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Supplementary data

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

Pooja Srivastava^{1,2*}, Ankur Kaul, Himanshu Ojha, Pravir Kumar², Anjani K Tiwari^{1*}

¹ Division of Cyclotron and Radiopharmaceutical Sciences, Institute of Nuclear Medicine and Allied Sciences, Brig. S. K. Mazumdar Road, Delhi-110054, India

² Molecular Neuroscience and Functional Genomics Laboratory, Department of Biotechnology, Delhi Technological University, Delhi 110042, India

Comparative docking studies

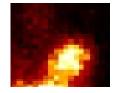
The affinity of MBIP towards TSPO has been validated through docking studies using wild type as well as mutant PDBs of TSPO. Wild type (4RYO and 4RYQ) as well as mutant (4UC1) PDBs were taken for docking studies from different sources such as BcTSPO and RsTSPO.

	Interaction sites for MBIP
4RYQ	Tyr19, Ser21, Ser22, Val23, Ile27, Tyr32, Gly44, Met45, Ile47, Gly48, Met49, Try51 , Phe55, Phe 90, Ser91, Gln94, Phe95, Trp138, Phe141, Ala142, Thr143, Leu145, Ser146
4RYO	Tyr19, Ser21, Ser22, Ile27, Arn29, Tyr32, Gly44, Ile47, Gly48, Try51, Ala52, Phe55, Asn87, Gln88, Phe90, Ser91, Gln94, Phe95, Cys107, Val110, Ala142,
4UC1	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	Glide	Glide	Glide	Glide	Glide	glide	glide	Glide
	gscore	lipo	hbond	evdw	ecoul	erotb	esite	emodel	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 99mTc-MBIP





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

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