Supporting Information

Comparison of Prostate Specific Membrane Antigen Ligands in Clinical Translation Research for Diagnosis of Prostate Cancer

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^{64}Cu-Labeled Inhibitors of Prostate-Specific Membrane Antigen for PET Imaging of Prostate Cancer

Sangeeta Ray Banerjee*†, Mrudula Pullambhatla†, Catherine A. Foss†, Sridhar Nimmagadda†, Riccardo Ferdani‡, Carolyn J. Anderson‡, Ronnie C. Mease†, and Martin G. Pomper†

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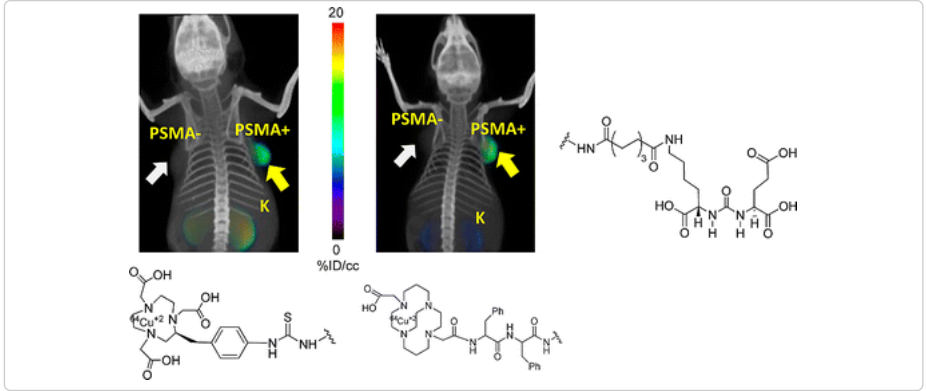

Prostate-specific membrane antigen (PSMA) is a well-recognized target for identification and therapy of a variety of cancers. Here we report five ^{64}Cu-labeled inhibitors of PSMA, [^{64}Cu]**3**–**7**, which are based on the lysine–glutamate urea scaffold and utilize a variety of macrocyclic chelators, namely NOTA(**3**), PCTA(**4**), Oxo-DO3A(**5**), CB-TE2A(**6**), and DOTA(**7**), in an effort to determine which provides the most suitable pharmacokinetics for in vivo PET imaging. [^{64}Cu]**3**–**7** were prepared in high radiochemical yield (60–90%) and purity (>95%). Positron emission tomography (PET) imaging studies of [^{64}Cu]**3**–**7** revealed specific accumulation in PSMA-expressing xenografts (PSMA+ PC3 PIP) relative to isogenic control tumor (PSMA– PC3 flu) and background tissue. The favorable kinetics and high image contrast provided by CB-TE2A chelated [^{64}Cu]**6** suggest it as the most promising among the candidates tested. That could be due to the higher stability of [^{64}Cu]CB-TE2A as compared with [^{64}Cu]NOTA, [^{64}Cu]PCTA, [^{64}Cu]Oxo-DO3A, and [^{64}Cu]DOTA chelates in vivo.

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