Supporting Information for RA-ART-07-2014-007004

Design, Synthesis and Preliminary evaluation of a novel SPECT DTPA-bistriazaspirodecanone conjugate for D_2 receptor imaging.

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Supporting Information Description

Fig. S1 -Two dimensional view of Spiperone 2 and 1-phenyl1,3,8-triazaspiro[4,5]decan-4-one with D₂ receptor. Fig. S2 -Two dimensional view of known Spiperone analogues 2 and 1-phenyl1,3,8-triazaspiro[4,5]decan-4-one with D₂ receptor Fig. S3 -Two dimensional views of known structurally 3 similar analogues and with D₂ receptor Fig. S4 -Radiochromatogram of ^{99m}Tc-DTPA-bis-(1-phenyl1,3,8-triazaspiro 4 [4,5]decan-4-one) Fig. S5- Radio-TLC of ^{99m}Tc labelled DTPA-bis-(1-phenyl1,3,8-4 triazaspiro[4,5]decan-4-one) after C-18 reversed phase extraction cartridge purification in 100% Acetone. Fig. S6. In vitro/in vivo stability of ^{99m}Tc-DTPA-bis-(1-phenyl1,3,8 triazaspiro 5 [4,5]decan-4-one)



Fig. S1 -Two dimensional view of Spiperone and 1-phenyl1,3,8-triazaspiro[4,5]decan-4-one with D_2 receptor.*



Fig. S2 -Two dimensional view of known Spiperone analogues and 1-phenyl1,3,8-triazaspiro[4,5]decan-4-one with D_2 receptor*



Fig. S3 -Two dimensional views of known structurally similar analogues and with D_2 receptor*

* Where green colored were hydrophobic, light blue were polar and red were positive charged residues. Pink lines represents hydrogen bonds, Green lines for pi-pi stacking.



Fig. S4 - Radiochromatogram of 99m Tc-DTPA-bis-(1-phenyl1,3,8-triazaspiro[4,5]decan-4-one) obtained with ITLC-SG paper strip developed in Acetone and 0.01% triethylamine showing one peaks after purification with C-18 reversed phase extraction cartridge.



Fig. S5-Radio-TLC of ^{99m}Tc labelled DTPA-bis-(1-phenyl1,3,8- triazaspiro[4,5]decan-4-one) after C-18 reversed phase extraction cartridge purification in 100% Acetone.



Fig. S6- *In vitro/in vivo* stability of ^{99m}Tc labelled DTPA-bis-(1-phenyl1,3,8-triazaspiro[4,5]decan-4-one)