

# Supporting information for the article:

## **Towards the functional oligomerisation state of tryptophane-rich sensory proteins**

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†The authors contributed equally.

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gi 163838662 re	1	MPESW	----	VP	-----	7	
gi 6978575 ref	1	MSQSW	----	VP	-----	7	
gi 296486947 tp	1	MAPPW	----	VP	-----	7	
gi 54400566 ref	1	MW	----	IP	-----	4	
gi 6690723 gb A	1	MNMDW	----	ALF	-----	8	
gi 294676238 re	1	MSLTL	----	F	-----	6	
gi 392243174 gb	1	MTDRV	----	SP	-----	7	
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gi 347834285 em	1	MDLNY	----	QVFTS		10	
gi 321312631 re	1	MKKI	----			4	
gi 11499070 ref	1	MNILK	----			5	
gi 77459036 ref	1	MVTF	----			4	
gi 7296190 gb A	1	MADRPCAGNILR				12	
gi 167656983 gb	1	MQVVI	----	NGRKGH	TIIVKY	-----	21
cons	1	*					33

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gi 163838662 re	8	-----	-----	AVGLTLVPSL		17
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gi 296486947 tp	8	-----	-----	AVGFTLLPSL		17
gi 54400566 ref	5	-----	-----	MLSLTALPHV		14
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gi 294676238 re	7	-----	-----	AVYFVACAC		15
gi 392243174 gb	8	-----	-----	RLPDDIPALGISLAAAV		25
gi 16226870 gb	29	ADDNKGKRDQKRA	-----	MAKRGLKSLTVAVAAPVL		59
gi 347834285 em	11	-----	I	SKNW	-----	25
gi 321312631 re	5	-----	-----	FG	AIAVFVITYAL	17
gi 11499070 ref	6	-----	-----	-----	LVASILAVLA	15
gi 77459036 ref	5	-----	-----	-----	LIFLIACGA	13
gi 7296190 gb A	13	-----	-----	-----	IAGAVILPNL	22
gi 167656983 gb	22	LSNAKGD	-----	NMKRNNKWL	-----	48
cons	34					66

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gi 163838662 re	18	GGFMGAYFVRGEGLRWYASLQKPSWHPPRWTLA	50
gi 6978575 ref	18	GGFMGAYFVRGEGLRWYASLQKPSWHPPRWTLA	50
gi 296486947 tp	18	GGFLGAQYTRGEGFRWYASLQKPPWHPPRWILA	50
gi 54400566 ref	15	GGIFGGIITRREVKTWYSTLNKPSWRPPNAAFP	47
gi 6690723 gb A	18	PATTGALLK---PDEWYDNLNKPWWNPPRWVFP	47
gi 294676238 re	16	AGATGAIIFS---PGAWYDSLKKPSWVPPNWLF	45
gi 392243174 gb	26	AAGVGGLAS-ANAAAQYGVLAQPSWAPPWVFG	57
gi 16226870 gb	60	VTLFATYFL-GTSDGYGNRAKSSSWIPPLWLLH	91
gi 347834285 em	26	GWFIGNSYK---PRKDYENKKQPKFHPPASAFG	55
gi 321312631 re	18	F-SAAGYLEF-PVDQEWYNSLKKPDWTPSGNAIG	48
gi 11499070 ref	16	IGFAGSFFTAQSVQOTWYAGVEKPFPTPPNWLF	48
gi 77459036 ref	14	AATTGMVFO---PGQWYAQLNKPFTPPNWVFP	43
gi 7296190 gb A	23	GGIYNGRLTRQHLQSWYANLKFPSFKPPNSVFA	55
gi 167656983 gb	49	IGMSSGLLA-GSFNEFFQKYNKPPLMPPSWVFP	80

cons	67		99
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gi 5911820 emb	51	PVWGTLYSAMGYGSYLVWKEGGFTE-KAVVPL	82
gi 163838662 re	51	PIWGTLYSAMGYGSYIVWKEGGFTE-DAMVPL	82
gi 6978575 ref	51	PIWGTLYSAMGYGSYIIWKEGGFTE-EAMVPL	82
gi 296486947 tp	51	PIWGTLYSAMGYGSYMIWKEGGFSK-EAVVPL	82
gi 54400566 ref	48	VVWTTLYTGMGYGSYLVWKEGGFTQ-DAMVPL	79
gi 6690723 gb A	48	LAWTSLYFLMSLAAMRVAQL-EGS-----GOAL	74
gi 294676238 re	46	VAWSTLYILMSISAARVSGL-AMENE-LAVLGL	76
gi 392243174 gb	58	PVWTVLYVLMGVAAWLVWRT-RP-PV-P-ASAL	86
gi 16226870 gb	92	TTCLASSGLMGLAAWLVWVD-GGFHK-K-PNAL	121
gi 347834285 em	56	PAWTLLEYLTMGYASHLAYKADPLMITNASRNGS	88
gi 321312631 re	49	IIWAILFALISLSAAIVYAA-FSFKG-A-KSFW	78
gi 11499070 ref	49	PAWTLLEYFLIGIVLYIAWEN--GFWN-DSRVK-	77
gi 77459036 ref	44	VAWTTIYLLLAWVGYRLTMI-PGS-----EMVL	70
gi 7296190 gb A	56	PMWISLYAGMGYGSYLVWRDGGGFAGEAAKLPL	88
gi 167656983 gb	81	VVWVILYAVMGVSAHLIHYSNAAGSI-K-RKLL	111

cons	100		132
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gi 163838662 re	83	GLYTGQLALNWAWPPIFFGARQMGWALADLLLV	115
gi 6978575 ref	83	GLYTGQLALNWAWPPIFFGARQMGWALVDLMLV	115
gi 296486947 tp	83	GLYAGQLALNWAWPPLFFGTRQMGWALVDLLLT	115
gi 54400566 ref	80	GLYGLQLALNWAWTPIFFGAHKIQLALIELLLM	112
gi 6690723 gb A	75	AFYAAQLAFNTLWTPVFFGMKRMATALAVVMVM	107
gi 294676238 re	77	AFWAVQIAVNTLWTPIFFGLHRLAGGMLVLVLL	109
gi 392243174 gb	87	TAYGIQLVLNALWTPLFFGLGWRGAALAEIVVL	119
gi 16226870 gb	122	YLYLAQFLLCVWDPVTFRVGSGVAGLAVWLGO	154
gi 347834285 em	89	ILYIAQLAANFAWMPLFYGLAKPKLALADLGIL	121
gi 321312631 re	79	FTLLINYVLNQAQFSYFQFTQKNLLAASLDCLLV	111
gi 11499070 ref	78	ATFFTQLGLNFLWSILFFGLQNLPLAGLVDIIAL	110
gi 77459036 ref	71	ALWAAQIALNTLWTPVFFGAQRIVAAMLILVLL	103
gi 7296190 gb A	89	IAYGTQLALNWAWTPIFFGQHNIKGGGLIDIVAL	121
gi 167656983 gb	112	MVYVWQLIVNFLWSIIFVRFELLWLAAADIVLL	144

cons	133	: . . .	165
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gi 163838662 re	116	SGVATATTLAWHRVSPPAARLLYPYLAWLAFAT	148
gi 6978575 ref	116	SGVATATTLAWHRVSPPAARLLYPYLAWLAFAT	148
gi 296486947 tp	116	GGMAAATAMAWHQVSPPAACLLYPYLAWLAFAA	148
gi 54400566 ref	113	SGTVAATMVSWYPIISRATLLMVPYMAWLCVAT	145
gi 6690723 gb A	108	WLFVAATMWAFFQLDTWAGVLFVPYLIWATAAT	140
gi 294676238 re	110	WLSVFATCVLFWSVDWLSGLMFVPYVIWVTVAG	142
gi 392243174 gb	120	WIALVVTIALFWVRSRVAAVLLLPYLVWTTFAA	152
gi 16226870 gb	155	SAALFGCYKAFNEISPVAGNLVKPCLAWAAFVA	187
gi 347834285 em	122	TGLVGWLAKTWWPLAPTASKWLI PYLAWLGYAG	154
gi 321312631 re	112	AITAIVLLIIAKKYSRIASYLLLPYFLWSAFAT	144
gi 11499070 ref	111	DIAVILTIVYIYH-HSKASLLLLPYLGWILFAS	142
gi 77459036 ref	104	WLVVAVMVVLALRLDVITGLILFPYLAWLCVAV	136
gi 7296190 gb A	122	TAAASACGVLFYRVNKTAGLLFVPYVAWLGAFAT	154
gi 167656983 gb	145	LVLIGIMILGFGKVNRIAGDINI PYFLWVAFAT	177

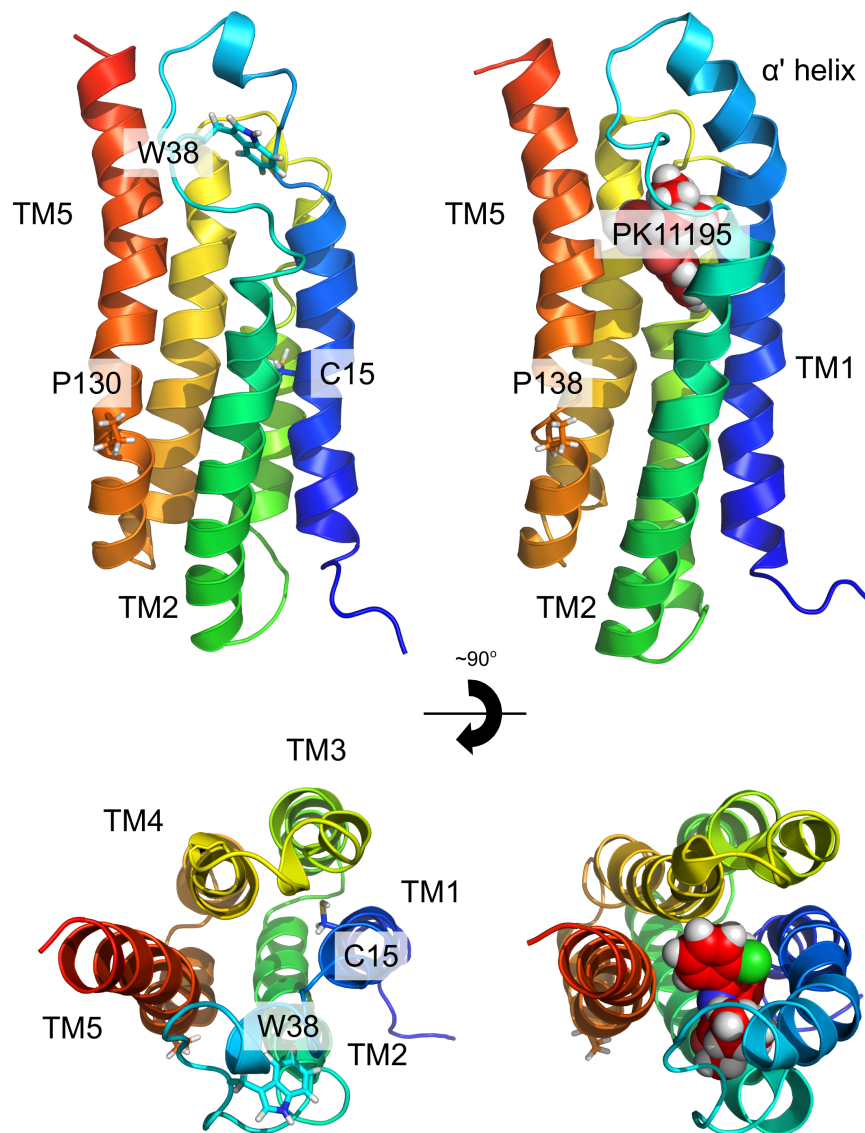
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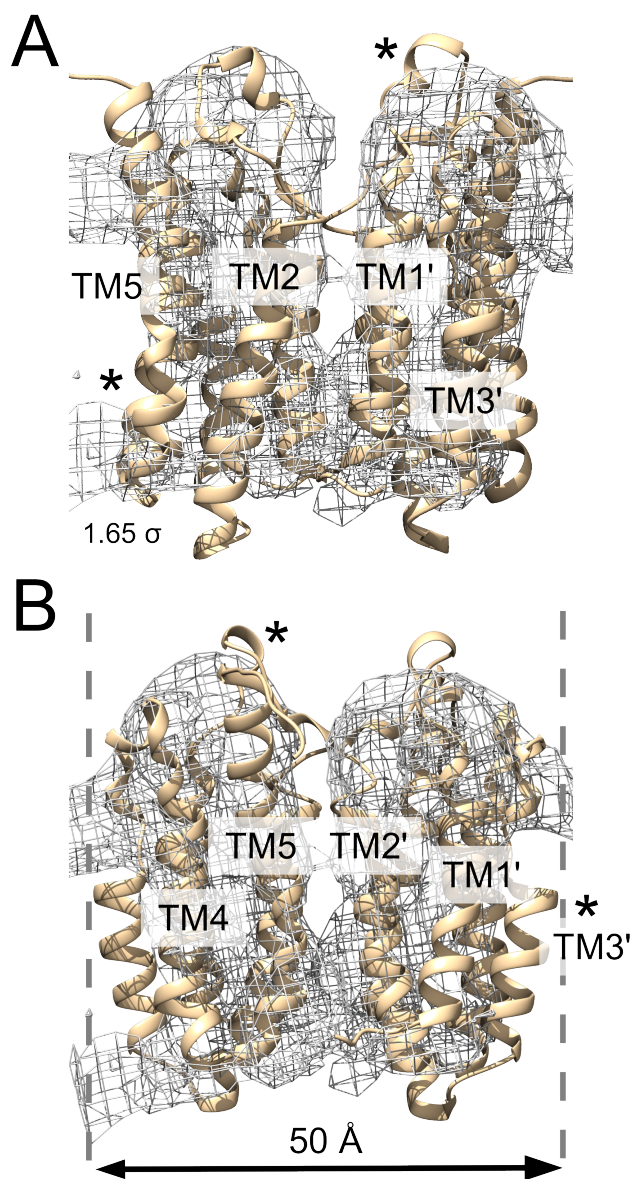
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gi 163838662 re	149	VLNYYVWRD	NSGRRGG	-----	SRLPE	169
gi 6978575 ref	149	MLNYYVWRD	NSGRRGG	-----	SRLTE	169
gi 296486947 tp	149	TLNYRMWQD	NQVRRSG	-----	RRLSE	169
gi 54400566 ref	146	SLNYCIWRD	NPEP	-----	KKED	162
gi 6690723 gb A	141	GLNFEAMRL	NWNRP	-----	EARA	158
gi 294676238 re	143	ALNFSVWRL	NPGEK	-----	PITL	160
gi 392243174 gb	153	CLNFAVWQL	NNTA	-----	AV	166
gi 16226870 gb	188	AVNVKLA		-----	VA	196
gi 347834285 em	155	YLNLYGYCLL		-----	N	164
gi 321312631 re	145	FLSFTINSM		-----	NL	155
gi 11499070 ref	143	ALNFAIYLLN		-----	A	153
gi 77459036 ref	137	ALNFSIMRNN	RAG	-----	YGS	152
gi 7296190 gb A	155	ALNYAIWKL	NPEKEQAPKDEEK	PSSSHAKSS		185
gi 167656983 gb	178	YLVNVA	TIFV	-----	N	187
<b>cons</b>	<b>199</b>					<b>229</b>

**Supporting Fig. S1.** Sequence alignment, as obtained from the T-COFFEE server, of TspO/PBR proteins from different organisms:

5911820 [Homo sapiens]  
163838662 [Mus musculus]  
6978575 [Rattus norvegicus]  
296486947 [Bos taurus]  
54400566 [Danio rerio]  
6690723 [Rhodobacter sphaeroides]  
294676238 [Rhodobacter capsulatus SB 1003]  
392243174 [Mycobacterium abscessus subsp. bolletii CCUG 48898 = JCM 15300]  
16226870 [Arabidopsis thaliana]  
347834285 [Schizosaccharomyces pombe]  
321312631 [Bacillus subtilis BSn5]  
11499070 [Archaeoglobus fulgidus DSM 4304]  
77459036 [Pseudomonas fluorescens Pf0-1]  
7296190 [Drosophila melanogaster]  
167656983 [Eubacterium siraeum DSM 15702]



**Supporting Fig. S2.** Comparison between the 3D model of a subunit of *RsTspO* (left column) and the 3D high-resolution structure of the *mTSPO*-PK 11195 complex (right column). The PK 11195 ligand is shown in spheres, trans-membrane helices are labelled. C15 and W38 of *RsTspO* and P130/P138 of *RsTspO/mTSPO* are shown in stick representation.



**Supporting Fig. S3.** Fit of two alternative (compared to Fig. 2(A)) dimeric arrangements to the electron density of *RsTspO*. (A) TM1TM2:TM2'TM1' similar to Fig. 2(A), but rotated by  $\sim 34^\circ$  around the C2 symmetry axis. In this model, TM5 is not placed well in the electron density (indicated by \*). (B) TM2TM5:TM5'TM2'. TM3 does not match the electron density and the overall dimension of the model is  $\sim 50$  Å.