

Supplemental Materials

Synthesis of BODIPY-TKI conjugates and investigation of their ability for targeting the Epidermal Growth Factor Receptor

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TABLE OF CONTENTS

Figures S1-S3: ¹ H NMR Spectra.....	S2
Figures S4-S7: Spectroscopic Data.....	S3
Figures S8-S10: HRMS Data	S6
Figure S11: Docked structure of erlotinib overlapped with the crystal structure of EGFR.....	S7
Figure S12: SPR of lapatinib binding to EGFR.....	S7
Figure S13: Lapatinib inhibition of EGFR Lapatinib.....	S8
Figure S14: Cytotoxicity in human HEP2 cells.....	S8

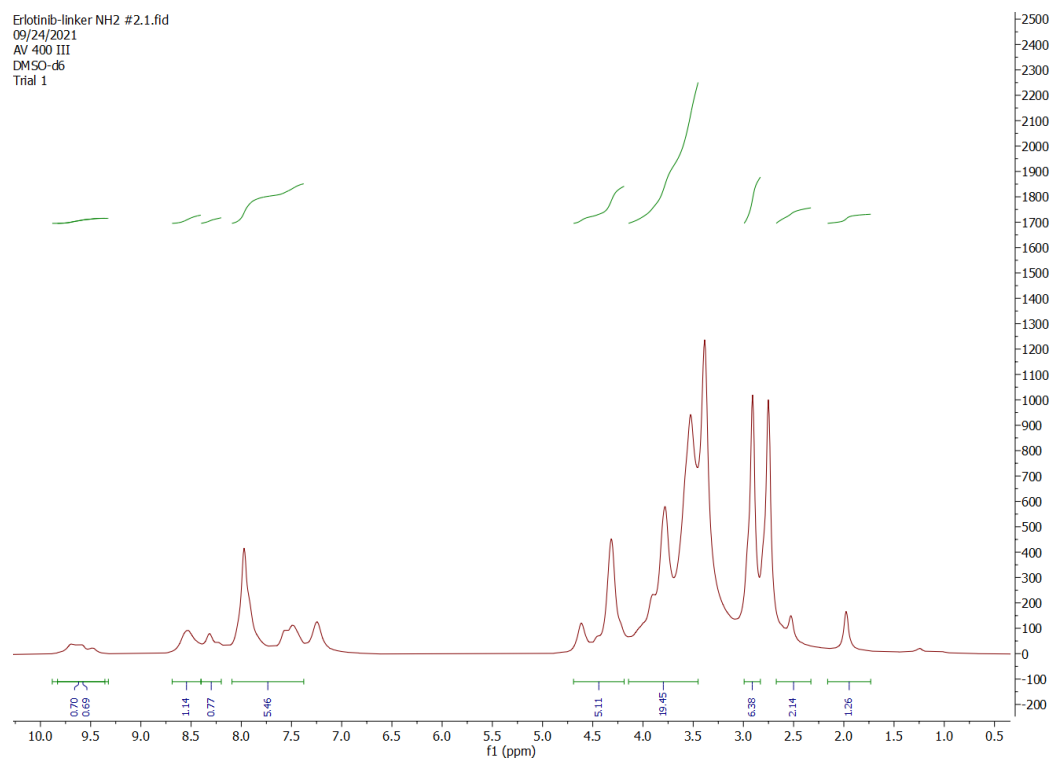


Figure S1. ^1H NMR of compound 4

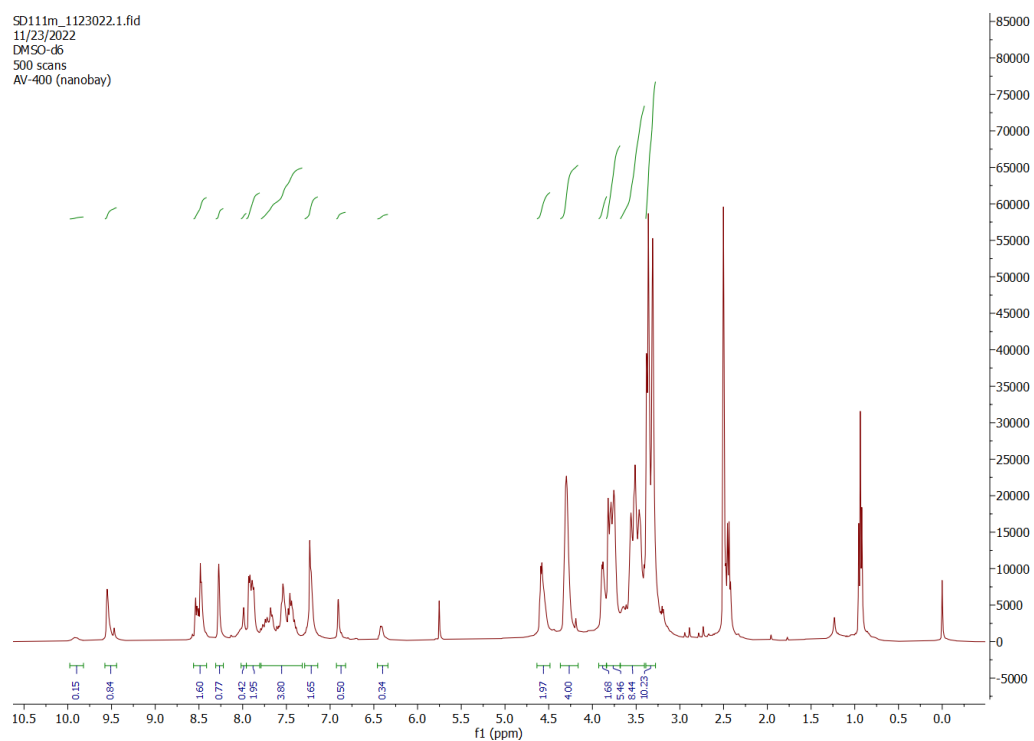


Figure S2. ^1H NMR of conjugate 5

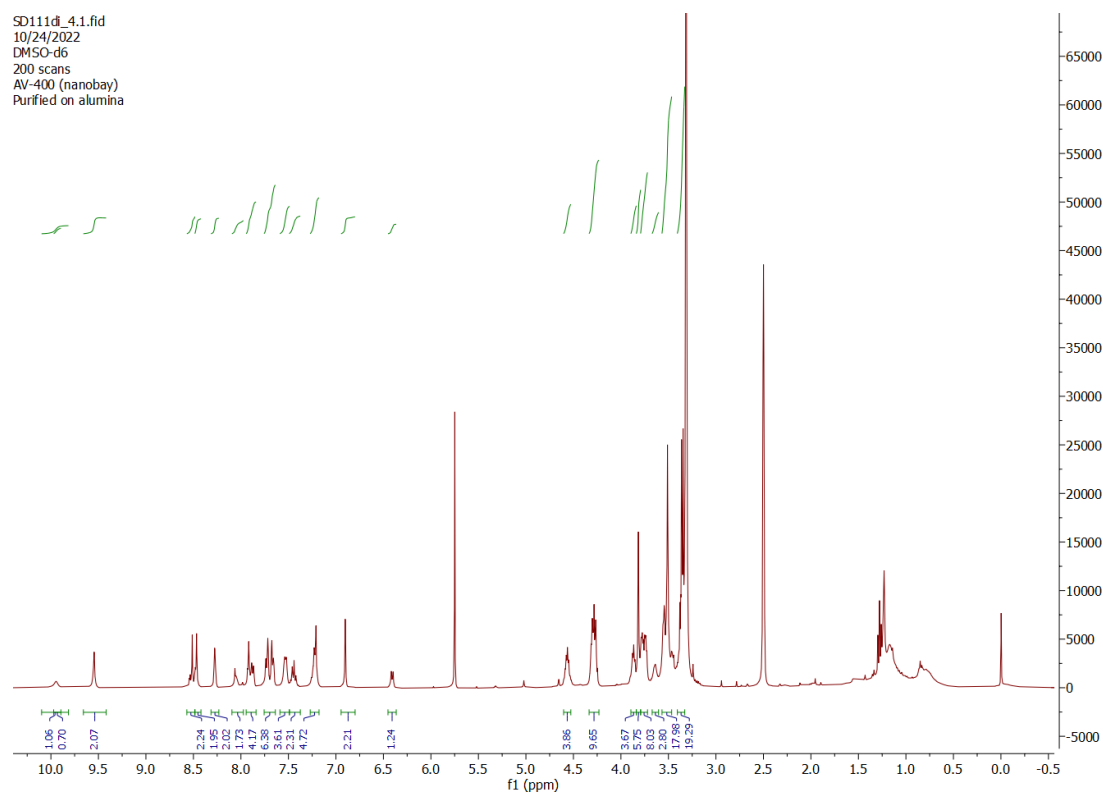


Figure S3. ^1H NMR of conjugate **6**

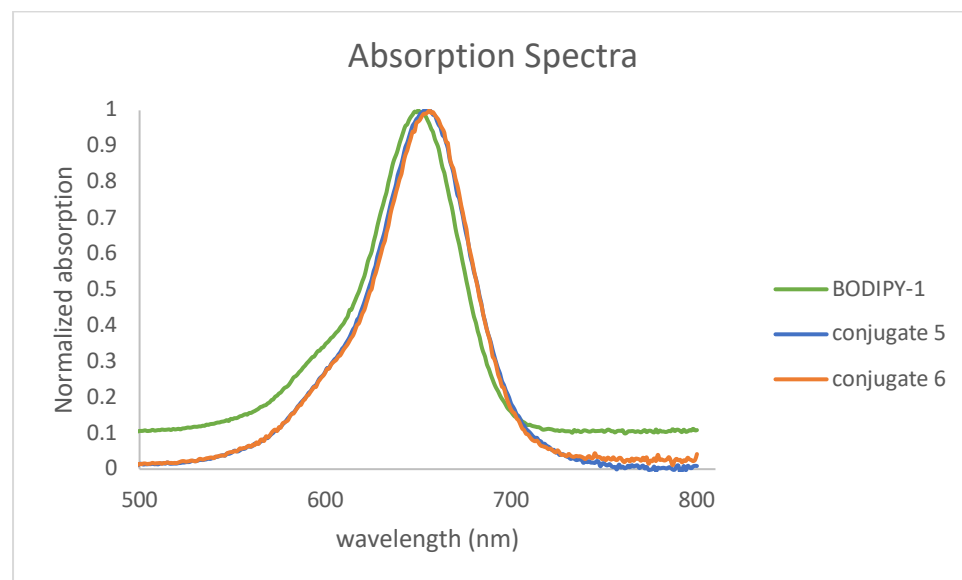


Figure S4. Normalized UV-Vis absorption spectra of BODIPY **1** and conjugates **5**, **6** in DMSO

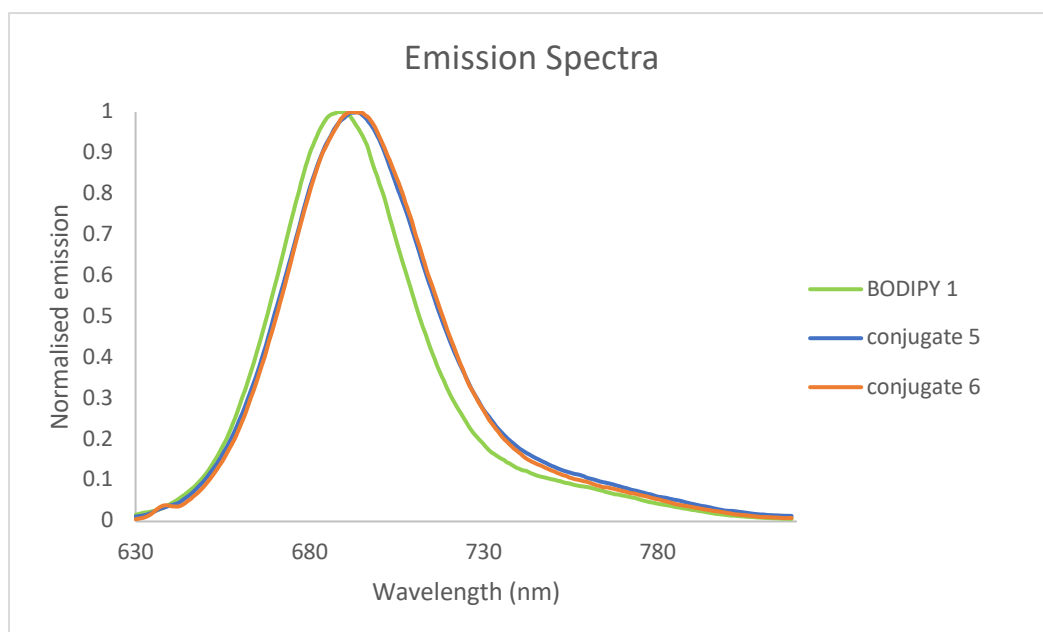


Figure S5. Normalized fluorescence emission spectra of BODIPY **1** and conjugates **5**, **6**

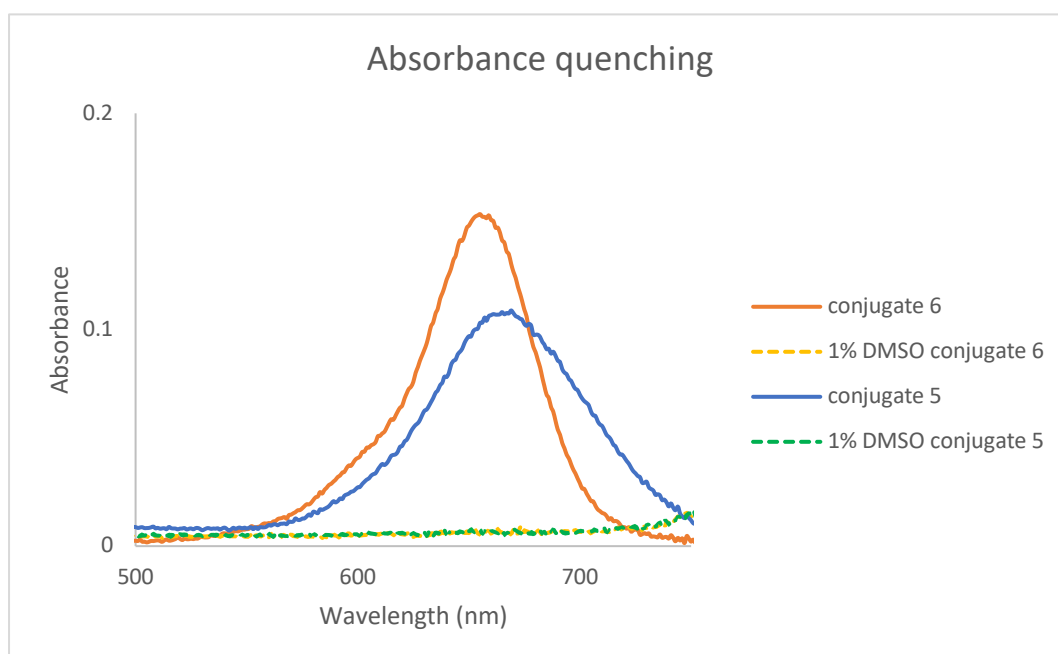


Figure S6. UV-Vis spectra of conjugates **5** and **6** at 1×10^{-5} M in a) DMSO solution (solid line), b) freshly prepared HEPES buffer solution containing 1% DMSO solution (dashed line)

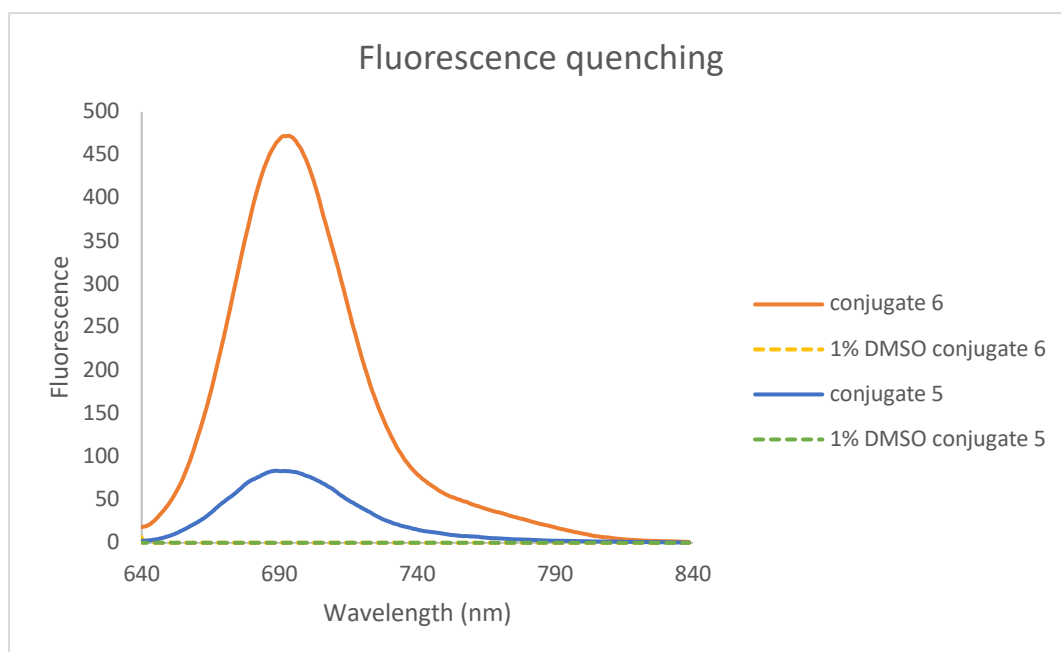


Figure S7. Fluorescence emission spectra of conjugates **5** and **6** at 1×10^{-5} M in a) DMSO solution (solid line), b) freshly prepared HEPES buffer solution containing 1% DMSO solution (dashed line)

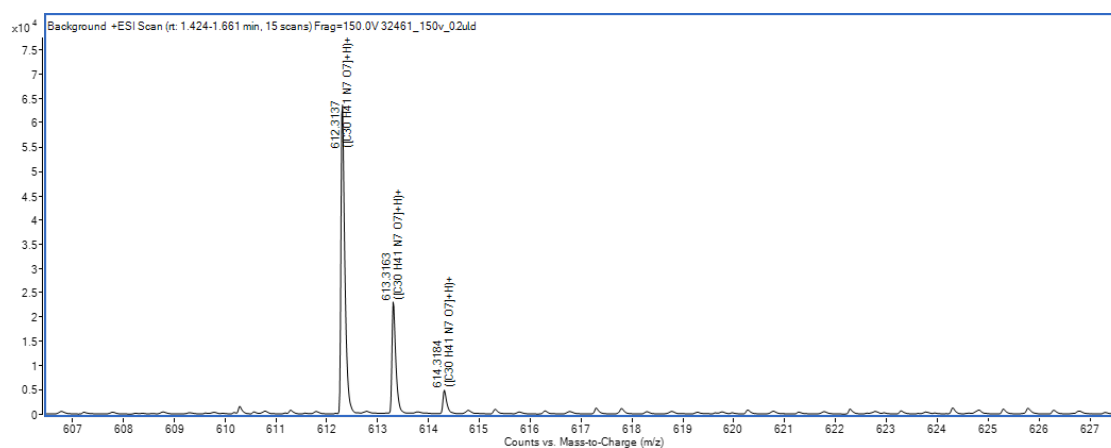


Figure S8. High-resolution mass spectrum (ESI-TOF) of compound **4**

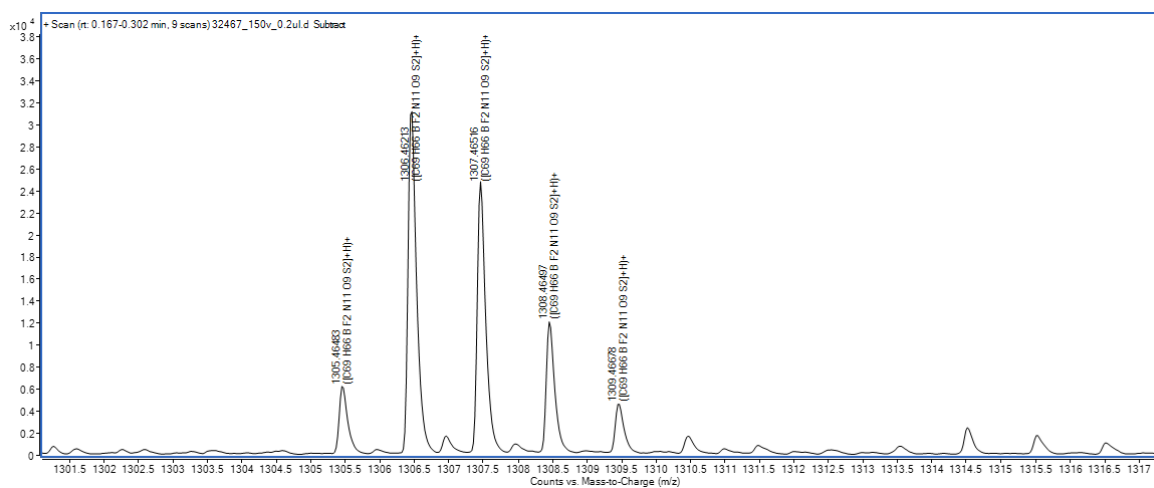


Figure S9. High-resolution mass spectrum (ESI-TOF) of conjugate **5**

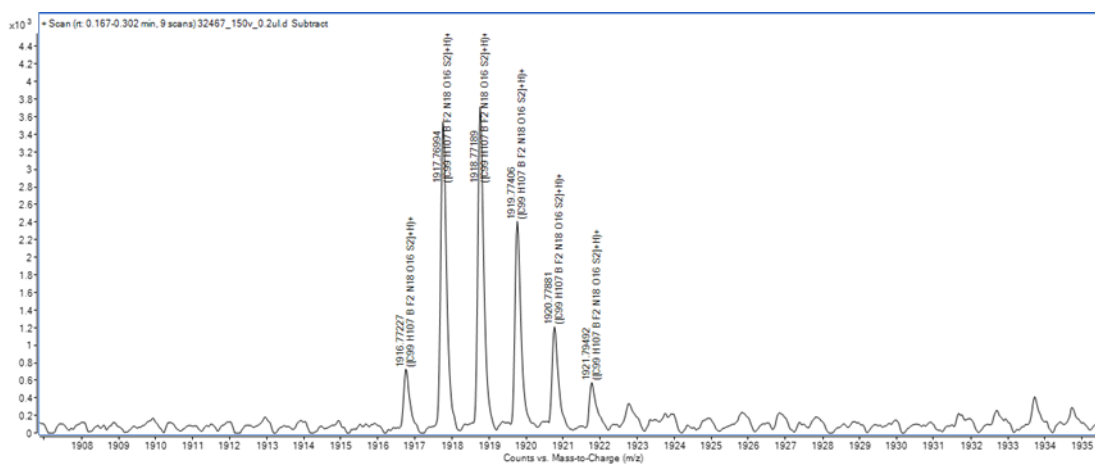


Figure S10. High-resolution mass spectrum (ESI-TOF) of conjugate **6**

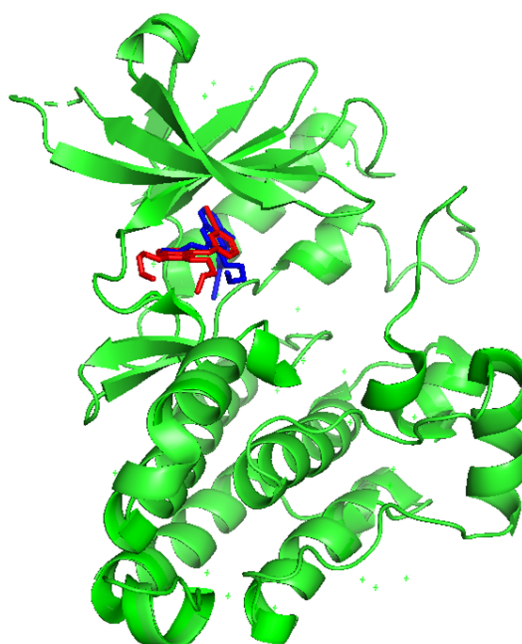


Figure S11. Low energy docked structure of erlotinib overlapped with the crystal structure of erlotinib EGFR kinase complex (PD ID: 4hjo). Red sticks, crystal structure of erlotinib, blue, docked structure of erlotinib.

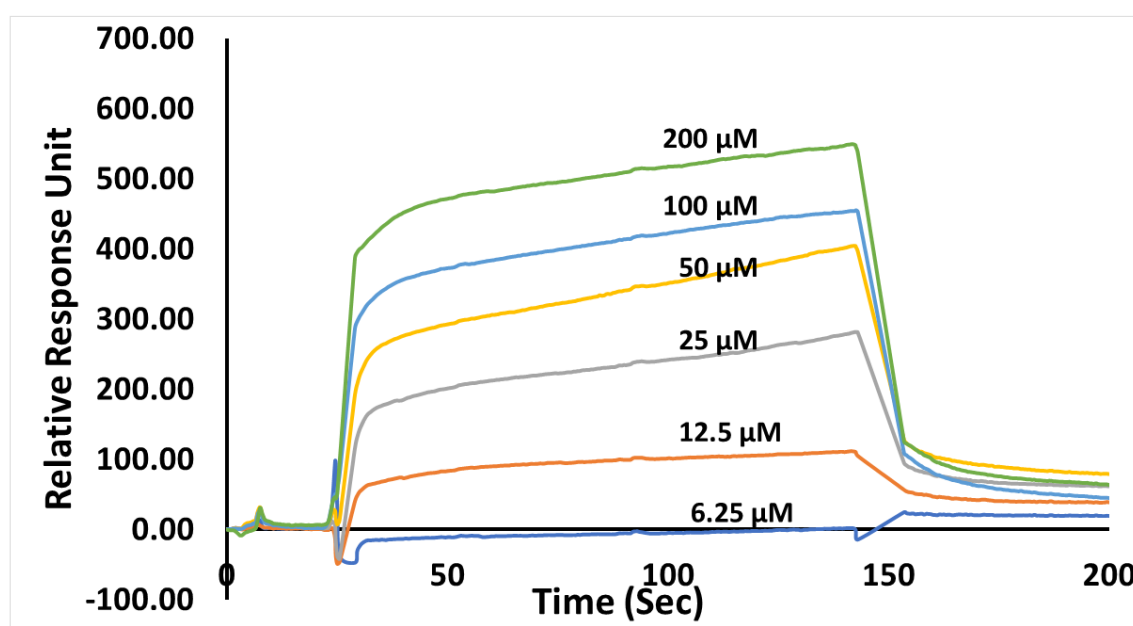


Figure S12. SPR analysis of binding of lapatinib a TKI to EGFR kinase domain is used as a positive control to evaluate the binding conjugates to EGFR kinase. Lapatinib is a kinase inhibitor of EGFR/HER2.

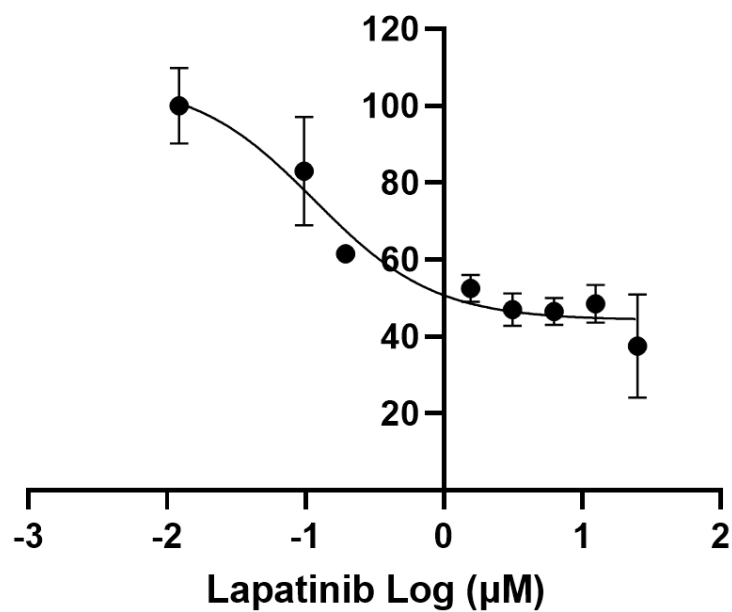


Figure S13. Inhibition of EGFR kinase activity assessed by kinase activity kit. Lapatinib is a known EGFR/HER2 kinase activity inhibitor. Dose dependent inhibition of kinase activity was observed.

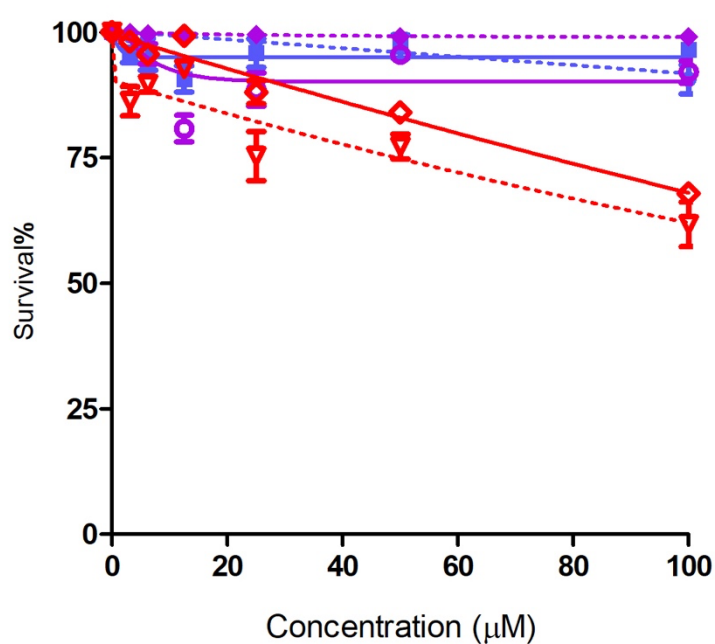


Figure S14. Dark (full line) and photocytotoxicity (1.5 J/cm^2 , dashed line) of BODIPY 1 (purple), conjugate 5 (red), and conjugate 6 (blue) in human HEp2 cells using a Cell Titer Blue assay.