *m/z* (%): 235 ($M^{+\bullet}$, 93), 219 (21), 218 (44), 217 (52), 205 (35), 203 (36), 192 (95), 191 (100), 179 (92), 163 (25), 156 (87), 155 (67), 128 (26).

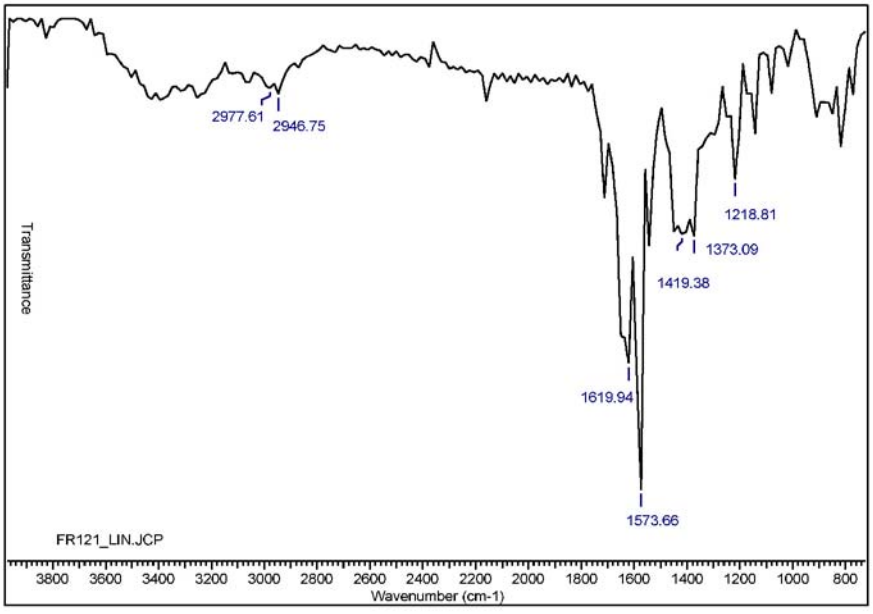

Figure S1. IR spectrum of 3-(2-((7-chloroquinolin-4-yl)amino)ethyl)-2-iminothiazolidin-4-one (**13**).

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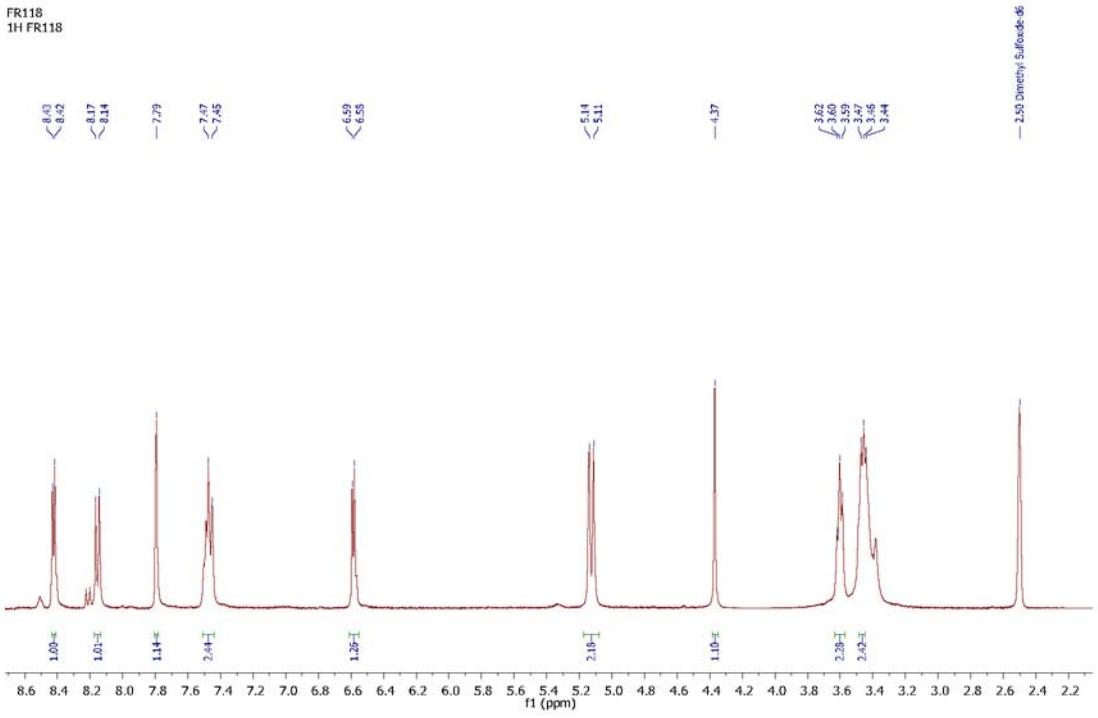

Figure S2. ^{1}H NMR spectrum of 3-(2-((7-chloroquinolin-4-yl)amino)ethyl)-2-iminothiazolidin-4-one (**13**).

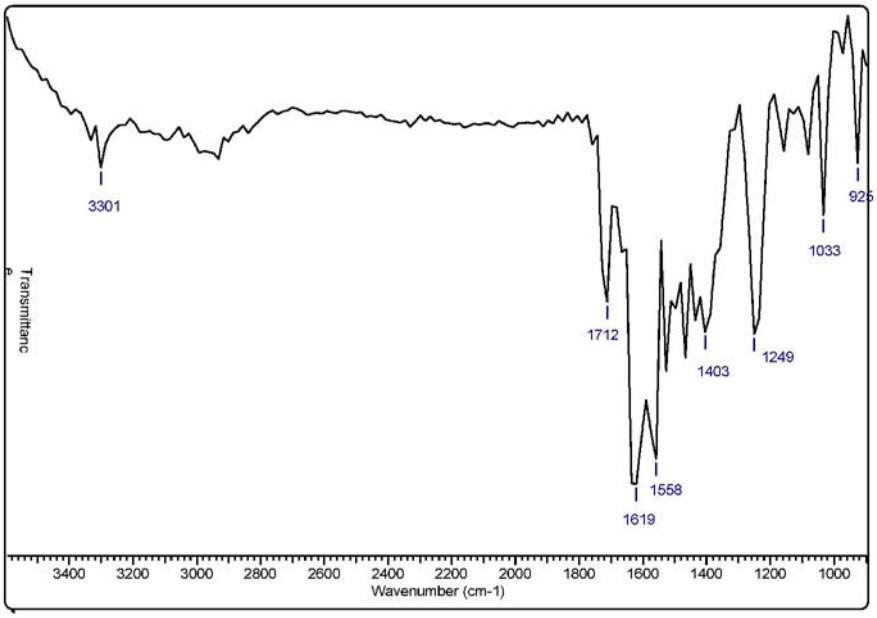

Figure S3. IR spectrum of 3-(3-((7-chloroquinolin-4-yl)amino)propyl)-2-iminothiazolidin-4-one (**14**).

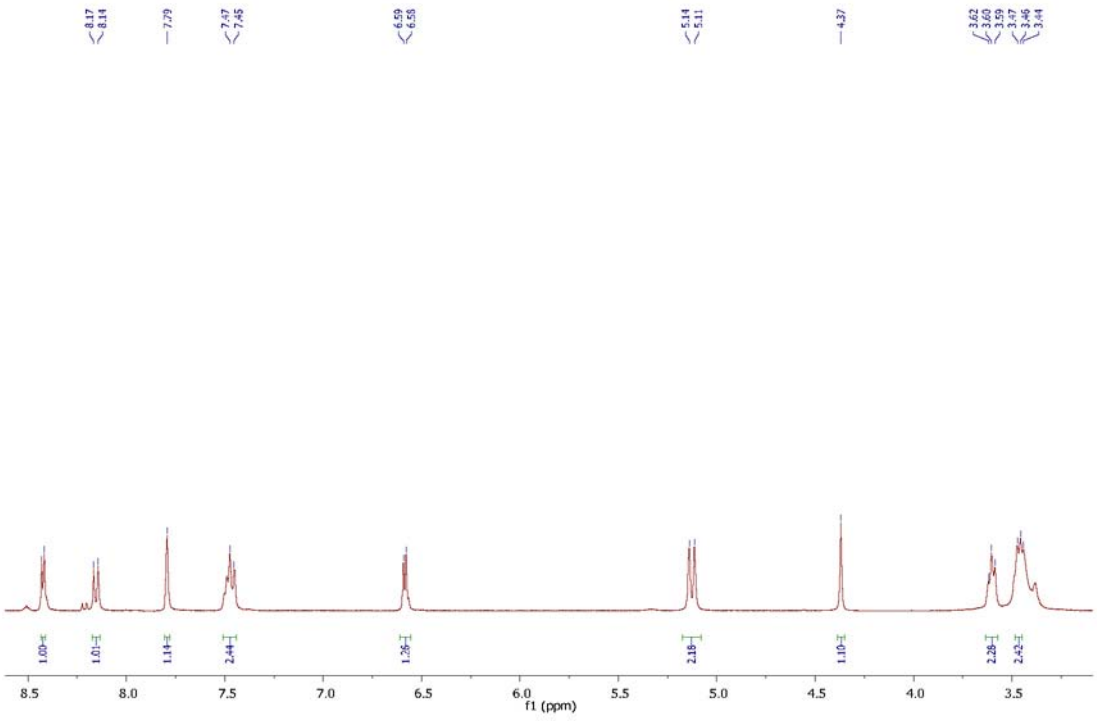

Figure S4. [1]H NMR spectrum of 3-(3-((7-chloroquinolin-4-yl)amino)propyl)-2-iminothiazolidin-4-one (**14**).

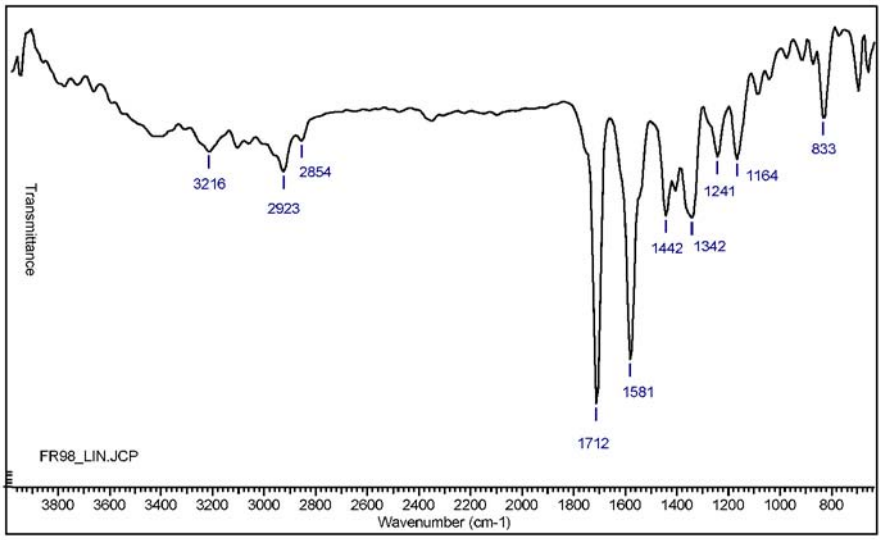

Figure S5. IR spectrum of 1-(2-((7-chloroquinolin-4-yl)amino)ethyl)-1*H*-pyrrole-2,5-dione (**15**).

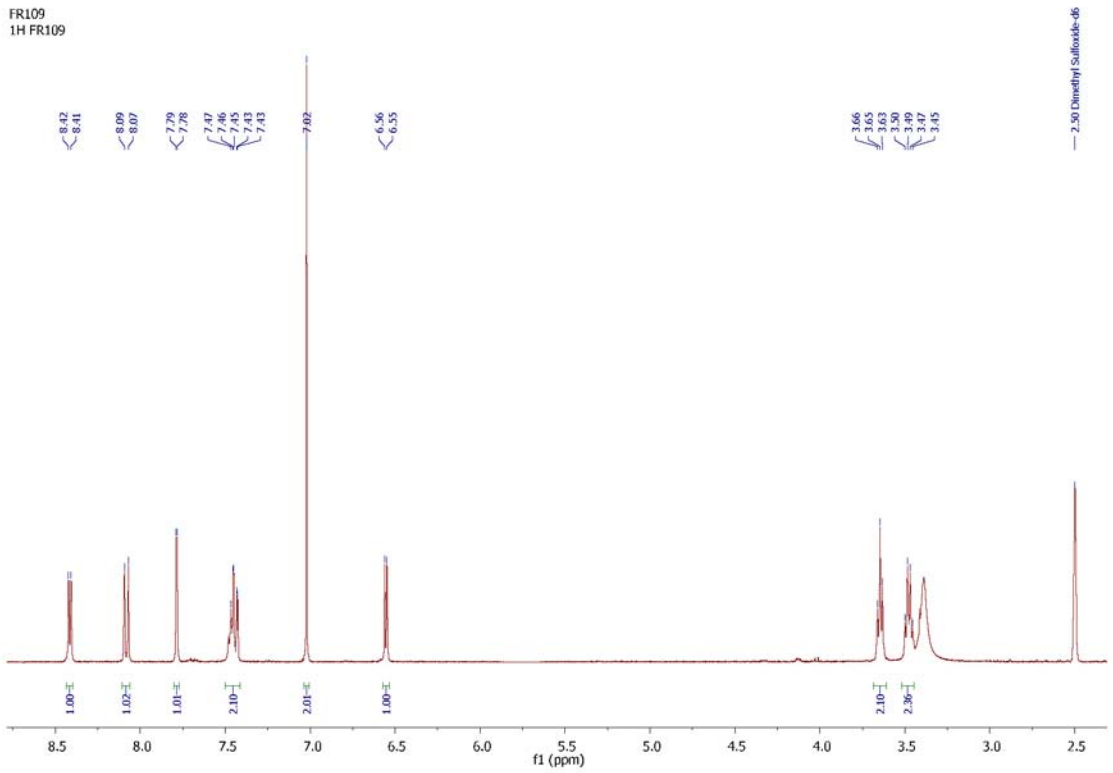

Figure S6. ^{1}H NMR spectrum of 1-(2-((7-chloroquinolin-4-yl)amino)ethyl)-1*H*-pyrrole-2,5-dione (**15**).

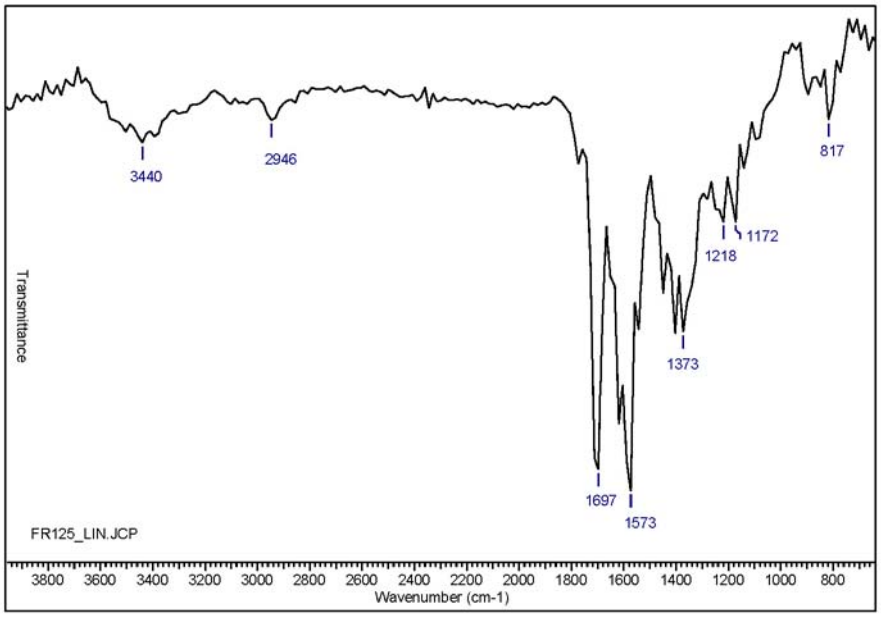

Figure S7. IR spectrum of 1-(2-((7-chloroquinolin-4-yl)amino)propyl)-1*H*-pyrrole-2,5-dione (**16**).

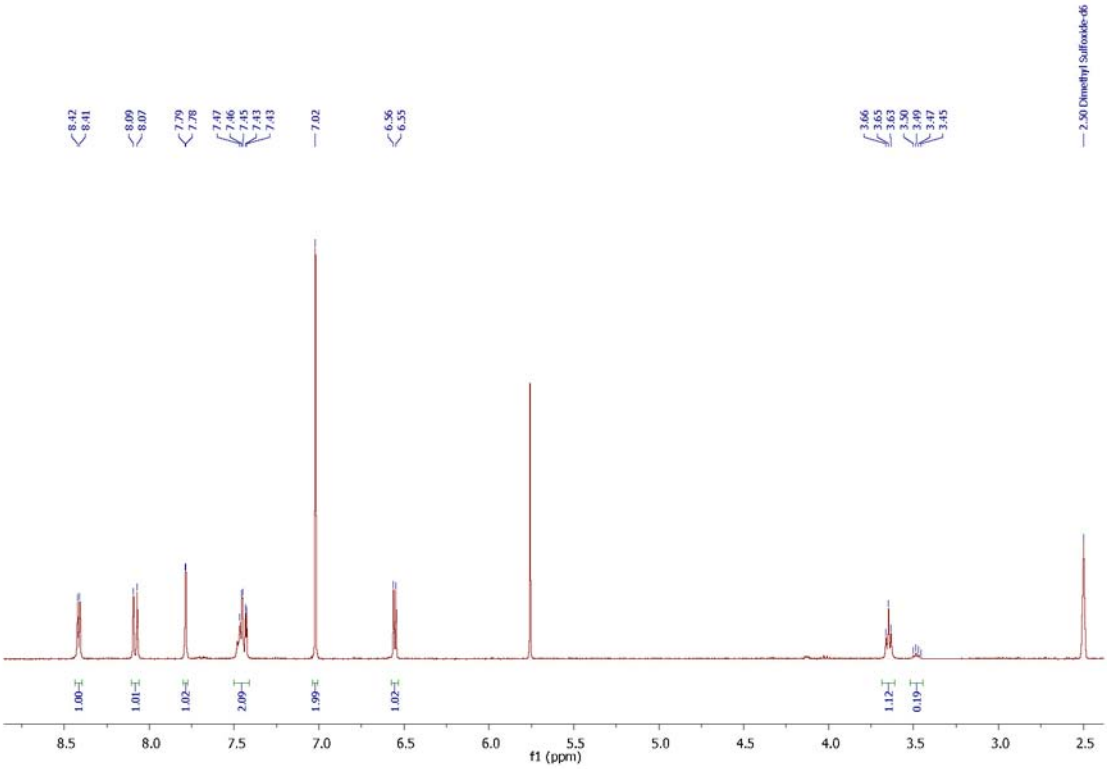

Figure S8. [1]H NMR spectrum of 1-(2-((7-chloroquinolin-4-yl)amino)propyl)-1*H*-pyrrole-2,5-dione (**16**).

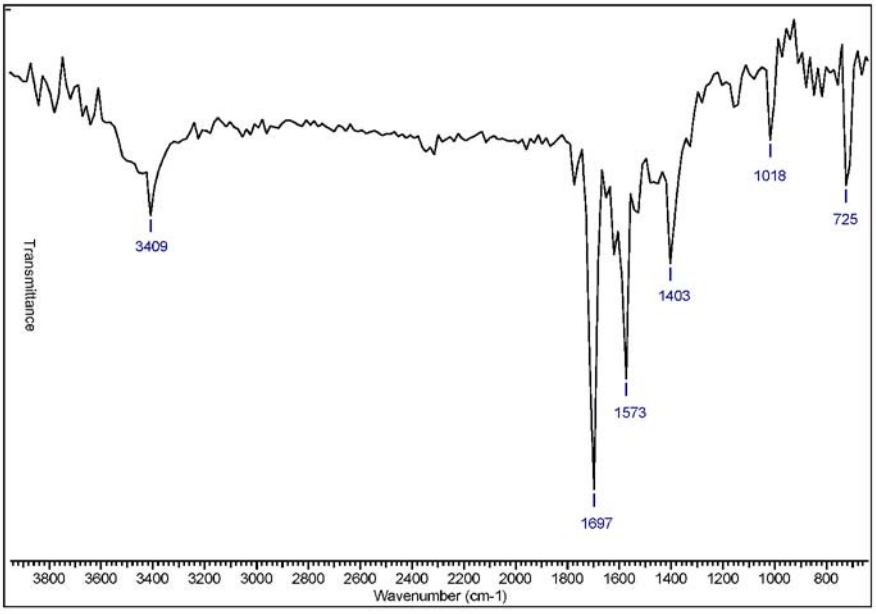

Figure S9. IR spectrum of 1-(2-((7-chloroquinolin-4-yl)amino)ethyl)-3-methyl-1*H*-pyrrol-2,5-dione (**17**).

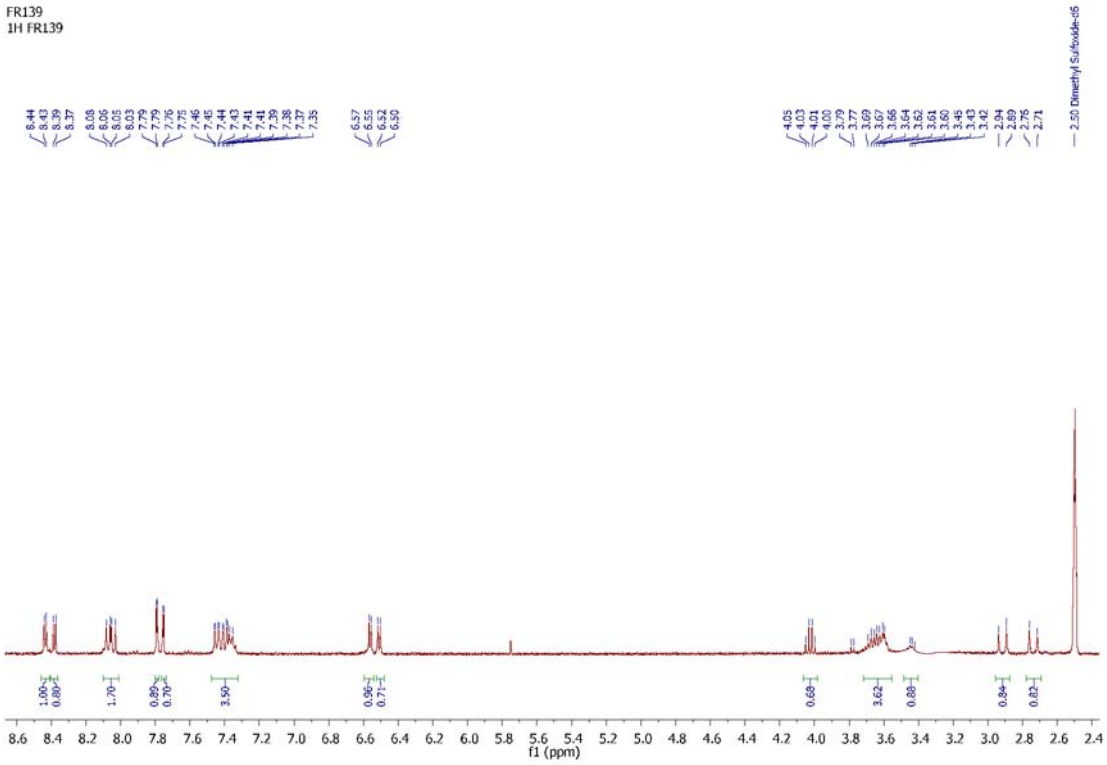

Figure S10. ^{1}H NMR spectrum of 1-(2-((7-chloroquinolin-4-yl)amino)ethyl)-3-methyl-1*H*-pyrrol-2,5-dione (**17**).

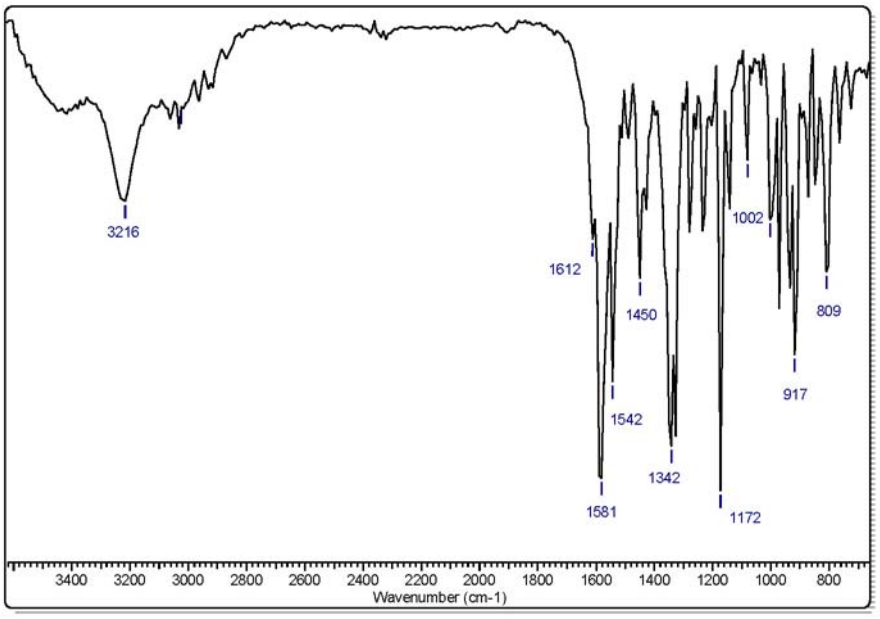

Figure S11. IR spectrum of 1-(2-((7-chloroquinolin-4-yl)amino)propyl)-3-methyl-1*H*-pyrrol-2,5-dione (**18**).

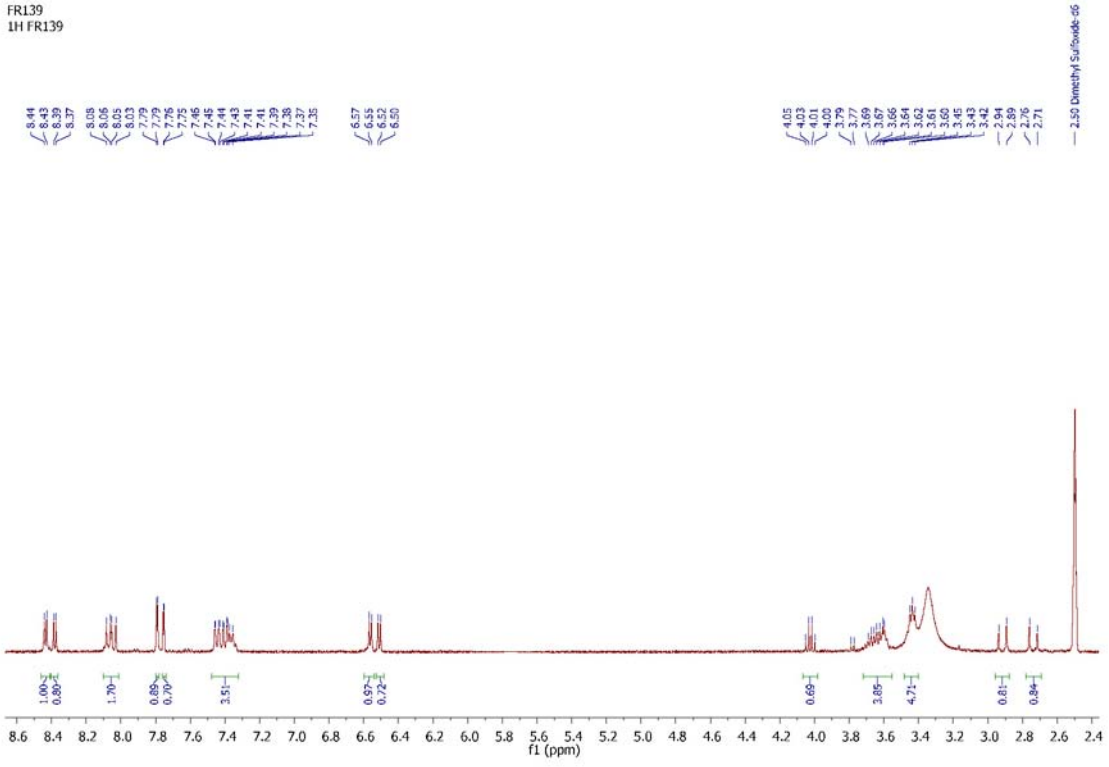

Figure S12. [1]H NMR spectrum of 1-(2-((7-chloroquinolin-4-yl)amino)propyl)-3-methyl-1*H*-pyrrol-2,5-dione (**18**).

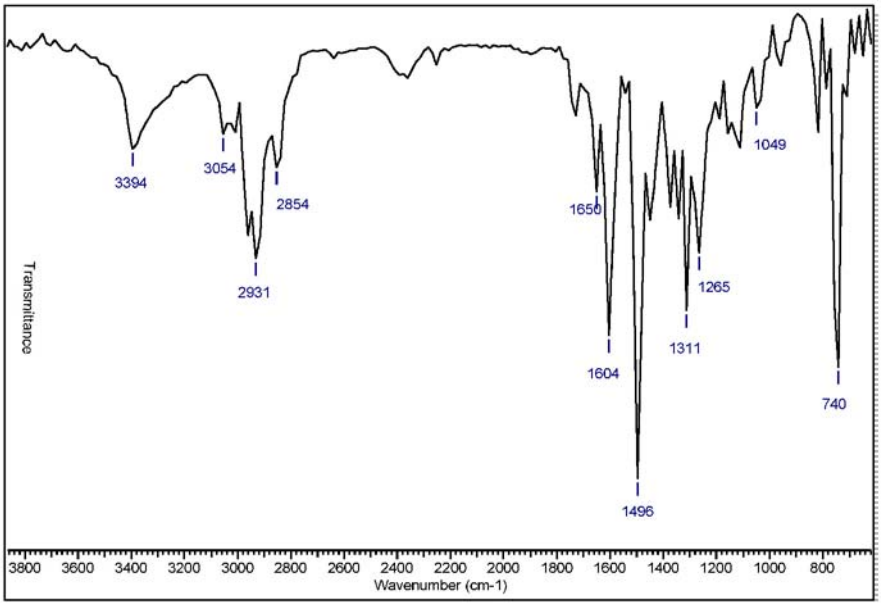

Figure S13. IR spectrum of 2-(2-((7-chloroquinolin-4-yl)amino)ethyl)-4,7-dihydro-1*H*-4,7-epoxyisoindole-1,3(2H)-dione (**19**).

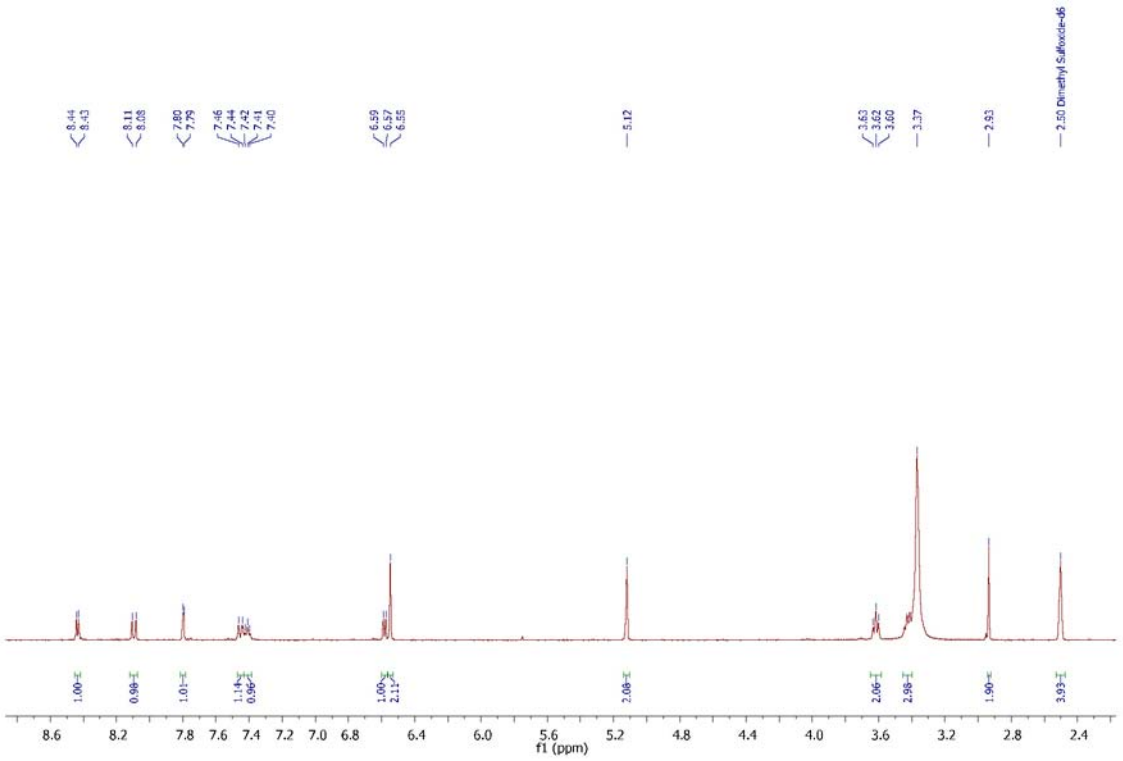

Figure S14. ^{1}H NMR spectrum of 2-(2-((7-chloroquinolin-4-yl)amino)ethyl)-4,7-dihydro-1*H*-4,7-epoxyisoindole-1,3(2H)-dione (**19**).

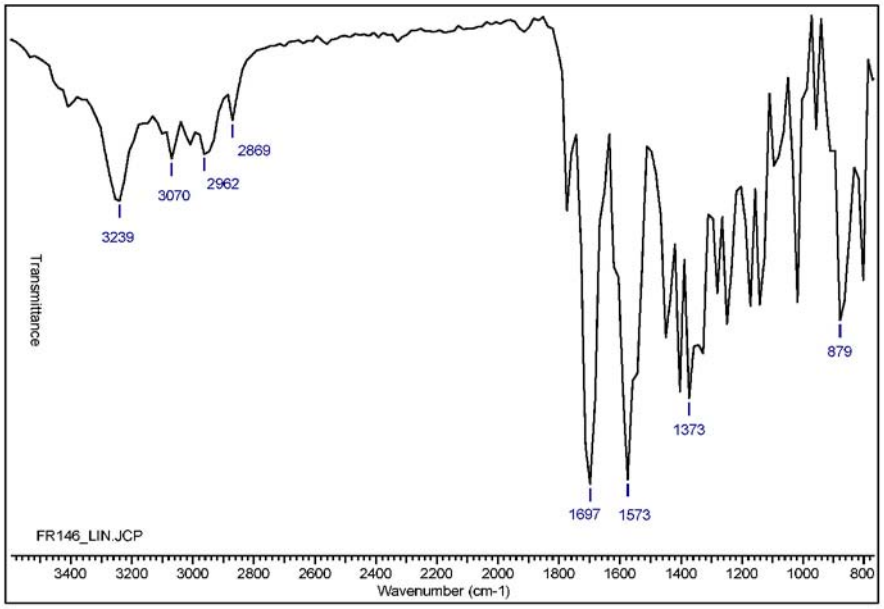

Figure S15. IR spectrum of 2-(3-((7-chloroquinolin-4-yl)amino)propyl)-4,7-dihydro-1*H*-4,7-epoxyisoindole-1,3(2H)-dione (**20**).

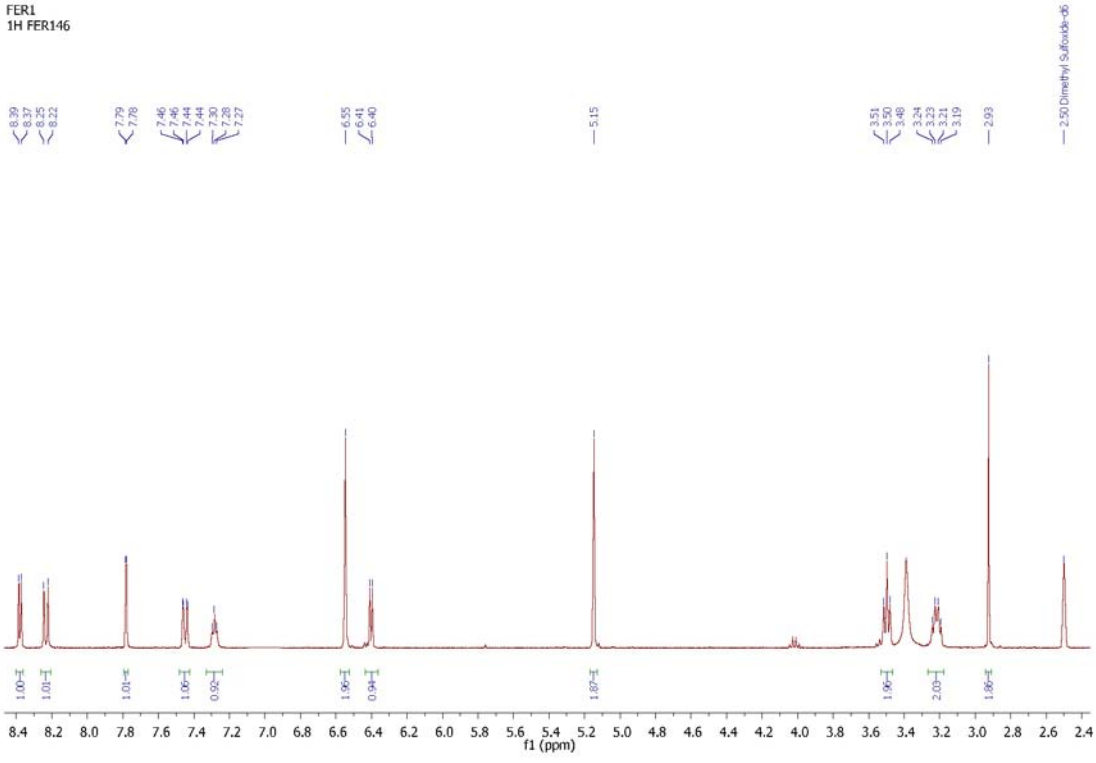

Figure S16. ^{1}H NMR spectrum of 2-(3-((7-chloroquinolin-4-yl)amino)propyl)-4,7-dihydro-1*H*-4,7-epoxyisoindole-1,3(2H)-dione (**20**).

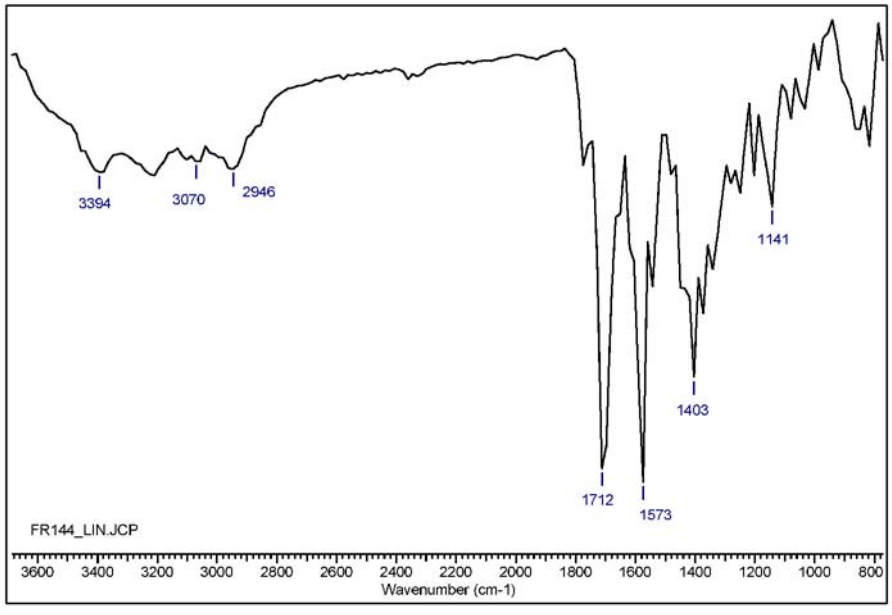

Figure S17. IR spectrum of 2-(3-((7-chloroquinolin-4-yl)amino)ethyl)isoindoline-1,3(2H)-dione (**21**).

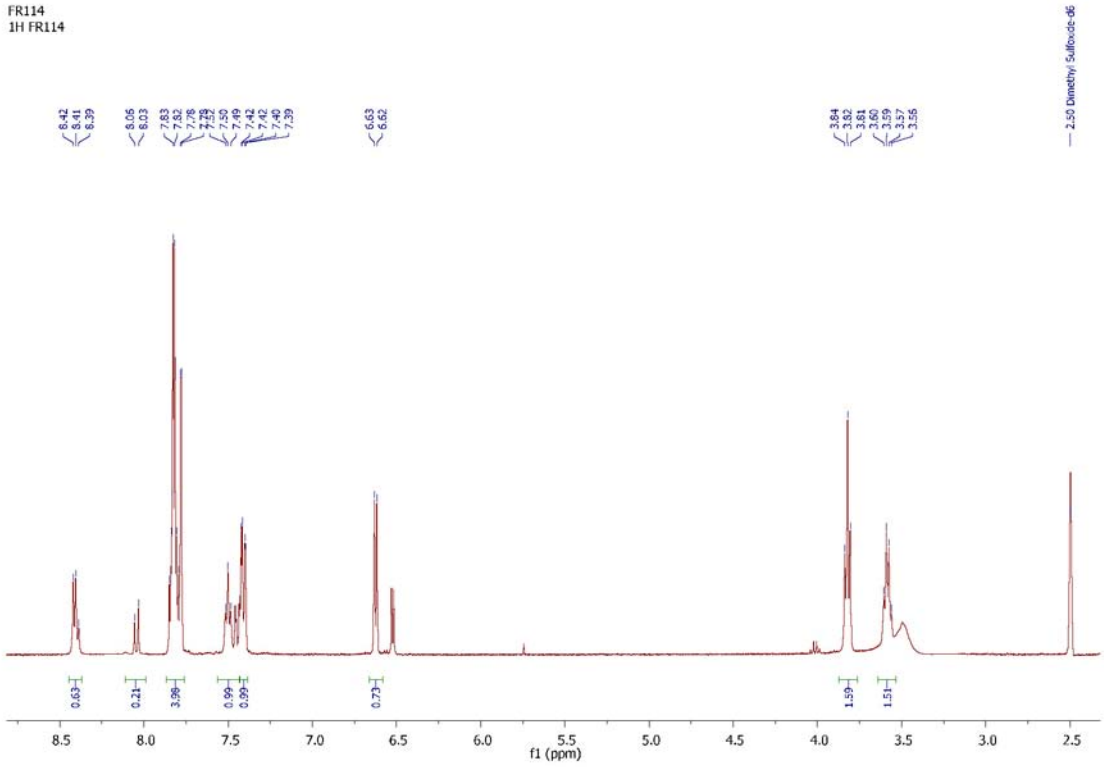

Figure S18. ^{1}H NMR spectrum of 2-(3-((7-chloroquinolin-4-yl)amino)ethyl)isoindoline-1,3(2H)-dione (**21**).

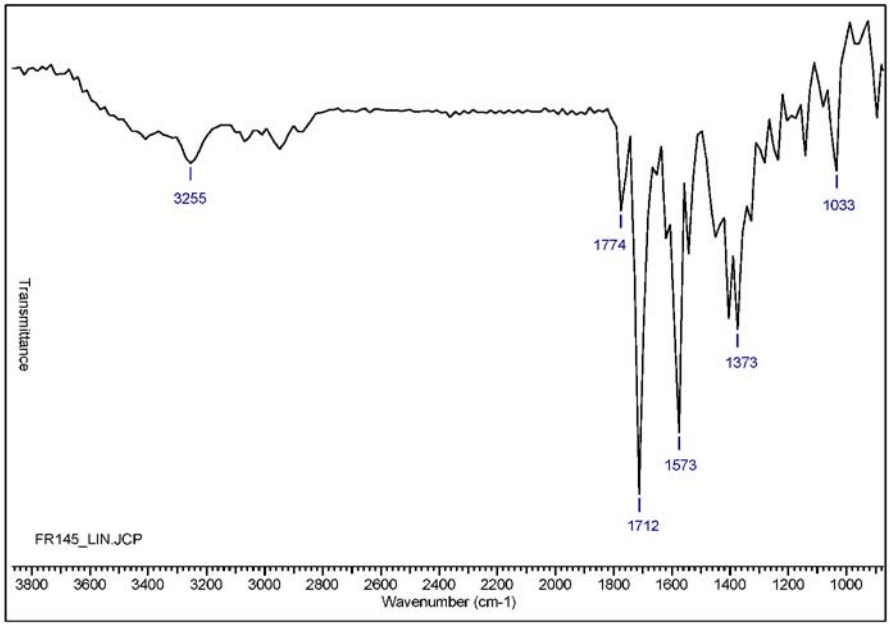

Figure S19. IR spectrum of 2-(3-((7-chloroquinolin-4-yl)amino)propyl)isoindoline-1,3(2H)-dione (**22**).

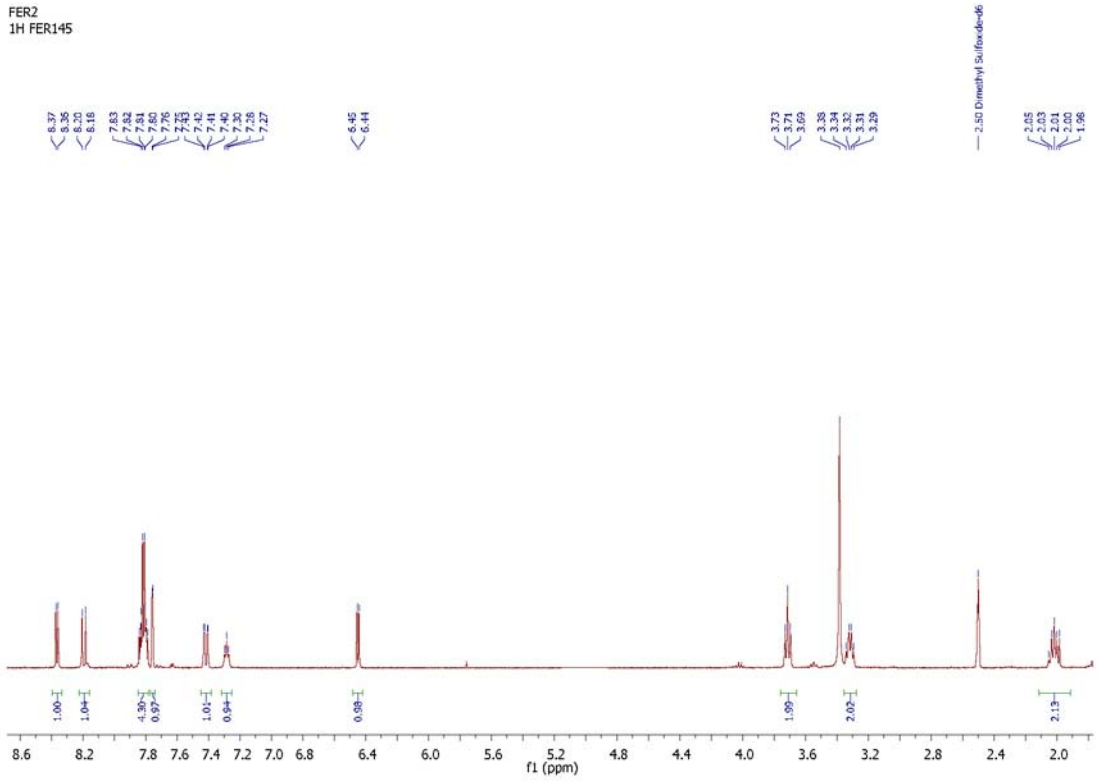

Figure S20. ^{1}H NMR spectrum of 2-(3-((7-chloroquinolin-4-yl)amino)propyl)isoindoline-1,3(2H)-dione (**22**).