Breast cancer continues to affect millions of people worldwide, and the hormone receptor +/human epidermal growth factor receptor 2- (HR+/HER2-) subtype is the most common. Work in recent years to develop selective cyclin-dependent kinase (CDK) 6 inhibitors has yielded promising results as a breast cancer therapy, but there is still an ongoing need to develop drug candidates that are safe and effective. This study, which builds on the experimental work of Chen et al. [*J. Med. Chem.* 2022, 65,15102-15122], aims to develop a density functional theory (DFT) quantitative structure-activity relationship (QSAR) model which can predict the effectiveness of CDK6 inhibitors based on single-molecule properties. Q-Chem computational chemistry software was used to perform electronic structure calculations and geometry optimizations for 29 drug candidates and several isolated side chain and linker groups at the ωB97X-D/6-31G level of theory. The results of these calculations provide physical and chemical information about these compounds which can be correlated to their effectiveness as CDK6 inhibitors. Preliminary results suggest that the polarity and van der Waals surface area of side chains and linker groups are strongly correlated with drug activity, and work is currently being done to optimize the fit and propose new drug candidates based on this QSAR model.