

## Supplementary data

### **Design, synthesis and biological evaluation of methyl-2-(2-(5-bromo benzoxazolone)acetamido)-3-(1*H*-indol-3-yl)propanoate: TSPO ligand for SPECT**

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## Comparative docking studies

The affinity of MBIP towards TSPO has been validated through docking studies using wild type as well as mutant PDBs of TSPO. Wild type (4RYO and 4RYQ) as well as mutant (4UC1) PDBs were taken for docking studies from different sources such as BcTSPO and RsTSPO.

Interaction sites for MBIP	
<b>4RYQ</b>	Tyr19, Ser21, Ser22, Val23, Ile27, Tyr32, Gly44, Met45, Ile47, Gly48, Met49, <b>Try51</b> , Phe55, Phe 90, Ser91, Gln94, Phe95, Trp138, Phe141, Ala142, Thr143, Leu145, Ser146
<b>4RYO</b>	Tyr19, Ser21, Ser22, Ile27, Arn29, Tyr32, Gly44, Ile47, Gly48, Try51, Ala52, Phe55, Asn87, Gln88, Phe90, Ser91, Gln94, Phe95, Cys107, Val110, Ala142,
<b>4UC1</b>	Ala19, Thr21, Gly22, Ala23, Leu25, Tyr31, Trp39, Asn40, Arg43, Trp44, Phe46, Pro47, Trp50, Thr51, Tyr54, Trp87, Thr88, Phe91, Phe92, Try139, Ala138, Leu142, Asn143

### Energetic of MBIP with two PDBs

	Glide gscore	Glide lipo	Glide hbond	Glide evdw	Glide ecoul	Glide erotb	glide esite	glide emodel	Glide energy
4RYQ	-6.922	-3.947	-0.320	-9.504	-5.659	0.453	0.000	-15.360	-15.163
4RYO	-7.011	-3.337	-0.360	-11.123	-5.885	0.453	-0.005	-25.190	-17.008

## SPECT image with $^{99m}\text{Tc}$ -MBIP



Blocking study of  $^{99m}\text{Tc}$  MBIP at 40 min in peripheral organ

**10 MIN POST INJECTION OF PK11195 (5 mg/kg)**