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Supporting information for article:

Structure determination of the human TRPV1 ankyrin-repeat domain under nonreducing conditions

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Table S1. Comparison of pharmacological properties between rTRPV1 and hTRPV1

| <i>Stimuli</i> | <i>rTRPV1 vs hTRPV1 sensitivity differences</i> | <i>Binding sites</i> |
|-----------------------|--|--------------------------------------|
| Capsaicin | EC ₅₀ no difference ^{s1, s2} | TM2-3 region ^{s3-s5} |
| I-RTX | IC ₅₀ rTRPV1 < IC ₅₀ hTRPV1 ^{s6} (to capsaicin) | TM2-3 region |
| Temperature | Activating temperatures no difference (42°C >) ^{s1, s2} | Highly controversial |
| Proton | Activating pH similar (hTRPV1(5.49), rTRPV1 (5.78)) ^{s1} | Outer TM5-6 (pore) ^{s7, s8} |
| Capsazepine | IC ₅₀ hTRPV1 < IC ₅₀ rTRPV1 ^{s1} (to capsaicin) | TM2-3 region ^{s9} |
| Ruthenium Red | IC ₅₀ hTRPV1 < IC ₅₀ rTRPV1 ^{s1} (to capsaicin) | Pore (blocker) |
| PPAHV | Agonist to rTRPV1 but inactive for hTRPV1 ^{s1} | TM2-4 region ^{s9} |

G S P N S S V A A S T E K T L R L Y D R R S I F E A V A Q N N C Q D L
E S L L L F L Q K S K K H L T D N E F K D P E T G K T C L L K A M L N
L H D G Q N T T I P L L L E I A R Q T D S L K E L V N A S Y T D S Y Y
K G Q T A L H I A I E R R N M A L V T L L V E N G A D V Q A A A H G D
F F K K T K G R P G F Y F G E L P L S L A A C T N Q L G I V K F L L Q
N S W Q T A D I S A R D S V G N T V L H A L V E V A D N T A D N T K F
V T S M Y N E I L I L G A K L H P T L K L E E L T N K K G M T P L A L
A A G T G K I G V L A Y I L Q R E I Q E P E C R H V D S S G R I V T D

Number of amino acids: 280

Molecular weight: 30778.14

Fig. S1. Amino acid sequence of hTRPV1-ARD.

The residue numbers from 101 to 365 were selected as the structure to be revealed. The underline indicates the amino acid sequence from hTRPV1 whereas the others are sequence from plasmid and the site remained after digestion by restriction enzymes.

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Rat      SVSA-GEKPPRLYDRRSIFD 119
Human    SVAASTEKTLRLYDRRSIFE 120
          **: * ** *****:

Rat      AVAQSNQCELESLLPFLQRSKKRLTDSEFKDPETGKTCLKAMLNLHNGQNDTIALLLDV 179
Human    AVAQNNCQDLESLLLFLQSKKHLTDNEFKDPETGKTCLKAMLNLHDGQNTTIPLLLEI 180
          ****.***:***** **:*:**:***.*****:*****:*** ** ***:

Rat      ARKTDLSLKQFVNASYTDSYYKGQTALHIAIERRNMTLVTLLEVENGADVQAAANGDFFKKT 239
Human    ARQTDLSLKELVNASYTDSYYKGQTALHIAIERRNMALVTLLVENGADVQAAAHGDFFKKT 240
          **:*****:*****:*****:*****:*****:*****:*****

Rat      KGRPGFYFGELPLSLAACTNQLAIVKFLQNSWQPADISARDSVGNTVLHALVEVADNTV 299
Human    KGRPGFYFGELPLSLAACTNQLGIVKFLQNSWQTADISARDSVGNTVLHALVEVADNTA 300
          *****:*****.***** *****

Rat      DNTKFVTSMYNEILILGAKLHPTLKLEEITNRKGLTPLALAASSGKIGVLAYILQREIHE 359
Human    DNTKFVTSMYNEILMLGAKLHPTLKLEELTNKGMTPLALAAGTGKIGVLAYILQREIQE 360
          *****:*****:***:**:*****.:*****:***

Rat      PECRH
Human    PECRH
          *****

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Fig. S2. Alignment of amino acid sequences of hTRPV1-ARD and rTRPV1-ARD.

The marks * indicates the same amino acid residues between human (residues 101-365) and rat (residues 101-364) proteins. The box indicates the region of finger loop 3 (residues 239-246 in human numbers).

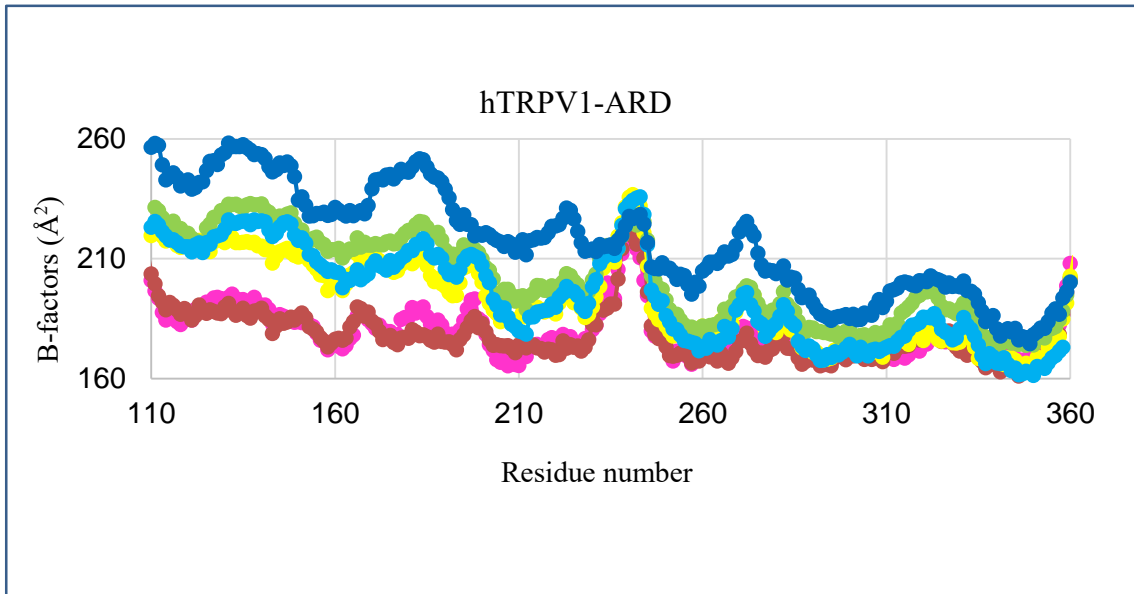


Fig. S3. The B-factor plot of the hTRPV1-ARD (chains A - F).

The horizontal and vertical axes indicate residue numbers and B-factors of $C\alpha$ atoms (\AA^2), respectively. The A, B, C, D, E and F chains are colored by magenta, orange, yellow, light green, cyan and blue, respectively.

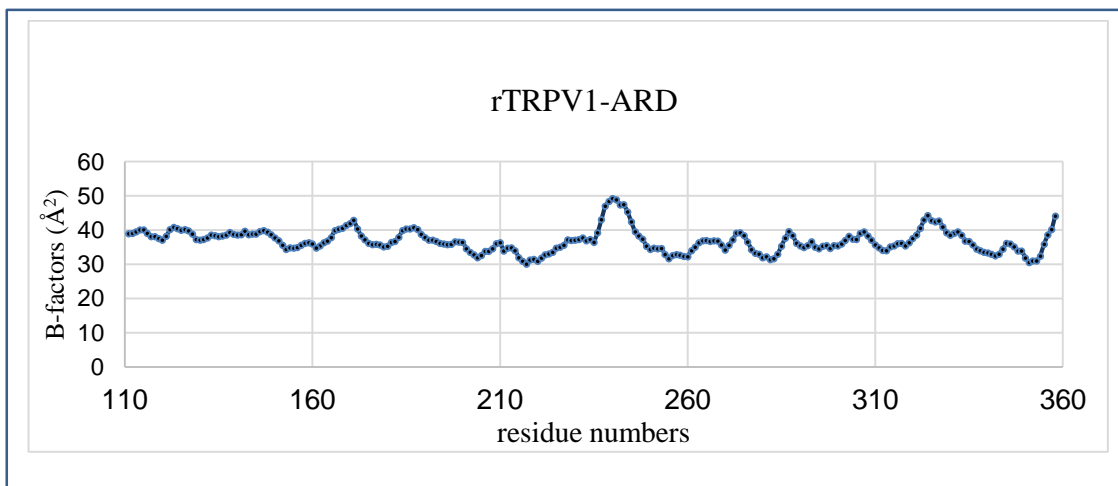


Fig. S4. The B-factor plot of the rTRPV1-ARD (PDB ID; 2PNM).
The horizontal and vertical axes indicate residue numbers and B-factors of C α atoms (Å²), respectively.

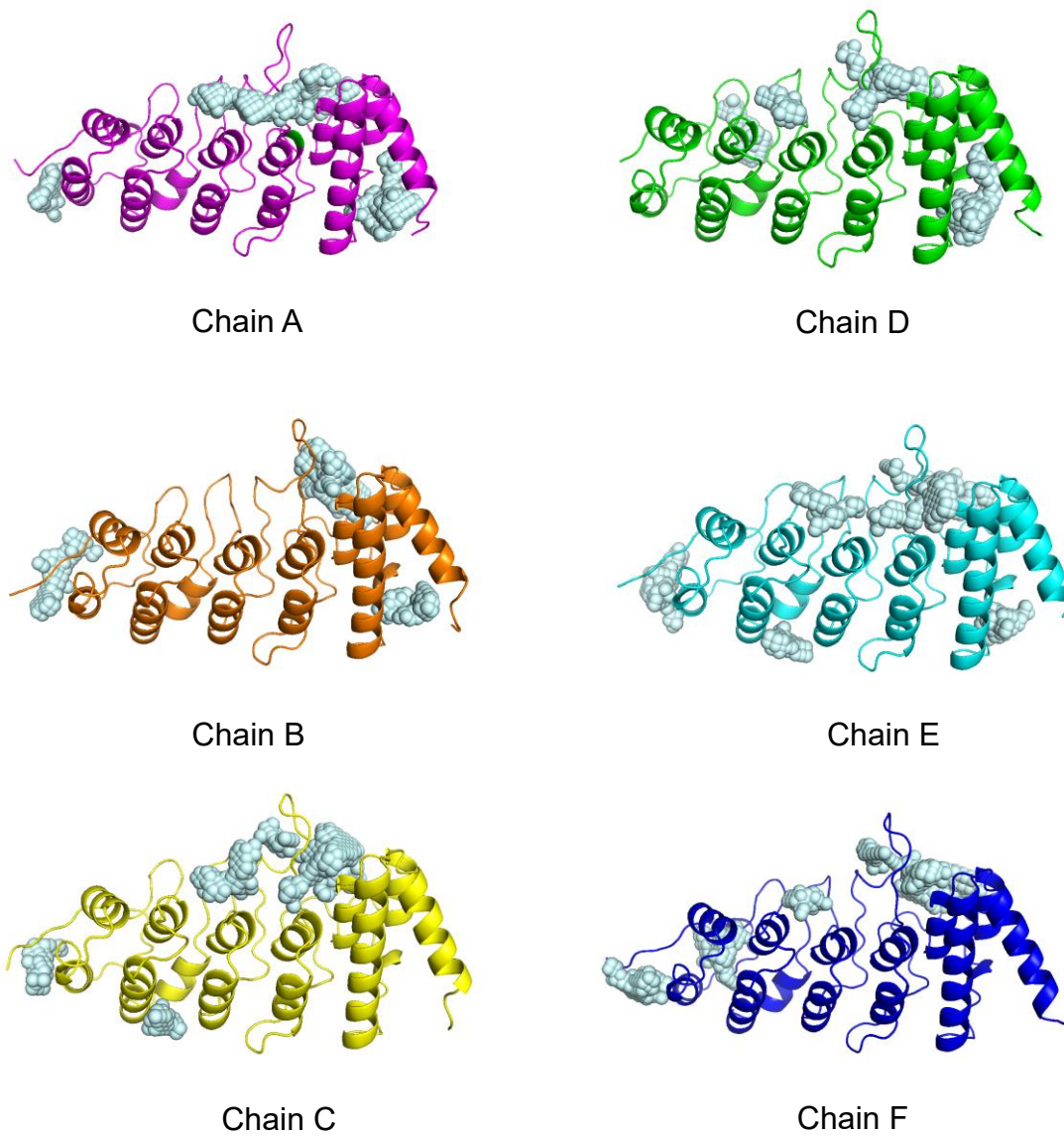


Fig. S5. Ligand-binding pockets of the hTRPV1-ARD (chains A - F). Mass of balls colored by light blue are candidates of the ligand-binding pockets. This was calculated using POCASA.

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