# ABSTRACT

**THESIS:** Structural and Anion Binding Studies of Synthesized Aryl Tetrazolones

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**DATE:** July 2017

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Compounds with tetrazolone ring system have found many applications in many scientific fields. However, these rings systems are photochemically labile. The broader goal of this research is to increase the photostability of tetrazolone based drugs, pesticides, and industrial products through cocrystallization. Tetrazolones offer a unique hydrogen bonding motif through their C=O and N-H groups that can interact with appropriately placed donor or acceptor on a neighboring molecule (coformer) in a cocrystal. This study could also allow the investigation of the possibility of tetrazolones as supramolecular synthons.

A series of monotetrazolones and bistetrazolones substituted with electron withdrawing groups were synthesized by 1,3-dipolar cycloaddition reactions of aryl isocyanates (commercially available or synthesized) with azidotrimethylsilane. The bisisocyanates needed for the synthesis of bistetrazolones were synthesized *in situ* by reacting corresponding anilines with triphosgene. The cocrystallization of the synthesized tetrazolones was studied with a series of coformers that included aliphatic and aromatic carboxylic acids as well as halogen bond donor,

1,4-diiodotetrafluorobenzene (2I4FB). One cocrystal was formed between *p*-methoxyphenyl tetrazolone and 2I4FB in which two tetrazolones form hydrogen bonded dimer and the neighboring dimers are held by halogen bonds with the -OMe group serving as a halogen bond acceptor and the –I atom on 2I4FB serving as a halogen bond donor resulting into 1D chains.

Furthermore, because of the ubiquitous role played by anions in biology, industry and environment, the anion binding ability of tetrazolones was also investigated with tetrabutylammonium acetate (TBAA), tetrabutylammonium bromide (TBAB) and tetrabutylammonium hydrosulfate ($TBAHSO_4$) by UV and NMR spectroscopy. Tetrazolones undergo proton transfer with tetrabutylammonium acetate (TBAA). However, no interactions were found with tetrabutylammonium bromide (TBAB), and tetrabutylammonium hydrosulfate ($TBAHSO_4$).