

## **S1 Supporting Information.**

### **Insights into the Binding Modes and Mechanism of Action of Atypical Retinoids as Ligands of SHP Receptor.**

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**Figure s1.** a) Verify3D plot of SHP<sub>DAX-1</sub> structure. b) Verify3D plot of SHP<sub>USP</sub> structure.

**Figure s2.** a) Verify3D plot of SHP<sub>RXR $\alpha$</sub>  structure. b) Verify3D plot of SHP<sub>RXR $\alpha$</sub> \* structure.

**Table s2.** Primers used for the mutagenesis assays.

## S2.

**Table s1.**

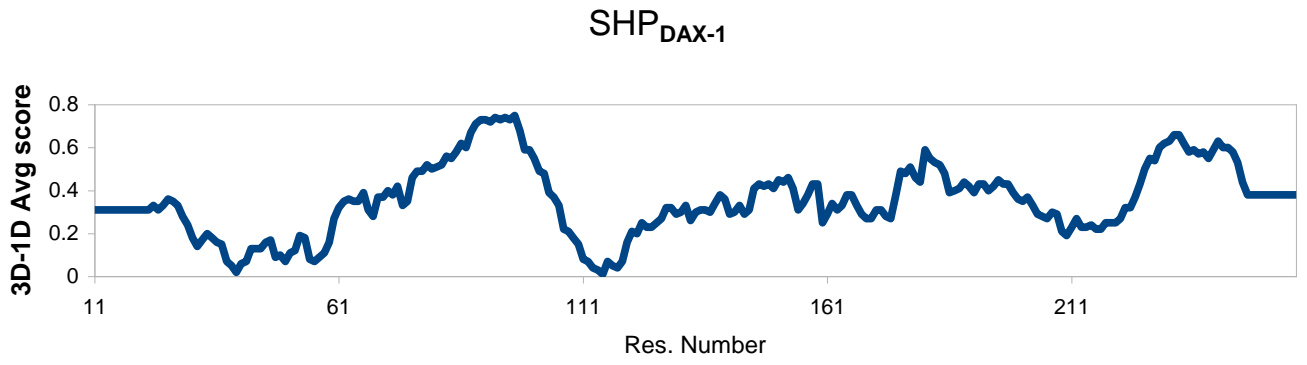
	<b>SHP<sub>DAX-1</sub></b>	<b>SHP<sub>USP</sub></b>	<b>SHP<sub>RXR<math>\alpha</math></sub></b>	<b>SHP<sub>RXR<math>\alpha</math></sub><sup>*</sup></b>
Template (pdb code)	3F5C	1G2N	1MV9	1DKF
Clash score <sup>a</sup>	2.85	9.93	6.53	10.97
Poor rotamers (%)	4.83%	4.83%	3.92%	4.37%
% Outliers in Ramachandran plot	2.47%	2.07%	3.77%	1.66%
% Favoured in Ramachandran plot	86.01%	84.71%	85.36%	87.72%
% Residue with bad bonds	0.00%	0.00%	0.00%	0.41%
% Residue with bad angles	2.04%	0.41%	1.24%	0.41%

<sup>a</sup>The clash score is an index of the number of serious steric overlaps (> 0.4 Å) occurring per 1000 atoms.

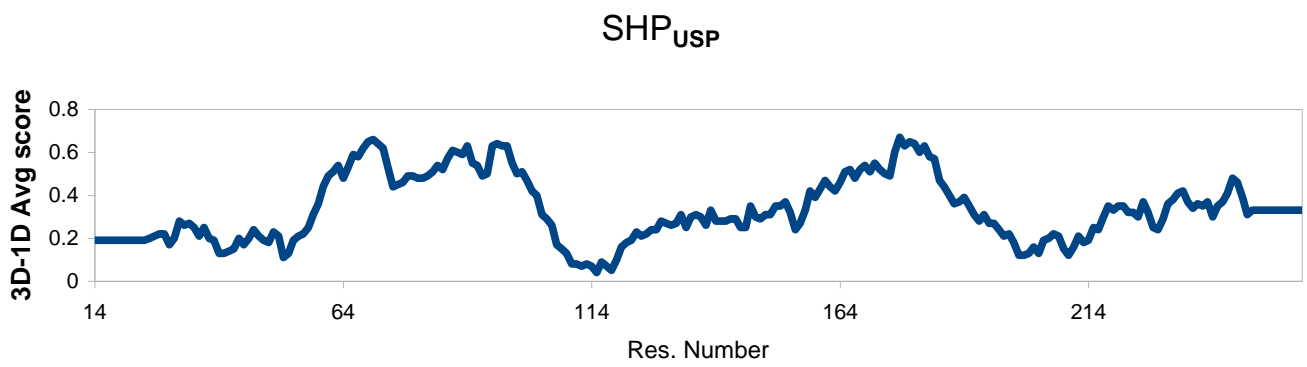
S3

Figure s1

a)



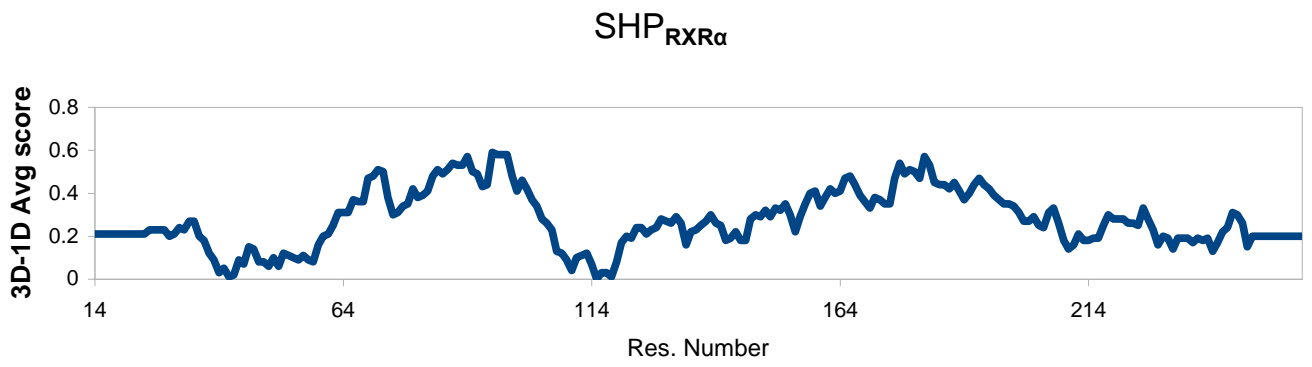
b)



S4

Figure s2

c)



d)

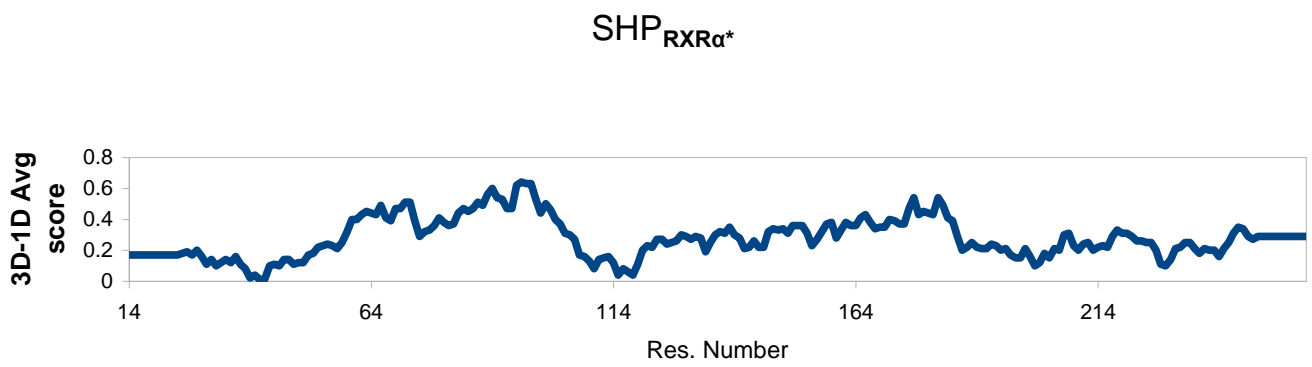


Table s2.

Primer	Sequence
R138D (F)	5'-ggCCAActgCCAgACgATCCCCAgCCCTCCCTg-3'
R138D (R)	5'-CAgggAgggCTggggATCgTCTggCagTTggCC-3'
R238D (F)	5'-CTgCTTggggACCTCTTCTTTgACCCTATCATTggAg-3'
R238D (R)	5'-CTCCAATgATAgggTCAAAgAAgAggTCCCCAAgCag-3'
R238A (F)	5'-CTgCTTggggACCTCTTCTTTgCCCCTATCATTggAg-3'
R238A (R)	5'-CTCCAATgATAggggCAAAgAAgAggTCCCCAAgCag-3'
R138A (F)	5'-CCAActgCCAgACgCACCCCAgCCCTCC-3'
R138A (R)	5'-ggAgggCTggggTgCgTCTggCagTTgg-3'
W92A (F)	5'-gCTgCAgggTTgCgCgggCCCCCTCTTC-3'
W92A (R)	5'-gAAgAgggggCCCgCgCAACCCTgCagC-3'
F96A (F)	5'-CTggggCCCCCTCgCCCTgCTTgggTTg-3'
F96A (R)	5'-CAACCCAAgCAgggCgAgggggCCCCAg-3'
W148A (F)	5'-CTggCTgCggTgCAggCgCTTCAATgCTgTCTg-3'
W148A (R)	5'-CAgACAgCATTgAAgCgCCTgCACCGCagCCAg-3'
R34A (F)	5'-CAAaggCTgTCCCCgCACCCCGTAgCCgC-3'
R34A (R)	5'-gCggCTACggggTgCggggACAgCCTTg-3'
Q134R (F)	5'-AgTggAggCagTggCagACTgCCAgACAgACC-3'
Q134R (R)	5'-ggTCTgTCTggCagTCTgCCTgCCTCCACT-3'
R34Q (F)	5'-ggCTgTCCCCCAACCCCGTAgCC-3'
R34Q (R)	5'-ggCTACggggTTgggggACAgCC-3'